Preparation of Ethynylsulfonamides and Study of Their Reactivity with Nucleophilic Amino Acids

Tatsuhiro Kyoya, [a] Hiroaki Ishida, [a] Toshiaki Saitoh, [b] and Toshimasa Itoh *[a]

[a]: *Laboratory of Drug Design and Medicinal Chemistry, Showa Pharmaceutical University, 3-2-1 Higashi-Tamagawagakuen, Machida, Tokyo 194-8543, Japan.*

[b]: *Division of Medicinal Informatics, Nihon Pharmaceutical University, 10281 Komuro, lna-machi, kitaadachi-gun, Saitama 362-0806 Japan.*

Supporting Information

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General Methods

Unless otherwise stated, reactions were performed under a nitrogen atmosphere using freshly dried solvents. Thin-layer chromatography (TLC) was performed using silica gel 70 F_{254} TLC Plate-*Wako* and were visualized by UV, *p*-anisaldehyde, Sonnenschein's reagent, or I_2 (5% silica gel) staining. Flash chromatography was performed using silica gel (40 - 50 μm particle size, spherical, neutral). Reverse-phase HPLC (RP-HPLC) was performed with a JASCO Gulliver system equipped with an Intelligent HPLC Pump PU-980 and an Intelligent UV/VIS Detector UV-970, and the eluent was detected by UV at 220 or 254 nm. For analytical RP-HPLC, a COSMOSIL 5C18-AR-II (4.6 × 250 mm) packed column was employed with linear gradients of acetonitrile and H_2O containing 0.1% (v/v) TFA with a flow rate of 1.0 mL $min^{-1.}$ For preparative RP-HPLC, a PEGASIL ODS (30 × 250 mm) packed column was employed with linear gradients of acetonitrile and H_2O containing 0.1% (v/v) TFA with a flow rate of 10 mL min^{-1}. NMR spectra were recorded on a JEOL ECZ400S (at 400 MHz for ^1H NMR and 101 MHz for ^{13}C NMR), and are reported relative to internal TMS (^1H, δ = 0.00) or DMSO-d_6 (^1H δ = 2.54), and $CDCl_3$ (^{13}C, δ = 77.0) or DMSO-d_6 (^{13}C = 39.5). Data for ^1H NMR spectra are reported as follows: chemical shift (δ ppm) (multiplicity, coupling constant (Hz), integration). Multiplicity and qualifier abbreviations are as follows: s = singlet, d = doublet, t = triplet, q = quartet, quin = quintet, sext = sextet, sep = septet, oct = octet, m = multiplet, br = broad. IR spectra were recorded on Jasco FT/IR-420 spectrometer (KBr tablet, NaCl plate), and Jasco FT/IR-4100 spectrometer (ATR). Absorbance abbreviations are as follows: vs = very strong, s = strong, m = medium, w = weak, br = broad. High-resolution mass spectrometry (HRMS) spectra were obtained with a JEOL AccuTOF LC-plus JMS-T100LP spectrometer (ESI), and JEOL JMS-700MS station (EI, FAB). FAB matrix is α-thioglycerol.

Abbreviations used:

DBU – 1,8-Diazabicyclo[5.4.0]undec-7-ene
DCC – Dicyclohexylcarbodiimide
DCM – Dichloromethane
DIPA – Diisopropylamine
DMAP – 4-Dimethylaminopyridine
DMF – *N*,*N*-Dimethylformamide
DMSO – Dimethylsulfoxide
HMDS – Hexamethyldisilazane
LDA – Lithium diisopropylamide
LHMDS – Lithium bis(trimethylsilyl)amide
MeI – Iodomethane
2-ME – 2-Mercaptoethanol
PBS – Phosphate-buffered saline
TFA – Trifluoroacetic acid
THF – Tetrahydrofuran

General Procedure for the Syntheses of Substrates

General Procedure 1A

2-Chloroethanesulfonyl chloride (4.08 g, 2.63 mL, 25 mmol) in DCM (25 mL), a solution of amine (27.5 mmol, 1.1 equiv.) and triethylamine (14.0 g, 10.5 mL, 75 mmol, 3.0 equiv.) in DCM (25 mL) was added dropwise at 0 °C over a period of 30 minutes. After the reaction mixture was stirred for 3 hours at room temperature, the reaction mixture was washed sequentially with 1 M HCl aqueous solution, distilled water, and then brine, and the organic layer was dried over Na_2SO_4. After concentration, chromatography was performed on the residue on a silica gel column to give *N*-substituted vinylsulfonamide (**3**).

General Procedure 1B

2-Chloroethanesulfonyl chloride (4.08 g, 2.63 mL, 25 mmol) and DMAP (28 mg, 0.25 mmol, 1.0 mol%) in DCM (25 mL), a solution of amine (27.5 mmol, 1.1 equiv.) and triethylamine (14.0 g, 10.5 mL, 75 mmol, 3.0 equiv.) in DCM (25 mL) was added dropwise at 0 °C over a period of 30 minutes. After the reaction mixture was stirred for 3 hours at 0 °C, the reaction mixture was washed sequentially with 1 M HCl aqueous solution, distilled water, and then brine, and the organic layer was dried over Na_2SO_4.After concentration, chromatography was performed on the residue on a silica gel column to give *N*-substituted vinylsulfonamide (**3**).

General Procedure 1C

The amine (27.5 mmol, 1.1 equiv.), triethylamine (14.0 g, 10.5 mL, 75 mmol, 3.0 equiv.) and DMAP (28 mg, 0.25 mmol, 1.0 mol%) were dissolved in DCM (100 mL). 2-Chloroethanesulfonyl chloride (4.08 g, 2.63 mL, 25 mmol) was added at 0 °C. After the reaction mixture was stirred for 3 hours at 0°C, the reaction mixture was washed sequentially with 1 M HCl aqueous solution, distilled water, and then brine, and the organic layer was dried over Na_2SO_4. After concentration, chromatography was performed on the residue on a silica gel column to give *N*-substituted vinylsulfonamide (**3**).

General Procedure 2

To a solution of the **3** (5 mmol) in DCM (10 mL) was added a solution of bromine (0.26 mL, 5.0 mmol, 1.0 equiv.) at 0 °C. The mixture was stirred at 0 °C for 5 minutes and warm to room temperature for 18 hours. the reaction mixture was quenched with saturated $Na_2S_2O_3$ aqueous solution (10 mL). After the reaction mixture had been washed three times with saturated $Na_2S_2O_3$ aqueous solution. After separation, the organic layer was dried over Na_2SO_4 and concentrated under reduced pressure. To a solution of the residue in DCM (20 mL) was added a solution of triethylamine (5.2 g, 0.71 mL, 5.5 mmol) in DCM (20 mL) over 30 min, and the reaction mixture was stirred at room temperature for 15

hours. The reaction mixture was washed three times with distilled water, once with brine, and the organic layer was dried over Na_2SO_4. After concentration, chromatography was performed on the residue on a silica gel column to give 1-bromo-*N*-substituted ethenylsulfonamide (**1**).

General Procedure 3A

To a stirred solution of the reactant (3 mmol) in dry THF (15 mL), LHMDS (10.5 mL, 1 M solution in THF, 3.5 equiv.) and dry THF (4.5 mL) ware added at −78 °C over 10–15 minutes. After the reaction mixture was stirred for 30 minutes at 0 °C, the mixture was quenched with 5 M HCl aqueous solution (10 mL) at 0 °C. To the reaction mixture, EtOAc (30 mL) and distilled water (50 mL) were added. The reaction mixture was extracted three times with EtOAc, washed once with brine, and the organic layer was dried over Na_2SO_4. After concentration, chromatography was performed on the residue on a silica gel column to give product *N*-substituted ethynylsulfonamide (**2**).

General Procedure 3B

To a stirred solution of the reactant (3 mmol) in dry THF (15 mL), LHMDS (7.5 mL, 1 M solution in THF, 2.5 equiv.) and dry THF (2.5 mL) ware added at −78 °C over 10–15 minutes. After the reaction mixture was stirred for 30 minutes at 0 °C, the mixture was quenched with 5 M HCl aqueous solution (10 mL) at 0 °C. To the reaction mixture, EtOAc (30 mL) and distilled water (50 mL) were added. The reaction mixture was extracted three times with EtOAc, washed once with brine, and the organic layer was dried over Na_2SO_4. After concentration, chromatography was performed on the residue on a silica gel column to give *N*-substituted ethynylsulfonamide (**2**).

General Procedure 3C

To a stirred solution of the reactant (3 mmol) in dry THF (15 mL), *t*-BuOK (10.5 mL, 1 M solution in THF, 3.5 equiv.) and dry THF (4.5 mL) ware added at −78 °C over 10–15 minutes. After the reaction mixture was stirred for 30 minutes at 0 °C, the mixture was quenched with 5 M HCl aqueous solution (10 mL) at 0 °C. To the reaction mixture, EtOAc (30 mL) and distilled water (50 mL) were added. The reaction mixture was extracted three times with EtOAc, washed once with brine, and the organic layer was dried over Na_2SO_4. After concentration, chromatography was performed on the residue on a silica gel column to give *N*-substituted ethynylsulfonamide (**2**).

General Procedure 4

To a stirred solution of the reactant (3 mmol) in dry THF (15 mL), LHMDS (10.5 mL, 1 M solution in THF, 3.5 equiv.) and dry THF (4.5 mL) were added at −78 °C over 10–15 minutes. The reaction mixture was then stirred for 30 minutes at 0 °C. MeI (69 μL, 1.1 equiv.) was added to the reaction mixture and stirred for 1 hour at room temperature. The mixture was quenched with 1 M HCl aqueous

solution (10 mL) at 0 °C. EtOAc (30 mL) and distilled water (50 mL) were added to the reaction mixture. The organic layer was extracted three times with EtOAc, washed once with brine, and dried over Na_2SO_4. After concentration, chromatography was performed on the residue on a silica gel column to give product.

General Procedure 5

To a solution of the reactant (0.50 mmol) in dry MeOH (3.0 mL) was added AcCl (11 μL) and stirred at room temperature for 30 min. The reaction mixture was diluted with 1,4-dioxane and concentrated in vacuo. After concentration, chromatography was performed on the residue on a silica gel column to give product.

General Procedure 6A

The amine (10 mmol), propiolic acid (**11**, 680 μL, 11 mmol) and DMAP (12.2 mg, 1.0 mol%) were added to DCM (20 mL) and the solution was cooled to 0 °C. To the reaction solution was then added dropwise a solution of DCC (2.27 g, 11 mmol, 1.1 equiv) in DCM (20 mL) and the reaction was allowed to warm to room temperature and stirred for 3 hours. After the reaction was completed, the reaction mixture was filtered through Celite pad and the solvent was removed in vacuo. After concentration, chromatography was performed on the residue on a silica gel column to give *N*-substituted ethynylamide (**13**).

General Procedure 7

A solution of reactant (0.50 mmol) in H_2O (2.5 mL) was added protected amino acid (Ac-AA-OMe) (0.50 mmol, 1.0 equiv.) at room temperature. The reaction mixture was diluted with EtOH and concentrated in vacuo. After concentration, chromatography was performed on the residue on a a silica gel column or preparative RP-HPLC to give product.

Water Solubility

A sufficient amount of the compound and 5.0% (v/v) MeCN in water was added, followed by vigorous stirring for 30 seconds. The mixture was then allowed to stand for 2 hours at 19°C to produce a saturated solution. The saturated solution was then diluted and its concentration was determined by UV absorption with reference to a previously prepared calibration curve.

NMR Experiments

CD_3CN solution

The reactant (300 μL, 40 mM solution in CD_3CN) and protected amino acid (Ac-AA-OMe) (300 μL, 60 mM solution in CD_3CN) were added to the NMR tube and mixed by shaking up and down, then the foam was removed by ultrasound. The reaction was then followed over time by ^{1}H-NMR.

H_2O or PBS solution

The reactant (300 μL, 40 mM solution in H_2O) and protected amino acid (Ac-AA-OMe) (300 μL, 60 mM solution in DMSO-d_6:H_2O = 19:1) were added to the NMR tube and mixed by shaking up and down, then the foam was removed by ultrasound. The reaction was then followed over time by NoD-NMR. (PBS solution instead of H_2O)

The following (1) and (2) was used for a single integrable peak on the NMR spectrum.

$$S_r + S_p = 1 \tag{1}$$

$$\frac{1}{C} = \frac{1}{20 \times 10^{-3} \times S_r} - \frac{1}{20 \times 10^{-3}} \tag{2}$$

C: $Reactants\ concentration$

S_r: $Integral\ value\ for\ reactants$

S_p: $Integral\ value\ for\ products$

Prot a $\frac{1}{C} - t$ of graph. Calculate reaction rate constant (k) from the gradient of the Approximate line of least squares method. To substitute k in (3).

$$t_{1/2} = \frac{1}{20 \times 10^{-3} \times k} \tag{3}$$

$t_{1/2}$: $Half - life\ of\ products$

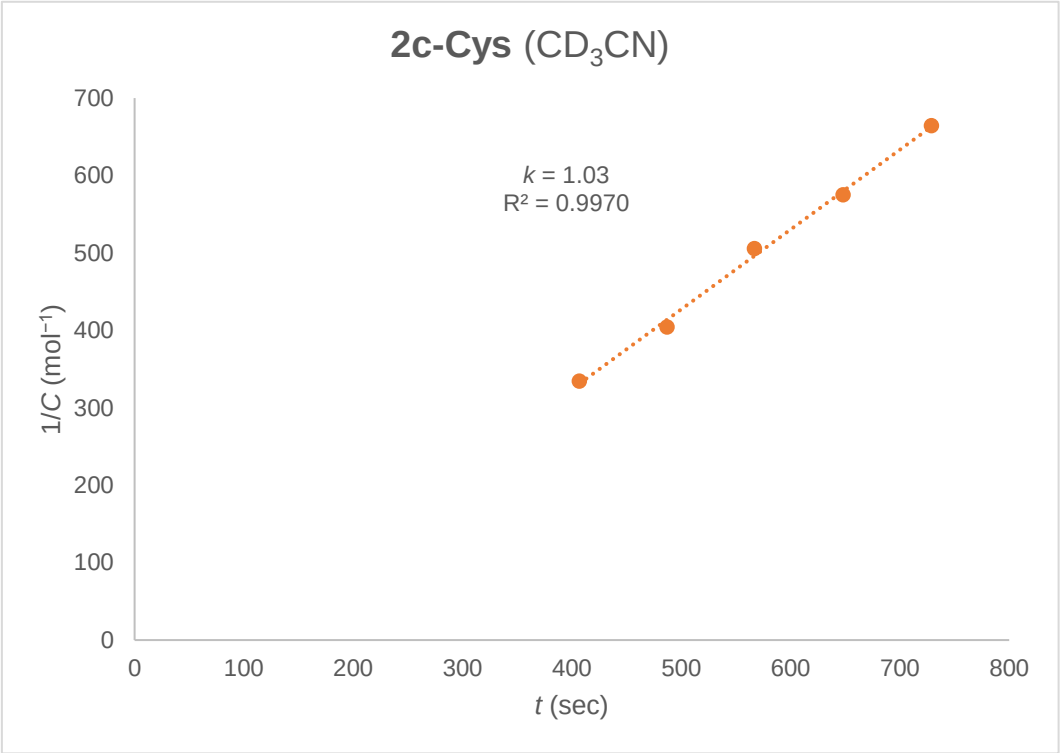
Conversion rate is calculated for (4).

$$Conversion\ rate = \frac{S_p}{S_r + S_p} \times 100 \tag{4}$$

Table S1. Results of reaction monitoring by NMR

Ac-AA-OMe	Cys			His			Ser			Tyr			Lys•HCl		
Solv.	CD_3CN	H_2O	PBS	CD_3CN	H_2O	PBS	CD_3CN	H_2O	PBS	CD_3CN	H_2O	PBS	CD_3CN[d]	H_2O	PBS
13	n.r.			n.r.			n.r.			n.r.			n.r.		
3b	n.r.			n.r.			n.r.			n.r.			n.r.		
2b	50 sec[a]			1300 min[a]			n.r.			n.r.			10% (48 h)[b]		
9b	n.r.			190 min[a]			n.r.			n.r.			22% (48 h)[b]		
2t	n.r.	42%[b] (52 h)	11 min[a]	n.r.	n.r.	n.r.	n.r.	n.r.	n.r.	n.r.	n.r.	n.r.	n.r.	n.r.	n.r.
15	n.r.	n.r.	52%[b] (46 h)	n.r.	n.r.	n.r.	n.r.	n.r.	n.r.	n.r.	n.r.	n.r.	n.r.	n.r.	n.r.
16	n.r.	63%[b] (48 h)	63 min[a]	n.r.	n.r.	n.r.	n.r.	n.r.	n.r.	n.r.	n.r.	n.r.	n.r.	n.r.	n.r.
8	n.r.	1.8 min[a]	< 50 sec[a]	1600 min[a]	3800 min[a]	230 min[a]	n.r.	n.r.	n.r.	n.r.	n.r.	n.r.	17% (48 h)[b]		13% (24 h)[b]
5	3.7 min[a]														
10	n.r.	24%[b] (50 h)	64 min[a]	n.r.	n.r.	n.r.	S	n.r.	n.r.	n.r.	n.r.	n.r.	n.r.	n.r.	n.r.
6		61 min[a]	40 min[a]		190 min[a]	360 min[a]		n.r.	n.r.		n.r.	n.r.		n.r.	22% (24 h)[b]
7		< 2.0 min[a]	< 50 sec[a]		190 min[a]	170 min[a]		n.r.	n.r.		n.r.	n.r.		5% (24 h)[b]	11% (24 h)[b]

Concentration: Amide or sulfonamide (20 mM) and protected amino acid (Ac-AA-OMe) (30 mM) were used. The analytical method involved CD_3CN for ^{1}H-NMR, and H_2O and PBS for NoD NMR (2.5 v/v% DMSO-d_6 added to H_2O and PBS). n.r.: no reaction. a: Half-life of amide or sulfonamide ($t_{1/2}$), c: The conversion rate (%) of the amide or sulfonamide was recorded as NMR yields for reactions with a half-life of more than 24 hours or those that stopped halfway., c: Solvent is CD_3CN:H_2O = 19:1.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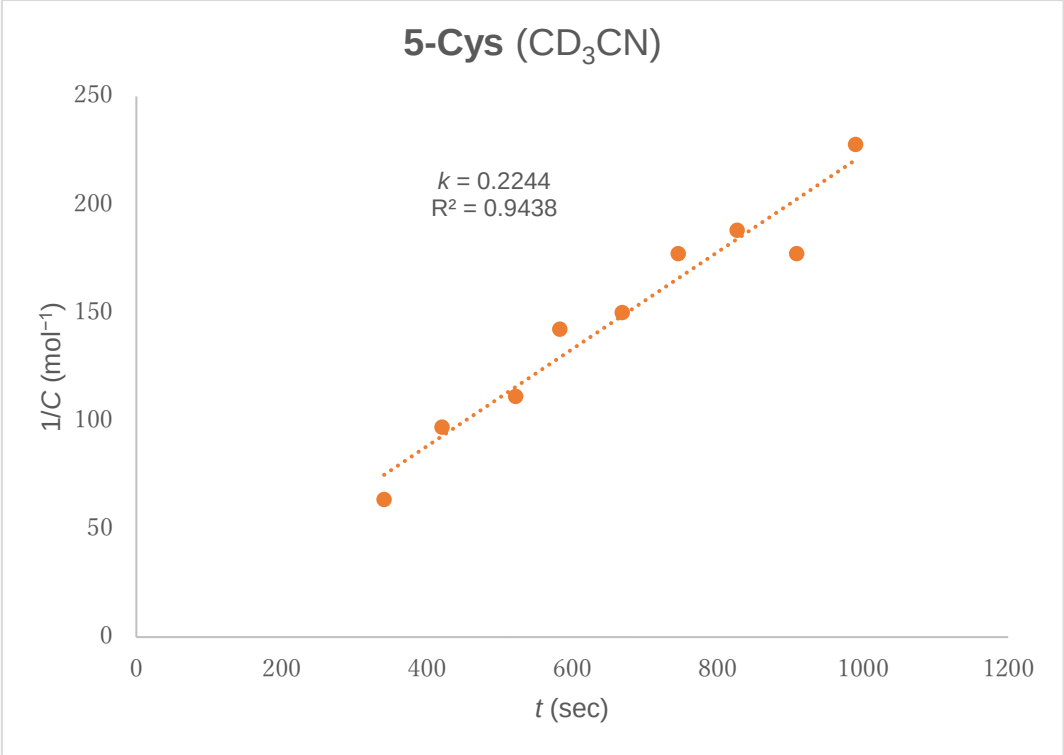
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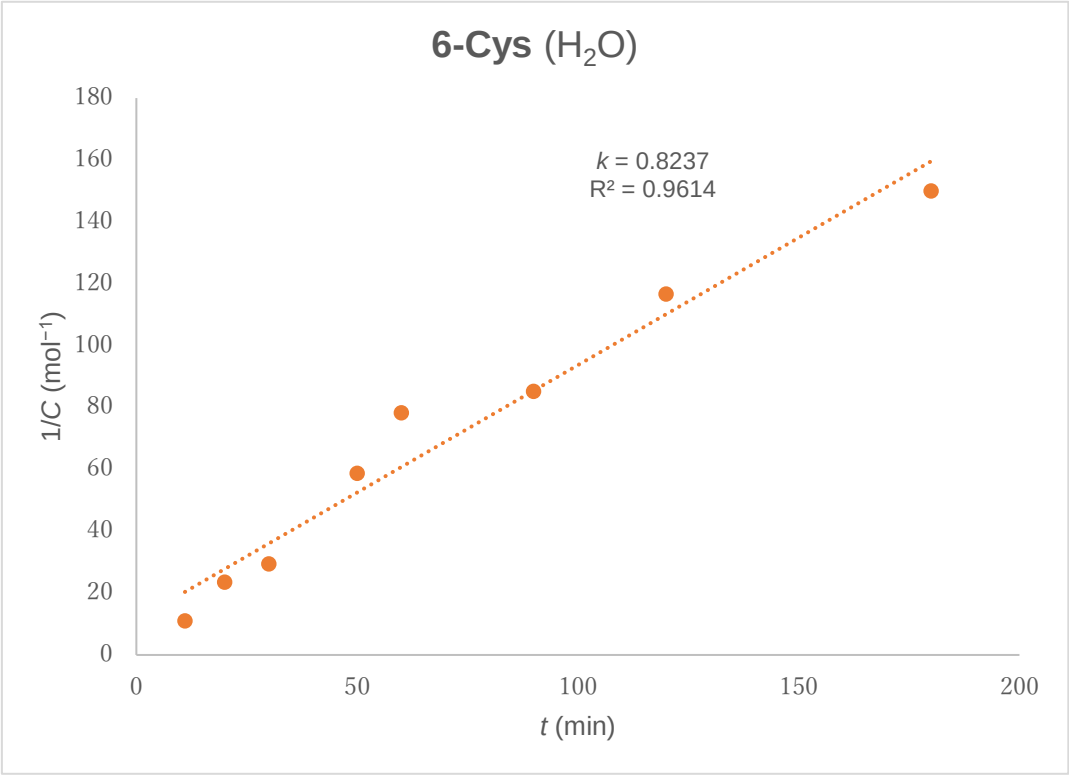
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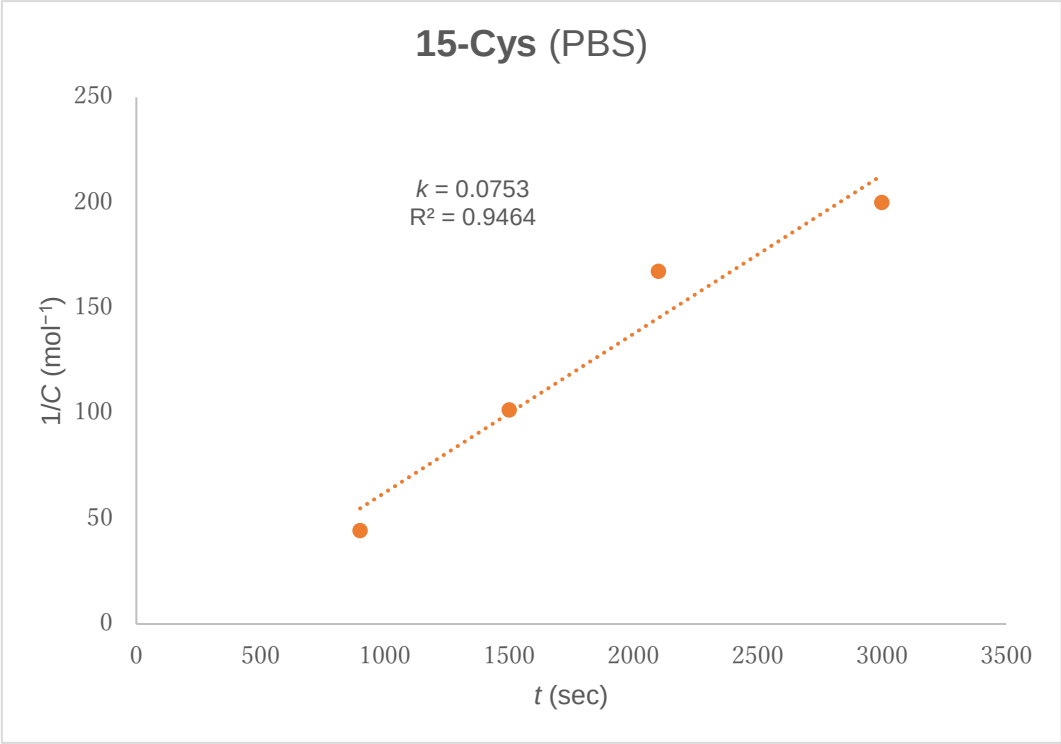
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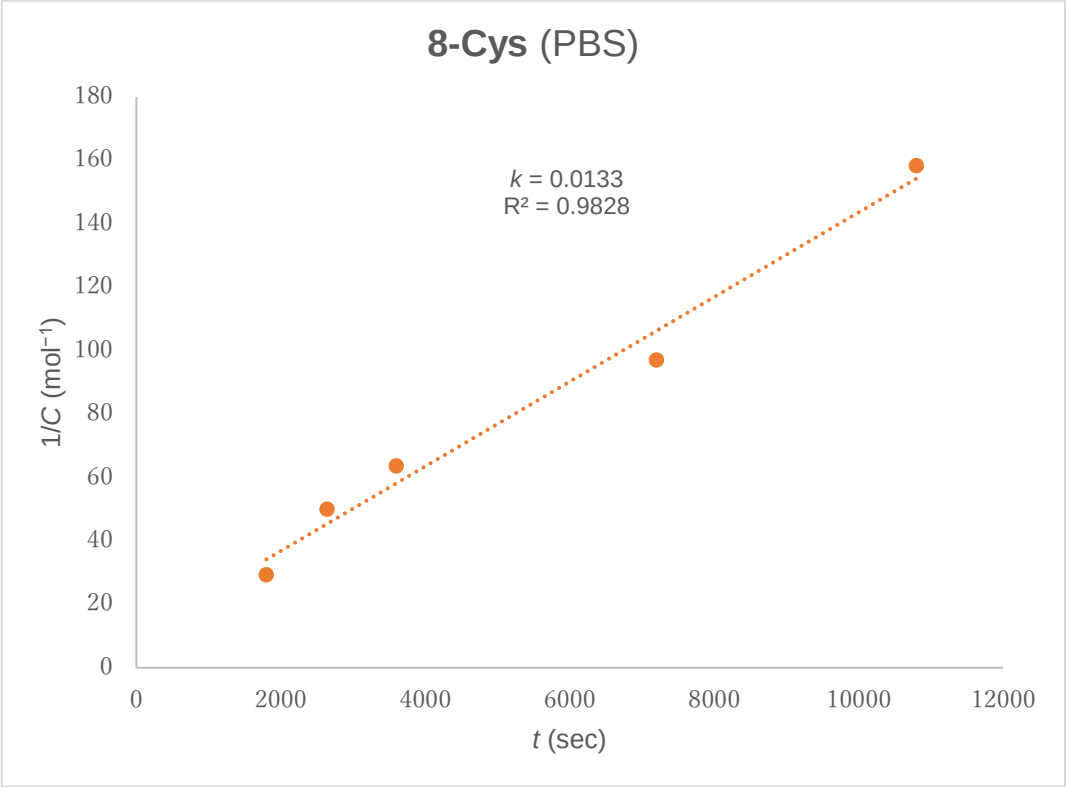
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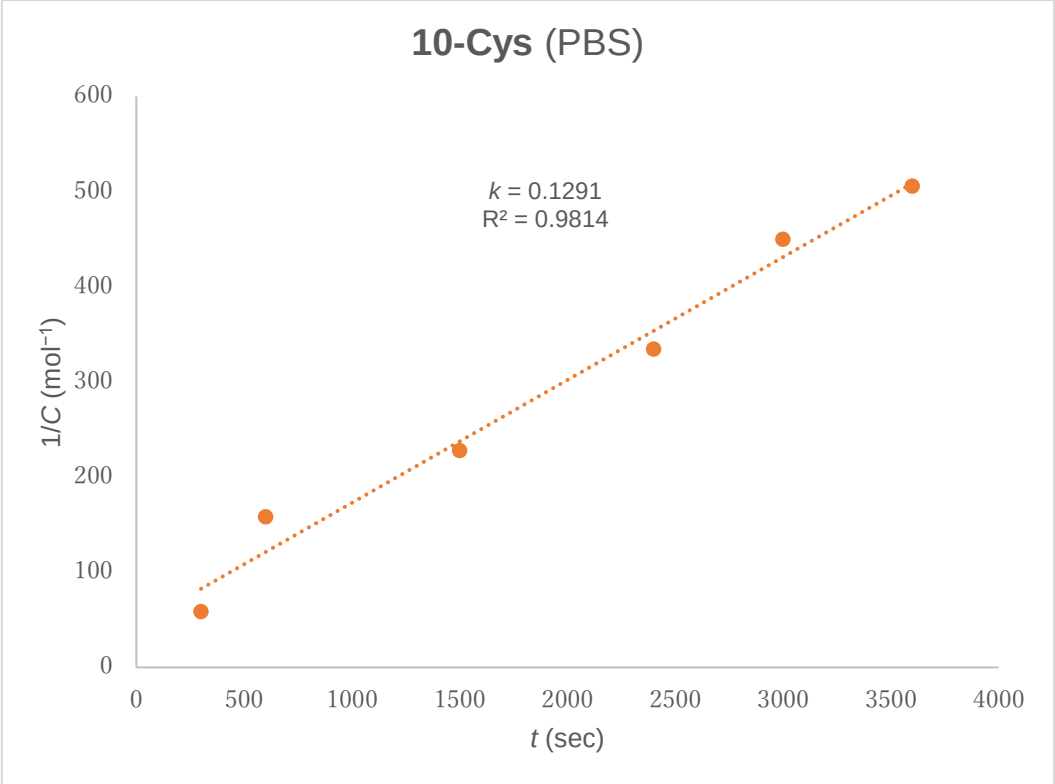
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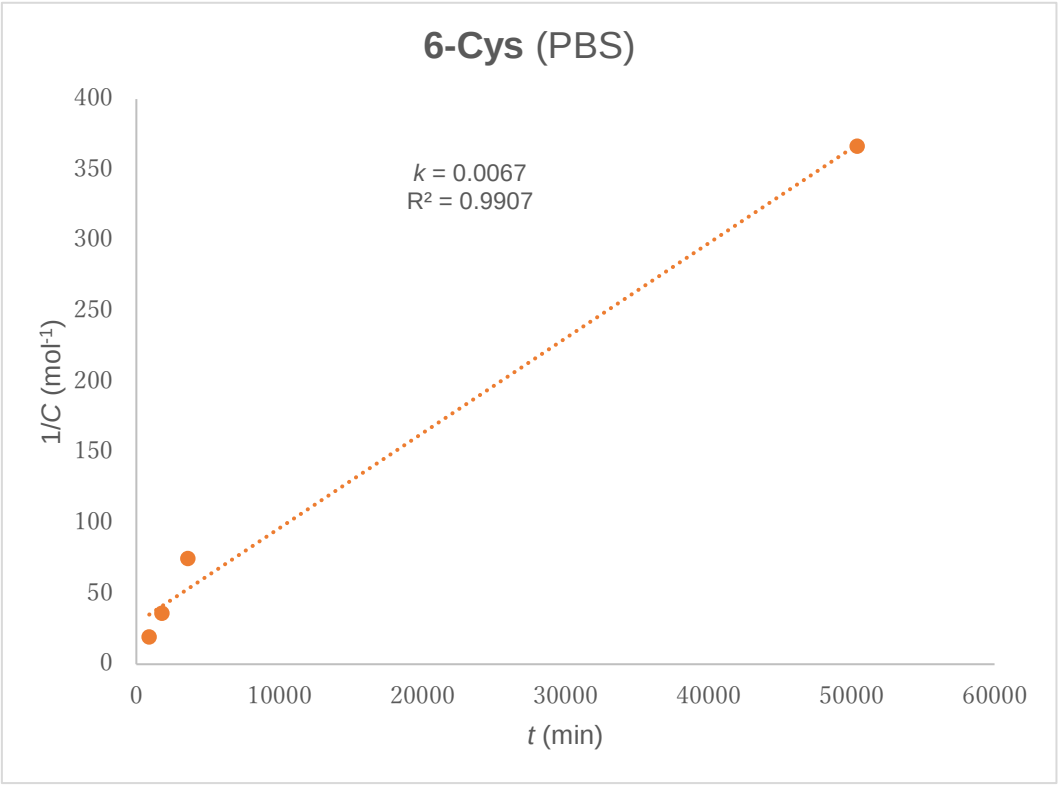
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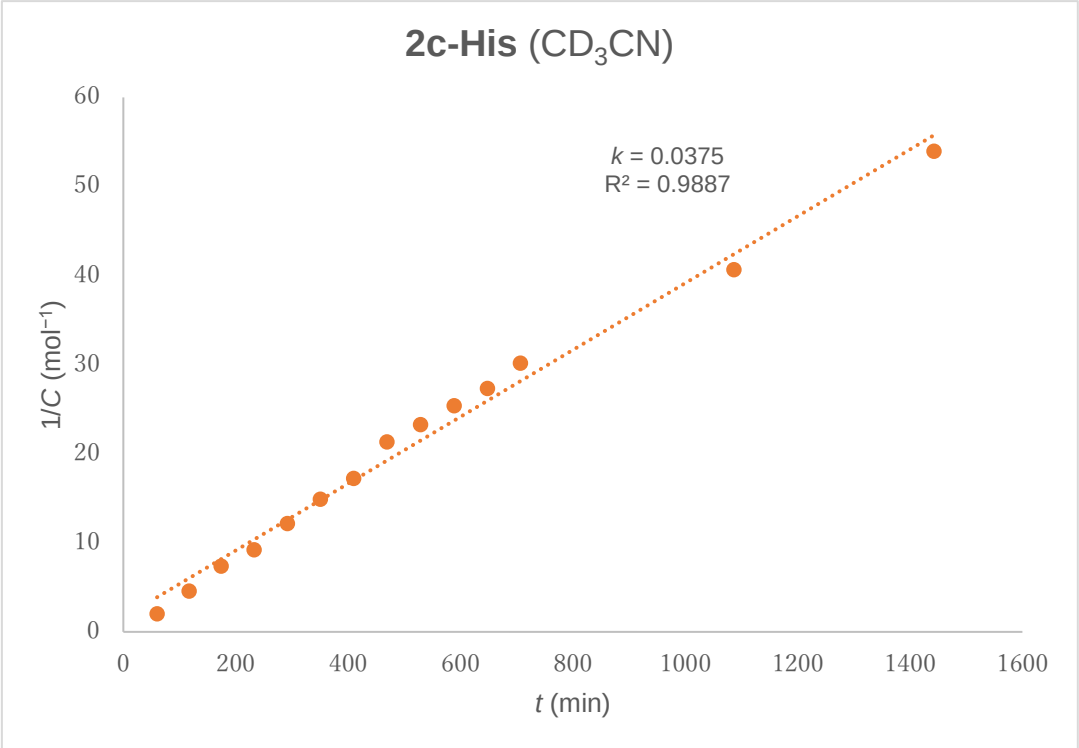
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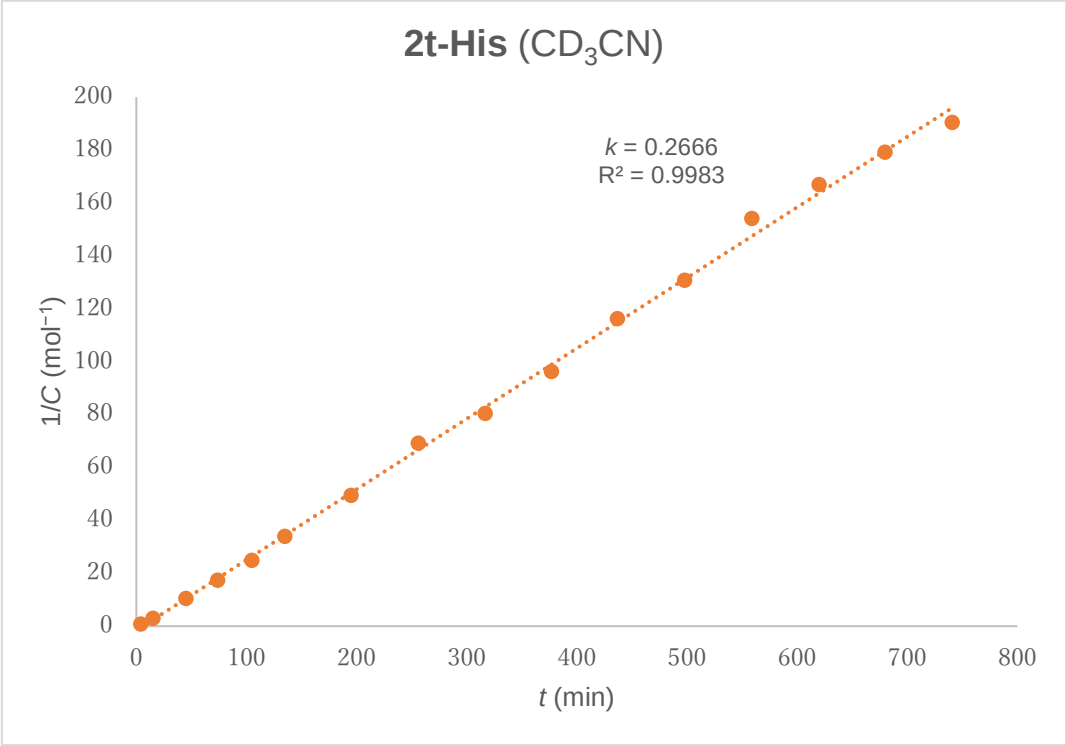
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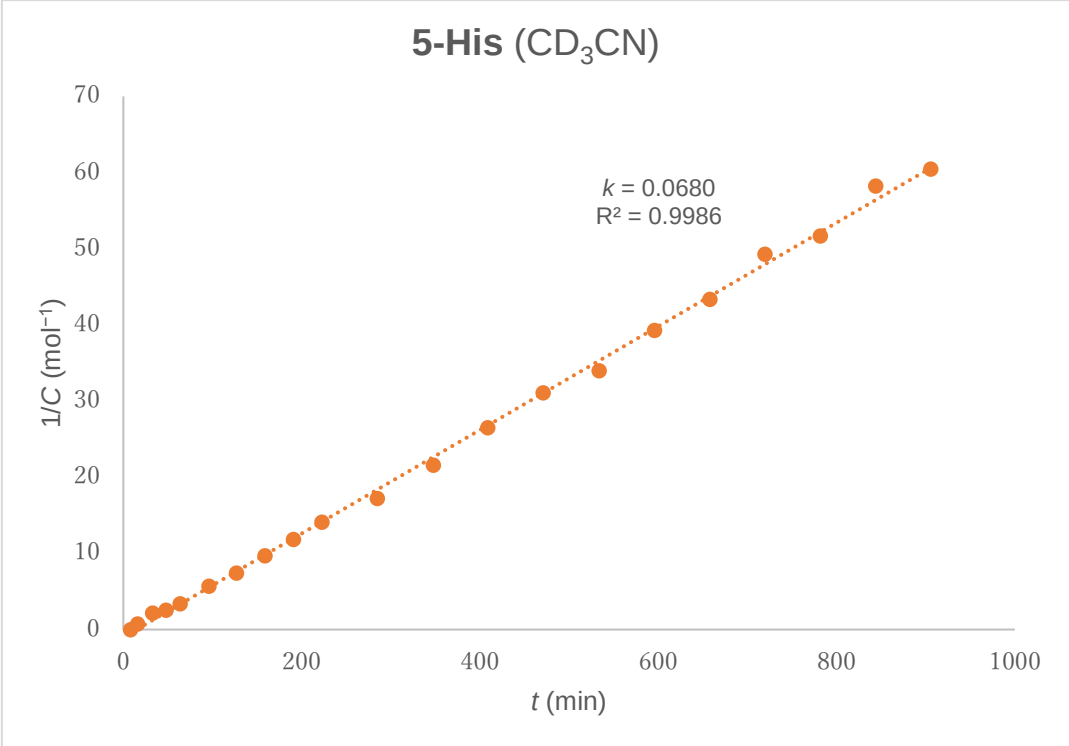
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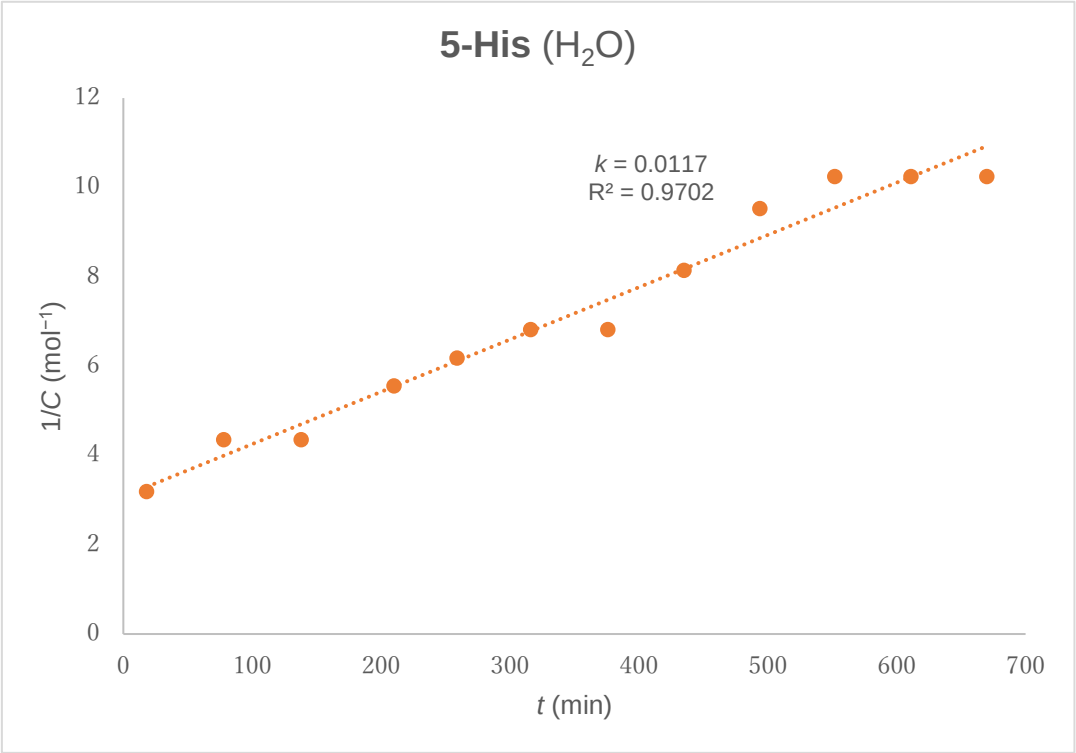
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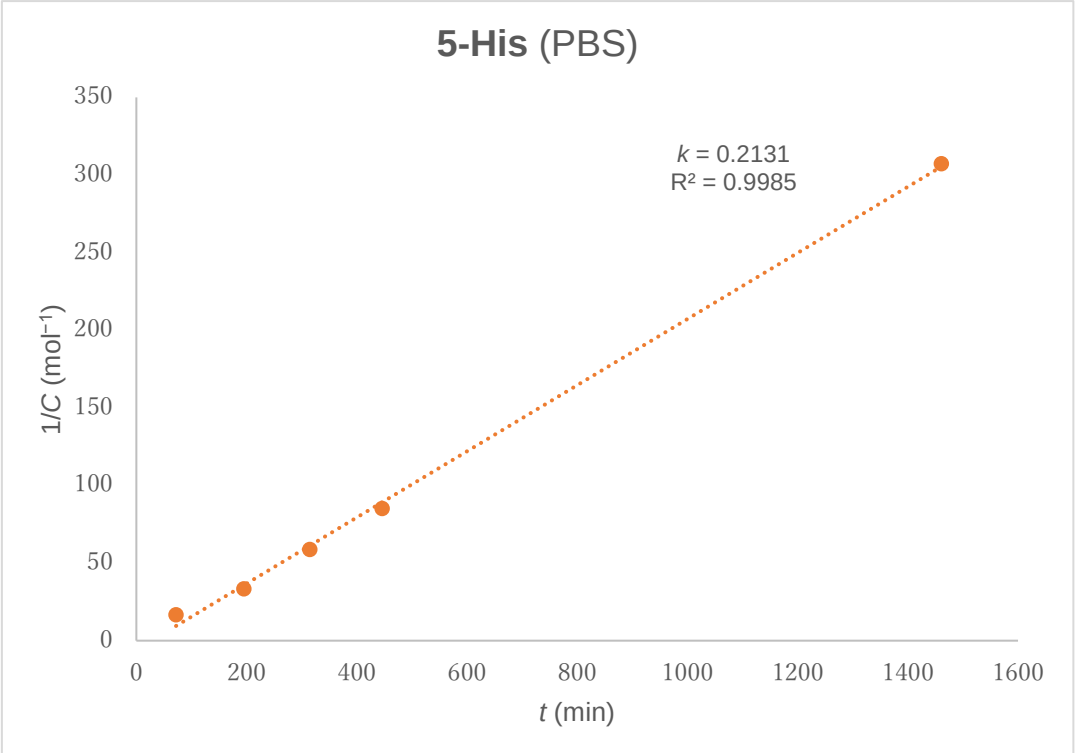
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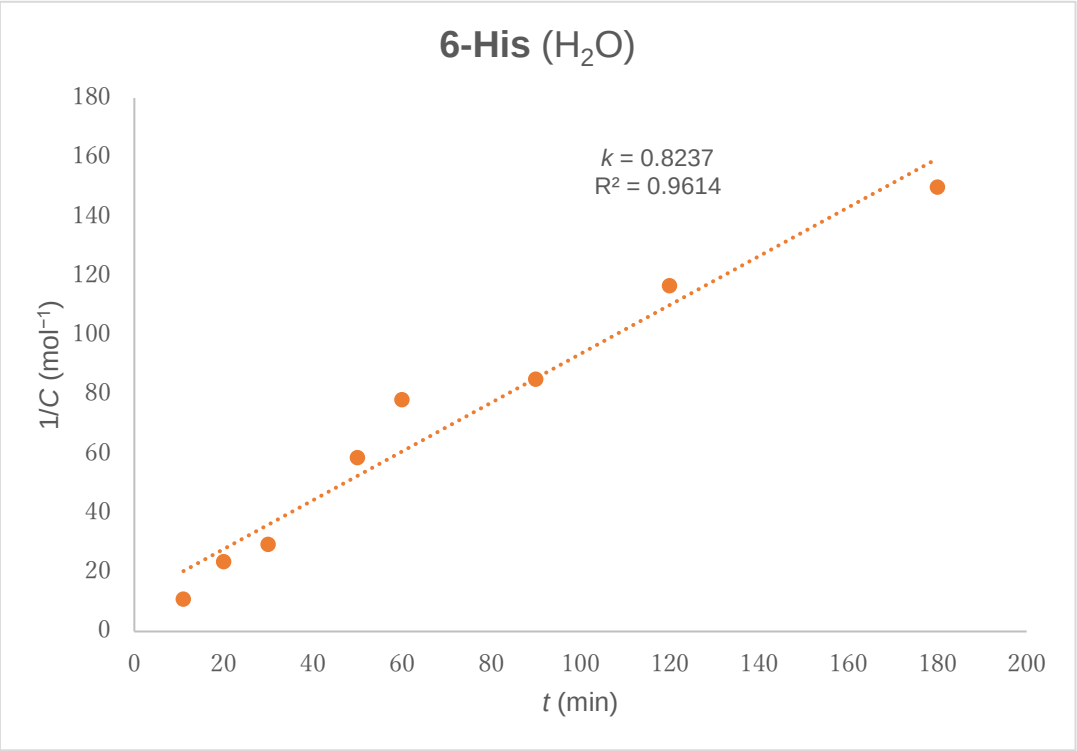
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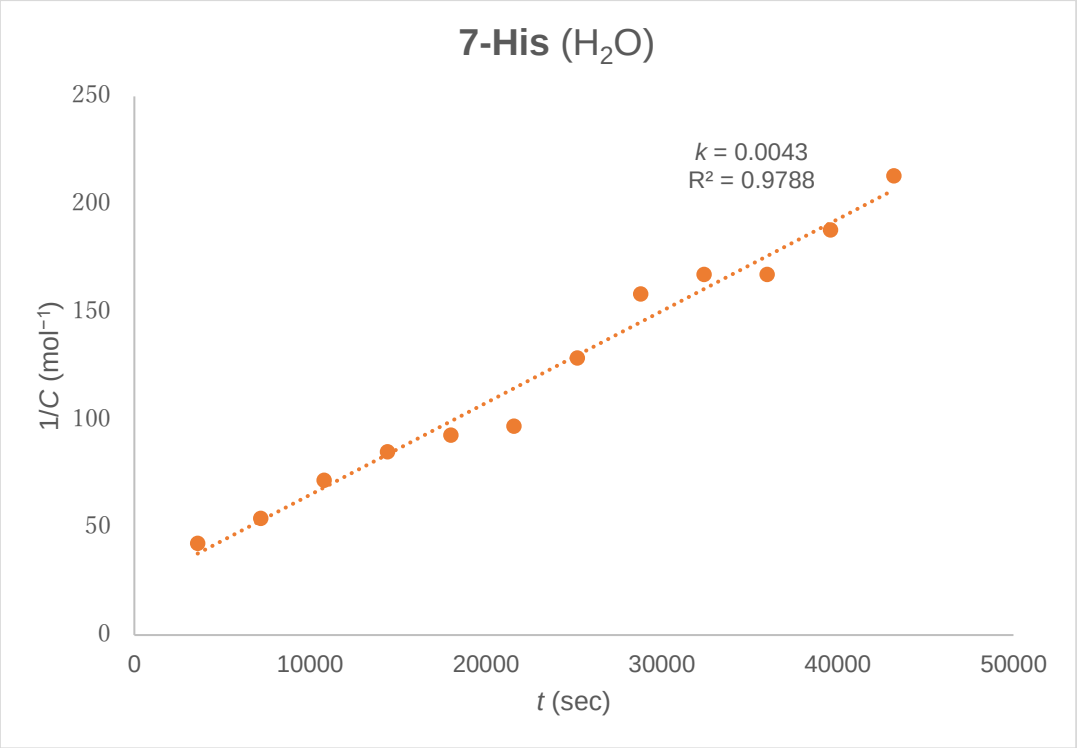
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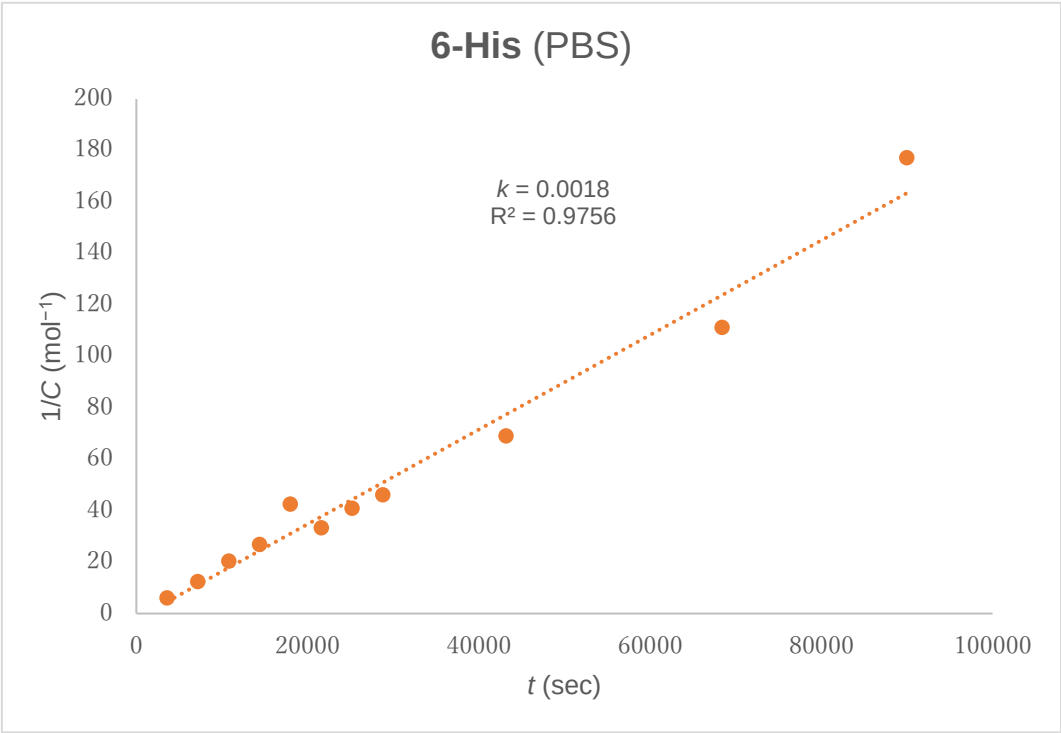
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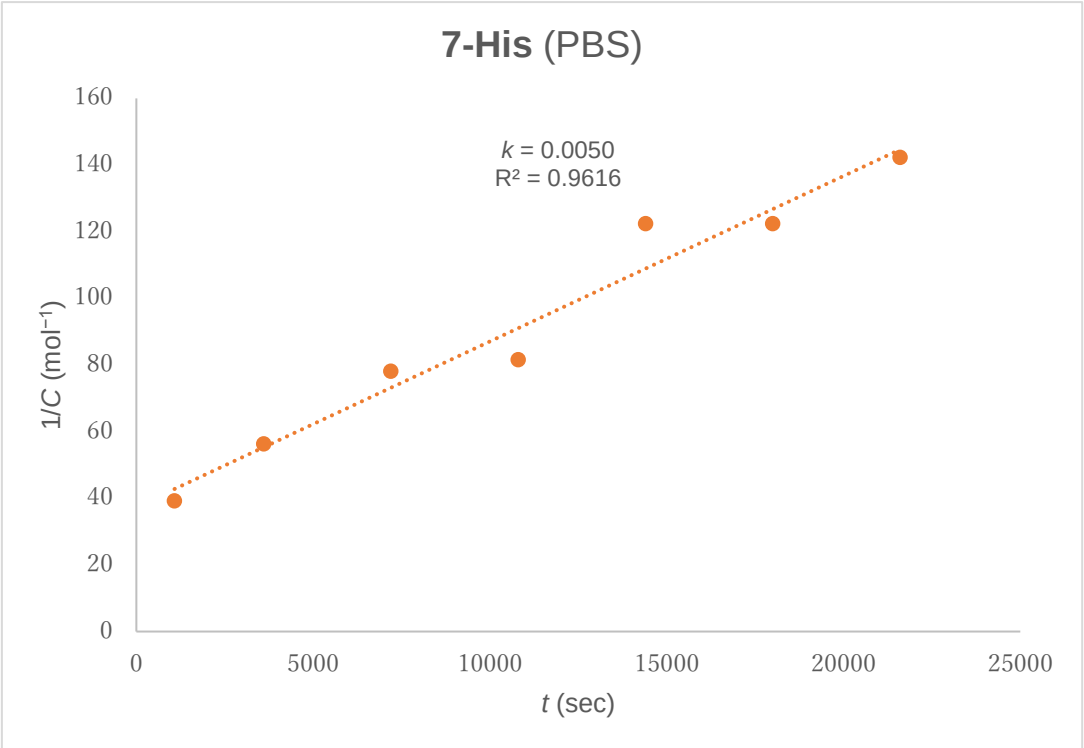
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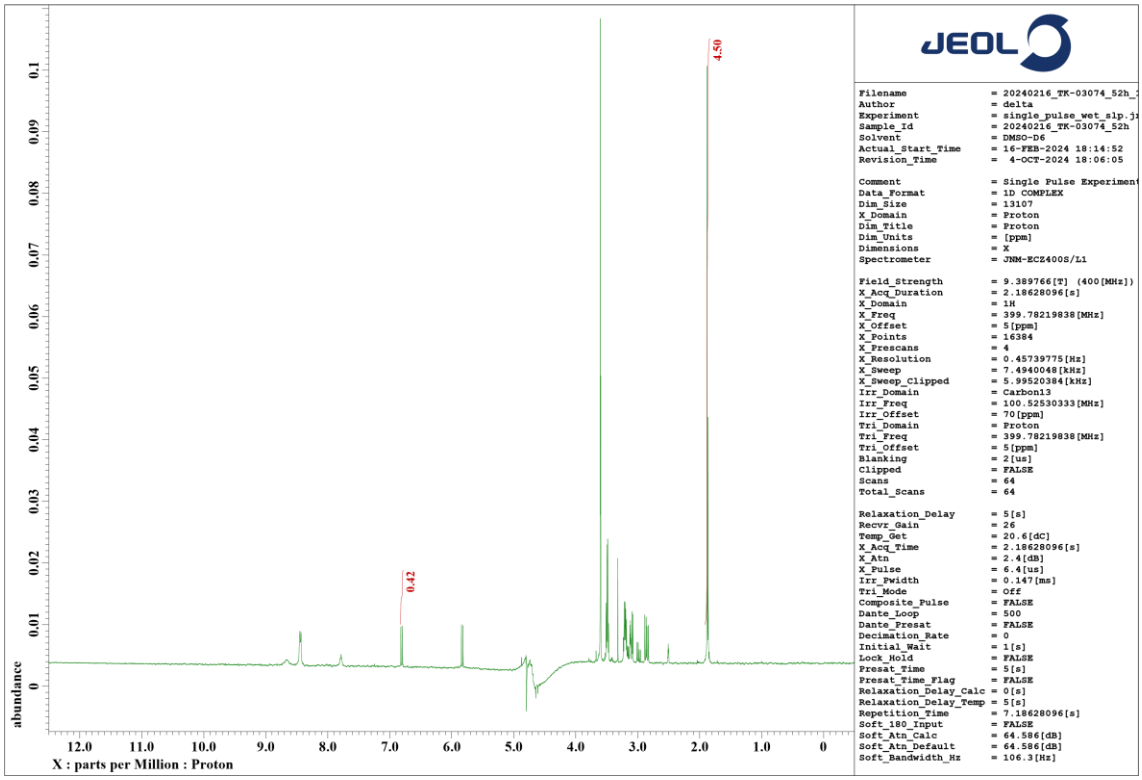
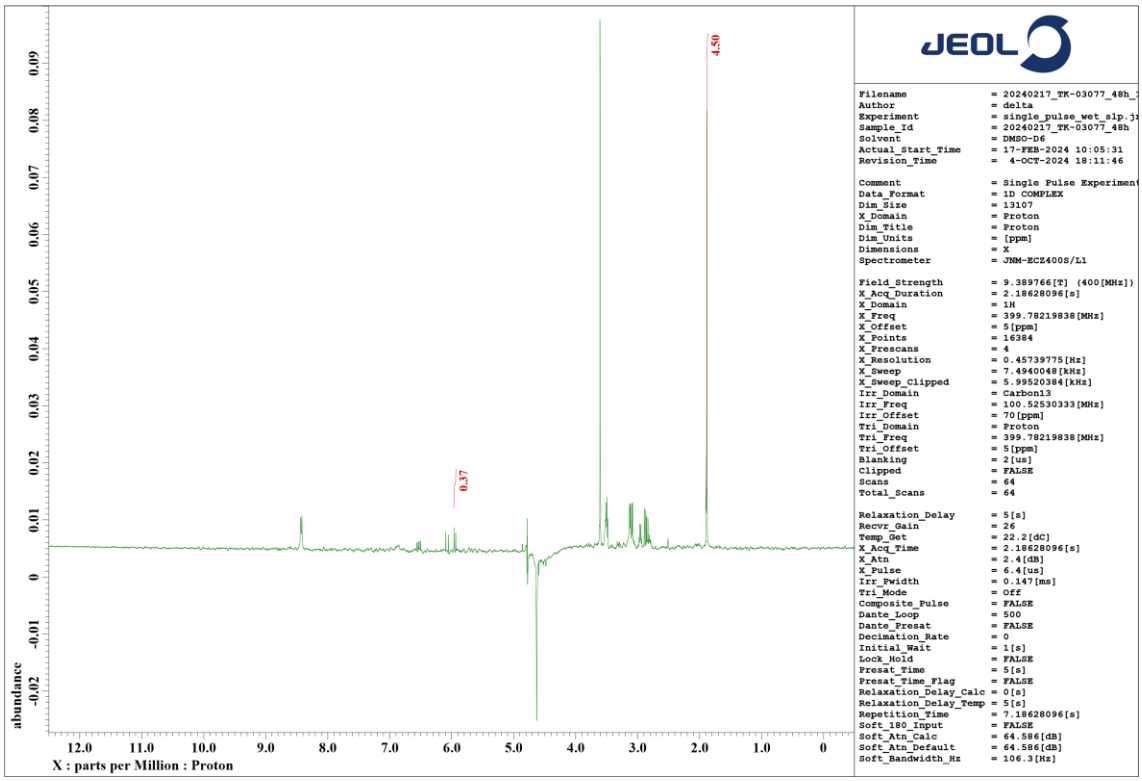
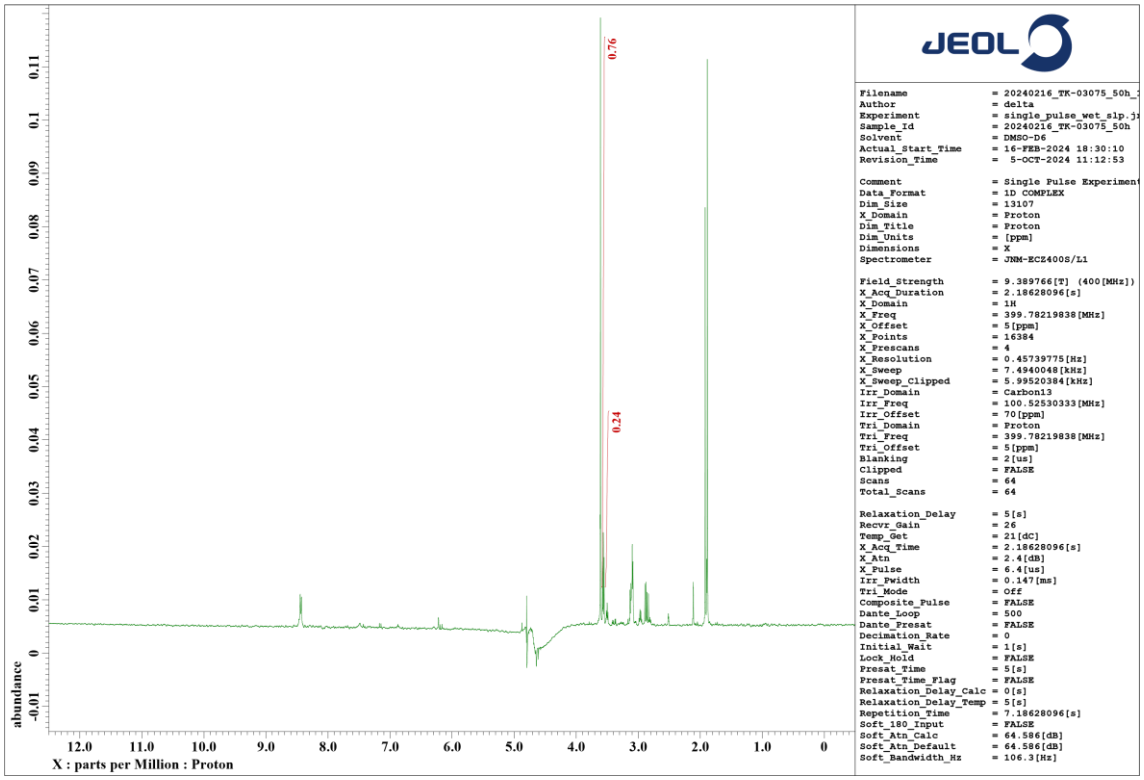
15-Cys (H_2O, 52 h)



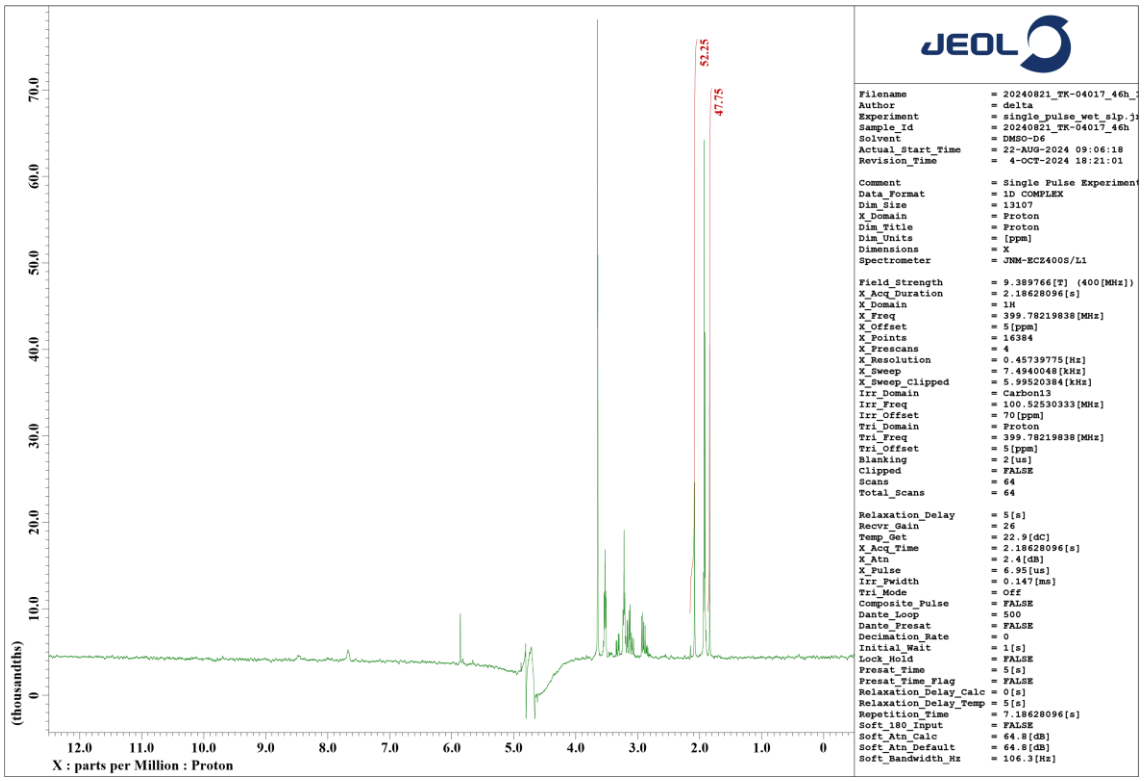
8-Cys (H_2O, 48 h)



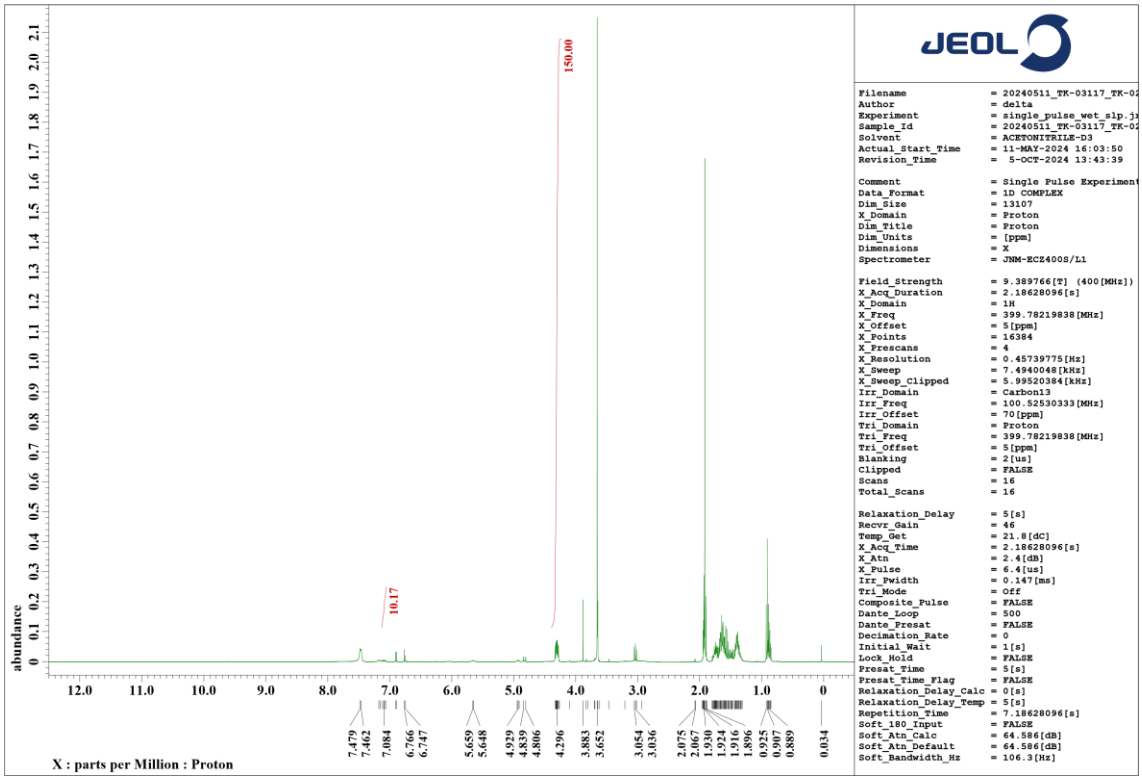
10-Cys (H_2O, 24 h)



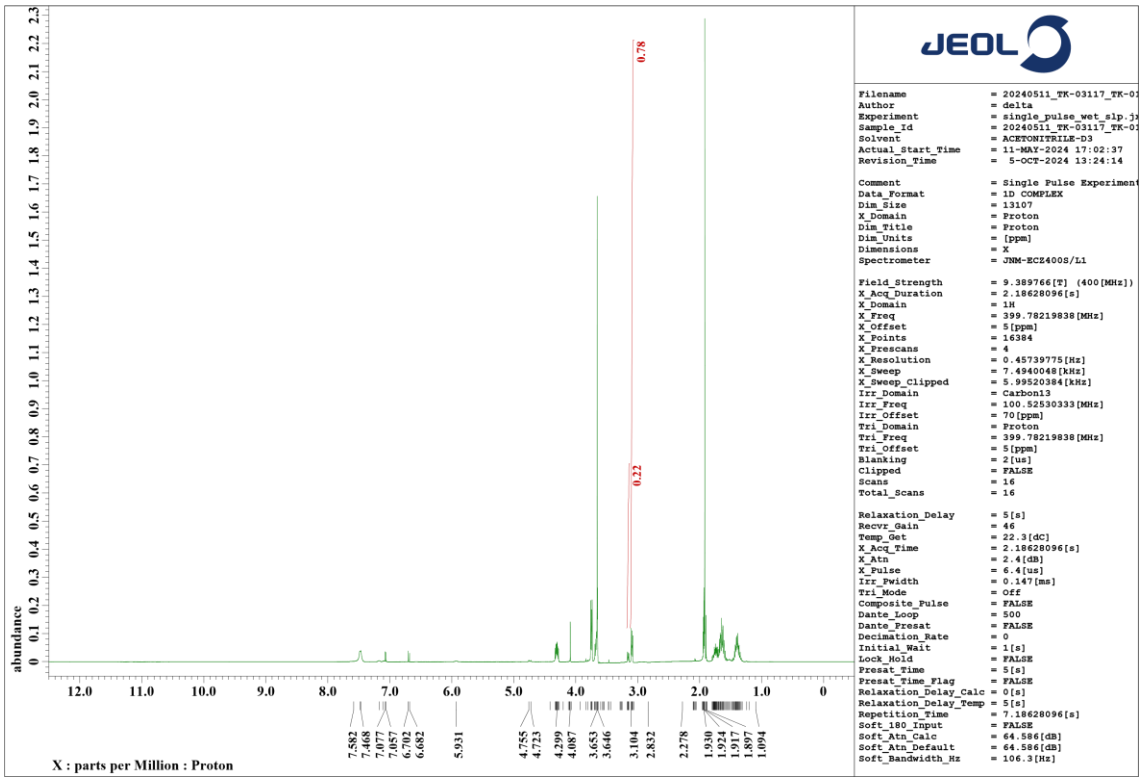
16-Cys (PBS, 46 h)



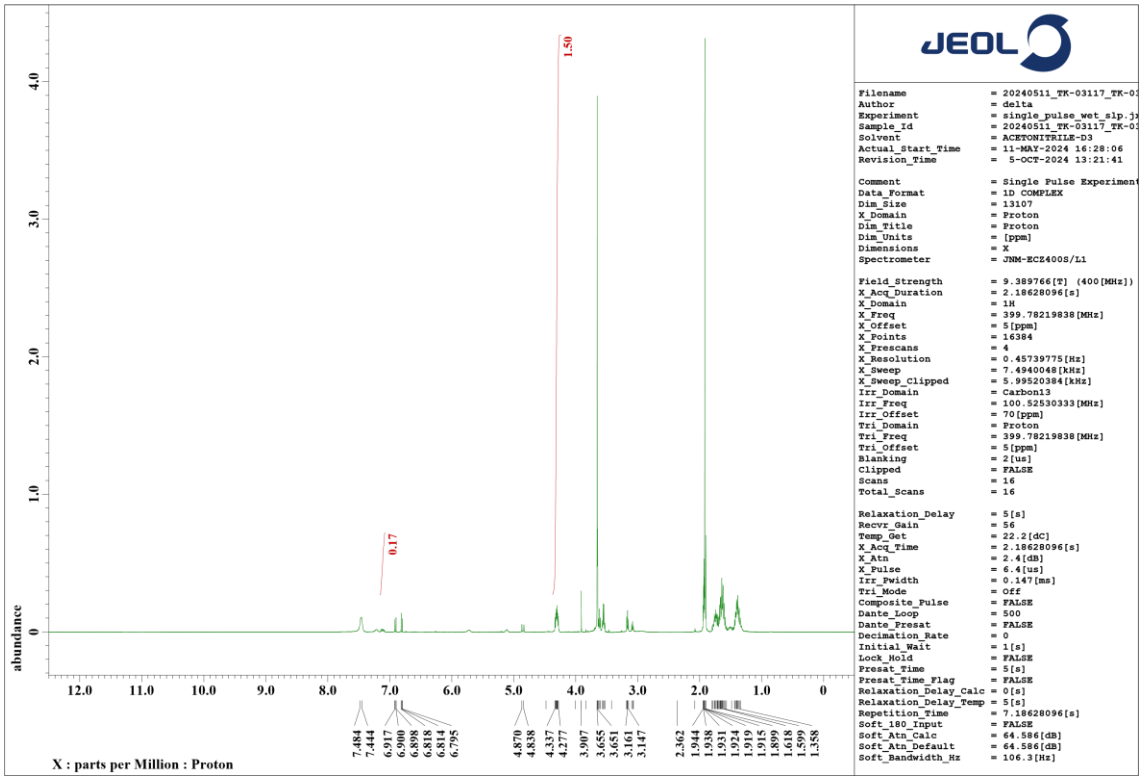
2c-Lys·HCl (CD_3CN, 48 h)



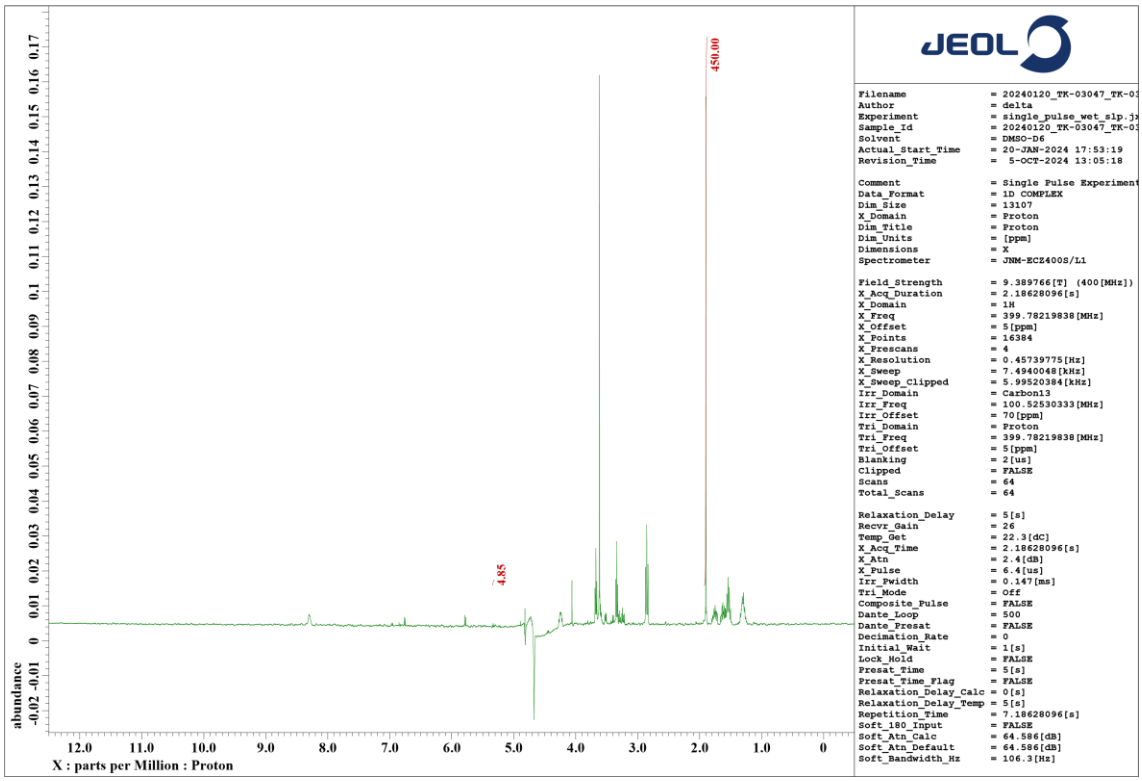
2t-Lys·HCl (CD_3CN, 48 h)



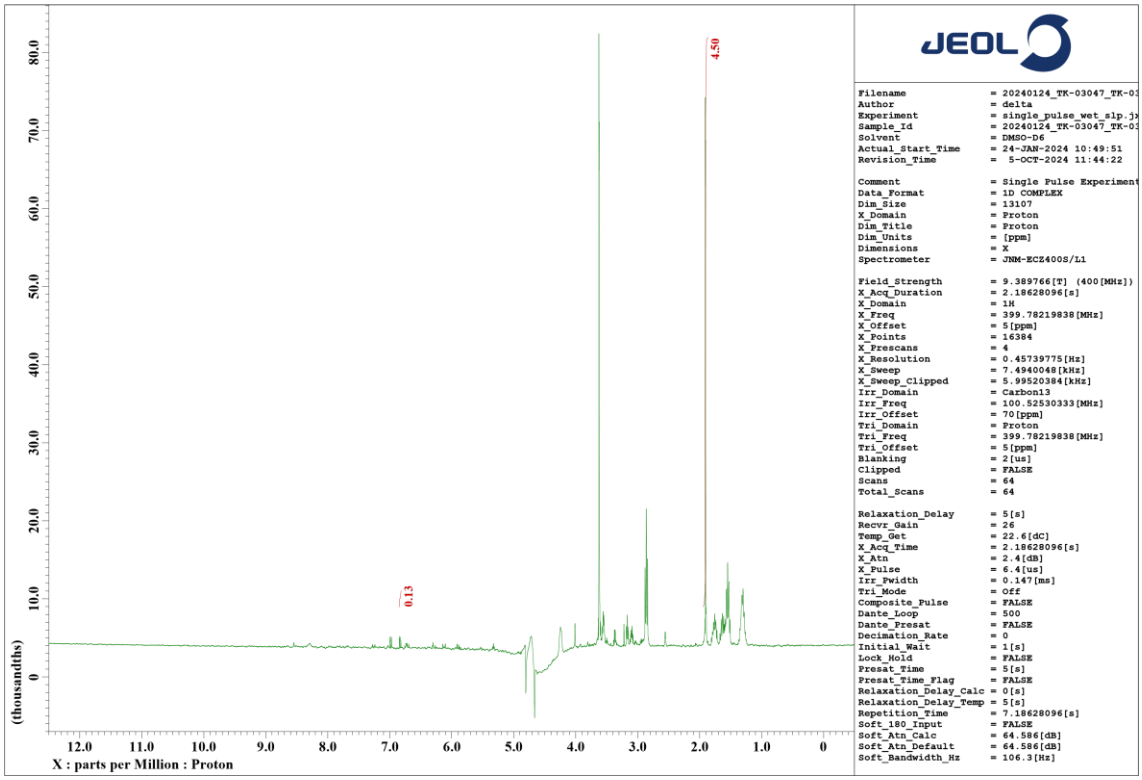
5-Lys·HCl (CD_3CN, 48 h)



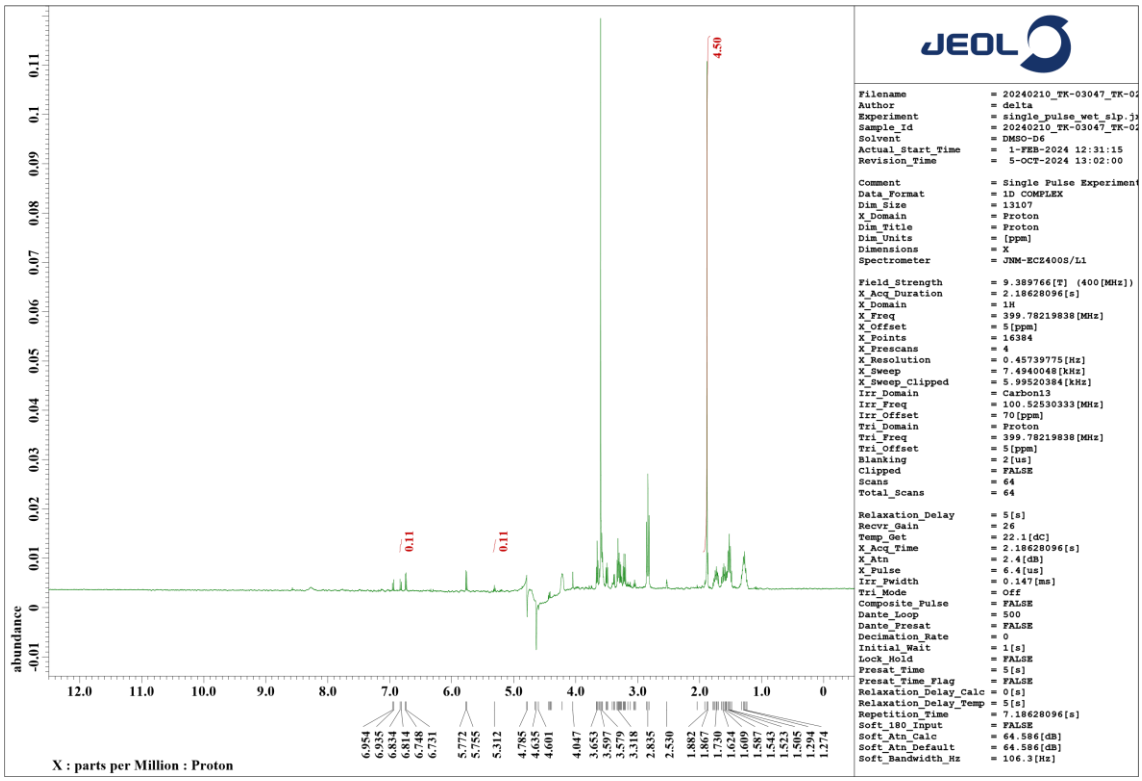
7-Lys·HCl (H_2O, 48 h)



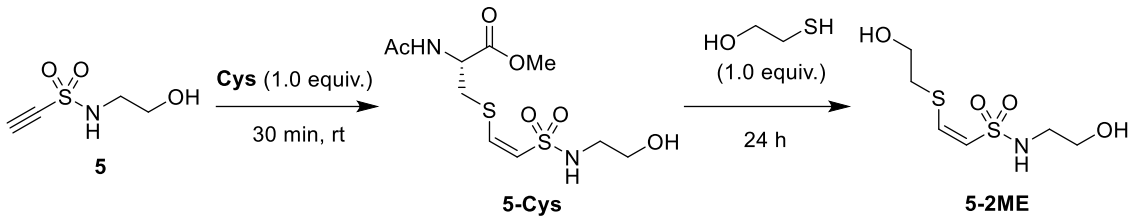
5-Lys·HCl (PBS, 48 h)



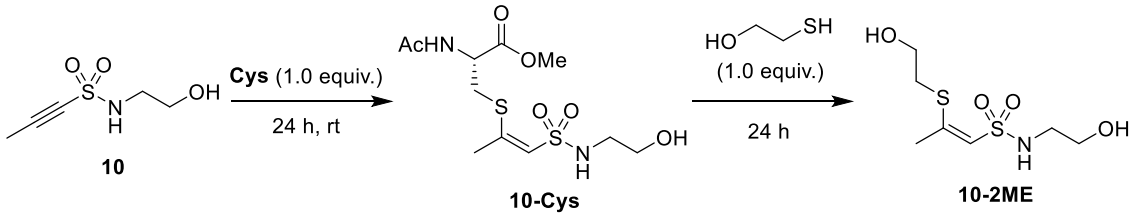
5-Lys·HCl (PBS, 48 h)



The reversibility of the conjugate addition



The **5** (300 μL, 40 mM solution in PBS) and **Cys** (300 μL, 40 mM solution in PBS) were added to the NMR tube and mixed by shaking up and down, then the foam was removed by ultrasound. The reaction mixture was allowed to stand at room temperature for 30 minutes. After, 2-mercaptoethanol (0.854 μL, 1.0 equiv.) was added, and the mixture was shaken up and down again. Foam was removed by ultrasound. The reaction mixture was subsequently allowed to stand at room temperature or 37 °C for 24 hours. DMSO-d_6 (15 μL) was added to the reaction mixture, and it was analyzed by NoD-NMR.



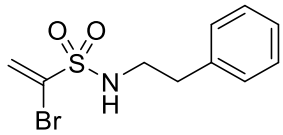
The **10** (300 μL, 40 mM solution in PBS) and **Cys** (300 μL, 40 mM solution in PBS) were added to the NMR tube and mixed by shaking up and down, then the foam was removed by ultrasound. The reaction mixture was allowed to stand at room temperature for 24 hours. After, 2-mercaptoethanol (0.854 μL, 1.0 equiv.) was added, and the mixture was shaken up and down again. Foam was removed by ultrasound. The reaction mixture was subsequently allowed to stand at room temperature or 37 °C for 24 hours. DMSO-d_6 (15 μL) was added to the reaction mixture, and it was analyzed by NoD-NMR.

Table S2 The reversibility of the conjugate addition

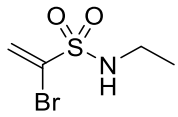
Entry	Sulfonamide	Temp. (°C)	**Cys** adducts:**2-ME** adducts
1	5	rt	No reaction
2	5	37	72:28
3	10	rt	No reaction
4	10	37	83:17

Cys adducts**:2-ME** adducts ratio by NMR

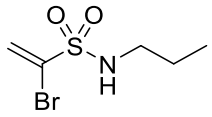
Characterization Data



1-Bromo-*N*-phenethylethene-1-sulfonamide (**1a**): Prepared as shown in general procedure 2; yellow oil; eluent (Hexane:EtOAc = 5:1, v/v); yield, 90%. FT-IR (ATR) ν cm^{-1}: 3303 (m), 3019 (w), 3028 (w), 2927 (w), 1604 (w), 1497 (w), 1455 (w), 1417 (w, 1337 (s), 1167 (s), 1095 (m), 1031 (w). ^{1}H-NMR (400 MHz, $CDCl_3$) δ 7.35–7.20 (m, 5H), 6.83 (d, J = 2.8 Hz, 1H), 6.19 (d, J = 2.8 Hz, 1H), 4.59 (br, 1H), 3.33 (q, J = 6.8 Hz, 2H), 2.90 (t, J = 6.8 Hz, 2H). ^{13}C-NMR (101 MHz, $CDCl_3$) δ 137.3, 128.9, 128.8, 128.4, 127.1, 127.0, 44.6, 35.8. LRMS (EI): m/z (%) 91 (81) [M – $C_3H_5NO_2SBr$], 198 (base peak) [M – C_7H_7], 289 (3) [M]. HRMS (EI): m/z calculated for $C_{10}H_{12}NO_2SBr$ 288.97721; found 288.9782 $[M]^+$ (error +3.4 ppm).

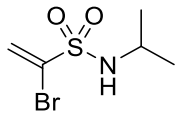


1-Bromo-*N*-ethylethene-1-sulfonamide (**1b**): Prepared as shown in general procedure 2; colorless oil; eluent (Hexane:EtOAc = 2:1, v/v); yield, 84%. FT-IR (NaCl) ν cm^{-1} : 3296 (s), 3113 (w), 2982 (m), 2939 (w), 2879 (w), 1604 (m), 1425 (s), 1333 (vs), 1165 (vs), 1093 (s), 949 (s), 860 (m), 783 (s), 600(s). ^{1}H-NMR (400 MHz, $CDCl_3$) δ 6.86 (d, J = 2.9 Hz, 1H), 6.22 (d, J = 2.9 Hz, 1H), 4.58 (br, 1H), 3.13 (qd, J = 7.2, 5.6 Hz, 2H), 1.25 (t, J = 7.2 Hz, 3H). ^{13}C-NMR (101 MHz, $CDCl_3$) δ 128.4, 127.3, 38.7, 15.1. LRMS (EI): m/z (%) 105 (21), [M – $C_2H_6NO_2S$], 134 (5), [M – Br], 198 (95) [M – CH_3], 213 (5) [M]. HRMS (EI): m/z calculated for $C_4H_8NO_2SBr$ 212.94529; found 212.9460 $[M]^+$ (error +0.5 ppm).

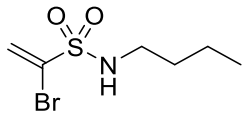


1-Bromo-*N*-propylethene-1-sulfonamide (**1c**): Prepared as shown in general procedure 2; colorless oil; eluent (Hexane:EtOAc = 4:1, v/v); yield, 89%. FT-IR (NaCl) ν cm^{-1}: 3300 (s), 3112 (w), 2968 (s), 2937 (m), 2877 (m), 1602 (m), 1423 (m), 1334 (s), 1245 (w), 1166 (s), 1092 (s), 1008 (m), 936 (m), 844 (w), 765 (m), 603 (m), 571 (w). ^{1}H-NMR (400 MHz, $CDCl_3$) δ 6.85 (d, J = 2.9 Hz, 1H), 6.21 (d, J = 2.9 Hz, 1H), 4.71 (br, 1H), 3.03 (td, J = 7.2, 6.0 Hz, 2H), 1.62 (sext, J = 7.2 Hz, 2H), 0.97 (t, J = 7.2 Hz, 3H). ^{13}C-NMR (101 MHz, $CDCl_3$) δ 128.3, 127.3, 45.3, 22.9, 11.1. LRMS (EI): m/z (%) 105

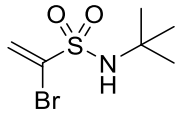
(12) [M – $C_3H_8NO_2S$], 198 (98) [M – C_2H_5], 227 (2) [M]. HRMS (EI): *m*/*z* calculated for $C_5H_{10}NO_2SBr$ 226.96156; found 226.9611 $[M]^+$ (error −2.1 ppm).



1-Bromo-*N*-isopropylethene-1-sulfonamide (**1d**): Prepared as shown in general procedure 2; off-white crystals; eluent (Hexane:EtOAc = 4:1, v/v); yield, 93%. FT-IR (KBr) *v* cm^{-1}: 3312 (s), 3294 (s), 3107 (w), 3013 (w), 2980 (m), 2933 (w), 1600 (w), 1464 (w), 1431 (m), 1392 (w), 1362 (w), 1339 (m), 1311 (m), 1162 (m), 1127 (s), 1090 (m), 1019 (m), 953 (m), 902(m), 832 (w), 757 (w), 719 (w), 607 (s), 569 (m). ^{1}H-NMR (400 MHz, $CDCl_3$) δ 6.86 (d, J = 2.9 Hz, 1H), 6.18 (d, J = 2.9 Hz, 1H), 4.59 (d, J = 6.0 Hz, 1H), 3.54 (oct, J = 6.4 Hz, 1H), 1.25 (d, J = 6.4 Hz, 6H). ^{13}C-NMR (101 MHz, $CDCl_3$) δ 128.3, 127.9, 47.0, 23.6. LRMS (EI): *m*/*z* (%) 105 (11) [M – $C_3H_8NO_2S$], 212 (99) [M – CH_3]. HRMS (EI): *m*/*z* calculated for $C_4H_7NO_2SBr$ 211.93809; found 211.9379 $[M - CH_3]^+$ (error −0.7 ppm).

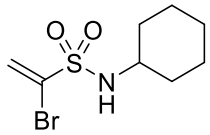


1-Bromo-*N*-butylethene-1-sulfonamide (**1e**): Prepared as shown in general procedure 2; yellow oil; eluent (Hexane:EtOAc = 4:1, v/v); yield, 90%. FT-IR (NaCl) *v* cm^{-1}: 3298 (s), 3112 (w), 2960 (s), 2935 (s), 2873 (m), 1603 (m), 1465 (m), 1427 (m), 1334 (s), 1165 (s), 1093 (m), 1034 (w), 937 (w), 760 (w), 603 (m), 574 (w). ^{1}H-NMR (400 MHz, $CDCl_3$) δ 6.85 (d, J = 2.9 Hz, 1H), 6.21 (d, J = 2.9 Hz, 1H), 4.69 (br, 1H), 3.05 (td, J = 6.7, 6.0 Hz, 2H), 1.57 (quin, J = 7.6 Hz, 2H), 1.39 (sext, J = 7.6 Hz, 2H), 0.94 (t, J = 7.3 Hz, 3H). ^{13}C-NMR (101 MHz, $CDCl_3$) δ 128.4, 127.2, 43.3, 31.5, 19.7, 13.5. LRMS (FAB): *m*/*z* (%) 242 (base peak) [M + H]. HRMS (FAB): *m*/*z* calculated for $C_6H_{13}NO_2SBr$ 241.98449; found 241.9851 $[M + H]^+$ (error +0.2 ppm).



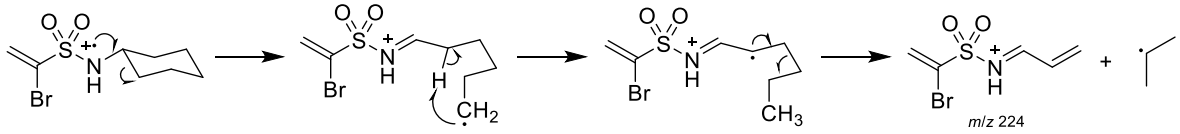
1-Bromo-*N*-(tert-butyl)ethene-1-sulfonamide (**1f**): Prepared as shown in general procedure 2; off-white crystals (cubic); eluent (Hexane:EtOAc = 4:1, v/v); yield, 92%. FT-IR (KBr) *v* cm^{-1}: 3273 (s), 3116 (w), 3030 (w), 2974 (m), 2875 (w), 1879 (w), 1604 (m), 1473 (w), 1435 (m), 1395 (m), 1369 (m), 1354 (w), 1323 (s), 1234 (m), 1211 (w), 1154 (s), 1090 (m), 1045 (w), 1014 (s), 939 (s), 867 (m), 769 (m), 701 (w), 611 (s), 583 (s). ^{1}H-NMR (400 MHz, $CDCl_3$) δ 6.85 (d, J = 2.9 Hz, 1H), 6.12 (d, J

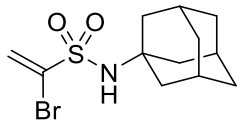
= 2.9 Hz, 1H), 4.67 (br, 1H), 1.37 (s, 9H). ^{13}C-NMR (101 MHz, $CDCl_3$) δ 131.2, 126.9, 55.4, 29.7. LRMS (EI): *m*/*z* (%) 226 (96) [M – CH_3]. HRMS (EI): *m*/*z* calculated for $C_5H_9NO_2SBr$ 225.95374; found 225.9542 $[M - CH_3]^+$ (error +2.0 ppm).



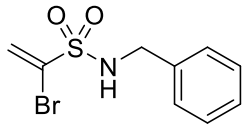
1-Bromo-*N*-cyclohexylethene-1-sulfonamide (**1g**): Prepared as shown in general procedure 2; off-white crystals; eluent (Hexane:EtOAc = 4:1, v/v); yield, 90%. FT-IR (KBr) *v* cm^{-1}: 3245 (s), 3109 (m), 3012 (w), 2935 (s), 2853 (m), 1603 (w), 1442 (m), 1353 (w), 1334 (s), 1166 (s), 1145 (m), 1100 (m), 1080 (s), 999 (w), 941 (m), 191 (w), 890 (m), 844 (w), 768 (m), 728 (w), 612 (s), 558 (s). ^{1}H-NMR (400 MHz, $CDCl_3$) δ 6.85 (d, *J* = 2.9 Hz, 1H), 6.17 (d, *J* = 2.9 Hz, 1H), 4.62 (d, *J* = 7.2 Hz, 1H), 3.25–3.16 (m, 1H), 2.03–1.96 (m, 2H), 1.74–1.68 (m, 2H), 1.62–1.54 (m, 1H), 1.38–1.13 (m, 5H). ^{13}C-NMR (101 MHz, $CDCl_3$) δ 128.6, 127.7, 53.4, 33.8, 25.1, 24.6. LRMS (EI): *m*/*z* (%) 98 [M – $C_2H_2NO_2SBr$], 224 (96) [M – C_3H_7], 267 (21) [M]. HRMS (EI): *m*/*z* calculated for $C_8H_{14}NO_2SBr$ 266.99286; found 266.9936 $[M]^+$ (error +2.6 ppm).

Note. McClafferty rearrangement.

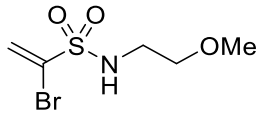




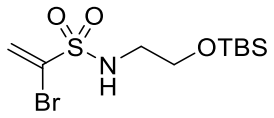
***N*-((3*s*,5*s*,7*s*)-Adamantan-1-yl)-1-bromoethene-1-sulfonamide** (**1h**): Prepared as shown in general procedure 2; off-white crystals; recrystallization (1,4-dioxane); yield, 82%. FT-IR (NaCl) *v* cm^{-1}: 3239 (s), 2955 (w), 2936 (m), 2903 (s), 2849 (w), 1604 (w), 1459 (m), 1450 (m), 1362 (m), 1346 (w), 1326 (s), 1254 (w), 1164 (s), 1120 (w), 1085 (m), 998 (m), 970 (w), 932 (m), 876 (w), 763 (m), 704 (w), 652 (w), 623 (m), 591 (m), 561 (m). ^{1}H-NMR (400 MHz, $CDCl_3$) δ 6.85 (d, *J* = 2.9 Hz, 1H), 6.10 (d, *J* = 2.9 Hz, 1H), 4.54 (br, 1H), 2.09 (br, 3H), 1.95 (d, *J* = 3.0 Hz, 6H), 1.65 (m, 6H). ^{13}C-NMR (101 MHz, $CDCl_3$) δ 131.8, 126.6, 55.8, 42.6, 35.8, 29.5. LRMS (ESI): *m*/*z* (%) 342 (28) [M + Na], 374 (96) [M + MeOH + Na] HRMS (ESI): *m*/*z* calculated for $C_{12}H_{18}NO_2NaSBr$ 342.01393; found 342.01544 $[M + Na]^+$ (error +4.41 ppm).



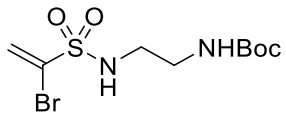
***N*-Benzyl-1-bromoethene-1-sulfonamide** (**1i**): Prepared as shown in general procedure 2; white crystals; eluent (Hexane:EtOAc = 4:1, v/v); yield, 84%. FT-IR (KBr) ν cm^{-1}: 3275 (s), 3119 (w), 3031 (w), 2872 (w), 1605 (m), 1496 (m), 1456 (m), 1415 (s), 1355 (m), 1333 (s), 1180 (m), 1089 (m), 1042 (m), 940 (m), 901 (m), 823 (w), 812 (w), 764 (s), 702 (s), 609 (s). ^{1}H-NMR (400 MHz, $CDCl_3$) δ 7.39–7.30 (m, 5H), 6.86 (d, J = 3.0 Hz, 1H), 6.21 (d, J = 3.0 Hz, 1H), 4.88 (br, 1H), 4.22 (d, J = 6.1 Hz, 2H). ^{13}C-NMR (101 MHz, $CDCl_3$) δ 135.6, 128.8, 128.7, 128.3, 128.1, 127.1, 47.7. LRMS (EI): m/z (%) 91 (22) [M – $C_2H_3NO_2SBr$], 106 (base peak) [M – $C_2H_2O_2SBr$], 275 (1) [M]. HRMS (EI): m/z calculated for $C_9H_{10}NO_2SBr$ 274.96156; found 274.9611 $[M]^+$ (error −1.7 ppm).



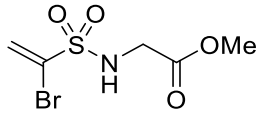
1-Bromo-*N*-(2-methoxyethyl)ethene-1-sulfonamide (**1j**): Prepared as shown in general procedure 2; colorless oil; eluent (Hexane:EtOAc = 2:1, v/v); yield, 81%. FT-IR (NaCl) ν cm^{-1}: 3605 (br), 3293 (br), 3112 (w), 2985 (w), 2932 (m), 2896 (m), 1603 (m), 1427 (m), 1390 (w), 1334 (s), 1197 (w), 1163 (s), 1124 (m), 1083 (s), 1025 (w), 945 (m), 867 (w), 801 (m), 759 (w), 600 (m). ^{1}H-NMR (400 MHz, $CDCl_3$) δ 6.85 (d, J = 2.9 Hz, 1H), 6.21 (d, J = 2.9 Hz, 1H), 5.09 (br, 1H), 3.53 (dd, J = 11.0, 6.1 Hz, 2H), 3.38 (s, 3H), 3.23 (td, J = 5.6, 4.4 Hz, 2H). ^{13}C-NMR (101 MHz, $CDCl_3$) δ 128.3, 127.3, 70.5, 58.9, 43.3. LRMS (FAB): m/z (%) 212 (93) [M – CH_3O], 224 (base peak) [M + H]. HRMS (FAB): m/z calculated for $C_{10}H_{11}NO_3SBr$ 243.96375; found 243.9642 $[M + H]^+$ (error −0.5 ppm).



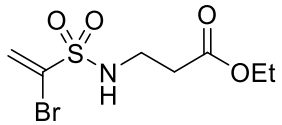
1-Bromo-*N*-(2-((*tert*-butyldimethylsilyl)oxy)ethyl)ethene-1-sulfonamide (**1k**): Prepared as shown in general procedure 2; colorless oil; eluent (Hexane:EtOAc = 9:1, v/v); yield, 77%. FT-IR (NaCl) ν cm^{-1}: 3304 (br), 3112 (w), 2953 (s), 2930 (s), 2884 (m), 2857 (s), 1604 (w), 1471 (m), 1407 (m), 1337 (s), 1256 (m), 1169 (s), 1093 (s), 1006 (w), 971 (m), 938 (m), 838 (s), 809 (m), 779 (m), 663 (w), 601 (m). ^{1}H-NMR (400 MHz, $CDCl_3$) δ 6.85 (d, J = 2.9 Hz, 1H), 6.22 (d, J = 2.9 Hz, 1H), 5.00 (br, 1H), 3.76 (t, J = 5.3 Hz, 2H), 3.15 (q, J = 5.3 Hz, 2H), 0.90 (s, 9H), 0.08 (s, 6H). ^{13}C-NMR (101 MHz, $CDCl_3$) δ 128.4, 127.1, 61.2, 45.7, 25.8, 18.2, -5.4. LRMS (ESI): m/z (%) 366 (95) [M + Na], 398 (34) [M + MeOH + Na], 709 (46) [2M + Na]. HRMS (ESI): m/z calculated for $C_{10}H_{22}NO_3NaSSiBr$ 366.01707; found 366.01732 $[M + Na]^+$ (error+0.67 ppm).



***tert*-Butyl (2-((1-bromovinyl)sulfonamido)ethyl)carbamate** (**1l**): Prepared as shown in general procedure 2; pale yellow oil; eluent (Hexane:EtOAc = 2:1, v/v); yield, 73%. FT-IR (NaCl) ν cm^{-1}: 3395 (m), 3310 (br), 3113 (w), 2979 (m), 2933 (w), 1691 (s), 1604 (w), 1519 (s), 1456 (w), 1394 (w), 1367 (m), 1336 (m), 1274 (w), 1254 (m), 1164 (s), 1099 (m), 939 (w), 915 (w), 733 (w). ^{1}H-NMR (400 MHz, $CDCl_3$) δ 6.84 (d, J = 2.9 Hz, 1H), 6.21 (d, J = 2.9 Hz, 1H), 5.57 (br, 1H), 4.92 (br, 1H), 3.32 (ddd, J = 11.2, 5.7 Hz, 2H), 3.20–3.16 (m, 2H), 1.45 (s, 9H). ^{13}C-NMR (101 MHz, $CDCl_3$) δ 156.8, 128.5, 127.1, 80.2, 44.4, 40.2, 28.4. LRMS (ESI): m/z (%) 295 (96) [M – C_4H_9 + H], 327 (33) [M + H], 351 (46) [M + Na], 679 (16) [2M + Na]. HRMS (ESI): m/z calculated for $C_9H_{17}NO_4NaSBr$ 350.99901; found 350.99946 [M + Na]$^+$ (error +1.28 ppm).

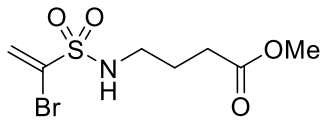


Methyl ((1-bromovinyl)sulfonyl)glycinate (**1m**): Prepared as shown in general procedure 2; colorless oil; eluent (Hexane:EtOAc = 3:1, v/v); yield, 21%. FT-IR (NaCl) ν cm^{-1}: 3624 (br), 3295 (br), 3114 (w), 3025 (w), 2956 (w), 1745 (s), 1603 (w), 1438 (m), 1339 (s), 1292 (w), 1221 (m), 1125 (m), 943 (w), 861 (m), 764 (w), 606 (m), 548 (w). ^{1}H-NMR (400 MHz, $CDCl_3$) δ 6.86 (d, J = 3.0 Hz, 1H), 6.22 (d, J = 3.0 Hz, 1H), 5.29 (br, 1H), 3.91 (d, J = 5.2 Hz, 2H), 3.81 (s, 3H). ^{13}C-NMR (101 MHz, $CDCl_3$) δ 168.9, 128.7, 126.8, 52.9, 44.5. LRMS (EI): m/z (%) 59 (10) [M – $C_3H_5NO_2SBr$], 105 (64) [M – $C_3H_6NO_4S$], 169 (8) [M – $C_3H_6NO_2$], 178 (86) [M – Br], 198 (base peak) [M – $C_2H_3O_2$], 228 (28) [M – CH_2O + H], 257 (1) [M], 258 (2) [M + H]. HRMS (EI): m/z calculated for $C_5H_9NO_4SBr$ 257.94302; found 257.9438 [M + H]$^+$ (error +0.7 ppm).

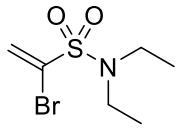


Ethyl 3-((1-bromovinyl)sulfonamido)propanoate (**1n**): Prepared as shown in general procedure 2; colorless oil; eluent (Hexane:EtOAc = 3:1, v/v); yield, 55%. FT-IR (NaCl) ν cm^{-1}: 3624 (br), 3292 (br), 3113 (w), 2984 (1604 (w), 1416 (m), 1378 (s), 1264 (m), 1193 (s), 1163 (s), 1096 (s), 1051 (m), 1026 (m), 943 (m), 819 (w), 787 (m), 600 (s), 569 (m). ^{1}H-NMR (400 MHz, $CDCl_3$) δ 6.86 (d, J = 2.9 Hz, 1H), 6.21 (d, J = 2.9 Hz, 1H), 5.41 (br, 1H), 4.19 (q, J = 7.1 Hz, 2H), 3.34 (q, J = 6.1 Hz, 2H), 2.63 (t, J = 5.9 Hz, 2H), 1.29 (t, J = 7.1 Hz, 3H). ^{13}C-NMR (101 MHz, $CDCl_3$) δ 172.0, 128.3, 127.5, 61.2,

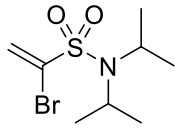
39.2, 34.0, 14.2. LRMS (FAB): *m*/*z* (%) 198 (52) [M – $C_4H_7O_2$], 242 (60) [M + H - C_2H_5O], 286 [M + H]. HRMS (FAB): *m*/*z* calculated for $C_7H_{13}NO_4SBr$ 285.97432; found 285.9736 $[M + H]^+$ (error −4.4 ppm).



Methyl 4-((1-bromovinyl)sulfonamido)butanoate (**1o**): Prepared as shown in general procedure 2; colorless oil; eluent (Hexane:EtOAc = 2:1, v/v); yield, 79%. FT-IR (ATR) *v* cm^{-1}: 3300 (br), 3114 (w), 2954 (m), 1734 (s), 1603 (w), 1439 (m), 1337 (s), 1261 (w), 1206 (w), 1166 (s), 1096 (m). ^{1}H-NMR (400 MHz, $CDCl_3$) δ 6.85 (d, J = 2.9 Hz, 1H), 6.21 (d, J = 2.9 Hz, 1H), 4.97 (t, J = 5.0 Hz, 1H), 3.70 (s, 3H), 3.13 (q, J = 6.5 Hz, 2H), 2.45 (t, J = 7.0 Hz, 2H), 1.92 (quin, J = 6.8 Hz, 2H). ^{13}C-NMR (101 MHz, $CDCl_3$) δ 173.6, 128.5, 127.2, 51.9, 43.0, 30.9, 24.6. LRMS (ESI): *m*/*z* (%) 309 (95) [M + Na]. HRMS (ESI): *m*/*z* calculated for $C_7H_{12}NO_4NaSBr$ 307.95681; found 307.95530 $[M + Na]^+$ (error −4.92 ppm).

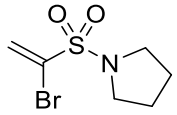


1-Bromo-*N*,*N*-diethylethene-1-sulfonamide (**1p**): Prepared as shown in general procedure 2; colorless oil; eluent (Hexane:EtOAc = 4:1, v/v); yield, 96%. FT-IR (NaCl) *v* cm^{-1}: 3111 (w), 2979 (m), 2938 (m), 2873 (w), 1601 (m), 1468 (m), 1385 (m), 1337 (s), 1298 (w), 1205 (s), 1181 (m), 1156 (s), 1090 (m), 1019 (s), 943 (m), 789 (m), 768 (m), 710 (w), 678 (m). ^{1}H-NMR (400 MHz, $CDCl_3$) δ 6.80 (d, J = 2.7 Hz, 1H), 6.14 (d, J = 2.7 Hz, 1H), 3.37 (q, J = 7.2 Hz, 4H), 1.23 (t, J = 7.2 Hz, 6H). ^{13}C-NMR (101 MHz, $CDCl_3$) δ 128.0, 127.6, 42.9, 14.3. LRMS (EI): *m*/*z* (%) 105 (11) [M – $C_4H_{10}NO_2S$], 198 (8) [M – CH_3 – C_2H_4], 226 (98) [M – CH_3], 241 (8) [M]. HRMS (EI): *m*/*z* calculated for $C_6H_{12}NO_2SBr$ 240.97721; found 240.9779 $[M]^+$ (error +3.0 ppm).

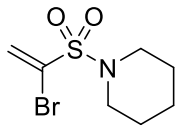


1-Bromo-*N*,*N*-diisopropylethene-1-sulfonamide (**1q**): Prepared as shown in general procedure 2; off-white crystals; eluent (Hexane:EtOAc = 5:1, v/v); yield, 97%. FT-IR (KBr) *v* cm^{-1}: 3106 (w), 2977 (m), 2937 (m), 2878 (w), 1598 (m), 1464 (m), 1409 (m), 1371 (m), 1331 (s), 1201 (s), 1169 (s), 1141 (s), 1122 (w), 983 (s), 942 (m), 887 (m), 760 (s), 708 (m), 657 (s), 587 (s), 568 (s), 529 (m). ^{1}H-NMR

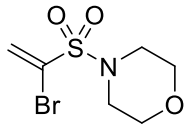
(400 MHz, $CDCl_3$) δ 6.83 (d, J = 2.6 Hz, 1H), 6.13 (d, J = 2.6 Hz, 1H), 3.79 (sep, J = 6.8 Hz, 2H), 1.35 (d, J = 6.8 Hz, 12H). ^{13}C-NMR (101 MHz, $CDCl_3$) δ 129.7, 127.7, 49.6, 22.2.
LRMS (EI): m/z (%) 105 (7) [M – $C_6H_{14}NO_2S$], 212 (base peak) [M – C_4H_9], 254 (46) [M – CH_3], 269 (2) [M]. HRMS (EI): m/z calculated for $C_7H_{13}NO_2SBr$ 253.98504; found 253.9860 [M - CH_3]$^+$ (error +3.6 ppm).



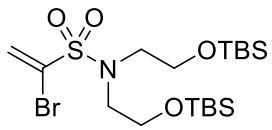
1-((1-Bromovinyl)sulfonyl)pyrrolidine (**1r**): Prepared as shown in general procedure 2; pale yellow crystals; eluent (Hexane:EtOAc = 4:1, v/v); yield, 92%. FT-IR (NaCl) v cm^{-1}: 3110 (w), 2979 (m), 2888 (m), 1600 (m), 1459 (w), 1343 (s), 1241 (m), 1203 (s), 1160 (s), 1098 (s), 1065 (s), 1014 (s), 938 (m), 777 (s), 698 (w), 615 (s), 573 (s), 504 (m). ^{1}H-NMR (400 MHz, $CDCl_3$) δ 6.80 (d, J = 2.7 Hz, 1H), 6.21 (d, J = 2.7 Hz, 1H), 3.49–3.43 (m, 4H), 2.02–1.94 (m, 4H). ^{13}C-NMR (101 MHz, $CDCl_3$) δ 128.6, 125.5, 48.9, 25.9. LRMS (EI): m/z (%) 70 (base peak) [M – $C_2H_2O_2SBr$], 105 (23) [M – $C_4H_8NO_2S$], 328 (40) [M – H], 329 (33) [M]. HRMS (EI): m/z calculated for $C_6H_{10}NO_2S^{79}Br$ 238.96156; found 238.9591 [M]$^+$ (error −10.1 ppm). HRMS (EI): m/z calculated for $C_6H_{10}NO_2S^{81}Br$ 240.95952; found 240.9591 [M]$^+$ (error −1.6 ppm).



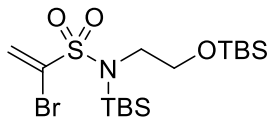
1-((1-Bromovinyl)sulfonyl)piperidine (**1s**): Prepared as shown in general procedure 2; pale yellow crystals; eluent (Hexane:EtOAc = 4:1, v/v); yield, 92%. FT-IR (NaCl) v cm^{-1}: 3110 (w), 2941 (s), 2857 (s), 1600 (m), 1453 (m), 1362 (vs), 1340 (vs), 1279 (m), 1219 (m), 1170 (vs), 1092 (s), 1051 (s), 945 (vs), 855 (w), 836 (w), 770 (s), 712 (s), 596 (vs). ^{1}H-NMR (400 MHz, $CDCl_3$) δ 6.77 (dd, J = 2.8, 0.4 Hz, 1H), 6.20 (d, J = 2.8 Hz, 1H), 3.31 (t, J = 5.3 Hz, 4H), 1.70–1.56 (m, 6H). ^{13}C-NMR (101 MHz, $CDCl_3$) δ 131.7, 127.8, 47.8, 25.6. LRMS (EI): m/z (%) 83 (base peak) [M – $C_2H_3O_2SBr$], 84 (35) [M – $C_2H_2O_2SBr$], 105 (12) [M – $C_5H_{10}NO_2S$], 212 (13) [M – C_3H_5], 252 (54) [M – H], 253 (59) [M]. HRMS (EI): m/z calculated for $C_7H_{12}NO_2S^{79}Br$ 252.97721; found 252.9735 [M]$^+$(error -14.8 ppm). HRMS (EI): m/z calculated for $C_7H_{12}NO_2S^{81}Br$ 254.97517; found 254.9761 [M]$^+$ (error +3.7 ppm).



4-((1-Bromovinyl)sulfonyl)morpholine (**1t**): Prepared as shown in general procedure 2; colorless crystals; eluent (Hexane:EtOAc = 4:1, v/v); yield, 90%. FT-IR (NaCl) ν cm^{-1}: 3110 (w), 2971 (w), 2920 (w), 2861 (w), 1600 (w), 1451 (m), 1348 (s), 1300 (w), 1262 (m), 1168 (s), 1114 (s), 1169 (m), 1014 (w), 954 (s), 848 (w), 774 (m), 714 (m), 613 (s), 530 (s). ^{1}H-NMR (400 MHz, $CDCl_3$) δ 6.82 (d, J = 2.9 Hz, 1H), 6.27 (d, J = 2.9 Hz, 1H), 3.78–3.75 (m, 4H), 3.38–3.35 (m, 4H). ^{13}C-NMR (101 MHz, $CDCl_3$) δ 129.2, 125.2, 66.6, 46.5. LRMS (EI): m/z (%) 85 (base peak) [M – $C_2H_2O_2SBr$], 105 (12) [M – $C_4H_8NO_3S$], 212 (21) [M – C_2H_4O + H], 255 (27) [M]. HRMS (EI): m/z calculated for $C_6H_{10}NO_3SBr$ 254.95648; found 254.9572 [M]$^+$ (error +2.7 ppm).

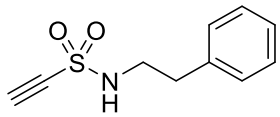


1-Bromo-*N*,*N*-bis(2-((*tert*-butyldimethylsilyl)oxy)ethyl)ethene-1-sulfonamide (**1u**): Prepared as shown in general procedure 2; colorless oil; eluent (Hexane:EtOAc = 19:1, v/v); yield, 77%. FT-IR (ATR) ν cm^{-1}: 3114 (m), 2958 (s), 2887 (s), 2860 (s), 1603 (w), 1472 (m), 1362 (m), 1258 (m), 1167 (m), 1111 (m), 1006 (m), 937 (m), 840 (m), 810 m), 780 (m). ^{1}H-NMR (400 MHz, $CDCl_3$) δ 6.82 (d, J = 2.8 Hz, 1H), 6.15 (d, J = 2.8 Hz, 1H), 3.79 (t, J = 6.3 Hz, 4H), 3.47 (t, J = 6.2 Hz, 4H), 0.89 (s, 18H), 0.07 (s, 12H). ^{13}C-NMR (101 MHz, $CDCl_3$) δ 127.8, 127.5, 77.3, 77.2, 77.0, 76.7, 62.1, 52.1, 25.9, 18.5, 18.2, 17.9, -5.4. LRMS (EI): m/z (%) 444 (base peak) [M – C_4H_9], 486 (13) [M – CH_3]. HRMS (EI): m/z calculated for $C_{17}H_{37}NO_4SiSBr$ 486.11652; found 486.1178 [M – CH_3]$^+$ (error +2.6 ppm).

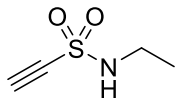


1-Bromo-*N*-(*tert*-butyldimethylsilyl)-*N*-(2-((*tert*-butyldimethylsilyl)oxy)ethyl)ethene-1-sulfonamide (**1v**): Prepared as shown in general procedure 2; colorless oil; eluent (Hexane:EtOAc = 19:1, v/v); yield, 47%. FT-IR (NaCl) ν cm^{-1}: 3112 (w), 2955 (s), 2931 (s), 2886 (s), 2859 (s), 2710 (w), 1602 (m), 1472 (s), 1407 (w), 1392 (m), 1338 (s), 1257 (s), 1162 (s), 1092 (s), 1038 (m), 1006 (m), 904 (s), 840 (s), 825 (s), 778 (s), 707 (w), 687 (m), 609 (s). ^{1}H-NMR (400 MHz, $CDCl_3$) δ 6.90 (d, J = 2.7 Hz, 1H), 6.20 (d, J = 2.7 Hz, 1H), 3.72 (t, J = 7.6 Hz, 2H), 3.27 (t, J = 7.6 Hz, 2H), 1.01 (s, 9H), 0.88 (s, 9H), 0.39 (s, 6H), 0.05 (s, 6H). ^{13}C-NMR (101 MHz, $CDCl_3$) δ 129.2, 128.9, 61.5, 49.0, 27.3,

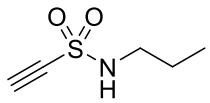
25.9, 19.7, 18.3, −2.9, −5.3. LRMS (EI): *m/z* (%) 400 (32) [M – C_4H_9], 442 (2) [M – CH_3]. HRMS (EI): *m/z* calculated for $C_{15}H_{33}NO_3Si_2SBr$ 442.09031; found 442.0913 [M – CH_3]$^+$ (error +2.3 ppm).



***N*-Phenethylethynesulfonamide** (**2a**): Prepared as shown in general procedure 3A; yellow oil; eluent (Hexane:EtOAc = 2:1, v/v); yield, 82%. UV (abs) λ_{max}: 206 nm (5%v/v MeCN in Water). FT-IR (ATR) *v* cm^{-1}: 3636 (m), 3269 (br), 3030 (w), 2933 (w), 2072 (s), 1604 (w), 1497 (w), 1445 (m), 1423 (m), 1353 (s), 1172 (s), 1075 (m). ^{1}H-NMR (400 MHz, $CDCl_3$) *δ* 7.36–7.20 (m, 5H), 4.74 (br, 1H), 3.49 (q, *J* = 6.8 Hz, 2H), 3.25 (s, 1H), 2.95 (t, *J* = 6.8 Hz, 2H). ^{13}C-NMR (101 MHz, $CDCl_3$) *δ* 137.2, 128.9, 128.8, 127.1, 78.3, 76.8, 44.6, 35.3. LRMS (EI): *m/z* (%) 91 (66) [M – $C_3H_4NO_2S$], 118 (base peak) [M – C_7H_7], 209 (6) [M]. HRMS (EI): *m/z* calculated for $C_{10}H_{11}NO_2S$ 209.05105; found 209.0512 [M]$^+$ (error +0.6 ppm).

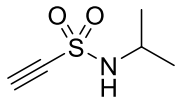


***N*-Ethylethynesulfonamide** (**2b**): Prepared as shown in general procedure 3A; yellow oil; eluent (Hexane:EtOAc = 2:1, v/v); yield, 91%. FT-IR (NaCl) *v* cm^{-1}: 3627 (w), 3265 (br), 2986 (m), 2942 (w), 2882 (w), 2071 (s), 1427 (s), 1340 (s), 1169 (s), 1062 (m), 958 (m), 868 (m), 777 (m), 695 (s), 573 (s). ^{1}H-NMR (400 MHz, $CDCl_3$) *δ* 4.71 (br, 1H), 3.30 (qd, *J* = 7.2, 6.0 Hz, 2H), 3.27 (s, 1H), 1.30 (t, *J* = 7.2 Hz, 3H). ^{13}C-NMR (101 MHz, $CDCl_3$) *δ* 78.4, 76.6, 38.8, 14.7. LRMS (EI): *m/z* (%) 44 (2) [M – C_2HO_2S], 89 (13)[M – C_2H_6N], 118 (base peak) [M – CH_3], 133 (4) [M]. HRMS (EI): *m/z* calculated for $C_4H_7NO_2S$ 133.01975; found 133.0198 [M]$^+$ (error +0.4 ppm).

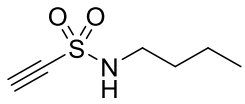


***N*-Propylethynesulfonamide** (**2c**): Prepared as shown in general procedure 3A; yellow oil; eluent (Hexane:EtOAc = 2:1, v/v); yield, 82%. FT-IR (NaCl) *v* cm^{-1}: 3269 (br), 2972 (m), 2939 (m), 2880 (m), 2071 (s), 1426 (m), 1342 (s), 1169 (s), 1074 (m), 1008 (w), 913 (m), 843 (w), 696 (s). ^{1}H-NMR (400 MHz, $CDCl_3$) *δ* 4.82 (br, 1H), 3.27 (s, 1H), 3.19 (ddd, *J* = 7.2, 6.4 Hz, 2H), 1.67 (sext, *J* = 7.2 Hz, 2H), 0.99 (t, *J* = 7.2 Hz, 3H). 1H-NMR (400 MHz, DMSO-d_6) *δ* 8.34 (t, *J* = 5.5 Hz, 1H), 5.74, 4.98 (s, 1H), 2.93 (td, *J* = 7.0, 5.7 Hz, 2H), 1.51 (sext, *J* = 7.3 Hz, 2H), 0.88 (t, *J* = 7.4 Hz, 3H). ^{13}C-NMR (101 MHz, $CDCl_3$) *δ* 78.4, 76.6, 45.4, 22.5, 11.1. LRMS (EI): *m/z* (%) 89 (6) [M – C_3H_8N], 118

(base peak) [M – C_2H_5], 147 (1) [M]. HRMS (EI): *m*/*z* calculated for $C_5H_9NO_2S$ 147.03540; found 147.0355 $[M]^+$ (error +0.7 ppm).

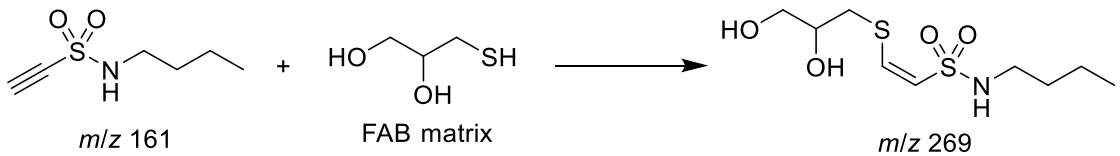


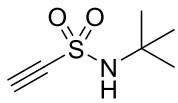
***N*-Isopropylethynesulfonamide** (**2d**): Prepared as shown in general procedure 3A; yellow oil; eluent (Hexane:EtOAc = 2:1, v/v); yield, 82%. UV (abs) λ_{max}: < 220 nm (5%v/v MeCN in Water). FT-IR (NaCl) *v* cm^{-1}: 3260 (br), 3978 (m), 2936 (w), 2879 (w), 2071 (s), 1428 (m), 1396 (s), 1372 (m), 1335 (m), 1232 (w), 1206 (w), 1158 (s), 1043 (w), 1007 (m), 931 (w), 865 (w), 758 (w), 698 (s). ^{1}H-NMR (400 MHz, $CDCl_3$) δ 4.71 (s, 1H), 3.76 (oct, *J* = 7.2, 6.8 Hz, 1H), 3.26 (s, 1H), 1.31 (d, *J* = 6.4 Hz, 6H). ^{13}C-NMR (101 MHz, $CDCl_3$) δ 79.5, 76.1, 47.3, 23.3. LRMS (EI): *m*/*z* (%) 89 (6) [M – C_2HO_2S], 132 (base peak) [M – CH_3], 146 (0.6) [M – H], 147(0.4) [M]. HRMS (EI): *m*/*z* calculated for $C_5H_9NO_2S$ 147.03540; found 147.0354 $[M]^+$ (error +0.3 ppm).



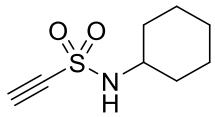
***N*-Butylethynesulfonamide** (**2e**): Prepared as shown in general procedure 3A; yellow oil; eluent (Hexane:EtOAc = 3:1, v/v); yield, 87%. FT-IR (ATR) *v* cm^{-1}: 3260 (br), 2962 (w), 2936 (w), 2875 (w), 2070 (m), 1465 (w), 1425 (m), 1341 (s), 1165 (s), 1119 (w), 1078 (m). ^{1}H-NMR (400 MHz, $CDCl_3$) δ 4.81 (br, 1H), 3.27 (s, 1H), 3.22 (ddd, *J* =6.0, 7.2 Hz, 2H), 1.62 (quin, *J* = 7.6 Hz, 2H), 1.41 (sext, *J* = 7.2 Hz, 2H), 0.95 (t, *J* = 7.2 Hz, 3H). ^{13}C-NMR (101 MHz, $CDCl_3$) δ 78.3, 76.7, 43.4, 31.1, 19.7, 13.5. LRMS (FAB): *m*/*z* (%) 74 (49) [M + H – C_2HO_2S], 162 (40) [M + H], 194 (36) [M + $C_3H_8O_2S$ – $C_3H_7O_2$], 270 (base peak) [M + $C_3H_8O_2S$ + H]. HRMS (FAB): *m*/*z* calculated for $C_6H_{12}NO_2S$ 162.05833; found 162.0590 $[M + H]^+$ (error +0.7 ppm).

Note:



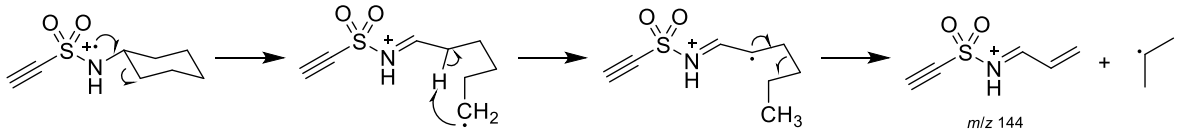


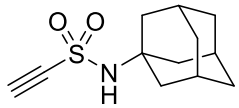
***N*-(tert-Butyl)ethynesulfonamide** (**2f**): Prepared as shown in general procedure 3A; off-white crystals; eluent (Hexane:EtOAc = 3:1, v/v); yield, 92%. FT-IR (NaCl) ν cm^{-1}: 3279 (br), 2979 (m), 2936 (w), 2874 (w), 2071 (s), 1428 (m), 1395 (s), 1372 (m), 1342 (s), 1232 (w), 1206 (w), 1158 (s), 1043 (w), 1007 (m), 931 (w), 865 (w), 758 (w), 698 (s), 595 (m). ^{1}H-NMR (400 MHz, $CDCl_3$) δ 4.87 (br, 1H), 3.24 (s, 1H), 1.45 (s, 9H). ^{13}C-NMR (101 MHz, $CDCl_3$) δ 81.3, 75.4, 56.1, 29.8. LRMS (EI): *m*/*z* (%) 146 (base peak) [M – CH_3]. HRMS (EI): *m*/*z* calculated for $C_5H_8NO_2S$ 146.02757; found 146.0275 $[M - CH_3]^+$ (error −0.9 ppm).



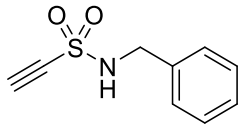
***N*-Cyclohexylethynesulfonamide** (**2g**): Prepared as shown in general procedure 3A; off-white crystals; eluent (Hexane:EtOAc = 3:1, v/v); yield, 93%. UV (abs) λ_{max}: < 220 nm (5%v/v MeCN in Water). ^{1}H-NMR (400 MHz, $CDCl_3$) δ 4.76 (d, J = 6.2 Hz, 1H), 3.50–3.41 (m, 1H), 3.25 (s, 1H), 2.11–2.05 (m, 2H), 1.78–1.73 (m, 2H), 1.63–1.57 (m, 1H), 1.43–1.15 (m, 5H). ^{13}C-NMR (101 MHz, $CDCl_3$) δ 79.7, 75.9, 53.7, 33.5, 25.1, 24.5. LRMS (EI): *m*/*z* (%) 98 (19) [M – C_2HO_2S], 144 (base peak) [M – C_3H_7], 187 (14) [M]. HRMS (EI): *m*/*z* calculated for $C_8H_{13}NO_2S$ 187.06670; found 187.0669 $[M]^+$ (error +1.0 ppm).

Note:

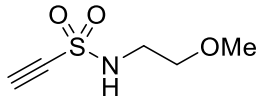




***N*-((3*s*,5*s*,7*s*)-Adamantan-1-yl)ethynesulfonamide** (**2h**): Prepared as shown in general procedure 3A; white crystals; eluent (Hexane:EtOAc = 4:1, v/v); yield, 65%. FT-IR (KBr) ν cm^{-1}: 3325 (s), 3229 (s), 2908 (s), 2888 (m), 2849 (m), 2067 (s), 1455 (w), 1424 (s), 1369 (s), 1353 (m), 1334 (s), 1321 (m), 1266 (w), 1155 (s), 1114 (w), 1006 (s), 972 (m), 886 (m), 746 (m), 723 (m), 694 (s), 561 (s). ^{1}H-NMR (400 MHz, $CDCl_3$) δ 4.77 (br, 1H), 3.24 (s, 1H), 2.13 (br, 3H), 2.04 (d, J = 3.0 Hz, 6H), 1.71–1.64 (m, 6H). ^{13}C-NMR (101 MHz, $CDCl_3$) δ 81.8, 75.3, 56.6, 42.7, 35.8, 29.5. LRMS (EI): *m*/*z* (%) 135 (83) [M – $C_2H_2NO_2S$], 239 (37) [M]. HRMS (EI): *m*/*z* calculated for $C_{12}H_{17}NO_2S$ 239.09800; found 239.0976 $[M]^+$ (error −1.8 ppm).

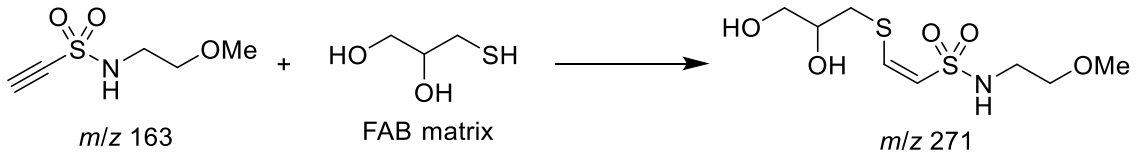


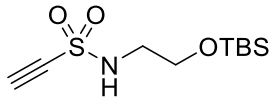
***N*-Benzylethynesulfonamide** (**2i**): Prepared as shown in general procedure 3A; colorless crystals; eluent (Hexane:EtOAc = 4:1, v/v); yield, 88%. FT-IR (NaCl) ν cm^{-1}: 3246 (w), 2946 (w), 2856 (w), 2063 (m), 1455 (w), 1366 (s), 1348 (s), 1318 (w), 1280 (w), 1214 (w), 1172 (s), 1149 (m), 1099 (w), 1055 (m), 1029 (w), 736 (s), 661 (s). ^{1}H-NMR (400 MHz, $CDCl_3$) δ 7.41–7.32 (m, 5H), 5.01 (br, 1H), 4.38 (d, J = 6.1 Hz, 2H), 3.29 (s, 1H). ^{13}C-NMR (101 MHz, $CDCl_3$) δ 135.1, 128.9, 128.4, 128.1, 78.2, 77.1, 47.8. LRMS (EI): *m*/*z* (%) 77 (55) [M – $C_3H_4NO_2S$], 91 (50) [M – $C_2H_2NO_2S$], 104 (base peak) [M – C_7H_7], 195 (40) [M]. HRMS (EI): *m*/*z* calculated for $C_9H_9NO_2S$ 195.03540; found 195.0349 [M]$^+$ (error −2.7 ppm).



***N*-(2-Methoxyethyl)ethynesulfonamide** (**2j**): Prepared as shown in general procedure 3A (The solvent used is Et_2O instead of THF); colorless oil; eluent (Hexane:EtOAc = 3:2, v/v); yield, 77%. FT-IR (NaCl) ν cm^{-1}: 3615 (br), 3255 (s), 2988 (w), 2935 (m), 2898 (m), 2839 (w), 2069 (s), 1628 (w), 1428 (s), 1391 (m), 1349 (s), 1241 (w), 1197 (m), 1169 (s), 1124 (s), 1081 (s), 1027 (m), 964 (m), 870 (w), 798 (w), 700 (s). ^{1}H-NMR (400 MHz, $CDCl_3$) δ 5.30 (s, 1H), 3.59 (dd, J = 5.3, 4.7 Hz, 2H), 3.39 (s, 3H), 3.38 (td, J = 5.8, 4.9 Hz, 2H), 3.29 (s, 1H). ^{13}C-NMR (101 MHz, $CDCl_3$) δ 78.2, 76.9, 69.8, 58.9, 43.4. LRMS (FAB): *m*/*z* (%) 164 (50) [M + H], 196 (22) [M + $C_3H_8O_2S$ – $C_3H_7O_2$], 272 (base peak) [M + $C_3H_8O_2S$ + H]. HRMS (FAB): *m*/*z* calculated for $C_5H_{11}NO_3S$ 164.03759; found 164.0376 [M + H]$^+$ (error −3.6 ppm).

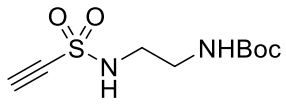
Note.



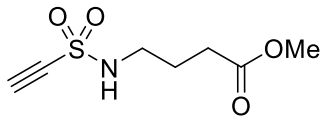


***N*-(2-((*tert*-Butyldimethylsilyl)oxy)ethyl)ethynesulfonamide** (**2k**): Prepared as shown in general procedure 3A (The solvent used is Et_2O instead of THF, and saturated citric acid aqueous solution

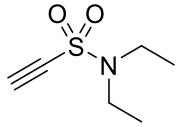
instead of 5 M HCl aqueous solution.); colorless oil; eluent (Hexane:EtOAc = 5:1, v/v); yield, 71%. FT-IR (NaCl) ν cm^{-1}: 3157 (s), 2954 (s), 2930 (s), 2884 (m), 2858 (s), 2070 (s), 1471 (m), 1411 (m), 1355 (s), 1257 (s), 1173 (s), 1117 (s), 1087 (s), 978 (m), 939 (w), 838 (s), 810 (m), 780 (s), 700 (m), 582 (w). ^{1}H-NMR (400 MHz, $CDCl_3$) δ 5.12 (br, 1H), 3.82–3.80 (m, 2H), 3.34–3.30 (m, 2H), 3.28 (s, 1H), 0.90 (s, 9H), 0.09 (s, 6H). ^{13}C-NMR (101 MHz, $CDCl_3$) δ 78.3, 76.8, 60.8, 45.7, 25.8, 18.3, −5.4. LRMS (ESI): *m*/*z* (%) 286 (67) [M + Na], 318(44) [M + MeOH + Na], 336 (base peak) [M + H_2O + MeOH + Na], 549 (24) [2M + Na]. HRMS (ESI): m/z calculated for $C_{10}H_{21}NO_3SSi$ 286.09091; found 286.08977 [M + Na]$^+$ (error −1.14 ppm).



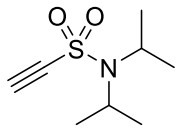
***tert*-Butyl (2-(ethynylsulfonamido)ethyl)carbamate** (**2l**): Prepared as shown in general procedure 3A; yellow gam; eluent (Hexane:EtOAc = 1:1, v/v); yield, 72%. FT-IR (NaCl) ν cm^{-1}: 3410 (m), 3253 (br), 2980 (m) 2935 (m), 2255 (w), 1091 (s), 1691 (s), 1521 (s), 1454 (m), 1394 (w), 1367 (s), 1351 (s), 1169 (s), 1091 (m), 947 (w), 913 (w), 859 (w), 782 (w), 701 (s), 574 (m). ^{1}H-NMR (400 MHz, $CDCl_3$) δ 5.97 (br, 1H), 4.94 (br, 1H), 3.38–3.31 (m, 4H), 3.27 (s, 1H), 1.45 (s, 9H). ^{13}C-NMR (101 MHz, $CDCl_3$) δ 157.0, 80.4, 78.4, 76.6, 44.6, 39.9, 28.3. LRMS (ESI): *m*/*z* (%) 215 (base peak) [M + H_2O – $C_4H_{10}O$ + Na], 271 (19) [M + Na], 519 (12) [2M + Na]. HRMS (ESI): *m*/*z* calculated for $C_9H_{16}N_2O_4NaS$ 271.07285; found 271.07281 [M + Na]$^+$ (error −0.13 ppm).



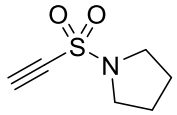
Methyl 4-(ethynylsulfonamido)butanoate (**2o**): Prepared as shown in general procedure 3C; colorless oil; eluent (Hexane:EtOAc = 2:1, v/v); yield, 20%. FT-IR (NaCl) ν cm^{-1}: 3255 (br), 2956 (w), 2069 (m), 1720 (m), 1439 (m), 1348 (s), 1261 (w), 1209 (w), 1164 (s), 1079 (m), 976 (w), 692 (s). ^{1}H-NMR (400 MHz, $CDCl_3$) δ 5.26 (br, 1H), 3.70 (s, 3H), 3.29 (td, J = 6.7, 6.2 Hz, 2H), 3.28 (s, 1H), 2.47 (t, J = 6.9 Hz, 2H), 1.97 (quin, J = 6.8 Hz, 2H). ^{13}C-NMR (101 MHz, $CDCl_3$) δ 173.7, 78.3, 76.8, 52.0, 43.1, 31.0, 24.2. LRMS (ESI): *m*/*z* (%) 228 (40) [M + Na]. HRMS (ESI): *m*/*z* calculated for $C_7H_{11}NO_4NaS$ 228.03065; found 228.03073 [M + Na]$^+$ (error +0.37 ppm).



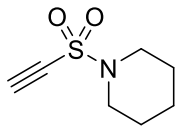
***N*,*N*-Diethylethynesulfonamide** (**2p**): Prepared as shown in general procedure 3B; pale yellow oil; eluent (Hexane:EtOAc = 4:1, v/v); yield, 91%. FT-IR (NaCl) ν cm^{-1}: 3251 (s), 2981 (s), 2941 (m), 2881 (m), 2066 (s), 1469 (m), 1363 (s), 1299 (m), 1205 (s), 1160 (s), 1098 (w), 1069 (w), 1019 (s), 945 (s), 787 (m), 727 (s), 659 (s), 529 (w). ^{1}H-NMR (400 MHz, $CDCl_3$) δ 3.34 (q, J = 7.2 Hz, 4H), 3.21 (s, 1H), 1.27 (t, J = 7.2 Hz, 6H). ^{13}C-NMR (101 MHz, $CDCl_3$) δ 78.7, 76.3, 42.9, 13.3. LRMS (EI): *m*/*z* (%) 89 (3) [M – $C_4H_{10}N$], 118 (48) [M – C_2H_5 – CH_3 + H], 146 (base peak) [M – CH_3], 161 (12) [M]. HRMS (EI): *m*/*z* calculated for $C_6H_{11}NO_2S$ 161.05105; found 161.0510 [M]$^+$ (error −0.3 ppm).



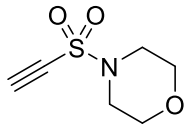
***N*,*N*-Diisopropylethynesulfonamide** (**2q**): Prepared as shown in general procedure 3B; colorless crystals; eluent (Hexane:EtOAc = 5:1, v/v); yield, 79%. UV (abs) λ_{max}: < 220 nm (5%v/v MeCN in Water). FT-IR (KBr) ν cm^{-1}: 3244 (s), 2981 (m), 2934 (w), 2880 (w), 2063 (s), 1469 (w), 1408 (m), 1373 (m), 1344 (s), 1203 (s), 1173 (s), 1139 (s), 1118 (s), 1018 (m), 989 (s), 887 (w), 714 (s), 641 (m), 565 (s), 535 (m), 480 (w), 455 (m). ^{1}H-NMR (400 MHz, $CDCl_3$) δ 3.91 (sep, J = 6.8 Hz, 2H), 3.18 (s, 1H), 1.37 (d, J = 6.8 Hz, 12H). ^{13}C-NMR (101 MHz, $CDCl_3$) δ 81.7, 74.9, 49.8, 21.3. LRMS (EI): *m*/*z* (%) 132 (base peak) [M – C_3H_7 – CH_3], 174 (31) [M – CH_3], 189 (4) [M]. HRMS (EI): *m*/*z* calculated for $C_8H_{15}NO_2S$ 189.08235; found 189.0826 [M]$^+$ (error +1.5 ppm).



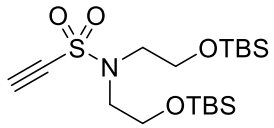
1-(Ethynylsulfonyl)pyrrolidine (**2r**): Prepared as shown in general procedure 3B; colorless oil; eluent (Hexane:EtOAc = 4:1, v/v); yield, 81%. UV (abs) λ_{max}: < 220 nm (5%v/v MeCN in Water). FT-IR (ATR) ν cm^{-1}: 3227 (br), 3107 (w), 3057 (w), 2978 (m), 2888 (m), 2063 (m), 1455 (w), 1337 (s), 1204 (m), 1150 (s), 1075 (s). 1010 (s), 735 (s), 668 (s). ^{1}H-NMR (400 MHz, $CDCl_3$) δ 3.42–3.38 (m, 4H), 3.21 (s, 1H), 2.01–1.94 (m, 4H). ^{13}C-NMR (101 MHz, $CDCl_3$) δ 76.9, 75.9, 48.7, 25.3. LRMS (EI): *m*/*z* (%) 42 (58) [M – $C_3H_3NO_2S$], 89 (12) [M – C_4H_8N], 118 (4) [M – C_3H_6 + H], 158 (base peak) [M – H], 159 (76) [M]. HRMS (EI): *m*/*z* calculated for $C_6H_9NO_2S$ 159.03540; found 159.0350 [M]$^+$ (error −2.7 ppm).



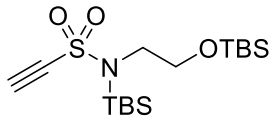
1-(Ethynylsulfonyl)piperidine (**2s**): Prepared as shown in general procedure 3B; colorless oil; eluent (Hexane:EtOAc = 4:1, v/v); yield, 89%. FT-IR (ATR) ν cm^{-1}: 3259 (br), 3065 (w), 2874 (w), 2069 (m), 1602 (m), 1425 (m), 1347 (s), 1164 (s), 1057 (m), 856 (w), 810 (m), 692 (s). ^{1}H-NMR (400 MHz, $CDCl_3$) δ 3.27 (s, 1H), 3.18 (t, J = 5.6 Hz, 4H), 1.74 (quin, J = 5.6 Hz, 4H), 1.60–1.54 (m, 2H). ^{13}C-NMR (101 MHz, $CDCl_3$) δ 78.1, 75.3, 47.1, 24.6, 23.3. LRMS (EI): m/z (%) 132 (40) [M – C_3H_6 + H], 172 (base peak) [M – H], 173 (60) [M]. HRMS (EI): m/z calculated for $C_7H_{11}NO_2S$ 173.05105; found 173.0507 $[M]^+$ (error −1.8 ppm).



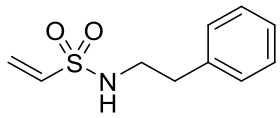
4-(Ethynylsulfonyl)morpholine (**2t**): Prepared as shown in general procedure 3B (The solvent used is Et_2O instead of THF); off-white crystals; eluent (Hexane:EtOAc = 2:1, v/v); yield, 75%. UV (abs) λ_{max}: < 220 nm (5%v/v MeCN in Water). FT-IR (NaCl) ν cm^{-1}: 3249 (m), 2973 (w), 2923 (m), 2862 (m), 2064 (s), 1455 (m), 1368 (s), 1300 (m), 1263 (s), 1218 (w), 1175 (s), 1114 (s), 1076 (s),1017 (w), 953 (s), 927 (w), 852 (w), 747 (s), 670 (m), 617 (m). ^{1}H-NMR (400 MHz, $CDCl_3$) δ 3.85–3.82 (m, 4H), 3.35 (s, 1H), 3.21–3.19 (m, 4H). ^{13}C-NMR (101 MHz, $CDCl_3$) δ 79.1, 74.4, 65.6, 46.1. LRMS (EI): m/z (%) 56 (91) [M – C_2HO_2S – CH_2O], 86 (base peak) [M – C_2HO_2S], 89 (21) [M – C_4H_8NO], 175 (52) [M]. HRMS (EI): m/z calculated for $C_6H_9NO_3S$ 175.03031; found 175.0300 $[M]^+$ (error −1.9 ppm).



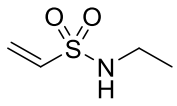
***N*,*N*-Bis(2-((*tert*-butyldimethylsilyl)oxy)ethyl)ethynesulfonamide** (**2u**): Prepared as shown in general procedure 3B (The solvent used is Et_2O instead of THF, and saturated citric acid aqueous solution instead of 5 M HCl aqueous solution.); colorless oil; eluent (Hexane:EtOAc = 9:1, v/v); yield, 96%. FT-IR (ATR) ν cm^{-1}: 3252 (w), 2953 (m), 2930 (m), 2885 (m), 2858 (m), 2066 (m), 1472 (w), 1464 (w), 1364 (m), 1254 (m), 1169 (m), 1104 (s), 1003 (m), 936 (w), 916 (w), 835 (s), 775 (s), 723 (s). ^{1}H-NMR (400 MHz, $CDCl_3$) δ 3.83 (t, J = 6.1 Hz, 4H), 3.46 (t, J = 6.0 Hz, 4H), 3.20 (s, 1H), 0.90 (s, 18H), 0.07 (s, 12H). ^{13}C-NMR (101 MHz, $CDCl_3$) δ 78.5, 76.2, 61.7, 52.1, 25.8, 18.2, −5.4. LRMS (EI): m/z (%) 364 (base peak) [M – C_4H_9], 406 (5) [M – CH_3]. HRMS (EI): m/z calculated for $C_{14}H_{30}NO_4Si_2S$ 364.14341; found 364.1427 $[M – C_4H_9]^+$ (error − 1.9 ppm).



***N*-(*tert*-Butyldimethylsilyl)-*N*-(2-((*tert*-butyldimethylsilyl)oxy)ethyl)ethynesulfonamide** (**2v**): Prepared as shown in general procedure 3B (The solvent used is Et_2O instead of THF, and saturated citric acid aqueous solution instead of 5 M HCl aqueous solution .); colorless oil; eluent (Hexane:EtOAc = 19:1, v/v); yield, 53%. FT-IR (ATR) ν cm^{-1}: 3546 (br), 3261 (br), 2956 (s), 2933 (s), 2887 (m), 2860 (m), 2072 (m), 1472 (m), 1414 (m), 1360 (m), 1258 (m), 1175 (s), 1087 (m). ^{1}H-NMR (400 MHz, $CDCl_3$) δ 3.83 (t, J = 7.2 Hz, 2H), 3.35 (t, J = 7.2 Hz, 2H), 3.19 (s, 1H), 0.99 (s, 9H), 0.90 (s, 9H), 0.39 (s, 6H), 0.07 (s, 6H). ^{13}C-NMR (101 MHz, $CDCl_3$) δ 80.3, 75.3, 61.8, 49.1, 26.9, 25.9, 19.7, 18.3, –3.2, -5.3. LRMS (EI): *m*/*z* (%) 320 [M – C_4H_9] (base peak), 362 [M – CH_3] (7). HRMS (EI): m/z calculated for $C_{15}H_{32}NO_3Si_2S$ 3362.16414; found 362.1628 $[M - CH_3]^+$ (error −3.9 ppm).

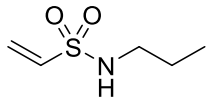


***N*-Phenethylvinylsulfonamide** (**3a**): Prepared as shown in general procedure 1C; pale yellow oil; eluent (Hexane:EtOAc = 2:1, v/v); yield, 91%. FT-IR (NaCl) ν cm^{-1}: 3290 (s), 3060 (m), 3028 (m), 2935 (m), 2871 (w), 1604 (w), 1496 (m), 1455 (m), 1327 (s), 1255 (w), 1149 (s), 1075 (m), 1030 (w), 970 (m), 901 (w), 818 (w), 751 (m), 701 (m), 660 (m), 546 (m). ^{1}H-NMR (400 MHz, $CDCl_3$) δ 7.34–7.18 (m, 5H), 6.39 (dd, J = 16.6, 9.8 Hz, 1H), 6.21 (d, J = 16.6 Hz, 1H), 5.89 (d, J = 9.8 Hz, 1H), 4.35 (br, 1H), 3.29 (q, J = 6.8 Hz, 2H), 2.86 (t, J = 6.8 Hz, 2H). ^{13}C-NMR (101 MHz, $CDCl_3$) δ 137.6, 135.7, 128.8, 126.9, 126.6, 44.1, 36.1. LRMS (EI): *m*/*z* (%) 91 (31) [M – $C_3H_6NO_2S$], 120 (base peak) [M – C_7H_7], 211 (4) [M]. HRMS (EI): *m*/*z* calculated for $C_{10}H_{13}NO_2S$ 211.06670; found 211.0669 $[M]^+$ (error +1.1 ppm).

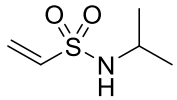


***N*-Ethylvinylsulfonamide** (**3b**): Prepared as shown in general procedure 1A; yellow oil; eluent (Hexane:EtOAc = 2:1, v/v); yield, 51%. FT-IR (NaCl) ν cm^{-1}: 3608 (w), 3266 (br), 3058 (w), 2982 (m), 2939 (w), 2880 (w), 1941 (w), 1426 (m), 1322 (s), 1151 (s), 1062 (m), 970 (s), 864 (w), 779 (m), 736 (m), 661 (w). ^{1}H-NMR (400 MHz, $CDCl_3$) δ 6.52 (dd, J = 16.8, 10.0 Hz, 1H), 6.26 (d, J = 16.8 Hz, 1H), 5.95 (d, J = 10.0 Hz, 1H), 4.26 (br, 1H), 3.10 (qd, J = 7.2, 6.0 Hz, 2H), 1.21 (t, J = 7.2 Hz, 3H). ^{13}C-NMR (101 MHz, $CDCl_3$) δ 135.9, 126.6, 38.0, 15.5. LRMS (EI): *m*/*z* (%) 27 (7) [M – $C_2H_6NO_2S$], 44 (6) [M – $C_2H_3O_2S$], 91 (32) [M – C_2H_6], 108 (1) [M – C_2H_3], 120 (base peak) [M –

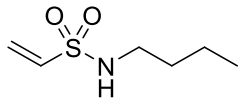
CH_3], 135 (5) [M]. HRMS (EI): *m*/*z* calculated for $C_4H_9NO_2S$ 135.03540; found 135.0352 $[M]^+$ (error −1.4 ppm).



***N*-Propylvinylsulfonamide** (**3c**): Prepared as shown in general procedure 1C; pale yellow oil; eluent (Hexane:EtOAc = 3:1, v/v); yield, 84%. FT-IR (NaCl) *v* cm^{-1}: 3595 (br), 3292 (s), 3108 (w), 3059 (w), 2969 (s), 2938 (s), 2878 (m), 1458 (m), 1426 (s), 1387 (s), 1325 (vs), 1255 (m), 1152 (vs), 1076 (s), 1004 (m), 970 (s), 842 (m), 737 (s), 661 (m). ^{1}H-NMR (400 MHz, $CDCl_3$) δ 6.52 (dd, J = 16.6, 10.0 Hz, 1H), 6.24 (d, J = 16.6 Hz, 1H), 5.94 (d, J = 10.0 Hz, 1H), 4.49 (br, 1H), 2.99 (q, J = 7.6 Hz, 2H), 1.58 (sext, J = 7.6 Hz, 2H), 0.95 (t, J = 7.6 Hz, 3H). ^{13}C-NMR (101 MHz, $CDCl_3$) δ 135.9, 126.5, 44.7, 23.2, 11.1. LRMS (EI): *m*/*z* (%) 91 (23) [M – C_3H_8N], 120 (base peak) [M – C_2H_5], 149 (3) [M]. HRMS (EI): *m*/*z* calculated for $C_5H_{11}NO_2S$ 149.05105; found 149.0506 $[M]^+$ (error −3.3 ppm).

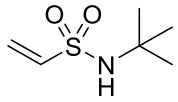


***N*-Isopropylvinylsulfonamide** (**3d**): Prepared as shown in general procedure 1A; yellow oil; eluent (Hexane:EtOAc = 3:2, v/v); yield, 65%. FT-IR (NaCl) *v* cm^{-1}: 3286 (vs), 3059 (w), 2976 (s), 2937 (m), 2878 (m), 1468 (m), 1427 (s), 1388 (m), 1329 (s), 1257 (m), 1136 (s), 1007 (s), 970 (s), 896 (s), 833 (w), 735 (s), 664 (s), 553 (m). ^{1}H-NMR (400 MHz, $CDCl_3$) δ 6.54 (dd, J = 16.6, 9.9 Hz, 1H), 6.25 (d, J = 16.5 Hz, 1H), 5.91 (d, J = 9.9 Hz, 1H), 4.40 (d, J = 5.5 Hz, 1H), 3.52 (oct, J = 6.4 Hz, 1H), 1.22 (d, J = 6.6 Hz, 6H). ^{13}C-NMR (101 MHz, $CDCl_3$) δ 137.0, 125.8, 46.1, 24.0. LRMS (EI): *m*/*z* (%) 90 (14) [M – C_3H_8N], 134 (base peak) [M – CH_3]. HRMS (EI): *m*/*z* calculated for $C_4H_8NO_2S$ 134.02757; found 134.0276 $[M – CH_3]^+$ (error −0.1 ppm).

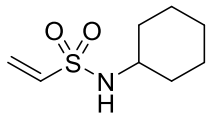


***N*-Butylvinylsulfonamide** (**3e**): Prepared as shown in general procedure 1A; pale yellow oil; eluent (Hexane:EtOAc = 3:1, v/v); yield, 79%. FT-IR (NaCl) *v* cm^{-1}: 3291 (s), 3107 (m), 3059 (w), 2961 (s), 2935 (s), 2874 (s), 1465 (m), 1426 (s), 1386 (s), 1327 (vs), 1256 (m), 1152 (vs), 1082 (s), 971 (s), 906 (m), 865 (m), 800 (m), 740 (s), 660 (s). ^{1}H-NMR (400 MHz, $CDCl_3$) δ 6.51 (dd, J = 16.6, 9.9 Hz, 1H), 6.23 (d, J = 16.6 Hz, 1H), 5.93 (d, J = 9.9 Hz, 1H), 4.51 (br, 1H), 2.99 (td, J = 7.2, 6.0 Hz, 2H), 1.54 (quin, J = 7.2 Hz, 2H), 1.37 (sext, J = 7.2 Hz, 2H), 0.91 (t, J = 7.2 Hz, 3H). ^{13}C-NMR (101 MHz,

$CDCl_3$) δ 135.8, 126.5, 42.7, 31.8, 19.7, 13.5. LRMS (FAB): *m/z* (%) 135 (10) [M + H – C_2H_5], 164 (base peak) [M + H], 327 (27) [2M + H]. HRMS (FAB): *m/z* calculated for $C_6H_{14}NO_2S$ 164.07398; found 164.0742 $[M + H]^+$ (error −2.1 ppm).

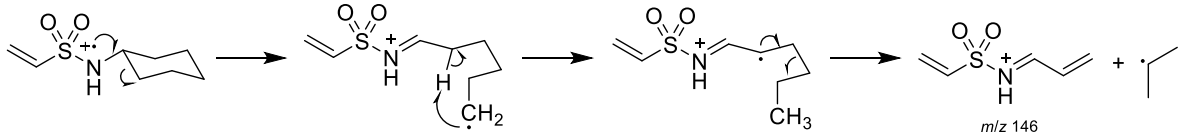


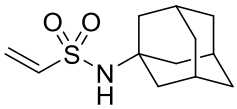
***N*-(tert-Butyl)vinylsulfonamide (3f)**: Prepared as shown in general procedure 1C; off-white crystals; eluent (Hexane:EtOAc = 3:1, v/v); yield, 79%. FT-IR (NaCl) *v* cm^{-1}: 3297 (s), 3101 (m), 3054 (m), 2986 (s), 2938 (m), 2878 (m), 1965 (w), 1469 (m), 1423 (m), 1372 (s), 1310 (s), 1259 (s), 1231 (s), 1204 (m), 1127 (s), 1047 (m), 1007 (s), 985 (s), 873 (s), 762 (s), 732 (s), 676 (s). ^{1}H-NMR (400 MHz, $CDCl_3$) δ 6.61 (dd, *J* = 16.5, 9.9 Hz, 1H), 6.23 (d, *J* = 16.5 Hz, 1H), 5.84 (d, *J* = 9.9 Hz, 1H), 4.47 (br, 1H), 1.35 (s, 9H). ^{13}C-NMR (101 MHz, $CDCl_3$) δ 139.5, 129.0, 128.2, 124.5, 54.6, 30.3. LRMS (EI): *m/z* (%) 91 (6) [M – $C_4H_{10}N$], 148 (base peak) [M – CH_3]. HRMS (EI): *m/z* calculated for $C_5H_{10}NO_2S$ 148.04322; found 148.0433 $[M – CH_3]^+$ (error +0.4 ppm).



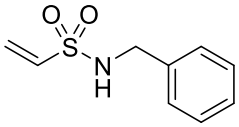
***N*-Cyclohexylvinylsulfonamide (3g)**: Prepared as shown in general procedure 1A; off-white crystals; eluent (Hexane:EtOAc = 3:1, v/v); yield, 84%. FT-IR (KBr) *v* cm^{-1}: 3269 (s), 3099 (w), 3049 (w), 2940 (s), 2857 (s), 2670 (w), 1610 (w), 1449 (s), 1391 (s), 1317 (s), 1256 (s), 1132 (m), 1085 (s), 986 (s), 927 (m), 890 (s), 842 (w), 733 (s), 673 (s), 588 (m). ^{1}H-NMR (400 MHz, $CDCl_3$) δ 6.54 (dd, *J* = 16.5, 9.9 Hz, 1H), 6.25 (d, *J* = 16.5 Hz, 1H), 5.89 (d, *J* = 9.9 Hz, 1H), 4.44 (d, *J* = 7.1 Hz, 1H), 3.22–3.13 (m, 1H), 1.96–1.93 (m, 2H), 1.75–1.67 (m, 2H), 1.60–1.54 (m, 1H), 1.37–1.11 (m, 5H). ^{13}C-NMR (101 MHz, $CDCl_3$) δ 137.2, 125.6, 52.6, 34.3, 25.1, 24.7. LRMS (EI): *m/z* (%) 91 (8) [M – $C_6H_{12}N$], 98 (13) [M – $C_2H_3O_2S$], 146 (base peak) [M – C_3H_7], 160 (4) [M – C_2H_5], 189 (14) [M]. HRMS (EI): *m/z* calculated for $C_8H_{15}NO_2S$ 189.08235; found 189.0822 $[M]^+$ (error −1.0 ppm).

Note: McClafferty rearrangement.

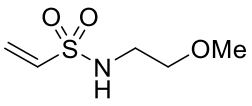




***N*-((3*s*,5*s*,7*s*)-Adamantan-1-yl)ethenesulfonamide** (**3h**): Prepared as shown in general procedure 1C; off-white crystals; eluent (Hexane:EtOAc = 3:1, v/v); yield, 81%. FT-IR (KBr) ν cm^{-1}: 3280 (s), 3099 (w), 3056 (w), 3982 (w), 3914 (s), 2869 (m), 2851 (m), 1455 (m), 1435 (s), 1387 (w), 1360 (m), 1344 (m), 1323 (s), 1288 (m), 1258 (m), 1152 (s), 1117 (m), 1088 (s), 993 (m), 976 (m), 964 (m), 872 (m), 815 (w), 776 (w), 740 (m), , 721 (w), 660 (m), 641 (w), 556 (m). ^{1}H-NMR (400 MHz, $CDCl_3$) δ 6.62 (dd, J = 16.5, 9.9 Hz, 1H), 6.23 (d, J = 16.5 Hz, 1H), 5.82 (d, J = 9.8 Hz, 1H), 4.25 (br, 1H), 2.09 (br, 3H), 1.92 (d, J = 2.9 Hz, 6H), 1.68–1.60 (m, 6H). ^{13}C-NMR (101 MHz, $CDCl_3$) δ 140.0, 124.3, 77.3, 77.0, 76.7, 55.1, 43.3, 35.9, 29.6. LRMS (ESI): *m*/*z* (%) 106 (base peak) [M – $C_{10}H_{15}$]136 (53) [M – $C_2H_4NO_2S$ + H], 264 (50) [M + Na]. HRMS (ESI): *m*/*z* calculated for $C_{12}H_{23}NO_2NaS$ 264.10342; found 264.10442 $[M + Na]^+$ (error +3.79 ppm).

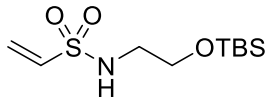


***N*-Benzylvinylsulfonamide** (**3i**): Prepared as shown in general procedure 1A; yellow crystals; eluent (Hexane:EtOAc = 2:1, v/v); yield, 70%. FT-IR (KBr) ν cm^{-1}: 3315 (br), 3101 (w), 3059 (w), 3033 (w), 1067 (w), 1497 (w), 1456 (m), 1426 (m), 1386 (m), 1323 (s), 1253 (w), 1147 (s), 1055 (m), 979 (m), 879 (w), 743 (m), 698 (m), 662 (m), 553 (m). ^{1}H-NMR (400 MHz, $CDCl_3$) δ 7.37−7.27 (m, 5H), 6.47 (dd, J = 16.6, 9.9 Hz, 1H), 6.24 (d, J = 16.5 Hz, 1H), 5.91 (d, J = 9.9 Hz, 1H), 4.76 (br, 1H), 4.20 (d, J = 6.2 Hz, 2H). ^{13}C-NMR (101 MHz, $CDCl_3$) δ 136.5, 136.0, 128.8, 128.1, 127.9, 126.8, 47.0. LRMS (EI): *m*/*z* (%) 77 (10) [M – $C_3H_6NO_2S$], 91 (19) [M – $C_2H_4NO_2S$], 106 (base peak) [M – C_7H_7], 197 (1) [M]. HRMS (EI): *m*/*z* calculated for $C_9H_{11}NO_2S$ 197.05105; found 197.0509 $[M]^+$ (error −0.7 ppm).

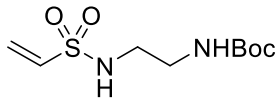


***N*-(2-Methoxyethyl)ethenesulfonamide** (**3j**): Prepared as shown in general procedure 1A; colorless oil; eluent (Hexane:EtOAc = 1:1, v/v); yield, 51%. FT-IR (NaCl) ν cm^{-1}: 3587 (br), 3284 (br), 3059 (w), 2934 (m), 2895 (m), 2934 (w), 1635 (w), 1426 (m), 1388 (m), 1327 (s), 1257 (w), 1197 (w), 1149 (s), 1126 (s), 1084 (s), 1027 (w), 967 (m), 869 (w), 797 (w), 735 (w), 660 (w). ^{1}H-NMR (400 MHz, $CDCl_3$) δ 6.54 (dd, J = 16.6, 9.9 Hz, 1H), 6.26 (d, J = 16.6 Hz, 1H), 5.96 (d, J = 9.9 Hz, 1H), 4.78 (br, 1H), 3.51 (t, J = 5.2 Hz, 2H), 3.36 (s, 3H), 3.20 (ddd, 2H). ^{13}C-NMR (101 MHz, $CDCl_3$) δ 135.9, 126.7, 70.8, 58.9, 42.7. LRMS (EI): *m*/*z* (%) 45 (base peak) [M – $C_3H_6NO_2S$], 74 (18) [M – $C_2H_3O_2S$],

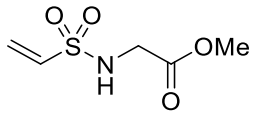
91 (45) [M – C_3H_8N], 120 (17) [M – C_2H_5O], 134 (45) [M – CH_3O]. HRMS (EI): *m*/*z* calculated for $C_3H_5NO_2S$ 120.01192; found 120.0117 [M – C_2H_5O]$^+$ (error −1.5 ppm).



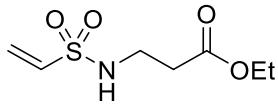
***N*-(2-((*tert*-Butyldimethylsilyl)oxy)ethyl)ethenesulfonamide** (**3k**): 2-Aminoethanol (1.66 mL, 1.1 equiv.), DMAP (28 mg, 1.0 mol%), Et_3N (18.8 mL, 5.0 equiv.), and *t*-butyldimethylsilyl (TBS) chloride (4.52 g, 1.2 equiv.) were added to DCM (100 mL) at 0 °C under N_2 and stirred for 1 hour. After **4** (2.62 mL, 1.0 equiv.) was added at 0 °C, and the reaction was stirred at 0 °C for 24 hours. After added PBS (100 mL, 1 M solution, pH 7.4), the reaction mixture was washed three times with distilled water, once with brine, and the organic layer was dried over Na_2SO_4. After concentration, chromatography was performed on the residue on a silica gel column (Hexane:EtOAc = 3:1, v/v) to give colorless oil **3k** (3.84g, 58%). FT-IR (NaCl) *v* cm^{-1}: 3295 (br), 2954 (s), 2930 (s), 2884 (m), 2858 (s), 1472 (m), 1387 (m), 1331 (s), 1256 (s), 1155 (s), 1088 (s), 1006 (w), 970 (s), 837 (s),779 (s), 734 (m), 662 (m). ^{1}H-NMR (400 MHz, $CDCl_3$) δ 6.54 (dd, *J* = 16.5, 9.9 Hz, 1H), 6.26 (d, *J* = 16.6 Hz, 1H), 5.95 (d, *J* = 9.9 Hz, 1H), 4.63 (s, 1H), 3.74–3.72 (m, 2H), 3.15–3.11 (m, 2H), 0.89 (s, 9H), 0.07 (s, 6H). 13C-NMR (101 MHz, $CDCl_3$) δ 135.9, 126.6, 61.7, 45.1, 25.9, 18.3, −5.4. LRMS (EI): *m*/*z* (%) 208 (base peak) [M – C_4H_9], 250 (12) [M – CH_3]. HRMS (EI): *m*/*z* calculated for $C_9H_{20}NO_3SiS$ 250.09332; found 250.0932 [M - CH_3]$^+$ (error −0.6 ppm).



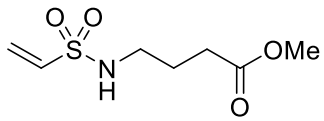
***tert*-Butyl (2-(vinylsulfonamido)ethyl)carbamate** (**3l**): Prepared as shown in general procedure 1A; colorless oil; eluent (Hexane:EtOAc = 1:1, v/v); yield, 61%. FT-IR (NaCl) *v* cm^{-1}: 3384 (br), 3298 (br), 3059 (w), 2979 (m), 2934 (w), 1693 (s), 1521 (s), 1455 (m), 1392 (m), 1367 (m), 1329 (s), 1275 (s), 1254 (s), 1151 (s), 1090 (m), 970 (m), 916 (m), 861 (w), 734 (s), 660 (m). ^{1}H-NMR (400 MHz, $CDCl_3$) δ 6.53 (dd, *J* = 16.5, 9.9 Hz, 1H), 6.25 (d, *J* = 16.5 Hz, 1H), 5.95 (d, *J* = 9.9 Hz, 1H), 5.09 (br, 1H), 4.94 (br, 1H), 3.29 (q, *J* = 5.8 Hz, 2H), 3.15 (q, *J* = 5.8 Hz, 2H), 1.45 (s, 9H). ^{13}C-NMR (101 MHz, $CDCl_3$) δ 156.6, 135.7, 126.7, 80.0, 43.5, 40.5, 28.3. LRMS (EI): *m*/*z* (%) 172 (15) [M + Na – $C_5H_{10}O_2$], 216 (base peak) [M + H – C_4H_9], 273 (47) [M + Na]. HRMS (ESI): *m*/*z* calculated for $C_9H_{18}N_2O_4NaS$ 273.08850; found 273.08960 [M + Na]$^+$ (error +4.05 ppm).



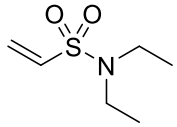
Methyl (vinylsulfonyl)glycinate (**3m**): Prepared as shown in general procedure 1C (Et_3N (4.0 equiv.)); colorless oil; eluent (Hexane:EtOAc = 1:1, v/v); yield, 71%. FT-IR (NaCl) ν cm^{-1}: 3617 (br), 3294 (br), 3062 (w), 2958 (w), 1748 (s), 1438 (m), 1388 (w), 1331 (s), 1220 (m), 1149 (s), 1063 (w), 976 (m), 855 (m), 740 (m), 652 (w). ^{1}H-NMR (400 MHz, $CDCl_3$) δ 6.56 (dd, J = 16.5, 9.9 Hz, 1H), 6.27 (d, J = 16.5 Hz, 1H), 5.96 (d, J = 9.9 Hz, 1H), 5.05 (br, 1H), 3.86 (d, J = 5.7 Hz, 2H), 3.78 (s, 3H). ^{13}C-NMR (101 MHz, $CDCl_3$) δ 169.9, 135.6, 127.2, 52.7, 43.9. LRMS (EI): m/z (%) 91 (22) [M – $C_3H_6NO_2$], 120 (base peak) [M – $C_2H_3O_2$], 179 (2) [M]. HRMS (EI): m/z calculated for $C_5H_9NO_4S$ 179.02523; found 179.0249 $[M]^+$ (error −1.8 ppm).



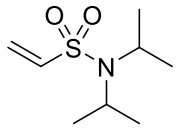
Ethyl 3-(vinylsulfonamido)propanoate (**3n**): Prepared as shown in general procedure 1C (Et_3N (4.0 equiv.)); colorless oil; eluent (Hexane:EtOAc = 1:1, v/v); yield, 99%. FT-IR (NaCl) ν cm^{-1}: 3603 (br), 3292 (br), 3059 (w), 1728 (s), 1422 (m), 1381 (m), 1329 (s), 1259 (m), 1191 (m), 1150 (s), 1092 (m), 1052 (m), 971 (m), 817 (w), 734 (m), 661 (w). ^{1}H-NMR (400 MHz, $CDCl_3$) δ 6.54 (dd, J = 16.6, 9.9 Hz, 1H), 6.27 (d, J = 16.6 Hz, 1H), 5.96 (d, J = 9.9 Hz, 1H), 5.01 (br, 1H), 4.17 (q, J = 7.1 Hz, 2H), 3.28 (q, J = 6.1 Hz, 2H), 2.62 (t, J = 5.9 Hz, 2H), 1.28 (t, J = 7.1 Hz, 3H). ^{13}C-NMR (101 MHz, $CDCl_3$) δ 172.1, 136.0, 126.8, 61.1, 38.6, 34.4, 14.2. LRMS (FAB): m/z (%) 91 (9) [M – $C_5H_{10}NO_2$], 120 (38) [M - $C_4H_8O_2$], 162 (45) [M – C_2H_5O], 208 (base peak) [M + H]. HRMS (FAB): m/z calculated for $C_7H_{13}NO_4S$ 208.06381; found 208.0644 $[M + H]^+$ (error +2.8 ppm).



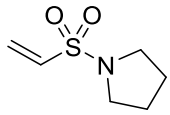
Methyl 4-(vinylsulfonamido)butanoate (**3o**): Prepared as shown in general procedure 1C (Et_3N (4.0 equiv.)); colorless oil; eluent (Hexane:EtOAc = 1:1, v/v); yield, 90%. FT-IR (NaCl) ν cm^{-1}: 3291 (br), 2953 (w), 1731 (s), 1437 (m), 1386 (m), 1324 (s), 1257 (m), 1203 (m), 1145 (s), 1079 (m), 968 (m), 896 (w), 836 (w), 734 (m), 659 (m). ^{1}H-NMR (400 MHz, $CDCl_3$) δ 6.52 (dd, J = 16.5, 9.9 Hz, 1H), 6.25 (d, J = 16.6 Hz, 1H), 5.96 (d, J = 9.9 Hz, 1H), 4.67 (br, 1H), 3.69 (s, 3H), 3.09 (q, J = 6.6 Hz, 2H), 2.43 (t, J = 7.1 Hz, 2H), 1.89 (quin, J = 6.9 Hz, 2H). ^{13}C-NMR (101 MHz, $CDCl_3$) δ 173.6, 135.8, 126.8, 51.8, 42.3, 30.9, 25.0. LRMS (ESI): m/z (%) 230 (41) [M + Na]. HRMS (ESI): m/z calculated for $C_7H_{13}NO_4NaS$ 230.04630; found 230.04676 $[M + Na]^+$ (error +2.0 ppm).



***N*,*N*-Diethylvinylsulfonamide** (**3p**): Prepared as shown in general procedure 1A; yellow oil; eluent (Hexane:EtOAc = 2:1, v/v); yield, 82%. FT-IR (NaCl) ν cm^{-1}: 3057 (br), 2978 (s), 2939 (s), 2879 (m), 1468 (m), 1385 (s), 1334 (vs), 1201 (vs), 1145 (vs), 1093 (w), 1018 (s), 970 (m), 935 (s), 786 (s), 750 (vs), 689 (s), 632 (w). ^{1}H-NMR (400 MHz, $CDCl_3$) δ 6.42 (dd, J = 16.5, 9.9 Hz, 1H), 6.20 (d, J = 16.5 Hz, 1H), 5.89 (d, J = 9.9 Hz, 1H), 3.23 (q, J = 7.1 Hz, 4H), 1.20 (t, J = 7.1 Hz, 6H). ^{13}C-NMR (101 MHz, $CDCl_3$) δ 135.5, 125.8, 41.7, 14.3. LRMS (EI): *m*/*z* (%) 91 [M – $C_4H_{10}N$] (13), 120 [M – C_2H_4 – CH_3] (6), 148 [M – CH_3] (base peak), 163 [M] (14). HRMS (EI): *m*/*z* calculated for $C_6H_{13}NO_2S$ 163.06670; found 163.0667 $[M]^+$ (error −0.1 ppm).

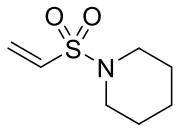


***N*,*N*-Diisopropylvinylsulfonamide** (**3q**): Prepared as shown in general procedure 1A; yellow oil; eluent (Hexane:EtOAc = 5:1, v/v); yield, 70%. FT-IR (KBr) ν cm^{-1}: 3099 (w), 3060 (w), 3005 (w), 2949 (s), 2934 (m), 2878 (w), 1931 (w), 1462 (m), 1409 (m), 1384 (m), 1369 (m), 1323 (s), 1263 (w), 1202 (s), 1185 (s), 1165 (s), 1128 (s), 1027 (m), 1185 (m), 980 (s), 885 (m), 862 (w), 740 (s), 683 (s), 620 (w), 570 (s), 530 (s). ^{1}H-NMR (400 MHz, $CDCl_3$) δ 6.45 (dd, J = 16.5, 9.8 Hz, 1H), 6.18 (d, J = 16.5 Hz, 1H), 5.79 (d, J = 9.8 Hz, 1H), 3.71 (sept, J = 6.8 Hz, 2H), 1.30 (d, J = 6.8 Hz, 12H). ^{13}C-NMR (101 MHz, $CDCl_3$) δ 138.4, 124.1, 48.4, 22.1. LRMS (EI): *m*/*z* (%) 134 (base peak) [M – C_3H_6 – CH_3], 176 (45) [M – CH_3], 191 (6) [M]. HRMS (EI): *m*/*z* calculated for $C_8H_{17}NO_2S$ 191.09800; found 191.0981 $[M]^+$ (error +0.8 ppm).

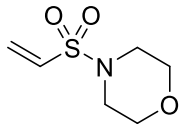


1-(Vinylsulfonyl)pyrrolidine (**3r**): Prepared as shown in general procedure 1A; yellow oil; eluent (Hexane:EtOAc = 2:1, v/v); yield, 70%. FT-IR (NaCl) ν cm^{-1}: 3056 (w), 2978 (m), 2882 (m), 1461 (w), 1386 (m), 1341 (s), 1256 (m), 1200 (m), 1150 (s), 1065 (m), 1008 (m), 973 (m), 769 (s), 718 (m), 661 (s). ^{1}H-NMR (400 MHz, $CDCl_3$) δ 6.48 (dd, J = 16.6, 9.9 Hz, 1H), 6.26 (d, J = 16.6 Hz, 1H), 6.01 (d, J = 9.9 Hz, 1H), 3.30–3.27 (m, 4H), 1.94–1.87 (m, 4H). ^{13}C-NMR (101 MHz, $CDCl_3$) δ 132.7, 128.0, 46.5, 25.3, 23.6. LRMS (EI): *m*/*z* (%) 42 (40) [M – $C_3H_5NO_2S$], 70 (base peak) [M – $C_2H_3O_2S$],

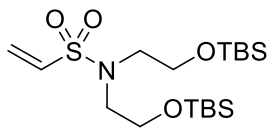
90 (8) [M – C_4H_8N], 160 (87) [M – H], 161 (70) [M]. HRMS (EI): *m/z* calculated for $C_6H_{11}NO_2S$ 161.05105; found 161.0516 $[M]^+$ (error +3.3 ppm).



1-(Vinylsulfonyl)piperidine (**3s**): Prepared as shown in general procedure 1A; off-white crystals; eluent (Hexane:EtOAc = 4:1, v/v); yield, 63%. FT-IR (KBr) *v* cm^{-1}: 2985 (w), 2942 (m), 2856 (m), 1469 (w), 1454 (w), 1385 (w), 1360 (m), 1339 (s), 1279 (w), 1261 (w), 1216 (w), 1163 (s), 1144 (m), 1106 (w), 1054 (m), 1028 (w), 971 (w), 931 (m), 859 (w), 839 (w), 757 (s), 693 (w), 657 (w). ^{1}H-NMR (400 MHz, $CDCl_3$) δ 6.42 (dd, J = 16.6, 9.9 Hz, 1H), 6.21 (d, J = 16.6 Hz, 1H), 6.01 (d, J = 9.9 Hz, 1H), 3.13 (t, J = 5.5 Hz, 4H), 1.66 (quin, J = 5.6 Hz, 4H), 1.57–1.51 (m, 2H). ^{13}C-NMR (101 MHz, $CDCl_3$) δ 131.7, 127.8, 47.8, 25.6. LRMS (EI): *m/z* (%) 83 (61) [M – $C_2H_3O_2S$ – H], 84 (32) [M – $C_2H_3O_2S$], 91 (12) [M – $C_5H_{10}N$], 134(19) [M – C_3H_6 + H], 174 (base peak) [M – H], 175 (71) [M]. HRMS (EI): *m/z* calculated for $C_7H_{13}NO_2S$ 175.06670; found 175.0669 $[M]^+$ (error +1.1 ppm).

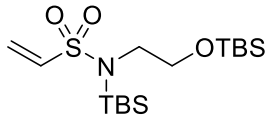


4-(Vinylsulfonyl)morpholine (**3t**): Prepared as shown in general procedure 1A; off-white crystals; eluent (Hexane:EtOAc = 1:1, v/v); yield, 58%. FT-IR (NaCl) *v* cm^{-1}: 3103 (w). 3060 (w), 2977 (w), 2923 (w), 2909 (w), 2871 (m), 1455 (m), 1394 (m), 1344 (s), 1330 (s), 1297 (w), 1259 (s), 1216 (w), 1152 (s), 1112 (s), 1072 (s), 1029 (w), 896 (s), 939 (s), 851 (w), 768 (s), 700 (w), 666 (s), 573 (w), 549 (m), 487 (m), 472 (w). ^{1}H-NMR (400 MHz, $CDCl_3$) δ 6.44 (dd, J = 16.6, 9.9 Hz, 1H), 6.27 (d, J = 16.6 Hz, 1H), 6.11 (d, J = 9.9 Hz, 1H), 3.78–3.76 (m, 4H), 3.16–3.13 (m, 4H). ^{13}C-NMR (101 MHz, $CDCl_3$) δ 131.7, 129.6, 66.2, 45.6. LRMS (EI): *m/z* (%) 56 (74) [M – $C_2H_3O_2S$ – CH_2O], 86 (base peak) [M – $C_2H_3O_2S$], 91 (33) [M – C_4H_8NO], 120 (15) [M – C_3H_5O], 134 (35) [M – C_2H_3O], 177 (57) [M]. HRMS (EI): *m/z* calculated for $C_6H_{11}NO_3S$ 177.04596; found 177.0456 $[M]^+$ (error −2.2 ppm).

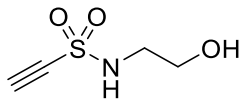


***N,N*-Bis(2-((*tert*-butyldimethylsilyl)oxy)ethyl)ethenesulfonamide** (**3u**): Prepared as shown in general procedure 1C (amine is **S2**); colorless oil; eluent (Hexane:EtOAc = 1:1, v/v); yield, 73%. FT-IR (NaCl) *v* cm^{-1}: 2954 (m), 2929 (m), 2884 (m), 2858 (m), 1472 (w), 1464 (w), 1387 (w), 1343 (m),

1254 (m), 1149 (m), 1100 (s), 1101 (m), 964 (m), 936 (m), 915 (m), 835 (s), 810 (m), 774 (s), 747(m). ^{1}H-NMR (400 MHz, $CDCl_3$) δ 6.53 (dd, J = 16.6, 9.9 Hz, 1H), 6.19 (d, J = 16.6 Hz, 1H), 5.86 (d, J = 9.9 Hz, 1H), 3.76 (t, J = 5.9 Hz, 4H), 3.35 (t, J = 5.9 Hz, 4H), 0.89 (s, 18H), 0.07 (s, 12H). ^{13}C-NMR (101 MHz, $CDCl_3$) δ 135.5, 125.5, 62.1, 50.6, 25.9, 18.2, -5.4. LRMS (EI): m/z (%) 366 (base peak) [M – C_4H_9], 408 (8) [M – CH_3]. HRMS (EI): m/z calculated for $C_{17}H_{38}NO_4Si_2S$ 408.20601; found 408.2075 [M – CH_3]$^+$ (error +3.5 ppm).



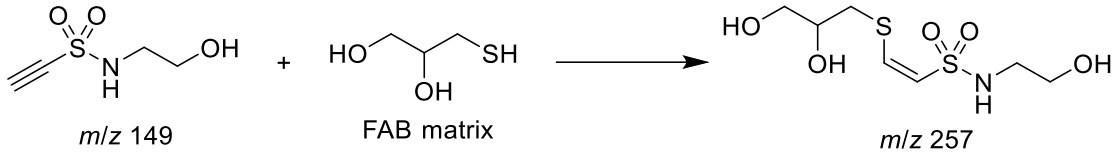
***N*-(*tert*-Butyldimethylsilyl)-*N*-(2-((*tert*-butyldimethylsilyl)oxy)ethyl)ethenesulfonamide** (**3v**): 2-Aminoethanol (1.66 mL, 1.1 equiv.), DMAP (28 mg, 1.0 mol%), Et_3N (18.8 mL, 5.0 equiv.), and *t*-butyldimethylsilyl (TBS) chloride (7.91 g, 2.1 equiv.) were added to DCM (100 mL) at 0 °C under N_2 and stirred for 1 hour. After **4** (2.62 mL, 1.0 equiv.) was added at 0 °C, and the reaction was stirred at 0 °C for 24 hours. After added PBS (100 mL, 1 M solution, pH 7.4), the reaction mixture was washed three times with distilled water, once with brine, and the organic layer was dried over Na_2SO_4. After concentration, chromatography was performed on the residue on a silica gel column (Hexane:EtOAc = 19:1, v/v) to give colorless oil **3v** (4.73 g, 52%). FT-IR (NaCl) ν cm^{-1}: 2955 (s), 2930 (s), 2886 (m), 2858 (s), 1472 (m), 1386 (w), 1362 (w), 1336 (s), 1257 (s), 1149 (s), 1085 (s), 1040 (w), 1006 (w), 965 (m), 903 (s), 840 (s), 825 (s), 813 (m), 778 (m), 741 (m), 666 (m). ^{1}H-NMR (400 MHz, $CDCl_3$) δ 6.49 (dd, J = 16.5, 9.9 Hz, 1H), 6.21 (d, J = 16.5 Hz, 1H), 5.86 (d, J = 9.8 Hz, 1H), 3.72 (t, J = 7.1 Hz, 2H), 3.20 (t, J = 7.2 Hz, 2H), 0.99 (s, 9H), 0.89 (s, 9H), 0.32 (s, 6H), 0.06 (s, 6H). ^{13}C-NMR (101 MHz, $CDCl_3$) δ 137.7, 125.2, 62.2, 48.5, 27.2, 25.9, 25.7, 19.5, 18.3, −2.9, −5.3. LRMS (EI): m/z (%) 322 (base peak) [M – C_4H_9], 364 (11) [M – CH_3]. HRMS (EI): m/z calculated for $C_{15}H_{34}NO_3Si_2S$ 364.17979; found 364.1809 [M – CH_3]$^+$ (error +3.0 ppm).

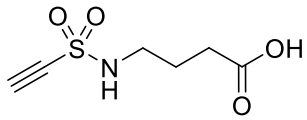


***N*-(2-Hydroxyethyl)ethynesulfonamide** (**5**): Prepared as shown in general procedure 5; colorless oil; eluent (EtOAc); yield, quant. FT-IR (NaCl) ν cm^{-1}: 3502 (m), 3234 (s), 3230 (br), 3151 (s), 3065 (w), 3029 (w), 2936 (m), 2886 (m), 2096 (s), 1604 (w), 1498 (m), 1455 (s), 1425 (m), 1331 (s), 1258 (w), 1221 (w), 1171 (s), 1112 (m), 1067 (m), 959 (m), 848 (w), 837 (w), 733 (m), 697 (s), 661 (w). ^{1}H-NMR (400 MHz, DMSO-d_6) δ 8.40 (br, 1H), 4.99 (s, 1H), 4.83 (t, J = 5.6 Hz, 1H), 3.50 (dd, J = 11.9, 6.1 Hz, 2H), 3.03 (t, J = 6.2 Hz, 2H). ^{13}C-NMR (101 MHz, DMSO-d_6) δ 79.8, 79.2, 59.4, 45.3. LRMS (FAB): m/z (%) 91 (base peak) [M + H – C_2H_6NO], 181 (21) [M + $C_3H_8O_2S$ – $C_3H_7O_2$], 258 (16) [M

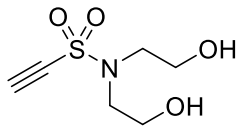
+ $C_3H_8O_2S$ + H]. HRMS (FAB): *m/z* calculated for $C_7H_{16}NO_5S_2$ 258.04644; found 258.0461 [M + $C_3H_8O_2S$]$^+$ (error −3.5 ppm).

Note: The exact mass of [M + H]$^+$ was measured at 5,000 resolution, including A+1 and A+2 peaks, with *m/z* and intensity nearly identical to theoretical values. HRMS (FAB): *m/z* calculated for $C_4H_8NO_3S$ 150.02194; found 150.0226 [M + H]$^+$ (error +0.7 ppm).



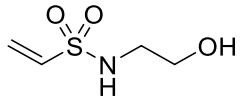


4-(Ethynylsulfonamido)butanoic acid (**6**): **2o** (410 mg, 2.0 mmol) were stirred for 24 h at room temperature in a 3:1 mixture of TFA/H_2O (10 mL). After evaporation of the volatile components, the crude residue was purified by column chromatography (Hexane:Et_2O:HCOOH = 1:2:0.015) to give colorless oil **6** (196 mg, 51%). FT-IR (KBr) *v* cm^{-1}: 3280 (m), 3242 (s), 3048 (br), 2982 (w), 2945 (w), 2069 (m), 1693 (s), 1465 (w), 1441 (m), 1415 (w), 1383 (w), 1350 (m), 1280 (m), 1219 (m), 1162 (s), 1085 (m), 1035 (w), 917 (w), 889 (m), 831 (m). ^{1}H-NMR (400 MHz, DMSO-*d*$_6$) *δ* 12.09 (br, 1H), 8.36 (t, *J* = 5.1 Hz, 1H), 4.97 (s, 1H), 2.98 (td, *J* = 6.9, 5.5 Hz, 2H), 2.25 (t, *J* = 7.3 Hz, 2H), 1.69 (quin, *J* = 7.2 Hz, 2H). ^{13}C-NMR (101 MHz, DMSO-*d*$_6$) *δ* 173.9, 79.9, 79.1, 42.1, 30.5, 24.0. LRMS (ESI): *m/z* (%) 190 (74) [M – H]. HRMS (ESI): *m/z* calculated for $C_6H_8NO_4S$ 190.01740; found 190.01671 [M – H]$^-$ (error −3.66 ppm).

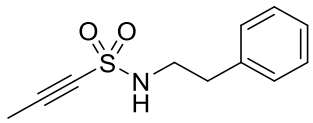


***N*,*N*-Bis(2-((*tert*-butyldimethylsilyl)oxy)ethyl)ethynesulfonamide** (**7**): Prepared as shown in general procedure 5; colorless oil; eluent (EtOAc); yield, quant. FT-IR (ATR) *v* cm^{-1}: 3300 (br), 3256 (m), 2951 (w), 2066 (m), 1606 (w), 1454 (s), 1364 (s), 1285 (w), 1254 (w), 1170 (s), 1077 (m). ^{1}H-NMR (400 MHz, DMSO-*d*$_6$) *δ* 5.11 (s, 1H), 4.92 (t, *J* = 5.5 Hz, 2H), 3.62–3.57 (dd, *J* = 6.3, 5.7 Hz, 4H), 3.28 (t, *J* = 6.2 Hz, 4H). ^{13}C-NMR (101 MHz, DMSO-*d*$_6$) *δ* 81.1, 77.6, 59.1, 51.5. LRMS (EI): *m/z* (%) 131 [M – CH_3O – CH_3O] (22), 162 [M – CH_3O] (base peak). HRMS (EI): *m/z* calculated for $C_5H_8NO_3S$ 162.2249; found 162.0232 [M – CH_3O]$^+$ (error +4.3 ppm).

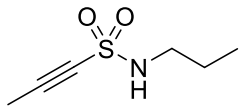
Note: Intramolecular reaction proceeds to produce **S1**.



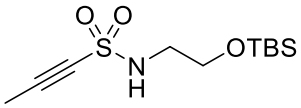
***N*-(2-Hydroxyethyl)ethenesulfonamide** (**8**): Prepared as shown in general procedure 5; colorless oil; eluent (Hexane:EtOAc = 1:3, v/v); yield, 92%. FT-IR (ATR) ν cm^{-1}: 3514 (br), 3300 (br), 3063 (w), 2936 (w), 2886 (w), 1424 (m), 1389 (m), 1328 (s), 1258 (w), 1154 (s), 1099 (m), 1060 (m), 972 (m). ^{1}H-NMR (400 MHz, DMSO-d_6) δ 7.23 (t, J = 5.7 Hz, 1H), 6.70 (dd, J = 16.6, 10.0 Hz, 1H), 6.01 (d, J = 16.6 Hz, 1H), 5.95 (d, J = 10.0 Hz, 1H), 4.73 (t, J = 5.6 Hz, 1H), 3.43 (td, J = 6.3, 5.7 Hz, 2H), 2.87 (q, J = 6.2 Hz, 2H). ^{13}C-NMR (101 MHz, DMSO-d_6) δ 137.0, 125.1, 60.1, 44.8. LRMS (EI): m/z (%) 60 [M – $C_2H_3O_2S$] (4), 91 [M – C_2H_6NO] (13), 120 [M – CH_3O] (46). HRMS (EI): m/z calculated for $C_3H_6NO_2S$ 120.01192; found 120.0120 [M – CH_3O]$^+$ (error +0.9 ppm).



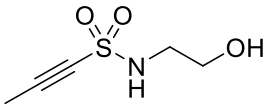
***N*-Phenethylprop-1-yne-1-sulfonamide** (**9a**): Prepared as shown in general procedure 4; colorless oil; eluent (Hexane:EtOAc = 2:1, v/v); yield, 51%. FT-IR (KBr) ν cm^{-1}: 3249 (s), 3033 (w), 2974 (w), 2937 (w), 2919 (w), 2211 (m), 1497 (w), 1468 (w), 1456 (w), 1431 (m), 1326 (s), 1163 (s), 1052 (s), 1031 (m), 942 (m), 910 (w), 771 (m), 753 (m), 705 (s), 558 (m), 497 (m). ^{1}H-NMR (400 MHz, $CDCl_3$) δ 7.36–7.21 (m, 5H), 4.59 (t, J = 5.7 Hz, 1H), 3.45 (td, J = 6.9, 6.3 Hz, 2H), 2.94 (t, J = 6.9 Hz, 2H), 2.04 (s, 3H). ^{13}C-NMR (101 MHz, $CDCl_3$) δ 137.5, 128.9, 128.8, 127.0, 88.5, 75.3, 44.6, 35.4, 3.9. LRMS (EI): m/z (%) 91 (78) [M – $C_4H_6NO_2S$], 132 (base peak) [M – C_7H_7], 223 (2) [M]. HRMS (EI): m/z calculated for $C_{11}H_{13}NO_2S$ 223.06670; found 223.0665 [M]$^+$ (error −0.8 ppm).



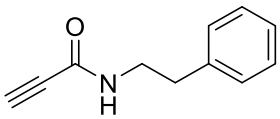
***N*-Propylprop-1-yne-1-sulfonamide** (**9b**): Prepared as shown in general procedure 4; colorless oil; eluent (Hexane:EtOAc = 2:1, v/v); yield, 62%. FT-IR (ATR) ν cm^{-1}: 3290 (br), 2970 (s), 2880 (m), 2219 (s), 1635 (w), 1460 (m), 1430 (m), 1170 (s). ^{1}H-NMR (400 MHz, $CDCl_3$) δ 4.64 (br, 1H), 3.15 (td, J = 7.1, 6.2 Hz, 2H), 2.06 (s, 3H), 1.65 (sext, J = 7.3 Hz, 2H), 0.99 (t, J = 7.4 Hz, 3H). ^{13}C-NMR (101 MHz, $CDCl_3$) δ 88.2, 75.4, 45.4, 22.6, 11.2, 3.9. LRMS (EI): m/z (%) 103 (32) [M – C_3H_8N], 132 (base peak) [M – C_2H_5], 146 (13) [M – CH_3], 161 (11) [M]. HRMS (EI): m/z calculated for $C_6H_{11}NO_2S$ 161.05105; found 161.0512 [M]$^+$ (error +0.8 ppm).



***N*-(2-((*tert*-Butyldimethylsilyl)oxy)ethyl)prop-1-yne-1-sulfonamide** (**9c**): Prepared as shown in general procedure 4; colorless oil; eluent (Hexane:EtOAc = 4:1, v/v); yield, 37%. FT-IR (NaCl) ν cm^{-1}: 3627 (br), 3296 (br), 2954 (s), 2930 (s), 2884 (s), 2858 (s), 2217 (s), 1471 (m), 1464 (m), 1411 (m), 1344 (s), 1257 (s), 1169 (s), 1088 (s), 1048 (m), 1007 (w), 973 (m), 939 (m), 838 (s), 810 (m), 780 (s), 718 (w), 645 (s). ^{1}H-NMR (400 MHz, $CDCl_3$) δ 4.96 (t, J = 5.0 Hz, 1H), 3.82–3.79 (m, 2H), 3.30–3.26 (m, 2H), 2.06 (s, 3H), 0.90 (s, 9H), 0.09 (s, 6H). ^{13}C-NMR (101 MHz, $CDCl_3$) δ 88.4, 75.3, 60.9, 45.7, 25.8, 18.3, 3.9, −5.4. LRMS (EI): m/z (%) 206 [M – C_4H_9 – CH_3] (14), 220 [M – C_4H_9] (base peak), 262 [M – CH_3] (6). HRMS (EI): m/z calculated for $C_{10}H_{20}NO_3SiS$ 262.09332; found 262.0940 [M – CH_3]$^+$ (error −2.6 ppm).



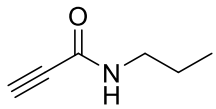
***N*-(2-Hydroxyethyl)prop-1-yne-1-sulfonamide** (**10**): Prepared as shown in general procedure 5; colorless oil; eluent (Hexane:EtOAc = 1:3, v/v); yield, quant. FT-IR (ATR) ν cm^{-1}: 3532 (br), 3301 (br), 2219 (s), 1636 (w), 1434 (m), 1337 (s), 1165 (s), 1052 (m). ^{1}H-NMR (400 MHz, $CDCl_3$) δ 5.45 (t, J = 5.4 Hz, 1H), 3.84 (dd, J = 4.7, 4.5 Hz, 2H), 3.36–3.32 (m, 2H), 2.32 (t, J = 4.4 Hz, 1H), 2.08 (s, 3H). ^{13}C-NMR (101 MHz, $CDCl_3$) δ 89.0, 75.1, 60.9, 45.5, 3.9. LRMS (FAB): m/z (%) 146 [M + H – H_2O] (30), 164 [M + H] (base peak). HRMS (FAB): m/z calculated for $C_5H_{10}NO_3S$ 164.03814; found 164.0377 [M + H]$^+$ (error −2.9 ppm).



***N*-Phenethylpropiolamide** (**13a**): Prepared as shown in general procedure 6A; pale yellow crystals; eluent (Hexane:EtOAc = 1:1, v/v); yield, 87%. FT-IR (NaCl) ν cm^{-1}: 3300 (m), 3274 (s), 3062 (w), 3029 (w), 2933 (w), 2109 (m), 1637 (vs), 1541 (s), 1497 (m), 1455 (m), 1362 (w), 1273 (m), 1199 (w), 747 (m), 699 (s). ^{1}H-NMR (400 MHz, $CDCl_3$) δ 7.35–7.31 (m, 2H), 7.27–7.19 (m, 3H), 5.93 (br, 1H), 3.57 (q, J = 6.9 Hz, 2H), 2.85 (t, J = 7.0 Hz, 2H), 2.75 (s, 1H). ^{13}C-NMR (101 MHz, $CDCl_3$) δ 152.1, 138.2, 128.8, 128.7, 126.9, 126.7, 79.2, 73.1, 44.6, 40.9, 36.9, 35.2, 34.0, 24.9. LRMS (EI): m/z (%) 53 (13) [M – $C_8H_{10}N$], 82 (19) [M – C_7H_7], 91 (22) [M – C_4H_4NO], 104 (base peak) [M – C_3H_3NO –

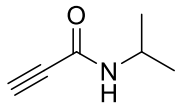
H], 173 (11) [M]. HRMS (EI): *m*/*z* calculated for $C_{11}H_{11}NO$ 173.08406; found 173.0841 $[M]^+$ (error +0.2 ppm).

Note: By ^1H NMR in $CDCl_3$, the compound is a 91:9 mixture of amide rotamers.



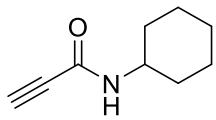
***N*-Propylpropiolamide** (**13b**): Prepared as shown in general procedure 6A; colorless oil; vacuum distillation (105 – 107 ºC/1.6 kPa); yield, 58%. FT-IR (NaCl) *v* cm^{-1}: 3250 (br), 3064 (w), 2966 (w), 2876 (w), 2108 (m), 1630 (vs), 1537 (s), 1452 (m), 1273 (s), 1150 (w), 942 (w). ^1H-NMR (400 MHz, $CDCl_3$, major rotamer) δ 6.01 (br, 1H), 3.28 (td, J = 7.1, 6.1 Hz, 2H), 2.78 (s, 1H), 1.57 (sext, J = 7.3 Hz, 2H), 0.96 (t, J = 7.4 Hz, 3H). ^{13}C-NMR (101 MHz, $CDCl_3$, major rotamer) δ 152.2, 79.2, 72.9, 41.6, 22.5, 11.3. LRMS (EI): *m*/*z* (%) 82 (14) [M – C_2H_5], 96 (34) [M – CH_3], 111 (17) [M]. HRMS (EI): *m*/*z* calculated for C_6H_9NO 111.06841; found 111.0688 $[M]^+$ (error +3.6 ppm).

Note: By ^1H NMR in $CDCl_3$, the compound is a 90:10 mixture of amide rotamers. By ^1H NMR in DMSO-d_6, the compound is a 94:6 mixture of amide rotamers.



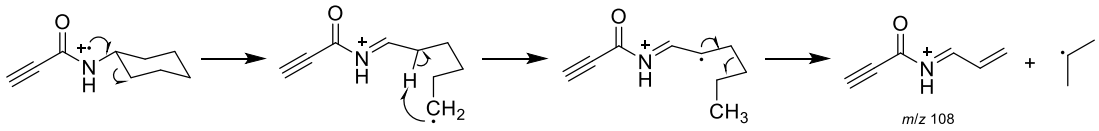
***N*-Isopropylpropiolamide** (**13c**): Prepared as shown in general procedure 6A; off-white crystals; eluent (Hexane:EtOAc = 2:1, v/v); yield, 43%. UV (abs) λ_{max}: 220 nm (5%v/v MeCN in Water). FT-IR (KBr) *v* cm^{-1}: 3205 (s), 3061 (m), 2980 (m), 2938 (w), 2826 (w), 2102 (s), 1643 (s), 1558 (s), 1468 (w), 1288 (m), 1156 (w), 979 (w), 921 (w), 762 (w), 719 (m), 608 (w). ^1H-NMR (400 MHz, $CDCl_3$, major rotamer) δ 5.78 (br, 1H), 4.18–4.07 (m, 1H), 2.75 (s, 1H), 1.19 (d, J = 6.6 Hz, 6H). ^{13}C-NMR (101 MHz, $CDCl_3$, major rotamer) δ 151.3, 77.5, 72.6, 42.1, 22.4. LRMS (EI): *m*/*z* (%) 82 (base peak) [M – C_2H_5], 95 (2) [M – CH_3]. HRMS (EI): *m*/*z* calculated for C_4H_4NO 82.0; found 82.0295 [M – $C_3H_5]^+$ (error +2.3 ppm).

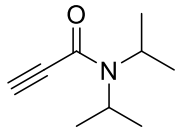
Note: ^1H NMR in $CDCl_3$, the compound is a 91:9 mixture of amide rotamers.



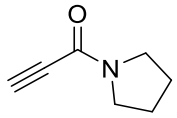
***N*-Cyclohexylpropiolamide** (**13d**): Prepared as shown in general procedure 6A; pale yellow crystals; eluent (Hexane:EtOAc = 3:1, v/v); yield, 43%. UV (abs) λ_{max}: 220 nm (5%v/v MeCN in Water). FT-IR (NaCl) ν cm^{-1}: 3301 (m), 3225 (m), 2933 (s), 2855 (m), 2104 (m), 1698 (s), 1631 (s), 1526 (s), 1452 (m), 1347 (m), 1236 (m), 1081 (w), 893 (w), 724 (m). ^{1}H-NMR (400 MHz, $CDCl_3$, major rotamer) δ 5.83 (br, 1H), 3.87–3.67 (m, 1H), 2.76 (s, 1H), 1.99–1.92 (m, 2H), 1.78–1.70 (m, 2H), 1.66–1.59 (m, 1H), 1.42–1.28 (m, 2H), 1.26–1.12 (m, 3H). ^{13}C-NMR (101 MHz, $CDCl_3$, major rotamer) δ 151.2, 77.6, 72.7, 48.9, 32.7, 25.4, 24.7. LRMS (EI): *m*/*z* (%) 53 (21) [M – $C_6H_{12}N$], 70 (base peak) [M – C_3HO – C_2H_4], 108 (79) [M – C_3H_7], 151 (14) [M]. HRMS (EI): *m*/*z* calculated for $C_9H_{13}NO$ 151.09971; found 151.0997 [M]$^+$ (error +0.0 ppm).

Note: ^{1}H NMR in $CDCl_3$, the compound is a 89:11 mixture of amide rotamers. McClafferty rearrangement.

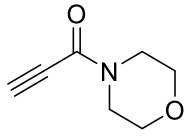




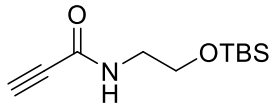
***N*,*N*-Diisopropylpropiolamide** (**13e**): Prepared as shown in general procedure 3B; colorless needles; eluent (Hexane:EtOAc = 3:1, v/v); yield, 77%. UV (abs) λ_{max}: 234 nm (5%v/v MeCN in Water). FT-IR (KBr) ν cm^{-1}: 3186 (s), 3003 (m), 2979 (s), 2936 (m), 2873 (w), 2091 (s), 1616 (s), 1446 (m), 1379 (m), 1370 (s), 1330 (s), 1208 (s), 1155 (m), 946 (w), 886 (w), 8957 (w), 774 (m), 741 (m), 588 (m). ^{1}H-NMR (400 MHz, $CDCl_3$) δ 4.60 (sep, J = 6.8 Hz, 1H), 3.60 (sep, J = 6.8 Hz, 1H), 3.03 (s, 1H), 1.39 (d, J = 6.8 Hz, 6H), 1.25 (d, J = 6.8 Hz, 6H). ^{13}C-NMR (101 MHz, $CDCl_3$) δ 152.3, 77.2, 77.1, 50.6, 45.8, 20.8, 19.9. LRMS (EI): *m*/*z* (%) 53 (20) [M – $C_6H_{14}N$], 96 (base peak) [M – C_3H_7 – CH_3 + H], 110 (37) [M – C_3H_7], 138 (49) [M – CH_3], 153 (36) [M]. HRMS (EI): *m*/*z* calculated for $C_9H_{15}NO$ 153.11536; found 153.1149 [M]$^+$ (error −3.0 ppm).



1-(Pyrrolidin-1-yl)prop-2-yn-1-one (**13f**): Prepared as shown in general procedure 6A; white crystals; eluent (Hexane:EtOAc = 1:1, v/v); yield, 85%. FT-IR (NaCl) ν cm^{-1}: 3180 (s), 2978 (w), 2884 (w), 2099 (s), 1640 (s), 1618 (vs), 1460 (w), 1431 (s), 1338 (w), 1192 (w), 780 (m), 727 (m), 641 (w). ^{1}H-NMR (400 MHz, $CDCl_3$) δ 3.68–3.65 (m, 2H), 3.51–3.47 (m, 2H), 3.05 (s, 1H), 2.00–1.89 (m, 4H). ^{13}C-NMR (101 MHz, $CDCl_3$) δ 151.4, 77.1, 76.8, 48.1, 45.3, 25.3, 24.6. LRMS (EI): *m*/*z* (%) 53 (15) [M – C_4H_8N] 70 (26) [M – C_3HO], 95 (21) [M – C_2H_4], 108 (11) [M – CH_3], 122 (71) [M – H], 123 (base peak) [M]. HRMS (EI): *m*/*z* calculated for C_7H_9NO 123.06841; found 123.0688 $[M]^+$ (error +3.0 ppm).

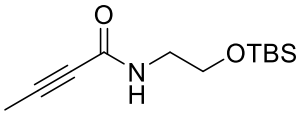


1-Morpholinoprop-2-yn-1-one (**13g**): Prepared as shown in general procedure 6A; white crystals; eluent (Hexane:EtOAc = 1:1, v/v); yield, 93%. UV (abs) λ_{max}: 236 nm (5%v/v MeCN in Water). FT-IR (KBr) ν cm^{-1}: 3181 (m), 2979 (w), 2926 (w), 2867 (w), 2103 (m), 1360 (s), 1442 (m), 1360 (w), 1331 (w), 1273 (m), 1240 (m), 1114 (m), 1039 (m), 959 (w), 844 (w), 774 (w), 745 (w), 557 (m). ^{1}H-NMR (400 MHz, $CDCl_3$) δ 3.80–3.77 (m, 2H), 3.74–3.64 (m, 6H), 3.17 (s, 1H). ^{13}C-NMR (101 MHz, $CDCl_3$) δ 151.9, 79.7, 75.0, 66.8, 66.3, 47.2, 41.9. LRMS (EI): *m*/*z* (%) 53 (80) [M – C_4H_8NO], 86 (76) [M – C_3HO], 124 (26) [M – CH_3], 139 (base peak) [M]. HRMS (EI): *m*/*z* calculated for C_7H_9NO 139.06333; found 139.0633 $[M]^+$ (error −0.4 ppm).

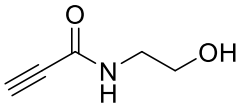


***N*-(2-((*tert*-Butyldimethylsilyl)oxy)ethyl)propiolamide** (**13h**): 2-Aminoethanol (605 µL, 10 mmol), DMAP (12 mg, 1.0 mol%), Et_3N (1.1 mL, 1.5 equiv.), and *t*-butyldimethylsilyl (TBS) chloride (1.8 g, 1.2 equiv.) were added to DCM (40 mL) at 0 °C under N_2 and stirred for 1 hour. After added saturated $NaHCO_3$ aqueous solution (100 mL). The reaction mixture was washed three times with distilled water, and the organic layer was dried over Na_2SO_4. After concentration. The reaction mixture, propiolic acid (**11**, 680 µL, 11 mmol) and DMAP (12.2 mg, 1.0 mol%) were added to DCM (20 mL) followed by and the solution was cooled to 0 ˚C. To this, a solution of DCC (2.27 g, 11 mmol, 1.1 equiv.) in DCM (20 mL) was added dropwise and the reaction was then allowed to warm to room temperature and stirred for 3 hour. Once complete, the reaction mixture was filtered through Celite, and the solvent

was then removed in vacuo. After concentration, chromatography was performed on the residue on a silica gel column eluent (Hexane:EtOAc = 3:1, v/v) to give yellow oil **13h** (820 mg, 36%). ^{1}H-NMR (400 MHz, DMSO-d_6) δ 8.35 (br, 1H), 3.89 (s, 1H), 3.60 (t, J = 6.2 Hz, 2H), 3.18 (q, J = 6.1 Hz, 2H), 0.87 (s, 9H), 0.04 (s, 5H). ^{13}C-NMR (101 MHz, DMSO-d_6) δ 151.4, 78.0, 74.7, 60.5, 41.1, 25.4, 17.5, −5.8. LRMS (ESI): m/z (%) 250 (base peak) [M + Na], 282 (16) [M + MeOH + Na]. HRMS (ESI): m/z calculated for $C_{11}H_{21}NO_2NaSi$ 250.12392; found 250.12356 $[M + Na]^+$ (error −1.47 ppm).

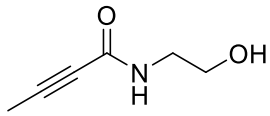


***N*-(2-((*tert*-Butyldimethylsilyl)oxy)ethyl)but-2-ynamide** (**14**): **12** instead of **11** in method **13h**; colorless oil; eluent (Hexane:EtOAc = 3:1, v/v); yield, 45%. FT-IR (NaCl) v cm^{-1}: 3276 (br), 3066 (w), 2953 (m), 2929 (m), 2883 (m), 2857 (m), 2257 (w), 2233 (w), 1631 (s), 1541 (m), 1471 (w), 1292 (m), 1253 (m), 1098 (s), 1007 (w), 939 (w), 877 (w), 834 (s), 775 (s). ^{1}H-NMR (400 MHz, DMSO-d_6, 393 K) δ 7.78 (br, 1H), 3.60 (t, J = 6.2 Hz, 2H), 3.18 (br, 2H), 2.85 (m, 2H), 1.91 (s, 3H), 0.87 (s, 9H), 0.04 (s, 6H). ^{13}C-NMR (101 MHz, DMSO-d_6, 393 K) δ 152.5, 82.1, 75.5, 60.9, 41.2, 25.7, 17.9, 2.9, −5.4. LRMS (EI): m/z (%) 67 (29) [M – $C_8H_{20}NOSi$], 184 (base peak) [M – C_4H_9], 226 (8) [M – CH_3]. HRMS (EI): m/z calculated for $C_{11}H_{20}NO_2Si$ 226.12633; found 226.1264 $[M – CH_3]^+$ (error +0.3 ppm).

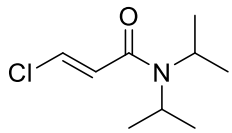


***N*-(2-Hydroxyethyl)propiolamide** (**15**): Prepared as shown in general procedure 5; white solids; eluent (EtOAc); yield, quant. FT-IR (NaCl) v cm^{-1}: 3255 (br), 3248 (s), 3059 (s), 2991 (w), 2963 (w), 2925 (w), 2878 (w), 2015 (m), 1634 (s), 1576 (m), 1463 (w), 1434 (m), 1353 (w), 1302 (m), 1260 (w), 1223 (w), 1107 (m), 1083 (w), 1055 (m), 913 (w), 848 (w), 810 (w), 726 (m), 694 (w). ^{1}H-NMR (400 MHz, DMSO-d_6, ma*J*or rotamer) δ 8.67 (br, 1H), 4.70 (t, J = 5.5 Hz, 1H), 4.09 (s, 1H), 3.39 (q, J = 6.0 Hz, 2H), 3.13 (q, J = 6.0 Hz, 2H). ^{13}C-NMR (101 MHz, DMSO-d_6, major rotamer) δ 151.4, 78.1, 74.7, 59.0, 41.5. LRMS (ESI): m/z (%) 136 (22) [M + Na], 249 (12) [2M + Na] HRMS (ESI): m/z calculated for $C_5H_7NO_2Na$ 136.03745; found 136.03691 $[M + Na]^+$ (error −3.96 ppm).

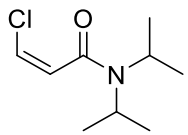
Note: By ^{1}H NMR in DMSO-d_6, the compound is a 95:5 mixture of amide rotamers.



***N*-(2-Hydroxyethyl)but-2-ynamide** (**16**): Prepared as shown in general procedure 5; white solids; eluent (EtOAc); yield, quant. FT-IR (ATR) ν cm^{-1}: 3278 (br), 3070 (w), 2931 (w), 2879 (w), 2260 (m), 2233 (m), 1635 (s), 1556 (m), 1439 (w), 1300 (m), 1069 (m). ^{1}H-NMR (400 MHz, DMSO-d_6, 373 K) δ 7.89 (br, 1H), 4.27 (br, 1H), 3.42 (q, J = 5.8 Hz, 2H), 3.14 (q, J = 5.7 Hz, 2H), 2.96 (s, 2H), 1.92 (s, 3H). ^{13}C-NMR (101 MHz, DMSO-d_6, 393 K) δ 152.2, 81.4, 75.2, 59.1, 41.4, 2.1. LRMS (EI): m/z (%) 67 (base peak) [M – C_2H_6NO], 96 (47) [M – CH_3O], 109 (6) [M – H_2O]. HRMS (EI): m/z calculated for C_6H_7NO 109.05276; found 109.0532 [M – H_2O]$^+$ (error +4.1 ppm).

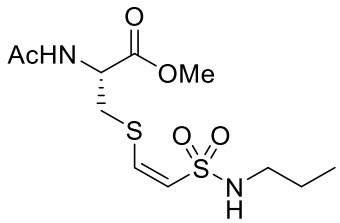


(*E*)-3-Chloro-*N*,*N*-diisopropylacrylamide (**17 (*E*)**): To a stirred solution of **11** (5.0 mmol) and dry DMF (0.97 mL, 1.5 equiv.) in dry DCM (15 mL), $(COCl)_2$ (2.45 mL, 2 M solution in DCM, 0.98 equiv.) was added at 0 °C. The reaction mixture was then stirred for 3 hours at room temperature. To a stirred solution of DIPA (2.1 mL, 3.0 equiv.) in DCM (5.0 mL), the reaction mixture was added dropwise over 10 minuts at 0 °C, was then stirred for 3 hours. The mixture was quenched with distilled water. The reaction mixture was washed with 5% NaOH aqueous solution, 1 M HCl aqueous solution, and brine. The organic layer was dried over Na_2SO_4. After concentration, chromatography was performed on the residue on a silica gel column (Hexane:EtOAc = 3:1, v/v) to give colorless oil **17 (*E*)** (545 mg, 57%). FT-IR (NaCl) ν cm^{-1}: 2970 (m), 2934 (w), 1637 (vs), 1584 (s), 1442 (s), 1372 (m), 1332 (s), 1206 (w), 1134 (w), 1045 (w), 930 (w), 859 (w), 740 (m), 607 (w). ^{1}H-NMR (400 MHz, $CDCl_3$) δ 7.17 (d, J = 12.8 Hz, 1H), 6.65 (d, J = 12.8 Hz, 1H), 3.95 (br, 1H), 3.77 (br, 1H), 1.35 (br, 6H), 1.27 (br, 6H). ^{13}C-NMR (101 MHz, $CDCl_3$) δ 163.4, 133.1, 126.7, 48.3, 45.9, 21.4, 20.5. LRMS (EI): m/z (%) 61 (3) [M – $C_7H_{14}NO$], 86 (base peak) [M – C_2H_2Cl – C_3H_7 + H], 89 (32) [M – $C_6H_{14}N$], 132 (11) [M – C_3H_7 – CH_3], 146 (14) [M – C_3H_7], 154 (51) [M – Cl], 174 (11) [M – CH_3], 189 (3) [M]. HRMS (EI): m/z calculated for $C_9H_{16}NOCl$ 189.09204; found 189.0927 [M]$^+$ (error +3.6 ppm).

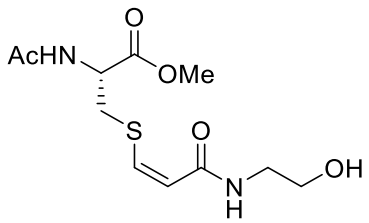


(*Z*)-3-Chloro-*N*,*N*-diisopropylacrylamide (**17 (*Z*)**): Prepared as shown in **17 (*Z*)**; colorless crystals; eluent (Hexane:EtOAc = 1:1, v/v); yield, 20%. FT-IR (NaCl) ν cm^{-1}: 2972 (m), 2935 (w), 1634 (vs), 1473 (w), 1443 (s), 1371 (m), 1348 (s), 1297 (m), 1214 (w), 1156 (w), 1135 (m), 1045 (w), 830 (w),

715 (w). ^{1}H-NMR (400 MHz, $CDCl_3$) δ 6.33 (d, J = 7.9 Hz, 1H), 6.28 (d, J = 7.9 Hz, 1H), 4.04 (sep, J = 6.8 Hz, 1H), 3.52 (sep, J = 6.8 Hz, 1H), 1.46 (d, J = 6.8 Hz, 6H), 1.21 (d, J = 6.8 Hz, 6H). ^{13}C-NMR (101 MHz, $CDCl_3$) δ 164.0, 127.2, 121.5, 50.3, 45.8, 21.1, 20.4. LRMS (EI): *m*/*z* (%) 61 (3) [M – $C_7H_{14}NO$], 86 (base peak) [M – C_2H_2Cl – C_3H_7 + H], 89 (31) [M – $C_6H_{14}N$], 132 (14) [M – C_3H_7 – CH_3], 146 (18) [M – C_3H_7], 154 (53) [M – Cl], 174 (8) [M – CH_3], 189 (3) [M]. HRMS (EI): *m*/*z* calculated for $C_9H_{16}NOCl$ 189.09204; found 189.0927 $[M]^+$ (error +0.5 ppm).

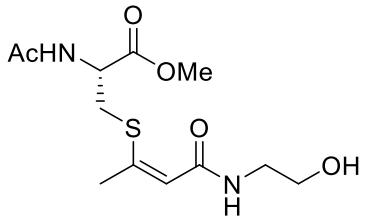


Methyl (*Z*)-*N*-acetyl-*S*-(2-(*N*-propylsulfamoyl)vinyl)-L-cysteinate (**2c-Cys**): Prepared as shown in general procedure 7; colorless crystals; silica gel column eluent (Hexane:EtOAc = 1:3, v/v); yield, 20% (isolated). FT-IR (NaCl) ν cm^{-1}: 3567 (br), 3287 (br), 3147 (w), 2965 (m), 2936 (w), 2877 (w), 2253 (w), 1742 (s), 1662 (s), 1553 (s), 1437 (m), 1374 (m), 1317 (s), 1220 (m), 1136 (s), 1076 (w), 1005 (w), 916 (w), 840 (w), 732 (m), 697 (m), 631 (w). ^{1}H-NMR (400 MHz, $CDCl_3$) δ 6.93 (d, J = 10.2 Hz, 1H), 6.43 (d, J = 6.8 Hz, 1H), 6.18 (d, J = 10.2 Hz, 1H), 4.86 (dt, J = 7.0, 4.6 Hz, 1H), 4.60 (t, J = 6.2 Hz, 1H), 3.80 (s, 3H), 3.32 (dd, J = 14.4, 4.8 Hz, 1H), 3.27 (dd, J = 14.4, 4.3 Hz, 1H), 3.03 (dt, J = 7.1, 6.3 Hz, 2H), 2.06 (s, 3H), 1.60 (sext, J = 7.1 Hz, 2H), 0.96 (t, J = 7.4 Hz, 3H). ^{13}C-NMR (101 MHz, $CDCl_3$) δ 170.2, 170.1, 143.2, 122.4, 53.1, 52.7, 44.7, 37.9, 23.3, 23.1, 11.2. LRMS (EI): *m*/*z* (%) 43 (54) [M − $C_8H_{13}N_2O_5S_2$], 58 (22) [M – $C_8H_{12}NO_5S_2$], 143 (55) [M – $C_2H_3O_2$ – $C_3H_8NO_2S$], 207 (base peak) [M – $C_2H_3O_2$ – C_3H_8N], 236 (76) [M – $C_2H_3O_2$ – C_2H_5], 265 (44) [M – $C_2H_3O_2$], 295 (3) [M – C_2H_5], 324 (6) [M]. HRMS (EI): *m*/*z* calculated for $C_{11}H_{20}N_2O_5S_2$ 324.08135; found 324.0810 $[M]^+$ (error −1.1 ppm).

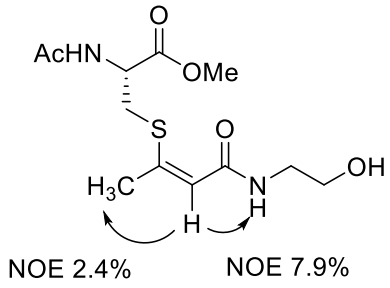


Methyl (*Z*)-*N*-acetyl-*S*-(3-((2-hydroxyethyl)amino)-3-oxoprop-1-en-1-yl)-L-cysteinate (**15-Cys**): Prepared as shown in general procedure 7; colorless crystals; silica gel column eluent ($CHCl_3$/Acetone = 1:1, v/v); yield, 13% (isolated). FT-IR (ATR) ν cm^{-1}: 3303 (br), 3075 (w), 3931 (w), 1744 (s), 1645 (s), 1578 (s(m 1540 (s), 1437 (m), 1375 (m), 1263 (m), 1221 (m), 1064 (m). ^{1}H-NMR (400 MHz, $CDCl_3$) δ 6.82 (d, J = 7.5 Hz, 1H), 6.76 (d, J = 9.9 Hz, 1H), 6.45 (t, J = 5.6 Hz, 1H), 5.84 (d, J = 9.9

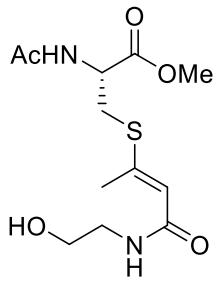
Hz, 1H), 4.87 (dt, *J* = 7.5, 4.8 Hz, 1H), 3.77 (s, 3H), 3.73 (d, *J* = 4.1 Hz, 2H), 3.45 (td, *J* = 5.5, 4.7 Hz, 2H), 3.33 (br, 1H), 3.27–3.18 (m, 2H), 2.04 (s, 3H).^{13}C-NMR (101 MHz, $CDCl_3$) δ 170.8, 170.4, 167.1, 144.7, 116.3, 61.9, 52.9, 52.5, 42.2, 38.3, 23.0. LRMS (EI): *m*/*z* (%) 313 (base peak) [M + Na]. HRMS (ESI): *m*/*z* calculated for $C_{11}H_{18}N_2O_5NaS$ 313.08341; found 313.08239 $[M + Na]^+$ (error −3.26 ppm).



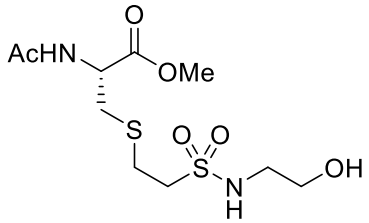
Methyl (*Z*)-*N*-acetyl-*S*-(4-((2-hydroxyethyl)amino)-4-oxobut-2-en-2-yl)-L-cysteinate (16-Cys (*Z*)): Prepared as shown in general procedure 7; colorless crystals; silica gel column eluent ($CHCl_3$/MeOH = 100:5, v/v); yield, 72% (isolated). FT-IR (KBr) *v* cm^{-1}: 3523 (m), 1401 (m), 3285 (br), 3077 (m), 2956 (m), 2886 (w), 1761 (m), 1737 (s), 1646 (s), 1631 (s), 1581 (s), 1552 (s), 1454 (m), 1438 (m), 1416 (m), 1372 (m), 1359 (m), 1372 (m), 1358 (m), 1300 (m), 1238 (s), 1198 (m), 1182 (m). ^{1}H-NMR (400 MHz, DMSO-d_6) δ 8.49 (d, *J* = 7.7 Hz, 1H), 7.73 (t, *J* = 5.7 Hz, 1H), 5.85 (s, 1H), 4.65 (t, *J* = 5.4 Hz, 1H), 4.38–4.33 (m, 1H), 3.65 (s, 3H), 3.37 (q, *J* = 5.9 Hz, 2H), 3.21 (dd, *J* = 13.3, 5.0 Hz, 1H), 3.10 (q, *J* = 6.0 Hz, 2H), 2.98 (dd, *J* = 13.3, 8.9 Hz, 1H), 2.12 (s, 3H), 1.86 (s, 3H). ^{13}C-NMR (101 MHz, DMSO-d_6) δ 171.0, 169.5, 165.3, 148.3, 116.2, 60.0, 52.4, 52.2, 41.2, 30.5, 23.2, 22.3. LRMS (ESI): *m*/*z* (%) 160 (18) [M – $C_6H_{10}NO_3$], 327 (base peak) [M + Na], 631 (6) [2M + Na]. HRMS (ESI): *m*/*z* calculated for $C_{12}H_{20}N_2O_5NaS$ 327.09906; found 327.09864 $[M + Na]^+$ (error −1.27 ppm).



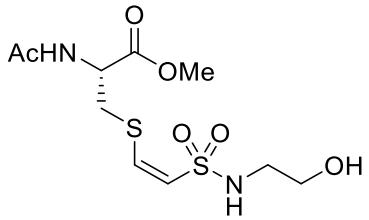
(DMSO-d_6)



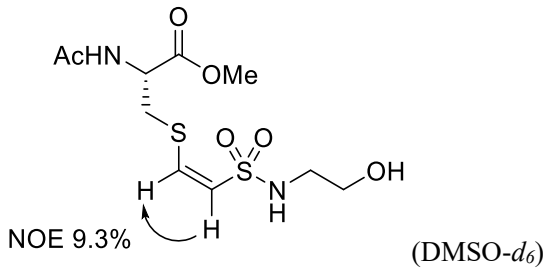
Methyl (*E*)-*N*-acetyl-*S*-(4-((2-hydroxyethyl)amino)-4-oxobut-2-en-2-yl)-L-cysteinate (16-Cys (*E*)): Prepared as shown in general procedure 7; colorless crystals; silica gel column eluent ($CHCl_3$/MeOH = 95:5, v/v); yield, 5% (isolated). FT-IR (ATR) ν cm^{-1}: 3291 (br), 3072 (w), 2930 (m), 1746 (s), 1645 (s), 1601 (s), 1540 (s), 1437 (m), 1377 (m), 1247 (m). ^{1}H-NMR (400 MHz, $CDCl_3$) δ 6.63 (d, J = 7.4 Hz, 1H), 6.57 (t, J = 5.4 Hz, 1H), 5.78 (s, 1H), 4.86–4.81 (m, 1H), 3.80 (s, 3H), 3.73 (t, J = 4.9 Hz, 2H), 3.44 (td, J = 5.7, 3.9 Hz, 2H), 3.21 (dd, J = 14.1, 6.5 Hz, 1H), 3.16 (dd, J = 14.2, 4.9 Hz, 1H), 2.40 (s, 3H), 2.17 (s, 1H), 2.04 (s, 3H). ^{13}C-NMR (101 MHz, $CDCl_3$) δ 170.9, 170.6, 166.4, 151.0, 112.9, 62.5, 53.0, 51.3, 42.3, 32.8, 23.1, 20.0. LRMS (ESI): m/z (%) 160 (16) [M – $C_6H_{10}NO_3$], 327 (bese peak) [M + Na], 631 (6) [2M + Na]. HRMS (ESI): m/z calculated for $C_{12}H_{20}N_2O_5NaS$ 327.09906; found 327.09772 $[M + Na]^+$ (error −4.10 ppm).



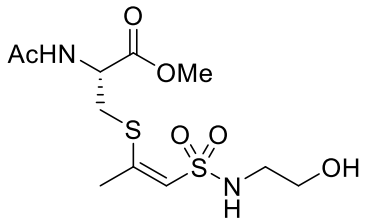
Methyl *N*-acetyl-*S*-(2-(*N*-(2-hydroxyethyl)sulfamoyl)ethyl)-L-cysteinate (8-Cys): Prepared as shown in general procedure 7; colorless crystals; silica gel column eluent ($CHCl_3$/MeOH = 95:5, v/v); yield, 61% (isolated). FT-IR (ATR) ν cm^{-1}: 3342 (br), 2955 (m), 1746 (s), 1660 (s), 1542 (m), 1438 (m), 1376 (m), 1325 (s), 1220 (m), 1147 (s). ^{1}H-NMR (400 MHz, $CDCl_3$) δ 6.46 (d, J = 7.5 Hz, 1H), 5.04 (t, J = 5.9 Hz, 1H), 4.85–4.80 (m, 1H), 3.81 (s, 3H), 3.77 (dd, J = 9.9, 5.1 Hz, 2H), 3.34–3.29 (m, 4H), 3.12 (t, J = 5.3 Hz, 1H), 3.09–2.89 (m, 4H), 2.08 (s, 3H). ^{13}C-NMR (101 MHz, DMSO-d_6) δ 171.2, 169.5, 79.2, 60.5, 52.1, 51.9, 51.5, 44.9, 32.6, 25.0, 22.3. LRMS (EI): m/z (%) 144 (base peak) [M – $C_4H_{10}NO_3S_2$], 204 (41) [M – $C_2H_6NO_6S$], 238 (3) [M – $C_2H_3O_2$ – CH_3O], 269 (8) [M – $C_2H_3O_2$], 283 (3) [M – C_2H_6O], 297 (5) [M – CH_3O]. HRMS (EI): m/z calculated for $C_9H_{17}N_2O_5S_2$ 297.05789; found 297.0576 $[M – CH_3O]^+$ (error −1.1 ppm).



Methyl (*Z*)-*N*-acetyl-*S*-(2-(*N*-(2-hydroxyethyl)sulfamoyl)vinyl)-L-cysteinate (**5-Cys**): Prepared as shown in general procedure 7; colorless crystals; silica gel column eluent ($CHCl_3$/MeOH = 95:5, v/v); yield, 39% (isolated). FT-IR (ATR) ν cm^{-1}: 3505 (br), 3298 (br), 2963 (m), 1742 (s), 1660 (s), 1556 (s), 1437 (m), 1375 (m), 1318 (s), 1263 (m), 1221 (m), 1143 (s), 1098 (m), 1054 (m). ^{1}H-NMR (400 MHz, DMSO-d_6) δ 8.47 (d, J = 7.9 Hz, 1H), 7.22 (d, J = 10.3 Hz, 1H), 7.16 (t, J = 5.9 Hz, 1H), 6.22 (d, J = 10.3 Hz, 1H), 4.71 (t, J = 5.5 Hz, 1H), 4.48 (td, J = 8.3, 5.1 Hz, 1H), 3.65 (s, 3H), 3.42 (dd, J = 11.6, 6.1 Hz, 2H), 3.20 (dd, J = 14.0, 5.1 Hz, 1H), 3.04 (dd, J = 14.0, 8.7 Hz, 1H), 2.88 (q, J = 6.2 Hz, 2H), 1.86 (s, 3H). ^{13}C-NMR (101 MHz, DMSO-d_6) δ 170.8, 169.6, 142.6, 121.6, 79.2, 60.1, 52.5, 52.3, 44.6, 35.8, 22.3. LRMS (ESI): m/z (%) 349 (base peak) [M + Na], 675 (10) [2M + Na]. HRMS (ESI): m/z calculated for $C_{10}H_{18}N_2O_6NaS$ 349.05040; found 349.04954 $[M + Na]^+$ (error −2.46 ppm).

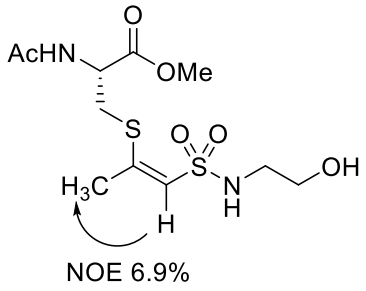


(DMSO-d_6)

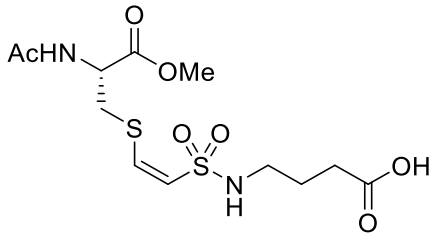


Methyl (*Z*)-*N*-acetyl-*S*-(1-(*N*-(2-hydroxyethyl)sulfamoyl)prop-1-en-2-yl)-L-cysteinate (**10-Cys**): Prepared as shown in general procedure 7; colorless crystals; preparative RP-HPLC eluent (MeOH/H_2O = 3:7, v/v); yield, 8% (isolated). FT-IR (KBr) ν cm^{-1}: 3360 (br), 3062 (w), 3955 (w), 2883 (w), 1741 (s), 1659 (s), 1558 (m), 1438 (m), 1375 (w), 1319 (s), 1282 (w), 1222 (w), 1142 (s), 1104 (w), 1058 (w), 1006 (w), 953 (w), 853 (w), 598 (m). ^{1}H-NMR (400 MHz, DMSO-d_6) δ 8.50 (d, J = 7.8 Hz, 1H), 7.00 (t, J = 6.0 Hz, 1H), 6.26 (d, J = 1.3 Hz, 1H), 4.70 (t, J = 5.6 Hz, 1H), 4.43–4.38 (td, J = 8.6, 5.0 Hz, 1H), 3.64 (s, 3H), 3.41 (dd, J = 12.0, 6.3 Hz, 2H), 3.29 (dd, J = 13.6, 5.1 Hz, 1H), 3.08 (dd, J = 13.6, 8.7 Hz, 1H), 2.89 (q, J = 6.3 Hz, 2H), 2.19 (d, J = 1.1 Hz, 3H), 1.86 (s, 3H). ^{13}C-NMR (101 MHz, DMSO-d_6) δ 170.7, 169.6, 148.8, 121.8, 60.1, 52.3, 52.1, 44.7, 30.9, 22.7, 22.3.

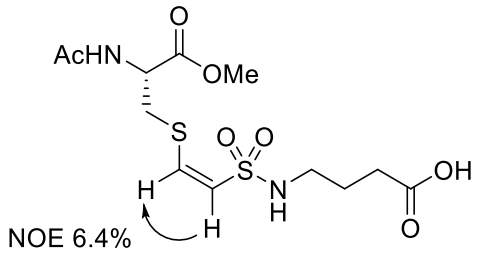
LRMS (ESI): *m*/*z* (%) 341 (10) [M + H], 363 (base peak) [M + Na], 703 (14) [2M + Na]. HRMS (ESI): *m*/*z* calculated for $C_{11}H_{20}N_2O_6NaS_2$ 363.06605; found 363.06578 $[M + Na]^+$ (error −0.74 ppm).



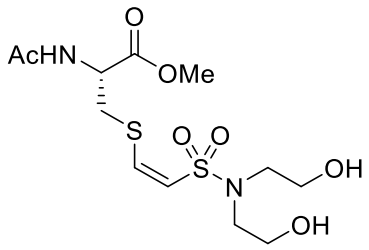
(DMSO-*d*$_6$)



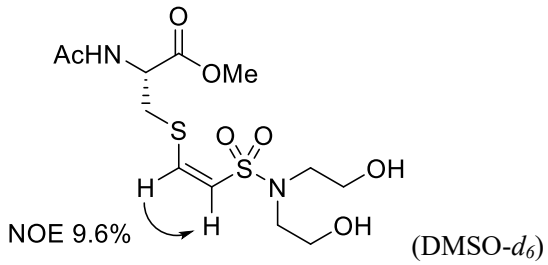
(*R*,*Z*)-4-((2-((2-Acetamido-3-methoxy-3-oxopropyl)thio)vinyl)sulfonamido)butanoic acid (6-Cys): Prepared as shown in general procedure 7; colorless gam; preparative RP-HPLC eluent (MeOH/H_2O = 3:7, v/v); yield, 44% (isolated). FT-IR (ATR) *v* cm^{-1}: 3534 (br), 3298 (br), 2960 (m), 1739 (s), 1661 (m), 1555 (s), 1436 (m), 1376 (m), 1319 (s), 1221 (m), 1142 (s), 705 (m). ^{1}H-NMR (400 MHz, DMSO-*d*$_6$) δ 12.06 (br, 1H), 8.45 (d, *J* = 7.9 Hz, 1H), 7.22 (d, *J* = 10.3 Hz, 1H), 7.24–7.22 (m, 1H), 6.18 (d, *J* = 10.3 Hz, 1H), 4.46 (td, *J* = 8.5, 5.1 Hz, 1H), 3.63 (s, 3H), 3.19 (dd, *J* = 14.0, 5.1 Hz, 1H), 3.02 (dd, *J* = 14.0, 8.7 Hz, 1H), 2.83 (td, *J* = 6.9, 5.8 Hz, 2H), 2.24 (t, *J* = 7.4 Hz, 2H), 1.85 (s, 3H), 1.64 (quin, *J* = 7.1 Hz, 2H). ^{13}C-NMR (101 MHz, DMSO-*d*$_6$) δ 174.1, 170.7, 169.5, 142.7, 121.4, 52.5, 52.2, 41.4, 35.8, 30.7, 24.7, 22.3. LRMS (ESI): *m*/*z* (%) 391 (base peak) [M + Na]. HRMS (ESI): *m*/*z* calculated for $C_{12}H_{20}N_2O_7NaS_2$ 391.06096; found 391.06069 $[M + Na]^+$ (error −0.68 ppm).



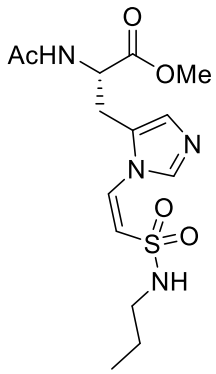
(DMSO-*d*$_6$)



Methyl (*Z*)-*N*-acetyl-*S*-(2-(*N*,*N*-bis(2-hydroxyethyl)sulfamoyl)vinyl)-L-cysteinate (**7-Cys**): Prepared as shown in general procedure 7; colorless gam; silica gel column eluent ($CHCl_3$/MeOH = 19:1, v/v); yield, 77% (isolated). FT-IR (ATR) ν cm^{-1}: 3615 (br), 3050 (w), 2952 (w), 2885 (w), 2258 (w), 2129 (w), 1741 (m), 1658 (m), 1550 (m), 1437 (m(, 1374 (w), 1321 (m), 1253 (w), 1219 (w), 1140 (s), 1074 (w), 1046 (m), 1024 (s), 992 (s), 915 (m), 826 (m). ^{1}H-NMR (400 MHz, DMSO-d_6) δ 8.47 (d, J = 7.9 Hz, 1H), 7.29 (d, J = 10.3 Hz, 1H), 6.36 (d, J = 10.3 Hz, 1H), 4.82 (t, J = 5.4 Hz, 2H), 4.49 (td, J = 8.3, 5.1 Hz, 1H), 3.65 (s, 3H), 3.51 (td, J = 6.2, 5.7 Hz, 4H), (dd, J = 14.0, 5.1 Hz, 5H), 3.16 (t, J = 6.3 Hz, 4H), 3.04 (dd, J = 14.0, 8.8 Hz, 1H), 1.86 (s, 3H). ^{13}C-NMR (101 MHz, DMSO-d_6) δ 170.8, 169.5, 143.5, 120.0, 59.7, 52.4, 52.2, 50.3, 35.7, 22.3. LRMS (EI): m/z (%) 371 (5) [M + H], 393 (base peak) [M + Na], 763 (15) [2M + Na]. HRMS (ESI): m/z calculated for $C_{12}H_{23}N_2O_7S_2$ 371.09467; found 371.09463 $[M + H]^+$ (error −0.09 ppm).

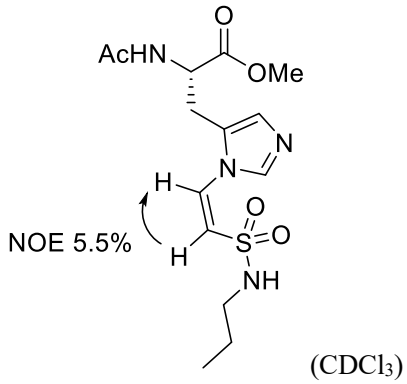


(DMSO-d_6)

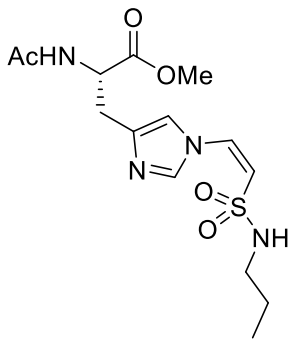


Methyl (*Z*)-N^{α}-acetyl-N^{π}-(2-(*N*-propylsulfamoyl)vinyl)-L-histidinate (**2b-His$^{\pi}$**): Prepared as shown in general procedure 7; colorless oil; preparative RP-HPLC eluent (MeOH/H_2O = 2:3, v/v); yield, 21% (isolated). FT-IR (KBr) ν cm^{-1}: 3367 (m), 3261 (br), 3061 (m), 2966 (m), 2877 (m), 1743 (s), 1661 (s), 1635 (s), 1540 (m), 1487 (m), 1439 (m), 1376 (m), 1324 (s), 1254 (m), 1221 (m), 1154 (m), 1103 (m),

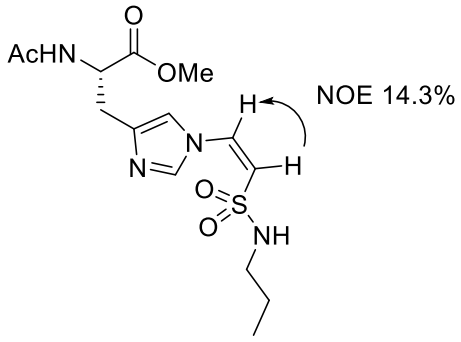
1077 (m), 1010 (m). ^{1}H-NMR (400 MHz, $CDCl_3$) δ 8.14 (s, 1H), 7.02 (d, J = 7.5 Hz, 1H), 6.95 (d, J = 9.5 Hz, 1H), 6.81 (d, J = 0.4 Hz, 1H), 6.80 (br, 1H), 6.36 (d, J = 9.6 Hz, 1H), 4.78 (dt, J = 7.5, 6.2 Hz, 1H), 3.76 (s, 3H), 3.22–3.12 (m, 2H), 3.04 (t, J = 6.2 Hz, 2H), 1.99 (s, 3H), 1.55 (sext, J = 7.3 Hz, 2H), 0.91 (t, J = 7.4 Hz, 3H). ^{13}C-NMR (101 MHz, $CDCl_3$) δ 171.2, 170.7, 139.5, 128.1, 126.9, 122.8, 52.8, 51.8, 44.8, 26.1, 23.2, 22.8, 11.1. LRMS (ESI): m/z (%) 257 (5) [M – $C_2H_3O_2$ – C_3H_7 + H], 300 (10) [M – $C_2H_3O_2$ + H], 317 (8) [M -C3H7 + 2H], 359 (base peak) [M + H], 381 (59) [M + Na], 739 (4) [2M +Na]. HRMS (ESI): m/z calculated for $C_{14}H_{22}N_4O_5NaS$ 381.12086; found 381.12157 [M + Na]$^+$ (error 1.85 ppm).



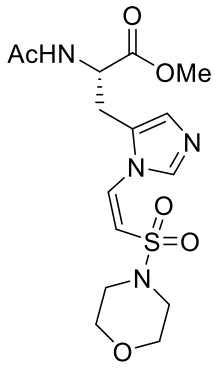
($CDCl_3$)



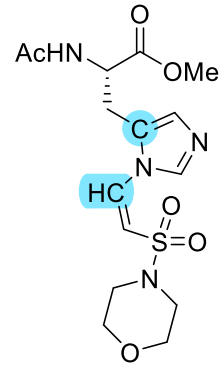
Methyl (*Z*)-N^{α}-acetyl-N^{τ}-(2-(*N*-propylsulfamoyl)vinyl)-L-histidinate (2b-His$^{\tau}$): Prepared as shown in general procedure 7; colorless oil; preparative RP-HPLC eluent (MeOH/H_2O = 2:3, v/v); yield, 45% (isolated). FT-IR (ATR) ν cm^{-1}: 3295 (br), 2968 (m), 2877 (m), 1741 (s), 1636 (s), 1539(m), 1498(s), 1437 (m), 1312 (s), 1243 (m), 1215 (m), 1155 (s), 1078 (m), 1026 (m). ^{1}H-NMR (400 MHz, $CDCl_3$) δ 7.75 (d, J = 1.4 Hz, 1H), 7.56 (d, J = 0.9 Hz, 1H), 6.95 (d, J = 10.1 Hz, 1H), 6.87 (d, J = 8.1 Hz, 1H), 6.09 (d, J = 10.1 Hz, 1H), 5.63 (t, J = 5.9 Hz, 1H), 4.90 (ddd, J = 8.1, 6.1, 4.8 Hz, 1H), 3.75 (s, 3H), 3.13–2.99 (m, 4H), 2.02 (s, 3H), 1.54 (sext, J = 7.3 Hz, 2H), 0.89 (t, J = 7.4 Hz, 3H). ^{13}C-NMR (101 MHz, $CDCl_3$) δ 172.2, 170.5, 139.2, 138.7, 128.4, 118.2, 117.9, 52.6, 51.9, 44.9, 30.2, 23.2, 23.1, 18.4, 11.1. LRMS (ESI): m/z (%) 257 (30) [M – $C_2H_3O_2$ – C_3H_7 + H], 300 (13) [M – $C_2H_3O_2$ + H], 317 (11) [M -C_3H_7 + 2H], 359 (21) [M + H], 381 (base peak) [M + Na], 739 (4) [2M +Na]. HRMS (ESI): m/z calculated for $C_{14}H_{23}N_4O_5S$ 359.13891; found 359.13860 [M + H]$^+$ (error −0.89 ppm).



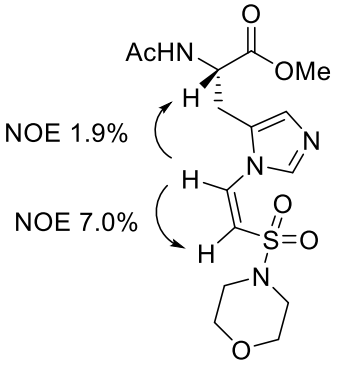
($CDCl_3$)



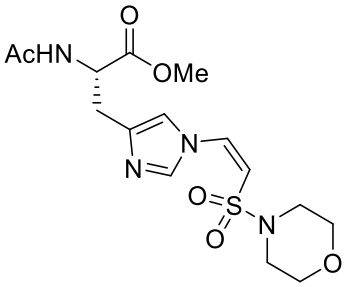
Methyl (*Z*)-N^{α}-acetyl-N^{π}-(2-(morpholinosulfonyl)vinyl)-L-histidinate (**2t-His$^{\pi}$**): Prepared as shown in general procedure 7; colorless gam; preparative RP-HPLC eluent (MeOH/H_2O = 2:3, v/v); yield, 45% (isolated). FT-IR (KBr) ν cm^{-1}: 3420 (br), 3144 (w), 3051 (w), 2925 (w), 3869 (w), 2600 (w), 1736 (m), 1675 (s), 1542 (m), 1438 (w), 1351 (m), 1303 (w), 1264 (m), 1203 (s), 1166 (s), 1137 (s), 1112 (m), 1076 (w), 956 (m), 835 (w), 800 (w), 739, (w), 722 (w). ^{1}H-NMR (400 MHz, DMSO-d_6) δ 8.96 (s, 1H), 8.50 (d, J = 7.8 Hz, 1H), 7.61 (d, J = 9.0 Hz, 1H), 7.38 (s, 1H), 7.23 (d, J = 9.0 Hz, 1H), 4.56 (td, J = 8.3, 5.4 Hz, 1H), 3.67–3.64 (m, 4H), 3.64 (s, 3H), 3.16–3.11 (m, 5H), 3.01 (dd, J = 15.8, 8.9 Hz, 1H), 1.84 (s, 3H). ^{13}C-NMR (101 MHz, DMSO-d_6) δ 171.0, 169.6, 137.3, 130.1, 125.4, 120.3, 65.5, 52.3, 50.6, 45.2, 25.1, 22.3. LRMS (ESI): m/z (%) 328 (6) [M – $C_2H_3O_2$ + H], 386 (base peak) [M + H], 409 (64) [M + Na]. HRMS (ESI): m/z calculated for $C_{15}H_{22}N_4O_6NaS$ 409.11577; found 409.11376 $[M + Na]^+$ (error −4.93 ppm).



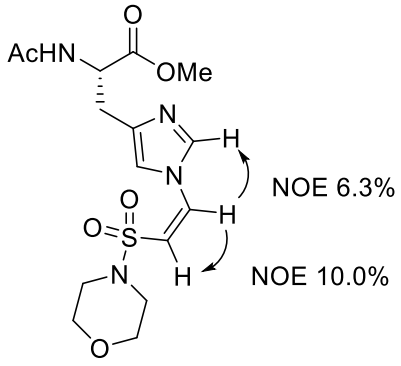
Overlaped 130.1 ppm
for ^{1}H-^{13}C HMBC



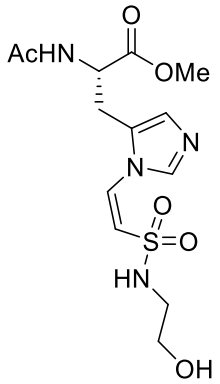
(DMSO-d_6)



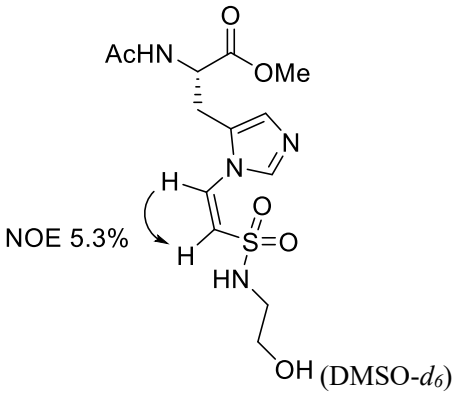
Methyl (*Z*)-N^{α}-acetyl-N^{τ}-(2-(morpholinosulfonyl)vinyl)-L-histidinate (2t-His$^{\tau}$): Prepared as shown in general procedure 7; colorless gam; preparative RP-HPLC eluent (MeOH/H_2O = 5:95–20:80, v/v); yield, 45% (isolated). FT-IR (KBr) ν cm^{-1}: 3333 (m), 3175 (w), 3139 (m), 3060 (w), 2982 (w), 2931 (w), 2898 (w), 2931 (w), 2898 (w), 1741 (s), 1650 (s), 1540 (s), 1376 (w), 1352 (m), 1333 (m), 1317 (m), 1264 (m), 1237 (m), 1186 (s), 1149 (s), 1131 (s), 1114 (s), 1176 (s), 1176 (m), 957 (m). ^{1}H-NMR (400 MHz, DMSO-d_6) δ 8.63 (d, J = 3.5 Hz, 1H), 8.34 (d, J = 7.8 Hz, 1H), 7.67 (s, 1H), 7.60 (d, J = 10.0 Hz, 1H), 6.71 (dd, J = 10.0, 2.7 Hz, 1H), 4.55 (td, J = 8.3, 5.5 Hz, 1H), 3.68–3.65 (m, 4H), 3.63 (s, 3H), 3.14–3.12 (m, 4H), 3.03 (dd, J = 14.8, 5.5 Hz, 1H), 2.92 (dd, J = 15.0, 8.8 Hz, 1H), 1.82 (s, 3H). ^{13}C-NMR (101 MHz, DMSO-d_6) δ 171.6, 169.5, 138.8, 134.9, 131.4, 118.5, 115.4, 65.4, 52.0, 51.4, 45.2, 28.1, 22.3. LRMS (ESI): m/z (%) 387 (13) [M + H], 409 (base peak) [M + Na], 795 (10) [2M + Na]. HRMS (ESI): m/z calculated for $C_{15}H_{22}N_4O_6NaS$ 409.11577; found 409.11393 [M + Na]$^{+}$ (error −4.51 ppm).

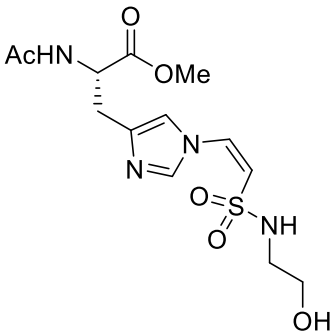


(DMSO-d_6)

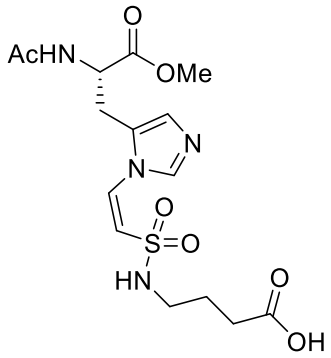


Methyl (*Z*)-N^{α}-acetyl-N^{π}-(2-(*N*-(2-hydroxyethyl)sulfamoyl)vinyl)-L-histidinate (5-His$^{\tau}$): Prepared as shown in general procedure 7; colorless gam; preparative RP-HPLC eluent (MeOH/H_2O = 5:95–15:85, v/v); yield, 13% (isolated). FT-IR (KBr) ν cm^{-1}: 3322 (s), 3196 (w), 3056 (w), 2959 (w), 2929 (w), 1753 (s), 1739 (s), 1655 (s), 1536 (s), 1435 (m), 1409 (w), 1371 (m), 1304 (m), 1269 (m), 1252 (m), 1233 (m), 1215 (m), ,1165 (m), 1130 w), 1044 (w), 1006 (m). ^{1}H-NMR (400 MHz, DMSO-d_6) δ 8.91 (s, 1H), 8.48 (d, J = 7.8 Hz, 1H), 7.87 (t, J = 5.7 Hz, 1H), 7.37–7.31 (m, 2H), 7.08 (d, J = 9.0 Hz, 1H), 4.55 (td, J = 8.3, 5.3 Hz, 1H), 3.62 (s, 3H), 3.44 (t, J = 5.9 Hz, 2H), 3.11 (dd, J = 15.8, 5.1 Hz, 1H), 3.04–2.96 (m, 3H), 1.82 (s, 3H).^{13}C-NMR (101 MHz, DMSO-d_6) δ 171.1, 169.7, 137.3, 129.9, 129.8, 126.3, 120.1, 60.2, 52.3, 50.6, 45.0, 25.1, 22.3. LRMS (ESI): m/z (%) 361 (20) [M + H], 383 (base peak) [M + Na], 743 (13) [2M + Na]. HRMS (ESI): m/z calculated for $C_{13}H_{20}N_4O_6NaS$ 383.10012; found 383.09829 $[M + Na]^+$ (error −4.80 ppm).

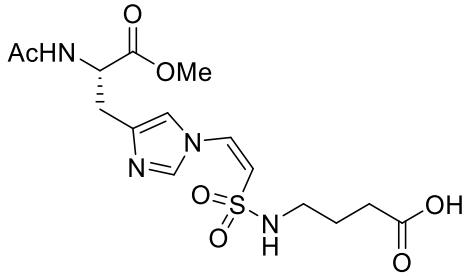




Methyl (*Z*)-N^{α}-acetyl-N^{τ}-(2-(*N*-(2-hydroxyethyl)sulfamoyl)vinyl)-L-histidinate (5-His$^{\tau}$): Prepared as shown in general procedure 7; colorless oil; preparative RP-HPLC eluent (MeOH/H_2O = 5:95–15:85, v/v); yield, 13% (isolated). FT-IR (KBr) ν cm^{-1}: 3398 (br), 2960 (w), 2877 (w), 1740 (m), 1675 (s), 1544 (m), 1502 (w), 1438 (m), 1377 (w), 1331 (m), 1203 (m), 1158 (m), 1052 (w), 1026 (w), 1002 (w), 832 (w), 801 (w), 764 (w), 721 (w), 687 (w), 623 (w). ^{1}H-NMR (400 MHz, DMSO-d_6) δ 8.55 (s, 1H), 8.33 (d, J = 7.7 Hz, 1H), 7.79 (t, J = 5.8 Hz, 1H), 7.64 (s, 1H), 7.38 (d, J = 10.0 Hz, 1H), 6.58 (d, J = 9.9 Hz, 1H), 4.57–4.51 (m, 1H), 3.62 (s, 3H), 3.46 (t, J = 6.0 Hz, 2H), 3.04–2.98 (m, 3H), 2.91 (dd, J = 14.8, 8.7 Hz, 1H), 1.83 (s, 3H). ^{13}C-NMR (101 MHz, DMSO-d_6) δ 171.7, 169.5, 138.6, 134.9, 128.1, 120.4, 118.7, 60.0, 52.0, 51.5, 45.0, 28.2, 22.3. LRMS (ESI): m/z (%) 361 (20) [M + H], 383 (base peak) [M + Na], 743 (13) [2M + Na]. HRMS (ESI): m/z calculated for $C_{13}H_{20}N_4O_6NaS$ 383.10012; found 383.09927 $[M + Na]^+$ (error −2.23 ppm).

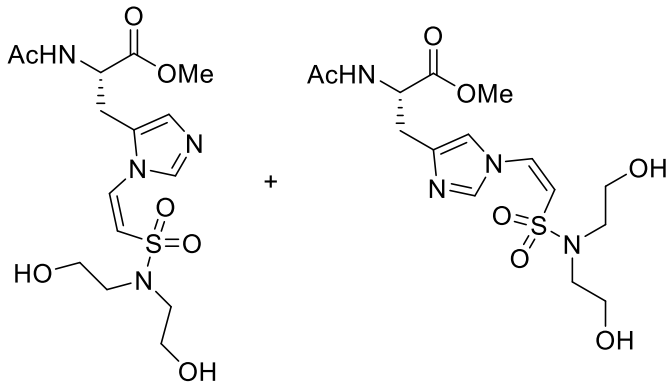


(*S*,*Z*)-4-((2-(5-(2-Acetamido-3-methoxy-3-oxopropyl)-1*H*-imidazol-1-yl)vinyl)sulfonamido)butanoic acid (**6-His$^{\pi}$**): Prepared as shown in general procedure 7; colorless oil; preparative RP-HPLC eluent (MeCN:H_2O:TFA = 1:9:0.01, v/v); yield, 9% (isolated). FT-IR (ATR) ν cm^{-1}: 3131 (br), 1727 (m), 1668 (s), 1544 (w), 1435 (w), 1333 (m), 1188 (s), 1149 (s), 1016 (s), 996 (s), 825 (m), 767 (m), 714 (m). ^{1}H-NMR (400 MHz, DMSO-d_6) δ 9.07 (s, 1H), 8.49 (d, J = 7.9 Hz, 1H), 7.91 (t, J = 5.7 Hz, 1H), 7.46 (s, 1H), 7.43 (d, J = 8.9 Hz, 1H), 7.17 (d, J = 8.9 Hz, 1H), 4.58 (td, J = 8.4, 5.2 Hz, 1H), 3.65 (s, 3H), 3.13 (dd, J = 15.8, 5.3 Hz, 1H), 3.04–2.95 (m, 3H), 2.27 (t, J = 7.3 Hz, 2H), 1.84 (s, 3H), 1.68 (quin, J = 7.2 Hz, 2H). ^{13}C-NMR (101 MHz, DMSO-d_6) δ 174.0, 171.0, 169.7, 137.1, 131.1, 130.3, 126.7, 118.9, 52.3, 50.5, 41.7, 30.5, 25.1, 24.9, 22.3. LRMS (ESI): m/z (%) 403 (68) [M + H], 425 (base peak) [M + Na]. HRMS (ESI): m/z calculated for $C_{15}H_{22}N_4O_7NaS$ 425.11069; found 425.10857 [M + Na]$^+$ (error −4.98 ppm).

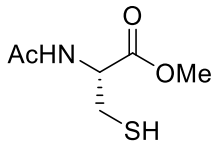


(*S*,*Z*)-4-((2-(4-(2-Acetamido-3-methoxy-3-oxopropyl)-1*H*-imidazol-1-yl)vinyl)sulfonamido)butanoic acid (**6-His$^{\tau}$**): Prepared as shown in general procedure 7; colorless oil; preparative RP-HPLC eluent (MeCN:H_2O:TFA = 1:9:0.01, v/v); yield, 10% (isolated). FT-IR (KBr) ν cm^{-1}: 3415 (br), 3273 (br), 3141 (w), 2874 (w), 2628 (w), 1734 (m), 1673 (s), 1544 (w), 1437 (w), 1376 (w), 1334 (m), 1202 (s), 1158 (s), 1084 (w), 1026 (w), 999 (w), 833 (m), 801 (m), 765 (m), 721 (m), 686 (m), 624 (m), 570 (m). ^{1}H-NMR (400 MHz, DMSO-d_6) δ 8.74 (s, 1H), 8.35 (d, J = 7.7 Hz, 1H), 7.83 (t, J = 5.7 Hz, 1H), 7.66 (s, 1H), 7.42 (d, J = 9.9 Hz, 1H), 6.65 (d, J = 9.8 Hz, 1H), 4.56 (td, J = 8.2, 5.7 Hz, 1H), 3.63 (s, 3H), 3.05 (dd, J = 14.9, 5.5 Hz, 1H), 3.00–2.89 (m, 3H), 2.26 (t, J = 7.3 Hz, 2H), 1.83 (s, 3H), 1.68 (quin, J = 7.1 Hz, 2H) ^{13}C-NMR (101 MHz, DMSO-d_6) δ 174.0, 171.5, 169.5, 138.3, 133.7, 128.3, 121.9, 119.1, 52.1, 51.4, 41.7, 30.6, 27.7, 24.8, 22.3. LRMS (ESI): m/z (%)

403 (16) [M + H], 425 (base peak) [M + Na], 827 (8) [2M + Na]. HRMS (ESI): *m*/*z* calculated for $C_{15}H_{22}N_4O_7NaS$ 425.11069; found 425.10910 $[M + Na]^+$ (error −3.74 ppm).

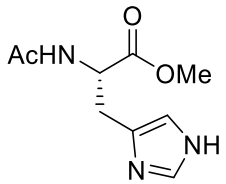


Methyl (*Z*)-N^{α}-acetyl-$N^{\pi\tau}$-(2-(*N*,*N*-bis(2-hydroxyethyl)sulfamoyl)vinyl)-L-histidinate (7-$His^{\pi,\tau}$): Prepared as shown in general procedure 7; colorless oil; preparative RP-HPLC eluent ($MeCN/H_2O$/TFA = 12.5:87.5:0.01, v/v); yield, 40% (π:τ = 1:4). FT-IR (KBr) *v* cm^{-1}: 3388 (br), 3060 (w), 2958 (w), 2882 (w), 1740 (m), 1675 (s), 1544 (m), 1503 (w), 1438 (w), 1375 (w), 1336 (m), 1203 (s), 1157 (s), 1074 (w), 1047 (w), 1001 (w), 924 (w), 836 (w), 801 (w), 761 (w), 723 (m). ^{1}H-NMR (400 MHz, DMSO-d_6, *π*-form) *δ* 8.53 (s, 1H), 8.25 (d, *J* = 7.8 Hz, 1H), 7.61 (s, 1H), 7.48 (d, *J* = 10.0 Hz, 1H), 6.70 (d, *J* = 10.0 Hz, 1H), 4.58–4.52 (m, 1H), 3.62 (s, 3H), 3.57 (t, *J* = 6.3 Hz, 2H), 3.32 (t, *J* = 6.0 Hz, 2H), 3.01–2.88 (m, 2H), 1.82 (s, 3H). ^{1}H-NMR (400 MHz, DMSO-d_6, *τ*-form) *δ* 8.61 (s, 1H), 8.34 (d, *J* = 7.8 Hz, 1H), 7.63 (s, 1H), 7.45 (d, *J* = 10.0 Hz, 1H), 6.75 (d, *J* = 10.0 Hz, 1H), 4.58–4.52 (m, 1H), 3.62 (s, 3H), 3.55 (t, *J* = 6.3 Hz, 2H), 3.28 (t, *J* = 6.0 Hz, 2H), 3.02 (dd, *J* = 14.9, 5.8 Hz, 1H), 2.93 (dd, *J* = 14.6, 8.7 Hz, 1H), 1.82 (s, 1H). ^{13}C-NMR (101 MHz, DMSO-d_6, *π*-form) *δ* 171.6, 169.5, 138.4, 134.1, 128.8, 120.4, 118.8, 59.3, 52.1, 51.4, 50.2, 40.1, 39.9, 39.7, 39.5, 39.3, 39.1, 38.9, 27.9, 22.3. ^{13}C-NMR (101 MHz, DMSO-d_6, *τ*-form) *δ* 171.6, 169.5, 138.4, 134.1, 128.8, 120.4, 118.8, 59.3, 52.1, 51.4, 50.2, 40.1, 39.9, 39.7, 39.5, 39.3, 39.1, 38.9, 27.9, 22.3. LRMS (ESI): *m*/*z* (%) 405 (11) [M + H], 427 (base peak) [M + Na], 831 (6) [2M + Na]. HRMS (ESI): *m*/*z* calculated for $C_{15}H_{24}N_4O_7NaS$ 427.12634; found 427.12623 $[M + Na]^+$ (error −0.26 ppm).

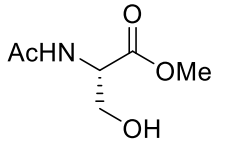


Methyl acetyl-L-cysteinate (Ac-Cys-OMe) (**Cys**): *N*-Acetyl-L-cysteine (10.0 mmol, 1.63 g) was dissolved distilled methanol (20 mL) in sealed tube. Acetyl chloride (0.2 mL) was added, and reaction was stirred 3 hours at 55°C. After evaporation of the solvent, and was added saturated $NaHCO_3$

aqueous solution (75 mL). The aqueous layer was extracted three times with EtOAc (150 mL), and dried over Na_2SO_4. After concentration, chromatography was performed on the residue on a silica gel column (Hexane:EtOAc = 1:1) to give light white solids **Cys** (1.18 g, yield 66%). FT-IR (NaCl) ν cm^{-1}: 3285 (br), 3060 (w), 2954 (w), 2849 (w), 2563 (w), 1742 (s), 1656 (s), 1541 (s), 1438 (m), 1374 (m), 1345 (m), 1312 (m), 1218 (s), 1179 (m), 1134 (m), 1039 8w), 714 (w). ^{1}H-NMR (400 MHz, $CDCl_3$) δ 6.43 (d, J = 3.0 Hz, 1H), 4.90 (dt, J = 7.4, 4.1 Hz, 1H), 3.80 (s, 3H), 3.02 (ddd, J = 9.0, 7.4, 3.0 Hz, 2H), 2.08 (s, 3H.), 1.35 (t, J = 9.0 Hz, 1H). ^{13}C-NMR (101 MHz, $CDCl_3$) δ 170.6, 169.9, 53.5, 52.9, 26.9, 23.2. LRMS (EI): m/z (%) 60 [M – C_4H_8NOS + H] (base peak), 118 [M – $C_2H_3O_2$] (25), 177 [M] (6). HRMS (EI): m/z calculated for $C_6H_{11}NO_3S$ 177.04596; found 177.0459 $[M]^+$ (error +0.34 ppm).

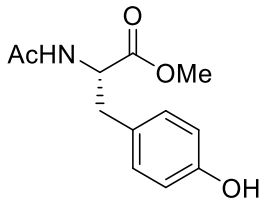


Methyl acetyl-L-histidinate (Ac-His-OMe) (**His**): A suspension of *N*-acetyl-L-histidine monohydride (2.15 g, 10.0 mmol) in dry MeOH (20 mL) was treated with thionyl chloride (2.18 mL, 3.0 equiv.) at 0 °C under an N_2 atmosphere. The reaction mixture was stirred at room temperature for 15 hours. After evaporation of the solvent, the residue was taken up in 4% NH_3 in MeOH (20 mL). After evaporating the solvent, acetone was added, and the mixture was filtered. After evaporating the solvent from the filtrate, the oily residue was purified via column chromatography on silica gel ($CHCl_3$/MeOH/NH_3 = 9:1:0.04) to give off-white solid **His** (1.88 g, 89%). FT-IR (KBr) ν cm^{-1}: 3338 (m), 3229 (m), 3192 (m), 3033 (m), 2960 (m), 2940 (m), 2863 (w), 1728 (s), 1658 (s), 1557 (s), 1493 (m), 1441 (m), 1376 (m), 1314 (m), 1267 (m), 1246 (s), 1143 (m), 1086 (w), 1064 (w), 1002 (m), 978 (m), 930 (w), 875 (w), 841 (w), 822 (w), 796 (w), 779 (w), 732 (w), 673 (w), 612 (m). ^{1}H-NMR (400 MHz, DMSO-d_6) δ 11.82 (br, 1H), 8.23 (d, J = 6.0 Hz, 1H), 7.51 (s, 1H), 6.81 (br, 1H), 4.44 (dt, J = 7.9, 5.3 Hz, 1H), 3.57 (s, 3H), 2.83 (dd, J = 14.2, 5.3 Hz, 1H), 2.76 (dd, J = 14.2, 8.1 Hz, 1H), 1.80 (s, 3H). ^{13}C-NMR (101 MHz, DMSO-d_6) δ 172.3, 169.3, 136.0, 134.9, 113.2, 52.5, 51.7, 29.8, 22.3. HRMS (ESI): m/z calculated for $C_9H_{13}N_3O_3Na$ 234.08546; found 234.08561 $[M + Na]^+$ (error +0.64 ppm).

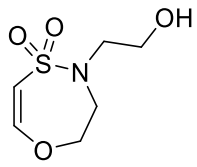


Methyl acetyl-L-serinate (Ac-Ser-OMe) (**Ser**): L-Serine methyl ester hydrochloride (1.556 g, 10.0 mmol) was dissolved in anhydrous DCM (50 mL). Et_3N (3.48 mL, 2.5 equiv.) was added at 0 °C for 30 minutes. Acetyl chloride (785 µL, 1.1 equiv.) was added at 0 °C, and the mixture was stirred at 0 °C

under an N_2 atmosphere for 2 h and filter the precipitated $Et_3N{\cdot}HCl$. Remove the solvent under reduce pressure and purify the residue by column chromatography on silica gel (EtOAc) to give colorless gam **Ser** (1.28 g, 79%). FT-IR (NaCl) ν cm^{-1}: 3311 (br), 3086 (m), 2956 (m), 2888 (w), 2249 (w), 1741 (s), 1655 (s), 1542 (s), 1438 (s), 1377 (s), 1348 (m), 1288 (m), 1226 (s), 1148 (m), 1080 (m), 982 (w), 917 (w), 856 (w), 732 (m). ^{1}H-NMR (400 MHz, $CDCl_3$) δ 6.58 (d, J = 5.4 Hz, 1H), 4.68 (dt, J = 7.4, 3.6 Hz, 1H), 3.99 (ddd, J = 11.2, 5.6, 4.0, 1H), 3.92 (ddd, J = 11.2, 5.6, 3.4 Hz, 1H), 3.80 (s, 3H), 2.91 (t, J = 5.9 Hz, 1H), 2.08 (s, 3H). ^{13}C-NMR (101 MHz, $CDCl_3$) δ 171.1, 170.8, 63.3, 54.7, 52.8, 23.1. LRMS (ESI): m/z (%) 184 (95) [M + Na], 345 (19) [2M + Na]. HRMS (ESI): m/z calculated for $C_6H_{11}NO_4Na$ 184.05858; found 184.05832 $[M + Na]^+$ (error −1.37 ppm).

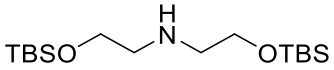


Methyl acetyl-L-tyrosinate (Ac-Tyr-OMe) (**Tyr**): *N*-Acetyl-L-tyrosine (1.12 g, 5.00 mmol) was dry MeOH (10 mL) in sealed tube. Acetyl chloride (33 μL) was added, and reaction was stirred 2 hours at 55°C. Remove the solvent under reduce pressure and purify the residue by column chromatography on silica gel (Hexane:EtOAc = 1:3) to give off-white solids **Tyr** (1.14 g, yield 96%). FT-IR (KBr) ν cm^{-1}: 3549 (m), 3351 (m), 3323 (s), 3273 (m), 3157 (br), 2957 (m), 2822 (m), 2749 (w), 2963 (w), 2615 (w), 2504 (w), 1731 (s), 1661 (s), 1615 (m), 1595 (m), 1547 (s), 1517 (s), 1450 (m), 1301 (m), 1378 (m), 1282 (m), 1240 (s), 1182 (m), 1173 (m), 1134 (m), 1110 (w), 1149 (m(, 1013 (m). ^{1}H-NMR (400 MHz, $CDCl_3$) δ 6.99 (s, 1H), 6.95–6.92 (m, 2H), 6.75–6.72 (m, 2H), 6.10 (d, J = 8.1 Hz, 1H), 4.87 (td, J = 7.0, 5.2 Hz, 1H), 3.74 (s, 3H), 3.08 (dd, J = 14.0, 5.6 Hz, 1H), 2.97 (dd, J = 14.1, 6.3 Hz, 1H), 1.99 (s, 3H). ^{13}C-NMR (101 MHz, $CDCl_3$) δ 172.3, 170.0, 155.2, 130.3, 127.4, 115.5, 53.3, 52.4, 37.2, 23.1. LRMS (EI): m/z (%) 107 (62) [M – $C_5H_8NO_3$], 178 (base peak) [M – $C_2H_3O_2$], 237 (6) [M]. HRMS (EI): m/z calculated for $C_{12}H_{15}NO_4$ 237.10011; found 237.1012 $[M]^+$ (error +4.8 ppm).



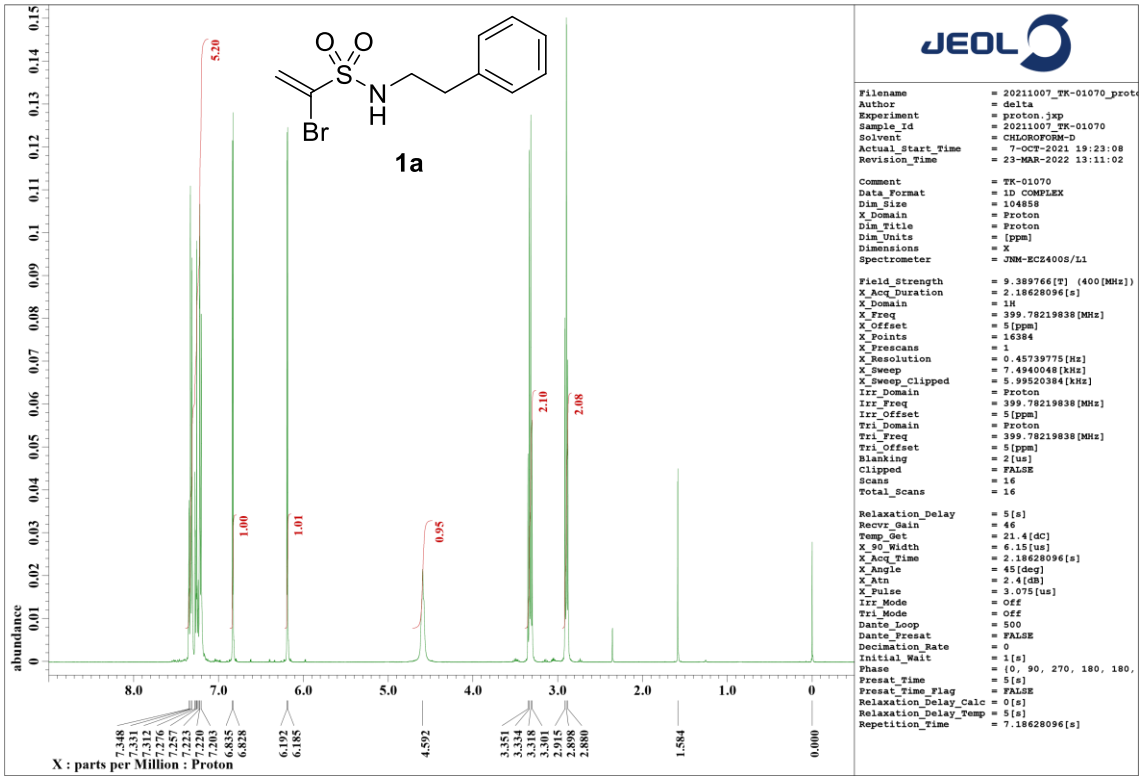
5-(2-Hydroxyethyl)-6,7-dihydro-5*H*-1,4,5-oxathiazepine 4,4-dioxide (S1): Prepared as shown in general procedure 7; colorless oil; silica gel column eluent ($CHCl_3$/MeOH = 9:1, v/v); yield, 5%. FT-IR (ATR) ν cm^{-1}: 3513 (br), 3069 (w), 2945 (w), 1605 (m), 1450 (w), 1317 (s), 1284 (m), 1255 (m), 1137 (s), 1082 (s), 963 (w), 913 (w), 823 (m), 708 (s). ^{1}H-NMR (400 MHz, $CDCl_3$) δ 6.69 (d, J = 6.9

Hz, 1H), 5.74 (d, J = 6.9 Hz, 1H), 4.65–4.62 (m, 2H), 3.80 (q, J = 5.0 Hz, 2H), 3.66–3.63 (m, 2H), 3.42 (t, J = 5.3 Hz, 2H), 2.17 (t, J = 5.0 Hz, 1H). ^{13}C-NMR (101 MHz, $CDCl_3$) δ 153.2, 110.1, 72.5, 61.5, 53.8, 51.0. LRMS (ESI): m/z (%) 194 (58) [M + H], 216 (34) [M + Na]. HRMS (ESI): m/z calculated for $C_6H_{12}NO_4S$ 194.04870; found 194.04876 $[M + H]^+$ (error +0.29 ppm).



Bis(2-((*tert*-butyldimethylsilyl)oxy)ethyl)amine (**S2**): Diethanolamine (2.63 g, 25 mmol), Et_3N (8.7 mL, 2.5 equiv.), and *t*-butyldimethylsilyl (TBS) chloride (8.65 g, 2.3 equiv.) were added to DCM (100 mL) at 0 °C under N_2 and stirred for 6 hours. The reaction mixture was washed three times with saturated $NaHCO_3$, and the organic layer was dried over Na_2SO_4. After concentration, chromatography was performed on the residue on a silica gel column (Hexane:EtOAc = 2:1, v/v) to give colorless oil **S2** (7.55 g, 90%). FT-IR (NaCl) ν cm^{-1}: 2954 (m), 2929 (m), 1885 (m), 1859 (m), 1471 (m), 1463 (m), 1254 (m), 1100 (s), 832 (s), 774 (s). ^{1}H-NMR (400 MHz, $CDCl_3$) δ 3.73 (t, J = 5.3 Hz, 4H), 2.73 (t, J = 5.3 Hz, 4H), 1.69 (br, 1H), 0.90 (s, 18H), 0.06 (s, 12H). ^{13}C-NMR (101 MHz, $CDCl_3$) δ 62.6, 51.8, 26.0, 18.3, −5.3. LRMS (EI): m/z (%) 334 (base peak) [M + H], 356 (23) [M +Na]. HRMS (ESI): m/z calculated for $C_{18}H_{40}NO_2Si_2$ 334.25976; found 334.26090 $[M + H]^+$ (error +3.41 ppm).

NMR spectra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Author = delta
Experiment = proton.jxp
Sample_Id = 20211007_TK-01070
Solvent = CHLOROFORM-D
Actual_Start_Time = 7-OCT-2021 19:23:08
Revision_Time = 23-MAR-2022 13:11:02
Comment = TK-01070
Data_Format = 1D COMPLEX
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Dim_Title = Proton
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Dimensions = X
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X_Acq_Duration = 2.18628096[s]
X_Domain = 1H
X_Freq = 399.78219838[MHz]
X_Offset = 5[ppm]
X_Points = 16384
X_Prescans = 1
X_Resolution = 0.45739775[Hz]
X_Sweep = 7.4940048[kHz]
X_Sweep_Clipped = 5.99520384[kHz]
Irr_Domain = Proton
Irr_Freq = 399.78219838[MHz]
Irr_Offset = 5[ppm]
Tri_Domain = Proton
Tri_Freq = 399.78219838[MHz]
Tri_Offset = 5[ppm]
Blanking = 2[us]
Clipped = FALSE
Scans = 16
Total_Scans = 16
Relaxation_Delay = 5[s]
Recvr_Gain = 46
Temp_Get = 21.4[dC]
X_90_Width = 6.15[us]
X_Acq_Time = 2.18628096[s]
X_Angle = 45[deg]
X_Atn = 2.4[dB]
X_Pulse = 3.075[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Loop = 500
Dante_Presat = FALSE
Decimation_Rate = 0
Initial_Wait = 1[s]
Phase = {0, 90, 270, 180, 180,
Presat_Time = 5[s]
Presat_Time_Flag = FALSE
Relaxation_Delay_Calc = 0[s]
Relaxation_Delay_Temp = 5[s]
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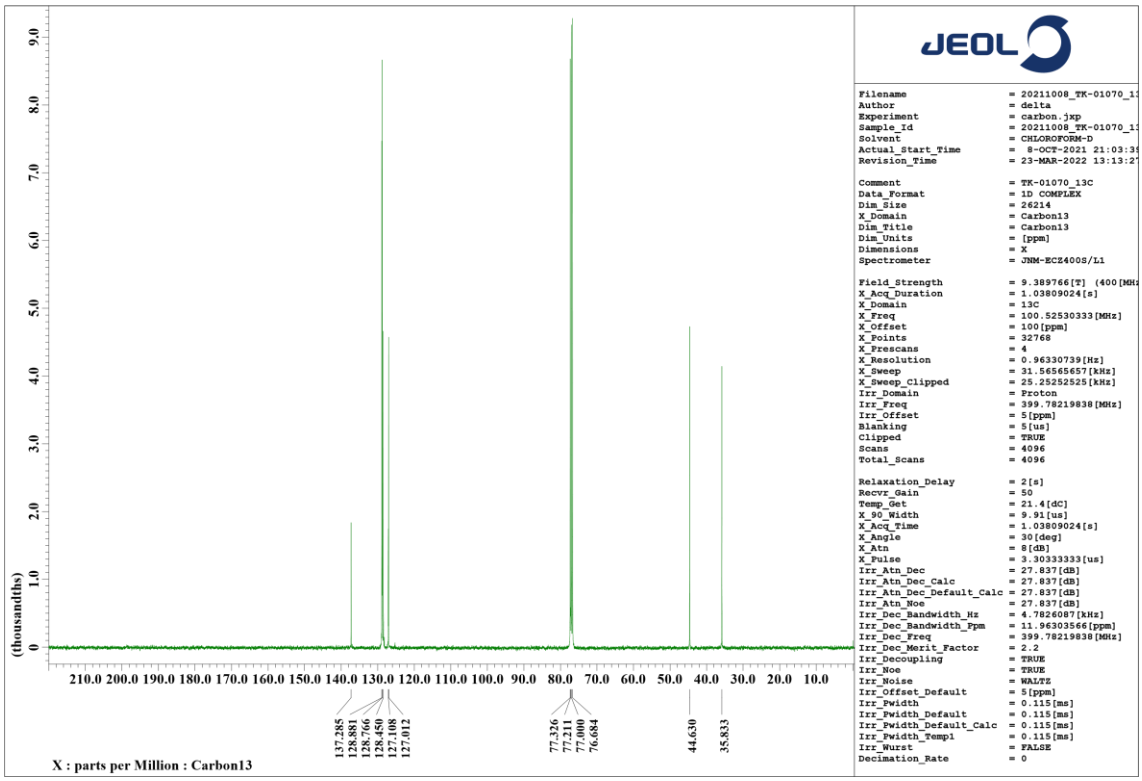
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Author = delta
Experiment = carbon.jxp
Sample_Id = 20211008_TK-01070_1
Solvent = CHLOROFORM-D
Actual_Start_Time = 8-OCT-2021 21:03:3
Revision_Time = 23-MAR-2022 13:13:2
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X_Acq_Duration = 1.03809024[s]
X_Domain = 13C
X_Freq = 100.52530333[MHz]
X_Offset = 100[ppm]
X_Points = 32768
X_Prescans = 4
X_Resolution = 0.96330739[Hz]
X_Sweep = 31.56565657[kHz]
X_Sweep_Clipped = 25.25252525[kHz]
Irr_Domain = Proton
Irr_Freq = 399.78219838[MHz]
Irr_Offset = 5[ppm]
Blanking = 5[us]
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Scans = 4096
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Relaxation_Delay = 2[s]
Recvr_Gain = 50
Temp_Get = 21.4[dC]
X_90_Width = 9.91[us]
X_Acq_Time = 1.03809024[s]
X_Angle = 30[deg]
X_Atn = 8[dB]
X_Pulse = 3.30333333[us]
Irr_Atn_Dec = 27.837[dB]
Irr_Atn_Dec_Calc = 27.837[dB]
Irr_Atn_Dec_Default_Calc = 27.837[dB]
Irr_Atn_Noe = 27.837[dB]
Irr_Dec_Bandwidth_Hz = 4.7826087[kHz]
Irr_Dec_Bandwidth_Ppm = 11.96303566[ppm]
Irr_Dec_Freq = 399.78219838[MHz]
Irr_Dec_Merit_Factor = 2.2
Irr_Decoupling = TRUE
Irr_Noe = TRUE
Irr_Noise = WALTZ
Irr_Offset_Default = 5[ppm]
Irr_Pwidth = 0.115[ms]
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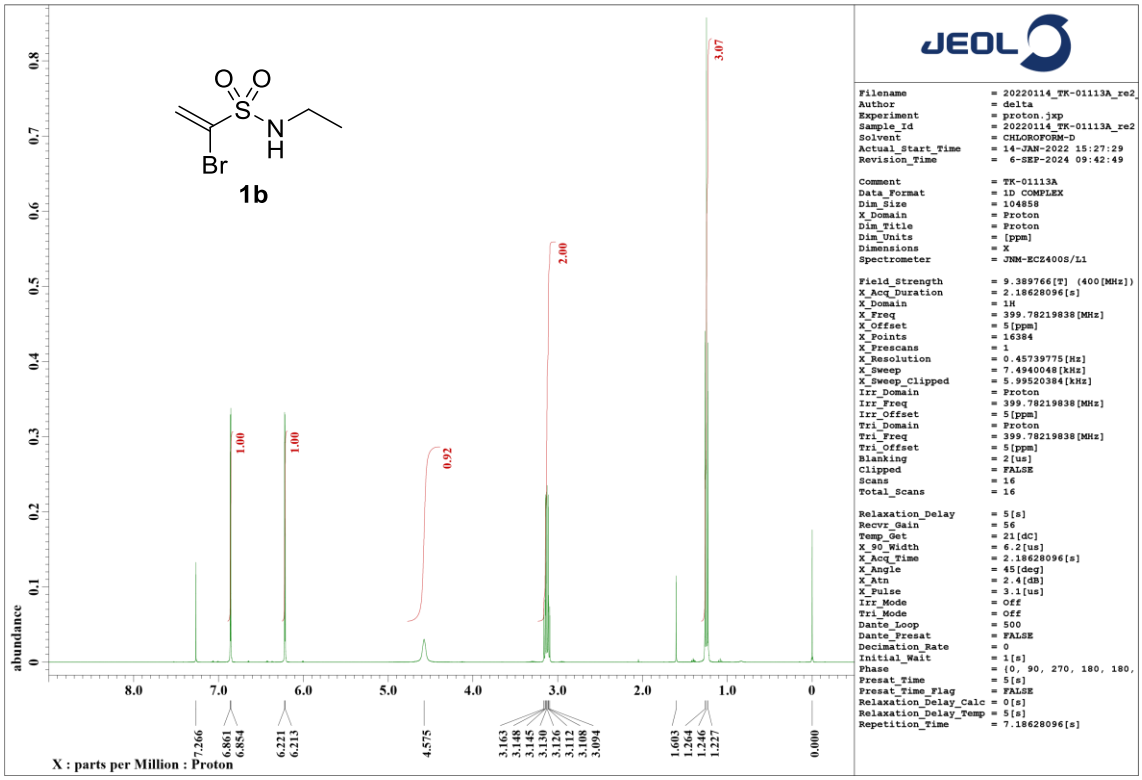
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6.854
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3.112
3.108
3.094
1.603
1.244
1.240
1.227
0.000
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Author = delta
Experiment = proton.jxp
Sample_Id = 20220114_TK-01113A_re2
Solvent = CHLOROFORM-D
Actual_Start_Time = 14-JAN-2022 15:27:29
Revision_Time = 6-SEP-2024 09:42:49
Comment = TK-01113A
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Dim_Title = Proton
Dim_Units = [ppm]
Dimensions = X
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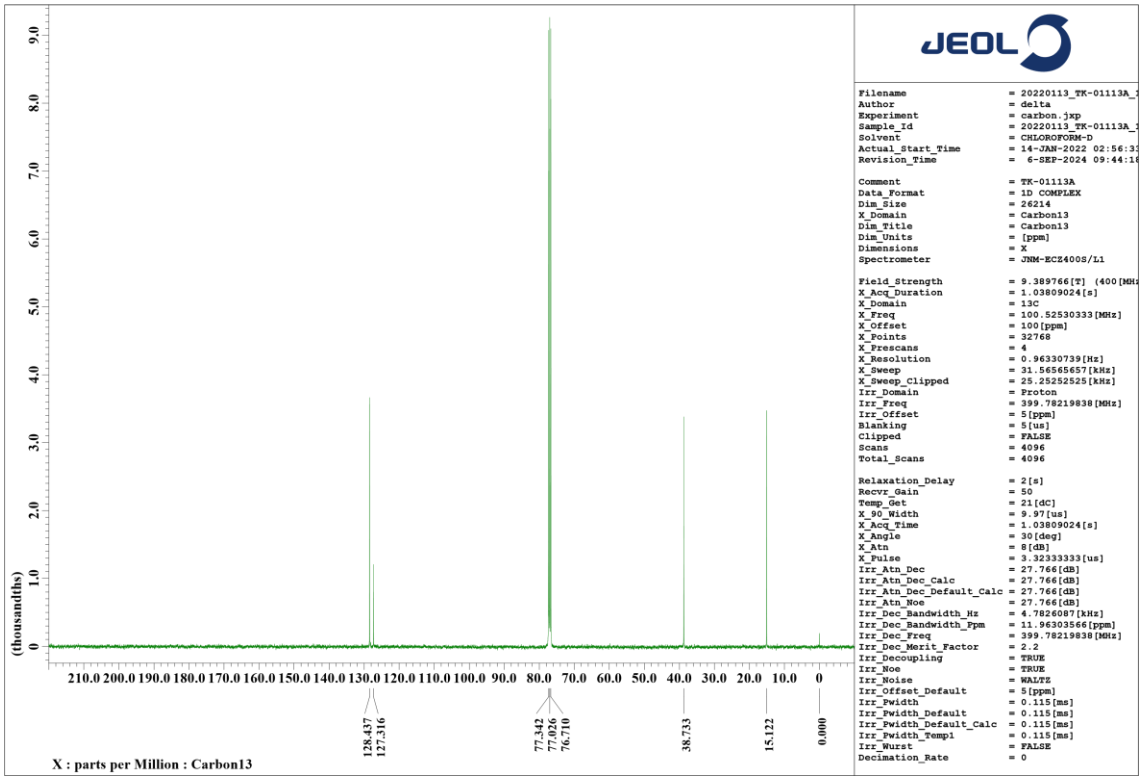
Field_Strength = 9.389766[T] (400[MHz])
X_Acq_Duration = 2.18628096[s]
X_Domain = 1H
X_Freq = 399.78219838[MHz]
X_Offset = 5[ppm]
X_Points = 16384
X_Prescans = 1
X_Resolution = 0.45739775[Hz]
X_Sweep = 7.4940048[kHz]
X_Sweep_Clipped = 5.99520384[kHz]
Irr_Domain = Proton
Irr_Freq = 399.78219838[MHz]
Irr_Offset = 5[ppm]
Tri_Domain = Proton
Tri_Freq = 399.78219838[MHz]
Tri_Offset = 5[ppm]
Blanking = 2[us]
Clipped = FALSE
Scans = 16
Total_Scans = 16
Relaxation_Delay = 5[s]
Recvr_Gain = 56
Temp_Get = 21[dC]
X_90_Width = 6.2[us]
X_Acq_Time = 2.18628096[s]
X_Angle = 45[deg]
X_Atn = 2.4[dB]
X_Pulse = 3.1[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Loop = 500
Dante_Presat = FALSE
Decimation_Rate = 0
Initial_Wait = 1[s]
Phase = (0, 90, 270, 180, 180,
Presat_Time = 5[s]
Presat_Time_Flag = FALSE
Relaxation_Delay_Calc = 0[s]
Relaxation_Delay_Temp = 5[s]
Repetition_Time = 7.18628096[s]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127.316
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77.026
76.710
38.733
15.122
0.000
Filename = 20220113_TK-01113A_1
Author = delta
Experiment = carbon.jxp
Sample_Id = 20220113_TK-01113A_1
Solvent = CHLOROFORM-D
Actual_Start_Time = 14-JAN-2022 02:56:31
Revision_Time = 6-SEP-2024 09:44:16
Comment = TK-01113A
Data_Format = 1D COMPLEX
Dim_Size = 26214
X_Domain = Carbon13
Dim_Title = Carbon13
Dim_Units = [ppm]
Dimensions = X
Spectrometer = JNM-ECZ400S/L1
Field_Strength = 9.389766[T] (400[MHz]
X_Acq_Duration = 1.03809024[s]
X_Domain = 13C
X_Freq = 100.52530333[MHz]
X_Offset = 100[ppm]
X_Points = 32768
X_Prescans = 4
X_Resolution = 0.96330739[Hz]
X_Sweep = 31.56565657[kHz]
X_Sweep_Clipped = 25.25252525[kHz]
Irr_Domain = Proton
Irr_Freq = 399.78219838[MHz]
Irr_Offset = 5[ppm]
Blanking = 5[us]
Clipped = FALSE
Scans = 4096
Total_Scans = 4096
Relaxation_Delay = 2[s]
Recvr_Gain = 50
Temp_Get = 21[dC]
X_90_Width = 9.97[us]
X_Acq_Time = 1.03809024[s]
X_Angle = 30[deg]
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Irr_Atn_Dec_Calc = 27.766[dB]
Irr_Atn_Dec_Default_Calc = 27.766[dB]
Irr_Atn_Noe = 27.766[dB]
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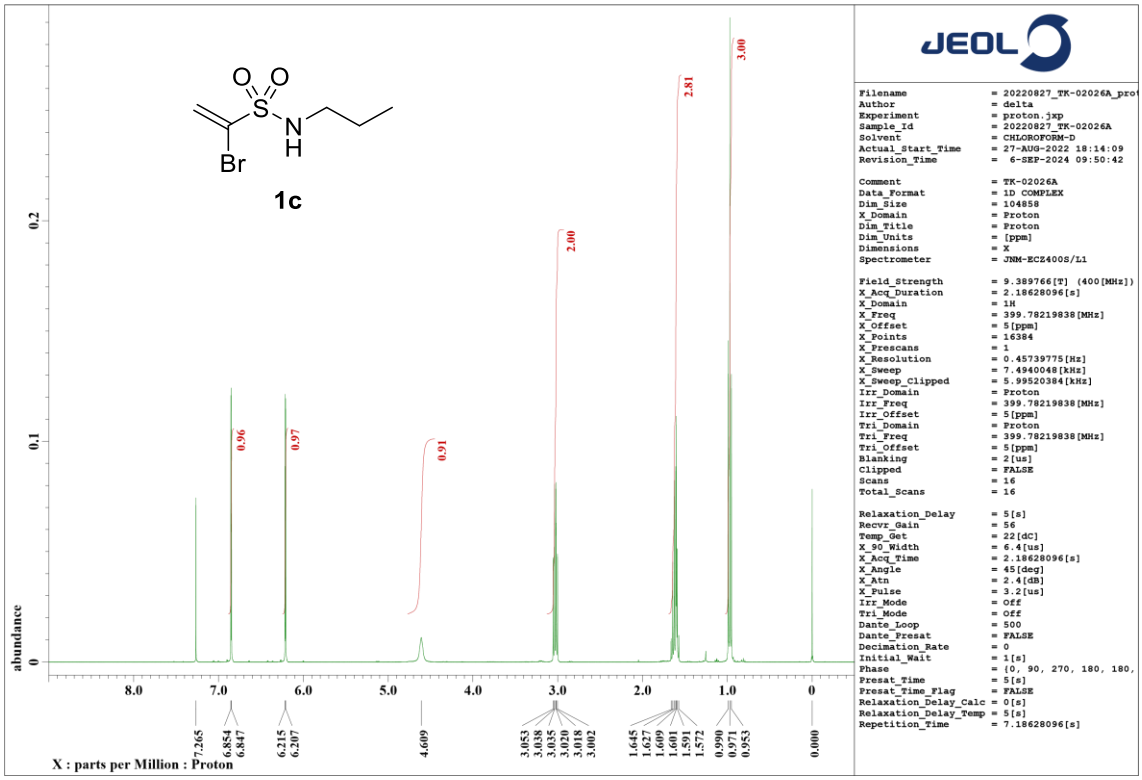
Irr_Dec_Bandwidth_Ppm = 11.96303566[ppm]
Irr_Dec_Freq = 399.78219838[MHz]
Irr_Dec_Merit_Factor = 2.2
Irr_Decoupling = TRUE
Irr_Noe = TRUE
Irr_Noise = WALTZ
Irr_Offset_Default = 5[ppm]
Irr_Pwidth = 0.115[ms]
Irr_Pwidth_Default = 0.115[ms]
Irr_Pwidth_Default_Calc = 0.115[ms]
Irr_Pwidth_Temp1 = 0.115[ms]
Irr_Wurst = FALSE
Decimation_Rate = 0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Author = delta
Experiment = proton.jxp
Sample_Id = 20220827_TK-02026A
Solvent = CHLOROFORM-D
Actual_Start_Time = 27-AUG-2022 18:14:09
Revision_Time = 6-SEP-2024 09:50:42
Comment = TK-02026A
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Dim_Title = Proton
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Field_Strength = 9.389766[T] (400[MHz])
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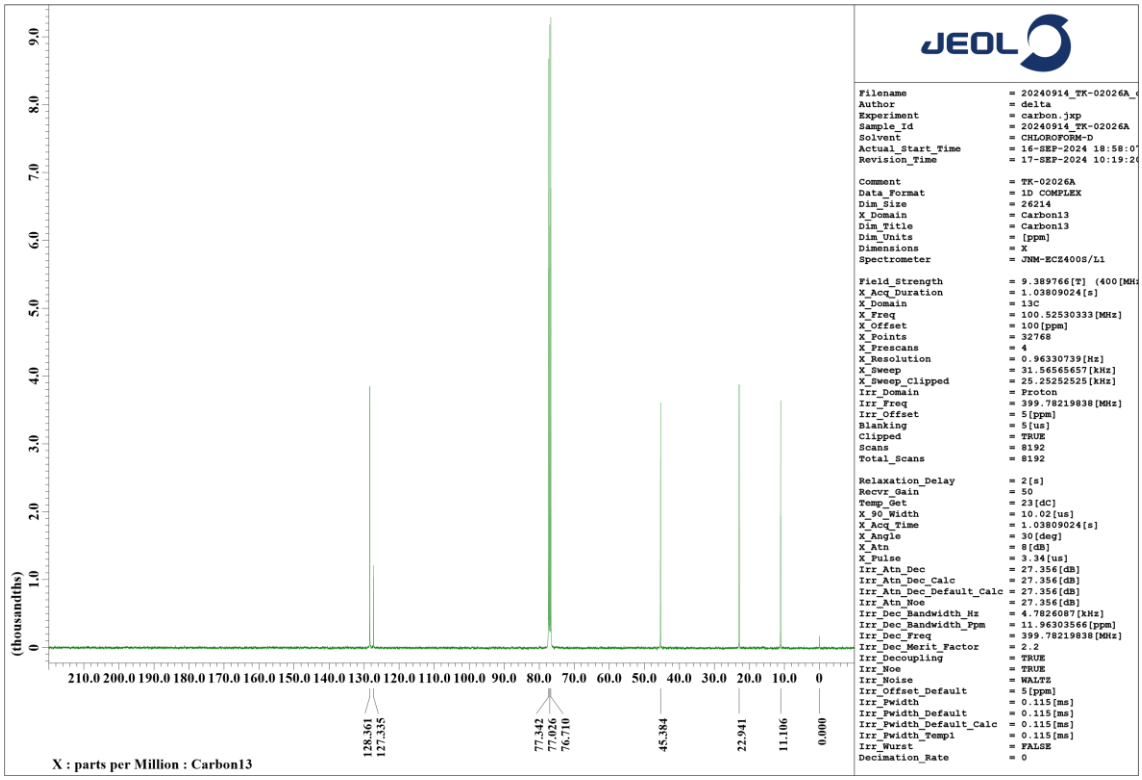
X_Freq = 399.78219838[MHz]
X_Offset = 5[ppm]
X_Points = 16384
X_Prescans = 1
X_Resolution = 0.45739775[Hz]
X_Sweep = 7.4940048[kHz]
X_Sweep_Clipped = 5.99520384[kHz]
Irr_Domain = Proton
Irr_Freq = 399.78219838[MHz]
Irr_Offset = 5[ppm]
Tri_Domain = Proton
Tri_Freq = 399.78219838[MHz]
Tri_Offset = 5[ppm]
Blanking = 2[us]
Clipped = FALSE
Scans = 16
Total_Scans = 16
Relaxation_Delay = 5[s]
Recvr_Gain = 56
Temp_Get = 22[dC]
X_90_Width = 6.4[us]
X_Acq_Time = 2.18628096[s]
X_Angle = 45[deg]
X_Atn = 2.4[dB]
X_Pulse = 3.2[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Loop = 500
Dante_Presat = FALSE
Decimation_Rate = 0
Initial_Wait = 1[s]
Phase = (0, 90, 270, 180, 180,
Presat_Time = 5[s]
Presat_Time_Flag = FALSE
Relaxation_Delay_Calc = 0[s]
Relaxation_Delay_Temp = 5[s]
Repetition_Time = 7.18628096[s]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Author = delta
Experiment = carbon.jxp
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Solvent = CHLOROFORM-D
Actual_Start_Time = 16-SEP-2024 18:58:0
Revision_Time = 17-SEP-2024 10:19:2
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Dimensions = X
Spectrometer = JNM-ECZ400S/L1
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X_Freq = 100.52530333[MHz]
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X_Points = 32768
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X_Resolution = 0.96330739[Hz]
X_Sweep = 31.56565657[kHz]
X_Sweep_Clipped = 25.25252525[kHz]
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Scans = 8192
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Relaxation_Delay = 2[s]
Recvr_Gain = 50
Temp_Get = 23[dC]
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X_Acq_Time = 1.03809024[s]
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X_Atn = 8[dB]
X_Pulse = 3.34[us]
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Irr_Atn_Dec_Calc = 27.356[dB]
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Irr_Atn_Noe = 27.356[dB]
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Irr_Dec_Bandwidth_Ppm = 11.96303566[ppm]
Irr_Dec_Freq = 399.78219838[MHz]
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Irr_Offset_Default = 5[ppm]
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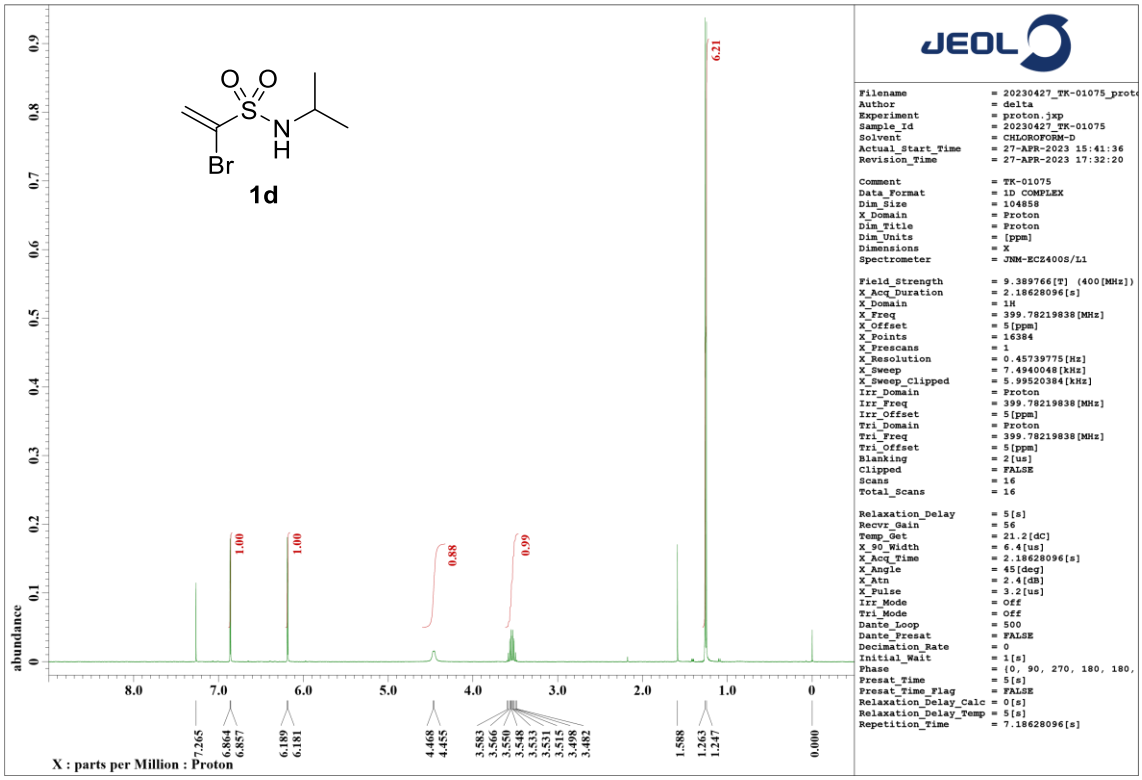
Irr_Wurst = FALSE
Decimation_Rate = 0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1.00
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Author = delta
Experiment = proton.jxp
Sample_Id = 20230427_TK-01075
Solvent = CHLOROFORM-D
Actual_Start_Time = 27-APR-2023 15:41:36
Revision_Time = 27-APR-2023 17:32:20
Comment = TK-01075
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Field_Strength = 9.389766[T] (400[MHz])
X_Acq_Duration = 2.18628096[s]
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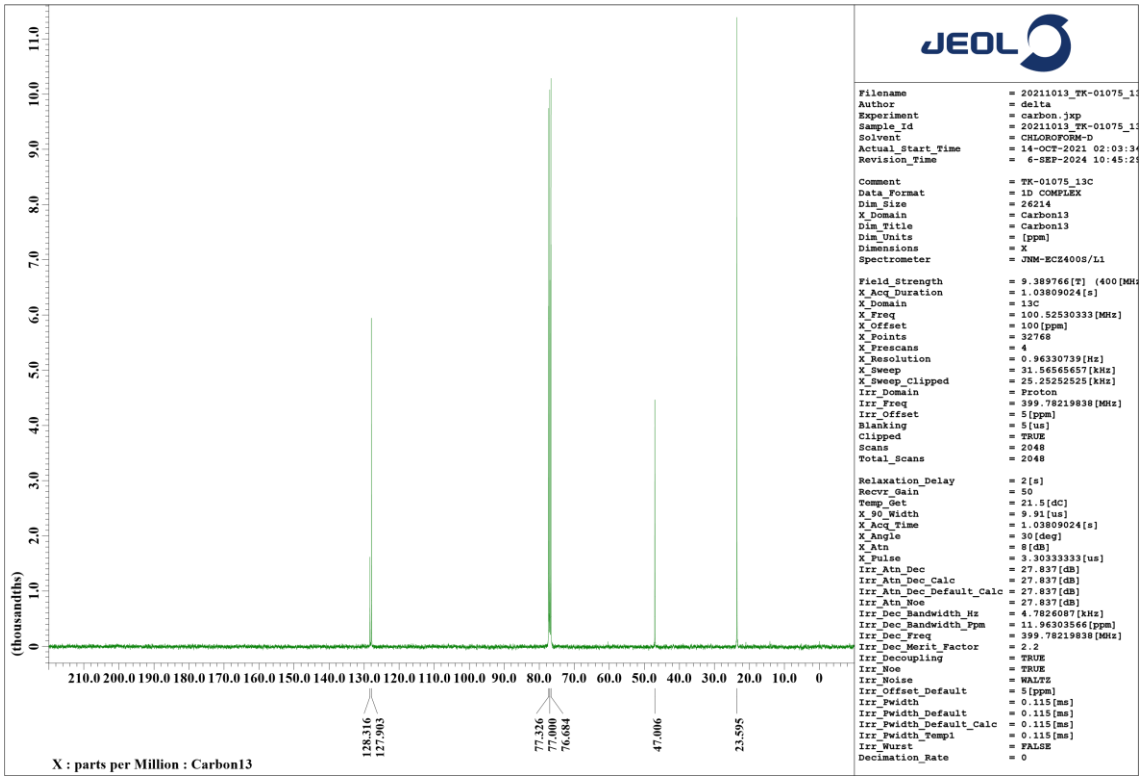
X_Freq = 399.78219838[MHz]
X_Offset = 5[ppm]
X_Points = 16384
X_Prescans = 1
X_Resolution = 0.45739775[Hz]
X_Sweep = 7.4940048[kHz]
X_Sweep_Clipped = 5.99520384[kHz]
Irr_Domain = Proton
Irr_Freq = 399.78219838[MHz]
Irr_Offset = 5[ppm]
Tri_Domain = Proton
Tri_Freq = 399.78219838[MHz]
Tri_Offset = 5[ppm]
Blanking = 2[us]
Clipped = FALSE
Scans = 16
Total_Scans = 16
Relaxation_Delay = 5[s]
Recvr_Gain = 56
Temp_Get = 21.2[dC]
X_90_Width = 6.4[us]
X_Acq_Time = 2.18628096[s]
X_Angle = 45[deg]
X_Atn = 2.4[dB]
X_Pulse = 3.2[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Loop = 500
Dante_Presat = FALSE
Decimation_Rate = 0
Initial_Wait = 1[s]
Phase = (0, 90, 270, 180, 180,
Presat_Time = 5[s]
Presat_Time_Flag = FALSE
Relaxation_Delay_Calc = 0[s]
Relaxation_Delay_Temp = 5[s]
Repetition_Time = 7.18628096[s]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Author = delta
Experiment = carbon.jxp
Sample_Id = 20211013_TK-01075_1
Solvent = CHLOROFORM-D
Actual_Start_Time = 14-OCT-2021 02:03:3
Revision_Time = 6-SEP-2024 10:45:2
Comment = TK-01075_13C
Data_Format = 1D COMPLEX
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X_Domain = Carbon13
Dim_Title = Carbon13
Dim_Units = [ppm]
Dimensions = X
Spectrometer = JNM-ECZ400S/L1
Field_Strength = 9.389766[T] (400[MH
X_Acq_Duration = 1.03809024[s]
X_Domain = 13C
X_Freq = 100.52530333[MHz]
X_Offset = 100[ppm]
X_Points = 32768
X_Prescans = 4
X_Resolution = 0.96330739[Hz]
X_Sweep = 31.56565657[kHz]
X_Sweep_Clipped = 25.25252525[kHz]
Irr_Domain = Proton
Irr_Freq = 399.78219838[MHz]
Irr_Offset = 5[ppm]
Blanking = 5[us]
Clipped = TRUE
Scans = 2048
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Relaxation_Delay = 2[s]
Recvr_Gain = 50
Temp_Get = 21.5[dC]
X_90_Width = 9.91[us]
X_Acq_Time = 1.03809024[s]
X_Angle = 30[deg]
X_Atn = 8[dB]
X_Pulse = 3.30333333[us]
Irr_Atn_Dec = 27.837[dB]
Irr_Atn_Dec_Calc = 27.837[dB]
Irr_Atn_Dec_Default_Calc = 27.837[dB]
Irr_Atn_Noe = 27.837[dB]
Irr_Dec_Bandwidth_Hz = 4.7826087[kHz]
Irr_Dec_Bandwidth_Ppm = 11.96303566[ppm]
Irr_Dec_Freq = 399.78219838[MHz]
Irr_Dec_Merit_Factor = 2.2
Irr_Decoupling = TRUE
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Irr_Noise = WALTZ
Irr_Offset_Default = 5[ppm]
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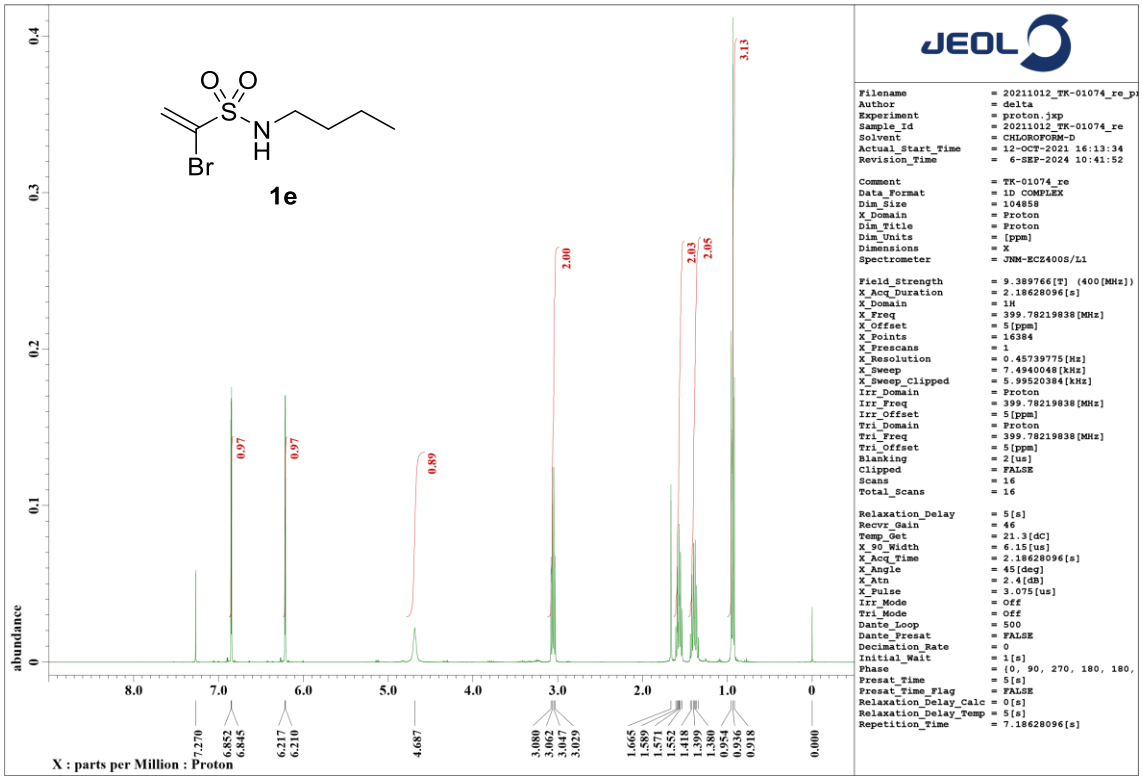
Decimation_Rate = 0



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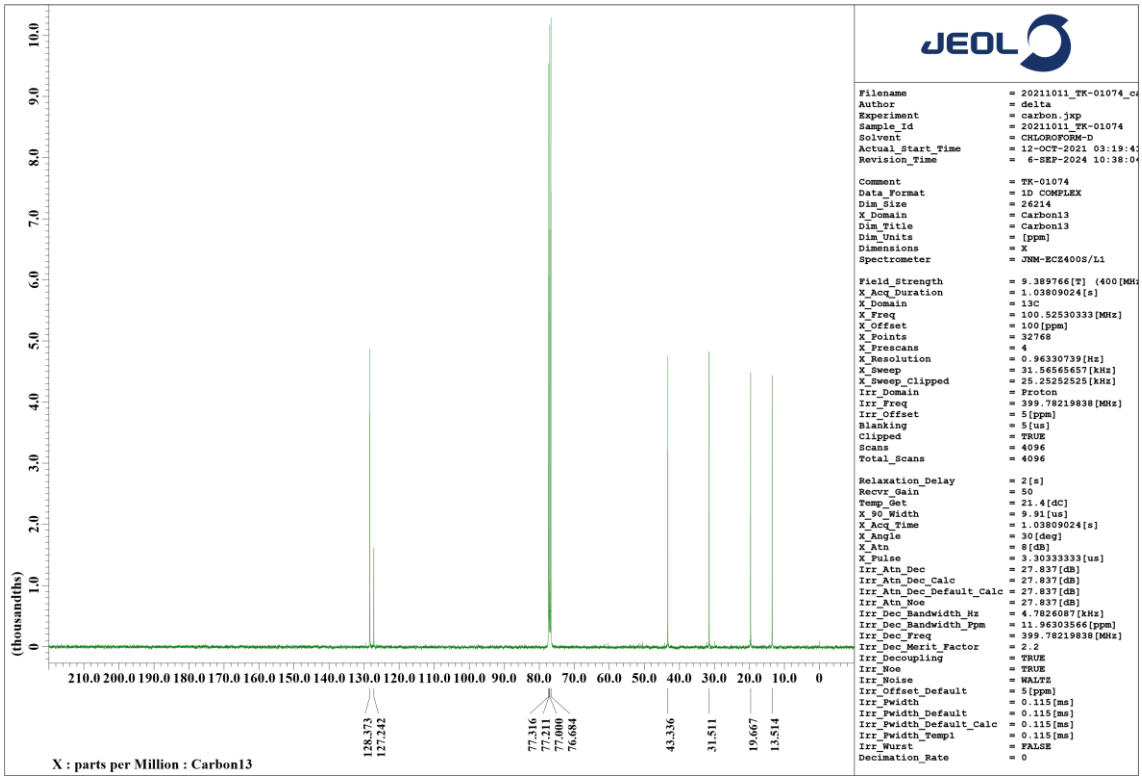
Author = delta
Experiment = proton.jxp
Sample_Id = 20211012_TK-01074_re
Solvent = CHLOROFORM-D
Actual_Start_Time = 12-OCT-2021 16:13:34
Revision_Time = 6-SEP-2024 10:41:52

Comment = TK-01074_re
Data_Format = 1D COMPLEX
Dim_Size = 104858
X_Domain = Proton
Dim_Title = Proton
Dim_Units = [ppm]
Dimensions = X
Spectrometer = JNM-ECZ400S/L1

Field_Strength = 9.389766[T] (400[MHz])
X_Acq_Duration = 2.18628096[s]
X_Domain = 1H
X_Freq = 399.78219838[MHz]
X_Offset = 5[ppm]
X_Points = 16384
X_Prescans = 1
X_Resolution = 0.45739775[Hz]
X_Sweep = 7.4940048[kHz]
X_Sweep_Clipped = 5.99520384[kHz]
Irr_Domain = Proton
Irr_Freq = 399.78219838[MHz]
Irr_Offset = 5[ppm]
Tri_Domain = Proton
Tri_Freq = 399.78219838[MHz]
Tri_Offset = 5[ppm]
Blanking = 2[us]
Clipped = FALSE
Scans = 16
Total_Scans = 16

Relaxation_Delay = 5[s]
Recvr_Gain = 46
Temp_Get = 21.3[dC]
X_90_Width = 6.15[us]
X_Acq_Time = 2.18628096[s]
X_Angle = 45[deg]
X_Atn = 2.4[dB]
X_Pulse = 3.075[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Loop = 500
Dante_Presat = FALSE
Decimation_Rate = 0
Initial_Wait = 1[s]
Phase = (0, 90, 270, 180, 180,
Presat_Time = 5[s]
Presat_Time_Flag = FALSE
Relaxation_Delay_Calc = 0[s]
Relaxation_Delay_Temp = 5[s]
Repetition_Time = 7.18628096[s]

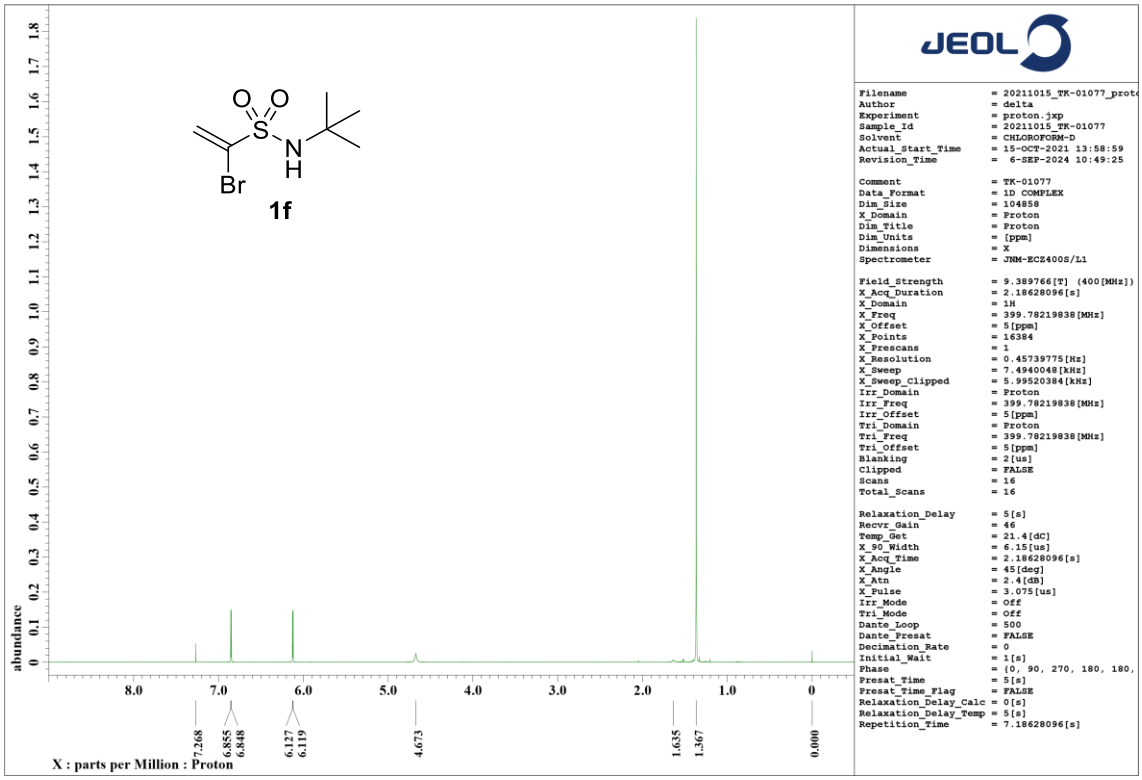


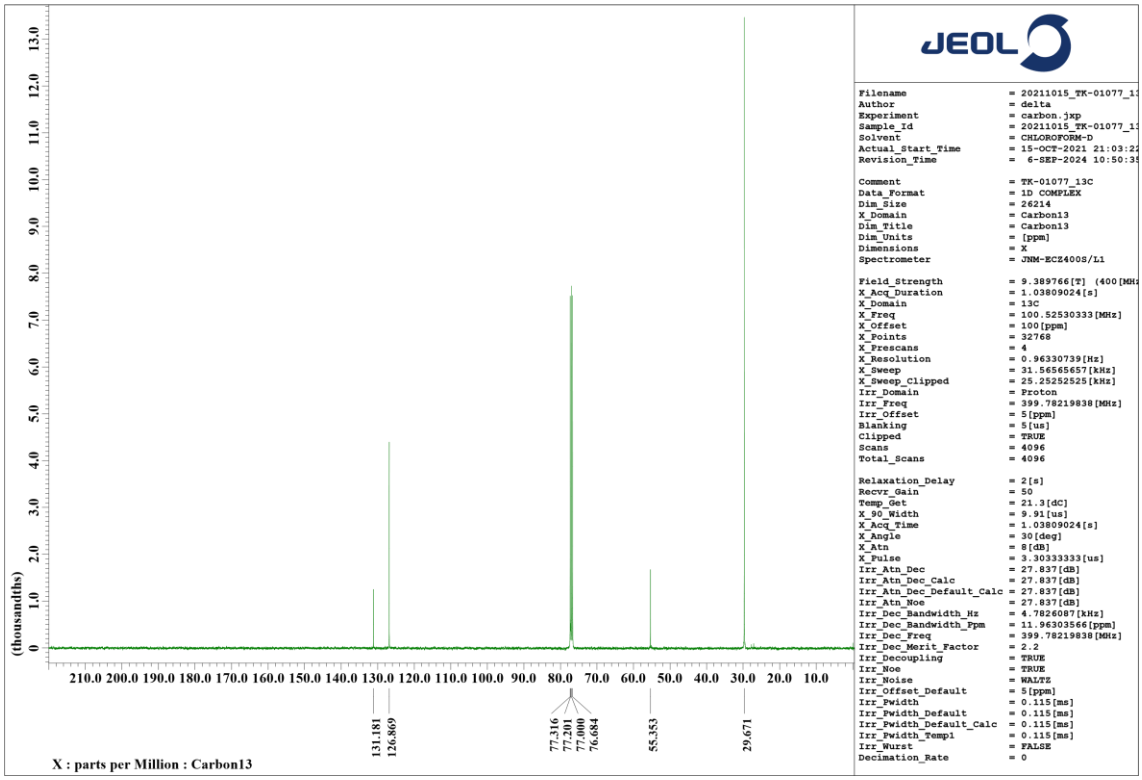
Filename = 20211011_TK-01074_c
Author = delta
Experiment = carbon.jxp
Sample_Id = 20211011_TK-01074
Solvent = CHLOROFORM-D
Actual_Start_Time = 12-OCT-2021 03:19:4
Revision_Time = 6-SEP-2024 10:38:0

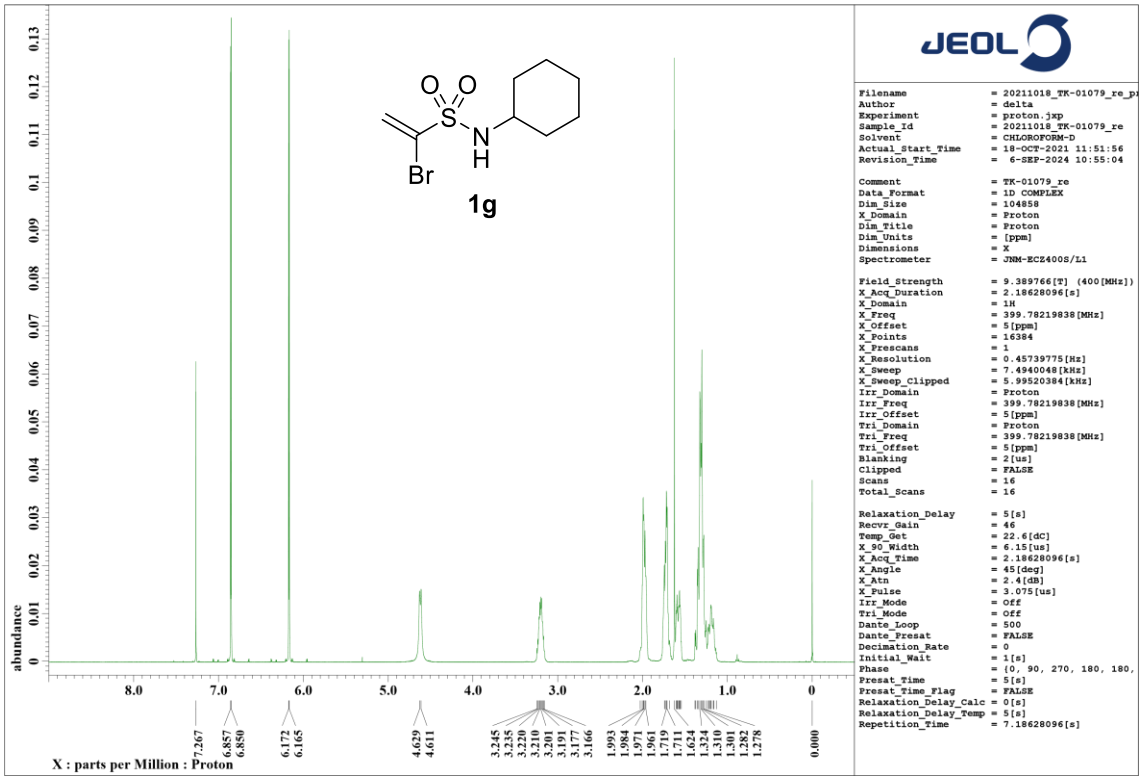
Comment = TK-01074
Data_Format = 1D COMPLEX
Dim_Size = 26214
X_Domain = Carbon13
Dim_Title = Carbon13
Dim_Units = [ppm]
Dimensions = X
Spectrometer = JNM-ECZ400S/L1

Field_Strength = 9.389766[T] (400[MH
X_Acq_Duration = 1.03809024[s]
X_Domain = 13C
X_Freq = 100.52530333[MHz]
X_Offset = 100[ppm]
X_Points = 32768
X_Prescans = 4
X_Resolution = 0.96330739[Hz]
X_Sweep = 31.56565657[kHz]
X_Sweep_Clipped = 25.25252525[kHz]
Irr_Domain = Proton
Irr_Freq = 399.78219838[MHz]
Irr_Offset = 5[ppm]
Blanking = 5[us]
Clipped = TRUE
Scans = 4096
Total_Scans = 4096

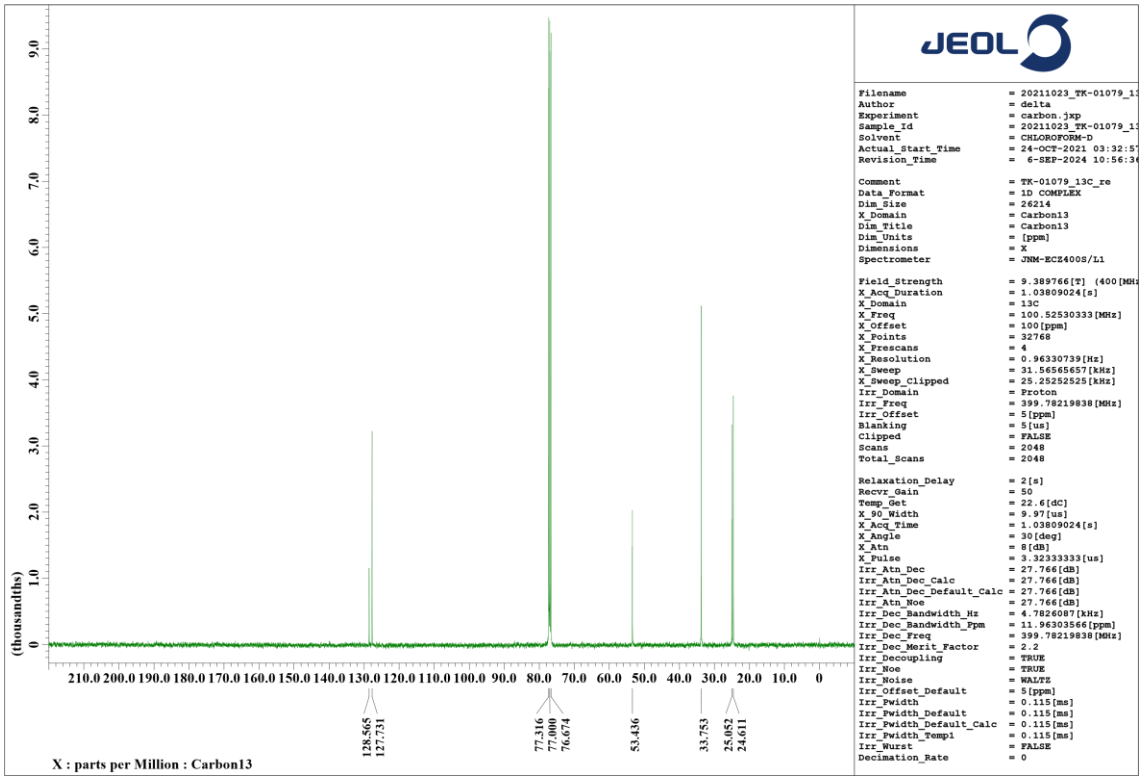
Relaxation_Delay = 2[s]
Recvr_Gain = 50
Temp_Get = 21.4[dC]
X_90_Width = 9.91[us]
X_Acq_Time = 1.03809024[s]
X_Angle = 30[deg]
X_Atn = 8[dB]
X_Pulse = 3.30333333[us]
Irr_Atn_Dec = 27.837[dB]
Irr_Atn_Dec_Calc = 27.837[dB]
Irr_Atn_Dec_Default_Calc = 27.837[dB]
Irr_Atn_Noe = 27.837[dB]
Irr_Dec_Bandwidth_Hz = 4.7826087[kHz]
Irr_Dec_Bandwidth_Ppm = 11.96303566[ppm]
Irr_Dec_Freq = 399.78219838[MHz]
Irr_Dec_Merit_Factor = 2.2
Irr_Decoupling = TRUE
Irr_Noe = TRUE
Irr_Noise = WALTZ
Irr_Offset_Default = 5[ppm]
Irr_Pwidth = 0.115[ms]
Irr_Pwidth_Default = 0.115[ms]
Irr_Pwidth_Default_Calc = 0.115[ms]
Irr_Pwidth_Temp1 = 0.115[ms]
Irr_Wurst = FALSE
Decimation_Rate = 0


1f
abundance
X : parts per Million : Proton
7.268
6.855
6.848
6.127
6.119
4.673
1.635
1.367
0.000

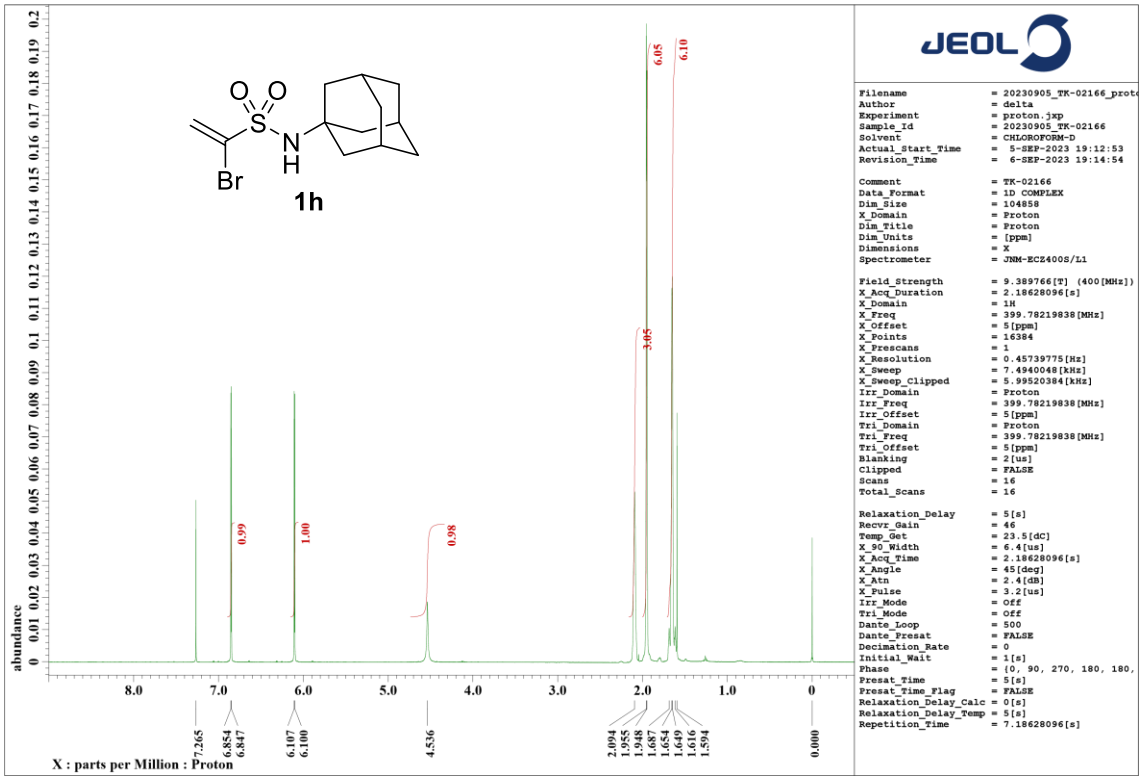

(thousandths)
X : parts per Million : Carbon13
131.181
126.869
77.316
77.201
77.000
76.684
55.353
29.671

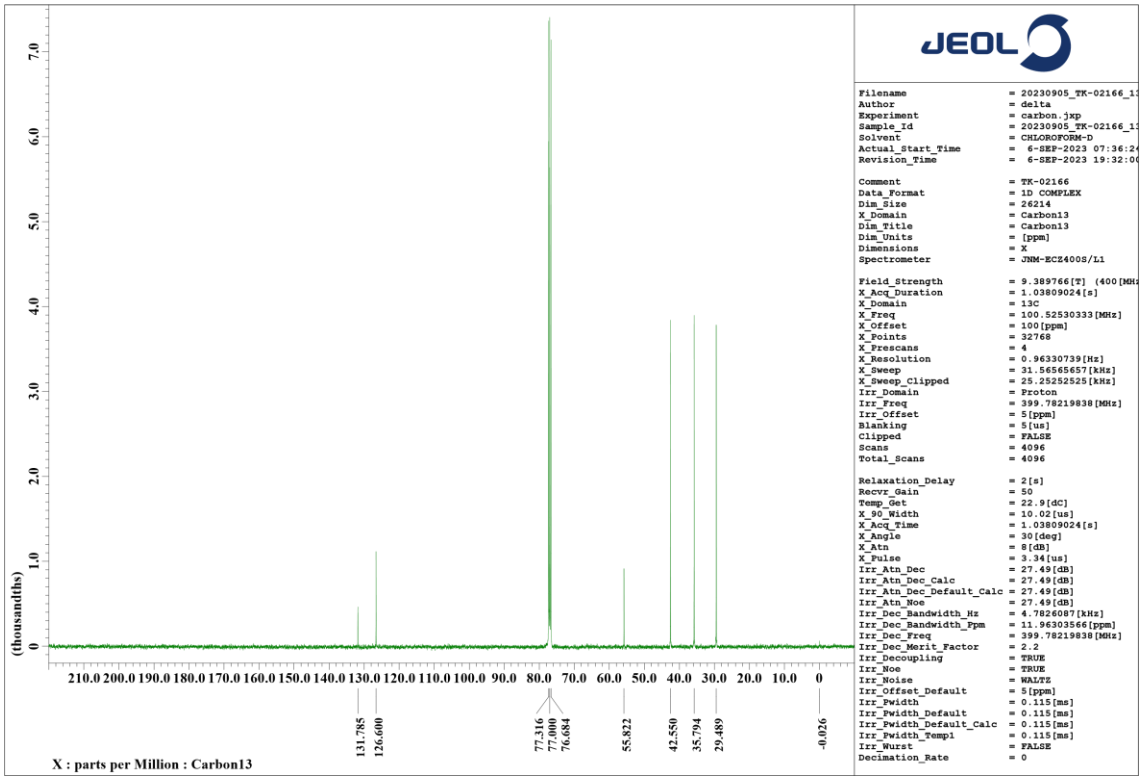


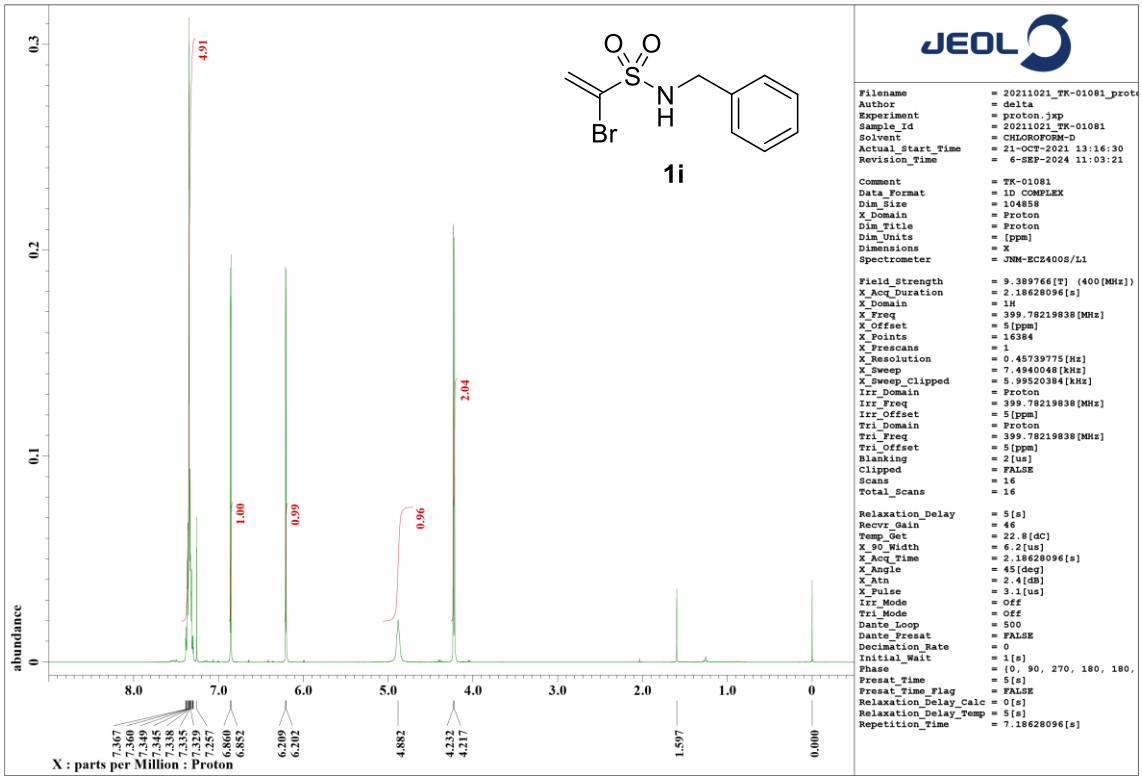

```
Filename                = 20211018_TK-01079_re_p
Author                  = delta
Experiment              = proton.jxp
Sample_Id               = 20211018_TK-01079_re
Solvent                 = CHLOROFORM-D
Actual_Start_Time       = 18-OCT-2021 11:51:56
Revision_Time           =  6-SEP-2024 10:55:04

Comment                 = TK-01079_re
Data_Format             = 1D COMPLEX
Dim_Size                = 104858
X_Domain                = Proton
Dim_Title               = Proton
Dim_Units               = [ppm]
Dimensions              = X
Spectrometer            = JNM-ECZ400S/L1

Field_Strength          = 9.389766[T] (400[MHz])
X_Acq_Duration          = 2.18628096[s]
X_Domain                = 1H
X_Freq                  = 399.78219838[MHz]
X_Offset                = 5[ppm]
X_Points                = 16384
X_Prescans              = 1
X_Resolution            = 0.45739775[Hz]
X_Sweep                 = 7.4940048[kHz]
X_Sweep_Clipped         = 5.99520384[kHz]
Irr_Domain              = Proton
Irr_Freq                = 399.78219838[MHz]
Irr_Offset              = 5[ppm]
Tri_Domain              = Proton
Tri_Freq                = 399.78219838[MHz]
Tri_Offset              = 5[ppm]
Blanking                = 2[us]
Clipped                 = FALSE
Scans                   = 16
Total_Scans             = 16

Relaxation_Delay        = 5[s]
Recvr_Gain              = 46
Temp_Get                = 22.6[dC]
X_90_Width              = 6.15[us]
X_Acq_Time              = 2.18628096[s]
X_Angle                 = 45[deg]
X_Atn                   = 2.4[dB]
X_Pulse                 = 3.075[us]
Irr_Mode                = Off
Tri_Mode                = Off
Dante_Loop              = 500
Dante_Presat            = FALSE
Decimation_Rate         = 0
Initial_Wait            = 1[s]
Phase                   = (0, 90, 270, 180, 180,
Presat_Time             = 5[s]
Presat_Time_Flag        = FALSE
Relaxation_Delay_Calc = 0[s]
Relaxation_Delay_Temp = 5[s]
Repetition_Time         = 7.18628096[s]
```

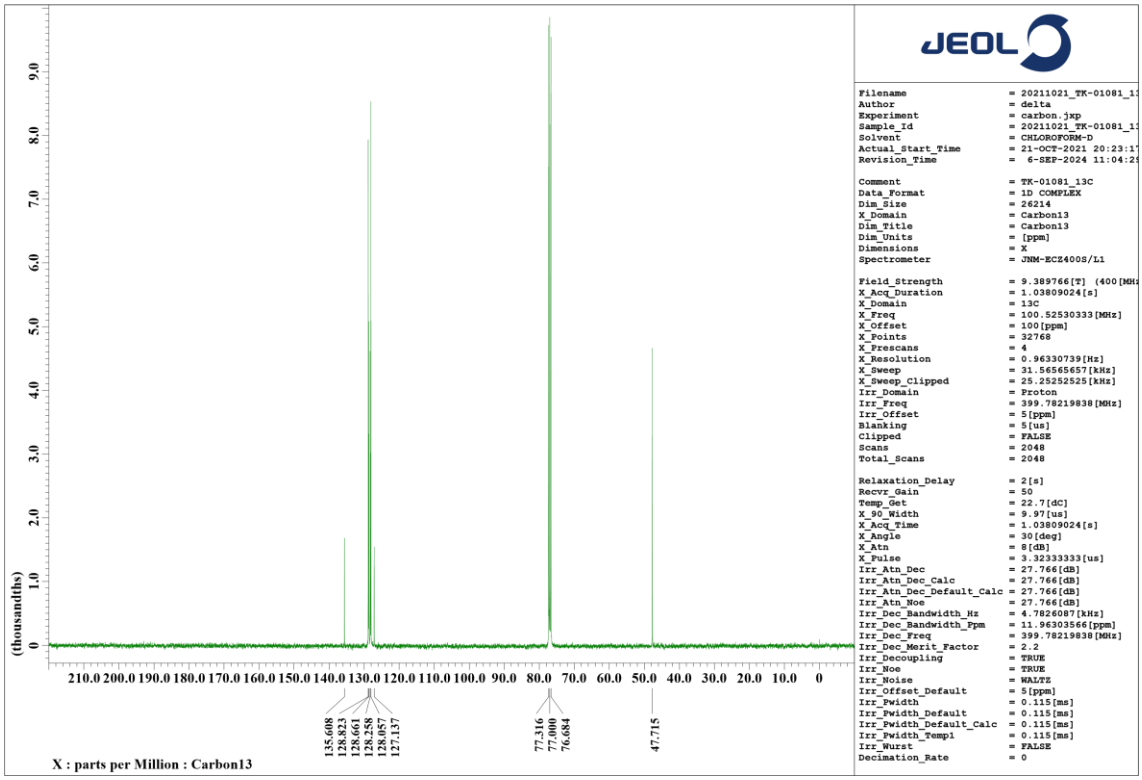


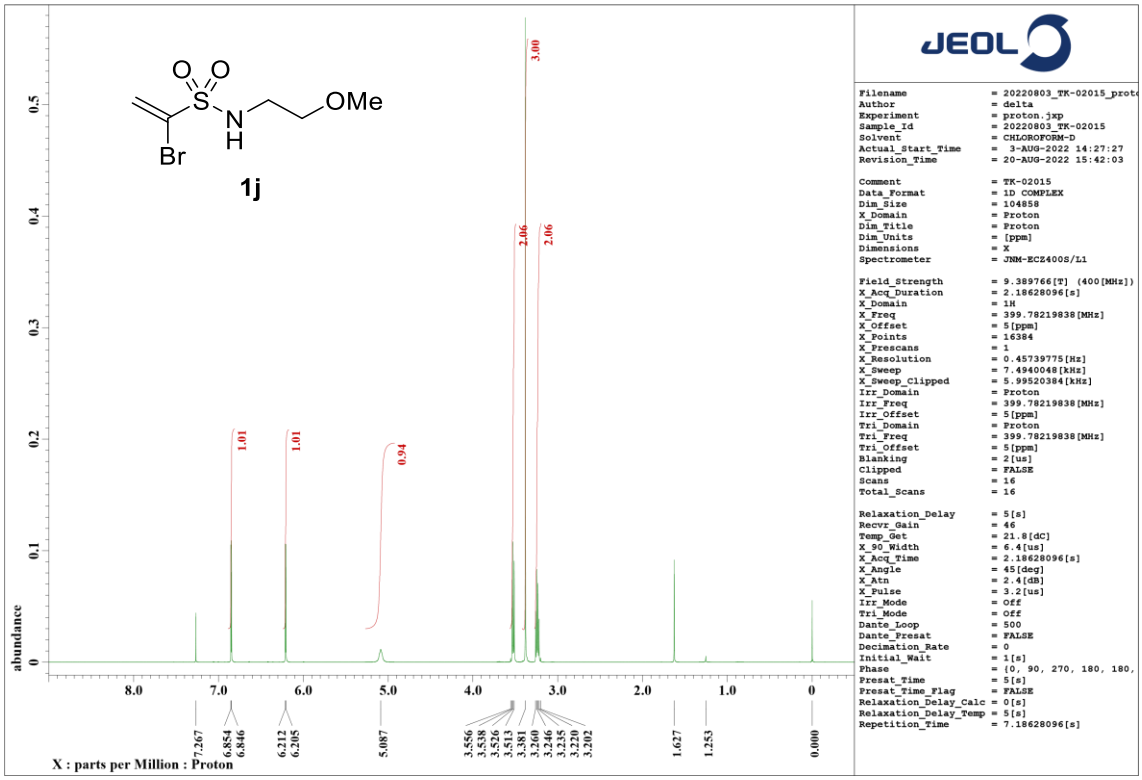

```
Filename                = 20211023_TK-01079_1
Author                  = delta
Experiment              = carbon.jxp
Sample_Id               = 20211023_TK-01079_1
Solvent                 = CHLOROFORM-D
Actual_Start_Time       = 24-OCT-2021 03:32:5
Revision_Time           =  6-SEP-2024 10:56:3

Comment                 = TK-01079_13C_re
Data_Format             = 1D COMPLEX
Dim_Size                = 26214
X_Domain                = Carbon13
Dim_Title               = Carbon13
Dim_Units               = [ppm]
Dimensions              = X
Spectrometer            = JNM-ECZ400S/L1

Field_Strength          = 9.389766[T] (400[MH
X_Acq_Duration          = 1.03809024[s]
X_Domain                = 13C
X_Freq                  = 100.52530333[MHz]
X_Offset                = 100[ppm]
X_Points                = 32768
X_Prescans              = 4
X_Resolution            = 0.96330739[Hz]
X_Sweep                 = 31.56565657[kHz]
X_Sweep_Clipped         = 25.25252525[kHz]
Irr_Domain              = Proton
Irr_Freq                = 399.78219838[MHz]
Irr_Offset              = 5[ppm]
Blanking                = 5[us]
Clipped                 = FALSE
Scans                   = 2048
Total_Scans             = 2048

Relaxation_Delay        = 2[s]
Recvr_Gain              = 50
Temp_Get                = 22.6[dC]
X_90_Width              = 9.97[us]
X_Acq_Time              = 1.03809024[s]
X_Angle                 = 30[deg]
X_Atn                   = 8[dB]
X_Pulse                 = 3.32333333[us]
Irr_Atn_Dec             = 27.766[dB]
Irr_Atn_Dec_Calc        = 27.766[dB]
Irr_Atn_Dec_Default_Calc = 27.766[dB]
Irr_Atn_Noe             = 27.766[dB]
Irr_Dec_Bandwidth_Hz    = 4.7826087[kHz]
Irr_Dec_Bandwidth_Ppm   = 11.96303566[ppm]
Irr_Dec_Freq            = 399.78219838[MHz]
Irr_Dec_Merit_Factor    = 2.2
Irr_Decoupling          = TRUE
Irr_Noe                 = TRUE
Irr_Noise               = WALTZ
Irr_Offset_Default      = 5[ppm]
Irr_Pwidth              = 0.115[ms]
Irr_Pwidth_Default      = 0.115[ms]
Irr_Pwidth_Default_Calc = 0.115[ms]
Irr_Pwidth_Temp1        = 0.115[ms]
Irr_Wurst               = FALSE
Decimation_Rate         = 0
```

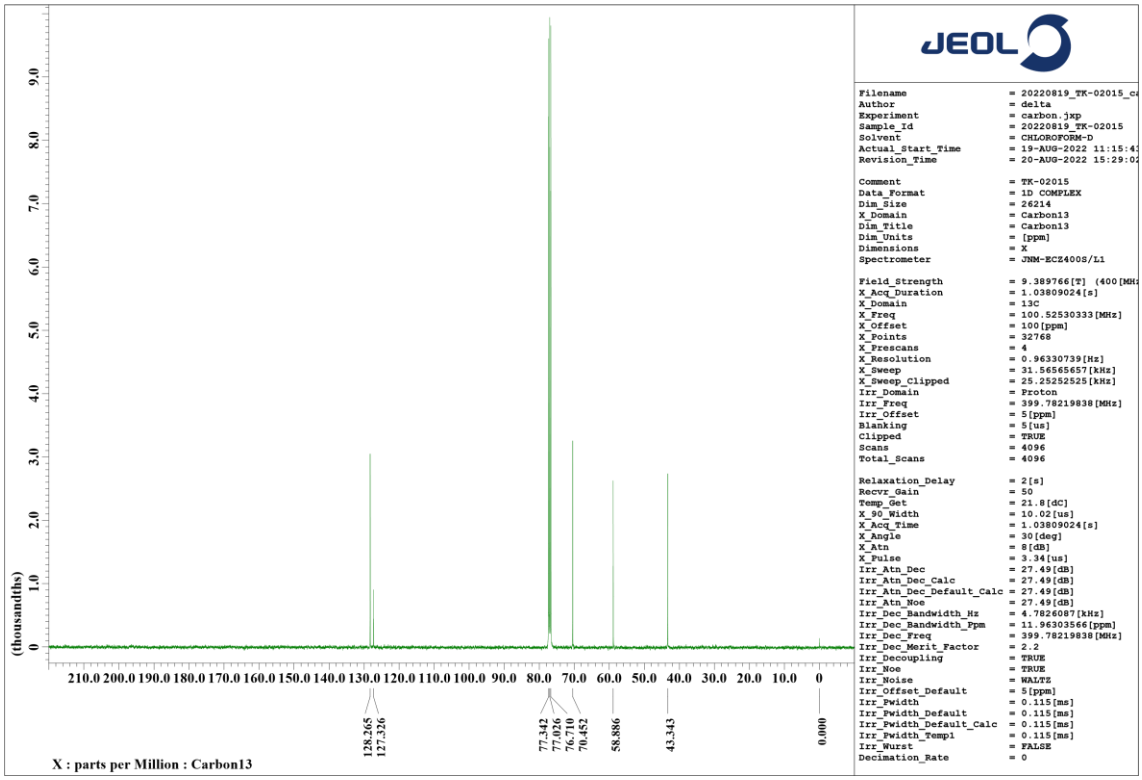

1h
abundance
X : parts per Million : Proton
7.265
6.854
6.847
6.107
6.100
4.536
2.094
1.955
1.948
1.687
1.654
1.649
1.616
1.594
0.000
0.99
1.00
0.98
3.05
6.05
6.10
Filename = 20230905_TK-02166_prot
Author = delta
Experiment = proton.jxp
Sample_Id = 20230905_TK-02166
Solvent = CHLOROFORM-D
Actual_Start_Time = 5-SEP-2023 19:12:53
Revision_Time = 6-SEP-2023 19:14:54
Comment = TK-02166
Data_Format = 1D COMPLEX
Dim_Size = 104858
X_Domain = Proton
Dim_Title = Proton
Dim_Units = [ppm]
Dimensions = X
Spectrometer = JNM-ECZ400S/L1
Field_Strength = 9.389766[T] (400[MHz])
X_Acq_Duration = 2.18628096[s]
X_Domain = 1H
X_Freq = 399.78219838[MHz]
X_Offset = 5[ppm]
X_Points = 16384
X_Prescans = 1
X_Resolution = 0.45739775[Hz]
X_Sweep = 7.4940048[kHz]
X_Sweep_Clipped = 5.99520384[kHz]
Irr_Domain = Proton
Irr_Freq = 399.78219838[MHz]
Irr_Offset = 5[ppm]
Tri_Domain = Proton
Tri_Freq = 399.78219838[MHz]
Tri_Offset = 5[ppm]
Blanking = 2[us]
Clipped = FALSE
Scans = 16
Total_Scans = 16
Relaxation_Delay = 5[s]
Recvr_Gain = 46
Temp_Get = 23.5[dC]
X_90_Width = 6.4[us]
X_Acq_Time = 2.18628096[s]
X_Angle = 45[deg]
X_Atn = 2.4[dB]
X_Pulse = 3.2[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Loop = 500
Dante_Presat = FALSE
Decimation_Rate = 0
Initial_Wait = 1[s]
Phase = (0, 90, 270, 180, 180,
Presat_Time = 5[s]
Presat_Time_Flag = FALSE
Relaxation_Delay_Calc = 0[s]
Relaxation_Delay_Temp = 5[s]
Repetition_Time = 7.18628096[s]

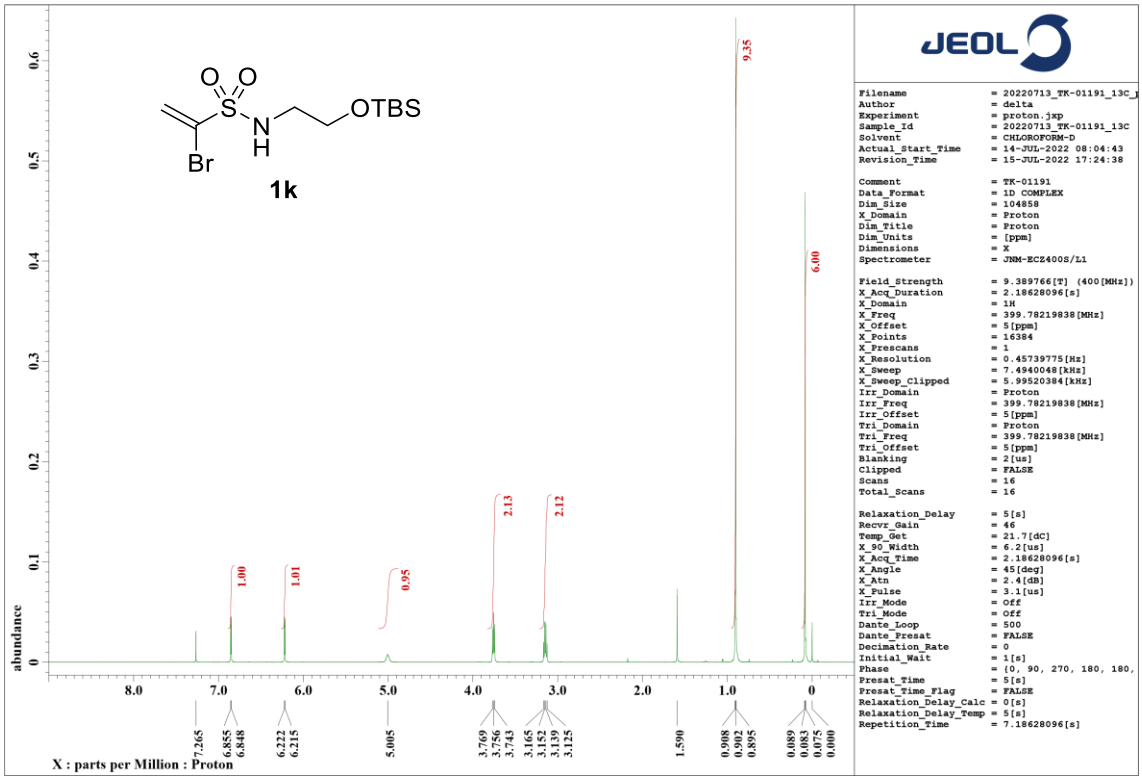

(thousandths)
X : parts per Million : Carbon13
131.785
126.600
77.316
77.000
76.684
55.822
42.550
35.794
29.489
-0.026
Filename = 20230905_TK-02166_1
Author = delta
Experiment = carbon.jxp
Sample_Id = 20230905_TK-02166_1
Solvent = CHLOROFORM-D
Actual_Start_Time = 6-SEP-2023 07:36:2
Revision_Time = 6-SEP-2023 19:32:0
Comment = TK-02166
Data_Format = 1D COMPLEX
Dim_Size = 26214
X_Domain = Carbon13
Dim_Title = Carbon13
Dim_Units = [ppm]
Dimensions = X
Spectrometer = JNM-ECZ400S/L1
Field_Strength = 9.389766[T] (400[MH
X_Acq_Duration = 1.03809024[s]
X_Domain = 13C
X_Freq = 100.52530333[MHz]
X_Offset = 100[ppm]
X_Points = 32768
X_Prescans = 4
X_Resolution = 0.96330739[Hz]
X_Sweep = 31.56565657[kHz]
X_Sweep_Clipped = 25.25252525[kHz]
Irr_Domain = Proton
Irr_Freq = 399.78219838[MHz]
Irr_Offset = 5[ppm]
Blanking = 5[us]
Clipped = FALSE
Scans = 4096
Total_Scans = 4096
Relaxation_Delay = 2[s]
Recvr_Gain = 50
Temp_Get = 22.9[dC]
X_90_Width = 10.02[us]
X_Acq_Time = 1.03809024[s]
X_Angle = 30[deg]
X_Atn = 8[dB]
X_Pulse = 3.34[us]
Irr_Atn_Dec = 27.49[dB]
Irr_Atn_Dec_Calc = 27.49[dB]
Irr_Atn_Dec_Default_Calc = 27.49[dB]
Irr_Atn_Noe = 27.49[dB]
Irr_Dec_Bandwidth_Hz = 4.78260087[kHz]
Irr_Dec_Bandwidth_Ppm = 11.96303566[ppm]
Irr_Dec_Freq = 399.78219838[MHz]
Irr_Dec_Merit_Factor = 2.2
Irr_Decoupling = TRUE
Irr_Noe = TRUE
Irr_Noise = WALTZ
Irr_Offset_Default = 5[ppm]
Irr_Pwidth = 0.115[ms]
Irr_Pwidth_Default = 0.115[ms]
Irr_Pwidth_Default_Calc = 0.115[ms]
Irr_Pwidth_Temp1 = 0.115[ms]
Irr_Wurst = FALSE
Decimation_Rate = 0

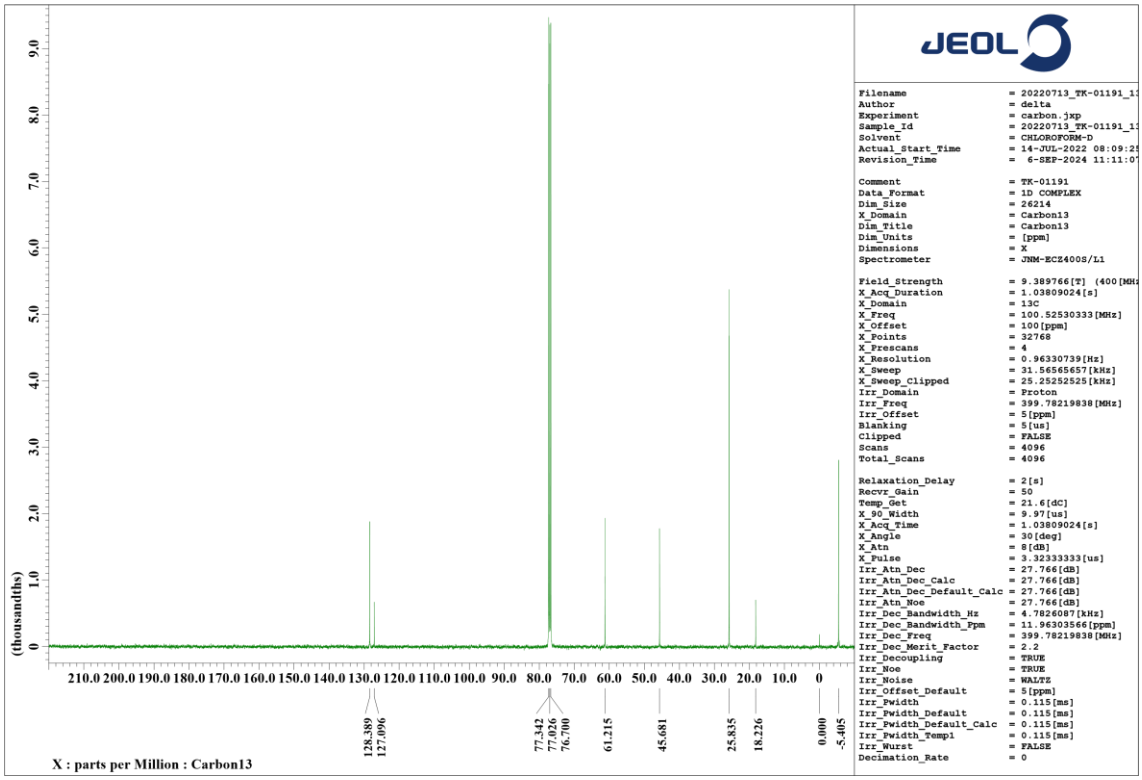

1i
4.91
1.00
0.99
0.96
2.04
abundance
X : parts per Million : Proton
7.367
7.360
7.349
7.345
7.338
7.335
7.329
7.257
6.860
6.852
6.209
6.202
4.882
4.232
4.217
1.597
0.000
Filename = 20211021_TK-01081_prot
Author = delta
Experiment = proton.jxp
Sample_Id = 20211021_TK-01081
Solvent = CHLOROFORM-D
Actual_Start_Time = 21-OCT-2021 13:16:30
Revision_Time = 6-SEP-2024 11:03:21
Comment = TK-01081
Data_Format = 1D COMPLEX
Dim_Size = 104858
X_Domain = Proton
Dim_Title = Proton
Dim_Units = [ppm]
Dimensions = X
Spectrometer = JNM-ECZ400S/L1
Field_Strength = 9.389766[T] (400[MHz])
X_Acq_Duration = 2.18628096[s]
X_Domain = 1H
X_Freq = 399.78219838[MHz]
X_Offset = 5[ppm]
X_Points = 16384
X_Prescans = 1
X_Resolution = 0.45739775[Hz]
X_Sweep = 7.4940048[kHz]
X_Sweep_Clipped = 5.99520384[kHz]
Irr_Domain = Proton
Irr_Freq = 399.78219838[MHz]
Irr_Offset = 5[ppm]
Tri_Domain = Proton
Tri_Freq = 399.78219838[MHz]
Tri_Offset = 5[ppm]
Blanking = 2[us]
Clipped = FALSE
Scans = 16
Total_Scans = 16
Relaxation_Delay = 5[s]
Recvr_Gain = 46
Temp_Get = 22.8[dC]
X_90_Width = 6.2[us]
X_Acq_Time = 2.18628096[s]
X_Angle = 45[deg]
X_Atn = 2.4[dB]
X_Pulse = 3.1[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Loop = 500
Dante_Presat = FALSE
Decimation_Rate = 0
Initial_Wait = 1[s]
Phase = (0, 90, 270, 180, 180,
Presat_Time = 5[s]
Presat_Time_Flag = FALSE
Relaxation_Delay_Calc = 0[s]
Relaxation_Delay_Temp = 5[s]
Repetition_Time = 7.18628096[s]

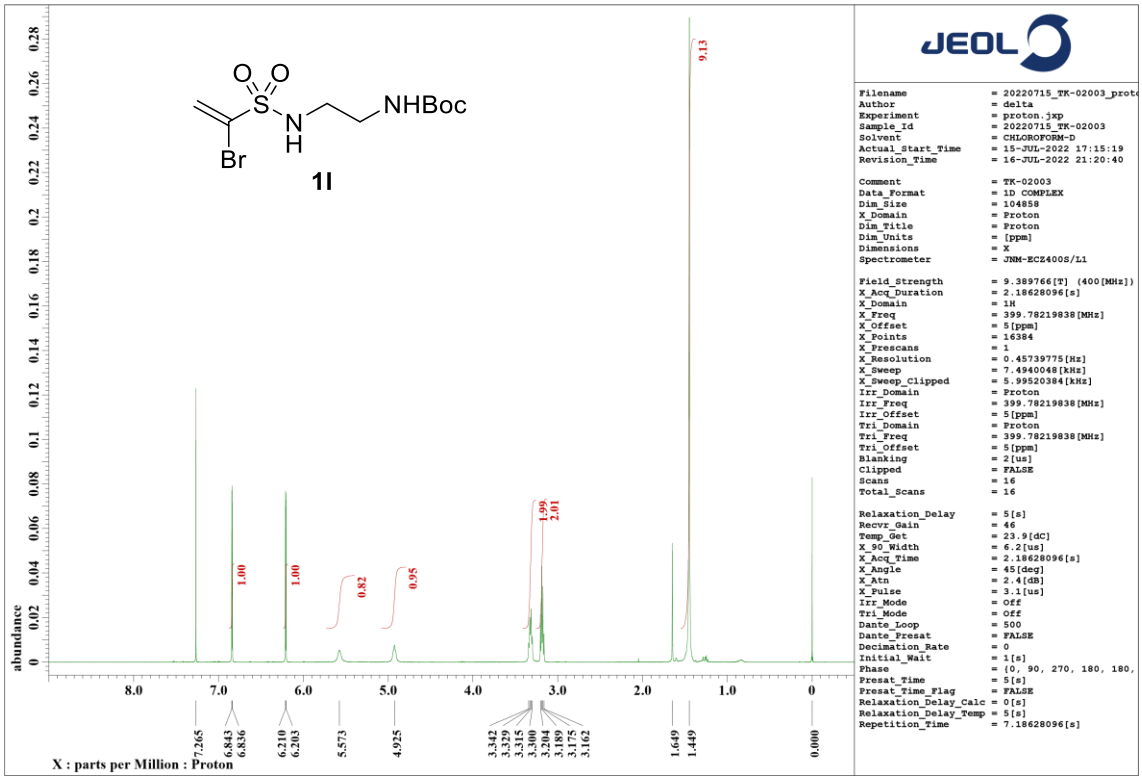

(thousandths)
X : parts per Million : Carbon13
135.608
128.823
128.661
128.258
128.057
127.137
77.316
77.000
76.684
47.715
Filename = 20211021_TK-01081_1
Author = delta
Experiment = carbon.jxp
Sample_Id = 20211021_TK-01081_1
Solvent = CHLOROFORM-D
Actual_Start_Time = 21-OCT-2021 20:23:1
Revision_Time = 6-SEP-2024 11:04:2
Comment = TK-01081_13C
Data_Format = 1D COMPLEX
Dim_Size = 26214
X_Domain = Carbon13
Dim_Title = Carbon13
Dim_Units = [ppm]
Dimensions = X
Spectrometer = JNM-ECZ400S/L1
Field_Strength = 9.389766[T] (400[MH
X_Acq_Duration = 1.03809024[s]
X_Domain = 13C
X_Freq = 100.52530333[MHz]
X_Offset = 100[ppm]
X_Points = 32768
X_Prescans = 4
X_Resolution = 0.96330739[Hz]
X_Sweep = 31.56565657[kHz]
X_Sweep_Clipped = 25.25252525[kHz]
Irr_Domain = Proton
Irr_Freq = 399.78219838[MHz]
Irr_Offset = 5[ppm]
Blanking = 5[us]
Clipped = FALSE
Scans = 2048
Total_Scans = 2048
Relaxation_Delay = 2[s]
Recvr_Gain = 50
Temp_Get = 22.7[dC]
X_90_Width = 9.97[us]
X_Acq_Time = 1.03809024[s]
X_Angle = 30[deg]
X_Atn = 8[dB]
X_Pulse = 3.32333333[us]
Irr_Atn_Dec = 27.766[dB]
Irr_Atn_Dec_Calc = 27.766[dB]
Irr_Atn_Dec_Default_Calc = 27.766[dB]
Irr_Atn_Noe = 27.766[dB]
Irr_Dec_Bandwidth_Hz = 4.7826087[kHz]
Irr_Dec_Bandwidth_Ppm = 11.96303566[ppm]
Irr_Dec_Freq = 399.78219838[MHz]
Irr_Dec_Merit_Factor = 2.2
Irr_Decoupling = TRUE
Irr_Noe = TRUE
Irr_Noise = WALTZ
Irr_Offset_Default = 5[ppm]
Irr_Pwidth = 0.115[ms]
Irr_Pwidth_Default = 0.115[ms]
Irr_Pwidth_Default_Calc = 0.115[ms]
Irr_Pwidth_Temp1 = 0.115[ms]
Irr_Wurst = FALSE
Decimation_Rate = 0

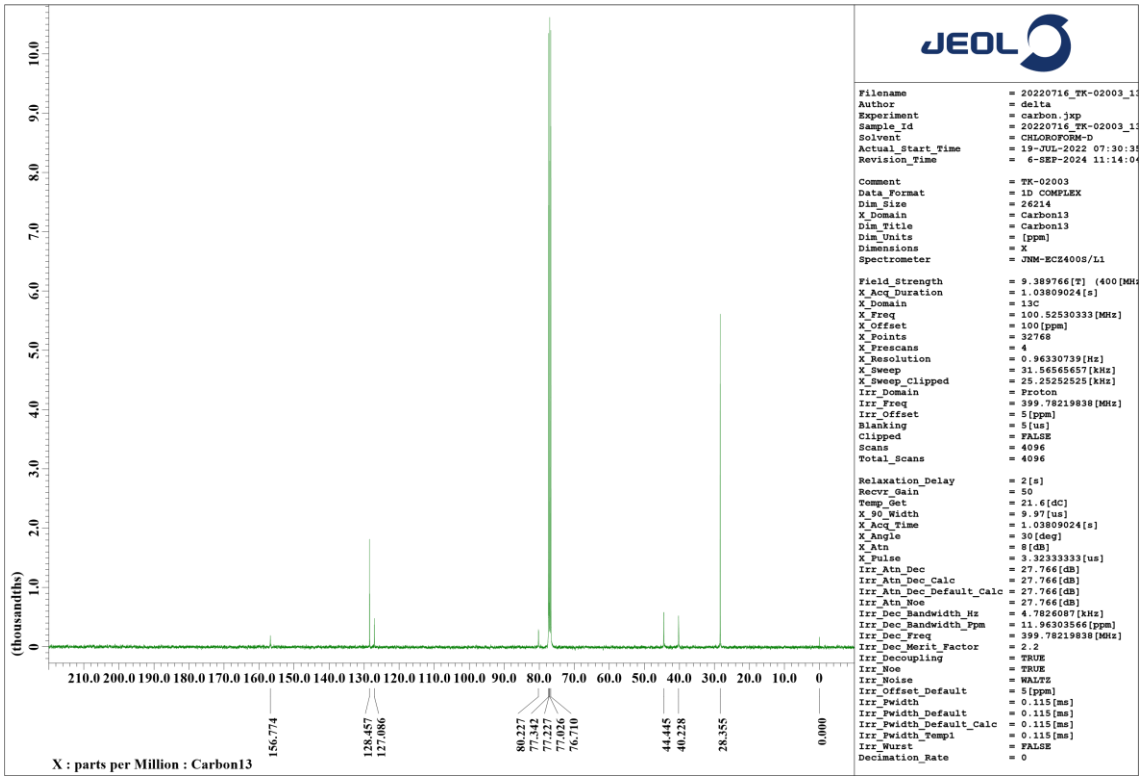

1j
abundance
X : parts per Million : Proton
Filename = 20220803_TK-02015_prot
Author = delta
Experiment = proton.jxp
Sample_Id = 20220803_TK-02015
Solvent = CHLOROFORM-D
Actual_Start_Time = 3-AUG-2022 14:27:27
Revision_Time = 20-AUG-2022 15:42:03
Comment = TK-02015
Data_Format = 1D COMPLEX
Dim_Size = 104858
X_Domain = Proton
Dim_Title = Proton
Dim_Units = [ppm]
Dimensions = X
Spectrometer = JNM-ECZ400S/L1
Field_Strength = 9.389766[T] (400[MHz])
X_Acq_Duration = 2.18628096[s]
X_Domain = 1H
X_Freq = 399.78219838[MHz]
X_Offset = 5[ppm]
X_Points = 16384
X_Prescans = 1
X_Resolution = 0.45739775[Hz]
X_Sweep = 7.4940048[kHz]
X_Sweep_Clipped = 5.99520384[kHz]
Irr_Domain = Proton
Irr_Freq = 399.78219838[MHz]
Irr_Offset = 5[ppm]
Tri_Domain = Proton
Tri_Freq = 399.78219838[MHz]
Tri_Offset = 5[ppm]
Blanking = 2[us]
Clipped = FALSE
Scans = 16
Total_Scans = 16
Relaxation_Delay = 5[s]
Recvr_Gain = 46
Temp_Get = 21.8[dC]
X_90_Width = 6.4[us]
X_Acq_Time = 2.18628096[s]
X_Angle = 45[deg]
X_Atn = 2.4[dB]
X_Pulse = 3.2[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Loop = 500
Dante_Presat = FALSE
Decimation_Rate = 0
Initial_Wait = 1[s]
Phase = (0, 90, 270, 180, 180,
Presat_Time = 5[s]
Presat_Time_Flag = FALSE
Relaxation_Delay_Calc = 0[s]
Relaxation_Delay_Temp = 5[s]
Repetition_Time = 7.18628096[s]

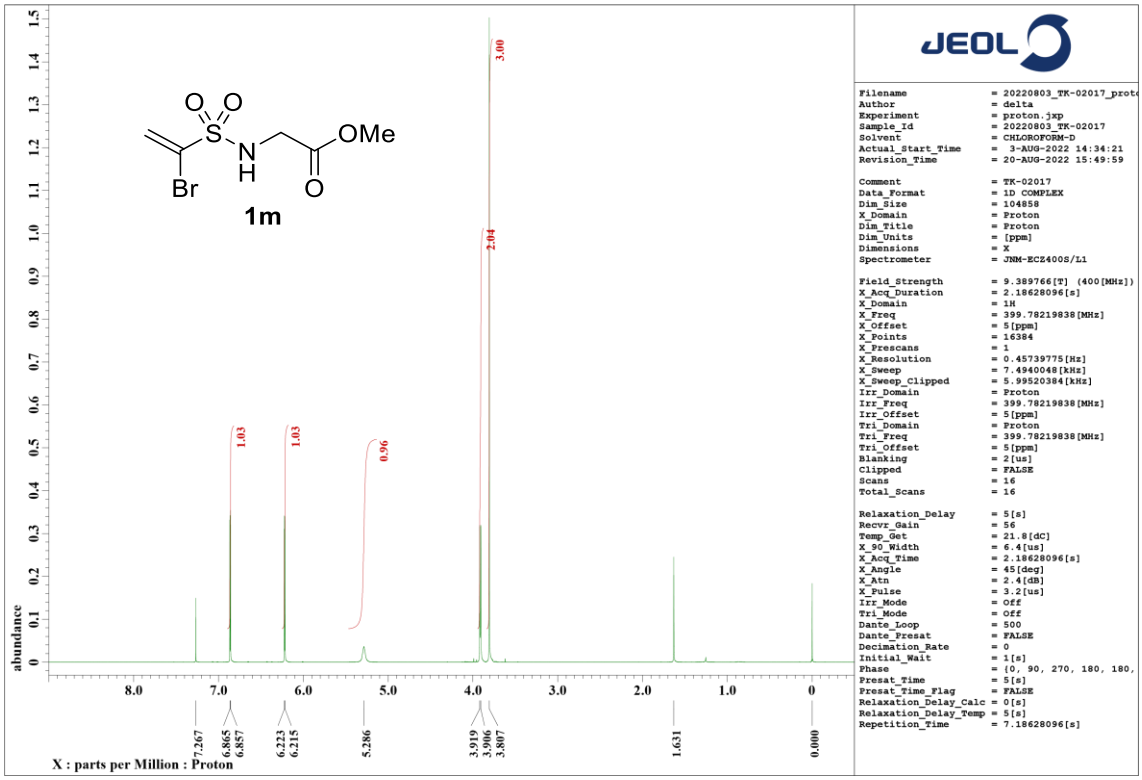

(thousandths)
X : parts per Million : Carbon13
Filename = 20220819_TK-02015_c
Author = delta
Experiment = carbon.jxp
Sample_Id = 20220819_TK-02015
Solvent = CHLOROFORM-D
Actual_Start_Time = 19-AUG-2022 11:15:4
Revision_Time = 20-AUG-2022 15:29:0
Comment = TK-02015
Data_Format = 1D COMPLEX
Dim_Size = 26214
X_Domain = Carbon13
Dim_Title = Carbon13
Dim_Units = [ppm]
Dimensions = X
Spectrometer = JNM-ECZ400S/L1
Field_Strength = 9.389766[T] (400[MH
X_Acq_Duration = 1.03809024[s]
X_Domain = 13C
X_Freq = 100.52530333[MHz]
X_Offset = 100[ppm]
X_Points = 32768
X_Prescans = 4
X_Resolution = 0.96330739[Hz]
X_Sweep = 31.56565657[kHz]
X_Sweep_Clipped = 25.25252525[kHz]
Irr_Domain = Proton
Irr_Freq = 399.78219838[MHz]
Irr_Offset = 5[ppm]
Blanking = 5[us]
Clipped = TRUE
Scans = 4096
Total_Scans = 4096
Relaxation_Delay = 2[s]
Recvr_Gain = 50
Temp_Get = 21.8[dC]
X_90_Width = 10.02[us]
X_Acq_Time = 1.03809024[s]
X_Angle = 30[deg]
X_Atn = 8[dB]
X_Pulse = 3.34[us]
Irr_Atn_Dec = 27.49[dB]
Irr_Atn_Dec_Calc = 27.49[dB]
Irr_Atn_Dec_Default_Calc = 27.49[dB]
Irr_Atn_Noe = 27.49[dB]
Irr_Dec_Bandwidth_Hz = 4.7826087[kHz]
Irr_Dec_Bandwidth_Ppm = 11.96303566[ppm]
Irr_Dec_Freq = 399.78219838[MHz]
Irr_Dec_Merit_Factor = 2.2
Irr_Decoupling = TRUE
Irr_Noe = TRUE
Irr_Noise = WALTZ
Irr_Offset_Default = 5[ppm]
Irr_Pwidth = 0.115[ms]
Irr_Pwidth_Default = 0.115[ms]
Irr_Pwidth_Default_Calc = 0.115[ms]
Irr_Pwidth_Temp1 = 0.115[ms]
Irr_Wurst = FALSE
Decimation_Rate = 0

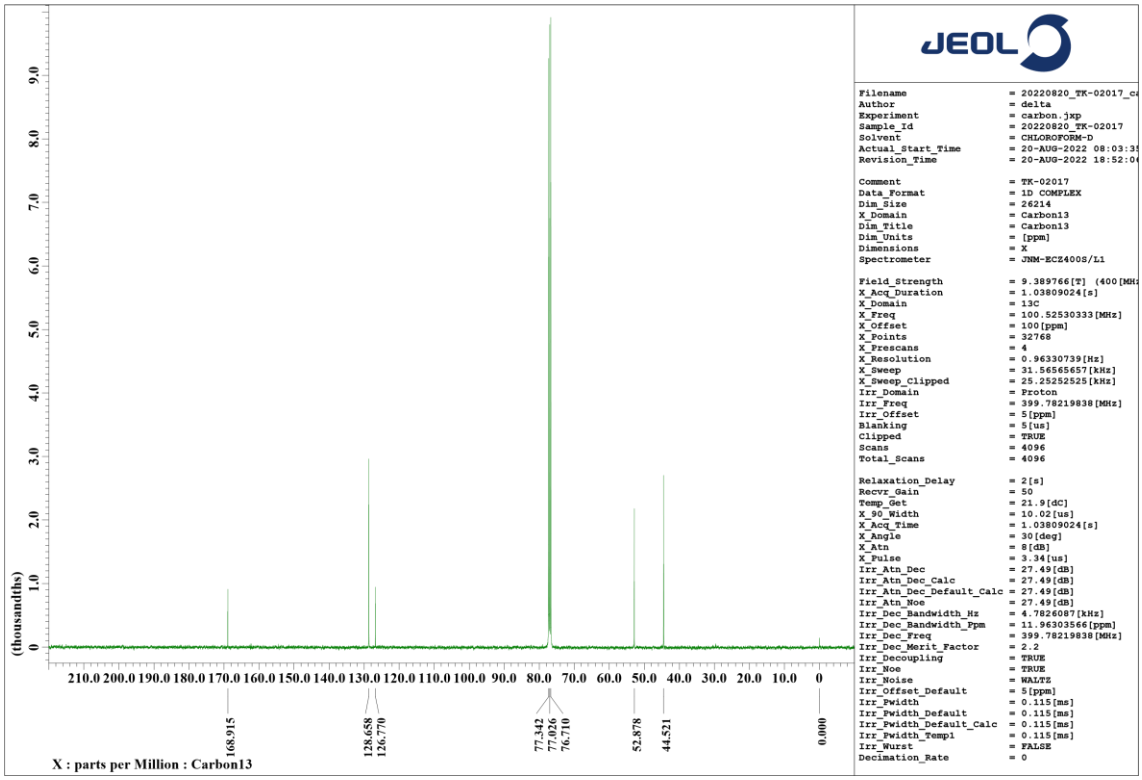

1k
OTBS
Br
9.35
6.00
2.13
2.12
1.00
1.01
0.95
abundance
X : parts per Million : Proton
JEOL

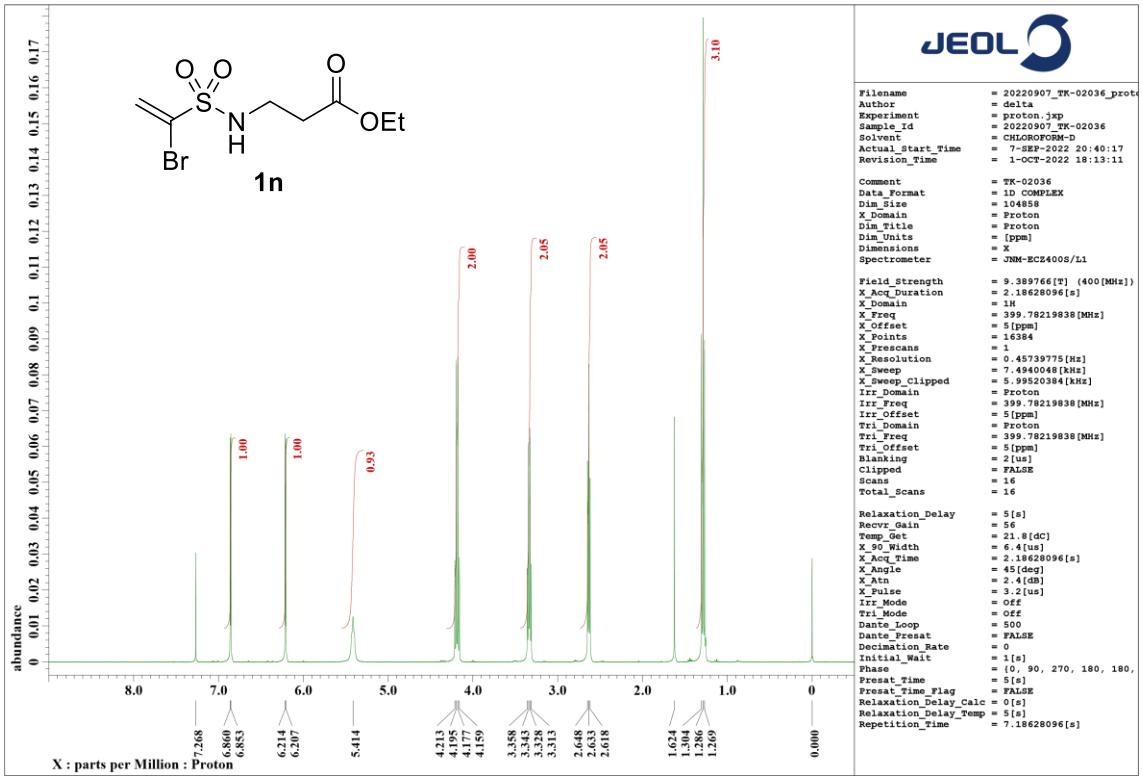

(thousandths)
X : parts per Million : Carbon13
JEOL


O
O
S
N
H
NHBoc
Br
1l
abundance
X : parts per Million : Proton
1.00
1.00
0.82
0.95
1.99
2.01
9.13
7.265
6.843
6.836
6.210
6.203
5.573
4.925
3.342
3.329
3.315
3.300
3.204
3.189
3.175
3.162
1.649
1.449
0.000
Filename = 20220715_TK-02003_prot
Author = delta
Experiment = proton.jxp
Sample_Id = 20220715_TK-02003
Solvent = CHLOROFORM-D
Actual_Start_Time = 15-JUL-2022 17:15:19
Revision_Time = 16-JUL-2022 21:20:40
Comment = TK-02003
Data_Format = 1D COMPLEX
Dim_Size = 104858
X_Domain = Proton
Dim_Title = Proton
Dim_Units = [ppm]
Dimensions = X
Spectrometer = JNM-ECZ400S/L1
Field_Strength = 9.389766[T] (400[MHz])
X_Acq_Duration = 2.18628096[s]
X_Domain = 1H
X_Freq = 399.78219838[MHz]
X_Offset = 5[ppm]
X_Points = 16384
X_Prescans = 1
X_Resolution = 0.45739775[Hz]
X_Sweep = 7.4940048[kHz]
X_Sweep_Clipped = 5.99520384[kHz]
Irr_Domain = Proton
Irr_Freq = 399.78219838[MHz]
Irr_Offset = 5[ppm]
Tri_Domain = Proton
Tri_Freq = 399.78219838[MHz]
Tri_Offset = 5[ppm]
Blanking = 2[us]
Clipped = FALSE
Scans = 16
Total_Scans = 16
Relaxation_Delay = 5[s]
Recvr_Gain = 46
Temp_Get = 23.9[dC]
X_90_Width = 6.2[us]
X_Acq_Time = 2.18628096[s]
X_Angle = 45[deg]
X_Atn = 2.4[dB]
X_Pulse = 3.1[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Loop = 500
Dante_Presat = FALSE
Decimation_Rate = 0
Initial_Wait = 1[s]
Phase = (0, 90, 270, 180, 180,
Presat_Time = 5[s]
Presat_Time_Flag = FALSE
Relaxation_Delay_Calc = 0[s]
Relaxation_Delay_Temp = 5[s]
Repetition_Time = 7.18628096[s]

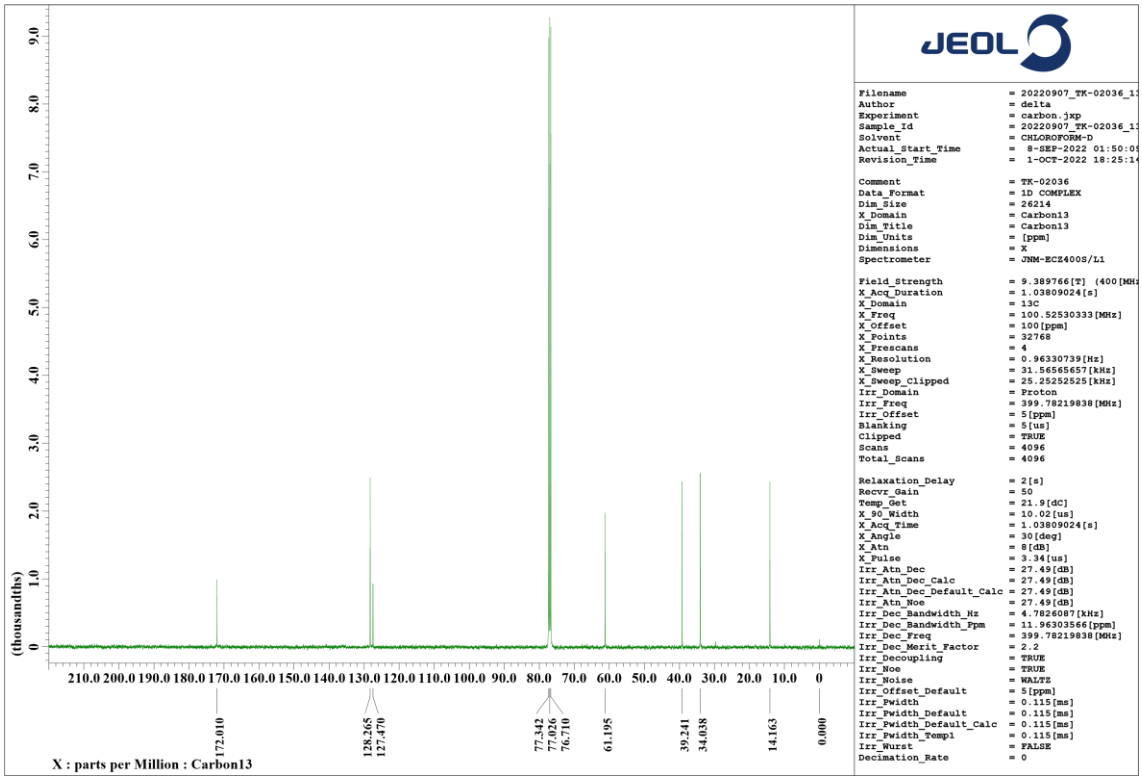

(thousandths)
X : parts per Million : Carbon13
156.774
128.457
127.086
80.237
77.342
77.237
77.026
76.710
44.445
40.228
28.355
0.000
Filename = 20220716_TK-02003_1
Author = delta
Experiment = carbon.jxp
Sample_Id = 20220716_TK-02003_1
Solvent = CHLOROFORM-D
Actual_Start_Time = 19-JUL-2022 07:30:3
Revision_Time = 6-SEP-2024 11:14:0
Comment = TK-02003
Data_Format = 1D COMPLEX
Dim_Size = 26214
X_Domain = Carbon13
Dim_Title = Carbon13
Dim_Units = [ppm]
Dimensions = X
Spectrometer = JNM-ECZ400S/L1
Field_Strength = 9.389766[T] (400[MH
X_Acq_Duration = 1.03809024[s]
X_Domain = 13C
X_Freq = 100.52530333[MHz]
X_Offset = 100[ppm]
X_Points = 32768
X_Prescans = 4
X_Resolution = 0.96330739[Hz]
X_Sweep = 31.56565657[kHz]
X_Sweep_Clipped = 25.25252525[kHz]
Irr_Domain = Proton
Irr_Freq = 399.78219838[MHz]
Irr_Offset = 5[ppm]
Blanking = 5[us]
Clipped = FALSE
Scans = 4096
Total_Scans = 4096
Relaxation_Delay = 2[s]
Recvr_Gain = 50
Temp_Get = 21.6[dC]
X_90_Width = 9.97[us]
X_Acq_Time = 1.03809024[s]
X_Angle = 30[deg]
X_Atn = 8[dB]
X_Pulse = 3.32333333[us]
Irr_Atn_Dec = 27.766[dB]
Irr_Atn_Dec_Calc = 27.766[dB]
Irr_Atn_Dec_Default_Calc = 27.766[dB]
Irr_Atn_Noe = 27.766[dB]
Irr_Dec_Bandwidth_Hz = 4.7826087[kHz]
Irr_Dec_Bandwidth_Ppm = 11.96303566[ppm]
Irr_Dec_Freq = 399.78219838[MHz]
Irr_Dec_Merit_Factor = 2.2
Irr_Decoupling = TRUE
Irr_Noe = TRUE
Irr_Noise = WALTZ
Irr_Offset_Default = 5[ppm]
Irr_Pwidth = 0.115[ms]
Irr_Pwidth_Default = 0.115[ms]
Irr_Pwidth_Default_Calc = 0.115[ms]
Irr_Pwidth_Temp1 = 0.115[ms]
Irr_Wurst = FALSE
Decimation_Rate = 0


1m
abundance
X : parts per Million : Proton
3.00
2.04
1.03
1.03
0.96
7.267
6.865
6.857
6.223
6.215
5.286
3.919
3.906
3.807
1.631
0.000

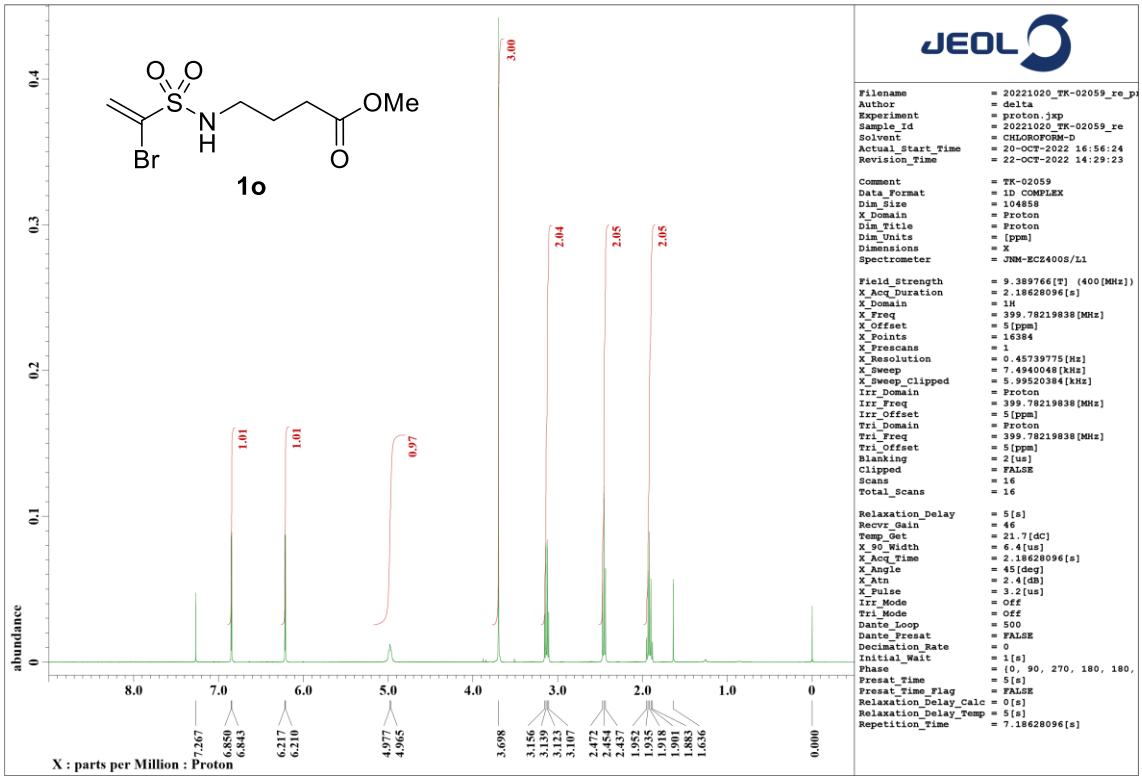

(thousandths)
X : parts per Million : Carbon13
168.915
128.658
126.770
77.342
77.026
76.710
52.878
44.521
0.000

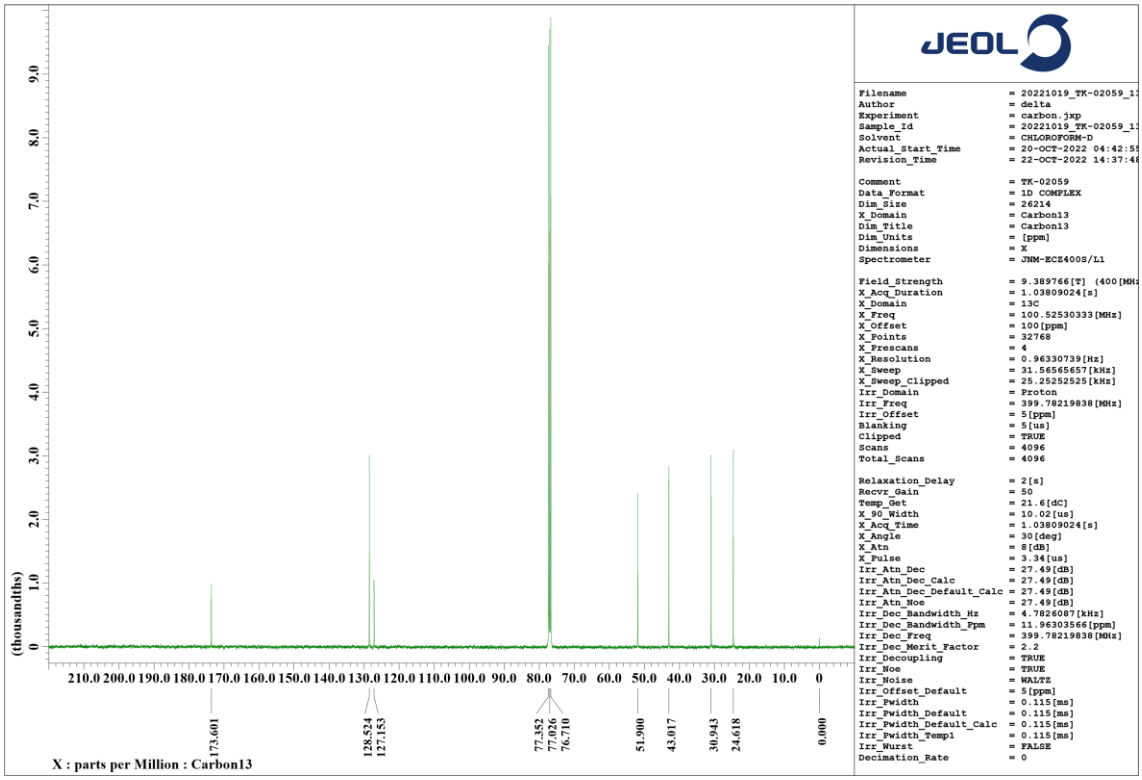


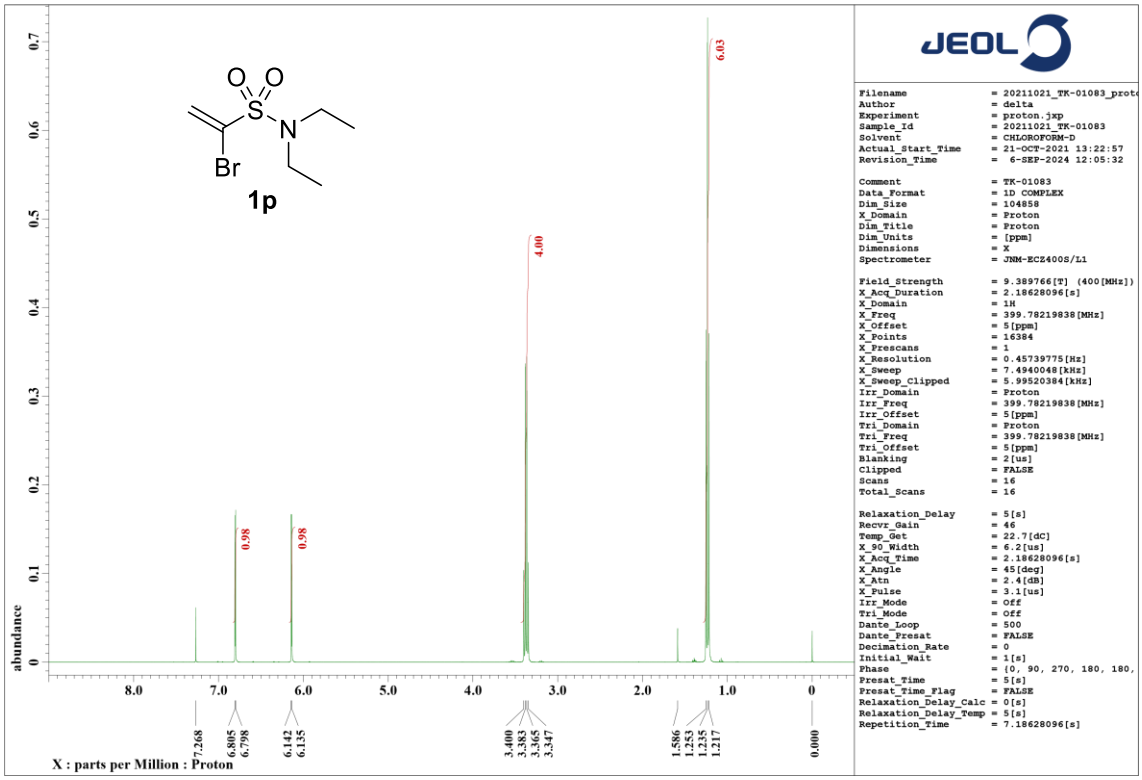

```
Filename                = 20220907_TK-02036_proto
Author                  = delta
Experiment              = proton.jxp
Sample_Id               = 20220907_TK-02036
Solvent                 = CHLOROFORM-D
Actual_Start_Time       =  7-SEP-2022 20:40:17
Revision_Time           =  1-OCT-2022 18:13:11

Comment                 = TK-02036
Data_Format             = 1D COMPLEX
Dim_Size                = 104858
X_Domain                = Proton
Dim_Title               = Proton
Dim_Units               = [ppm]
Dimensions              = X
Spectrometer            = JNM-ECZ400S/L1

Field_Strength          = 9.389766[T] (400[MHz])
X_Acq_Duration          = 2.18628096[s]
X_Domain                = 1H
X_Freq                  = 399.78219838[MHz]
X_Offset                = 5[ppm]
X_Points                = 16384
X_Prescans              = 1
X_Resolution            = 0.45739775[Hz]
X_Sweep                 = 7.4940048[kHz]
X_Sweep_Clipped         = 5.99520384[kHz]
Irr_Domain              = Proton
Irr_Freq                = 399.78219838[MHz]
Irr_Offset              = 5[ppm]
Tri_Domain              = Proton
Tri_Freq                = 399.78219838[MHz]
Tri_Offset              = 5[ppm]
Blanking                = 2[us]
Clipped                 = FALSE
Scans                   = 16
Total_Scans             = 16

Relaxation_Delay        = 5[s]
Recvr_Gain              = 56
Temp_Get                = 21.8[dC]
X_90_Width              = 6.4[us]
X_Acq_Time              = 2.18628096[s]
X_Angle                 = 45[deg]
X_Atn                   = 2.4[dB]
X_Pulse                 = 3.2[us]
Irr_Mode                = Off
Tri_Mode                = Off
Dante_Loop              = 500
Dante_Presat            = FALSE
Decimation_Rate         = 0
Initial_Wait            = 1[s]
Phase                   = (0, 90, 270, 180, 180,
Presat_Time             = 5[s]
Presat_Time_Flag        = FALSE
Relaxation_Delay_Calc   = 0[s]
Relaxation_Delay_Temp   = 5[s]
Repetition_Time         = 7.18628096[s]
```

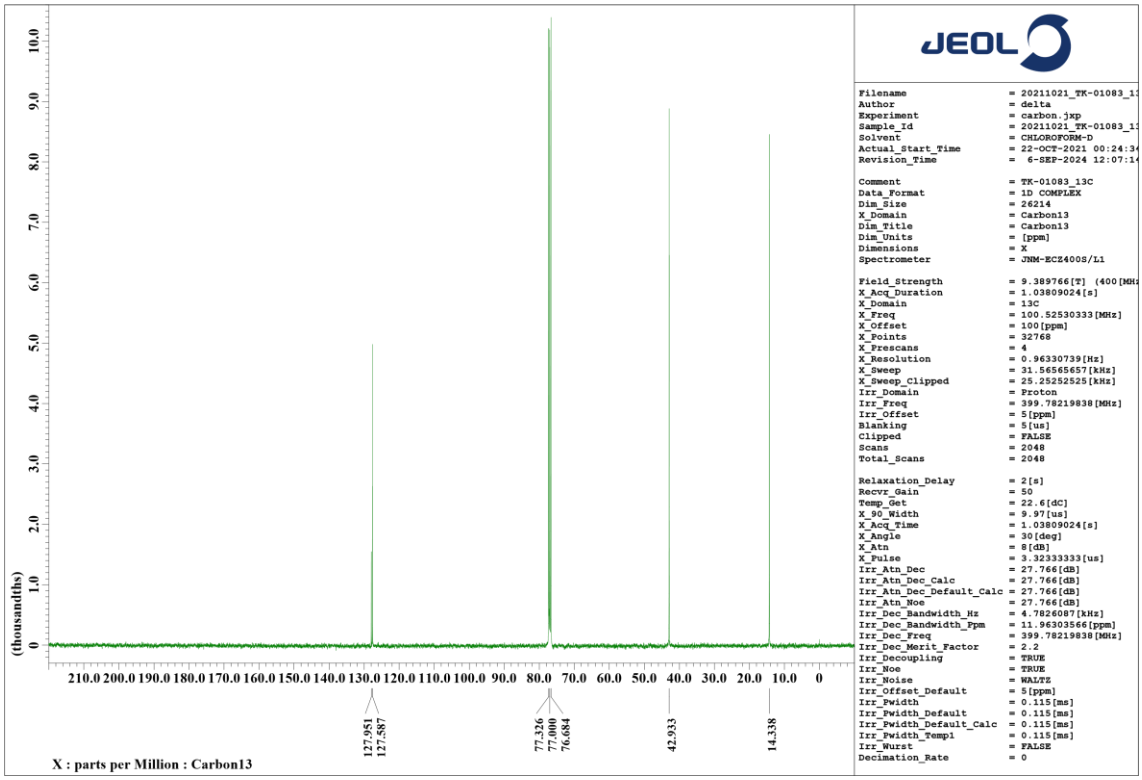


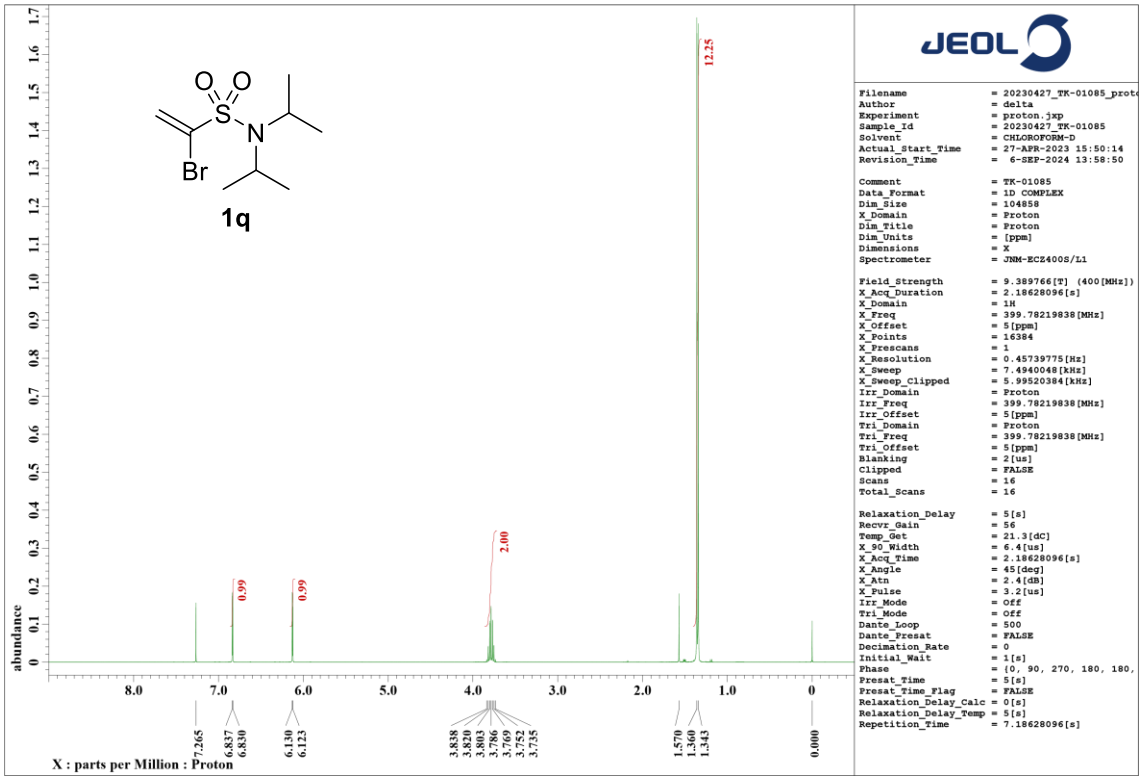

```
Filename                = 20220907_TK-02036_1
Author                  = delta
Experiment              = carbon.jxp
Sample_Id               = 20220907_TK-02036_1
Solvent                 = CHLOROFORM-D
Actual_Start_Time       =  8-SEP-2022 01:50:0
Revision_Time           =  1-OCT-2022 18:25:1

Comment                 = TK-02036
Data_Format             = 1D COMPLEX
Dim_Size                = 26214
X_Domain                = Carbon13
Dim_Title               = Carbon13
Dim_Units               = [ppm]
Dimensions              = X
Spectrometer            = JNM-ECZ400S/L1

Field_Strength          = 9.389766[T] (400[MH
X_Acq_Duration          = 1.03809024[s]
X_Domain                = 13C
X_Freq                  = 100.52530333[MHz]
X_Offset                = 100[ppm]
X_Points                = 32768
X_Prescans              = 4
X_Resolution            = 0.96330739[Hz]
X_Sweep                 = 31.56565657[kHz]
X_Sweep_Clipped         = 25.25252525[kHz]
Irr_Domain              = Proton
Irr_Freq                = 399.78219838[MHz]
Irr_Offset              = 5[ppm]
Blanking                = 5[us]
Clipped                 = TRUE
Scans                   = 4096
Total_Scans             = 4096

Relaxation_Delay        = 2[s]
Recvr_Gain              = 50
Temp_Get                = 21.9[dC]
X_90_Width              = 10.02[us]
X_Acq_Time              = 1.03809024[s]
X_Angle                 = 30[deg]
X_Atn                   = 8[dB]
X_Pulse                 = 3.34[us]
Irr_Atn_Dec             = 27.49[dB]
Irr_Atn_Dec_Calc        = 27.49[dB]
Irr_Atn_Dec_Default_Calc = 27.49[dB]
Irr_Atn_Noe             = 27.49[dB]
Irr_Dec_Bandwidth_Hz    = 4.78260087[kHz]
Irr_Dec_Bandwidth_Ppm   = 11.96303566[ppm]
Irr_Dec_Freq            = 399.78219838[MHz]
Irr_Dec_Merit_Factor    = 2.2
Irr_Decoupling          = TRUE
Irr_Noe                 = TRUE
Irr_Noise               = WALTZ
Irr_Offset_Default      = 5[ppm]
Irr_Pwidth              = 0.115[ms]
Irr_Pwidth_Default      = 0.115[ms]
Irr_Pwidth_Default_Calc = 0.115[ms]
Irr_Pwidth_Temp1        = 0.115[ms]
Irr_Wurst               = FALSE
Decimation_Rate         = 0
```

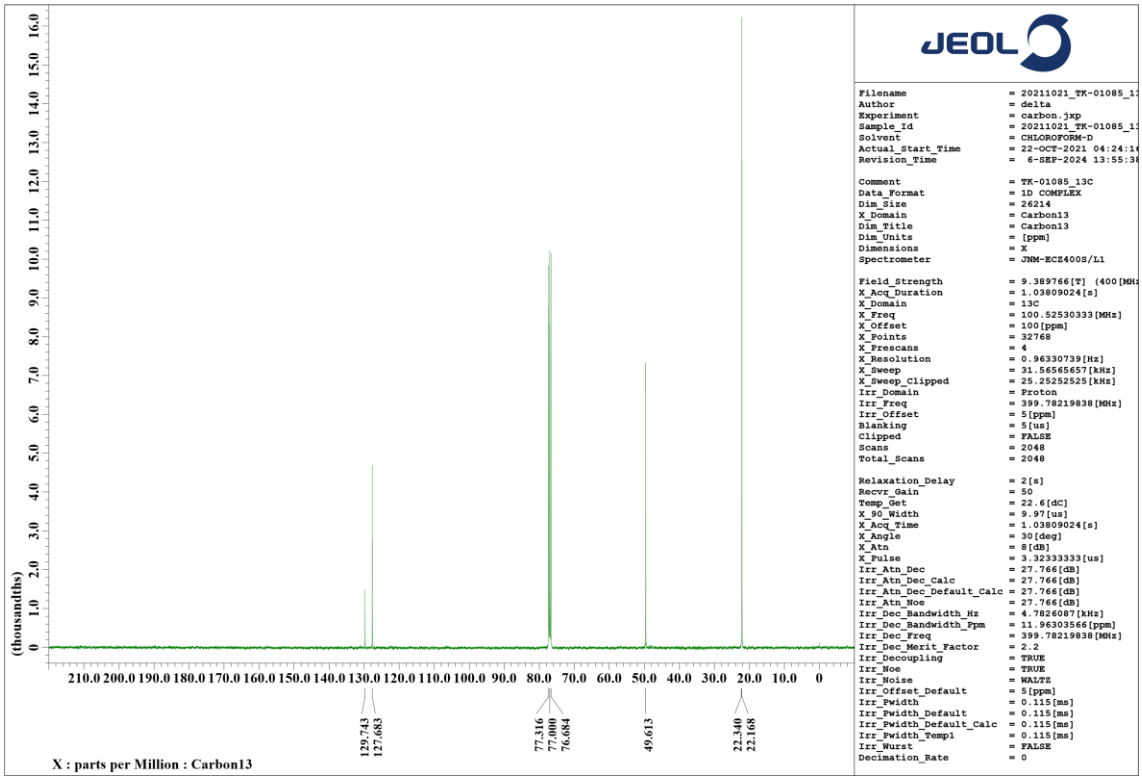

1o
X : parts per Million : Proton
abundance

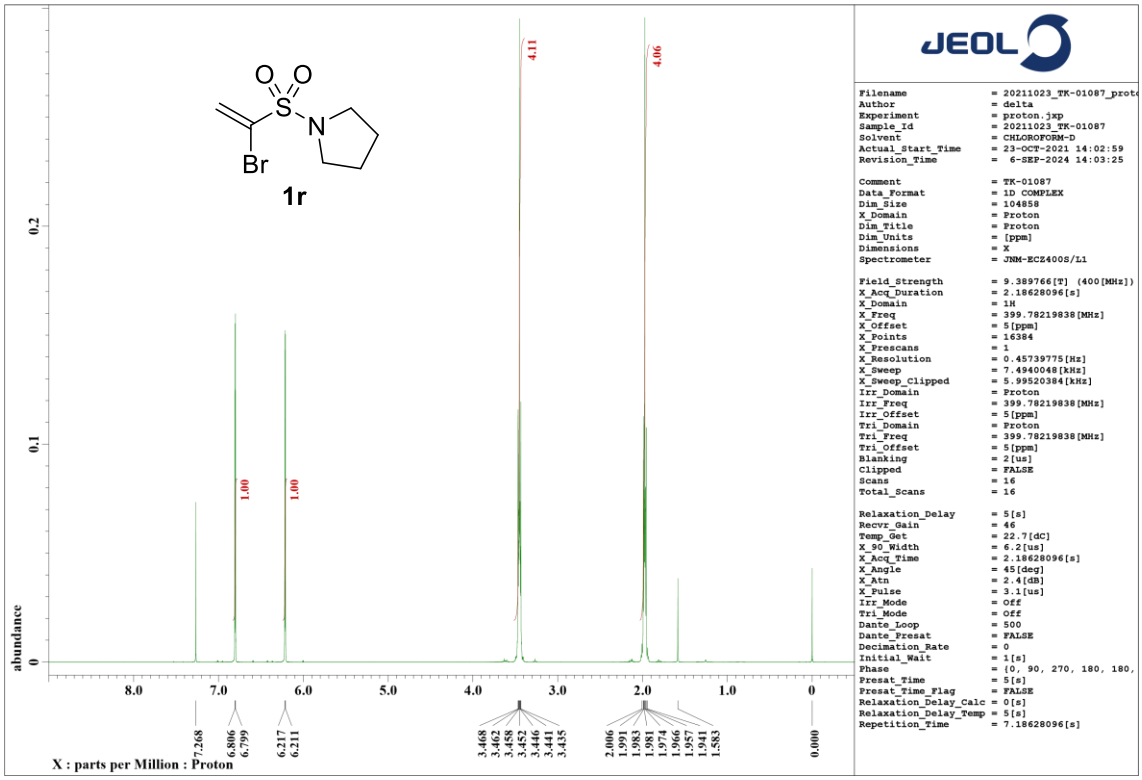

X : parts per Million : Carbon13
(thousandths)


1p
Br
O
O
S
N
6.03
4.00
0.98
0.98
abundance
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
7.268
6.805
6.798
6.142
6.135
3.400
3.383
3.365
3.347
1.586
1.253
1.235
1.217
0.000
X : parts per Million : Proton
JEOL
Filename = 20211021_TK-01083_prot
Author = delta
Experiment = proton.jxp
Sample_Id = 20211021_TK-01083
Solvent = CHLOROFORM-D
Actual_Start_Time = 21-OCT-2021 13:22:57
Revision_Time = 6-SEP-2024 12:05:32
Comment = TK-01083
Data_Format = 1D COMPLEX
Dim_Size = 104858
X_Domain = Proton
Dim_Title = Proton
Dim_Units = [ppm]
Dimensions = X
Spectrometer = JNM-ECZ400S/L1
Field_Strength = 9.389766[T] (400[MHz])
X_Acq_Duration = 2.18628096[s]
X_Domain = 1H
X_Freq = 399.78219838[MHz]
X_Offset = 5[ppm]
X_Points = 16384
X_Prescans = 1
X_Resolution = 0.45739775[Hz]
X_Sweep = 7.4940048[kHz]
X_Sweep_Clipped = 5.99520384[kHz]
Irr_Domain = Proton
Irr_Freq = 399.78219838[MHz]
Irr_Offset = 5[ppm]
Tri_Domain = Proton
Tri_Freq = 399.78219838[MHz]
Tri_Offset = 5[ppm]
Blanking = 2[us]
Clipped = FALSE
Scans = 16
Total_Scans = 16
Relaxation_Delay = 5[s]
Recvr_Gain = 46
Temp_Get = 22.7[dC]
X_90_Width = 6.2[us]
X_Acq_Time = 2.18628096[s]
X_Angle = 45[deg]
X_Atn = 2.4[dB]
X_Pulse = 3.1[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Loop = 500
Dante_Presat = FALSE
Decimation_Rate = 0
Initial_Wait = 1[s]
Phase = (0, 90, 270, 180, 180,
Presat_Time = 5[s]
Presat_Time_Flag = FALSE
Relaxation_Delay_Calc = 0[s]
Relaxation_Delay_Temp = 5[s]
Repetition_Time = 7.18628096[s]

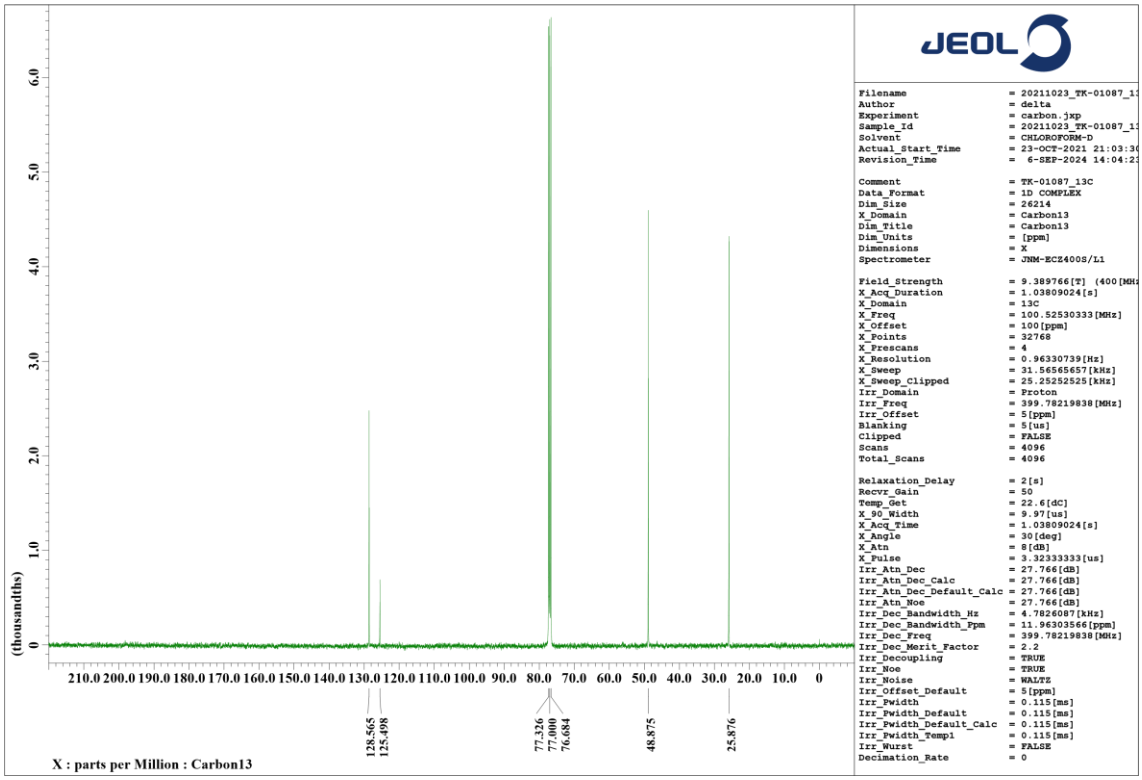

(thousandths)
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
210.0 200.0 190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0
127.951
127.587
77.326
77.000
76.684
42.933
14.338
X : parts per Million : Carbon13
JEOL
Filename = 20211021_TK-01083_1
Author = delta
Experiment = carbon.jxp
Sample_Id = 20211021_TK-01083_1
Solvent = CHLOROFORM-D
Actual_Start_Time = 22-OCT-2021 00:24:3
Revision_Time = 6-SEP-2024 12:07:1
Comment = TK-01083_13C
Data_Format = 1D COMPLEX
Dim_Size = 26214
X_Domain = Carbon13
Dim_Title = Carbon13
Dim_Units = [ppm]
Dimensions = X
Spectrometer = JNM-ECZ400S/L1
Field_Strength = 9.389766[T] (400[MH
X_Acq_Duration = 1.03809024[s]
X_Domain = 13C
X_Freq = 100.52530333[MHz]
X_Offset = 100[ppm]
X_Points = 32768
X_Prescans = 4
X_Resolution = 0.96330739[Hz]
X_Sweep = 31.56565657[kHz]
X_Sweep_Clipped = 25.25252525[kHz]
Irr_Domain = Proton
Irr_Freq = 399.78219838[MHz]
Irr_Offset = 5[ppm]
Blanking = 5[us]
Clipped = FALSE
Scans = 2048
Total_Scans = 2048
Relaxation_Delay = 2[s]
Recvr_Gain = 50
Temp_Get = 22.6[dC]
X_90_Width = 9.97[us]
X_Acq_Time = 1.03809024[s]
X_Angle = 30[deg]
X_Atn = 8[dB]
X_Pulse = 3.32333333[us]
Irr_Atn_Dec = 27.766[dB]
Irr_Atn_Dec_Calc = 27.766[dB]
Irr_Atn_Dec_Default_Calc = 27.766[dB]
Irr_Atn_Noe = 27.766[dB]
Irr_Dec_Bandwidth_Hz = 4.7826087[kHz]
Irr_Dec_Bandwidth_Ppm = 11.96303566[ppm]
Irr_Dec_Freq = 399.78219838[MHz]
Irr_Dec_Merit_Factor = 2.2
Irr_Decoupling = TRUE
Irr_Noe = TRUE
Irr_Noise = WALTZ
Irr_Offset_Default = 5[ppm]
Irr_Pwidth = 0.115[ms]
Irr_Pwidth_Default = 0.115[ms]
Irr_Pwidth_Default_Calc = 0.115[ms]
Irr_Pwidth_Temp1 = 0.115[ms]
Irr_Wurst = FALSE
Decimation_Rate = 0


1q
abundance
X : parts per Million : Proton
12.25
2.00
0.99
0.99
7.265
6.837
6.830
6.130
6.123
3.838
3.820
3.803
3.786
3.769
3.752
3.735
1.570
1.360
1.343
0.000

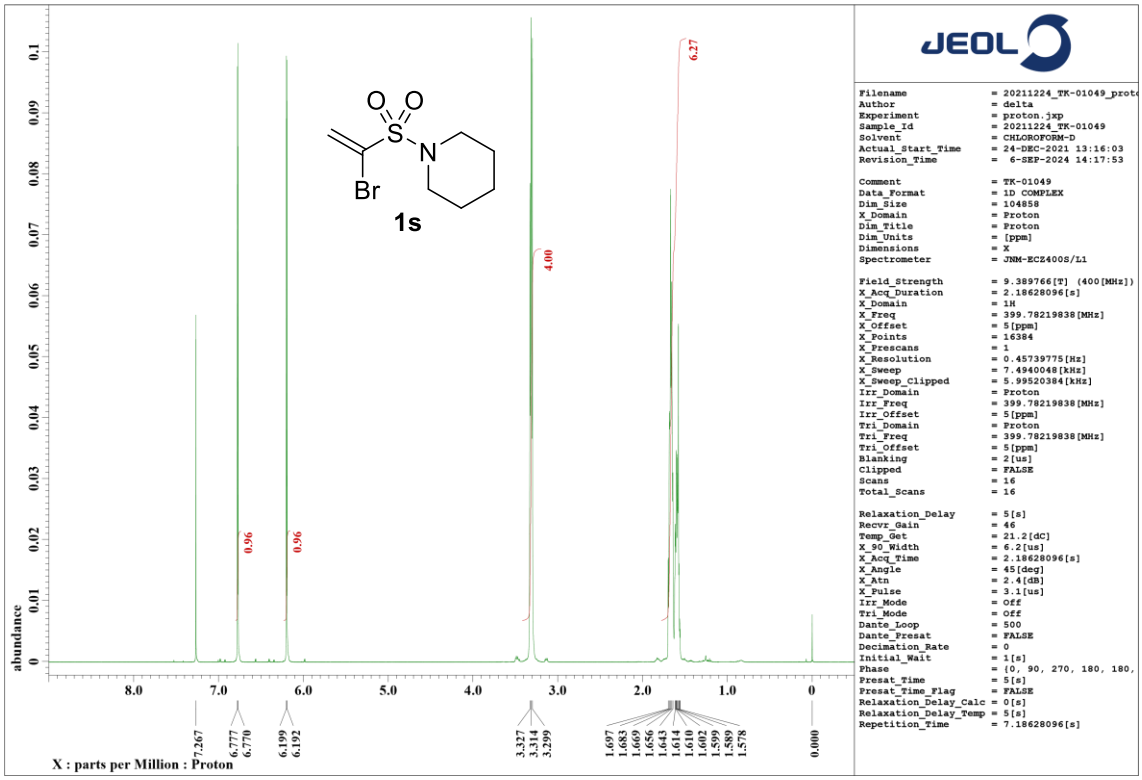

(thousandths)
X : parts per Million : Carbon13
129.743
127.683
77.316
77.000
76.684
49.613
22.340
22.168

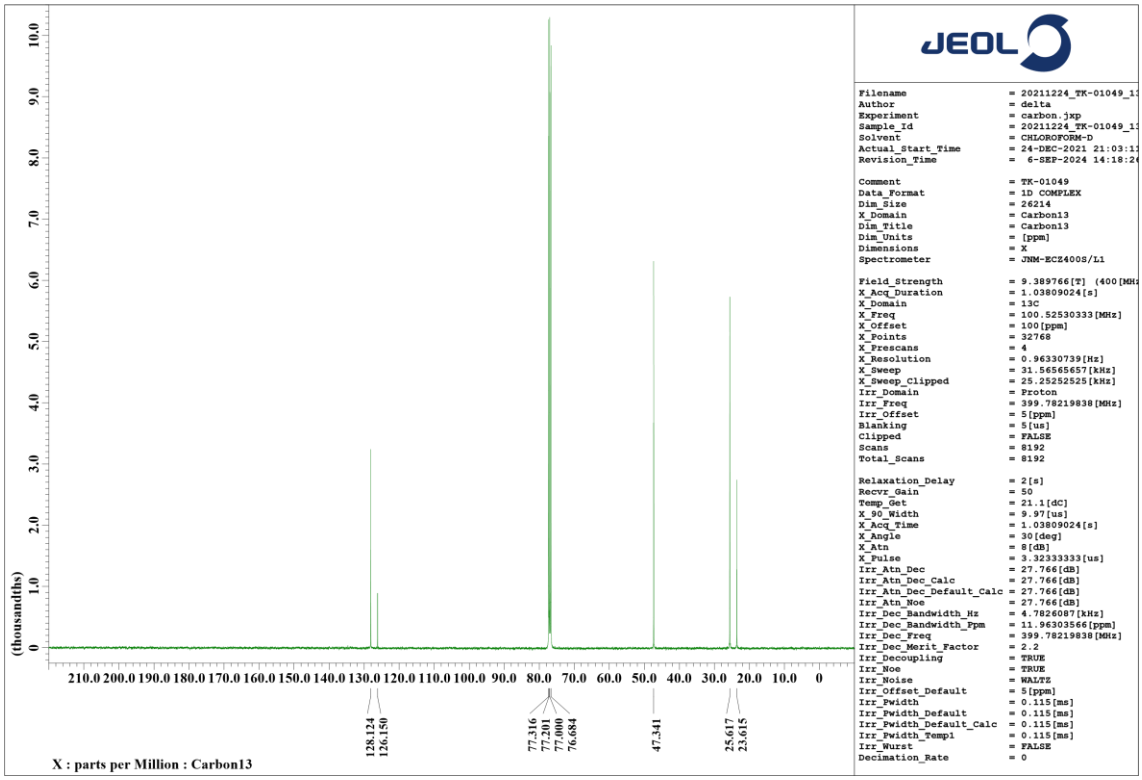


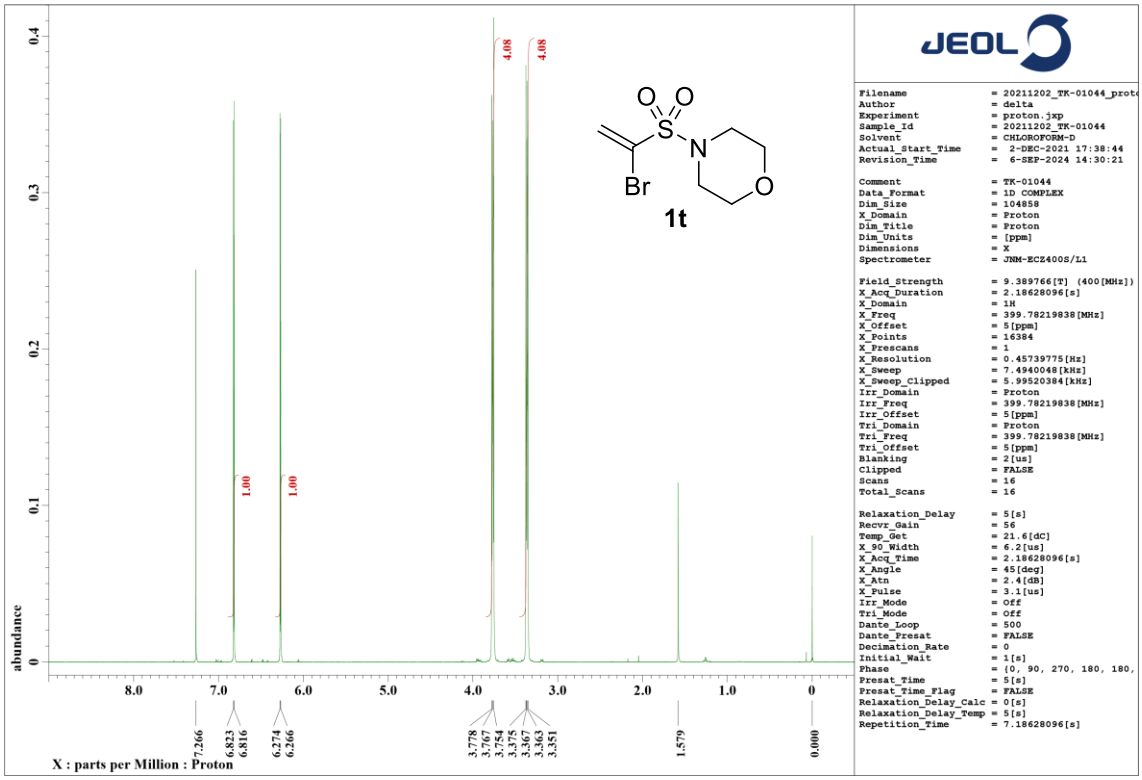

```
Filename                = 20211023_TK-01087_proto
Author                  = delta
Experiment              = proton.jxp
Sample_Id               = 20211023_TK-01087
Solvent                 = CHLOROFORM-D
Actual_Start_Time       = 23-OCT-2021 14:02:59
Revision_Time           =  6-SEP-2024 14:03:25

Comment                 = TK-01087
Data_Format             = 1D COMPLEX
Dim_Size                = 104858
X_Domain                = Proton
Dim_Title               = Proton
Dim_Units               = [ppm]
Dimensions              = X
Spectrometer            = JNM-ECZ400S/L1

Field_Strength          = 9.389766[T] (400[MHz])
X_Acq_Duration          = 2.18628096[s]
X_Domain                = 1H
X_Freq                  = 399.78219838[MHz]
X_Offset                = 5[ppm]
X_Points                = 16384
X_Prescans              = 1
X_Resolution            = 0.45739775[Hz]
X_Sweep                 = 7.4940048[kHz]
X_Sweep_Clipped         = 5.99520384[kHz]
Irr_Domain              = Proton
Irr_Freq                = 399.78219838[MHz]
Irr_Offset              = 5[ppm]
Tri_Domain              = Proton
Tri_Freq                = 399.78219838[MHz]
Tri_Offset              = 5[ppm]
Blanking                = 2[us]
Clipped                 = FALSE
Scans                   = 16
Total_Scans             = 16

Relaxation_Delay        = 5[s]
Recvr_Gain              = 46
Temp_Get                = 22.7[dC]
X_90_Width              = 6.2[us]
X_Acq_Time              = 2.18628096[s]
X_Angle                 = 45[deg]
X_Atn                   = 2.4[dB]
X_Pulse                 = 3.1[us]
Irr_Mode                = Off
Tri_Mode                = Off
Dante_Loop              = 500
Dante_Presat            = FALSE
Decimation_Rate         = 0
Initial_Wait            = 1[s]
Phase                   = (0, 90, 270, 180, 180,
Presat_Time             = 5[s]
Presat_Time_Flag        = FALSE
Relaxation_Delay_Calc   = 0[s]
Relaxation_Delay_Temp   = 5[s]
Repetition_Time         = 7.18628096[s]
```

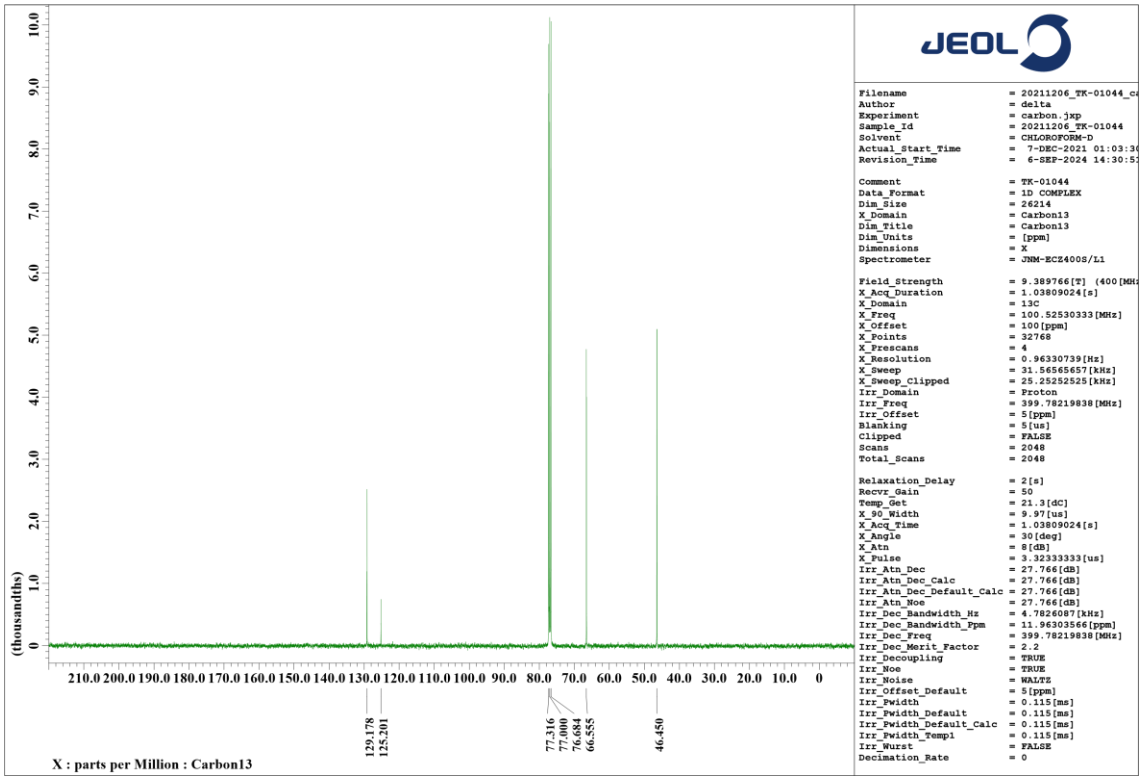


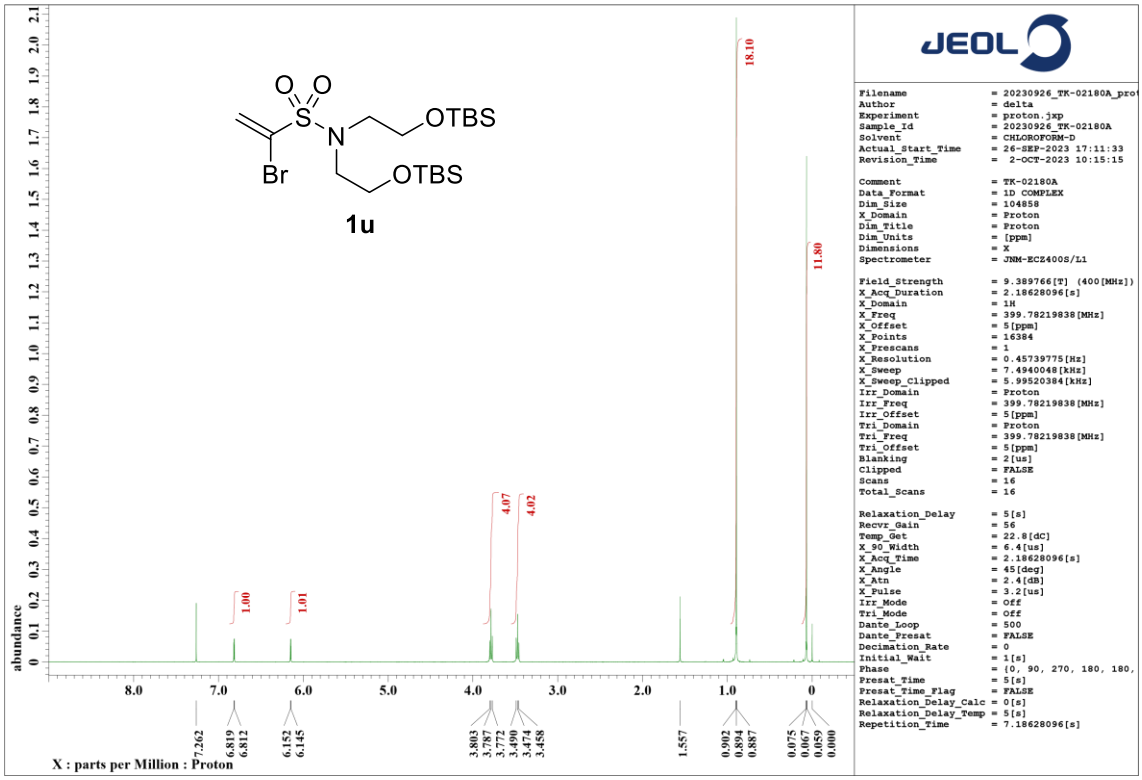

```
Filename                = 20211023_TK-01087_13
Author                  = delta
Experiment              = carbon.jxp
Sample_Id               = 20211023_TK-01087_13
Solvent                 = CHLOROFORM-D
Actual_Start_Time       = 23-OCT-2021 21:03:36
Revision_Time           =  6-SEP-2024 14:04:23

Comment                 = TK-01087_13C
Data_Format             = 1D COMPLEX
Dim_Size                = 26214
X_Domain                = Carbon13
Dim_Title               = Carbon13
Dim_Units               = [ppm]
Dimensions              = X
Spectrometer            = JNM-ECZ400S/L1

Field_Strength          = 9.389766[T] (400[MHz]
X_Acq_Duration          = 1.03809024[s]
X_Domain                = 13C
X_Freq                  = 100.52530333[MHz]
X_Offset                = 100[ppm]
X_Points                = 32768
X_Prescans              = 4
X_Resolution            = 0.96330739[Hz]
X_Sweep                 = 31.56565657[kHz]
X_Sweep_Clipped         = 25.25252525[kHz]
Irr_Domain              = Proton
Irr_Freq                = 399.78219838[MHz]
Irr_Offset              = 5[ppm]
Blanking                = 5[us]
Clipped                 = FALSE
Scans                   = 4096
Total_Scans             = 4096

Relaxation_Delay        = 2[s]
Recvr_Gain              = 50
Temp_Get                = 22.6[dC]
X_90_Width              = 9.97[us]
X_Acq_Time              = 1.03809024[s]
X_Angle                 = 30[deg]
X_Atn                   = 8[dB]
X_Pulse                 = 3.32333333[us]
Irr_Atn_Dec             = 27.766[dB]
Irr_Atn_Dec_Calc        = 27.766[dB]
Irr_Atn_Dec_Default_Calc = 27.766[dB]
Irr_Atn_Noe             = 27.766[dB]
Irr_Dec_Bandwidth_Hz    = 4.7826087[kHz]
Irr_Dec_Bandwidth_Ppm   = 11.96303566[ppm]
Irr_Dec_Freq            = 399.78219838[MHz]
Irr_Dec_Merit_Factor    = 2.2
Irr_Decoupling          = TRUE
Irr_Noe                 = TRUE
Irr_Noise               = WALTZ
Irr_Offset_Default      = 5[ppm]
Irr_Pwidth              = 0.115[ms]
Irr_Pwidth_Default      = 0.115[ms]
Irr_Pwidth_Default_Calc = 0.115[ms]
Irr_Pwidth_Temp1        = 0.115[ms]
Irr_Wurst               = FALSE
Decimation_Rate         = 0
```

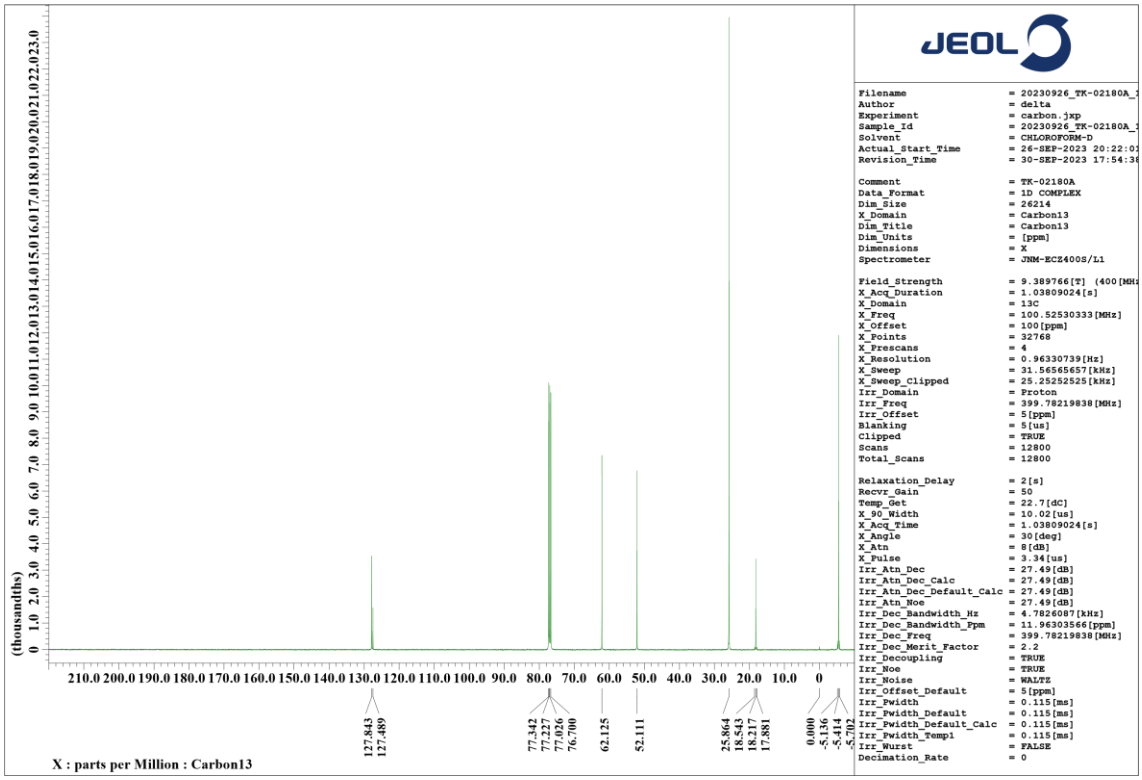

1s
abundance
X : parts per Million : Proton
6.27
4.00
0.96
0.96
7.267
6.777
6.770
6.199
6.192
3.327
3.314
3.299
1.697
1.683
1.669
1.656
1.643
1.614
1.610
1.602
1.589
1.578
0.000
Filename = 20211224_TK-01049_prot
Author = delta
Experiment = proton.jxp
Sample_Id = 20211224_TK-01049
Solvent = CHLOROFORM-D
Actual_Start_Time = 24-DEC-2021 13:16:03
Revision_Time = 6-SEP-2024 14:17:53
Comment = TK-01049
Data_Format = 1D COMPLEX
Dim_Size = 104858
X_Domain = Proton
Dim_Title = Proton
Dim_Units = [ppm]
Dimensions = X
Spectrometer = JNM-ECZ400S/L1
Field_Strength = 9.389766[T] (400[MHz])
X_Acq_Duration = 2.18628096[s]
X_Domain = 1H
X_Freq = 399.78219838[MHz]
X_Offset = 5[ppm]
X_Points = 16384
X_Prescans = 1
X_Resolution = 0.45739775[Hz]
X_Sweep = 7.4940048[kHz]
X_Sweep_Clipped = 5.99520384[kHz]
Irr_Domain = Proton
Irr_Freq = 399.78219838[MHz]
Irr_Offset = 5[ppm]
Tri_Domain = Proton
Tri_Freq = 399.78219838[MHz]
Tri_Offset = 5[ppm]
Blanking = 2[us]
Clipped = FALSE
Scans = 16
Total_Scans = 16
Relaxation_Delay = 5[s]
Recvr_Gain = 46
Temp_Get = 21.2[dC]
X_90_Width = 6.2[us]
X_Acq_Time = 2.18628096[s]
X_Angle = 45[deg]
X_Atn = 2.4[dB]
X_Pulse = 3.1[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Loop = 500
Dante_Presat = FALSE
Decimation_Rate = 0
Initial_Wait = 1[s]
Phase = (0, 90, 270, 180, 180,
Presat_Time = 5[s]
Presat_Time_Flag = FALSE
Relaxation_Delay_Calc = 0[s]
Relaxation_Delay_Temp = 5[s]
Repetition_Time = 7.18628096[s]

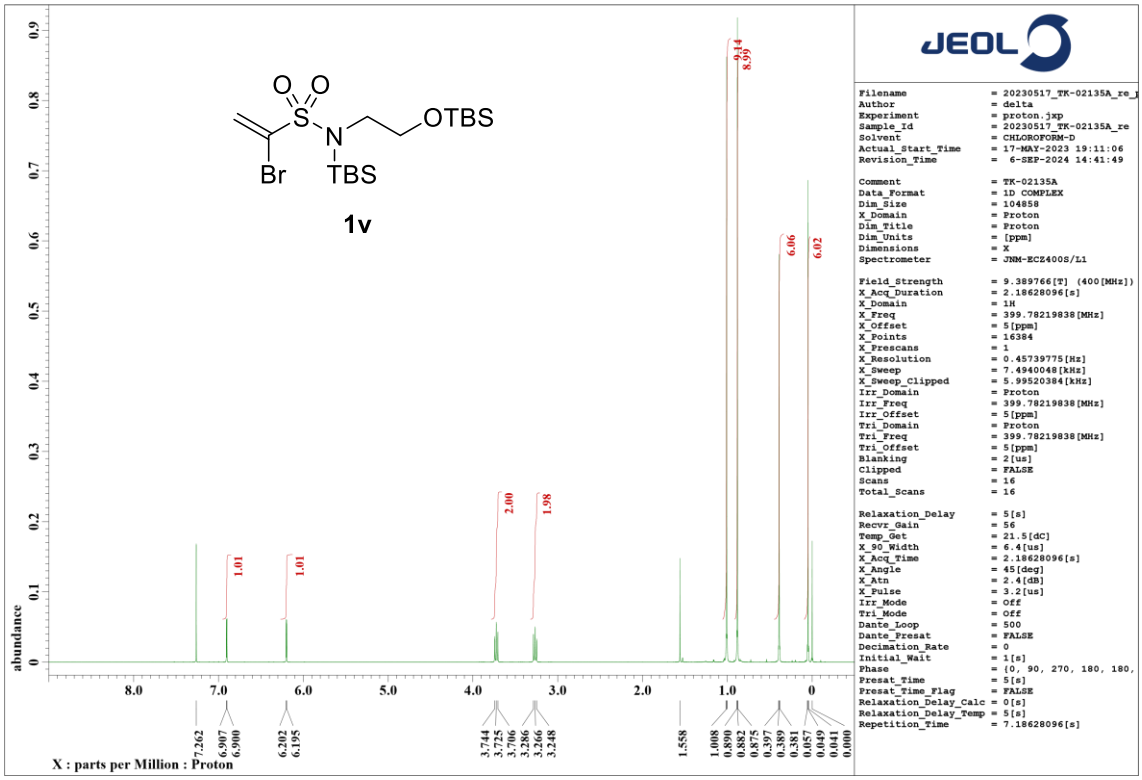

(thousandths)
X : parts per Million : Carbon13
128.124
126.150
77.316
77.201
77.000
76.684
47.341
25.617
23.615
Filename = 20211224_TK-01049_1
Author = delta
Experiment = carbon.jxp
Sample_Id = 20211224_TK-01049_1
Solvent = CHLOROFORM-D
Actual_Start_Time = 24-DEC-2021 21:03:1
Revision_Time = 6-SEP-2024 14:18:2
Comment = TK-01049
Data_Format = 1D COMPLEX
Dim_Size = 26214
X_Domain = Carbon13
Dim_Title = Carbon13
Dim_Units = [ppm]
Dimensions = X
Spectrometer = JNM-ECZ400S/L1
Field_Strength = 9.389766[T] (400[MH
X_Acq_Duration = 1.03809024[s]
X_Domain = 13C
X_Freq = 100.52530333[MHz]
X_Offset = 100[ppm]
X_Points = 32768
X_Prescans = 4
X_Resolution = 0.96330739[Hz]
X_Sweep = 31.56565657[kHz]
X_Sweep_Clipped = 25.25252525[kHz]
Irr_Domain = Proton
Irr_Freq = 399.78219838[MHz]
Irr_Offset = 5[ppm]
Blanking = 5[us]
Clipped = FALSE
Scans = 8192
Total_Scans = 8192
Relaxation_Delay = 2[s]
Recvr_Gain = 50
Temp_Get = 21.1[dC]
X_90_Width = 9.97[us]
X_Acq_Time = 1.03809024[s]
X_Angle = 30[deg]
X_Atn = 8[dB]
X_Pulse = 3.32333333[us]
Irr_Atn_Dec = 27.766[dB]
Irr_Atn_Dec_Calc = 27.766[dB]
Irr_Atn_Dec_Default_Calc = 27.766[dB]
Irr_Atn_Noe = 27.766[dB]
Irr_Dec_Bandwidth_Hz = 4.7826087[kHz]
Irr_Dec_Bandwidth_Ppm = 11.96303566[ppm]
Irr_Dec_Freq = 399.78219838[MHz]
Irr_Dec_Merit_Factor = 2.2
Irr_Decoupling = TRUE
Irr_Noe = TRUE
Irr_Noise = WALTZ
Irr_Offset_Default = 5[ppm]
Irr_Pwidth = 0.115[ms]
Irr_Pwidth_Default = 0.115[ms]
Irr_Pwidth_Default_Calc = 0.115[ms]
Irr_Pwidth_Temp1 = 0.115[ms]
Irr_Wurst = FALSE
Decimation_Rate = 0

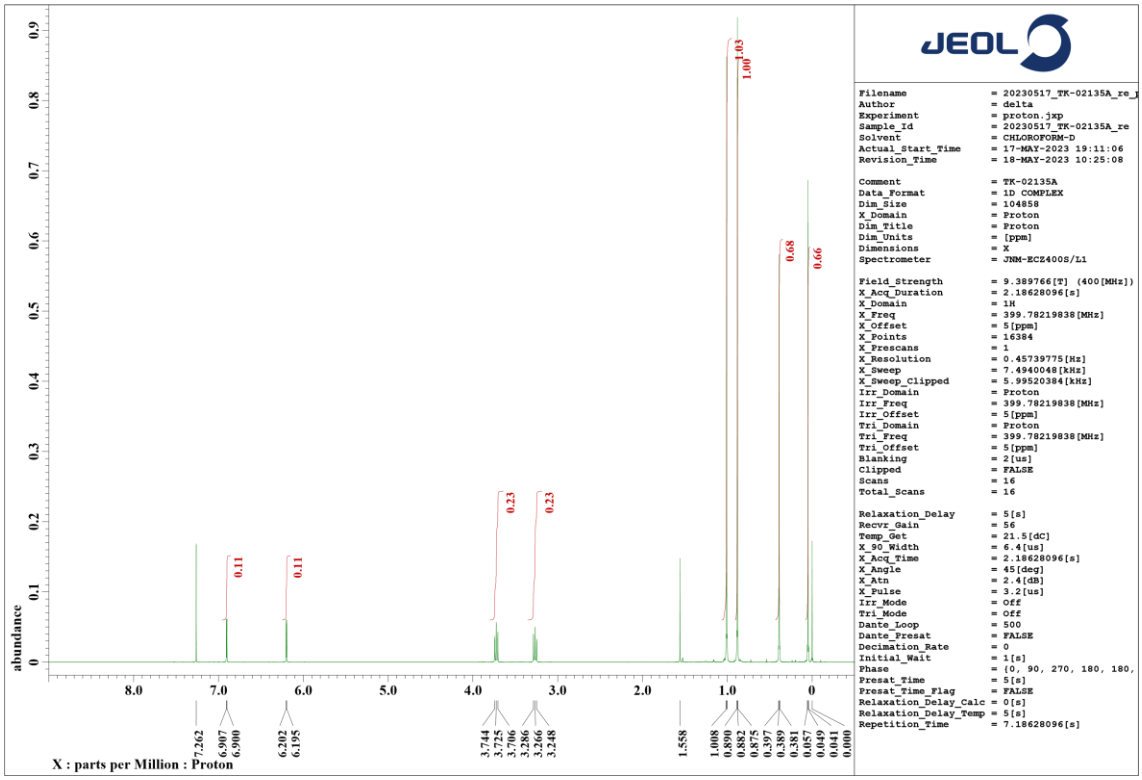

4.08
4.08
1.00
1.00
1t
abundance
X : parts per Million : Proton
7.266
6.823
6.816
6.274
6.266
3.778
3.767
3.754
3.375
3.367
3.363
3.351
1.579
0.000

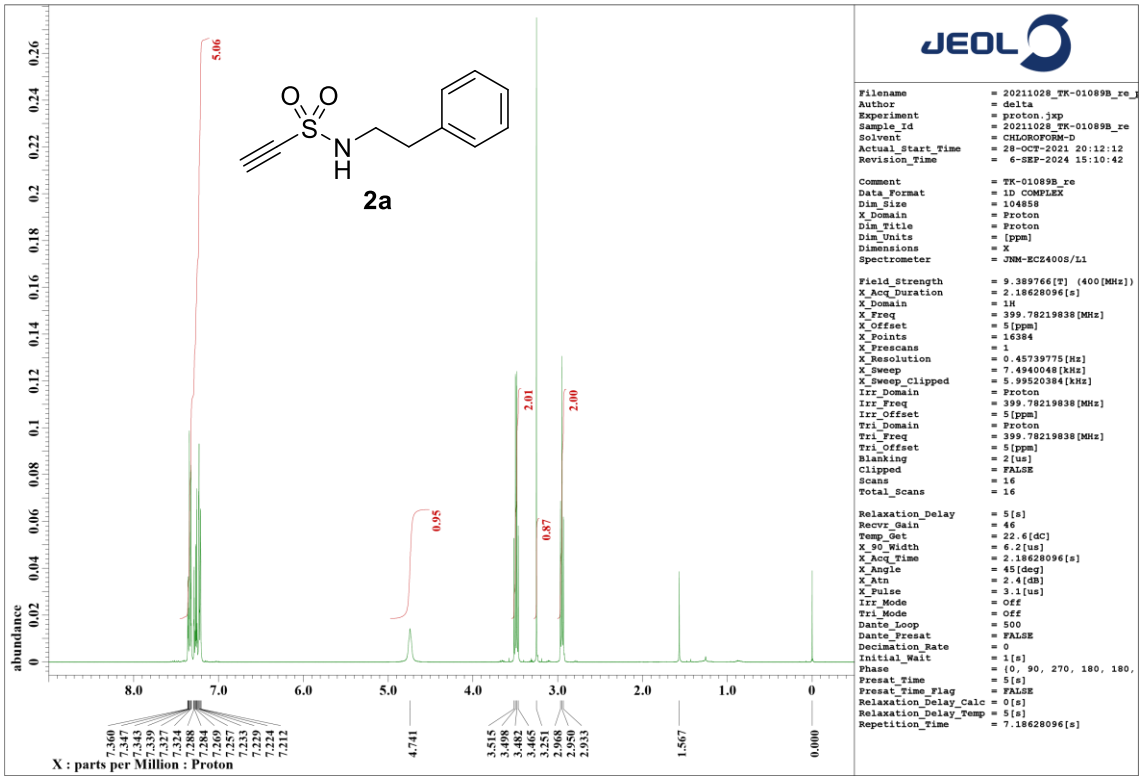

(thousandths)
X : parts per Million : Carbon13
129.178
125.201
77.316
77.000
76.684
66.555
46.450

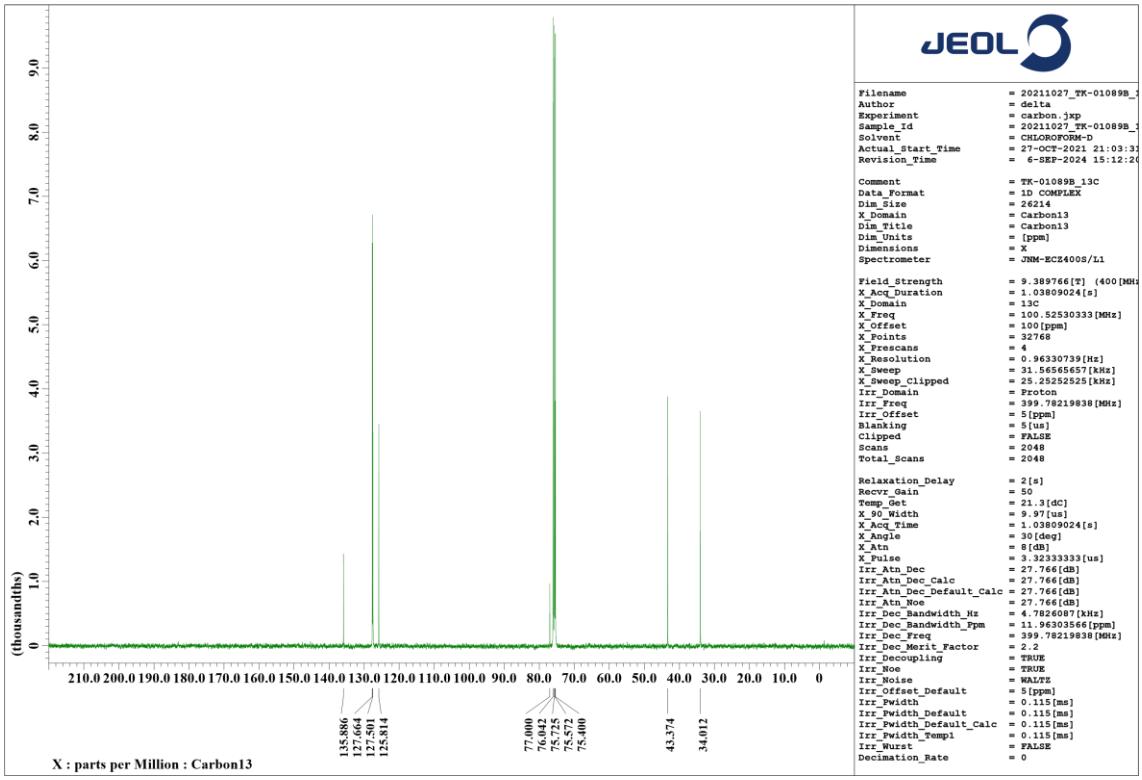

O
O
S
N
OTBS
Br
OTBS
1u
abundance
X : parts per Million : Proton
7.262
6.819
6.812
6.152
6.145
3.803
3.787
3.772
3.490
3.474
3.458
1.557
0.902
0.894
0.887
0.075
0.067
0.059
0.000
1.00
1.01
4.07
4.02
18.10
11.80
JEOL
Filename = 20230926_TK-02180A_pro
Author = delta
Experiment = proton.jxp
Sample_Id = 20230926_TK-02180A
Solvent = CHLOROFORM-D
Actual_Start_Time = 26-SEP-2023 17:11:33
Revision_Time = 2-OCT-2023 10:15:15
Comment = TK-02180A
Data_Format = 1D COMPLEX
Dim_Size = 104858
X_Domain = Proton
Dim_Title = Proton
Dim_Units = [ppm]
Dimensions = X
Spectrometer = JNM-ECZ400S/L1
Field_Strength = 9.389766[T] (400[MHz])
X_Acq_Duration = 2.18628096[s]
X_Domain = 1H
X_Freq = 399.78219838[MHz]
X_Offset = 5[ppm]
X_Points = 16384
X_Prescans = 1
X_Resolution = 0.45739775[Hz]
X_Sweep = 7.4940048[kHz]
X_Sweep_Clipped = 5.99520384[kHz]
Irr_Domain = Proton
Irr_Freq = 399.78219838[MHz]
Irr_Offset = 5[ppm]
Tri_Domain = Proton
Tri_Freq = 399.78219838[MHz]
Tri_Offset = 5[ppm]
Blanking = 2[us]
Clipped = FALSE
Scans = 16
Total_Scans = 16
Relaxation_Delay = 5[s]
Recvr_Gain = 56
Temp_Get = 22.8[dC]
X_90_Width = 6.4[us]
X_Acq_Time = 2.18628096[s]
X_Angle = 45[deg]
X_Atn = 2.4[dB]
X_Pulse = 3.2[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Loop = 500
Dante_Presat = FALSE
Decimation_Rate = 0
Initial_Wait = 1[s]
Phase = (0, 90, 270, 180, 180,
Presat_Time = 5[s]
Presat_Time_Flag = FALSE
Relaxation_Delay_Calc = 0[s]
Relaxation_Delay_Temp = 5[s]
Repetition_Time = 7.18628096[s]

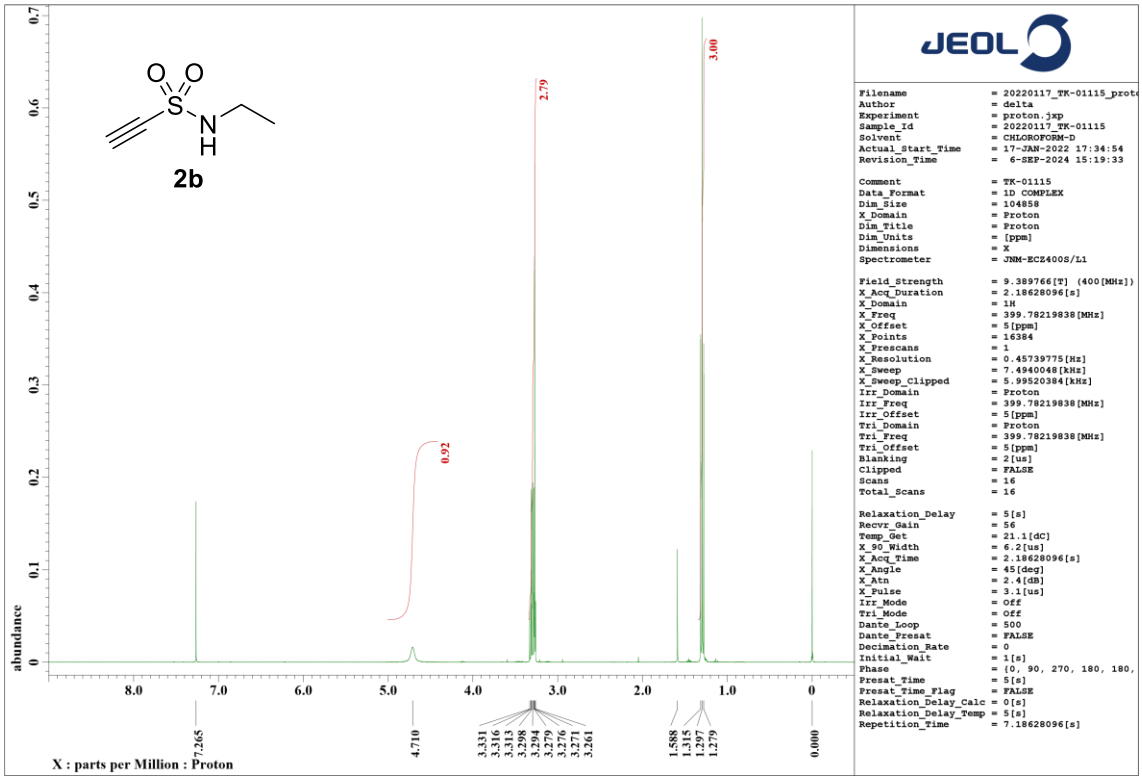

(thousandths)
X : parts per Million : Carbon13
127.843
127.489
77.342
77.227
77.026
76.700
62.125
52.111
25.864
18.543
18.217
17.881
0.000
-5.136
-5.414
-5.702
JEOL
Filename = 20230926_TK-02180A_1
Author = delta
Experiment = carbon.jxp
Sample_Id = 20230926_TK-02180A_1
Solvent = CHLOROFORM-D
Actual_Start_Time = 26-SEP-2023 20:22:01
Revision_Time = 30-SEP-2023 17:54:36
Comment = TK-02180A
Data_Format = 1D COMPLEX
Dim_Size = 26214
X_Domain = Carbon13
Dim_Title = Carbon13
Dim_Units = [ppm]
Dimensions = X
Spectrometer = JNM-ECZ400S/L1
Field_Strength = 9.389766[T] (400[MHz
X_Acq_Duration = 1.03809024[s]
X_Domain = 13C
X_Freq = 100.52530333[MHz]
X_Offset = 100[ppm]
X_Points = 32768
X_Prescans = 4
X_Resolution = 0.96330739[Hz]
X_Sweep = 31.56565657[kHz]
X_Sweep_Clipped = 25.25252525[kHz]
Irr_Domain = Proton
Irr_Freq = 399.78219838[MHz]
Irr_Offset = 5[ppm]
Blanking = 5[us]
Clipped = TRUE
Scans = 12800
Total_Scans = 12800
Relaxation_Delay = 2[s]
Recvr_Gain = 50
Temp_Get = 22.7[dC]
X_90_Width = 10.02[us]
X_Acq_Time = 1.03809024[s]
X_Angle = 30[deg]
X_Atn = 8[dB]
X_Pulse = 3.34[us]
Irr_Atn_Dec = 27.49[dB]
Irr_Atn_Dec_Calc = 27.49[dB]
Irr_Atn_Dec_Default_Calc = 27.49[dB]
Irr_Atn_Noe = 27.49[dB]
Irr_Dec_Bandwidth_Hz = 4.78260587[kHz]
Irr_Dec_Bandwidth_Ppm = 11.96303566[ppm]
Irr_Dec_Freq = 399.78219838[MHz]
Irr_Dec_Merit_Factor = 2.2
Irr_Decoupling = TRUE
Irr_Noe = TRUE
Irr_Noise = WALTZ
Irr_Offset_Default = 5[ppm]
Irr_Pwidth = 0.115[ms]
Irr_Pwidth_Default = 0.115[ms]
Irr_Pwidth_Default_Calc = 0.115[ms]
Irr_Pwidth_Temp1 = 0.115[ms]
Irr_Wurst = FALSE
Decimation_Rate = 0

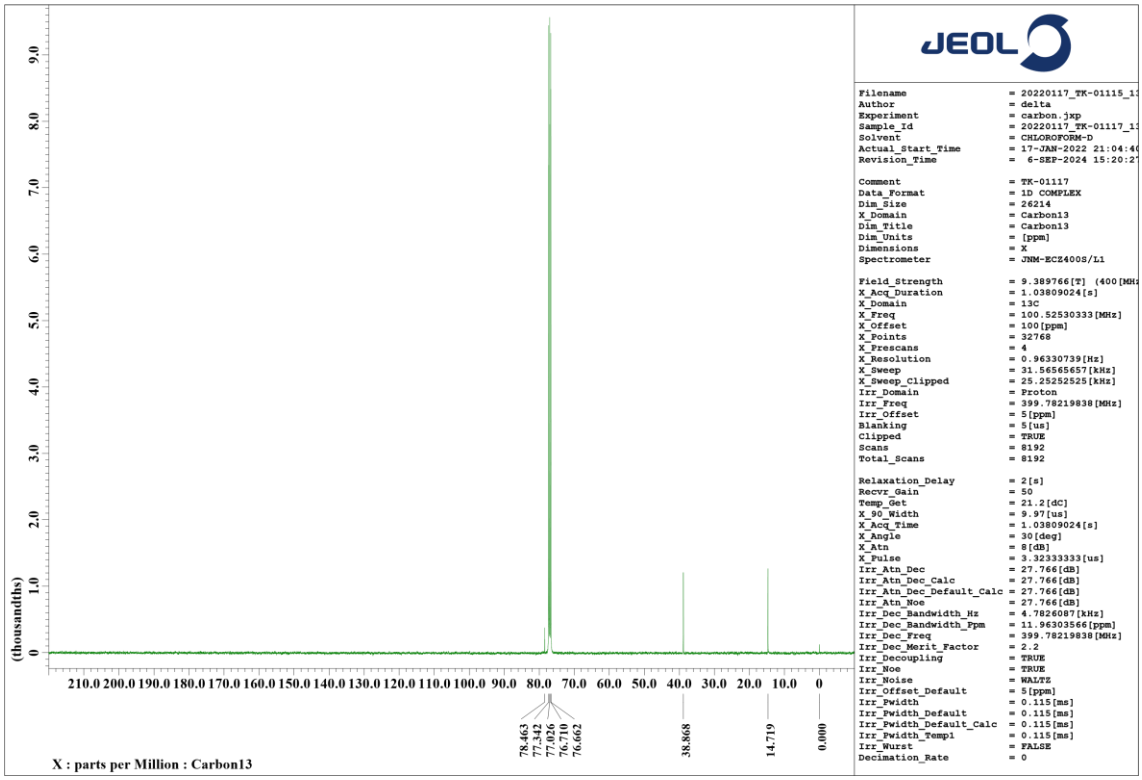

O
O
S
N
OTBS
Br
TBS
1v
abundance
X : parts per Million : Proton
JEOL
Filename = 20230517_TK-02135A_re_1
Author = delta
Experiment = proton.jxp
Sample_Id = 20230517_TK-02135A_re
Solvent = CHLOROFORM-D
Actual_Start_Time = 17-MAY-2023 19:11:06
Revision_Time = 6-SEP-2024 14:41:49
Comment = TK-02135A
Data_Format = 1D COMPLEX
Dim_Size = 104858
X_Domain = Proton
Dim_Title = Proton
Dim_Units = [ppm]
Dimensions = X
Spectrometer = JNM-ECZ400S/L1
Field_Strength = 9.389766[T] (400[MHz])
X_Acq_Duration = 2.18628096[s]
X_Domain = 1H
X_Freq = 399.78219838[MHz]
X_Offset = 5[ppm]
X_Points = 16384
X_Prescans = 1
X_Resolution = 0.45739775[Hz]
X_Sweep = 7.4940048[kHz]
X_Sweep_Clipped = 5.99520384[kHz]
Irr_Domain = Proton
Irr_Freq = 399.78219838[MHz]
Irr_Offset = 5[ppm]
Tri_Domain = Proton
Tri_Freq = 399.78219838[MHz]
Tri_Offset = 5[ppm]
Blanking = 2[us]
Clipped = FALSE
Scans = 16
Total_Scans = 16
Relaxation_Delay = 5[s]
Recvr_Gain = 56
Temp_Get = 21.5[dC]
X_90_Width = 6.4[us]
X_Acq_Time = 2.18628096[s]
X_Angle = 45[deg]
X_Atn = 2.4[dB]
X_Pulse = 3.2[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Loop = 500
Dante_Presat = FALSE
Decimation_Rate = 0
Initial_Wait = 1[s]
Phase = {0, 90, 270, 180, 180,
Presat_Time = 5[s]
Presat_Time_Flag = FALSE
Relaxation_Delay_Calc = 0[s]
Relaxation_Delay_Temp = 5[s]
Repetition_Time = 7.18628096[s]

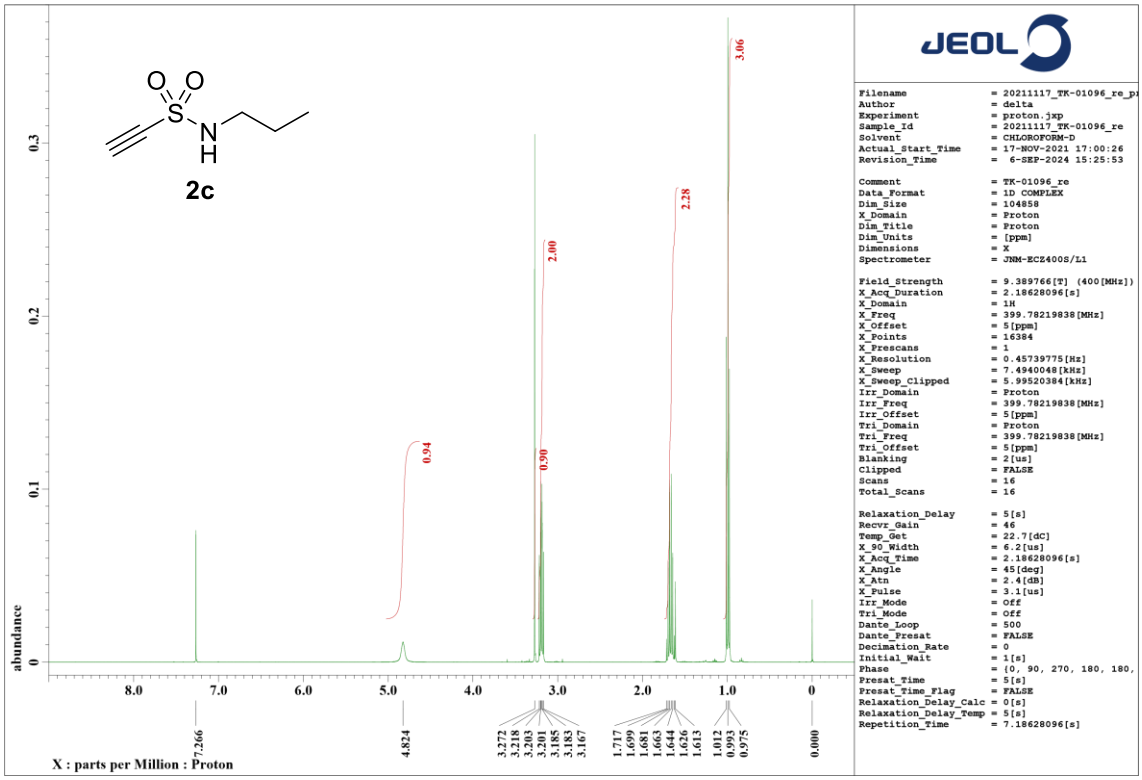

abundance
X : parts per Million : Proton
JEOL
Filename = 20230517_TK-02135A_re_1
Author = delta
Experiment = proton.jxp
Sample_Id = 20230517_TK-02135A_re
Solvent = CHLOROFORM-D
Actual_Start_Time = 17-MAY-2023 19:11:06
Revision_Time = 18-MAY-2023 10:25:08
Comment = TK-02135A
Data_Format = 1D COMPLEX
Dim_Size = 104858
X_Domain = Proton
Dim_Title = Proton
Dim_Units = [ppm]
Dimensions = X
Spectrometer = JNM-ECZ400S/L1
Field_Strength = 9.389766[T] (400[MHz])
X_Acq_Duration = 2.18628096[s]
X_Domain = 1H
X_Freq = 399.78219838[MHz]
X_Offset = 5[ppm]
X_Points = 16384
X_Prescans = 1
X_Resolution = 0.45739775[Hz]
X_Sweep = 7.4940048[kHz]
X_Sweep_Clipped = 5.99520384[kHz]
Irr_Domain = Proton
Irr_Freq = 399.78219838[MHz]
Irr_Offset = 5[ppm]
Tri_Domain = Proton
Tri_Freq = 399.78219838[MHz]
Tri_Offset = 5[ppm]
Blanking = 2[us]
Clipped = FALSE
Scans = 16
Total_Scans = 16
Relaxation_Delay = 5[s]
Recvr_Gain = 56
Temp_Get = 21.5[dC]
X_90_Width = 6.4[us]
X_Acq_Time = 2.18628096[s]
X_Angle = 45[deg]
X_Atn = 2.4[dB]
X_Pulse = 3.2[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Loop = 500
Dante_Presat = FALSE
Decimation_Rate = 0
Initial_Wait = 1[s]
Phase = {0, 90, 270, 180, 180,
Presat_Time = 5[s]
Presat_Time_Flag = FALSE
Relaxation_Delay_Calc = 0[s]
Relaxation_Delay_Temp = 5[s]
Repetition_Time = 7.18628096[s]

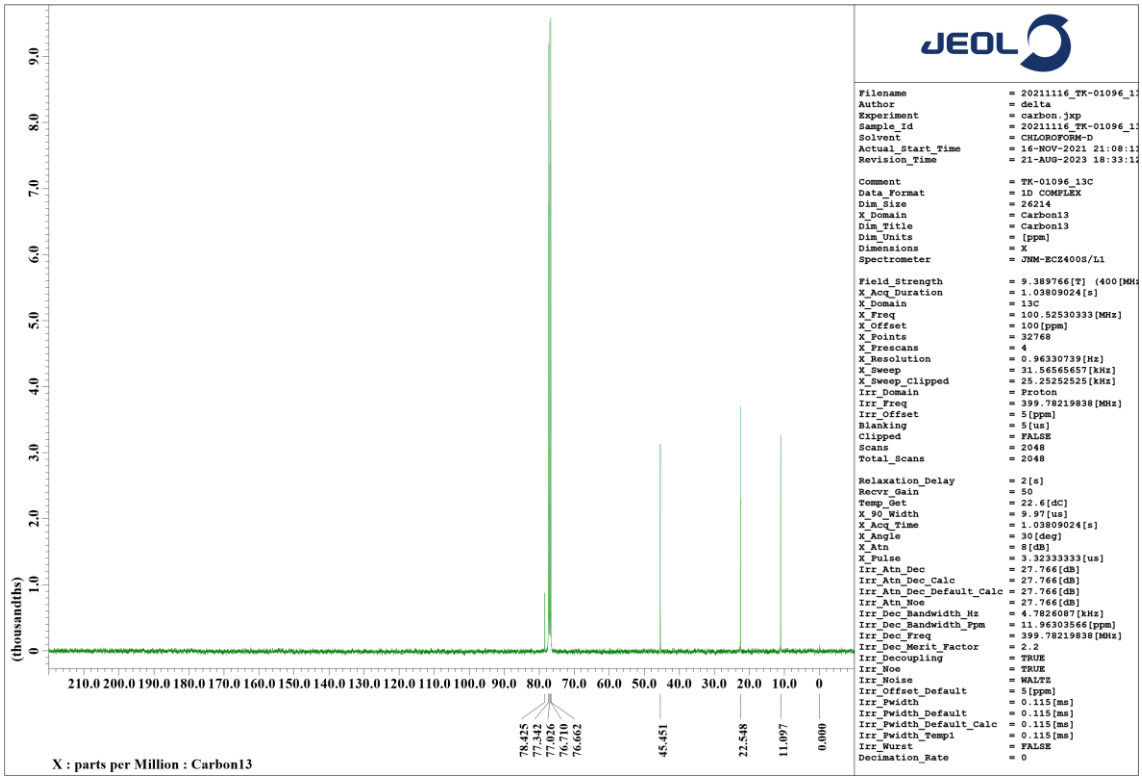

2a
5.06
2.01
2.00
0.95
0.87
abundance
X : parts per Million : Proton
Filename = 20211028_TK-01089B_re_1
Author = delta
Experiment = proton.jxp
Sample_Id = 20211028_TK-01089B_re
Solvent = CHLOROFORM-D
Actual_Start_Time = 28-OCT-2021 20:12:12
Revision_Time = 6-SEP-2024 15:10:42
Comment = TK-01089B_re
Data_Format = 1D COMPLEX
Dim_Size = 104858
X_Domain = Proton
Dim_Title = Proton
Dim_Units = [ppm]
Dimensions = X
Spectrometer = JNM-ECZ400S/L1
Field_Strength = 9.389766[T] (400[MHz])
X_Acq_Duration = 2.18628096[s]
X_Domain = 1H
X_Freq = 399.78219838[MHz]
X_Offset = 5[ppm]
X_Points = 16384
X_Prescans = 1
X_Resolution = 0.45739775[Hz]
X_Sweep = 7.4940048[kHz]
X_Sweep_Clipped = 5.99520384[kHz]
Irr_Domain = Proton
Irr_Freq = 399.78219838[MHz]
Irr_Offset = 5[ppm]
Tri_Domain = Proton
Tri_Freq = 399.78219838[MHz]
Tri_Offset = 5[ppm]
Blanking = 2[us]
Clipped = FALSE
Scans = 16
Total_Scans = 16
Relaxation_Delay = 5[s]
Recvr_Gain = 46
Temp_Get = 22.6[dC]
X_90_Width = 6.2[us]
X_Acq_Time = 2.18628096[s]
X_Angle = 45[deg]
X_Atn = 2.4[dB]
X_Pulse = 3.1[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Loop = 500
Dante_Presat = FALSE
Decimation_Rate = 0
Initial_Wait = 1[s]
Phase = (0, 90, 270, 180, 180,
Presat_Time = 5[s]
Presat_Time_Flag = FALSE
Relaxation_Delay_Calc = 0[s]
Relaxation_Delay_Temp = 5[s]
Repetition_Time = 7.18628096[s]

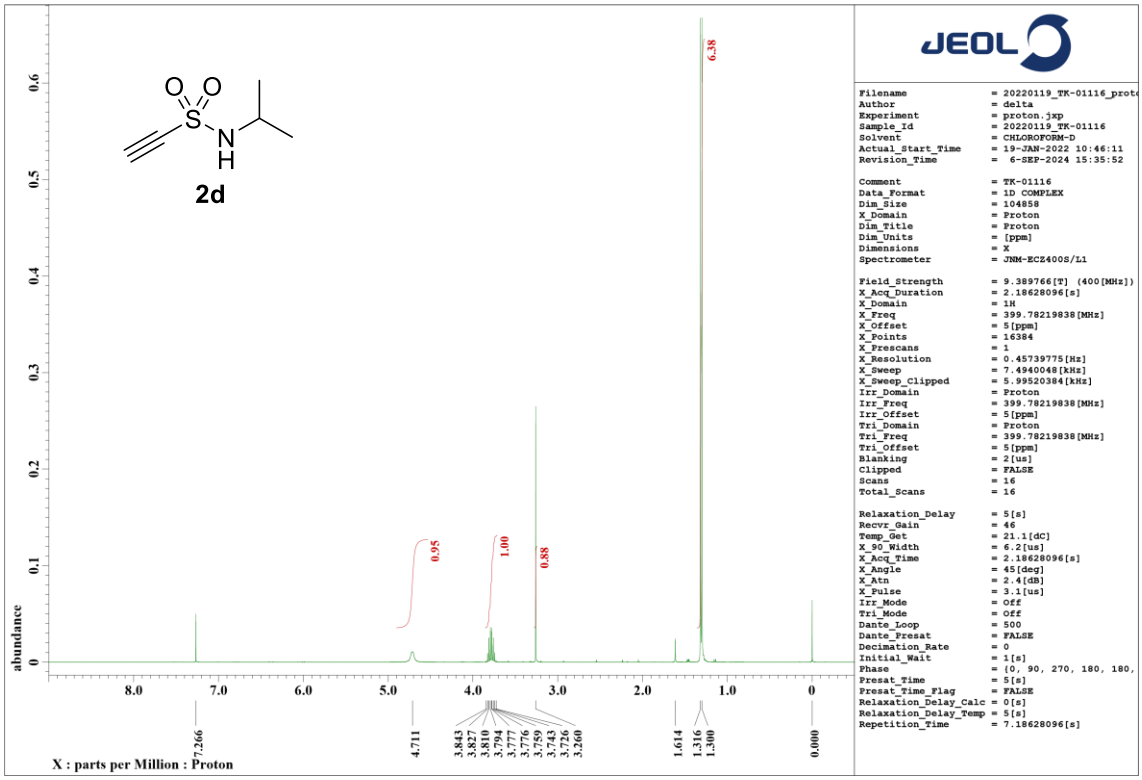

(thousandths)
X : parts per Million : Carbon13
Filename = 20211027_TK-01089B_1
Author = delta
Experiment = carbon.jxp
Sample_Id = 20211027_TK-01089B_1
Solvent = CHLOROFORM-D
Actual_Start_Time = 27-OCT-2021 21:03:31
Revision_Time = 6-SEP-2024 15:12:20
Comment = TK-01089B_13C
Data_Format = 1D COMPLEX
Dim_Size = 26214
X_Domain = Carbon13
Dim_Title = Carbon13
Dim_Units = [ppm]
Dimensions = X
Spectrometer = JNM-ECZ400S/L1
Field_Strength = 9.389766[T] (400[MHz
X_Acq_Duration = 1.03809024[s]
X_Domain = 13C
X_Freq = 100.52530333[MHz]
X_Offset = 100[ppm]
X_Points = 32768
X_Prescans = 4
X_Resolution = 0.96330739[Hz]
X_Sweep = 31.56565657[kHz]
X_Sweep_Clipped = 25.25252525[kHz]
Irr_Domain = Proton
Irr_Freq = 399.78219838[MHz]
Irr_Offset = 5[ppm]
Blanking = 5[us]
Clipped = FALSE
Scans = 2048
Total_Scans = 2048
Relaxation_Delay = 2[s]
Recvr_Gain = 50
Temp_Get = 21.3[dC]
X_90_Width = 9.97[us]
X_Acq_Time = 1.03809024[s]
X_Angle = 30[deg]
X_Atn = 8[dB]
X_Pulse = 3.32333333[us]
Irr_Atn_Dec = 27.766[dB]
Irr_Atn_Dec_Calc = 27.766[dB]
Irr_Atn_Dec_Default_Calc = 27.766[dB]
Irr_Atn_Noe = 27.766[dB]
Irr_Dec_Bandwidth_Hz = 4.7826087[kHz]
Irr_Dec_Bandwidth_Ppm = 11.96303566[ppm]
Irr_Dec_Freq = 399.78219838[MHz]
Irr_Dec_Merit_Factor = 2.2
Irr_Decoupling = TRUE
Irr_Noe = TRUE
Irr_Noise = WALTZ
Irr_Offset_Default = 5[ppm]
Irr_Pwidth = 0.115[ms]
Irr_Pwidth_Default = 0.115[ms]
Irr_Pwidth_Default_Calc = 0.115[ms]
Irr_Pwidth_Temp1 = 0.115[ms]
Irr_Wurst = FALSE
Decimation_Rate = 0

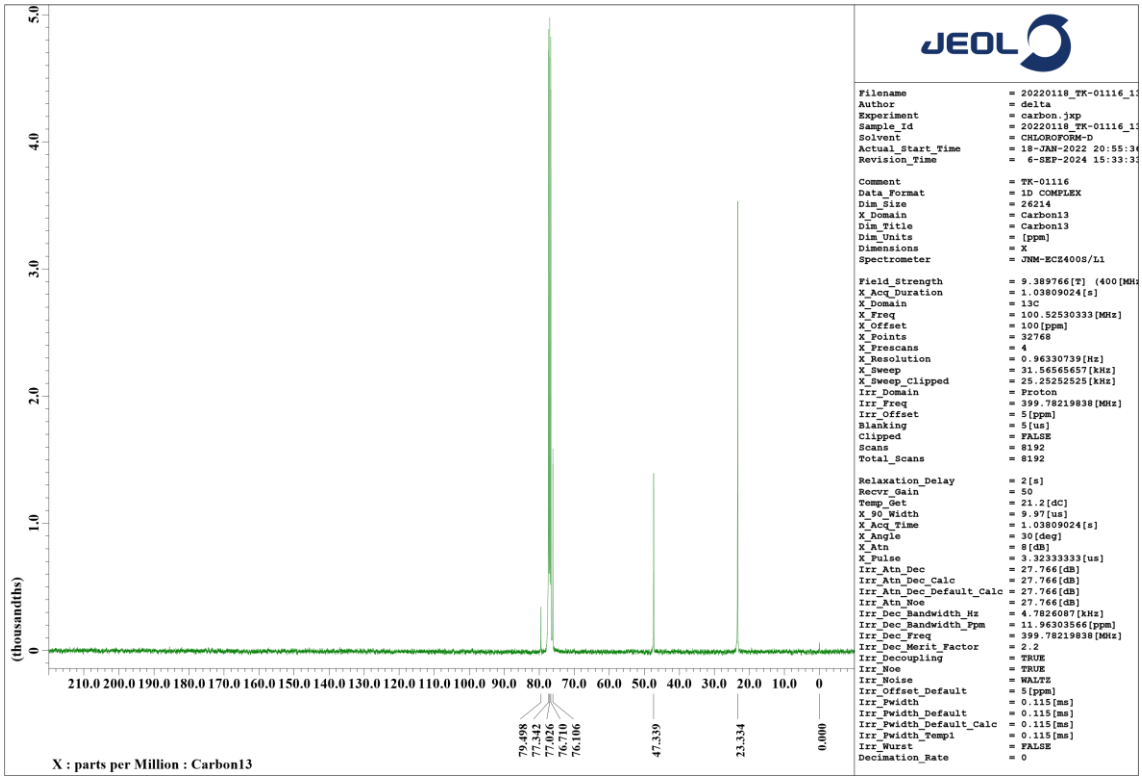

2b
abundance
X : parts per Million : Proton
2.79
3.00
0.92
7.265
4.710
3.331
3.316
3.313
3.298
3.294
3.279
3.276
3.261
1.588
1.315
1.297
1.279
0.000
Filename = 20220117_TK-01115_prot
Author = delta
Experiment = proton.jxp
Sample_Id = 20220117_TK-01115
Solvent = CHLOROFORM-D
Actual_Start_Time = 17-JAN-2022 17:34:54
Revision_Time = 6-SEP-2024 15:19:33
Comment = TK-01115
Data_Format = 1D COMPLEX
Dim_Size = 104858
X_Domain = Proton
Dim_Title = Proton
Dim_Units = [ppm]
Dimensions = X
Spectrometer = JNM-ECZ400S/L1
Field_Strength = 9.389766[T] (400[MHz])
X_Acq_Duration = 2.18628096[s]
X_Domain = 1H
X_Freq = 399.78219838[MHz]
X_Offset = 5[ppm]
X_Points = 16384
X_Prescans = 1
X_Resolution = 0.45739775[Hz]
X_Sweep = 7.4940048[kHz]
X_Sweep_Clipped = 5.99520384[kHz]
Irr_Domain = Proton
Irr_Freq = 399.78219838[MHz]
Irr_Offset = 5[ppm]
Tri_Domain = Proton
Tri_Freq = 399.78219838[MHz]
Tri_Offset = 5[ppm]
Blanking = 2[us]
Clipped = FALSE
Scans = 16
Total_Scans = 16
Relaxation_Delay = 5[s]
Recvr_Gain = 56
Temp_Get = 21.1[dC]
X_90_Width = 6.2[us]
X_Acq_Time = 2.18628096[s]
X_Angle = 45[deg]
X_Atn = 2.4[dB]
X_Pulse = 3.1[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Loop = 500
Dante_Presat = FALSE
Decimation_Rate = 0
Initial_Wait = 1[s]
Phase = (0, 90, 270, 180, 180,
Presat_Time = 5[s]
Presat_Time_Flag = FALSE
Relaxation_Delay_Calc = 0[s]
Relaxation_Delay_Temp = 5[s]
Repetition_Time = 7.18628096[s]

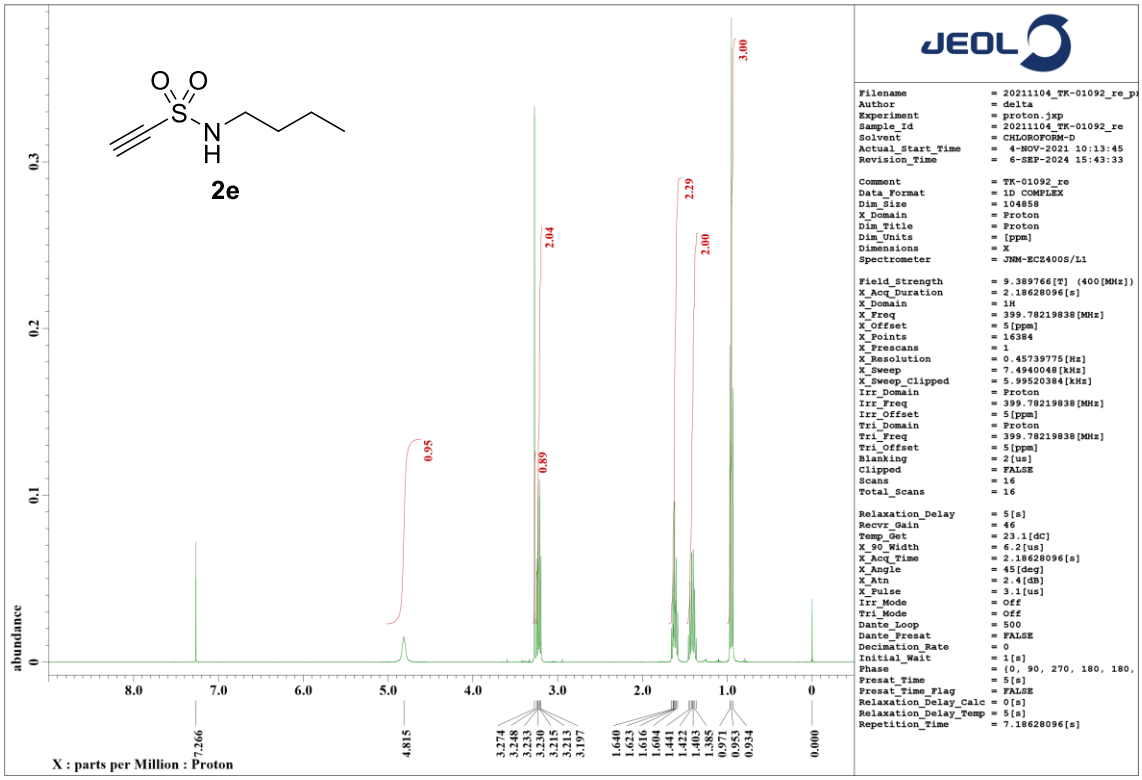

(thousandths)
X : parts per Million : Carbon13
78.463
77.342
77.026
76.710
76.662
38.868
14.719
0.000
Filename = 20220117_TK-01115_1
Author = delta
Experiment = carbon.jxp
Sample_Id = 20220117_TK-01117_1
Solvent = CHLOROFORM-D
Actual_Start_Time = 17-JAN-2022 21:04:4
Revision_Time = 6-SEP-2024 15:20:2
Comment = TK-01117
Data_Format = 1D COMPLEX
Dim_Size = 26214
X_Domain = Carbon13
Dim_Title = Carbon13
Dim_Units = [ppm]
Dimensions = X
Spectrometer = JNM-ECZ400S/L1
Field_Strength = 9.389766[T] (400[MH
X_Acq_Duration = 1.03809024[s]
X_Domain = 13C
X_Freq = 100.52530333[MHz]
X_Offset = 100[ppm]
X_Points = 32768
X_Prescans = 4
X_Resolution = 0.96330739[Hz]
X_Sweep = 31.56565657[kHz]
X_Sweep_Clipped = 25.25252525[kHz]
Irr_Domain = Proton
Irr_Freq = 399.78219838[MHz]
Irr_Offset = 5[ppm]
Blanking = 5[us]
Clipped = TRUE
Scans = 8192
Total_Scans = 8192
Relaxation_Delay = 2[s]
Recvr_Gain = 50
Temp_Get = 21.2[dC]
X_90_Width = 9.97[us]
X_Acq_Time = 1.03809024[s]
X_Angle = 30[deg]
X_Atn = 8[dB]
X_Pulse = 3.32333333[us]
Irr_Atn_Dec = 27.766[dB]
Irr_Atn_Dec_Calc = 27.766[dB]
Irr_Atn_Dec_Default_Calc = 27.766[dB]
Irr_Atn_Noe = 27.766[dB]
Irr_Dec_Bandwidth_Hz = 4.7826087[kHz]
Irr_Dec_Bandwidth_Ppm = 11.96303566[ppm]
Irr_Dec_Freq = 399.78219838[MHz]
Irr_Dec_Merit_Factor = 2.2
Irr_Decoupling = TRUE
Irr_Noe = TRUE
Irr_Noise = WALTZ
Irr_Offset_Default = 5[ppm]
Irr_Pwidth = 0.115[ms]
Irr_Pwidth_Default = 0.115[ms]
Irr_Pwidth_Default_Calc = 0.115[ms]
Irr_Pwidth_Temp1 = 0.115[ms]
Irr_Wurst = FALSE
Decimation_Rate = 0

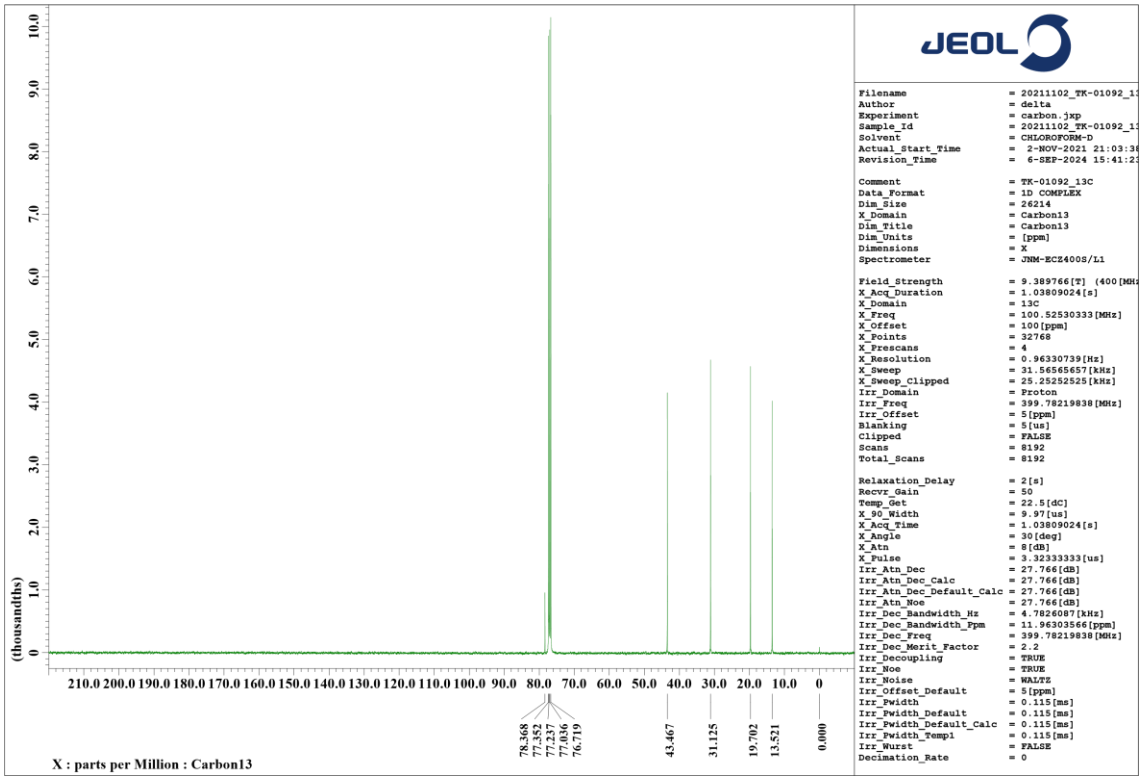

2c
abundance
X : parts per Million : Proton
7.266
4.824
3.272
3.218
3.203
3.201
3.185
3.183
3.167
1.717
1.699
1.681
1.663
1.644
1.626
1.613
1.012
0.993
0.975
0.000
0.94
0.90
2.00
2.28
3.06
JEOL
Filename = 20211117_TK-01096_re_p
Author = delta
Experiment = proton.jxp
Sample_Id = 20211117_TK-01096_re
Solvent = CHLOROFORM-D
Actual_Start_Time = 17-NOV-2021 17:00:26
Revision_Time = 6-SEP-2024 15:25:53
Comment = TK-01096_re
Data_Format = 1D COMPLEX
Dim_Size = 104858
X_Domain = Proton
Dim_Title = Proton
Dim_Units = [ppm]
Dimensions = X
Spectrometer = JNM-ECZ400S/L1
Field_Strength = 9.389766[T] (400[MHz])
X_Acq_Duration = 2.18628096[s]
X_Domain = 1H
X_Freq = 399.78219838[MHz]
X_Offset = 5[ppm]
X_Points = 16384
X_Prescans = 1
X_Resolution = 0.45739775[Hz]
X_Sweep = 7.4940048[kHz]
X_Sweep_Clipped = 5.99520384[kHz]
Irr_Domain = Proton
Irr_Freq = 399.78219838[MHz]
Irr_Offset = 5[ppm]
Tri_Domain = Proton
Tri_Freq = 399.78219838[MHz]
Tri_Offset = 5[ppm]
Blanking = 2[us]
Clipped = FALSE
Scans = 16
Total_Scans = 16
Relaxation_Delay = 5[s]
Recvr_Gain = 46
Temp_Get = 22.7[dC]
X_90_Width = 6.2[us]
X_Acq_Time = 2.18628096[s]
X_Angle = 45[deg]
X_Atn = 2.4[dB]
X_Pulse = 3.1[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Loop = 500
Dante_Presat = FALSE
Decimation_Rate = 0
Initial_Wait = 1[s]
Phase = (0, 90, 270, 180, 180,
Presat_Time = 5[s]
Presat_Time_Flag = FALSE
Relaxation_Delay_Calc = 0[s]
Relaxation_Delay_Temp = 5[s]
Repetition_Time = 7.18628096[s]

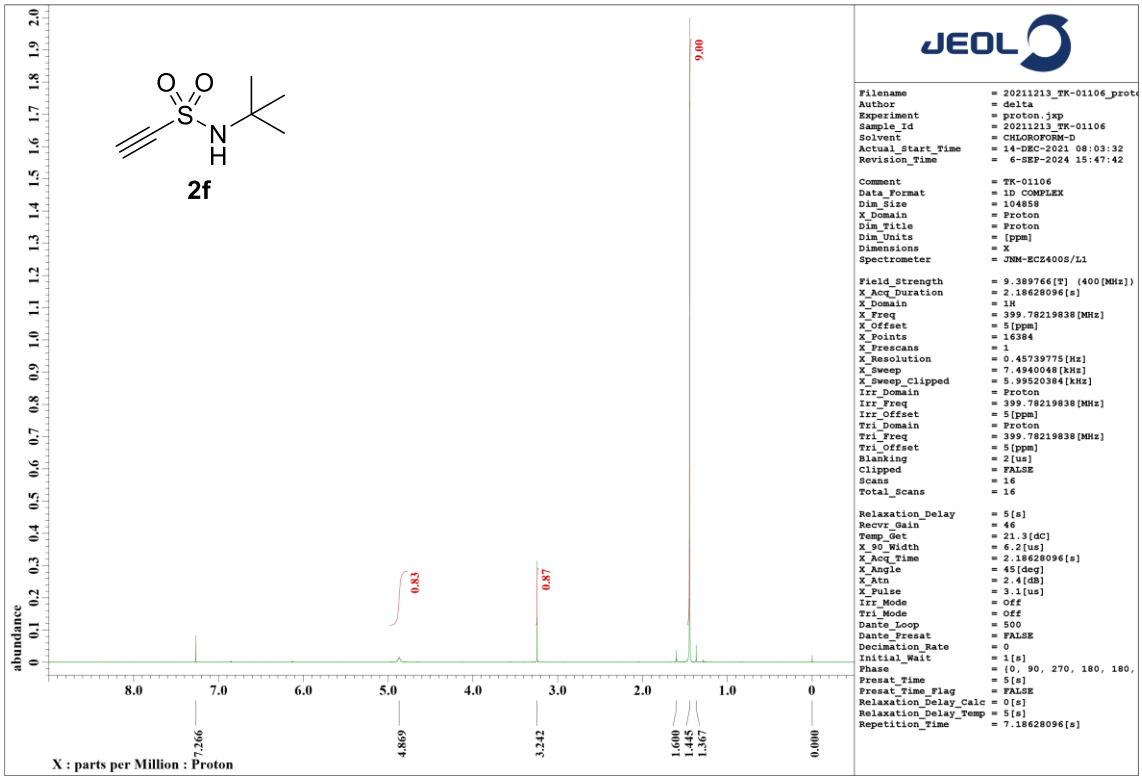

(thousandths)
X : parts per Million : Carbon13
78.425
77.342
77.026
76.710
76.662
45.451
22.548
11.097
0.000
JEOL
Filename = 20211116_TK-01096_1
Author = delta
Experiment = carbon.jxp
Sample_Id = 20211116_TK-01096_1
Solvent = CHLOROFORM-D
Actual_Start_Time = 16-NOV-2021 21:08:1
Revision_Time = 21-AUG-2023 18:33:1
Comment = TK-01096_13C
Data_Format = 1D COMPLEX
Dim_Size = 26214
X_Domain = Carbon13
Dim_Title = Carbon13
Dim_Units = [ppm]
Dimensions = X
Spectrometer = JNM-ECZ400S/L1
Field_Strength = 9.389766[T] (400[MH
X_Acq_Duration = 1.03809024[s]
X_Domain = 13C
X_Freq = 100.52530333[MHz]
X_Offset = 100[ppm]
X_Points = 32768
X_Prescans = 4
X_Resolution = 0.96330739[Hz]
X_Sweep = 31.56565657[kHz]
X_Sweep_Clipped = 25.25252525[kHz]
Irr_Domain = Proton
Irr_Freq = 399.78219838[MHz]
Irr_Offset = 5[ppm]
Blanking = 5[us]
Clipped = FALSE
Scans = 2048
Total_Scans = 2048
Relaxation_Delay = 2[s]
Recvr_Gain = 50
Temp_Get = 22.6[dC]
X_90_Width = 9.97[us]
X_Acq_Time = 1.03809024[s]
X_Angle = 30[deg]
X_Atn = 8[dB]
X_Pulse = 3.32333333[us]
Irr_Atn_Dec = 27.766[dB]
Irr_Atn_Dec_Calc = 27.766[dB]
Irr_Atn_Dec_Default_Calc = 27.766[dB]
Irr_Atn_Noe = 27.766[dB]
Irr_Dec_Bandwidth_Hz = 4.7826087[kHz]
Irr_Dec_Bandwidth_Ppm = 11.96303566[ppm]
Irr_Dec_Freq = 399.78219838[MHz]
Irr_Dec_Merit_Factor = 2.2
Irr_Decoupling = TRUE
Irr_Noe = TRUE
Irr_Noise = WALTZ
Irr_Offset_Default = 5[ppm]
Irr_Pwidth = 0.115[ms]
Irr_Pwidth_Default = 0.115[ms]
Irr_Pwidth_Default_Calc = 0.115[ms]
Irr_Pwidth_Temp1 = 0.115[ms]
Irr_Wurst = FALSE
Decimation_Rate = 0

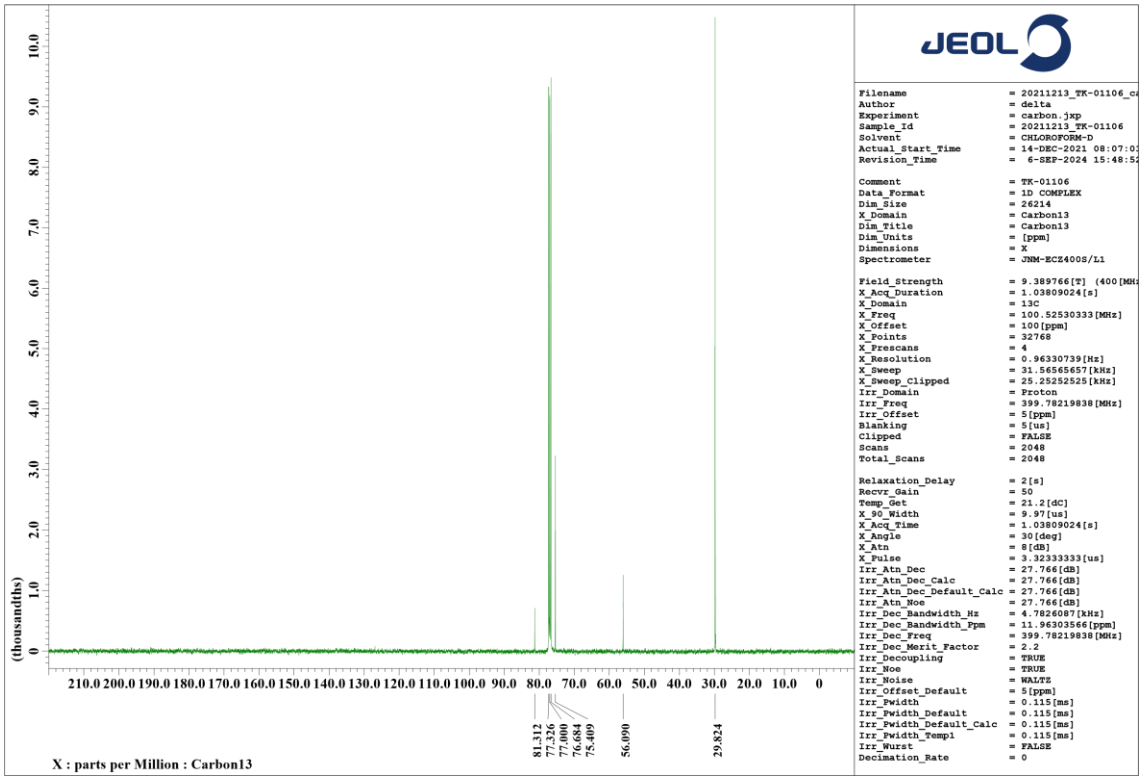

2d
6.38
0.95
1.00
0.88
abundance
X : parts per Million : Proton
7.266
4.711
3.843
3.827
3.810
3.794
3.777
3.776
3.759
3.743
3.726
3.260
1.614
1.316
1.300
0.000
Filename = 20220119_TK-01116_prot
Author = delta
Experiment = proton.jxp
Sample_Id = 20220119_TK-01116
Solvent = CHLOROFORM-D
Actual_Start_Time = 19-JAN-2022 10:46:11
Revision_Time = 6-SEP-2024 15:35:52
Comment = TK-01116
Data_Format = 1D COMPLEX
Dim_Size = 104858
X_Domain = Proton
Dim_Title = Proton
Dim_Units = [ppm]
Dimensions = X
Spectrometer = JNM-ECZ400S/L1
Field_Strength = 9.389766[T] (400[MHz])
X_Acq_Duration = 2.18628096[s]
X_Domain = 1H
X_Freq = 399.78219838[MHz]
X_Offset = 5[ppm]
X_Points = 16384
X_Prescans = 1
X_Resolution = 0.45739775[Hz]
X_Sweep = 7.4940048[kHz]
X_Sweep_Clipped = 5.99520384[kHz]
Irr_Domain = Proton
Irr_Freq = 399.78219838[MHz]
Irr_Offset = 5[ppm]
Tri_Domain = Proton
Tri_Freq = 399.78219838[MHz]
Tri_Offset = 5[ppm]
Blanking = 2[us]
Clipped = FALSE
Scans = 16
Total_Scans = 16
Relaxation_Delay = 5[s]
Recvr_Gain = 46
Temp_Get = 21.1[dC]
X_90_Width = 6.2[us]
X_Acq_Time = 2.18628096[s]
X_Angle = 45[deg]
X_Atn = 2.4[dB]
X_Pulse = 3.1[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Loop = 500
Dante_Presat = FALSE
Decimation_Rate = 0
Initial_Wait = 1[s]
Phase = (0, 90, 270, 180, 180,
Presat_Time = 5[s]
Presat_Time_Flag = FALSE
Relaxation_Delay_Calc = 0[s]
Relaxation_Delay_Temp = 5[s]
Repetition_Time = 7.18628096[s]

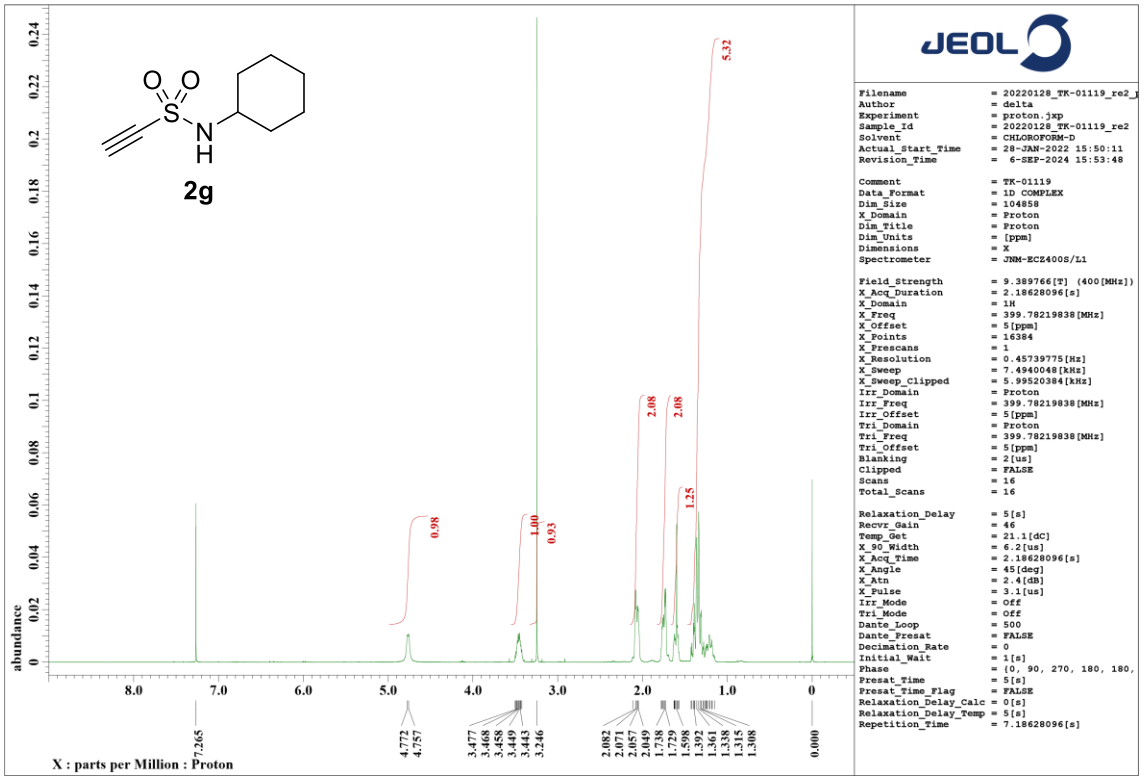

(thousandths)
X : parts per Million : Carbon13
79.498
77.342
77.026
76.710
76.106
47.339
23.334
0.000
Filename = 20220118_TK-01116_1
Author = delta
Experiment = carbon.jxp
Sample_Id = 20220119_TK-01116_1
Solvent = CHLOROFORM-D
Actual_Start_Time = 18-JAN-2022 20:55:3
Revision_Time = 6-SEP-2024 15:33:3
Comment = TK-01116
Data_Format = 1D COMPLEX
Dim_Size = 26214
X_Domain = Carbon13
Dim_Title = Carbon13
Dim_Units = [ppm]
Dimensions = X
Spectrometer = JNM-ECZ400S/L1
Field_Strength = 9.389766[T] (400[MH
X_Acq_Duration = 1.03809024[s]
X_Domain = 13C
X_Freq = 100.52530333[MHz]
X_Offset = 100[ppm]
X_Points = 32768
X_Prescans = 4
X_Resolution = 0.96330739[Hz]
X_Sweep = 31.56565657[kHz]
X_Sweep_Clipped = 25.25252525[kHz]
Irr_Domain = Proton
Irr_Freq = 399.78219838[MHz]
Irr_Offset = 5[ppm]
Blanking = 5[us]
Clipped = FALSE
Scans = 8192
Total_Scans = 8192
Relaxation_Delay = 2[s]
Recvr_Gain = 50
Temp_Get = 21.2[dC]
X_90_Width = 9.97[us]
X_Acq_Time = 1.03809024[s]
X_Angle = 30[deg]
X_Atn = 8[dB]
X_Pulse = 3.32333333[us]
Irr_Atn_Dec = 27.766[dB]
Irr_Atn_Dec_Calc = 27.766[dB]
Irr_Atn_Dec_Default_Calc = 27.766[dB]
Irr_Atn_Noe = 27.766[dB]
Irr_Dec_Bandwidth_Hz = 4.7826087[kHz]
Irr_Dec_Bandwidth_Ppm = 11.96303566[ppm]
Irr_Dec_Freq = 399.78219838[MHz]
Irr_Dec_Merit_Factor = 2.2
Irr_Decoupling = TRUE
Irr_Noe = TRUE
Irr_Noise = WALTZ
Irr_Offset_Default = 5[ppm]
Irr_Pwidth = 0.115[ms]
Irr_Pwidth_Default = 0.115[ms]
Irr_Pwidth_Default_Calc = 0.115[ms]
Irr_Pwidth_Temp1 = 0.115[ms]
Irr_Wurst = FALSE
Decimation_Rate = 0

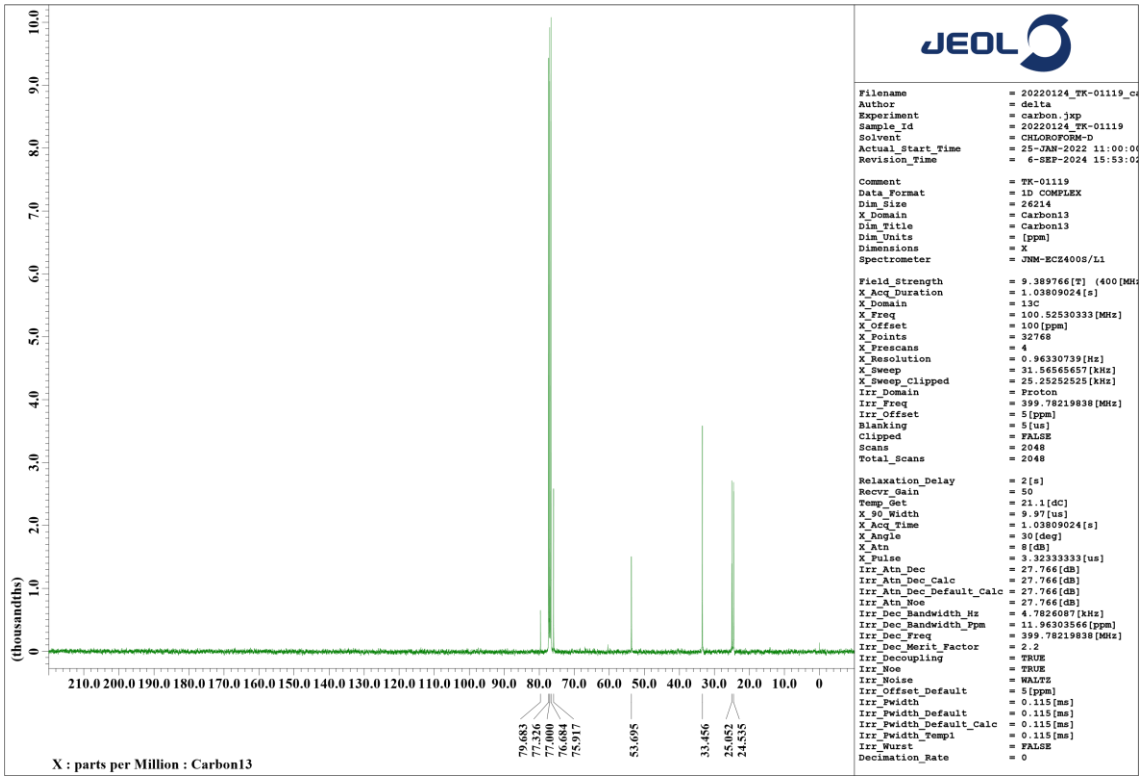

2e
abundance
X : parts per Million : Proton
3.00
2.29
2.04
2.00
0.95
0.89
7.266
4.815
3.274
3.248
3.233
3.230
3.215
3.213
3.197
1.640
1.623
1.616
1.604
1.441
1.422
1.403
1.385
0.971
0.953
0.934
0.000
Filename = 20211104_TK-01092_re_p
Author = delta
Experiment = proton.jxp
Sample_Id = 20211104_TK-01092_re
Solvent = CHLOROFORM-D
Actual_Start_Time = 4-NOV-2021 10:13:45
Revision_Time = 6-SEP-2024 15:43:33
Comment = TK-01092_re
Data_Format = 1D COMPLEX
Dim_Size = 104858
X_Domain = Proton
Dim_Title = Proton
Dim_Units = [ppm]
Dimensions = X
Spectrometer = JNM-ECZ400S/L1
Field_Strength = 9.389766[T] (400[MHz])
X_Acq_Duration = 2.18628096[s]
X_Domain = 1H
X_Freq = 399.78219838[MHz]
X_Offset = 5[ppm]
X_Points = 16384
X_Prescans = 1
X_Resolution = 0.45739775[Hz]
X_Sweep = 7.4940048[kHz]
X_Sweep_Clipped = 5.99520384[kHz]
Irr_Domain = Proton
Irr_Freq = 399.78219838[MHz]
Irr_Offset = 5[ppm]
Tri_Domain = Proton
Tri_Freq = 399.78219838[MHz]
Tri_Offset = 5[ppm]
Blanking = 2[us]
Clipped = FALSE
Scans = 16
Total_Scans = 16
Relaxation_Delay = 5[s]
Recvr_Gain = 46
Temp_Get = 23.1[dC]
X_90_Width = 6.2[us]
X_Acq_Time = 2.18628096[s]
X_Angle = 45[deg]
X_Atn = 2.4[dB]
X_Pulse = 3.1[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Loop = 500
Dante_Presat = FALSE
Decimation_Rate = 0
Initial_Wait = 1[s]
Phase = (0, 90, 270, 180, 180,
Presat_Time = 5[s]
Presat_Time_Flag = FALSE
Relaxation_Delay_Calc = 0[s]
Relaxation_Delay_Temp = 5[s]
Repetition_Time = 7.18628096[s]

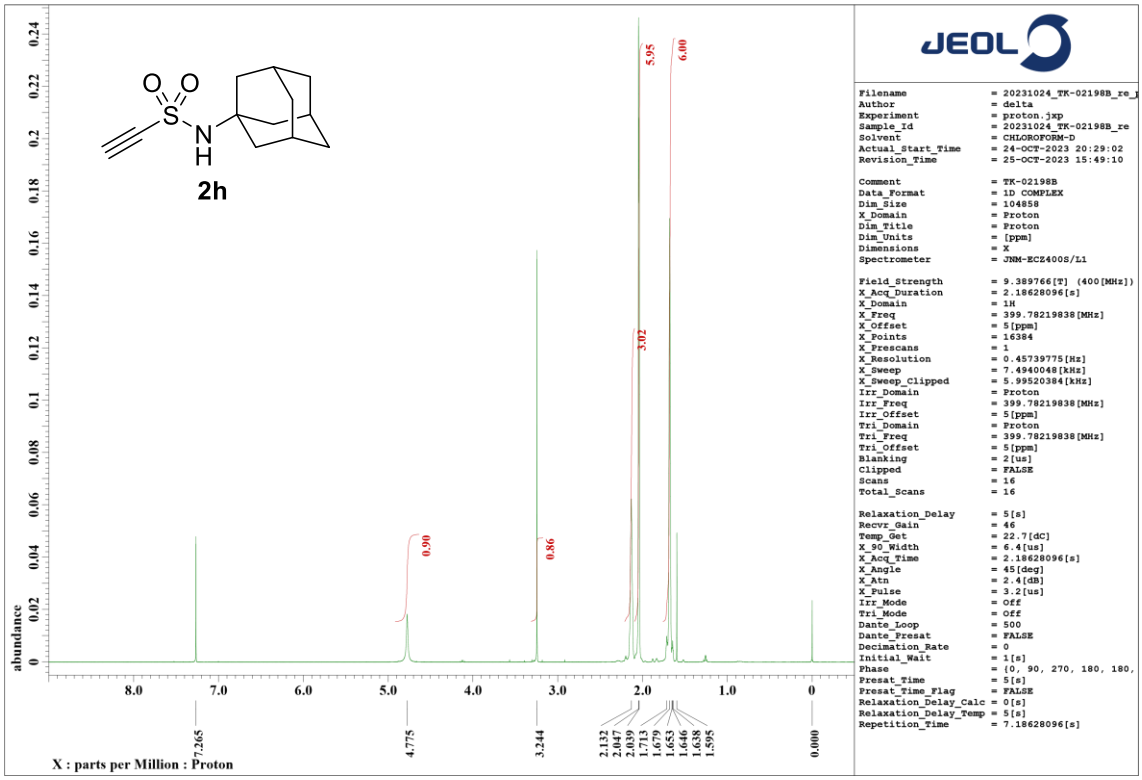

(thousandths)
X : parts per Million : Carbon13
78.368
77.352
77.237
77.036
76.719
43.467
31.125
19.702
13.521
0.000
Filename = 20211102_TK-01092_1
Author = delta
Experiment = carbon.jxp
Sample_Id = 20211102_TK-01092_1
Solvent = CHLOROFORM-D
Actual_Start_Time = 2-NOV-2021 21:03:3
Revision_Time = 6-SEP-2024 15:41:2
Comment = TK-01092_13C
Data_Format = 1D COMPLEX
Dim_Size = 26214
X_Domain = Carbon13
Dim_Title = Carbon13
Dim_Units = [ppm]
Dimensions = X
Spectrometer = JNM-ECZ400S/L1
Field_Strength = 9.389766[T] (400[MH
X_Acq_Duration = 1.03809024[s]
X_Domain = 13C
X_Freq = 100.52530333[MHz]
X_Offset = 100[ppm]
X_Points = 32768
X_Prescans = 4
X_Resolution = 0.96330739[Hz]
X_Sweep = 31.56565657[kHz]
X_Sweep_Clipped = 25.25252525[kHz]
Irr_Domain = Proton
Irr_Freq = 399.78219838[MHz]
Irr_Offset = 5[ppm]
Blanking = 5[us]
Clipped = FALSE
Scans = 8192
Total_Scans = 8192
Relaxation_Delay = 2[s]
Recvr_Gain = 50
Temp_Get = 22.5[dC]
X_90_Width = 9.97[us]
X_Acq_Time = 1.03809024[s]
X_Angle = 30[deg]
X_Atn = 8[dB]
X_Pulse = 3.32333333[us]
Irr_Atn_Dec = 27.766[dB]
Irr_Atn_Dec_Calc = 27.766[dB]
Irr_Atn_Dec_Default_Calc = 27.766[dB]
Irr_Atn_Noe = 27.766[dB]
Irr_Dec_Bandwidth_Hz = 4.7826087[kHz]
Irr_Dec_Bandwidth_Ppm = 11.96303566[ppm]
Irr_Dec_Freq = 399.78219838[MHz]
Irr_Dec_Merit_Factor = 2.2
Irr_Decoupling = TRUE
Irr_Noe = TRUE
Irr_Noise = WALTZ
Irr_Offset_Default = 5[ppm]
Irr_Pwidth = 0.115[ms]
Irr_Pwidth_Default = 0.115[ms]
Irr_Pwidth_Default_Calc = 0.115[ms]
Irr_Pwidth_Temp1 = 0.115[ms]
Irr_Wurst = FALSE
Decimation_Rate = 0

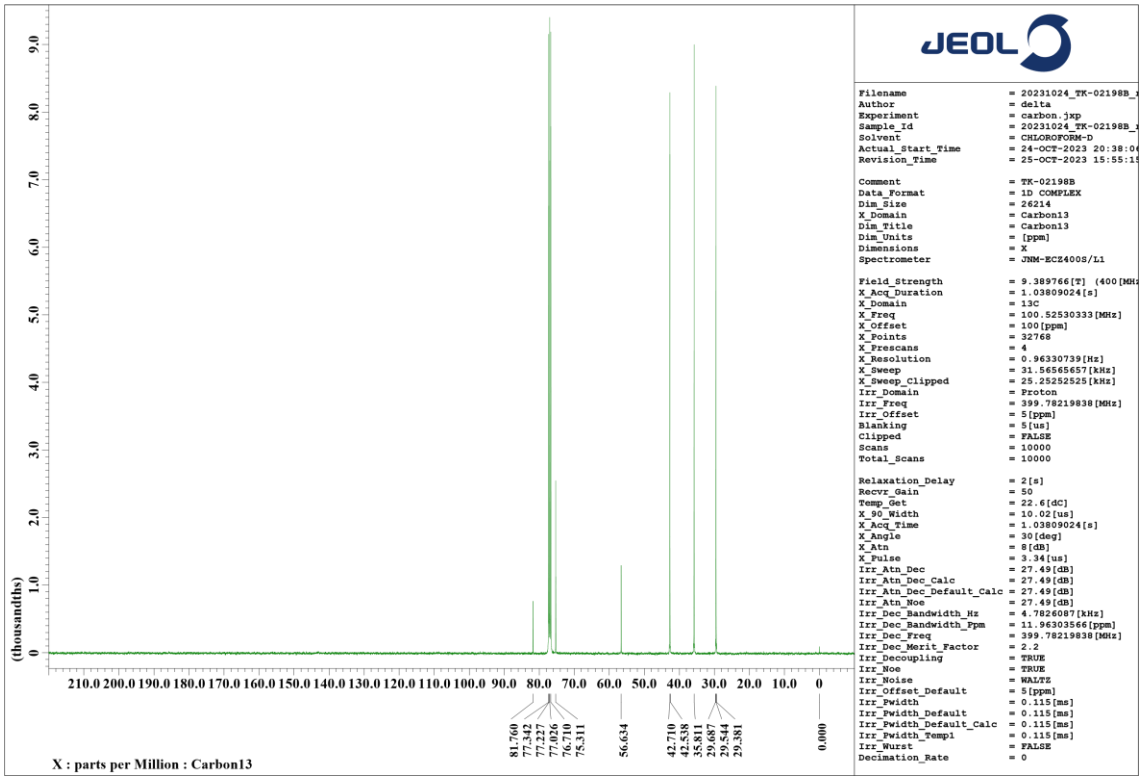

2f
9.00
0.83
0.87
abundance
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
7.266
4.869
3.242
1.600
1.445
1.367
0.000
X : parts per Million : Proton
JEOL
Filename = 20211213_TK-01106_prot
Author = delta
Experiment = proton.jxp
Sample_Id = 20211213_TK-01106
Solvent = CHLOROFORM-D
Actual_Start_Time = 14-DEC-2021 08:03:32
Revision_Time = 6-SEP-2024 15:47:42
Comment = TK-01106
Data_Format = 1D COMPLEX
Dim_Size = 104858
X_Domain = Proton
Dim_Title = Proton
Dim_Units = [ppm]
Dimensions = X
Spectrometer = JNM-ECZ400S/L1
Field_Strength = 9.389766[T] (400[MHz])
X_Acq_Duration = 2.18628096[s]
X_Domain = 1H
X_Freq = 399.78219838[MHz]
X_Offset = 5[ppm]
X_Points = 16384
X_Prescans = 1
X_Resolution = 0.45739775[Hz]
X_Sweep = 7.4940048[kHz]
X_Sweep_Clipped = 5.99520384[kHz]
Irr_Domain = Proton
Irr_Freq = 399.78219838[MHz]
Irr_Offset = 5[ppm]
Tri_Domain = Proton
Tri_Freq = 399.78219838[MHz]
Tri_Offset = 5[ppm]
Blanking = 2[us]
Clipped = FALSE
Scans = 16
Total_Scans = 16
Relaxation_Delay = 5[s]
Recvr_Gain = 46
Temp_Get = 21.3[dC]
X_90_Width = 6.2[us]
X_Acq_Time = 2.18628096[s]
X_Angle = 45[deg]
X_Atn = 2.4[dB]
X_Pulse = 3.1[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Loop = 500
Dante_Presat = FALSE
Decimation_Rate = 0
Initial_Wait = 1[s]
Phase = (0, 90, 270, 180, 180,
Presat_Time = 5[s]
Presat_Time_Flag = FALSE
Relaxation_Delay_Calc = 0[s]
Relaxation_Delay_Temp = 5[s]
Repetition_Time = 7.18628096[s]

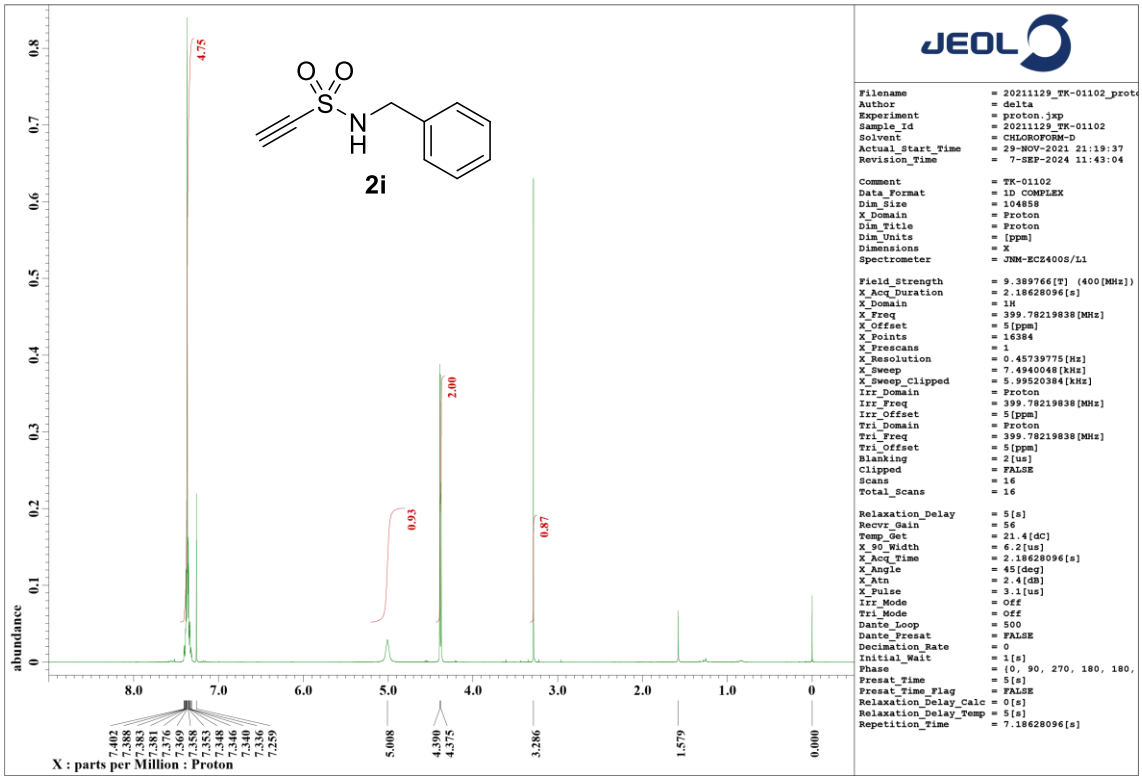

(thousandths)
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
210.0 200.0 190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0
81.312
77.326
77.000
76.684
75.409
56.090
29.824
X : parts per Million : Carbon13
JEOL
Filename = 20211213_TK-01106_c
Author = delta
Experiment = carbon.jxp
Sample_Id = 20211213_TK-01106
Solvent = CHLOROFORM-D
Actual_Start_Time = 14-DEC-2021 08:07:0
Revision_Time = 6-SEP-2024 15:48:5
Comment = TK-01106
Data_Format = 1D COMPLEX
Dim_Size = 26214
X_Domain = Carbon13
Dim_Title = Carbon13
Dim_Units = [ppm]
Dimensions = X
Spectrometer = JNM-ECZ400S/L1
Field_Strength = 9.389766[T] (400[MH
X_Acq_Duration = 1.03809024[s]
X_Domain = 13C
X_Freq = 100.52530333[MHz]
X_Offset = 100[ppm]
X_Points = 32768
X_Prescans = 4
X_Resolution = 0.96330739[Hz]
X_Sweep = 31.56565657[kHz]
X_Sweep_Clipped = 25.25252525[kHz]
Irr_Domain = Proton
Irr_Freq = 399.78219838[MHz]
Irr_Offset = 5[ppm]
Blanking = 5[us]
Clipped = FALSE
Scans = 2048
Total_Scans = 2048
Relaxation_Delay = 2[s]
Recvr_Gain = 50
Temp_Get = 21.2[dC]
X_90_Width = 9.97[us]
X_Acq_Time = 1.03809024[s]
X_Angle = 30[deg]
X_Atn = 8[dB]
X_Pulse = 3.32333333[us]
Irr_Atn_Dec = 27.766[dB]
Irr_Atn_Dec_Calc = 27.766[dB]
Irr_Atn_Dec_Default_Calc = 27.766[dB]
Irr_Atn_Noe = 27.766[dB]
Irr_Dec_Bandwidth_Hz = 4.7826087[kHz]
Irr_Dec_Bandwidth_Ppm = 11.96303566[ppm]
Irr_Dec_Freq = 399.78219838[MHz]
Irr_Dec_Merit_Factor = 2.2
Irr_Decoupling = TRUE
Irr_Noe = TRUE
Irr_Noise = WALTZ
Irr_Offset_Default = 5[ppm]
Irr_Pwidth = 0.115[ms]
Irr_Pwidth_Default = 0.115[ms]
Irr_Pwidth_Default_Calc = 0.115[ms]
Irr_Pwidth_Temp1 = 0.115[ms]
Irr_Wurst = FALSE
Decimation_Rate = 0

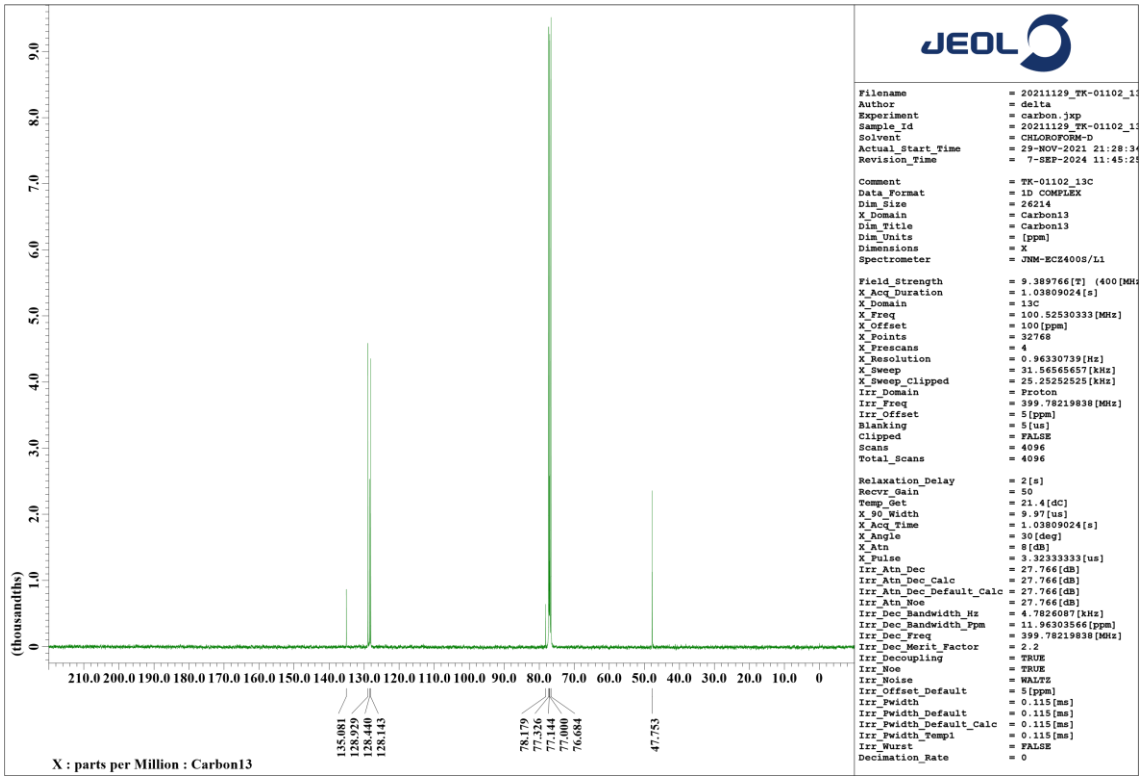

2g
abundance
X : parts per Million : Proton
0.98
1.00
0.93
2.08
2.08
1.25
5.32
7.265
4.772
4.757
3.477
3.468
3.458
3.449
3.443
3.246
2.082
2.071
2.057
2.049
1.738
1.729
1.598
1.392
1.361
1.338
1.315
1.308
0.000
Filename = 20220128_TK-01119_re2_
Author = delta
Experiment = proton.jxp
Sample_Id = 20220128_TK-01119_re2
Solvent = CHLOROFORM-D
Actual_Start_Time = 28-JAN-2022 15:50:11
Revision_Time = 6-SEP-2024 15:53:48
Comment = TK-01119
Data_Format = 1D COMPLEX
Dim_Size = 104858
X_Domain = Proton
Dim_Title = Proton
Dim_Units = [ppm]
Dimensions = X
Spectrometer = JNM-ECZ400S/L1
Field_Strength = 9.389766[T] (400[MHz])
X_Acq_Duration = 2.18628096[s]
X_Domain = 1H
X_Freq = 399.78219838[MHz]
X_Offset = 5[ppm]
X_Points = 16384
X_Prescans = 1
X_Resolution = 0.45739775[Hz]
X_Sweep = 7.4940048[kHz]
X_Sweep_Clipped = 5.99520384[kHz]
Irr_Domain = Proton
Irr_Freq = 399.78219838[MHz]
Irr_Offset = 5[ppm]
Tri_Domain = Proton
Tri_Freq = 399.78219838[MHz]
Tri_Offset = 5[ppm]
Blanking = 2[us]
Clipped = FALSE
Scans = 16
Total_Scans = 16
Relaxation_Delay = 5[s]
Recvr_Gain = 46
Temp_Get = 21.1[dC]
X_90_Width = 6.2[us]
X_Acq_Time = 2.18628096[s]
X_Angle = 45[deg]
X_Atn = 2.4[dB]
X_Pulse = 3.1[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Loop = 500
Dante_Presat = FALSE
Decimation_Rate = 0
Initial_Wait = 1[s]
Phase = (0, 90, 270, 180, 180,
Presat_Time = 5[s]
Presat_Time_Flag = FALSE
Relaxation_Delay_Calc = 0[s]
Relaxation_Delay_Temp = 5[s]
Repetition_Time = 7.18628096[s]

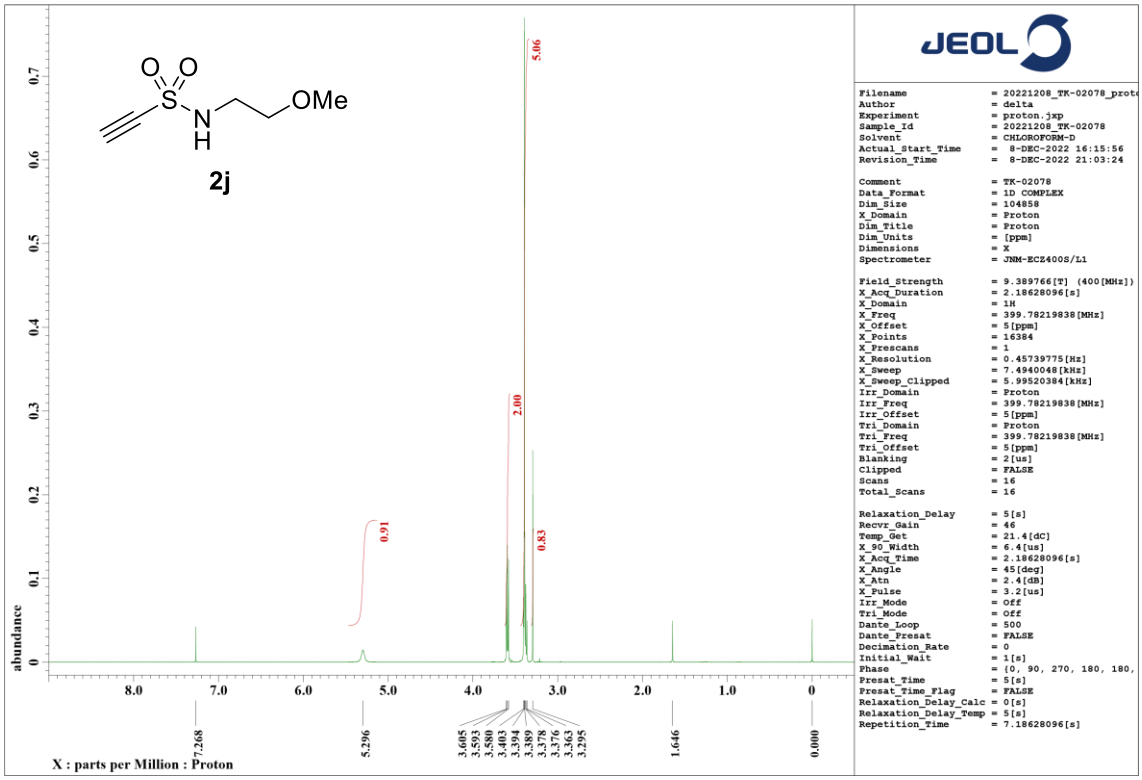

(thousandths)
X : parts per Million : Carbon13
79.683
77.326
77.000
76.684
75.917
53.695
33.456
25.052
24.535
Filename = 20220124_TK-01119_c
Author = delta
Experiment = carbon.jxp
Sample_Id = 20220124_TK-01119
Solvent = CHLOROFORM-D
Actual_Start_Time = 25-JAN-2022 11:00:0
Revision_Time = 6-SEP-2024 15:53:0
Comment = TK-01119
Data_Format = 1D COMPLEX
Dim_Size = 26214
X_Domain = Carbon13
Dim_Title = Carbon13
Dim_Units = [ppm]
Dimensions = X
Spectrometer = JNM-ECZ400S/L1
Field_Strength = 9.389766[T] (400[MH
X_Acq_Duration = 1.03809024[s]
X_Domain = 13C
X_Freq = 100.52530333[MHz]
X_Offset = 100[ppm]
X_Points = 32768
X_Prescans = 4
X_Resolution = 0.96330739[Hz]
X_Sweep = 31.56565657[kHz]
X_Sweep_Clipped = 25.25252525[kHz]
Irr_Domain = Proton
Irr_Freq = 399.78219838[MHz]
Irr_Offset = 5[ppm]
Blanking = 5[us]
Clipped = FALSE
Scans = 2048
Total_Scans = 2048
Relaxation_Delay = 2[s]
Recvr_Gain = 50
Temp_Get = 21.1[dC]
X_90_Width = 9.97[us]
X_Acq_Time = 1.03809024[s]
X_Angle = 30[deg]
X_Atn = 8[dB]
X_Pulse = 3.32333333[us]
Irr_Atn_Dec = 27.766[dB]
Irr_Atn_Dec_Calc = 27.766[dB]
Irr_Atn_Dec_Default_Calc = 27.766[dB]
Irr_Atn_Noe = 27.766[dB]
Irr_Dec_Bandwidth_Hz = 4.7826087[kHz]
Irr_Dec_Bandwidth_Ppm = 11.96303566[ppm]
Irr_Dec_Freq = 399.78219838[MHz]
Irr_Dec_Merit_Factor = 2.2
Irr_Decoupling = TRUE
Irr_Noe = TRUE
Irr_Noise = WALTZ
Irr_Offset_Default = 5[ppm]
Irr_Pwidth = 0.115[ms]
Irr_Pwidth_Default = 0.115[ms]
Irr_Pwidth_Default_Calc = 0.115[ms]
Irr_Pwidth_Temp1 = 0.115[ms]
Irr_Wurst = FALSE
Decimation_Rate = 0

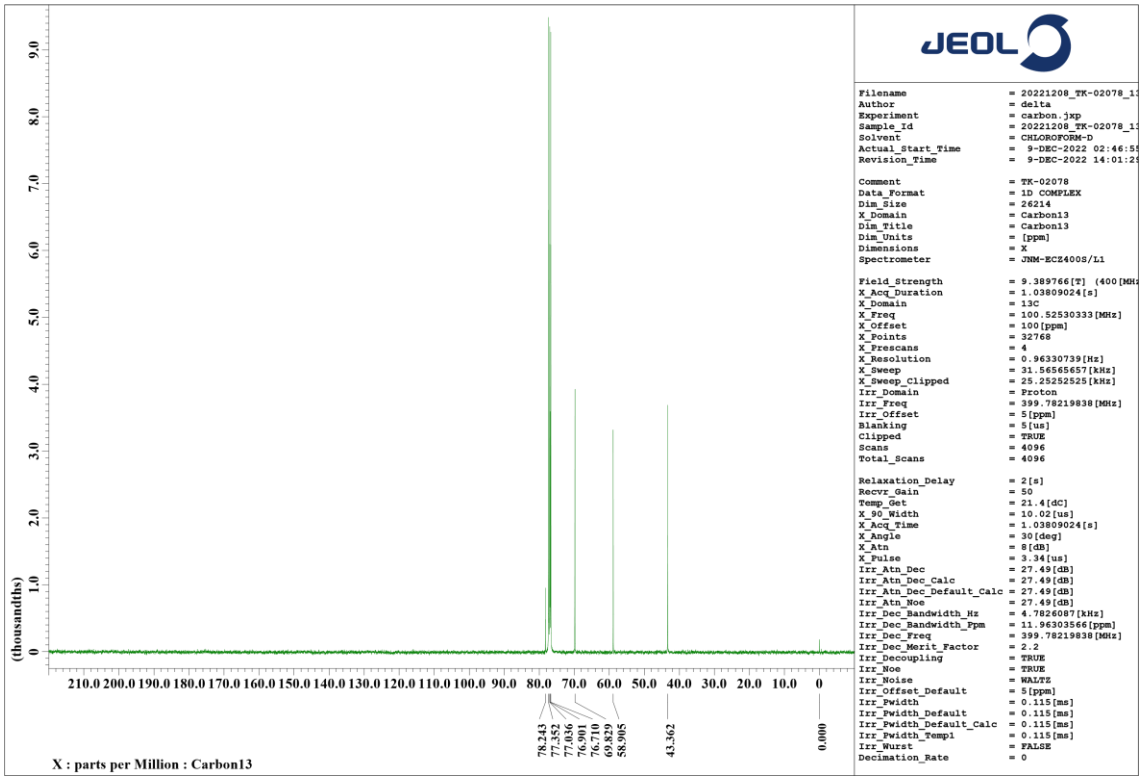

2h
abundance
X : parts per Million : Proton
5.95
6.00
3.02
0.90
0.86
7.265
4.775
3.244
2.132
2.047
2.039
1.713
1.679
1.653
1.646
1.638
1.595
0.000

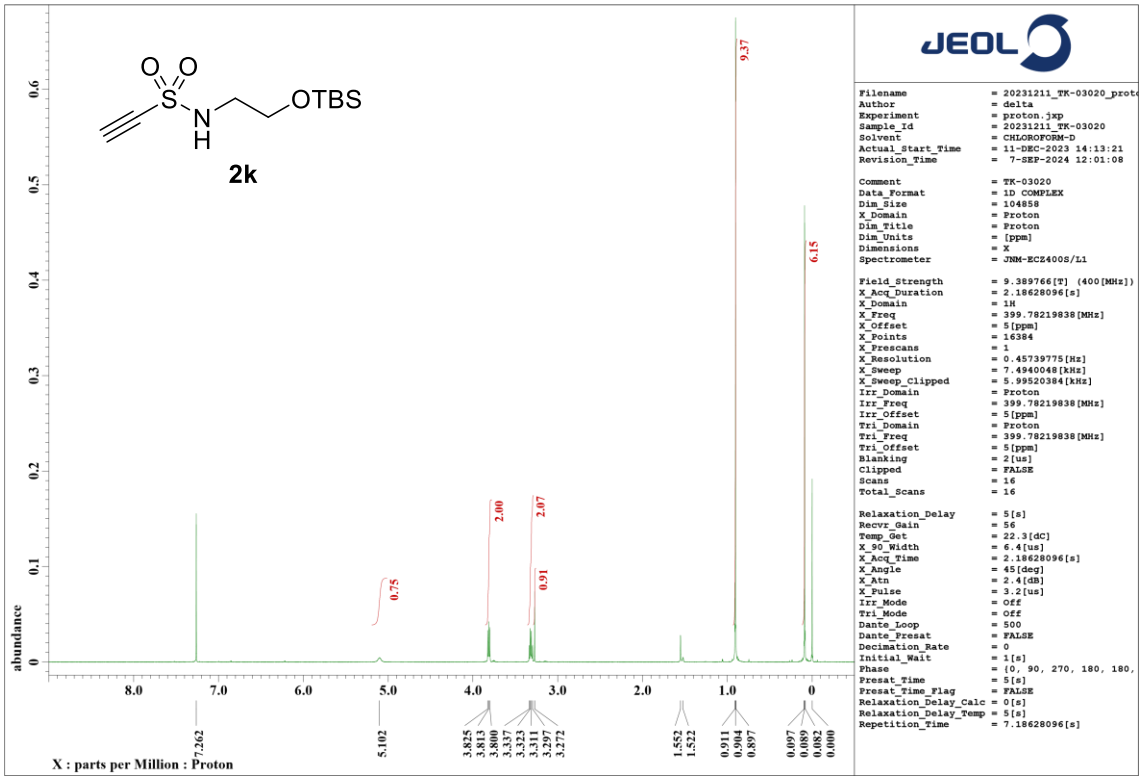

(thousandths)
X : parts per Million : Carbon13
81.760
77.342
77.227
77.026
76.710
75.311
56.634
42.710
42.538
35.811
29.687
29.544
29.381
0.000

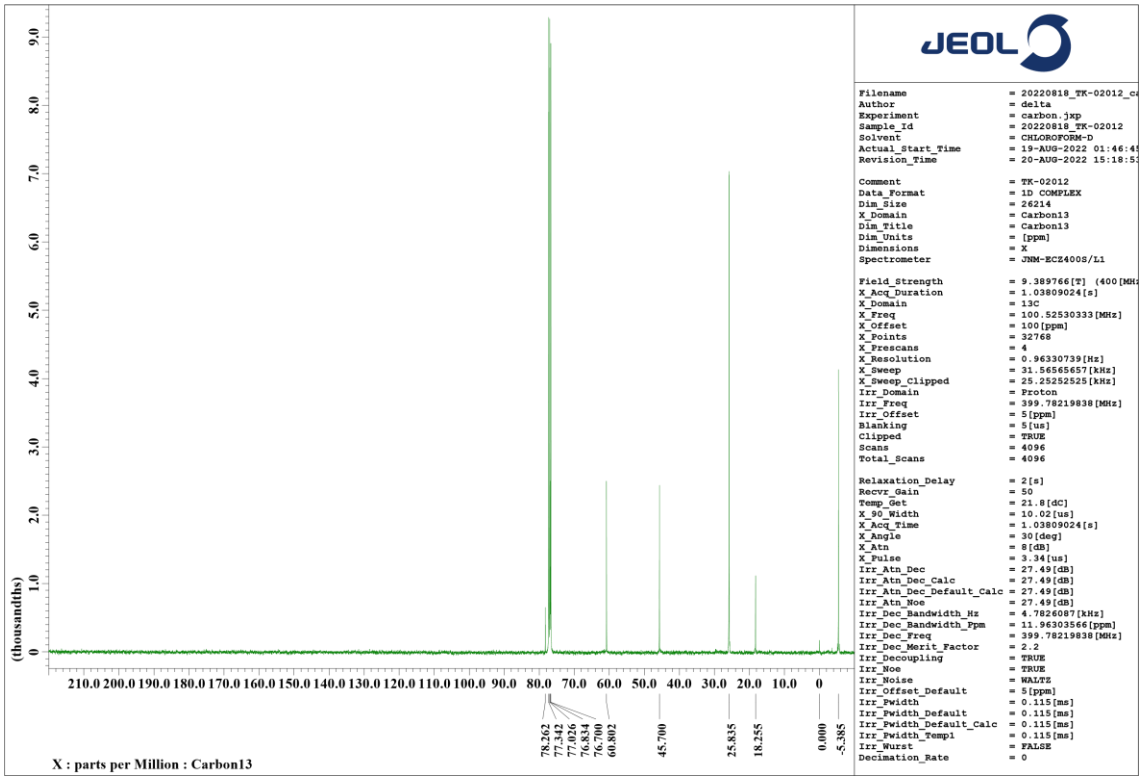

4.75
2.00
0.93
0.87
2i
abundance
X : parts per Million : Proton
7.402
7.388
7.383
7.381
7.376
7.369
7.358
7.353
7.348
7.346
7.340
7.336
7.259
5.008
4.390
4.375
3.286
1.579
0.000
Filename = 20211129_TK-01102_prot
Author = delta
Experiment = proton.jxp
Sample_Id = 20211129_TK-01102
Solvent = CHLOROFORM-D
Actual_Start_Time = 29-NOV-2021 21:19:37
Revision_Time = 7-SEP-2024 11:43:04
Comment = TK-01102
Data_Format = 1D COMPLEX
Dim_Size = 104858
X_Domain = Proton
Dim_Title = Proton
Dim_Units = [ppm]
Dimensions = X
Spectrometer = JNM-ECZ400S/L1
Field_Strength = 9.389766[T] (400[MHz])
X_Acq_Duration = 2.18628096[s]
X_Domain = 1H
X_Freq = 399.78219838[MHz]
X_Offset = 5[ppm]
X_Points = 16384
X_Prescans = 1
X_Resolution = 0.45739775[Hz]
X_Sweep = 7.4940048[kHz]
X_Sweep_Clipped = 5.99520384[kHz]
Irr_Domain = Proton
Irr_Freq = 399.78219838[MHz]
Irr_Offset = 5[ppm]
Tri_Domain = Proton
Tri_Freq = 399.78219838[MHz]
Tri_Offset = 5[ppm]
Blanking = 2[us]
Clipped = FALSE
Scans = 16
Total_Scans = 16
Relaxation_Delay = 5[s]
Recvr_Gain = 56
Temp_Get = 21.4[dC]
X_90_Width = 6.2[us]
X_Acq_Time = 2.18628096[s]
X_Angle = 45[deg]
X_Atn = 2.4[dB]
X_Pulse = 3.1[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Loop = 500
Dante_Presat = FALSE
Decimation_Rate = 0
Initial_Wait = 1[s]
Phase = (0, 90, 270, 180, 180,
Presat_Time = 5[s]
Presat_Time_Flag = FALSE
Relaxation_Delay_Calc = 0[s]
Relaxation_Delay_Temp = 5[s]
Repetition_Time = 7.18628096[s]

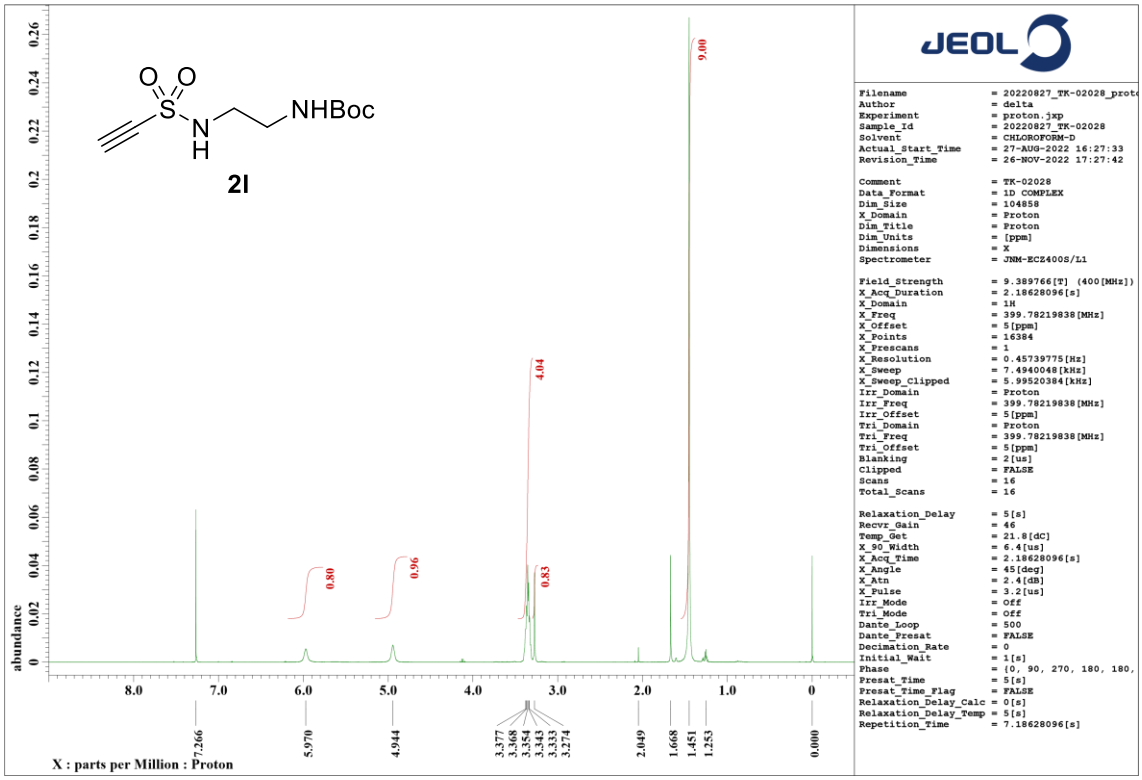

(thousandths)
X : parts per Million : Carbon13
135.081
128.929
128.440
128.143
78.179
77.326
77.144
77.000
76.684
47.753
Filename = 20211129_TK-01102_1
Author = delta
Experiment = carbon.jxp
Sample_Id = 20211129_TK-01102_1
Solvent = CHLOROFORM-D
Actual_Start_Time = 29-NOV-2021 21:28:3
Revision_Time = 7-SEP-2024 11:45:2
Comment = TK-01102_13C
Data_Format = 1D COMPLEX
Dim_Size = 26214
X_Domain = Carbon13
Dim_Title = Carbon13
Dim_Units = [ppm]
Dimensions = X
Spectrometer = JNM-ECZ400S/L1
Field_Strength = 9.389766[T] (400[MH
X_Acq_Duration = 1.03809024[s]
X_Domain = 13C
X_Freq = 100.52530333[MHz]
X_Offset = 100[ppm]
X_Points = 32768
X_Prescans = 4
X_Resolution = 0.96330739[Hz]
X_Sweep = 31.56565657[kHz]
X_Sweep_Clipped = 25.25252525[kHz]
Irr_Domain = Proton
Irr_Freq = 399.78219838[MHz]
Irr_Offset = 5[ppm]
Blanking = 5[us]
Clipped = FALSE
Scans = 4096
Total_Scans = 4096
Relaxation_Delay = 2[s]
Recvr_Gain = 50
Temp_Get = 21.4[dC]
X_90_Width = 9.97[us]
X_Acq_Time = 1.03809024[s]
X_Angle = 30[deg]
X_Atn = 8[dB]
X_Pulse = 3.32333333[us]
Irr_Atn_Dec = 27.766[dB]
Irr_Atn_Dec_Calc = 27.766[dB]
Irr_Atn_Dec_Default_Calc = 27.766[dB]
Irr_Atn_Noe = 27.766[dB]
Irr_Dec_Bandwidth_Hz = 4.7826087[kHz]
Irr_Dec_Bandwidth_Ppm = 11.96303566[ppm]
Irr_Dec_Freq = 399.78219838[MHz]
Irr_Dec_Merit_Factor = 2.2
Irr_Decoupling = TRUE
Irr_Noe = TRUE
Irr_Noise = WALTZ
Irr_Offset_Default = 5[ppm]
Irr_Pwidth = 0.115[ms]
Irr_Pwidth_Default = 0.115[ms]
Irr_Pwidth_Default_Calc = 0.115[ms]
Irr_Pwidth_Temp1 = 0.115[ms]
Irr_Wurst = FALSE
Decimation_Rate = 0

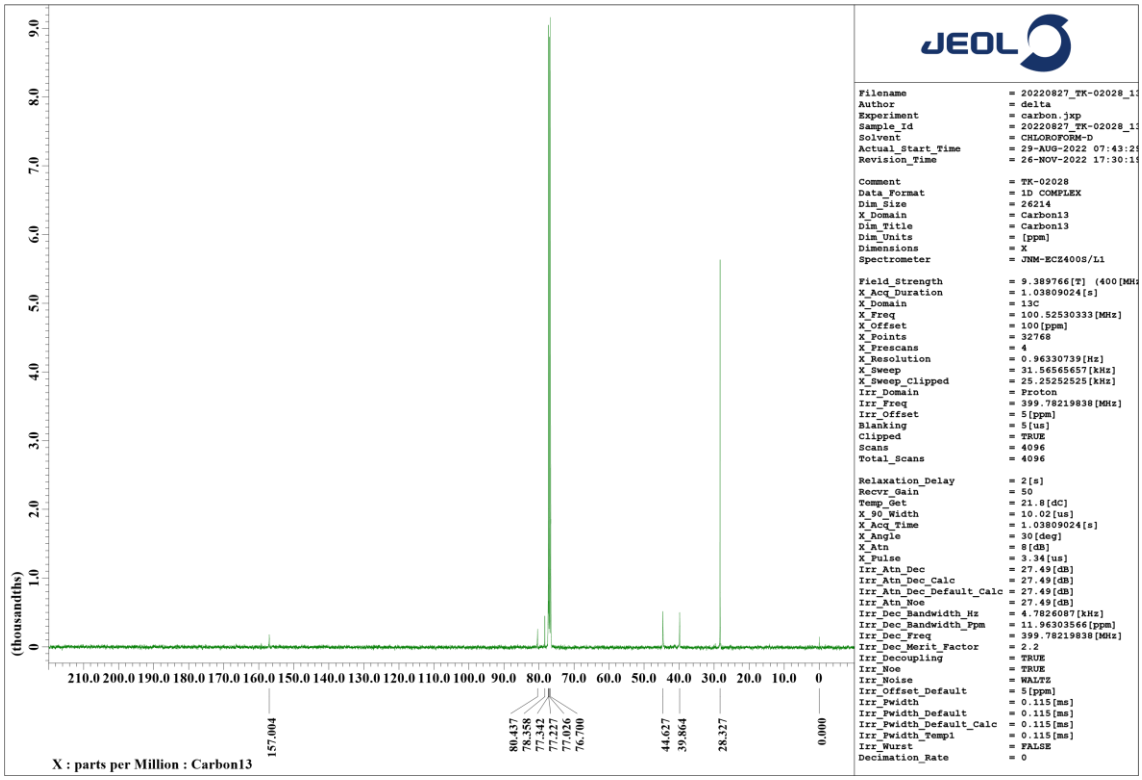

2j
abundance
X : parts per Million : Proton
5.06
2.00
0.91
0.83
7.268
5.296
3.605
3.593
3.580
3.403
3.394
3.389
3.378
3.376
3.363
3.295
1.646
0.000

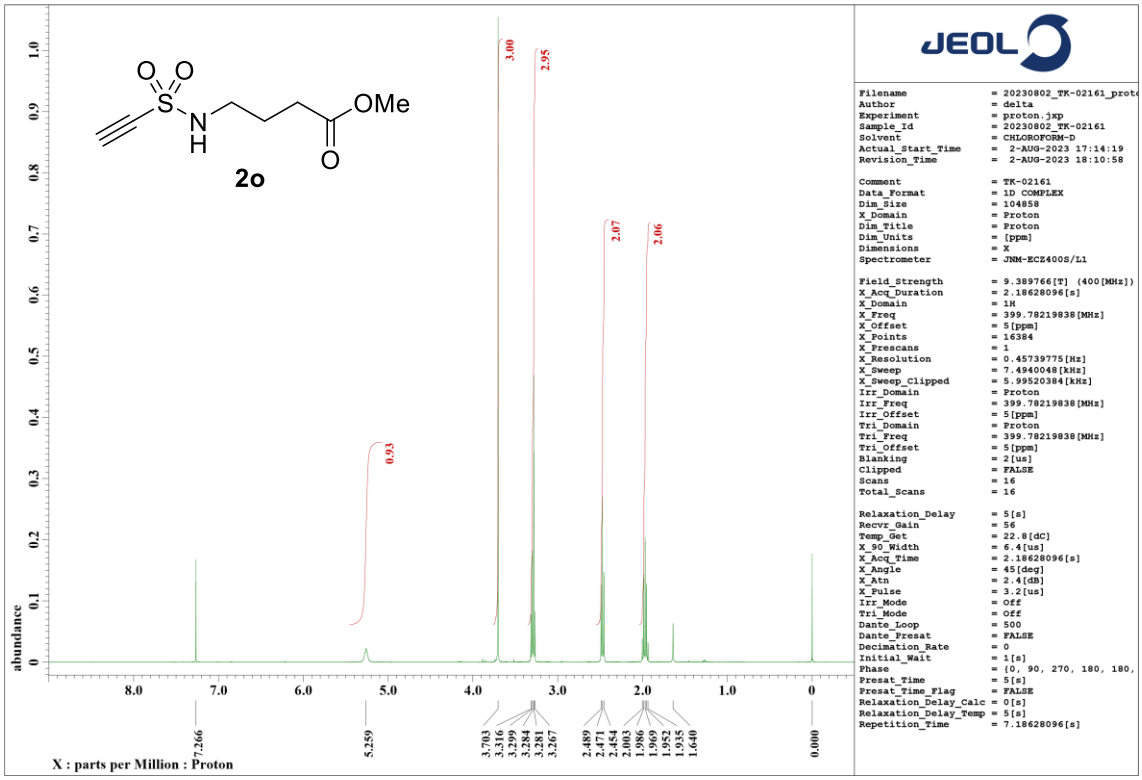

(thousandths)
X : parts per Million : Carbon13
78.243
77.352
77.036
76.901
76.710
69.829
58.905
43.362
0.000

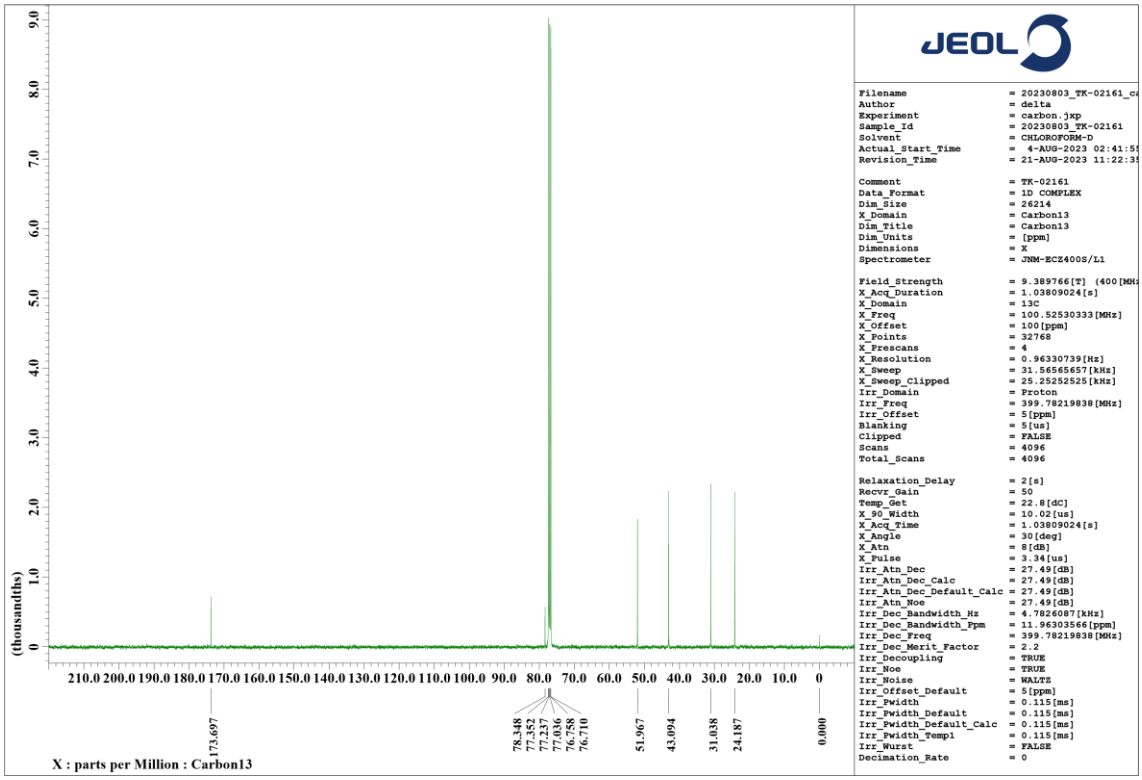

OTBS
2k
9.37
6.15
2.00
2.07
0.91
0.75
abundance
X : parts per Million : Proton
JEOL

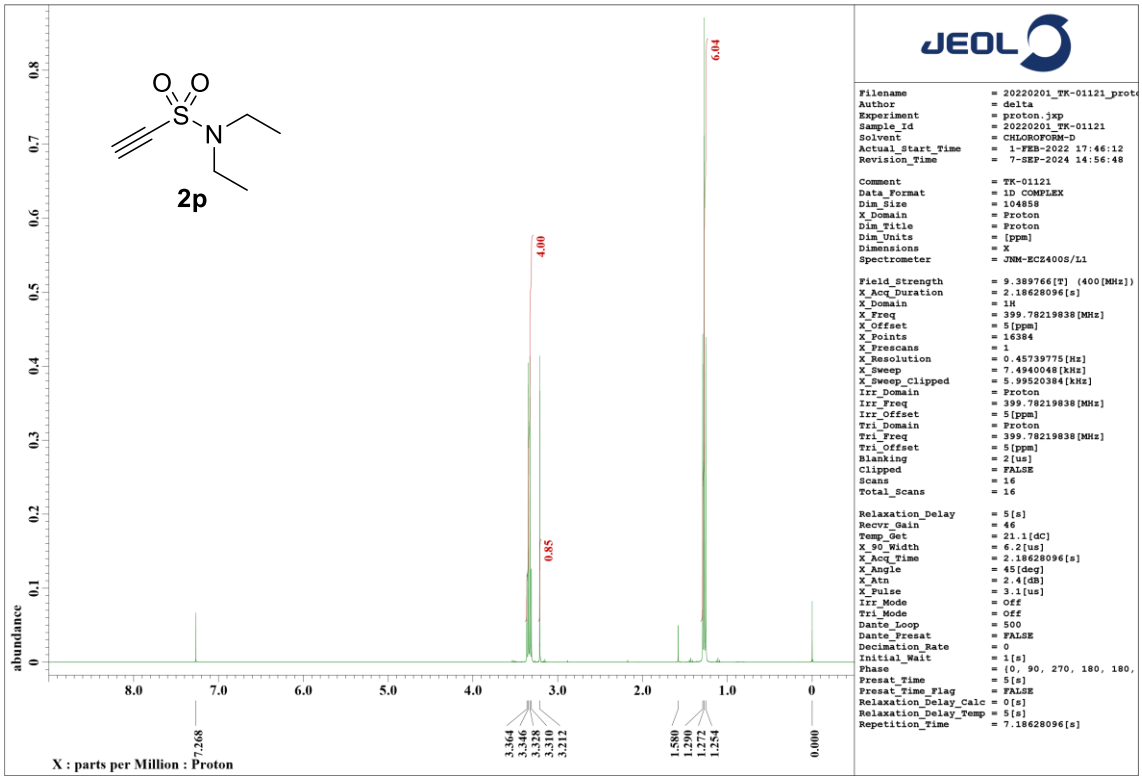

(thousandths)
X : parts per Million : Carbon13
JEOL

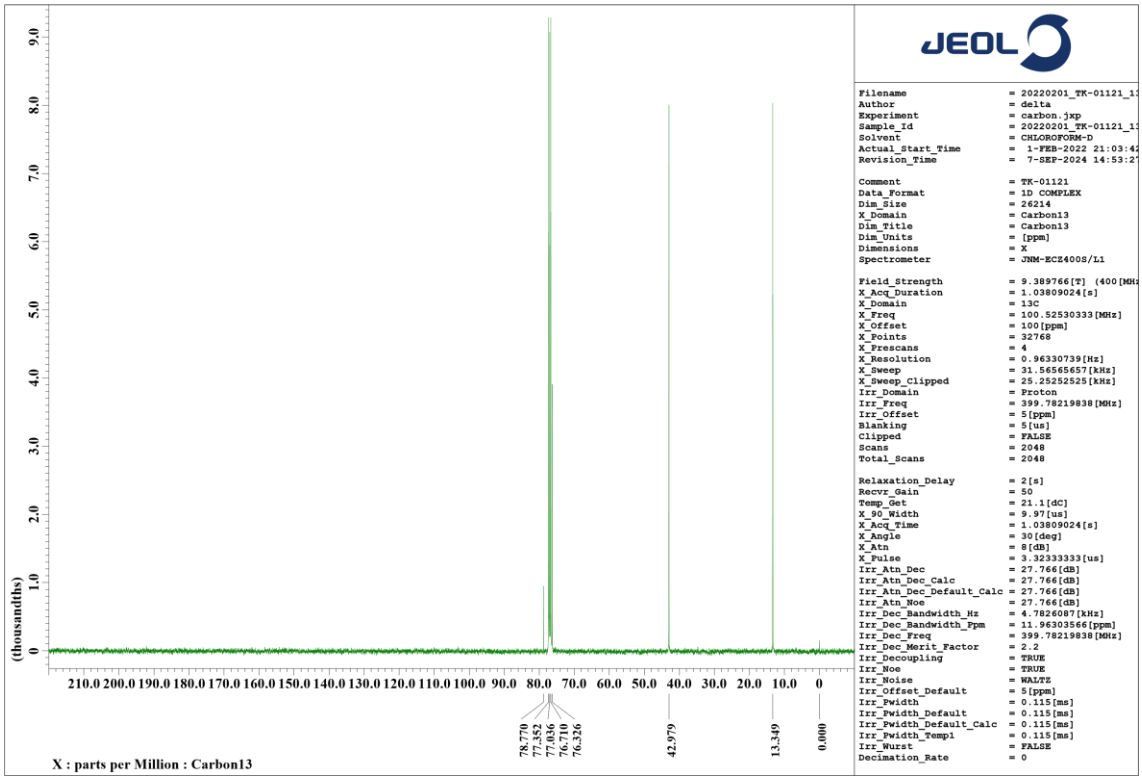

NHBoc
2l
abundance
X : parts per Million : Proton
9.00
4.04
0.80
0.96
0.83
7.266
5.970
4.944
3.377
3.368
3.354
3.343
3.333
3.274
2.049
1.668
1.451
1.253
0.000
JEOL
Filename = 20220827_TK-02028_prot
Author = delta
Experiment = proton.jxp
Sample_Id = 20220827_TK-02028
Solvent = CHLOROFORM-D
Actual_Start_Time = 27-AUG-2022 16:27:33
Revision_Time = 26-NOV-2022 17:27:42
Comment = TK-02028
Data_Format = 1D COMPLEX
Dim_Size = 104858
X_Domain = Proton
Dim_Title = Proton
Dim_Units = [ppm]
Dimensions = X
Spectrometer = JNM-ECZ400S/L1
Field_Strength = 9.389766[T] (400[MHz])
X_Acq_Duration = 2.18628096[s]
X_Domain = 1H
X_Freq = 399.78219838[MHz]
X_Offset = 5[ppm]
X_Points = 16384
X_Prescans = 1
X_Resolution = 0.45739775[Hz]
X_Sweep = 7.4940048[kHz]
X_Sweep_Clipped = 5.99520384[kHz]
Irr_Domain = Proton
Irr_Freq = 399.78219838[MHz]
Irr_Offset = 5[ppm]
Tri_Domain = Proton
Tri_Freq = 399.78219838[MHz]
Tri_Offset = 5[ppm]
Blanking = 2[us]
Clipped = FALSE
Scans = 16
Total_Scans = 16
Relaxation_Delay = 5[s]
Recvr_Gain = 46
Temp_Get = 21.8[dC]
X_90_Width = 6.4[us]
X_Acq_Time = 2.18628096[s]
X_Angle = 45[deg]
X_Atn = 2.4[dB]
X_Pulse = 3.2[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Loop = 500
Dante_Presat = FALSE
Decimation_Rate = 0
Initial_Wait = 1[s]
Phase = (0, 90, 270, 180, 180,
Presat_Time = 5[s]
Presat_Time_Flag = FALSE
Relaxation_Delay_Calc = 0[s]
Relaxation_Delay_Temp = 5[s]
Repetition_Time = 7.18628096[s]

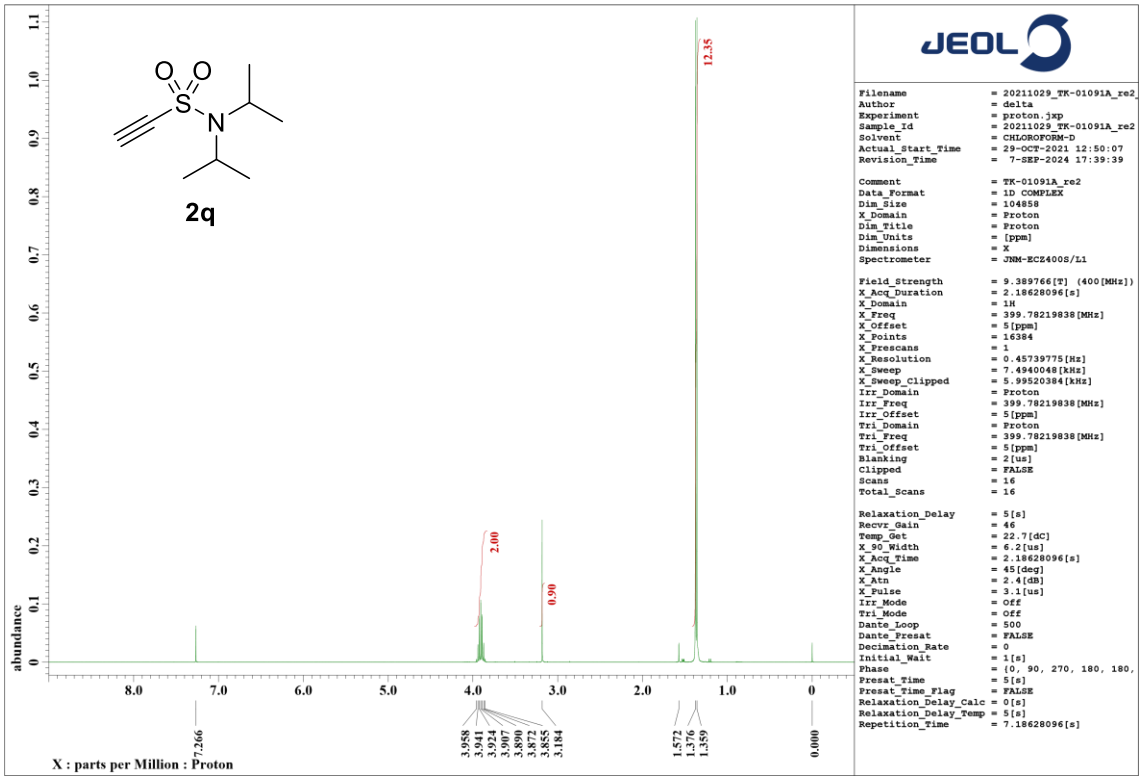

(thousandths)
X : parts per Million : Carbon13
157.004
80.437
78.358
77.342
77.227
77.026
76.700
44.627
39.864
28.327
0.000
JEOL
Filename = 20220827_TK-02028_1
Author = delta
Experiment = carbon.jxp
Sample_Id = 20220827_TK-02028_1
Solvent = CHLOROFORM-D
Actual_Start_Time = 29-AUG-2022 07:43:2
Revision_Time = 26-NOV-2022 17:30:1
Comment = TK-02028
Data_Format = 1D COMPLEX
Dim_Size = 26214
X_Domain = Carbon13
Dim_Title = Carbon13
Dim_Units = [ppm]
Dimensions = X
Spectrometer = JNM-ECZ400S/L1
Field_Strength = 9.389766[T] (400[MH
X_Acq_Duration = 1.03809024[s]
X_Domain = 13C
X_Freq = 100.52530333[MHz]
X_Offset = 100[ppm]
X_Points = 32768
X_Prescans = 4
X_Resolution = 0.96330739[Hz]
X_Sweep = 31.56565657[kHz]
X_Sweep_Clipped = 25.25252525[kHz]
Irr_Domain = Proton
Irr_Freq = 399.78219838[MHz]
Irr_Offset = 5[ppm]
Blanking = 5[us]
Clipped = TRUE
Scans = 4096
Total_Scans = 4096
Relaxation_Delay = 2[s]
Recvr_Gain = 50
Temp_Get = 21.8[dC]
X_90_Width = 10.02[us]
X_Acq_Time = 1.03809024[s]
X_Angle = 30[deg]
X_Atn = 8[dB]
X_Pulse = 3.34[us]
Irr_Atn_Dec = 27.49[dB]
Irr_Atn_Dec_Calc = 27.49[dB]
Irr_Atn_Dec_Default_Calc = 27.49[dB]
Irr_Atn_Noe = 27.49[dB]
Irr_Dec_Bandwidth_Hz = 4.7826087[kHz]
Irr_Dec_Bandwidth_Ppm = 11.96303566[ppm]
Irr_Dec_Freq = 399.78219838[MHz]
Irr_Dec_Merit_Factor = 2.2
Irr_Decoupling = TRUE
Irr_Noe = TRUE
Irr_Noise = WALTZ
Irr_Offset_Default = 5[ppm]
Irr_Pwidth = 0.115[ms]
Irr_Pwidth_Default = 0.115[ms]
Irr_Pwidth_Default_Calc = 0.115[ms]
Irr_Pwidth_Temp1 = 0.115[ms]
Irr_Wurst = FALSE
Decimation_Rate = 0


2o
3.00
2.95
2.07
2.06
0.93
abundance
X : parts per Million : Proton
7.266
5.259
3.703
3.316
3.299
3.284
3.281
3.267
2.489
2.471
2.454
2.003
1.986
1.969
1.952
1.935
1.640
0.000


(thousandths)
X : parts per Million : Carbon13
173.697
78.348
77.352
77.237
77.036
76.758
76.710
51.967
43.094
31.038
24.187
0.000

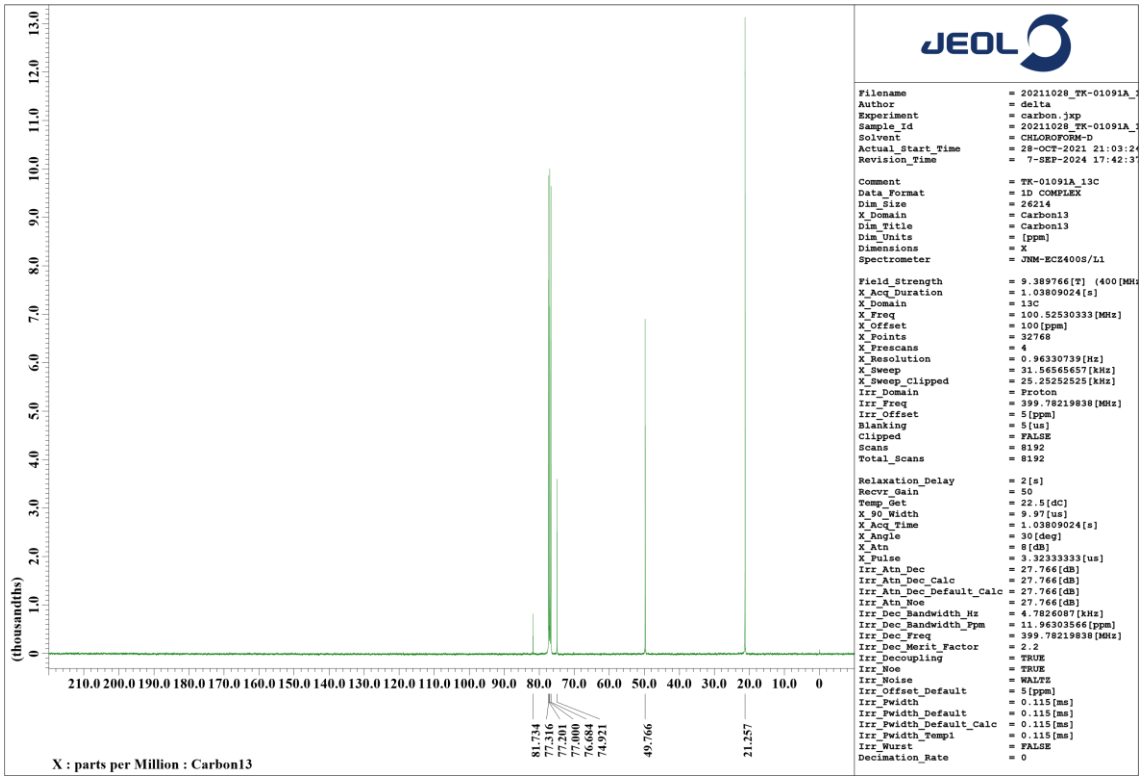

2p
6.04
4.00
0.85
abundance
X : parts per Million : Proton
7.268
3.364
3.346
3.328
3.310
3.212
1.580
1.270
1.272
1.254
0.000
Filename = 20220201_TK-01121_prot
Author = delta
Experiment = proton.jxp
Sample_Id = 20220201_TK-01121
Solvent = CHLOROFORM-D
Actual_Start_Time = 1-FEB-2022 17:46:12
Revision_Time = 7-SEP-2024 14:56:48
Comment = TK-01121
Data_Format = 1D COMPLEX
Dim_Size = 104858
X_Domain = Proton
Dim_Title = Proton
Dim_Units = [ppm]
Dimensions = X
Spectrometer = JNM-ECZ400S/L1
Field_Strength = 9.389766[T] (400[MHz])
X_Acq_Duration = 2.18628096[s]
X_Domain = 1H
X_Freq = 399.78219838[MHz]
X_Offset = 5[ppm]
X_Points = 16384
X_Prescans = 1
X_Resolution = 0.45739775[Hz]
X_Sweep = 7.4940048[kHz]
X_Sweep_Clipped = 5.99520384[kHz]
Irr_Domain = Proton
Irr_Freq = 399.78219838[MHz]
Irr_Offset = 5[ppm]
Tri_Domain = Proton
Tri_Freq = 399.78219838[MHz]
Tri_Offset = 5[ppm]
Blanking = 2[us]
Clipped = FALSE
Scans = 16
Total_Scans = 16
Relaxation_Delay = 5[s]
Recvr_Gain = 46
Temp_Get = 21.1[dC]
X_90_Width = 6.2[us]
X_Acq_Time = 2.18628096[s]
X_Angle = 45[deg]
X_Atn = 2.4[dB]
X_Pulse = 3.1[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Loop = 500
Dante_Presat = FALSE
Decimation_Rate = 0
Initial_Wait = 1[s]
Phase = (0, 90, 270, 180, 180,
Presat_Time = 5[s]
Presat_Time_Flag = FALSE
Relaxation_Delay_Calc = 0[s]
Relaxation_Delay_Temp = 5[s]
Repetition_Time = 7.18628096[s]


(thousandths)
X : parts per Million : Carbon13
78.770
77.352
77.036
76.710
76.326
42.979
13.349
0.000
Filename = 20220201_TK-01121_1
Author = delta
Experiment = carbon.jxp
Sample_Id = 20220201_TK-01121_1
Solvent = CHLOROFORM-D
Actual_Start_Time = 1-FEB-2022 21:03:4
Revision_Time = 7-SEP-2024 14:53:2
Comment = TK-01121
Data_Format = 1D COMPLEX
Dim_Size = 26214
X_Domain = Carbon13
Dim_Title = Carbon13
Dim_Units = [ppm]
Dimensions = X
Spectrometer = JNM-ECZ400S/L1
Field_Strength = 9.389766[T] (400[MH
X_Acq_Duration = 1.03809024[s]
X_Domain = 13C
X_Freq = 100.52530333[MHz]
X_Offset = 100[ppm]
X_Points = 32768
X_Prescans = 4
X_Resolution = 0.96330739[Hz]
X_Sweep = 31.56565657[kHz]
X_Sweep_Clipped = 25.25252525[kHz]
Irr_Domain = Proton
Irr_Freq = 399.78219838[MHz]
Irr_Offset = 5[ppm]
Blanking = 5[us]
Clipped = FALSE
Scans = 2048
Total_Scans = 2048
Relaxation_Delay = 2[s]
Recvr_Gain = 50
Temp_Get = 21.1[dC]
X_90_Width = 9.97[us]
X_Acq_Time = 1.03809024[s]
X_Angle = 30[deg]
X_Atn = 8[dB]
X_Pulse = 3.32333333[us]
Irr_Atn_Dec = 27.766[dB]
Irr_Atn_Dec_Calc = 27.766[dB]
Irr_Atn_Dec_Default_Calc = 27.766[dB]
Irr_Atn_Noe = 27.766[dB]
Irr_Dec_Bandwidth_Hz = 4.7826087[kHz]
Irr_Dec_Bandwidth_Ppm = 11.96303566[ppm]
Irr_Dec_Freq = 399.78219838[MHz]
Irr_Dec_Merit_Factor = 2.2
Irr_Decoupling = TRUE
Irr_Noe = TRUE
Irr_Noise = WALTZ
Irr_Offset_Default = 5[ppm]
Irr_Pwidth = 0.115[ms]
Irr_Pwidth_Default = 0.115[ms]
Irr_Pwidth_Default_Calc = 0.115[ms]
Irr_Pwidth_Temp1 = 0.115[ms]
Irr_Wurst = FALSE
Decimation_Rate = 0



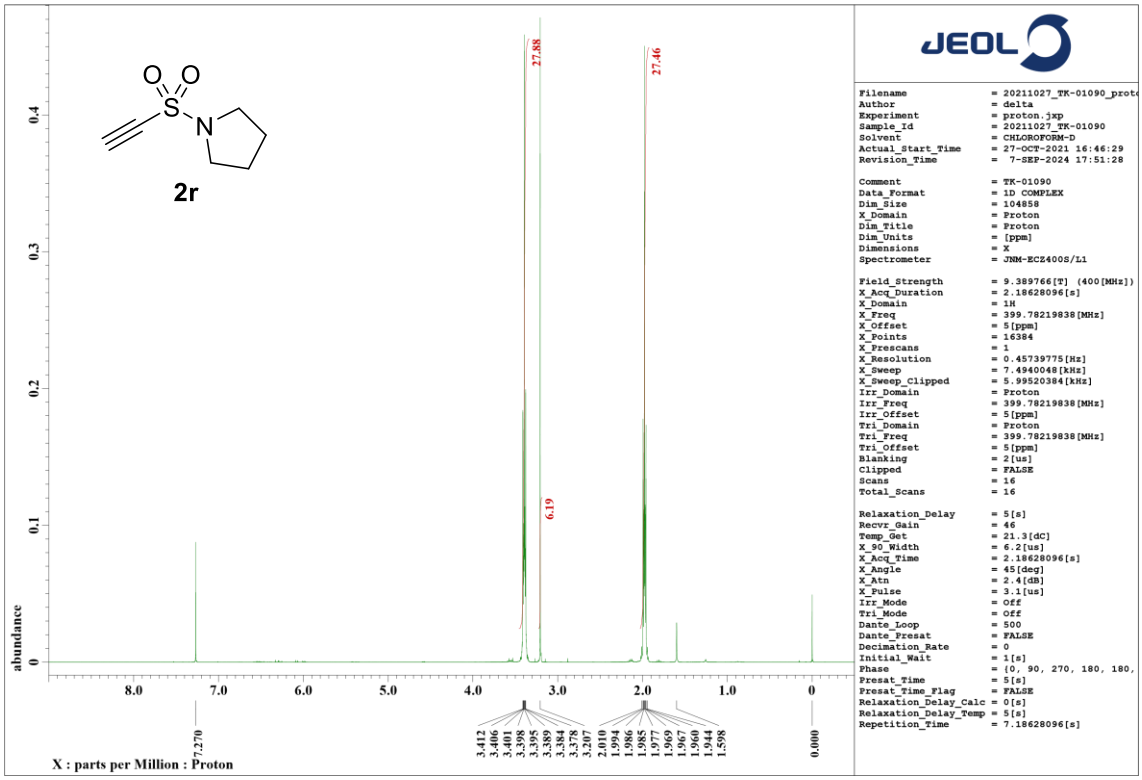
JEOL

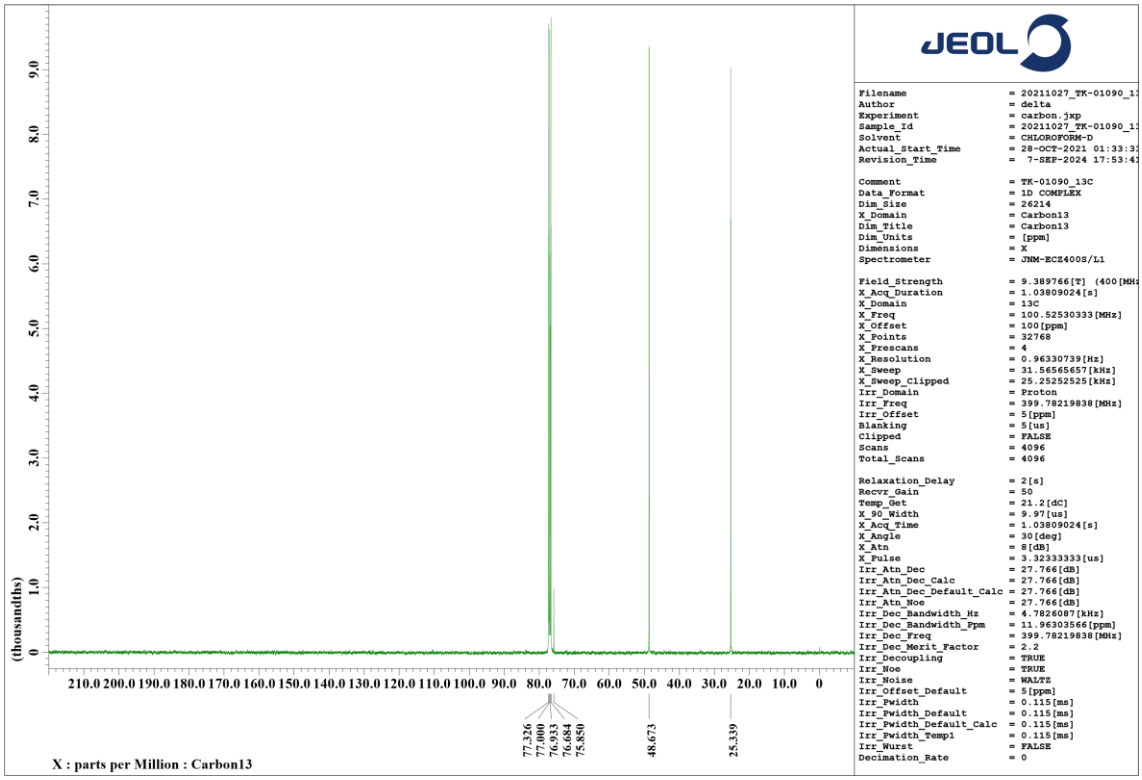
```
Filename                = 20211029_TK-01091A_re2_
Author                  = delta
Experiment              = proton.jxp
Sample_Id               = 20211029_TK-01091A_re2
Solvent                 = CHLOROFORM-D
Actual_Start_Time       = 29-OCT-2021 12:50:07
Revision_Time           =  7-SEP-2024 17:39:39

Comment                 = TK-01091A_re2
Data_Format             = 1D COMPLEX
Dim_Size                = 104858
X_Domain                = Proton
Dim_Title               = Proton
Dim_Units               = [ppm]
Dimensions              = X
Spectrometer            = JNM-ECZ400S/L1

Field_Strength          = 9.389766[T] (400[MHz])
X_Acq_Duration          = 2.18628096[s]
X_Domain                = 1H
X_Freq                  = 399.78219838[MHz]
X_Offset                = 5[ppm]
X_Points                = 16384
X_Prescans              = 1
X_Resolution            = 0.45739775[Hz]
X_Sweep                 = 7.4940048[kHz]
X_Sweep_Clipped         = 5.99520384[kHz]
Irr_Domain              = Proton
Irr_Freq                = 399.78219838[MHz]
Irr_Offset              = 5[ppm]
Tri_Domain              = Proton
Tri_Freq                = 399.78219838[MHz]
Tri_Offset              = 5[ppm]
Blanking                = 2[us]
Clipped                 = FALSE
Scans                   = 16
Total_Scans             = 16

Relaxation_Delay        = 5[s]
Recvr_Gain              = 46
Temp_Get                = 22.7[dC]
X_90_Width              = 6.2[us]
X_Acq_Time              = 2.18628096[s]
X_Angle                 = 45[deg]
X_Atn                   = 2.4[dB]
X_Pulse                 = 3.1[us]
Irr_Mode                = Off
Tri_Mode                = Off
Dante_Loop              = 500
Dante_Presat            = FALSE
Decimation_Rate         = 0
Initial_Wait            = 1[s]
Phase                   = (0, 90, 270, 180, 180,
Presat_Time             = 5[s]
Presat_Time_Flag        = FALSE
Relaxation_Delay_Calc   = 0[s]
Relaxation_Delay_Temp   = 5[s]
Repetition_Time         = 7.18628096[s]
```

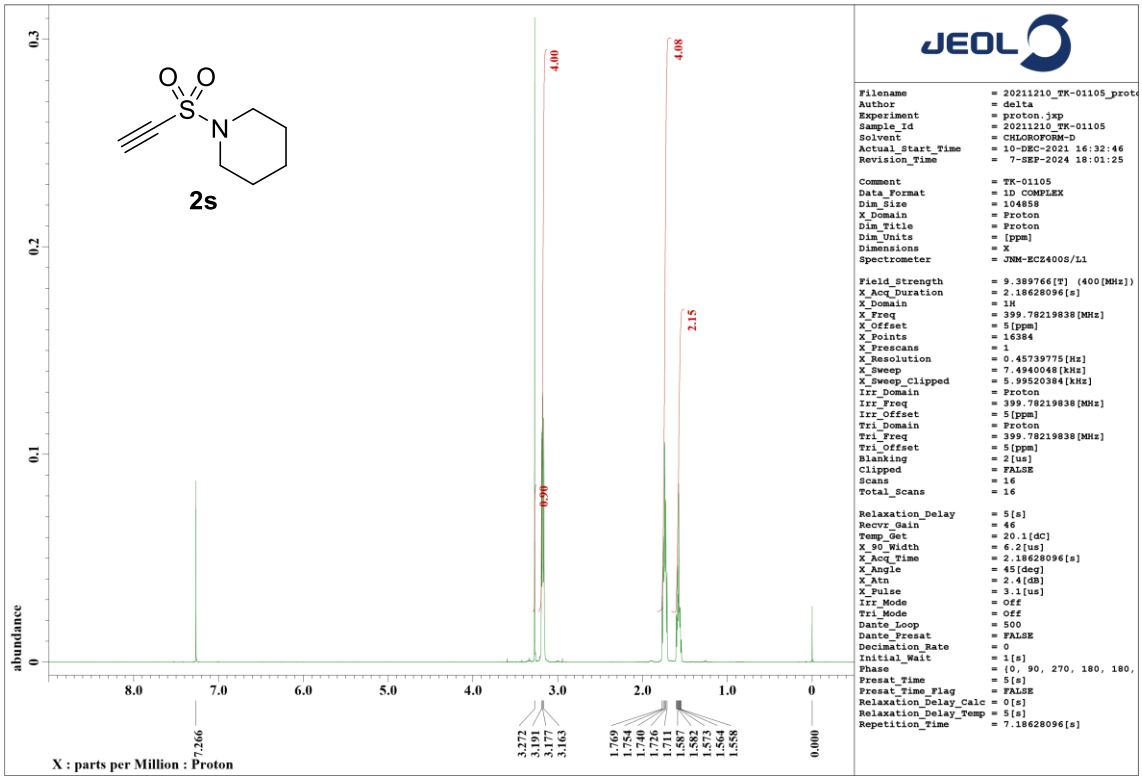


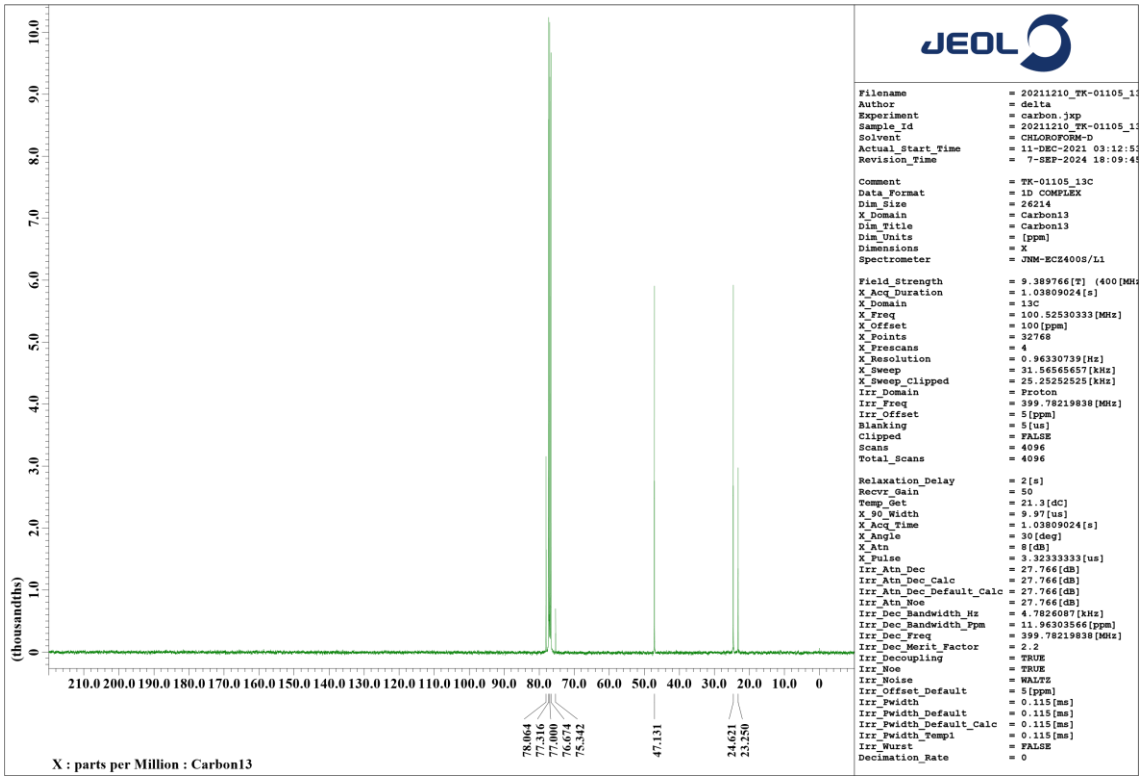
JEOL

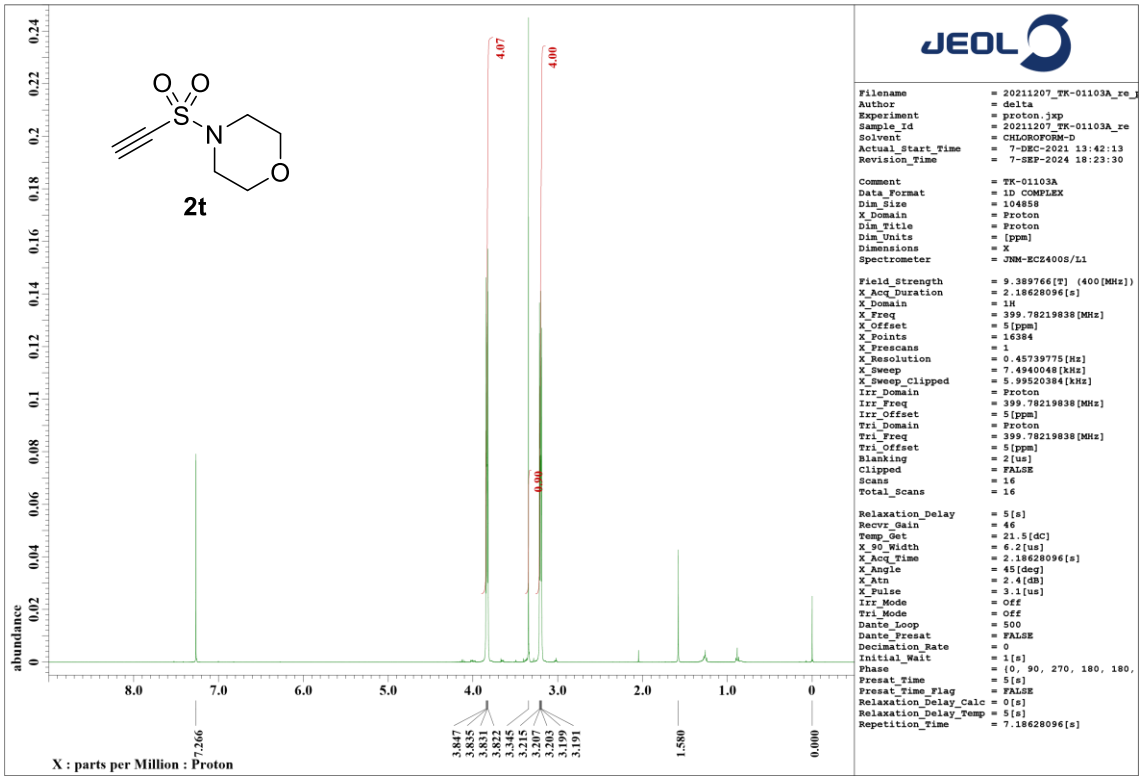
```
Filename                = 20211028_TK-01091A_1
Author                  = delta
Experiment              = carbon.jxp
Sample_Id               = 20211028_TK-01091A_1
Solvent                 = CHLOROFORM-D
Actual_Start_Time       = 28-OCT-2021 21:03:24
Revision_Time           =  7-SEP-2024 17:42:37

Comment                 = TK-01091A_13C
Data_Format             = 1D COMPLEX
Dim_Size                = 26214
X_Domain                = Carbon13
Dim_Title               = Carbon13
Dim_Units               = [ppm]
Dimensions              = X
Spectrometer            = JNM-ECZ400S/L1

Field_Strength          = 9.389766[T] (400[MHz
X_Acq_Duration          = 1.03809024[s]
X_Domain                = 13C
X_Freq                  = 100.52530333[MHz]
X_Offset                = 100[ppm]
X_Points                = 32768
X_Prescans              = 4
X_Resolution            = 0.96330739[Hz]
X_Sweep                 = 31.56565657[kHz]
X_Sweep_Clipped         = 25.25252525[kHz]
Irr_Domain              = Proton
Irr_Freq                = 399.78219838[MHz]
Irr_Offset              = 5[ppm]
Blanking                = 5[us]
Clipped                 = FALSE
Scans                   = 8192
Total_Scans             = 8192

Relaxation_Delay        = 2[s]
Recvr_Gain              = 50
Temp_Get                = 22.5[dC]
X_90_Width              = 9.97[us]
X_Acq_Time              = 1.03809024[s]
X_Angle                 = 30[deg]
X_Atn                   = 8[dB]
X_Pulse                 = 3.32333333[us]
Irr_Atn_Dec             = 27.766[dB]
Irr_Atn_Dec_Calc        = 27.766[dB]
Irr_Atn_Dec_Default_Calc = 27.766[dB]
Irr_Atn_Noe             = 27.766[dB]
Irr_Dec_Bandwidth_Hz    = 4.7826087[kHz]
Irr_Dec_Bandwidth_Ppm   = 11.96303566[ppm]
Irr_Dec_Freq            = 399.78219838[MHz]
Irr_Dec_Merit_Factor    = 2.2
Irr_Decoupling          = TRUE
Irr_Noe                 = TRUE
Irr_Noise               = WALTZ
Irr_Offset_Default      = 5[ppm]
Irr_Pwidth              = 0.115[ms]
Irr_Pwidth_Default      = 0.115[ms]
Irr_Pwidth_Default_Calc = 0.115[ms]
Irr_Pwidth_Temp1        = 0.115[ms]
Irr_Wurst               = FALSE
Decimation_Rate         = 0
```

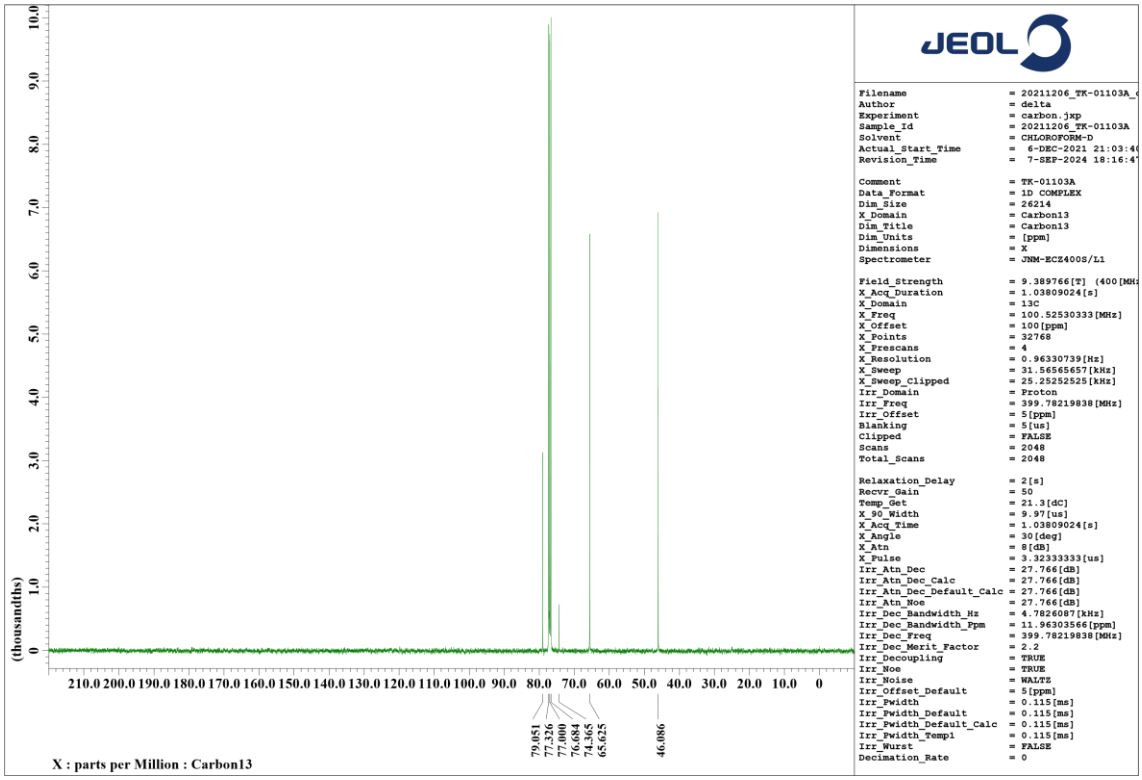

2r
abundance
X : parts per Million : Proton
27.88
27.46
6.19
7.270
3.412
3.406
3.401
3.398
3.395
3.389
3.384
3.378
3.207
2.010
1.994
1.986
1.985
1.977
1.969
1.967
1.960
1.944
1.598
0.000
Filename = 20211027_TK-01090_prot
Author = delta
Experiment = proton.jxp
Sample_Id = 20211027_TK-01090
Solvent = CHLOROFORM-D
Actual_Start_Time = 27-OCT-2021 16:46:29
Revision_Time = 7-SEP-2024 17:51:28
Comment = TK-01090
Data_Format = 1D COMPLEX
Dim_Size = 104858
X_Domain = Proton
Dim_Title = Proton
Dim_Units = [ppm]
Dimensions = X
Spectrometer = JNM-ECZ400S/L1
Field_Strength = 9.389766[T] (400[MHz])
X_Acq_Duration = 2.18628096[s]
X_Domain = 1H
X_Freq = 399.78219838[MHz]
X_Offset = 5[ppm]
X_Points = 16384
X_Prescans = 1
X_Resolution = 0.45739775[Hz]
X_Sweep = 7.4940048[kHz]
X_Sweep_Clipped = 5.99520384[kHz]
Irr_Domain = Proton
Irr_Freq = 399.78219838[MHz]
Irr_Offset = 5[ppm]
Tri_Domain = Proton
Tri_Freq = 399.78219838[MHz]
Tri_Offset = 5[ppm]
Blanking = 2[us]
Clipped = FALSE
Scans = 16
Total_Scans = 16
Relaxation_Delay = 5[s]
Recvr_Gain = 46
Temp_Get = 21.3[dC]
X_90_Width = 6.2[us]
X_Acq_Time = 2.18628096[s]
X_Angle = 45[deg]
X_Atn = 2.4[dB]
X_Pulse = 3.1[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Loop = 500
Dante_Presat = FALSE
Decimation_Rate = 0
Initial_Wait = 1[s]
Phase = (0, 90, 270, 180, 180,
Presat_Time = 5[s]
Presat_Time_Flag = FALSE
Relaxation_Delay_Calc = 0[s]
Relaxation_Delay_Temp = 5[s]
Repetition_Time = 7.18628096[s]

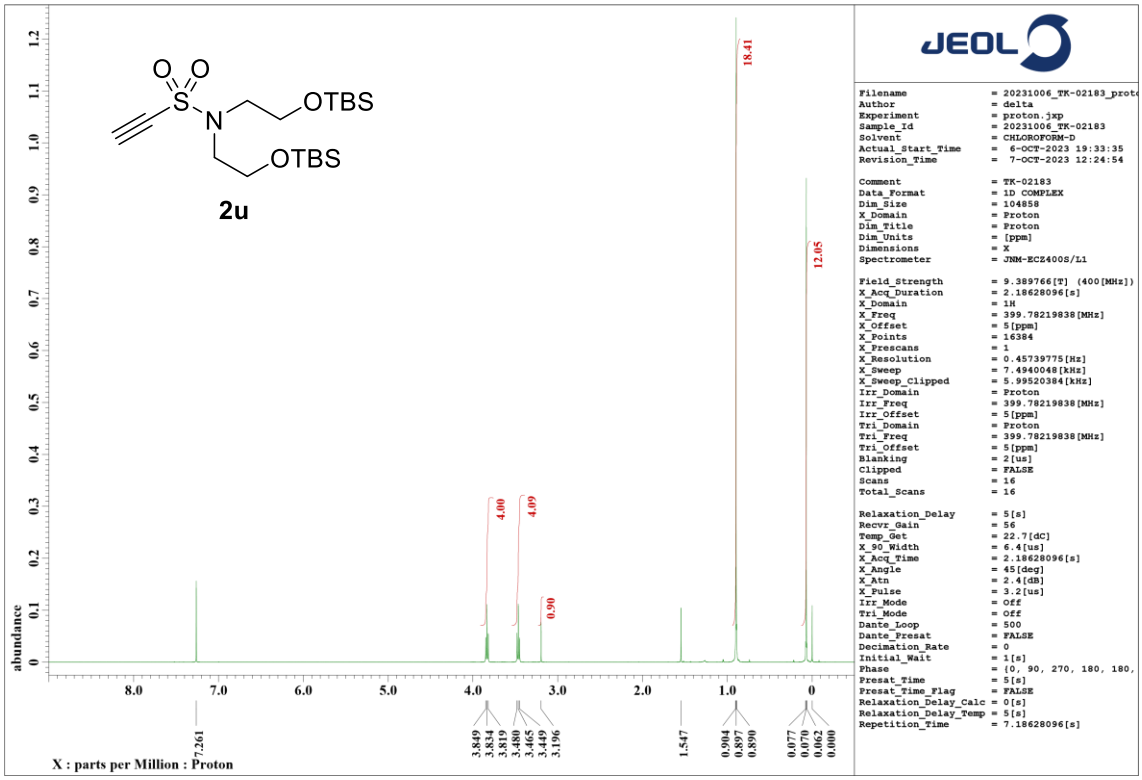

(thousandths)
X : parts per Million : Carbon13
77.326
77.000
76.933
76.684
75.850
48.673
25.339
Filename = 20211027_TK-01090_1
Author = delta
Experiment = carbon.jxp
Sample_Id = 20211027_TK-01090_1
Solvent = CHLOROFORM-D
Actual_Start_Time = 28-OCT-2021 01:33:3
Revision_Time = 7-SEP-2024 17:53:4
Comment = TK-01090_13C
Data_Format = 1D COMPLEX
Dim_Size = 26214
X_Domain = Carbon13
Dim_Title = Carbon13
Dim_Units = [ppm]
Dimensions = X
Spectrometer = JNM-ECZ400S/L1
Field_Strength = 9.389766[T] (400[MH
X_Acq_Duration = 1.03809024[s]
X_Domain = 13C
X_Freq = 100.52530333[MHz]
X_Offset = 100[ppm]
X_Points = 32768
X_Prescans = 4
X_Resolution = 0.96330739[Hz]
X_Sweep = 31.56565657[kHz]
X_Sweep_Clipped = 25.25252525[kHz]
Irr_Domain = Proton
Irr_Freq = 399.78219838[MHz]
Irr_Offset = 5[ppm]
Blanking = 5[us]
Clipped = FALSE
Scans = 4096
Total_Scans = 4096
Relaxation_Delay = 2[s]
Recvr_Gain = 50
Temp_Get = 21.2[dC]
X_90_Width = 9.97[us]
X_Acq_Time = 1.03809024[s]
X_Angle = 30[deg]
X_Atn = 8[dB]
X_Pulse = 3.32333333[us]
Irr_Atn_Dec = 27.766[dB]
Irr_Atn_Dec_Calc = 27.766[dB]
Irr_Atn_Dec_Default_Calc = 27.766[dB]
Irr_Atn_Noe = 27.766[dB]
Irr_Dec_Bandwidth_Hz = 4.7826087[kHz]
Irr_Dec_Bandwidth_Ppm = 11.96303566[ppm]
Irr_Dec_Freq = 399.78219838[MHz]
Irr_Dec_Merit_Factor = 2.2
Irr_Decoupling = TRUE
Irr_Noe = TRUE
Irr_Noise = WALTZ
Irr_Offset_Default = 5[ppm]
Irr_Pwidth = 0.115[ms]
Irr_Pwidth_Default = 0.115[ms]
Irr_Pwidth_Default_Calc = 0.115[ms]
Irr_Pwidth_Temp1 = 0.115[ms]
Irr_Wurst = FALSE
Decimation_Rate = 0

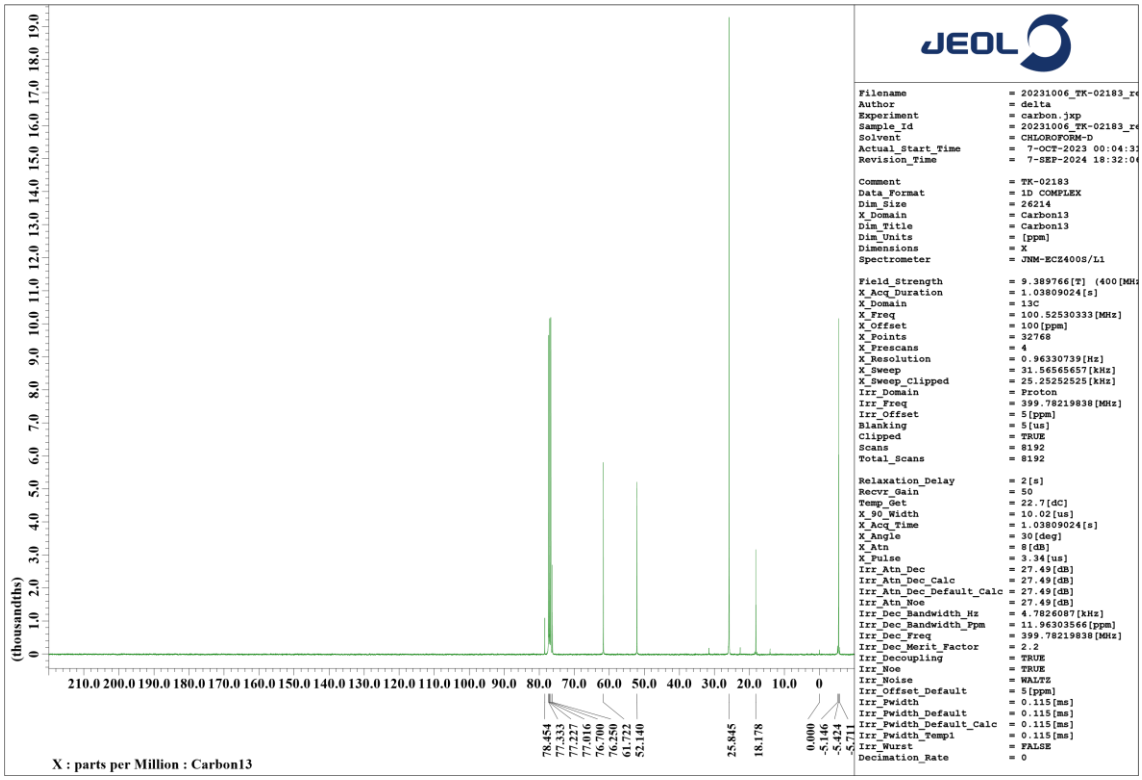

2s
4.00
4.08
2.15
0.90
abundance
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
7.266
3.272
3.191
3.177
3.163
1.769
1.754
1.740
1.726
1.711
1.587
1.582
1.573
1.564
1.558
0.000
X : parts per Million : Proton
JEOL
Filename = 20211210_TK-01105_prot
Author = delta
Experiment = proton.jxp
Sample_Id = 20211210_TK-01105
Solvent = CHLOROFORM-D
Actual_Start_Time = 10-DEC-2021 16:32:46
Revision_Time = 7-SEP-2024 18:01:25
Comment = TK-01105
Data_Format = 1D COMPLEX
Dim_Size = 104858
X_Domain = Proton
Dim_Title = Proton
Dim_Units = [ppm]
Dimensions = X
Spectrometer = JNM-ECZ400S/L1
Field_Strength = 9.389766[T] (400[MHz])
X_Acq_Duration = 2.18628096[s]
X_Domain = 1H
X_Freq = 399.78219838[MHz]
X_Offset = 5[ppm]
X_Points = 16384
X_Prescans = 1
X_Resolution = 0.45739775[Hz]
X_Sweep = 7.4940048[kHz]
X_Sweep_Clipped = 5.99520384[kHz]
Irr_Domain = Proton
Irr_Freq = 399.78219838[MHz]
Irr_Offset = 5[ppm]
Tri_Domain = Proton
Tri_Freq = 399.78219838[MHz]
Tri_Offset = 5[ppm]
Blanking = 2[us]
Clipped = FALSE
Scans = 16
Total_Scans = 16
Relaxation_Delay = 5[s]
Recvr_Gain = 46
Temp_Get = 20.1[dC]
X_90_Width = 6.2[us]
X_Acq_Time = 2.18628096[s]
X_Angle = 45[deg]
X_Atn = 2.4[dB]
X_Pulse = 3.1[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Loop = 500
Dante_Presat = FALSE
Decimation_Rate = 0
Initial_Wait = 1[s]
Phase = (0, 90, 270, 180, 180,
Presat_Time = 5[s]
Presat_Time_Flag = FALSE
Relaxation_Delay_Calc = 0[s]
Relaxation_Delay_Temp = 5[s]
Repetition_Time = 7.18628096[s]

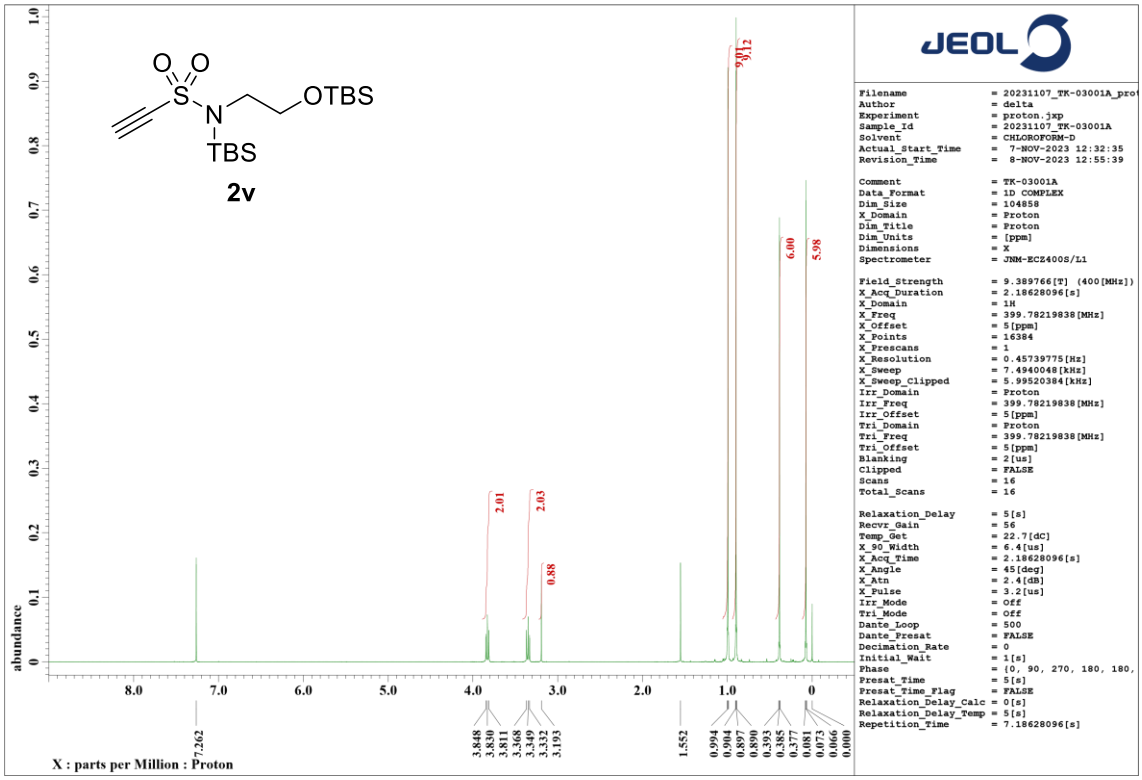

(thousandths)
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
210.0 200.0 190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0
78.064
77.316
77.000
76.674
75.342
47.131
24.621
23.250
X : parts per Million : Carbon13
JEOL
Filename = 20211210_TK-01105_1
Author = delta
Experiment = carbon.jxp
Sample_Id = 20211210_TK-01105_1
Solvent = CHLOROFORM-D
Actual_Start_Time = 11-DEC-2021 03:12:5
Revision_Time = 7-SEP-2024 18:09:4
Comment = TK-01105_13C
Data_Format = 1D COMPLEX
Dim_Size = 26214
X_Domain = Carbon13
Dim_Title = Carbon13
Dim_Units = [ppm]
Dimensions = X
Spectrometer = JNM-ECZ400S/L1
Field_Strength = 9.389766[T] (400[MH
X_Acq_Duration = 1.03809024[s]
X_Domain = 13C
X_Freq = 100.52530333[MHz]
X_Offset = 100[ppm]
X_Points = 32768
X_Prescans = 4
X_Resolution = 0.96330739[Hz]
X_Sweep = 31.56565657[kHz]
X_Sweep_Clipped = 25.25252525[kHz]
Irr_Domain = Proton
Irr_Freq = 399.78219838[MHz]
Irr_Offset = 5[ppm]
Blanking = 5[us]
Clipped = FALSE
Scans = 4096
Total_Scans = 4096
Relaxation_Delay = 2[s]
Recvr_Gain = 50
Temp_Get = 21.3[dC]
X_90_Width = 9.97[us]
X_Acq_Time = 1.03809024[s]
X_Angle = 30[deg]
X_Atn = 8[dB]
X_Pulse = 3.32333333[us]
Irr_Atn_Dec = 27.766[dB]
Irr_Atn_Dec_Calc = 27.766[dB]
Irr_Atn_Dec_Default_Calc = 27.766[dB]
Irr_Atn_Noe = 27.766[dB]
Irr_Dec_Bandwidth_Hz = 4.7826087[kHz]
Irr_Dec_Bandwidth_Ppm = 11.96303566[ppm]
Irr_Dec_Freq = 399.78219838[MHz]
Irr_Dec_Merit_Factor = 2.2
Irr_Decoupling = TRUE
Irr_Noe = TRUE
Irr_Noise = WALTZ
Irr_Offset_Default = 5[ppm]
Irr_Pwidth = 0.115[ms]
Irr_Pwidth_Default = 0.115[ms]
Irr_Pwidth_Default_Calc = 0.115[ms]
Irr_Pwidth_Temp1 = 0.115[ms]
Irr_Wurst = FALSE
Decimation_Rate = 0

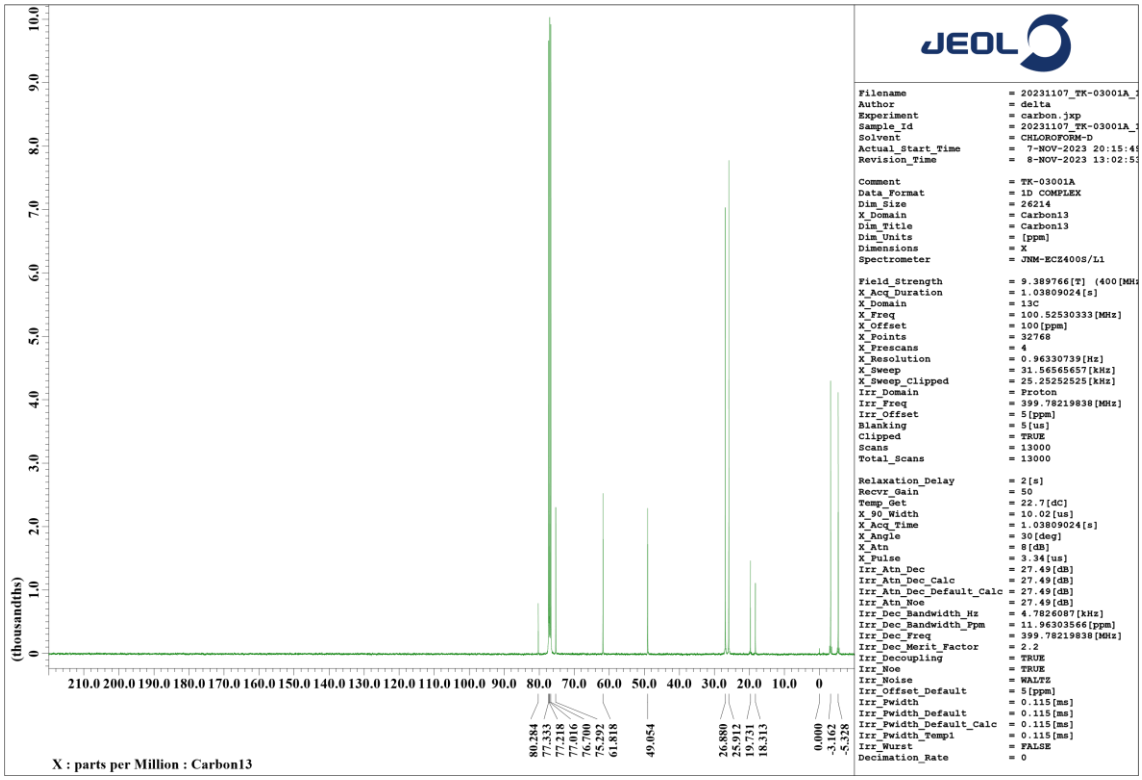

2t
4.07
4.00
0.00
abundance
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
7.266
3.847
3.835
3.831
3.822
3.345
3.215
3.207
3.203
3.199
3.191
1.580
0.000
X : parts per Million : Proton
JEOL
Filename = 20211207_TK-01103A_re_
Author = delta
Experiment = proton.jxp
Sample_Id = 20211207_TK-01103A_re
Solvent = CHLOROFORM-D
Actual_Start_Time = 7-DEC-2021 13:42:13
Revision_Time = 7-SEP-2024 18:23:30
Comment = TK-01103A
Data_Format = 1D COMPLEX
Dim_Size = 104858
X_Domain = Proton
Dim_Title = Proton
Dim_Units = [ppm]
Dimensions = X
Spectrometer = JNM-ECZ400S/L1
Field_Strength = 9.389766[T] (400[MHz])
X_Acq_Duration = 2.18628096[s]
X_Domain = 1H
X_Freq = 399.78219838[MHz]
X_Offset = 5[ppm]
X_Points = 16384
X_Prescans = 1
X_Resolution = 0.45739775[Hz]
X_Sweep = 7.4940048[kHz]
X_Sweep_Clipped = 5.99520384[kHz]
Irr_Domain = Proton
Irr_Freq = 399.78219838[MHz]
Irr_Offset = 5[ppm]
Tri_Domain = Proton
Tri_Freq = 399.78219838[MHz]
Tri_Offset = 5[ppm]
Blanking = 2[us]
Clipped = FALSE
Scans = 16
Total_Scans = 16
Relaxation_Delay = 5[s]
Recvr_Gain = 46
Temp_Get = 21.5[dC]
X_90_Width = 6.2[us]
X_Acq_Time = 2.18628096[s]
X_Angle = 45[deg]
X_Atn = 2.4[dB]
X_Pulse = 3.1[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Loop = 500
Dante_Presat = FALSE
Decimation_Rate = 0
Initial_Wait = 1[s]
Phase = (0, 90, 270, 180, 180,
Presat_Time = 5[s]
Presat_Time_Flag = FALSE
Relaxation_Delay_Calc = 0[s]
Relaxation_Delay_Temp = 5[s]
Repetition_Time = 7.18628096[s]

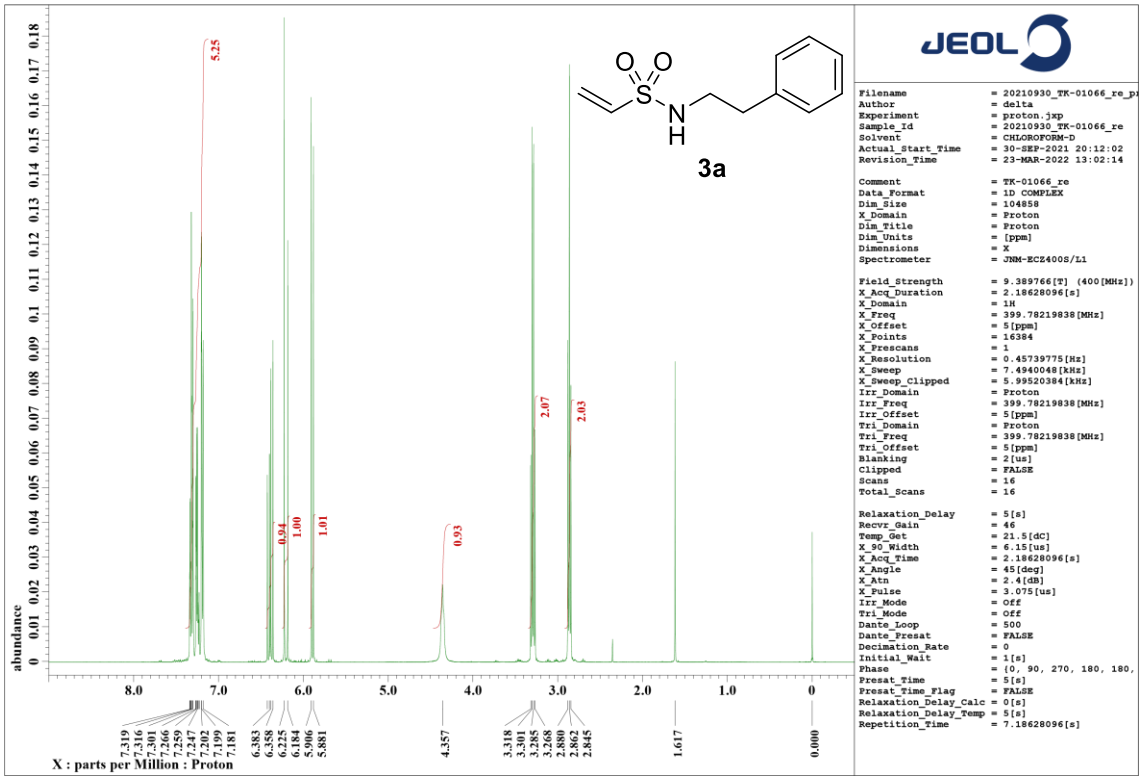

(thousandths)
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
210.0 200.0 190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0
79.051
77.326
77.000
76.684
74.365
65.625
46.086
X : parts per Million : Carbon13
JEOL
Filename = 20211206_TK-01103A_
Author = delta
Experiment = carbon.jxp
Sample_Id = 20211206_TK-01103A
Solvent = CHLOROFORM-D
Actual_Start_Time = 6-DEC-2021 21:03:4
Revision_Time = 7-SEP-2024 18:16:4
Comment = TK-01103A
Data_Format = 1D COMPLEX
Dim_Size = 26214
X_Domain = Carbon13
Dim_Title = Carbon13
Dim_Units = [ppm]
Dimensions = X
Spectrometer = JNM-ECZ400S/L1
Field_Strength = 9.389766[T] (400[MH
X_Acq_Duration = 1.03809024[s]
X_Domain = 13C
X_Freq = 100.52530333[MHz]
X_Offset = 100[ppm]
X_Points = 32768
X_Prescans = 4
X_Resolution = 0.96330739[Hz]
X_Sweep = 31.56565657[kHz]
X_Sweep_Clipped = 25.25252525[kHz]
Irr_Domain = Proton
Irr_Freq = 399.78219838[MHz]
Irr_Offset = 5[ppm]
Blanking = 5[us]
Clipped = FALSE
Scans = 2048
Total_Scans = 2048
Relaxation_Delay = 2[s]
Recvr_Gain = 50
Temp_Get = 21.3[dC]
X_90_Width = 9.97[us]
X_Acq_Time = 1.03809024[s]
X_Angle = 30[deg]
X_Atn = 8[dB]
X_Pulse = 3.32333333[us]
Irr_Atn_Dec = 27.766[dB]
Irr_Atn_Dec_Calc = 27.766[dB]
Irr_Atn_Dec_Default_Calc = 27.766[dB]
Irr_Atn_Noe = 27.766[dB]
Irr_Dec_Bandwidth_Hz = 4.7826087[kHz]
Irr_Dec_Bandwidth_Ppm = 11.96303566[ppm]
Irr_Dec_Freq = 399.78219838[MHz]
Irr_Dec_Merit_Factor = 2.2
Irr_Decoupling = TRUE
Irr_Noe = TRUE
Irr_Noise = WALTZ
Irr_Offset_Default = 5[ppm]
Irr_Pwidth = 0.115[ms]
Irr_Pwidth_Default = 0.115[ms]
Irr_Pwidth_Default_Calc = 0.115[ms]
Irr_Pwidth_Temp1 = 0.115[ms]
Irr_Wurst = FALSE
Decimation_Rate = 0

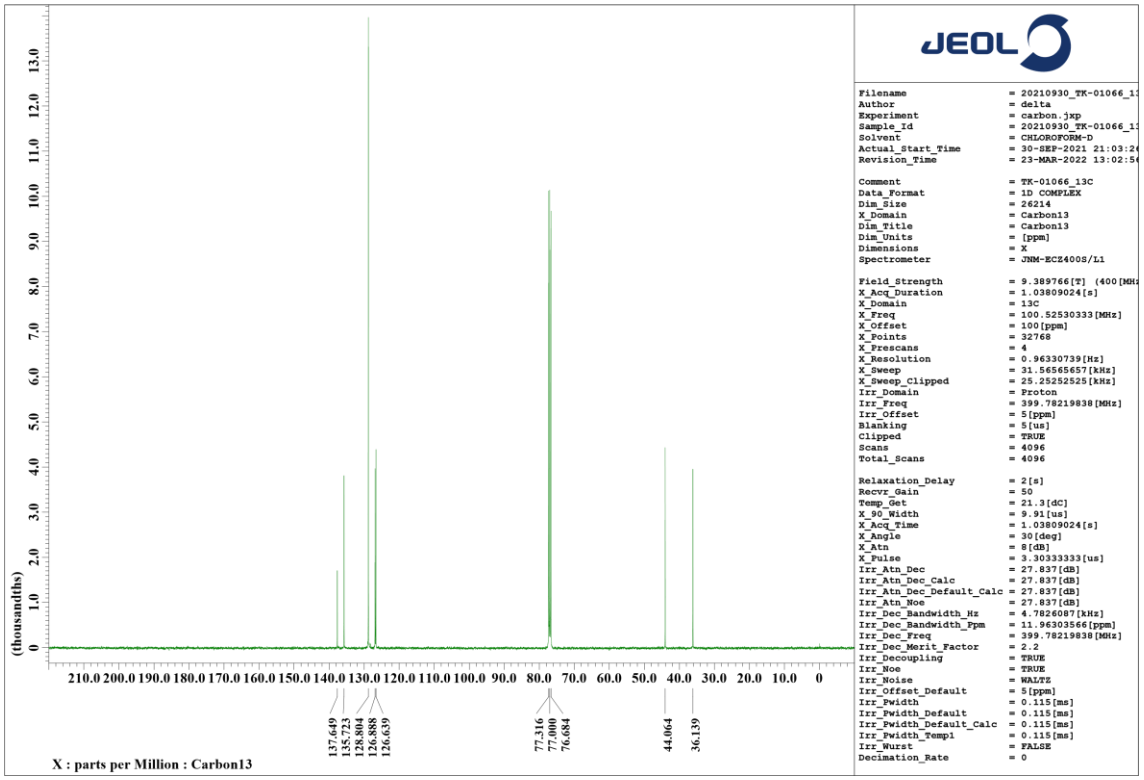

OTBS
OTBS
2u
abundance
X : parts per Million : Proton
JEOL

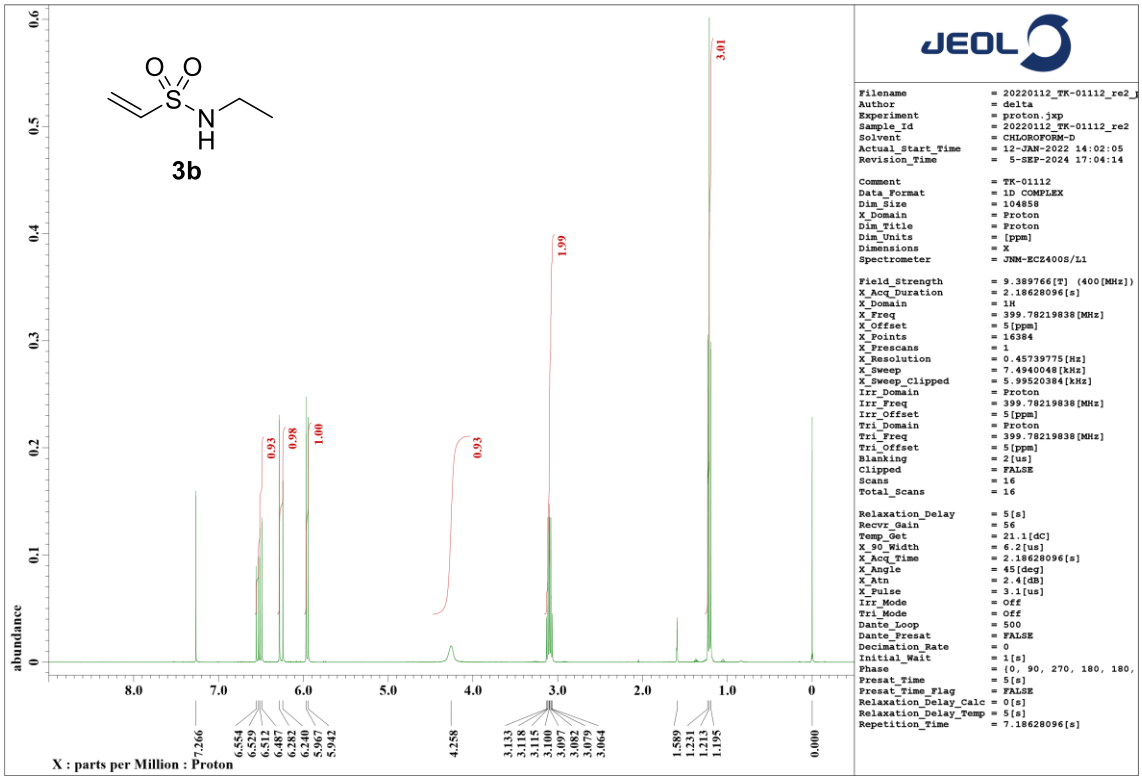

(thousandths)
X : parts per Million : Carbon13
JEOL

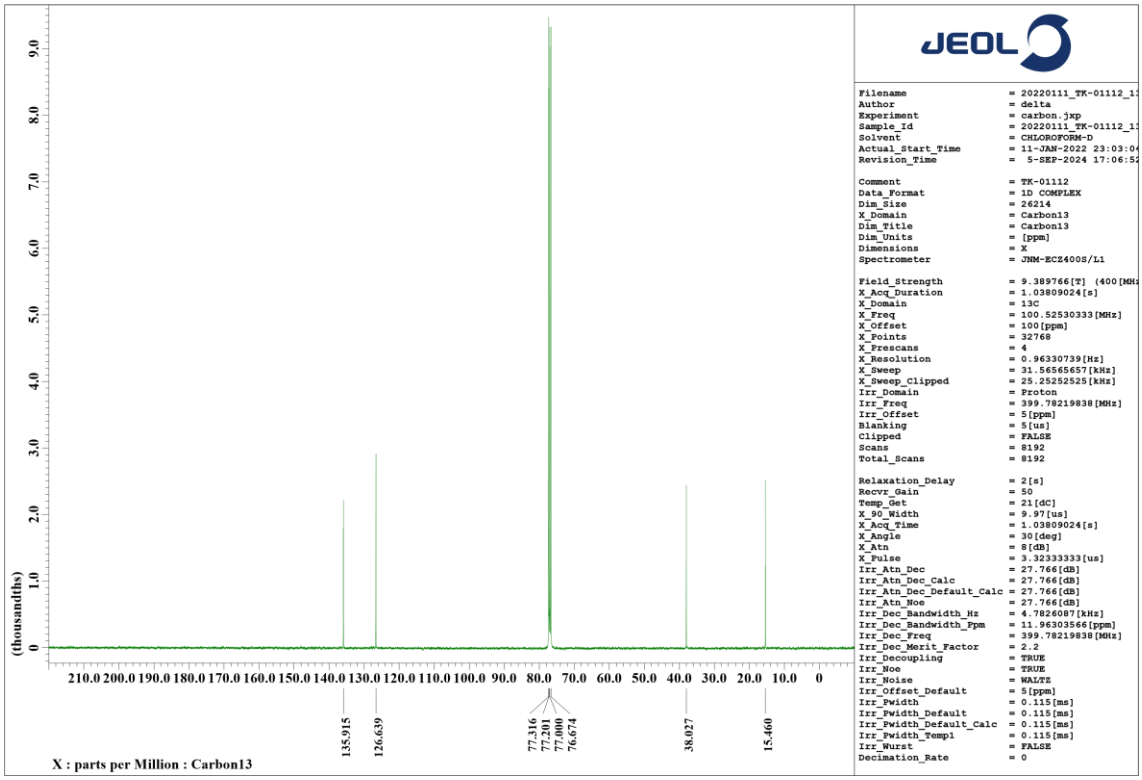

O
O
S
N
OTBS
TBS
2v
abundance
X : parts per Million : Proton
9.12
9.01
6.00
5.98
2.01
2.03
0.88
7.262
3.848
3.830
3.811
3.368
3.349
3.332
3.193
1.552
0.994
0.904
0.897
0.890
0.393
0.385
0.377
0.081
0.073
0.066
0.000
JEOL
Filename = 20231107_TK-03001A_pro
Author = delta
Experiment = proton.jxp
Sample_Id = 20231107_TK-03001A
Solvent = CHLOROFORM-D
Actual_Start_Time = 7-NOV-2023 12:32:35
Revision_Time = 8-NOV-2023 12:55:39
Comment = TK-03001A
Data_Format = 1D COMPLEX
Dim_Size = 104858
X_Domain = Proton
Dim_Title = Proton
Dim_Units = [ppm]
Dimensions = X
Spectrometer = JNM-ECZ400S/L1
Field_Strength = 9.389766[T] (400[MHz])
X_Acq_Duration = 2.18628096[s]
X_Domain = 1H
X_Freq = 399.78219838[MHz]
X_Offset = 5[ppm]
X_Points = 16384
X_Prescans = 1
X_Resolution = 0.45739775[Hz]
X_Sweep = 7.4940048[kHz]
X_Sweep_Clipped = 5.99520384[kHz]
Irr_Domain = Proton
Irr_Freq = 399.78219838[MHz]
Irr_Offset = 5[ppm]
Tri_Domain = Proton
Tri_Freq = 399.78219838[MHz]
Tri_Offset = 5[ppm]
Blanking = 2[us]
Clipped = FALSE
Scans = 16
Total_Scans = 16
Relaxation_Delay = 5[s]
Recvr_Gain = 56
Temp_Get = 22.7[dC]
X_90_Width = 6.4[us]
X_Acq_Time = 2.18628096[s]
X_Angle = 45[deg]
X_Atn = 2.4[dB]
X_Pulse = 3.2[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Loop = 500
Dante_Presat = FALSE
Decimation_Rate = 0
Initial_Wait = 1[s]
Phase = (0, 90, 270, 180, 180,
Presat_Time = 5[s]
Presat_Time_Flag = FALSE
Relaxation_Delay_Calc = 0[s]
Relaxation_Delay_Temp = 5[s]
Repetition_Time = 7.18628096[s]

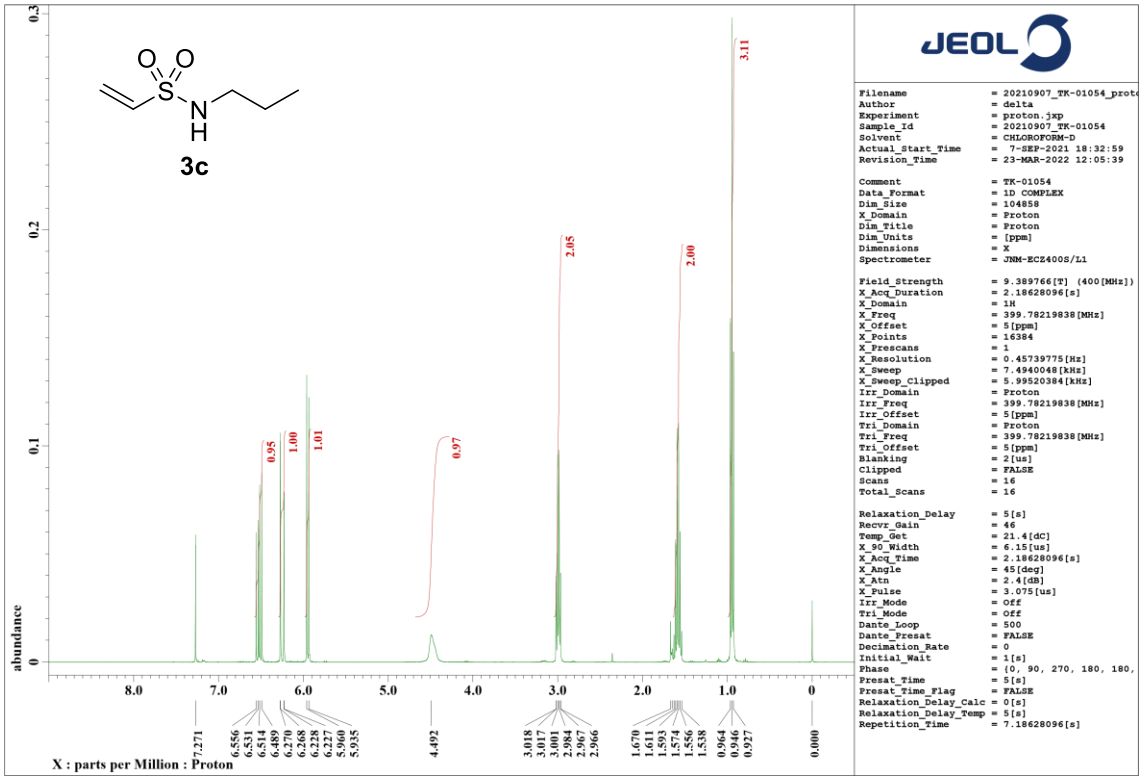

(thousandths)
X : parts per Million : Carbon13
80.284
77.333
77.218
77.016
76.700
75.292
61.818
49.054
26.880
25.912
19.731
18.313
0.000
-3.162
-5.328
JEOL
Filename = 20231107_TK-03001A_1
Author = delta
Experiment = carbon.jxp
Sample_Id = 20231107_TK-03001A_1
Solvent = CHLOROFORM-D
Actual_Start_Time = 7-NOV-2023 20:15:4
Revision_Time = 8-NOV-2023 13:02:5
Comment = TK-03001A
Data_Format = 1D COMPLEX
Dim_Size = 26214
X_Domain = Carbon13
Dim_Title = Carbon13
Dim_Units = [ppm]
Dimensions = X
Spectrometer = JNM-ECZ400S/L1
Field_Strength = 9.389766[T] (400[MH
X_Acq_Duration = 1.03809024[s]
X_Domain = 13C
X_Freq = 100.52530333[MHz]
X_Offset = 100[ppm]
X_Points = 32768
X_Prescans = 4
X_Resolution = 0.96330739[Hz]
X_Sweep = 31.56565657[kHz]
X_Sweep_Clipped = 25.25252525[kHz]
Irr_Domain = Proton
Irr_Freq = 399.78219838[MHz]
Irr_Offset = 5[ppm]
Blanking = 5[us]
Clipped = TRUE
Scans = 13000
Total_Scans = 13000
Relaxation_Delay = 2[s]
Recvr_Gain = 50
Temp_Get = 22.7[dC]
X_90_Width = 10.02[us]
X_Acq_Time = 1.03809024[s]
X_Angle = 30[deg]
X_Atn = 8[dB]
X_Pulse = 3.34[us]
Irr_Atn_Dec = 27.49[dB]
Irr_Atn_Dec_Calc = 27.49[dB]
Irr_Atn_Dec_Default_Calc = 27.49[dB]
Irr_Atn_Noe = 27.49[dB]
Irr_Dec_Bandwidth_Hz = 4.78260087[kHz]
Irr_Dec_Bandwidth_Ppm = 11.96303566[ppm]
Irr_Dec_Freq = 399.78219838[MHz]
Irr_Dec_Merit_Factor = 2.2
Irr_Decoupling = TRUE
Irr_Noe = TRUE
Irr_Noise = WALTZ
Irr_Offset_Default = 5[ppm]
Irr_Pwidth = 0.115[ms]
Irr_Pwidth_Default = 0.115[ms]
Irr_Pwidth_Default_Calc = 0.115[ms]
Irr_Pwidth_Temp1 = 0.115[ms]
Irr_Wurst = FALSE
Decimation_Rate = 0

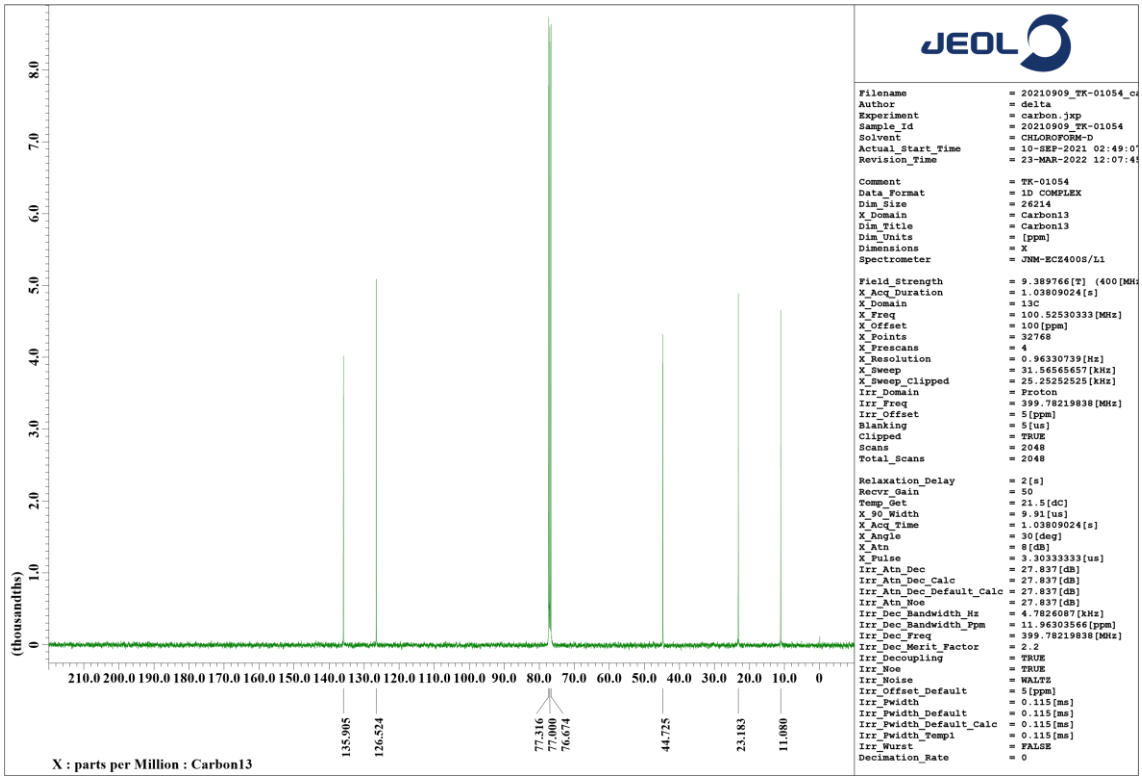

3a
5.25
0.94
1.00
1.01
0.93
2.07
2.03
abundance
X : parts per Million : Proton
Filename = 20210930_TK-01066_re_p
Author = delta
Experiment = proton.jxp
Sample_Id = 20210930_TK-01066_re
Solvent = CHLOROFORM-D
Actual_Start_Time = 30-SEP-2021 20:12:02
Revision_Time = 23-MAR-2022 13:02:14
Comment = TK-01066_re
Data_Format = 1D COMPLEX
Dim_Size = 104858
X_Domain = Proton
Dim_Title = Proton
Dim_Units = [ppm]
Dimensions = X
Spectrometer = JNM-ECZ400S/L1
Field_Strength = 9.389766[T] (400[MHz])
X_Acq_Duration = 2.18628096[s]
X_Domain = 1H
X_Freq = 399.78219838[MHz]
X_Offset = 5[ppm]
X_Points = 16384
X_Prescans = 1
X_Resolution = 0.45739775[Hz]
X_Sweep = 7.4940048[kHz]
X_Sweep_Clipped = 5.99520384[kHz]
Irr_Domain = Proton
Irr_Freq = 399.78219838[MHz]
Irr_Offset = 5[ppm]
Tri_Domain = Proton
Tri_Freq = 399.78219838[MHz]
Tri_Offset = 5[ppm]
Blanking = 2[us]
Clipped = FALSE
Scans = 16
Total_Scans = 16
Relaxation_Delay = 5[s]
Recvr_Gain = 46
Temp_Get = 21.5[dC]
X_90_Width = 6.15[us]
X_Acq_Time = 2.18628096[s]
X_Angle = 45[deg]
X_Atn = 2.4[dB]
X_Pulse = 3.075[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Loop = 500
Dante_Presat = FALSE
Decimation_Rate = 0
Initial_Wait = 1[s]
Phase = (0, 90, 270, 180, 180,
Presat_Time = 5[s]
Presat_Time_Flag = FALSE
Relaxation_Delay_Calc = 0[s]
Relaxation_Delay_Temp = 5[s]
Repetition_Time = 7.18628096[s]

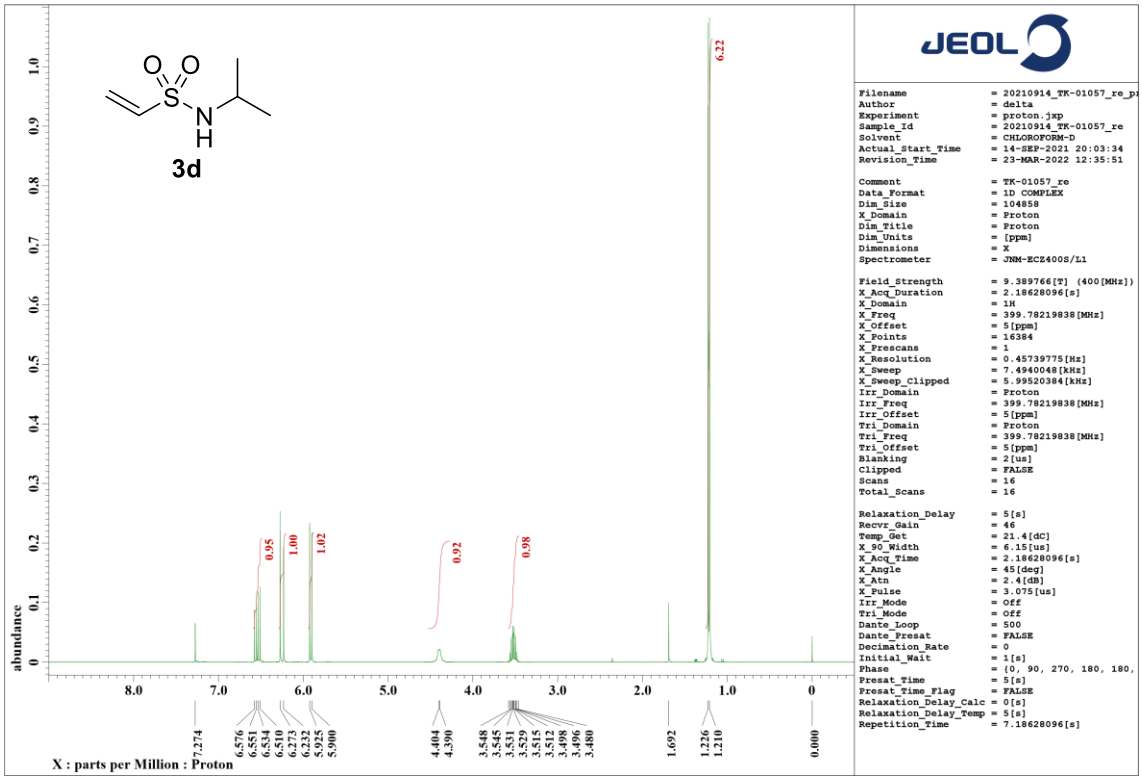

(thousandths)
X : parts per Million : Carbon13
Filename = 20210930_TK-01066_1
Author = delta
Experiment = carbon.jxp
Sample_Id = 20210930_TK-01066_1
Solvent = CHLOROFORM-D
Actual_Start_Time = 30-SEP-2021 21:03:2
Revision_Time = 23-MAR-2022 13:02:5
Comment = TK-01066_13C
Data_Format = 1D COMPLEX
Dim_Size = 26214
X_Domain = Carbon13
Dim_Title = Carbon13
Dim_Units = [ppm]
Dimensions = X
Spectrometer = JNM-ECZ400S/L1
Field_Strength = 9.389766[T] (400[MH
X_Acq_Duration = 1.03809024[s]
X_Domain = 13C
X_Freq = 100.52530333[MHz]
X_Offset = 100[ppm]
X_Points = 32768
X_Prescans = 4
X_Resolution = 0.96330739[Hz]
X_Sweep = 31.56565657[kHz]
X_Sweep_Clipped = 25.25252525[kHz]
Irr_Domain = Proton
Irr_Freq = 399.78219838[MHz]
Irr_Offset = 5[ppm]
Blanking = 5[us]
Clipped = TRUE
Scans = 4096
Total_Scans = 4096
Relaxation_Delay = 2[s]
Recvr_Gain = 50
Temp_Get = 21.3[dC]
X_90_Width = 9.91[us]
X_Acq_Time = 1.03809024[s]
X_Angle = 30[deg]
X_Atn = 8[dB]
X_Pulse = 3.30333333[us]
Irr_Atn_Dec = 27.837[dB]
Irr_Atn_Dec_Calc = 27.837[dB]
Irr_Atn_Dec_Default_Calc = 27.837[dB]
Irr_Atn_Noe = 27.837[dB]
Irr_Dec_Bandwidth_Hz = 4.7826087[kHz]
Irr_Dec_Bandwidth_Ppm = 11.96303566[ppm]
Irr_Dec_Freq = 399.78219838[MHz]
Irr_Dec_Merit_Factor = 2.2
Irr_Decoupling = TRUE
Irr_Noe = TRUE
Irr_Noise = WALTZ
Irr_Offset_Default = 5[ppm]
Irr_Pwidth = 0.115[ms]
Irr_Pwidth_Default = 0.115[ms]
Irr_Pwidth_Default_Calc = 0.115[ms]
Irr_Pwidth_Temp1 = 0.115[ms]
Irr_Wurst = FALSE
Decimation_Rate = 0

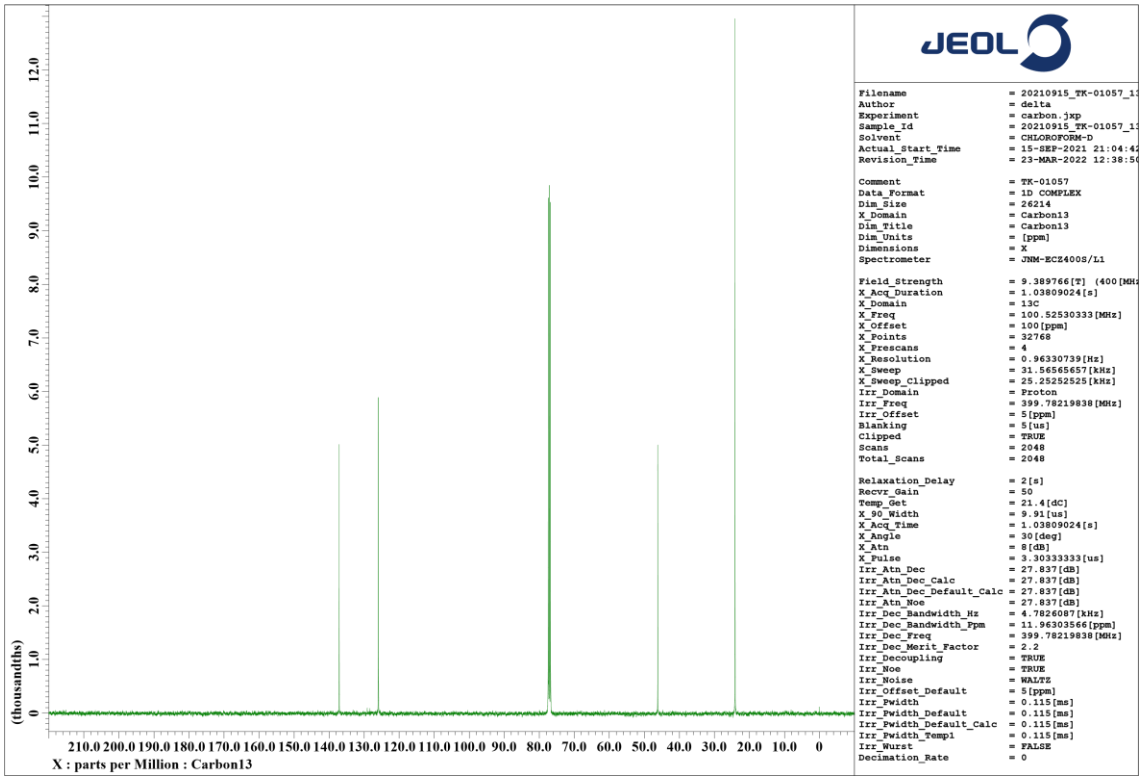

3b
abundance
X : parts per Million : Proton
7.266
6.554
6.529
6.512
6.487
6.282
6.240
5.967
5.942
4.258
3.133
3.118
3.115
3.100
3.097
3.082
3.079
3.064
1.589
1.231
1.213
1.195
0.000
0.93
0.98
1.00
0.93
1.99
3.01
JEOL
Filename = 20220112_TK-01112_re2_
Author = delta
Experiment = proton.jxp
Sample_Id = 20220112_TK-01112_re2
Solvent = CHLOROFORM-D
Actual_Start_Time = 12-JAN-2022 14:02:05
Revision_Time = 5-SEP-2024 17:04:14
Comment = TK-01112
Data_Format = 1D COMPLEX
Dim_Size = 104858
X_Domain = Proton
Dim_Title = Proton
Dim_Units = [ppm]
Dimensions = X
Spectrometer = JNM-ECZ400S/L1
Field_Strength = 9.389766[T] (400[MHz])
X_Acq_Duration = 2.18628096[s]
X_Domain = 1H
X_Freq = 399.78219838[MHz]
X_Offset = 5[ppm]
X_Points = 16384
X_Prescans = 1
X_Resolution = 0.45739775[Hz]
X_Sweep = 7.4940048[kHz]
X_Sweep_Clipped = 5.99520384[kHz]
Irr_Domain = Proton
Irr_Freq = 399.78219838[MHz]
Irr_Offset = 5[ppm]
Tri_Domain = Proton
Tri_Freq = 399.78219838[MHz]
Tri_Offset = 5[ppm]
Blanking = 2[us]
Clipped = FALSE
Scans = 16
Total_Scans = 16
Relaxation_Delay = 5[s]
Recvr_Gain = 56
Temp_Get = 21.1[dC]
X_90_Width = 6.2[us]
X_Acq_Time = 2.18628096[s]
X_Angle = 45[deg]
X_Atn = 2.4[dB]
X_Pulse = 3.1[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Loop = 500
Dante_Presat = FALSE
Decimation_Rate = 0
Initial_Wait = 1[s]
Phase = (0, 90, 270, 180, 180,
Presat_Time = 5[s]
Presat_Time_Flag = FALSE
Relaxation_Delay_Calc = 0[s]
Relaxation_Delay_Temp = 5[s]
Repetition_Time = 7.18628096[s]

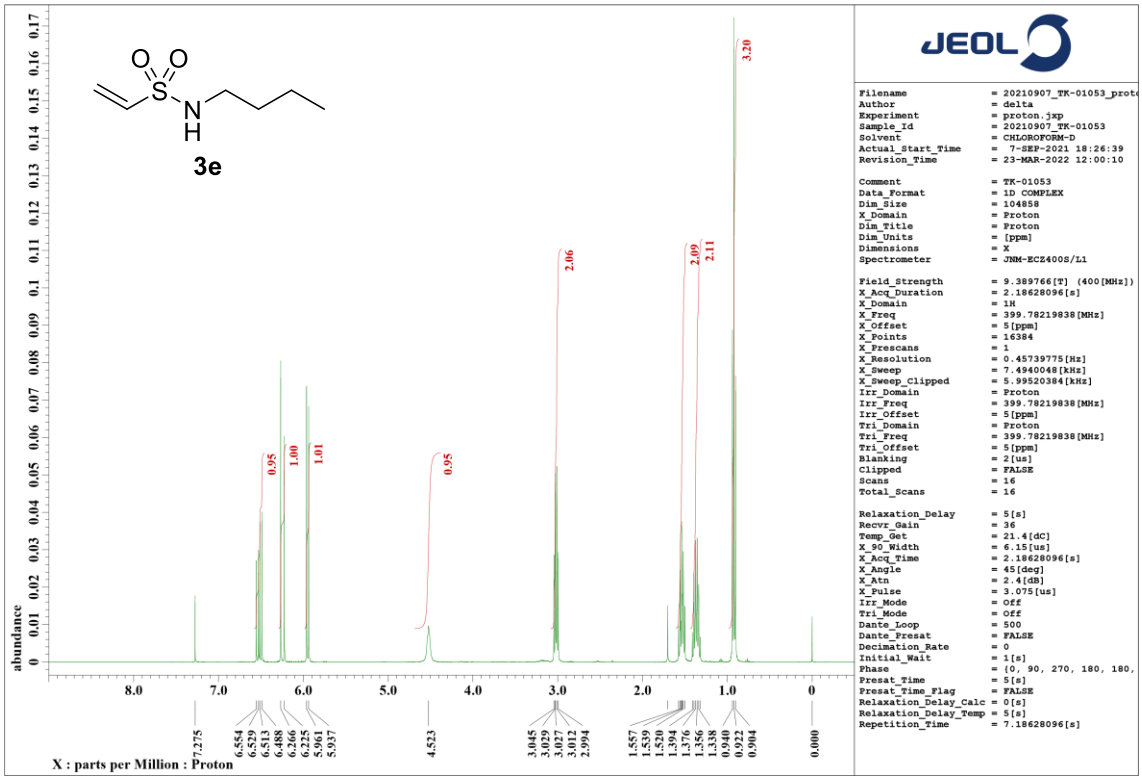

(thousandths)
X : parts per Million : Carbon13
135.915
126.639
77.316
77.201
77.000
76.674
38.027
15.460
JEOL
Filename = 20220111_TK-01112_1
Author = delta
Experiment = carbon.jxp
Sample_Id = 20220111_TK-01112_1
Solvent = CHLOROFORM-D
Actual_Start_Time = 11-JAN-2022 23:03:0
Revision_Time = 5-SEP-2024 17:06:5
Comment = TK-01112
Data_Format = 1D COMPLEX
Dim_Size = 26214
X_Domain = Carbon13
Dim_Title = Carbon13
Dim_Units = [ppm]
Dimensions = X
Spectrometer = JNM-ECZ400S/L1
Field_Strength = 9.389766[T] (400[MH
X_Acq_Duration = 1.03809024[s]
X_Domain = 13C
X_Freq = 100.52530333[MHz]
X_Offset = 100[ppm]
X_Points = 32768
X_Prescans = 4
X_Resolution = 0.96330739[Hz]
X_Sweep = 31.56565657[kHz]
X_Sweep_Clipped = 25.25252525[kHz]
Irr_Domain = Proton
Irr_Freq = 399.78219838[MHz]
Irr_Offset = 5[ppm]
Blanking = 5[us]
Clipped = FALSE
Scans = 8192
Total_Scans = 8192
Relaxation_Delay = 2[s]
Recvr_Gain = 50
Temp_Get = 21[dC]
X_90_Width = 9.97[us]
X_Acq_Time = 1.03809024[s]
X_Angle = 30[deg]
X_Atn = 8[dB]
X_Pulse = 3.32333333[us]
Irr_Atn_Dec = 27.766[dB]
Irr_Atn_Dec_Calc = 27.766[dB]
Irr_Atn_Dec_Default_Calc = 27.766[dB]
Irr_Atn_Noe = 27.766[dB]
Irr_Dec_Bandwidth_Hz = 4.7826087[kHz]
Irr_Dec_Bandwidth_Ppm = 11.96303566[ppm]
Irr_Dec_Freq = 399.78219838[MHz]
Irr_Dec_Merit_Factor = 2.2
Irr_Decoupling = TRUE
Irr_Noe = TRUE
Irr_Noise = WALTZ
Irr_Offset_Default = 5[ppm]
Irr_Pwidth = 0.115[ms]
Irr_Pwidth_Default = 0.115[ms]
Irr_Pwidth_Default_Calc = 0.115[ms]
Irr_Pwidth_Temp1 = 0.115[ms]
Irr_Wurst = FALSE
Decimation_Rate = 0

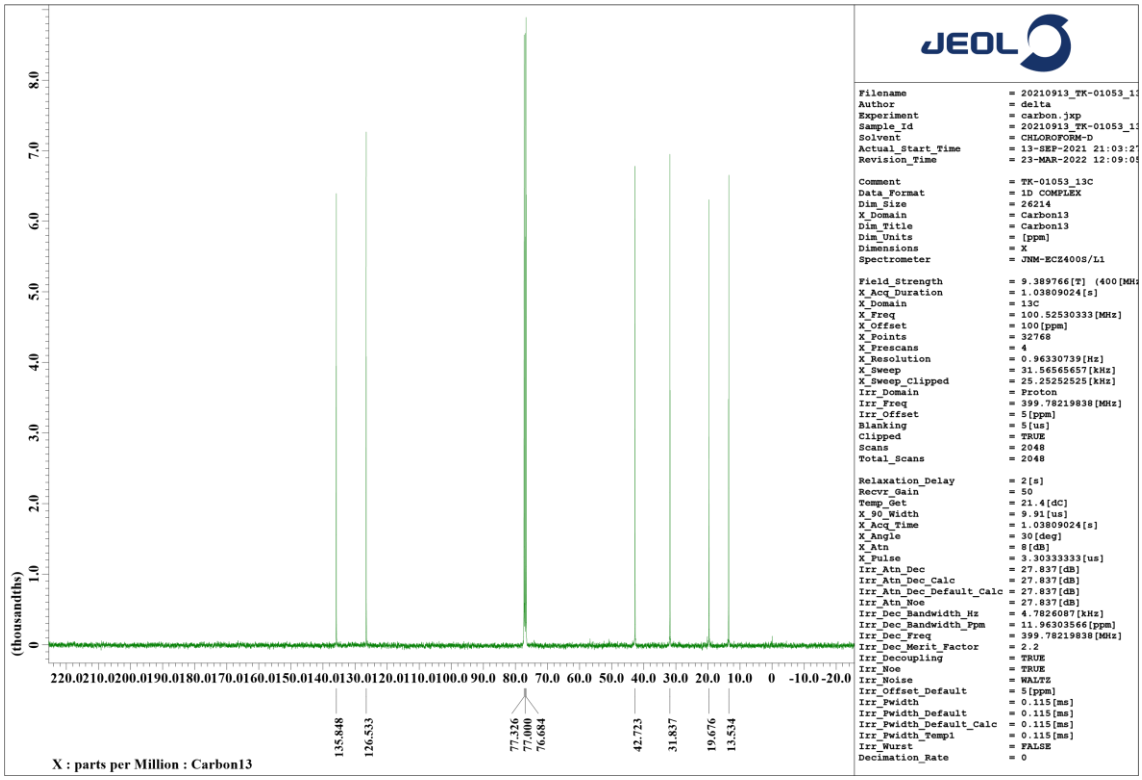

3c
abundance
X : parts per Million : Proton
7.271
6.556
6.531
6.514
6.489
6.270
6.268
6.228
6.227
5.960
5.935
4.492
3.018
3.017
3.001
2.984
2.967
2.966
1.670
1.611
1.593
1.574
1.556
1.538
0.964
0.946
0.927
0.000
0.95
1.00
1.01
0.97
2.05
2.00
3.11
Filename = 20210907_TK-01054_prot
Author = delta
Experiment = proton.jxp
Sample_Id = 20210907_TK-01054
Solvent = CHLOROFORM-D
Actual_Start_Time = 7-SEP-2021 18:32:59
Revision_Time = 23-MAR-2022 12:05:39
Comment = TK-01054
Data_Format = 1D COMPLEX
Dim_Size = 104858
X_Domain = Proton
Dim_Title = Proton
Dim_Units = [ppm]
Dimensions = X
Spectrometer = JNM-ECZ400S/L1
Field_Strength = 9.389766[T] (400[MHz])
X_Acq_Duration = 2.18628096[s]
X_Domain = 1H
X_Freq = 399.78219838[MHz]
X_Offset = 5[ppm]
X_Points = 16384
X_Prescans = 1
X_Resolution = 0.45739775[Hz]
X_Sweep = 7.4940048[kHz]
X_Sweep_Clipped = 5.99520384[kHz]
Irr_Domain = Proton
Irr_Freq = 399.78219838[MHz]
Irr_Offset = 5[ppm]
Tri_Domain = Proton
Tri_Freq = 399.78219838[MHz]
Tri_Offset = 5[ppm]
Blanking = 2[us]
Clipped = FALSE
Scans = 16
Total_Scans = 16
Relaxation_Delay = 5[s]
Recvr_Gain = 46
Temp_Get = 21.4[dC]
X_90_Width = 6.15[us]
X_Acq_Time = 2.18628096[s]
X_Angle = 45[deg]
X_Atn = 2.4[dB]
X_Pulse = 3.075[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Loop = 500
Dante_Presat = FALSE
Decimation_Rate = 0
Initial_Wait = 1[s]
Phase = (0, 90, 270, 180, 180,
Presat_Time = 5[s]
Presat_Time_Flag = FALSE
Relaxation_Delay_Calc = 0[s]
Relaxation_Delay_Temp = 5[s]
Repetition_Time = 7.18628096[s]

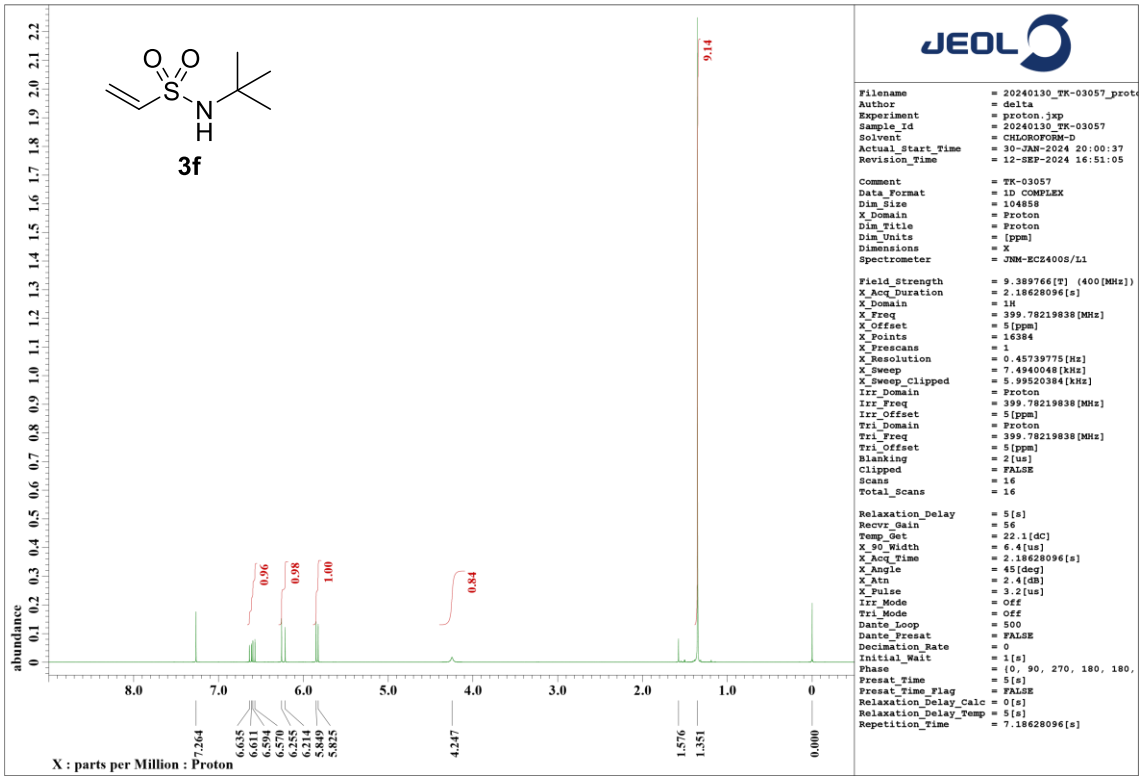

(thousandths)
X : parts per Million : Carbon13
135.905
126.524
77.316
77.000
76.674
44.725
23.183
11.080
Filename = 20210909_TK-01054_c
Author = delta
Experiment = carbon.jxp
Sample_Id = 20210909_TK-01054
Solvent = CHLOROFORM-D
Actual_Start_Time = 10-SEP-2021 02:49:0
Revision_Time = 23-MAR-2022 12:07:4
Comment = TK-01054
Data_Format = 1D COMPLEX
Dim_Size = 26214
X_Domain = Carbon13
Dim_Title = Carbon13
Dim_Units = [ppm]
Dimensions = X
Spectrometer = JNM-ECZ400S/L1
Field_Strength = 9.389766[T] (400[MH
X_Acq_Duration = 1.03809024[s]
X_Domain = 13C
X_Freq = 100.52530333[MHz]
X_Offset = 100[ppm]
X_Points = 32768
X_Prescans = 4
X_Resolution = 0.96330739[Hz]
X_Sweep = 31.56565657[kHz]
X_Sweep_Clipped = 25.25252525[kHz]
Irr_Domain = Proton
Irr_Freq = 399.78219838[MHz]
Irr_Offset = 5[ppm]
Blanking = 5[us]
Clipped = TRUE
Scans = 2048
Total_Scans = 2048
Relaxation_Delay = 2[s]
Recvr_Gain = 50
Temp_Get = 21.5[dC]
X_90_Width = 9.91[us]
X_Acq_Time = 1.03809024[s]
X_Angle = 30[deg]
X_Atn = 8[dB]
X_Pulse = 3.30333333[us]
Irr_Atn_Dec = 27.837[dB]
Irr_Atn_Dec_Calc = 27.837[dB]
Irr_Atn_Dec_Default_Calc = 27.837[dB]
Irr_Atn_Noe = 27.837[dB]
Irr_Dec_Bandwidth_Hz = 4.7826087[kHz]
Irr_Dec_Bandwidth_Ppm = 11.96303566[ppm]
Irr_Dec_Freq = 399.78219838[MHz]
Irr_Dec_Merit_Factor = 2.2
Irr_Decoupling = TRUE
Irr_Noe = TRUE
Irr_Noise = WALTZ
Irr_Offset_Default = 5[ppm]
Irr_Pwidth = 0.115[ms]
Irr_Pwidth_Default = 0.115[ms]
Irr_Pwidth_Default_Calc = 0.115[ms]
Irr_Pwidth_Temp1 = 0.115[ms]
Irr_Wurst = FALSE
Decimation_Rate = 0


3d
abundance
X : parts per Million : Proton
6.22
0.95
1.00
1.02
0.92
0.98
7.274
6.576
6.551
6.534
6.510
6.273
6.232
5.925
5.900
4.404
4.390
3.548
3.545
3.531
3.529
3.515
3.512
3.498
3.496
3.480
1.692
1.226
1.210
0.000
Filename = 20210914_TK-01057_re_p
Author = delta
Experiment = proton.jxp
Sample_Id = 20210914_TK-01057_re
Solvent = CHLOROFORM-D
Actual_Start_Time = 14-SEP-2021 20:03:34
Revision_Time = 23-MAR-2022 12:35:51
Comment = TK-01057_re
Data_Format = 1D COMPLEX
Dim_Size = 104858
X_Domain = Proton
Dim_Title = Proton
Dim_Units = [ppm]
Dimensions = X
Spectrometer = JNM-ECZ400S/L1
Field_Strength = 9.389766[T] (400[MHz])
X_Acq_Duration = 2.18628096[s]
X_Domain = 1H
X_Freq = 399.78219838[MHz]
X_Offset = 5[ppm]
X_Points = 16384
X_Prescans = 1
X_Resolution = 0.45739775[Hz]
X_Sweep = 7.4940048[kHz]
X_Sweep_Clipped = 5.99520384[kHz]
Irr_Domain = Proton
Irr_Freq = 399.78219838[MHz]
Irr_Offset = 5[ppm]
Tri_Domain = Proton
Tri_Freq = 399.78219838[MHz]
Tri_Offset = 5[ppm]
Blanking = 2[us]
Clipped = FALSE
Scans = 16
Total_Scans = 16
Relaxation_Delay = 5[s]
Recvr_Gain = 46
Temp_Get = 21.4[dC]
X_90_Width = 6.15[us]
X_Acq_Time = 2.18628096[s]
X_Angle = 45[deg]
X_Atn = 2.4[dB]
X_Pulse = 3.075[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Loop = 500
Dante_Presat = FALSE
Decimation_Rate = 0
Initial_Wait = 1[s]
Phase = (0, 90, 270, 180, 180,
Presat_Time = 5[s]
Presat_Time_Flag = FALSE
Relaxation_Delay_Calc = 0[s]
Relaxation_Delay_Temp = 5[s]
Repetition_Time = 7.18628096[s]

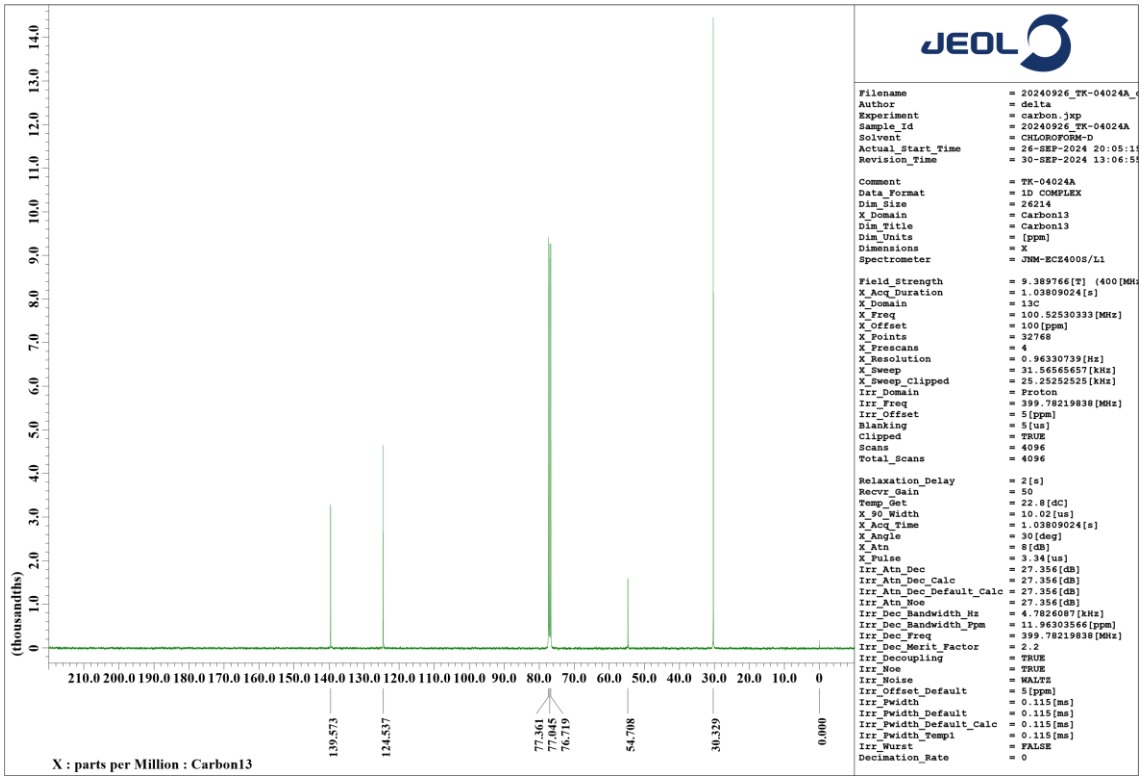

(thousandths)
X : parts per Million : Carbon13
Filename = 20210915_TK-01057_1
Author = delta
Experiment = carbon.jxp
Sample_Id = 20210915_TK-01057_1
Solvent = CHLOROFORM-D
Actual_Start_Time = 15-SEP-2021 21:04:4
Revision_Time = 23-MAR-2022 12:38:5
Comment = TK-01057
Data_Format = 1D COMPLEX
Dim_Size = 26214
X_Domain = Carbon13
Dim_Title = Carbon13
Dim_Units = [ppm]
Dimensions = X
Spectrometer = JNM-ECZ400S/L1
Field_Strength = 9.389766[T] (400[MH
X_Acq_Duration = 1.03809024[s]
X_Domain = 13C
X_Freq = 100.52530333[MHz]
X_Offset = 100[ppm]
X_Points = 32768
X_Prescans = 4
X_Resolution = 0.96330739[Hz]
X_Sweep = 31.56565657[kHz]
X_Sweep_Clipped = 25.25252525[kHz]
Irr_Domain = Proton
Irr_Freq = 399.78219838[MHz]
Irr_Offset = 5[ppm]
Blanking = 5[us]
Clipped = TRUE
Scans = 2048
Total_Scans = 2048
Relaxation_Delay = 2[s]
Recvr_Gain = 50
Temp_Get = 21.4[dC]
X_90_Width = 9.91[us]
X_Acq_Time = 1.03809024[s]
X_Angle = 30[deg]
X_Atn = 8[dB]
X_Pulse = 3.30333333[us]
Irr_Atn_Dec = 27.837[dB]
Irr_Atn_Dec_Calc = 27.837[dB]
Irr_Atn_Dec_Default_Calc = 27.837[dB]
Irr_Atn_Noe = 27.837[dB]
Irr_Dec_Bandwidth_Hz = 4.7826087[kHz]
Irr_Dec_Bandwidth_Ppm = 11.96303566[ppm]
Irr_Dec_Freq = 399.78219838[MHz]
Irr_Dec_Merit_Factor = 2.2
Irr_Decoupling = TRUE
Irr_Noe = TRUE
Irr_Noise = WALTZ
Irr_Offset_Default = 5[ppm]
Irr_Pwidth = 0.115[ms]
Irr_Pwidth_Default = 0.115[ms]
Irr_Pwidth_Default_Calc = 0.115[ms]
Irr_Pwidth_Temp1 = 0.115[ms]
Irr_Wurst = FALSE
Decimation_Rate = 0


3e
abundance
X : parts per Million : Proton
7.275
6.554
6.529
6.513
6.488
6.266
6.225
5.961
5.937
4.523
3.045
3.029
3.027
3.012
2.994
1.557
1.539
1.530
1.394
1.376
1.356
1.338
0.940
0.922
0.904
0.000
0.95
1.00
1.01
0.95
2.06
2.09
2.11
3.20
Filename = 20210907_TK-01053_prot
Author = delta
Experiment = proton.jxp
Sample_Id = 20210907_TK-01053
Solvent = CHLOROFORM-D
Actual_Start_Time = 7-SEP-2021 18:26:39
Revision_Time = 23-MAR-2022 12:00:10
Comment = TK-01053
Data_Format = 1D COMPLEX
Dim_Size = 104858
X_Domain = Proton
Dim_Title = Proton
Dim_Units = [ppm]
Dimensions = X
Spectrometer = JNM-ECZ400S/L1
Field_Strength = 9.389766[T] (400[MHz])
X_Acq_Duration = 2.18628096[s]
X_Domain = 1H
X_Freq = 399.78219838[MHz]
X_Offset = 5[ppm]
X_Points = 16384
X_Prescans = 1
X_Resolution = 0.45739775[Hz]
X_Sweep = 7.4940048[kHz]
X_Sweep_Clipped = 5.99520384[kHz]
Irr_Domain = Proton
Irr_Freq = 399.78219838[MHz]
Irr_Offset = 5[ppm]
Tri_Domain = Proton
Tri_Freq = 399.78219838[MHz]
Tri_Offset = 5[ppm]
Blanking = 2[us]
Clipped = FALSE
Scans = 16
Total_Scans = 16
Relaxation_Delay = 5[s]
Recvr_Gain = 36
Temp_Get = 21.4[dC]
X_90_Width = 6.15[us]
X_Acq_Time = 2.18628096[s]
X_Angle = 45[deg]
X_Atn = 2.4[dB]
X_Pulse = 3.075[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Loop = 500
Dante_Presat = FALSE
Decimation_Rate = 0
Initial_Wait = 1[s]
Phase = (0, 90, 270, 180, 180,
Presat_Time = 5[s]
Presat_Time_Flag = FALSE
Relaxation_Delay_Calc = 0[s]
Relaxation_Delay_Temp = 5[s]
Repetition_Time = 7.18628096[s]

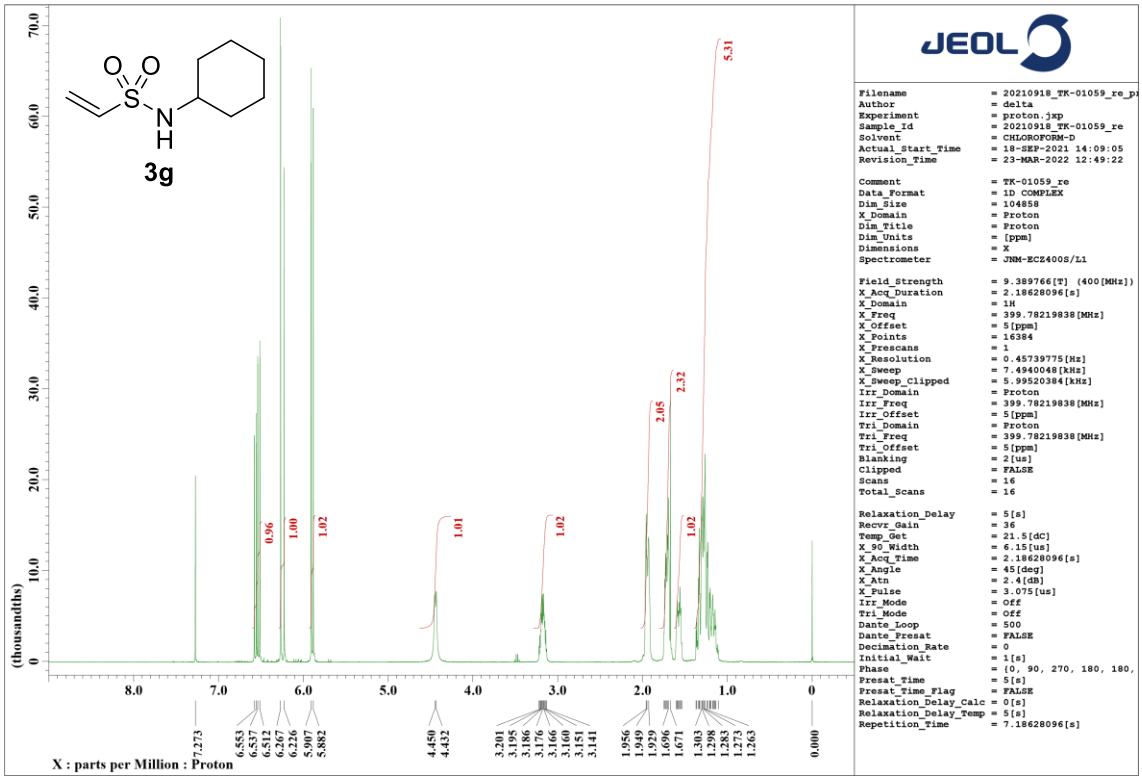

(thousandths)
X : parts per Million : Carbon13
135.848
126.533
77.326
77.000
76.684
42.723
31.837
19.676
13.534
Filename = 20210913_TK-01053_1
Author = delta
Experiment = carbon.jxp
Sample_Id = 20210913_TK-01053_1
Solvent = CHLOROFORM-D
Actual_Start_Time = 13-SEP-2021 21:03:2
Revision_Time = 23-MAR-2022 12:09:0
Comment = TK-01053_13C
Data_Format = 1D COMPLEX
Dim_Size = 26214
X_Domain = Carbon13
Dim_Title = Carbon13
Dim_Units = [ppm]
Dimensions = X
Spectrometer = JNM-ECZ400S/L1
Field_Strength = 9.389766[T] (400[MH
X_Acq_Duration = 1.03809024[s]
X_Domain = 13C
X_Freq = 100.52530333[MHz]
X_Offset = 100[ppm]
X_Points = 32768
X_Prescans = 4
X_Resolution = 0.96330739[Hz]
X_Sweep = 31.56565657[kHz]
X_Sweep_Clipped = 25.25252525[kHz]
Irr_Domain = Proton
Irr_Freq = 399.78219838[MHz]
Irr_Offset = 5[ppm]
Blanking = 5[us]
Clipped = TRUE
Scans = 2048
Total_Scans = 2048
Relaxation_Delay = 2[s]
Recvr_Gain = 50
Temp_Get = 21.4[dC]
X_90_Width = 9.91[us]
X_Acq_Time = 1.03809024[s]
X_Angle = 30[deg]
X_Atn = 8[dB]
X_Pulse = 3.30333333[us]
Irr_Atn_Dec = 27.837[dB]
Irr_Atn_Dec_Calc = 27.837[dB]
Irr_Atn_Dec_Default_Calc = 27.837[dB]
Irr_Atn_Noe = 27.837[dB]
Irr_Dec_Bandwidth_Hz = 4.7826087[kHz]
Irr_Dec_Bandwidth_Ppm = 11.96303566[ppm]
Irr_Dec_Freq = 399.78219838[MHz]
Irr_Dec_Merit_Factor = 2.2
Irr_Decoupling = TRUE
Irr_Noe = TRUE
Irr_Noise = WALTZ
Irr_Offset_Default = 5[ppm]
Irr_Pwidth = 0.115[ms]
Irr_Pwidth_Default = 0.115[ms]
Irr_Pwidth_Default_Calc = 0.115[ms]
Irr_Pwidth_Temp1 = 0.115[ms]
Irr_Wurst = FALSE
Decimation_Rate = 0

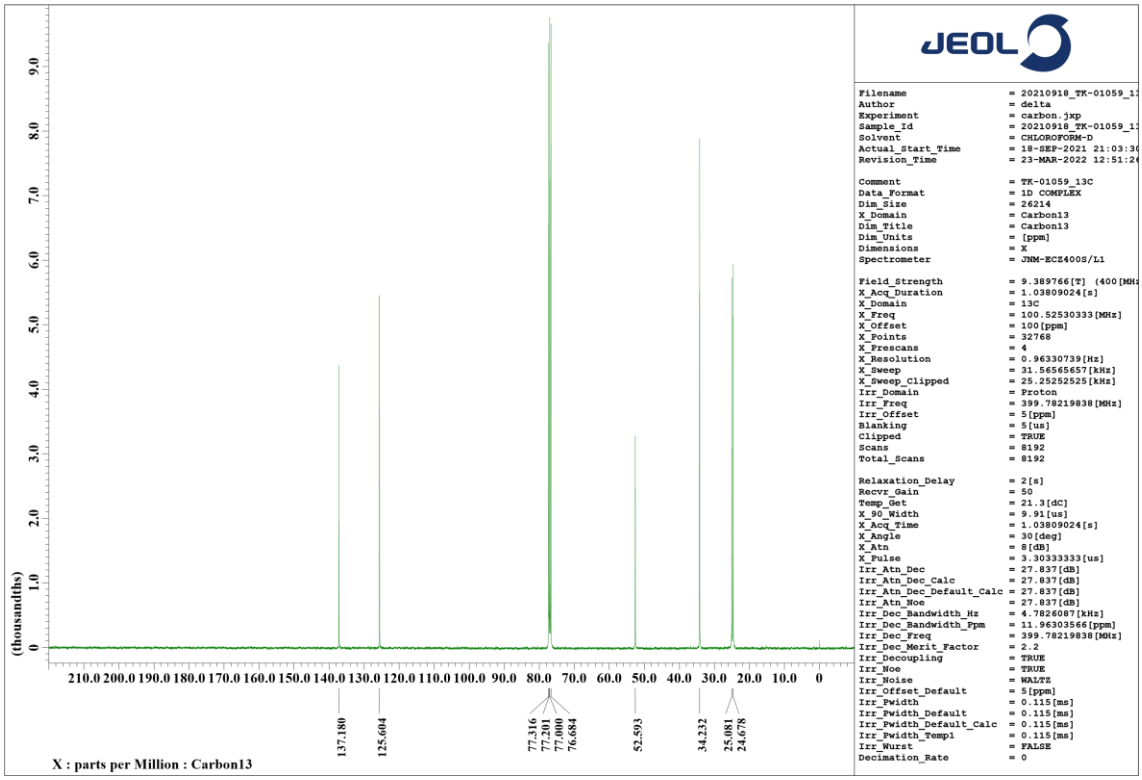


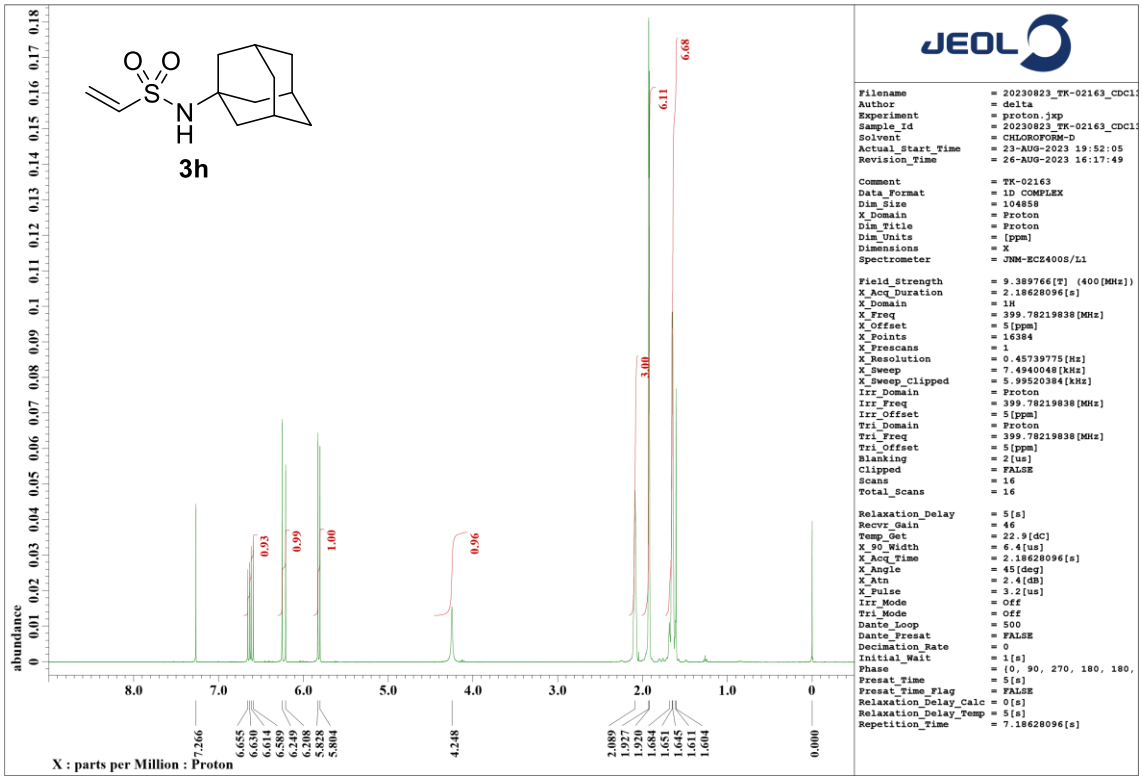

```
Filename                = 20240130_TK-03057_proto
Author                  = delta
Experiment              = proton.jxp
Sample_Id               = 20240130_TK-03057
Solvent                 = CHLOROFORM-D
Actual_Start_Time       = 30-JAN-2024 20:00:37
Revision_Time           = 12-SEP-2024 16:51:05

Comment                 = TK-03057
Data_Format             = 1D COMPLEX
Dim_Size                = 104858
X_Domain                = Proton
Dim_Title               = Proton
Dim_Units               = [ppm]
Dimensions              = X
Spectrometer            = JNM-ECZ400S/L1

Field_Strength          = 9.389766[T] (400[MHz])
X_Acq_Duration          = 2.18628096[s]
X_Domain                = 1H
X_Freq                  = 399.78219838[MHz]
X_Offset                = 5[ppm]
X_Points                = 16384
X_Prescans              = 1
X_Resolution            = 0.45739775[Hz]
X_Sweep                 = 7.4940048[kHz]
X_Sweep_Clipped         = 5.99520384[kHz]
Irr_Domain              = Proton
Irr_Freq                = 399.78219838[MHz]
Irr_Offset              = 5[ppm]
Tri_Domain              = Proton
Tri_Freq                = 399.78219838[MHz]
Tri_Offset              = 5[ppm]
Blanking                = 2[us]
Clipped                 = FALSE
Scans                   = 16
Total_Scans             = 16

Relaxation_Delay        = 5[s]
Recvr_Gain              = 56
Temp_Get                = 22.1[dC]
X_90_Width              = 6.4[us]
X_Acq_Time              = 2.18628096[s]
X_Angle                 = 45[deg]
X_Atn                   = 2.4[dB]
X_Pulse                 = 3.2[us]
Irr_Mode                = Off
Tri_Mode                = Off
Dante_Loop              = 500
Dante_Presat            = FALSE
Decimation_Rate         = 0
Initial_Wait            = 1[s]
Phase                   = (0, 90, 270, 180, 180,
Presat_Time             = 5[s]
Presat_Time_Flag        = FALSE
Relaxation_Delay_Calc   = 0[s]
Relaxation_Delay_Temp   = 5[s]
Repetition_Time         = 7.18628096[s]
```

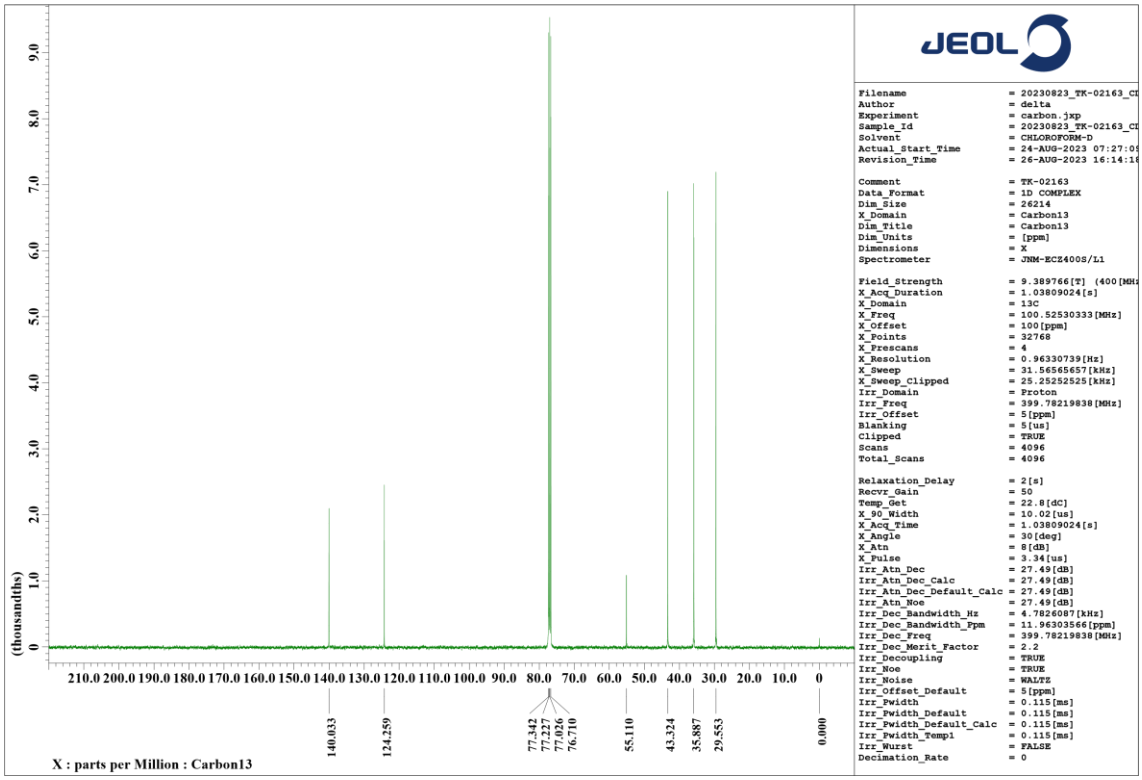


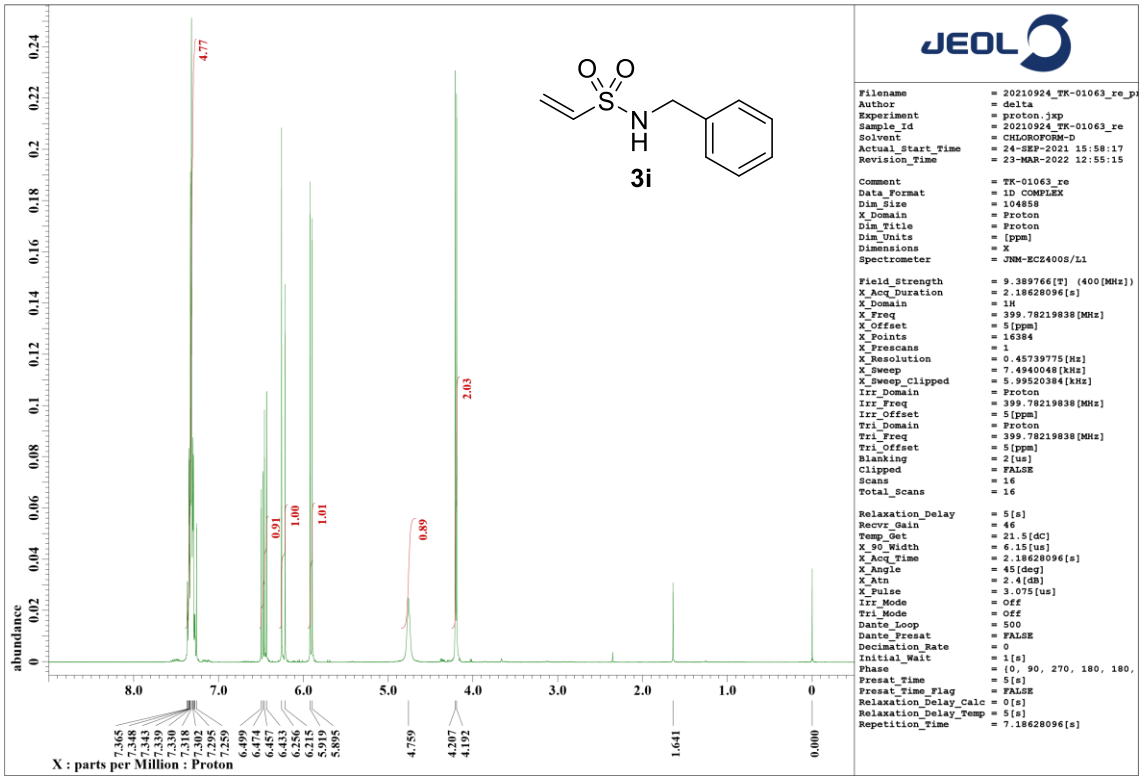

```
Filename                = 20240926_TK-04024A_
Author                  = delta
Experiment              = carbon.jxp
Sample_Id               = 20240926_TK-04024A
Solvent                 = CHLOROFORM-D
Actual_Start_Time       = 26-SEP-2024 20:05:1
Revision_Time           = 30-SEP-2024 13:06:5

Comment                 = TK-04024A
Data_Format             = 1D COMPLEX
Dim_Size                = 26214
X_Domain                = Carbon13
Dim_Title               = Carbon13
Dim_Units               = [ppm]
Dimensions              = X
Spectrometer            = JNM-ECZ400S/L1

Field_Strength          = 9.389766[T] (400[MH
X_Acq_Duration          = 1.03809024[s]
X_Domain                = 13C
X_Freq                  = 100.52530333[MHz]
X_Offset                = 100[ppm]
X_Points                = 32768
X_Prescans              = 4
X_Resolution            = 0.96330739[Hz]
X_Sweep                 = 31.56565657[kHz]
X_Sweep_Clipped         = 25.25252525[kHz]
Irr_Domain              = Proton
Irr_Freq                = 399.78219838[MHz]
Irr_Offset              = 5[ppm]
Blanking                = 5[us]
Clipped                 = TRUE
Scans                   = 4096
Total_Scans             = 4096

Relaxation_Delay        = 2[s]
Recvr_Gain              = 50
Temp_Get                = 22.8[dC]
X_90_Width              = 10.02[us]
X_Acq_Time              = 1.03809024[s]
X_Angle                 = 30[deg]
X_Atn                   = 8[dB]
X_Pulse                 = 3.34[us]
Irr_Atn_Dec             = 27.356[dB]
Irr_Atn_Dec_Calc        = 27.356[dB]
Irr_Atn_Dec_Default_Calc = 27.356[dB]
Irr_Atn_Noe             = 27.356[dB]
Irr_Dec_Bandwidth_Hz    = 4.7826087[kHz]
Irr_Dec_Bandwidth_Ppm   = 11.96303566[ppm]
Irr_Dec_Freq            = 399.78219838[MHz]
Irr_Dec_Merit_Factor    = 2.2
Irr_Decoupling          = TRUE
Irr_Noe                 = TRUE
Irr_Noise               = WALTZ
Irr_Offset_Default      = 5[ppm]
Irr_Pwidth              = 0.115[ms]
Irr_Pwidth_Default      = 0.115[ms]
Irr_Pwidth_Default_Calc = 0.115[ms]
Irr_Pwidth_Temp1        = 0.115[ms]
Irr_Wurst               = FALSE
Decimation_Rate         = 0
```

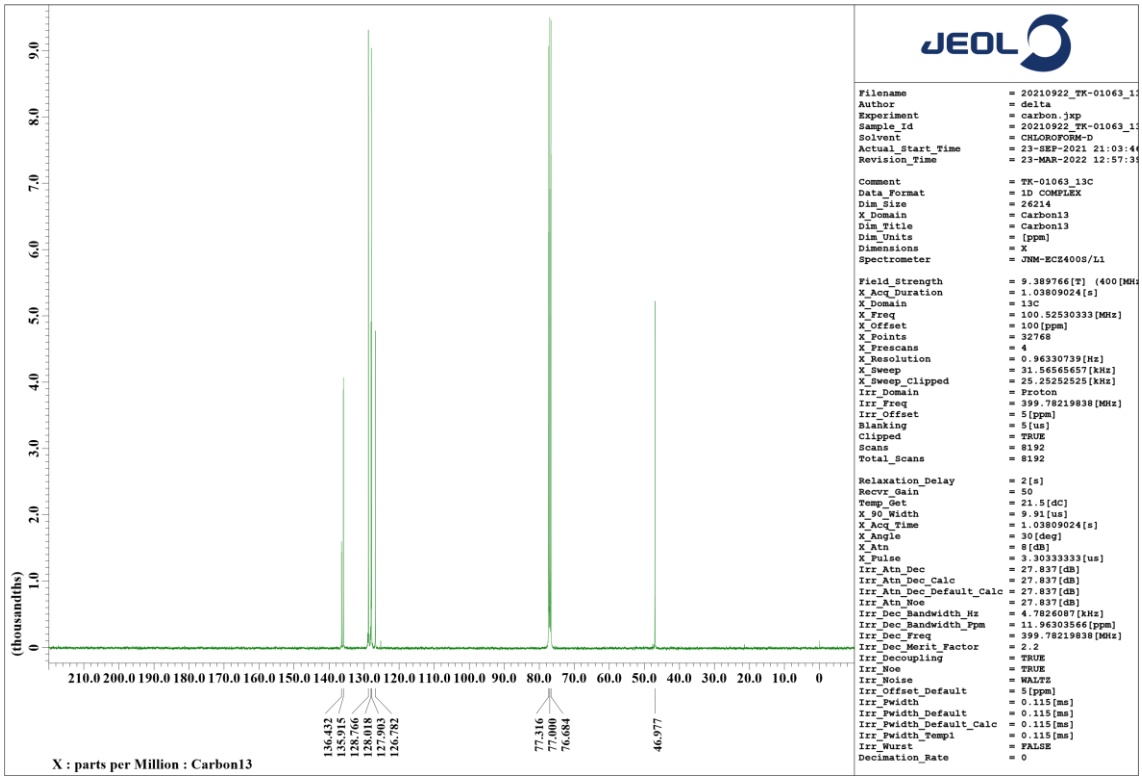

3g
(thousandths)
X : parts per Million : Proton
0.96
1.00
1.02
1.01
1.02
2.05
2.32
1.02
5.31
7.273
6.553
6.537
6.512
6.267
6.226
5.907
5.882
4.450
4.432
3.201
3.195
3.186
3.176
3.166
3.160
3.151
3.141
1.956
1.949
1.929
1.696
1.671
1.303
1.298
1.283
1.273
1.263
0.000
Filename = 20210918_TK-01059_re_p
Author = delta
Experiment = proton.jxp
Sample_Id = 20210918_TK-01059_re
Solvent = CHLOROFORM-D
Actual_Start_Time = 18-SEP-2021 14:09:05
Revision_Time = 23-MAR-2022 12:49:22
Comment = TK-01059_re
Data_Format = 1D COMPLEX
Dim_Size = 104858
X_Domain = Proton
Dim_Title = Proton
Dim_Units = [ppm]
Dimensions = X
Spectrometer = JNM-ECZ400S/L1
Field_Strength = 9.389766[T] (400[MHz])
X_Acq_Duration = 2.18628096[s]
X_Domain = 1H
X_Freq = 399.78219838[MHz]
X_Offset = 5[ppm]
X_Points = 16384
X_Prescans = 1
X_Resolution = 0.45739775[Hz]
X_Sweep = 7.4940048[kHz]
X_Sweep_Clipped = 5.99520384[kHz]
Irr_Domain = Proton
Irr_Freq = 399.78219838[MHz]
Irr_Offset = 5[ppm]
Tri_Domain = Proton
Tri_Freq = 399.78219838[MHz]
Tri_Offset = 5[ppm]
Blanking = 2[us]
Clipped = FALSE
Scans = 16
Total_Scans = 16
Relaxation_Delay = 5[s]
Recvr_Gain = 36
Temp_Get = 21.5[dC]
X_90_Width = 6.15[us]
X_Acq_Time = 2.18628096[s]
X_Angle = 45[deg]
X_Atn = 2.4[dB]
X_Pulse = 3.075[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Loop = 500
Dante_Presat = FALSE
Decimation_Rate = 0
Initial_Wait = 1[s]
Phase = (0, 90, 270, 180, 180,
Presat_Time = 5[s]
Presat_Time_Flag = FALSE
Relaxation_Delay_Calc = 0[s]
Relaxation_Delay_Temp = 5[s]
Repetition_Time = 7.18628096[s]

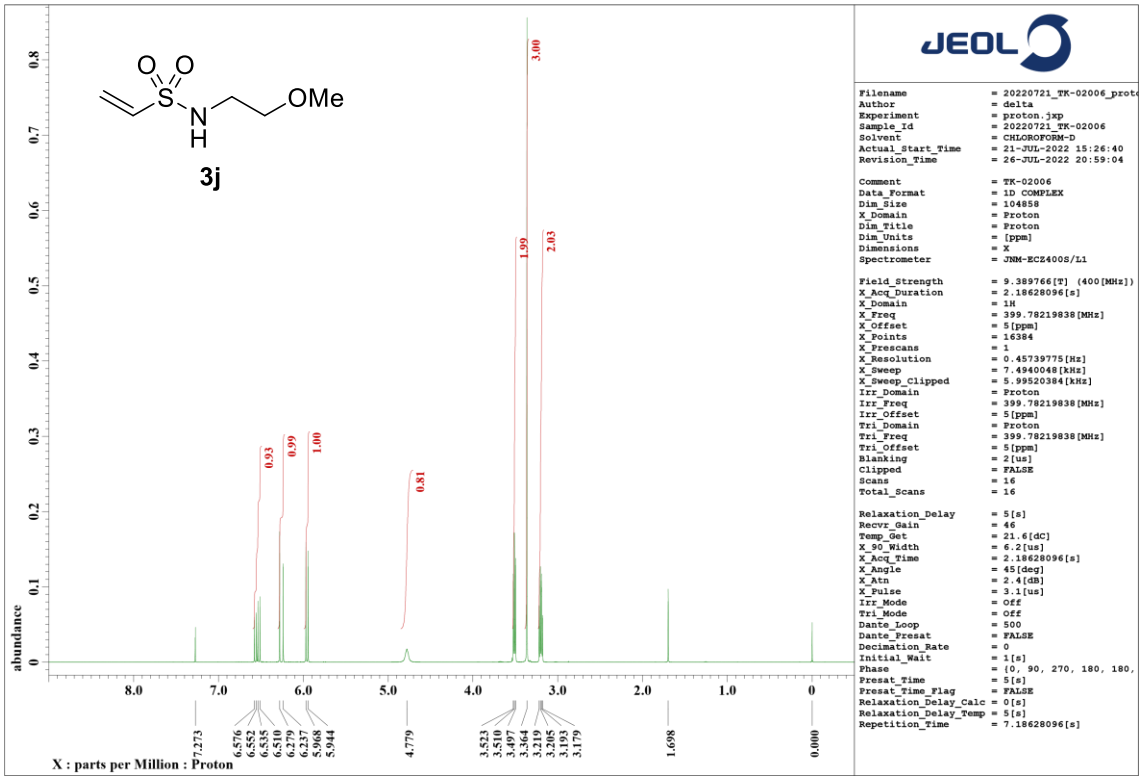

(thousandths)
X : parts per Million : Carbon13
137.180
125.604
77.316
77.201
77.000
76.684
52.593
34.232
25.081
24.678
Filename = 20210918_TK-01059_1
Author = delta
Experiment = carbon.jxp
Sample_Id = 20210918_TK-01059_1
Solvent = CHLOROFORM-D
Actual_Start_Time = 18-SEP-2021 21:03:3
Revision_Time = 23-MAR-2022 12:51:2
Comment = TK-01059_13C
Data_Format = 1D COMPLEX
Dim_Size = 26214
X_Domain = Carbon13
Dim_Title = Carbon13
Dim_Units = [ppm]
Dimensions = X
Spectrometer = JNM-ECZ400S/L1
Field_Strength = 9.389766[T] (400[MH
X_Acq_Duration = 1.03809024[s]
X_Domain = 13C
X_Freq = 100.52530333[MHz]
X_Offset = 100[ppm]
X_Points = 32768
X_Prescans = 4
X_Resolution = 0.96330739[Hz]
X_Sweep = 31.56565657[kHz]
X_Sweep_Clipped = 25.25252525[kHz]
Irr_Domain = Proton
Irr_Freq = 399.78219838[MHz]
Irr_Offset = 5[ppm]
Blanking = 5[us]
Clipped = TRUE
Scans = 8192
Total_Scans = 8192
Relaxation_Delay = 2[s]
Recvr_Gain = 50
Temp_Get = 21.3[dC]
X_90_Width = 9.91[us]
X_Acq_Time = 1.03809024[s]
X_Angle = 30[deg]
X_Atn = 8[dB]
X_Pulse = 3.30333333[us]
Irr_Atn_Dec = 27.837[dB]
Irr_Atn_Dec_Calc = 27.837[dB]
Irr_Atn_Dec_Default_Calc = 27.837[dB]
Irr_Atn_Noe = 27.837[dB]
Irr_Dec_Bandwidth_Hz = 4.7826087[kHz]
Irr_Dec_Bandwidth_Ppm = 11.96303566[ppm]
Irr_Dec_Freq = 399.78219838[MHz]
Irr_Dec_Merit_Factor = 2.2
Irr_Decoupling = TRUE
Irr_Noe = TRUE
Irr_Noise = WALTZ
Irr_Offset_Default = 5[ppm]
Irr_Pwidth = 0.115[ms]
Irr_Pwidth_Default = 0.115[ms]
Irr_Pwidth_Default_Calc = 0.115[ms]
Irr_Pwidth_Temp1 = 0.115[ms]
Irr_Wurst = FALSE
Decimation_Rate = 0

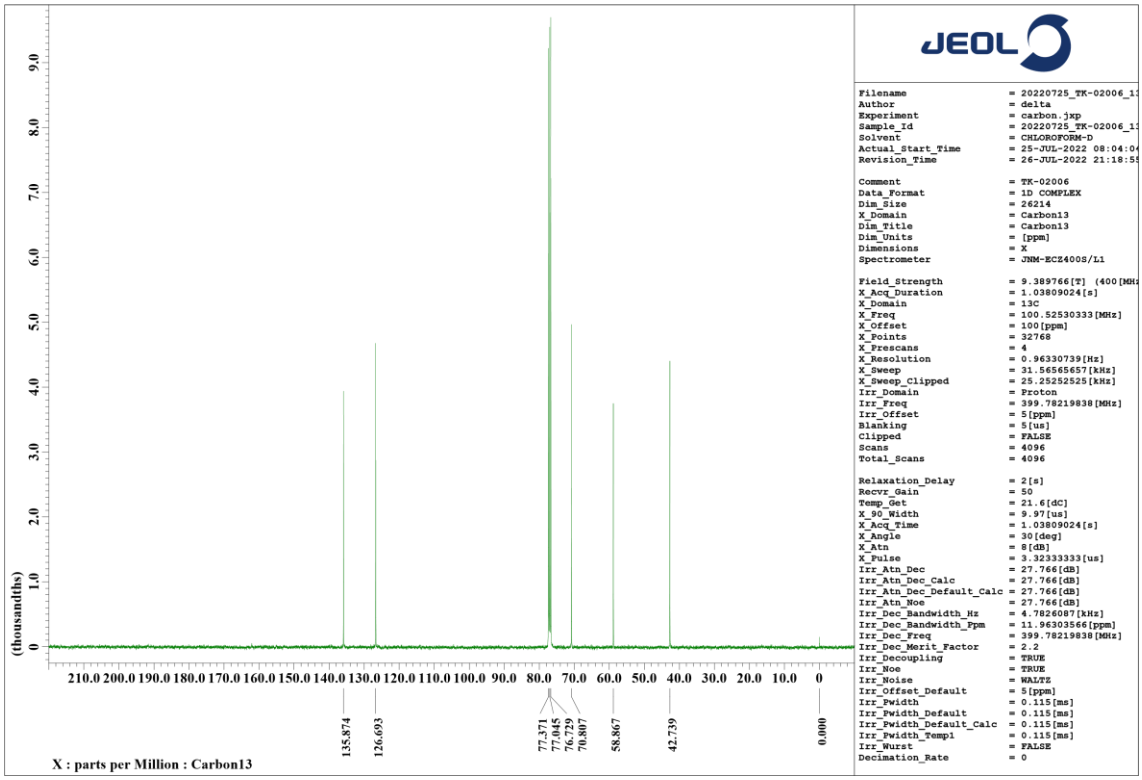

3h
abundance
X : parts per Million : Proton
7.266
6.655
6.630
6.614
6.589
6.249
6.208
5.828
5.804
4.248
2.089
1.927
1.920
1.684
1.651
1.645
1.611
1.604
0.000
0.93
0.99
1.00
0.96
3.00
6.11
6.68
Filename = 20230823_TK-02163_CDCl3
Author = delta
Experiment = proton.jxp
Sample_Id = 20230823_TK-02163_CDCl3
Solvent = CHLOROFORM-D
Actual_Start_Time = 23-AUG-2023 19:52:05
Revision_Time = 26-AUG-2023 16:17:49
Comment = TK-02163
Data_Format = 1D COMPLEX
Dim_Size = 104858
X_Domain = Proton
Dim_Title = Proton
Dim_Units = [ppm]
Dimensions = X
Spectrometer = JNM-ECZ400S/L1
Field_Strength = 9.389766[T] (400[MHz])
X_Acq_Duration = 2.18628096[s]
X_Domain = 1H
X_Freq = 399.78219838[MHz]
X_Offset = 5[ppm]
X_Points = 16384
X_Prescans = 1
X_Resolution = 0.45739775[Hz]
X_Sweep = 7.4940048[kHz]
X_Sweep_Clipped = 5.99520384[kHz]
Irr_Domain = Proton
Irr_Freq = 399.78219838[MHz]
Irr_Offset = 5[ppm]
Tri_Domain = Proton
Tri_Freq = 399.78219838[MHz]
Tri_Offset = 5[ppm]
Blanking = 2[us]
Clipped = FALSE
Scans = 16
Total_Scans = 16
Relaxation_Delay = 5[s]
Recvr_Gain = 46
Temp_Get = 22.9[dC]
X_90_Width = 6.4[us]
X_Acq_Time = 2.18628096[s]
X_Angle = 45[deg]
X_Atn = 2.4[dB]
X_Pulse = 3.2[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Loop = 500
Dante_Presat = FALSE
Decimation_Rate = 0
Initial_Wait = 1[s]
Phase = (0, 90, 270, 180, 180,
Presat_Time = 5[s]
Presat_Time_Flag = FALSE
Relaxation_Delay_Calc = 0[s]
Relaxation_Delay_Temp = 5[s]
Repetition_Time = 7.18628096[s]

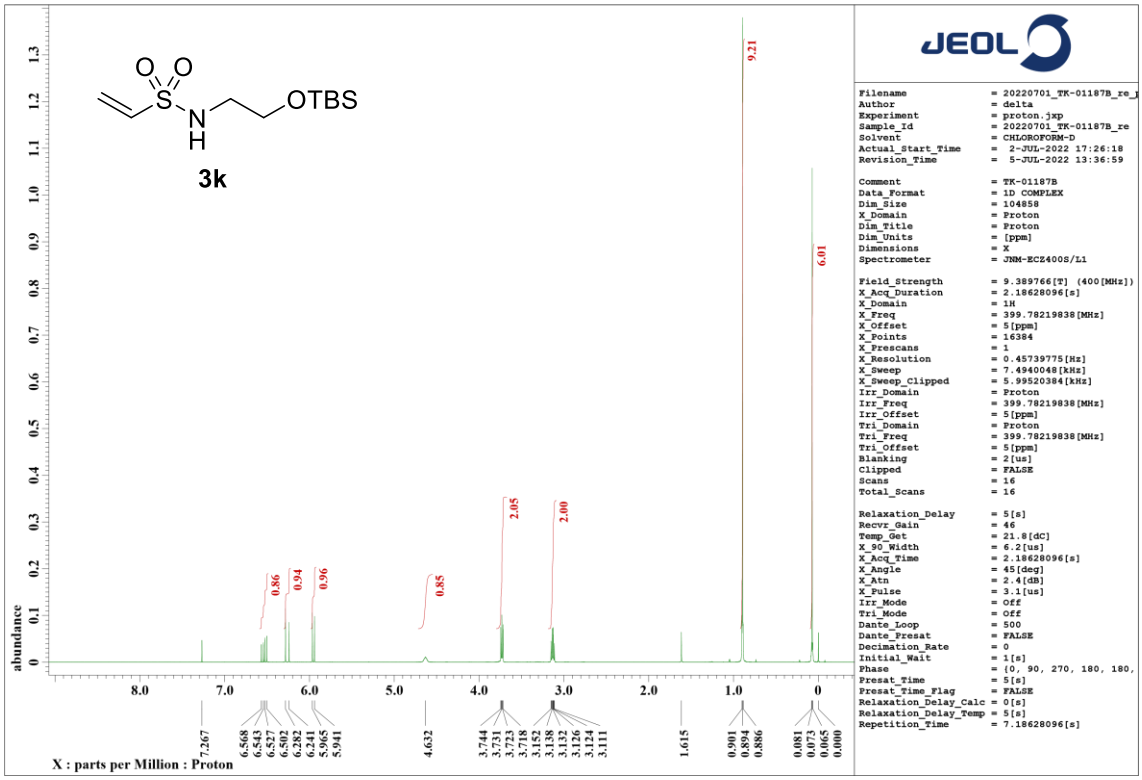

(thousandths)
X : parts per Million : Carbon13
140.033
124.259
77.342
77.227
77.026
76.710
55.110
43.324
35.887
29.553
0.000
Filename = 20230823_TK-02163_CD
Author = delta
Experiment = carbon.jxp
Sample_Id = 20230823_TK-02163_CD
Solvent = CHLOROFORM-D
Actual_Start_Time = 24-AUG-2023 07:27:0
Revision_Time = 26-AUG-2023 16:14:1
Comment = TK-02163
Data_Format = 1D COMPLEX
Dim_Size = 26214
X_Domain = Carbon13
Dim_Title = Carbon13
Dim_Units = [ppm]
Dimensions = X
Spectrometer = JNM-ECZ400S/L1
Field_Strength = 9.389766[T] (400[MH
X_Acq_Duration = 1.03809024[s]
X_Domain = 13C
X_Freq = 100.52530333[MHz]
X_Offset = 100[ppm]
X_Points = 32768
X_Prescans = 4
X_Resolution = 0.96330739[Hz]
X_Sweep = 31.56565657[kHz]
X_Sweep_Clipped = 25.25252525[kHz]
Irr_Domain = Proton
Irr_Freq = 399.78219838[MHz]
Irr_Offset = 5[ppm]
Blanking = 5[us]
Clipped = TRUE
Scans = 4096
Total_Scans = 4096
Relaxation_Delay = 2[s]
Recvr_Gain = 50
Temp_Get = 22.8[dC]
X_90_Width = 10.02[us]
X_Acq_Time = 1.03809024[s]
X_Angle = 30[deg]
X_Atn = 8[dB]
X_Pulse = 3.34[us]
Irr_Atn_Dec = 27.49[dB]
Irr_Atn_Dec_Calc = 27.49[dB]
Irr_Atn_Dec_Default_Calc = 27.49[dB]
Irr_Atn_Noe = 27.49[dB]
Irr_Dec_Bandwidth_Hz = 4.7826087[kHz]
Irr_Dec_Bandwidth_Ppm = 11.96303566[ppm]
Irr_Dec_Freq = 399.78219838[MHz]
Irr_Dec_Merit_Factor = 2.2
Irr_Decoupling = TRUE
Irr_Noe = TRUE
Irr_Noise = WALTZ
Irr_Offset_Default = 5[ppm]
Irr_Pwidth = 0.115[ms]
Irr_Pwidth_Default = 0.115[ms]
Irr_Pwidth_Default_Calc = 0.115[ms]
Irr_Pwidth_Temp1 = 0.115[ms]
Irr_Wurst = FALSE
Decimation_Rate = 0

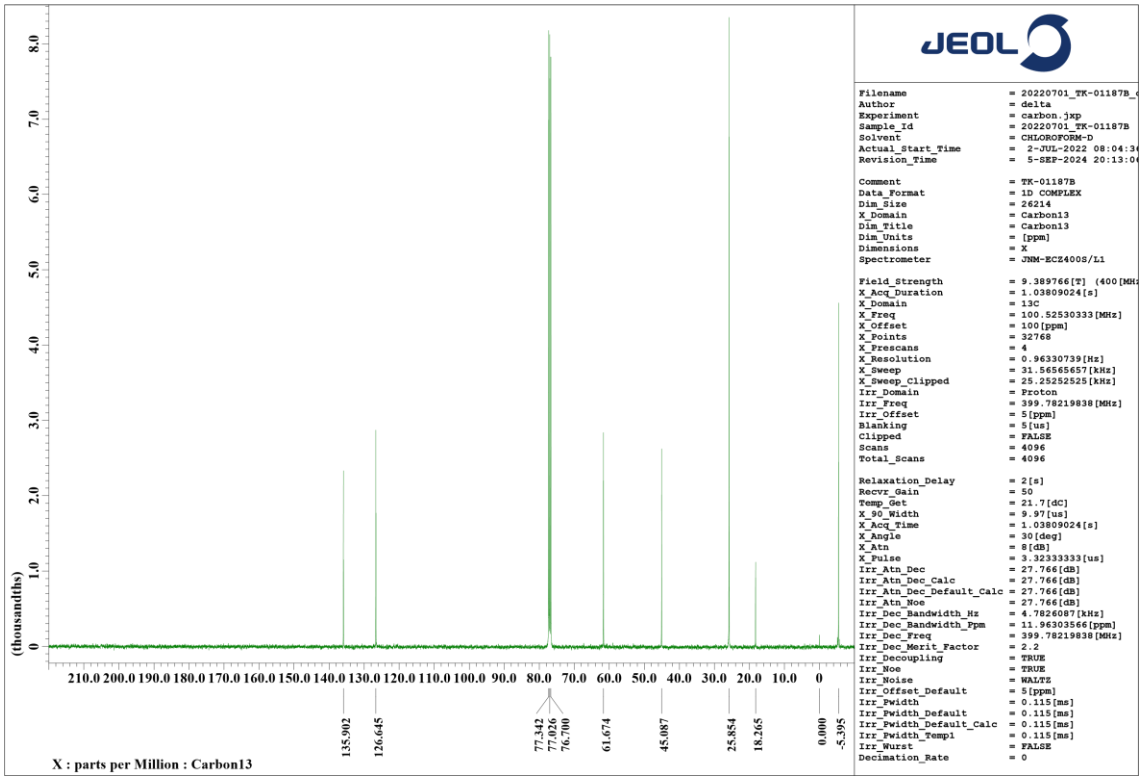

4.77
2.03
0.91
1.00
1.01
0.89
3i
abundance
X : parts per Million : Proton
7.365
7.348
7.343
7.339
7.330
7.318
7.302
7.295
7.259
6.499
6.474
6.457
6.433
6.256
6.215
5.919
5.895
4.759
4.207
4.192
1.641
0.000
Filename = 20210924_TK-01063_re_p
Author = delta
Experiment = proton.jxp
Sample_Id = 20210924_TK-01063_re
Solvent = CHLOROFORM-D
Actual_Start_Time = 24-SEP-2021 15:58:17
Revision_Time = 23-MAR-2022 12:55:15
Comment = TK-01063_re
Data_Format = 1D COMPLEX
Dim_Size = 104858
X_Domain = Proton
Dim_Title = Proton
Dim_Units = [ppm]
Dimensions = X
Spectrometer = JNM-ECZ400S/L1
Field_Strength = 9.389766[T] (400[MHz])
X_Acq_Duration = 2.18628096[s]
X_Domain = 1H
X_Freq = 399.78219838[MHz]
X_Offset = 5[ppm]
X_Points = 16384
X_Prescans = 1
X_Resolution = 0.45739775[Hz]
X_Sweep = 7.4940048[kHz]
X_Sweep_Clipped = 5.99520384[kHz]
Irr_Domain = Proton
Irr_Freq = 399.78219838[MHz]
Irr_Offset = 5[ppm]
Tri_Domain = Proton
Tri_Freq = 399.78219838[MHz]
Tri_Offset = 5[ppm]
Blanking = 2[us]
Clipped = FALSE
Scans = 16
Total_Scans = 16
Relaxation_Delay = 5[s]
Recvr_Gain = 46
Temp_Get = 21.5[dC]
X_90_Width = 6.15[us]
X_Acq_Time = 2.18628096[s]
X_Angle = 45[deg]
X_Atn = 2.4[dB]
X_Pulse = 3.075[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Loop = 500
Dante_Presat = FALSE
Decimation_Rate = 0
Initial_Wait = 1[s]
Phase = (0, 90, 270, 180, 180,
Presat_Time = 5[s]
Presat_Time_Flag = FALSE
Relaxation_Delay_Calc = 0[s]
Relaxation_Delay_Temp = 5[s]
Repetition_Time = 7.18628096[s]

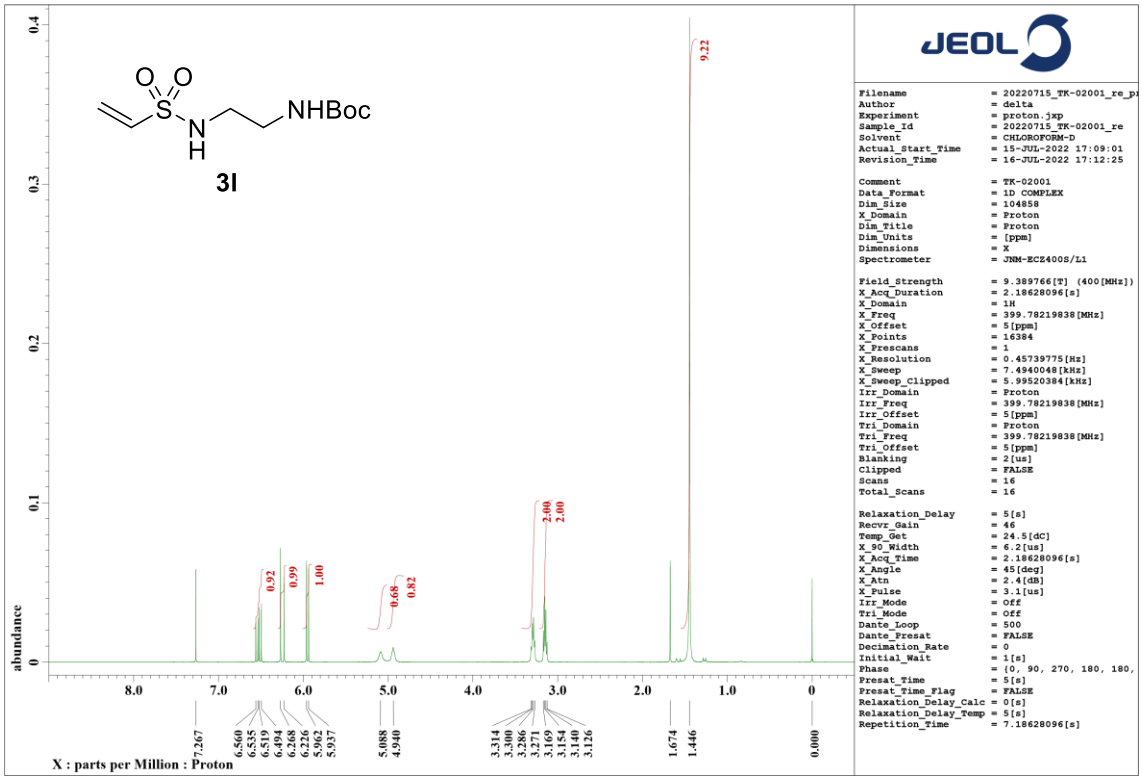

(thousandths)
X : parts per Million : Carbon13
136.432
135.915
128.766
128.018
127.903
126.782
77.316
77.000
76.684
46.977
Filename = 20210922_TK-01063_1
Author = delta
Experiment = carbon.jxp
Sample_Id = 20210922_TK-01063_1
Solvent = CHLOROFORM-D
Actual_Start_Time = 23-SEP-2021 21:03:4
Revision_Time = 23-MAR-2022 12:57:3
Comment = TK-01063_13C
Data_Format = 1D COMPLEX
Dim_Size = 26214
X_Domain = Carbon13
Dim_Title = Carbon13
Dim_Units = [ppm]
Dimensions = X
Spectrometer = JNM-ECZ400S/L1
Field_Strength = 9.389766[T] (400[MH
X_Acq_Duration = 1.03809024[s]
X_Domain = 13C
X_Freq = 100.52530333[MHz]
X_Offset = 100[ppm]
X_Points = 32768
X_Prescans = 4
X_Resolution = 0.96330739[Hz]
X_Sweep = 31.56565657[kHz]
X_Sweep_Clipped = 25.25252525[kHz]
Irr_Domain = Proton
Irr_Freq = 399.78219838[MHz]
Irr_Offset = 5[ppm]
Blanking = 5[us]
Clipped = TRUE
Scans = 8192
Total_Scans = 8192
Relaxation_Delay = 2[s]
Recvr_Gain = 50
Temp_Get = 21.5[dC]
X_90_Width = 9.91[us]
X_Acq_Time = 1.03809024[s]
X_Angle = 30[deg]
X_Atn = 8[dB]
X_Pulse = 3.30333333[us]
Irr_Atn_Dec = 27.837[dB]
Irr_Atn_Dec_Calc = 27.837[dB]
Irr_Atn_Dec_Default_Calc = 27.837[dB]
Irr_Atn_Noe = 27.837[dB]
Irr_Dec_Bandwidth_Hz = 4.7826087[kHz]
Irr_Dec_Bandwidth_Ppm = 11.96303566[ppm]
Irr_Dec_Freq = 399.78219838[MHz]
Irr_Dec_Merit_Factor = 2.2
Irr_Decoupling = TRUE
Irr_Noe = TRUE
Irr_Noise = WALTZ
Irr_Offset_Default = 5[ppm]
Irr_Pwidth = 0.115[ms]
Irr_Pwidth_Default = 0.115[ms]
Irr_Pwidth_Default_Calc = 0.115[ms]
Irr_Pwidth_Temp1 = 0.115[ms]
Irr_Wurst = FALSE
Decimation_Rate = 0

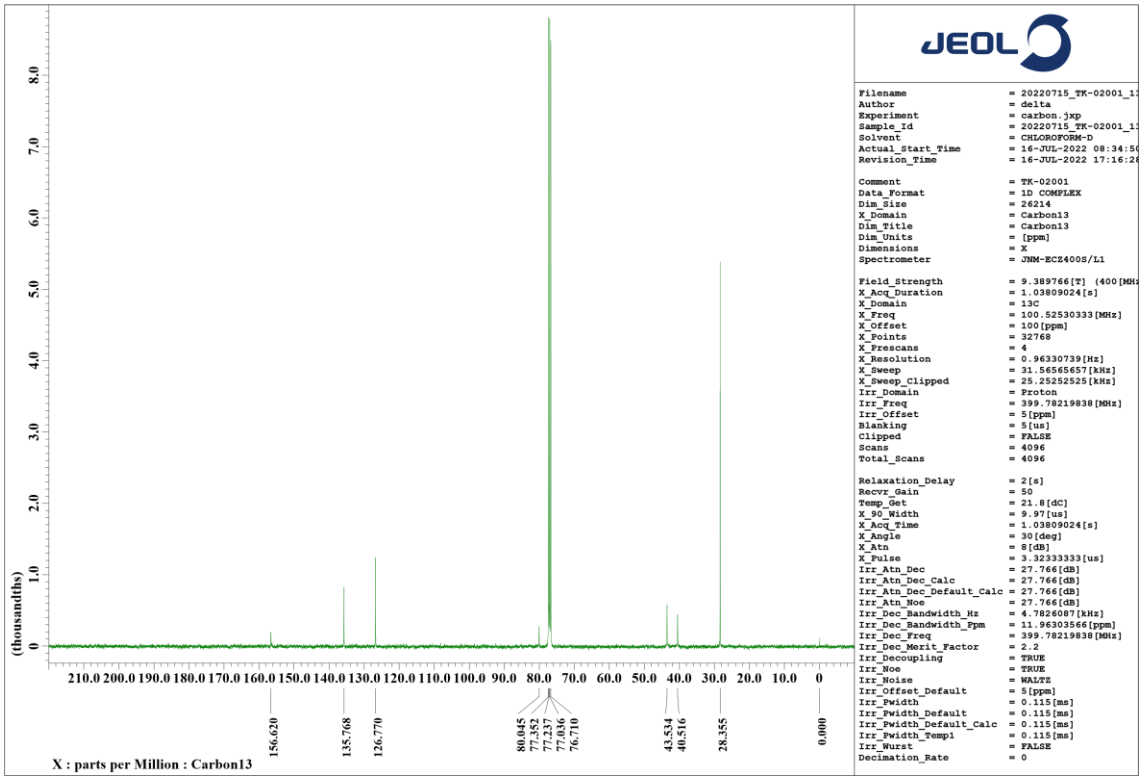

3j
abundance
X : parts per Million : Proton
JEOL
Filename = 20220721_TK-02006_prot
Author = delta
Experiment = proton.jxp
Sample_Id = 20220721_TK-02006
Solvent = CHLOROFORM-D
Actual_Start_Time = 21-JUL-2022 15:26:40
Revision_Time = 26-JUL-2022 20:59:04
Comment = TK-02006
Data_Format = 1D COMPLEX
Dim_Size = 104858
X_Domain = Proton
Dim_Title = Proton
Dim_Units = [ppm]
Dimensions = X
Spectrometer = JNM-ECZ400S/L1
Field_Strength = 9.389766[T] (400[MHz])
X_Acq_Duration = 2.18628096[s]
X_Domain = 1H
X_Freq = 399.78219838[MHz]
X_Offset = 5[ppm]
X_Points = 16384
X_Prescans = 1
X_Resolution = 0.45739775[Hz]
X_Sweep = 7.4940048[kHz]
X_Sweep_Clipped = 5.99520384[kHz]
Irr_Domain = Proton
Irr_Freq = 399.78219838[MHz]
Irr_Offset = 5[ppm]
Tri_Domain = Proton
Tri_Freq = 399.78219838[MHz]
Tri_Offset = 5[ppm]
Blanking = 2[us]
Clipped = FALSE
Scans = 16
Total_Scans = 16
Relaxation_Delay = 5[s]
Recvr_Gain = 46
Temp_Get = 21.6[dC]
X_90_Width = 6.2[us]
X_Acq_Time = 2.18628096[s]
X_Angle = 45[deg]
X_Atn = 2.4[dB]
X_Pulse = 3.1[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Loop = 500
Dante_Presat = FALSE
Decimation_Rate = 0
Initial_Wait = 1[s]
Phase = (0, 90, 270, 180, 180,
Presat_Time = 5[s]
Presat_Time_Flag = FALSE
Relaxation_Delay_Calc = 0[s]
Relaxation_Delay_Temp = 5[s]
Repetition_Time = 7.18628096[s]

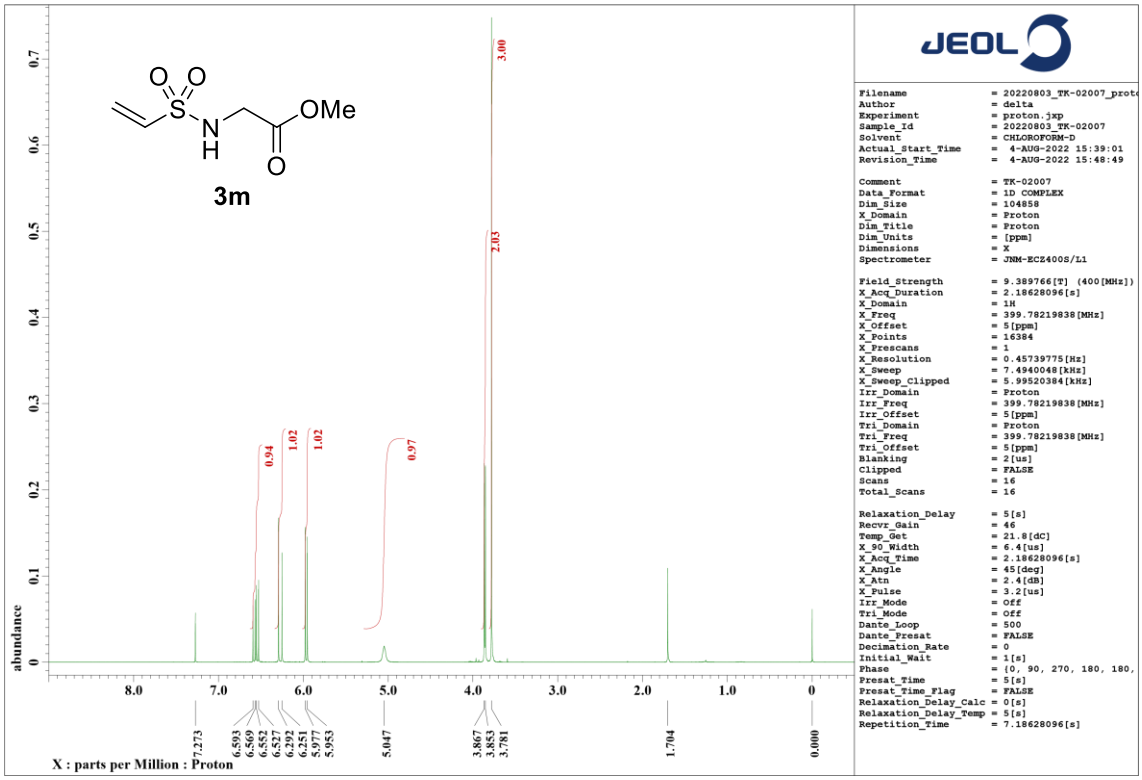

(thousandths)
X : parts per Million : Carbon13
JEOL
Filename = 20220725_TK-02006_1
Author = delta
Experiment = carbon.jxp
Sample_Id = 20220725_TK-02006_1
Solvent = CHLOROFORM-D
Actual_Start_Time = 25-JUL-2022 08:04:0
Revision_Time = 26-JUL-2022 21:18:5
Comment = TK-02006
Data_Format = 1D COMPLEX
Dim_Size = 26214
X_Domain = Carbon13
Dim_Title = Carbon13
Dim_Units = [ppm]
Dimensions = X
Spectrometer = JNM-ECZ400S/L1
Field_Strength = 9.389766[T] (400[MH
X_Acq_Duration = 1.03809024[s]
X_Domain = 13C
X_Freq = 100.52530333[MHz]
X_Offset = 100[ppm]
X_Points = 32768
X_Prescans = 4
X_Resolution = 0.96330739[Hz]
X_Sweep = 31.56565657[kHz]
X_Sweep_Clipped = 25.25252525[kHz]
Irr_Domain = Proton
Irr_Freq = 399.78219838[MHz]
Irr_Offset = 5[ppm]
Blanking = 5[us]
Clipped = FALSE
Scans = 4096
Total_Scans = 4096
Relaxation_Delay = 2[s]
Recvr_Gain = 50
Temp_Get = 21.6[dC]
X_90_Width = 9.97[us]
X_Acq_Time = 1.03809024[s]
X_Angle = 30[deg]
X_Atn = 8[dB]
X_Pulse = 3.32333333[us]
Irr_Atn_Dec = 27.766[dB]
Irr_Atn_Dec_Calc = 27.766[dB]
Irr_Atn_Dec_Default_Calc = 27.766[dB]
Irr_Atn_Noe = 27.766[dB]
Irr_Dec_Bandwidth_Hz = 4.7826087[kHz]
Irr_Dec_Bandwidth_Ppm = 11.96303566[ppm]
Irr_Dec_Freq = 399.78219838[MHz]
Irr_Dec_Merit_Factor = 2.2
Irr_Decoupling = TRUE
Irr_Noe = TRUE
Irr_Noise = WALTZ
Irr_Offset_Default = 5[ppm]
Irr_Pwidth = 0.115[ms]
Irr_Pwidth_Default = 0.115[ms]
Irr_Pwidth_Default_Calc = 0.115[ms]
Irr_Pwidth_Temp1 = 0.115[ms]
Irr_Wurst = FALSE
Decimation_Rate = 0

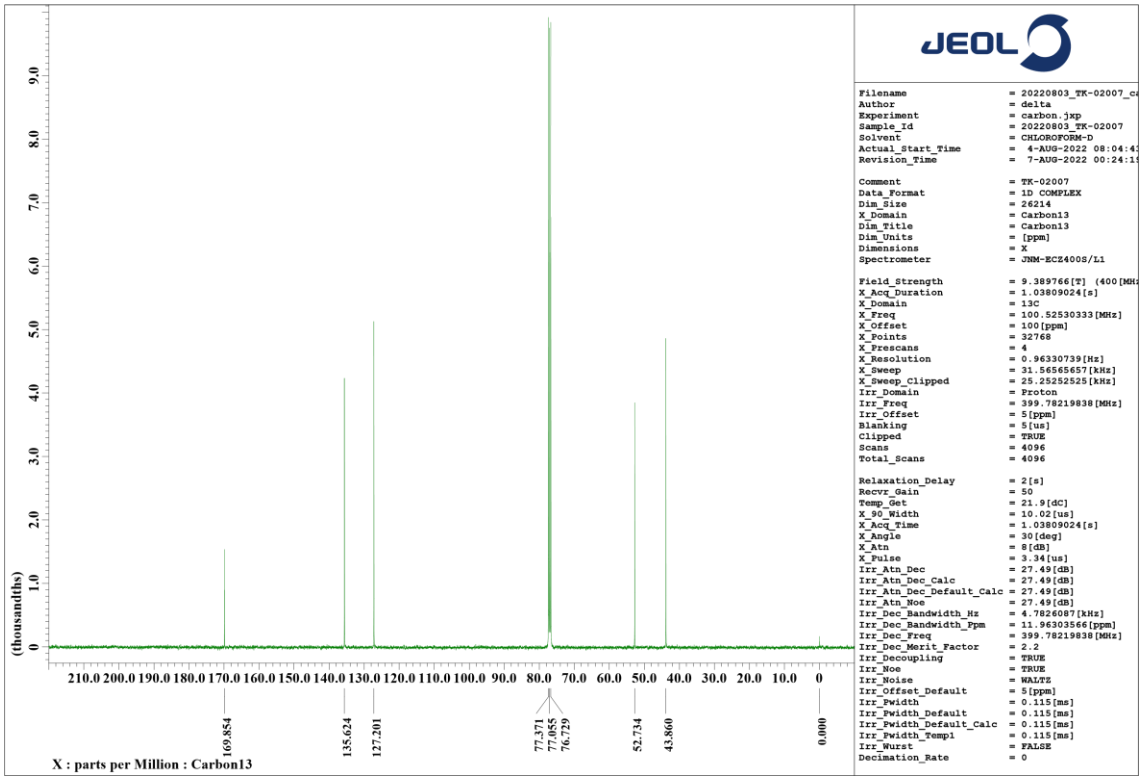

OTBS
3k
abundance
X : parts per Million : Proton
9.21
6.01
2.05
2.00
0.86
0.94
0.96
0.85
7.267
6.568
6.543
6.527
6.502
6.282
6.241
6.065
5.941
4.632
3.744
3.731
3.723
3.718
3.152
3.138
3.132
3.126
3.114
3.111
1.615
0.901
0.894
0.886
0.081
0.073
0.065
0.000
Filename = 20220701_TK-01187B_re_
Author = delta
Experiment = proton.jxp
Sample_Id = 20220701_TK-01187B_re
Solvent = CHLOROFORM-D
Actual_Start_Time = 2-JUL-2022 17:26:18
Revision_Time = 5-JUL-2022 13:36:59
Comment = TK-01187B
Data_Format = 1D COMPLEX
Dim_Size = 104858
X_Domain = Proton
Dim_Title = Proton
Dim_Units = [ppm]
Dimensions = X
Spectrometer = JNM-ECZ400S/L1
Field_Strength = 9.389766[T] (400[MHz])
X_Acq_Duration = 2.18628096[s]
X_Domain = 1H
X_Freq = 399.78219838[MHz]
X_Offset = 5[ppm]
X_Points = 16384
X_Prescans = 1
X_Resolution = 0.45739775[Hz]
X_Sweep = 7.4940048[kHz]
X_Sweep_Clipped = 5.99520384[kHz]
Irr_Domain = Proton
Irr_Freq = 399.78219838[MHz]
Irr_Offset = 5[ppm]
Tri_Domain = Proton
Tri_Freq = 399.78219838[MHz]
Tri_Offset = 5[ppm]
Blanking = 2[us]
Clipped = FALSE
Scans = 16
Total_Scans = 16
Relaxation_Delay = 5[s]
Recvr_Gain = 46
Temp_Get = 21.8[dC]
X_90_Width = 6.2[us]
X_Acq_Time = 2.18628096[s]
X_Angle = 45[deg]
X_Atn = 2.4[dB]
X_Pulse = 3.1[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Loop = 500
Dante_Presat = FALSE
Decimation_Rate = 0
Initial_Wait = 1[s]
Phase = (0, 90, 270, 180, 180,
Presat_Time = 5[s]
Presat_Time_Flag = FALSE
Relaxation_Delay_Calc = 0[s]
Relaxation_Delay_Temp = 5[s]
Repetition_Time = 7.18628096[s]

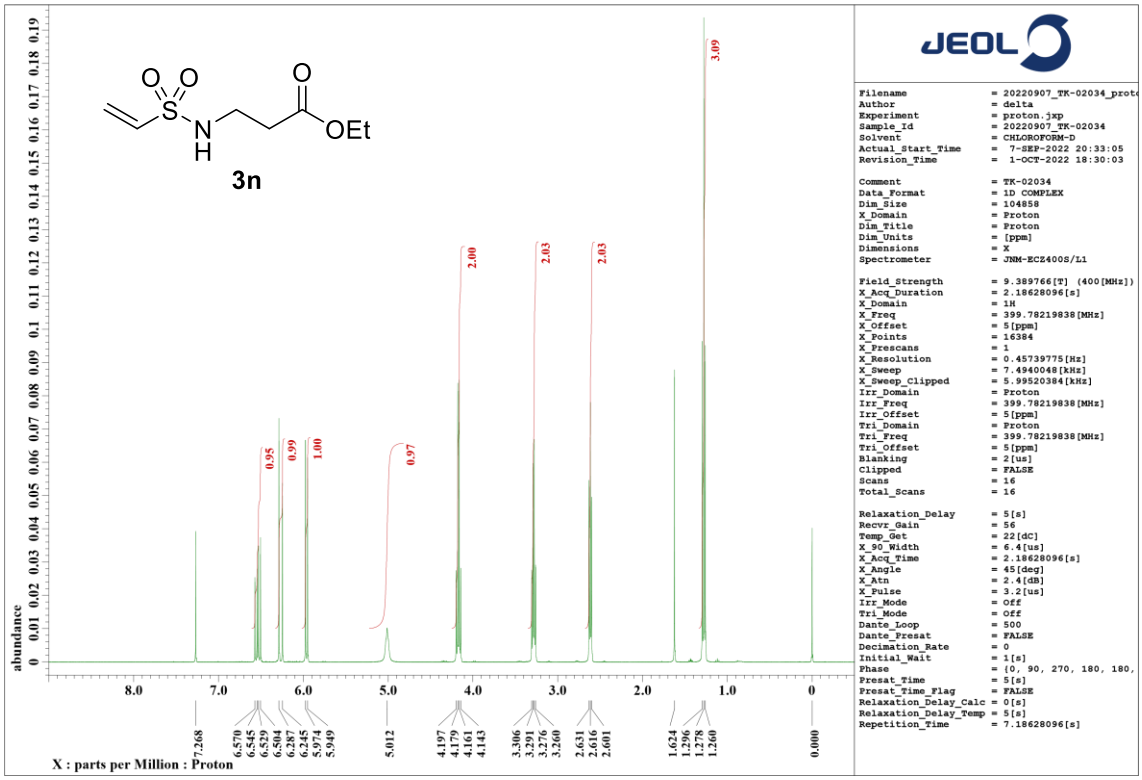

(thousandths)
X : parts per Million : Carbon13
135.902
126.645
77.342
77.026
76.700
61.674
45.087
25.854
18.265
0.000
-5.395
Filename = 20220701_TK-01187B_
Author = delta
Experiment = carbon.jxp
Sample_Id = 20220701_TK-01187B
Solvent = CHLOROFORM-D
Actual_Start_Time = 2-JUL-2022 08:04:3
Revision_Time = 5-SEP-2024 20:13:0
Comment = TK-01187B
Data_Format = 1D COMPLEX
Dim_Size = 26214
X_Domain = Carbon13
Dim_Title = Carbon13
Dim_Units = [ppm]
Dimensions = X
Spectrometer = JNM-ECZ400S/L1
Field_Strength = 9.389766[T] (400[MH
X_Acq_Duration = 1.03809024[s]
X_Domain = 13C
X_Freq = 100.52530333[MHz]
X_Offset = 100[ppm]
X_Points = 32768
X_Prescans = 4
X_Resolution = 0.96330739[Hz]
X_Sweep = 31.56565657[kHz]
X_Sweep_Clipped = 25.25252525[kHz]
Irr_Domain = Proton
Irr_Freq = 399.78219838[MHz]
Irr_Offset = 5[ppm]
Blanking = 5[us]
Clipped = FALSE
Scans = 4096
Total_Scans = 4096
Relaxation_Delay = 2[s]
Recvr_Gain = 50
Temp_Get = 21.7[dC]
X_90_Width = 9.97[us]
X_Acq_Time = 1.03809024[s]
X_Angle = 30[deg]
X_Atn = 8[dB]
X_Pulse = 3.32333333[us]
Irr_Atn_Dec = 27.766[dB]
Irr_Atn_Dec_Calc = 27.766[dB]
Irr_Atn_Dec_Default_Calc = 27.766[dB]
Irr_Atn_Noe = 27.766[dB]
Irr_Dec_Bandwidth_Hz = 4.7826087[kHz]
Irr_Dec_Bandwidth_Ppm = 11.96303566[ppm]
Irr_Dec_Freq = 399.78219838[MHz]
Irr_Dec_Merit_Factor = 2.2
Irr_Decoupling = TRUE
Irr_Noe = TRUE
Irr_Noise = WALTZ
Irr_Offset_Default = 5[ppm]
Irr_Pwidth = 0.115[ms]
Irr_Pwidth_Default = 0.115[ms]
Irr_Pwidth_Default_Calc = 0.115[ms]
Irr_Pwidth_Temp1 = 0.115[ms]
Irr_Wurst = FALSE
Decimation_Rate = 0

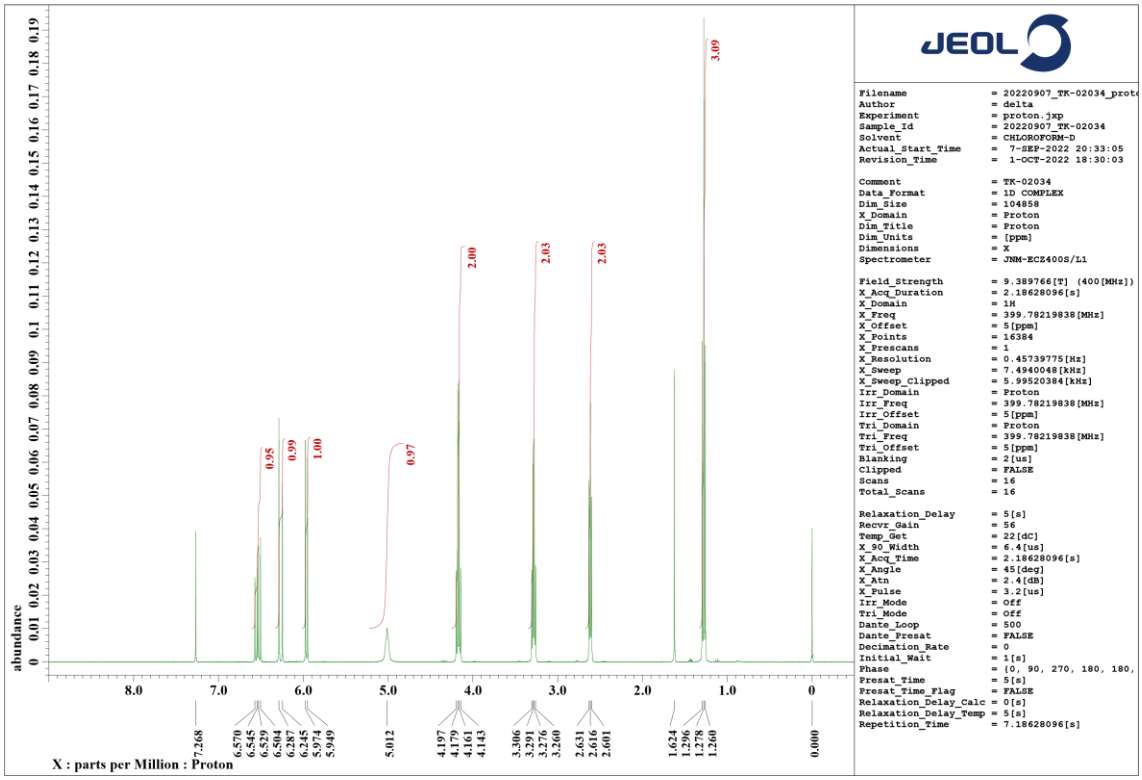

NHBoc
3l
abundance
X : parts per Million : Proton
9.22
2.00
2.00
0.92
0.99
1.00
0.68
0.82
7.267
6.560
6.535
6.519
6.494
6.268
6.226
5.962
5.937
5.088
4.940
3.314
3.300
3.286
3.271
3.169
3.154
3.140
3.126
1.674
1.446
0.000
JEOL
Filename = 20220715_TK-02001_re_p
Author = delta
Experiment = proton.jxp
Sample_Id = 20220715_TK-02001_re
Solvent = CHLOROFORM-D
Actual_Start_Time = 15-JUL-2022 17:09:01
Revision_Time = 16-JUL-2022 17:12:25
Comment = TK-02001
Data_Format = 1D COMPLEX
Dim_Size = 104858
X_Domain = Proton
Dim_Title = Proton
Dim_Units = [ppm]
Dimensions = X
Spectrometer = JNM-ECZ400S/L1
Field_Strength = 9.389766[T] (400[MHz])
X_Acq_Duration = 2.18628096[s]
X_Domain = 1H
X_Freq = 399.78219838[MHz]
X_Offset = 5[ppm]
X_Points = 16384
X_Prescans = 1
X_Resolution = 0.45739775[Hz]
X_Sweep = 7.4940048[kHz]
X_Sweep_Clipped = 5.99520384[kHz]
Irr_Domain = Proton
Irr_Freq = 399.78219838[MHz]
Irr_Offset = 5[ppm]
Tri_Domain = Proton
Tri_Freq = 399.78219838[MHz]
Tri_Offset = 5[ppm]
Blanking = 2[us]
Clipped = FALSE
Scans = 16
Total_Scans = 16
Relaxation_Delay = 5[s]
Recvr_Gain = 46
Temp_Get = 24.5[dC]
X_90_Width = 6.2[us]
X_Acq_Time = 2.18628096[s]
X_Angle = 45[deg]
X_Atn = 2.4[dB]
X_Pulse = 3.1[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Loop = 500
Dante_Presat = FALSE
Decimation_Rate = 0
Initial_Wait = 1[s]
Phase = (0, 90, 270, 180, 180,
Presat_Time = 5[s]
Presat_Time_Flag = FALSE
Relaxation_Delay_Calc = 0[s]
Relaxation_Delay_Temp = 5[s]
Repetition_Time = 7.18628096[s]

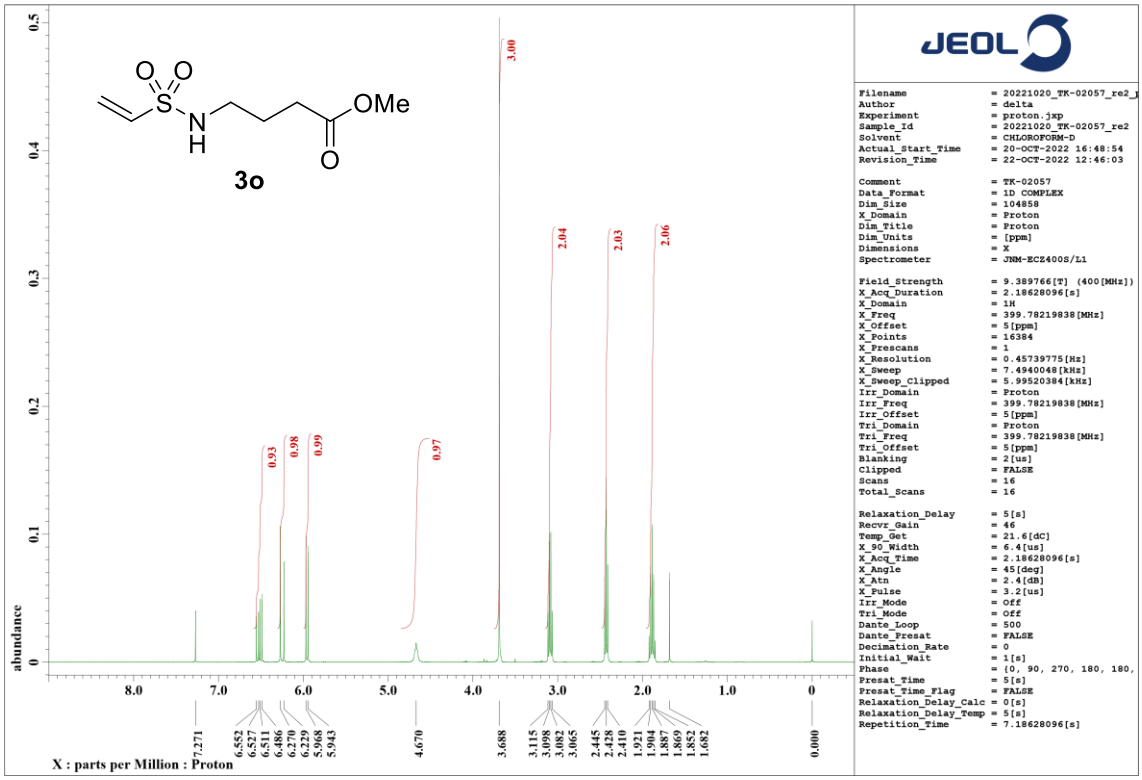

(thousandths)
X : parts per Million : Carbon13
156.620
135.768
126.770
80.045
77.432
77.217
77.036
76.710
43.534
40.516
28.355
0.000
JEOL
Filename = 20220715_TK-02001_1
Author = delta
Experiment = carbon.jxp
Sample_Id = 20220715_TK-02001_1
Solvent = CHLOROFORM-D
Actual_Start_Time = 16-JUL-2022 08:34:5
Revision_Time = 16-JUL-2022 17:16:2
Comment = TK-02001
Data_Format = 1D COMPLEX
Dim_Size = 26214
X_Domain = Carbon13
Dim_Title = Carbon13
Dim_Units = [ppm]
Dimensions = X
Spectrometer = JNM-ECZ400S/L1
Field_Strength = 9.389766[T] (400[MH
X_Acq_Duration = 1.03809024[s]
X_Domain = 13C
X_Freq = 100.52530333[MHz]
X_Offset = 100[ppm]
X_Points = 32768
X_Prescans = 4
X_Resolution = 0.96330739[Hz]
X_Sweep = 31.56565657[kHz]
X_Sweep_Clipped = 25.25252525[kHz]
Irr_Domain = Proton
Irr_Freq = 399.78219838[MHz]
Irr_Offset = 5[ppm]
Blanking = 5[us]
Clipped = FALSE
Scans = 4096
Total_Scans = 4096
Relaxation_Delay = 2[s]
Recvr_Gain = 50
Temp_Get = 21.8[dC]
X_90_Width = 9.97[us]
X_Acq_Time = 1.03809024[s]
X_Angle = 30[deg]
X_Atn = 8[dB]
X_Pulse = 3.32333333[us]
Irr_Atn_Dec = 27.766[dB]
Irr_Atn_Dec_Calc = 27.766[dB]
Irr_Atn_Dec_Default_Calc = 27.766[dB]
Irr_Atn_Noe = 27.766[dB]
Irr_Dec_Bandwidth_Hz = 4.7826087[kHz]
Irr_Dec_Bandwidth_Ppm = 11.96303566[ppm]
Irr_Dec_Freq = 399.78219838[MHz]
Irr_Dec_Merit_Factor = 2.2
Irr_Decoupling = TRUE
Irr_Noe = TRUE
Irr_Noise = WALTZ
Irr_Offset_Default = 5[ppm]
Irr_Pwidth = 0.115[ms]
Irr_Pwidth_Default = 0.115[ms]
Irr_Pwidth_Default_Calc = 0.115[ms]
Irr_Pwidth_Temp1 = 0.115[ms]
Irr_Wurst = FALSE
Decimation_Rate = 0

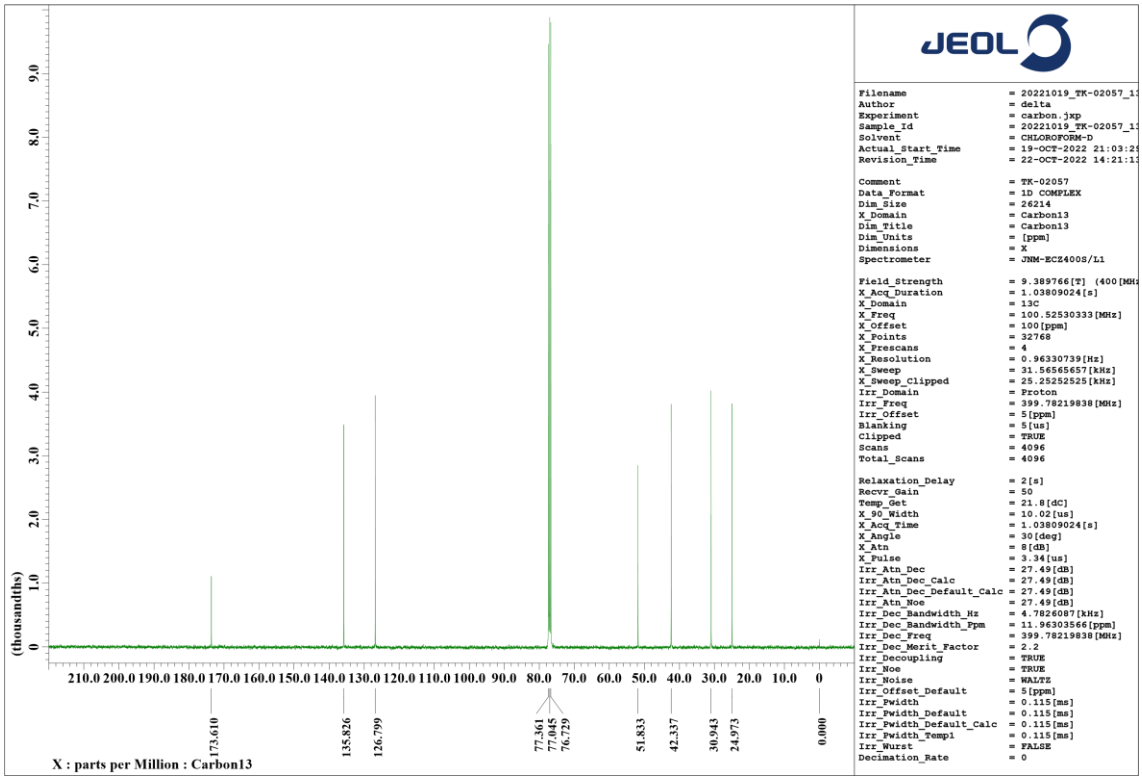

3m
abundance
X : parts per Million : Proton
7.273
6.593
6.569
6.552
6.527
6.292
6.251
5.977
5.953
5.047
3.867
3.853
3.781
1.704
0.000
0.94
1.02
1.02
0.97
2.03
3.00

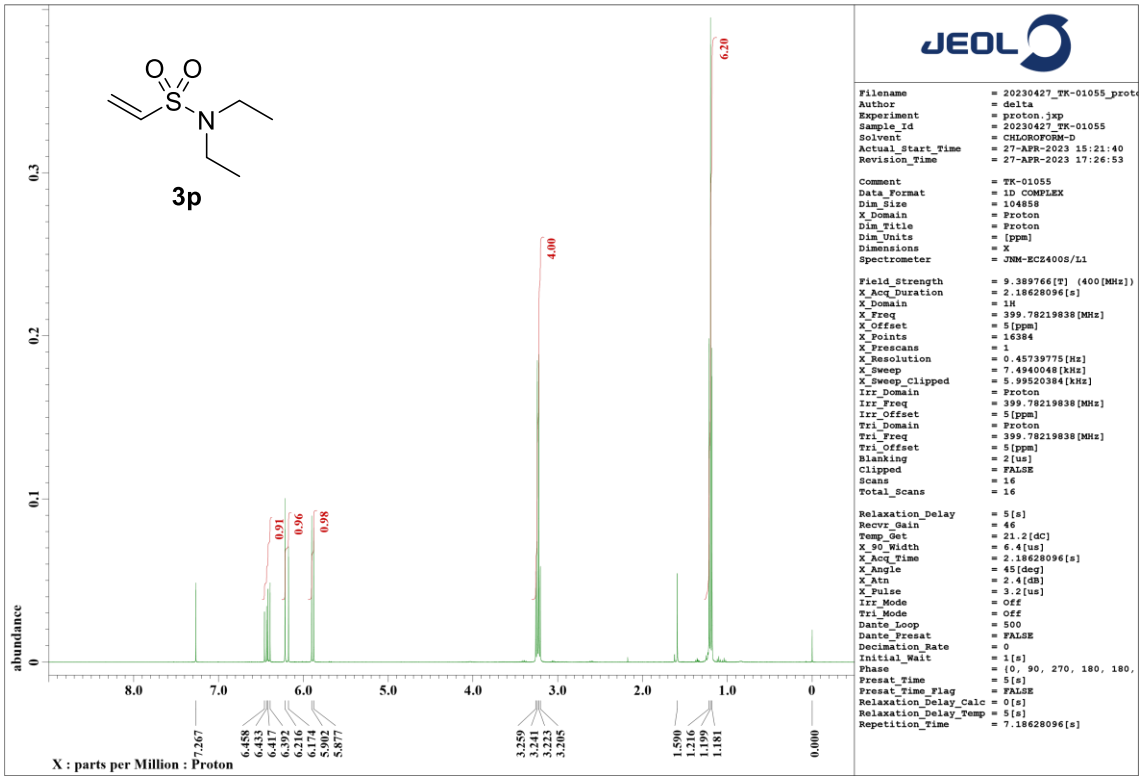

(thousandths)
X : parts per Million : Carbon13
169.854
135.624
127.201
77.371
77.055
76.729
52.734
43.860
0.000

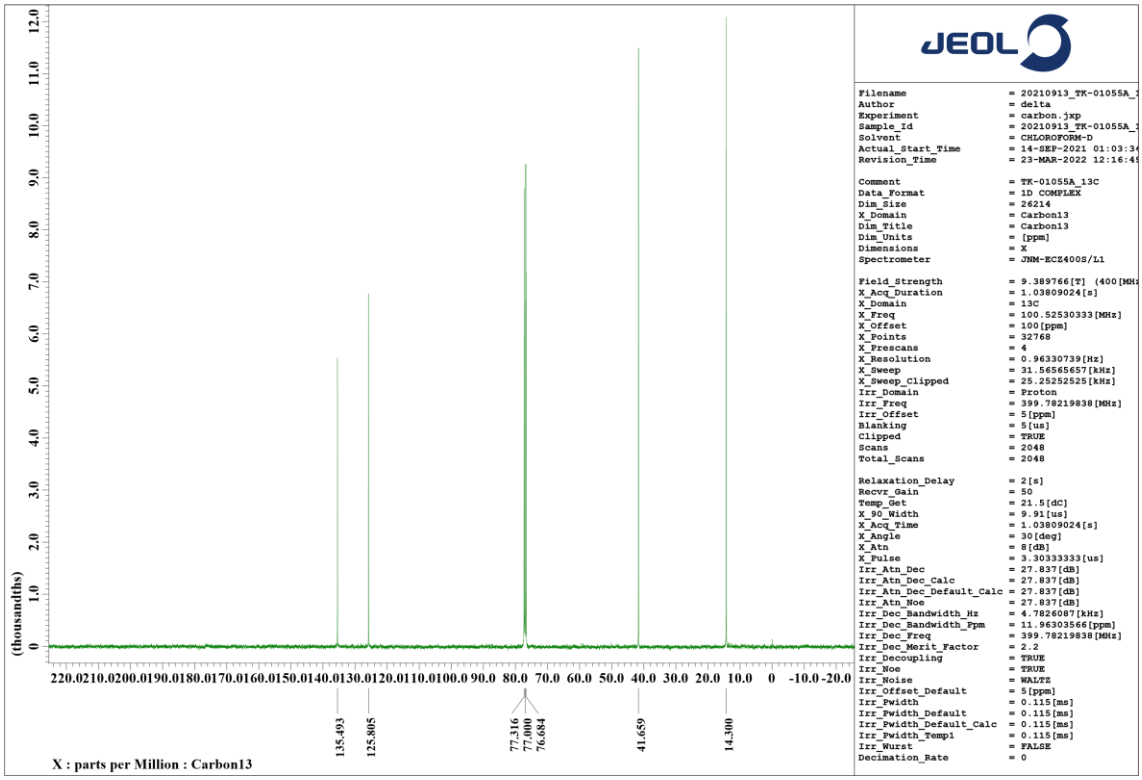

3n
abundance
X : parts per Million : Proton
0.95
0.99
1.00
0.97
2.00
2.03
2.03
3.09
7.268
6.570
6.545
6.529
6.504
6.287
6.245
5.974
5.949
5.012
4.197
4.179
4.161
4.143
3.306
3.291
3.276
3.260
2.631
2.616
2.601
1.624
1.296
1.278
1.260
0.000
Filename = 20220907_TK-02034_prot
Author = delta
Experiment = proton.jxp
Sample_Id = 20220907_TK-02034
Solvent = CHLOROFORM-D
Actual_Start_Time = 7-SEP-2022 20:33:05
Revision_Time = 1-OCT-2022 18:30:03
Comment = TK-02034
Data_Format = 1D COMPLEX
Dim_Size = 104858
X_Domain = Proton
Dim_Title = Proton
Dim_Units = [ppm]
Dimensions = X
Spectrometer = JNM-ECZ400S/L1
Field_Strength = 9.389766[T] (400[MHz])
X_Acq_Duration = 2.18628096[s]
X_Domain = 1H
X_Freq = 399.78219838[MHz]
X_Offset = 5[ppm]
X_Points = 16384
X_Prescans = 1
X_Resolution = 0.45739775[Hz]
X_Sweep = 7.4940048[kHz]
X_Sweep_Clipped = 5.99520384[kHz]
Irr_Domain = Proton
Irr_Freq = 399.78219838[MHz]
Irr_Offset = 5[ppm]
Tri_Domain = Proton
Tri_Freq = 399.78219838[MHz]
Tri_Offset = 5[ppm]
Blanking = 2[us]
Clipped = FALSE
Scans = 16
Total_Scans = 16
Relaxation_Delay = 5[s]
Recvr_Gain = 56
Temp_Get = 22[dC]
X_90_Width = 6.4[us]
X_Acq_Time = 2.18628096[s]
X_Angle = 45[deg]
X_Atn = 2.4[dB]
X_Pulse = 3.2[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Loop = 500
Dante_Presat = FALSE
Decimation_Rate = 0
Initial_Wait = 1[s]
Phase = {0, 90, 270, 180, 180,
Presat_Time = 5[s]
Presat_Time_Flag = FALSE
Relaxation_Delay_Calc = 0[s]
Relaxation_Delay_Temp = 5[s]
Repetition_Time = 7.18628096[s]

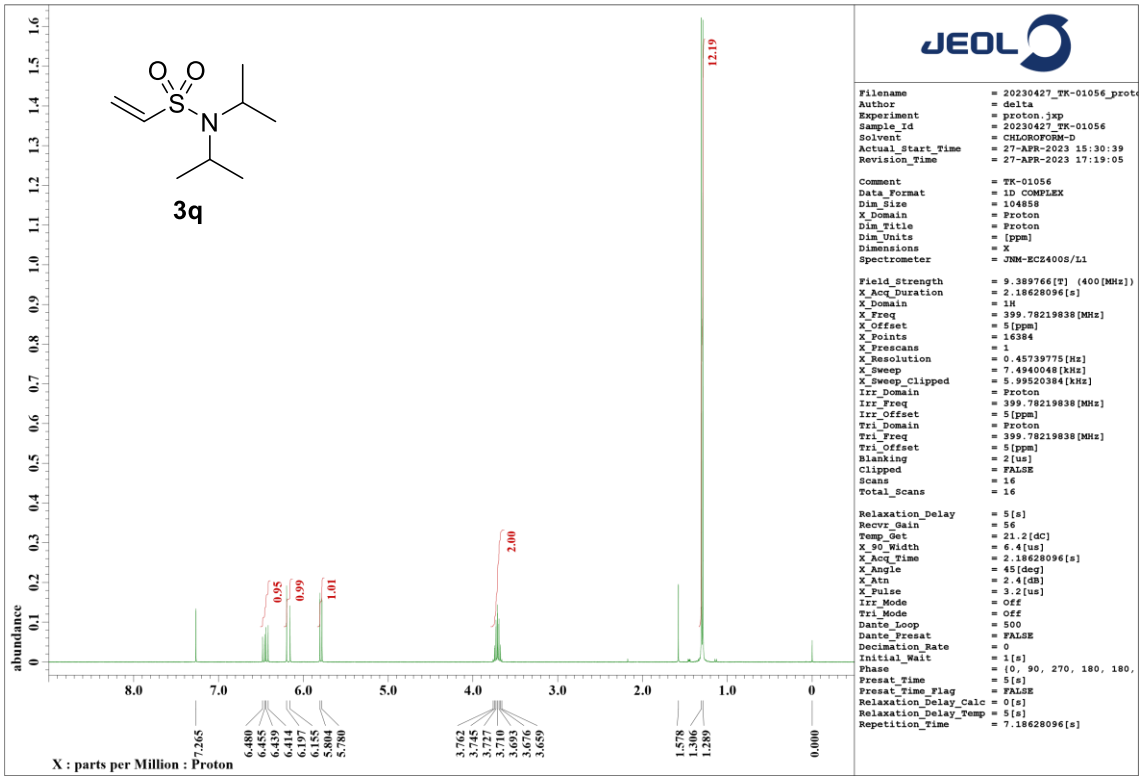

abundance
X : parts per Million : Proton
0.95
0.99
1.00
0.97
2.00
2.03
2.03
3.09
7.268
6.570
6.545
6.529
6.504
6.287
6.245
5.974
5.949
5.012
4.197
4.179
4.161
4.143
3.306
3.291
3.276
3.260
2.631
2.616
2.601
1.624
1.296
1.278
1.260
0.000
Filename = 20220907_TK-02034_prot
Author = delta
Experiment = proton.jxp
Sample_Id = 20220907_TK-02034
Solvent = CHLOROFORM-D
Actual_Start_Time = 7-SEP-2022 20:33:05
Revision_Time = 1-OCT-2022 18:30:03
Comment = TK-02034
Data_Format = 1D COMPLEX
Dim_Size = 104858
X_Domain = Proton
Dim_Title = Proton
Dim_Units = [ppm]
Dimensions = X
Spectrometer = JNM-ECZ400S/L1
Field_Strength = 9.389766[T] (400[MHz])
X_Acq_Duration = 2.18628096[s]
X_Domain = 1H
X_Freq = 399.78219838[MHz]
X_Offset = 5[ppm]
X_Points = 16384
X_Prescans = 1
X_Resolution = 0.45739775[Hz]
X_Sweep = 7.4940048[kHz]
X_Sweep_Clipped = 5.99520384[kHz]
Irr_Domain = Proton
Irr_Freq = 399.78219838[MHz]
Irr_Offset = 5[ppm]
Tri_Domain = Proton
Tri_Freq = 399.78219838[MHz]
Tri_Offset = 5[ppm]
Blanking = 2[us]
Clipped = FALSE
Scans = 16
Total_Scans = 16
Relaxation_Delay = 5[s]
Recvr_Gain = 56
Temp_Get = 22[dC]
X_90_Width = 6.4[us]
X_Acq_Time = 2.18628096[s]
X_Angle = 45[deg]
X_Atn = 2.4[dB]
X_Pulse = 3.2[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Loop = 500
Dante_Presat = FALSE
Decimation_Rate = 0
Initial_Wait = 1[s]
Phase = {0, 90, 270, 180, 180,
Presat_Time = 5[s]
Presat_Time_Flag = FALSE
Relaxation_Delay_Calc = 0[s]
Relaxation_Delay_Temp = 5[s]
Repetition_Time = 7.18628096[s]

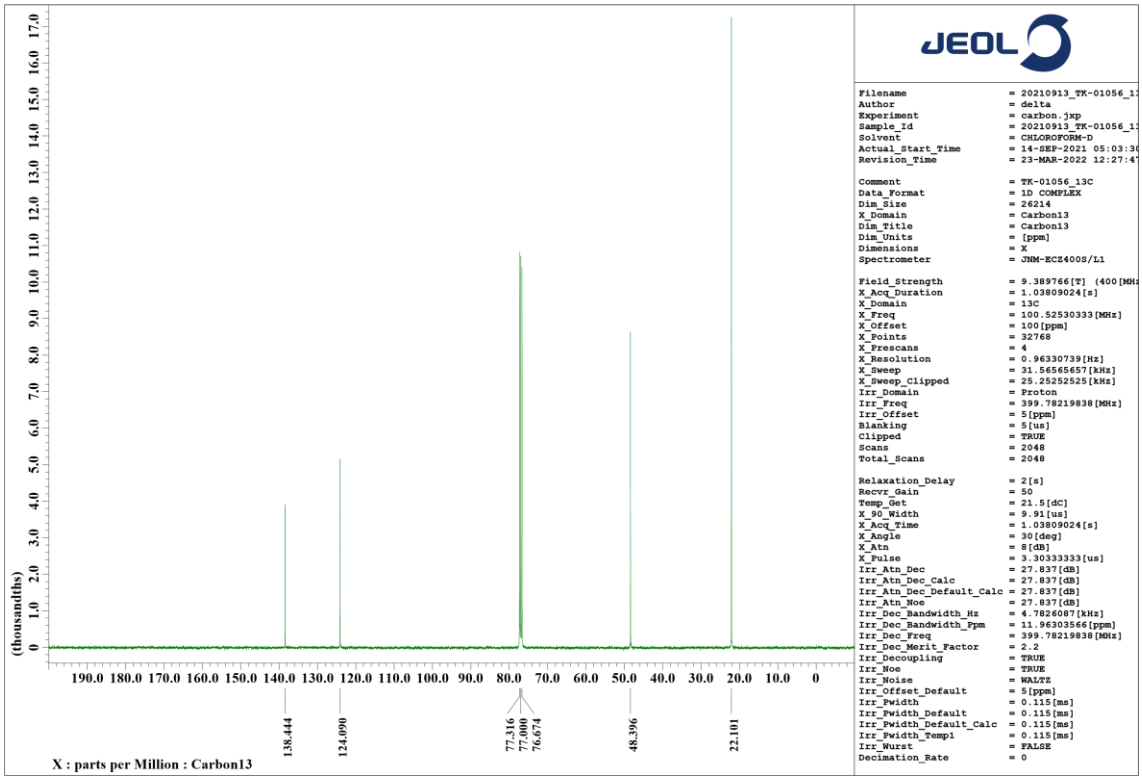

3o
abundance
X : parts per Million : Proton
JEOL

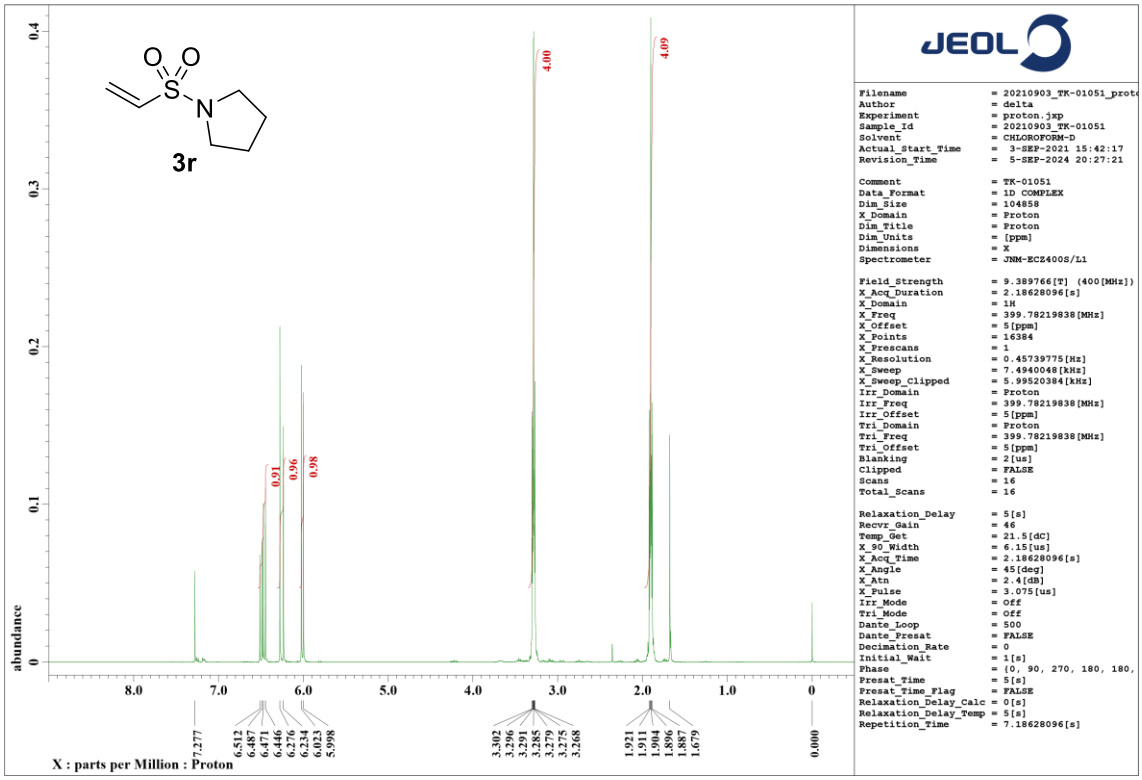

(thousandths)
X : parts per Million : Carbon13
JEOL

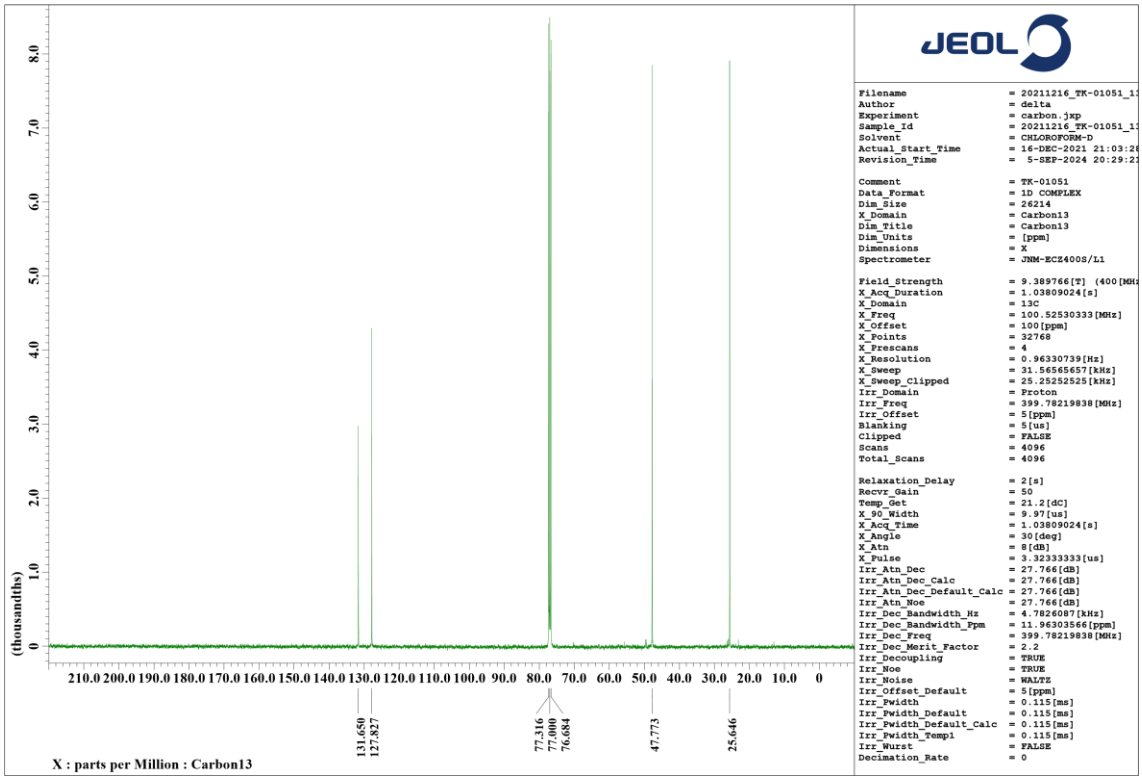

3p
abundance
X : parts per Million : Proton
6.20
4.00
0.91
0.96
0.98
7.267
6.458
6.433
6.417
6.392
6.216
6.174
5.902
5.877
3.259
3.241
3.223
3.205
1.590
1.216
1.199
1.181
0.000
JEOL
Filename = 20230427_TK-01055_prot
Author = delta
Experiment = proton.jxp
Sample_Id = 20230427_TK-01055
Solvent = CHLOROFORM-D
Actual_Start_Time = 27-APR-2023 15:21:40
Revision_Time = 27-APR-2023 17:26:53
Comment = TK-01055
Data_Format = 1D COMPLEX
Dim_Size = 104858
X_Domain = Proton
Dim_Title = Proton
Dim_Units = [ppm]
Dimensions = X
Spectrometer = JNM-ECZ400S/L1
Field_Strength = 9.389766[T] (400[MHz])
X_Acq_Duration = 2.18628096[s]
X_Domain = 1H
X_Freq = 399.78219838[MHz]
X_Offset = 5[ppm]
X_Points = 16384
X_Prescans = 1
X_Resolution = 0.45739775[Hz]
X_Sweep = 7.4940048[kHz]
X_Sweep_Clipped = 5.99520384[kHz]
Irr_Domain = Proton
Irr_Freq = 399.78219838[MHz]
Irr_Offset = 5[ppm]
Tri_Domain = Proton
Tri_Freq = 399.78219838[MHz]
Tri_Offset = 5[ppm]
Blanking = 2[us]
Clipped = FALSE
Scans = 16
Total_Scans = 16
Relaxation_Delay = 5[s]
Recvr_Gain = 46
Temp_Get = 21.2[dC]
X_90_Width = 6.4[us]
X_Acq_Time = 2.18628096[s]
X_Angle = 45[deg]
X_Atn = 2.4[dB]
X_Pulse = 3.2[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Loop = 500
Dante_Presat = FALSE
Decimation_Rate = 0
Initial_Wait = 1[s]
Phase = (0, 90, 270, 180, 180,
Presat_Time = 5[s]
Presat_Time_Flag = FALSE
Relaxation_Delay_Calc = 0[s]
Relaxation_Delay_Temp = 5[s]
Repetition_Time = 7.18628096[s]

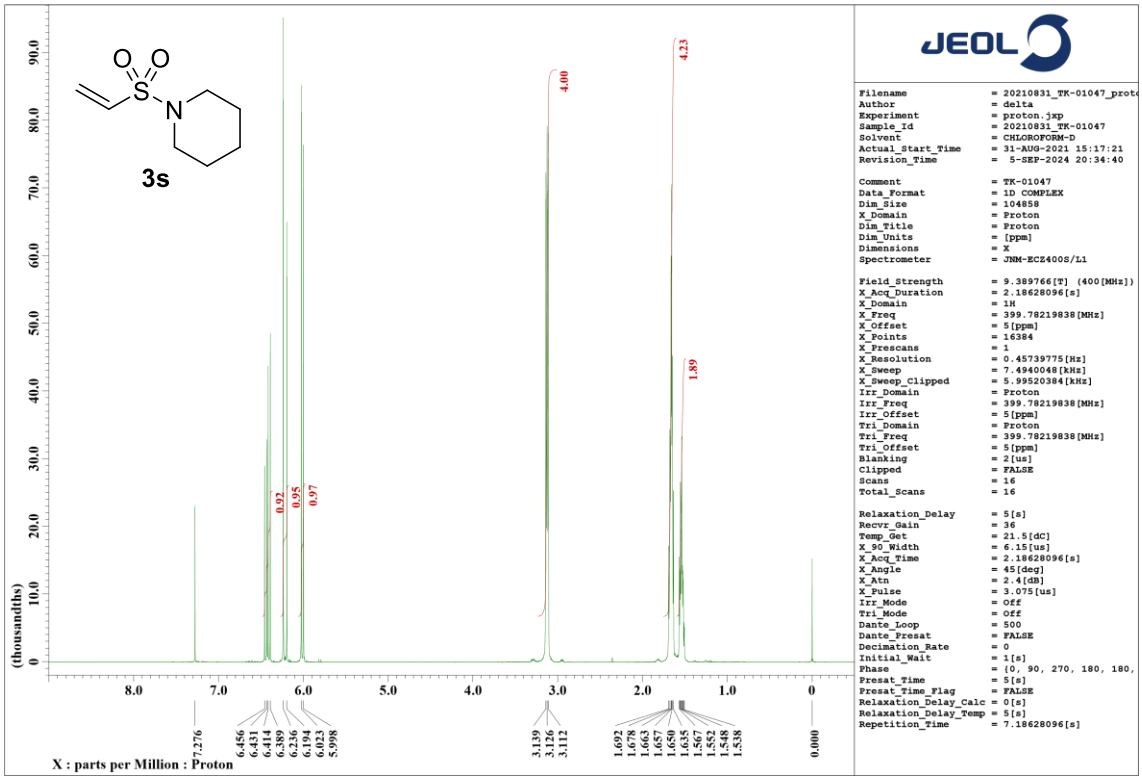

(thousandths)
X : parts per Million : Carbon13
135.493
125.805
77.316
77.000
76.684
41.659
14.300
JEOL
Filename = 20210913_TK-01055A_1
Author = delta
Experiment = carbon.jxp
Sample_Id = 20210913_TK-01055A_1
Solvent = CHLOROFORM-D
Actual_Start_Time = 14-SEP-2021 01:03:3
Revision_Time = 23-MAR-2022 12:16:4
Comment = TK-01055A_13C
Data_Format = 1D COMPLEX
Dim_Size = 26214
X_Domain = Carbon13
Dim_Title = Carbon13
Dim_Units = [ppm]
Dimensions = X
Spectrometer = JNM-ECZ400S/L1
Field_Strength = 9.389766[T] (400[MH
X_Acq_Duration = 1.03809024[s]
X_Domain = 13C
X_Freq = 100.52530333[MHz]
X_Offset = 100[ppm]
X_Points = 32768
X_Prescans = 4
X_Resolution = 0.96330739[Hz]
X_Sweep = 31.56565657[kHz]
X_Sweep_Clipped = 25.25252525[kHz]
Irr_Domain = Proton
Irr_Freq = 399.78219838[MHz]
Irr_Offset = 5[ppm]
Blanking = 5[us]
Clipped = TRUE
Scans = 2048
Total_Scans = 2048
Relaxation_Delay = 2[s]
Recvr_Gain = 50
Temp_Get = 21.5[dC]
X_90_Width = 9.91[us]
X_Acq_Time = 1.03809024[s]
X_Angle = 30[deg]
X_Atn = 8[dB]
X_Pulse = 3.30333333[us]
Irr_Atn_Dec = 27.837[dB]
Irr_Atn_Dec_Calc = 27.837[dB]
Irr_Atn_Dec_Default_Calc = 27.837[dB]
Irr_Atn_Noe = 27.837[dB]
Irr_Dec_Bandwidth_Hz = 4.7826087[kHz]
Irr_Dec_Bandwidth_Ppm = 11.96303566[ppm]
Irr_Dec_Freq = 399.78219838[MHz]
Irr_Dec_Merit_Factor = 2.2
Irr_Decoupling = TRUE
Irr_Noe = TRUE
Irr_Noise = WALTZ
Irr_Offset_Default = 5[ppm]
Irr_Pwidth = 0.115[ms]
Irr_Pwidth_Default = 0.115[ms]
Irr_Pwidth_Default_Calc = 0.115[ms]
Irr_Pwidth_Temp1 = 0.115[ms]
Irr_Wurst = FALSE
Decimation_Rate = 0

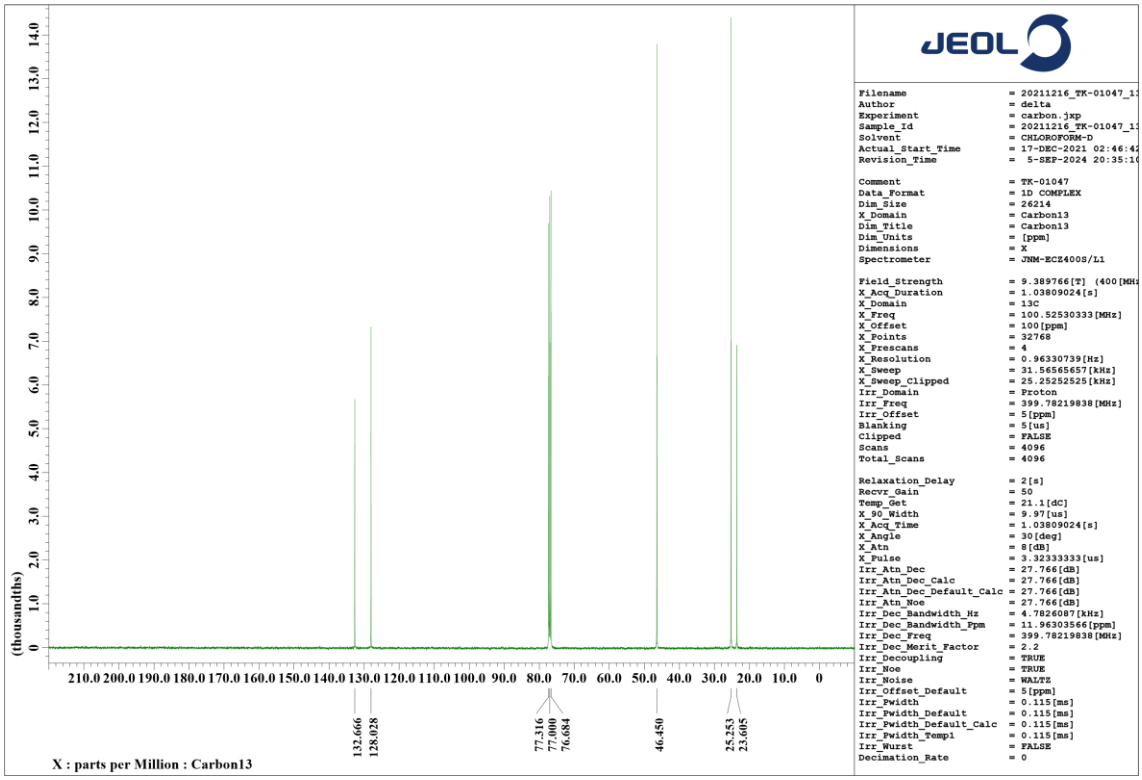

3q
12.19
2.00
0.95
0.99
1.01
abundance
X : parts per Million : Proton
7.265
6.480
6.455
6.439
6.414
6.197
6.155
5.804
5.780
3.762
3.745
3.727
3.710
3.693
3.676
3.659
1.578
1.306
1.289
0.000

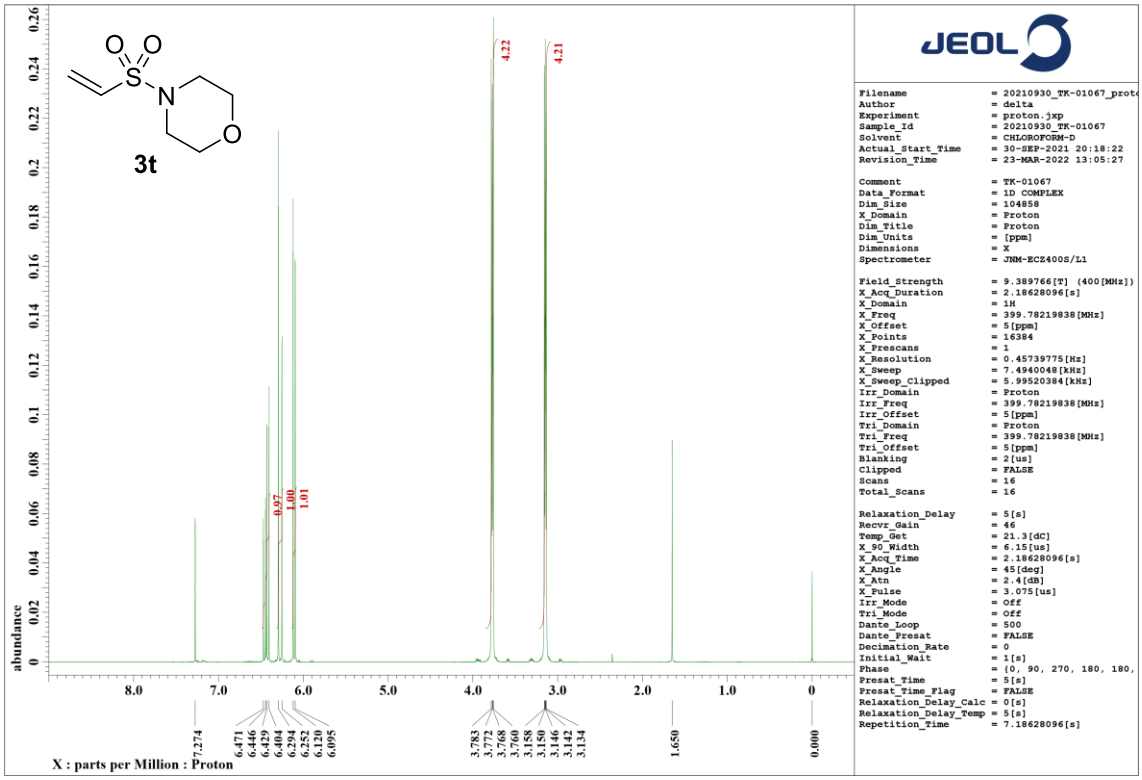

(thousandths)
X : parts per Million : Carbon13
138.444
124.090
77.316
77.000
76.674
48.396
22.101

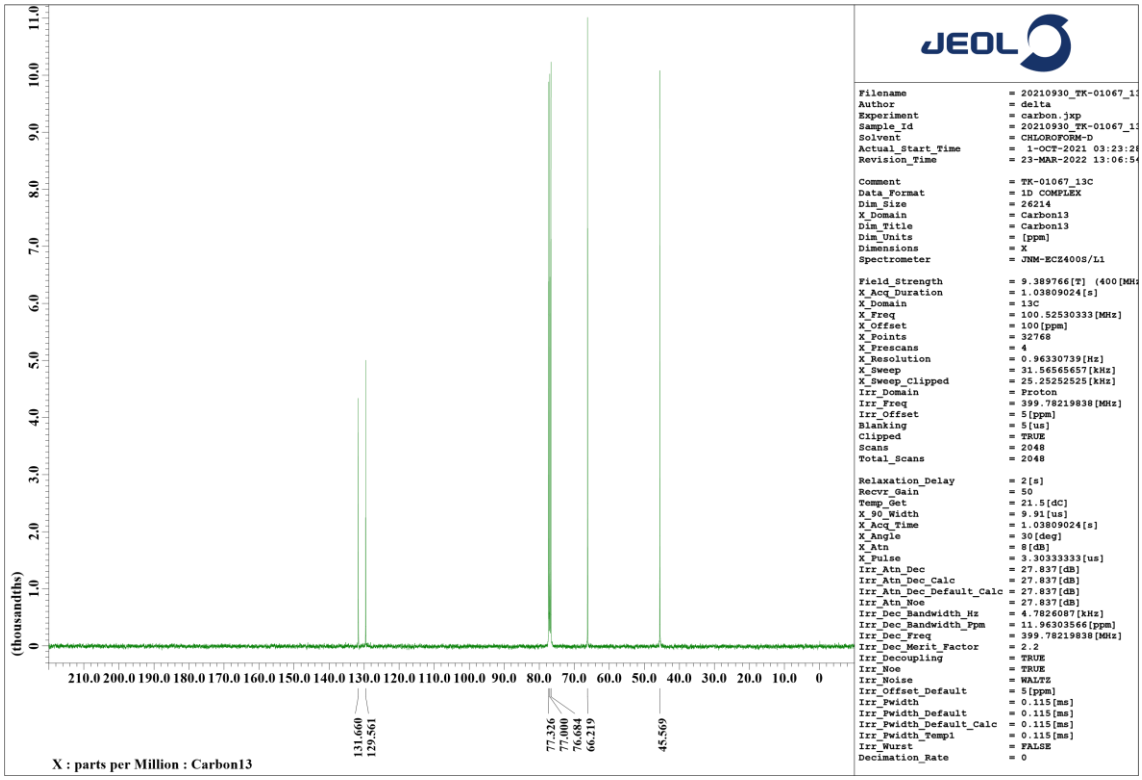

3r
4.00
4.09
0.91
0.96
0.98
abundance
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
7.277
6.512
6.487
6.471
6.446
6.276
6.234
6.023
5.998
3.302
3.296
3.291
3.285
3.279
3.275
3.268
1.921
1.911
1.904
1.896
1.887
1.679
0.000
X : parts per Million : Proton
JEOL
Filename = 20210903_TK-01051_prot
Author = delta
Experiment = proton.jxp
Sample_Id = 20210903_TK-01051
Solvent = CHLOROFORM-D
Actual_Start_Time = 3-SEP-2021 15:42:17
Revision_Time = 5-SEP-2024 20:27:21
Comment = TK-01051
Data_Format = 1D COMPLEX
Dim_Size = 104858
X_Domain = Proton
Dim_Title = Proton
Dim_Units = [ppm]
Dimensions = X
Spectrometer = JNM-ECZ400S/L1
Field_Strength = 9.389766[T] (400[MHz])
X_Acq_Duration = 2.18628096[s]
X_Domain = 1H
X_Freq = 399.78219838[MHz]
X_Offset = 5[ppm]
X_Points = 16384
X_Prescans = 1
X_Resolution = 0.45739775[Hz]
X_Sweep = 7.4940048[kHz]
X_Sweep_Clipped = 5.99520384[kHz]
Irr_Domain = Proton
Irr_Freq = 399.78219838[MHz]
Irr_Offset = 5[ppm]
Tri_Domain = Proton
Tri_Freq = 399.78219838[MHz]
Tri_Offset = 5[ppm]
Blanking = 2[us]
Clipped = FALSE
Scans = 16
Total_Scans = 16
Relaxation_Delay = 5[s]
Recvr_Gain = 46
Temp_Get = 21.5[dC]
X_90_Width = 6.15[us]
X_Acq_Time = 2.18628096[s]
X_Angle = 45[deg]
X_Atn = 2.4[dB]
X_Pulse = 3.075[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Loop = 500
Dante_Presat = FALSE
Decimation_Rate = 0
Initial_Wait = 1[s]
Phase = (0, 90, 270, 180, 180,
Presat_Time = 5[s]
Presat_Time_Flag = FALSE
Relaxation_Delay_Calc = 0[s]
Relaxation_Delay_Temp = 5[s]
Repetition_Time = 7.18628096[s]

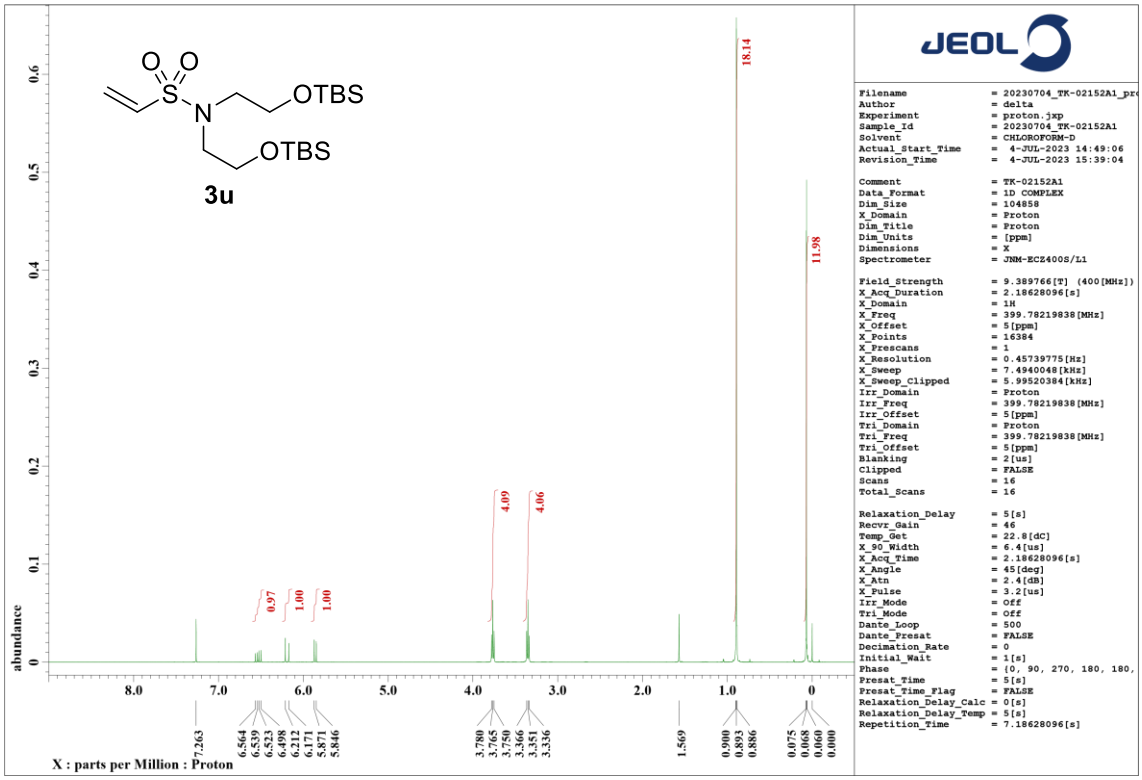

(thousandths)
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
210.0 200.0 190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0
131.650
127.827
77.316
77.000
76.684
47.773
25.646
X : parts per Million : Carbon13
JEOL
Filename = 20211216_TK-01051_1
Author = delta
Experiment = carbon.jxp
Sample_Id = 20211216_TK-01051_1
Solvent = CHLOROFORM-D
Actual_Start_Time = 16-DEC-2021 21:03:2
Revision_Time = 5-SEP-2024 20:29:2
Comment = TK-01051
Data_Format = 1D COMPLEX
Dim_Size = 26214
X_Domain = Carbon13
Dim_Title = Carbon13
Dim_Units = [ppm]
Dimensions = X
Spectrometer = JNM-ECZ400S/L1
Field_Strength = 9.389766[T] (400[MH
X_Acq_Duration = 1.03809024[s]
X_Domain = 13C
X_Freq = 100.52530333[MHz]
X_Offset = 100[ppm]
X_Points = 32768
X_Prescans = 4
X_Resolution = 0.96330739[Hz]
X_Sweep = 31.56565657[kHz]
X_Sweep_Clipped = 25.25252525[kHz]
Irr_Domain = Proton
Irr_Freq = 399.78219838[MHz]
Irr_Offset = 5[ppm]
Blanking = 5[us]
Clipped = FALSE
Scans = 4096
Total_Scans = 4096
Relaxation_Delay = 2[s]
Recvr_Gain = 50
Temp_Get = 21.2[dC]
X_90_Width = 9.97[us]
X_Acq_Time = 1.03809024[s]
X_Angle = 30[deg]
X_Atn = 8[dB]
X_Pulse = 3.32333333[us]
Irr_Atn_Dec = 27.766[dB]
Irr_Atn_Dec_Calc = 27.766[dB]
Irr_Atn_Dec_Default_Calc = 27.766[dB]
Irr_Atn_Noe = 27.766[dB]
Irr_Dec_Bandwidth_Hz = 4.7826087[kHz]
Irr_Dec_Bandwidth_Ppm = 11.96303566[ppm]
Irr_Dec_Freq = 399.78219838[MHz]
Irr_Dec_Merit_Factor = 2.2
Irr_Decoupling = TRUE
Irr_Noe = TRUE
Irr_Noise = WALTZ
Irr_Offset_Default = 5[ppm]
Irr_Pwidth = 0.115[ms]
Irr_Pwidth_Default = 0.115[ms]
Irr_Pwidth_Default_Calc = 0.115[ms]
Irr_Pwidth_Temp1 = 0.115[ms]
Irr_Wurst = FALSE
Decimation_Rate = 0

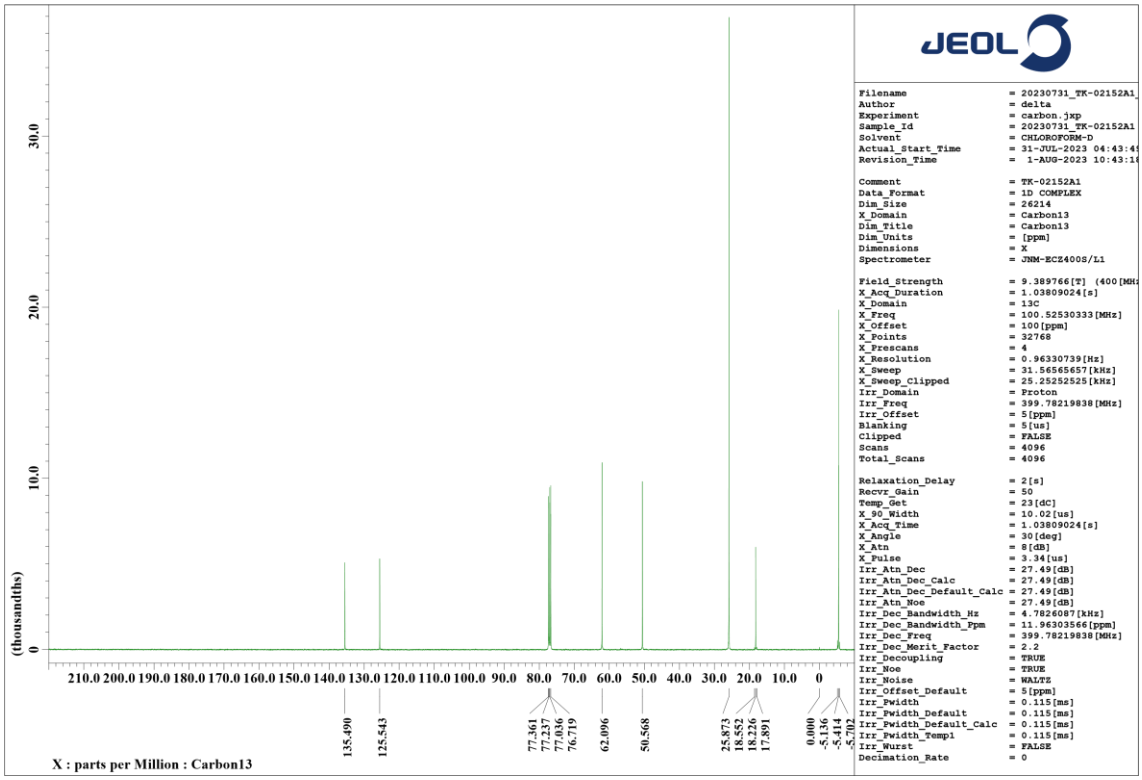

3s
4.23
4.00
1.89
0.92
0.95
0.97
X : parts per Million : Proton
Filename = 20210831_TK-01047_prot
Author = delta
Experiment = proton.jxp
Sample_Id = 20210831_TK-01047
Solvent = CHLOROFORM-D
Actual_Start_Time = 31-AUG-2021 15:17:21
Revision_Time = 5-SEP-2024 20:34:40
Comment = TK-01047
Data_Format = 1D COMPLEX
Dim_Size = 104858
X_Domain = Proton
Dim_Title = Proton
Dim_Units = [ppm]
Dimensions = X
Spectrometer = JNM-ECZ400S/L1
Field_Strength = 9.389766[T] (400[MHz])
X_Acq_Duration = 2.18628096[s]
X_Domain = 1H
X_Freq = 399.78219838[MHz]
X_Offset = 5[ppm]
X_Points = 16384
X_Prescans = 1
X_Resolution = 0.45739775[Hz]
X_Sweep = 7.4940048[kHz]
X_Sweep_Clipped = 5.99520384[kHz]
Irr_Domain = Proton
Irr_Freq = 399.78219838[MHz]
Irr_Offset = 5[ppm]
Tri_Domain = Proton
Tri_Freq = 399.78219838[MHz]
Tri_Offset = 5[ppm]
Blanking = 2[us]
Clipped = FALSE
Scans = 16
Total_Scans = 16
Relaxation_Delay = 5[s]
Recvr_Gain = 36
Temp_Get = 21.5[dC]
X_90_Width = 6.15[us]
X_Acq_Time = 2.18628096[s]
X_Angle = 45[deg]
X_Atn = 2.4[dB]
X_Pulse = 3.075[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Loop = 500
Dante_Presat = FALSE
Decimation_Rate = 0
Initial_Wait = 1[s]
Phase = (0, 90, 270, 180, 180,
Presat_Time = 5[s]
Presat_Time_Flag = FALSE
Relaxation_Delay_Calc = 0[s]
Relaxation_Delay_Temp = 5[s]
Repetition_Time = 7.18628096[s]

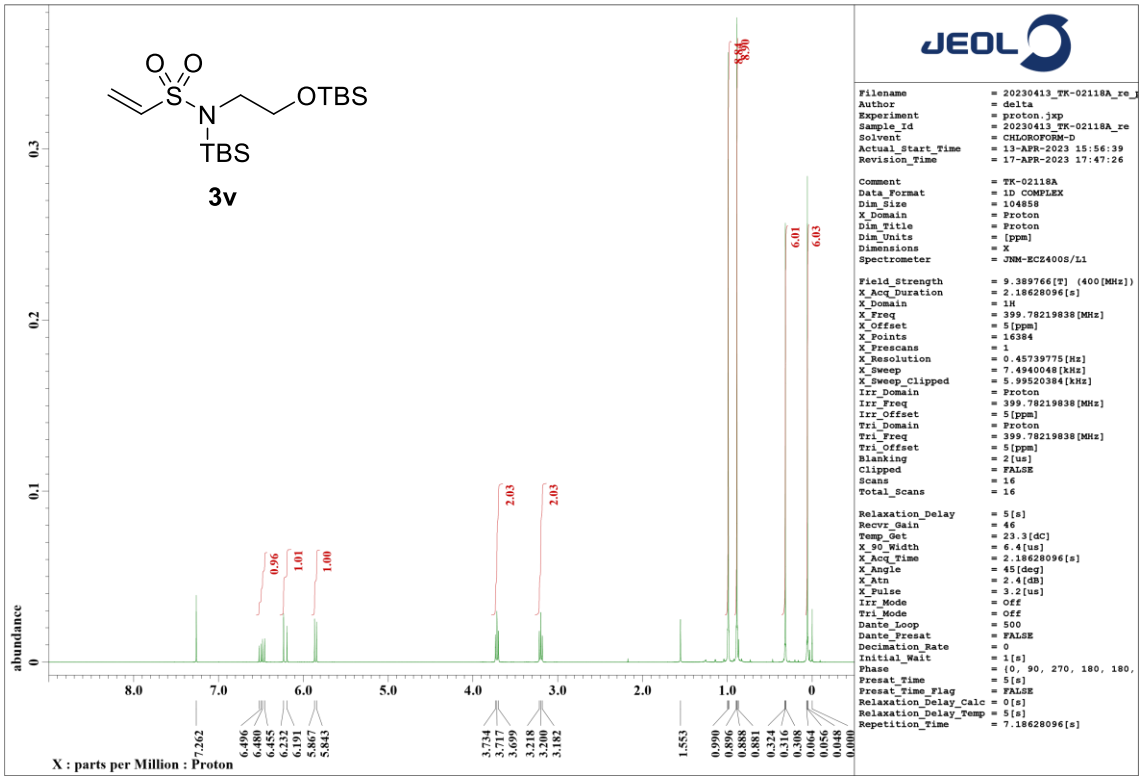

X : parts per Million : Carbon13
Filename = 20211216_TK-01047_1
Author = delta
Experiment = carbon.jxp
Sample_Id = 20211216_TK-01047_1
Solvent = CHLOROFORM-D
Actual_Start_Time = 17-DEC-2021 02:46:4
Revision_Time = 5-SEP-2024 20:35:1
Comment = TK-01047
Data_Format = 1D COMPLEX
Dim_Size = 26214
X_Domain = Carbon13
Dim_Title = Carbon13
Dim_Units = [ppm]
Dimensions = X
Spectrometer = JNM-ECZ400S/L1
Field_Strength = 9.389766[T] (400[MH
X_Acq_Duration = 1.03809024[s]
X_Domain = 13C
X_Freq = 100.52530333[MHz]
X_Offset = 100[ppm]
X_Points = 32768
X_Prescans = 4
X_Resolution = 0.96330739[Hz]
X_Sweep = 31.56565657[kHz]
X_Sweep_Clipped = 25.25252525[kHz]
Irr_Domain = Proton
Irr_Freq = 399.78219838[MHz]
Irr_Offset = 5[ppm]
Blanking = 5[us]
Clipped = FALSE
Scans = 4096
Total_Scans = 4096
Relaxation_Delay = 2[s]
Recvr_Gain = 50
Temp_Get = 21.1[dC]
X_90_Width = 9.97[us]
X_Acq_Time = 1.03809024[s]
X_Angle = 30[deg]
X_Atn = 8[dB]
X_Pulse = 3.32333333[us]
Irr_Atn_Dec = 27.766[dB]
Irr_Atn_Dec_Calc = 27.766[dB]
Irr_Atn_Dec_Default_Calc = 27.766[dB]
Irr_Atn_Noe = 27.766[dB]
Irr_Dec_Bandwidth_Hz = 4.7826087[kHz]
Irr_Dec_Bandwidth_Ppm = 11.96303566[ppm]
Irr_Dec_Freq = 399.78219838[MHz]
Irr_Dec_Merit_Factor = 2.2
Irr_Decoupling = TRUE
Irr_Noe = TRUE
Irr_Noise = WALTZ
Irr_Offset_Default = 5[ppm]
Irr_Pwidth = 0.115[ms]
Irr_Pwidth_Default = 0.115[ms]
Irr_Pwidth_Default_Calc = 0.115[ms]
Irr_Pwidth_Temp1 = 0.115[ms]
Irr_Wurst = FALSE
Decimation_Rate = 0

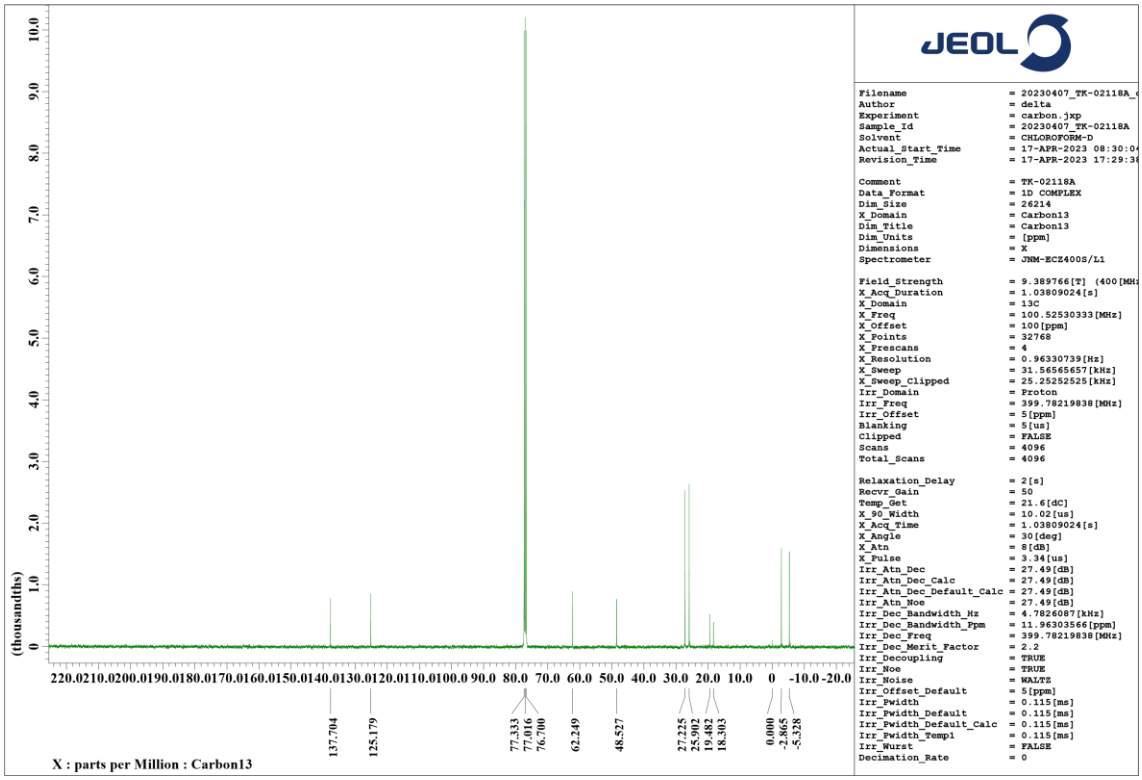

3t
4.22
4.21
0.97
1.00
1.01
abundance
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
7.274
6.471
6.446
6.429
6.404
6.294
6.252
6.120
6.095
3.783
3.772
3.768
3.760
3.158
3.150
3.146
3.142
3.134
1.650
0.000
X : parts per Million : Proton
JEOL
Filename = 20210930_TK-01067_prot
Author = delta
Experiment = proton.jxp
Sample_Id = 20210930_TK-01067
Solvent = CHLOROFORM-D
Actual_Start_Time = 30-SEP-2021 20:18:22
Revision_Time = 23-MAR-2022 13:05:27
Comment = TK-01067
Data_Format = 1D COMPLEX
Dim_Size = 104858
X_Domain = Proton
Dim_Title = Proton
Dim_Units = [ppm]
Dimensions = X
Spectrometer = JNM-ECZ400S/L1
Field_Strength = 9.389766[T] (400[MHz])
X_Acq_Duration = 2.18628096[s]
X_Domain = 1H
X_Freq = 399.78219838[MHz]
X_Offset = 5[ppm]
X_Points = 16384
X_Prescans = 1
X_Resolution = 0.45739775[Hz]
X_Sweep = 7.4940048[kHz]
X_Sweep_Clipped = 5.99520384[kHz]
Irr_Domain = Proton
Irr_Freq = 399.78219838[MHz]
Irr_Offset = 5[ppm]
Tri_Domain = Proton
Tri_Freq = 399.78219838[MHz]
Tri_Offset = 5[ppm]
Blanking = 2[us]
Clipped = FALSE
Scans = 16
Total_Scans = 16
Relaxation_Delay = 5[s]
Recvr_Gain = 46
Temp_Get = 21.3[dC]
X_90_Width = 6.15[us]
X_Acq_Time = 2.18628096[s]
X_Angle = 45[deg]
X_Atn = 2.4[dB]
X_Pulse = 3.075[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Loop = 500
Dante_Presat = FALSE
Decimation_Rate = 0
Initial_Wait = 1[s]
Phase = (0, 90, 270, 180, 180,
Presat_Time = 5[s]
Presat_Time_Flag = FALSE
Relaxation_Delay_Calc = 0[s]
Relaxation_Delay_Temp = 5[s]
Repetition_Time = 7.18628096[s]

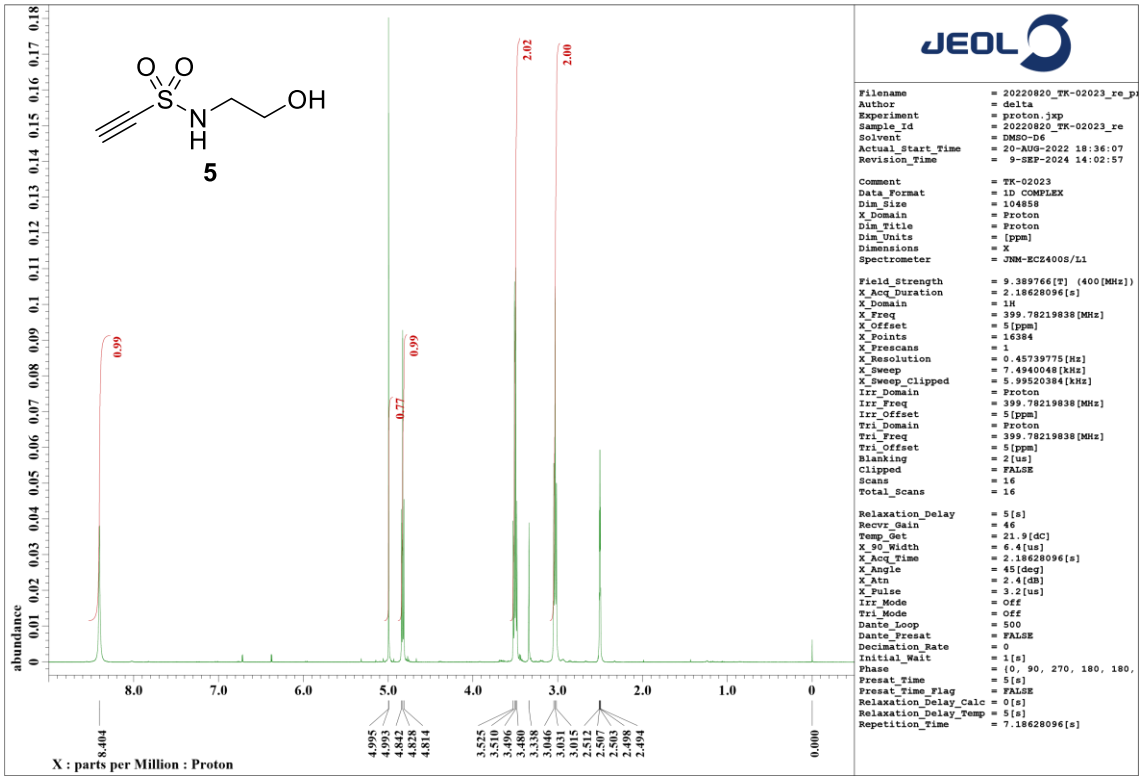

(thousandths)
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
210.0 200.0 190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0
131.660
129.561
77.326
77.000
76.684
66.219
45.569
X : parts per Million : Carbon13
JEOL
Filename = 20210930_TK-01067_1
Author = delta
Experiment = carbon.jxp
Sample_Id = 20210930_TK-01067_1
Solvent = CHLOROFORM-D
Actual_Start_Time = 1-OCT-2021 03:23:2
Revision_Time = 23-MAR-2022 13:06:5
Comment = TK-01067_13C
Data_Format = 1D COMPLEX
Dim_Size = 26214
X_Domain = Carbon13
Dim_Title = Carbon13
Dim_Units = [ppm]
Dimensions = X
Spectrometer = JNM-ECZ400S/L1
Field_Strength = 9.389766[T] (400[MH
X_Acq_Duration = 1.03809024[s]
X_Domain = 13C
X_Freq = 100.52530333[MHz]
X_Offset = 100[ppm]
X_Points = 32768
X_Prescans = 4
X_Resolution = 0.96330739[Hz]
X_Sweep = 31.56565657[kHz]
X_Sweep_Clipped = 25.25252525[kHz]
Irr_Domain = Proton
Irr_Freq = 399.78219838[MHz]
Irr_Offset = 5[ppm]
Blanking = 5[us]
Clipped = TRUE
Scans = 2048
Total_Scans = 2048
Relaxation_Delay = 2[s]
Recvr_Gain = 50
Temp_Get = 21.5[dC]
X_90_Width = 9.91[us]
X_Acq_Time = 1.03809024[s]
X_Angle = 30[deg]
X_Atn = 8[dB]
X_Pulse = 3.30333333[us]
Irr_Atn_Dec = 27.837[dB]
Irr_Atn_Dec_Calc = 27.837[dB]
Irr_Atn_Dec_Default_Calc = 27.837[dB]
Irr_Atn_Noe = 27.837[dB]
Irr_Dec_Bandwidth_Hz = 4.7826087[kHz]
Irr_Dec_Bandwidth_Ppm = 11.96303566[ppm]
Irr_Dec_Freq = 399.78219838[MHz]
Irr_Dec_Merit_Factor = 2.2
Irr_Decoupling = TRUE
Irr_Noe = TRUE
Irr_Noise = WALTZ
Irr_Offset_Default = 5[ppm]
Irr_Pwidth = 0.115[ms]
Irr_Pwidth_Default = 0.115[ms]
Irr_Pwidth_Default_Calc = 0.115[ms]
Irr_Pwidth_Temp1 = 0.115[ms]
Irr_Wurst = FALSE
Decimation_Rate = 0

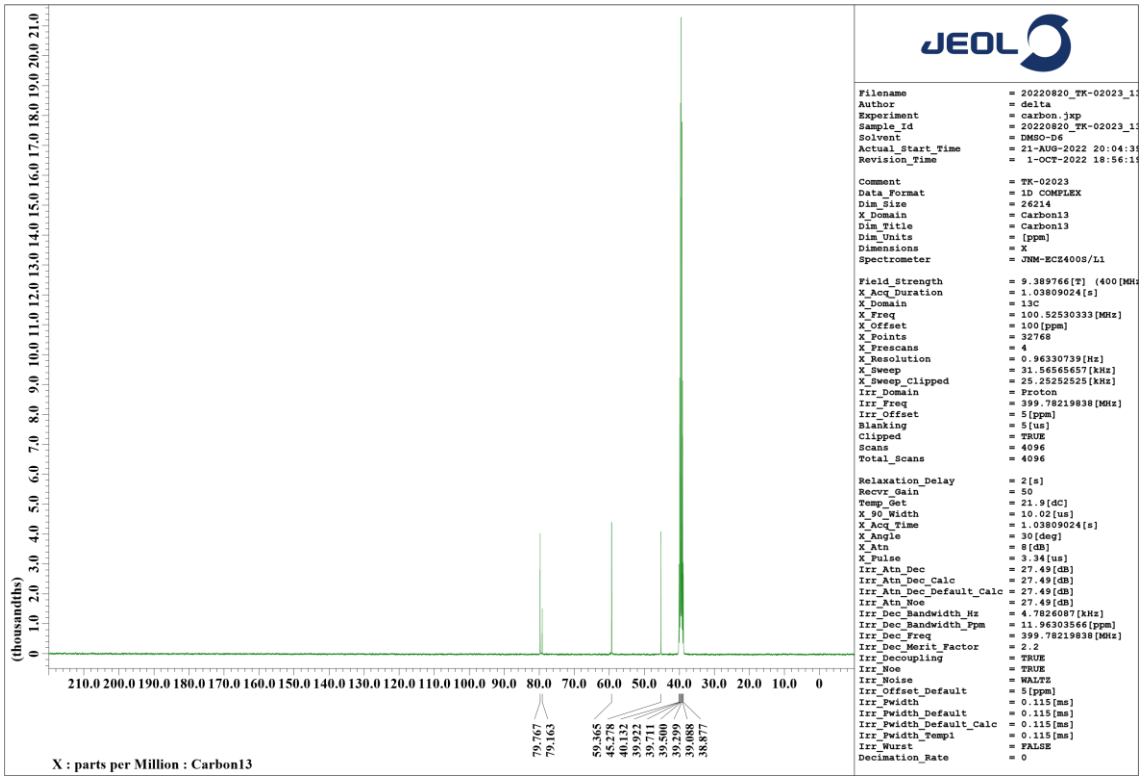

OTBS
OTBS
3u
abundance
X : parts per Million : Proton
18.14
11.98
4.09
4.06
0.97
1.00
1.00
7.263
6.564
6.539
6.523
6.498
6.171
5.871
5.846
3.780
3.765
3.750
3.366
3.351
3.336
1.569
0.900
0.893
0.886
0.075
0.068
0.060
0.000
JEOL
Filename = 20230704_TK-02152A1_pr
Author = delta
Experiment = proton.jxp
Sample_Id = 20230704_TK-02152A1
Solvent = CHLOROFORM-D
Actual_Start_Time = 4-JUL-2023 14:49:06
Revision_Time = 4-JUL-2023 15:39:04
Comment = TK-02152A1
Data_Format = 1D COMPLEX
Dim_Size = 104858
X_Domain = Proton
Dim_Title = Proton
Dim_Units = [ppm]
Dimensions = X
Spectrometer = JNM-ECZ400S/L1
Field_Strength = 9.389766[T] (400[MHz])
X_Acq_Duration = 2.18628096[s]
X_Domain = 1H
X_Freq = 399.78219838[MHz]
X_Offset = 5[ppm]
X_Points = 16384
X_Prescans = 1
X_Resolution = 0.45739775[Hz]
X_Sweep = 7.4940048[kHz]
X_Sweep_Clipped = 5.99520384[kHz]
Irr_Domain = Proton
Irr_Freq = 399.78219838[MHz]
Irr_Offset = 5[ppm]
Tri_Domain = Proton
Tri_Freq = 399.78219838[MHz]
Tri_Offset = 5[ppm]
Blanking = 2[us]
Clipped = FALSE
Scans = 16
Total_Scans = 16
Relaxation_Delay = 5[s]
Recvr_Gain = 46
Temp_Get = 22.8[dC]
X_90_Width = 6.4[us]
X_Acq_Time = 2.18628096[s]
X_Angle = 45[deg]
X_Atn = 2.4[dB]
X_Pulse = 3.2[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Loop = 500
Dante_Presat = FALSE
Decimation_Rate = 0
Initial_Wait = 1[s]
Phase = (0, 90, 270, 180, 180,
Presat_Time = 5[s]
Presat_Time_Flag = FALSE
Relaxation_Delay_Calc = 0[s]
Relaxation_Delay_Temp = 5[s]
Repetition_Time = 7.18628096[s]

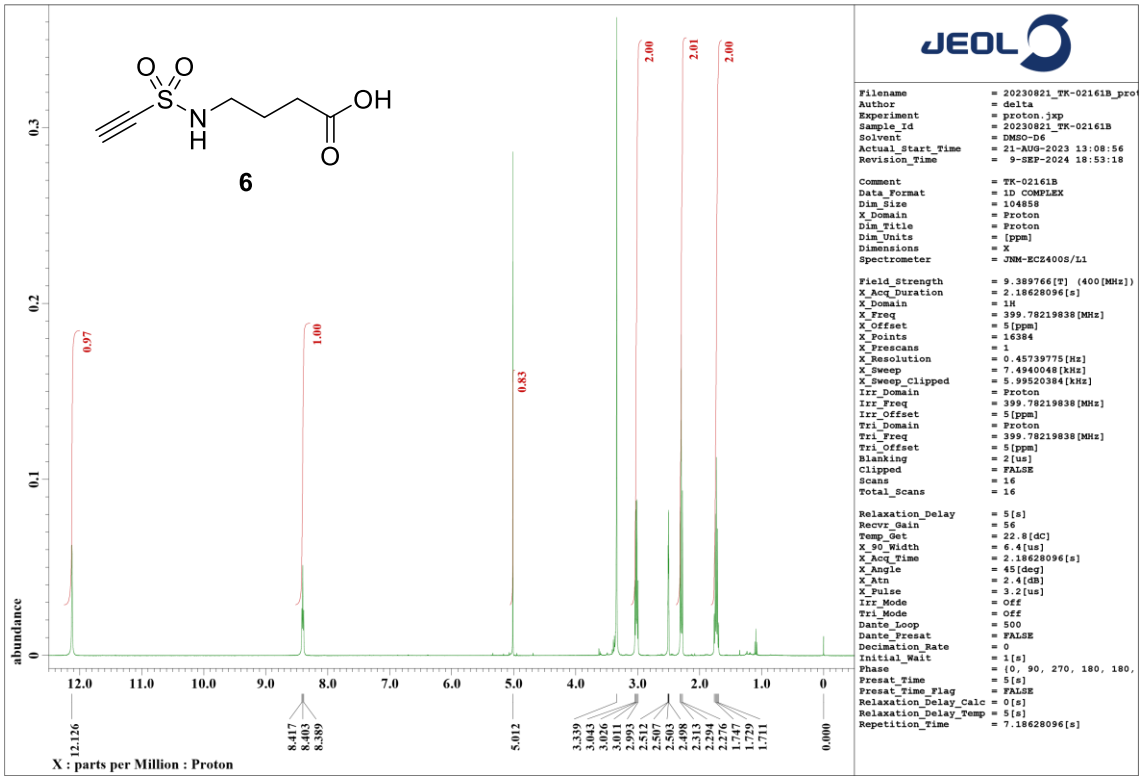

(thousandths)
X : parts per Million : Carbon13
135.490
125.543
77.361
77.237
77.036
76.719
62.096
50.568
25.873
18.552
18.226
17.891
0.000
-5.136
-5.414
-5.702
JEOL
Filename = 20230731_TK-02152A1_
Author = delta
Experiment = carbon.jxp
Sample_Id = 20230731_TK-02152A1
Solvent = CHLOROFORM-D
Actual_Start_Time = 31-JUL-2023 04:43:4
Revision_Time = 1-AUG-2023 10:43:1
Comment = TK-02152A1
Data_Format = 1D COMPLEX
Dim_Size = 26214
X_Domain = Carbon13
Dim_Title = Carbon13
Dim_Units = [ppm]
Dimensions = X
Spectrometer = JNM-ECZ400S/L1
Field_Strength = 9.389766[T] (400[MH
X_Acq_Duration = 1.03809024[s]
X_Domain = 13C
X_Freq = 100.52530333[MHz]
X_Offset = 100[ppm]
X_Points = 32768
X_Prescans = 4
X_Resolution = 0.96330739[Hz]
X_Sweep = 31.56565657[kHz]
X_Sweep_Clipped = 25.25252525[kHz]
Irr_Domain = Proton
Irr_Freq = 399.78219838[MHz]
Irr_Offset = 5[ppm]
Blanking = 5[us]
Clipped = FALSE
Scans = 4096
Total_Scans = 4096
Relaxation_Delay = 2[s]
Recvr_Gain = 50
Temp_Get = 23[dC]
X_90_Width = 10.02[us]
X_Acq_Time = 1.03809024[s]
X_Angle = 30[deg]
X_Atn = 8[dB]
X_Pulse = 3.34[us]
Irr_Atn_Dec = 27.49[dB]
Irr_Atn_Dec_Calc = 27.49[dB]
Irr_Atn_Dec_Default_Calc = 27.49[dB]
Irr_Atn_Noe = 27.49[dB]
Irr_Dec_Bandwidth_Hz = 4.7826087[kHz]
Irr_Dec_Bandwidth_Ppm = 11.96303566[ppm]
Irr_Dec_Freq = 399.78219838[MHz]
Irr_Dec_Merit_Factor = 2.2
Irr_Decoupling = TRUE
Irr_Noe = TRUE
Irr_Noise = WALTZ
Irr_Offset_Default = 5[ppm]
Irr_Pwidth = 0.115[ms]
Irr_Pwidth_Default = 0.115[ms]
Irr_Pwidth_Default_Calc = 0.115[ms]
Irr_Pwidth_Temp1 = 0.115[ms]
Irr_Wurst = FALSE
Decimation_Rate = 0

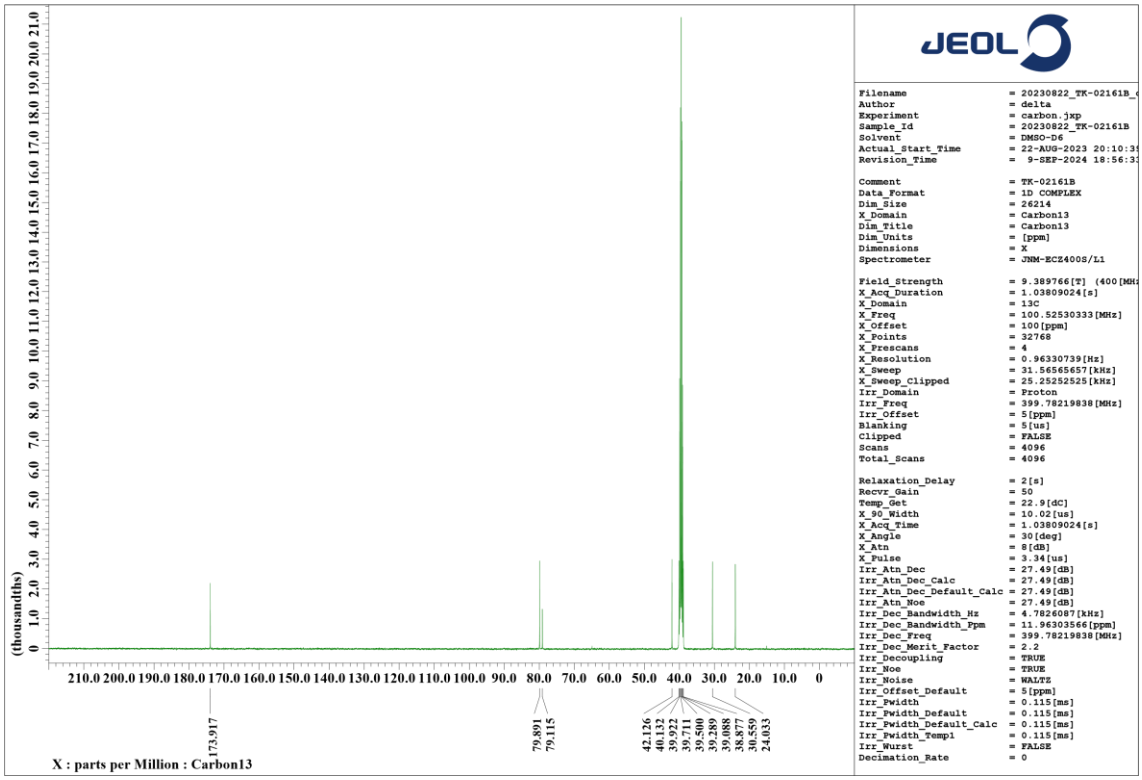

O
O
S
N
OTBS
TBS
3v
abundance
X : parts per Million : Proton
JEOL
Filename = 20230413_TK-02118A_re_
Author = delta
Experiment = proton.jxp
Sample_Id = 20230413_TK-02118A_re
Solvent = CHLOROFORM-D
Actual_Start_Time = 13-APR-2023 15:56:39
Revision_Time = 17-APR-2023 17:47:26
Comment = TK-02118A
Data_Format = 1D COMPLEX
Dim_Size = 104858
X_Domain = Proton
Dim_Title = Proton
Dim_Units = [ppm]
Dimensions = X
Spectrometer = JNM-ECZ400S/L1
Field_Strength = 9.389766[T] (400[MHz])
X_Acq_Duration = 2.18628096[s]
X_Domain = 1H
X_Freq = 399.78219838[MHz]
X_Offset = 5[ppm]
X_Points = 16384
X_Prescans = 1
X_Resolution = 0.45739775[Hz]
X_Sweep = 7.4940048[kHz]
X_Sweep_Clipped = 5.99520384[kHz]
Irr_Domain = Proton
Irr_Freq = 399.78219838[MHz]
Irr_Offset = 5[ppm]
Tri_Domain = Proton
Tri_Freq = 399.78219838[MHz]
Tri_Offset = 5[ppm]
Blanking = 2[us]
Clipped = FALSE
Scans = 16
Total_Scans = 16
Relaxation_Delay = 5[s]
Recvr_Gain = 46
Temp_Get = 23.3[dC]
X_90_Width = 6.4[us]
X_Acq_Time = 2.18628096[s]
X_Angle = 45[deg]
X_Atn = 2.4[dB]
X_Pulse = 3.2[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Loop = 500
Dante_Presat = FALSE
Decimation_Rate = 0
Initial_Wait = 1[s]
Phase = (0, 90, 270, 180, 180,
Presat_Time = 5[s]
Presat_Time_Flag = FALSE
Relaxation_Delay_Calc = 0[s]
Relaxation_Delay_Temp = 5[s]
Repetition_Time = 7.18628096[s]

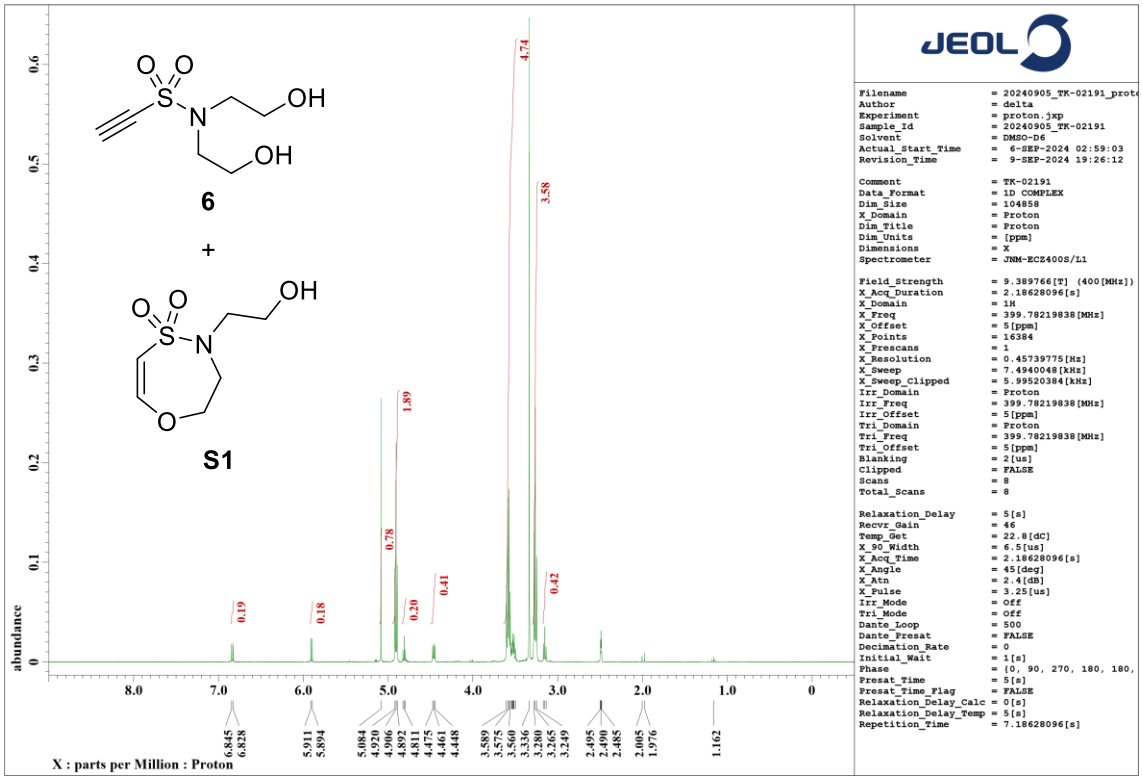

(thousandths)
X : parts per Million : Carbon13
JEOL
Filename = 20230407_TK-02118A_
Author = delta
Experiment = carbon.jxp
Sample_Id = 20230407_TK-02118A
Solvent = CHLOROFORM-D
Actual_Start_Time = 17-APR-2023 08:30:0
Revision_Time = 17-APR-2023 17:29:3
Comment = TK-02118A
Data_Format = 1D COMPLEX
Dim_Size = 26214
X_Domain = Carbon13
Dim_Title = Carbon13
Dim_Units = [ppm]
Dimensions = X
Spectrometer = JNM-ECZ400S/L1
Field_Strength = 9.389766[T] (400[MH
X_Acq_Duration = 1.03809024[s]
X_Domain = 13C
X_Freq = 100.52530333[MHz]
X_Offset = 100[ppm]
X_Points = 32768
X_Prescans = 4
X_Resolution = 0.96330739[Hz]
X_Sweep = 31.56565657[kHz]
X_Sweep_Clipped = 25.25252525[kHz]
Irr_Domain = Proton
Irr_Freq = 399.78219838[MHz]
Irr_Offset = 5[ppm]
Blanking = 5[us]
Clipped = FALSE
Scans = 4096
Total_Scans = 4096
Relaxation_Delay = 2[s]
Recvr_Gain = 50
Temp_Get = 21.6[dC]
X_90_Width = 10.02[us]
X_Acq_Time = 1.03809024[s]
X_Angle = 30[deg]
X_Atn = 8[dB]
X_Pulse = 3.34[us]
Irr_Atn_Dec = 27.49[dB]
Irr_Atn_Dec_Calc = 27.49[dB]
Irr_Atn_Dec_Default_Calc = 27.49[dB]
Irr_Atn_Noe = 27.49[dB]
Irr_Dec_Bandwidth_Hz = 4.78260587[kHz]
Irr_Dec_Bandwidth_Ppm = 11.96303566[ppm]
Irr_Dec_Freq = 399.78219838[MHz]
Irr_Dec_Merit_Factor = 2.2
Irr_Decoupling = TRUE
Irr_Noe = TRUE
Irr_Noise = WALTZ
Irr_Offset_Default = 5[ppm]
Irr_Pwidth = 0.115[ms]
Irr_Pwidth_Default = 0.115[ms]
Irr_Pwidth_Default_Calc = 0.115[ms]
Irr_Pwidth_Temp1 = 0.115[ms]
Irr_Wurst = FALSE
Decimation_Rate = 0

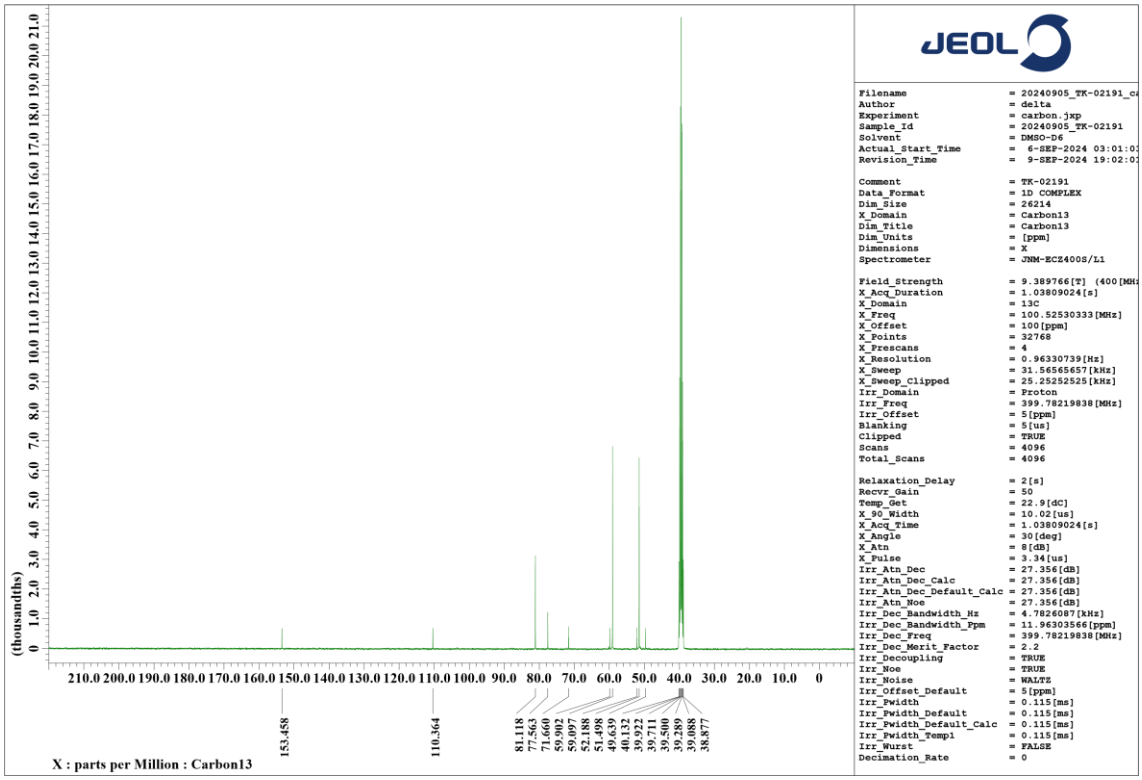

5
abundance
X : parts per Million : Proton
8.404
4.995
4.993
4.842
4.828
4.814
3.525
3.510
3.496
3.480
3.338
3.046
3.031
3.015
2.512
2.507
2.503
2.498
2.494
0.000
0.99
0.77
0.99
2.02
2.00

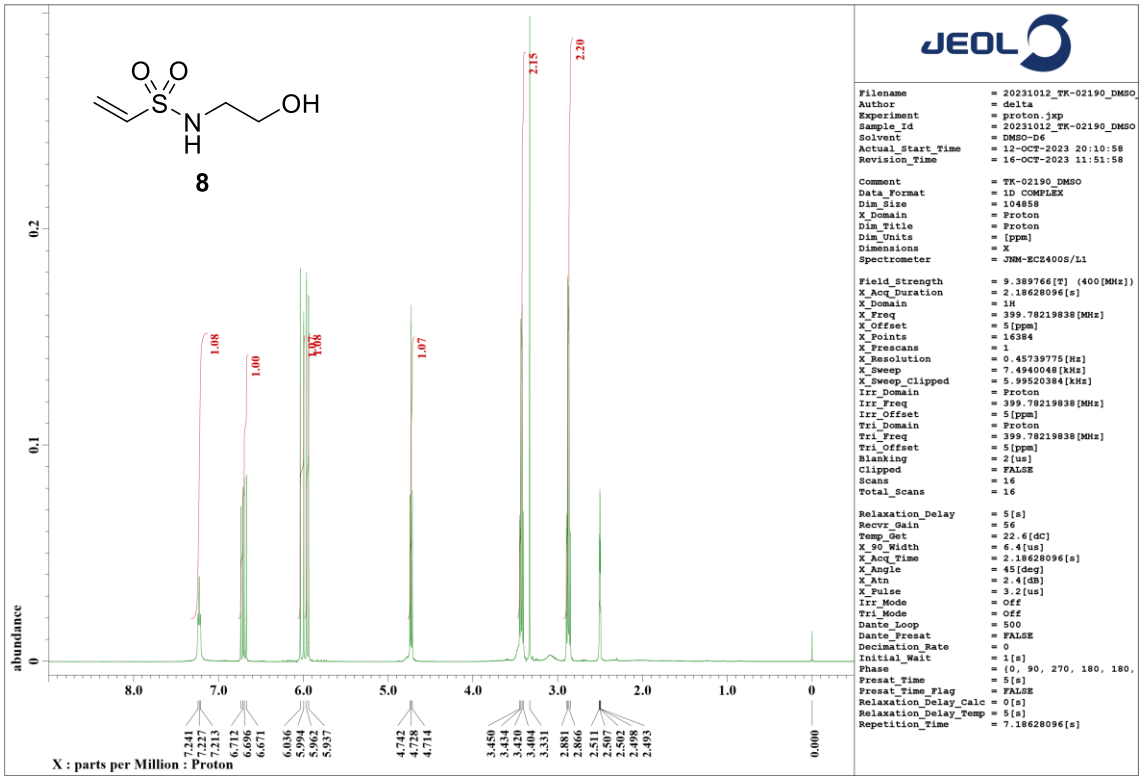

(thousandths)
X : parts per Million : Carbon13
79.767
79.163
59.365
45.278
40.132
39.922
39.711
39.500
39.299
39.088
38.877

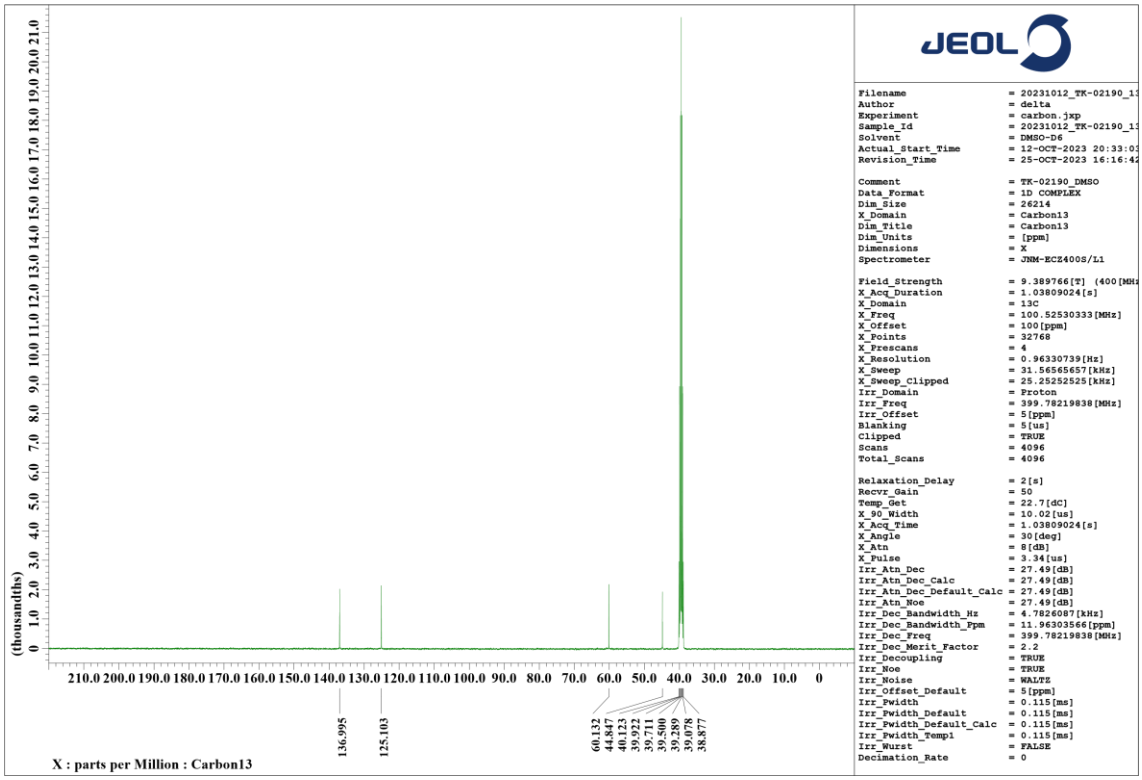

6
abundance
X : parts per Million : Proton
Filename = 20230821_TK-02161B_pro
Author = delta
Experiment = proton.jxp
Sample_Id = 20230821_TK-02161B
Solvent = DMSO-D6
Actual_Start_Time = 21-AUG-2023 13:08:56
Revision_Time = 9-SEP-2024 18:53:18
Comment = TK-02161B
Data_Format = 1D COMPLEX
Dim_Size = 104858
X_Domain = Proton
Dim_Title = Proton
Dim_Units = [ppm]
Dimensions = X
Spectrometer = JNM-ECZ400S/L1
Field_Strength = 9.389766[T] (400[MHz])
X_Acq_Duration = 2.18628096[s]
X_Domain = 1H
X_Freq = 399.78219838[MHz]
X_Offset = 5[ppm]
X_Points = 16384
X_Prescans = 1
X_Resolution = 0.45739775[Hz]
X_Sweep = 7.4940048[kHz]
X_Sweep_Clipped = 5.99520384[kHz]
Irr_Domain = Proton
Irr_Freq = 399.78219838[MHz]
Irr_Offset = 5[ppm]
Tri_Domain = Proton
Tri_Freq = 399.78219838[MHz]
Tri_Offset = 5[ppm]
Blanking = 2[us]
Clipped = FALSE
Scans = 16
Total_Scans = 16
Relaxation_Delay = 5[s]
Recvr_Gain = 56
Temp_Get = 22.8[dC]
X_90_Width = 6.4[us]
X_Acq_Time = 2.18628096[s]
X_Angle = 45[deg]
X_Atn = 2.4[dB]
X_Pulse = 3.2[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Loop = 500
Dante_Presat = FALSE
Decimation_Rate = 0
Initial_Wait = 1[s]
Phase = (0, 90, 270, 180, 180,
Presat_Time = 5[s]
Presat_Time_Flag = FALSE
Relaxation_Delay_Calc = 0[s]
Relaxation_Delay_Temp = 5[s]
Repetition_Time = 7.18628096[s]

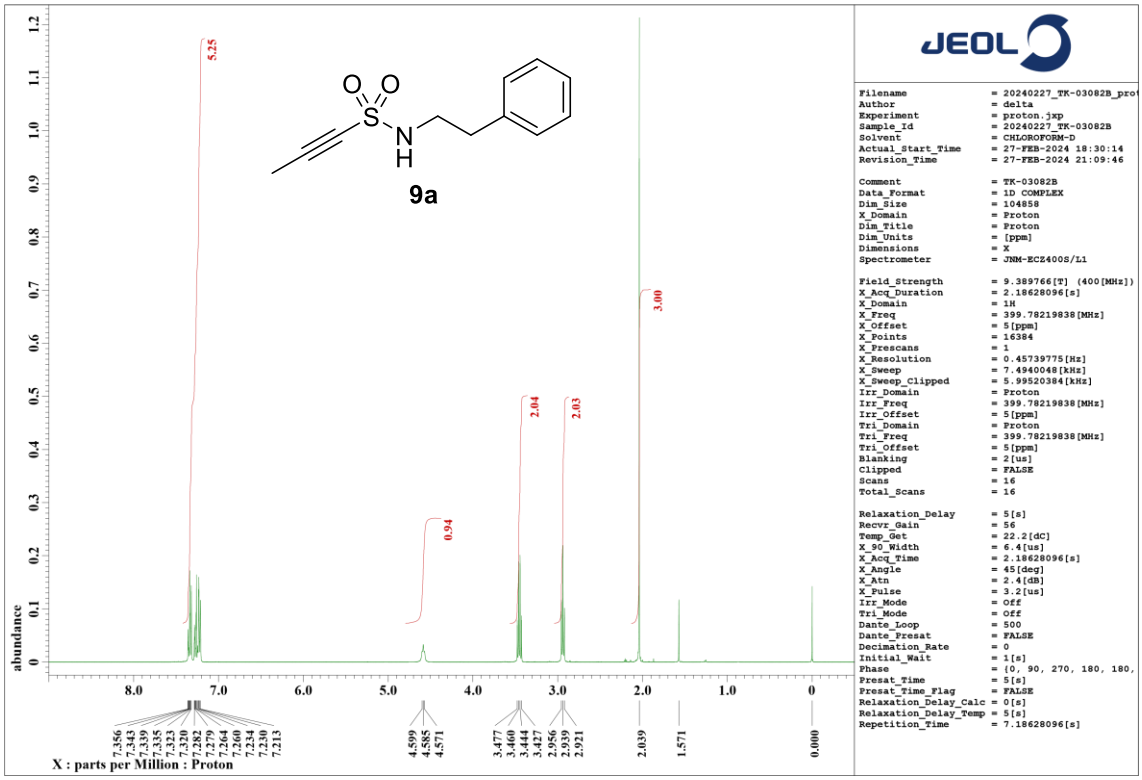

(thousandths)
X : parts per Million : Carbon13
Filename = 20230822_TK-02161B_
Author = delta
Experiment = carbon.jxp
Sample_Id = 20230822_TK-02161B
Solvent = DMSO-D6
Actual_Start_Time = 22-AUG-2023 20:10:3
Revision_Time = 9-SEP-2024 18:56:3
Comment = TK-02161B
Data_Format = 1D COMPLEX
Dim_Size = 26214
X_Domain = Carbon13
Dim_Title = Carbon13
Dim_Units = [ppm]
Dimensions = X
Spectrometer = JNM-ECZ400S/L1
Field_Strength = 9.389766[T] (400[MH
X_Acq_Duration = 1.03809024[s]
X_Domain = 13C
X_Freq = 100.52530333[MHz]
X_Offset = 100[ppm]
X_Points = 32768
X_Prescans = 4
X_Resolution = 0.96330739[Hz]
X_Sweep = 31.56565657[kHz]
X_Sweep_Clipped = 25.25252525[kHz]
Irr_Domain = Proton
Irr_Freq = 399.78219838[MHz]
Irr_Offset = 5[ppm]
Blanking = 5[us]
Clipped = FALSE
Scans = 4096
Total_Scans = 4096
Relaxation_Delay = 2[s]
Recvr_Gain = 50
Temp_Get = 22.9[dC]
X_90_Width = 10.02[us]
X_Acq_Time = 1.03809024[s]
X_Angle = 30[deg]
X_Atn = 8[dB]
X_Pulse = 3.34[us]
Irr_Atn_Dec = 27.49[dB]
Irr_Atn_Dec_Calc = 27.49[dB]
Irr_Atn_Dec_Default_Calc = 27.49[dB]
Irr_Atn_Noe = 27.49[dB]
Irr_Dec_Bandwidth_Hz = 4.78260871[kHz]
Irr_Dec_Bandwidth_Ppm = 11.96303566[ppm]
Irr_Dec_Freq = 399.78219838[MHz]
Irr_Dec_Merit_Factor = 2.2
Irr_Decoupling = TRUE
Irr_Noe = TRUE
Irr_Noise = WALTZ
Irr_Offset_Default = 5[ppm]
Irr_Pwidth = 0.115[ms]
Irr_Pwidth_Default = 0.115[ms]
Irr_Pwidth_Default_Calc = 0.115[ms]
Irr_Pwidth_Temp1 = 0.115[ms]
Irr_Wurst = FALSE
Decimation_Rate = 0

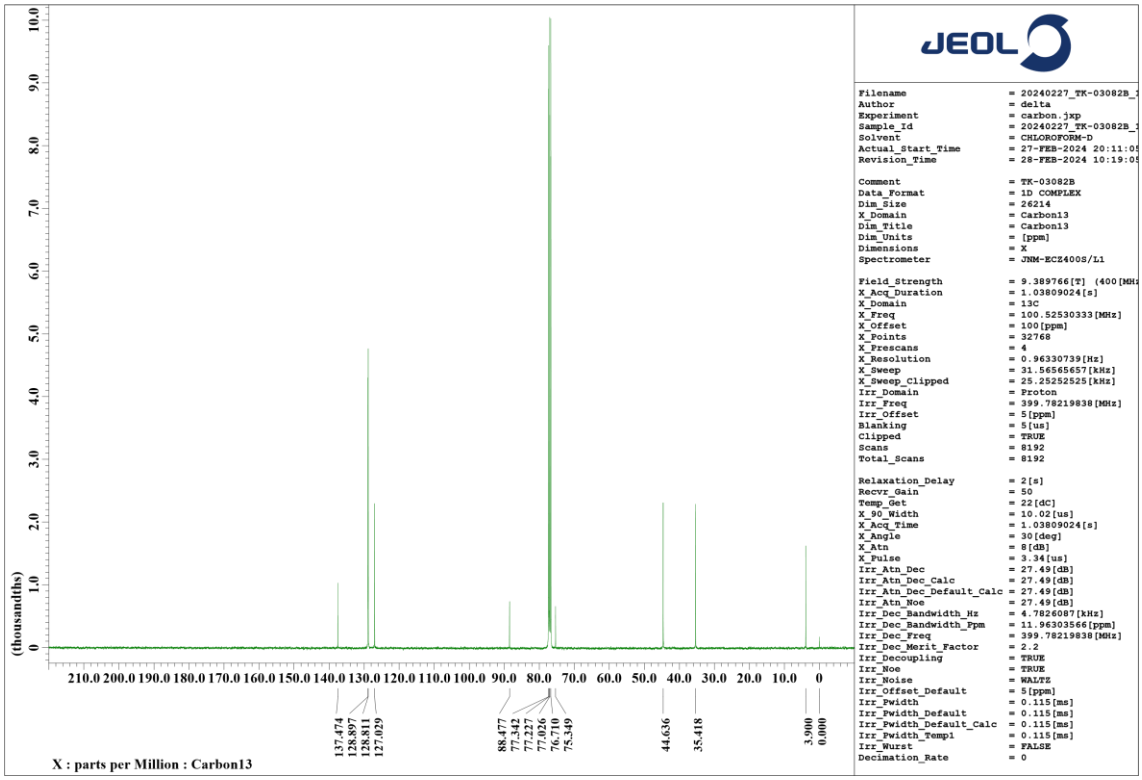

6
+
S1
abundance
X : parts per Million : Proton
4.74
3.58
1.89
0.78
0.41
0.42
0.19
0.18
0.20
JEOL
Filename = 20240905_TK-02191_prot
Author = delta
Experiment = proton.jxp
Sample_Id = 20240905_TK-02191
Solvent = DMSO-D6
Actual_Start_Time = 6-SEP-2024 02:59:03
Revision_Time = 9-SEP-2024 19:26:12
Comment = TK-02191
Data_Format = 1D COMPLEX
Dim_Size = 104858
X_Domain = Proton
Dim_Title = Proton
Dim_Units = [ppm]
Dimensions = X
Spectrometer = JNM-ECZ400S/L1
Field_Strength = 9.389766[T] (400[MHz])
X_Acq_Duration = 2.18628096[s]
X_Domain = 1H
X_Freq = 399.78219838[MHz]
X_Offset = 5[ppm]
X_Points = 16384
X_Prescans = 1
X_Resolution = 0.45739775[Hz]
X_Sweep = 7.4940048[kHz]
X_Sweep_Clipped = 5.99520384[kHz]
Irr_Domain = Proton
Irr_Freq = 399.78219838[MHz]
Irr_Offset = 5[ppm]
Tri_Domain = Proton
Tri_Freq = 399.78219838[MHz]
Tri_Offset = 5[ppm]
Blanking = 2[us]
Clipped = FALSE
Scans = 8
Total_Scans = 8
Relaxation_Delay = 5[s]
Recvr_Gain = 46
Temp_Get = 22.8[dC]
X_90_Width = 6.5[us]
X_Acq_Time = 2.18628096[s]
X_Angle = 45[deg]
X_Atn = 2.4[dB]
X_Pulse = 3.25[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Loop = 500
Dante_Presat = FALSE
Decimation_Rate = 0
Initial_Wait = 1[s]
Phase = (0, 90, 270, 180, 180,
Presat_Time = 5[s]
Presat_Time_Flag = FALSE
Relaxation_Delay_Calc = 0[s]
Relaxation_Delay_Temp = 5[s]
Repetition_Time = 7.18628096[s]

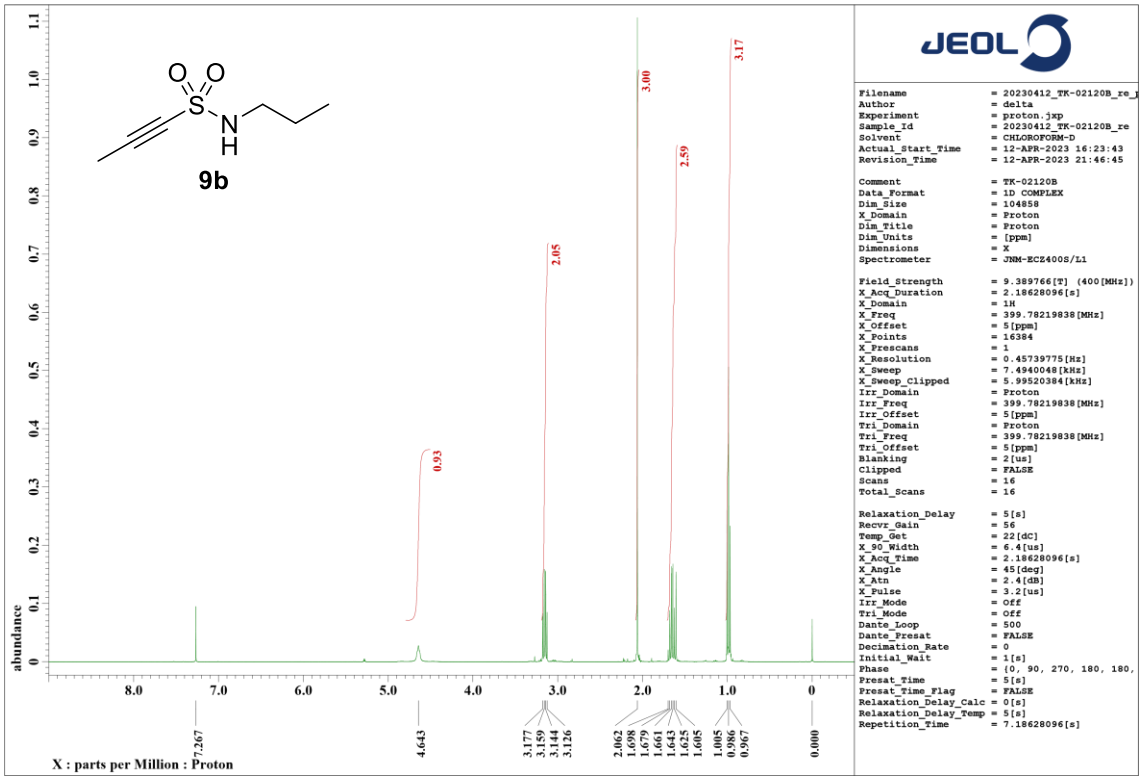

(thousandths)
X : parts per Million : Carbon13
153.458
110.364
81.118
77.563
71.660
59.902
59.097
52.188
51.498
49.639
40.132
39.922
39.711
39.500
39.289
39.088
38.877
JEOL
Filename = 20240905_TK-02191_c
Author = delta
Experiment = carbon.jxp
Sample_Id = 20240905_TK-02191
Solvent = DMSO-D6
Actual_Start_Time = 6-SEP-2024 03:01:0
Revision_Time = 9-SEP-2024 19:02:0
Comment = TK-02191
Data_Format = 1D COMPLEX
Dim_Size = 26214
X_Domain = Carbon13
Dim_Title = Carbon13
Dim_Units = [ppm]
Dimensions = X
Spectrometer = JNM-ECZ400S/L1
Field_Strength = 9.389766[T] (400[MH
X_Acq_Duration = 1.03809024[s]
X_Domain = 13C
X_Freq = 100.52530333[MHz]
X_Offset = 100[ppm]
X_Points = 32768
X_Prescans = 4
X_Resolution = 0.96330739[Hz]
X_Sweep = 31.56565657[kHz]
X_Sweep_Clipped = 25.25252525[kHz]
Irr_Domain = Proton
Irr_Freq = 399.78219838[MHz]
Irr_Offset = 5[ppm]
Blanking = 5[us]
Clipped = TRUE
Scans = 4096
Total_Scans = 4096
Relaxation_Delay = 2[s]
Recvr_Gain = 50
Temp_Get = 22.9[dC]
X_90_Width = 10.02[us]
X_Acq_Time = 1.03809024[s]
X_Angle = 30[deg]
X_Atn = 8[dB]
X_Pulse = 3.34[us]
Irr_Atn_Dec = 27.356[dB]
Irr_Atn_Dec_Calc = 27.356[dB]
Irr_Atn_Dec_Default_Calc = 27.356[dB]
Irr_Atn_Noe = 27.356[dB]
Irr_Dec_Bandwidth_Hz = 4.7826087[kHz]
Irr_Dec_Bandwidth_Ppm = 11.96303566[ppm]
Irr_Dec_Freq = 399.78219838[MHz]
Irr_Dec_Merit_Factor = 2.2
Irr_Decoupling = TRUE
Irr_Noe = TRUE
Irr_Noise = WALTZ
Irr_Offset_Default = 5[ppm]
Irr_Pwidth = 0.115[ms]
Irr_Pwidth_Default = 0.115[ms]
Irr_Pwidth_Default_Calc = 0.115[ms]
Irr_Pwidth_Temp1 = 0.115[ms]
Irr_Wurst = FALSE
Decimation_Rate = 0

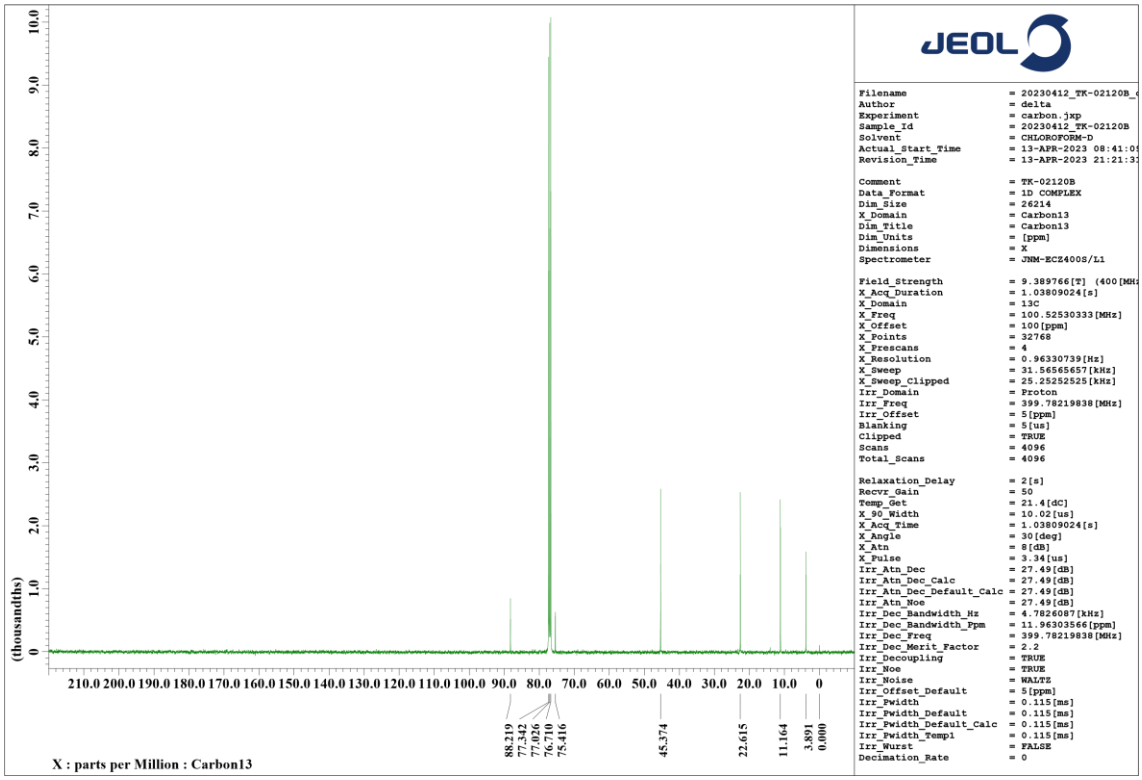

8
abundance
X : parts per Million : Proton
Filename = 20231012_TK-02190_DMSO_
Author = delta
Experiment = proton.jxp
Sample_Id = 20231012_TK-02190_DMSO
Solvent = DMSO-D6
Actual_Start_Time = 12-OCT-2023 20:10:58
Revision_Time = 16-OCT-2023 11:51:58
Comment = TK-02190_DMSO
Data_Format = 1D COMPLEX
Dim_Size = 104858
X_Domain = Proton
Dim_Title = Proton
Dim_Units = [ppm]
Dimensions = X
Spectrometer = JNM-ECZ400S/L1
Field_Strength = 9.389766[T] (400[MHz])
X_Acq_Duration = 2.18628096[s]
X_Domain = 1H
X_Freq = 399.78219838[MHz]
X_Offset = 5[ppm]
X_Points = 16384
X_Prescans = 1
X_Resolution = 0.45739775[Hz]
X_Sweep = 7.4940048[kHz]
X_Sweep_Clipped = 5.99520384[kHz]
Irr_Domain = Proton
Irr_Freq = 399.78219838[MHz]
Irr_Offset = 5[ppm]
Tri_Domain = Proton
Tri_Freq = 399.78219838[MHz]
Tri_Offset = 5[ppm]
Blanking = 2[us]
Clipped = FALSE
Scans = 16
Total_Scans = 16
Relaxation_Delay = 5[s]
Recvr_Gain = 56
Temp_Get = 22.6[dC]
X_90_Width = 6.4[us]
X_Acq_Time = 2.18628096[s]
X_Angle = 45[deg]
X_Atn = 2.4[dB]
X_Pulse = 3.2[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Loop = 500
Dante_Presat = FALSE
Decimation_Rate = 0
Initial_Wait = 1[s]
Phase = (0, 90, 270, 180, 180,
Presat_Time = 5[s]
Presat_Time_Flag = FALSE
Relaxation_Delay_Calc = 0[s]
Relaxation_Delay_Temp = 5[s]
Repetition_Time = 7.18628096[s]

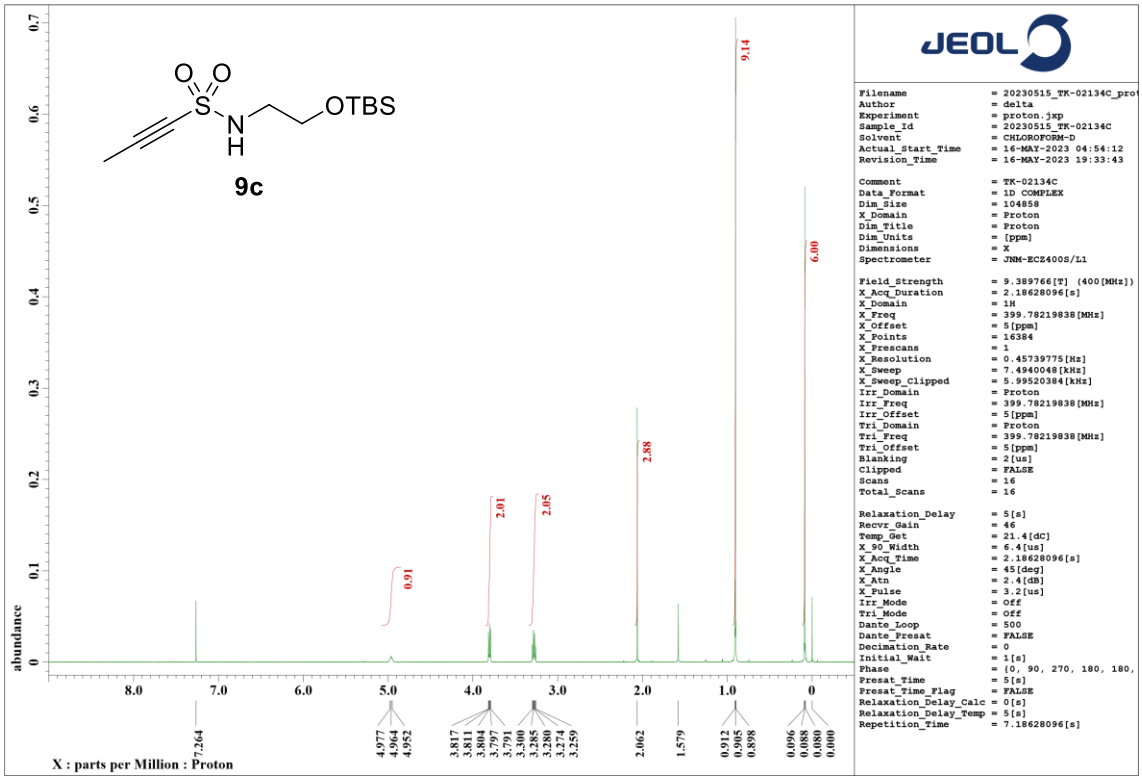

(thousandths)
X : parts per Million : Carbon13
Filename = 20231012_TK-02190_1
Author = delta
Experiment = carbon.jxp
Sample_Id = 20231012_TK-02190_1
Solvent = DMSO-D6
Actual_Start_Time = 12-OCT-2023 20:33:0
Revision_Time = 25-OCT-2023 16:16:4
Comment = TK-02190_DMSO
Data_Format = 1D COMPLEX
Dim_Size = 26214
X_Domain = Carbon13
Dim_Title = Carbon13
Dim_Units = [ppm]
Dimensions = X
Spectrometer = JNM-ECZ400S/L1
Field_Strength = 9.389766[T] (400[MH
X_Acq_Duration = 1.03809024[s]
X_Domain = 13C
X_Freq = 100.52530333[MHz]
X_Offset = 100[ppm]
X_Points = 32768
X_Prescans = 4
X_Resolution = 0.96330739[Hz]
X_Sweep = 31.56565657[kHz]
X_Sweep_Clipped = 25.25252525[kHz]
Irr_Domain = Proton
Irr_Freq = 399.78219838[MHz]
Irr_Offset = 5[ppm]
Blanking = 5[us]
Clipped = TRUE
Scans = 4096
Total_Scans = 4096
Relaxation_Delay = 2[s]
Recvr_Gain = 50
Temp_Get = 22.7[dC]
X_90_Width = 10.02[us]
X_Acq_Time = 1.03809024[s]
X_Angle = 30[deg]
X_Atn = 8[dB]
X_Pulse = 3.34[us]
Irr_Atn_Dec = 27.49[dB]
Irr_Atn_Dec_Calc = 27.49[dB]
Irr_Atn_Dec_Default_Calc = 27.49[dB]
Irr_Atn_Noe = 27.49[dB]
Irr_Dec_Bandwidth_Hz = 4.7826087[kHz]
Irr_Dec_Bandwidth_Ppm = 11.96303566[ppm]
Irr_Dec_Freq = 399.78219838[MHz]
Irr_Dec_Merit_Factor = 2.2
Irr_Decoupling = TRUE
Irr_Noe = TRUE
Irr_Noise = WALTZ
Irr_Offset_Default = 5[ppm]
Irr_Pwidth = 0.115[ms]
Irr_Pwidth_Default = 0.115[ms]
Irr_Pwidth_Default_Calc = 0.115[ms]
Irr_Pwidth_Temp1 = 0.115[ms]
Irr_Wurst = FALSE
Decimation_Rate = 0

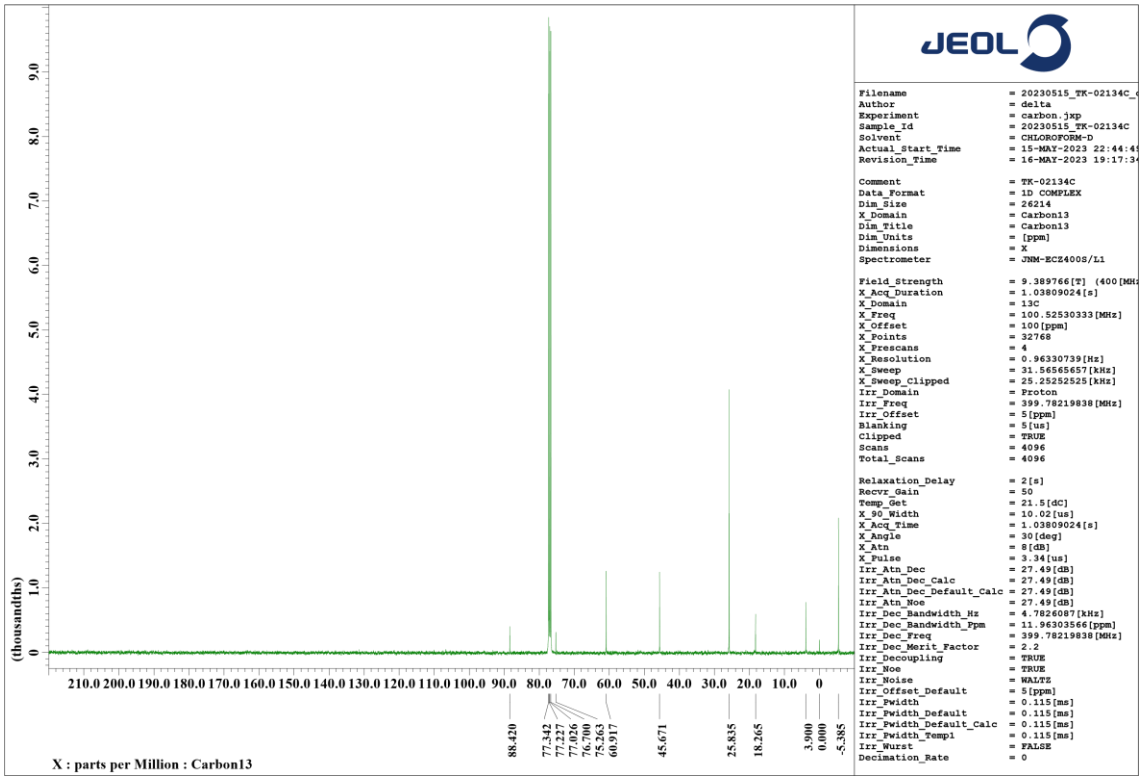

9a
5.25
0.94
2.04
2.03
3.00
abundance
X : parts per Million : Proton
Filename = 20240227_TK-03082B_pro
Author = delta
Experiment = proton.jxp
Sample_Id = 20240227_TK-03082B
Solvent = CHLOROFORM-D
Actual_Start_Time = 27-FEB-2024 18:30:14
Revision_Time = 27-FEB-2024 21:09:46
Comment = TK-03082B
Data_Format = 1D COMPLEX
Dim_Size = 104858
X_Domain = Proton
Dim_Title = Proton
Dim_Units = [ppm]
Dimensions = X
Spectrometer = JNM-ECZ400S/L1
Field_Strength = 9.389766[T] (400[MHz])
X_Acq_Duration = 2.18628096[s]
X_Domain = 1H
X_Freq = 399.78219838[MHz]
X_Offset = 5[ppm]
X_Points = 16384
X_Prescans = 1
X_Resolution = 0.45739775[Hz]
X_Sweep = 7.4940048[kHz]
X_Sweep_Clipped = 5.99520384[kHz]
Irr_Domain = Proton
Irr_Freq = 399.78219838[MHz]
Irr_Offset = 5[ppm]
Tri_Domain = Proton
Tri_Freq = 399.78219838[MHz]
Tri_Offset = 5[ppm]
Blanking = 2[us]
Clipped = FALSE
Scans = 16
Total_Scans = 16
Relaxation_Delay = 5[s]
Recvr_Gain = 56
Temp_Get = 22.2[dC]
X_90_Width = 6.4[us]
X_Acq_Time = 2.18628096[s]
X_Angle = 45[deg]
X_Atn = 2.4[dB]
X_Pulse = 3.2[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Loop = 500
Dante_Presat = FALSE
Decimation_Rate = 0
Initial_Wait = 1[s]
Phase = (0, 90, 270, 180, 180,
Presat_Time = 5[s]
Presat_Time_Flag = FALSE
Relaxation_Delay_Calc = 0[s]
Relaxation_Delay_Temp = 5[s]
Repetition_Time = 7.18628096[s]

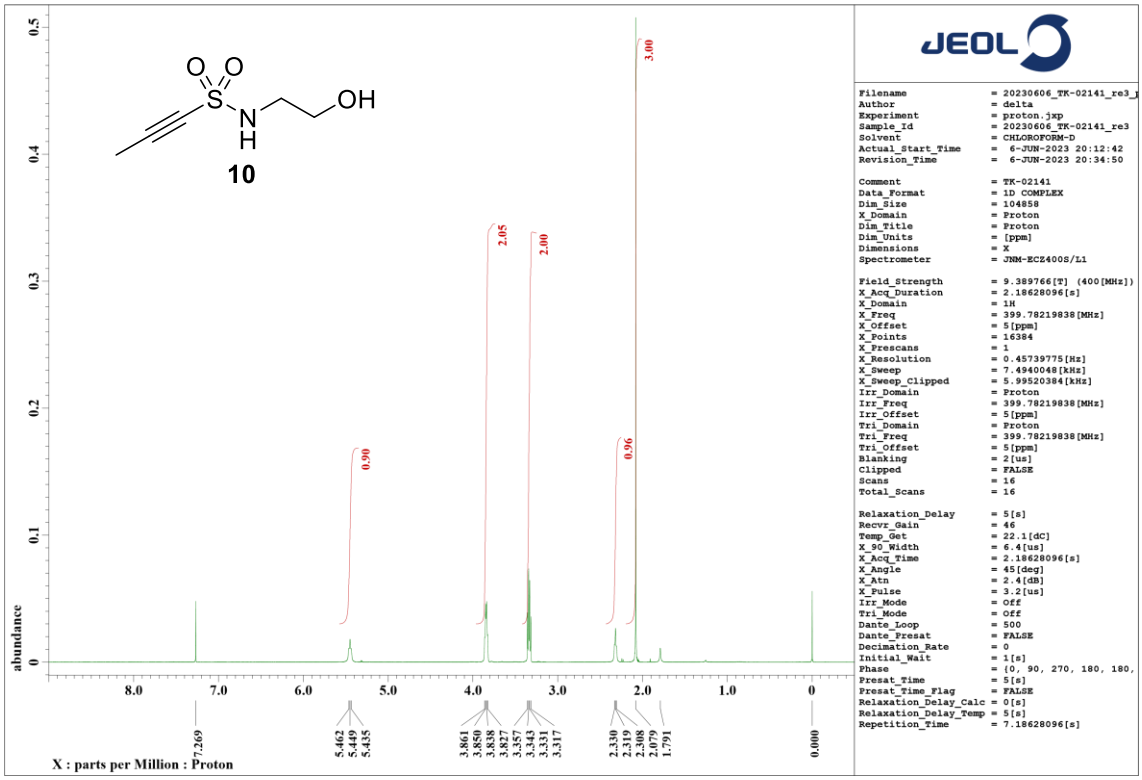

(thousandths)
X : parts per Million : Carbon13
Filename = 20240227_TK-03082B_1
Author = delta
Experiment = carbon.jxp
Sample_Id = 20240227_TK-03082B_1
Solvent = CHLOROFORM-D
Actual_Start_Time = 27-FEB-2024 20:11:05
Revision_Time = 28-FEB-2024 10:19:05
Comment = TK-03082B
Data_Format = 1D COMPLEX
Dim_Size = 26214
X_Domain = Carbon13
Dim_Title = Carbon13
Dim_Units = [ppm]
Dimensions = X
Spectrometer = JNM-ECZ400S/L1
Field_Strength = 9.389766[T] (400[MHz
X_Acq_Duration = 1.03809024[s]
X_Domain = 13C
X_Freq = 100.52530333[MHz]
X_Offset = 100[ppm]
X_Points = 32768
X_Prescans = 4
X_Resolution = 0.96330739[Hz]
X_Sweep = 31.56565657[kHz]
X_Sweep_Clipped = 25.25252525[kHz]
Irr_Domain = Proton
Irr_Freq = 399.78219838[MHz]
Irr_Offset = 5[ppm]
Blanking = 5[us]
Clipped = TRUE
Scans = 8192
Total_Scans = 8192
Relaxation_Delay = 2[s]
Recvr_Gain = 50
Temp_Get = 22[dC]
X_90_Width = 10.02[us]
X_Acq_Time = 1.03809024[s]
X_Angle = 30[deg]
X_Atn = 8[dB]
X_Pulse = 3.34[us]
Irr_Atn_Dec = 27.49[dB]
Irr_Atn_Dec_Calc = 27.49[dB]
Irr_Atn_Dec_Default_Calc = 27.49[dB]
Irr_Atn_Noe = 27.49[dB]
Irr_Dec_Bandwidth_Hz = 4.78260087[kHz]
Irr_Dec_Bandwidth_Ppm = 11.96303566[ppm]
Irr_Dec_Freq = 399.78219838[MHz]
Irr_Dec_Merit_Factor = 2.2
Irr_Decoupling = TRUE
Irr_Noe = TRUE
Irr_Noise = WALTZ
Irr_Offset_Default = 5[ppm]
Irr_Pwidth = 0.115[ms]
Irr_Pwidth_Default = 0.115[ms]
Irr_Pwidth_Default_Calc = 0.115[ms]
Irr_Pwidth_Temp1 = 0.115[ms]
Irr_Wurst = FALSE
Decimation_Rate = 0

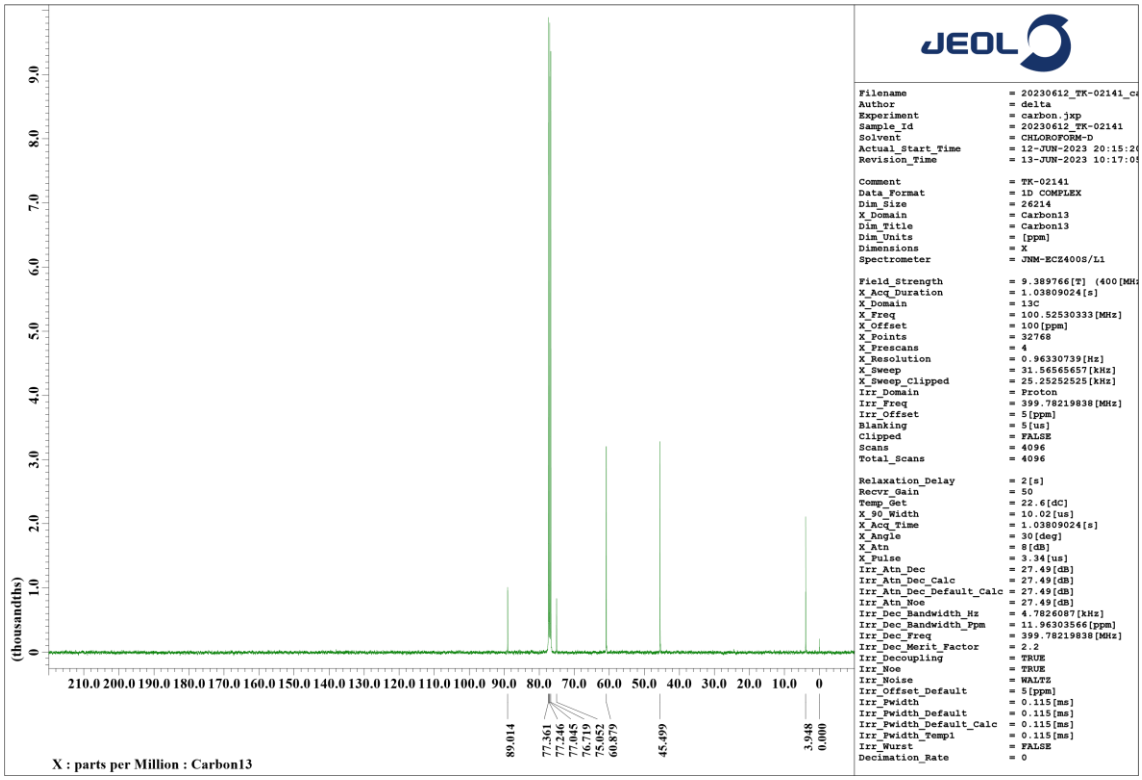

9b
abundance
X : parts per Million : Proton
7.267
4.643
3.177
3.159
3.144
3.126
2.062
1.698
1.679
1.661
1.643
1.625
1.605
1.005
0.986
0.967
0.000
0.93
2.05
3.00
2.59
3.17
JEOL
Filename = 20230412_TK-02120B_re_
Author = delta
Experiment = proton.jxp
Sample_Id = 20230412_TK-02120B_re
Solvent = CHLOROFORM-D
Actual_Start_Time = 12-APR-2023 16:23:43
Revision_Time = 12-APR-2023 21:46:45
Comment = TK-02120B
Data_Format = 1D COMPLEX
Dim_Size = 104858
X_Domain = Proton
Dim_Title = Proton
Dim_Units = [ppm]
Dimensions = X
Spectrometer = JNM-ECZ400S/L1
Field_Strength = 9.389766[T] (400[MHz])
X_Acq_Duration = 2.18628096[s]
X_Domain = 1H
X_Freq = 399.78219838[MHz]
X_Offset = 5[ppm]
X_Points = 16384
X_Prescans = 1
X_Resolution = 0.45739775[Hz]
X_Sweep = 7.4940048[kHz]
X_Sweep_Clipped = 5.99520384[kHz]
Irr_Domain = Proton
Irr_Freq = 399.78219838[MHz]
Irr_Offset = 5[ppm]
Tri_Domain = Proton
Tri_Freq = 399.78219838[MHz]
Tri_Offset = 5[ppm]
Blanking = 2[us]
Clipped = FALSE
Scans = 16
Total_Scans = 16
Relaxation_Delay = 5[s]
Recvr_Gain = 56
Temp_Get = 22[dC]
X_90_Width = 6.4[us]
X_Acq_Time = 2.18628096[s]
X_Angle = 45[deg]
X_Atn = 2.4[dB]
X_Pulse = 3.2[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Loop = 500
Dante_Presat = FALSE
Decimation_Rate = 0
Initial_Wait = 1[s]
Phase = (0, 90, 270, 180, 180,
Presat_Time = 5[s]
Presat_Time_Flag = FALSE
Relaxation_Delay_Calc = 0[s]
Relaxation_Delay_Temp = 5[s]
Repetition_Time = 7.18628096[s]

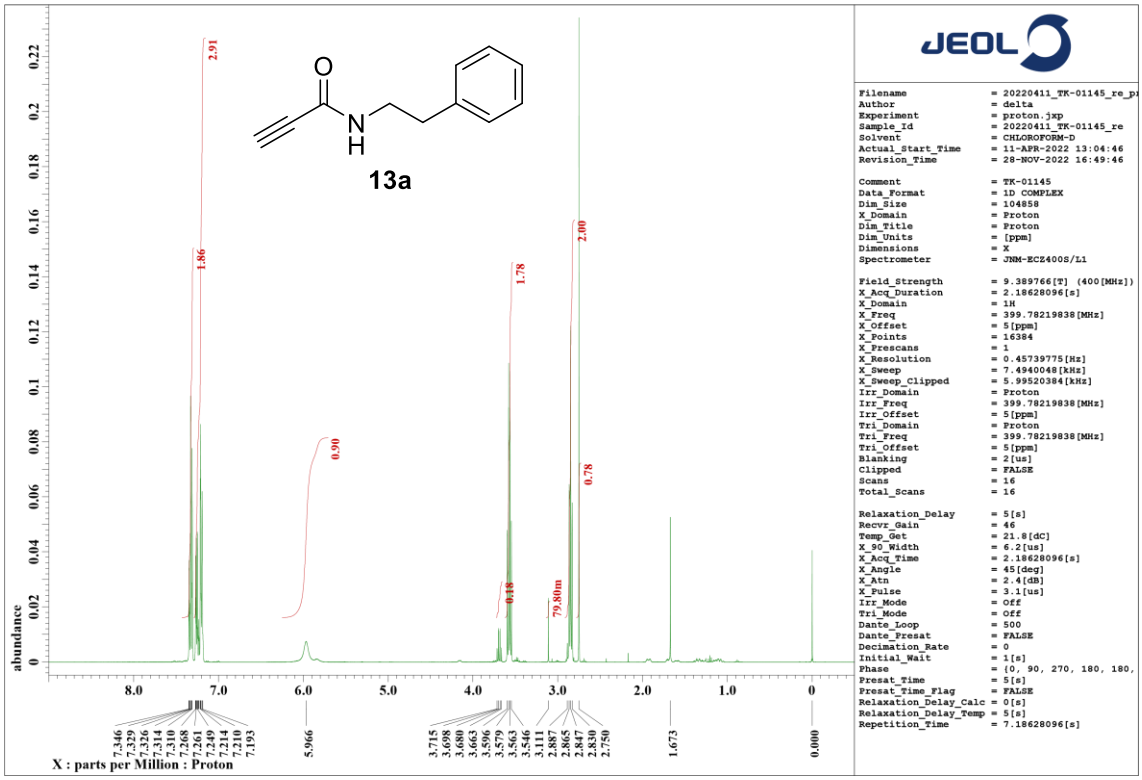

(thousandths)
X : parts per Million : Carbon13
88.219
77.342
77.026
76.710
75.416
45.374
22.615
11.164
3.891
0.000
JEOL
Filename = 20230412_TK-02120B_
Author = delta
Experiment = carbon.jxp
Sample_Id = 20230412_TK-02120B
Solvent = CHLOROFORM-D
Actual_Start_Time = 13-APR-2023 08:41:0
Revision_Time = 13-APR-2023 21:21:3
Comment = TK-02120B
Data_Format = 1D COMPLEX
Dim_Size = 26214
X_Domain = Carbon13
Dim_Title = Carbon13
Dim_Units = [ppm]
Dimensions = X
Spectrometer = JNM-ECZ400S/L1
Field_Strength = 9.389766[T] (400[MHz
X_Acq_Duration = 1.03809024[s]
X_Domain = 13C
X_Freq = 100.52530333[MHz]
X_Offset = 100[ppm]
X_Points = 32768
X_Prescans = 4
X_Resolution = 0.96330739[Hz]
X_Sweep = 31.56565657[kHz]
X_Sweep_Clipped = 25.25252525[kHz]
Irr_Domain = Proton
Irr_Freq = 399.78219838[MHz]
Irr_Offset = 5[ppm]
Blanking = 5[us]
Clipped = TRUE
Scans = 4096
Total_Scans = 4096
Relaxation_Delay = 2[s]
Recvr_Gain = 50
Temp_Get = 21.4[dC]
X_90_Width = 10.02[us]
X_Acq_Time = 1.03809024[s]
X_Angle = 30[deg]
X_Atn = 8[dB]
X_Pulse = 3.34[us]
Irr_Atn_Dec = 27.49[dB]
Irr_Atn_Dec_Calc = 27.49[dB]
Irr_Atn_Dec_Default_Calc = 27.49[dB]
Irr_Atn_Noe = 27.49[dB]
Irr_Dec_Bandwidth_Hz = 4.7826087[kHz]
Irr_Dec_Bandwidth_Ppm = 11.96303566[ppm]
Irr_Dec_Freq = 399.78219838[MHz]
Irr_Dec_Merit_Factor = 2.2
Irr_Decoupling = TRUE
Irr_Noe = TRUE
Irr_Noise = WALTZ
Irr_Offset_Default = 5[ppm]
Irr_Pwidth = 0.115[ms]
Irr_Pwidth_Default = 0.115[ms]
Irr_Pwidth_Default_Calc = 0.115[ms]
Irr_Pwidth_Temp1 = 0.115[ms]
Irr_Wurst = FALSE
Decimation_Rate = 0

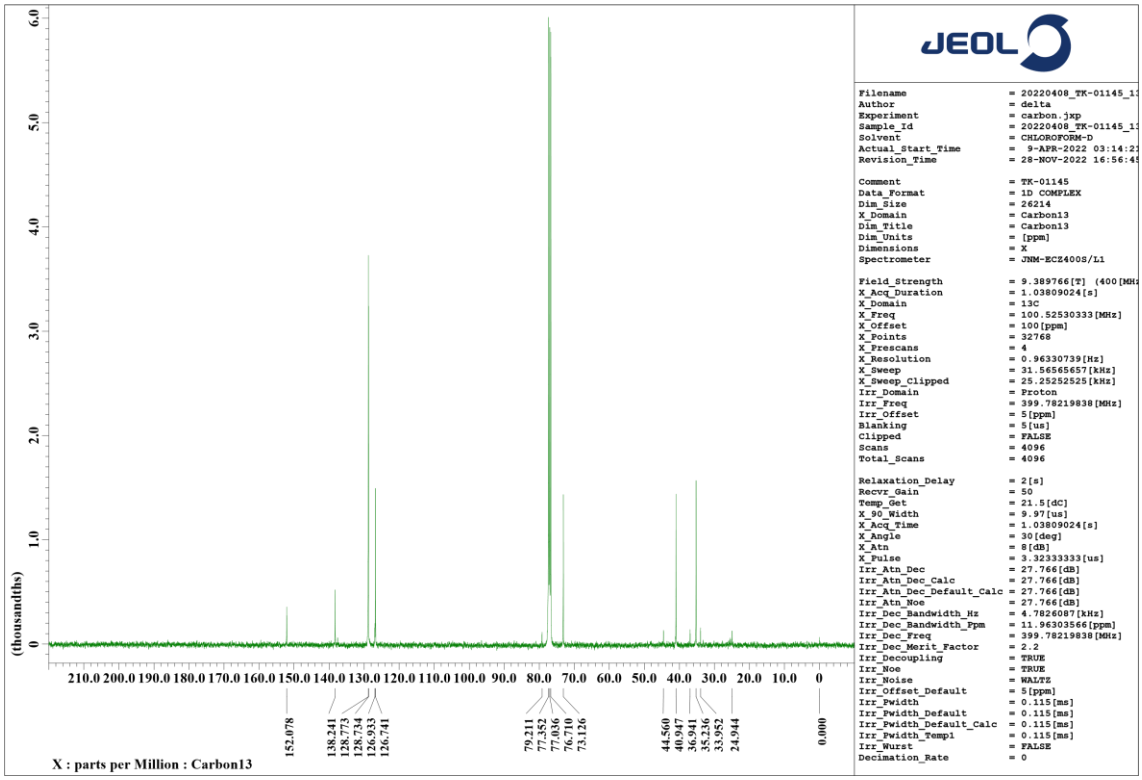

OTBS
9c
abundance
X : parts per Million : Proton
9.14
6.00
2.88
2.01
2.05
0.91
7.264
4.977
4.964
4.952
3.817
3.811
3.804
3.797
3.791
3.300
3.285
3.280
3.274
3.259
2.062
1.579
0.912
0.905
0.898
0.096
0.088
0.080
0.000
Filename = 20230515_TK-02134C_pro
Author = delta
Experiment = proton.jxp
Sample_Id = 20230515_TK-02134C
Solvent = CHLOROFORM-D
Actual_Start_Time = 16-MAY-2023 04:54:12
Revision_Time = 16-MAY-2023 19:33:43
Comment = TK-02134C
Data_Format = 1D COMPLEX
Dim_Size = 104858
X_Domain = Proton
Dim_Title = Proton
Dim_Units = [ppm]
Dimensions = X
Spectrometer = JNM-ECZ400S/L1
Field_Strength = 9.389766[T] (400[MHz])
X_Acq_Duration = 2.18628096[s]
X_Domain = 1H
X_Freq = 399.78219838[MHz]
X_Offset = 5[ppm]
X_Points = 16384
X_Prescans = 1
X_Resolution = 0.45739775[Hz]
X_Sweep = 7.4940048[kHz]
X_Sweep_Clipped = 5.99520384[kHz]
Irr_Domain = Proton
Irr_Freq = 399.78219838[MHz]
Irr_Offset = 5[ppm]
Tri_Domain = Proton
Tri_Freq = 399.78219838[MHz]
Tri_Offset = 5[ppm]
Blanking = 2[us]
Clipped = FALSE
Scans = 16
Total_Scans = 16
Relaxation_Delay = 5[s]
Recvr_Gain = 46
Temp_Get = 21.4[dC]
X_90_Width = 6.4[us]
X_Acq_Time = 2.18628096[s]
X_Angle = 45[deg]
X_Atn = 2.4[dB]
X_Pulse = 3.2[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Loop = 500
Dante_Presat = FALSE
Decimation_Rate = 0
Initial_Wait = 1[s]
Phase = (0, 90, 270, 180, 180,
Presat_Time = 5[s]
Presat_Time_Flag = FALSE
Relaxation_Delay_Calc = 0[s]
Relaxation_Delay_Temp = 5[s]
Repetition_Time = 7.18628096[s]

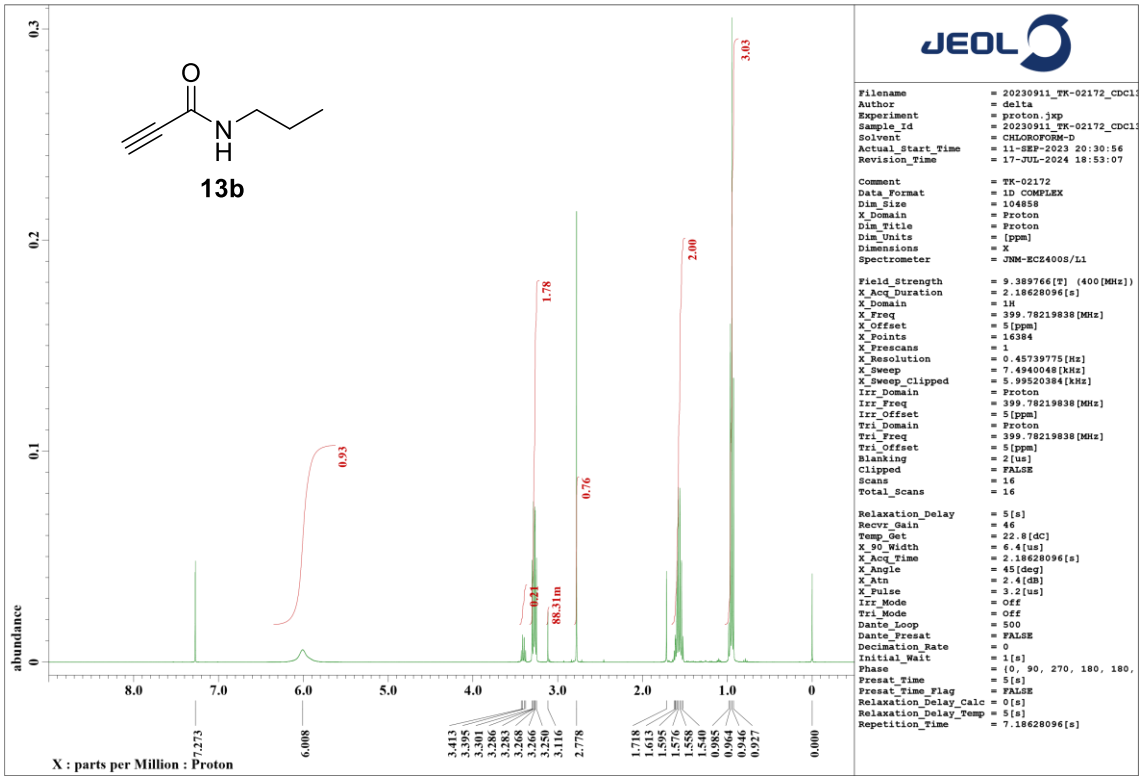

(thousandths)
X : parts per Million : Carbon13
88.420
77.342
77.227
77.026
76.700
75.263
60.917
45.671
25.835
18.265
3.900
0.000
-5.385
Filename = 20230515_TK-02134C_
Author = delta
Experiment = carbon.jxp
Sample_Id = 20230515_TK-02134C
Solvent = CHLOROFORM-D
Actual_Start_Time = 15-MAY-2023 22:44:4
Revision_Time = 16-MAY-2023 19:17:3
Comment = TK-02134C
Data_Format = 1D COMPLEX
Dim_Size = 26214
X_Domain = Carbon13
Dim_Title = Carbon13
Dim_Units = [ppm]
Dimensions = X
Spectrometer = JNM-ECZ400S/L1
Field_Strength = 9.389766[T] (400[MH
X_Acq_Duration = 1.03809024[s]
X_Domain = 13C
X_Freq = 100.52530333[MHz]
X_Offset = 100[ppm]
X_Points = 32768
X_Prescans = 4
X_Resolution = 0.96330739[Hz]
X_Sweep = 31.56565657[kHz]
X_Sweep_Clipped = 25.25252525[kHz]
Irr_Domain = Proton
Irr_Freq = 399.78219838[MHz]
Irr_Offset = 5[ppm]
Blanking = 5[us]
Clipped = TRUE
Scans = 4096
Total_Scans = 4096
Relaxation_Delay = 2[s]
Recvr_Gain = 50
Temp_Get = 21.5[dC]
X_90_Width = 10.02[us]
X_Acq_Time = 1.03809024[s]
X_Angle = 30[deg]
X_Atn = 8[dB]
X_Pulse = 3.34[us]
Irr_Atn_Dec = 27.49[dB]
Irr_Atn_Dec_Calc = 27.49[dB]
Irr_Atn_Dec_Default_Calc = 27.49[dB]
Irr_Atn_Noe = 27.49[dB]
Irr_Dec_Bandwidth_Hz = 4.7826087[kHz]
Irr_Dec_Bandwidth_Ppm = 11.96303566[ppm]
Irr_Dec_Freq = 399.78219838[MHz]
Irr_Dec_Merit_Factor = 2.2
Irr_Decoupling = TRUE
Irr_Noe = TRUE
Irr_Noise = WALTZ
Irr_Offset_Default = 5[ppm]
Irr_Pwidth = 0.115[ms]
Irr_Pwidth_Default = 0.115[ms]
Irr_Pwidth_Default_Calc = 0.115[ms]
Irr_Pwidth_Temp1 = 0.115[ms]
Irr_Wurst = FALSE
Decimation_Rate = 0

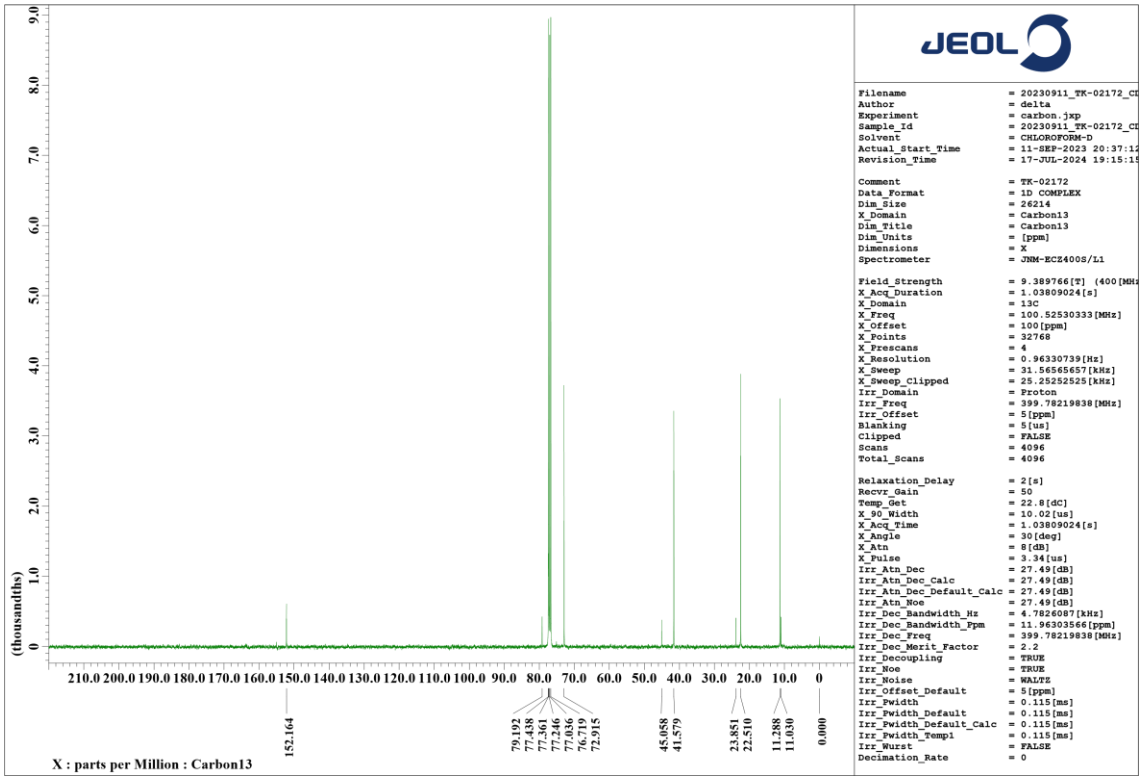

O
O
S
N
H
OH
10
abundance
0.5
0.4
0.3
0.2
0.1
0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
0.90
2.05
2.00
0.96
3.00
7.269
5.462
5.449
5.435
3.861
3.850
3.838
3.827
3.357
3.343
3.331
3.317
2.330
2.319
2.308
2.079
1.791
0.000
X : parts per Million : Proton
JEOL
Filename = 20230606_TK-02141_re3_
Author = delta
Experiment = proton.jxp
Sample_Id = 20230606_TK-02141_re3
Solvent = CHLOROFORM-D
Actual_Start_Time = 6-JUN-2023 20:12:42
Revision_Time = 6-JUN-2023 20:34:50
Comment = TK-02141
Data_Format = 1D COMPLEX
Dim_Size = 104858
X_Domain = Proton
Dim_Title = Proton
Dim_Units = [ppm]
Dimensions = X
Spectrometer = JNM-ECZ400S/L1
Field_Strength = 9.389766[T] (400[MHz])
X_Acq_Duration = 2.18628096[s]
X_Domain = 1H
X_Freq = 399.78219838[MHz]
X_Offset = 5[ppm]
X_Points = 16384
X_Prescans = 1
X_Resolution = 0.45739775[Hz]
X_Sweep = 7.4940048[kHz]
X_Sweep_Clipped = 5.99520384[kHz]
Irr_Domain = Proton
Irr_Freq = 399.78219838[MHz]
Irr_Offset = 5[ppm]
Tri_Domain = Proton
Tri_Freq = 399.78219838[MHz]
Tri_Offset = 5[ppm]
Blanking = 2[us]
Clipped = FALSE
Scans = 16
Total_Scans = 16
Relaxation_Delay = 5[s]
Recvr_Gain = 46
Temp_Get = 22.1[dC]
X_90_Width = 6.4[us]
X_Acq_Time = 2.18628096[s]
X_Angle = 45[deg]
X_Atn = 2.4[dB]
X_Pulse = 3.2[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Loop = 500
Dante_Presat = FALSE
Decimation_Rate = 0
Initial_Wait = 1[s]
Phase = (0, 90, 270, 180, 180,
Presat_Time = 5[s]
Presat_Time_Flag = FALSE
Relaxation_Delay_Calc = 0[s]
Relaxation_Delay_Temp = 5[s]
Repetition_Time = 7.18628096[s]

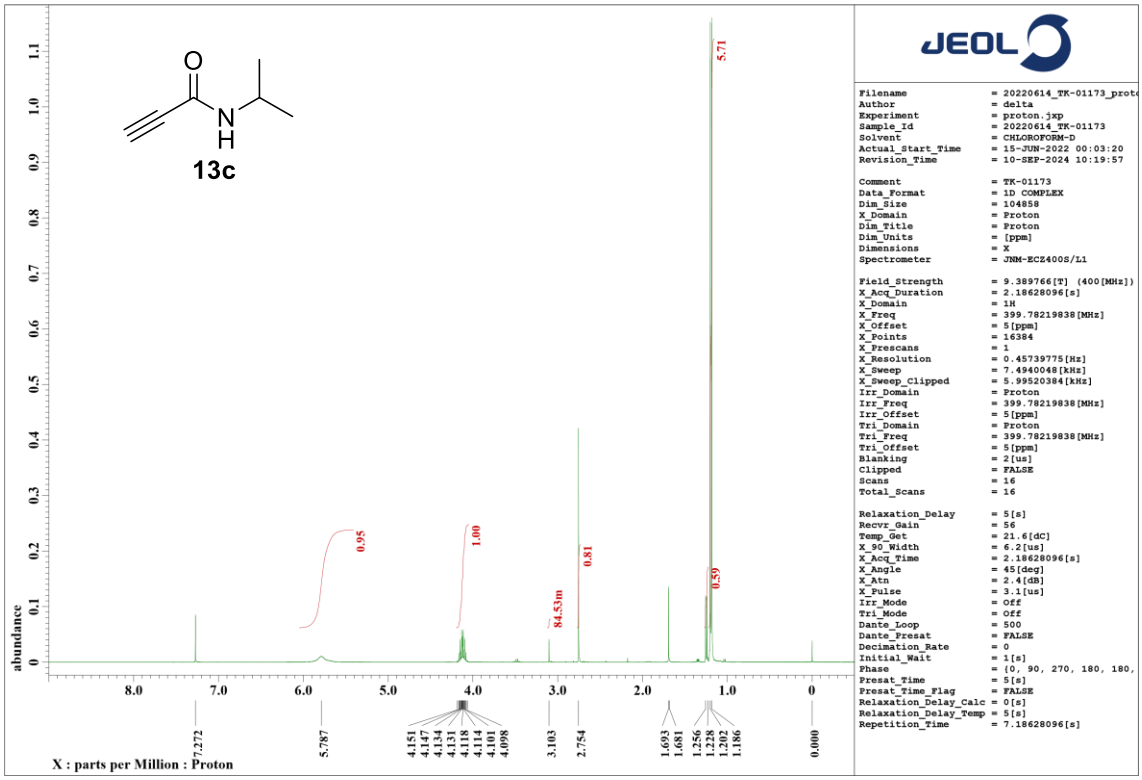

(thousandths)
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
210.0 200.0 190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0
89.014
77.361
77.246
77.045
76.719
75.052
60.879
45.499
3.948
0.000
X : parts per Million : Carbon13
JEOL
Filename = 20230612_TK-02141_c
Author = delta
Experiment = carbon.jxp
Sample_Id = 20230612_TK-02141
Solvent = CHLOROFORM-D
Actual_Start_Time = 12-JUN-2023 20:15:2
Revision_Time = 13-JUN-2023 10:17:0
Comment = TK-02141
Data_Format = 1D COMPLEX
Dim_Size = 26214
X_Domain = Carbon13
Dim_Title = Carbon13
Dim_Units = [ppm]
Dimensions = X
Spectrometer = JNM-ECZ400S/L1
Field_Strength = 9.389766[T] (400[MH
X_Acq_Duration = 1.03809024[s]
X_Domain = 13C
X_Freq = 100.52530333[MHz]
X_Offset = 100[ppm]
X_Points = 32768
X_Prescans = 4
X_Resolution = 0.96330739[Hz]
X_Sweep = 31.56565657[kHz]
X_Sweep_Clipped = 25.25252525[kHz]
Irr_Domain = Proton
Irr_Freq = 399.78219838[MHz]
Irr_Offset = 5[ppm]
Blanking = 5[us]
Clipped = FALSE
Scans = 4096
Total_Scans = 4096
Relaxation_Delay = 2[s]
Recvr_Gain = 50
Temp_Get = 22.6[dC]
X_90_Width = 10.02[us]
X_Acq_Time = 1.03809024[s]
X_Angle = 30[deg]
X_Atn = 8[dB]
X_Pulse = 3.34[us]
Irr_Atn_Dec = 27.49[dB]
Irr_Atn_Dec_Calc = 27.49[dB]
Irr_Atn_Dec_Default_Calc = 27.49[dB]
Irr_Atn_Noe = 27.49[dB]
Irr_Dec_Bandwidth_Hz = 4.78260087[kHz]
Irr_Dec_Bandwidth_Ppm = 11.96303566[ppm]
Irr_Dec_Freq = 399.78219838[MHz]
Irr_Dec_Merit_Factor = 2.2
Irr_Decoupling = TRUE
Irr_Noe = TRUE
Irr_Noise = WALTZ
Irr_Offset_Default = 5[ppm]
Irr_Pwidth = 0.115[ms]
Irr_Pwidth_Default = 0.115[ms]
Irr_Pwidth_Default_Calc = 0.115[ms]
Irr_Pwidth_Temp1 = 0.115[ms]
Irr_Wurst = FALSE
Decimation_Rate = 0

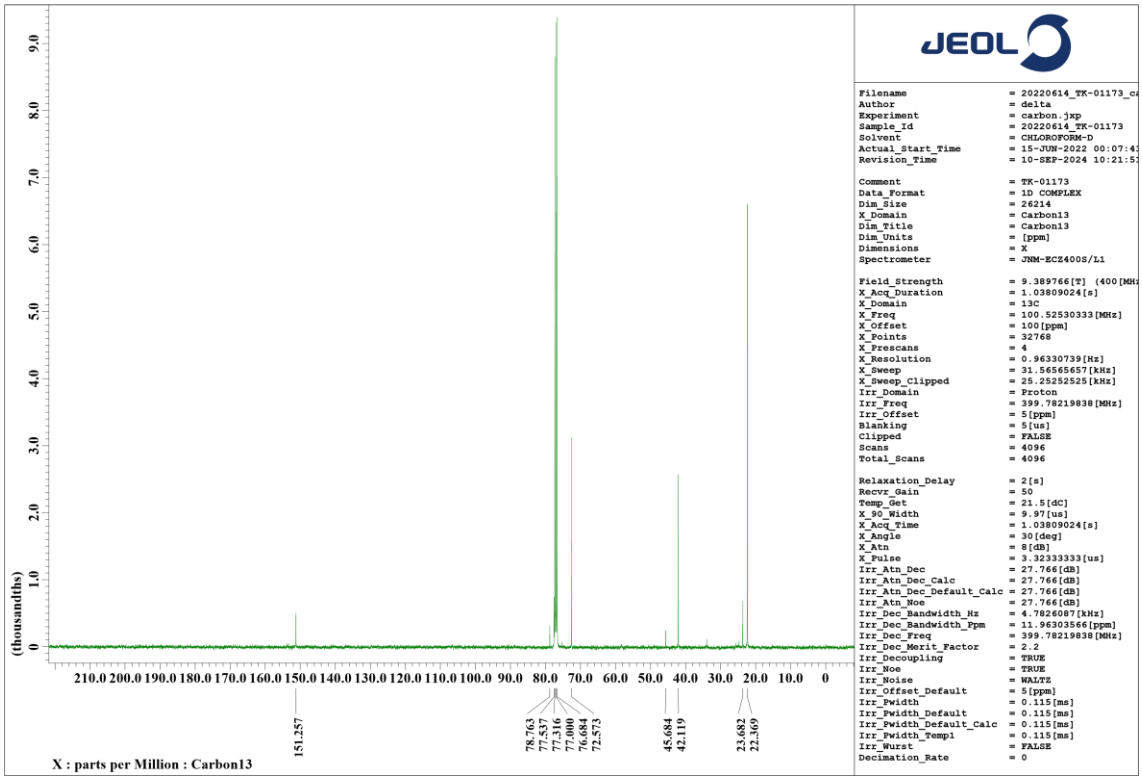

13a
abundance
X : parts per Million : Proton
Filename = 20220411_TK-01145_re_p
Author = delta
Experiment = proton.jxp
Sample_Id = 20220411_TK-01145_re
Solvent = CHLOROFORM-D
Actual_Start_Time = 11-APR-2022 13:04:46
Revision_Time = 28-NOV-2022 16:49:46
Comment = TK-01145
Data_Format = 1D COMPLEX
Dim_Size = 104858
X_Domain = Proton
Dim_Title = Proton
Dim_Units = [ppm]
Dimensions = X
Spectrometer = JNM-ECZ400S/L1
Field_Strength = 9.389766[T] (400[MHz])
X_Acq_Duration = 2.18628096[s]
X_Domain = 1H
X_Freq = 399.78219838[MHz]
X_Offset = 5[ppm]
X_Points = 16384
X_Prescans = 1
X_Resolution = 0.45739775[Hz]
X_Sweep = 7.4940048[kHz]
X_Sweep_Clipped = 5.99520384[kHz]
Irr_Domain = Proton
Irr_Freq = 399.78219838[MHz]
Irr_Offset = 5[ppm]
Tri_Domain = Proton
Tri_Freq = 399.78219838[MHz]
Tri_Offset = 5[ppm]
Blanking = 2[us]
Clipped = FALSE
Scans = 16
Total_Scans = 16
Relaxation_Delay = 5[s]
Recvr_Gain = 46
Temp_Get = 21.8[dC]
X_90_Width = 6.2[us]
X_Acq_Time = 2.18628096[s]
X_Angle = 45[deg]
X_Atn = 2.4[dB]
X_Pulse = 3.1[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Loop = 500
Dante_Presat = FALSE
Decimation_Rate = 0
Initial_Wait = 1[s]
Phase = (0, 90, 270, 180, 180,
Presat_Time = 5[s]
Presat_Time_Flag = FALSE
Relaxation_Delay_Calc = 0[s]
Relaxation_Delay_Temp = 5[s]
Repetition_Time = 7.18628096[s]

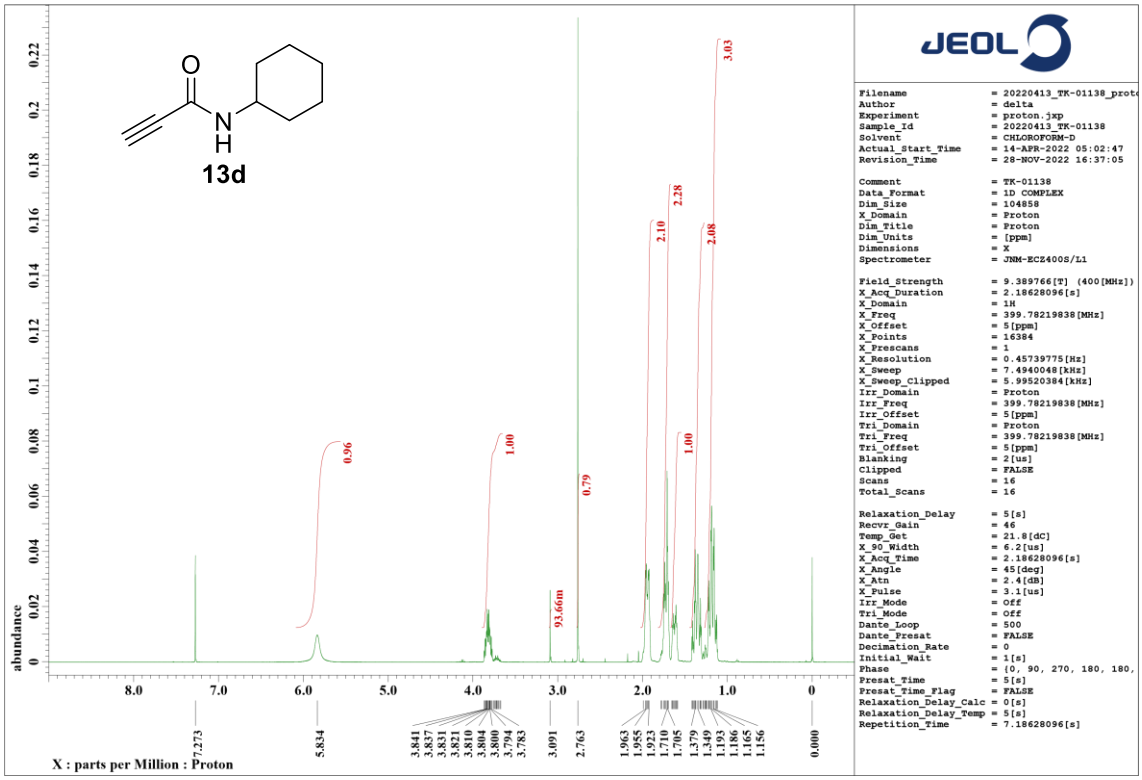

(thousandths)
X : parts per Million : Carbon13
Filename = 20220408_TK-01145_1
Author = delta
Experiment = carbon.jxp
Sample_Id = 20220408_TK-01145_1
Solvent = CHLOROFORM-D
Actual_Start_Time = 9-APR-2022 03:14:2
Revision_Time = 28-NOV-2022 16:56:4
Comment = TK-01145
Data_Format = 1D COMPLEX
Dim_Size = 26214
X_Domain = Carbon13
Dim_Title = Carbon13
Dim_Units = [ppm]
Dimensions = X
Spectrometer = JNM-ECZ400S/L1
Field_Strength = 9.389766[T] (400[MH
X_Acq_Duration = 1.03809024[s]
X_Domain = 13C
X_Freq = 100.52530333[MHz]
X_Offset = 100[ppm]
X_Points = 32768
X_Prescans = 4
X_Resolution = 0.96330739[Hz]
X_Sweep = 31.56565657[kHz]
X_Sweep_Clipped = 25.25252525[kHz]
Irr_Domain = Proton
Irr_Freq = 399.78219838[MHz]
Irr_Offset = 5[ppm]
Blanking = 5[us]
Clipped = FALSE
Scans = 4096
Total_Scans = 4096
Relaxation_Delay = 2[s]
Recvr_Gain = 50
Temp_Get = 21.5[dC]
X_90_Width = 9.97[us]
X_Acq_Time = 1.03809024[s]
X_Angle = 30[deg]
X_Atn = 8[dB]
X_Pulse = 3.32333333[us]
Irr_Atn_Dec = 27.766[dB]
Irr_Atn_Dec_Calc = 27.766[dB]
Irr_Atn_Dec_Default_Calc = 27.766[dB]
Irr_Atn_Noe = 27.766[dB]
Irr_Dec_Bandwidth_Hz = 4.7826087[kHz]
Irr_Dec_Bandwidth_Ppm = 11.96303566[ppm]
Irr_Dec_Freq = 399.78219838[MHz]
Irr_Dec_Merit_Factor = 2.2
Irr_Decoupling = TRUE
Irr_Noe = TRUE
Irr_Noise = WALTZ
Irr_Offset_Default = 5[ppm]
Irr_Pwidth = 0.115[ms]
Irr_Pwidth_Default = 0.115[ms]
Irr_Pwidth_Default_Calc = 0.115[ms]
Irr_Pwidth_Temp1 = 0.115[ms]
Irr_Wurst = FALSE
Decimation_Rate = 0

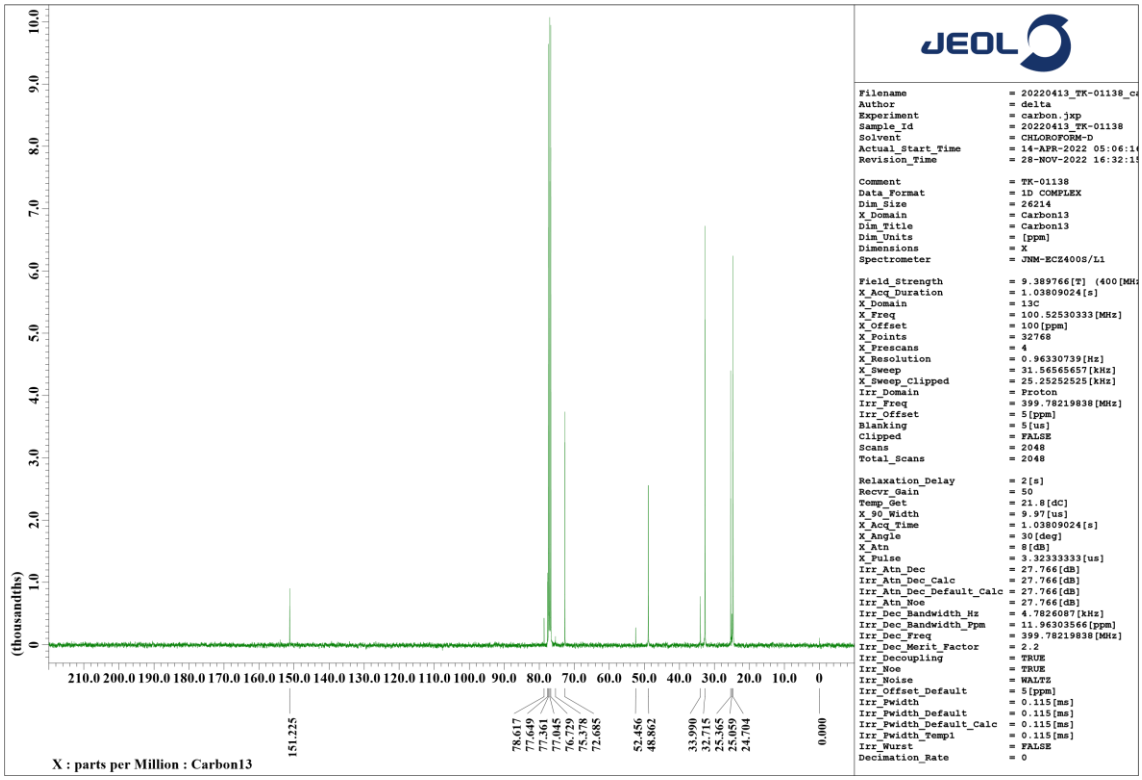

13b
abundance
X : parts per Million : Proton
0.93
1.78
0.21
88.31m
0.76
2.00
3.03
Filename = 20230911_TK-02172_CDCl3
Author = delta
Experiment = proton.jxp
Sample_Id = 20230911_TK-02172_CDCl3
Solvent = CHLOROFORM-D
Actual_Start_Time = 11-SEP-2023 20:30:56
Revision_Time = 17-JUL-2024 18:53:07
Comment = TK-02172
Data_Format = 1D COMPLEX
Dim_Size = 104858
X_Domain = Proton
Dim_Title = Proton
Dim_Units = [ppm]
Dimensions = X
Spectrometer = JNM-ECZ400S/L1
Field_Strength = 9.389766[T] (400[MHz])
X_Acq_Duration = 2.18628096[s]
X_Domain = 1H
X_Freq = 399.78219838[MHz]
X_Offset = 5[ppm]
X_Points = 16384
X_Prescans = 1
X_Resolution = 0.45739775[Hz]
X_Sweep = 7.4940048[kHz]
X_Sweep_Clipped = 5.99520384[kHz]
Irr_Domain = Proton
Irr_Freq = 399.78219838[MHz]
Irr_Offset = 5[ppm]
Tri_Domain = Proton
Tri_Freq = 399.78219838[MHz]
Tri_Offset = 5[ppm]
Blanking = 2[us]
Clipped = FALSE
Scans = 16
Total_Scans = 16
Relaxation_Delay = 5[s]
Recvr_Gain = 46
Temp_Get = 22.8[dC]
X_90_Width = 6.4[us]
X_Acq_Time = 2.18628096[s]
X_Angle = 45[deg]
X_Atn = 2.4[dB]
X_Pulse = 3.2[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Loop = 500
Dante_Presat = FALSE
Decimation_Rate = 0
Initial_Wait = 1[s]
Phase = (0, 90, 270, 180, 180,
Presat_Time = 5[s]
Presat_Time_Flag = FALSE
Relaxation_Delay_Calc = 0[s]
Relaxation_Delay_Temp = 5[s]
Repetition_Time = 7.18628096[s]

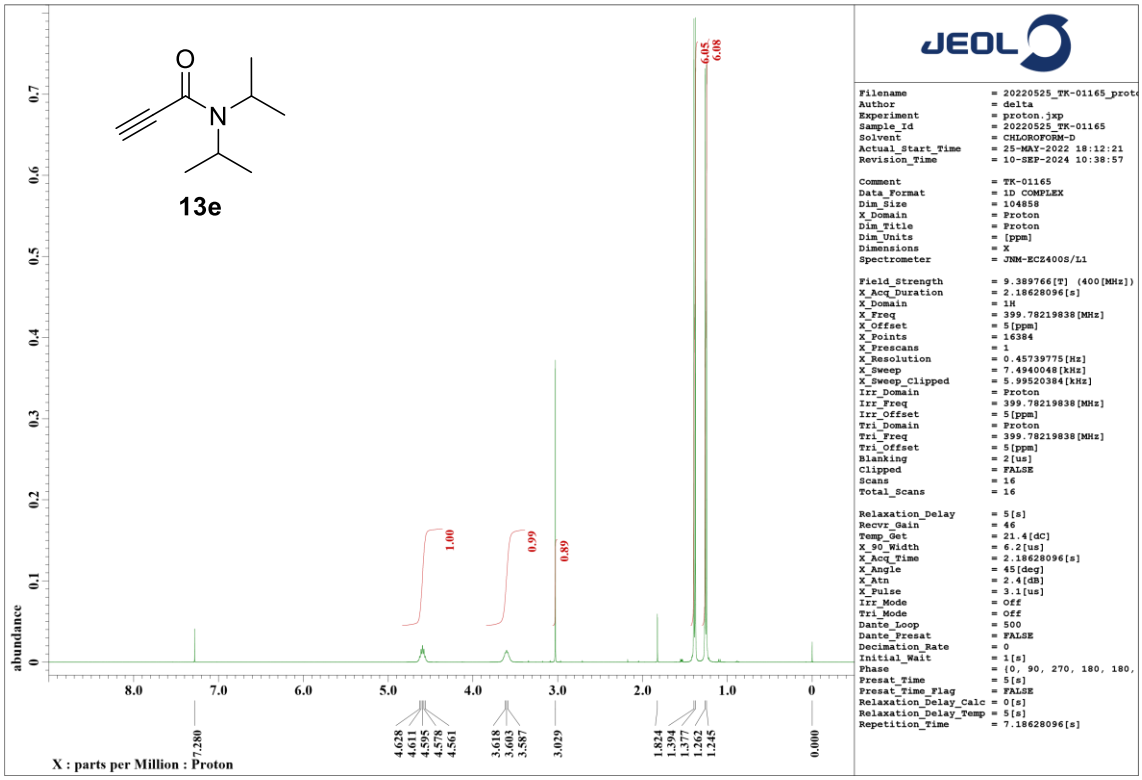

(thousandths)
X : parts per Million : Carbon13
Filename = 20230911_TK-02172_CD
Author = delta
Experiment = carbon.jxp
Sample_Id = 20230911_TK-02172_CD
Solvent = CHLOROFORM-D
Actual_Start_Time = 11-SEP-2023 20:37:12
Revision_Time = 17-JUL-2024 19:15:15
Comment = TK-02172
Data_Format = 1D COMPLEX
Dim_Size = 26214
X_Domain = Carbon13
Dim_Title = Carbon13
Dim_Units = [ppm]
Dimensions = X
Spectrometer = JNM-ECZ400S/L1
Field_Strength = 9.389766[T] (400[MHz
X_Acq_Duration = 1.03809024[s]
X_Domain = 13C
X_Freq = 100.52530333[MHz]
X_Offset = 100[ppm]
X_Points = 32768
X_Prescans = 4
X_Resolution = 0.96330739[Hz]
X_Sweep = 31.56565657[kHz]
X_Sweep_Clipped = 25.25252525[kHz]
Irr_Domain = Proton
Irr_Freq = 399.78219838[MHz]
Irr_Offset = 5[ppm]
Blanking = 5[us]
Clipped = FALSE
Scans = 4096
Total_Scans = 4096
Relaxation_Delay = 2[s]
Recvr_Gain = 50
Temp_Get = 22.8[dC]
X_90_Width = 10.02[us]
X_Acq_Time = 1.03809024[s]
X_Angle = 30[deg]
X_Atn = 8[dB]
X_Pulse = 3.34[us]
Irr_Atn_Dec = 27.49[dB]
Irr_Atn_Dec_Calc = 27.49[dB]
Irr_Atn_Dec_Default_Calc = 27.49[dB]
Irr_Atn_Noe = 27.49[dB]
Irr_Dec_Bandwidth_Hz = 4.78260087[kHz]
Irr_Dec_Bandwidth_Ppm = 11.96303566[ppm]
Irr_Dec_Freq = 399.78219838[MHz]
Irr_Dec_Merit_Factor = 2.2
Irr_Decoupling = TRUE
Irr_Noe = TRUE
Irr_Noise = WALTZ
Irr_Offset_Default = 5[ppm]
Irr_Pwidth = 0.115[ms]
Irr_Pwidth_Default = 0.115[ms]
Irr_Pwidth_Default_Calc = 0.115[ms]
Irr_Pwidth_Temp1 = 0.115[ms]
Irr_Wurst = FALSE
Decimation_Rate = 0

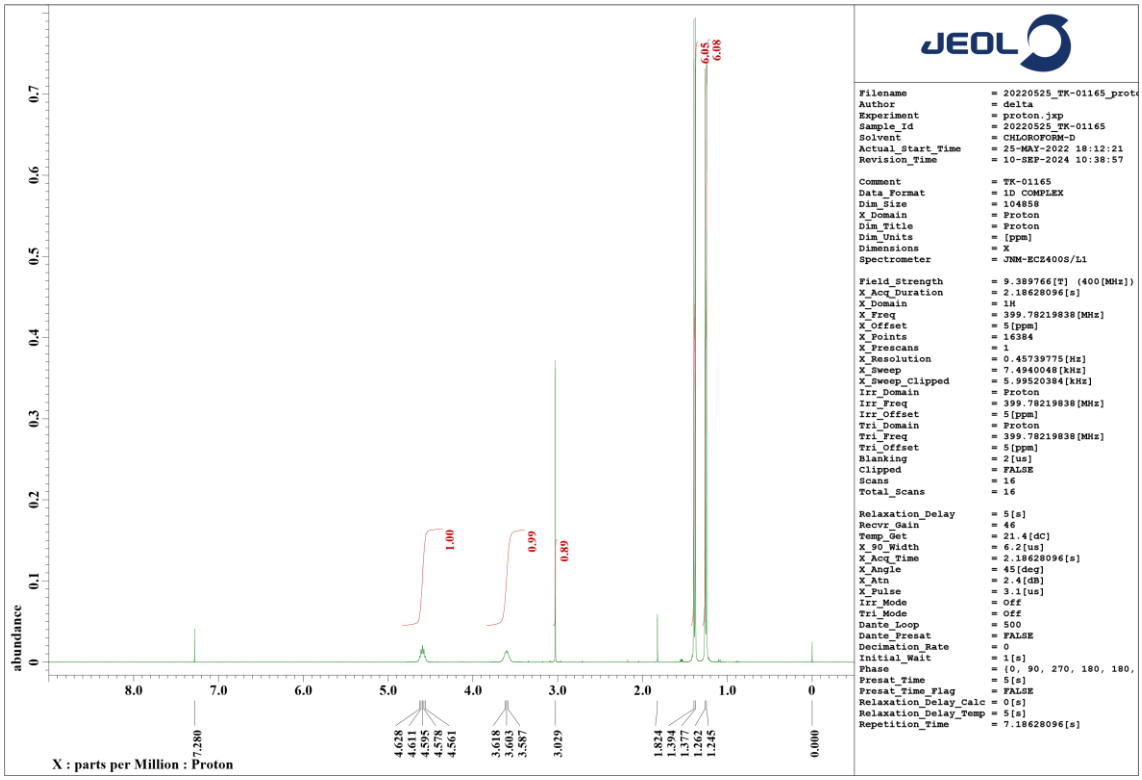

13c
abundance
X : parts per Million : Proton
5.71
1.00
0.95
0.81
0.59
84.53m
7.272
5.787
4.151
4.147
4.134
4.131
4.118
4.114
4.101
4.098
3.103
2.754
1.693
1.681
1.256
1.228
1.202
1.186
0.000
Filename = 20220614_TK-01173_prot
Author = delta
Experiment = proton.jxp
Sample_Id = 20220614_TK-01173
Solvent = CHLOROFORM-D
Actual_Start_Time = 15-JUN-2022 00:03:20
Revision_Time = 10-SEP-2024 10:19:57
Comment = TK-01173
Data_Format = 1D COMPLEX
Dim_Size = 104858
X_Domain = Proton
Dim_Title = Proton
Dim_Units = [ppm]
Dimensions = X
Spectrometer = JNM-ECZ400S/L1
Field_Strength = 9.389766[T] (400[MHz])
X_Acq_Duration = 2.18628096[s]
X_Domain = 1H
X_Freq = 399.78219838[MHz]
X_Offset = 5[ppm]
X_Points = 16384
X_Prescans = 1
X_Resolution = 0.45739775[Hz]
X_Sweep = 7.4940048[kHz]
X_Sweep_Clipped = 5.99520384[kHz]
Irr_Domain = Proton
Irr_Freq = 399.78219838[MHz]
Irr_Offset = 5[ppm]
Tri_Domain = Proton
Tri_Freq = 399.78219838[MHz]
Tri_Offset = 5[ppm]
Blanking = 2[us]
Clipped = FALSE
Scans = 16
Total_Scans = 16
Relaxation_Delay = 5[s]
Recvr_Gain = 56
Temp_Get = 21.6[dC]
X_90_Width = 6.2[us]
X_Acq_Time = 2.18628096[s]
X_Angle = 45[deg]
X_Atn = 2.4[dB]
X_Pulse = 3.1[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Loop = 500
Dante_Presat = FALSE
Decimation_Rate = 0
Initial_Wait = 1[s]
Phase = (0, 90, 270, 180, 180,
Presat_Time = 5[s]
Presat_Time_Flag = FALSE
Relaxation_Delay_Calc = 0[s]
Relaxation_Delay_Temp = 5[s]
Repetition_Time = 7.18628096[s]

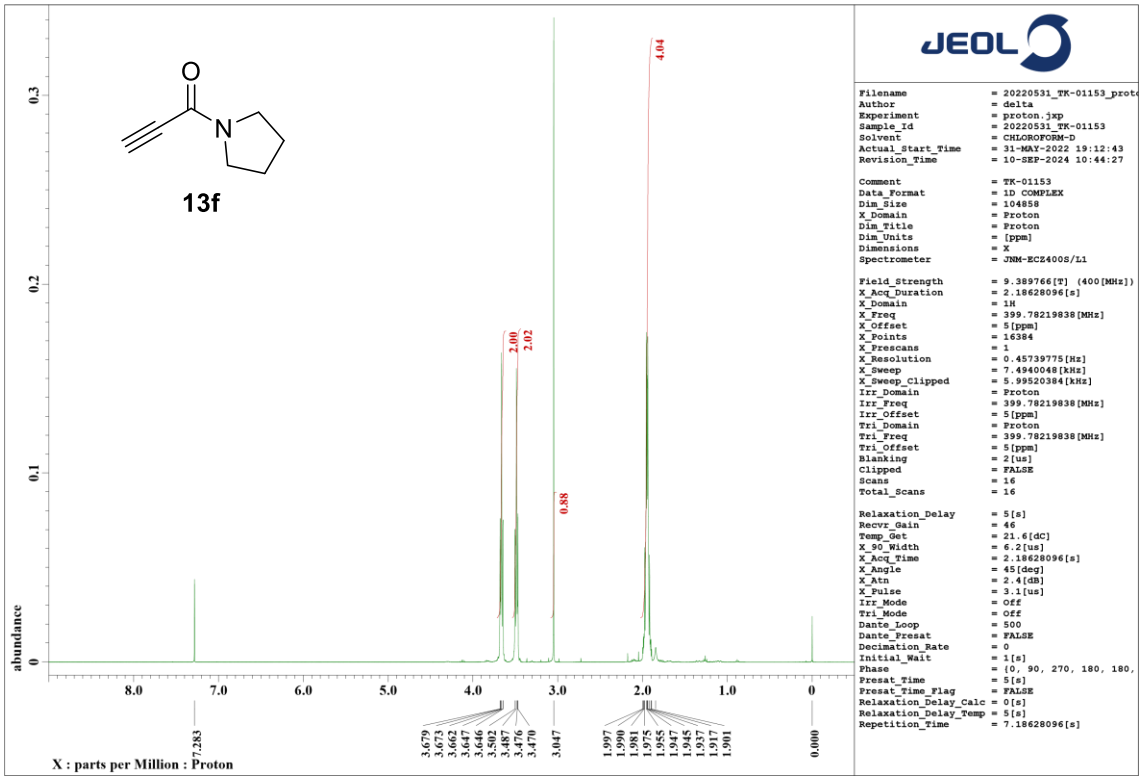

(thousandths)
X : parts per Million : Carbon13
151.257
78.763
77.537
77.316
77.000
76.684
72.573
45.684
42.119
23.682
22.369
Filename = 20220614_TK-01173_c
Author = delta
Experiment = carbon.jxp
Sample_Id = 20220614_TK-01173
Solvent = CHLOROFORM-D
Actual_Start_Time = 15-JUN-2022 00:07:4
Revision_Time = 10-SEP-2024 10:21:5
Comment = TK-01173
Data_Format = 1D COMPLEX
Dim_Size = 26214
X_Domain = Carbon13
Dim_Title = Carbon13
Dim_Units = [ppm]
Dimensions = X
Spectrometer = JNM-ECZ400S/L1
Field_Strength = 9.389766[T] (400[MH
X_Acq_Duration = 1.03809024[s]
X_Domain = 13C
X_Freq = 100.52530333[MHz]
X_Offset = 100[ppm]
X_Points = 32768
X_Prescans = 4
X_Resolution = 0.96330739[Hz]
X_Sweep = 31.56565657[kHz]
X_Sweep_Clipped = 25.25252525[kHz]
Irr_Domain = Proton
Irr_Freq = 399.78219838[MHz]
Irr_Offset = 5[ppm]
Blanking = 5[us]
Clipped = FALSE
Scans = 4096
Total_Scans = 4096
Relaxation_Delay = 2[s]
Recvr_Gain = 50
Temp_Get = 21.5[dC]
X_90_Width = 9.97[us]
X_Acq_Time = 1.03809024[s]
X_Angle = 30[deg]
X_Atn = 8[dB]
X_Pulse = 3.32333333[us]
Irr_Atn_Dec = 27.766[dB]
Irr_Atn_Dec_Calc = 27.766[dB]
Irr_Atn_Dec_Default_Calc = 27.766[dB]
Irr_Atn_Noe = 27.766[dB]
Irr_Dec_Bandwidth_Hz = 4.7826087[kHz]
Irr_Dec_Bandwidth_Ppm = 11.96303566[ppm]
Irr_Dec_Freq = 399.78219838[MHz]
Irr_Dec_Merit_Factor = 2.2
Irr_Decoupling = TRUE
Irr_Noe = TRUE
Irr_Noise = WALTZ
Irr_Offset_Default = 5[ppm]
Irr_Pwidth = 0.115[ms]
Irr_Pwidth_Default = 0.115[ms]
Irr_Pwidth_Default_Calc = 0.115[ms]
Irr_Pwidth_Temp1 = 0.115[ms]
Irr_Wurst = FALSE
Decimation_Rate = 0

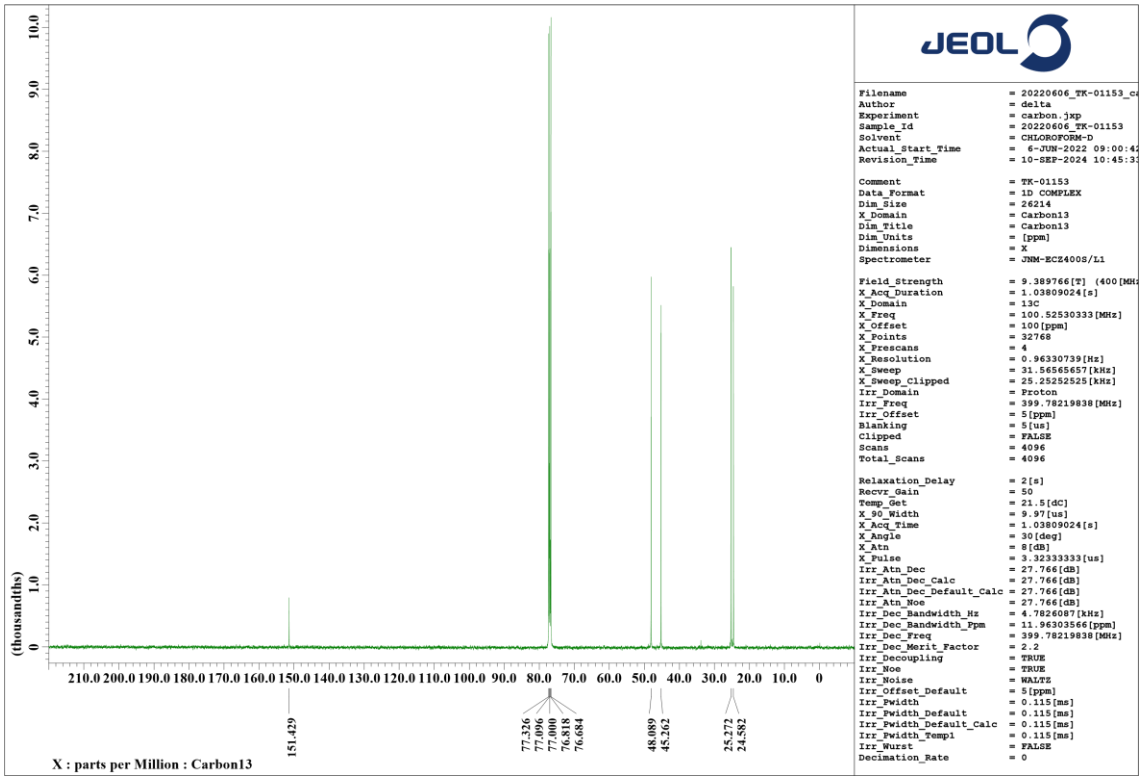

O
N
H
13d
abundance
X : parts per Million : Proton
0.96
1.00
0.79
93.66m
2.10
2.28
2.08
1.00
3.03
Filename = 20220413_TK-01138_prot
Author = delta
Experiment = proton.jxp
Sample_Id = 20220413_TK-01138
Solvent = CHLOROFORM-D
Actual_Start_Time = 14-APR-2022 05:02:47
Revision_Time = 28-NOV-2022 16:37:05
Comment = TK-01138
Data_Format = 1D COMPLEX
Dim_Size = 104858
X_Domain = Proton
Dim_Title = Proton
Dim_Units = [ppm]
Dimensions = X
Spectrometer = JNM-ECZ400S/L1
Field_Strength = 9.389766[T] (400[MHz])
X_Acq_Duration = 2.18628096[s]
X_Domain = 1H
X_Freq = 399.78219838[MHz]
X_Offset = 5[ppm]
X_Points = 16384
X_Prescans = 1
X_Resolution = 0.45739775[Hz]
X_Sweep = 7.4940048[kHz]
X_Sweep_Clipped = 5.99520384[kHz]
Irr_Domain = Proton
Irr_Freq = 399.78219838[MHz]
Irr_Offset = 5[ppm]
Tri_Domain = Proton
Tri_Freq = 399.78219838[MHz]
Tri_Offset = 5[ppm]
Blanking = 2[us]
Clipped = FALSE
Scans = 16
Total_Scans = 16
Relaxation_Delay = 5[s]
Recvr_Gain = 46
Temp_Get = 21.8[dC]
X_90_Width = 6.2[us]
X_Acq_Time = 2.18628096[s]
X_Angle = 45[deg]
X_Atn = 2.4[dB]
X_Pulse = 3.1[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Loop = 500
Dante_Presat = FALSE
Decimation_Rate = 0
Initial_Wait = 1[s]
Phase = (0, 90, 270, 180, 180,
Presat_Time = 5[s]
Presat_Time_Flag = FALSE
Relaxation_Delay_Calc = 0[s]
Relaxation_Delay_Temp = 5[s]
Repetition_Time = 7.18628096[s]

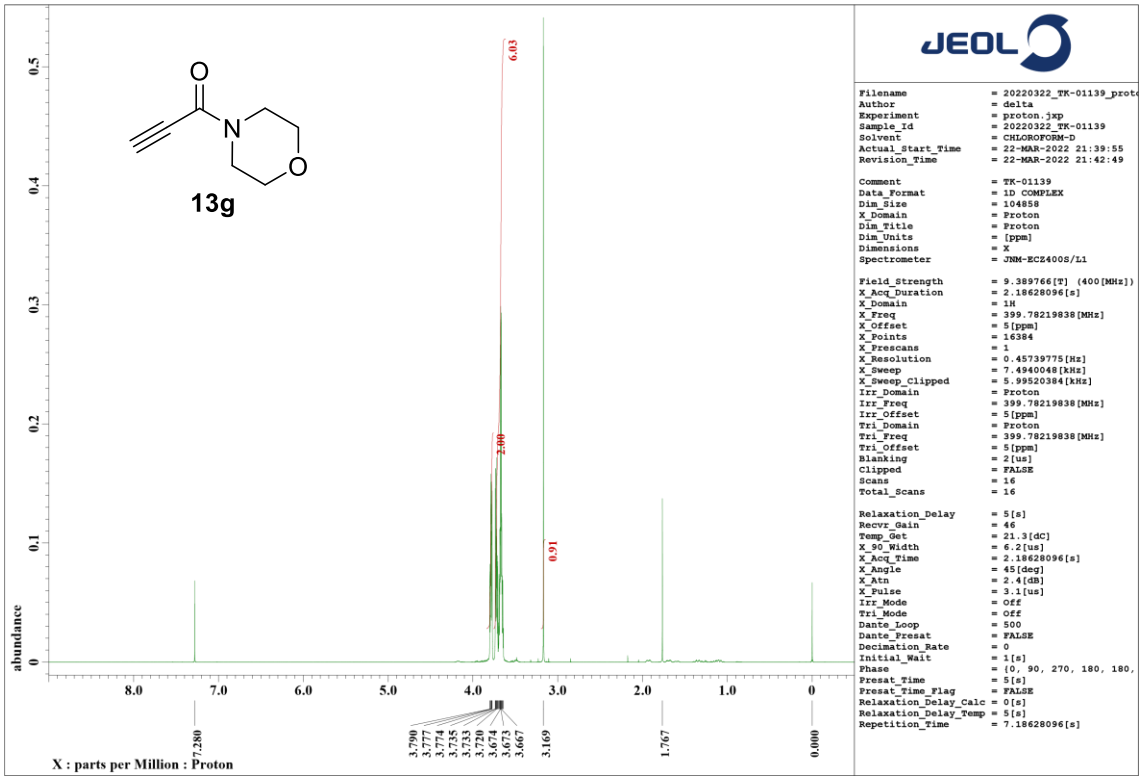

(thousandths)
X : parts per Million : Carbon13
Filename = 20220413_TK-01138_c
Author = delta
Experiment = carbon.jxp
Sample_Id = 20220413_TK-01138
Solvent = CHLOROFORM-D
Actual_Start_Time = 14-APR-2022 05:06:1
Revision_Time = 28-NOV-2022 16:32:1
Comment = TK-01138
Data_Format = 1D COMPLEX
Dim_Size = 26214
X_Domain = Carbon13
Dim_Title = Carbon13
Dim_Units = [ppm]
Dimensions = X
Spectrometer = JNM-ECZ400S/L1
Field_Strength = 9.389766[T] (400[MH
X_Acq_Duration = 1.03809024[s]
X_Domain = 13C
X_Freq = 100.52530333[MHz]
X_Offset = 100[ppm]
X_Points = 32768
X_Prescans = 4
X_Resolution = 0.96330739[Hz]
X_Sweep = 31.56565657[kHz]
X_Sweep_Clipped = 25.25252525[kHz]
Irr_Domain = Proton
Irr_Freq = 399.78219838[MHz]
Irr_Offset = 5[ppm]
Blanking = 5[us]
Clipped = FALSE
Scans = 2048
Total_Scans = 2048
Relaxation_Delay = 2[s]
Recvr_Gain = 50
Temp_Get = 21.8[dC]
X_90_Width = 9.97[us]
X_Acq_Time = 1.03809024[s]
X_Angle = 30[deg]
X_Atn = 8[dB]
X_Pulse = 3.32333333[us]
Irr_Atn_Dec = 27.766[dB]
Irr_Atn_Dec_Calc = 27.766[dB]
Irr_Atn_Dec_Default_Calc = 27.766[dB]
Irr_Atn_Noe = 27.766[dB]
Irr_Dec_Bandwidth_Hz = 4.7826087[kHz]
Irr_Dec_Bandwidth_Ppm = 11.96303566[ppm]
Irr_Dec_Freq = 399.78219838[MHz]
Irr_Dec_Merit_Factor = 2.2
Irr_Decoupling = TRUE
Irr_Noe = TRUE
Irr_Noise = WALTZ
Irr_Offset_Default = 5[ppm]
Irr_Pwidth = 0.115[ms]
Irr_Pwidth_Default = 0.115[ms]
Irr_Pwidth_Default_Calc = 0.115[ms]
Irr_Pwidth_Temp1 = 0.115[ms]
Irr_Wurst = FALSE
Decimation_Rate = 0

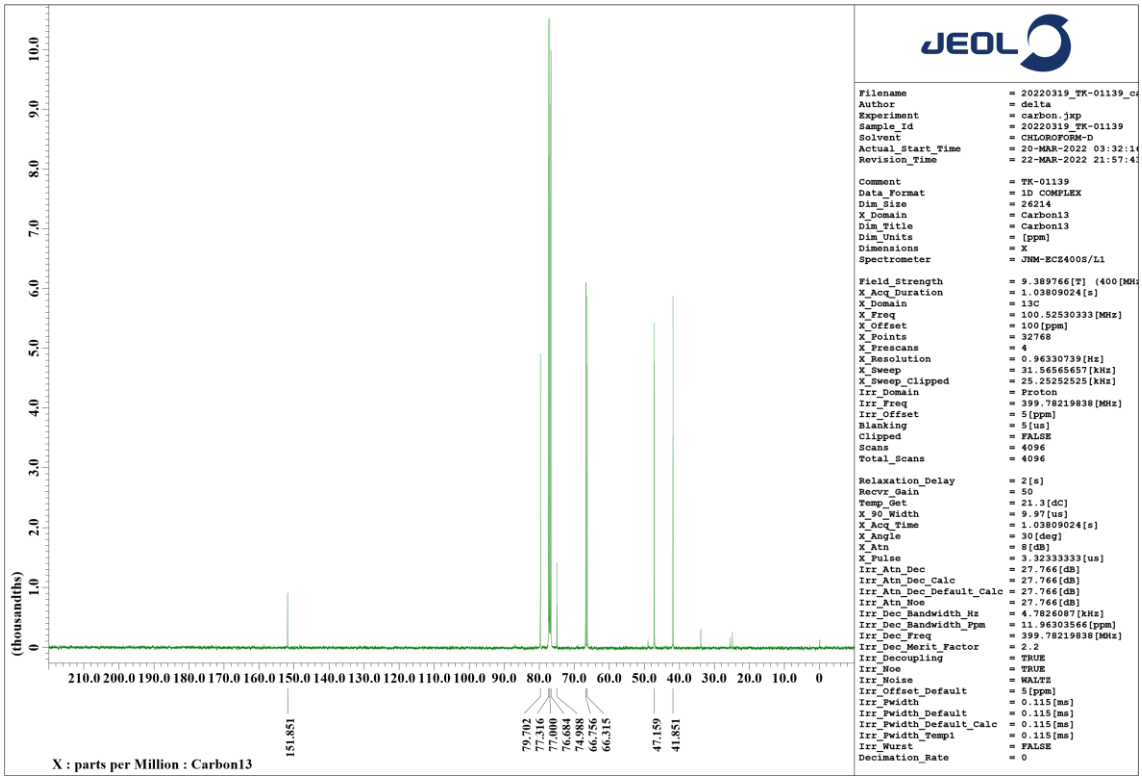

13e
6.05
6.08
1.00
0.99
0.89
abundance
X : parts per Million : Proton
7.280
4.628
4.611
4.595
4.578
4.561
3.618
3.603
3.587
3.029
1.824
1.394
1.377
1.262
1.245
0.000
Filename = 20220525_TK-01165_prot
Author = delta
Experiment = proton.jxp
Sample_Id = 20220525_TK-01165
Solvent = CHLOROFORM-D
Actual_Start_Time = 25-MAY-2022 18:12:21
Revision_Time = 10-SEP-2024 10:38:57
Comment = TK-01165
Data_Format = 1D COMPLEX
Dim_Size = 104858
X_Domain = Proton
Dim_Title = Proton
Dim_Units = [ppm]
Dimensions = X
Spectrometer = JNM-ECZ400S/L1
Field_Strength = 9.389766[T] (400[MHz])
X_Acq_Duration = 2.18628096[s]
X_Domain = 1H
X_Freq = 399.78219838[MHz]
X_Offset = 5[ppm]
X_Points = 16384
X_Prescans = 1
X_Resolution = 0.45739775[Hz]
X_Sweep = 7.4940048[kHz]
X_Sweep_Clipped = 5.99520384[kHz]
Irr_Domain = Proton
Irr_Freq = 399.78219838[MHz]
Irr_Offset = 5[ppm]
Tri_Domain = Proton
Tri_Freq = 399.78219838[MHz]
Tri_Offset = 5[ppm]
Blanking = 2[us]
Clipped = FALSE
Scans = 16
Total_Scans = 16
Relaxation_Delay = 5[s]
Recvr_Gain = 46
Temp_Get = 21.4[dC]
X_90_Width = 6.2[us]
X_Acq_Time = 2.18628096[s]
X_Angle = 45[deg]
X_Atn = 2.4[dB]
X_Pulse = 3.1[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Loop = 500
Dante_Presat = FALSE
Decimation_Rate = 0
Initial_Wait = 1[s]
Phase = {0, 90, 270, 180, 180,
Presat_Time = 5[s]
Presat_Time_Flag = FALSE
Relaxation_Delay_Calc = 0[s]
Relaxation_Delay_Temp = 5[s]
Repetition_Time = 7.18628096[s]

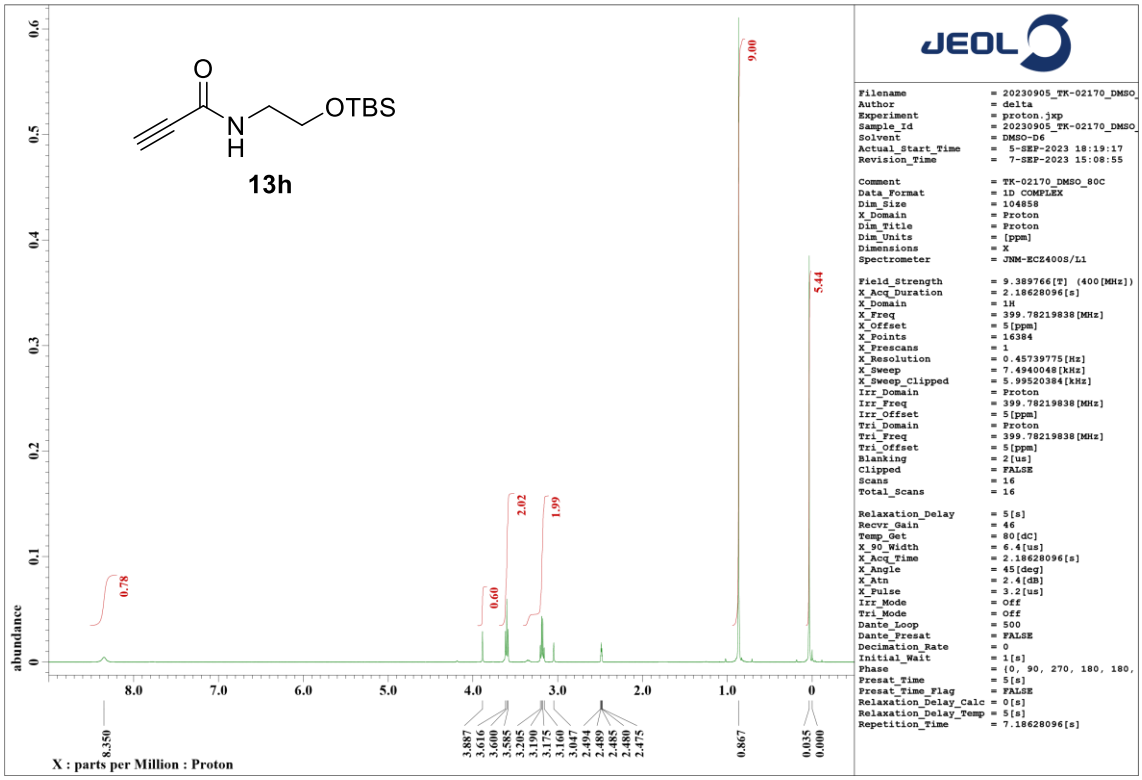

6.05
6.08
1.00
0.99
0.89
abundance
X : parts per Million : Proton
7.280
4.628
4.611
4.595
4.578
4.561
3.618
3.603
3.587
3.029
1.824
1.394
1.377
1.262
1.245
0.000
Filename = 20220525_TK-01165_prot
Author = delta
Experiment = proton.jxp
Sample_Id = 20220525_TK-01165
Solvent = CHLOROFORM-D
Actual_Start_Time = 25-MAY-2022 18:12:21
Revision_Time = 10-SEP-2024 10:38:57
Comment = TK-01165
Data_Format = 1D COMPLEX
Dim_Size = 104858
X_Domain = Proton
Dim_Title = Proton
Dim_Units = [ppm]
Dimensions = X
Spectrometer = JNM-ECZ400S/L1
Field_Strength = 9.389766[T] (400[MHz])
X_Acq_Duration = 2.18628096[s]
X_Domain = 1H
X_Freq = 399.78219838[MHz]
X_Offset = 5[ppm]
X_Points = 16384
X_Prescans = 1
X_Resolution = 0.45739775[Hz]
X_Sweep = 7.4940048[kHz]
X_Sweep_Clipped = 5.99520384[kHz]
Irr_Domain = Proton
Irr_Freq = 399.78219838[MHz]
Irr_Offset = 5[ppm]
Tri_Domain = Proton
Tri_Freq = 399.78219838[MHz]
Tri_Offset = 5[ppm]
Blanking = 2[us]
Clipped = FALSE
Scans = 16
Total_Scans = 16
Relaxation_Delay = 5[s]
Recvr_Gain = 46
Temp_Get = 21.4[dC]
X_90_Width = 6.2[us]
X_Acq_Time = 2.18628096[s]
X_Angle = 45[deg]
X_Atn = 2.4[dB]
X_Pulse = 3.1[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Loop = 500
Dante_Presat = FALSE
Decimation_Rate = 0
Initial_Wait = 1[s]
Phase = {0, 90, 270, 180, 180,
Presat_Time = 5[s]
Presat_Time_Flag = FALSE
Relaxation_Delay_Calc = 0[s]
Relaxation_Delay_Temp = 5[s]
Repetition_Time = 7.18628096[s]

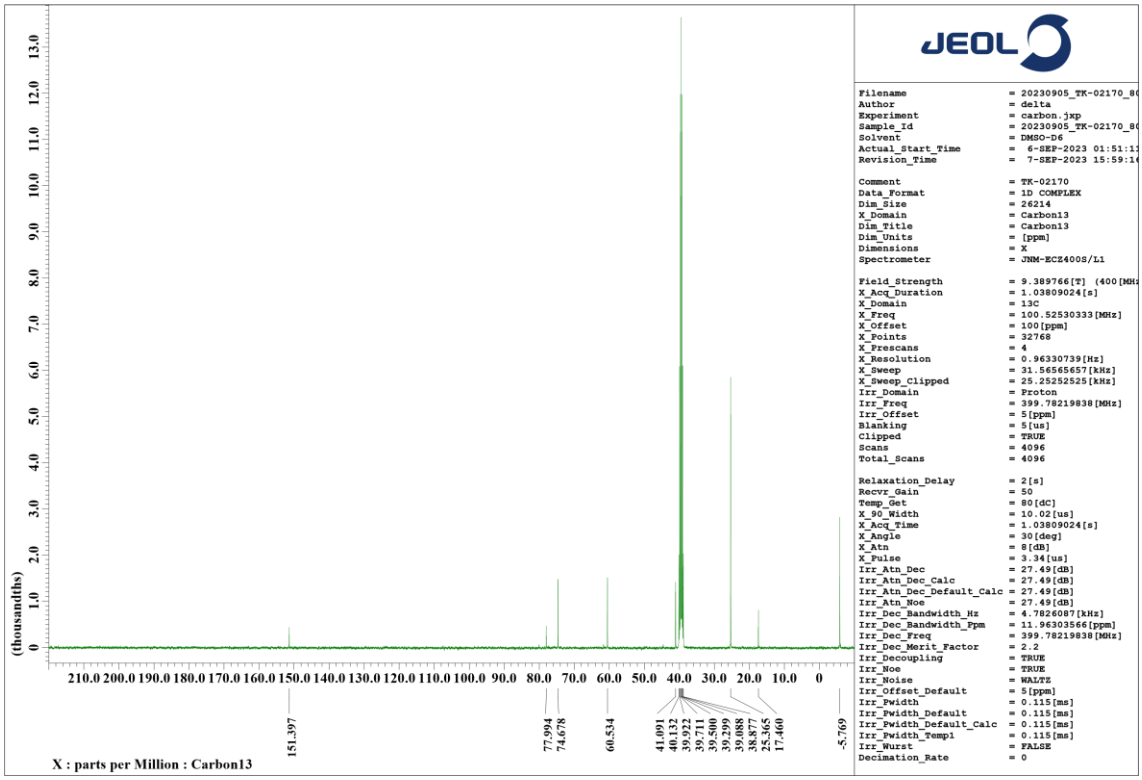

13f
abundance
X : parts per Million : Proton
4.04
2.00
2.02
0.88
7.283
3.679
3.673
3.662
3.647
3.646
3.502
3.487
3.476
3.470
3.047
1.997
1.990
1.981
1.975
1.955
1.947
1.945
1.937
1.917
1.901
0.000
Filename = 20220531_TK-01153_prot
Author = delta
Experiment = proton.jxp
Sample_Id = 20220531_TK-01153
Solvent = CHLOROFORM-D
Actual_Start_Time = 31-MAY-2022 19:12:43
Revision_Time = 10-SEP-2024 10:44:27
Comment = TK-01153
Data_Format = 1D COMPLEX
Dim_Size = 104858
X_Domain = Proton
Dim_Title = Proton
Dim_Units = [ppm]
Dimensions = X
Spectrometer = JNM-ECZ400S/L1
Field_Strength = 9.389766[T] (400[MHz])
X_Acq_Duration = 2.18628096[s]
X_Domain = 1H
X_Freq = 399.78219838[MHz]
X_Offset = 5[ppm]
X_Points = 16384
X_Prescans = 1
X_Resolution = 0.45739775[Hz]
X_Sweep = 7.4940048[kHz]
X_Sweep_Clipped = 5.99520384[kHz]
Irr_Domain = Proton
Irr_Freq = 399.78219838[MHz]
Irr_Offset = 5[ppm]
Tri_Domain = Proton
Tri_Freq = 399.78219838[MHz]
Tri_Offset = 5[ppm]
Blanking = 2[us]
Clipped = FALSE
Scans = 16
Total_Scans = 16
Relaxation_Delay = 5[s]
Recvr_Gain = 46
Temp_Get = 21.6[dC]
X_90_Width = 6.2[us]
X_Acq_Time = 2.18628096[s]
X_Angle = 45[deg]
X_Atn = 2.4[dB]
X_Pulse = 3.1[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Loop = 500
Dante_Presat = FALSE
Decimation_Rate = 0
Initial_Wait = 1[s]
Phase = (0, 90, 270, 180, 180,
Presat_Time = 5[s]
Presat_Time_Flag = FALSE
Relaxation_Delay_Calc = 0[s]
Relaxation_Delay_Temp = 5[s]
Repetition_Time = 7.18628096[s]

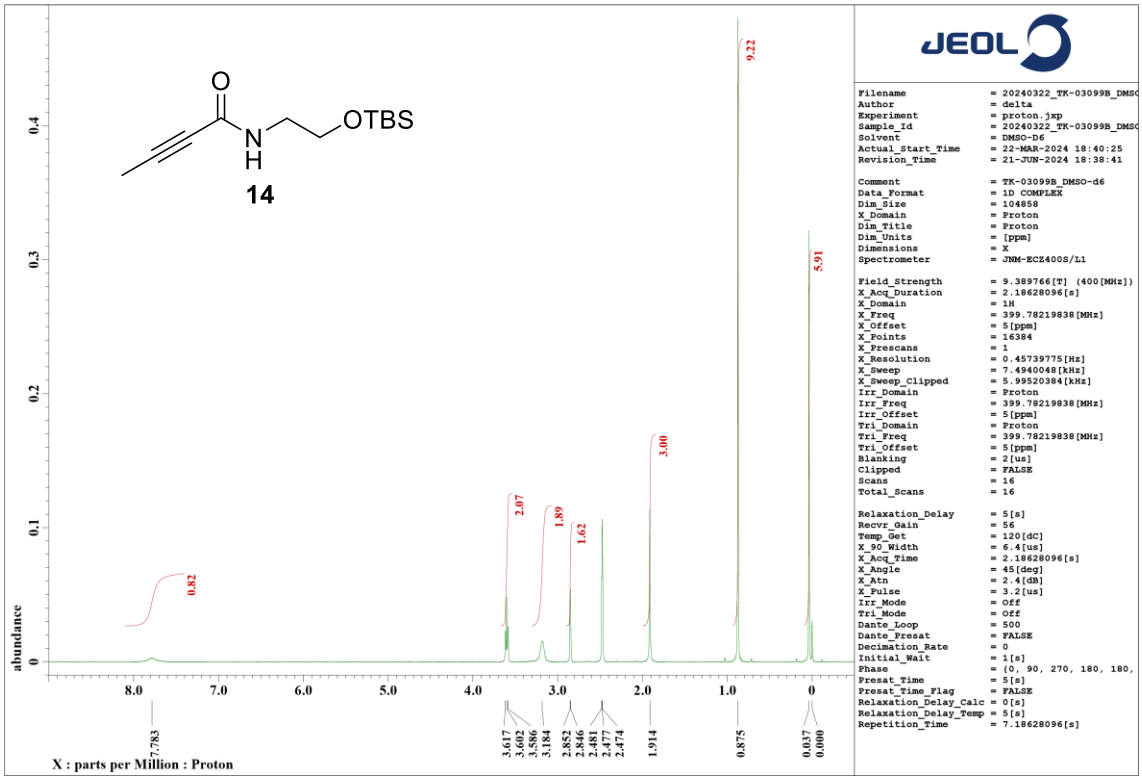

(thousandths)
X : parts per Million : Carbon13
151.429
77.326
77.096
77.000
76.818
76.684
48.089
45.262
25.272
24.582
Filename = 20220606_TK-01153_c
Author = delta
Experiment = carbon.jxp
Sample_Id = 20220606_TK-01153
Solvent = CHLOROFORM-D
Actual_Start_Time = 6-JUN-2022 09:00:4
Revision_Time = 10-SEP-2024 10:45:3
Comment = TK-01153
Data_Format = 1D COMPLEX
Dim_Size = 26214
X_Domain = Carbon13
Dim_Title = Carbon13
Dim_Units = [ppm]
Dimensions = X
Spectrometer = JNM-ECZ400S/L1
Field_Strength = 9.389766[T] (400[MH
X_Acq_Duration = 1.03809024[s]
X_Domain = 13C
X_Freq = 100.52530333[MHz]
X_Offset = 100[ppm]
X_Points = 32768
X_Prescans = 4
X_Resolution = 0.96330739[Hz]
X_Sweep = 31.56565657[kHz]
X_Sweep_Clipped = 25.25252525[kHz]
Irr_Domain = Proton
Irr_Freq = 399.78219838[MHz]
Irr_Offset = 5[ppm]
Blanking = 5[us]
Clipped = FALSE
Scans = 4096
Total_Scans = 4096
Relaxation_Delay = 2[s]
Recvr_Gain = 50
Temp_Get = 21.5[dC]
X_90_Width = 9.97[us]
X_Acq_Time = 1.03809024[s]
X_Angle = 30[deg]
X_Atn = 8[dB]
X_Pulse = 3.32333333[us]
Irr_Atn_Dec = 27.766[dB]
Irr_Atn_Dec_Calc = 27.766[dB]
Irr_Atn_Dec_Default_Calc = 27.766[dB]
Irr_Atn_Noe = 27.766[dB]
Irr_Dec_Bandwidth_Hz = 4.7826087[kHz]
Irr_Dec_Bandwidth_Ppm = 11.96303566[ppm]
Irr_Dec_Freq = 399.78219838[MHz]
Irr_Dec_Merit_Factor = 2.2
Irr_Decoupling = TRUE
Irr_Noe = TRUE
Irr_Noise = WALTZ
Irr_Offset_Default = 5[ppm]
Irr_Pwidth = 0.115[ms]
Irr_Pwidth_Default = 0.115[ms]
Irr_Pwidth_Default_Calc = 0.115[ms]
Irr_Pwidth_Temp1 = 0.115[ms]
Irr_Wurst = FALSE
Decimation_Rate = 0

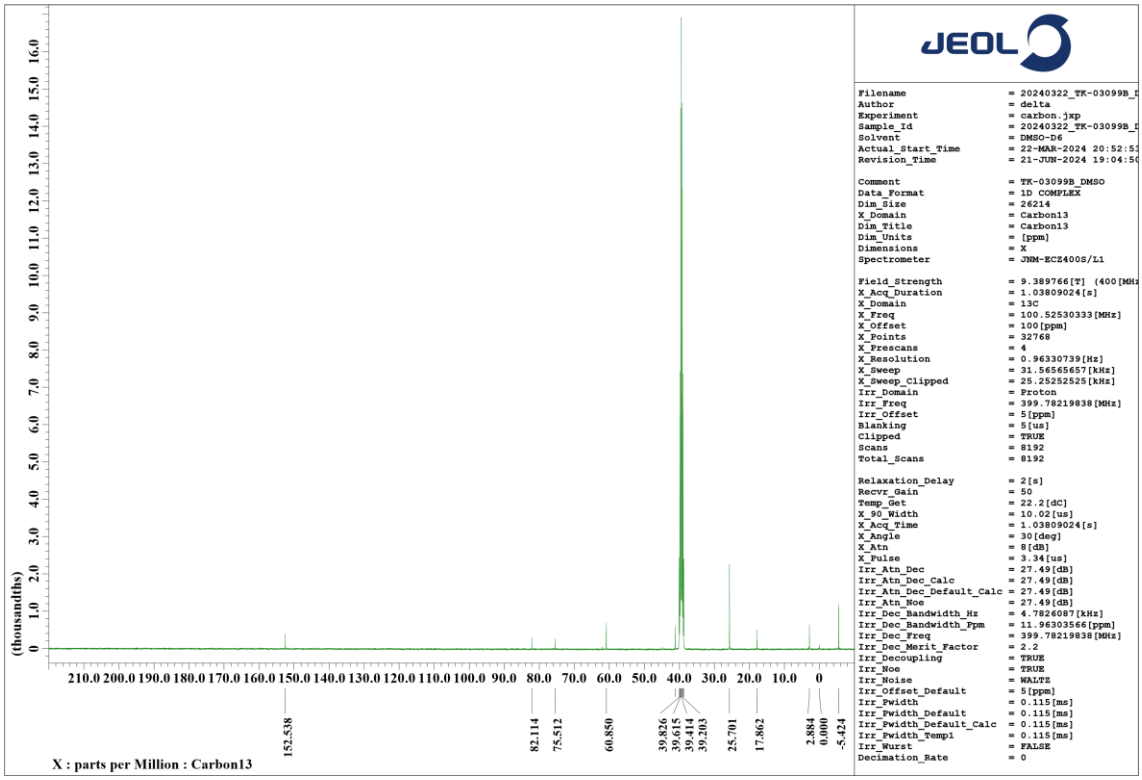

13g
6.03
2.00
0.91
abundance
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
7.280
3.790
3.777
3.774
3.735
3.733
3.720
3.674
3.673
3.667
3.169
1.767
0.000
X : parts per Million : Proton
JEOL
Filename = 20220322_TK-01139_prot
Author = delta
Experiment = proton.jxp
Sample_Id = 20220322_TK-01139
Solvent = CHLOROFORM-D
Actual_Start_Time = 22-MAR-2022 21:39:55
Revision_Time = 22-MAR-2022 21:42:49
Comment = TK-01139
Data_Format = 1D COMPLEX
Dim_Size = 104858
X_Domain = Proton
Dim_Title = Proton
Dim_Units = [ppm]
Dimensions = X
Spectrometer = JNM-ECZ400S/L1
Field_Strength = 9.389766[T] (400[MHz])
X_Acq_Duration = 2.18628096[s]
X_Domain = 1H
X_Freq = 399.78219838[MHz]
X_Offset = 5[ppm]
X_Points = 16384
X_Prescans = 1
X_Resolution = 0.45739775[Hz]
X_Sweep = 7.4940048[kHz]
X_Sweep_Clipped = 5.99520384[kHz]
Irr_Domain = Proton
Irr_Freq = 399.78219838[MHz]
Irr_Offset = 5[ppm]
Tri_Domain = Proton
Tri_Freq = 399.78219838[MHz]
Tri_Offset = 5[ppm]
Blanking = 2[us]
Clipped = FALSE
Scans = 16
Total_Scans = 16
Relaxation_Delay = 5[s]
Recvr_Gain = 46
Temp_Get = 21.3[dC]
X_90_Width = 6.2[us]
X_Acq_Time = 2.18628096[s]
X_Angle = 45[deg]
X_Atn = 2.4[dB]
X_Pulse = 3.1[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Loop = 500
Dante_Presat = FALSE
Decimation_Rate = 0
Initial_Wait = 1[s]
Phase = (0, 90, 270, 180, 180,
Presat_Time = 5[s]
Presat_Time_Flag = FALSE
Relaxation_Delay_Calc = 0[s]
Relaxation_Delay_Temp = 5[s]
Repetition_Time = 7.18628096[s]

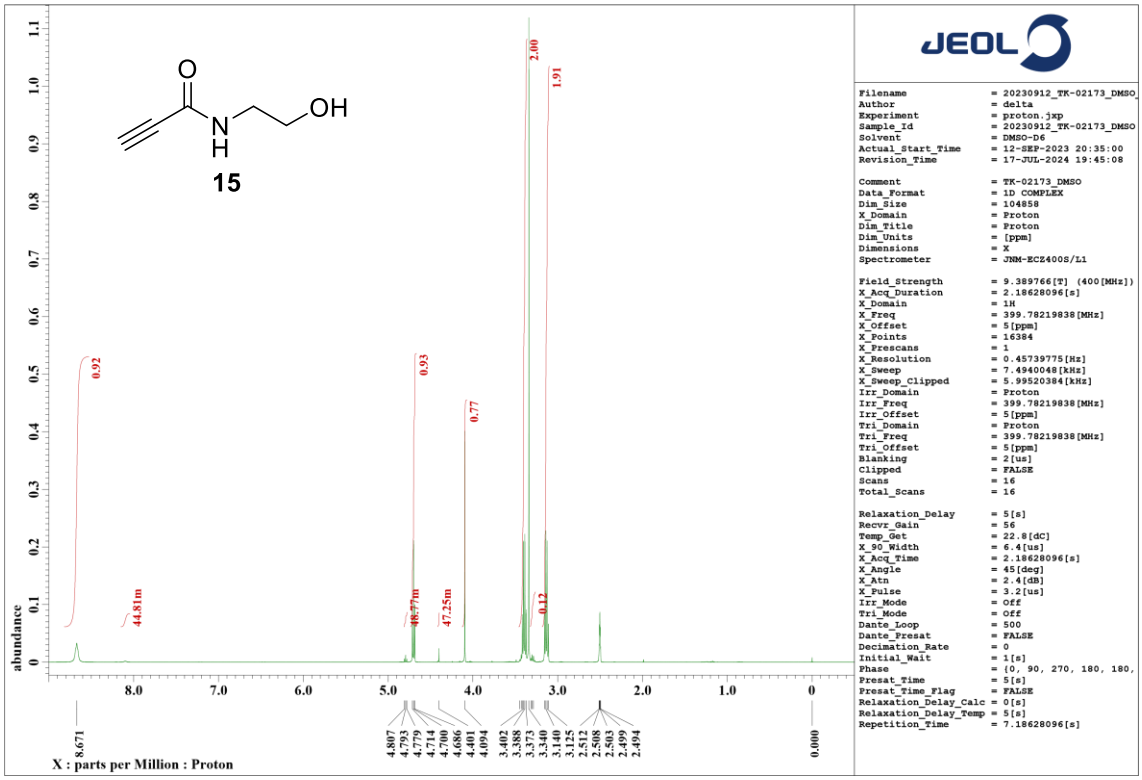

(thousandths)
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
210.0 200.0 190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0
151.851
79.702
77.316
77.000
76.684
74.988
66.756
66.315
47.159
41.851
X : parts per Million : Carbon13
JEOL
Filename = 20220319_TK-01139_c
Author = delta
Experiment = carbon.jxp
Sample_Id = 20220319_TK-01139
Solvent = CHLOROFORM-D
Actual_Start_Time = 20-MAR-2022 03:32:1
Revision_Time = 22-MAR-2022 21:57:4
Comment = TK-01139
Data_Format = 1D COMPLEX
Dim_Size = 26214
X_Domain = Carbon13
Dim_Title = Carbon13
Dim_Units = [ppm]
Dimensions = X
Spectrometer = JNM-ECZ400S/L1
Field_Strength = 9.389766[T] (400[MH
X_Acq_Duration = 1.03809024[s]
X_Domain = 13C
X_Freq = 100.52530333[MHz]
X_Offset = 100[ppm]
X_Points = 32768
X_Prescans = 4
X_Resolution = 0.96330739[Hz]
X_Sweep = 31.56565657[kHz]
X_Sweep_Clipped = 25.25252525[kHz]
Irr_Domain = Proton
Irr_Freq = 399.78219838[MHz]
Irr_Offset = 5[ppm]
Blanking = 5[us]
Clipped = FALSE
Scans = 4096
Total_Scans = 4096
Relaxation_Delay = 2[s]
Recvr_Gain = 50
Temp_Get = 21.3[dC]
X_90_Width = 9.97[us]
X_Acq_Time = 1.03809024[s]
X_Angle = 30[deg]
X_Atn = 8[dB]
X_Pulse = 3.32333333[us]
Irr_Atn_Dec = 27.766[dB]
Irr_Atn_Dec_Calc = 27.766[dB]
Irr_Atn_Dec_Default_Calc = 27.766[dB]
Irr_Atn_Noe = 27.766[dB]
Irr_Dec_Bandwidth_Hz = 4.7826087[kHz]
Irr_Dec_Bandwidth_Ppm = 11.96303566[ppm]
Irr_Dec_Freq = 399.78219838[MHz]
Irr_Dec_Merit_Factor = 2.2
Irr_Decoupling = TRUE
Irr_Noe = TRUE
Irr_Noise = WALTZ
Irr_Offset_Default = 5[ppm]
Irr_Pwidth = 0.115[ms]
Irr_Pwidth_Default = 0.115[ms]
Irr_Pwidth_Default_Calc = 0.115[ms]
Irr_Pwidth_Temp1 = 0.115[ms]
Irr_Wurst = FALSE
Decimation_Rate = 0

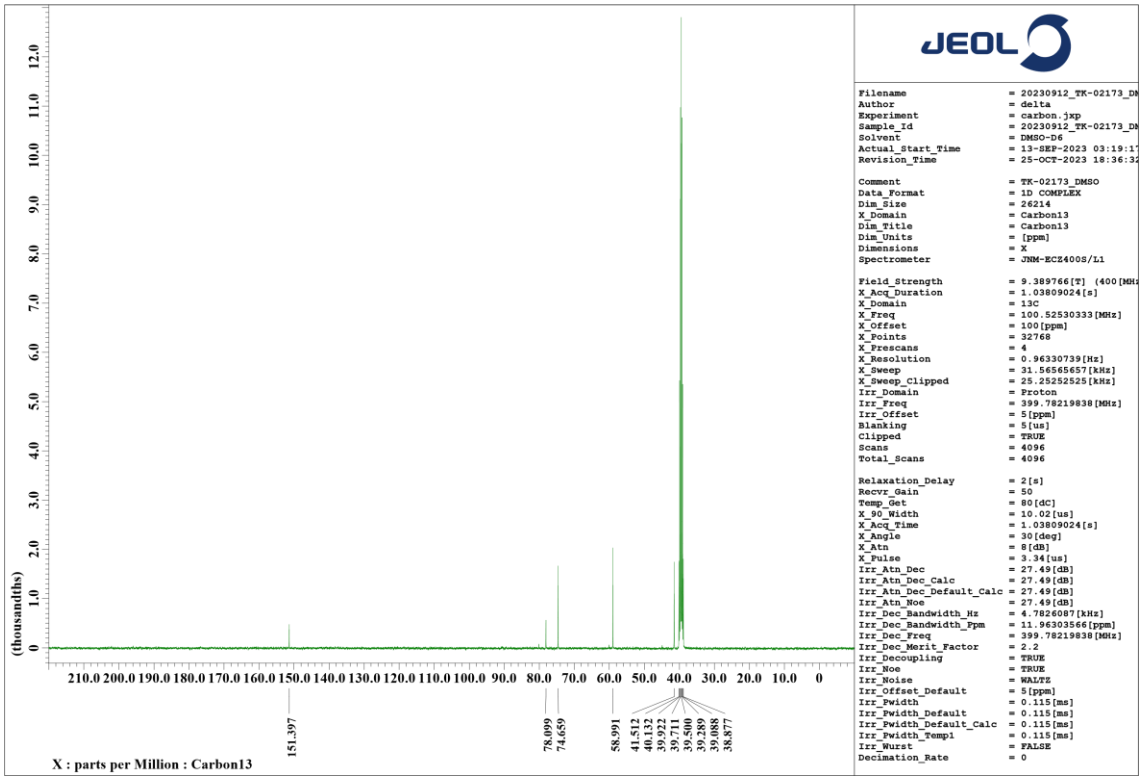

O
N
H
OTBS
13h
abundance
X : parts per Million : Proton
JEOL
Filename = 20230905_TK-02170_DMSO_
Author = delta
Experiment = proton.jxp
Sample_Id = 20230905_TK-02170_DMSO_
Solvent = DMSO-D6
Actual_Start_Time = 5-SEP-2023 18:19:17
Revision_Time = 7-SEP-2023 15:08:55
Comment = TK-02170_DMSO_80C
Data_Format = 1D COMPLEX
Dim_Size = 104858
X_Domain = Proton
Dim_Title = Proton
Dim_Units = [ppm]
Dimensions = X
Spectrometer = JNM-ECZ400S/L1
Field_Strength = 9.389766[T] (400[MHz])
X_Acq_Duration = 2.18628096[s]
X_Domain = 1H
X_Freq = 399.78219838[MHz]
X_Offset = 5[ppm]
X_Points = 16384
X_Prescans = 1
X_Resolution = 0.45739775[Hz]
X_Sweep = 7.4940048[kHz]
X_Sweep_Clipped = 5.99520384[kHz]
Irr_Domain = Proton
Irr_Freq = 399.78219838[MHz]
Irr_Offset = 5[ppm]
Tri_Domain = Proton
Tri_Freq = 399.78219838[MHz]
Tri_Offset = 5[ppm]
Blanking = 2[us]
Clipped = FALSE
Scans = 16
Total_Scans = 16
Relaxation_Delay = 5[s]
Recvr_Gain = 46
Temp_Get = 80[dC]
X_90_Width = 6.4[us]
X_Acq_Time = 2.18628096[s]
X_Angle = 45[deg]
X_Atn = 2.4[dB]
X_Pulse = 3.2[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Loop = 500
Dante_Presat = FALSE
Decimation_Rate = 0
Initial_Wait = 1[s]
Phase = (0, 90, 270, 180, 180,
Presat_Time = 5[s]
Presat_Time_Flag = FALSE
Relaxation_Delay_Calc = 0[s]
Relaxation_Delay_Temp = 5[s]
Repetition_Time = 7.18628096[s]

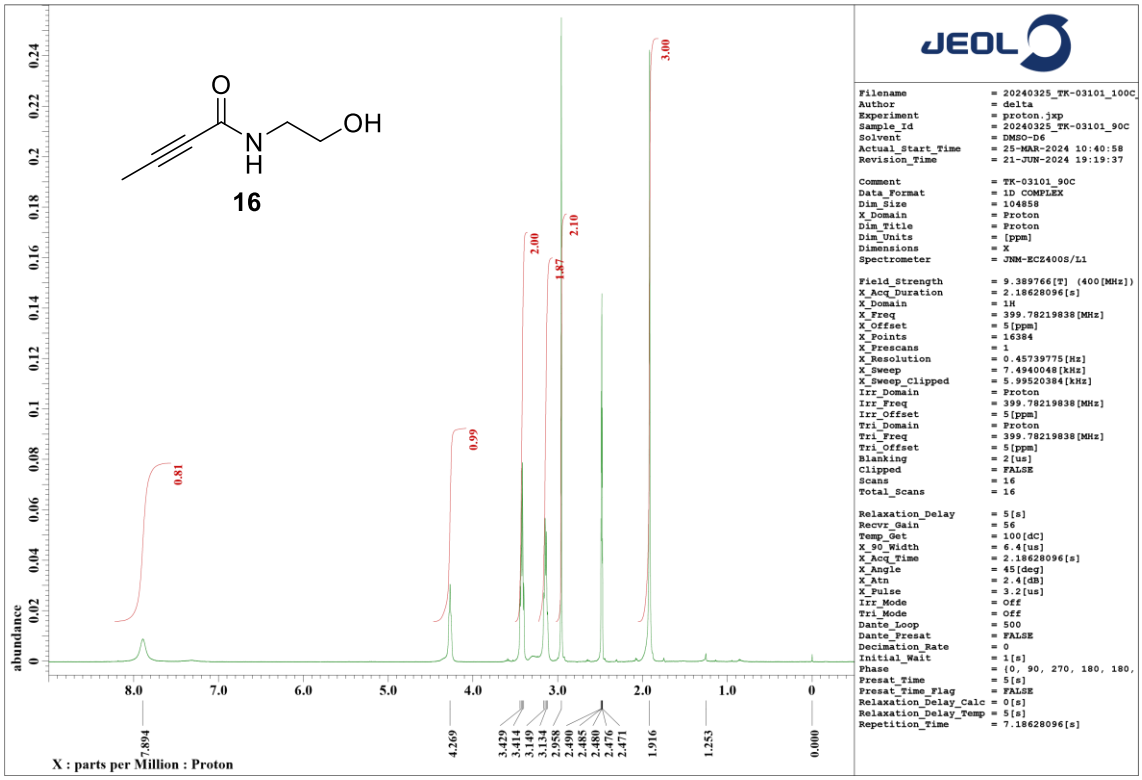

(thousandths)
X : parts per Million : Carbon13
JEOL
Filename = 20230905_TK-02170_8
Author = delta
Experiment = carbon.jxp
Sample_Id = 20230905_TK-02170_8
Solvent = DMSO-D6
Actual_Start_Time = 6-SEP-2023 01:51:1
Revision_Time = 7-SEP-2023 15:59:1
Comment = TK-02170
Data_Format = 1D COMPLEX
Dim_Size = 26214
X_Domain = Carbon13
Dim_Title = Carbon13
Dim_Units = [ppm]
Dimensions = X
Spectrometer = JNM-ECZ400S/L1
Field_Strength = 9.389766[T] (400[MH
X_Acq_Duration = 1.03809024[s]
X_Domain = 13C
X_Freq = 100.52530333[MHz]
X_Offset = 100[ppm]
X_Points = 32768
X_Prescans = 4
X_Resolution = 0.96330739[Hz]
X_Sweep = 31.56565657[kHz]
X_Sweep_Clipped = 25.25252525[kHz]
Irr_Domain = Proton
Irr_Freq = 399.78219838[MHz]
Irr_Offset = 5[ppm]
Blanking = 5[us]
Clipped = TRUE
Scans = 4096
Total_Scans = 4096
Relaxation_Delay = 2[s]
Recvr_Gain = 50
Temp_Get = 80[dC]
X_90_Width = 10.02[us]
X_Acq_Time = 1.03809024[s]
X_Angle = 30[deg]
X_Atn = 8[dB]
X_Pulse = 3.34[us]
Irr_Atn_Dec = 27.49[dB]
Irr_Atn_Dec_Calc = 27.49[dB]
Irr_Atn_Dec_Default_Calc = 27.49[dB]
Irr_Atn_Noe = 27.49[dB]
Irr_Dec_Bandwidth_Hz = 4.78260871[kHz]
Irr_Dec_Bandwidth_Ppm = 11.96303566[ppm]
Irr_Dec_Freq = 399.78219838[MHz]
Irr_Dec_Merit_Factor = 2.2
Irr_Decoupling = TRUE
Irr_Noe = TRUE
Irr_Noise = WALTZ
Irr_Offset_Default = 5[ppm]
Irr_Pwidth = 0.115[ms]
Irr_Pwidth_Default = 0.115[ms]
Irr_Pwidth_Default_Calc = 0.115[ms]
Irr_Pwidth_Temp1 = 0.115[ms]
Irr_Wurst = FALSE
Decimation_Rate = 0

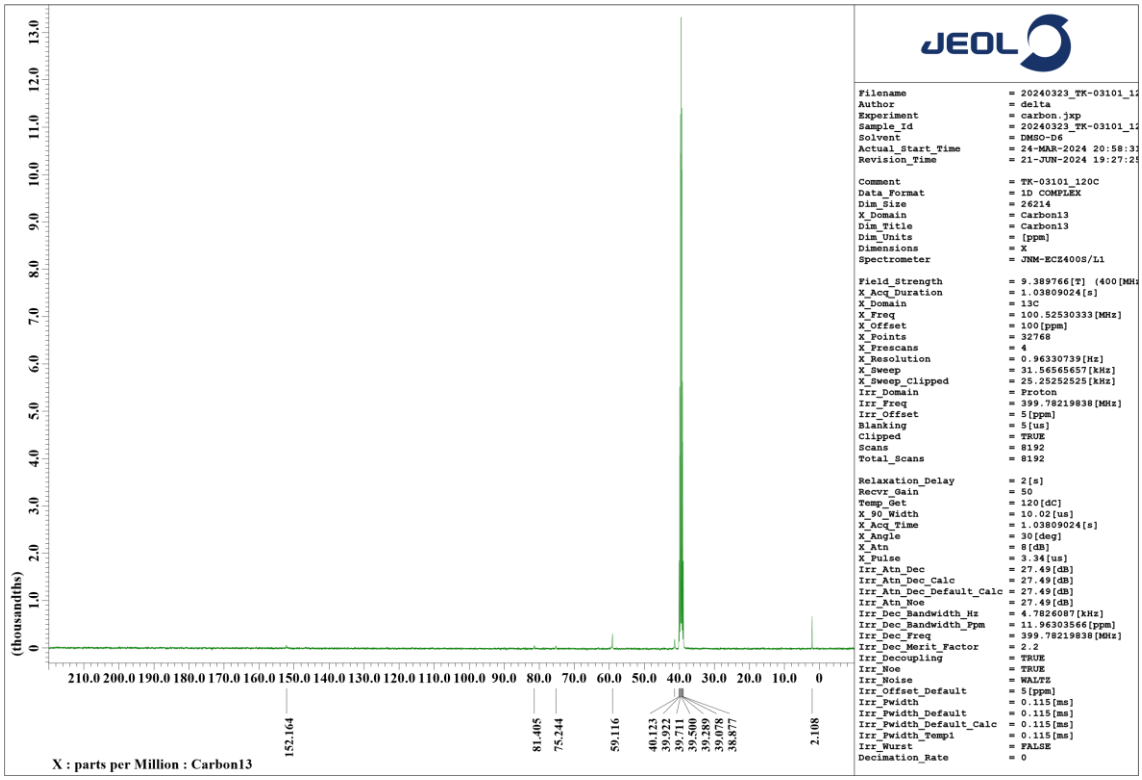

O
N
H
OTBS
14
abundance
X : parts per Million : Proton
9.22
5.91
3.00
2.07
1.89
1.62
0.82
Filename = 20240322_TK-03099B_DMSO
Author = delta
Experiment = proton.jxp
Sample_Id = 20240322_TK-03099B_DMSO
Solvent = DMSO-D6
Actual_Start_Time = 22-MAR-2024 18:40:25
Revision_Time = 21-JUN-2024 18:38:41
Comment = TK-03099B_DMSO-d6
Data_Format = 1D COMPLEX
Dim_Size = 104858
X_Domain = Proton
Dim_Title = Proton
Dim_Units = [ppm]
Dimensions = X
Spectrometer = JNM-ECZ400S/L1
Field_Strength = 9.389766[T] (400[MHz])
X_Acq_Duration = 2.18628096[s]
X_Domain = 1H
X_Freq = 399.78219838[MHz]
X_Offset = 5[ppm]
X_Points = 16384
X_Prescans = 1
X_Resolution = 0.45739775[Hz]
X_Sweep = 7.4940048[kHz]
X_Sweep_Clipped = 5.99520384[kHz]
Irr_Domain = Proton
Irr_Freq = 399.78219838[MHz]
Irr_Offset = 5[ppm]
Tri_Domain = Proton
Tri_Freq = 399.78219838[MHz]
Tri_Offset = 5[ppm]
Blanking = 2[us]
Clipped = FALSE
Scans = 16
Total_Scans = 16
Relaxation_Delay = 5[s]
Recvr_Gain = 56
Temp_Get = 120[dC]
X_90_Width = 6.4[us]
X_Acq_Time = 2.18628096[s]
X_Angle = 45[deg]
X_Atn = 2.4[dB]
X_Pulse = 3.2[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Loop = 500
Dante_Presat = FALSE
Decimation_Rate = 0
Initial_Wait = 1[s]
Phase = (0, 90, 270, 180, 180,
Presat_Time = 5[s]
Presat_Time_Flag = FALSE
Relaxation_Delay_Calc = 0[s]
Relaxation_Delay_Temp = 5[s]
Repetition_Time = 7.18628096[s]

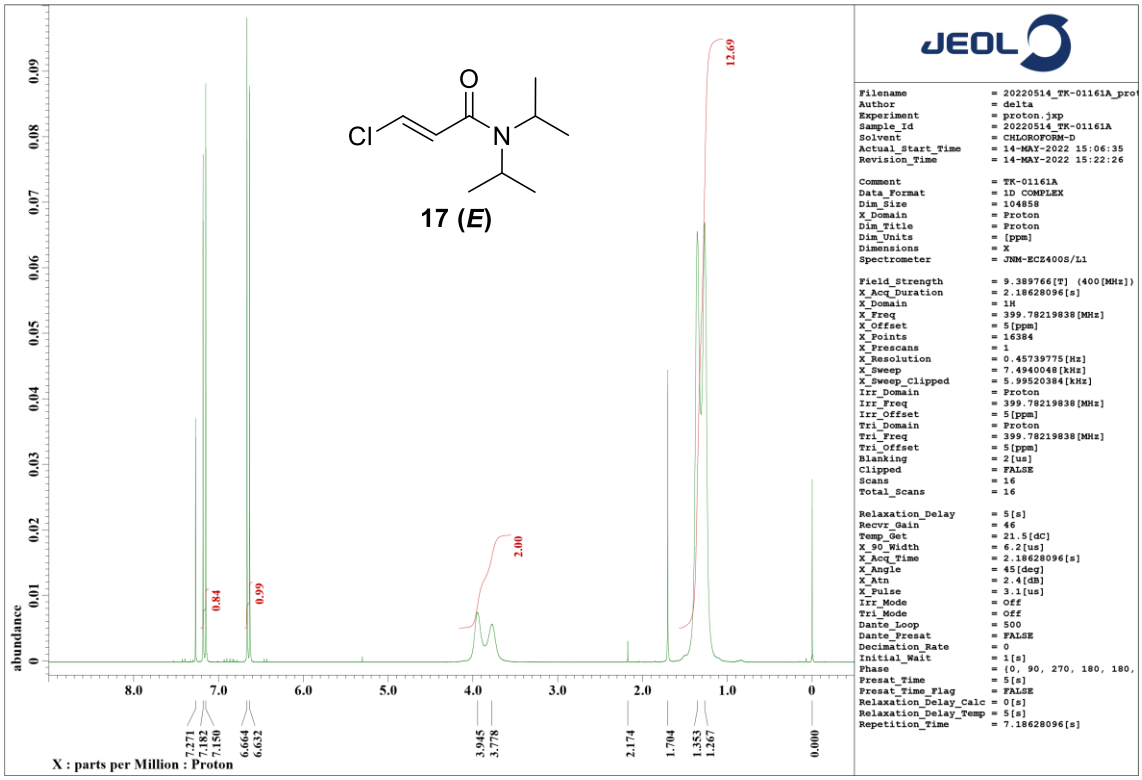

(thousandths)
X : parts per Million : Carbon13
Filename = 20240322_TK-03099B_D
Author = delta
Experiment = carbon.jxp
Sample_Id = 20240322_TK-03099B_D
Solvent = DMSO-D6
Actual_Start_Time = 22-MAR-2024 20:52:51
Revision_Time = 21-JUN-2024 19:04:50
Comment = TK-03099B_DMSO
Data_Format = 1D COMPLEX
Dim_Size = 26214
X_Domain = Carbon13
Dim_Title = Carbon13
Dim_Units = [ppm]
Dimensions = X
Spectrometer = JNM-ECZ400S/L1
Field_Strength = 9.389766[T] (400[MHz
X_Acq_Duration = 1.03809024[s]
X_Domain = 13C
X_Freq = 100.52530333[MHz]
X_Offset = 100[ppm]
X_Points = 32768
X_Prescans = 4
X_Resolution = 0.96330739[Hz]
X_Sweep = 31.56565657[kHz]
X_Sweep_Clipped = 25.25252525[kHz]
Irr_Domain = Proton
Irr_Freq = 399.78219838[MHz]
Irr_Offset = 5[ppm]
Blanking = 5[us]
Clipped = TRUE
Scans = 8192
Total_Scans = 8192
Relaxation_Delay = 2[s]
Recvr_Gain = 50
Temp_Get = 22.2[dC]
X_90_Width = 10.02[us]
X_Acq_Time = 1.03809024[s]
X_Angle = 30[deg]
X_Atn = 8[dB]
X_Pulse = 3.34[us]
Irr_Atn_Dec = 27.49[dB]
Irr_Atn_Dec_Calc = 27.49[dB]
Irr_Atn_Dec_Default_Calc = 27.49[dB]
Irr_Atn_Noe = 27.49[dB]
Irr_Dec_Bandwidth_Hz = 4.78226087[kHz]
Irr_Dec_Bandwidth_Ppm = 11.96303566[ppm]
Irr_Dec_Freq = 399.78219838[MHz]
Irr_Dec_Merit_Factor = 2.2
Irr_Decoupling = TRUE
Irr_Noe = TRUE
Irr_Noise = WALTZ
Irr_Offset_Default = 5[ppm]
Irr_Pwidth = 0.115[ms]
Irr_Pwidth_Default = 0.115[ms]
Irr_Pwidth_Default_Calc = 0.115[ms]
Irr_Pwidth_Temp1 = 0.115[ms]
Irr_Wurst = FALSE
Decimation_Rate = 0

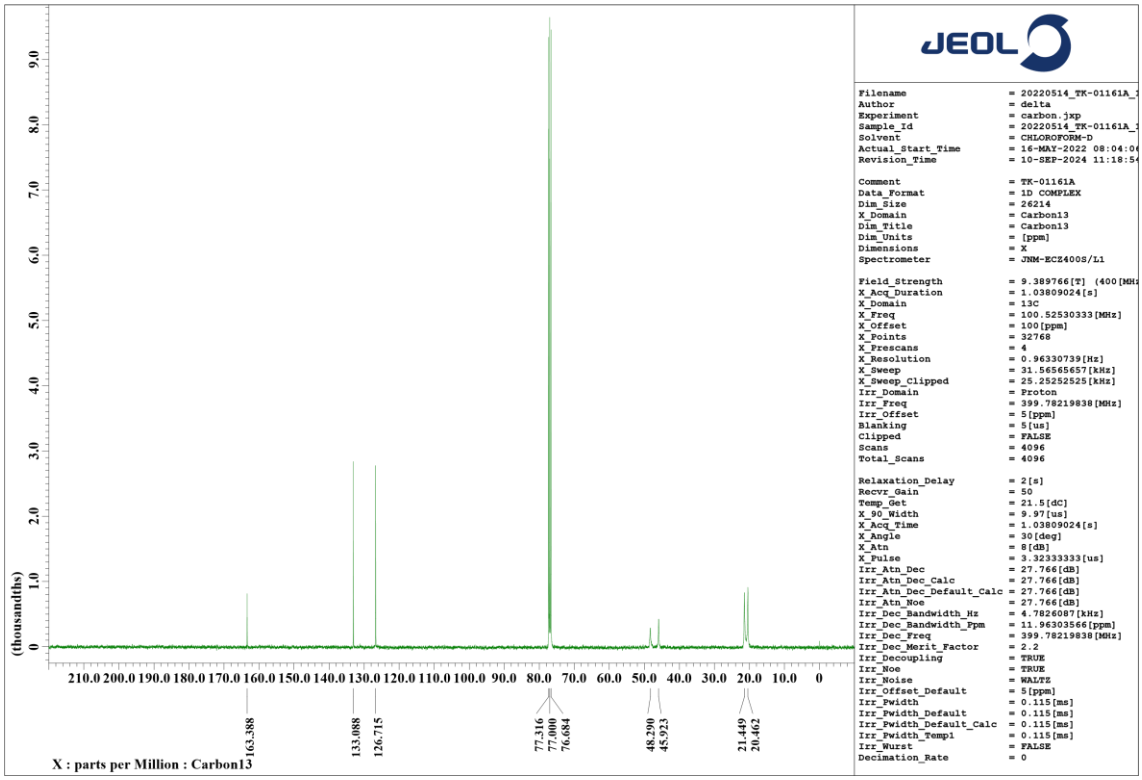

O
N
H
OH
15
abundance
X : parts per Million : Proton
0.92
44.81m
48.77m
0.93
47.25m
0.77
2.00
1.91
0.12
8.671
4.807
4.793
4.779
4.714
4.700
4.686
4.401
4.094
3.402
3.388
3.373
3.340
3.140
3.125
2.512
2.508
2.503
2.499
2.494
0.000
Filename = 20230912_TK-02173_DMSO_
Author = delta
Experiment = proton.jxp
Sample_Id = 20230912_TK-02173_DMSO
Solvent = DMSO-D6
Actual_Start_Time = 12-SEP-2023 20:35:00
Revision_Time = 17-JUL-2024 19:45:08
Comment = TK-02173_DMSO
Data_Format = 1D COMPLEX
Dim_Size = 104858
X_Domain = Proton
Dim_Title = Proton
Dim_Units = [ppm]
Dimensions = X
Spectrometer = JNM-ECZ400S/L1
Field_Strength = 9.389766[T] (400[MHz])
X_Acq_Duration = 2.18628096[s]
X_Domain = 1H
X_Freq = 399.78219838[MHz]
X_Offset = 5[ppm]
X_Points = 16384
X_Prescans = 1
X_Resolution = 0.45739775[Hz]
X_Sweep = 7.4940048[kHz]
X_Sweep_Clipped = 5.99520384[kHz]
Irr_Domain = Proton
Irr_Freq = 399.78219838[MHz]
Irr_Offset = 5[ppm]
Tri_Domain = Proton
Tri_Freq = 399.78219838[MHz]
Tri_Offset = 5[ppm]
Blanking = 2[us]
Clipped = FALSE
Scans = 16
Total_Scans = 16
Relaxation_Delay = 5[s]
Recvr_Gain = 56
Temp_Get = 22.8[dC]
X_90_Width = 6.4[us]
X_Acq_Time = 2.18628096[s]
X_Angle = 45[deg]
X_Atn = 2.4[dB]
X_Pulse = 3.2[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Loop = 500
Dante_Presat = FALSE
Decimation_Rate = 0
Initial_Wait = 1[s]
Phase = (0, 90, 270, 180, 180,
Presat_Time = 5[s]
Presat_Time_Flag = FALSE
Relaxation_Delay_Calc = 0[s]
Relaxation_Delay_Temp = 5[s]
Repetition_Time = 7.18628096[s]

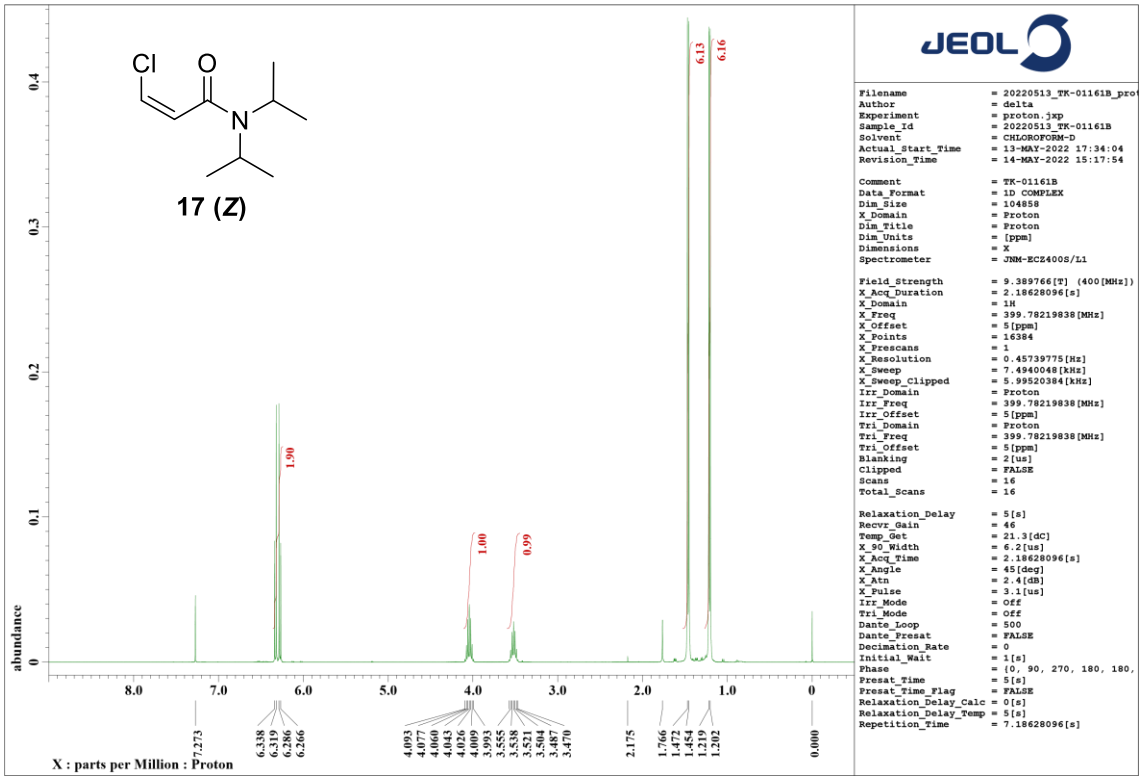

(thousandths)
X : parts per Million : Carbon13
151.397
78.099
74.659
58.991
41.512
40.132
39.922
39.711
39.500
39.289
39.088
38.877
Filename = 20230912_TK-02173_DM
Author = delta
Experiment = carbon.jxp
Sample_Id = 20230912_TK-02173_DM
Solvent = DMSO-D6
Actual_Start_Time = 13-SEP-2023 03:19:1
Revision_Time = 25-OCT-2023 18:36:3
Comment = TK-02173_DMSO
Data_Format = 1D COMPLEX
Dim_Size = 26214
X_Domain = Carbon13
Dim_Title = Carbon13
Dim_Units = [ppm]
Dimensions = X
Spectrometer = JNM-ECZ400S/L1
Field_Strength = 9.389766[T] (400[MH
X_Acq_Duration = 1.03809024[s]
X_Domain = 13C
X_Freq = 100.52530333[MHz]
X_Offset = 100[ppm]
X_Points = 32768
X_Prescans = 4
X_Resolution = 0.96330739[Hz]
X_Sweep = 31.56565657[kHz]
X_Sweep_Clipped = 25.25252525[kHz]
Irr_Domain = Proton
Irr_Freq = 399.78219838[MHz]
Irr_Offset = 5[ppm]
Blanking = 5[us]
Clipped = TRUE
Scans = 4096
Total_Scans = 4096
Relaxation_Delay = 2[s]
Recvr_Gain = 50
Temp_Get = 80[dC]
X_90_Width = 10.02[us]
X_Acq_Time = 1.03809024[s]
X_Angle = 30[deg]
X_Atn = 8[dB]
X_Pulse = 3.34[us]
Irr_Atn_Dec = 27.49[dB]
Irr_Atn_Dec_Calc = 27.49[dB]
Irr_Atn_Dec_Default_Calc = 27.49[dB]
Irr_Atn_Noe = 27.49[dB]
Irr_Dec_Bandwidth_Hz = 4.7826087[kHz]
Irr_Dec_Bandwidth_Ppm = 11.96303566[ppm]
Irr_Dec_Freq = 399.78219838[MHz]
Irr_Dec_Merit_Factor = 2.2
Irr_Decoupling = TRUE
Irr_Noe = TRUE
Irr_Noise = WALTZ
Irr_Offset_Default = 5[ppm]
Irr_Pwidth = 0.115[ms]
Irr_Pwidth_Default = 0.115[ms]
Irr_Pwidth_Default_Calc = 0.115[ms]
Irr_Pwidth_Temp1 = 0.115[ms]
Irr_Wurst = FALSE
Decimation_Rate = 0

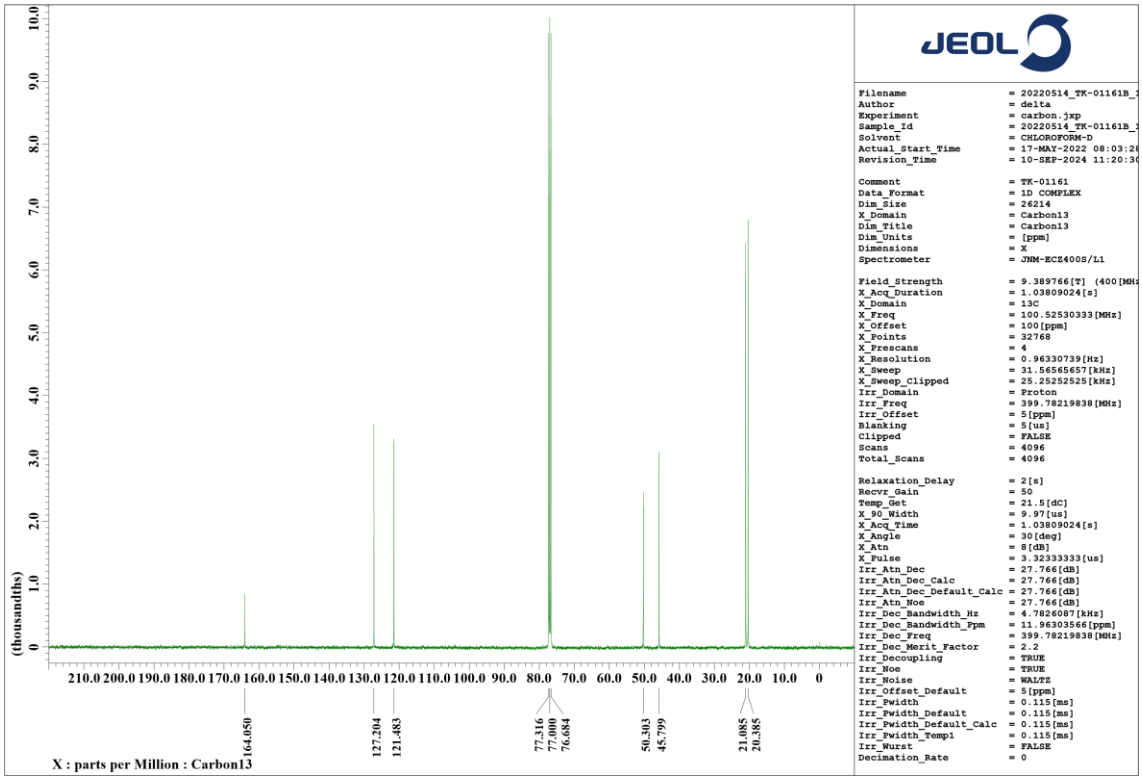

O
N
H
OH
16
abundance
0.81
0.99
2.00
1.87
2.10
3.00
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
7.894
4.269
3.429
3.414
3.149
3.134
2.958
2.490
2.485
2.480
2.476
2.471
1.916
1.253
0.000
X : parts per Million : Proton
JEOL
Filename = 20240325_TK-03101_100C_
Author = delta
Experiment = proton.jxp
Sample_Id = 20240325_TK-03101_90C
Solvent = DMSO-D6
Actual_Start_Time = 25-MAR-2024 10:40:58
Revision_Time = 21-JUN-2024 19:19:37
Comment = TK-03101_90C
Data_Format = 1D COMPLEX
Dim_Size = 104858
X_Domain = Proton
Dim_Title = Proton
Dim_Units = [ppm]
Dimensions = X
Spectrometer = JNM-ECZ400S/L1
Field_Strength = 9.389766[T] (400[MHz])
X_Acq_Duration = 2.18628096[s]
X_Domain = 1H
X_Freq = 399.78219838[MHz]
X_Offset = 5[ppm]
X_Points = 16384
X_Prescans = 1
X_Resolution = 0.45739775[Hz]
X_Sweep = 7.4940048[kHz]
X_Sweep_Clipped = 5.99520384[kHz]
Irr_Domain = Proton
Irr_Freq = 399.78219838[MHz]
Irr_Offset = 5[ppm]
Tri_Domain = Proton
Tri_Freq = 399.78219838[MHz]
Tri_Offset = 5[ppm]
Blanking = 2[us]
Clipped = FALSE
Scans = 16
Total_Scans = 16
Relaxation_Delay = 5[s]
Recvr_Gain = 56
Temp_Get = 100[dC]
X_90_Width = 6.4[us]
X_Acq_Time = 2.18628096[s]
X_Angle = 45[deg]
X_Atn = 2.4[dB]
X_Pulse = 3.2[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Loop = 500
Dante_Presat = FALSE
Decimation_Rate = 0
Initial_Wait = 1[s]
Phase = (0, 90, 270, 180, 180,
Presat_Time = 5[s]
Presat_Time_Flag = FALSE
Relaxation_Delay_Calc = 0[s]
Relaxation_Delay_Temp = 5[s]
Repetition_Time = 7.18628096[s]

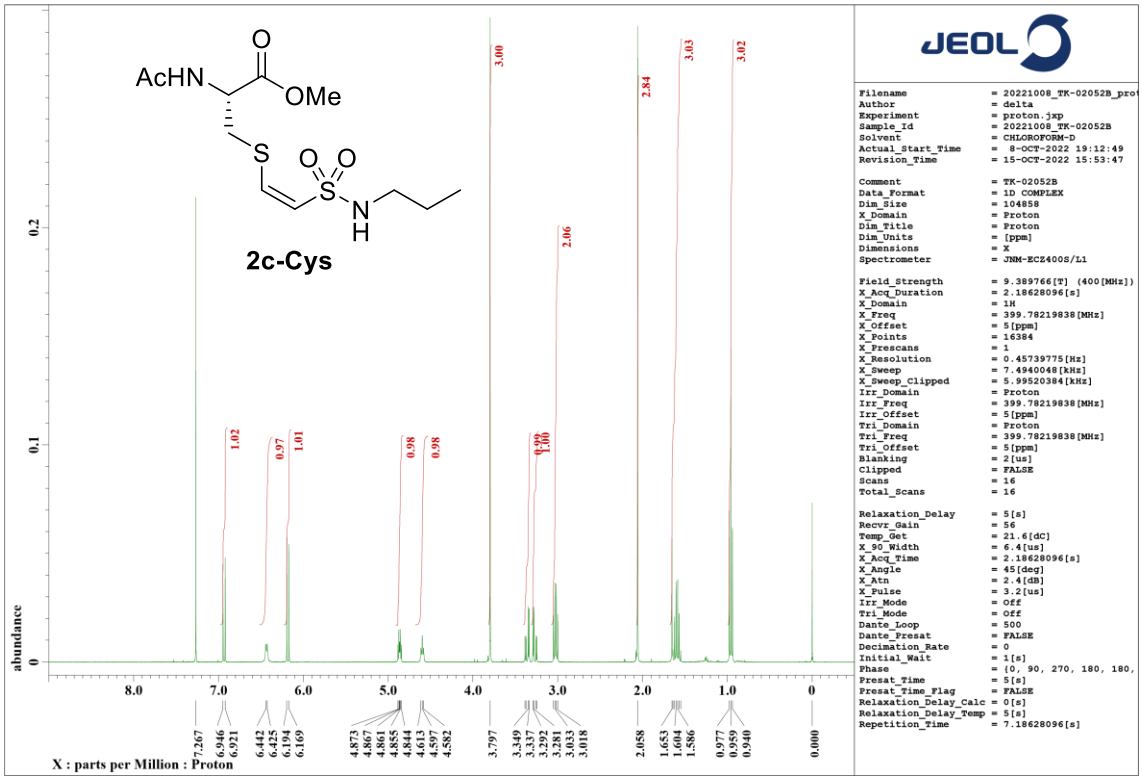

(thousandths)
13.0
12.0
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
210.0 200.0 190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0
152.164
81.405
75.244
59.116
40.123
39.922
39.711
39.500
39.289
39.078
38.877
2.108
X : parts per Million : Carbon13
JEOL
Filename = 20240323_TK-03101_12
Author = delta
Experiment = carbon.jxp
Sample_Id = 20240323_TK-03101_12
Solvent = DMSO-D6
Actual_Start_Time = 24-MAR-2024 20:58:31
Revision_Time = 21-JUN-2024 19:27:25
Comment = TK-03101_120C
Data_Format = 1D COMPLEX
Dim_Size = 26214
X_Domain = Carbon13
Dim_Title = Carbon13
Dim_Units = [ppm]
Dimensions = X
Spectrometer = JNM-ECZ400S/L1
Field_Strength = 9.389766[T] (400[MHz
X_Acq_Duration = 1.03809024[s]
X_Domain = 13C
X_Freq = 100.52530333[MHz]
X_Offset = 100[ppm]
X_Points = 32768
X_Prescans = 4
X_Resolution = 0.96330739[Hz]
X_Sweep = 31.56565657[kHz]
X_Sweep_Clipped = 25.25252525[kHz]
Irr_Domain = Proton
Irr_Freq = 399.78219838[MHz]
Irr_Offset = 5[ppm]
Blanking = 5[us]
Clipped = TRUE
Scans = 8192
Total_Scans = 8192
Relaxation_Delay = 2[s]
Recvr_Gain = 50
Temp_Get = 120[dC]
X_90_Width = 10.02[us]
X_Acq_Time = 1.03809024[s]
X_Angle = 30[deg]
X_Atn = 8[dB]
X_Pulse = 3.34[us]
Irr_Atn_Dec = 27.49[dB]
Irr_Atn_Dec_Calc = 27.49[dB]
Irr_Atn_Dec_Default_Calc = 27.49[dB]
Irr_Atn_Noe = 27.49[dB]
Irr_Dec_Bandwidth_Hz = 4.7826087[kHz]
Irr_Dec_Bandwidth_Ppm = 11.96303566[ppm]
Irr_Dec_Freq = 399.78219838[MHz]
Irr_Dec_Merit_Factor = 2.2
Irr_Decoupling = TRUE
Irr_Noe = TRUE
Irr_Noise = WALTZ
Irr_Offset_Default = 5[ppm]
Irr_Pwidth = 0.115[ms]
Irr_Pwidth_Default = 0.115[ms]
Irr_Pwidth_Default_Calc = 0.115[ms]
Irr_Pwidth_Temp1 = 0.115[ms]
Irr_Wurst = FALSE
Decimation_Rate = 0

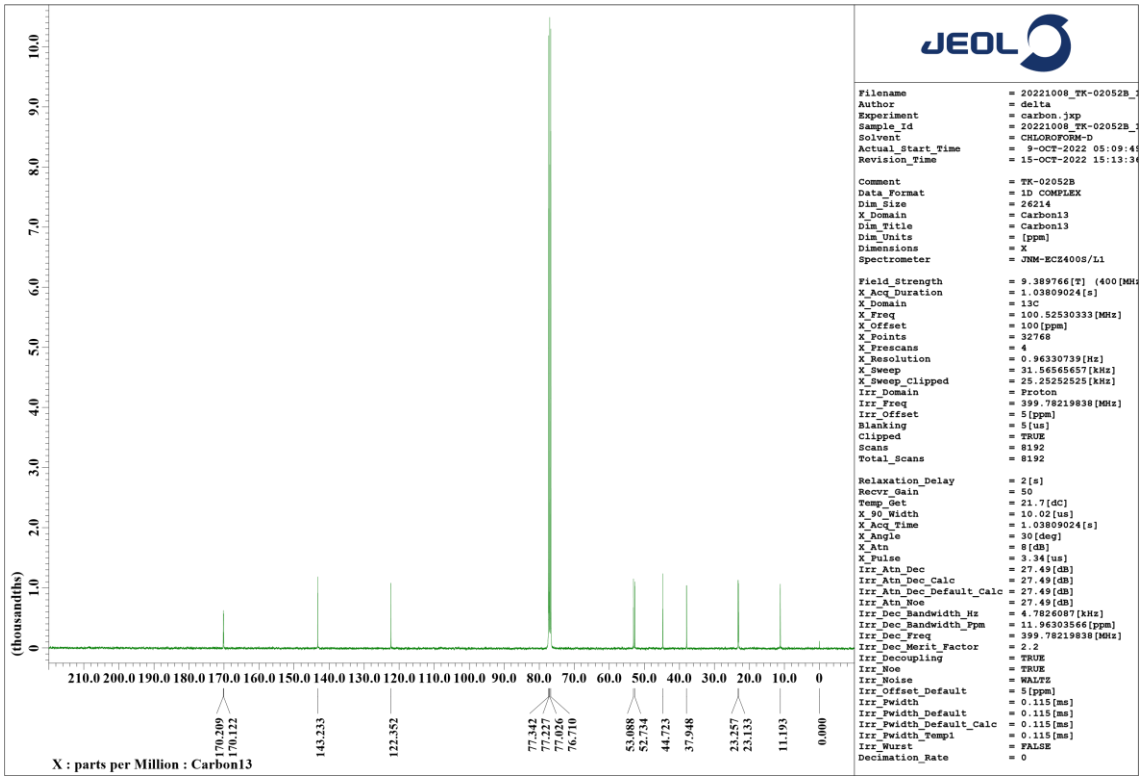

Cl
O
N
17 (E)
abundance
X : parts per Million : Proton
12.69
2.00
0.84
0.99
7.271
7.182
7.150
6.664
6.632
3.945
3.778
2.174
1.704
1.353
1.267
0.000

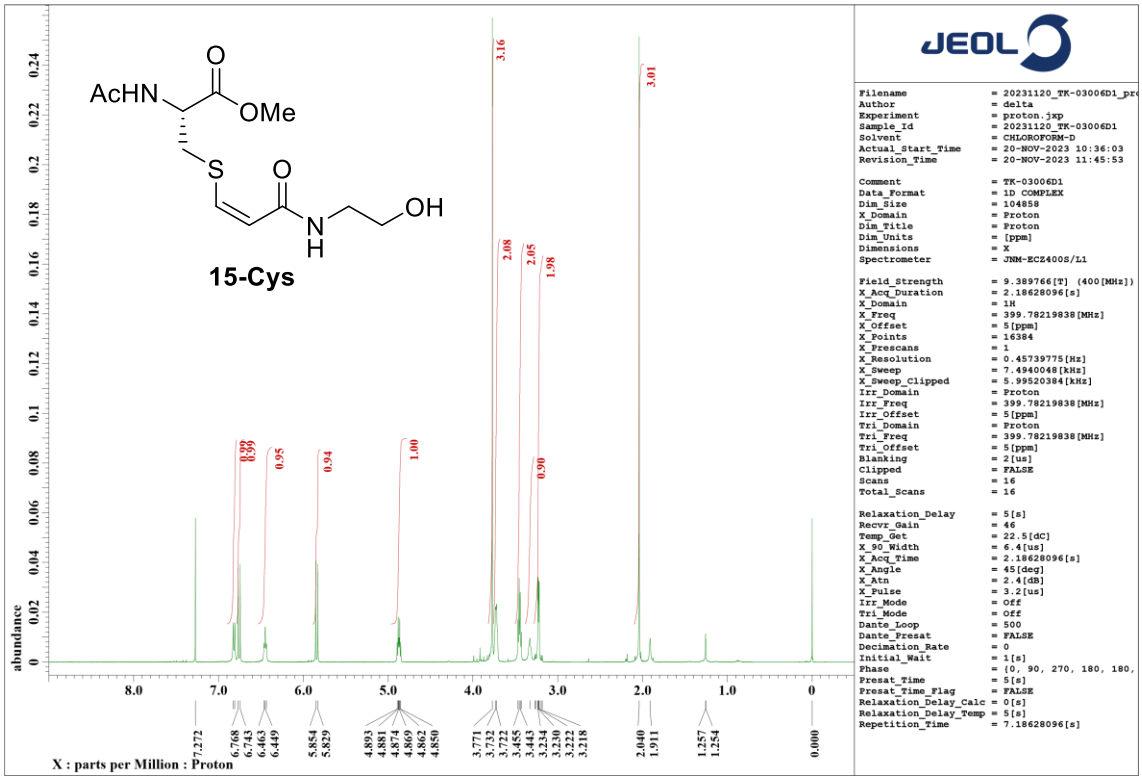

(thousandths)
X : parts per Million : Carbon13
163.388
133.088
126.715
77.316
77.000
76.684
48.290
45.923
21.449
20.462

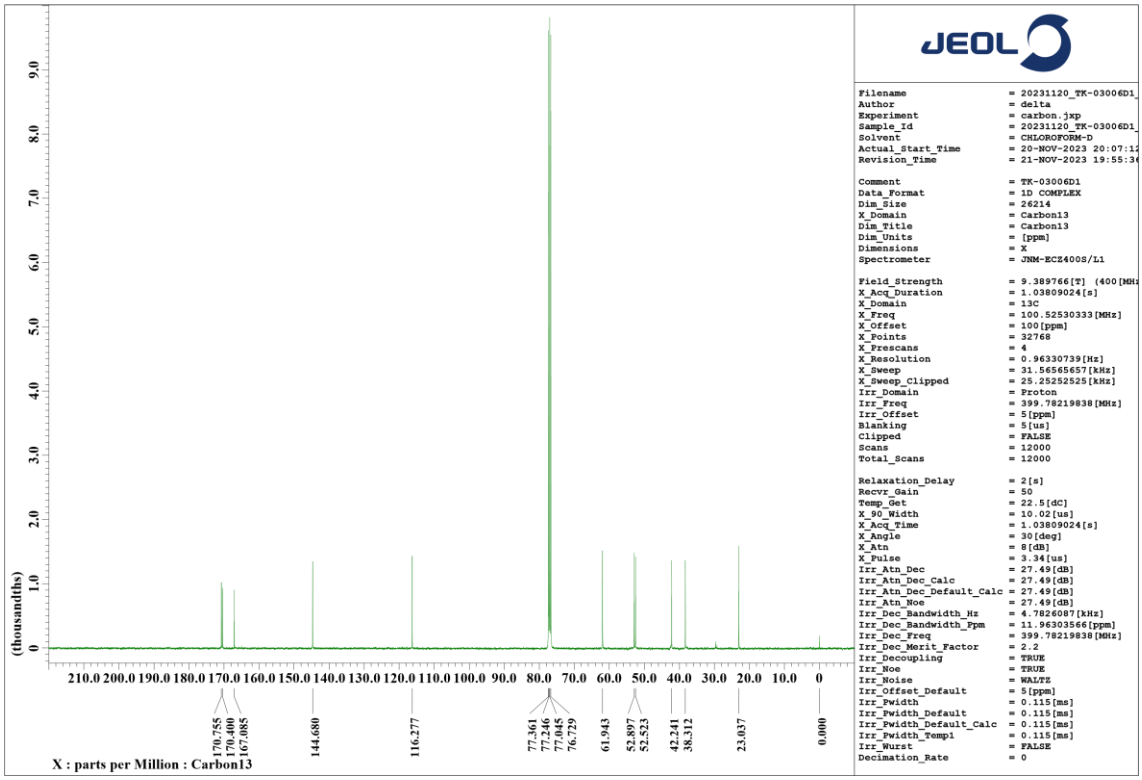

Cl
O
N
17 (Z)
abundance
X : parts per Million : Proton
6.13
6.16
1.90
1.00
0.99
7.273
6.338
6.319
6.286
6.266
4.093
4.077
4.060
4.043
4.026
4.009
3.993
3.555
3.538
3.521
3.504
3.487
3.470
2.175
1.766
1.472
1.454
1.219
1.202
0.000
Filename = 20220513_TK-01161B_pro
Author = delta
Experiment = proton.jxp
Sample_Id = 20220513_TK-01161B
Solvent = CHLOROFORM-D
Actual_Start_Time = 13-MAY-2022 17:34:04
Revision_Time = 14-MAY-2022 15:17:54
Comment = TK-01161B
Data_Format = 1D COMPLEX
Dim_Size = 104858
X_Domain = Proton
Dim_Title = Proton
Dim_Units = [ppm]
Dimensions = X
Spectrometer = JNM-ECZ400S/L1
Field_Strength = 9.389766[T] (400[MHz])
X_Acq_Duration = 2.18628096[s]
X_Domain = 1H
X_Freq = 399.78219838[MHz]
X_Offset = 5[ppm]
X_Points = 16384
X_Prescans = 1
X_Resolution = 0.45739775[Hz]
X_Sweep = 7.4940048[kHz]
X_Sweep_Clipped = 5.99520384[kHz]
Irr_Domain = Proton
Irr_Freq = 399.78219838[MHz]
Irr_Offset = 5[ppm]
Tri_Domain = Proton
Tri_Freq = 399.78219838[MHz]
Tri_Offset = 5[ppm]
Blanking = 2[us]
Clipped = FALSE
Scans = 16
Total_Scans = 16
Relaxation_Delay = 5[s]
Recvr_Gain = 46
Temp_Get = 21.3[dC]
X_90_Width = 6.2[us]
X_Acq_Time = 2.18628096[s]
X_Angle = 45[deg]
X_Atn = 2.4[dB]
X_Pulse = 3.1[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Loop = 500
Dante_Presat = FALSE
Decimation_Rate = 0
Initial_Wait = 1[s]
Phase = (0, 90, 270, 180, 180,
Presat_Time = 5[s]
Presat_Time_Flag = FALSE
Relaxation_Delay_Calc = 0[s]
Relaxation_Delay_Temp = 5[s]
Repetition_Time = 7.18628096[s]

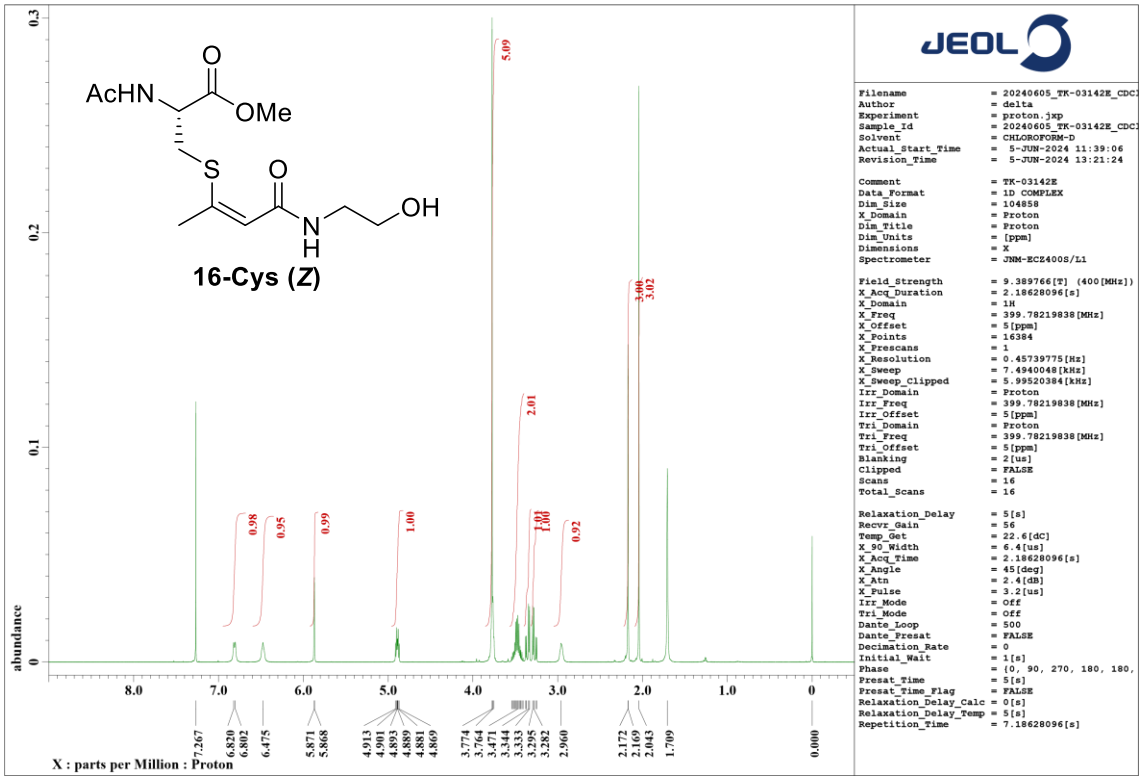

(thousandths)
X : parts per Million : Carbon13
164.050
127.204
121.483
77.316
77.000
76.684
50.303
45.799
21.085
20.385
Filename = 20220514_TK-01161B_1
Author = delta
Experiment = carbon.jxp
Sample_Id = 20220514_TK-01161B_1
Solvent = CHLOROFORM-D
Actual_Start_Time = 17-MAY-2022 08:03:26
Revision_Time = 10-SEP-2024 11:20:30
Comment = TK-01161
Data_Format = 1D COMPLEX
Dim_Size = 26214
X_Domain = Carbon13
Dim_Title = Carbon13
Dim_Units = [ppm]
Dimensions = X
Spectrometer = JNM-ECZ400S/L1
Field_Strength = 9.389766[T] (400[MHz
X_Acq_Duration = 1.03809024[s]
X_Domain = 13C
X_Freq = 100.52530333[MHz]
X_Offset = 100[ppm]
X_Points = 32768
X_Prescans = 4
X_Resolution = 0.96330739[Hz]
X_Sweep = 31.56565657[kHz]
X_Sweep_Clipped = 25.25252525[kHz]
Irr_Domain = Proton
Irr_Freq = 399.78219838[MHz]
Irr_Offset = 5[ppm]
Blanking = 5[us]
Clipped = FALSE
Scans = 4096
Total_Scans = 4096
Relaxation_Delay = 2[s]
Recvr_Gain = 50
Temp_Get = 21.5[dC]
X_90_Width = 9.97[us]
X_Acq_Time = 1.03809024[s]
X_Angle = 30[deg]
X_Atn = 8[dB]
X_Pulse = 3.32333333[us]
Irr_Atn_Dec = 27.766[dB]
Irr_Atn_Dec_Calc = 27.766[dB]
Irr_Atn_Dec_Default_Calc = 27.766[dB]
Irr_Atn_Noe = 27.766[dB]
Irr_Dec_Bandwidth_Hz = 4.7826087[kHz]
Irr_Dec_Bandwidth_Ppm = 11.96303566[ppm]
Irr_Dec_Freq = 399.78219838[MHz]
Irr_Dec_Merit_Factor = 2.2
Irr_Decoupling = TRUE
Irr_Noe = TRUE
Irr_Noise = WALTZ
Irr_Offset_Default = 5[ppm]
Irr_Pwidth = 0.115[ms]
Irr_Pwidth_Default = 0.115[ms]
Irr_Pwidth_Default_Calc = 0.115[ms]
Irr_Pwidth_Temp1 = 0.115[ms]
Irr_Wurst = FALSE
Decimation_Rate = 0

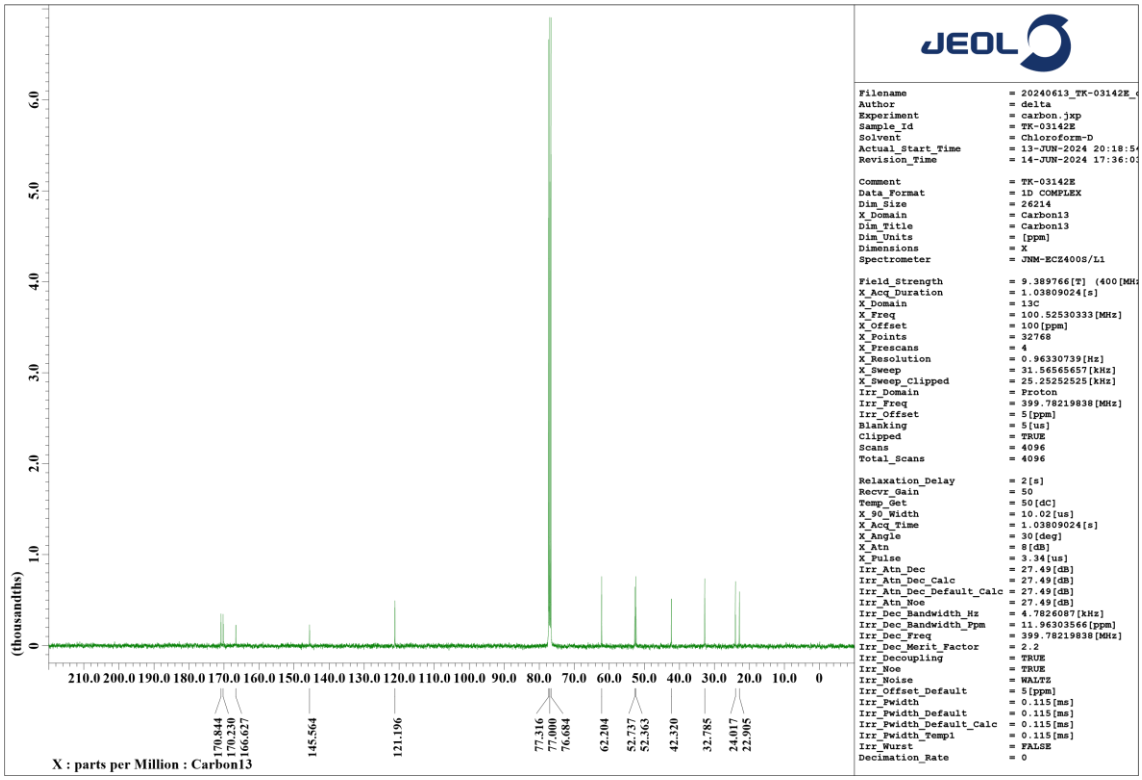

AcHN
OMe
S
O
O
S
N
H
2c-Cys
abundance
X : parts per Million : Proton
JEOL
Filename = 20221008_TK-02052B_pro
Author = delta
Experiment = proton.jxp
Sample_Id = 20221008_TK-02052B
Solvent = CHLOROFORM-D
Actual_Start_Time = 8-OCT-2022 19:12:49
Revision_Time = 15-OCT-2022 15:53:47
Comment = TK-02052B
Data_Format = 1D COMPLEX
Dim_Size = 104858
X_Domain = Proton
Dim_Title = Proton
Dim_Units = [ppm]
Dimensions = X
Spectrometer = JNM-ECZ400S/L1
Field_Strength = 9.389766[T] (400[MHz])
X_Acq_Duration = 2.18628096[s]
X_Domain = 1H
X_Freq = 399.78219838[MHz]
X_Offset = 5[ppm]
X_Points = 16384
X_Prescans = 1
X_Resolution = 0.45739775[Hz]
X_Sweep = 7.4940048[kHz]
X_Sweep_Clipped = 5.99520384[kHz]
Irr_Domain = Proton
Irr_Freq = 399.78219838[MHz]
Irr_Offset = 5[ppm]
Tri_Domain = Proton
Tri_Freq = 399.78219838[MHz]
Tri_Offset = 5[ppm]
Blanking = 2[us]
Clipped = FALSE
Scans = 16
Total_Scans = 16
Relaxation_Delay = 5[s]
Recvr_Gain = 56
Temp_Get = 21.6[dC]
X_90_Width = 6.4[us]
X_Acq_Time = 2.18628096[s]
X_Angle = 45[deg]
X_Atn = 2.4[dB]
X_Pulse = 3.2[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Loop = 500
Dante_Presat = FALSE
Decimation_Rate = 0
Initial_Wait = 1[s]
Phase = (0, 90, 270, 180, 180,
Presat_Time = 5[s]
Presat_Time_Flag = FALSE
Relaxation_Delay_Calc = 0[s]
Relaxation_Delay_Temp = 5[s]
Repetition_Time = 7.18628096[s]

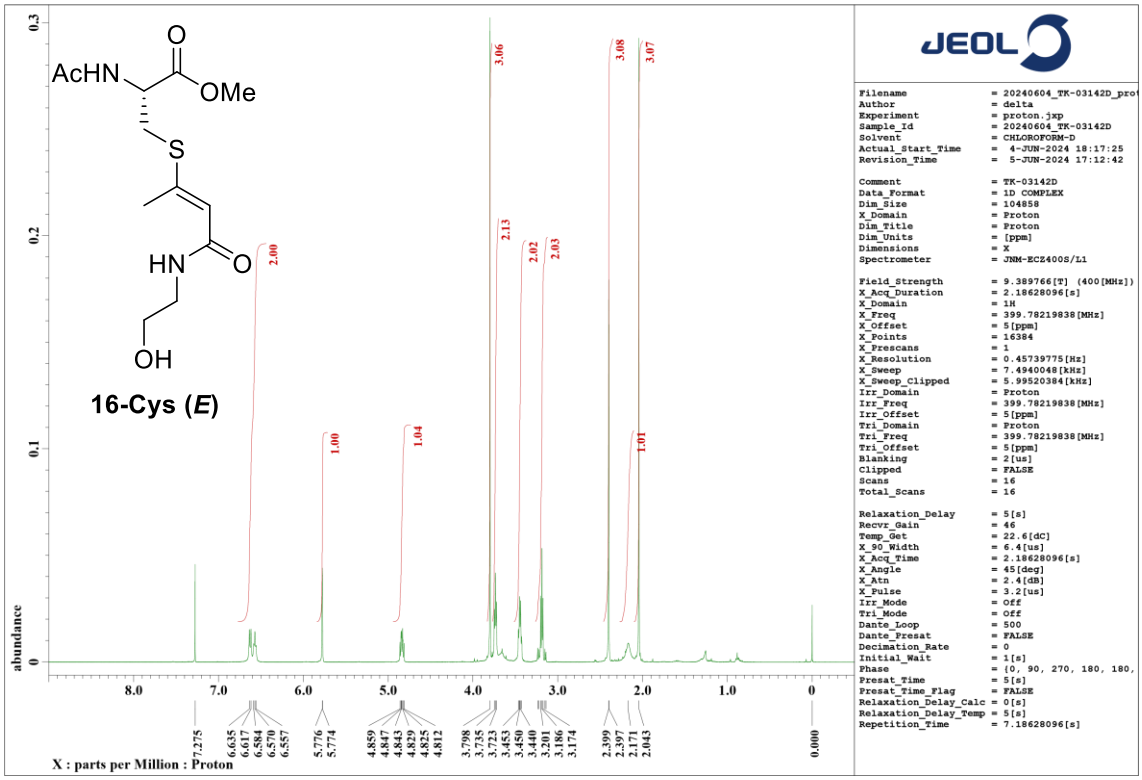

(thousandths)
X : parts per Million : Carbon13
JEOL
Filename = 20221008_TK-02052B_1
Author = delta
Experiment = carbon.jxp
Sample_Id = 20221008_TK-02052B_1
Solvent = CHLOROFORM-D
Actual_Start_Time = 9-OCT-2022 05:09:4
Revision_Time = 15-OCT-2022 15:13:3
Comment = TK-02052B
Data_Format = 1D COMPLEX
Dim_Size = 26214
X_Domain = Carbon13
Dim_Title = Carbon13
Dim_Units = [ppm]
Dimensions = X
Spectrometer = JNM-ECZ400S/L1
Field_Strength = 9.389766[T] (400[MH
X_Acq_Duration = 1.03809024[s]
X_Domain = 13C
X_Freq = 100.52530333[MHz]
X_Offset = 100[ppm]
X_Points = 32768
X_Prescans = 4
X_Resolution = 0.96330739[Hz]
X_Sweep = 31.56565657[kHz]
X_Sweep_Clipped = 25.25252525[kHz]
Irr_Domain = Proton
Irr_Freq = 399.78219838[MHz]
Irr_Offset = 5[ppm]
Blanking = 5[us]
Clipped = TRUE
Scans = 8192
Total_Scans = 8192
Relaxation_Delay = 2[s]
Recvr_Gain = 50
Temp_Get = 21.7[dC]
X_90_Width = 10.02[us]
X_Acq_Time = 1.03809024[s]
X_Angle = 30[deg]
X_Atn = 8[dB]
X_Pulse = 3.34[us]
Irr_Atn_Dec = 27.49[dB]
Irr_Atn_Dec_Calc = 27.49[dB]
Irr_Atn_Dec_Default_Calc = 27.49[dB]
Irr_Atn_Noe = 27.49[dB]
Irr_Dec_Bandwidth_Hz = 4.7826087[kHz]
Irr_Dec_Bandwidth_Ppm = 11.96303566[ppm]
Irr_Dec_Freq = 399.78219838[MHz]
Irr_Dec_Merit_Factor = 2.2
Irr_Decoupling = TRUE
Irr_Noe = TRUE
Irr_Noise = WALTZ
Irr_Offset_Default = 5[ppm]
Irr_Pwidth = 0.115[ms]
Irr_Pwidth_Default = 0.115[ms]
Irr_Pwidth_Default_Calc = 0.115[ms]
Irr_Pwidth_Temp1 = 0.115[ms]
Irr_Wurst = FALSE
Decimation_Rate = 0

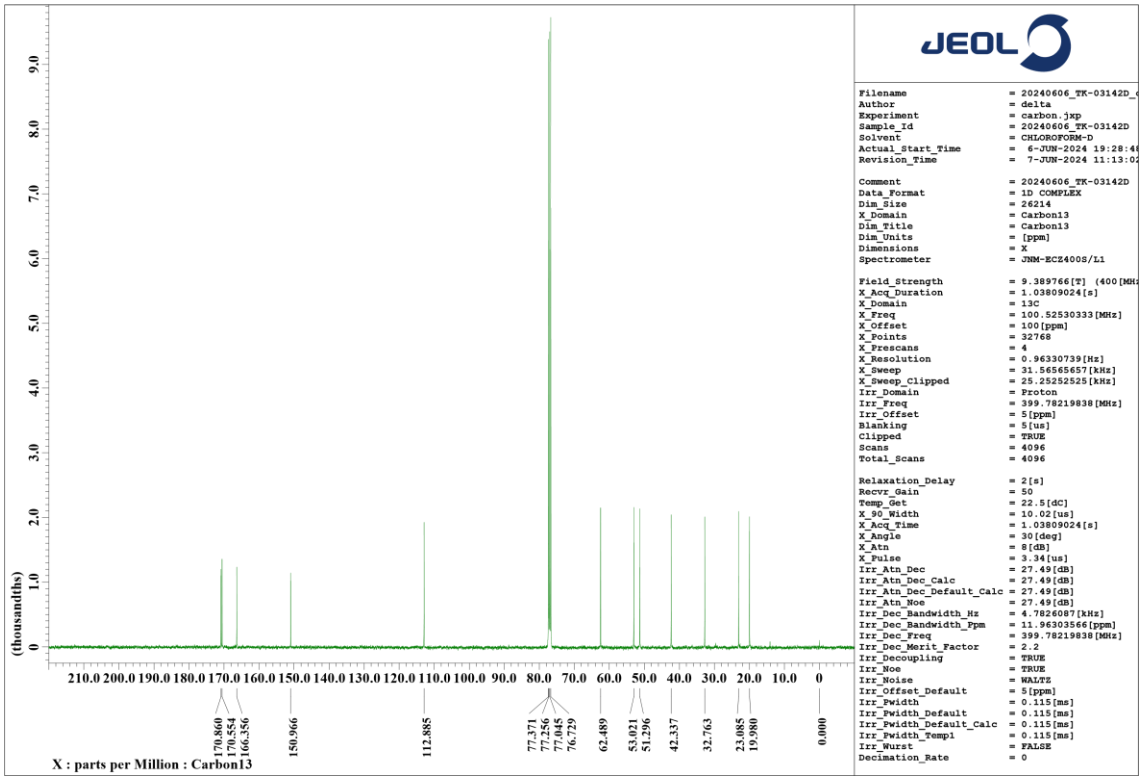

AcHN
O
OMe
S
O
N
H
OH
15-Cys
3.16
3.01
2.08
2.05
1.98
0.95
0.94
1.00
0.90
abundance
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
X : parts per Million : Proton
7.272
6.768
6.743
6.463
6.449
5.854
5.829
4.893
4.881
4.874
4.869
4.862
4.850
3.771
3.732
3.722
3.455
3.443
3.234
3.230
3.222
3.218
2.040
1.911
1.257
1.254
0.000
JEOL
Filename = 20231120_TK-03006D1_pr
Author = delta
Experiment = proton.jxp
Sample_Id = 20231120_TK-03006D1
Solvent = CHLOROFORM-D
Actual_Start_Time = 20-NOV-2023 10:36:03
Revision_Time = 20-NOV-2023 11:45:53
Comment = TK-03006D1
Data_Format = 1D COMPLEX
Dim_Size = 104858
X_Domain = Proton
Dim_Title = Proton
Dim_Units = [ppm]
Dimensions = X
Spectrometer = JNM-ECZ400S/L1
Field_Strength = 9.389766[T] (400[MHz])
X_Acq_Duration = 2.18628096[s]
X_Domain = 1H
X_Freq = 399.78219838[MHz]
X_Offset = 5[ppm]
X_Points = 16384
X_Prescans = 1
X_Resolution = 0.45739775[Hz]
X_Sweep = 7.4940048[kHz]
X_Sweep_Clipped = 5.99520384[kHz]
Irr_Domain = Proton
Irr_Freq = 399.78219838[MHz]
Irr_Offset = 5[ppm]
Tri_Domain = Proton
Tri_Freq = 399.78219838[MHz]
Tri_Offset = 5[ppm]
Blanking = 2[us]
Clipped = FALSE
Scans = 16
Total_Scans = 16
Relaxation_Delay = 5[s]
Recvr_Gain = 46
Temp_Get = 22.5[dC]
X_90_Width = 6.4[us]
X_Acq_Time = 2.18628096[s]
X_Angle = 45[deg]
X_Atn = 2.4[dB]
X_Pulse = 3.2[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Loop = 500
Dante_Presat = FALSE
Decimation_Rate = 0
Initial_Wait = 1[s]
Phase = (0, 90, 270, 180, 180,
Presat_Time = 5[s]
Presat_Time_Flag = FALSE
Relaxation_Delay_Calc = 0[s]
Relaxation_Delay_Temp = 5[s]
Repetition_Time = 7.18628096[s]

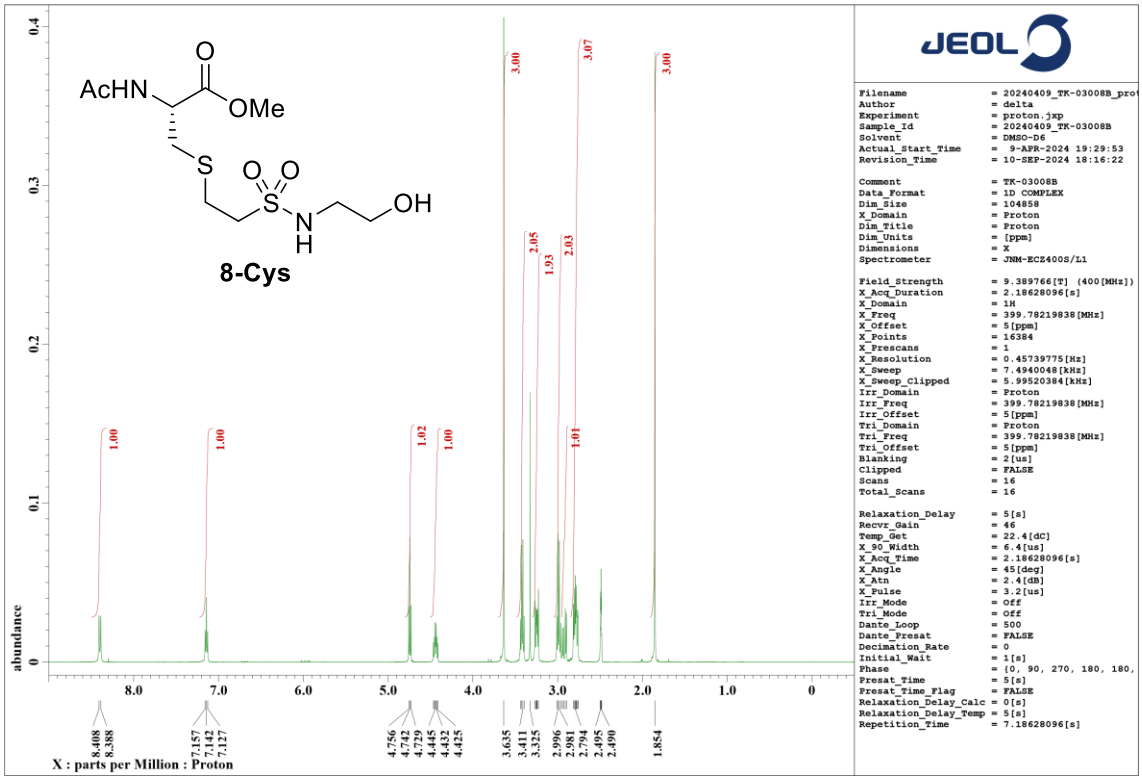

(thousandths)
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
210.0 200.0 190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0
X : parts per Million : Carbon13
170.755
170.400
167.085
144.680
116.277
77.361
77.246
77.045
76.729
61.943
52.897
52.523
42.241
38.312
23.037
0.000
JEOL
Filename = 20231120_TK-03006D1_
Author = delta
Experiment = carbon.jxp
Sample_Id = 20231120_TK-03006D1_
Solvent = CHLOROFORM-D
Actual_Start_Time = 20-NOV-2023 20:07:1
Revision_Time = 21-NOV-2023 19:55:3
Comment = TK-03006D1
Data_Format = 1D COMPLEX
Dim_Size = 26214
X_Domain = Carbon13
Dim_Title = Carbon13
Dim_Units = [ppm]
Dimensions = X
Spectrometer = JNM-ECZ400S/L1
Field_Strength = 9.389766[T] (400[MH
X_Acq_Duration = 1.03809024[s]
X_Domain = 13C
X_Freq = 100.52530333[MHz]
X_Offset = 100[ppm]
X_Points = 32768
X_Prescans = 4
X_Resolution = 0.96330739[Hz]
X_Sweep = 31.56565657[kHz]
X_Sweep_Clipped = 25.25252525[kHz]
Irr_Domain = Proton
Irr_Freq = 399.78219838[MHz]
Irr_Offset = 5[ppm]
Blanking = 5[us]
Clipped = FALSE
Scans = 12000
Total_Scans = 12000
Relaxation_Delay = 2[s]
Recvr_Gain = 50
Temp_Get = 22.5[dC]
X_90_Width = 10.02[us]
X_Acq_Time = 1.03809024[s]
X_Angle = 30[deg]
X_Atn = 8[dB]
X_Pulse = 3.34[us]
Irr_Atn_Dec = 27.49[dB]
Irr_Atn_Dec_Calc = 27.49[dB]
Irr_Atn_Dec_Default_Calc = 27.49[dB]
Irr_Atn_Noe = 27.49[dB]
Irr_Dec_Bandwidth_Hz = 4.7826087[kHz]
Irr_Dec_Bandwidth_Ppm = 11.96303566[ppm]
Irr_Dec_Freq = 399.78219838[MHz]
Irr_Dec_Merit_Factor = 2.2
Irr_Decoupling = TRUE
Irr_Noe = TRUE
Irr_Noise = WALTZ
Irr_Offset_Default = 5[ppm]
Irr_Pwidth = 0.115[ms]
Irr_Pwidth_Default = 0.115[ms]
Irr_Pwidth_Default_Calc = 0.115[ms]
Irr_Pwidth_Temp1 = 0.115[ms]
Irr_Wurst = FALSE
Decimation_Rate = 0

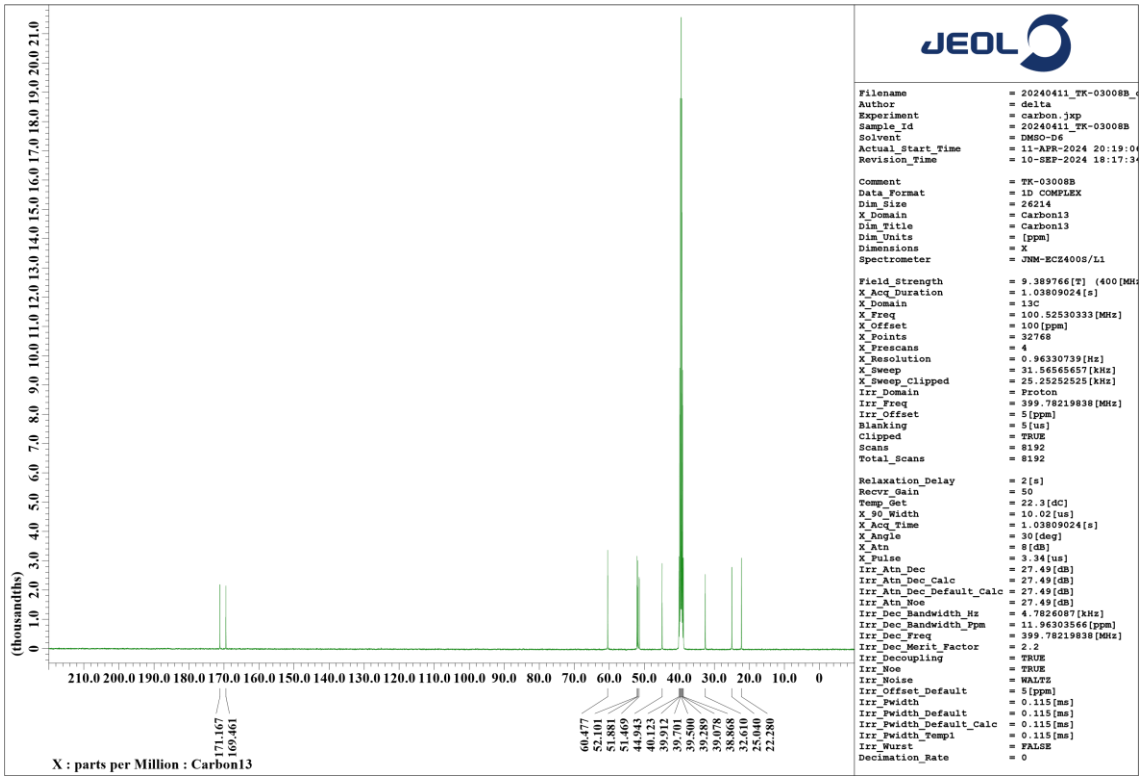

AcHN
OMe
S
O
N
H
OH
16-Cys (Z)
abundance
X : parts per Million : Proton
JEOL

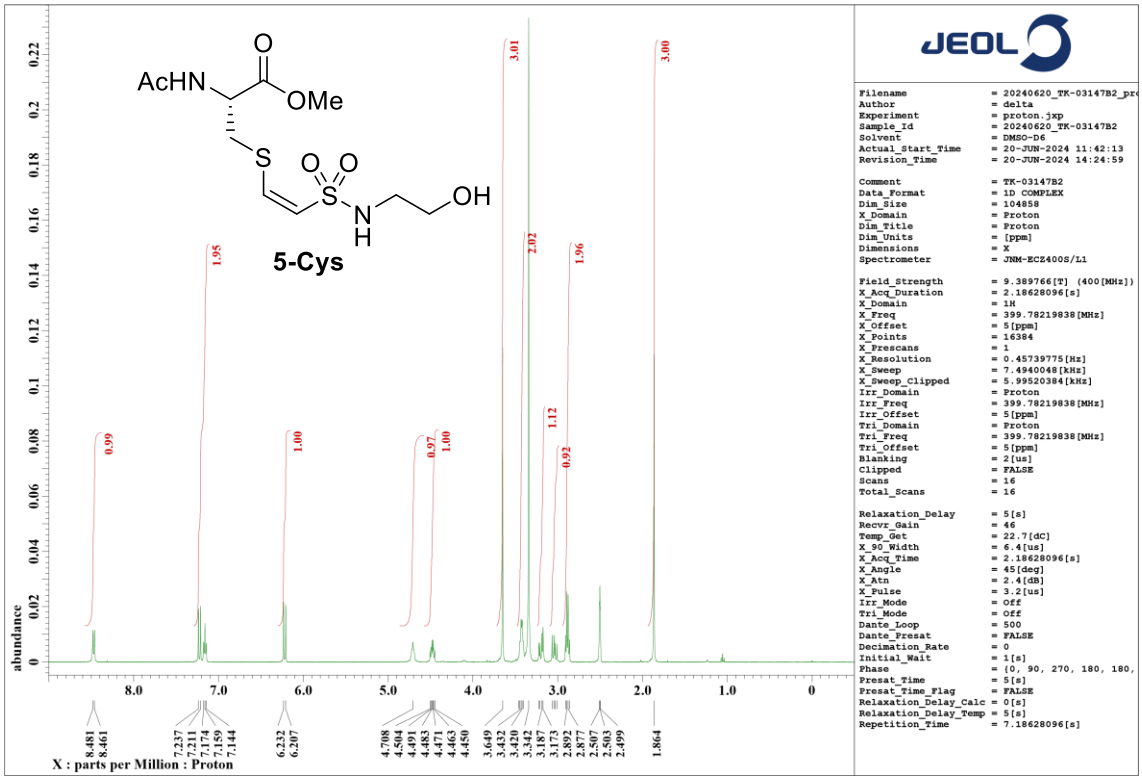

(thousandths)
X : parts per Million : Carbon13
JEOL

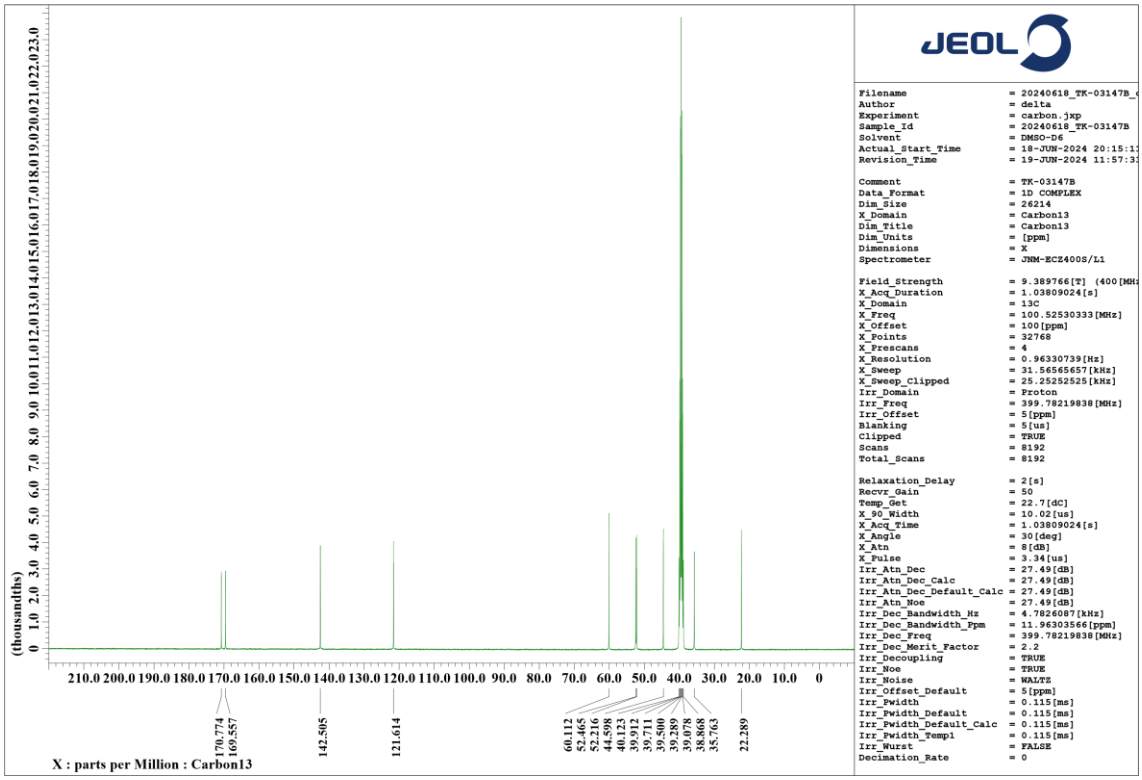

AcHN
OMe
S
HN
O
OH
16-Cys (E)
abundance
X : parts per Million : Proton
JEOL
Filename = 20240604_TK-03142D_pro
Author = delta
Experiment = proton.jxp
Sample_Id = 20240604_TK-03142D
Solvent = CHLOROFORM-D
Actual_Start_Time = 4-JUN-2024 18:17:25
Revision_Time = 5-JUN-2024 17:12:42
Comment = TK-03142D
Data_Format = 1D COMPLEX
Dim_Size = 104858
X_Domain = Proton
Dim_Title = Proton
Dim_Units = [ppm]
Dimensions = X
Spectrometer = JNM-ECZ400S/L1
Field_Strength = 9.389766[T] (400[MHz])
X_Acq_Duration = 2.18628096[s]
X_Domain = 1H
X_Freq = 399.78219838[MHz]
X_Offset = 5[ppm]
X_Points = 16384
X_Prescans = 1
X_Resolution = 0.45739775[Hz]
X_Sweep = 7.4940048[kHz]
X_Sweep_Clipped = 5.99520384[kHz]
Irr_Domain = Proton
Irr_Freq = 399.78219838[MHz]
Irr_Offset = 5[ppm]
Tri_Domain = Proton
Tri_Freq = 399.78219838[MHz]
Tri_Offset = 5[ppm]
Blanking = 2[us]
Clipped = FALSE
Scans = 16
Total_Scans = 16
Relaxation_Delay = 5[s]
Recvr_Gain = 46
Temp_Get = 22.6[dC]
X_90_Width = 6.4[us]
X_Acq_Time = 2.18628096[s]
X_Angle = 45[deg]
X_Atn = 2.4[dB]
X_Pulse = 3.2[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Loop = 500
Dante_Presat = FALSE
Decimation_Rate = 0
Initial_Wait = 1[s]
Phase = (0, 90, 270, 180, 180,
Presat_Time = 5[s]
Presat_Time_Flag = FALSE
Relaxation_Delay_Calc = 0[s]
Relaxation_Delay_Temp = 5[s]
Repetition_Time = 7.18628096[s]

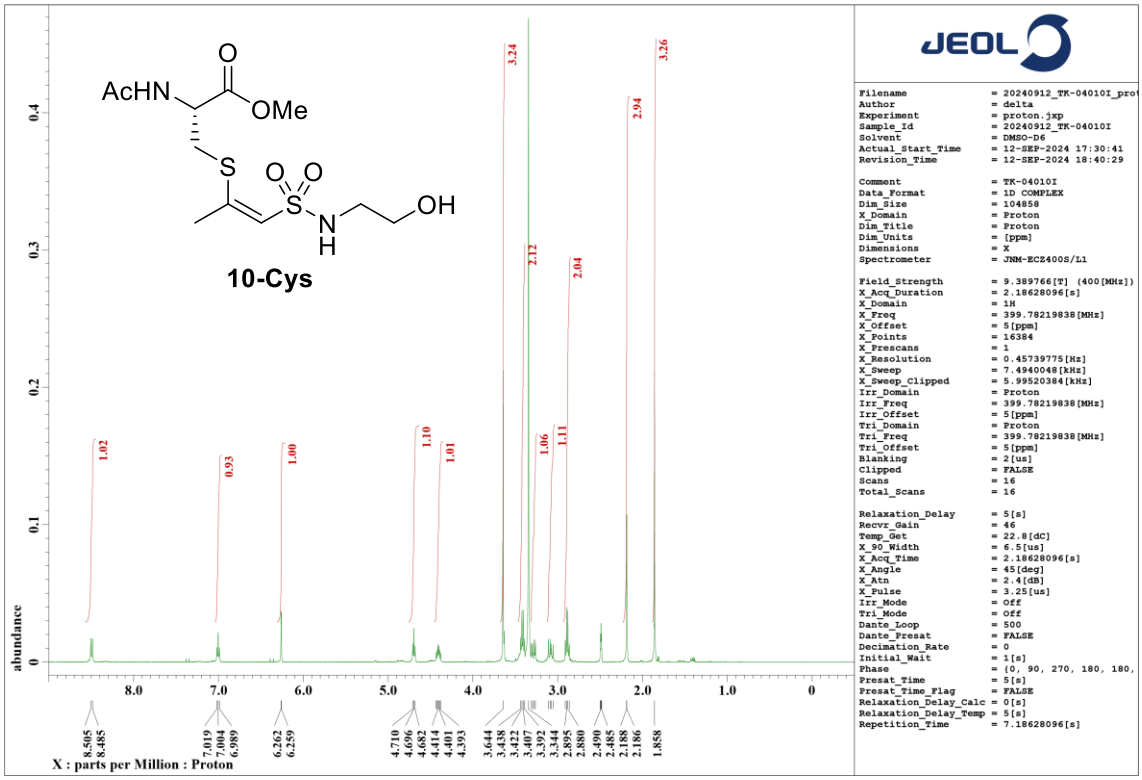

(thousandths)
X : parts per Million : Carbon13
JEOL
Filename = 20240606_TK-03142D_
Author = delta
Experiment = carbon.jxp
Sample_Id = 20240606_TK-03142D
Solvent = CHLOROFORM-D
Actual_Start_Time = 6-JUN-2024 19:28:4
Revision_Time = 7-JUN-2024 11:13:0
Comment = 20240606_TK-03142D
Data_Format = 1D COMPLEX
Dim_Size = 26214
X_Domain = Carbon13
Dim_Title = Carbon13
Dim_Units = [ppm]
Dimensions = X
Spectrometer = JNM-ECZ400S/L1
Field_Strength = 9.389766[T] (400[MH
X_Acq_Duration = 1.03809024[s]
X_Domain = 13C
X_Freq = 100.52530333[MHz]
X_Offset = 100[ppm]
X_Points = 32768
X_Prescans = 4
X_Resolution = 0.96330739[Hz]
X_Sweep = 31.56565657[kHz]
X_Sweep_Clipped = 25.25252525[kHz]
Irr_Domain = Proton
Irr_Freq = 399.78219838[MHz]
Irr_Offset = 5[ppm]
Blanking = 5[us]
Clipped = TRUE
Scans = 4096
Total_Scans = 4096
Relaxation_Delay = 2[s]
Recvr_Gain = 50
Temp_Get = 22.5[dC]
X_90_Width = 10.02[us]
X_Acq_Time = 1.03809024[s]
X_Angle = 30[deg]
X_Atn = 8[dB]
X_Pulse = 3.34[us]
Irr_Atn_Dec = 27.49[dB]
Irr_Atn_Dec_Calc = 27.49[dB]
Irr_Atn_Dec_Default_Calc = 27.49[dB]
Irr_Atn_Noe = 27.49[dB]
Irr_Dec_Bandwidth_Hz = 4.7826087[kHz]
Irr_Dec_Bandwidth_Ppm = 11.96303566[ppm]
Irr_Dec_Freq = 399.78219838[MHz]
Irr_Dec_Merit_Factor = 2.2
Irr_Decoupling = TRUE
Irr_Noe = TRUE
Irr_Noise = WALTZ
Irr_Offset_Default = 5[ppm]
Irr_Pwidth = 0.115[ms]
Irr_Pwidth_Default = 0.115[ms]
Irr_Pwidth_Default_Calc = 0.115[ms]
Irr_Pwidth_Temp1 = 0.115[ms]
Irr_Wurst = FALSE
Decimation_Rate = 0

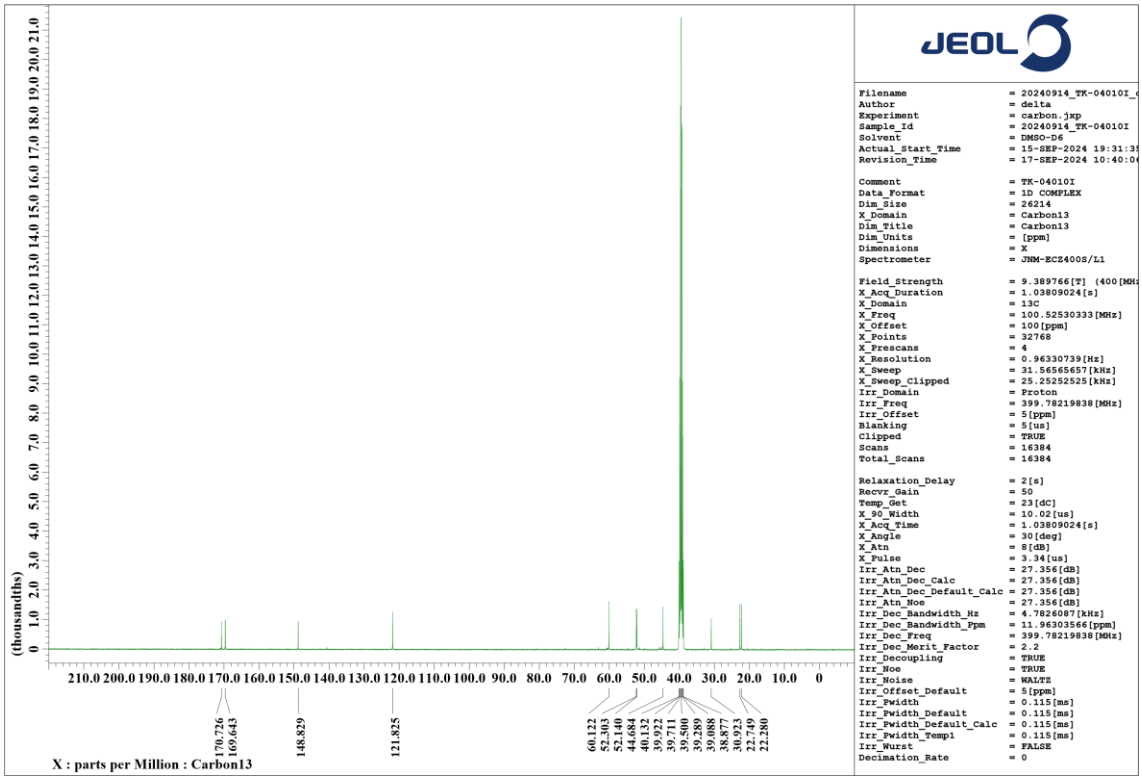

AcHN
O
OMe
S
O
O
S
N
H
OH
8-Cys
abundance
X : parts per Million : Proton
JEOL

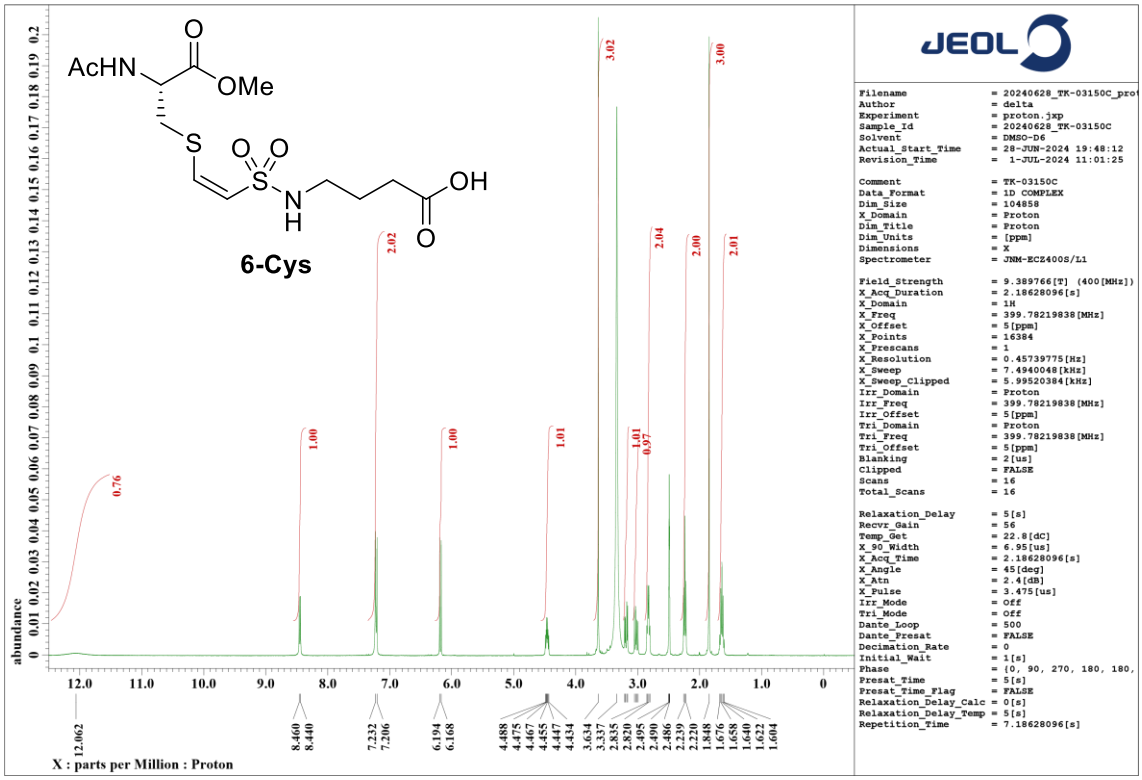

(thousandths)
X : parts per Million : Carbon13
JEOL

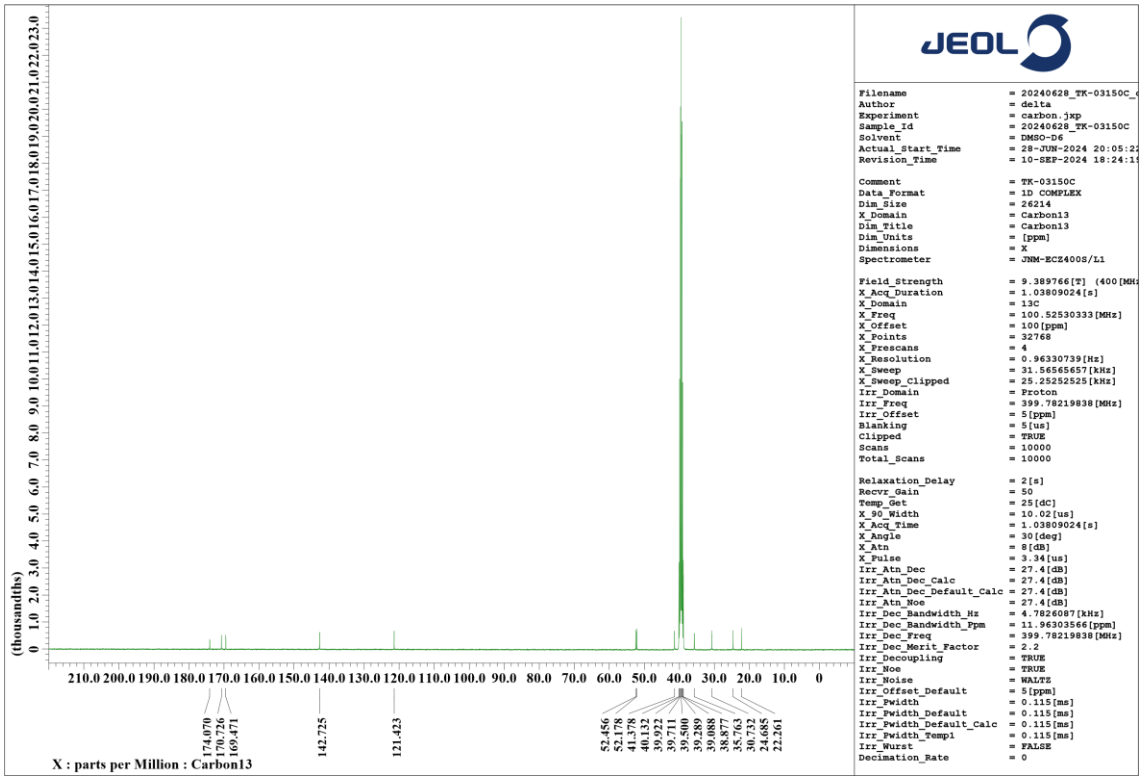

AcHN
O
OMe
S
O
O
S
N
H
OH
5-Cys
abundance
X : parts per Million : Proton
JEOL
Filename = 20240620_TK-03147B2_pr
Author = delta
Experiment = proton.jxp
Sample_Id = 20240620_TK-03147B2
Solvent = DMSO-D6
Actual_Start_Time = 20-JUN-2024 11:42:13
Revision_Time = 20-JUN-2024 14:24:59
Comment = TK-03147B2
Data_Format = 1D COMPLEX
Dim_Size = 104858
X_Domain = Proton
Dim_Title = Proton
Dim_Units = [ppm]
Dimensions = X
Spectrometer = JNM-ECZ400S/L1
Field_Strength = 9.389766[T] (400[MHz])
X_Acq_Duration = 2.18628096[s]
X_Domain = 1H
X_Freq = 399.78219838[MHz]
X_Offset = 5[ppm]
X_Points = 16384
X_Prescans = 1
X_Resolution = 0.45739775[Hz]
X_Sweep = 7.4940048[kHz]
X_Sweep_Clipped = 5.99520384[kHz]
Irr_Domain = Proton
Irr_Freq = 399.78219838[MHz]
Irr_Offset = 5[ppm]
Tri_Domain = Proton
Tri_Freq = 399.78219838[MHz]
Tri_Offset = 5[ppm]
Blanking = 2[us]
Clipped = FALSE
Scans = 16
Total_Scans = 16
Relaxation_Delay = 5[s]
Recvr_Gain = 46
Temp_Get = 22.7[dC]
X_90_Width = 6.4[us]
X_Acq_Time = 2.18628096[s]
X_Angle = 45[deg]
X_Atn = 2.4[dB]
X_Pulse = 3.2[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Loop = 500
Dante_Presat = FALSE
Decimation_Rate = 0
Initial_Wait = 1[s]
Phase = (0, 90, 270, 180, 180,
Presat_Time = 5[s]
Presat_Time_Flag = FALSE
Relaxation_Delay_Calc = 0[s]
Relaxation_Delay_Temp = 5[s]
Repetition_Time = 7.18628096[s]

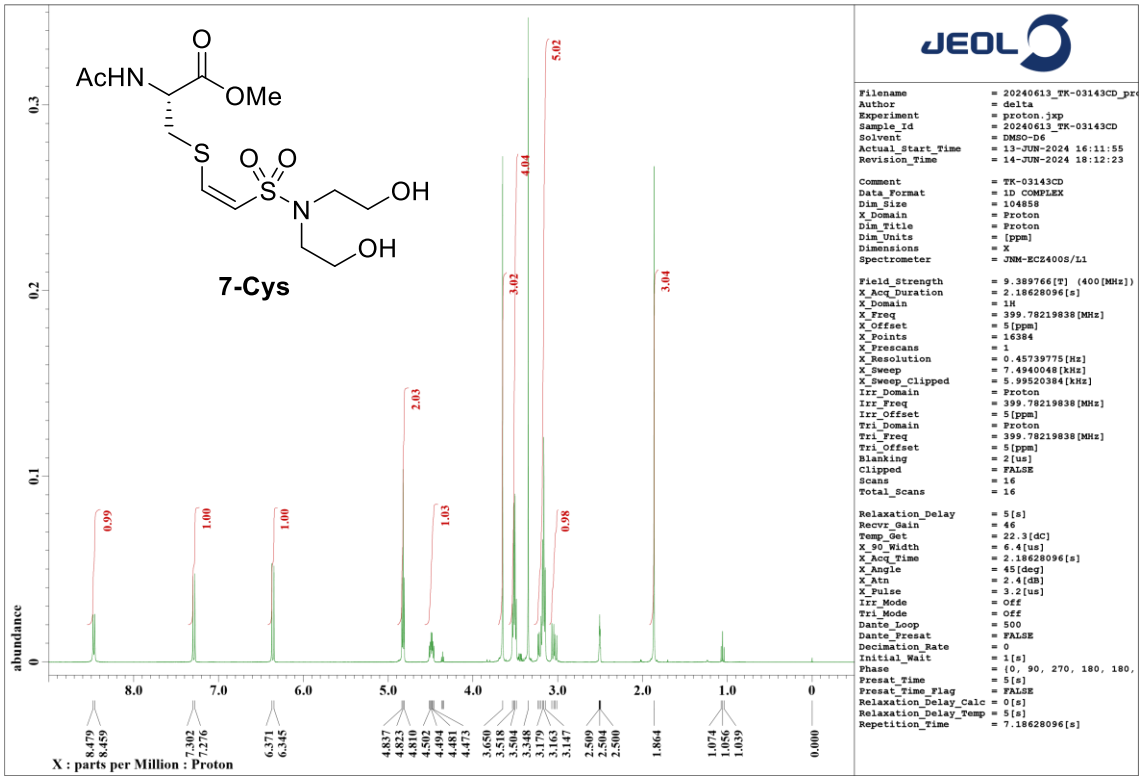

(thousandths)
X : parts per Million : Carbon13
JEOL
Filename = 20240618_TK-03147B_
Author = delta
Experiment = carbon.jxp
Sample_Id = 20240618_TK-03147B
Solvent = DMSO-D6
Actual_Start_Time = 18-JUN-2024 20:15:1
Revision_Time = 19-JUN-2024 11:57:3
Comment = TK-03147B
Data_Format = 1D COMPLEX
Dim_Size = 26214
X_Domain = Carbon13
Dim_Title = Carbon13
Dim_Units = [ppm]
Dimensions = X
Spectrometer = JNM-ECZ400S/L1
Field_Strength = 9.389766[T] (400[MH
X_Acq_Duration = 1.03809024[s]
X_Domain = 13C
X_Freq = 100.52530333[MHz]
X_Offset = 100[ppm]
X_Points = 32768
X_Prescans = 4
X_Resolution = 0.96330739[Hz]
X_Sweep = 31.56565657[kHz]
X_Sweep_Clipped = 25.25252525[kHz]
Irr_Domain = Proton
Irr_Freq = 399.78219838[MHz]
Irr_Offset = 5[ppm]
Blanking = 5[us]
Clipped = TRUE
Scans = 8192
Total_Scans = 8192
Relaxation_Delay = 2[s]
Recvr_Gain = 50
Temp_Get = 22.7[dC]
X_90_Width = 10.02[us]
X_Acq_Time = 1.03809024[s]
X_Angle = 30[deg]
X_Atn = 8[dB]
X_Pulse = 3.34[us]
Irr_Atn_Dec = 27.49[dB]
Irr_Atn_Dec_Calc = 27.49[dB]
Irr_Atn_Dec_Default_Calc = 27.49[dB]
Irr_Atn_Noe = 27.49[dB]
Irr_Dec_Bandwidth_Hz = 4.7826087[kHz]
Irr_Dec_Bandwidth_Ppm = 11.96303566[ppm]
Irr_Dec_Freq = 399.78219838[MHz]
Irr_Dec_Merit_Factor = 2.2
Irr_Decoupling = TRUE
Irr_Noe = TRUE
Irr_Noise = WALTZ
Irr_Offset_Default = 5[ppm]
Irr_Pwidth = 0.115[ms]
Irr_Pwidth_Default = 0.115[ms]
Irr_Pwidth_Default_Calc = 0.115[ms]
Irr_Pwidth_Temp1 = 0.115[ms]
Irr_Wurst = FALSE
Decimation_Rate = 0

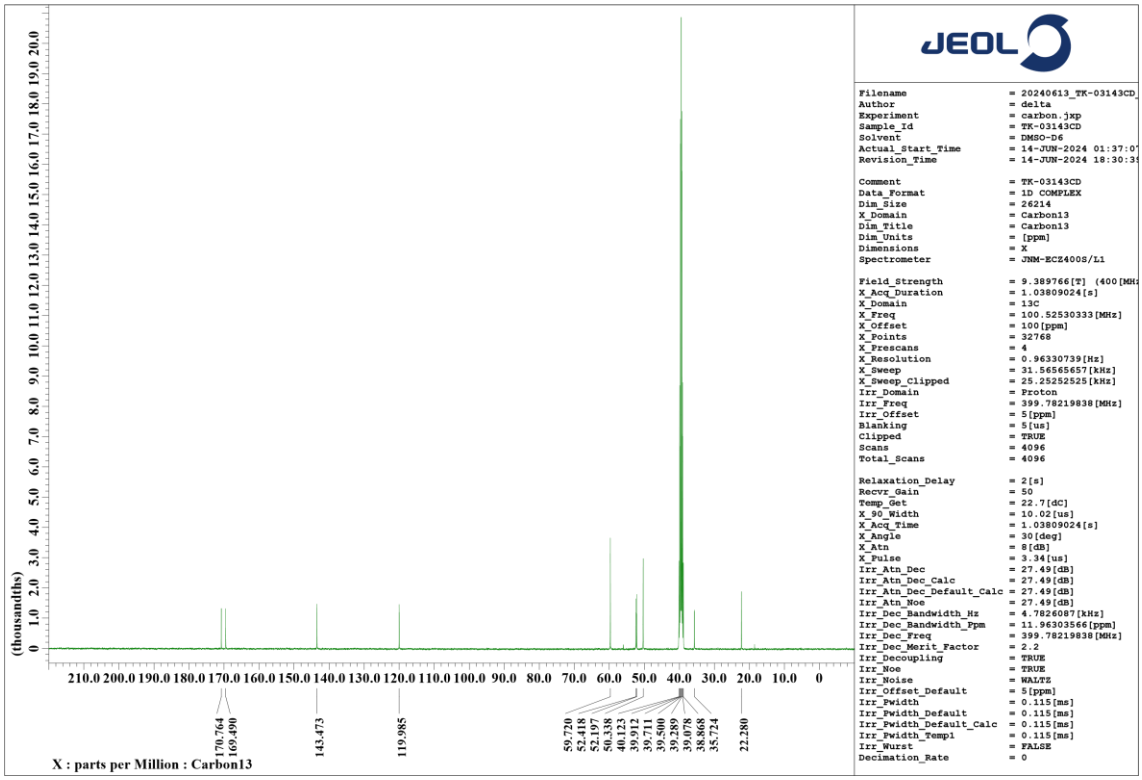

AcHN
OMe
S
O
O
S
N
H
OH
10-Cys
abundance
X : parts per Million : Proton
JEOL
Filename = 20240912_TK-04010I_pro
Author = delta
Experiment = proton.jxp
Sample_Id = 20240912_TK-04010I
Solvent = DMSO-D6
Actual_Start_Time = 12-SEP-2024 17:30:41
Revision_Time = 12-SEP-2024 18:40:29
Comment = TK-04010I
Data_Format = 1D COMPLEX
Dim_Size = 104858
X_Domain = Proton
Dim_Title = Proton
Dim_Units = [ppm]
Dimensions = X
Spectrometer = JNM-ECZ400S/L1
Field_Strength = 9.389766[T] (400[MHz])
X_Acq_Duration = 2.18628096[s]
X_Domain = 1H
X_Freq = 399.78219838[MHz]
X_Offset = 5[ppm]
X_Points = 16384
X_Prescans = 1
X_Resolution = 0.45739775[Hz]
X_Sweep = 7.4940048[kHz]
X_Sweep_Clipped = 5.99520384[kHz]
Irr_Domain = Proton
Irr_Freq = 399.78219838[MHz]
Irr_Offset = 5[ppm]
Tri_Domain = Proton
Tri_Freq = 399.78219838[MHz]
Tri_Offset = 5[ppm]
Blanking = 2[us]
Clipped = FALSE
Scans = 16
Total_Scans = 16
Relaxation_Delay = 5[s]
Recvr_Gain = 46
Temp_Get = 22.8[dC]
X_90_Width = 6.5[us]
X_Acq_Time = 2.18628096[s]
X_Angle = 45[deg]
X_Atn = 2.4[dB]
X_Pulse = 3.25[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Loop = 500
Dante_Presat = FALSE
Decimation_Rate = 0
Initial_Wait = 1[s]
Phase = (0, 90, 270, 180, 180,
Presat_Time = 5[s]
Presat_Time_Flag = FALSE
Relaxation_Delay_Calc = 0[s]
Relaxation_Delay_Temp = 5[s]
Repetition_Time = 7.18628096[s]

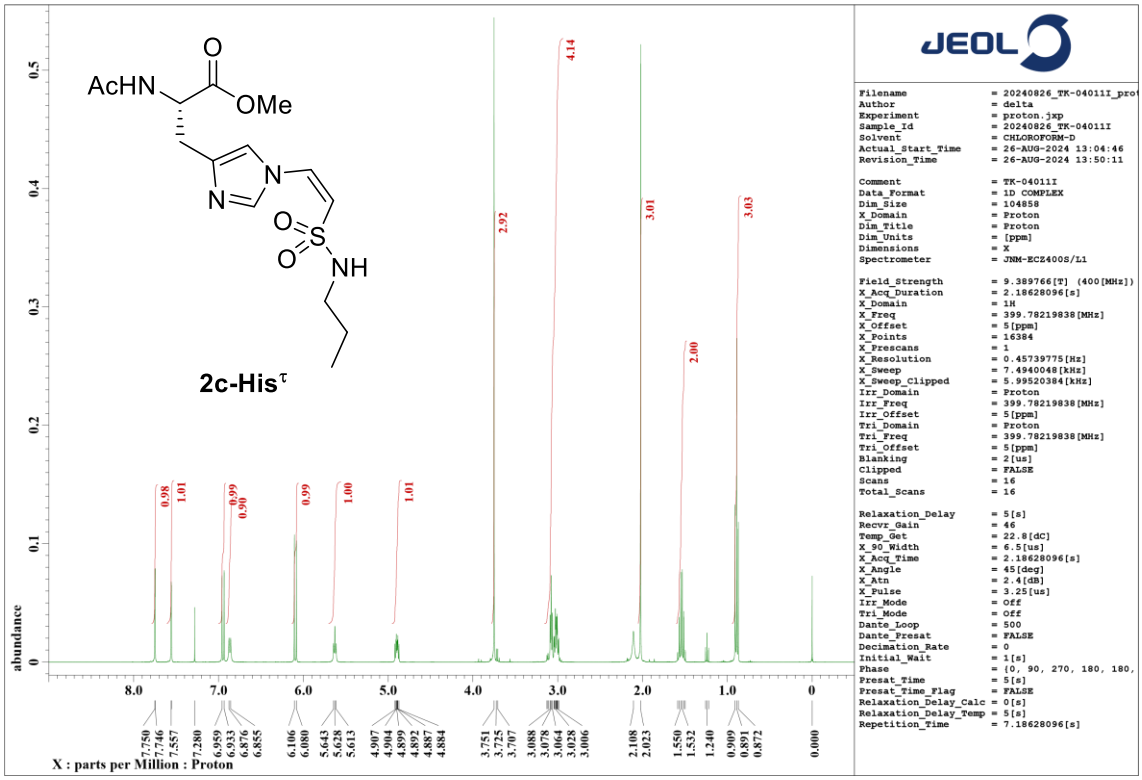

(thousandths)
X : parts per Million : Carbon13
JEOL
Filename = 20240914_TK-04010I_
Author = delta
Experiment = carbon.jxp
Sample_Id = 20240914_TK-04010I
Solvent = DMSO-D6
Actual_Start_Time = 15-SEP-2024 19:31:3
Revision_Time = 17-SEP-2024 10:40:0
Comment = TK-04010I
Data_Format = 1D COMPLEX
Dim_Size = 26214
X_Domain = Carbon13
Dim_Title = Carbon13
Dim_Units = [ppm]
Dimensions = X
Spectrometer = JNM-ECZ400S/L1
Field_Strength = 9.389766[T] (400[MH
X_Acq_Duration = 1.03809024[s]
X_Domain = 13C
X_Freq = 100.52530333[MHz]
X_Offset = 100[ppm]
X_Points = 32768
X_Prescans = 4
X_Resolution = 0.96330739[Hz]
X_Sweep = 31.56565657[kHz]
X_Sweep_Clipped = 25.25252525[kHz]
Irr_Domain = Proton
Irr_Freq = 399.78219838[MHz]
Irr_Offset = 5[ppm]
Blanking = 5[us]
Clipped = TRUE
Scans = 16384
Total_Scans = 16384
Relaxation_Delay = 2[s]
Recvr_Gain = 50
Temp_Get = 23[dC]
X_90_Width = 10.02[us]
X_Acq_Time = 1.03809024[s]
X_Angle = 30[deg]
X_Atn = 8[dB]
X_Pulse = 3.34[us]
Irr_Atn_Dec = 27.356[dB]
Irr_Atn_Dec_Calc = 27.356[dB]
Irr_Atn_Dec_Default_Calc = 27.356[dB]
Irr_Atn_Noe = 27.356[dB]
Irr_Dec_Bandwidth_Hz = 4.7826087[kHz]
Irr_Dec_Bandwidth_Ppm = 11.96303566[ppm]
Irr_Dec_Freq = 399.78219838[MHz]
Irr_Dec_Merit_Factor = 2.2
Irr_Decoupling = TRUE
Irr_Noe = TRUE
Irr_Noise = WALTZ
Irr_Offset_Default = 5[ppm]
Irr_Pwidth = 0.115[ms]
Irr_Pwidth_Default = 0.115[ms]
Irr_Pwidth_Default_Calc = 0.115[ms]
Irr_Pwidth_Temp1 = 0.115[ms]
Irr_Wurst = FALSE
Decimation_Rate = 0

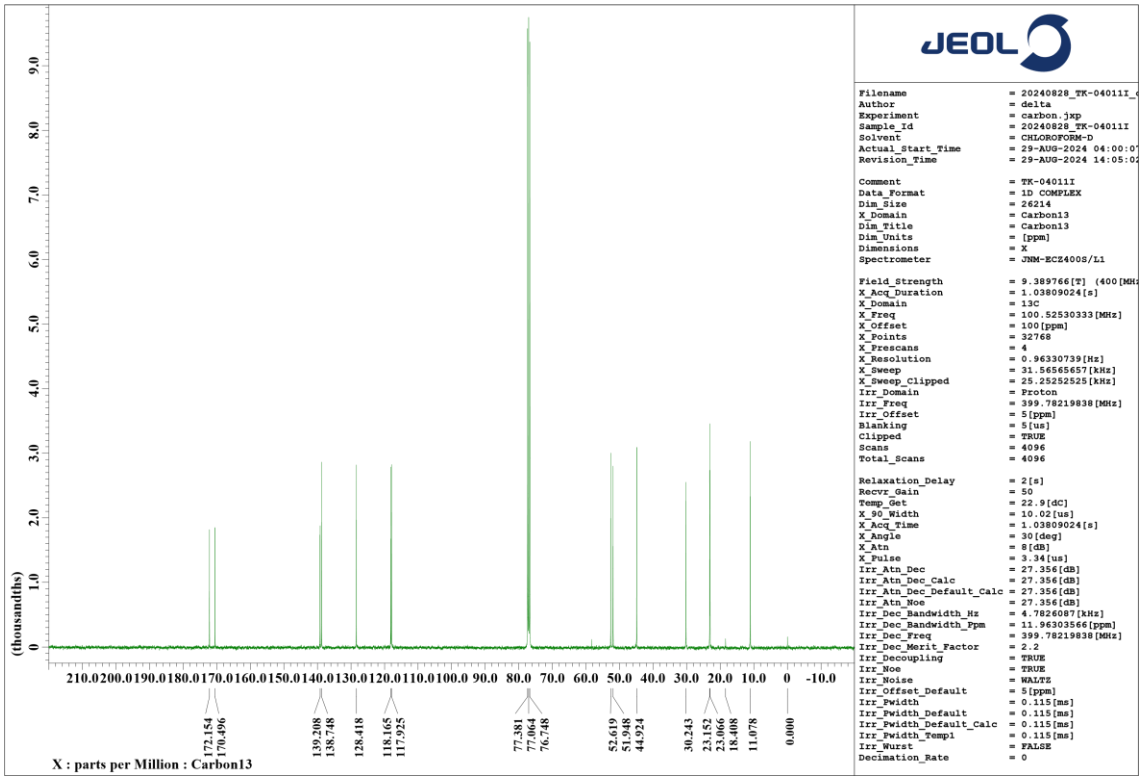

AcHN
OMe
S
O
O
S
N
H
OH
O
6-Cys
abundance
X : parts per Million : Proton
12.062
8.460
8.440
7.232
7.206
6.194
6.168
4.488
4.475
4.467
4.455
4.447
4.434
3.634
3.337
2.835
2.820
2.495
2.490
2.486
2.239
2.220
1.848
1.676
1.658
1.640
1.622
1.604
0.76
1.00
2.02
1.00
1.01
3.02
1.01
0.97
2.04
2.00
3.00
2.01
JEOL
Filename = 20240628_TK-03150C_pro
Author = delta
Experiment = proton.jxp
Sample_Id = 20240628_TK-03150C
Solvent = DMSO-D6
Actual_Start_Time = 28-JUN-2024 19:48:12
Revision_Time = 1-JUL-2024 11:01:25
Comment = TK-03150C
Data_Format = 1D COMPLEX
Dim_Size = 104858
X_Domain = Proton
Dim_Title = Proton
Dim_Units = [ppm]
Dimensions = X
Spectrometer = JNM-ECZ400S/L1
Field_Strength = 9.389766[T] (400[MHz])
X_Acq_Duration = 2.18628096[s]
X_Domain = 1H
X_Freq = 399.78219838[MHz]
X_Offset = 5[ppm]
X_Points = 16384
X_Prescans = 1
X_Resolution = 0.45739775[Hz]
X_Sweep = 7.4940048[kHz]
X_Sweep_Clipped = 5.99520384[kHz]
Irr_Domain = Proton
Irr_Freq = 399.78219838[MHz]
Irr_Offset = 5[ppm]
Tri_Domain = Proton
Tri_Freq = 399.78219838[MHz]
Tri_Offset = 5[ppm]
Blanking = 2[us]
Clipped = FALSE
Scans = 16
Total_Scans = 16
Relaxation_Delay = 5[s]
Recvr_Gain = 56
Temp_Get = 22.8[dC]
X_90_Width = 6.95[us]
X_Acq_Time = 2.18628096[s]
X_Angle = 45[deg]
X_Atn = 2.4[dB]
X_Pulse = 3.475[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Loop = 500
Dante_Presat = FALSE
Decimation_Rate = 0
Initial_Wait = 1[s]
Phase = (0, 90, 270, 180, 180,
Presat_Time = 5[s]
Presat_Time_Flag = FALSE
Relaxation_Delay_Calc = 0[s]
Relaxation_Delay_Temp = 5[s]
Repetition_Time = 7.18628096[s]

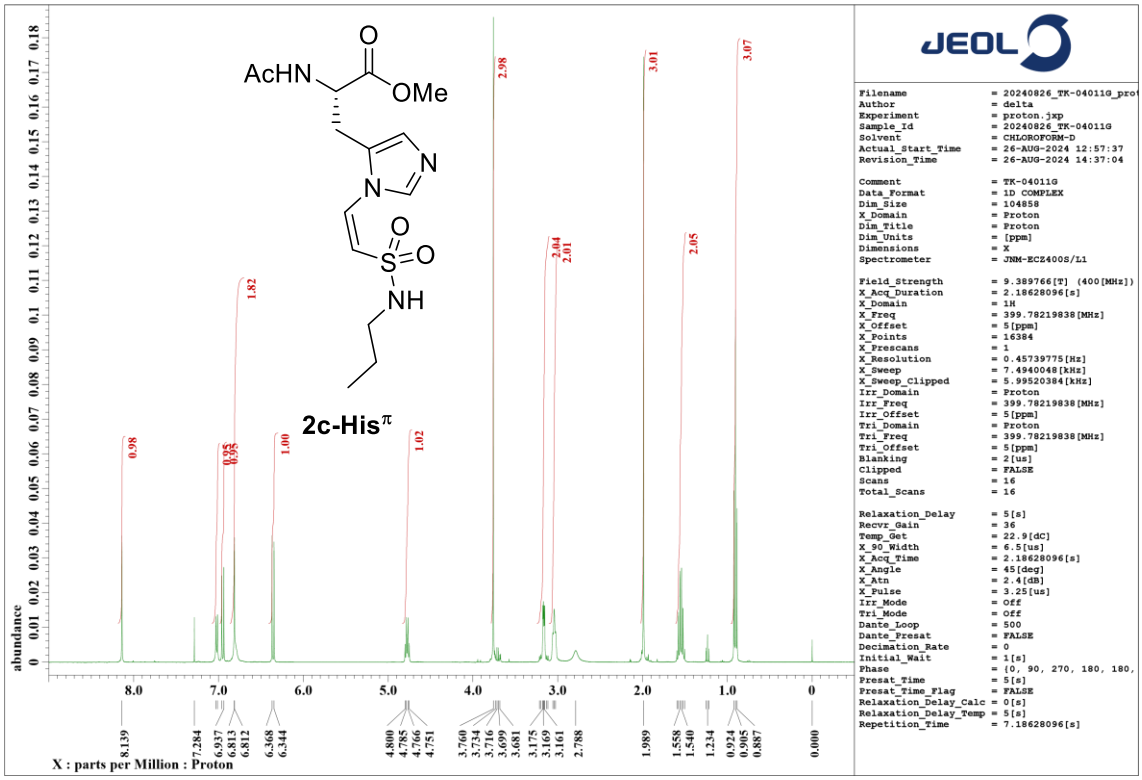

(thousandths)
X : parts per Million : Carbon13
174.070
170.726
169.471
142.725
121.423
52.456
52.178
40.133
39.922
39.711
39.500
39.289
39.088
38.877
35.763
30.732
24.685
22.261
JEOL
Filename = 20240628_TK-03150C_
Author = delta
Experiment = carbon.jxp
Sample_Id = 20240628_TK-03150C
Solvent = DMSO-D6
Actual_Start_Time = 28-JUN-2024 20:05:2
Revision_Time = 10-SEP-2024 18:24:1
Comment = TK-03150C
Data_Format = 1D COMPLEX
Dim_Size = 26214
X_Domain = Carbon13
Dim_Title = Carbon13
Dim_Units = [ppm]
Dimensions = X
Spectrometer = JNM-ECZ400S/L1
Field_Strength = 9.389766[T] (400[MH
X_Acq_Duration = 1.03809024[s]
X_Domain = 13C
X_Freq = 100.52530333[MHz]
X_Offset = 100[ppm]
X_Points = 32768
X_Prescans = 4
X_Resolution = 0.96330739[Hz]
X_Sweep = 31.56565657[kHz]
X_Sweep_Clipped = 25.25252525[kHz]
Irr_Domain = Proton
Irr_Freq = 399.78219838[MHz]
Irr_Offset = 5[ppm]
Blanking = 5[us]
Clipped = TRUE
Scans = 10000
Total_Scans = 10000
Relaxation_Delay = 2[s]
Recvr_Gain = 50
Temp_Get = 25[dC]
X_90_Width = 10.02[us]
X_Acq_Time = 1.03809024[s]
X_Angle = 30[deg]
X_Atn = 8[dB]
X_Pulse = 3.34[us]
Irr_Atn_Dec = 27.4[dB]
Irr_Atn_Dec_Calc = 27.4[dB]
Irr_Atn_Dec_Default_Calc = 27.4[dB]
Irr_Atn_Noe = 27.4[dB]
Irr_Dec_Bandwidth_Hz = 4.7826087[kHz]
Irr_Dec_Bandwidth_Ppm = 11.96303566[ppm]
Irr_Dec_Freq = 399.78219838[MHz]
Irr_Dec_Merit_Factor = 2.2
Irr_Decoupling = TRUE
Irr_Noe = TRUE
Irr_Noise = WALTZ
Irr_Offset_Default = 5[ppm]
Irr_Pwidth = 0.115[ms]
Irr_Pwidth_Default = 0.115[ms]
Irr_Pwidth_Default_Calc = 0.115[ms]
Irr_Pwidth_Temp1 = 0.115[ms]
Irr_Wurst = FALSE
Decimation_Rate = 0


AcHN
OMe
S
O
O
S
N
OH
OH
7-Cys
abundance
X : parts per Million : Proton
Filename = 20240613_TK-03143CD_pr
Author = delta
Experiment = proton.jxp
Sample_Id = 20240613_TK-03143CD
Solvent = DMSO-D6
Actual_Start_Time = 13-JUN-2024 16:11:55
Revision_Time = 14-JUN-2024 18:12:23
Comment = TK-03143CD
Data_Format = 1D COMPLEX
Dim_Size = 104858
X_Domain = Proton
Dim_Title = Proton
Dim_Units = [ppm]
Dimensions = X
Spectrometer = JNM-ECZ400S/L1
Field_Strength = 9.389766[T] (400[MHz])
X_Acq_Duration = 2.18628096[s]
X_Domain = 1H
X_Freq = 399.78219838[MHz]
X_Offset = 5[ppm]
X_Points = 16384
X_Prescans = 1
X_Resolution = 0.45739775[Hz]
X_Sweep = 7.4940048[kHz]
X_Sweep_Clipped = 5.99520384[kHz]
Irr_Domain = Proton
Irr_Freq = 399.78219838[MHz]
Irr_Offset = 5[ppm]
Tri_Domain = Proton
Tri_Freq = 399.78219838[MHz]
Tri_Offset = 5[ppm]
Blanking = 2[us]
Clipped = FALSE
Scans = 16
Total_Scans = 16
Relaxation_Delay = 5[s]
Recvr_Gain = 46
Temp_Get = 22.3[dC]
X_90_Width = 6.4[us]
X_Acq_Time = 2.18628096[s]
X_Angle = 45[deg]
X_Atn = 2.4[dB]
X_Pulse = 3.2[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Loop = 500
Dante_Presat = FALSE
Decimation_Rate = 0
Initial_Wait = 1[s]
Phase = (0, 90, 270, 180, 180,
Presat_Time = 5[s]
Presat_Time_Flag = FALSE
Relaxation_Delay_Calc = 0[s]
Relaxation_Delay_Temp = 5[s]
Repetition_Time = 7.18628096[s]


(thousandths)
X : parts per Million : Carbon13
Filename = 20240613_TK-03143CD_
Author = delta
Experiment = carbon.jxp
Sample_Id = TK-03143CD
Solvent = DMSO-D6
Actual_Start_Time = 14-JUN-2024 01:37:0
Revision_Time = 14-JUN-2024 18:30:3
Comment = TK-03143CD
Data_Format = 1D COMPLEX
Dim_Size = 26214
X_Domain = Carbon13
Dim_Title = Carbon13
Dim_Units = [ppm]
Dimensions = X
Spectrometer = JNM-ECZ400S/L1
Field_Strength = 9.389766[T] (400[MH
X_Acq_Duration = 1.03809024[s]
X_Domain = 13C
X_Freq = 100.52530333[MHz]
X_Offset = 100[ppm]
X_Points = 32768
X_Prescans = 4
X_Resolution = 0.96330739[Hz]
X_Sweep = 31.56565657[kHz]
X_Sweep_Clipped = 25.25252525[kHz]
Irr_Domain = Proton
Irr_Freq = 399.78219838[MHz]
Irr_Offset = 5[ppm]
Blanking = 5[us]
Clipped = TRUE
Scans = 4096
Total_Scans = 4096
Relaxation_Delay = 2[s]
Recvr_Gain = 50
Temp_Get = 22.7[dC]
X_90_Width = 10.02[us]
X_Acq_Time = 1.03809024[s]
X_Angle = 30[deg]
X_Atn = 8[dB]
X_Pulse = 3.34[us]
Irr_Atn_Dec = 27.49[dB]
Irr_Atn_Dec_Calc = 27.49[dB]
Irr_Atn_Dec_Default_Calc = 27.49[dB]
Irr_Atn_Noe = 27.49[dB]
Irr_Dec_Bandwidth_Hz = 4.7826087[kHz]
Irr_Dec_Bandwidth_Ppm = 11.96303566[ppm]
Irr_Dec_Freq = 399.78219838[MHz]
Irr_Dec_Merit_Factor = 2.2
Irr_Decoupling = TRUE
Irr_Noe = TRUE
Irr_Noise = WALTZ
Irr_Offset_Default = 5[ppm]
Irr_Pwidth = 0.115[ms]
Irr_Pwidth_Default = 0.115[ms]
Irr_Pwidth_Default_Calc = 0.115[ms]
Irr_Pwidth_Temp1 = 0.115[ms]
Irr_Wurst = FALSE
Decimation_Rate = 0


AcHN
OMe
O
N
N
O
S
O
NH
2c-His$^{\tau}$
abundance
X : parts per Million : Proton
JEOL
Filename = 20240826_TK-04011I_pro
Author = delta
Experiment = proton.jxp
Sample_Id = 20240826_TK-04011I
Solvent = CHLOROFORM-D
Actual_Start_Time = 26-AUG-2024 13:04:46
Revision_Time = 26-AUG-2024 13:50:11
Comment = TK-04011I
Data_Format = 1D COMPLEX
Dim_Size = 104858
X_Domain = Proton
Dim_Title = Proton
Dim_Units = [ppm]
Dimensions = X
Spectrometer = JNM-ECZ400S/L1
Field_Strength = 9.389766[T] (400[MHz])
X_Acq_Duration = 2.18628096[s]
X_Domain = 1H
X_Freq = 399.78219838[MHz]
X_Offset = 5[ppm]
X_Points = 16384
X_Prescans = 1
X_Resolution = 0.45739775[Hz]
X_Sweep = 7.4940048[kHz]
X_Sweep_Clipped = 5.99520384[kHz]
Irr_Domain = Proton
Irr_Freq = 399.78219838[MHz]
Irr_Offset = 5[ppm]
Tri_Domain = Proton
Tri_Freq = 399.78219838[MHz]
Tri_Offset = 5[ppm]
Blanking = 2[us]
Clipped = FALSE
Scans = 16
Total_Scans = 16
Relaxation_Delay = 5[s]
Recvr_Gain = 46
Temp_Get = 22.8[dC]
X_90_Width = 6.5[us]
X_Acq_Time = 2.18628096[s]
X_Angle = 45[deg]
X_Atn = 2.4[dB]
X_Pulse = 3.25[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Loop = 500
Dante_Presat = FALSE
Decimation_Rate = 0
Initial_Wait = 1[s]
Phase = (0, 90, 270, 180, 180,
Presat_Time = 5[s]
Presat_Time_Flag = FALSE
Relaxation_Delay_Calc = 0[s]
Relaxation_Delay_Temp = 5[s]
Repetition_Time = 7.18628096[s]


(thousandths)
X : parts per Million : Carbon13
JEOL
Filename = 20240828_TK-04011I_
Author = delta
Experiment = carbon.jxp
Sample_Id = 20240828_TK-04011I
Solvent = CHLOROFORM-D
Actual_Start_Time = 29-AUG-2024 04:00:0
Revision_Time = 29-AUG-2024 14:05:0
Comment = TK-04011I
Data_Format = 1D COMPLEX
Dim_Size = 26214
X_Domain = Carbon13
Dim_Title = Carbon13
Dim_Units = [ppm]
Dimensions = X
Spectrometer = JNM-ECZ400S/L1
Field_Strength = 9.389766[T] (400[MH
X_Acq_Duration = 1.03809024[s]
X_Domain = 13C
X_Freq = 100.52530333[MHz]
X_Offset = 100[ppm]
X_Points = 32768
X_Prescans = 4
X_Resolution = 0.96330739[Hz]
X_Sweep = 31.56565657[kHz]
X_Sweep_Clipped = 25.25252525[kHz]
Irr_Domain = Proton
Irr_Freq = 399.78219838[MHz]
Irr_Offset = 5[ppm]
Blanking = 5[us]
Clipped = TRUE
Scans = 4096
Total_Scans = 4096
Relaxation_Delay = 2[s]
Recvr_Gain = 50
Temp_Get = 22.9[dC]
X_90_Width = 10.02[us]
X_Acq_Time = 1.03809024[s]
X_Angle = 30[deg]
X_Atn = 8[dB]
X_Pulse = 3.34[us]
Irr_Atn_Dec = 27.356[dB]
Irr_Atn_Dec_Calc = 27.356[dB]
Irr_Atn_Dec_Default_Calc = 27.356[dB]
Irr_Atn_Noe = 27.356[dB]
Irr_Dec_Bandwidth_Hz = 4.7826087[kHz]
Irr_Dec_Bandwidth_Ppm = 11.96303566[ppm]
Irr_Dec_Freq = 399.78219838[MHz]
Irr_Dec_Merit_Factor = 2.2
Irr_Decoupling = TRUE
Irr_Noe = TRUE
Irr_Noise = WALTZ
Irr_Offset_Default = 5[ppm]
Irr_Pwidth = 0.115[ms]
Irr_Pwidth_Default = 0.115[ms]
Irr_Pwidth_Default_Calc = 0.115[ms]
Irr_Pwidth_Temp1 = 0.115[ms]
Irr_Wurst = FALSE
Decimation_Rate = 0


AcHN
OMe
N
N
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S
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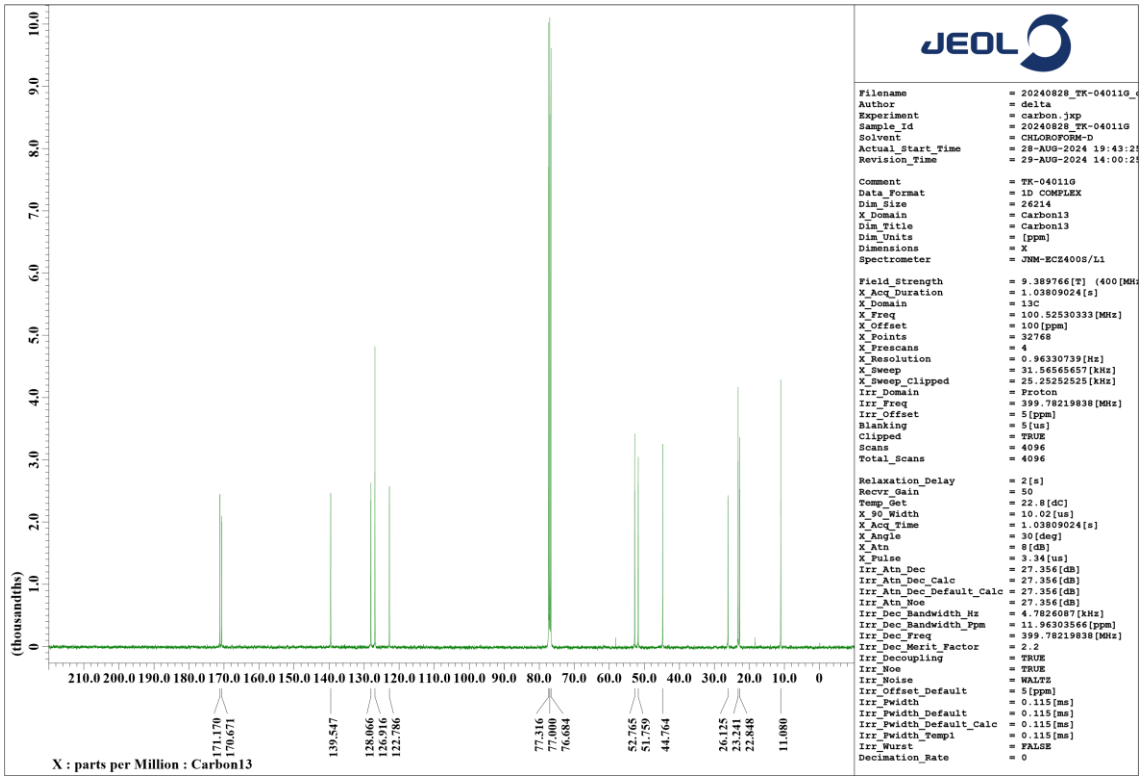
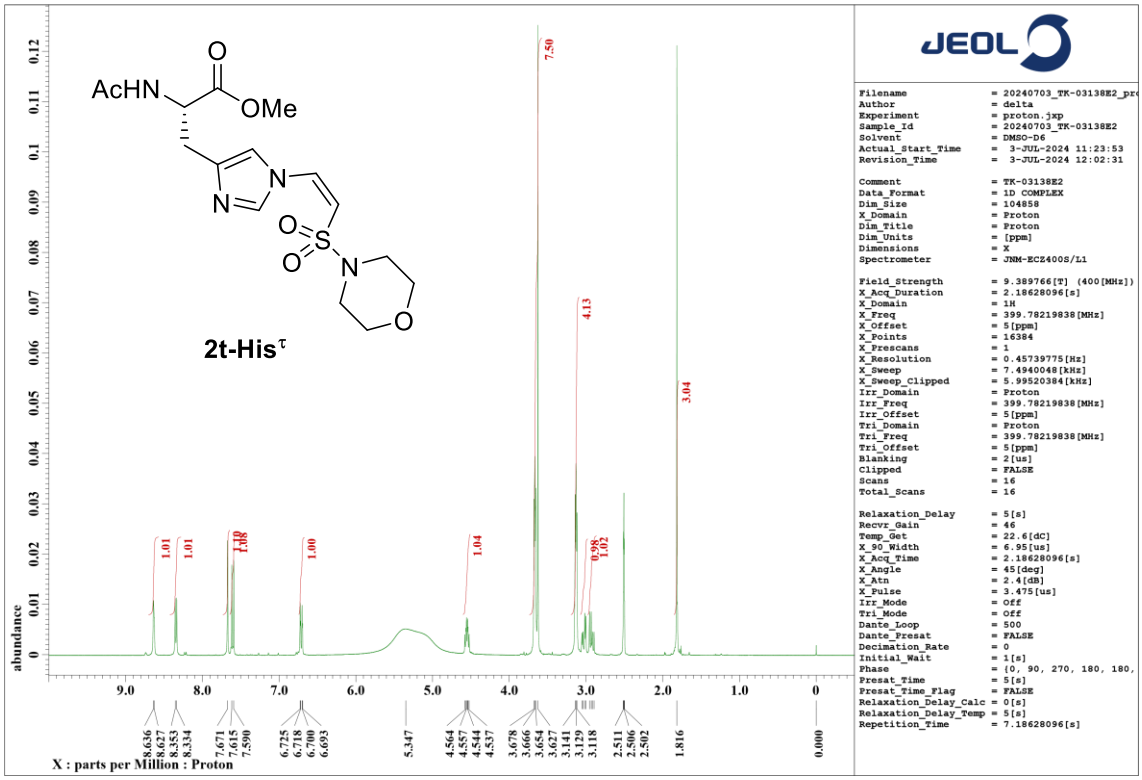
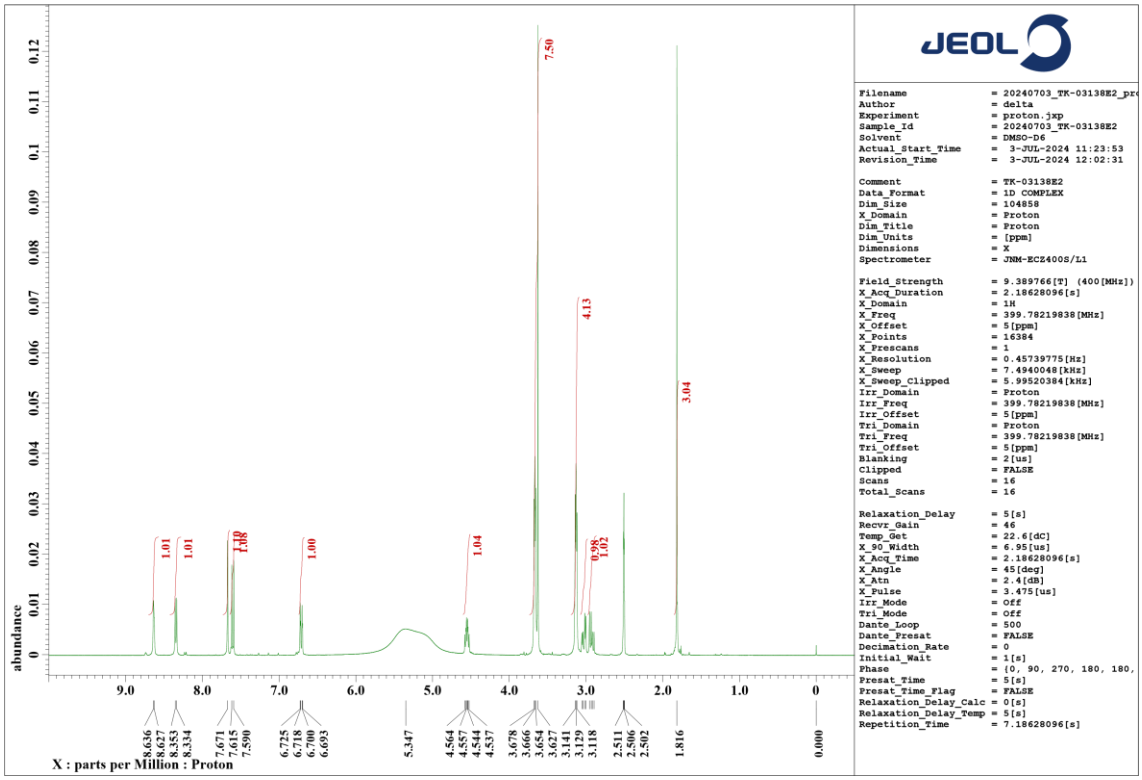
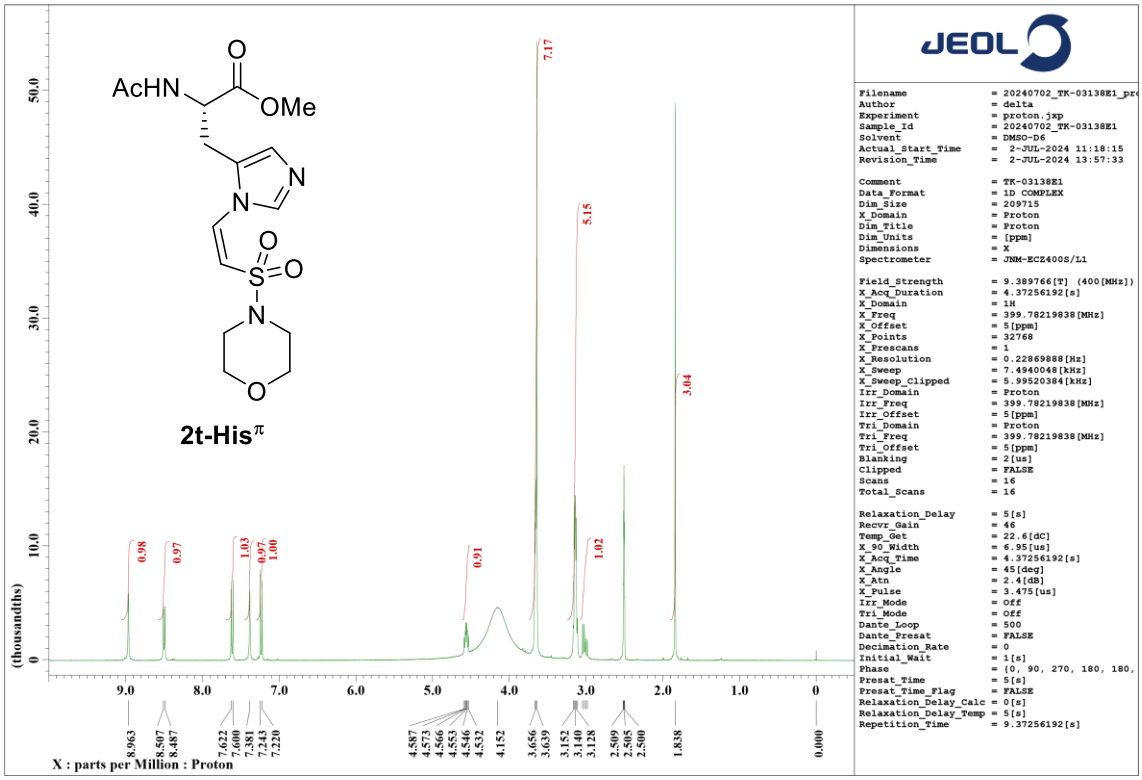
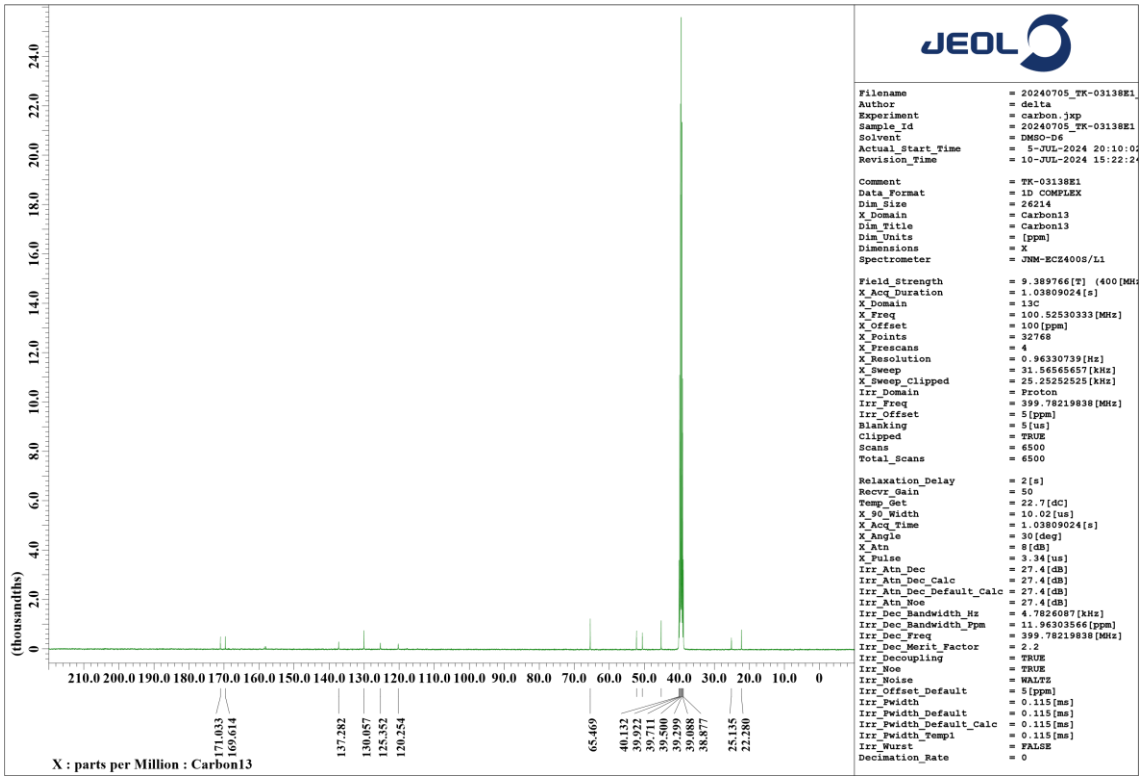
NH
2c-His$^{\pi}$
abundance
X : parts per Million : Proton
JEOL
Filename = 20240826_TK-04011G_pro
Author = delta
Experiment = proton.jxp
Sample_Id = 20240826_TK-04011G
Solvent = CHLOROFORM-D
Actual_Start_Time = 26-AUG-2024 12:57:37
Revision_Time = 26-AUG-2024 14:37:04
Comment = TK-04011G
Data_Format = 1D COMPLEX
Dim_Size = 104858
X_Domain = Proton
Dim_Title = Proton
Dim_Units = [ppm]
Dimensions = X
Spectrometer = JNM-ECZ400S/L1
Field_Strength = 9.389766[T] (400[MHz])
X_Acq_Duration = 2.18628096[s]
X_Domain = 1H
X_Freq = 399.78219838[MHz]
X_Offset = 5[ppm]
X_Points = 16384
X_Prescans = 1
X_Resolution = 0.45739775[Hz]
X_Sweep = 7.4940048[kHz]
X_Sweep_Clipped = 5.99520384[kHz]
Irr_Domain = Proton
Irr_Freq = 399.78219838[MHz]
Irr_Offset = 5[ppm]
Tri_Domain = Proton
Tri_Freq = 399.78219838[MHz]
Tri_Offset = 5[ppm]
Blanking = 2[us]
Clipped = FALSE
Scans = 16
Total_Scans = 16
Relaxation_Delay = 5[s]
Recvr_Gain = 36
Temp_Get = 22.9[dC]
X_90_Width = 6.5[us]
X_Acq_Time = 2.18628096[s]
X_Angle = 45[deg]
X_Atn = 2.4[dB]
X_Pulse = 3.25[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Loop = 500
Dante_Presat = FALSE
Decimation_Rate = 0
Initial_Wait = 1[s]
Phase = (0, 90, 270, 180, 180,
Presat_Time = 5[s]
Presat_Time_Flag = FALSE
Relaxation_Delay_Calc = 0[s]
Relaxation_Delay_Temp = 5[s]
Repetition_Time = 7.18628096[s]

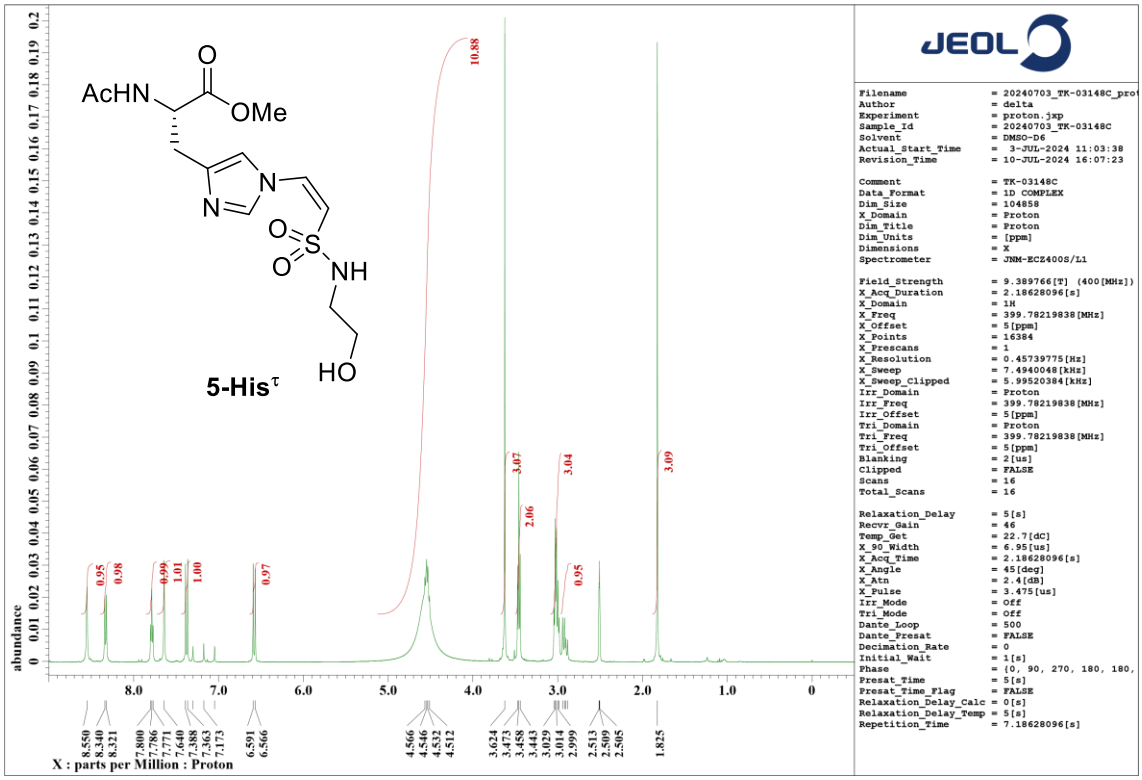

(thousandths)
X : parts per Million : Carbon13
JEOL
Filename = 20240828_TK-04011G_
Author = delta
Experiment = carbon.jxp
Sample_Id = 20240828_TK-04011G
Solvent = CHLOROFORM-D
Actual_Start_Time = 28-AUG-2024 19:43:2
Revision_Time = 29-AUG-2024 14:00:2
Comment = TK-04011G
Data_Format = 1D COMPLEX
Dim_Size = 26214
X_Domain = Carbon13
Dim_Title = Carbon13
Dim_Units = [ppm]
Dimensions = X
Spectrometer = JNM-ECZ400S/L1
Field_Strength = 9.389766[T] (400[MH
X_Acq_Duration = 1.03809024[s]
X_Domain = 13C
X_Freq = 100.52530333[MHz]
X_Offset = 100[ppm]
X_Points = 32768
X_Prescans = 4
X_Resolution = 0.96330739[Hz]
X_Sweep = 31.56565657[kHz]
X_Sweep_Clipped = 25.25252525[kHz]
Irr_Domain = Proton
Irr_Freq = 399.78219838[MHz]
Irr_Offset = 5[ppm]
Blanking = 5[us]
Clipped = TRUE
Scans = 4096
Total_Scans = 4096
Relaxation_Delay = 2[s]
Recvr_Gain = 50
Temp_Get = 22.8[dC]
X_90_Width = 10.02[us]
X_Acq_Time = 1.03809024[s]
X_Angle = 30[deg]
X_Atn = 8[dB]
X_Pulse = 3.34[us]
Irr_Atn_Dec = 27.356[dB]
Irr_Atn_Dec_Calc = 27.356[dB]
Irr_Atn_Dec_Default_Calc = 27.356[dB]
Irr_Atn_Noe = 27.356[dB]
Irr_Dec_Bandwidth_Hz = 4.7826087[kHz]
Irr_Dec_Bandwidth_Ppm = 11.96303566[ppm]
Irr_Dec_Freq = 399.78219838[MHz]
Irr_Dec_Merit_Factor = 2.2
Irr_Decoupling = TRUE
Irr_Noe = TRUE
Irr_Noise = WALTZ
Irr_Offset_Default = 5[ppm]
Irr_Pwidth = 0.115[ms]
Irr_Pwidth_Default = 0.115[ms]
Irr_Pwidth_Default_Calc = 0.115[ms]
Irr_Pwidth_Temp1 = 0.115[ms]
Irr_Wurst = FALSE
Decimation_Rate = 0

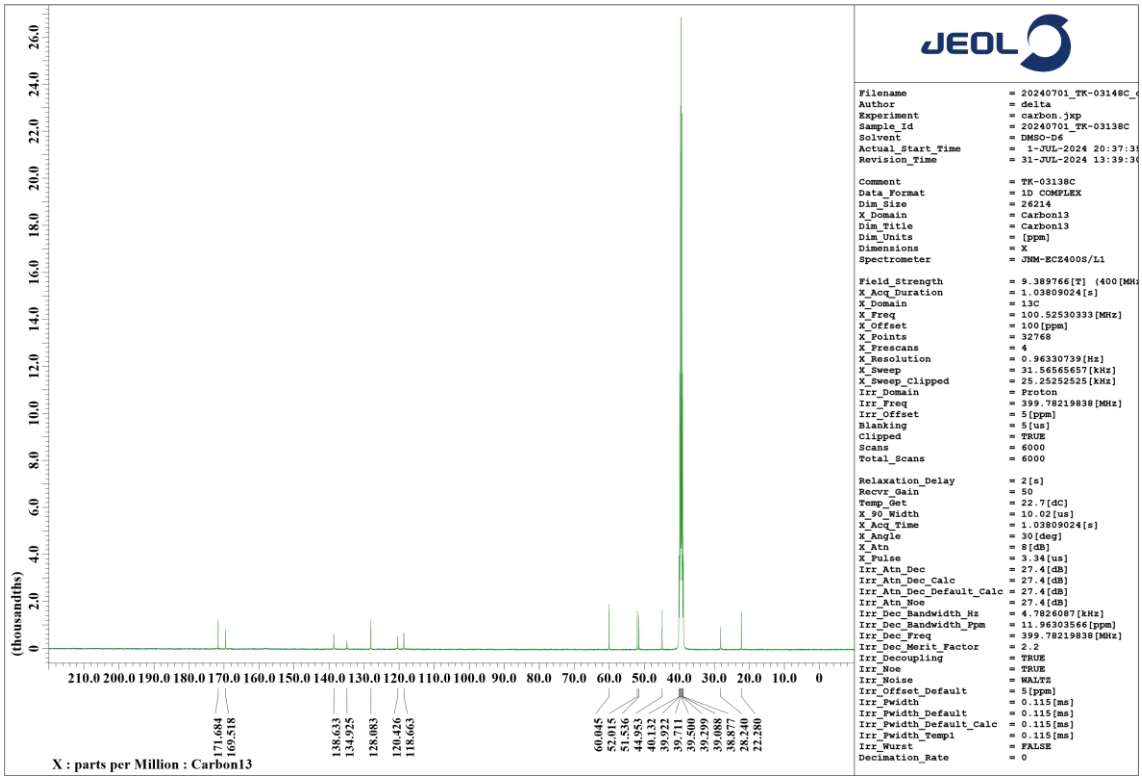

AcHN
O
OMe
N
N
O
S
O
N
O
2t-His$^{\tau}$
7.50
4.13
3.04
1.01
1.01
1.10
1.08
1.00
1.04
0.98
1.02
abundance
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
8.636
8.627
8.353
8.334
7.671
7.615
7.590
6.725
6.718
6.700
6.693
5.347
4.564
4.557
4.544
4.537
3.678
3.666
3.654
3.627
3.141
3.129
3.118
2.511
2.506
2.502
1.816
0.000
X : parts per Million : Proton
JEOL
Filename = 20240703_TK-03138E2_pr
Author = delta
Experiment = proton.jxp
Sample_Id = 20240703_TK-03138E2
Solvent = DMSO-D6
Actual_Start_Time = 3-JUL-2024 11:23:53
Revision_Time = 3-JUL-2024 12:02:31
Comment = TK-03138E2
Data_Format = 1D COMPLEX
Dim_Size = 104858
X_Domain = Proton
Dim_Title = Proton
Dim_Units = [ppm]
Dimensions = X
Spectrometer = JNM-ECZ400S/L1
Field_Strength = 9.389766[T] (400[MHz])
X_Acq_Duration = 2.18628096[s]
X_Domain = 1H
X_Freq = 399.78219838[MHz]
X_Offset = 5[ppm]
X_Points = 16384
X_Prescans = 1
X_Resolution = 0.45739775[Hz]
X_Sweep = 7.4940048[kHz]
X_Sweep_Clipped = 5.99520384[kHz]
Irr_Domain = Proton
Irr_Freq = 399.78219838[MHz]
Irr_Offset = 5[ppm]
Tri_Domain = Proton
Tri_Freq = 399.78219838[MHz]
Tri_Offset = 5[ppm]
Blanking = 2[us]
Clipped = FALSE
Scans = 16
Total_Scans = 16
Relaxation_Delay = 5[s]
Recvr_Gain = 46
Temp_Get = 22.6[dC]
X_90_Width = 6.95[us]
X_Acq_Time = 2.18628096[s]
X_Angle = 45[deg]
X_Atn = 2.4[dB]
X_Pulse = 3.475[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Loop = 500
Dante_Presat = FALSE
Decimation_Rate = 0
Initial_Wait = 1[s]
Phase = {0, 90, 270, 180, 180,
Presat_Time = 5[s]
Presat_Time_Flag = FALSE
Relaxation_Delay_Calc = 0[s]
Relaxation_Delay_Temp = 5[s]
Repetition_Time = 7.18628096[s]

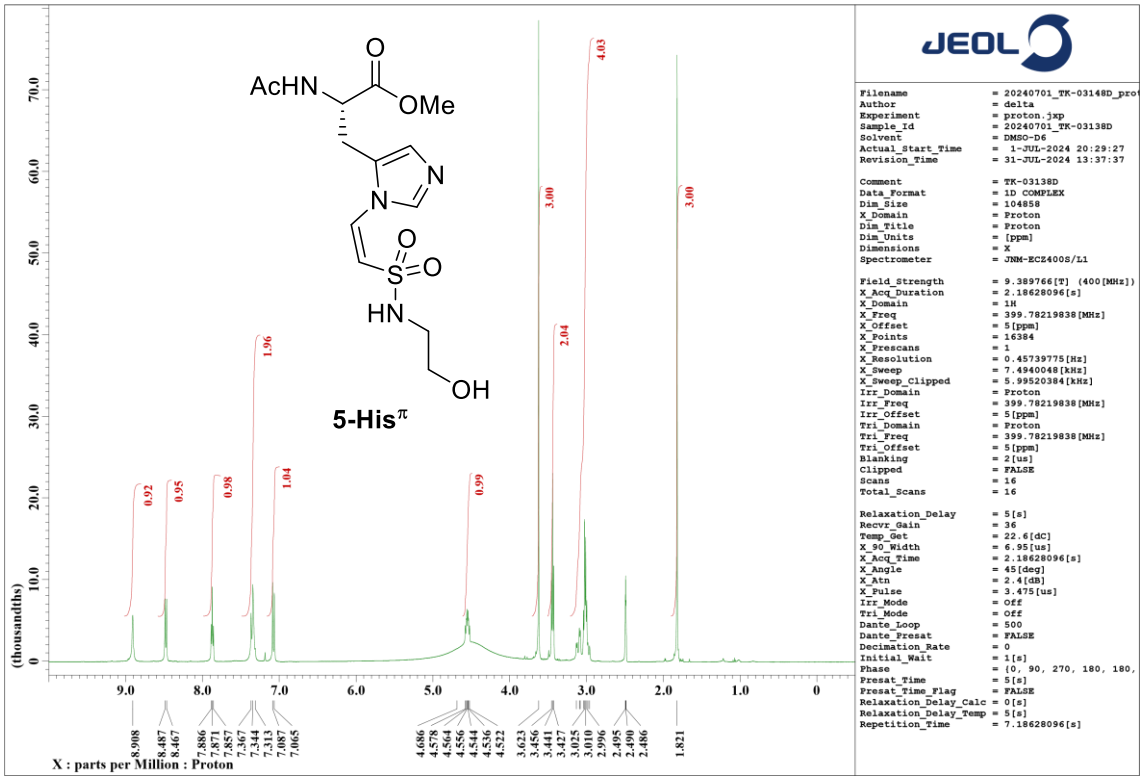

7.50
4.13
3.04
1.01
1.01
1.10
1.08
1.00
1.04
0.98
1.02
abundance
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
8.636
8.627
8.353
8.334
7.671
7.615
7.590
6.725
6.718
6.700
6.693
5.347
4.564
4.557
4.544
4.537
3.678
3.666
3.654
3.627
3.141
3.129
3.118
2.511
2.506
2.502
1.816
0.000
X : parts per Million : Proton
JEOL
Filename = 20240703_TK-03138E2_pr
Author = delta
Experiment = proton.jxp
Sample_Id = 20240703_TK-03138E2
Solvent = DMSO-D6
Actual_Start_Time = 3-JUL-2024 11:23:53
Revision_Time = 3-JUL-2024 12:02:31
Comment = TK-03138E2
Data_Format = 1D COMPLEX
Dim_Size = 104858
X_Domain = Proton
Dim_Title = Proton
Dim_Units = [ppm]
Dimensions = X
Spectrometer = JNM-ECZ400S/L1
Field_Strength = 9.389766[T] (400[MHz])
X_Acq_Duration = 2.18628096[s]
X_Domain = 1H
X_Freq = 399.78219838[MHz]
X_Offset = 5[ppm]
X_Points = 16384
X_Prescans = 1
X_Resolution = 0.45739775[Hz]
X_Sweep = 7.4940048[kHz]
X_Sweep_Clipped = 5.99520384[kHz]
Irr_Domain = Proton
Irr_Freq = 399.78219838[MHz]
Irr_Offset = 5[ppm]
Tri_Domain = Proton
Tri_Freq = 399.78219838[MHz]
Tri_Offset = 5[ppm]
Blanking = 2[us]
Clipped = FALSE
Scans = 16
Total_Scans = 16
Relaxation_Delay = 5[s]
Recvr_Gain = 46
Temp_Get = 22.6[dC]
X_90_Width = 6.95[us]
X_Acq_Time = 2.18628096[s]
X_Angle = 45[deg]
X_Atn = 2.4[dB]
X_Pulse = 3.475[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Loop = 500
Dante_Presat = FALSE
Decimation_Rate = 0
Initial_Wait = 1[s]
Phase = {0, 90, 270, 180, 180,
Presat_Time = 5[s]
Presat_Time_Flag = FALSE
Relaxation_Delay_Calc = 0[s]
Relaxation_Delay_Temp = 5[s]
Repetition_Time = 7.18628096[s]

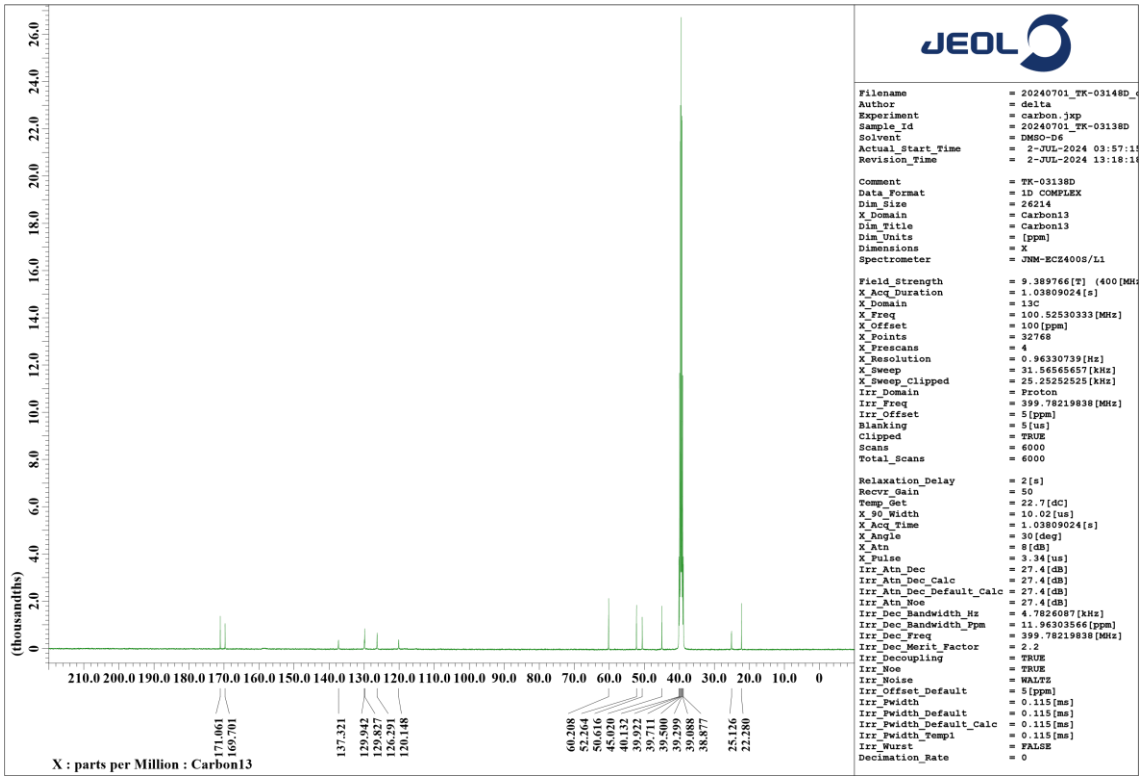

AcHN
OMe
2t-His$^{\pi}$
X : parts per Million : Proton
Filename = 20240702_TK-03138E1_pr
Author = delta
Experiment = proton.jxp
Sample_Id = 20240702_TK-03138E1
Solvent = DMSO-D6
Actual_Start_Time = 2-JUL-2024 11:18:15
Revision_Time = 2-JUL-2024 13:57:33
Comment = TK-03138E1
Data_Format = 1D COMPLEX
Dim_Size = 209715
X_Domain = Proton
Dim_Title = Proton
Dim_Units = [ppm]
Dimensions = X
Spectrometer = JNM-ECZ400S/L1
Field_Strength = 9.389766[T] (400[MHz])
X_Acq_Duration = 4.37256192[s]
X_Domain = 1H
X_Freq = 399.78219838[MHz]
X_Offset = 5[ppm]
X_Points = 32768
X_Prescans = 1
X_Resolution = 0.22869888[Hz]
X_Sweep = 7.4940048[kHz]
X_Sweep_Clipped = 5.99520384[kHz]
Irr_Domain = Proton
Irr_Freq = 399.78219838[MHz]
Irr_Offset = 5[ppm]
Tri_Domain = Proton
Tri_Freq = 399.78219838[MHz]
Tri_Offset = 5[ppm]
Blanking = 2[us]
Clipped = FALSE
Scans = 16
Total_Scans = 16
Relaxation_Delay = 5[s]
Recvr_Gain = 46
Temp_Get = 22.6[dC]
X_90_Width = 6.95[us]
X_Acq_Time = 4.37256192[s]
X_Angle = 45[deg]
X_Atn = 2.4[dB]
X_Pulse = 3.475[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Loop = 500
Dante_Presat = FALSE
Decimation_Rate = 0
Initial_Wait = 1[s]
Phase = (0, 90, 270, 180, 180,
Presat_Time = 5[s]
Presat_Time_Flag = FALSE
Relaxation_Delay_Calc = 0[s]
Relaxation_Delay_Temp = 5[s]
Repetition_Time = 9.37256192[s]

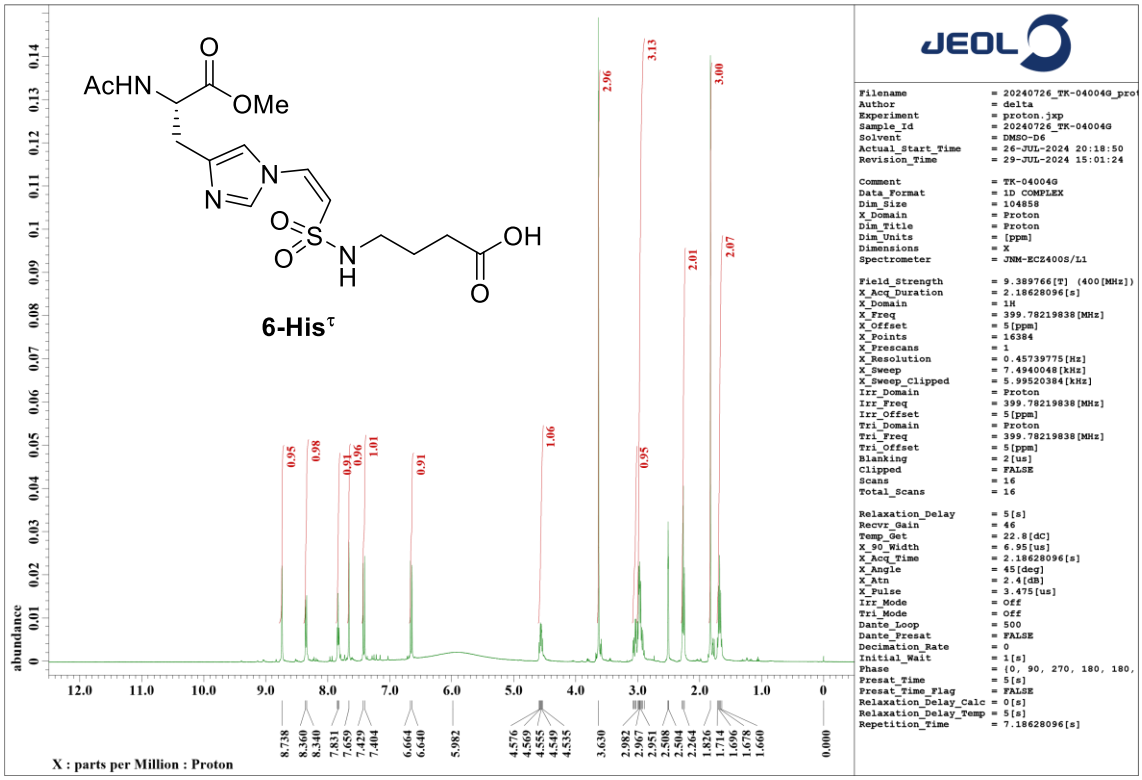

X : parts per Million : Carbon13
Filename = 20240705_TK-03138E1_
Author = delta
Experiment = carbon.jxp
Sample_Id = 20240705_TK-03138E1
Solvent = DMSO-D6
Actual_Start_Time = 5-JUL-2024 20:10:0
Revision_Time = 10-JUL-2024 15:22:2
Comment = TK-03138E1
Data_Format = 1D COMPLEX
Dim_Size = 26214
X_Domain = Carbon13
Dim_Title = Carbon13
Dim_Units = [ppm]
Dimensions = X
Spectrometer = JNM-ECZ400S/L1
Field_Strength = 9.389766[T] (400[MH
X_Acq_Duration = 1.03809024[s]
X_Domain = 13C
X_Freq = 100.52530333[MHz]
X_Offset = 100[ppm]
X_Points = 32768
X_Prescans = 4
X_Resolution = 0.96330739[Hz]
X_Sweep = 31.56565657[kHz]
X_Sweep_Clipped = 25.25252525[kHz]
Irr_Domain = Proton
Irr_Freq = 399.78219838[MHz]
Irr_Offset = 5[ppm]
Blanking = 5[us]
Clipped = TRUE
Scans = 6500
Total_Scans = 6500
Relaxation_Delay = 2[s]
Recvr_Gain = 50
Temp_Get = 22.7[dC]
X_90_Width = 10.02[us]
X_Acq_Time = 1.03809024[s]
X_Angle = 30[deg]
X_Atn = 8[dB]
X_Pulse = 3.34[us]
Irr_Atn_Dec = 27.4[dB]
Irr_Atn_Dec_Calc = 27.4[dB]
Irr_Atn_Dec_Default_Calc = 27.4[dB]
Irr_Atn_Noe = 27.4[dB]
Irr_Dec_Bandwidth_Hz = 4.7826087[kHz]
Irr_Dec_Bandwidth_Ppm = 11.96303566[ppm]
Irr_Dec_Freq = 399.78219838[MHz]
Irr_Dec_Merit_Factor = 2.2
Irr_Decoupling = TRUE
Irr_Noe = TRUE
Irr_Noise = WALTZ
Irr_Offset_Default = 5[ppm]
Irr_Pwidth = 0.115[ms]
Irr_Pwidth_Default = 0.115[ms]
Irr_Pwidth_Default_Calc = 0.115[ms]
Irr_Pwidth_Temp1 = 0.115[ms]
Irr_Wurst = FALSE
Decimation_Rate = 0

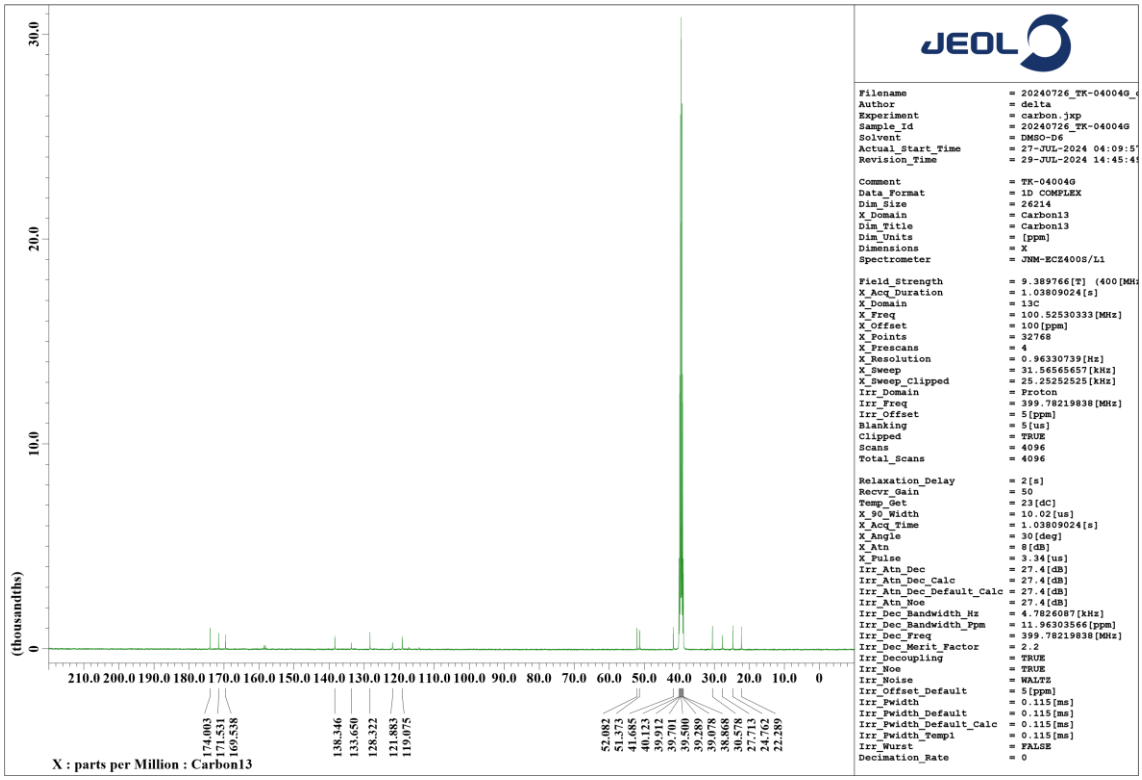

AcHN
O
OMe
N
N
O
S
O
NH
HO
5-His$^{\tau}$
abundance
X : parts per Million : Proton
10.88
3.07
2.06
3.04
3.09
0.95
0.98
0.99
1.01
1.00
0.97
0.95
JEOL
Filename = 20240703_TK-03148C_pro
Author = delta
Experiment = proton.jxp
Sample_Id = 20240703_TK-03148C
Solvent = DMSO-D6
Actual_Start_Time = 3-JUL-2024 11:03:38
Revision_Time = 10-JUL-2024 16:07:23
Comment = TK-03148C
Data_Format = 1D COMPLEX
Dim_Size = 104858
X_Domain = Proton
Dim_Title = Proton
Dim_Units = [ppm]
Dimensions = X
Spectrometer = JNM-ECZ400S/L1
Field_Strength = 9.389766[T] (400[MHz])
X_Acq_Duration = 2.18628096[s]
X_Domain = 1H
X_Freq = 399.78219838[MHz]
X_Offset = 5[ppm]
X_Points = 16384
X_Prescans = 1
X_Resolution = 0.45739775[Hz]
X_Sweep = 7.4940048[kHz]
X_Sweep_Clipped = 5.99520384[kHz]
Irr_Domain = Proton
Irr_Freq = 399.78219838[MHz]
Irr_Offset = 5[ppm]
Tri_Domain = Proton
Tri_Freq = 399.78219838[MHz]
Tri_Offset = 5[ppm]
Blanking = 2[us]
Clipped = FALSE
Scans = 16
Total_Scans = 16
Relaxation_Delay = 5[s]
Recvr_Gain = 46
Temp_Get = 22.7[dC]
X_90_Width = 6.95[us]
X_Acq_Time = 2.18628096[s]
X_Angle = 45[deg]
X_Atn = 2.4[dB]
X_Pulse = 3.475[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Loop = 500
Dante_Presat = FALSE
Decimation_Rate = 0
Initial_Wait = 1[s]
Phase = (0, 90, 270, 180, 180,
Presat_Time = 5[s]
Presat_Time_Flag = FALSE
Relaxation_Delay_Calc = 0[s]
Relaxation_Delay_Temp = 5[s]
Repetition_Time = 7.18628096[s]

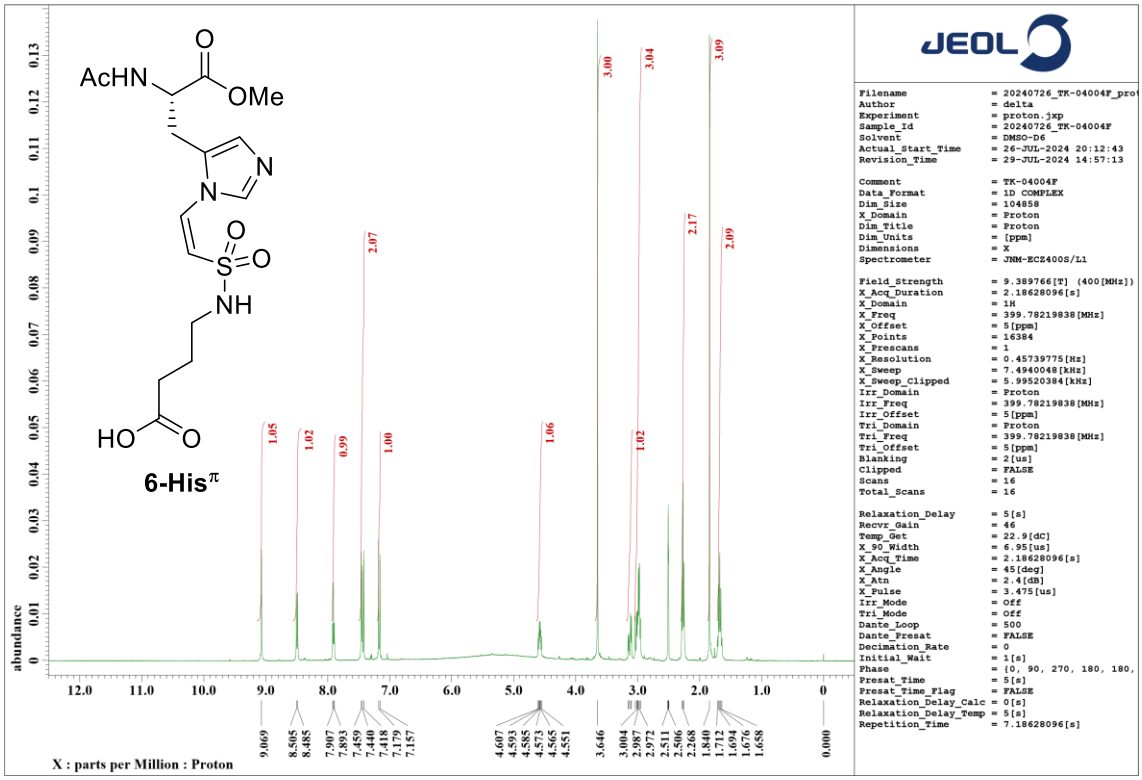

(thousandths)
X : parts per Million : Carbon13
JEOL
Filename = 20240701_TK-03148C_
Author = delta
Experiment = carbon.jxp
Sample_Id = 20240701_TK-03138C
Solvent = DMSO-D6
Actual_Start_Time = 1-JUL-2024 20:37:3
Revision_Time = 31-JUL-2024 13:39:3
Comment = TK-03138C
Data_Format = 1D COMPLEX
Dim_Size = 26214
X_Domain = Carbon13
Dim_Title = Carbon13
Dim_Units = [ppm]
Dimensions = X
Spectrometer = JNM-ECZ400S/L1
Field_Strength = 9.389766[T] (400[MH
X_Acq_Duration = 1.03809024[s]
X_Domain = 13C
X_Freq = 100.52530333[MHz]
X_Offset = 100[ppm]
X_Points = 32768
X_Prescans = 4
X_Resolution = 0.96330739[Hz]
X_Sweep = 31.56565657[kHz]
X_Sweep_Clipped = 25.25252525[kHz]
Irr_Domain = Proton
Irr_Freq = 399.78219838[MHz]
Irr_Offset = 5[ppm]
Blanking = 5[us]
Clipped = TRUE
Scans = 6000
Total_Scans = 6000
Relaxation_Delay = 2[s]
Recvr_Gain = 50
Temp_Get = 22.7[dC]
X_90_Width = 10.02[us]
X_Acq_Time = 1.03809024[s]
X_Angle = 30[deg]
X_Atn = 8[dB]
X_Pulse = 3.34[us]
Irr_Atn_Dec = 27.4[dB]
Irr_Atn_Dec_Calc = 27.4[dB]
Irr_Atn_Dec_Default_Calc = 27.4[dB]
Irr_Atn_Noe = 27.4[dB]
Irr_Dec_Bandwidth_Hz = 4.7826087[kHz]
Irr_Dec_Bandwidth_Ppm = 11.96303566[ppm]
Irr_Dec_Freq = 399.78219838[MHz]
Irr_Dec_Merit_Factor = 2.2
Irr_Decoupling = TRUE
Irr_Noe = TRUE
Irr_Noise = WALTZ
Irr_Offset_Default = 5[ppm]
Irr_Pwidth = 0.115[ms]
Irr_Pwidth_Default = 0.115[ms]
Irr_Pwidth_Default_Calc = 0.115[ms]
Irr_Pwidth_Temp1 = 0.115[ms]
Irr_Wurst = FALSE
Decimation_Rate = 0

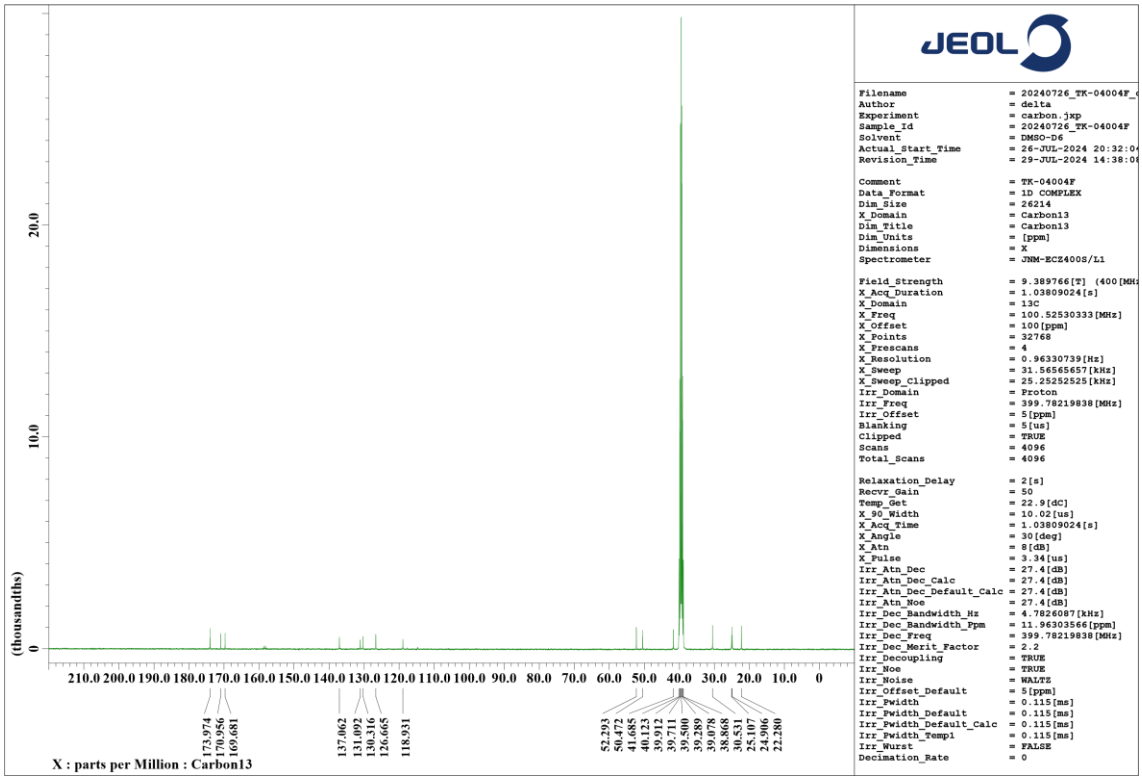

AcHN
OMe
HN
OH
5-His$^{\pi}$
X : parts per Million : Proton
(thousandths)

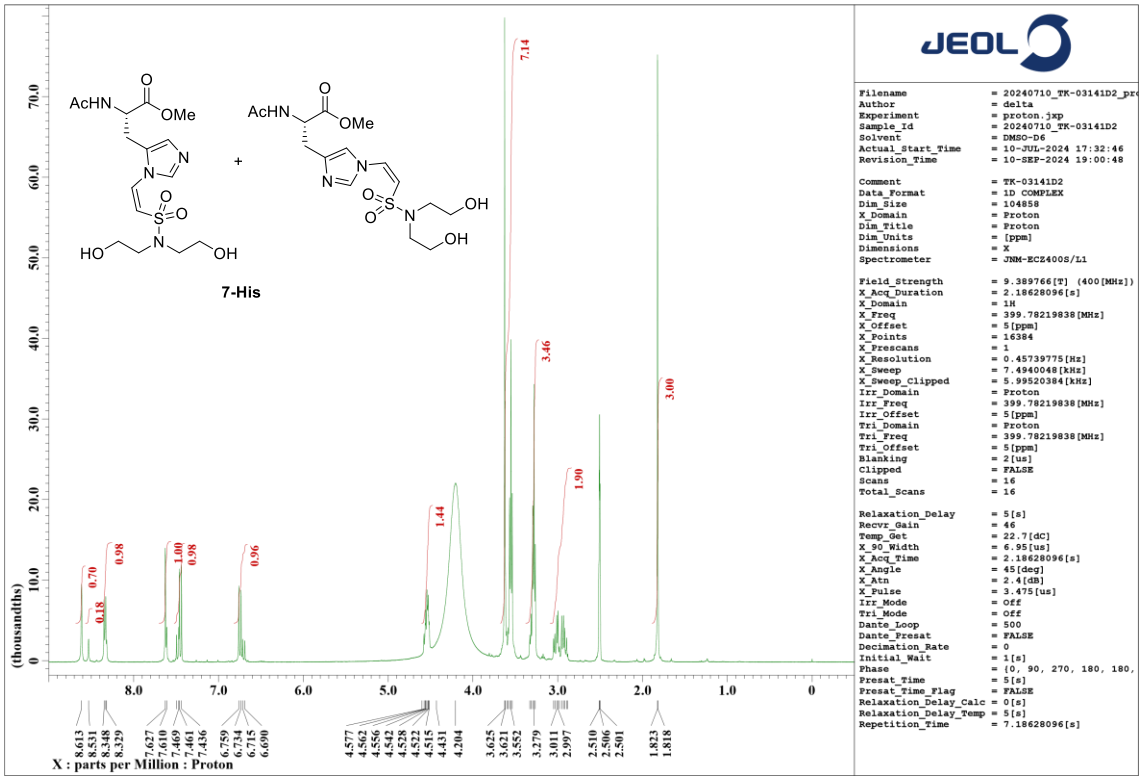

X : parts per Million : Carbon13
(thousandths)

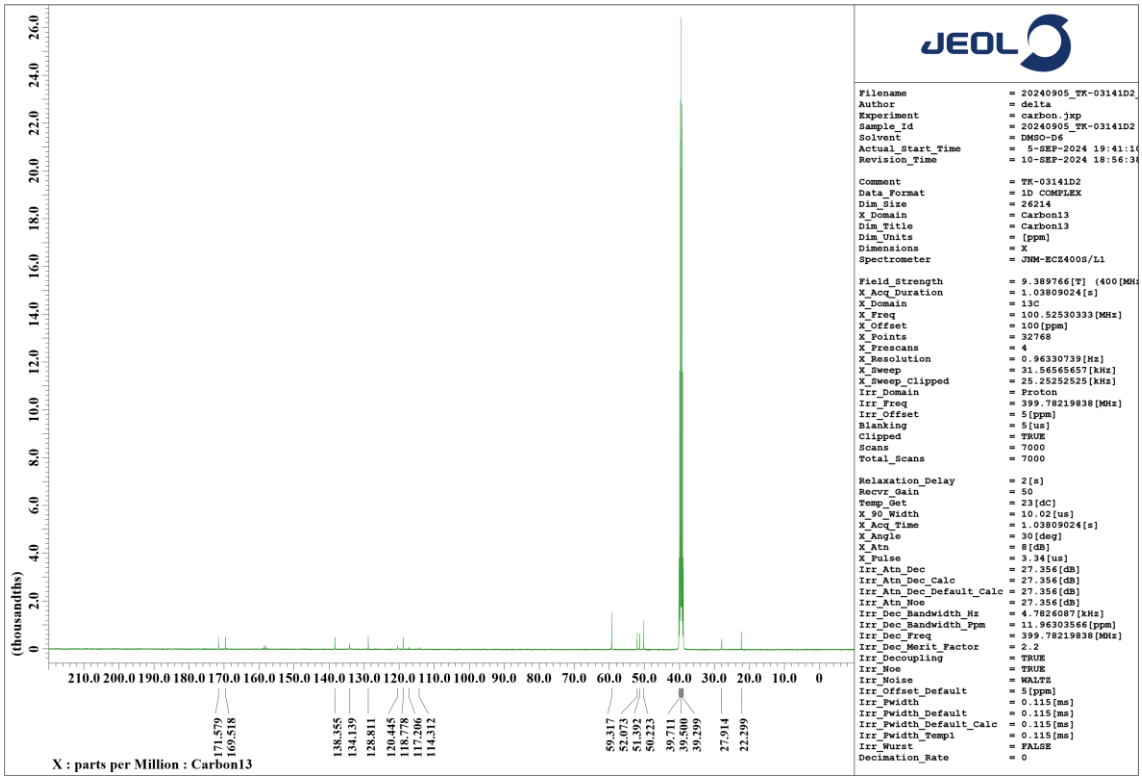

AcHN
OMe
O
N
N
O
S
O
N
H
OH
O
6-His$^{\tau}$
2.96
3.13
3.00
2.01
2.07
0.95
0.98
0.91
0.96
1.01
0.91
1.06
0.95
abundance
12.0 11.0 10.0 9.0 8.0 7.0 6.0 5.0 4.0 3.0 2.0 1.0 0
8.738 8.360 8.340 7.831 7.659 7.429 7.404 6.664 6.640 5.982 4.576 4.569 4.555 4.549 4.535 3.630 2.982 2.967 2.951 2.508 2.504 2.264 1.826 1.714 1.696 1.678 1.660 0.000
X : parts per Million : Proton
JEOL
Filename = 20240726_TK-04004G_pro
Author = delta
Experiment = proton.jxp
Sample_Id = 20240726_TK-04004G
Solvent = DMSO-D6
Actual_Start_Time = 26-JUL-2024 20:18:50
Revision_Time = 29-JUL-2024 15:01:24
Comment = TK-04004G
Data_Format = 1D COMPLEX
Dim_Size = 104858
X_Domain = Proton
Dim_Title = Proton
Dim_Units = [ppm]
Dimensions = X
Spectrometer = JNM-ECZ400S/L1
Field_Strength = 9.389766[T] (400[MHz])
X_Acq_Duration = 2.18628096[s]
X_Domain = 1H
X_Freq = 399.78219838[MHz]
X_Offset = 5[ppm]
X_Points = 16384
X_Prescans = 1
X_Resolution = 0.45739775[Hz]
X_Sweep = 7.4940048[kHz]
X_Sweep_Clipped = 5.99520384[kHz]
Irr_Domain = Proton
Irr_Freq = 399.78219838[MHz]
Irr_Offset = 5[ppm]
Tri_Domain = Proton
Tri_Freq = 399.78219838[MHz]
Tri_Offset = 5[ppm]
Blanking = 2[us]
Clipped = FALSE
Scans = 16
Total_Scans = 16
Relaxation_Delay = 5[s]
Recvr_Gain = 46
Temp_Get = 22.8[dC]
X_90_Width = 6.95[us]
X_Acq_Time = 2.18628096[s]
X_Angle = 45[deg]
X_Atn = 2.4[dB]
X_Pulse = 3.475[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Loop = 500
Dante_Presat = FALSE
Decimation_Rate = 0
Initial_Wait = 1[s]
Phase = (0, 90, 270, 180, 180,
Presat_Time = 5[s]
Presat_Time_Flag = FALSE
Relaxation_Delay_Calc = 0[s]
Relaxation_Delay_Temp = 5[s]
Repetition_Time = 7.18628096[s]

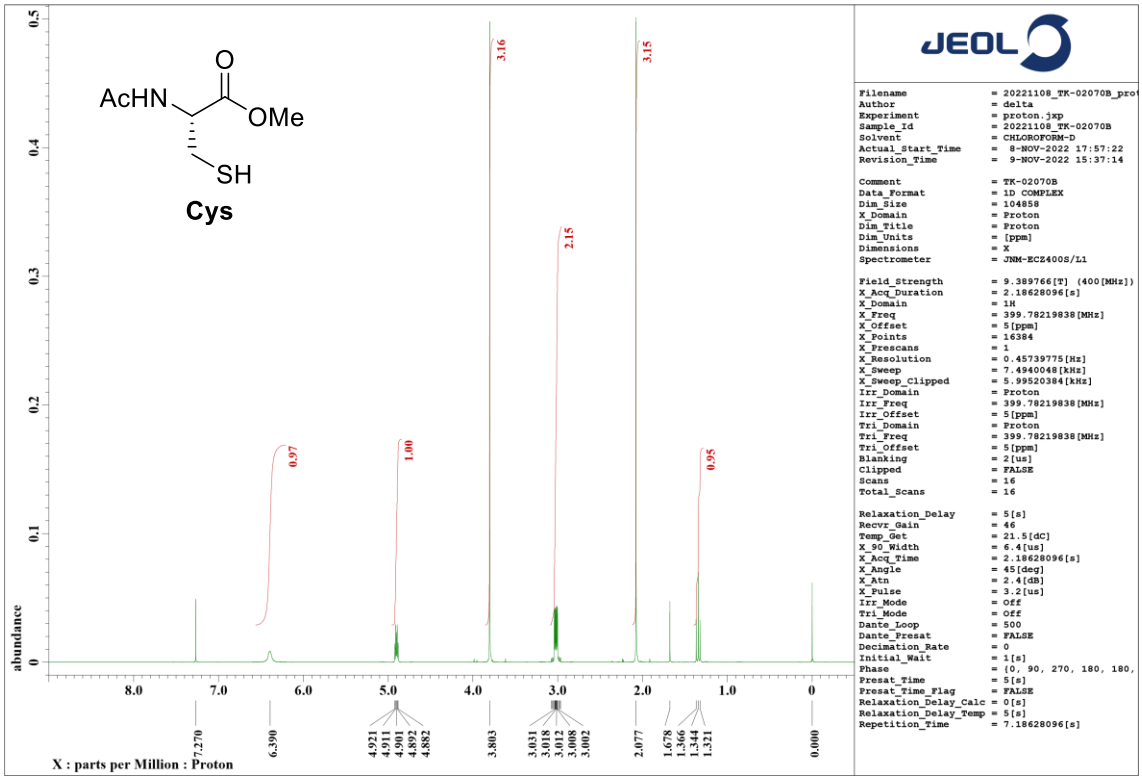

(thousandths)
30.0 20.0 10.0 0
210.0 200.0 190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0
174.003 171.531 169.538 138.346 133.650 128.322 121.883 119.075 52.082 51.373 41.685 40.121 39.912 39.701 39.500 39.289 39.078 38.868 30.578 27.713 24.762 22.289
X : parts per Million : Carbon13
JEOL
Filename = 20240726_TK-04004G_
Author = delta
Experiment = carbon.jxp
Sample_Id = 20240726_TK-04004G
Solvent = DMSO-D6
Actual_Start_Time = 27-JUL-2024 04:09:5
Revision_Time = 29-JUL-2024 14:45:4
Comment = TK-04004G
Data_Format = 1D COMPLEX
Dim_Size = 26214
X_Domain = Carbon13
Dim_Title = Carbon13
Dim_Units = [ppm]
Dimensions = X
Spectrometer = JNM-ECZ400S/L1
Field_Strength = 9.389766[T] (400[MH
X_Acq_Duration = 1.03809024[s]
X_Domain = 13C
X_Freq = 100.52530333[MHz]
X_Offset = 100[ppm]
X_Points = 32768
X_Prescans = 4
X_Resolution = 0.96330739[Hz]
X_Sweep = 31.56565657[kHz]
X_Sweep_Clipped = 25.25252525[kHz]
Irr_Domain = Proton
Irr_Freq = 399.78219838[MHz]
Irr_Offset = 5[ppm]
Blanking = 5[us]
Clipped = TRUE
Scans = 4096
Total_Scans = 4096
Relaxation_Delay = 2[s]
Recvr_Gain = 50
Temp_Get = 23[dC]
X_90_Width = 10.02[us]
X_Acq_Time = 1.03809024[s]
X_Angle = 30[deg]
X_Atn = 8[dB]
X_Pulse = 3.34[us]
Irr_Atn_Dec = 27.4[dB]
Irr_Atn_Dec_Calc = 27.4[dB]
Irr_Atn_Dec_Default_Calc = 27.4[dB]
Irr_Atn_Noe = 27.4[dB]
Irr_Dec_Bandwidth_Hz = 4.7826087[kHz]
Irr_Dec_Bandwidth_Ppm = 11.96303566[ppm]
Irr_Dec_Freq = 399.78219838[MHz]
Irr_Dec_Merit_Factor = 2.2
Irr_Decoupling = TRUE
Irr_Noe = TRUE
Irr_Noise = WALTZ
Irr_Offset_Default = 5[ppm]
Irr_Pwidth = 0.115[ms]
Irr_Pwidth_Default = 0.115[ms]
Irr_Pwidth_Default_Calc = 0.115[ms]
Irr_Pwidth_Temp1 = 0.115[ms]
Irr_Wurst = FALSE
Decimation_Rate = 0

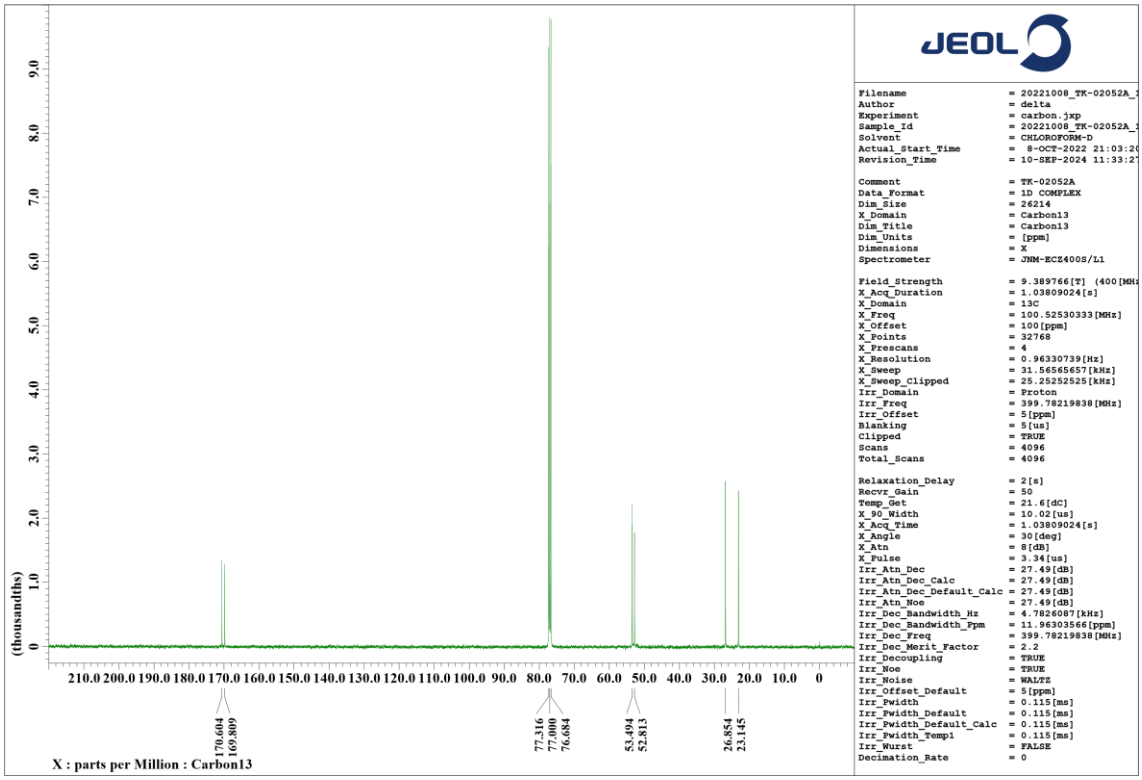

AcHN
OMe
N
N
O
S
O
NH
HO
O
6-His$^{\pi}$
abundance
X : parts per Million : Proton
Filename = 20240726_TK-04004F_pro
Author = delta
Experiment = proton.jxp
Sample_Id = 20240726_TK-04004F
Solvent = DMSO-D6
Actual_Start_Time = 26-JUL-2024 20:12:43
Revision_Time = 29-JUL-2024 14:57:13
Comment = TK-04004F
Data_Format = 1D COMPLEX
Dim_Size = 104858
X_Domain = Proton
Dim_Title = Proton
Dim_Units = [ppm]
Dimensions = X
Spectrometer = JNM-ECZ400S/L1
Field_Strength = 9.389766[T] (400[MHz])
X_Acq_Duration = 2.18628096[s]
X_Domain = 1H
X_Freq = 399.78219838[MHz]
X_Offset = 5[ppm]
X_Points = 16384
X_Prescans = 1
X_Resolution = 0.45739775[Hz]
X_Sweep = 7.4940048[kHz]
X_Sweep_Clipped = 5.99520384[kHz]
Irr_Domain = Proton
Irr_Freq = 399.78219838[MHz]
Irr_Offset = 5[ppm]
Tri_Domain = Proton
Tri_Freq = 399.78219838[MHz]
Tri_Offset = 5[ppm]
Blanking = 2[us]
Clipped = FALSE
Scans = 16
Total_Scans = 16
Relaxation_Delay = 5[s]
Recvr_Gain = 46
Temp_Get = 22.9[dC]
X_90_Width = 6.95[us]
X_Acq_Time = 2.18628096[s]
X_Angle = 45[deg]
X_Atn = 2.4[dB]
X_Pulse = 3.475[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Loop = 500
Dante_Presat = FALSE
Decimation_Rate = 0
Initial_Wait = 1[s]
Phase = (0, 90, 270, 180, 180,
Presat_Time = 5[s]
Presat_Time_Flag = FALSE
Relaxation_Delay_Calc = 0[s]
Relaxation_Delay_Temp = 5[s]
Repetition_Time = 7.18628096[s]

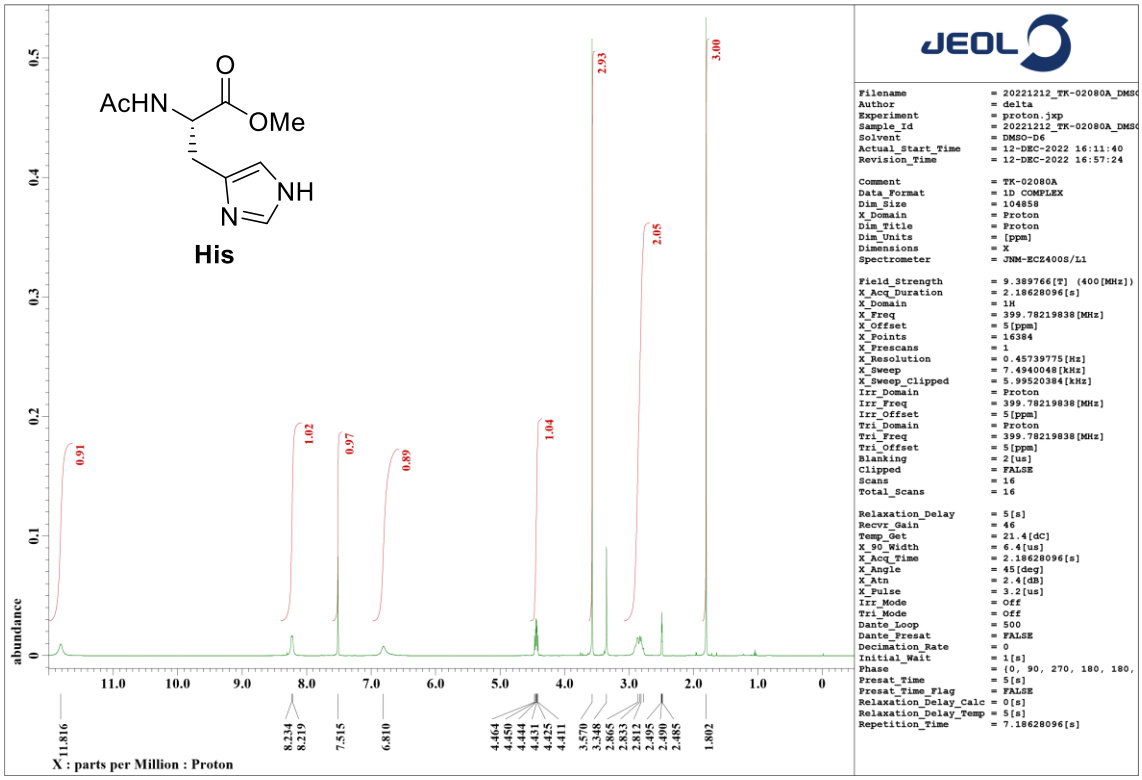

(thousandths)
X : parts per Million : Carbon13
Filename = 20240726_TK-04004F_
Author = delta
Experiment = carbon.jxp
Sample_Id = 20240726_TK-04004F
Solvent = DMSO-D6
Actual_Start_Time = 26-JUL-2024 20:32:0
Revision_Time = 29-JUL-2024 14:38:0
Comment = TK-04004F
Data_Format = 1D COMPLEX
Dim_Size = 26214
X_Domain = Carbon13
Dim_Title = Carbon13
Dim_Units = [ppm]
Dimensions = X
Spectrometer = JNM-ECZ400S/L1
Field_Strength = 9.389766[T] (400[MH
X_Acq_Duration = 1.03809024[s]
X_Domain = 13C
X_Freq = 100.52530333[MHz]
X_Offset = 100[ppm]
X_Points = 32768
X_Prescans = 4
X_Resolution = 0.96330739[Hz]
X_Sweep = 31.56565657[kHz]
X_Sweep_Clipped = 25.25252525[kHz]
Irr_Domain = Proton
Irr_Freq = 399.78219838[MHz]
Irr_Offset = 5[ppm]
Blanking = 5[us]
Clipped = TRUE
Scans = 4096
Total_Scans = 4096
Relaxation_Delay = 2[s]
Recvr_Gain = 50
Temp_Get = 22.9[dC]
X_90_Width = 10.02[us]
X_Acq_Time = 1.03809024[s]
X_Angle = 30[deg]
X_Atn = 8[dB]
X_Pulse = 3.34[us]
Irr_Atn_Dec = 27.4[dB]
Irr_Atn_Dec_Calc = 27.4[dB]
Irr_Atn_Dec_Default_Calc = 27.4[dB]
Irr_Atn_Noe = 27.4[dB]
Irr_Dec_Bandwidth_Hz = 4.7826087[kHz]
Irr_Dec_Bandwidth_Ppm = 11.96303566[ppm]
Irr_Dec_Freq = 399.78219838[MHz]
Irr_Dec_Merit_Factor = 2.2
Irr_Decoupling = TRUE
Irr_Noe = TRUE
Irr_Noise = WALTZ
Irr_Offset_Default = 5[ppm]
Irr_Pwidth = 0.115[ms]
Irr_Pwidth_Default = 0.115[ms]
Irr_Pwidth_Default_Calc = 0.115[ms]
Irr_Pwidth_Temp1 = 0.115[ms]
Irr_Wurst = FALSE
Decimation_Rate = 0

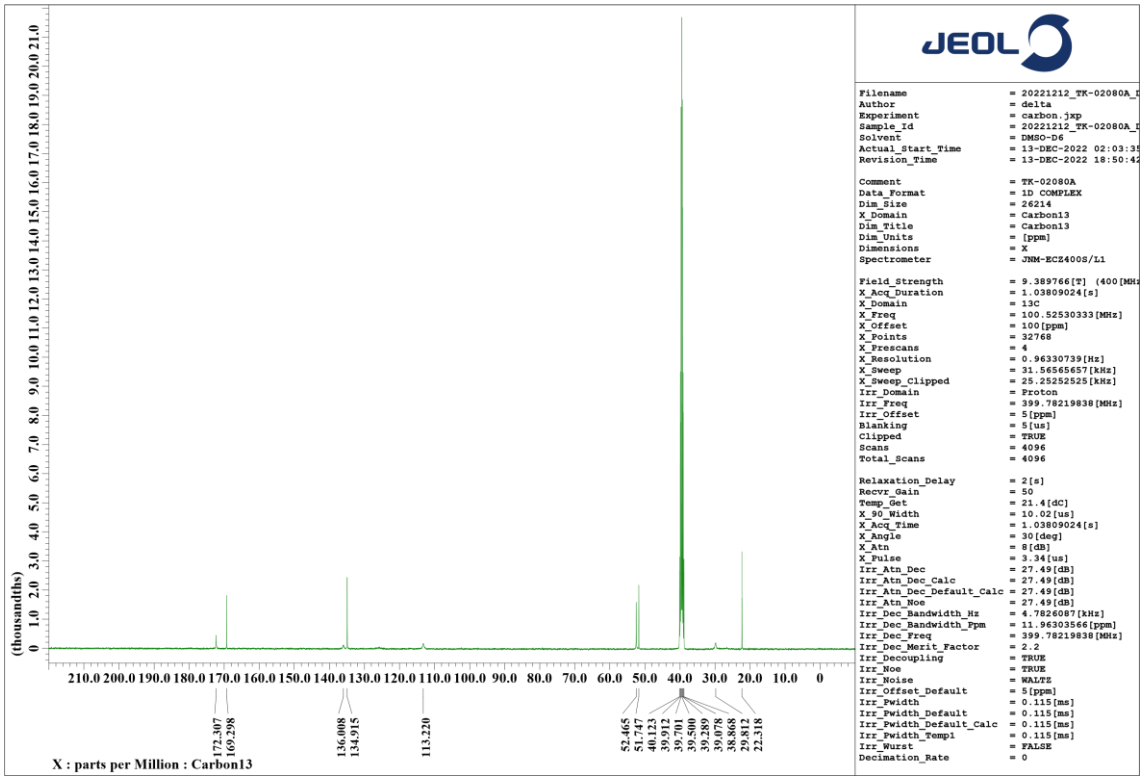

AcHN
OMe
HO
OH
7-His
7.14
3.46
3.00
1.90
1.44
0.98
1.00
0.98
0.96
0.70
0.18
(thousandths)
X : parts per Million : Proton
Filename = 20240710_TK-03141D2_pr
Author = delta
Experiment = proton.jxp
Sample_Id = 20240710_TK-03141D2
Solvent = DMSO-D6
Actual_Start_Time = 10-JUL-2024 17:32:46
Revision_Time = 10-SEP-2024 19:00:48
Comment = TK-03141D2
Data_Format = 1D COMPLEX
Dim_Size = 104858
X_Domain = Proton
Dim_Title = Proton
Dim_Units = [ppm]
Dimensions = X
Spectrometer = JNM-ECZ400S/L1
Field_Strength = 9.389766[T] (400[MHz])
X_Acq_Duration = 2.18628096[s]
X_Domain = 1H
X_Freq = 399.78219838[MHz]
X_Offset = 5[ppm]
X_Points = 16384
X_Prescans = 1
X_Resolution = 0.45739775[Hz]
X_Sweep = 7.4940048[kHz]
X_Sweep_Clipped = 5.99520384[kHz]
Irr_Domain = Proton
Irr_Freq = 399.78219838[MHz]
Irr_Offset = 5[ppm]
Tri_Domain = Proton
Tri_Freq = 399.78219838[MHz]
Tri_Offset = 5[ppm]
Blanking = 2[us]
Clipped = FALSE
Scans = 16
Total_Scans = 16
Relaxation_Delay = 5[s]
Recvr_Gain = 46
Temp_Get = 22.7[dC]
X_90_Width = 6.95[us]
X_Acq_Time = 2.18628096[s]
X_Angle = 45[deg]
X_Atn = 2.4[dB]
X_Pulse = 3.475[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Loop = 500
Dante_Presat = FALSE
Decimation_Rate = 0
Initial_Wait = 1[s]
Phase = (0, 90, 270, 180, 180,
Presat_Time = 5[s]
Presat_Time_Flag = FALSE
Relaxation_Delay_Calc = 0[s]
Relaxation_Delay_Temp = 5[s]
Repetition_Time = 7.18628096[s]

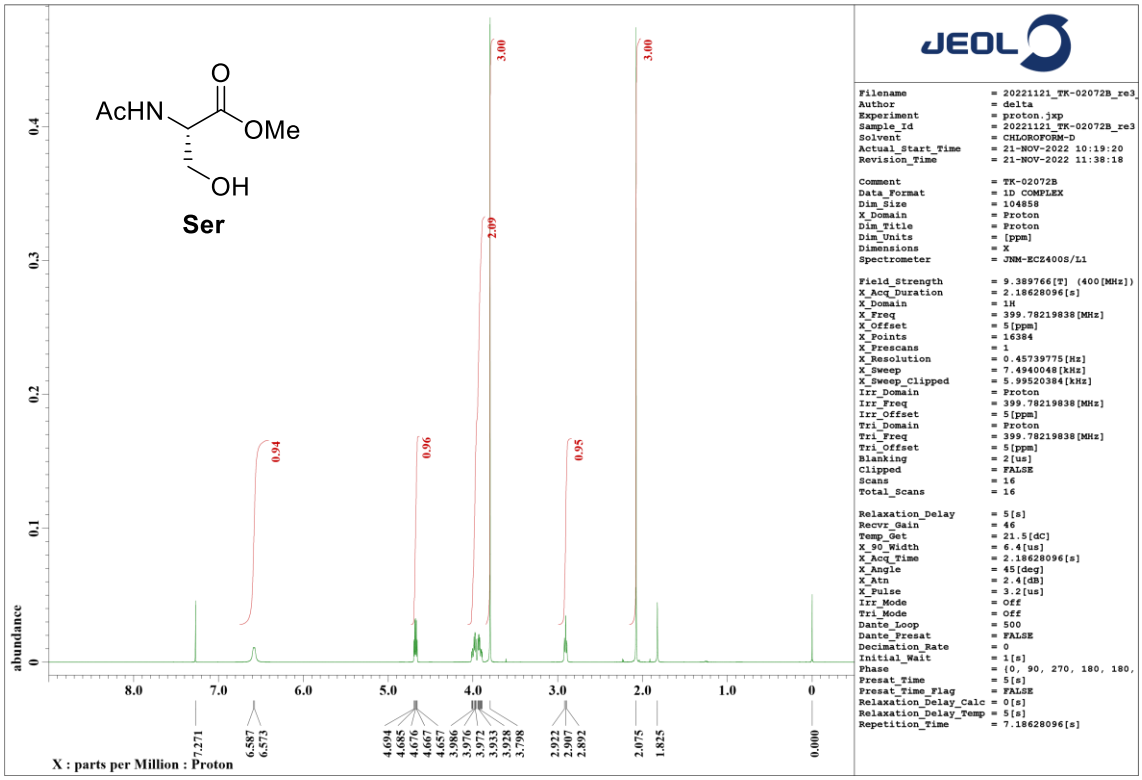

(thousandths)
X : parts per Million : Carbon13
Filename = 20240905_TK-03141D2_
Author = delta
Experiment = carbon.jxp
Sample_Id = 20240905_TK-03141D2
Solvent = DMSO-D6
Actual_Start_Time = 5-SEP-2024 19:41:1
Revision_Time = 10-SEP-2024 18:56:3
Comment = TK-03141D2
Data_Format = 1D COMPLEX
Dim_Size = 26214
X_Domain = Carbon13
Dim_Title = Carbon13
Dim_Units = [ppm]
Dimensions = X
Spectrometer = JNM-ECZ400S/L1
Field_Strength = 9.389766[T] (400[MH
X_Acq_Duration = 1.03809024[s]
X_Domain = 13C
X_Freq = 100.52530333[MHz]
X_Offset = 100[ppm]
X_Points = 32768
X_Prescans = 4
X_Resolution = 0.96330739[Hz]
X_Sweep = 31.56565657[kHz]
X_Sweep_Clipped = 25.25252525[kHz]
Irr_Domain = Proton
Irr_Freq = 399.78219838[MHz]
Irr_Offset = 5[ppm]
Blanking = 5[us]
Clipped = TRUE
Scans = 7000
Total_Scans = 7000
Relaxation_Delay = 2[s]
Recvr_Gain = 50
Temp_Get = 23[dC]
X_90_Width = 10.02[us]
X_Acq_Time = 1.03809024[s]
X_Angle = 30[deg]
X_Atn = 8[dB]
X_Pulse = 3.34[us]
Irr_Atn_Dec = 27.356[dB]
Irr_Atn_Dec_Calc = 27.356[dB]
Irr_Atn_Dec_Default_Calc = 27.356[dB]
Irr_Atn_Noe = 27.356[dB]
Irr_Dec_Bandwidth_Hz = 4.7826087[kHz]
Irr_Dec_Bandwidth_Ppm = 11.96303566[ppm]
Irr_Dec_Freq = 399.78219838[MHz]
Irr_Dec_Merit_Factor = 2.2
Irr_Decoupling = TRUE
Irr_Noe = TRUE
Irr_Noise = WALTZ
Irr_Offset_Default = 5[ppm]
Irr_Pwidth = 0.115[ms]
Irr_Pwidth_Default = 0.115[ms]
Irr_Pwidth_Default_Calc = 0.115[ms]
Irr_Pwidth_Temp1 = 0.115[ms]
Irr_Wurst = FALSE
Decimation_Rate = 0

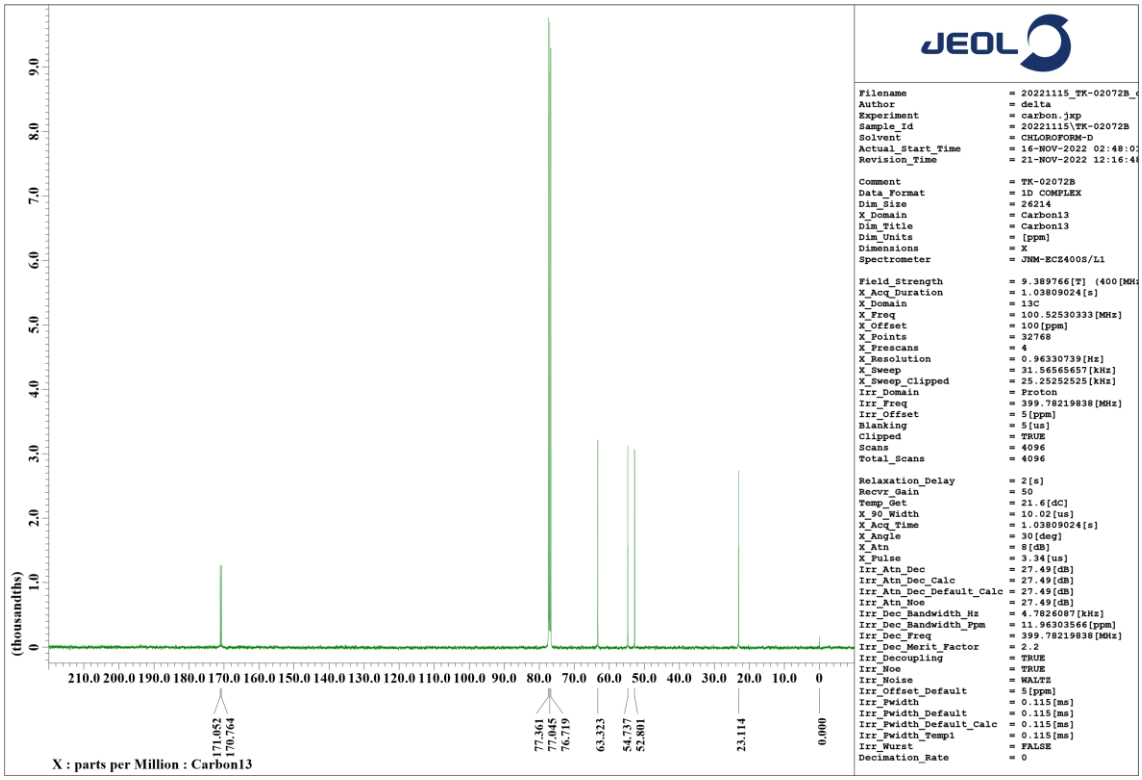

AcHN
O
OMe
SH
Cys
3.16
3.15
2.15
0.97
1.00
0.95
abundance
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
7.270
6.390
4.921
4.911
4.901
4.892
4.882
3.803
3.031
3.018
3.012
3.008
3.002
2.077
1.678
1.366
1.344
1.321
0.000
X : parts per Million : Proton
JEOL
Filename = 20221108_TK-02070B_pro
Author = delta
Experiment = proton.jxp
Sample_Id = 20221108_TK-02070B
Solvent = CHLOROFORM-D
Actual_Start_Time = 8-NOV-2022 17:57:22
Revision_Time = 9-NOV-2022 15:37:14
Comment = TK-02070B
Data_Format = 1D COMPLEX
Dim_Size = 104858
X_Domain = Proton
Dim_Title = Proton
Dim_Units = [ppm]
Dimensions = X
Spectrometer = JNM-ECZ400S/L1
Field_Strength = 9.389766[T] (400[MHz])
X_Acq_Duration = 2.18628096[s]
X_Domain = 1H
X_Freq = 399.78219838[MHz]
X_Offset = 5[ppm]
X_Points = 16384
X_Prescans = 1
X_Resolution = 0.45739775[Hz]
X_Sweep = 7.4940048[kHz]
X_Sweep_Clipped = 5.99520384[kHz]
Irr_Domain = Proton
Irr_Freq = 399.78219838[MHz]
Irr_Offset = 5[ppm]
Tri_Domain = Proton
Tri_Freq = 399.78219838[MHz]
Tri_Offset = 5[ppm]
Blanking = 2[us]
Clipped = FALSE
Scans = 16
Total_Scans = 16
Relaxation_Delay = 5[s]
Recvr_Gain = 46
Temp_Get = 21.5[dC]
X_90_Width = 6.4[us]
X_Acq_Time = 2.18628096[s]
X_Angle = 45[deg]
X_Atn = 2.4[dB]
X_Pulse = 3.2[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Loop = 500
Dante_Presat = FALSE
Decimation_Rate = 0
Initial_Wait = 1[s]
Phase = (0, 90, 270, 180, 180,
Presat_Time = 5[s]
Presat_Time_Flag = FALSE
Relaxation_Delay_Calc = 0[s]
Relaxation_Delay_Temp = 5[s]
Repetition_Time = 7.18628096[s]

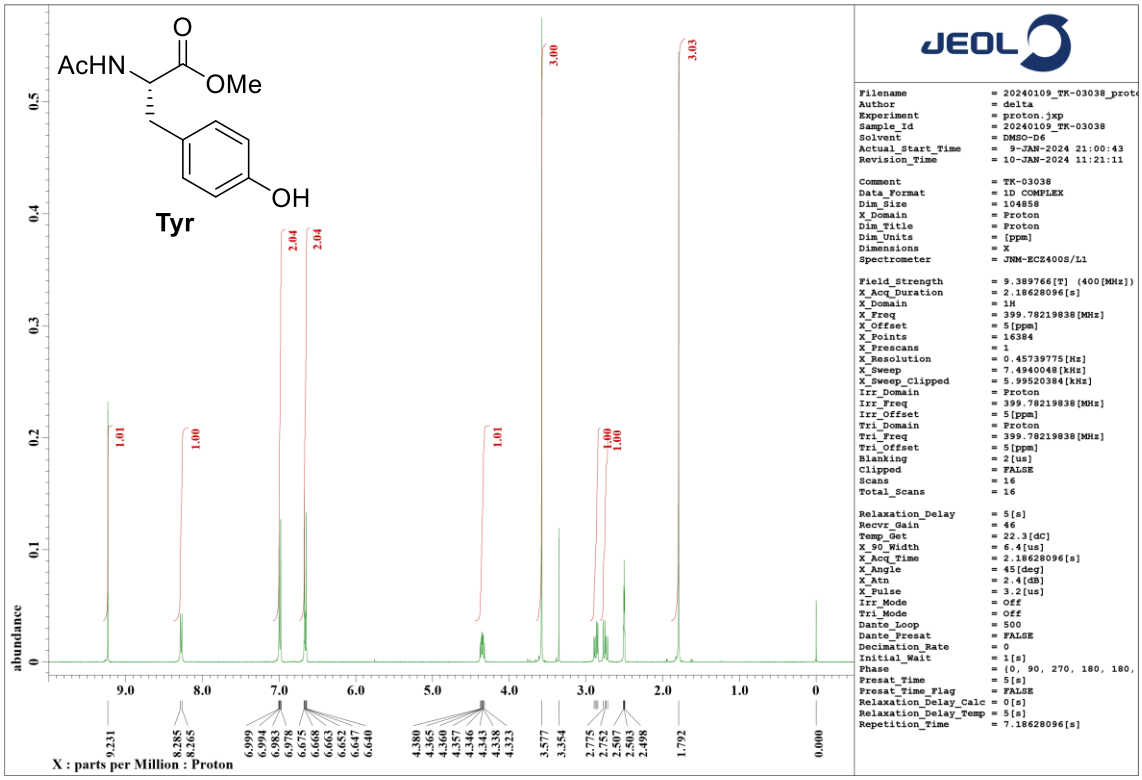

(thousandths)
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
210.0 200.0 190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0
170.604
169.809
77.316
77.000
76.684
53.494
52.813
26.854
23.145
X : parts per Million : Carbon13
JEOL
Filename = 20221008_TK-02052A_1
Author = delta
Experiment = carbon.jxp
Sample_Id = 20221008_TK-02052A_1
Solvent = CHLOROFORM-D
Actual_Start_Time = 8-OCT-2022 21:03:20
Revision_Time = 10-SEP-2024 11:33:27
Comment = TK-02052A
Data_Format = 1D COMPLEX
Dim_Size = 26214
X_Domain = Carbon13
Dim_Title = Carbon13
Dim_Units = [ppm]
Dimensions = X
Spectrometer = JNM-ECZ400S/L1
Field_Strength = 9.389766[T] (400[MHz]
X_Acq_Duration = 1.03809024[s]
X_Domain = 13C
X_Freq = 100.52530333[MHz]
X_Offset = 100[ppm]
X_Points = 32768
X_Prescans = 4
X_Resolution = 0.96330739[Hz]
X_Sweep = 31.56565657[kHz]
X_Sweep_Clipped = 25.25252525[kHz]
Irr_Domain = Proton
Irr_Freq = 399.78219838[MHz]
Irr_Offset = 5[ppm]
Blanking = 5[us]
Clipped = TRUE
Scans = 4096
Total_Scans = 4096
Relaxation_Delay = 2[s]
Recvr_Gain = 50
Temp_Get = 21.6[dC]
X_90_Width = 10.02[us]
X_Acq_Time = 1.03809024[s]
X_Angle = 30[deg]
X_Atn = 8[dB]
X_Pulse = 3.34[us]
Irr_Atn_Dec = 27.49[dB]
Irr_Atn_Dec_Calc = 27.49[dB]
Irr_Atn_Dec_Default_Calc = 27.49[dB]
Irr_Atn_Noe = 27.49[dB]
Irr_Dec_Bandwidth_Hz = 4.7826087[kHz]
Irr_Dec_Bandwidth_Ppm = 11.96303566[ppm]
Irr_Dec_Freq = 399.78219838[MHz]
Irr_Dec_Merit_Factor = 2.2
Irr_Decoupling = TRUE
Irr_Noe = TRUE
Irr_Noise = WALTZ
Irr_Offset_Default = 5[ppm]
Irr_Pwidth = 0.115[ms]
Irr_Pwidth_Default = 0.115[ms]
Irr_Pwidth_Default_Calc = 0.115[ms]
Irr_Pwidth_Temp1 = 0.115[ms]
Irr_Wurst = FALSE
Decimation_Rate = 0

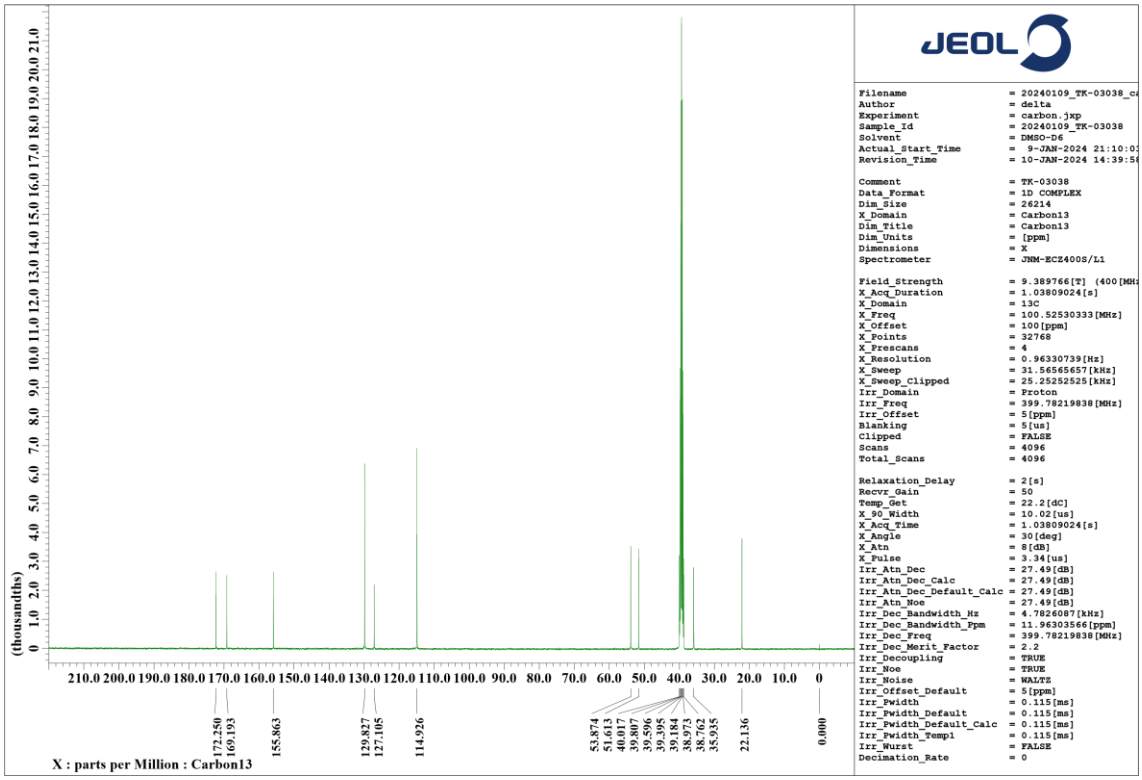

AcHN
O
OMe
NH
N
His
abundance
X : parts per Million : Proton
0.91
1.02
0.97
0.89
1.04
2.93
2.05
3.00
11.816
8.234
8.219
7.515
6.810
4.464
4.450
4.444
4.431
4.425
4.411
3.570
3.348
2.865
2.833
2.812
2.495
2.490
2.485
1.802
JEOL
Filename = 20221212_TK-02080A_DMSO
Author = delta
Experiment = proton.jxp
Sample_Id = 20221212_TK-02080A_DMSO
Solvent = DMSO-D6
Actual_Start_Time = 12-DEC-2022 16:11:40
Revision_Time = 12-DEC-2022 16:57:24
Comment = TK-02080A
Data_Format = 1D COMPLEX
Dim_Size = 104858
X_Domain = Proton
Dim_Title = Proton
Dim_Units = [ppm]
Dimensions = X
Spectrometer = JNM-ECZ400S/L1
Field_Strength = 9.389766[T] (400[MHz])
X_Acq_Duration = 2.18628096[s]
X_Domain = 1H
X_Freq = 399.78219838[MHz]
X_Offset = 5[ppm]
X_Points = 16384
X_Prescans = 1
X_Resolution = 0.45739775[Hz]
X_Sweep = 7.4940048[kHz]
X_Sweep_Clipped = 5.99520384[kHz]
Irr_Domain = Proton
Irr_Freq = 399.78219838[MHz]
Irr_Offset = 5[ppm]
Tri_Domain = Proton
Tri_Freq = 399.78219838[MHz]
Tri_Offset = 5[ppm]
Blanking = 2[us]
Clipped = FALSE
Scans = 16
Total_Scans = 16
Relaxation_Delay = 5[s]
Recvr_Gain = 46
Temp_Get = 21.4[dC]
X_90_Width = 6.4[us]
X_Acq_Time = 2.18628096[s]
X_Angle = 45[deg]
X_Atn = 2.4[dB]
X_Pulse = 3.2[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Loop = 500
Dante_Presat = FALSE
Decimation_Rate = 0
Initial_Wait = 1[s]
Phase = (0, 90, 270, 180, 180,
Presat_Time = 5[s]
Presat_Time_Flag = FALSE
Relaxation_Delay_Calc = 0[s]
Relaxation_Delay_Temp = 5[s]
Repetition_Time = 7.18628096[s]

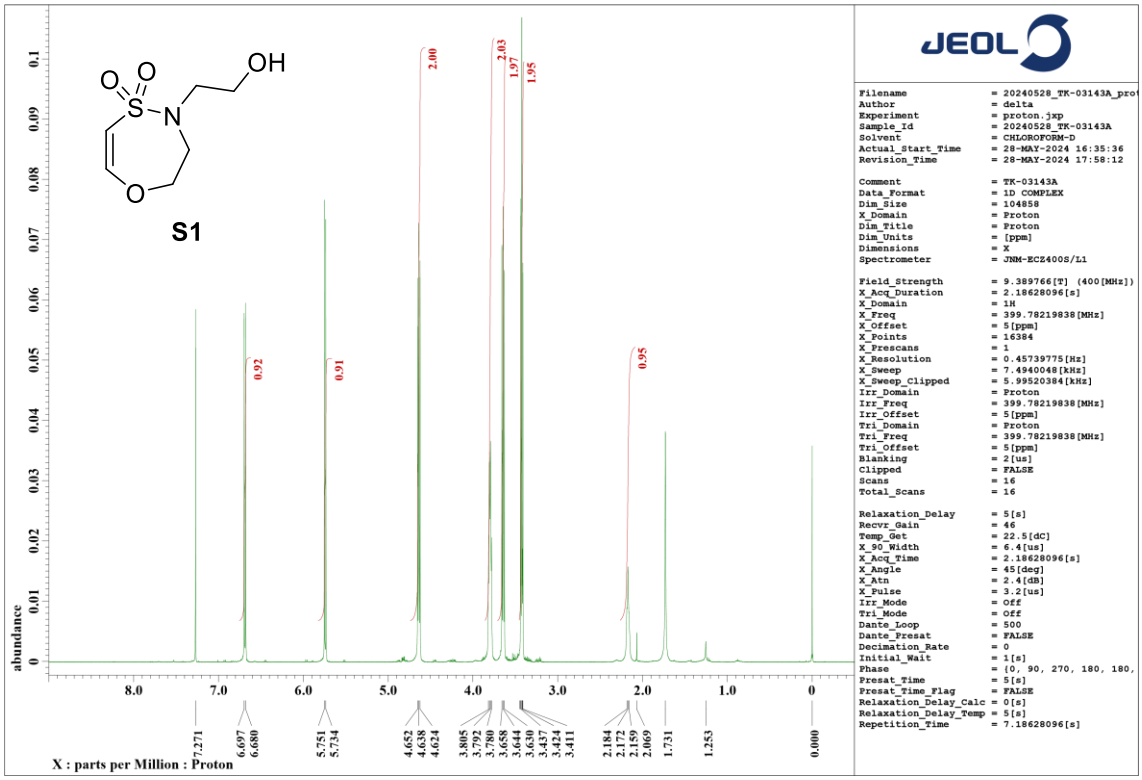

(thousandths)
X : parts per Million : Carbon13
172.307
169.298
136.008
134.915
113.220
52.465
51.747
40.123
39.912
39.701
39.500
39.289
39.078
38.868
23.812
22.318
JEOL
Filename = 20221212_TK-02080A_D
Author = delta
Experiment = carbon.jxp
Sample_Id = 20221212_TK-02080A_D
Solvent = DMSO-D6
Actual_Start_Time = 13-DEC-2022 02:03:35
Revision_Time = 13-DEC-2022 18:50:42
Comment = TK-02080A
Data_Format = 1D COMPLEX
Dim_Size = 26214
X_Domain = Carbon13
Dim_Title = Carbon13
Dim_Units = [ppm]
Dimensions = X
Spectrometer = JNM-ECZ400S/L1
Field_Strength = 9.389766[T] (400[MHz
X_Acq_Duration = 1.03809024[s]
X_Domain = 13C
X_Freq = 100.52530333[MHz]
X_Offset = 100[ppm]
X_Points = 32768
X_Prescans = 4
X_Resolution = 0.96330739[Hz]
X_Sweep = 31.56565657[kHz]
X_Sweep_Clipped = 25.25252525[kHz]
Irr_Domain = Proton
Irr_Freq = 399.78219838[MHz]
Irr_Offset = 5[ppm]
Blanking = 5[us]
Clipped = TRUE
Scans = 4096
Total_Scans = 4096
Relaxation_Delay = 2[s]
Recvr_Gain = 50
Temp_Get = 21.4[dC]
X_90_Width = 10.02[us]
X_Acq_Time = 1.03809024[s]
X_Angle = 30[deg]
X_Atn = 8[dB]
X_Pulse = 3.34[us]
Irr_Atn_Dec = 27.49[dB]
Irr_Atn_Dec_Calc = 27.49[dB]
Irr_Atn_Dec_Default_Calc = 27.49[dB]
Irr_Atn_Noe = 27.49[dB]
Irr_Dec_Bandwidth_Hz = 4.7826087[kHz]
Irr_Dec_Bandwidth_Ppm = 11.96303566[ppm]
Irr_Dec_Freq = 399.78219838[MHz]
Irr_Dec_Merit_Factor = 2.2
Irr_Decoupling = TRUE
Irr_Noe = TRUE
Irr_Noise = WALTZ
Irr_Offset_Default = 5[ppm]
Irr_Pwidth = 0.115[ms]
Irr_Pwidth_Default = 0.115[ms]
Irr_Pwidth_Default_Calc = 0.115[ms]
Irr_Pwidth_Temp1 = 0.115[ms]
Irr_Wurst = FALSE
Decimation_Rate = 0

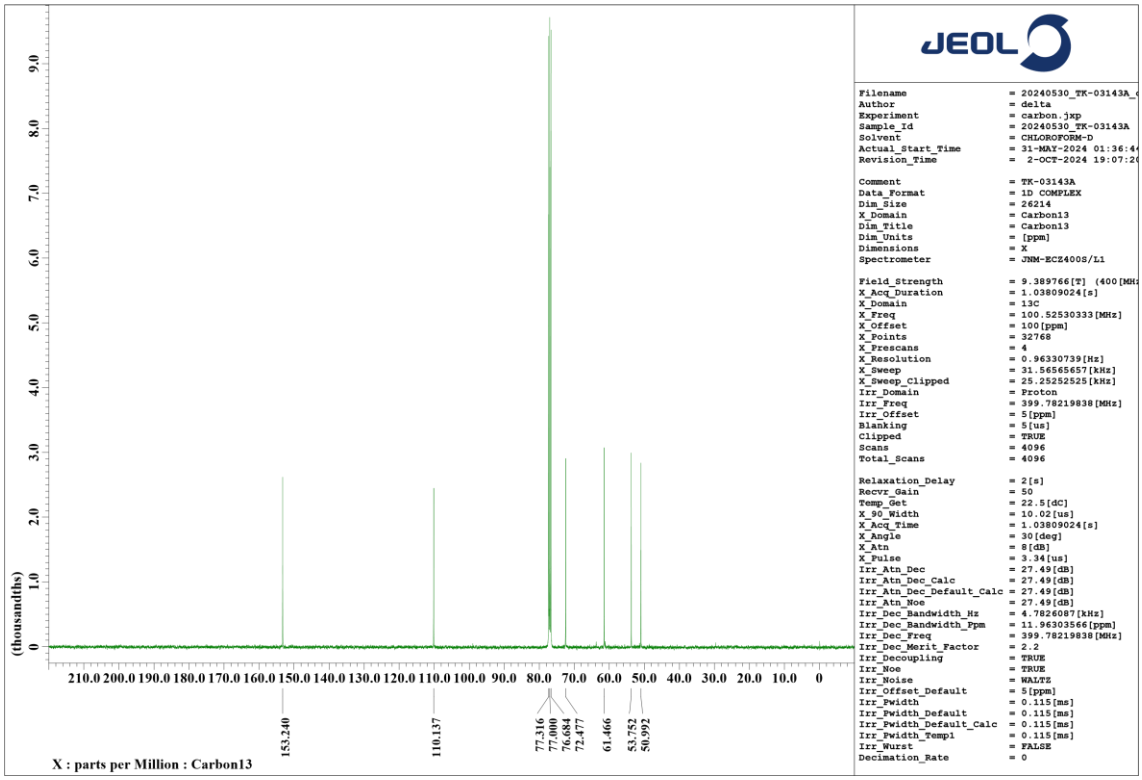

AcHN
O
OMe
OH
Ser
3.00
2.09
3.00
0.94
0.96
0.95
abundance
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
7.271
6.587
6.573
4.694
4.685
4.676
4.667
4.657
3.986
3.976
3.972
3.933
3.928
3.798
2.922
2.907
2.892
2.075
1.825
0.000
X : parts per Million : Proton
JEOL
Filename = 20221121_TK-02072B_re3_
Author = delta
Experiment = proton.jxp
Sample_Id = 20221121_TK-02072B_re3
Solvent = CHLOROFORM-D
Actual_Start_Time = 21-NOV-2022 10:19:20
Revision_Time = 21-NOV-2022 11:38:18
Comment = TK-02072B
Data_Format = 1D COMPLEX
Dim_Size = 104858
X_Domain = Proton
Dim_Title = Proton
Dim_Units = [ppm]
Dimensions = X
Spectrometer = JNM-ECZ400S/L1
Field_Strength = 9.389766[T] (400[MHz])
X_Acq_Duration = 2.18628096[s]
X_Domain = 1H
X_Freq = 399.78219838[MHz]
X_Offset = 5[ppm]
X_Points = 16384
X_Prescans = 1
X_Resolution = 0.45739775[Hz]
X_Sweep = 7.4940048[kHz]
X_Sweep_Clipped = 5.99520384[kHz]
Irr_Domain = Proton
Irr_Freq = 399.78219838[MHz]
Irr_Offset = 5[ppm]
Tri_Domain = Proton
Tri_Freq = 399.78219838[MHz]
Tri_Offset = 5[ppm]
Blanking = 2[us]
Clipped = FALSE
Scans = 16
Total_Scans = 16
Relaxation_Delay = 5[s]
Recvr_Gain = 46
Temp_Get = 21.5[dC]
X_90_Width = 6.4[us]
X_Acq_Time = 2.18628096[s]
X_Angle = 45[deg]
X_Atn = 2.4[dB]
X_Pulse = 3.2[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Loop = 500
Dante_Presat = FALSE
Decimation_Rate = 0
Initial_Wait = 1[s]
Phase = (0, 90, 270, 180, 180,
Presat_Time = 5[s]
Presat_Time_Flag = FALSE
Relaxation_Delay_Calc = 0[s]
Relaxation_Delay_Temp = 5[s]
Repetition_Time = 7.18628096[s]

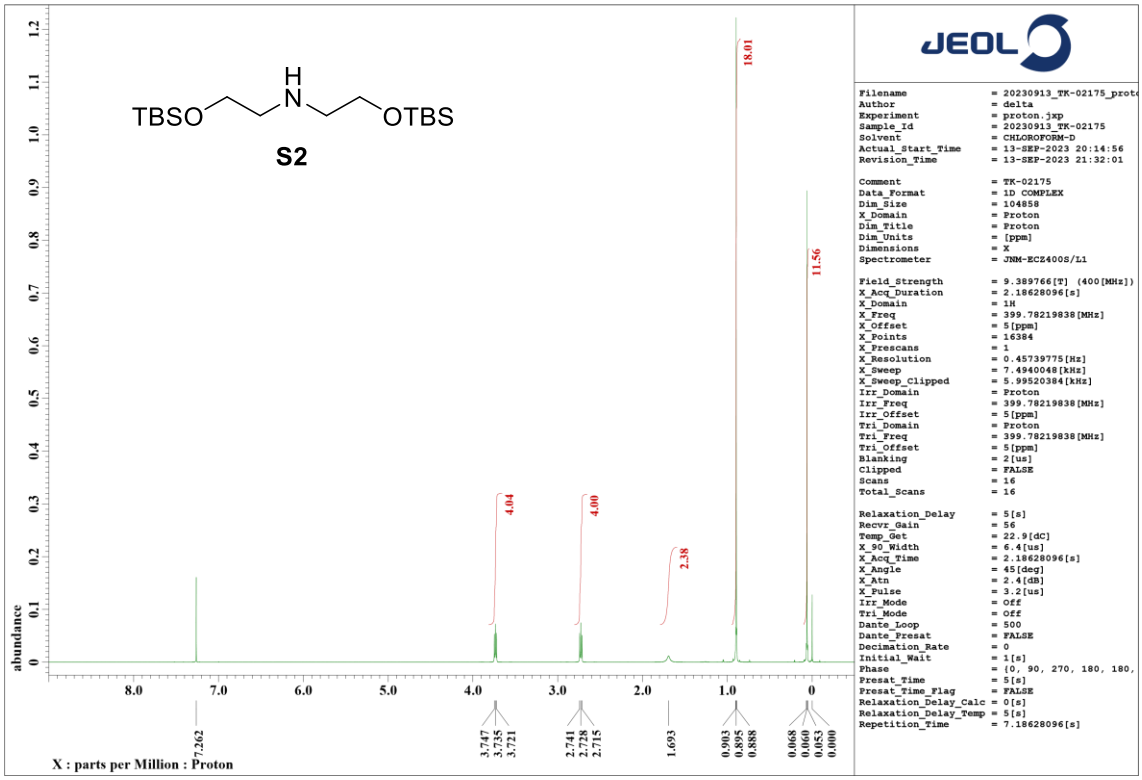

(thousandths)
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
210.0 200.0 190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0
171.052
170.764
77.361
77.045
76.719
63.323
54.737
52.801
23.114
0.000
X : parts per Million : Carbon13
JEOL
Filename = 20221115_TK-02072B_
Author = delta
Experiment = carbon.jxp
Sample_Id = 20221115\TK-02072B
Solvent = CHLOROFORM-D
Actual_Start_Time = 16-NOV-2022 02:48:0
Revision_Time = 21-NOV-2022 12:16:4
Comment = TK-02072B
Data_Format = 1D COMPLEX
Dim_Size = 26214
X_Domain = Carbon13
Dim_Title = Carbon13
Dim_Units = [ppm]
Dimensions = X
Spectrometer = JNM-ECZ400S/L1
Field_Strength = 9.389766[T] (400[MH
X_Acq_Duration = 1.03809024[s]
X_Domain = 13C
X_Freq = 100.52530333[MHz]
X_Offset = 100[ppm]
X_Points = 32768
X_Prescans = 4
X_Resolution = 0.96330739[Hz]
X_Sweep = 31.56565657[kHz]
X_Sweep_Clipped = 25.25252525[kHz]
Irr_Domain = Proton
Irr_Freq = 399.78219838[MHz]
Irr_Offset = 5[ppm]
Blanking = 5[us]
Clipped = TRUE
Scans = 4096
Total_Scans = 4096
Relaxation_Delay = 2[s]
Recvr_Gain = 50
Temp_Get = 21.6[dC]
X_90_Width = 10.02[us]
X_Acq_Time = 1.03809024[s]
X_Angle = 30[deg]
X_Atn = 8[dB]
X_Pulse = 3.34[us]
Irr_Atn_Dec = 27.49[dB]
Irr_Atn_Dec_Calc = 27.49[dB]
Irr_Atn_Dec_Default_Calc = 27.49[dB]
Irr_Atn_Noe = 27.49[dB]
Irr_Dec_Bandwidth_Hz = 4.7826087[kHz]
Irr_Dec_Bandwidth_Ppm = 11.96303566[ppm]
Irr_Dec_Freq = 399.78219838[MHz]
Irr_Dec_Merit_Factor = 2.2
Irr_Decoupling = TRUE
Irr_Noe = TRUE
Irr_Noise = WALTZ
Irr_Offset_Default = 5[ppm]
Irr_Pwidth = 0.115[ms]
Irr_Pwidth_Default = 0.115[ms]
Irr_Pwidth_Default_Calc = 0.115[ms]
Irr_Pwidth_Temp1 = 0.115[ms]
Irr_Wurst = FALSE
Decimation_Rate = 0

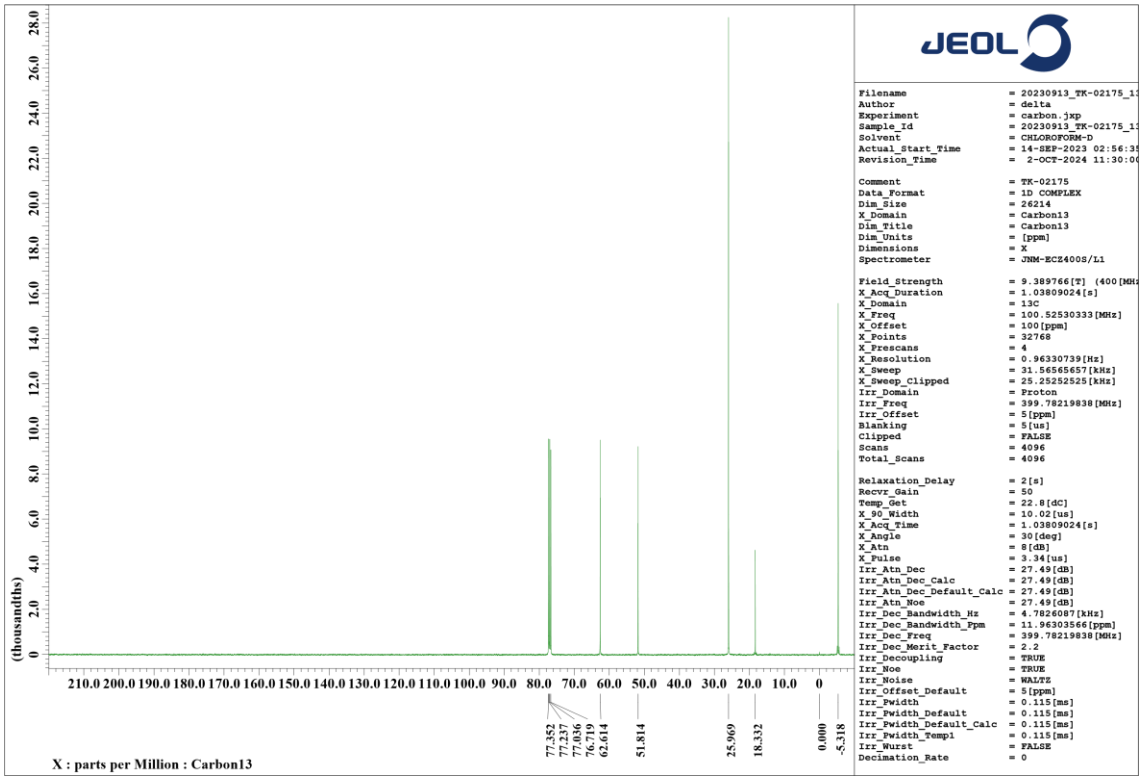

AcHN
O
OMe
OH
Tyr
abundance
X : parts per Million : Proton
Filename = 20240109_TK-03038_prot
Author = delta
Experiment = proton.jxp
Sample_Id = 20240109_TK-03038
Solvent = DMSO-D6
Actual_Start_Time = 9-JAN-2024 21:00:43
Revision_Time = 10-JAN-2024 11:21:11
Comment = TK-03038
Data_Format = 1D COMPLEX
Dim_Size = 104858
X_Domain = Proton
Dim_Title = Proton
Dim_Units = [ppm]
Dimensions = X
Spectrometer = JNM-ECZ400S/L1
Field_Strength = 9.389766[T] (400[MHz])
X_Acq_Duration = 2.18628096[s]
X_Domain = 1H
X_Freq = 399.78219838[MHz]
X_Offset = 5[ppm]
X_Points = 16384
X_Prescans = 1
X_Resolution = 0.45739775[Hz]
X_Sweep = 7.4940048[kHz]
X_Sweep_Clipped = 5.99520384[kHz]
Irr_Domain = Proton
Irr_Freq = 399.78219838[MHz]
Irr_Offset = 5[ppm]
Tri_Domain = Proton
Tri_Freq = 399.78219838[MHz]
Tri_Offset = 5[ppm]
Blanking = 2[us]
Clipped = FALSE
Scans = 16
Total_Scans = 16
Relaxation_Delay = 5[s]
Recvr_Gain = 46
Temp_Get = 22.3[dC]
X_90_Width = 6.4[us]
X_Acq_Time = 2.18628096[s]
X_Angle = 45[deg]
X_Atn = 2.4[dB]
X_Pulse = 3.2[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Loop = 500
Dante_Presat = FALSE
Decimation_Rate = 0
Initial_Wait = 1[s]
Phase = (0, 90, 270, 180, 180,
Presat_Time = 5[s]
Presat_Time_Flag = FALSE
Relaxation_Delay_Calc = 0[s]
Relaxation_Delay_Temp = 5[s]
Repetition_Time = 7.18628096[s]


(thousandths)
X : parts per Million : Carbon13
Filename = 20240109_TK-03038_c
Author = delta
Experiment = carbon.jxp
Sample_Id = 20240109_TK-03038
Solvent = DMSO-D6
Actual_Start_Time = 9-JAN-2024 21:10:0
Revision_Time = 10-JAN-2024 14:39:5
Comment = TK-03038
Data_Format = 1D COMPLEX
Dim_Size = 26214
X_Domain = Carbon13
Dim_Title = Carbon13
Dim_Units = [ppm]
Dimensions = X
Spectrometer = JNM-ECZ400S/L1
Field_Strength = 9.389766[T] (400[MH
X_Acq_Duration = 1.03809024[s]
X_Domain = 13C
X_Freq = 100.52530333[MHz]
X_Offset = 100[ppm]
X_Points = 32768
X_Prescans = 4
X_Resolution = 0.96330739[Hz]
X_Sweep = 31.56565657[kHz]
X_Sweep_Clipped = 25.25252525[kHz]
Irr_Domain = Proton
Irr_Freq = 399.78219838[MHz]
Irr_Offset = 5[ppm]
Blanking = 5[us]
Clipped = FALSE
Scans = 4096
Total_Scans = 4096
Relaxation_Delay = 2[s]
Recvr_Gain = 50
Temp_Get = 22.2[dC]
X_90_Width = 10.02[us]
X_Acq_Time = 1.03809024[s]
X_Angle = 30[deg]
X_Atn = 8[dB]
X_Pulse = 3.34[us]
Irr_Atn_Dec = 27.49[dB]
Irr_Atn_Dec_Calc = 27.49[dB]
Irr_Atn_Dec_Default_Calc = 27.49[dB]
Irr_Atn_Noe = 27.49[dB]
Irr_Dec_Bandwidth_Hz = 4.7826087[kHz]
Irr_Dec_Bandwidth_Ppm = 11.96303566[ppm]
Irr_Dec_Freq = 399.78219838[MHz]
Irr_Dec_Merit_Factor = 2.2
Irr_Decoupling = TRUE
Irr_Noe = TRUE
Irr_Noise = WALTZ
Irr_Offset_Default = 5[ppm]
Irr_Pwidth = 0.115[ms]
Irr_Pwidth_Default = 0.115[ms]
Irr_Pwidth_Default_Calc = 0.115[ms]
Irr_Pwidth_Temp1 = 0.115[ms]
Irr_Wurst = FALSE
Decimation_Rate = 0


S1
abundance
X : parts per Million : Proton
2.00
2.03
1.97
1.95
0.92
0.91
0.95
7.271
6.697
6.680
5.751
5.734
4.652
4.638
4.624
3.805
3.792
3.780
3.658
3.644
3.630
3.437
3.424
3.411
2.184
2.172
2.159
2.069
1.731
1.253
0.000
Filename = 20240528_TK-03143A_pro
Author = delta
Experiment = proton.jxp
Sample_Id = 20240528_TK-03143A
Solvent = CHLOROFORM-D
Actual_Start_Time = 28-MAY-2024 16:35:36
Revision_Time = 28-MAY-2024 17:58:12
Comment = TK-03143A
Data_Format = 1D COMPLEX
Dim_Size = 104858
X_Domain = Proton
Dim_Title = Proton
Dim_Units = [ppm]
Dimensions = X
Spectrometer = JNM-ECZ400S/L1
Field_Strength = 9.389766[T] (400[MHz])
X_Acq_Duration = 2.18628096[s]
X_Domain = 1H
X_Freq = 399.78219838[MHz]
X_Offset = 5[ppm]
X_Points = 16384
X_Prescans = 1
X_Resolution = 0.45739775[Hz]
X_Sweep = 7.4940048[kHz]
X_Sweep_Clipped = 5.99520384[kHz]
Irr_Domain = Proton
Irr_Freq = 399.78219838[MHz]
Irr_Offset = 5[ppm]
Tri_Domain = Proton
Tri_Freq = 399.78219838[MHz]
Tri_Offset = 5[ppm]
Blanking = 2[us]
Clipped = FALSE
Scans = 16
Total_Scans = 16
Relaxation_Delay = 5[s]
Recvr_Gain = 46
Temp_Get = 22.5[dC]
X_90_Width = 6.4[us]
X_Acq_Time = 2.18628096[s]
X_Angle = 45[deg]
X_Atn = 2.4[dB]
X_Pulse = 3.2[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Loop = 500
Dante_Presat = FALSE
Decimation_Rate = 0
Initial_Wait = 1[s]
Phase = (0, 90, 270, 180, 180,
Presat_Time = 5[s]
Presat_Time_Flag = FALSE
Relaxation_Delay_Calc = 0[s]
Relaxation_Delay_Temp = 5[s]
Repetition_Time = 7.18628096[s]


(thousandths)
X : parts per Million : Carbon13
153.240
110.137
77.316
77.000
76.684
72.477
61.466
53.752
50.992
Filename = 20240530_TK-03143A_
Author = delta
Experiment = carbon.jxp
Sample_Id = 20240530_TK-03143A
Solvent = CHLOROFORM-D
Actual_Start_Time = 31-MAY-2024 01:36:4
Revision_Time = 2-OCT-2024 19:07:2
Comment = TK-03143A
Data_Format = 1D COMPLEX
Dim_Size = 26214
X_Domain = Carbon13
Dim_Title = Carbon13
Dim_Units = [ppm]
Dimensions = X
Spectrometer = JNM-ECZ400S/L1
Field_Strength = 9.389766[T] (400[MH
X_Acq_Duration = 1.03809024[s]
X_Domain = 13C
X_Freq = 100.52530333[MHz]
X_Offset = 100[ppm]
X_Points = 32768
X_Prescans = 4
X_Resolution = 0.96330739[Hz]
X_Sweep = 31.56565657[kHz]
X_Sweep_Clipped = 25.25252525[kHz]
Irr_Domain = Proton
Irr_Freq = 399.78219838[MHz]
Irr_Offset = 5[ppm]
Blanking = 5[us]
Clipped = TRUE
Scans = 4096
Total_Scans = 4096
Relaxation_Delay = 2[s]
Recvr_Gain = 50
Temp_Get = 22.5[dC]
X_90_Width = 10.02[us]
X_Acq_Time = 1.03809024[s]
X_Angle = 30[deg]
X_Atn = 8[dB]
X_Pulse = 3.34[us]
Irr_Atn_Dec = 27.49[dB]
Irr_Atn_Dec_Calc = 27.49[dB]
Irr_Atn_Dec_Default_Calc = 27.49[dB]
Irr_Atn_Noe = 27.49[dB]
Irr_Dec_Bandwidth_Hz = 4.7826087[kHz]
Irr_Dec_Bandwidth_Ppm = 11.96303566[ppm]
Irr_Dec_Freq = 399.78219838[MHz]
Irr_Dec_Merit_Factor = 2.2
Irr_Decoupling = TRUE
Irr_Noe = TRUE
Irr_Noise = WALTZ
Irr_Offset_Default = 5[ppm]
Irr_Pwidth = 0.115[ms]
Irr_Pwidth_Default = 0.115[ms]
Irr_Pwidth_Default_Calc = 0.115[ms]
Irr_Pwidth_Temp1 = 0.115[ms]
Irr_Wurst = FALSE
Decimation_Rate = 0


TBSO
H
N
OTBS
S2
abundance
X : parts per Million : Proton
18.01
11.56
4.04
4.00
2.38
7.262
3.747
3.735
3.721
2.741
2.728
2.715
1.693
0.903
0.895
0.888
0.068
0.060
0.053
0.000
JEOL
Filename = 20230913_TK-02175_prot
Author = delta
Experiment = proton.jxp
Sample_Id = 20230913_TK-02175
Solvent = CHLOROFORM-D
Actual_Start_Time = 13-SEP-2023 20:14:56
Revision_Time = 13-SEP-2023 21:32:01
Comment = TK-02175
Data_Format = 1D COMPLEX
Dim_Size = 104858
X_Domain = Proton
Dim_Title = Proton
Dim_Units = [ppm]
Dimensions = X
Spectrometer = JNM-ECZ400S/L1
Field_Strength = 9.389766[T] (400[MHz])
X_Acq_Duration = 2.18628096[s]
X_Domain = 1H
X_Freq = 399.78219838[MHz]
X_Offset = 5[ppm]
X_Points = 16384
X_Prescans = 1
X_Resolution = 0.45739775[Hz]
X_Sweep = 7.4940048[kHz]
X_Sweep_Clipped = 5.99520384[kHz]
Irr_Domain = Proton
Irr_Freq = 399.78219838[MHz]
Irr_Offset = 5[ppm]
Tri_Domain = Proton
Tri_Freq = 399.78219838[MHz]
Tri_Offset = 5[ppm]
Blanking = 2[us]
Clipped = FALSE
Scans = 16
Total_Scans = 16
Relaxation_Delay = 5[s]
Recvr_Gain = 56
Temp_Get = 22.9[dC]
X_90_Width = 6.4[us]
X_Acq_Time = 2.18628096[s]
X_Angle = 45[deg]
X_Atn = 2.4[dB]
X_Pulse = 3.2[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Loop = 500
Dante_Presat = FALSE
Decimation_Rate = 0
Initial_Wait = 1[s]
Phase = (0, 90, 270, 180, 180,
Presat_Time = 5[s]
Presat_Time_Flag = FALSE
Relaxation_Delay_Calc = 0[s]
Relaxation_Delay_Temp = 5[s]
Repetition_Time = 7.18628096[s]


(thousandths)
X : parts per Million : Carbon13
77.352
77.237
77.036
76.719
62.614
51.814
25.969
18.332
0.000
-5.318
JEOL
Filename = 20230913_TK-02175_1
Author = delta
Experiment = carbon.jxp
Sample_Id = 20230913_TK-02175_1
Solvent = CHLOROFORM-D
Actual_Start_Time = 14-SEP-2023 02:56:3
Revision_Time = 2-OCT-2024 11:30:0
Comment = TK-02175
Data_Format = 1D COMPLEX
Dim_Size = 26214
X_Domain = Carbon13
Dim_Title = Carbon13
Dim_Units = [ppm]
Dimensions = X
Spectrometer = JNM-ECZ400S/L1
Field_Strength = 9.389766[T] (400[MH
X_Acq_Duration = 1.03809024[s]
X_Domain = 13C
X_Freq = 100.52530333[MHz]
X_Offset = 100[ppm]
X_Points = 32768
X_Prescans = 4
X_Resolution = 0.96330739[Hz]
X_Sweep = 31.56565657[kHz]
X_Sweep_Clipped = 25.25252525[kHz]
Irr_Domain = Proton
Irr_Freq = 399.78219838[MHz]
Irr_Offset = 5[ppm]
Blanking = 5[us]
Clipped = FALSE
Scans = 4096
Total_Scans = 4096
Relaxation_Delay = 2[s]
Recvr_Gain = 50
Temp_Get = 22.8[dC]
X_90_Width = 10.02[us]
X_Acq_Time = 1.03809024[s]
X_Angle = 30[deg]
X_Atn = 8[dB]
X_Pulse = 3.34[us]
Irr_Atn_Dec = 27.49[dB]
Irr_Atn_Dec_Calc = 27.49[dB]
Irr_Atn_Dec_Default_Calc = 27.49[dB]
Irr_Atn_Noe = 27.49[dB]
Irr_Dec_Bandwidth_Hz = 4.7826087[kHz]
Irr_Dec_Bandwidth_Ppm = 11.96303566[ppm]
Irr_Dec_Freq = 399.78219838[MHz]
Irr_Dec_Merit_Factor = 2.2
Irr_Decoupling = TRUE
Irr_Noe = TRUE
Irr_Noise = WALTZ
Irr_Offset_Default = 5[ppm]
Irr_Pwidth = 0.115[ms]
Irr_Pwidth_Default = 0.115[ms]
Irr_Pwidth_Default_Calc = 0.115[ms]
Irr_Pwidth_Temp1 = 0.115[ms]
Irr_Wurst = FALSE
Decimation_Rate = 0