

Supporting Information
For

Regioselective Synthesis of Functionalized Pyrazole-Chalcones via Base Mediated Reaction of Diazo Compounds with Pyrylium Salts

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Comment [N]: spelling corrected

1. General Information

Until mentioned otherwise, all reactions were carried out under nitrogen atmosphere in flame-dried glassware. All reactions were monitored by Thin Layer Chromatography (TLC) and visualization was effected with UV and/or by developing in iodine. Melting points were recorded on a Precision melting point apparatus and are uncorrected. NMR spectra were recorded on a Bruker Avance spectrometer at 300/400/500 MHz (^1H), 75/100/125 MHz (^{13}C), 121/162 MHz (^{31}P) and 282/376 MHz (^{19}F). Chemical shifts are reported in δ (ppm) relative to TMS as the internal standard for ^1H and ^{13}C . To describe spin multiplicity, standard abbreviations such as s, d, t, q, m, dd referring to singlet, doublet, triplet, quartet, multiplet and doublet of doublet respectively, are used. The ESI-HRMS spectra were recorded on Agilent 6520- Q-ToF/MS system.

The starting substrates i.e. trisubstituted-pyrylium tetrafluoroborate salts¹ and diazo compounds² were synthesized according to standard protocols. All other chemicals and catalysts were purchased from commercial sources and used as received.

2. General Procedures

General procedure for the reaction of 2,4,6-trisubstituted pyrylium tetrafluoroborate salts **1** with diazo compounds **2**

In an oven dried 25 mL round bottom flask equipped with a magnetic stirring bar, the trisubstituted pyrylium tetrafluoroborate salt **1** (0.4 mmol) and diazo substrate **2** (0.2 mmol) were dissolved in anhydrous CH_3CN (5.0 mL) followed by dropwise addition of DBU (0.4 mL, 0.3 mmol) in the reaction mixture. The resulting reaction mixture was stirred at room temperature until reaction completion (2-6 h; TLC monitoring). The reaction mixture was concentrated under reduced pressure and diluted with water (10 mL). The crude product was extracted with dichloromethane (10 mL x 3) and the organic layer was washed with brine (5 mL x 3), dried over Na_2SO_4 and concentrated under reduced pressure. The crude product was purified by column chromatography on neutral silica gel (100-200 mesh) using hexane/ethyl acetate as eluent to afford the pure product **3**.

General procedure for conversion of pyrazole-chalcones **3** into indenyl-pyrazoles **4**

In an oven dried 25 mL round bottom flask equipped with a magnetic stirring bar, the sulfonylated pyrazole-chalcone **3** (0.1 mmol) and NaBH_4 (15 mg, 0.4 mmol) were taken in toluene (5.0 mL). The reaction mixture was stirred at room temperature until reaction completion (2-4 h; TLC monitoring) and 1N acetic acid (2.0 mL, excess) was added. After stirring at room temperature for additional 15 minutes, the reaction mixture was diluted with water (5 mL) and extracted with ethyl acetate (5 mL x 3). The organic layer was washed with brine (5 mL x 3), dried over Na_2SO_4 and concentrated under reduced pressure. The crude product was purified by column chromatography on neutral silica gel (100-200 mesh) using hexane/ethyl acetate as eluent to afford the pure product **4**.

3. Details of Variable Temperature NMR Experiments

In order to record ^1H NMR at variable temperatures, a 33.3 mM solution of **3c** was prepared freshly and NMR was recorded at 223K, 300K and 323K (Figure 1). The singlets at 3.80 ppm and 3.75 ppm are for -OMe group in the major and minor isomers, respectively which are

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little shielded at. The “doublets” for PO(OMe)₂ group in major and minor isomers are not resolved well at 223 and 300K, either due to slow intermediate exchange causing peak-broadening or due to shielding of the minor doublet (notably, the -OMe peak in the minor isomer is also shielded at 223K). However at 323 K, both the doublets for minor as well as for the major tautomer are well resolved and appear at 3.68 ppm ($^3J_{\text{H-P}} = 11.3$ Hz) and 3.66 ppm ($^3J_{\text{H-P}} = 11.4$ Hz), respectively.³

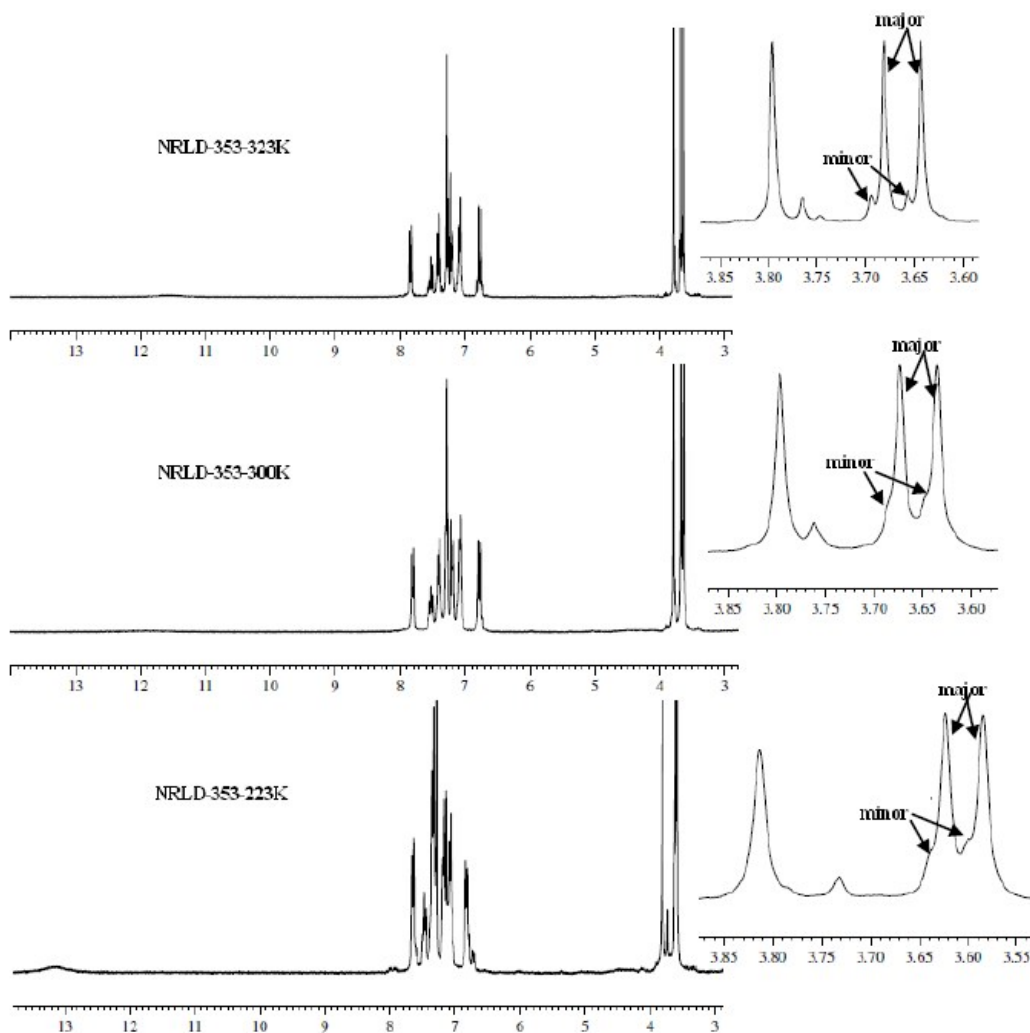


Figure 1. ¹H NMR spectrum of **3c** recorded at variable temperatures

4. Details of X-ray Analysis of **3a**

A good quality single crystal of compound **3a** of size 0.20 x 0.19 x 0.16 mm, was selected under a polarizing microscope and mounted on a glass fibre for data collection. Single crystal X-ray data for compound **3a** was collected on the Rigaku Kappa 3 circle diffractometer equipped with the AFC-12 goniometer and enhanced sensitivity (HG) Saturn724+ CCD detector in the 4x4 bin mode using the monochromated Mo-K α radiation generated from the microfocus sealed tube MicroMax-003 X-ray generator equipped with specially designed confocal multilayer optics. Data collection was performed using ω -scans of 0.5 $^\circ$ steps at 293(2) K. Cell determination, data collection and data reduction was performed using the Rigaku CrystalClear-SM Expert 2.1 b24 software.⁴ Structure solution and refinement were performed by using SHELX-97.⁵ Refinement of coordinates and anisotropic thermal

parameters of non-hydrogen atoms were carried out by the full-matrix least-squares method. The hydrogen atoms attached to carbon atoms were generated with idealized geometries and isotropically refined using a riding model.

Crystallization: Crystals of compound **3a** were grown from the solvent DCM:MeOH (1:3) by slow evaporation method (Figure 2; Table 1).

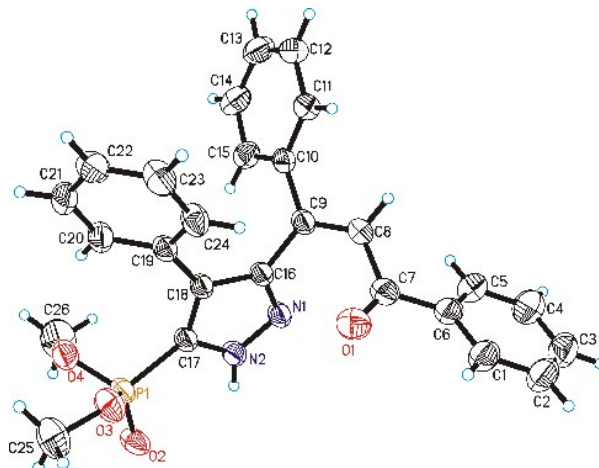


Figure 2. ORTEP diagram drawn with molecule of solvent of crystallization with 30% ellipsoid probability for non-H atoms of the crystal structure of compound **3a** determined at 293 K

Table 1 Crystal data and structure refinement details for **3a**

Compound	3a
Empirical formula	C ₂₆ H ₂₃ N ₂ O ₄ P
Formula weight	458.43
Crystal System	Triclinic
Space group	<i>P</i> -1
<i>a</i> (Å)	8.83667(15)
<i>b</i> (Å)	12.0256(2)
<i>c</i> (Å)	12.1039(2)
<i>α</i> (°)	83.6482(15)
<i>β</i> (°)	74.9958(16)
<i>γ</i> (°)	70.8882(16)
<i>V</i> (Å ³)	1173.43(4)
<i>Z</i>	2
<i>D_c</i> (g/cm ³)	1.297
<i>F</i> ₀₀₀	480
<i>μ</i> (mm ⁻¹)	1.328
<i>θ</i> _{max} (°)	72.72
Total reflections	10050
Unique reflections	4092
Reflections [<i>I</i> > 2σ(<i>I</i>)]	3651
Parameters	305
<i>R</i> _{int}	0.1042
Goodness-of-fit	1.067
<i>R</i> [<i>F</i> ² > 2σ(<i>F</i> ²)]	0.0753
<i>wR</i> (<i>F</i> ² , all data)	0.2172
CCDC No.	2038874

5. References

- (1) For preparation of trisubstituted-pyrylium tetrafluoroborate salts, see: (a) C. T. F. Salfeena, Basavaraja, K. T. Ashitha, V. P. Kumar, S. Varughese, C. H. Suresh, B. S. Sashidhar, *Chem. Commun.* **2018**, *54*, 12463-12466; (b) L. E. E. Broeckx, S. Gven, F. J. L. Heutz, M. Lutz, D. Vogt, C. Muller, *Chem. Eur. J.* **2013**, *19*, 13087-13098; (c) Y. Zhao, B. Huang, C. Yang, B. Li, B. Gou, W. Xia, *ACS Catal.* **2017**, *7*, 2446-2451; (d) B. Breit, R. Winde, T. Mackewitz, R. Paciello, K. Harms, *Chem. Eur. J.* **2001**, *7*, 3106-3121; (e) T. W. Greulich, C. G. Daniliuc, A. Studer, *Org. Lett.* **2015**, *17*, 254-257.
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- (3) R. Muruganatham, I. Namboothiri, *J. Org. Chem.* **2010**, *75*, 2197-2205
- (4) CrystalClear 2.1, Rigaku Corporation, Tokyo, Japan
- (5) G. M. Sheldrick, *Acta Crystallogr. Sect. A* **2008**, *64*, 112-122

6. Characterization Data

Dimethyl (Z)-(3-(3-oxo-1,3-diphenylprop-1-en-1-yl)-4-phenyl-1H-pyrazol-5-yl)phosphonate (3a)

White solid; isolated yield 72% (66 mg). R_f 0.50 (70% EtOAc/hexane); Mp 159-160 °C; ^1H NMR (300 MHz, CDCl_3) δ 7.76 (d, $J = 7.5$ Hz, 2H), 7.45 (t, $J = 7.3$ Hz, 1H), 7.32 (t, $J = 7.6$ Hz, 2H), 7.14-7.24 (m merged with solvent peak, 6H), 7.06-7.09 (m, 2H), 6.96-7.01 (m, 3H), 3.55 (d, $^3J_{\text{H-P}} = 11.4$ Hz, 6H); ^{13}C NMR (75 MHz, CDCl_3) δ 191.60, 143.52, 139.12, 137.74, 132.96, 130.76, 129.80, 129.49, 128.67, 128.42, 128.38, 128.16, 128.02, 127.79, 127.66, 127.26, 53.16 (d, $^2J_{\text{C-P}} = 5.3$ Hz); ^{31}P NMR (162 MHz, CDCl_3) δ 10.90 (s); HRMS for $\text{C}_{26}\text{H}_{23}\text{N}_2\text{O}_4\text{P}$: calcd. (MH^+): 459.1468, found: 459.1464

Selected X-ray crystallographic data for 3a, $\text{C}_{26}\text{H}_{23}\text{N}_2\text{O}_4\text{P}$, $M = 458.43$, Triclinic, $P -1$, $a = 8.83667(15)$ Å, $b = 12.0256(2)$ Å, $c = 12.1039(2)$ Å, $V = 1173.43(4)$ Å³, $\alpha = 83.6482(15)$ °, $\beta = 74.9958(16)$ °, $\gamma = 70.8882(16)$ °, $Z = 2$, $D_c = 1.297$ g/cm³, $\mu(\text{Mo-K}\alpha) = 1.328$ mm⁻¹, $F(000) = 480$, Reflections collected: Unique 10050/4092 [$R(\text{int}) = 0.1042$]. Final R indices [$I > 2\sigma(I)$], $R_1 = 0.0753$, $wR_2 = 0.2172$.

Dimethyl (Z)-(3-(3-oxo-3-phenyl-1-(p-tolyl)prop-1-en-1-yl)-4-phenyl-1H-pyrazol-5-yl)phosphonate (3b)

Yellow solid; isolated yield 69% (65 mg). R_f 0.50 (70% EtOAc/hexane); Mp 151-153 °C; ^1H NMR (300 MHz, CDCl_3) δ 7.76 (d, $J = 7.5$ Hz, 2H), 7.46-7.50 (m, 1H), 7.33-7.38 (m, 2H), 7.13-7.21 (m, 5H), 7.03 (br s, 5H), 3.61 (d, $^3J_{\text{H-P}} = 11.4$ Hz, 6H), 2.28 (s, 3H); ^{13}C NMR (75 MHz, CDCl_3) δ 191.44, 143.49, 139.80, 137.85, 136.21, 132.73, 130.80, 129.71, 129.14, 128.56, 128.25, 127.96, 127.88, 127.60, 127.13, 126.74, 53.10 (d, $^2J_{\text{C-P}} = 5.5$ Hz), 21.20; ^{31}P NMR (121 MHz, CDCl_3) δ 10.97 (s); HRMS for $\text{C}_{27}\text{H}_{25}\text{N}_2\text{O}_4\text{P}$: calcd. (MH^+): 473.1625, found: 473.1630

Dimethyl (Z)-(3-(1-(4-methoxyphenyl)-3-oxo-3-phenylprop-1-en-1-yl)-4-phenyl-1H-pyrazol-5-yl)phosphonate (3c)

Yellow solid; isolated yield 64% (62 mg). R_f 0.50 (80% EtOAc/hexane); Mp 84-92°C; ^1H NMR (300 MHz, CDCl_3): (major/minor in 1:0.70 ratio) δ 12.30 (br s, 1H), 7.75 (d, $J = 7.3$ Hz, 2H, major), 7.56 (d, $J = 7.4$ Hz, 2H, minor), 7.44-7.49 (m, 2H, minor), 7.26-7.37 (merged with solvent peak, 10H), 7.12-7.18 (m, 5H), 7.05-7.07 (m, 4H), 6.74-6.79 (m, 3H), 6.67 (d, $J = 8.3$ Hz, 2H, minor), 3.76 (s, 3H, major), 3.70 (s, 3H, minor), 3.61 (d, $^3J_{\text{H-P}} = 11.4$ Hz, 12H); ^{13}C NMR (75 MHz, CDCl_3) δ 192.07, 191.28, 160.88, 159.98, 143.27, 138.04, 137.73, 132.71, 132.69, 131.47, 131.38, 131.05, 130.81, 130.07, 129.70, 129.47, 128.63, 128.52, 128.38, 128.29, 128.23, 127.95, 127.81, 127.65, 127.22, 126.43, 125.59, 113.92, 113.45, 55.35, 55.18, 53.14 (d, $^2J_{\text{C-P}} = 5.5$ Hz); ^{31}P NMR (162 MHz, CDCl_3): (major/minor in 1:0.66 ratio) δ 10.95 (s, major), 10.20 (s, minor); HRMS for $\text{C}_{27}\text{H}_{25}\text{N}_2\text{O}_5\text{P}$: calcd. (MH^+): 489.1574, found: 489.1576

Dimethyl (Z)-(3-(1-(4-chlorophenyl)-3-oxo-3-phenylprop-1-en-1-yl)-4-phenyl-1H-pyrazol-5-yl)phosphonate (3d)

Yellow solid; isolated yield 50% (49 mg). R_f 0.50 (65% EtOAc/hexane); Mp 113-115°C; ^1H NMR (400 MHz, CDCl_3) δ 7.71 (d, $J = 7.3$ Hz, 2H), 7.42 (t, $J = 7.4$ Hz, 1H), 7.30 (t, $J = 7.7$ Hz, 2H), 7.09-7.18 (m merged with solvent peak, 5H), 7.04-7.07 (m, 2H), 6.98-7.01 (m, 3H), 3.52 (d, $^3J_{\text{H-P}} = 11.5$ Hz, 6H); ^{13}C NMR (100 MHz, CDCl_3) δ 191.46, 142.61, 137.62, 137.58, 135.45, 132.99, 130.60, 129.67, 129.21, 128.63, 128.59, 128.38, 128.14, 127.91, 127.75, 127.41, 53.17 (d, $^2J_{\text{C-P}} = 5.3$ Hz); ^{31}P NMR (162 MHz, CDCl_3): (major/minor in 1:0.04 ratio) δ 12.92 (s, minor), 10.45 (s, major); HRMS for $\text{C}_{26}\text{H}_{22}\text{ClN}_2\text{O}_4\text{P}$: calcd. (MH^+): 493.1078, found: 493.1079

Dimethyl (Z)-(3-(1-(4-bromophenyl)-3-oxo-3-phenylprop-1-en-1-yl)-4-phenyl-1H-pyrazol-5-yl)phosphonate (3e)

White solid; isolated yield 48% (51 mg). R_f 0.50 (65% EtOAc/hexane); Mp 130-132 °C; ^1H NMR (300 MHz, CDCl_3): (minor tautomer in traces) δ 7.70-7.73 (m, 2H), 7.40-7.46 (m, 1H), 7.25-7.33 (m, 4H), 7.10-7.12 (m, 2H), 7.05-7.08 (m, 3H), 6.99-7.02 (m, 3H), 3.53 (d, $^3J_{\text{H-P}} = 11.5$ Hz, 6H); ^{13}C NMR (75 MHz, CDCl_3) δ 191.43, 142.67, 138.03, 137.56, 132.95, 131.52, 130.55, 129.63, 129.42, 128.60, 128.33, 128.07, 127.91, 127.74, 127.38, 123.75, 53.15 (d, $^2J_{\text{C-P}} = 5.5$ Hz); ^{31}P NMR (121 MHz, CDCl_3): (major/minor in 1:0.03 ratio) δ 12.95 (s, minor), 10.41 (s, major); HRMS for $\text{C}_{26}\text{H}_{22}\text{BrN}_2\text{O}_4\text{P}$: calcd. (MH^+): 537.0573, found: 537.0578

Dimethyl (Z)-(4-(4-methoxyphenyl)-3-(3-(4-methoxyphenyl)-3-oxo-1-phenylprop-1-en-1-yl)-1H-pyrazol-5-yl)phosphonate (3f)

Yellow solid; isolated yield 65% (67 mg). R_f 0.50 (85% EtOAc/hexane); Mp 84-86 °C; ^1H NMR (300 MHz, CDCl_3): (major/minor in 1:0.24 ratio) δ 7.78 (d, $J = 7.9$ Hz, 2H, major), 7.55-7.63 (m, 2H, minor), 7.19-7.43 (m merged with solvent peak, 13H), 7.05 (d, $J = 8.1$ Hz, 2H, major), 6.85 (d, $J = 8.2$ Hz, 2H, major), 6.66-6.80 (m, 3H, minor), 6.56 (d, $J = 8.2$ Hz, 2H, major), 3.85 (s, 3H, major), 3.80 (s, 3H, minor), 3.72 (d, $^3J_{\text{H-P}} = 11.5$ Hz, 6H, minor), 3.65, 3.61 (s, 3H, major and d, 6H major merged together); ^{13}C NMR (75 MHz, CDCl_3) δ

191.08, 163.51, 158.66, 142.38, 139.30, 131.04, 131.00, 130.64, 130.59, 129.28, 128.38, 128.15, 127.93, 123.06, 113.53, 113.14, 55.46, 54.95, 53.10 (d, $^2J_{C-P} = 5.6$ Hz); ^{31}P NMR (121 MHz, $CDCl_3$): (major/minor in 1:0.09 ratio) δ 13.47 (s, minor), 11.50 (s, major); HRMS for $C_{28}H_{27}N_2O_6P$: calcd. (MH⁺): 519.1679, found: 519.1682

Dimethyl (Z)-(3-(1,3-bis(4-methoxyphenyl)-3-oxoprop-1-en-1-yl)-4-(4-methoxyphenyl)-1H-pyrazol-5-yl)phosphonate (3g)

Yellow solid; isolated yield 61% (67 mg). R_f 0.50 (90% EtOAc/hexane); Mp 77-80 °C; 1H NMR (400 MHz, $CDCl_3$): (major/minor in 1:0.12 ratio) δ 7.79 (m appearing as d, $J = 8.8$ Hz, 2H, major), 7.54-7.57 (m, 2H, minor), 7.33-7.36 (m, 2H, minor), 7.22-7.26 (m merged with solvent peak, 2H, major), 7.17-7.19 (s, 1H, major merged with m, 1H, minor), 7.06-7.09 (m, 2H, major), 6.89-6.91 (m, 3H, minor), 6.84-6.88 (m, 2H, major), 6.73-6.77 (m, 2H, major merged with m, 2H, minor), 6.56-6.60 (m, 2H, major), 3.86 (s, 3H, major), 3.81 (s, 3H, minor), 3.80 (s, 3H, minor), 3.78 (s, 3H, major), 3.75 (s, 3H, minor), 3.67 (d, $^3J_{H-P} = 11.4$ Hz, 6H, minor), 3.67 (s, 3H, major), 3.65 (d, $^3J_{H-P} = 11.4$ Hz, 6H, major); ^{13}C NMR (100 MHz, $CDCl_3$) δ 189.86, 163.42, 160.73, 158.67, 142.09, 131.57, 131.26, 130.96, 130.88, 129.41, 127.93, 127.72, 126.11, 123.12, 113.91, 113.52, 113.18, 55.48, 55.37, 54.98, 53.13 (d, $^2J_{C-P} = 5.6$ Hz); ^{31}P NMR (162 MHz, $CDCl_3$): (major/minor in 1:0.13 ratio) δ 11.60 (s, major), 10.77 (s, minor); HRMS for $C_{29}H_{29}N_2O_7P$: calcd. (MH⁺): 549.1785, found: 549.1776

Dimethyl (Z)-(3-(1-(4-methoxyphenyl)-3-oxo-3-(p-tolyl)prop-1-en-1-yl)-4-(p-tolyl)-1H-pyrazol-5-yl)phosphonate (3h)

Yellow solid; isolated yield 67% (69 mg). R_f 0.50 (70% EtOAc/hexane); Mp 84-92 °C; 1H NMR (300 MHz, $CDCl_3$): (major/minor in 1:0.25 ratio) δ 7.67 (d, $J = 7.6$ Hz, 2H, major), 7.47 (d, $J = 7.8$ Hz, 2H, minor), 7.26-7.29 (m, 5H), 7.15-7.18 (m merged with solvent peak, 6H), 7.04-7.09 (m, 4H), 6.84-6.87 (m appearing as d, $J = 7.6$ Hz, 3H), 6.73-6.79 (m, 4H), 3.79 (s, 3H, major), 3.75 (s, 3H, minor), 3.64 (d, $^3J_{H-P} = 11.4$ Hz, 12H), 2.39 (s, 3H, major), 2.37 (s, 3H, minor), 2.34 (s, 3H, minor), 2.17 (s, 3H, major); ^{13}C NMR (75 MHz, $CDCl_3$) δ 191.62, 190.88, 160.80, 159.93, 143.54, 143.48, 142.67, 137.56, 136.74, 135.43, 135.28, 131.59, 130.97, 129.93, 129.58, 129.43, 129.18, 128.96, 128.90, 128.83, 128.73, 128.41, 128.23, 127.77, 126.63, 125.88, 113.91, 113.49, 55.36, 55.19, 53.14 (d, $^2J_{C-P} = 5.6$ Hz), 53.11 (d, $^2J_{C-P} = 5.5$ Hz), 21.65, 21.61, 21.28, 21.08; ^{31}P NMR (162 MHz, $CDCl_3$): (major/minor in 1:0.60 ratio) δ 11.31 (s, major), 10.53 (s, minor); HRMS for $C_{29}H_{29}N_2O_5P$: calcd. (MH⁺): 517.1887, found: 517.1883

Diethyl (Z)-(3-(3-oxo-1,3-diphenylprop-1-en-1-yl)-4-phenyl-1H-pyrazol-5-yl)phosphonate (3i)

Yellow solid; isolated yield 47% (46 mg). R_f 0.50 (70% EtOAc/hexane); Mp 133-135 °C; 1H NMR (400 MHz, $CDCl_3$) δ 12.25 (br s, 1H), 7.76 (t, $J = 6.9$ Hz, 2H), 7.43-7.47 (m, 1H), 7.29-7.35 (m, 4H), 7.21-7.24 (m, 3H), 7.14-7.17 (m merged with solvent peak, 3H), 7.01-7.03 (m, 3H), 3.85-4.05 (m, 4H), 1.08 (t, $^4J_{H-P} = 6.9$ Hz, 6H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 191.64, 139.25, 137.79, 132.67, 130.95, 129.80, 129.34, 128.60, 128.34, 128.21, 128.07, 127.95, 127.81, 127.66, 127.54, 127.09, 62.80 (d, $^2J_{C-P} = 5.2$ Hz), 15.91 (d, $^2J_{C-P} = 6.8$ Hz);

^{31}P NMR (162 MHz, CDCl_3) δ 7.37 (s); HRMS for $\text{C}_{28}\text{H}_{27}\text{N}_2\text{O}_4\text{P}$: calcd. (MH^+): 487.1781, found: 487.1780

Diethyl (Z)-(3-(1-(4-methoxyphenyl)-3-oxo-3-phenylprop-1-en-1-yl)-4-phenyl-1H-pyrazol-5-yl)phosphonate (3j)

Yellow solid; isolated yield 43% (44 mg). R_f 0.50 (80% EtOAc/hexane); Mp 147-150 °C; ^1H NMR (300 MHz, CDCl_3): (major/minor in 1:0.13 ratio) δ 7.78 (d, $J = 7.5$ Hz, 2H, maj), 7.53-7.56 (m, 2H, min), 7.48 (t, $J = 7.2$ Hz, 1H, maj), 7.34-7.39 (m, 4H), 7.18-7.29 (m merged with solvent peak, 12H), 7.05-7.10 (m, 5H), 6.70-6.77 (m, 4H), 3.88-4.11 (m, 8H), 3.77 (s, 3H, maj), 3.73 (s, 3H, min), 1.13 (t, $J = 7.1$ Hz, 12H); ^{13}C NMR (75 MHz, CDCl_3) δ 191.36, 160.75, 159.75, 143.72, 138.09, 132.42, 131.56, 131.08, 131.02, 130.11, 129.70, 129.39, 128.64, 128.46, 128.11, 127.86, 127.55, 127.05, 126.32, 125.43, 113.83, 113.19, 62.80 (d, $^2J_{\text{C-P}} = 5.3$ Hz), 55.30, 55.10, 15.89 (d, $^3J_{\text{C-P}} = 6.9$ Hz); ^{31}P NMR (121 MHz, CDCl_3): (major/minor in 1:0.03 ratio) δ 9.29 (s, minor), 7.52 (s, major); HRMS for $\text{C}_{29}\text{H}_{29}\text{N}_2\text{O}_5\text{P}$: calcd. (MH^+): 517.1887, found: 517.1882

Diethyl (Z)-(3-(1-(4-chlorophenyl)-3-oxo-3-phenylprop-1-en-1-yl)-4-phenyl-1H-pyrazol-5-yl)phosphonate (3k)

White solid; isolated yield 36% (37 mg). R_f 0.50 (65% EtOAc/hexane); Mp 157-159°C; ^1H NMR (300 MHz, CDCl_3) δ 12.38 (br s, 1H), 7.78 (d, $J = 7.1$ Hz, 2H), 7.46-7.51 (m, 1H), 7.36 (t, $J = 7.4$ Hz, 2H), 7.15-7.24 (m merged with solvent peak, 7H), 7.07-7.08 (br m, 3H), 3.88-4.07 (m, 4H), 1.11 (t, $^4J_{\text{H-P}} = 6.9$ Hz, 6H); ^{13}C NMR (75 MHz, CDCl_3) δ 191.49, 142.87, 137.69, 137.66, 135.35, 132.83, 130.76, 129.72, 129.17, 128.60, 128.55, 128.28, 128.07, 127.86, 127.82, 127.67, 127.28, 62.89 (d, $^2J_{\text{C-P}} = 5.4$ Hz), 15.91 (d, $^2J_{\text{C-P}} = 6.8$ Hz); ^{31}P NMR (162 MHz, CDCl_3) δ 7.04 (s); HRMS for $\text{C}_{28}\text{H}_{26}\text{ClN}_2\text{O}_4\text{P}$: calcd. (MH^+): 521.1391, found: 521.1384

(Z)-1,3-Diphenyl-3-(4-phenyl-5-(phenylsulfonyl)-1H-pyrazol-3-yl)prop-2-en-1-one (3l)

White solid; isolated yield 70% (69 mg). R_f 0.50 (40% EtOAc/hexane); Mp 181-183 °C; ^1H NMR (400 MHz, CDCl_3) δ 12.79 (br s, 1H), 7.87 (d, $J = 7.4$ Hz, 2H), 7.63 (d, $J = 7.4$ Hz, 2H), 7.48-7.59 (m, 2H), 7.29-7.46 (m, 5H), 7.18-7.22 (br m merged with solvent peak, 5H), 6.92-7.04 (m, 5H); ^{13}C NMR (100 MHz, CDCl_3) δ 191.44, 149.45, 142.11, 140.51, 140.23, 138.64, 137.22, 133.60, 133.22, 130.73, 129.54, 129.21, 128.78, 128.64, 128.44, 128.38, 128.10, 127.50, 127.36, 123.83; HRMS for $\text{C}_{30}\text{H}_{22}\text{N}_2\text{O}_3\text{S}$: calcd. (MH^+): 491.1424, found: 491.1427

(Z)-1-phenyl-3-(4-phenyl-5-(phenylsulfonyl)-1H-pyrazol-3-yl)-3-p-tolylprop-2-en-1-one (3m)

White solid; isolated yield 73% (74 mg). R_f 0.50 (40% EtOAc/hexane); Mp 173-176 °C; ^1H NMR (300 MHz, CDCl_3) δ 12.45 (br s, 1H), 7.65 (d, $J = 7.8$ Hz, 2H), 7.47 (d, $J = 7.6$ Hz, 2H), 7.30-7.41 (m, 2H), 7.12-7.27 (m, 4H), 7.02 (s, 1H), 6.91 (d, $J = 8.2$ Hz, 2H), 6.74-6.87 (m, 7H), 2.13 (s, 3H); ^{13}C NMR (75 MHz, CDCl_3) δ 191.35, 142.04, 140.59, 139.93, 137.37, 135.74, 133.46, 133.20, 130.72, 129.29, 129.11, 128.71, 128.65, 128.57, 128.11, 128.03,

127.53, 127.33, 123.73, 21.16; HRMS for C₃₁H₂₄N₂O₃S: calcd. (MH⁺): 505.1580, found: 505.1586

(Z)-3-(4-methoxyphenyl)-1-phenyl-3-(4-phenyl-5-(phenylsulfonyl)-1H-pyrazol-3-yl)prop-2-en-1-one (3n)

Yellow solid; isolated yield 60% (62 mg). *R_f* 0.50 (50% EtOAc/hexane); Mp 159-161 °C; ¹H NMR (300 MHz, CDCl₃) δ 12.49 (br s, 1H), 7.78 (d, *J* = 7.4 Hz, 2H), 7.61 (d, *J* = 7.5 Hz, 2H), 7.45-7.54 (m, 2H), 7.26-7.40 (m merged with solvent peak, 4H), 7.11-7.14 (m, 3H), 6.95-7.03 (m, 5H), 7.68 (d, *J* = 8.5 Hz, 2H), 3.74 (s, 3H); ¹³C NMR (100 MHz, CDCl₃) δ 191.23, 160.91, 141.58, 140.57, 137.47, 133.33, 133.20, 130.87, 130.65, 129.59, 129.32, 128.64, 128.51, 128.08, 127.49, 127.41, 126.45, 126.41, 123.50, 113.96, 55.40; HRMS for C₃₁H₂₄N₂O₄S: calcd. (MH⁺): 521.1530, found: 521.1533

(Z)-3-(4-(methylthio)phenyl)-1-phenyl-3-(4-phenyl-5-(phenylsulfonyl)-1H-pyrazol-3-yl)prop-2-en-1-one (3o)

Yellow solid; isolated yield 48% (51 mg). *R_f* 0.50 (50% EtOAc/hexane); Mp 94-98 °C; ¹H NMR (300 MHz, CDCl₃): (major/minor in 1:0.26 ratio) δ 12.46 (br s, 1H), 7.78 (d, *J* = 7.5 Hz, 2H, major), 7.60 (d, *J* = 7.6 Hz, 2H major + 2H minor), 7.42-7.54 (m, 5H), 7.22-7.44 (m merged with solvent peak, 10H), 7.17 (br s, 4H, minor), 6.90-7.09 (m, 14H), 6.77 (s, 1H, minor), 2.41 (s, 3H, major), 2.39 (s, 3H, minor); ¹³C NMR (75 MHz, CDCl₃) δ 191.28, 191.25, 141.52, 141.26, 140.53, 140.33, 137.34, 137.23, 134.99, 133.48, 133.24, 133.14, 130.72, 130.68, 129.85, 129.72, 129.23, 128.83, 128.69, 128.68, 128.58, 128.39, 128.17, 128.07, 127.55, 127.44, 127.32, 127.21, 125.89, 125.77, 123.66, 121.91, 15.36, 15.20; HRMS for C₃₁H₂₄N₂O₃S₂: calcd. (MH⁺): 537.1301, found: 537.1295

(Z)-3-(4-Chlorophenyl)-1-phenyl-3-(4-phenyl-5-(phenylsulfonyl)-1H-pyrazol-3-yl)prop-2-en-1-one (3p)

White solid; isolated yield 52% (54 mg). *R_f* 0.50 (40% EtOAc/hexane); Mp 190-192 °C; ¹H NMR (400 MHz, CDCl₃) δ 12.99 (br s, 1H), 7.86 (d, *J* = 7.4 Hz, 2H), 7.54-7.59 (m, 3H), 7.40-7.49 (m, 3H), 7.16 (s, 1H), 7.07 (br s, 5H), 6.99 (t, *J* = 7.4 Hz, 2H), 6.87 (d, *J* = 7.2 Hz, 2H); ¹³C NMR (100 MHz, CDCl₃) δ 191.33, 140.99, 140.40, 137.09, 135.59, 133.71, 133.29, 130.66, 129.37, 129.07, 128.77, 128.68, 128.67, 128.58, 128.53, 128.04, 127.67, 127.50, 123.80; HRMS for C₃₀H₂₁ClN₂O₃S: calcd. (MH⁺): 525.1034, found: 525.1031

(Z)-3-(4-bromophenyl)-1-phenyl-3-(4-phenyl-5-(phenylsulfonyl)-1H-pyrazol-3-yl)prop-2-en-1-one (3q)

White solid; isolated yield 51% (58 mg). *R_f* 0.50 (40% EtOAc/hexane); Mp 166-168 °C; ¹H NMR (300 MHz, CDCl₃) δ 12.96 (br s, 1H), 7.84 (d, *J* = 6.8 Hz, 2H), 7.54-7.61 (m, 3H), 7.40-7.50 (m, 3H), 7.27-7.35 (m, 4H), 7.02-7.09 (m, 5H), 6.90 (d, *J* = 6.3 Hz, 2H); ¹³C NMR (75 MHz, CDCl₃) δ 191.29, 140.89, 140.36, 137.48, 136.98, 133.62, 133.23, 131.50, 130.58, 129.52, 128.99, 128.69, 128.63, 128.58, 128.49, 127.97, 127.61, 127.45, 123.86, 123.67; HRMS for C₃₀H₂₁BrN₂O₃S: calcd. (MH⁺): 569.0529, found: 569.0536

(Z)-3-(4-fluorophenyl)-1-phenyl-3-(4-phenyl-5-(phenylsulfonyl)-1H-pyrazol-3-yl)prop-2-en-1-one (3r)

White solid; isolated yield 37% (38 mg). R_f 0.50 (40% EtOAc/hexane); Mp 202-204 °C; ^1H NMR (300 MHz, CDCl_3) δ 12.86 (br s, 1H), 7.85 (d, $J = 7.5$ Hz, 2H), 7.57 (d, $J = 7.6$ Hz, 2H), 7.88-7.54 (m, 4H), 7.24-7.31 (m merged with solvent peak, 2H), 7.08-7.13 (m, 3H), 7.02 (d, $J = 7.1$ Hz, 1H), 6.94-6.99 (m, 2H), 6.85-6.88 (m appearing as br d, 2H), 6.75-6.80 (m, 2H); ^{13}C NMR (75 MHz, DMSO-d_6) δ 189.61, 163.05 (d, $J_{\text{C-F}} = 246.7$ Hz), 148.30, 140.76, 139.90, 138.61, 137.17, 134.04, 133.68, 133.19, 129.87 (d, $J_{\text{C-F}} = 8.8$ Hz), 129.75, 129.62, 129.21, 128.46, 128.37, 128.07, 127.51, 127.34, 120.72, 115.79 (d, $J_{\text{C-F}} = 21.7$ Hz); HRMS for $\text{C}_{30}\text{H}_{21}\text{FN}_2\text{O}_3\text{S}$: calcd. (MH^+): 509.1330, found: 509.1323

(Z)-3-(3-methoxyphenyl)-1-phenyl-3-(4-phenyl-5-(phenylsulfonyl)-1H-pyrazol-3-yl)prop-2-en-1-one (3s)

Yellow solid; isolated yield 54% (56 mg). R_f 0.50 (50% EtOAc/hexane); Mp 75-77°C; ^1H NMR (300 MHz, CDCl_3) δ 12.49 (br s, 1H), 7.77 (d, $J = 7.5$ Hz, 2H), 7.52 (d, $J = 8.0$ Hz, 2H), 7.31-7.47 (m, 4H), 7.20-7.25 (m, 2H), 7.11 (s, 1H), 6.82-7.00 (m, 6H), 6.62-6.69 (m, 2H), 6.55 (s, 1H), 3.61 (s, 3H); ^{13}C NMR (75 MHz, CDCl_3) δ 191.45, 159.24, 142.05, 140.50, 140.00, 137.22, 133.67, 133.23, 130.73, 129.48, 129.27, 128.81, 128.66, 128.50, 128.36, 128.20, 128.08, 127.51, 127.32, 123.96, 120.73, 115.06, 113.94, 55.34; HRMS for $\text{C}_{31}\text{H}_{24}\text{N}_2\text{O}_4\text{S}$: calcd. (MH^+): 521.1530, found: 521.1522

(Z)-3-(3-Chlorophenyl)-1-phenyl-3-(4-phenyl-5-(phenylsulfonyl)-1H-pyrazol-3-yl)prop-2-en-1-one (3t)

White solid; isolated yield 46% (48 mg). R_f 0.50 (40% EtOAc/hexane); Mp 171-173 °C; ^1H NMR (300 MHz, CDCl_3) δ 13.14 (br s, 1H), 7.87 (d, $J = 7.4$ Hz, 2H), 7.53-7.58 (m, 3H), 7.40-7.47 (m, 3H), 7.24-7.31 (m merged with solvent peak, 2H), 6.96-7.14 (m, 8H), 6.86 (d, $J = 6.6$ Hz, 2H); ^{13}C NMR (75 MHz, CDCl_3) δ 191.38, 141.12, 140.41, 140.37, 137.11, 134.26, 133.92, 133.30, 130.74, 129.58, 129.28, 129.11, 128.90, 128.79, 128.68, 128.37, 128.11, 127.71, 127.40, 126.36, 124.26; HRMS for $\text{C}_{30}\text{H}_{21}\text{ClN}_2\text{O}_3\text{S}$: calcd. (MH^+): 525.1034, found: 525.1026

(Z)-1-(4-methoxyphenyl)-3-(4-(4-methoxyphenyl)-5-(phenylsulfonyl)-1H-pyrazol-3-yl)-3-phenylprop-2-en-1-one (3u)

Yellow solid; isolated yield 67% (74 mg). R_f 0.50 (55% EtOAc/hexane); Mp 232-234 °C; ^1H NMR (300 MHz, CDCl_3) δ 12.70 (br s, 1H), 7.74-7.79 (m, 2H), 7.55-7.57 (m, 2H), 7.38-7.43 (m, 1H), 7.23-7.28 (m, 2H), 7.07-7.13 (m, 6H), 6.78-6.83 (m, 2H), 6.73-6.77 (m, 2H), 6.39-6.43 (m, 2H), 3.80 (s, 3H), 3.60 (s, 3H); ^{13}C NMR (75 MHz, CDCl_3) δ 189.94, 164.02, 158.88, 141.35, 140.69, 138.93, 133.18, 131.99, 131.28, 130.21, 129.30, 128.81, 128.65, 128.35, 128.11, 123.57, 121.54, 113.85, 112.92, 55.56, 55.09; HRMS for $\text{C}_{32}\text{H}_{26}\text{N}_2\text{O}_5\text{S}$: calcd. (MH^+): 551.1635, found: 551.1632

(Z)-1-(4-methoxyphenyl)-3-(4-(4-methoxyphenyl)-5-(phenylsulfonyl)-1H-pyrazol-3-yl)-3-(p-tolyl)prop-2-en-1-one (3v)

Yellow solid; isolated yield 70% (79 mg). R_f 0.50 (55% EtOAc/hexane); Mp 215-217 °C; ^1H NMR (300 MHz, CDCl_3) δ 12.50 (br s, 1H), 7.74-7.78 (m, 2H), 7.57-7.60 (m, 2H), 7.39-7.45 (m, 1H), 7.26-7.30 (m, 2H), 7.08 (s, 1H), 6.98, 6.89 (ABq, $J_{\text{AB}} = 8.2$ Hz, 4H), 6.80-6.84 (m, 2H), 6.74-6.79 (m, 2H), 6.40-6.45 (m, 2H), 3.81 (s, 3H), 3.62 (s, 3H), 2.20 (s, 3H); ^{13}C NMR (75 MHz, CDCl_3) δ 189.89, 163.90, 158.91, 141.15, 140.76, 139.64, 135.99, 133.17, 131.96, 131.19, 130.32, 129.11, 128.66, 128.12, 128.02, 127.95, 123.37, 121.62, 113.78, 112.91, 55.55, 55.08, 21.17; HRMS for $\text{C}_{33}\text{H}_{28}\text{N}_2\text{O}_5\text{S}$: calcd. (MH^+): 565.1792, found: 565.1794

(Z)-1,3-bis(4-methoxyphenyl)-3-(4-(4-methoxyphenyl)-5-(phenylsulfonyl)-1H-pyrazol-3-yl)prop-2-en-1-one (3w)

White solid; isolated yield 63% (73 mg). R_f 0.50 (60% EtOAc/hexane); Mp 232-235 °C; ^1H NMR (300 MHz, CDCl_3) δ 12.48 (br s, 1H), 7.68 (d, $J = 8.9$ Hz, 2H), 7.56 (d, $J = 7.4$ Hz, 2H), 7.40 (t, $J = 7.4$ Hz, 1H), 7.25 (t, $J = 7.8$ Hz, 2H), 7.01-7.04 (m, 3H), 6.74-6.79 (m, 4H), 6.61 (d, $J = 8.7$ Hz, 2H), 6.42 (d, $J = 8.7$ Hz, 2H), 3.77 (s, 3H), 3.67 (s, 3H), 3.59 (s, 3H); ^{13}C NMR (75 MHz, CDCl_3) δ 189.77, 163.80, 160.72, 158.86, 140.78, 140.71, 133.15, 131.90, 131.10, 130.40, 129.52, 128.64, 128.09, 126.91, 123.22, 121.62, 113.92, 113.71, 112.95, 55.51, 55.38, 55.04; HRMS for $\text{C}_{33}\text{H}_{28}\text{N}_2\text{O}_6\text{S}$: calcd. (MH^+): 581.1741, found: 581.1741

(Z)-3-(5-(phenylsulfonyl)-4-p-tolyl-1H-pyrazol-3-yl)-1,3-dip-tolylprop-2-en-1-one (3x)

Yellow solid; isolated yield 30% (32 mg). R_f 0.50 (40% EtOAc/hexane); Mp 184-186 °C; ^1H NMR (300 MHz, CDCl_3) δ 12.53 (br s, 1H), 7.64 (br d, $J = 5.7$ Hz, 4H), 7.47 (t, $J = 7.2$ Hz, 1H), 7.32 (t, $J = 7.4$ Hz, 2H), 7.15 (d, $J = 7.9$ Hz, 2H), 7.12 (s, 1H), 7.06, 6.97 (ABq, $J_{\text{AB}} = 7.7$ Hz, 4H), 6.79, 6.73 (ABq, $J_{\text{AB}} = 7.6$ Hz, 4H), 2.39 (s, 3H), 2.26 (s, 3H), 2.15 (s, 3H); ^{13}C NMR (75 MHz, CDCl_3) δ 190.94, 144.32, 141.37, 140.77, 139.80, 137.02, 135.86, 134.76, 133.13, 130.54, 129.12, 128.88, 128.63, 128.12, 128.08, 128.01, 127.76, 126.27, 123.61, 21.73, 21.17, 21.08; HRMS for $\text{C}_{33}\text{H}_{28}\text{N}_2\text{O}_3\text{S}$: calcd. (MH^+): 533.1893, found: 533.1892

(Z)-3-(4-methoxyphenyl)-3-(5-(phenylsulfonyl)-4-(p-tolyl)-1H-pyrazol-3-yl)-1-(p-tolyl)prop-2-en-1-one (3y)

White solid; isolated yield 58% (64 mg). R_f 0.50 (50% EtOAc/hexane); Mp 218-220 °C; ^1H NMR (300 MHz, CDCl_3) δ 12.37 (br s, 1H), 7.58 (d, $J = 7.4$ Hz, 4H), 7.41 (t, $J = 7.5$ Hz, 1H), 7.26 (t, $J = 7.6$ Hz, 2H), 7.03-7.09 (m, 5H), 6.74, 6.68 (ABq, $J_{\text{AB}} = 7.9$ Hz, 4H), 6.62 (d, $J = 8.5$ Hz, 2H), 3.68 (s, 3H), 2.32 (s, 3H), 2.08 (s, 3H); ^{13}C NMR (75 MHz, CDCl_3) δ 190.79, 160.81, 144.17, 140.99, 140.72, 137.00, 134.87, 133.11, 131.03, 130.47, 129.52, 129.08, 128.79, 128.61, 128.10, 128.08, 126.68, 126.27, 123.44, 113.91, 55.37, 21.69, 21.06; HRMS for $\text{C}_{33}\text{H}_{28}\text{N}_2\text{O}_4\text{S}$: calcd. (MH^+): 549.1843, found: 549.1843

(Z)-1-(4-chlorophenyl)-3-(4-(4-chlorophenyl)-5-(phenylsulfonyl)-1H-pyrazol-3-yl)-3-(4-methoxyphenyl)prop-2-en-1-one (3z)

White solid; isolated yield 49% (58 mg). R_f 0.50 (50% EtOAc/hexane); Mp 210-212 °C; ^1H NMR (400 MHz, CDCl_3) δ 12.17 (br s, 1H), 7.58-7.60 (m, 4H), 7.43-7.47 (m, 1H), 7.26-7.33 (m, 4H), 7.05 (m appearing as d, $J = 8.8$ Hz, 2H), 7.01 (s, 1H), 6.88, 6.81 (ABq, $J_{\text{AB}} = 8.5$ Hz,

4H), 6.67 (m appearing as d, $J = 8.8$ Hz, 2H), 3.71 (s, 3H); ^{13}C NMR (75 MHz, CDCl_3) δ 189.73, 161.32, 141.61, 140.40, 140.04, 135.50, 133.84, 133.45, 131.91, 130.51, 129.88, 129.60, 128.85, 128.81, 128.06, 127.83, 127.78, 125.82, 122.12, 114.22, 55.48; HRMS for $\text{C}_{31}\text{H}_{22}\text{Cl}_2\text{N}_2\text{O}_4\text{S}$: calcd. (MH^+): 589.0750, found: 589.0752

(Z)-4-(4-methyl-5-(phenylsulfonyl)-1H-pyrazol-3-yl)-4-phenylbut-3-en-2-one (3za)

White solid; isolated yield 53% (39 mg). R_f 0.50 (40% EtOAc/hexane); Mp 188-191 °C; ^1H NMR (400 MHz, CDCl_3) δ 13.15 (br s, 1H), 7.93-7.95 (m, 2H), 7.51-7.55 (m, 1H), 7.43-7.47 (m, 2H), 7.30-7.39 (m, 3H), 7.17-7.19 (m merged with solvent peak, 2H), 6.49 (s, 1H), 2.25 (s, 3H), 1.59 (s, 3H); ^{13}C NMR (100 MHz, CDCl_3) δ 199.25, 141.48, 141.10, 139.12, 133.41, 129.84, 129.11, 129.07, 128.98, 127.97, 127.86, 119.46, 31.15, 9.39; HRMS for $\text{C}_{20}\text{H}_{18}\text{N}_2\text{O}_3\text{S}$: calcd. (MH^+): 367.1111, found: 367.1106

(Z)-4-(4-methyl-5-(phenylsulfonyl)-1H-pyrazol-3-yl)pent-3-en-2-one (3zb; major isomer) & (Z)-4-(4-methyl-3-(phenylsulfonyl)-1H-pyrazol-5-yl)pent-3-en-2-one (3zb; minor isomer)

Major isomer: White solid; isolated yield 24% (15 mg). R_f 0.50 (40% EtOAc/hexane); Mp 136-138 °C; ^1H NMR (400 MHz, CDCl_3) δ 11.58 (br s, 1H), 7.91 (d, $J = 7.2$ Hz, 2H), 7.52-7.55 (m, 1H), 7.43-7.47 (m, 2H), 6.33 (s, 1H), 2.37 (s, 3H), 2.26 (s, 3H), 2.19 (s, 3H); ^{13}C NMR (125 MHz, CDCl_3) δ 198.64, 141.00, 140.84, 133.67, 129.29, 127.67, 127.24, 115.97, 32.21, 17.90, 9.43; HRMS for $\text{C}_{15}\text{H}_{16}\text{N}_2\text{O}_3\text{S}$: calcd. (MH^+): 305.0954, found: 305.0956

Minor-isomer: Colorless liquid; isolated yield 8% (5 mg). R_f 0.50 (45% EtOAc/hexane); ^1H NMR (400 MHz, CDCl_3) δ 14.27 (br s, 1H), 7.95 (d, $J = 5.0$ Hz, 2H), 7.45-7.52 (m, 3H), 6.27 (s, 1H), 2.41 (s, 3H), 2.26 (s, 3H), 2.22 (s, 3H); ^{13}C NMR (100 MHz, CDCl_3) δ 199.05, 150.60, 141.26, 140.13, 139.34, 133.37, 129.08, 127.86, 127.06, 118.25, 31.60, 25.65, 10.48; HRMS for $\text{C}_{15}\text{H}_{16}\text{N}_2\text{O}_3\text{S}$: calcd. (MH^+): 305.0954, found: 305.0952

(Z)-1,3-diphenyl-3-(4-phenyl-5-tosyl-1H-pyrazol-3-yl)prop-2-en-1-one (3zc)

White solid; isolated yield 72% (73 mg). R_f 0.50 (40% EtOAc/hexane); Mp 218-220 °C; ^1H NMR (300 MHz, CDCl_3) δ 12.56 (br s, 1H), 7.77-7.80 (m, 2H), 7.45-7.51 (m, 1H), 7.43 (d, $J = 8.3$ Hz, 2H), 7.35 (t, $J = 7.8$ Hz, 2H), 7.03-7.11 (m, 8H), 6.84-6.94 (m, 5H), 2.27 (s, 3H); ^{13}C NMR (75 MHz, CDCl_3) δ 191.40, 144.18, 142.27, 138.70, 137.57, 137.25, 133.59, 130.75, 129.45, 129.31, 128.78, 128.63, 128.41, 128.32, 128.17, 128.12, 127.43, 127.30, 123.76, 21.56; HRMS for $\text{C}_{31}\text{H}_{24}\text{N}_2\text{O}_3\text{S}$: calcd. (MH^+): 505.1580, found: 505.1581

(Z)-1,3-diphenyl-3-(4-phenyl-5-(trifluoromethyl)-1H-pyrazol-3-yl)prop-2-en-1-one (3zd)

White solid; isolated yield 39% (33 mg). R_f 0.50 (15% EtOAc/hexane); Mp 148-150 °C; ^1H NMR (300 MHz, CDCl_3) δ 12.38 (s, 1H), 7.88 (d, $J = 7.4$ Hz, 2H), 7.57 (t, $J = 7.2$ Hz, 1H), 7.44 (t, $J = 7.5$ Hz, 2H), 7.21-7.26 (m merged with solvent peak, 6H), 6.99 (br s, 5H); ^{13}C NMR (125 MHz, CDCl_3) δ 191.47, 141.71, 139.12, 138.73, 137.14, 133.55, 129.90, 129.86, 129.70, 128.74, 128.58, 128.50, 128.38, 128.09, 127.69, 127.30, 122.22, 121.44 (q, $J_{\text{C-F}} = 268.8$ Hz); ^{19}F NMR (282 MHz, CDCl_3) δ -59.45 (s); HRMS for $\text{C}_{25}\text{H}_{17}\text{F}_3\text{N}_2\text{O}$: calcd. (MH^+): 419.1366, found: 419.1359

(Z)-3-(4-methoxyphenyl)-1-phenyl-3-(4-phenyl-5-(trifluoromethyl)-1H-pyrazol-3-yl)prop-2-en-1-one (3ze)

Yellow solid; isolated yield 35% (31 mg). R_f 0.50 (25% EtOAc/hexane); Mp 136-138 °C; ^1H NMR (300 MHz, CDCl_3): (major/minor in 1:0.33 ratio) δ 12.15 (br s, 1H), 7.76 (d, $J = 7.4$ Hz, 2H, major), 7.49-7.54 (m, 2H), 7.35-7.46 (m, 6H), 7.19-7.29 (m, 7H), 7.01 (br s, 7H), 6.77-6.83 (m, 3H, minor), 6.73 (d, $J = 8.6$ Hz, 2H, major), 6.61-6.66 (m, 1H, minor), 3.76 (s, 3H, major), 3.74 (s, 3H, minor); ^{13}C NMR (75 MHz, CDCl_3) δ 191.38, 191.23, 161.02, 160.46, 141.27, 139.39, 139.28, 137.41, 133.29, 133.01, 130.98, 130.94, 130.47, 130.13, 129.95, 129.81, 129.56, 128.85, 128.60, 128.52, 128.48, 128.35, 128.24, 127.71, 127.36, 127.26, 126.48, 126.32, 121.93, 120.46, 119.67 (q appearing as t, $J_{\text{C-F}} = 268.2$ Hz), 114.03, 113.98, 55.39, 55.24; ^{19}F NMR (376 MHz, CDCl_3): (major/minor in 1:0.34 ratio) δ -59.42 (s, major), -59.97 (s, minor); HRMS for $\text{C}_{26}\text{H}_{19}\text{F}_3\text{N}_2\text{O}_2$: calcd. (MH^+): 449.1471, found: 449.1466

4-Phenyl-3-(1-phenyl-1H-inden-1-yl)-5-(phenylsulfonyl)-1H-pyrazole (4a)

White fluffy solid; isolated yield 94% (45 mg). R_f 0.50 (50% EtOAc/hexane); Mp 80-82 °C; ^1H NMR (300 MHz, CDCl_3) δ 12.10 (br s, 1H), 7.68 (d, $J = 7.6$ Hz, 2H), 7.52 (t, $J = 7.4$ Hz, 1H), 7.34 (t, $J = 7.8$ Hz, 2H), 7.24-7.26 (m merged with solvent peak, 2H), 7.13-7.19 (m, 7H), 7.02-7.11 (m, 5H), 6.30 (d, $J = 9.1$ Hz, 1H), 5.16 (d, $J = 9.1$ Hz, 1H); ^{13}C NMR (75 MHz, CDCl_3) δ 148.78, 141.76, 141.49, 140.33, 138.43, 136.20, 133.43, 131.18, 130.30, 129.17, 128.81, 128.56, 128.35, 128.30, 128.02, 127.92, 127.84, 127.78, 126.90, 125.90, 122.22, 71.38; HRMS for $\text{C}_{30}\text{H}_{22}\text{N}_2\text{O}_2\text{S}$: calcd. (MH^+): 475.1475, found: 475.1470

4-Phenyl-5-(phenylsulfonyl)-3-(1-(p-tolyl)-1H-inden-1-yl)-1H-pyrazole (4b)

White fluffy solid; isolated yield 94% (46 mg). R_f 0.50 (50% EtOAc/hexane); Mp 106-108 °C; ^1H NMR (300 MHz, CDCl_3) δ 7.71 (d, $J = 7.6$ Hz, 2H), 7.53 (t, $J = 7.5$ Hz, 1H), 7.36 (t, $J = 7.7$ Hz, 2H), 7.12-7.24 (m merged with solvent peak, 9H), 6.96 (s, 4H), 6.26 (d, $J = 9.2$ Hz, 1H), 5.10 (d, $J = 9.2$ Hz, 1H), 2.25 (s, 3H); ^{13}C NMR (75 MHz, CDCl_3) δ 141.83, 140.44, 138.35, 135.63, 135.22, 133.43, 131.41, 130.80, 130.32, 129.30, 129.13, 128.82, 128.53, 128.07, 127.92, 127.72, 127.63, 127.42, 127.35, 126.93, 126.72, 125.88, 122.11, 71.42, 21.10; HRMS for $\text{C}_{31}\text{H}_{24}\text{N}_2\text{O}_2\text{S}$: calcd. (MH^+): 489.1631, found: 489.1630

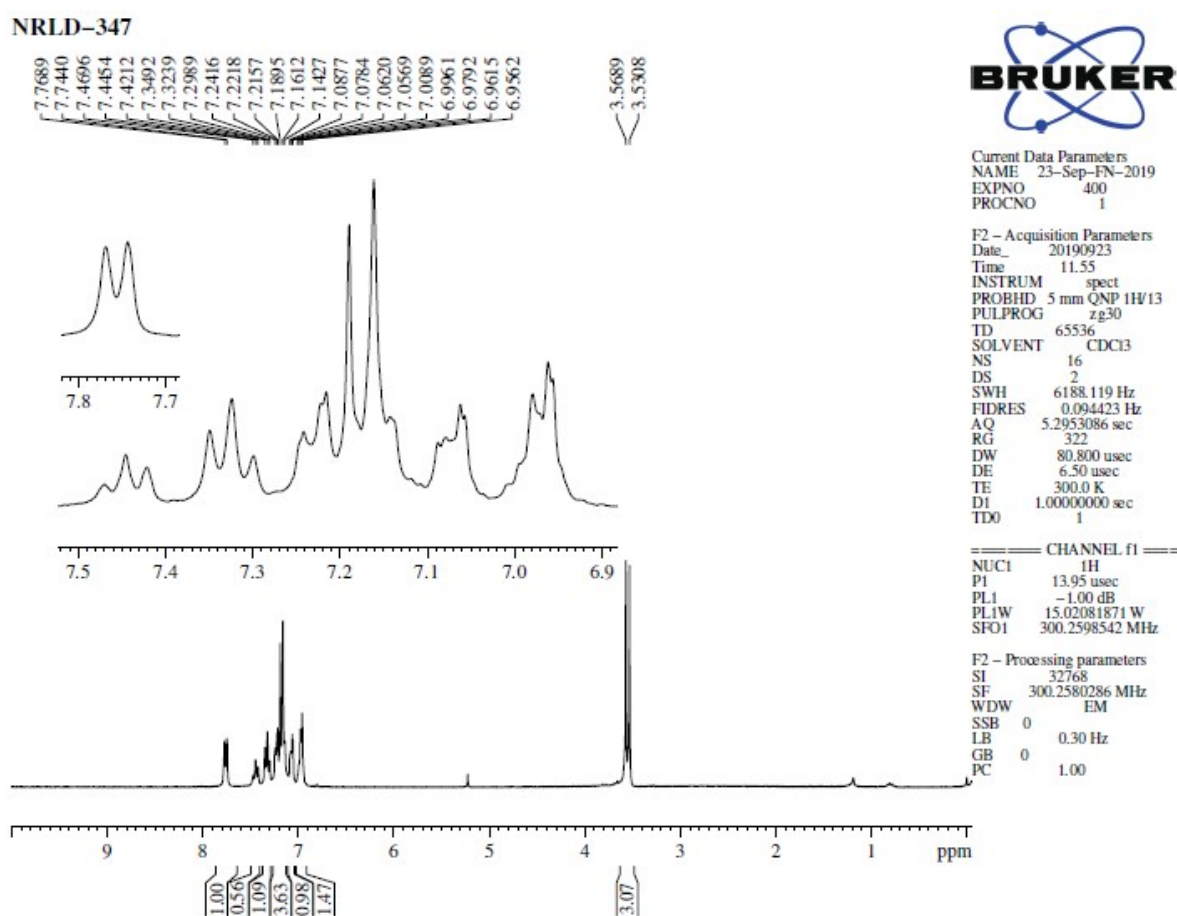
3-(1-(4-Methoxyphenyl)-1H-inden-1-yl)-4-phenyl-5-(phenylsulfonyl)-1H-pyrazole (4c)

White fluffy solid; isolated yield 90% (45 mg). R_f 0.50 (60% EtOAc/hexane); Mp 91-93 °C; ^1H NMR (300 MHz, CDCl_3) δ 12.16 (br s, 1H), 7.69 (d, $J = 7.5$ Hz, 2H), 7.52 (t, $J = 7.4$ Hz, 1H), 7.35 (t, $J = 7.8$ Hz, 2H), 7.09-7.24 (m merged with solvent peak, 10H), 6.98 (d, $J = 8.7$ Hz, 2H), 6.67 (d, $J = 8.7$ Hz, 2H), 6.20 (d, $J = 9.1$ Hz, 1H), 5.10 (d, $J = 9.2$ Hz, 1H), 3.72 (s, 3H); ^{13}C NMR (125 MHz, CDCl_3) δ 159.71, 148.82, 141.98, 141.57, 140.44, 134.24, 133.40, 131.00, 130.49, 130.29, 129.29, 128.80, 128.51, 128.09, 128.03, 127.92, 127.88, 127.67, 125.89, 122.10, 113.81, 71.50, 55.26; HRMS for $\text{C}_{31}\text{H}_{24}\text{N}_2\text{O}_3\text{S}$: calcd. (MH^+): 505.1580, found: 505.1573

3-(6-Methoxy-1-(p-tolyl)-1H-inden-1-yl)-4-(4-methoxyphenyl)-5-(phenylsulfonyl)-1H-pyrazole (4d)

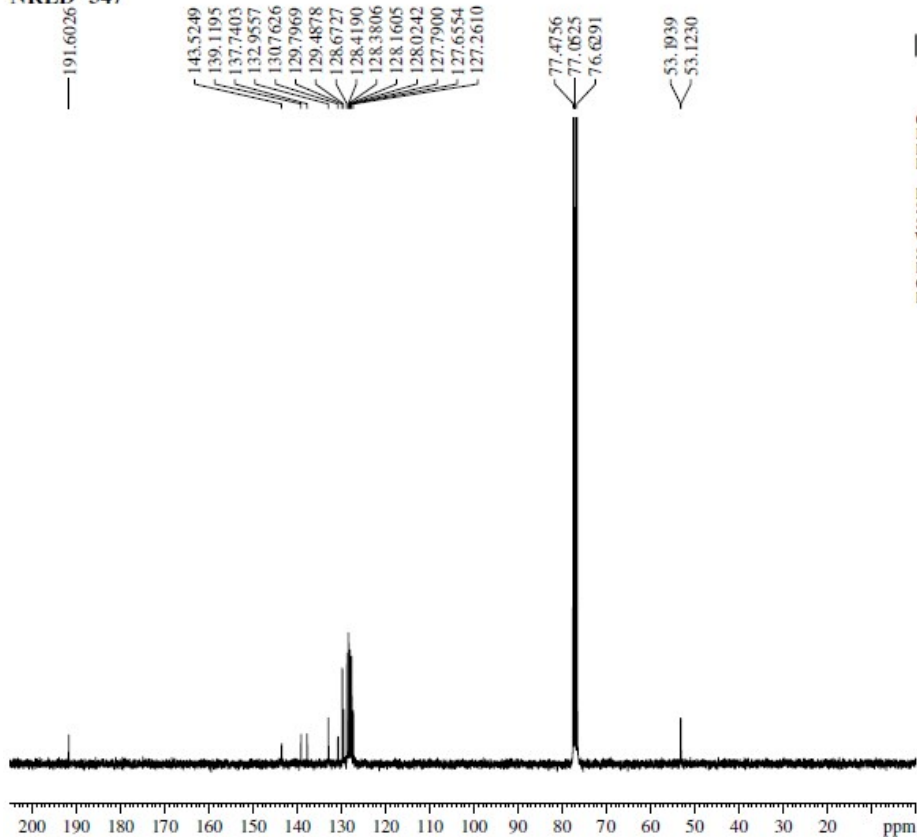
White fluffy solid; isolated yield 92% (50 mg). R_f 0.50 (60% EtOAc/hexane); Mp 104-108 °C; ^1H NMR (300 MHz, CDCl_3) δ 7.72-7.75 (m, 2H), 7.51-7.56 (m, 1H), 7.36-7.41 (m, 2H), 7.04-7.08 (m, 3H), 6.97 (s, 4H), 6.77-6.80 (m, 2H), 6.67-6.70 (m, 2H), 6.28 (d, $J = 9.2$ Hz, 1H), 5.03 (d, $J = 9.2$ Hz, 1H), 3.77 (s, 3H), 3.75(s, 3H), 2.26 (s, 3H); ^{13}C NMR (75 MHz, CDCl_3) δ 159.30, 159.23, 148.87, 141.33, 140.54, 138.34, 135.59, 135.16, 134.05, 133.40, 131.47, 130.53, 129.15, 128.80, 128.11, 127.23, 126.69, 121.84, 121.40, 113.98, 113.44, 71.14, 55.28, 55.17, 21.08; HRMS for $\text{C}_{33}\text{H}_{28}\text{N}_2\text{O}_4\text{S}$: calcd. (MH^+): 549.1843, found: 549.1839

7. Copies of ^1H , ^{13}C , ^{31}P & ^{19}F NMR Spectra



S1: ^1H NMR spectrum of **3a**

NRLD-347

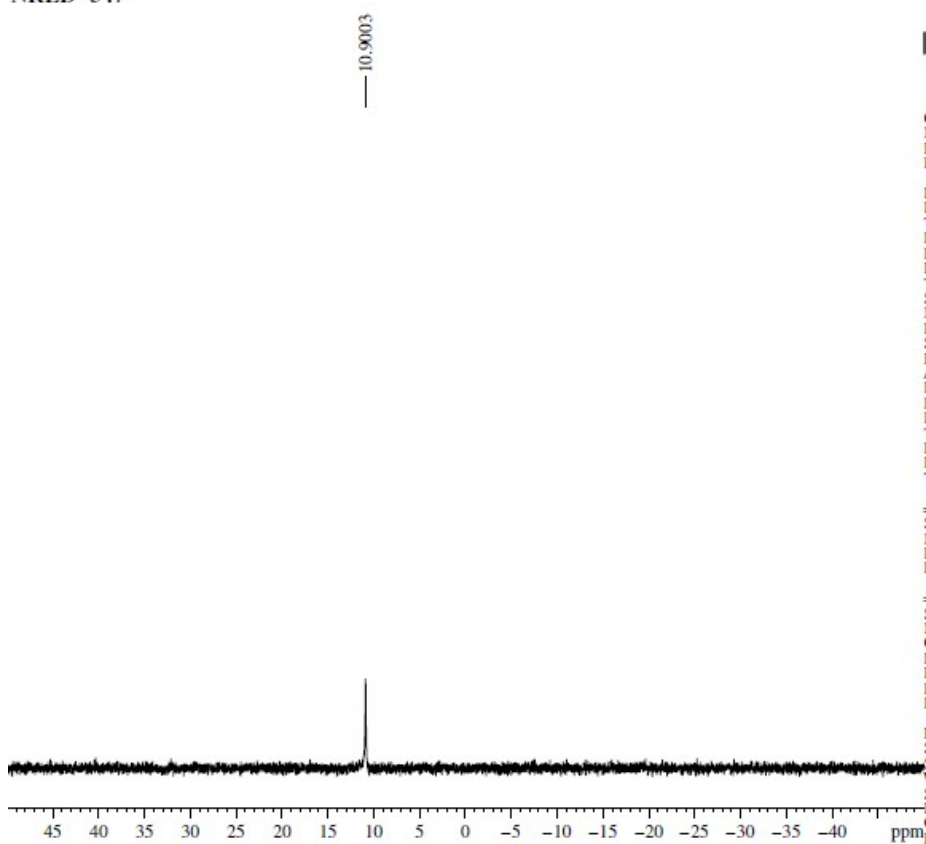


Current Data Parameters
NAME 28-Aug-FN-2019
EXPNO 570
PROCNO 1

F2 - Processing parameters
SI 32768
SF 75.4999324 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

S2: ¹³C NMR spectrum of 3a

NRLD-347



Current Data Parameters
NAME 24-Dec-AN-2019
EXPNO 320
PROCNO 1

F2 - Acquisition Parameters
Date_ 20191224
Time 22.08
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 16
DS 4
SWH 64102.563 Hz
FIDRES 0.978127 Hz
AQ 0.5111808 sec
RG 201.48
DW 7.800 usec
DE 6.50 usec
TE 303.1 K
D1 2.0000000 sec
D11 0.0300000 sec
TD0 1

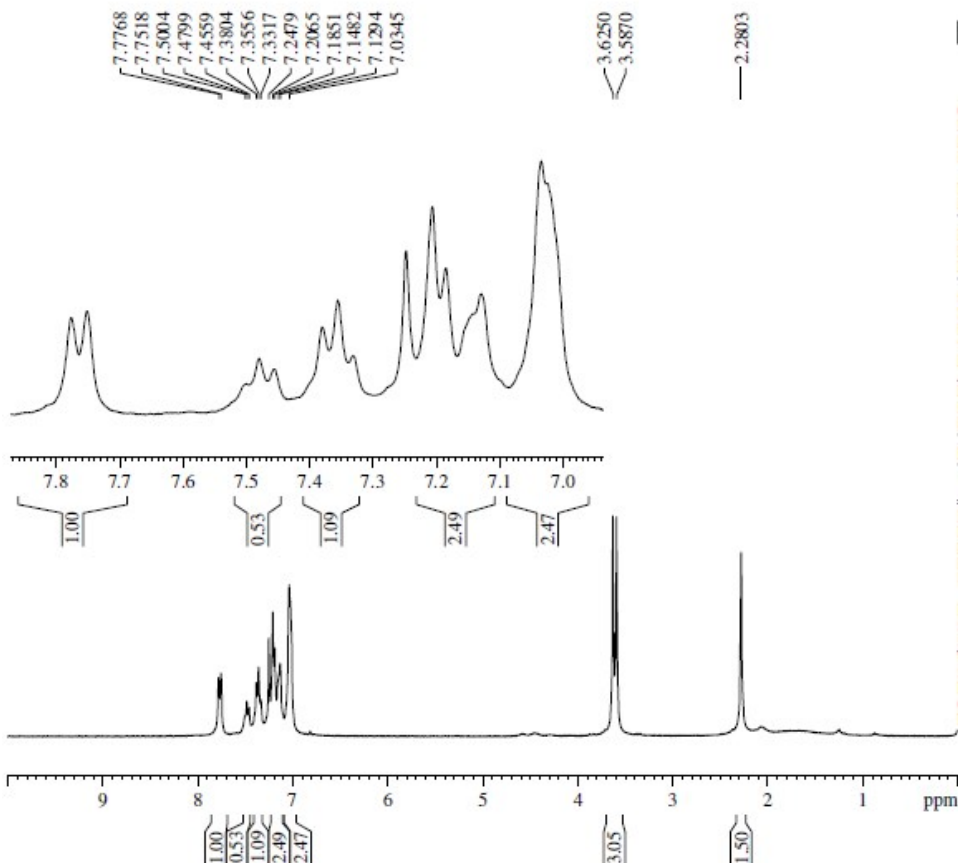
==== CHANNEL f1 ====
SFO1 161.9798402 MHz
NUC1 31P
P1 15.00 usec
PLW1 12.0000000 W

==== CHANNEL f2 ====
SFO2 400.1621006 MHz
NUC2 1H
CPDPRG2 waltz16
PCPD2 90.00 usec
PLW2 13.0000000 W
PLW12 0.27963999 W
PLW13 0.22651000 W

F2 - Processing parameters
SI 32768
SF 161.9879400 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

S3: ³¹P NMR spectrum of 3a

NRLD-412



Current Data Parameters
NAME 01-July-AN-2020
EXPNO 360
PROCNO 1

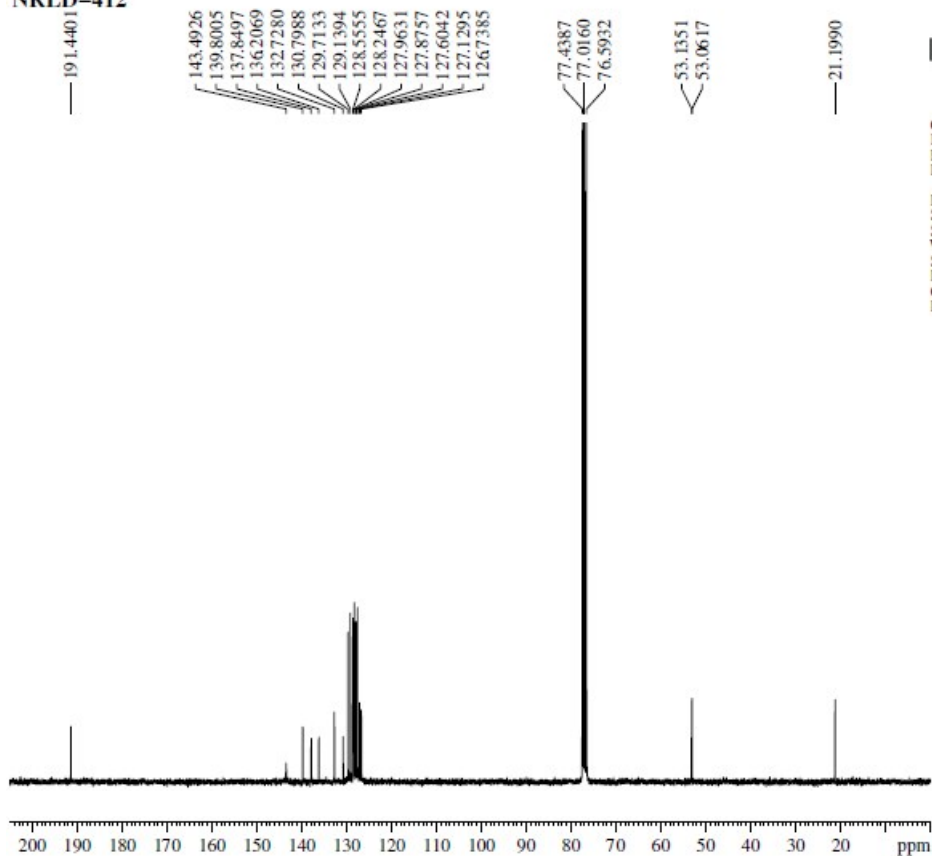
F2 - Acquisition Parameters
Date_ 20200701
Time 16.05
INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 6188.119 Hz
FIDRES 0.094423 Hz
AQ 5.2953086 sec
RG 287
DW 80.800 usec
DE 6.50 usec
TE 300.0 K
D1 1.0000000 sec
TDO 1

==== CHANNEL f1 ====
NUC1 1H
P1 13.95 usec
PL1 -1.00 dB
PL1W 15.02081871 W
SFO1 300.2598542 MHz

F2 - Processing parameters
SI 32768
SF 300.2580111 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

S4: ¹H NMR spectrum of 3b

NRLD-412

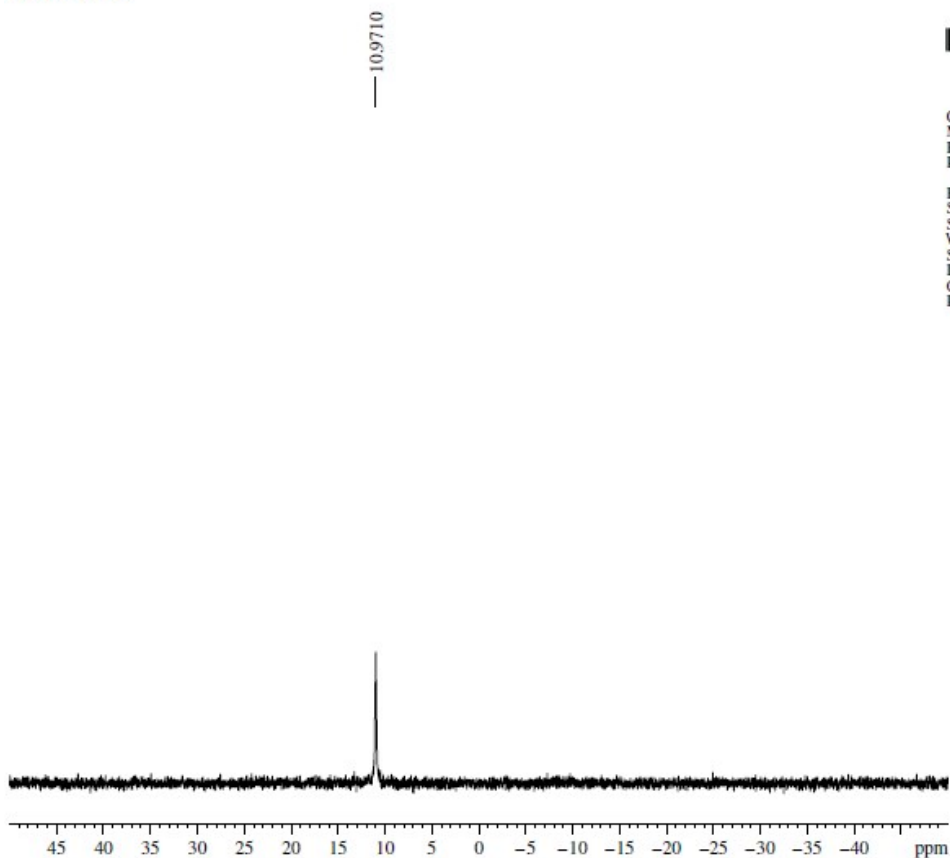


Current Data Parameters
NAME 07-Feb-AN-2020
EXPNO 440
PROCNO 1

F2 - Processing parameters
SI 32768
SF 75.4999359 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

S5: ¹³C NMR spectrum of 3b

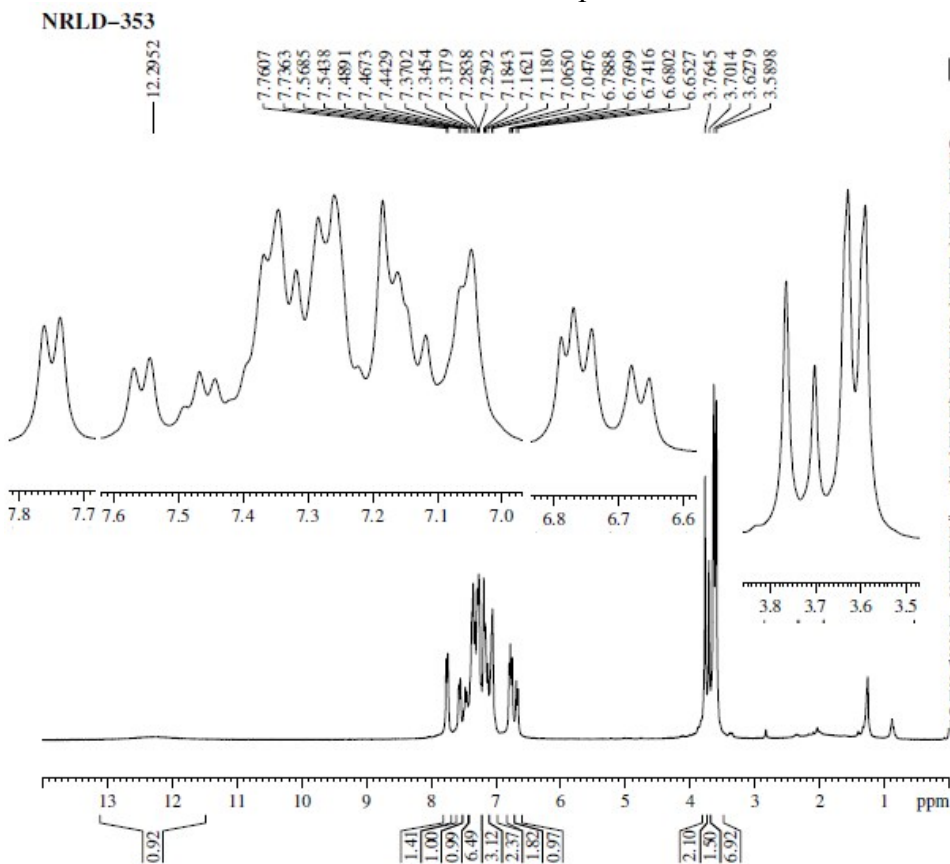
NRLD-412



Current Data Parameters
NAME 07-Feb-AN-2020
EXPNO 430
PROCNO 1

F2 - Processing parameters
SI 32768
SF 121.5466660 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

S6: ³¹P NMR spectrum of 3b



Current Data Parameters
NAME 30-Sept-FN-2019
EXPNO 430
PROCNO 1

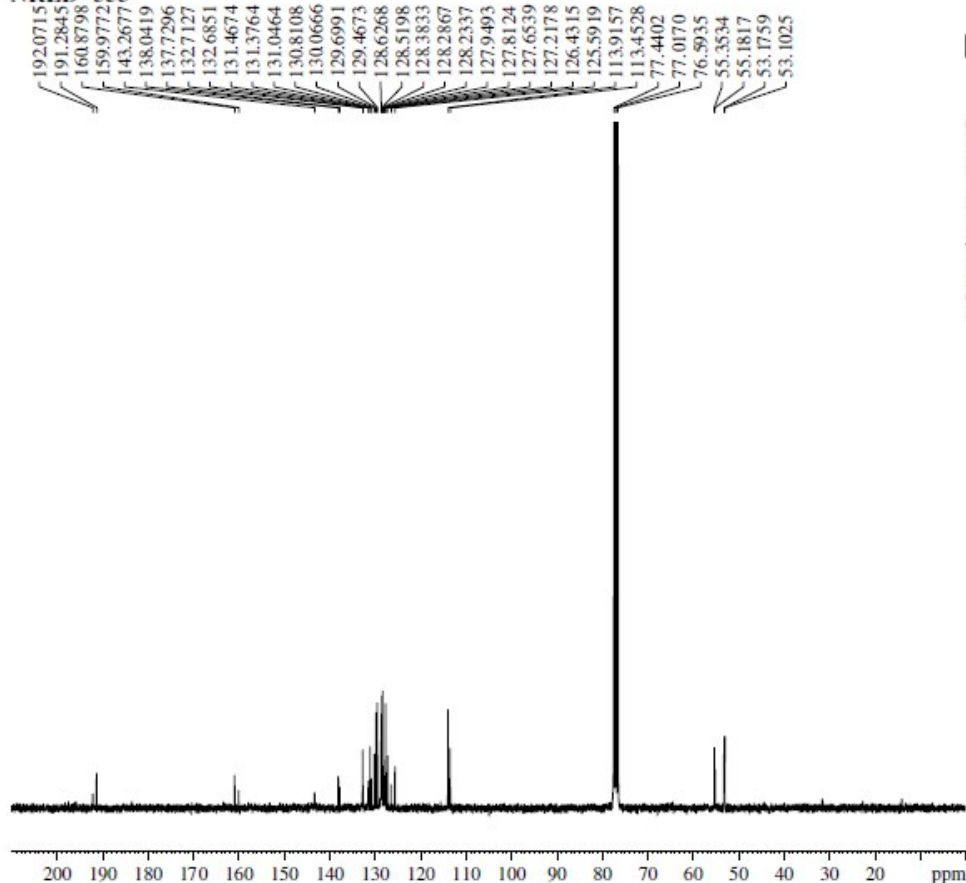
F2 - Acquisition Parameters
Date_ 20190930
Time 11.11
INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 6188.119 Hz
FIDRES 0.094423 Hz
AQ 5.2953086 sec
RG 181
DW 80.800 usec
DE 6.50 usec
TE 300.0 K
D1 1.0000000 sec
TD0 1

==== CHANNEL f1 ====
NUC1 1H
P1 13.95 usec
PL1 -1.00 dB
PL1W 15.02081871 W
SFO1 300.2598542 MHz

F2 - Processing parameters
SI 32768
SF 300.2580071 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

S7: ¹H NMR spectrum of 3c

NRLD-353

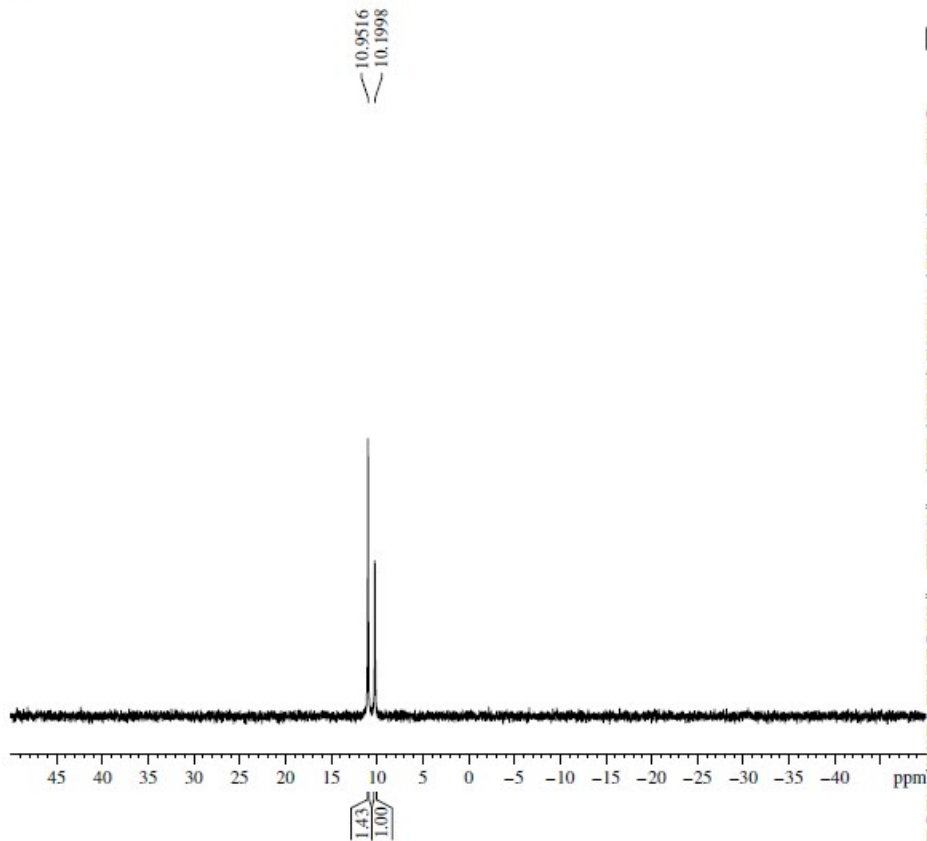


Current Data Parameters
NAME 10-Oct-FN-2019
EXPNO 490
PROCNO 1

F2 - Processing parameters
SI 32768
SF 75.4999349 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

S8: ¹³C NMR spectrum of 3c

NRLD-353



Current Data Parameters
NAME 23-Dec-AN-2019
EXPNO 340
PROCNO 1

F2 - Acquisition Parameters
Date_ 20191223
Time 22.46
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zpg30
TD 65536
SOLVENT CDCl3
NS 16
DS 4
SWH 64102.563 Hz
FIDRES 0.978127 Hz
AQ 0.5111808 sec
RG 201.48
DW 7.800 usec
DE 6.50 usec
TE 303.1 K
D1 2.0000000 sec
D11 0.0300000 sec
TD0 1

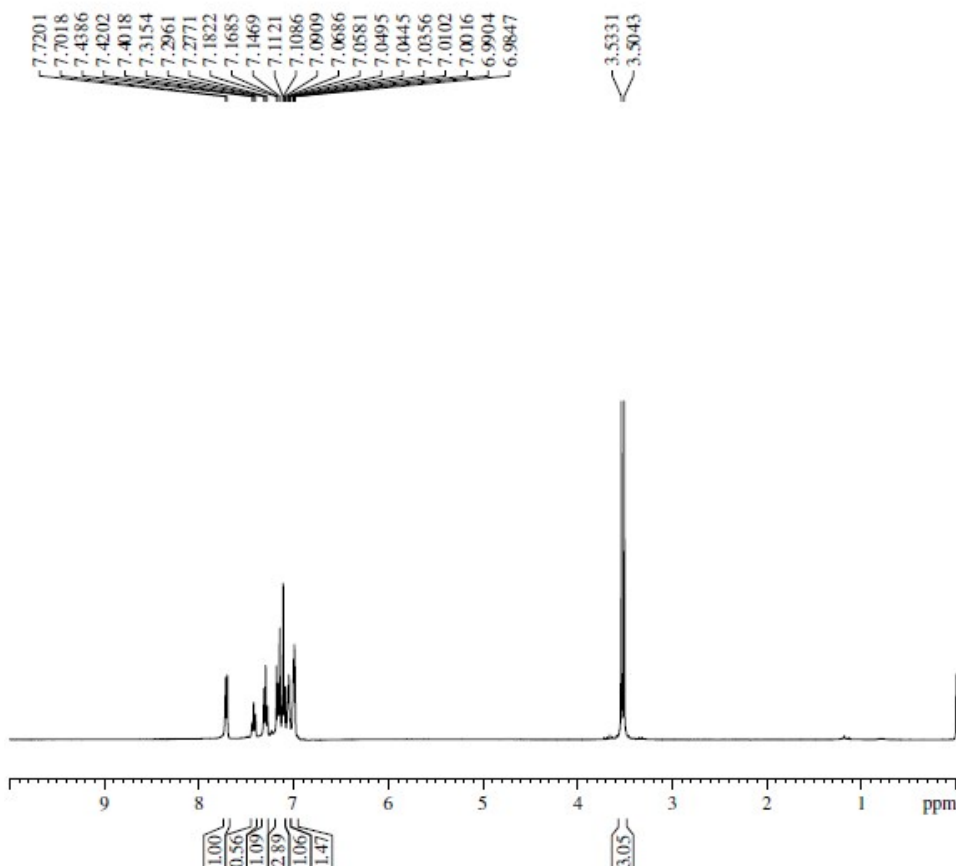
==== CHANNEL f1 ====
SFO1 161.9798402 MHz
NUC1 31P
P1 15.00 usec
PLW1 12.0000000 W

==== CHANNEL f2 ====
SFO2 400.1621006 MHz
NUC2 1H
CPDPRG2 waltz16
PCPD2 90.00 usec
PLW2 13.0000000 W
PLW12 0.27963999 W
PLW13 0.22651000 W

F2 - Processing parameters
SI 32768
SF 161.9879400 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

S9: ³¹P NMR spectrum of 3c

NRLD 377



Current Data Parameters
 NAME 30-Oct-FN-2019
 EXPNO 390
 PROCNO 1

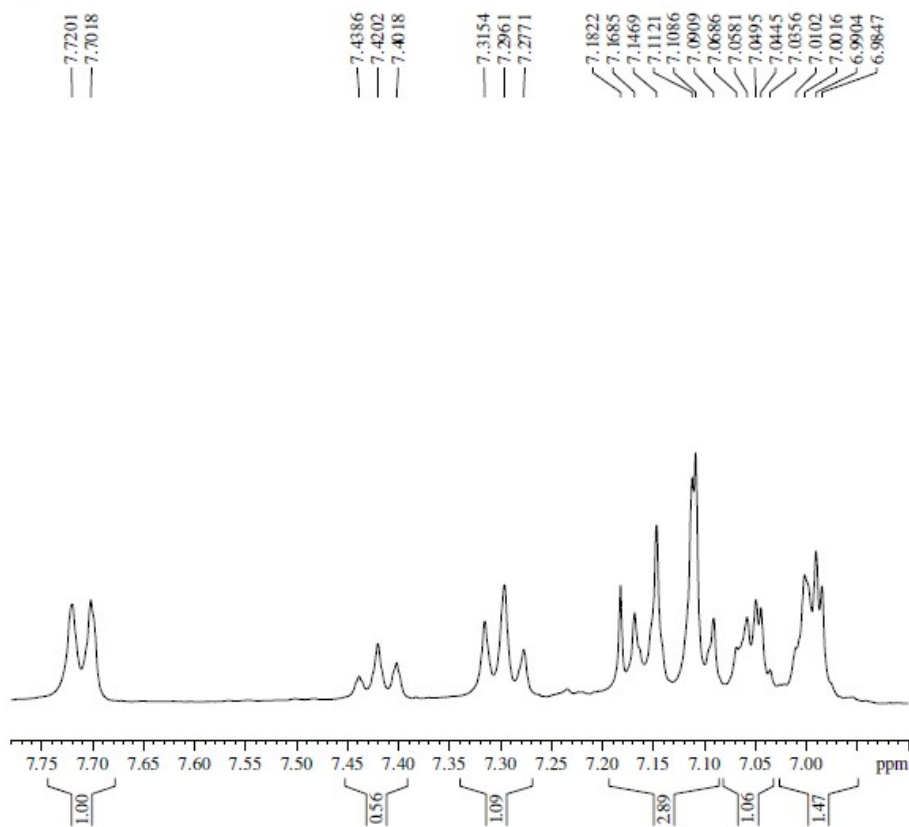
F2 - Acquisition Parameters
 Date_ 20191030
 Time 16.13
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 32
 DS 0
 SWH 9615.385 Hz
 FIDRES 0.146719 Hz
 AQ 3.4078720 sec
 RG 129.57
 DW 52.000 usec
 DE 6.50 usec
 TE 300.0 K
 D1 1.00000000 sec
 TDO 1

==== CHANNEL f1 ====
 SFO1 400.1629712 MHz
 NUC1 1H
 P1 13.20 usec
 PLW1 13.00000000 W

F2 - Processing parameters
 SI 65536
 SF 400.1605409 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

S10: ¹H NMR spectrum of 3d

NRLD 377



Current Data Parameters
 NAME 30-Oct-FN-2019
 EXPNO 390
 PROCNO 1

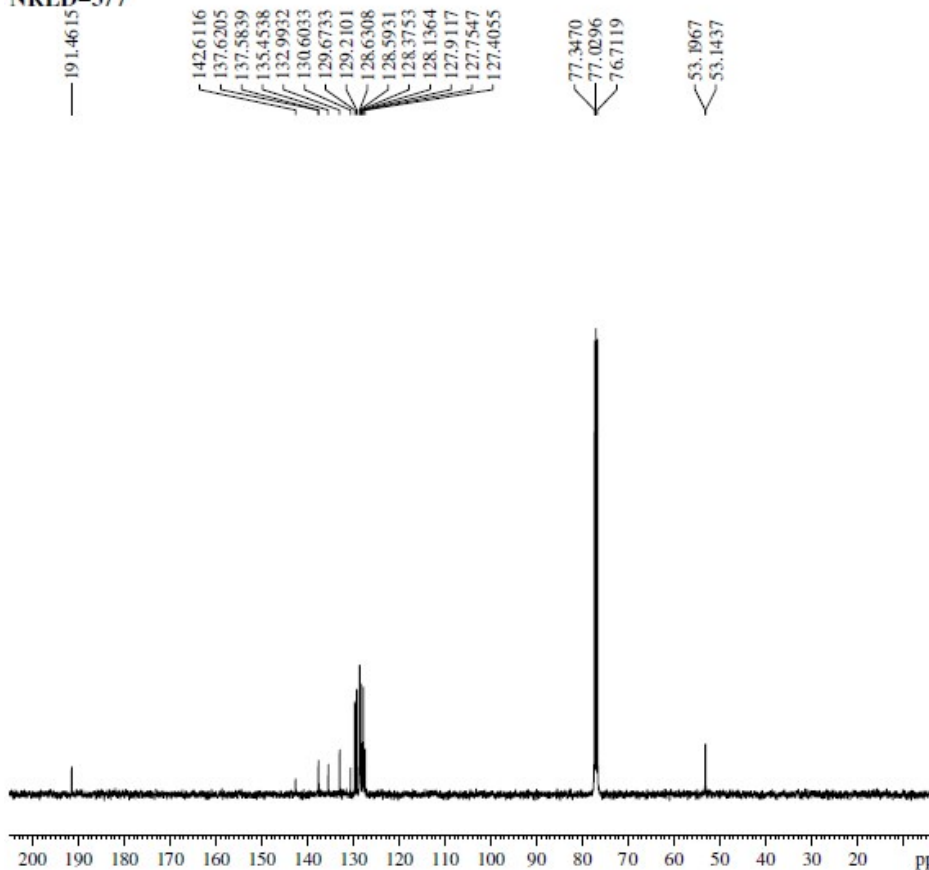
F2 - Acquisition Parameters
 Date_ 20191030
 Time 16.13
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 32
 DS 0
 SWH 9615.385 Hz
 FIDRES 0.146719 Hz
 AQ 3.4078720 sec
 RG 129.57
 DW 52.000 usec
 DE 6.50 usec
 TE 300.0 K
 D1 1.00000000 sec
 TDO 1

==== CHANNEL f1 ====
 SFO1 400.1629712 MHz
 NUC1 1H
 P1 13.20 usec
 PLW1 13.00000000 W

F2 - Processing parameters
 SI 65536
 SF 400.1605409 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

S11: ¹H NMR spectrum of 3d (expansion)

NRLD-377



Current Data Parameters
 NAME 30-Oct-FN-2019
 EXPNO 310
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20191031
 Time 13.52
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 4096
 DS 4
 SWH 24038.461 Hz
 FIDRES 0.366798 Hz
 AQ 1.3631488 sec
 RG 201.48
 DW 20.800 usec
 DE 6.50 usec
 TE 300.2 K
 D1 2.0000000 sec
 D11 0.0300000 sec
 TDO 1

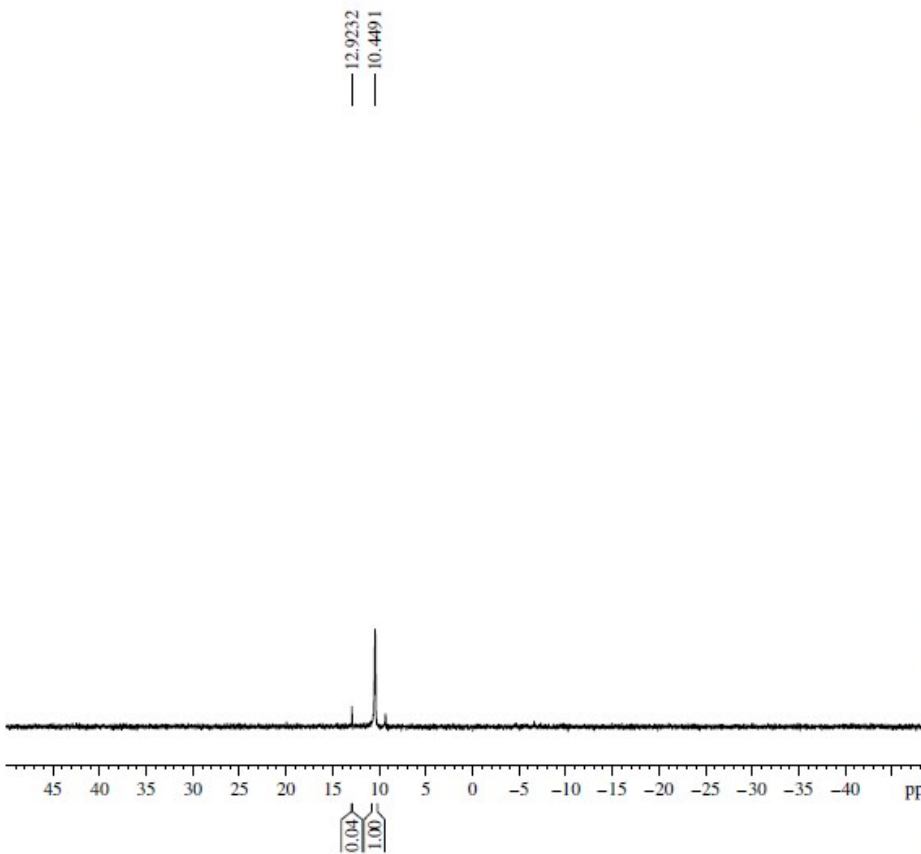
==== CHANNEL f1 ====
 SFO1 100.6304993 MHz
 NUC1 13C
 P1 9.90 usec
 PLW1 53.0000000 W

==== CHANNEL f2 ====
 SFO2 400.1621006 MHz
 NUC2 1H
 CPDPRG2 waltz16
 PCPD2 90.00 usec
 PLW2 13.0000000 W
 PLW12 0.27963999 W
 PLW13 0.22651000 W

F2 - Processing parameters
 SI 32768
 SF 100.6204380 MHz
 WDW EM
 SSB 0
 LB 3.00 Hz
 GB 0
 PC 1.40

S12: 13C NMR spectrum of 3d

NRLD 377



Current Data Parameters
 NAME 10-July-FN-2020
 EXPNO 570
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20200710
 Time 19.38
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 32
 DS 4
 SWH 64102.563 Hz
 FIDRES 0.978127 Hz
 AQ 0.5111808 sec
 RG 201.48
 DW 7.800 usec
 DE 6.50 usec
 TE 303.1 K
 D1 2.0000000 sec
 D11 0.0300000 sec
 TDO 1

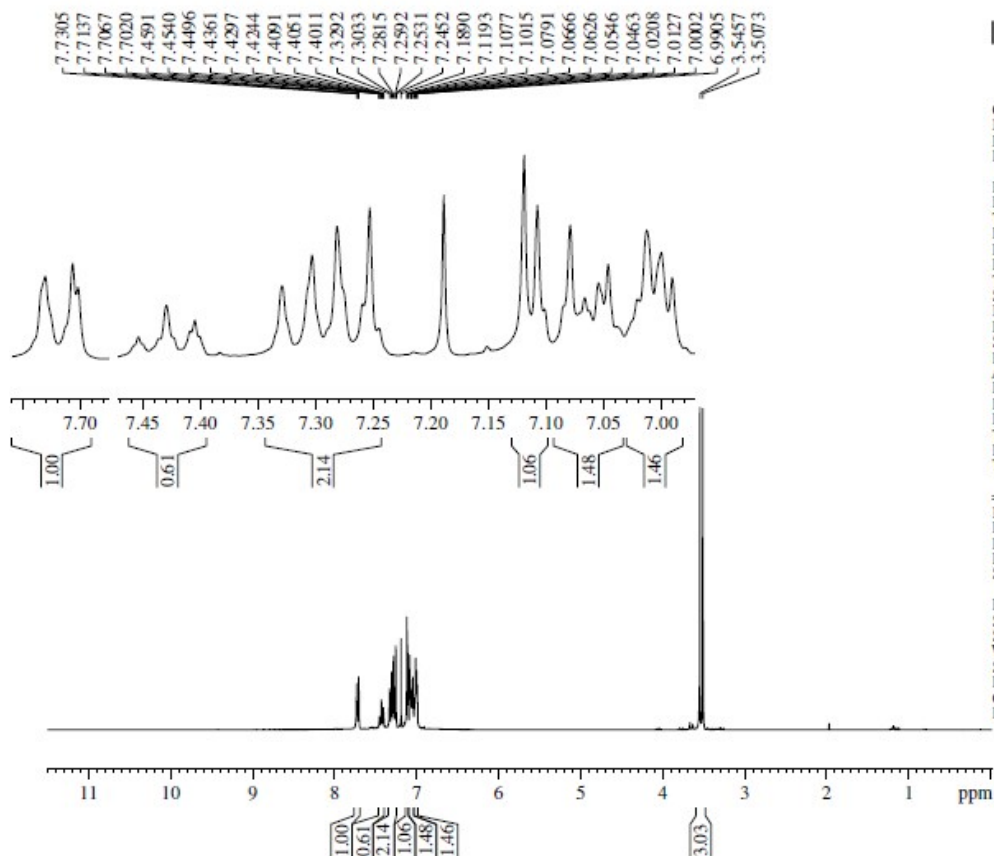
==== CHANNEL f1 ====
 SFO1 161.9798402 MHz
 NUC1 31P
 P1 15.00 usec
 PLW1 12.0000000 W

==== CHANNEL f2 ====
 SFO2 400.1621006 MHz
 NUC2 1H
 CPDPRG2 waltz16
 PCPD2 90.00 usec
 PLW2 13.0000000 W
 PLW12 0.27963999 W
 PLW13 0.22651000 W

F2 - Processing parameters
 SI 32768
 SF 161.9879400 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

S13: 31P NMR spectrum of 3d

NRLD-401



Current Data Parameters
NAME 24-Jan-FN-2020
EXPNO 540
PROCNO 1

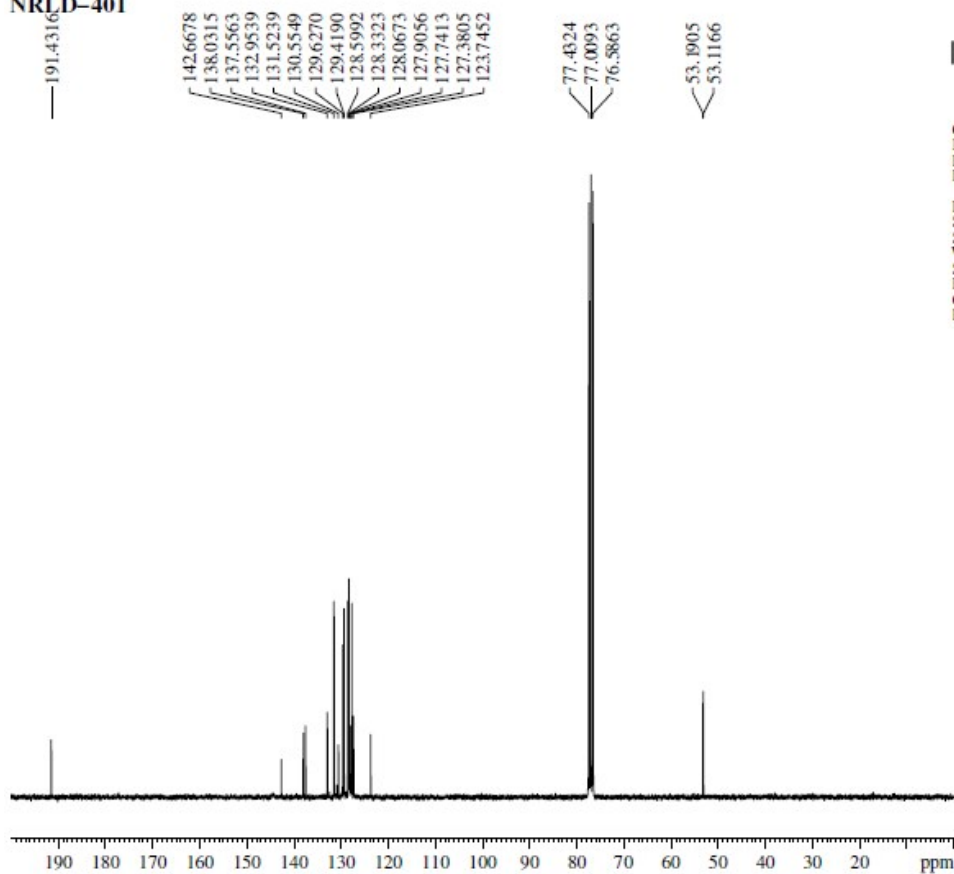
F2 - Acquisition Parameters
Date_ 20200124
Time 12.15
INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 6188.119 Hz
FIDRES 0.094423 Hz
AQ 5.2953086 sec
RG 256
DW 80.800 usec
DE 6.50 usec
TE 300.0 K
D1 1.00000000 sec
TD0 1

==== CHANNEL f1 ====
NUC1 1H
P1 13.95 usec
PL1 -1.00 dB
PL1W 15.02081871 W
SFO1 300.2598542 MHz

F2 - Processing parameters
SI 32768
SF 300.2580287 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

S14: ¹H NMR spectrum of 3e

NRLD-401

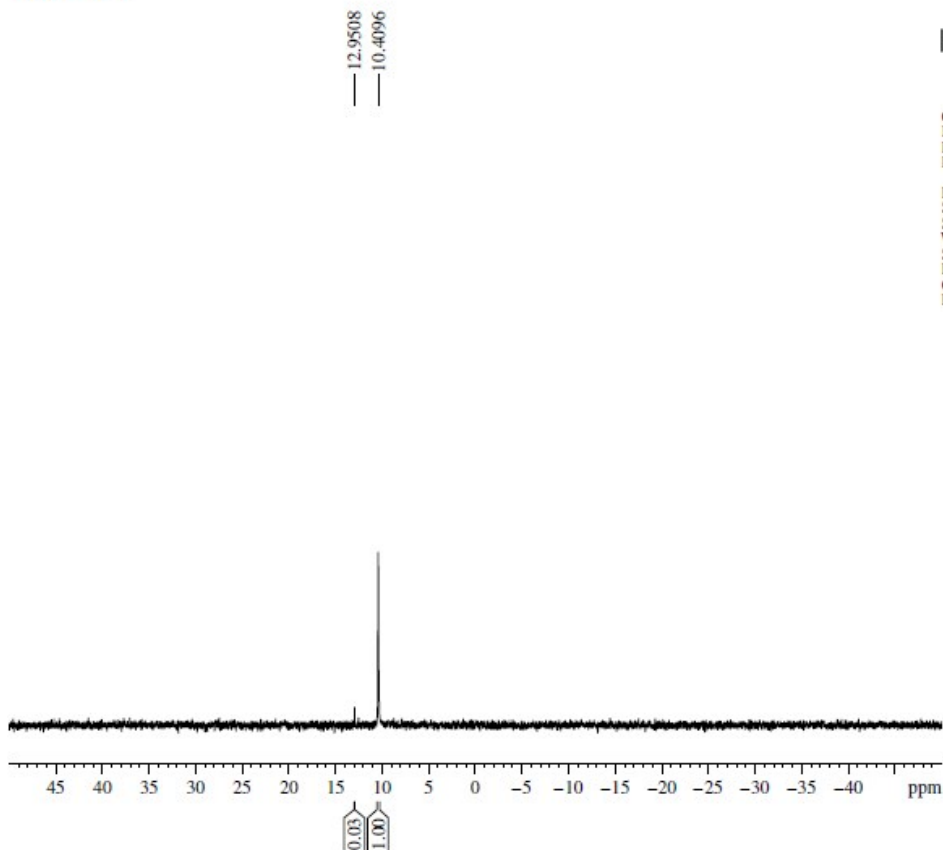


Current Data Parameters
NAME 24-Jan-FN-2020
EXPNO 550
PROCNO 1

F2 - Processing parameters
SI 32768
SF 75.4999369 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

S15: ¹³C NMR spectrum of 3e

NRLD-401



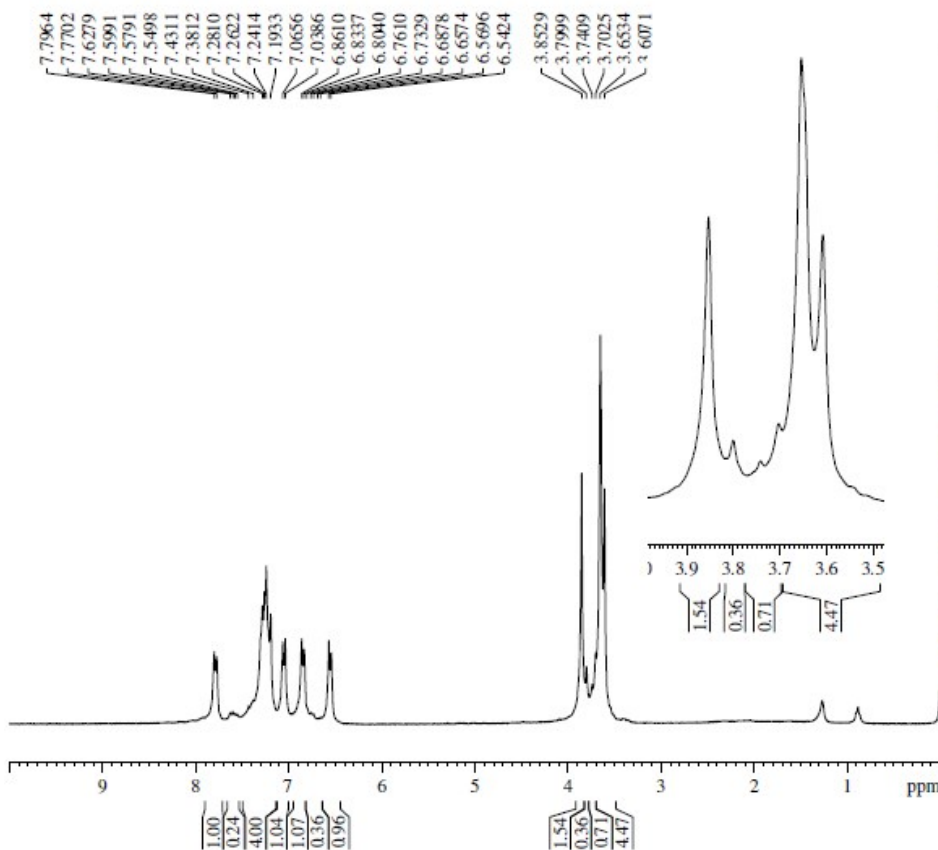
S16: ³¹P NMR spectrum of 3e



Current Data Parameters
NAME 24-Jan-FN-2020
EXPNO 580
PROCNO 1

F2 - Processing parameters
SI 32768
SF 121.5466660 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

NRLD-410



S17: ¹H NMR spectrum of 3f



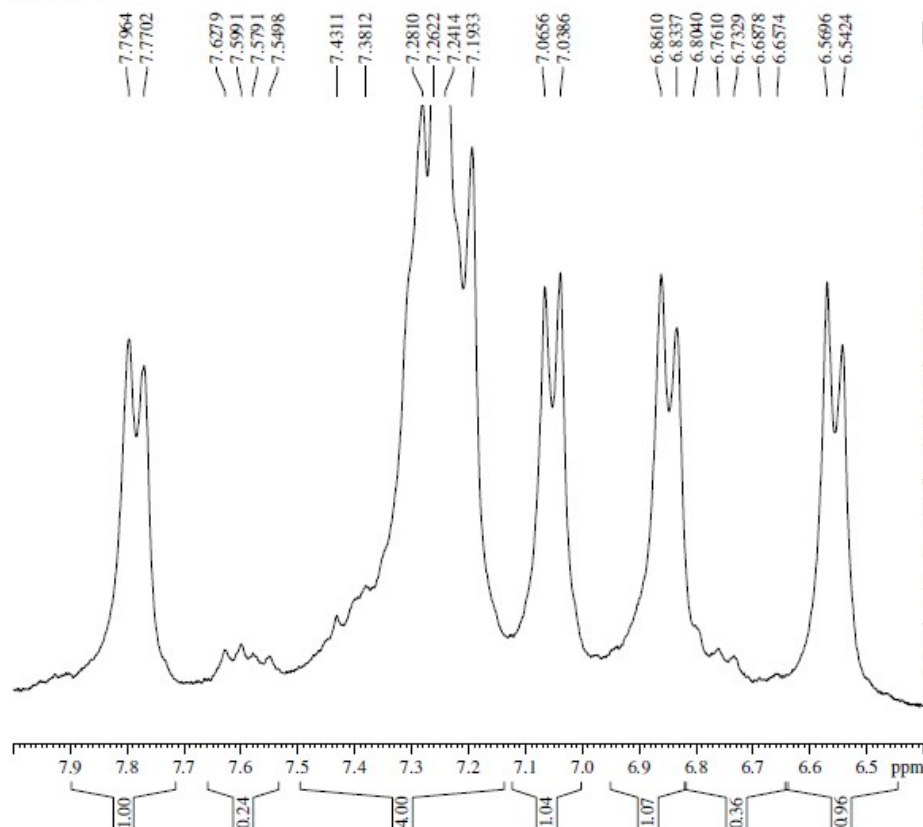
Current Data Parameters
NAME 13-Mar-AN-2020
EXPNO 330
PROCNO 1

F2 - Acquisition Parameters
Date_ 20200313
Time 16.29
INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 6188.119 Hz
FIDRES 0.094423 Hz
AQ 5.2953086 sec
RG 228
DW 80.800 usec
DE 6.50 usec
TE 300.0 K
D1 1.00000000 sec
TD0 1

==== CHANNEL f1 ====
NUC1 1H
P1 13.95 usec
PL1 -1.00 dB
PL1W 15.02081871 W
SFO1 300.2598542 MHz

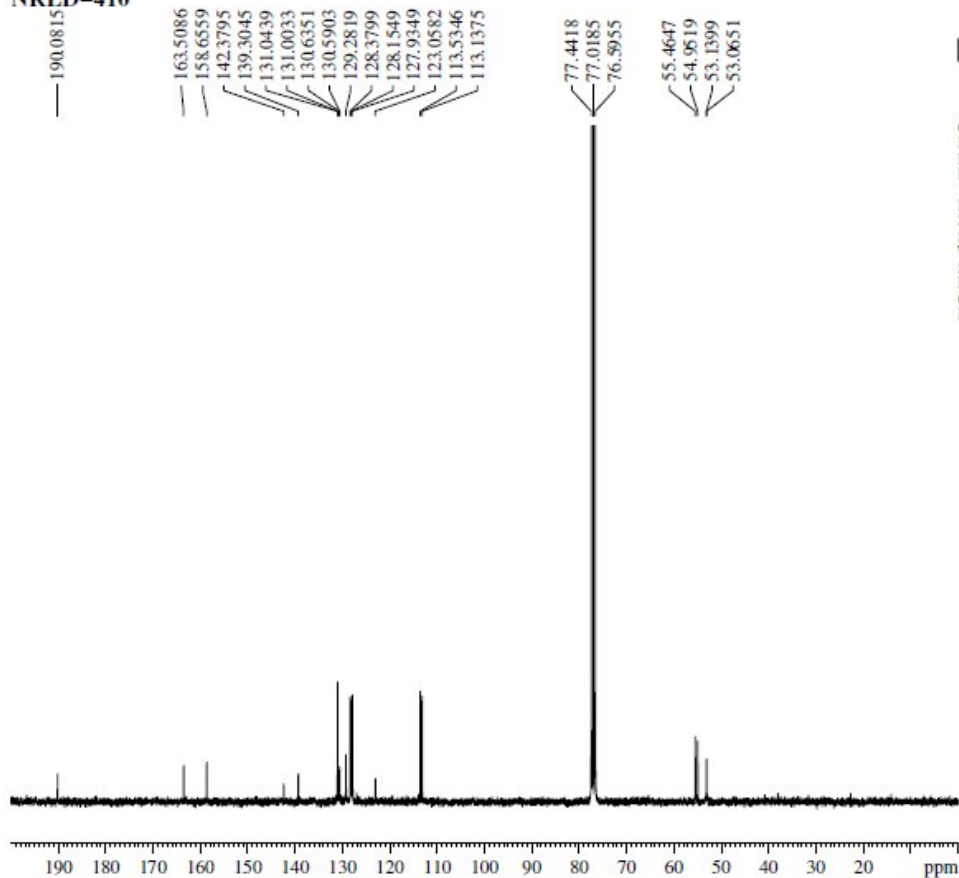
F2 - Processing parameters
SI 32768
SF 300.2580063 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

NRLD-410



S18: ¹H NMR spectrum of 3f (expansion)

NRLD-410



S19: ¹³C NMR spectrum of 3f



Current Data Parameters
NAME 13-Mar-AN-2020
EXPNO 330
PROCNO 1

F2 - Acquisition Parameters
Date_ 20200313
Time 16.29
INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 6188.119 Hz
FIDRES 0.094423 Hz
AQ 5.2953086 sec
RG 228
DW 80.800 usec
DE 6.50 usec
TE 300.0 K
D1 1.00000000 sec
TDO 1

==== CHANNEL f1 ====
NUC1 1H
PI 13.95 usec
PL1 -1.00 dB
PL1W 15.02081871 W
SFO1 300.2598542 MHz

F2 - Processing parameters
SI 32768
SF 300.2580063 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



Current Data Parameters
NAME 13-Mar-AN-2020
EXPNO 340
PROCNO 1

F2 - Processing parameters
SI 32768
SF 75.4999351 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

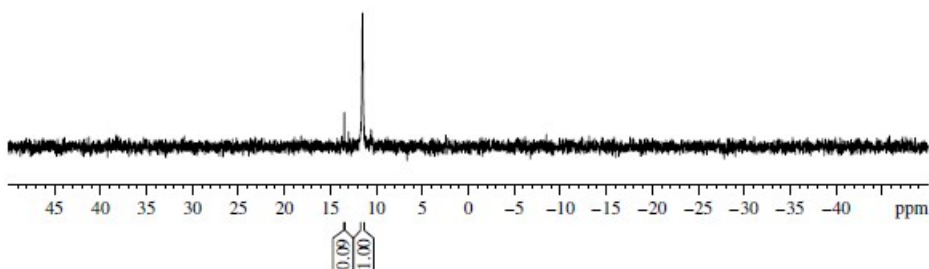
NRLD-410

13.4650
11.5010



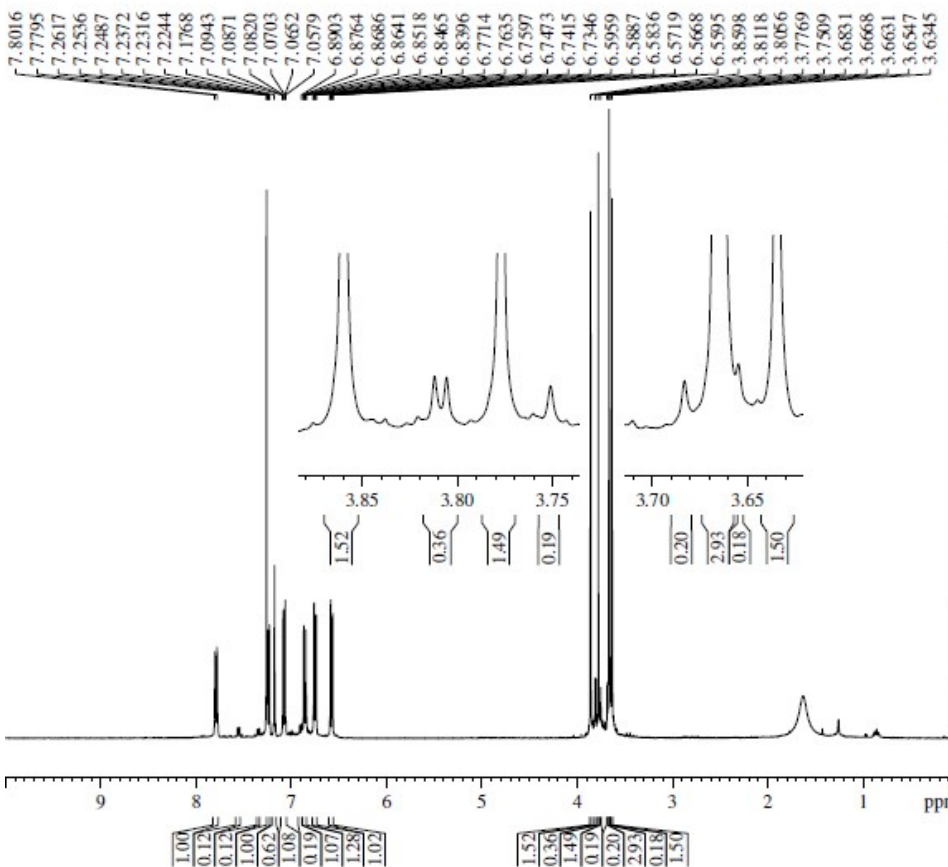
Current Data Parameters
NAME 17-Mar-AN-2020
EXPNO 350
PROCNO 1

F2 - Processing parameters
SI 32768
SF 121.5466660 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



S20: ³¹P NMR spectrum of 3f

NRLD 384



Current Data Parameters
NAME 04-Nov-FN-2019
EXPNO 490
PROCNO 1

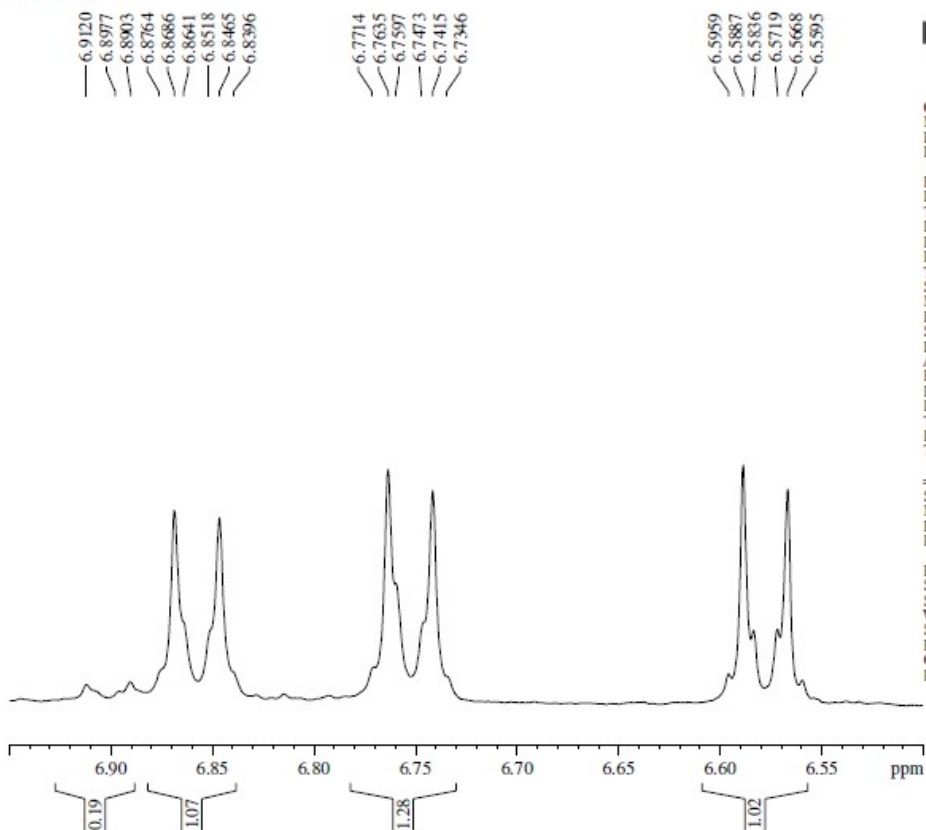
F2 - Acquisition Parameters
Date_ 20191104
Time 16.35
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 32
DS 0
SWH 9615.385 Hz
FIDRES 0.146719 Hz
AQ 3.4078720 sec
RG 159.22
DW 52.000 usec
DE 6.50 usec
TE 300.0 K
D1 1.00000000 sec
TD0 1

==== CHANNEL f1 ====
SFO1 400.1629712 MHz
NUC1 1H
P1 13.20 usec
PLW1 13.00000000 W

F2 - Processing parameters
SI 65536
SF 400.1605089 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

S21: ¹H NMR spectrum of 3g

NRLD 384



S22: ¹H NMR spectrum of 3g (expansion)



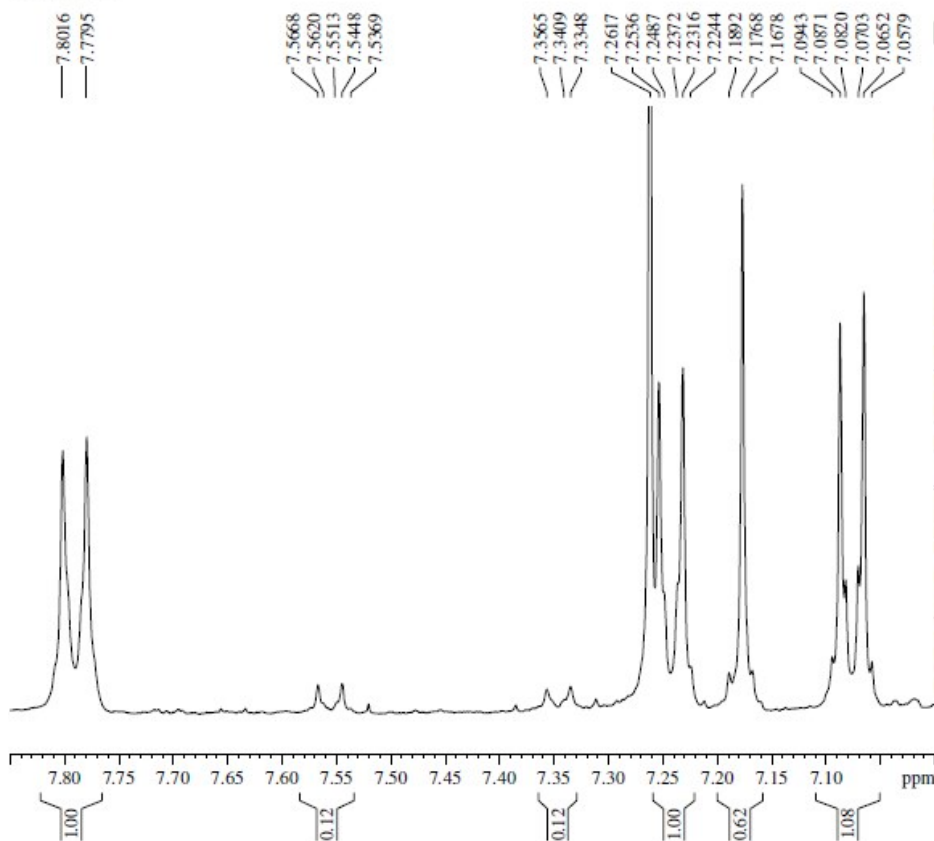
Current Data Parameters
NAME 04-Nov-FN-2019
EXPNO 490
PROCNO 1

F2 - Acquisition Parameters
Date_ 20191104
Time 16.35
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 32
DS 0
SWH 9615.385 Hz
FIDRES 0.146719 Hz
AQ 3.4078720 sec
RG 159.22
DW 52.000 usec
DE 6.50 usec
TE 300.0 K
D1 1.00000000 sec
TD0 1

==== CHANNEL f1 ====
SFO1 400.1629712 MHz
NUC1 1H
P1 13.20 usec
PLW1 13.00000000 W

F2 - Processing parameters
SI 65536
SF 400.1605089 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

NRLD 384



S23: ¹H NMR spectrum of 3g (expansion)



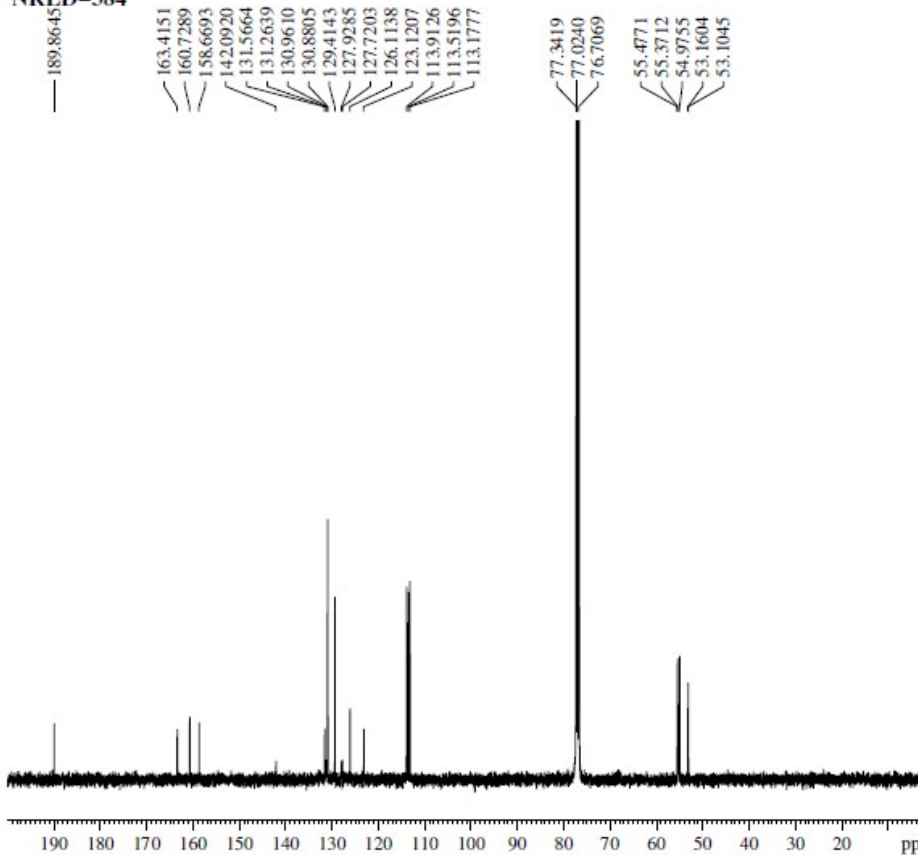
Current Data Parameters
NAME 04-Nov-FN-2019
EXPNO 490
PROCNO 1

F2 - Acquisition Parameters
Date_ 20191104
Time 16.35
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 32
DS 0
SWH 9615.385 Hz
FIDRES 0.146719 Hz
AQ 3.4078720 sec
RG 159.22
DW 52.000 usec
DE 6.50 usec
TE 300.0 K
D1 1.00000000 sec
TD0 1

==== CHANNEL f1 ====
SFO1 400.1629712 MHz
NUC1 1H
P1 13.20 usec
PLW1 13.00000000 W

F2 - Processing parameters
SI 65536
SF 400.1605089 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

NRLD-384



Current Data Parameters
 NAME 04-Nov-AN-2019
 EXPNO 350
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20191105
 Time 4.43
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 4096
 DS 4
 SWH 24038.461 Hz
 FIDRES 0.366798 Hz
 AQ 1.3631488 sec
 RG 201.48
 DW 20.800 usec
 DE 6.50 usec
 TE 300.0 K
 D1 2.0000000 sec
 D11 0.0300000 sec
 TD0 1

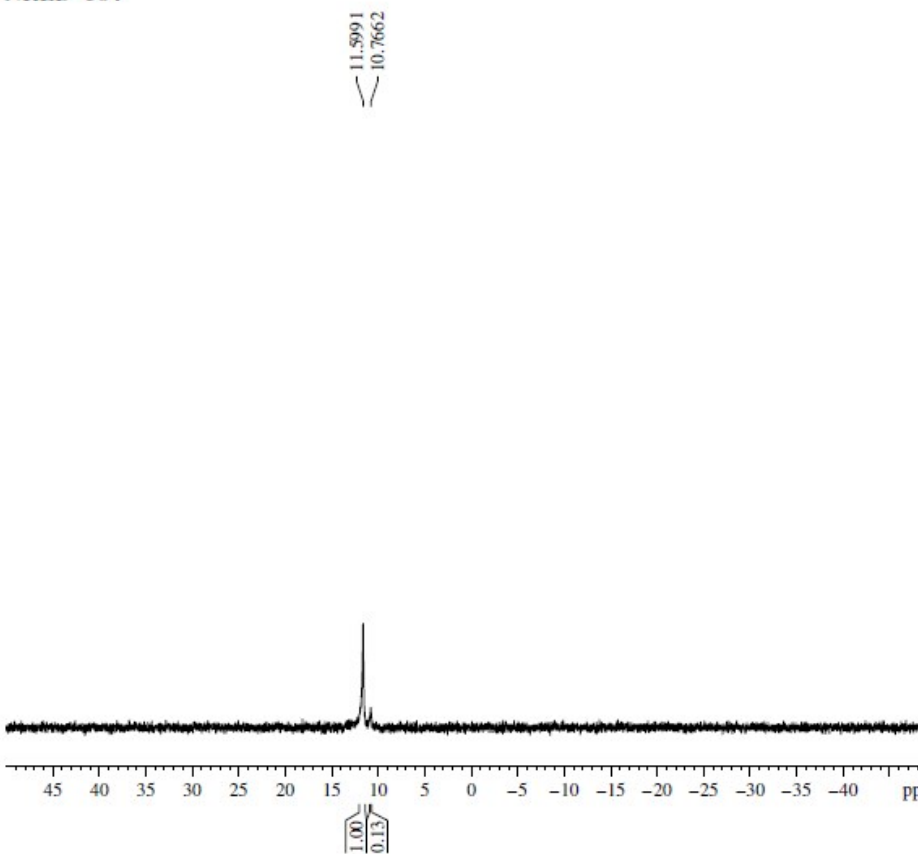
==== CHANNEL f1 ====
 SFO1 100.6304993 MHz
 NUC1 13C
 P1 9.90 usec
 PLW1 53.0000000 W

==== CHANNEL f2 ====
 SFO2 400.1621006 MHz
 NUC2 1H
 CPDPRG2 waltz16
 PCPD2 90.00 usec
 PLW2 13.0000000 W
 PLW12 0.27963999 W
 PLW13 0.22651000 W

F2 - Processing parameters
 SI 32768
 SF 100.6204374 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

S24: ¹³C NMR spectrum of 3g

NRLD-384



Current Data Parameters
 NAME 13-May-FN-2019
 EXPNO 490
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20200513
 Time 16.31
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 16
 DS 4
 SWH 64102.563 Hz
 FIDRES 0.978127 Hz
 AQ 0.5111808 sec
 RG 201.48
 DW 7.800 usec
 DE 6.50 usec
 TE 300.1 K
 D1 2.0000000 sec
 D11 0.0300000 sec
 TD0 1

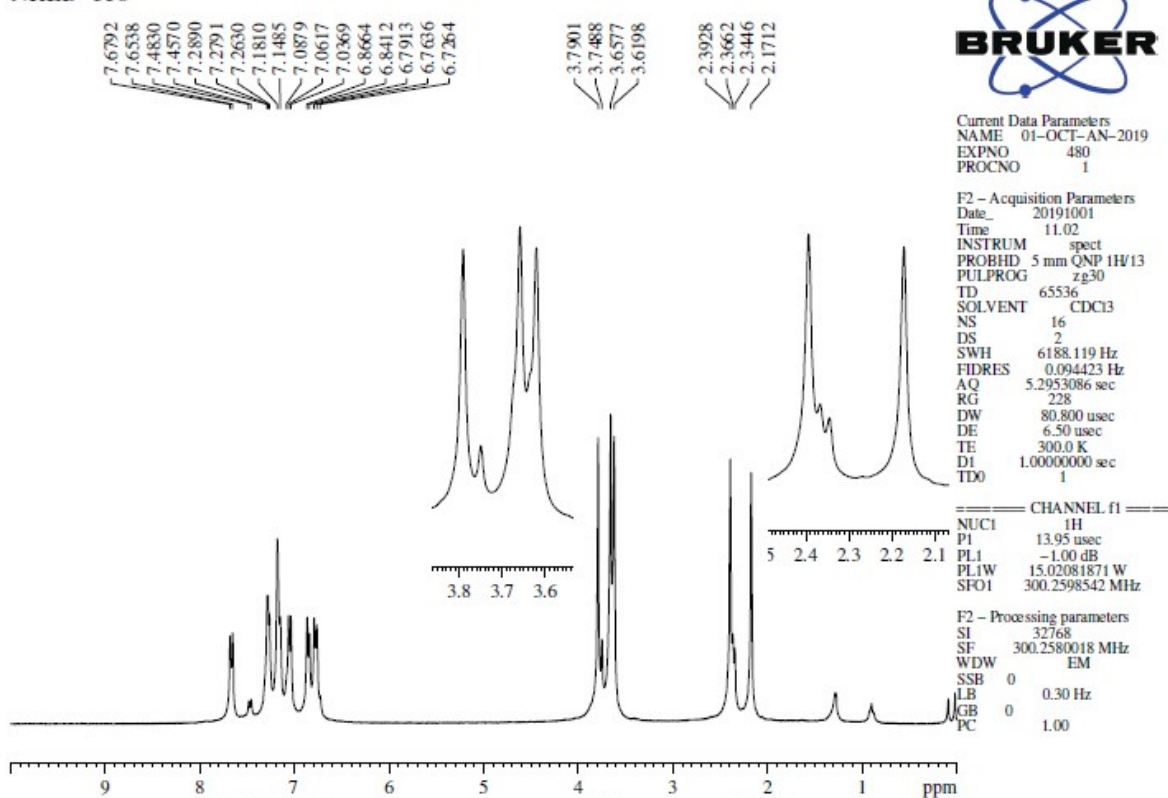
==== CHANNEL f1 ====
 SFO1 161.9798402 MHz
 NUC1 31P
 P1 15.00 usec
 PLW1 12.0000000 W

==== CHANNEL f2 ====
 SFO2 400.1621006 MHz
 NUC2 1H
 CPDPRG2 waltz16
 PCPD2 90.00 usec
 PLW2 13.0000000 W
 PLW12 0.27963999 W
 PLW13 0.22651000 W

F2 - Processing parameters
 SI 32768
 SF 161.9879400 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

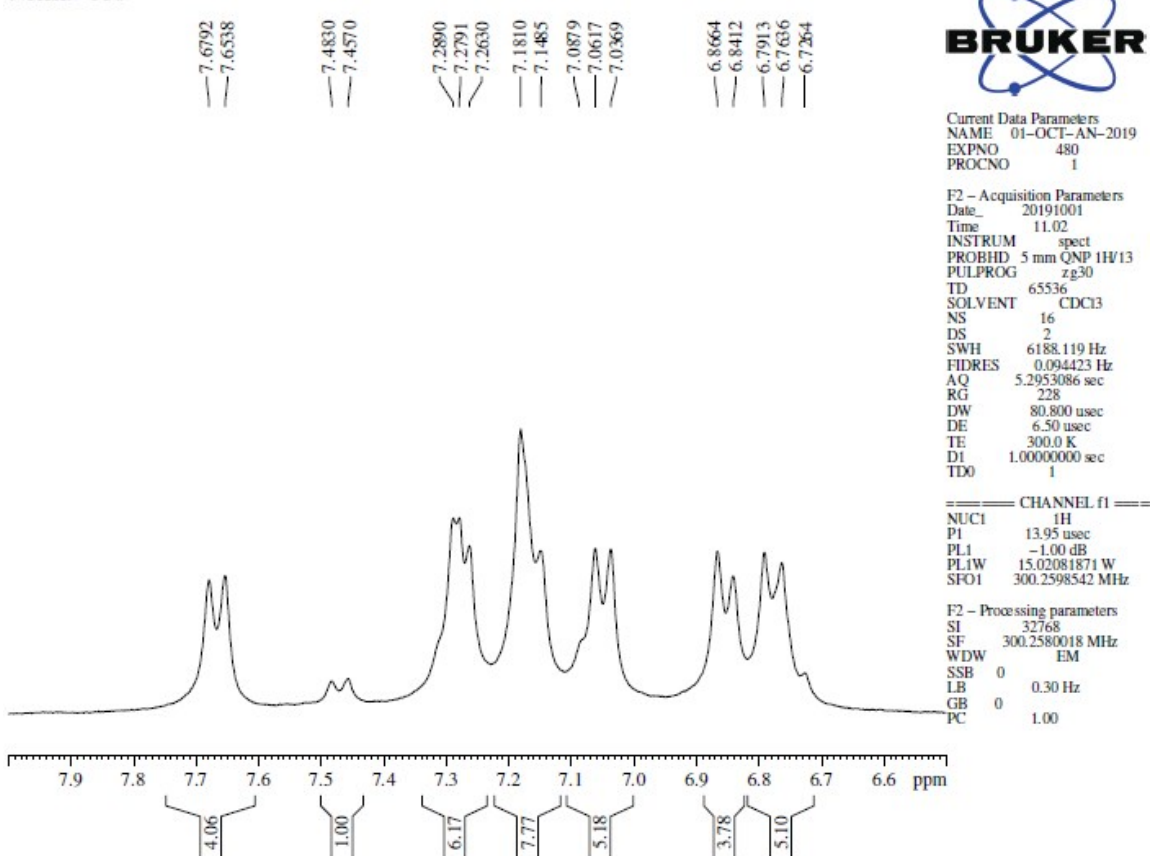
S25: ³¹P NMR spectrum of 3g

NRLD-358

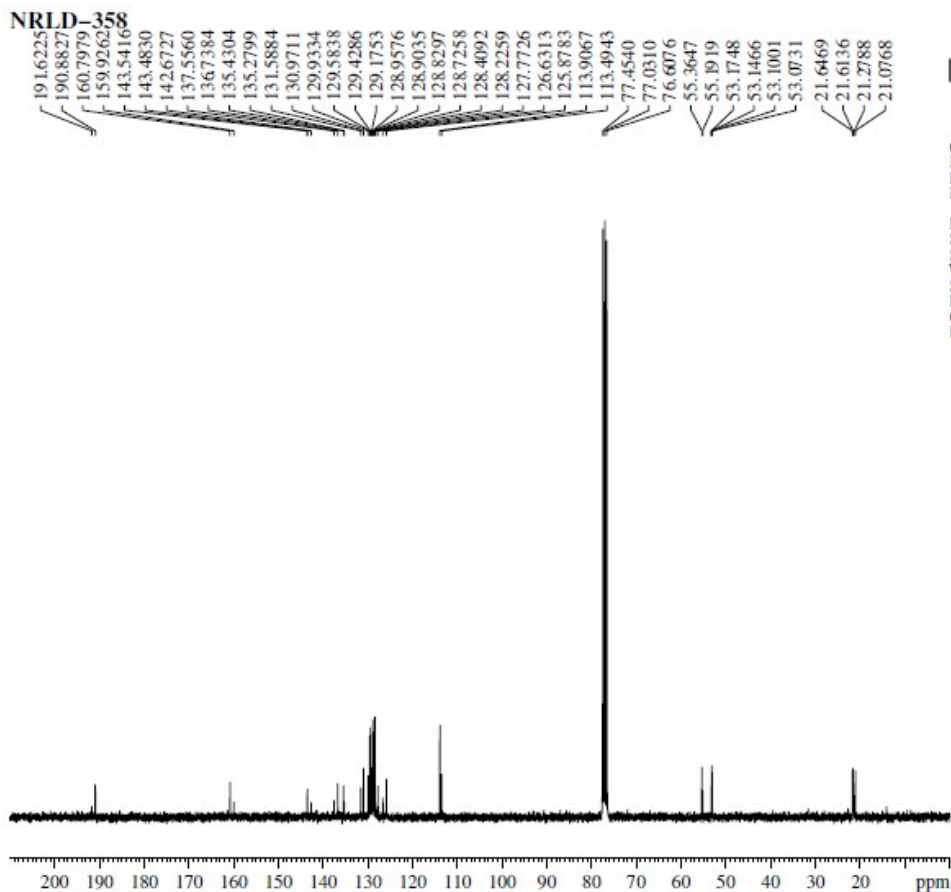


S26: ¹H NMR spectrum of 3h

NRLD-358



S27: ¹H NMR spectrum of 3h (expansion)

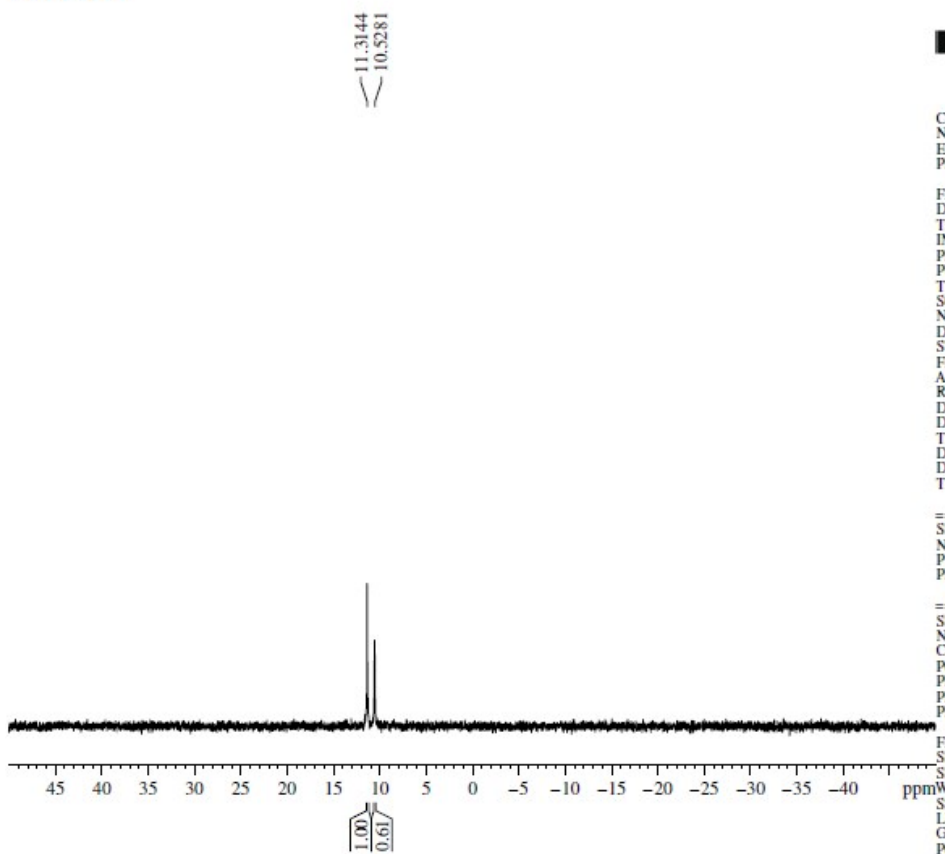


Current Data Parameters
NAME 10-Oct-FN-2019
EXPNO 500
PROCNO 1

F2 - Processing parameters
SI 32768
SF 75.4999340 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

S28: ¹³C NMR spectrum of 3h

NRLD-358



Current Data Parameters
NAME 26-Dec-AN-2019
EXPNO 540
PROCNO 1

F2 - Acquisition Parameters
Date_ 20191226
Time 21.20
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 16
DS 4
SWH 64102.563 Hz
FIDRES 0.978127 Hz
AQ 0.511808 sec
RG 201.48
DW 7.800 usec
DE 6.50 usec
TE 303.1 K
D1 2.0000000 sec
D11 0.0300000 sec
TD0 1

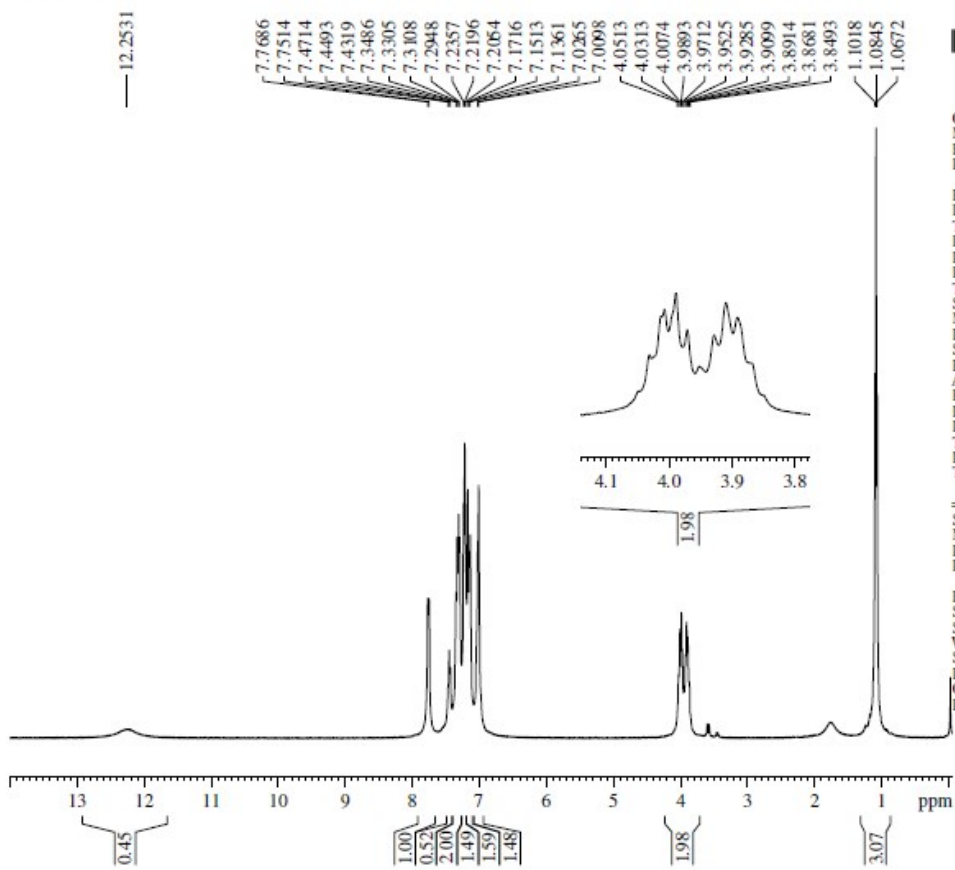
==== CHANNEL f1 ====
SFO1 161.9798402 MHz
NUC1 31P
P1 15.00 usec
PLW1 12.00000000 W

==== CHANNEL f2 ====
SFO2 400.1621006 MHz
NUC2 1H
CPDPRG2 waltz16
PCPD2 90.00 usec
PLW2 13.00000000 W
PLW12 0.27963999 W
PLW13 0.22651000 W

F2 - Processing parameters
SI 32768
SF 161.9879400 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

S29: ³¹P NMR spectrum of 3h

NRLD 392



Current Data Parameters
 NAME 13-Jan-FN-2020
 EXPNO 500
 PROCNO 1

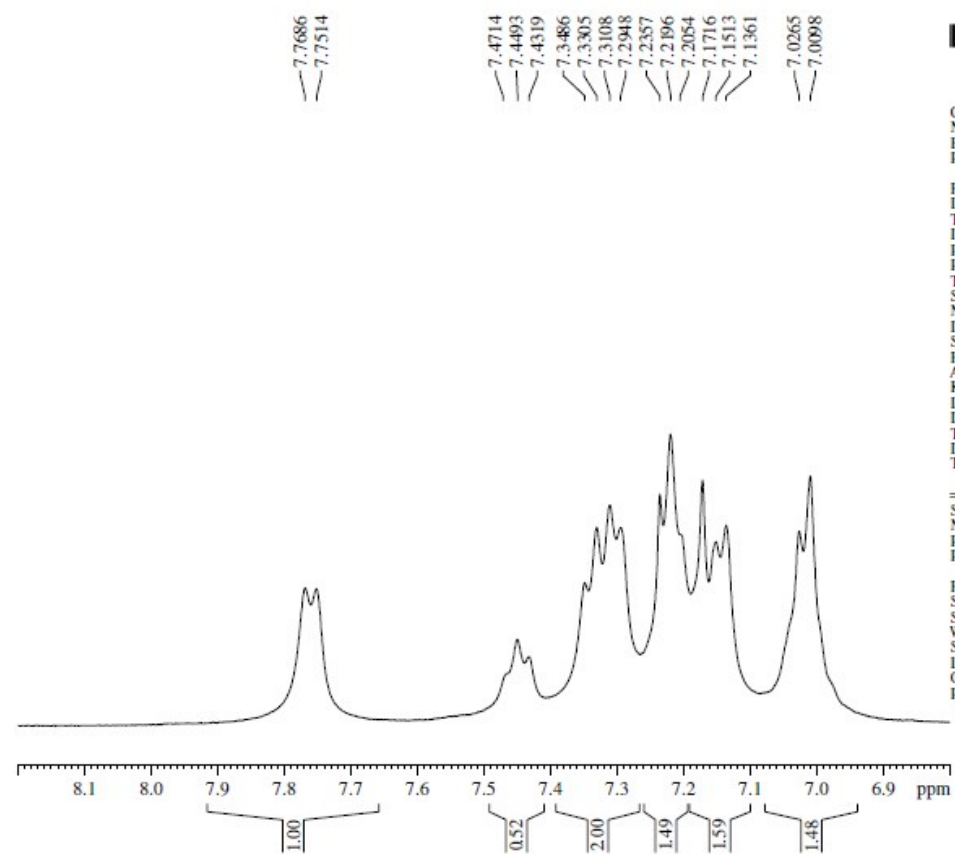
F2 - Acquisition Parameters
 Date_ 20200113
 Time 17.12
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 8
 DS 0
 SWH 9615.385 Hz
 FIDRES 0.146719 Hz
 AQ 3.4078720 sec
 RG 100.41
 DW 52.000 usec
 DE 6.50 usec
 TE 303.0 K
 DI 1.00000000 sec
 TDO 1

==== CHANNEL f1 ====
 SFO1 400.1629712 MHz
 NUC1 1H
 P1 13.20 usec
 PLW1 13.00000000 W

F2 - Processing parameters
 SI 65536
 SF 400.1605188 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

S30: ¹H NMR spectrum of 3i

NRLD 392



Current Data Parameters
 NAME 13-Jan-FN-2020
 EXPNO 500
 PROCNO 1

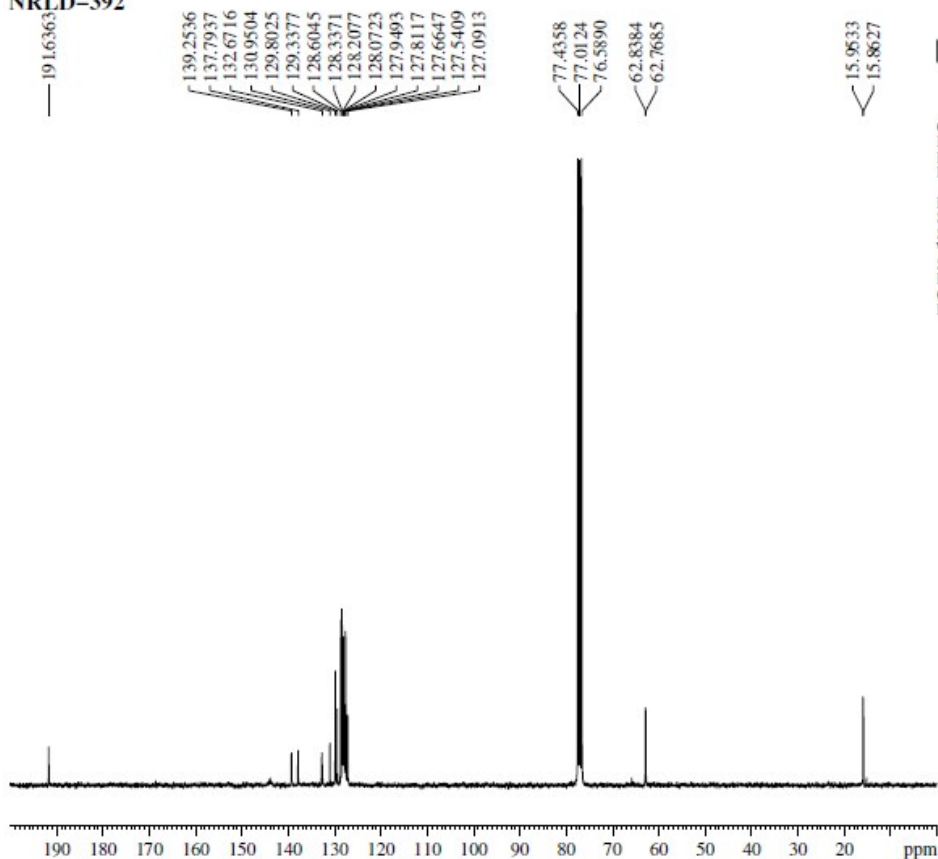
F2 - Acquisition Parameters
 Date_ 20200113
 Time 17.12
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 8
 DS 0
 SWH 9615.385 Hz
 FIDRES 0.146719 Hz
 AQ 3.4078720 sec
 RG 100.41
 DW 52.000 usec
 DE 6.50 usec
 TE 303.0 K
 DI 1.00000000 sec
 TDO 1

==== CHANNEL f1 ====
 SFO1 400.1629712 MHz
 NUC1 1H
 P1 13.20 usec
 PLW1 13.00000000 W

F2 - Processing parameters
 SI 65536
 SF 400.1605188 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

S31: ¹H NMR spectrum of 3i (expansion)

NRLD-392

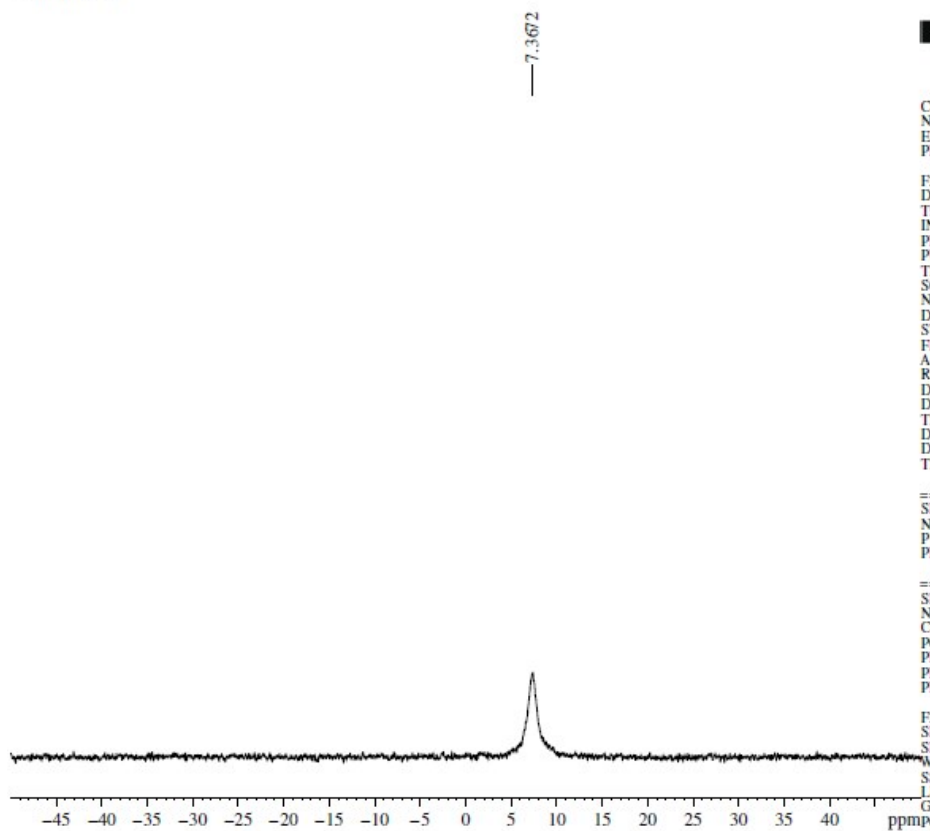


Current Data Parameters
NAME 21-Jan-AN-2020
EXPNO 410
PROCNO 1

F2 - Processing parameters
SI 32768
SF 75.4999363 MHz
WDW EM
SSB 0
LB 2.00 Hz
GB 0
PC 1.40

S32: ¹³C NMR spectrum of 3i

NRLD 392



Current Data Parameters
NAME 13-Jan-FN-2020
EXPNO 560
PROCNO 1

F2 - Acquisition Parameters
Date_ 20200113
Time 17.14
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 32
DS 4
SWH 64102.563 Hz
FIDRES 0.978127 Hz
AQ 0.5111808 sec
RG 201.48
DW 7.800 usec
DE 6.50 usec
TE 303.1 K
D1 2.0000000 sec
D11 0.0300000 sec
TD0 1

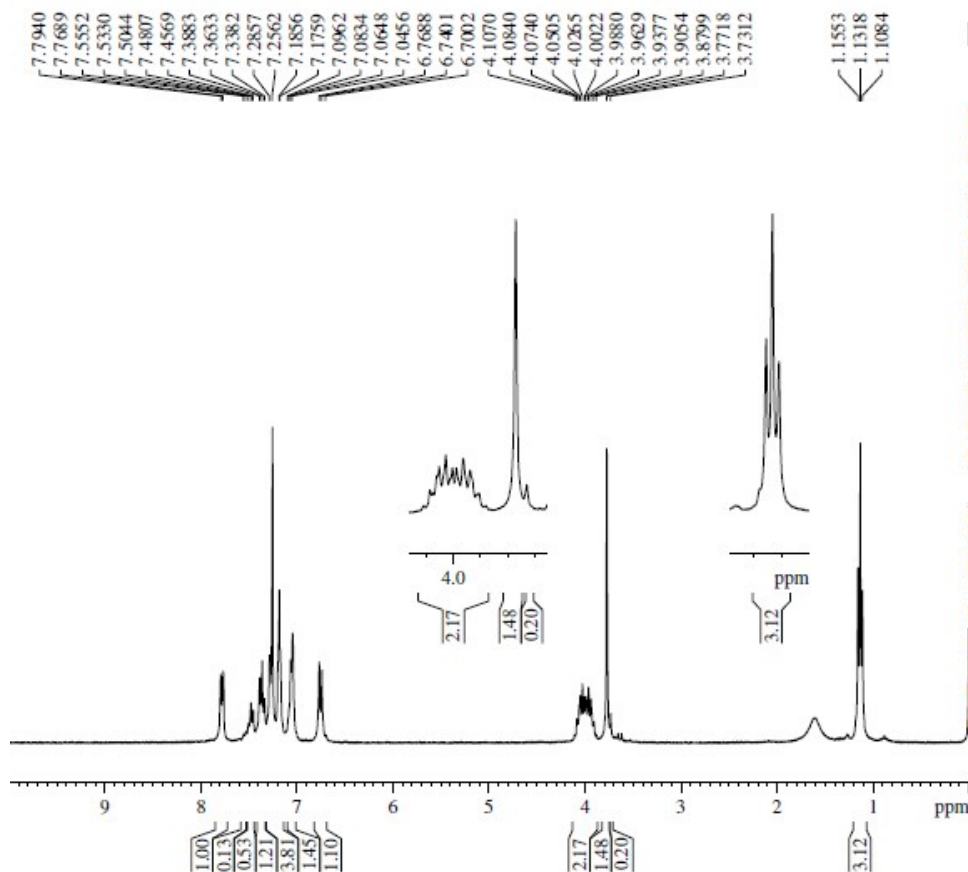
==== CHANNEL f1 ====
SFO1 161.9798402 MHz
NUC1 31P
P1 15.00 usec
PLW1 12.00000000 W

==== CHANNEL f2 ====
SFO2 400.1621006 MHz
NUC2 1H
CPDPRG2 waltz16
PCPD2 90.00 usec
PLW2 13.00000000 W
PLW12 0.27963999 W
PLW13 0.22651000 W

F2 - Processing parameters
SI 32768
SF 161.9879400 MHz
WDW EM
SSB 0
LB 6.00 Hz
GB 0
PC 1.40

S33: ³¹P NMR spectrum of 3i

NRLD-393



Current Data Parameters
 NAME 24-Jan-FN-2020
 EXPNO 520
 PROCNO 1

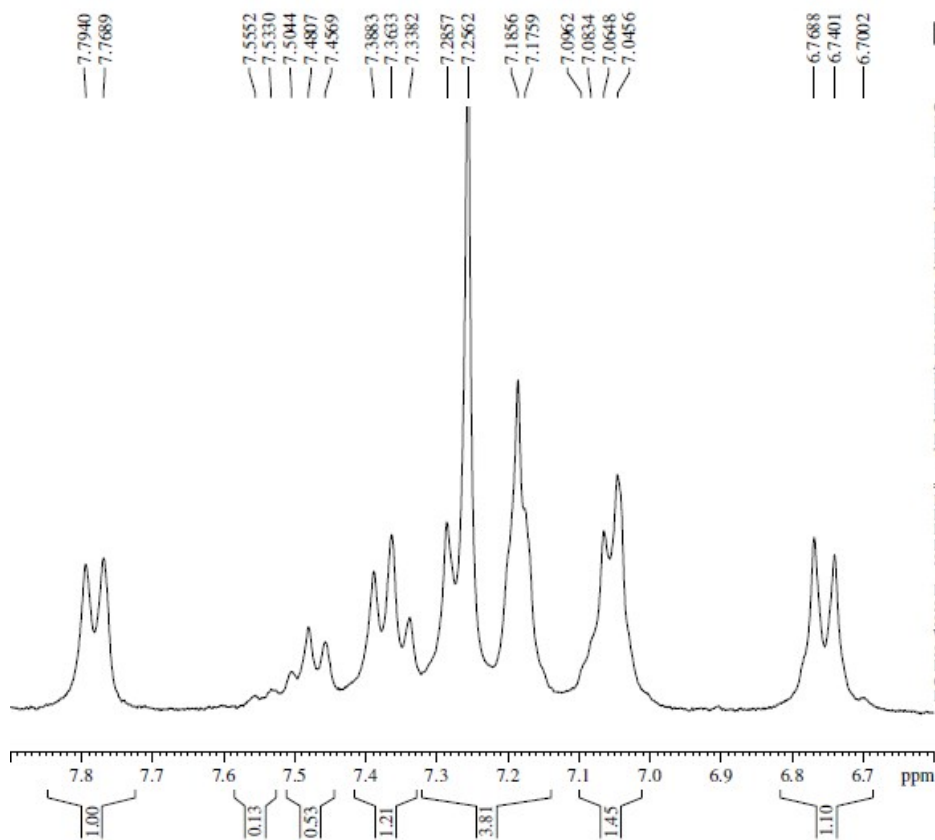
F2 - Acquisition Parameters
 Date_ 20200124
 Time 11.22
 INSTRUM spect
 PROBHD 5 mm QNP 1H/13
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 16
 DS 2
 SWH 6188.119 Hz
 FIDRES 0.094423 Hz
 AQ 5.2953086 sec
 RG 322
 DW 80.800 usec
 DE 6.50 usec
 TE 300.0 K
 D1 1.00000000 sec
 TDO 1

==== CHANNEL f1 ====
 NUC1 1H
 P1 13.95 usec
 PL1 -1.00 dB
 PL1W 15.02081871 W
 SFO1 300.2598542 MHz

F2 - Processing parameters
 SI 32768
 SF 300.2580085 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

S34: ¹H NMR spectrum of 3j

NRLD-393



Current Data Parameters
 NAME 24-Jan-FN-2020
 EXPNO 520
 PROCNO 1

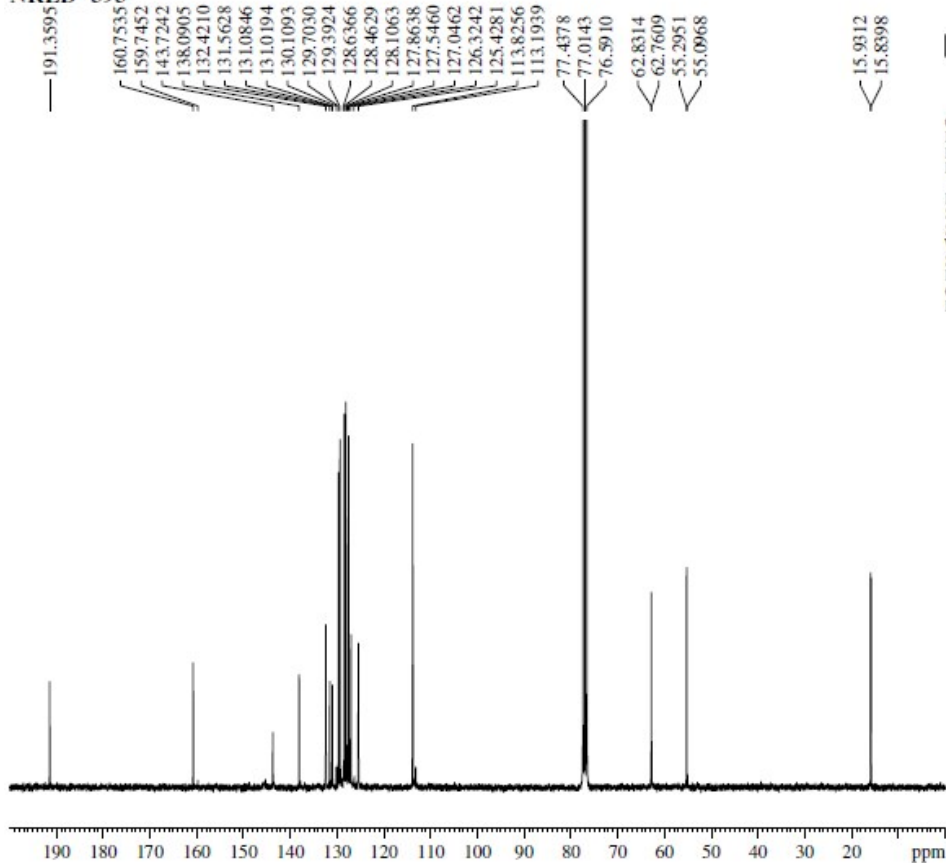
F2 - Acquisition Parameters
 Date_ 20200124
 Time 11.22
 INSTRUM spect
 PROBHD 5 mm QNP 1H/13
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 16
 DS 2
 SWH 6188.119 Hz
 FIDRES 0.094423 Hz
 AQ 5.2953086 sec
 RG 322
 DW 80.800 usec
 DE 6.50 usec
 TE 300.0 K
 D1 1.00000000 sec
 TDO 1

==== CHANNEL f1 ====
 NUC1 1H
 P1 13.95 usec
 PL1 -1.00 dB
 PL1W 15.02081871 W
 SFO1 300.2598542 MHz

F2 - Processing parameters
 SI 32768
 SF 300.2580085 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

S35: ¹H NMR spectrum of 3j (expansion)

NRLD-393

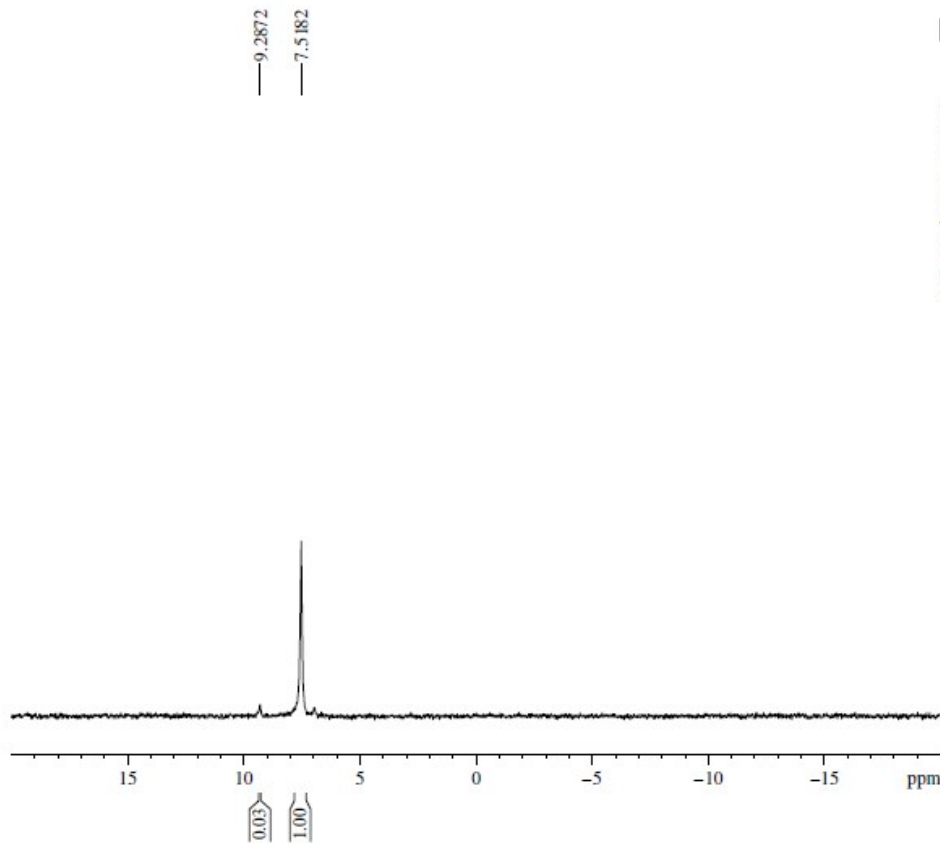


Current Data Parameters
NAME 21-Jan-FN-2020
EXPNO 430
PROCNO 1

F2 - Processing parameters
SI 32768
SF 75.4999383 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

S36: ¹³C NMR spectrum of 3j

NRLD-393

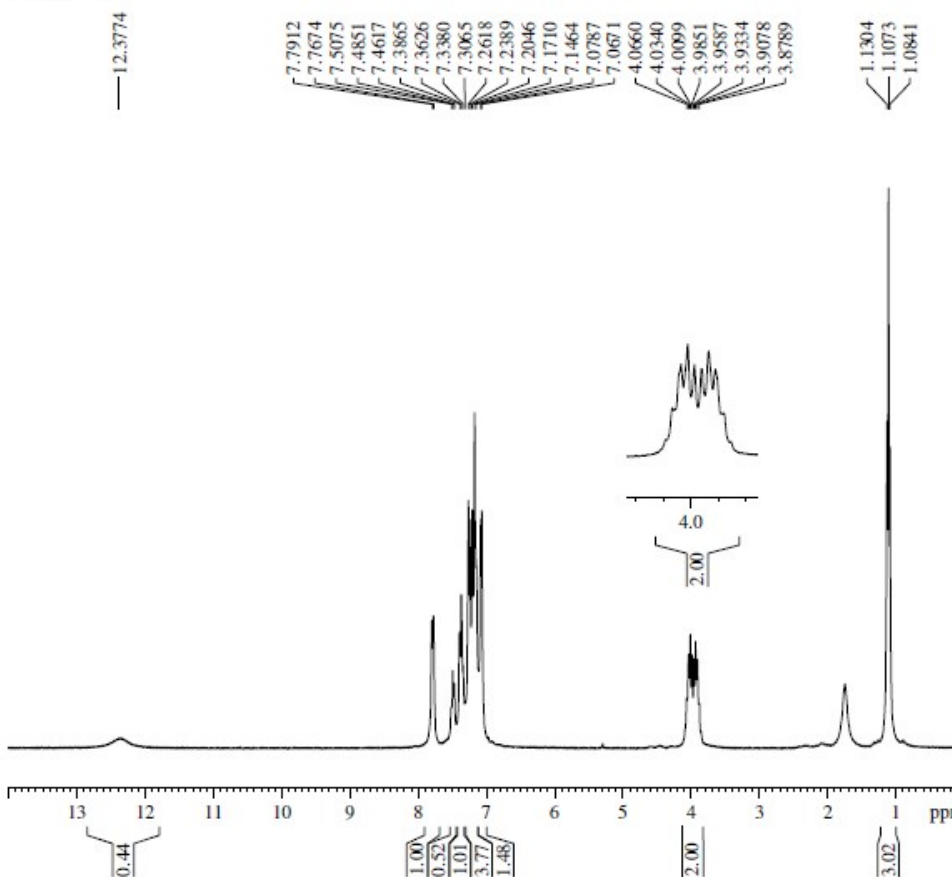


Current Data Parameters
NAME 21-Jan-FN-2020
EXPNO 420
PROCNO 1

F2 - Processing parameters
SI 32768
SF 121.5466660 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

S37: ³¹P NMR spectrum of 3j

NRLD-439



Current Data Parameters
 NAME 29-JUNE-AN-2020
 EXPNO 380
 PROCNO 1

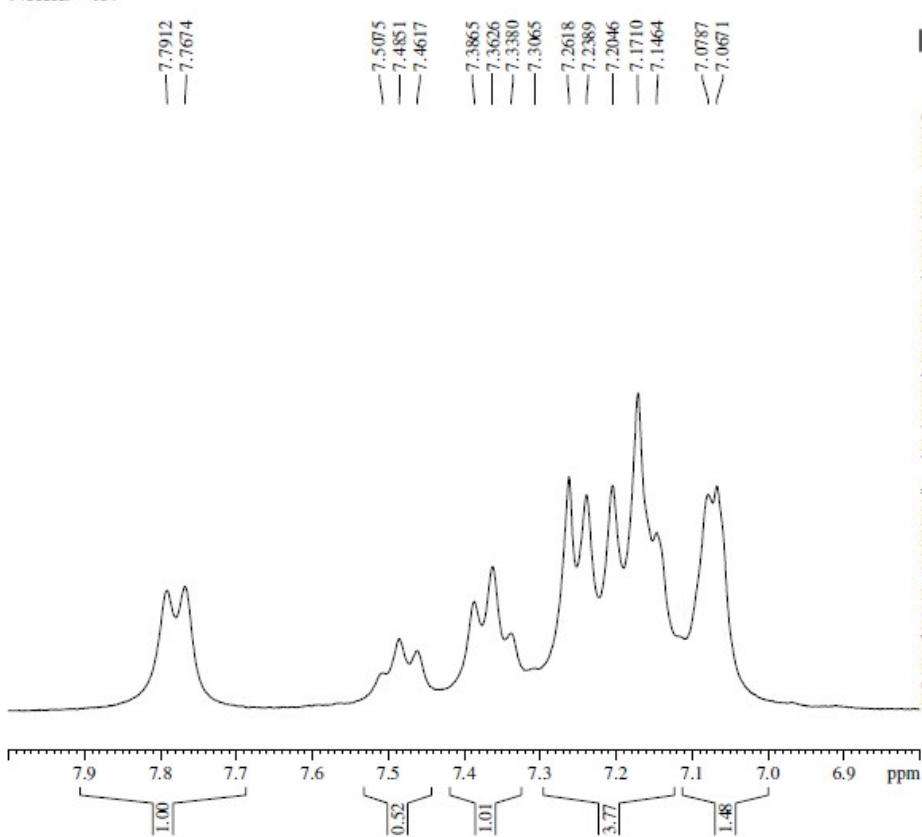
F2 - Acquisition Parameters
 Date_ 20200629
 Time 16.22
 INSTRUM spect
 PROBHD 5 mm QNP 1H/13
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 16
 DS 2
 SWH 6188.119 Hz
 FIDRES 0.094423 Hz
 AQ 5.2953086 sec
 RG 256
 DW 80.800 usec
 DE 6.50 usec
 TE 300.0 K
 D1 1.00000000 sec
 TDO 1

==== CHANNEL f1 ====
 NUC1 1H
 P1 13.95 usec
 PL1 -1.00 dB
 PL1W 15.02081871 W
 SFO1 300.2598542 MHz

F2 - Processing parameters
 SI 32768
 SF 300.2580069 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

S38: ¹H NMR spectrum of 3k

NRLD-439



Current Data Parameters
 NAME 29-JUNE-AN-2020
 EXPNO 380
 PROCNO 1

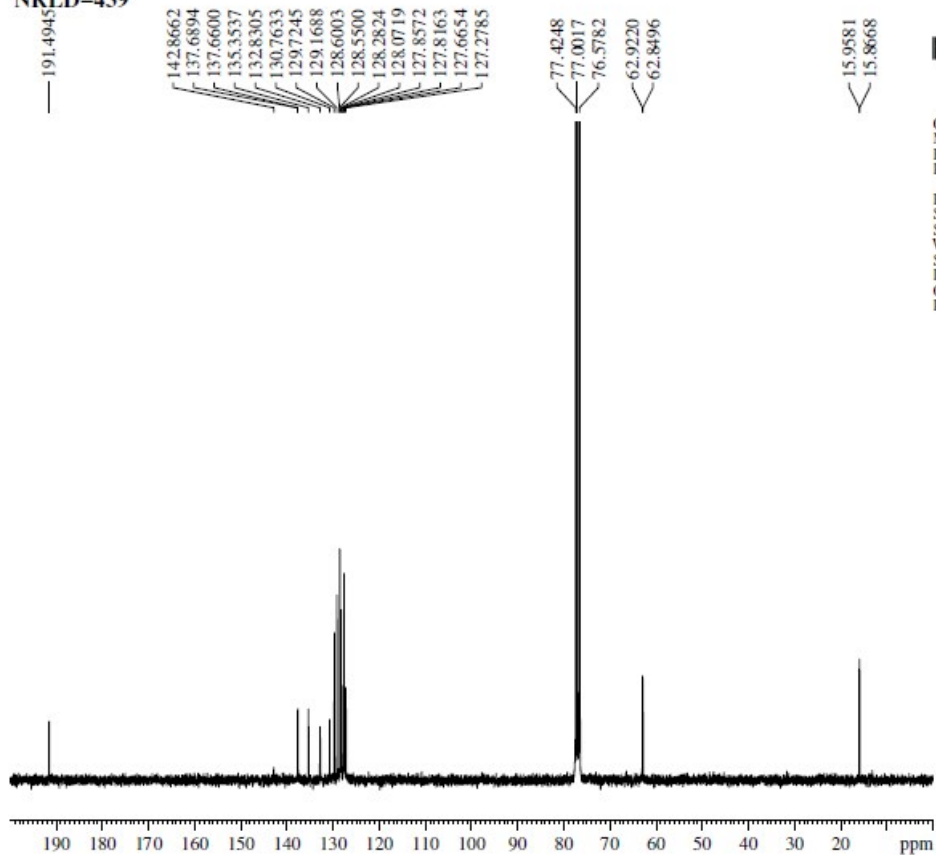
F2 - Acquisition Parameters
 Date_ 20200629
 Time 16.22
 INSTRUM spect
 PROBHD 5 mm QNP 1H/13
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 16
 DS 2
 SWH 6188.119 Hz
 FIDRES 0.094423 Hz
 AQ 5.2953086 sec
 RG 256
 DW 80.800 usec
 DE 6.50 usec
 TE 300.0 K
 D1 1.00000000 sec
 TDO 1

==== CHANNEL f1 ====
 NUC1 1H
 P1 13.95 usec
 PL1 -1.00 dB
 PL1W 15.02081871 W
 SFO1 300.2598542 MHz

F2 - Processing parameters
 SI 32768
 SF 300.2580069 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

S39: ¹H NMR spectrum of 3k (expansion)

NRLD-439

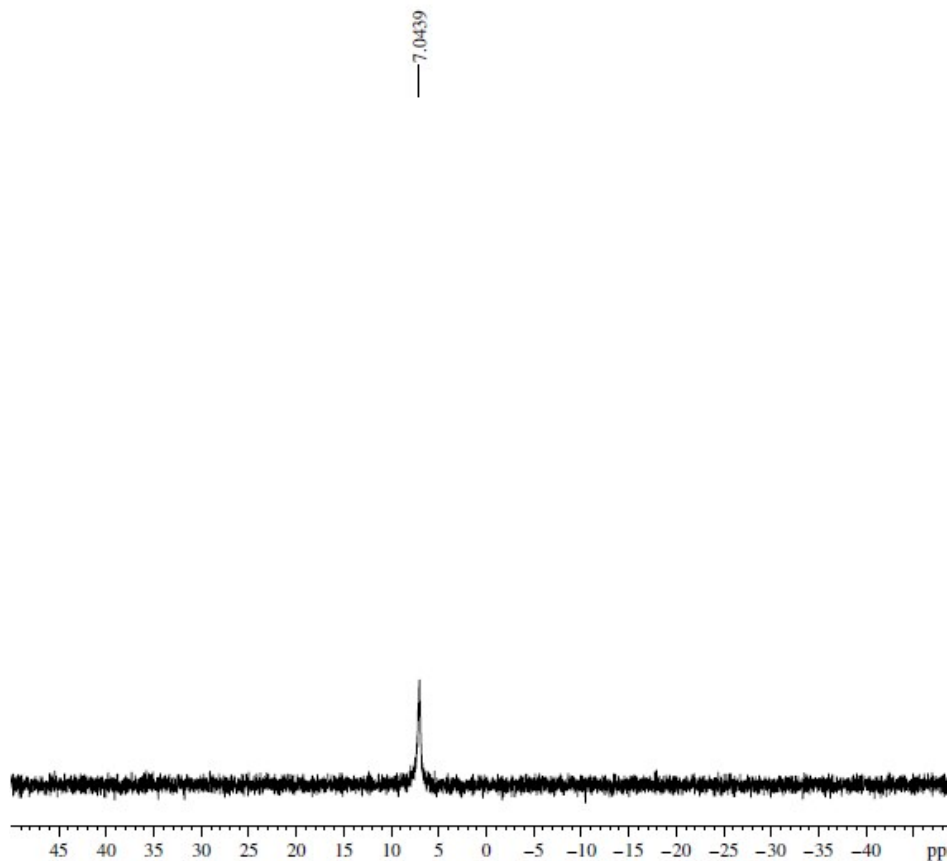


Current Data Parameters
 NAME 30-June-AN-2020
 EXPNO 310
 PROCNO 1

F2 - Processing parameters
 SI 32768
 SF 75.4999361 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

S40: 13C NMR spectrum of 3k

NRLD 439



Current Data Parameters
 NAME 24-July-FN-2020
 EXPNO 560
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20200724
 Time 17.47
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 32
 DS 4
 SWH 64102.563 Hz
 FIDRES 0.978127 Hz
 AQ 0.5111808 sec
 RG 201.48
 DW 7.800 usec
 DE 6.50 usec
 TE 300.1 K
 D1 2.0000000 sec
 D11 0.03000000 sec
 TD0 1

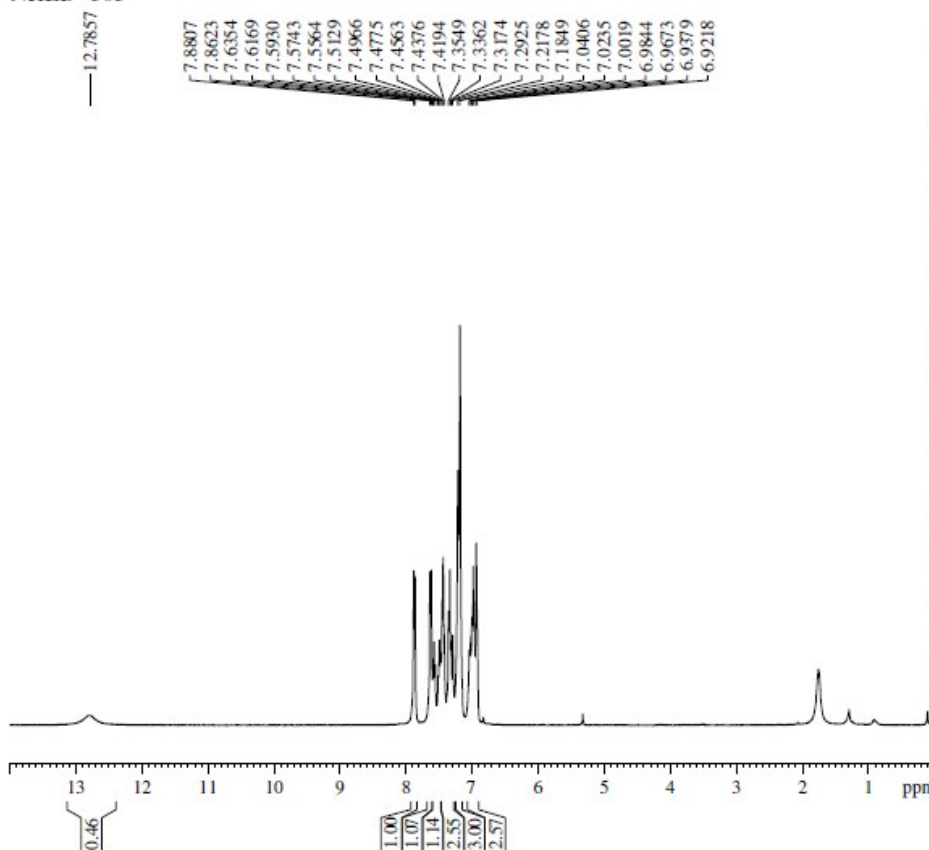
==== CHANNEL f1 ====
 SFO1 161.9798402 MHz
 NUC1 31P
 P1 15.00 usec
 PLW1 12.00000000 W

==== CHANNEL f2 ====
 SFO2 400.1621006 MHz
 NUC2 1H
 CPDPRG2 waltz16
 PCPD2 90.00 usec
 PLW2 13.00000000 W
 PLW12 0.27963999 W
 PLW13 0.22651000 W

F2 - Processing parameters
 SI 32768
 SF 161.9879400 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

S41: 31P NMR spectrum of 3k

NRLD-363



Current Data Parameters
 NAME 04-Nov-AN-2019
 EXPNO 360
 PROCNO 1

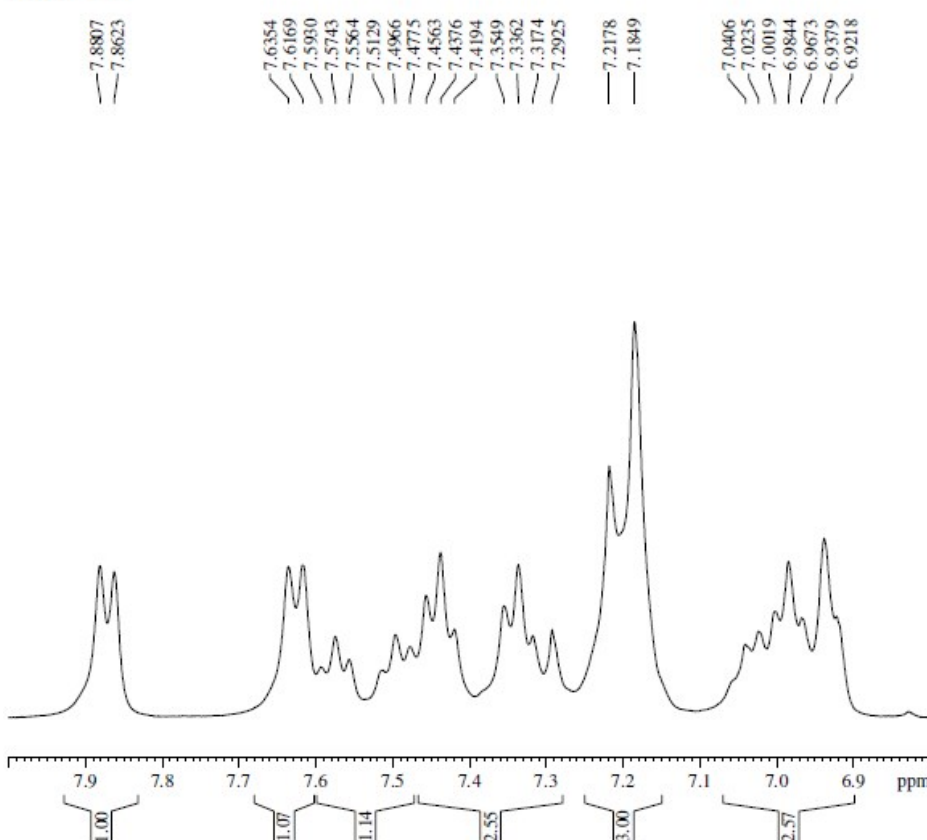
F2 - Acquisition Parameters
 Date_ 700101
 Time 5.30
 INSTRUM
 PROBHD
 PULPROG zg30
 TD 65536
 SOLVENT
 NS 16
 DS 2
 SWH 8012.820 Hz
 FIDRES 0.122266 Hz
 AQ 4.0894465 sec
 RG 32
 DW 62.400 usec
 DE 6.50 usec
 TE 298.0 K
 D1 1.00000000 sec
 TD0 1

==== CHANNEL f1 ====
 SFO1 400.1629712 MHz
 NUC1 1H
 P1 10.00 usec
 PLW1 0 W

F2 - Processing parameters
 SI 65536
 SF 400.1604974 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

S42: ¹H NMR spectrum of 31

NRLD-363



Current Data Parameters
 NAME 04-Nov-AN-2019
 EXPNO 360
 PROCNO 1

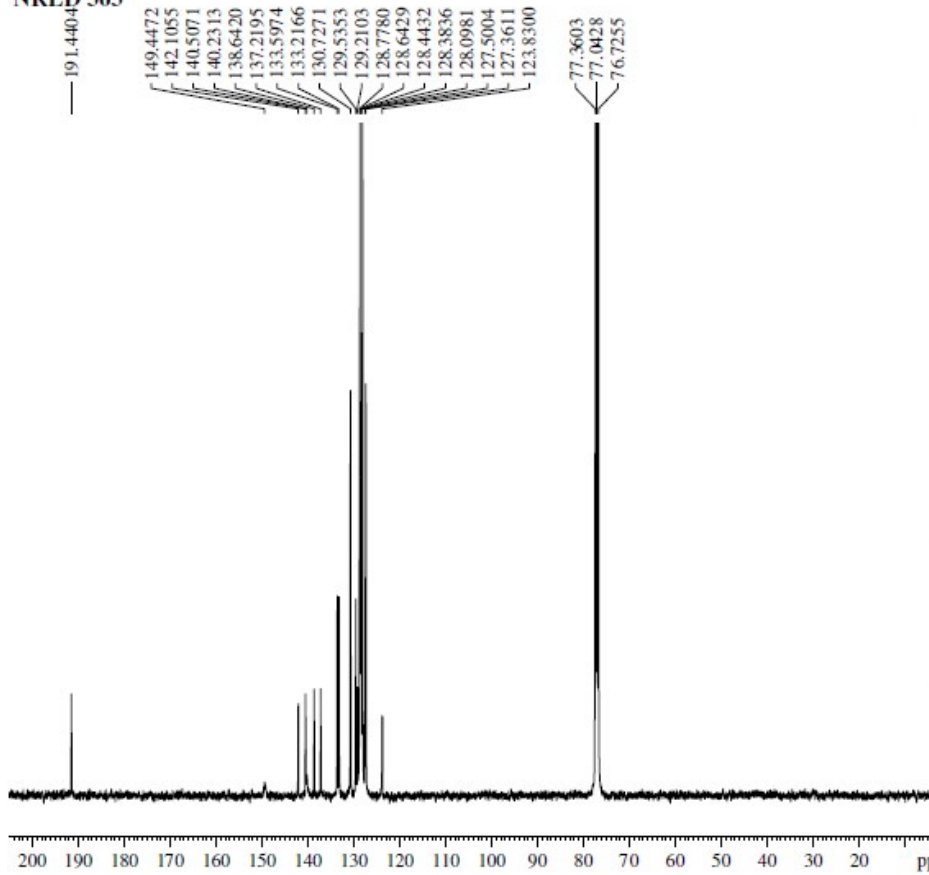
F2 - Acquisition Parameters
 Date_ 700101
 Time 5.30
 INSTRUM
 PROBHD
 PULPROG zg30
 TD 65536
 SOLVENT
 NS 16
 DS 2
 SWH 8012.820 Hz
 FIDRES 0.122266 Hz
 AQ 4.0894465 sec
 RG 32
 DW 62.400 usec
 DE 6.50 usec
 TE 298.0 K
 D1 1.00000000 sec
 TD0 1

==== CHANNEL f1 ====
 SFO1 400.1629712 MHz
 NUC1 1H
 P1 10.00 usec
 PLW1 0 W

F2 - Processing parameters
 SI 65536
 SF 400.1604974 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

S43: ¹H NMR spectrum of 31 (expansion)

NRLD 363



Current Data Parameters
 NAME 30-Oct-FN-2019
 EXPNO 410
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20191031
 Time 7.21
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zgpg30
 TD 65536
 SOLVENT CDC13
 NS 4096
 DS 0
 SWH 32051.281 Hz
 FIDRES 0.489064 Hz
 AQ 1.0223616 sec
 RG 201.48
 DW 15.600 usec
 DE 6.50 usec
 TE 300.0 K
 D1 2.0000000 sec
 D11 0.03000000 sec
 TDO 1

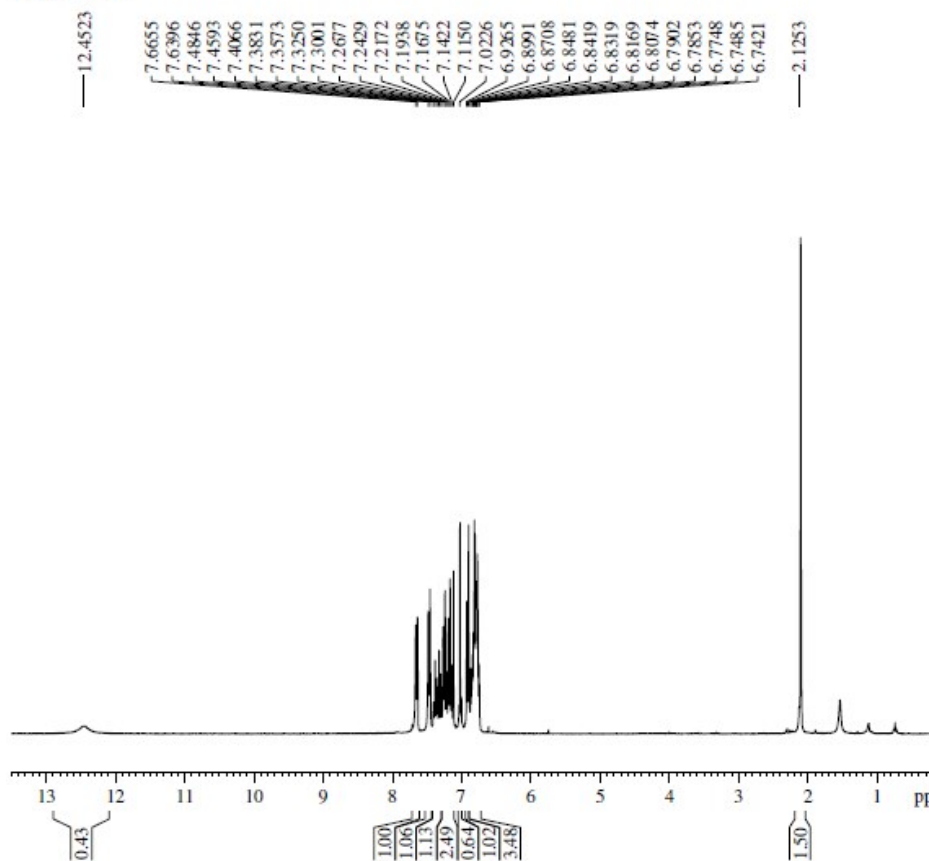
==== CHANNEL f1 ====
 SFO1 100.6304993 MHz
 NUC1 13C
 P1 9.90 usec
 PLW1 53.0000000 W

==== CHANNEL f2 ====
 SFO2 400.1621006 MHz
 NUC2 1H
 CPDPRG2 waltz16
 PCPD2 90.00 usec
 PLW2 13.0000000 W
 PLW12 0.27963999 W
 PLW13 0.22651000 W

F2 - Processing parameters
 SI 32768
 SF 100.6204380 MHz
 WDW EM
 SSB 0
 LB 3.00 Hz
 GB 0
 PC 1.40

S44: ¹³C NMR spectrum of 3l

NRLD-413



Current Data Parameters
 NAME 06-Feb-AN-2020
 EXPNO 330
 PROCNO 1

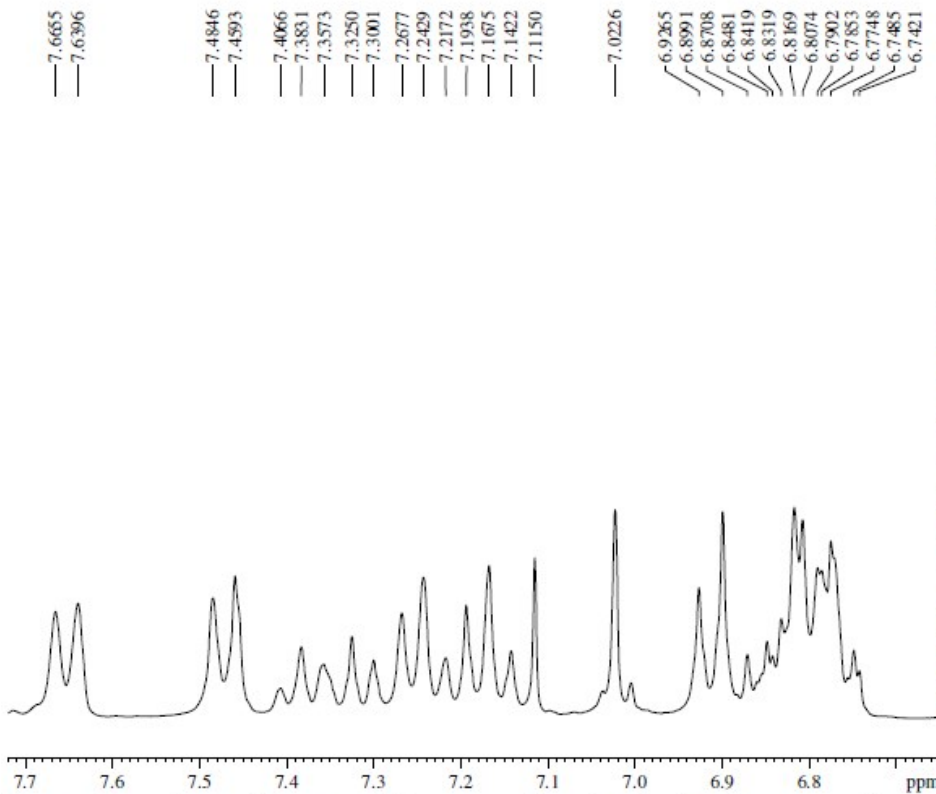
F2 - Acquisition Parameters
 Date_ 20200206
 Time 16.03
 INSTRUM spect
 PROBHD 5 mm QNP 1H/13
 PULPROG zg30
 TD 65536
 SOLVENT CDC13
 NS 16
 DS 2
 SWH 6188.119 Hz
 FIDRES 0.094423 Hz
 AQ 5.2953086 sec
 RG 203
 DW 80.800 usec
 DE 6.50 usec
 TE 300.0 K
 D1 1.0000000 sec
 TDO 1

==== CHANNEL f1 ====
 NUC1 1H
 P1 13.95 usec
 PL1 -1.00 dB
 PL1W 15.02081871 W
 SFO1 300.2598542 MHz

F2 - Processing parameters
 SI 32768
 SF 300.2580509 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

S45: ¹H NMR spectrum of 3m

NRLD-413



Current Data Parameters
 NAME 06-Feb-AN-2020
 EXPNO 330
 PROCNO 1

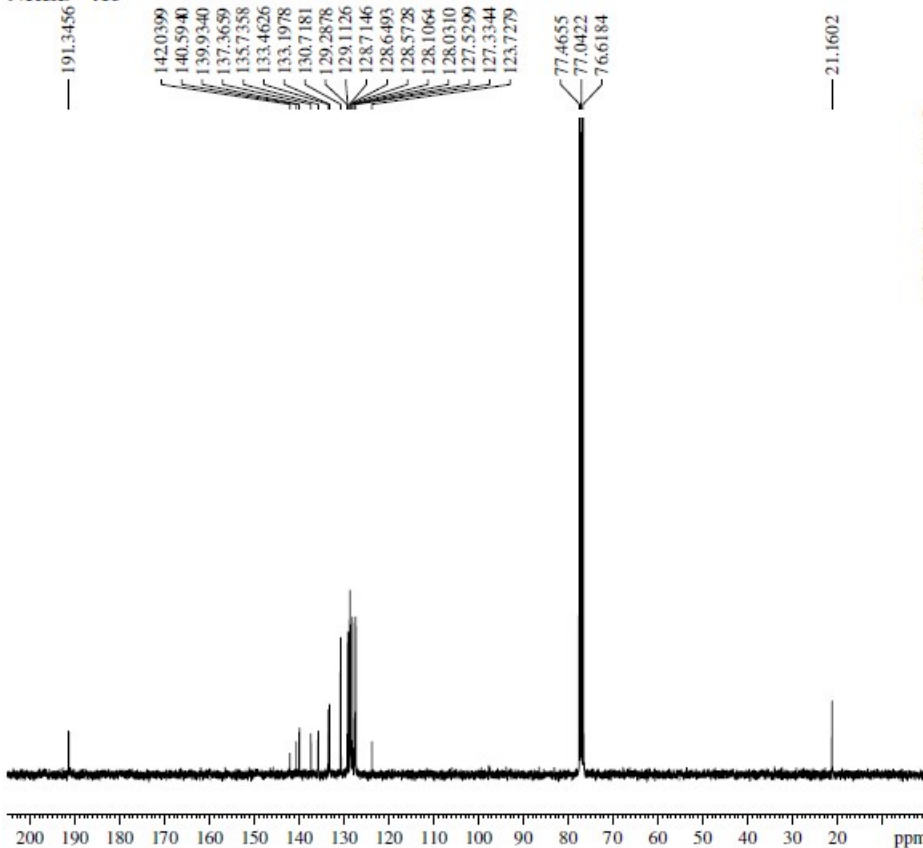
F2 - Acquisition Parameters
 Date_ 20200206
 Time 16.03
 INSTRUM spect
 PROBHD 5 mm QNP 1H/13
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 16
 DS 2
 SWH 6188.119 Hz
 FIDRES 0.094423 Hz
 AQ 5.2953086 sec
 RG 203
 DW 80.800 usec
 DE 6.50 usec
 TE 300.0 K
 D1 1.00000000 sec
 TD0 1

==== CHANNEL f1 ====
 NUC1 1H
 P1 13.95 usec
 PL1 -1.00 dB
 PL1W 15.02081871 W
 SFO1 300.2598542 MHz

F2 - Processing parameters
 SI 32768
 SF 300.2580509 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

S46: ¹H NMR spectrum of 3m (expansion)

NRLD-413

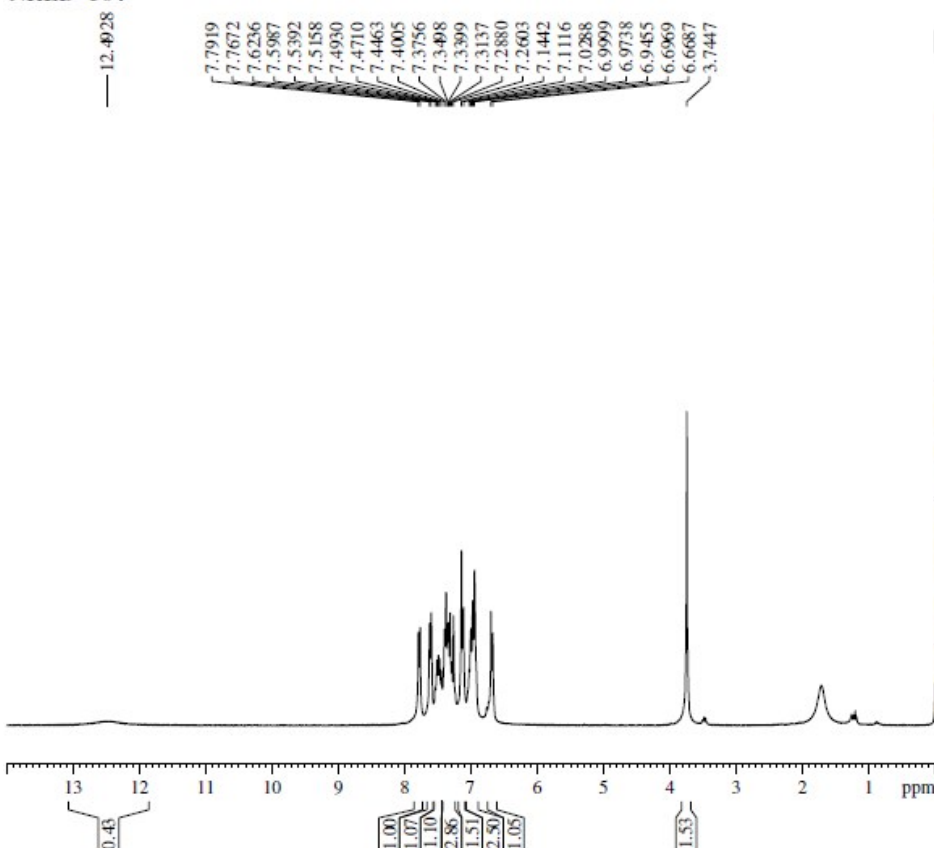


Current Data Parameters
 NAME 06-Feb-AN-2020
 EXPNO 340
 PROCNO 1

F2 - Processing parameters
 SI 32768
 SF 75.4999337 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

S47: ¹³C NMR spectrum of 3m

NRLD-364



S48: ¹H NMR spectrum of 3n



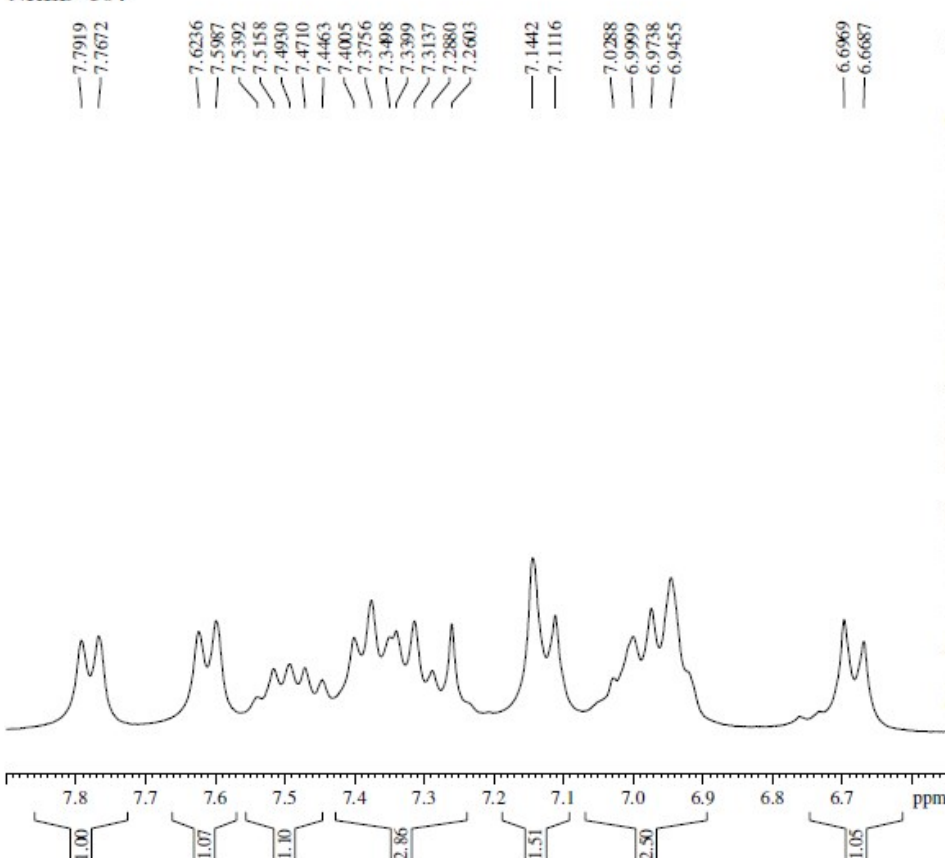
Current Data Parameters
NAME 25-June-AN-2020
EXPNO 510
PROCNO 1

F2 - Acquisition Parameters
Date_ 20200625
Time 15.49
INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 6188.119 Hz
FIDRES 0.094423 Hz
AQ 5.2953086 sec
RG 228
DW 80.800 usec
DE 6.50 usec
TE 300.0 K
D1 1.00000000 sec
TD0 1

==== CHANNEL f1 ====
NUC1 1H
P1 13.95 usec
PL1 -1.00 dB
PL1W 15.02081871 W
SFO1 300.2598542 MHz

F2 - Processing parameters
SI 32768
SF 300.2580074 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

NRLD-364



S49: ¹H NMR spectrum of 3n (expansion)



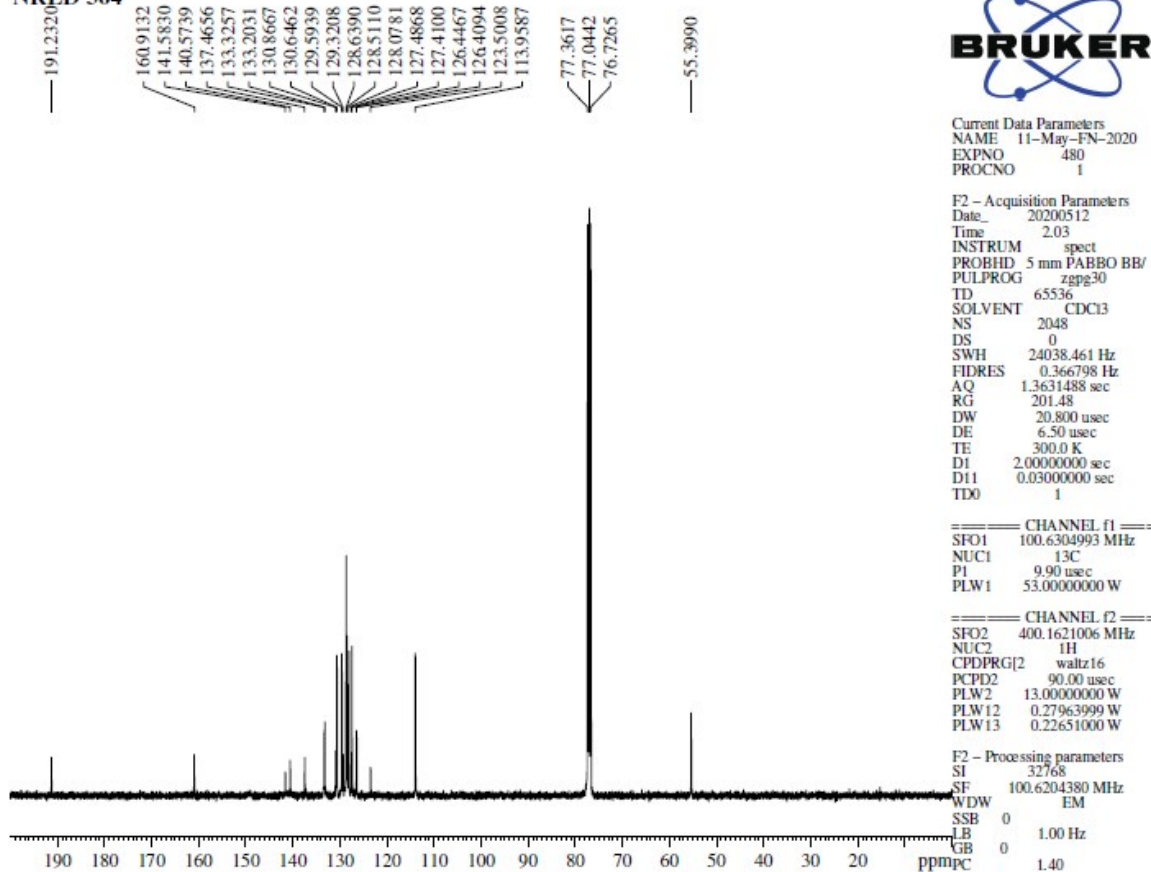
Current Data Parameters
NAME 25-June-AN-2020
EXPNO 510
PROCNO 1

F2 - Acquisition Parameters
Date_ 20200625
Time 15.49
INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 6188.119 Hz
FIDRES 0.094423 Hz
AQ 5.2953086 sec
RG 228
DW 80.800 usec
DE 6.50 usec
TE 300.0 K
D1 1.00000000 sec
TD0 1

==== CHANNEL f1 ====
NUC1 1H
P1 13.95 usec
PL1 -1.00 dB
PL1W 15.02081871 W
SFO1 300.2598542 MHz

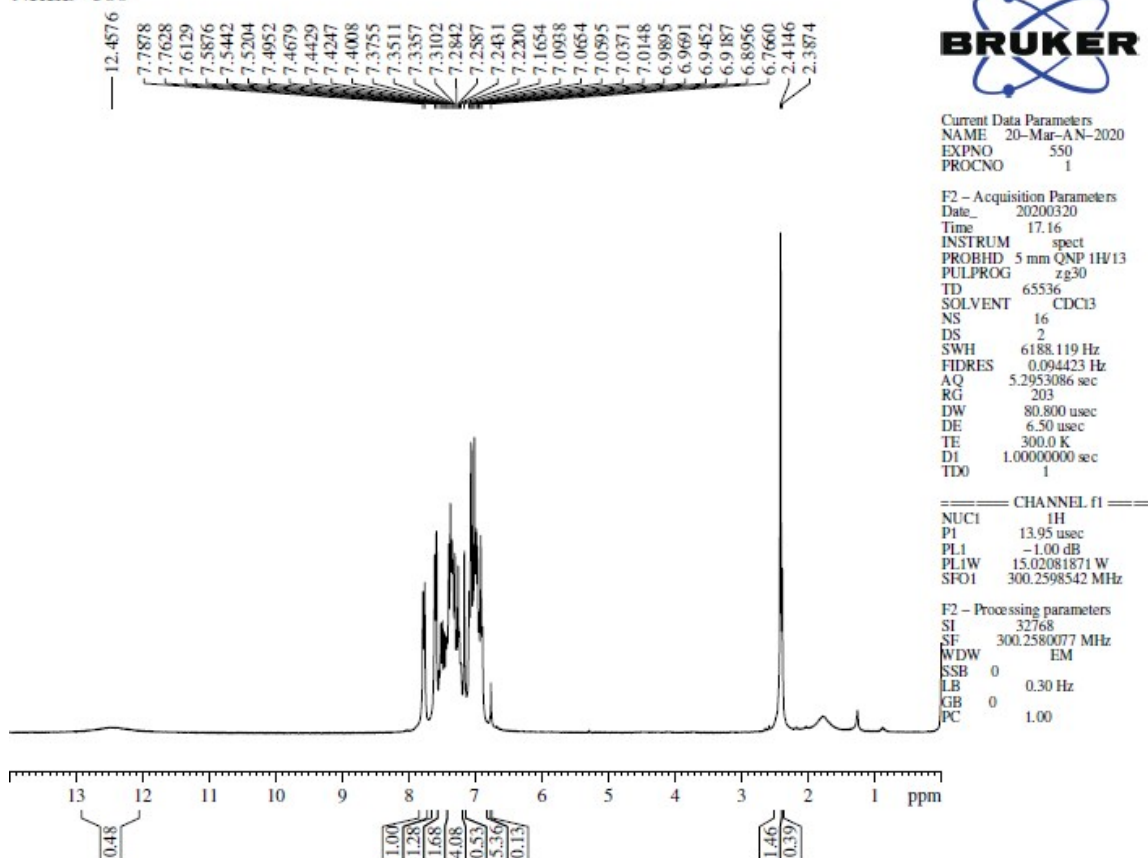
F2 - Processing parameters
SI 32768
SF 300.2580074 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

NRLD 364



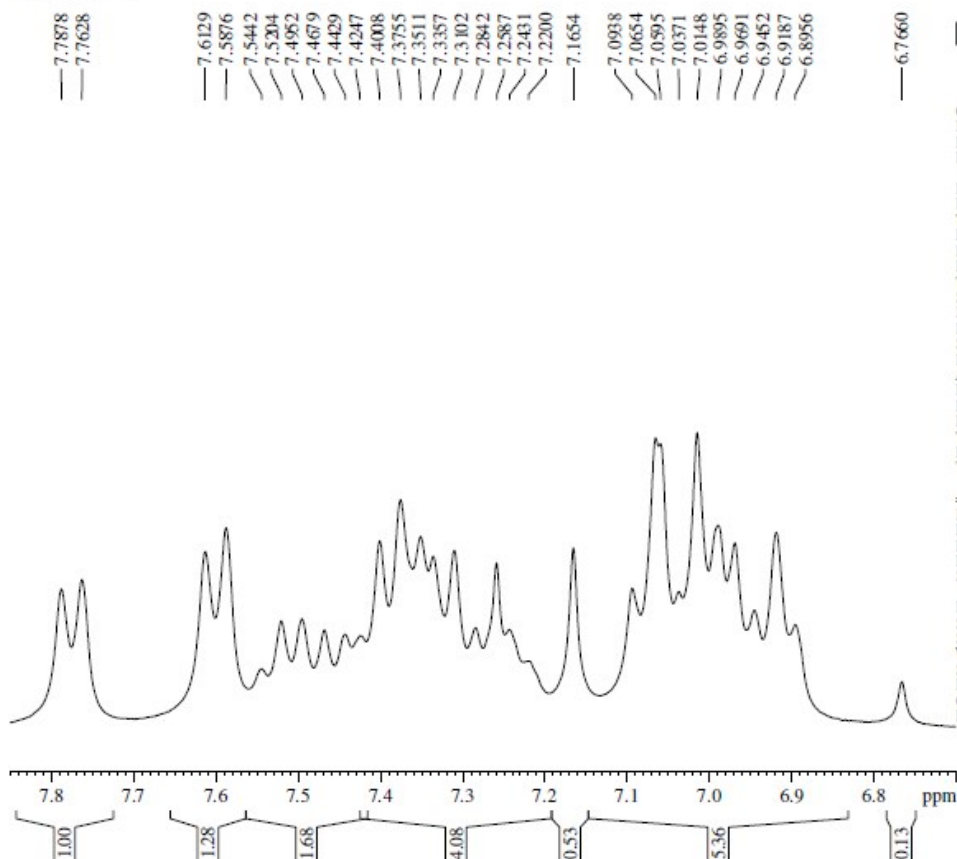
S50: ¹³C NMR spectrum of 3n

NRLD-386



S51: ¹H NMR spectrum of 3o

NRLD-386



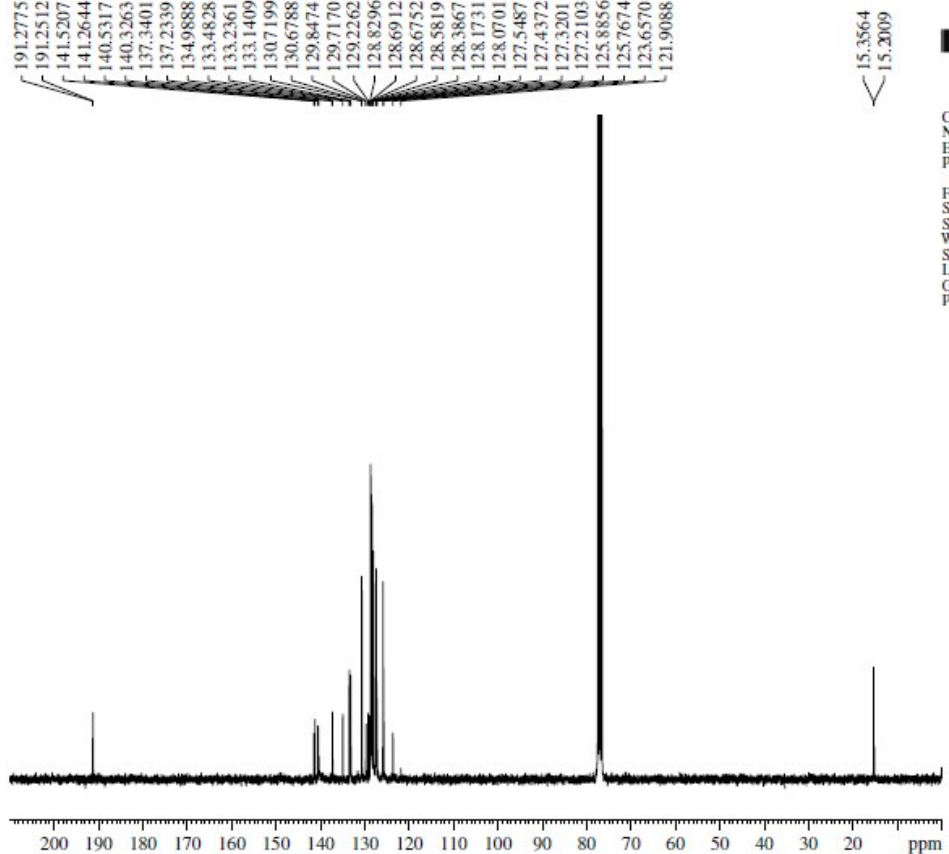
Current Data Parameters
NAME 20-Mar-AN-2020
EXPNO 550
PROCNO 1

F2 - Acquisition Parameters
Date_ 20200320
Time 17.16
INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 6188.119 Hz
FIDRES 0.094423 Hz
AQ 5.2953086 sec
RG 203
DW 80.800 usec
DE 6.50 usec
TE 300.0 K
D1 1.0000000 sec
TD0 1

==== CHANNEL f1 ====
NUC1 1H
P1 13.95 usec
PL1 -1.00 dB
PL1W 15.02081871 W
SFO1 300.2598542 MHz

F2 - Processing parameters
SI 32768
SF 300.2580077 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

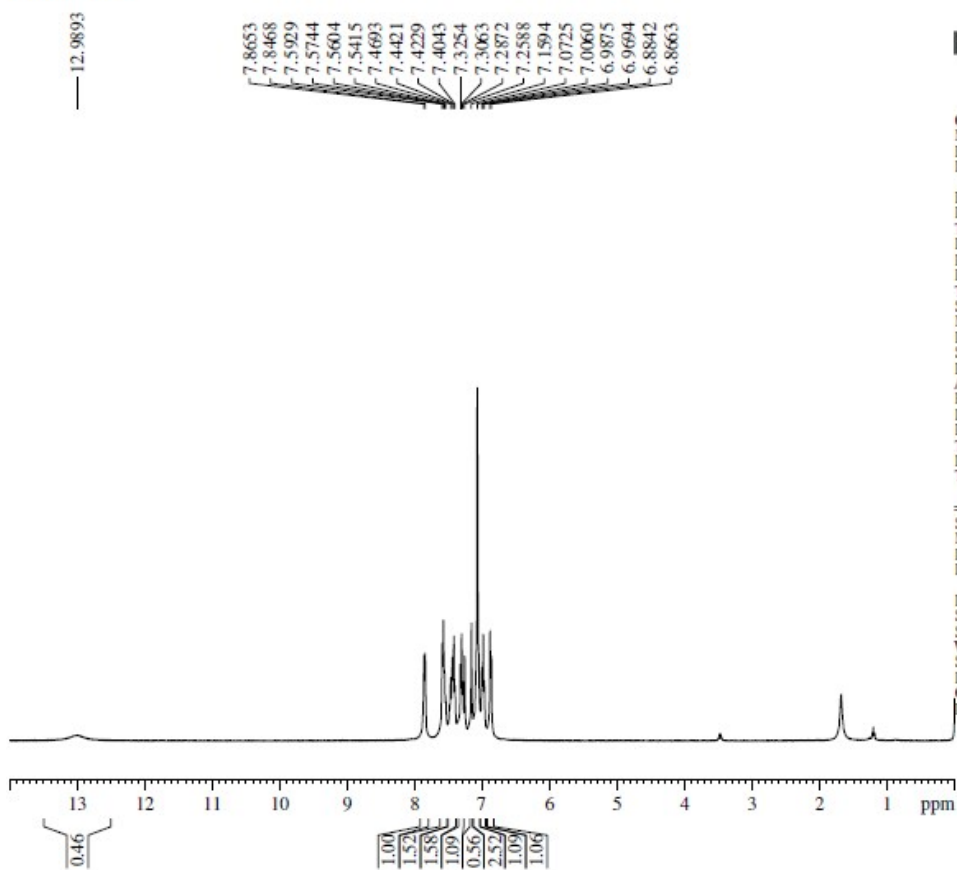
NRLD-386



Current Data Parameters
NAME 20-Mar-AN-2020
EXPNO 560
PROCNO 1

F2 - Processing parameters
SI 32768
SF 75.4999340 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

NRLD-376



S54: ¹H NMR spectrum of 3p



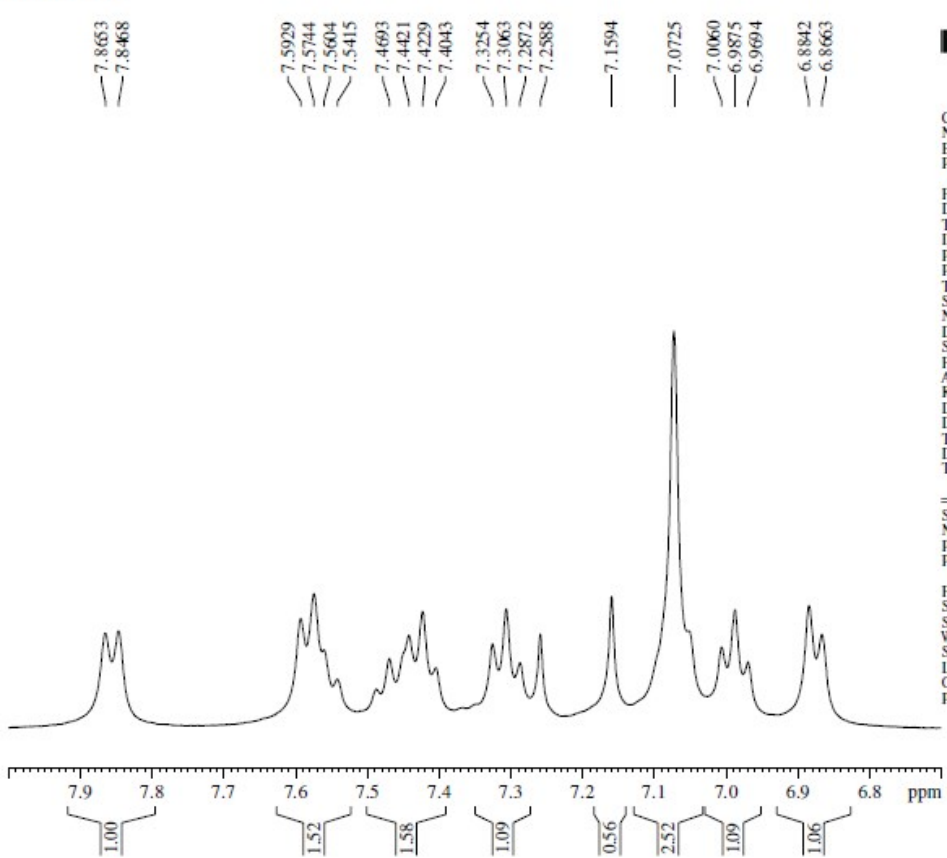
Current Data Parameters
 NAME 11-May-FN-2020
 EXPNO 460
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20200511
 Time 17.09
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zg30
 TD 65536
 SOLVENT CDC13
 NS 8
 DS 0
 SWH 9615.385 Hz
 FIDRES 0.146719 Hz
 AQ 3.4078720 sec
 RG 129.57
 DW 52.000 usec
 DE 6.50 usec
 TE 300.0 K
 D1 1.00000000 sec
 TD0 1

==== CHANNEL f1 ====
 SFO1 400.1629712 MHz
 NUC1 1H
 P1 13.20 usec
 PLW1 13.00000000 W

F2 - Processing parameters
 SI 65536
 SF 400.1605104 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

NRLD-376



S55: ¹H NMR spectrum of 3p (expansion)



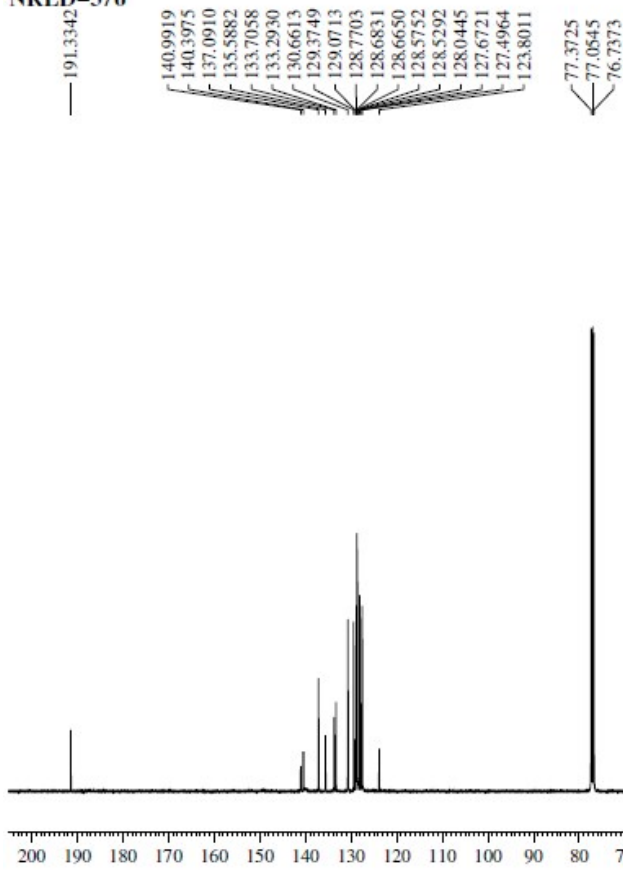
Current Data Parameters
 NAME 11-May-FN-2020
 EXPNO 460
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20200511
 Time 17.09
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zg30
 TD 65536
 SOLVENT CDC13
 NS 8
 DS 0
 SWH 9615.385 Hz
 FIDRES 0.146719 Hz
 AQ 3.4078720 sec
 RG 129.57
 DW 52.000 usec
 DE 6.50 usec
 TE 300.0 K
 D1 1.00000000 sec
 TD0 1

==== CHANNEL f1 ====
 SFO1 400.1629712 MHz
 NUC1 1H
 P1 13.20 usec
 PLW1 13.00000000 W

F2 - Processing parameters
 SI 65536
 SF 400.1605104 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

NRLD-376



Current Data Parameters
 NAME 31-OCT-AN-2019
 EXPNO 370
 PROCNO 1

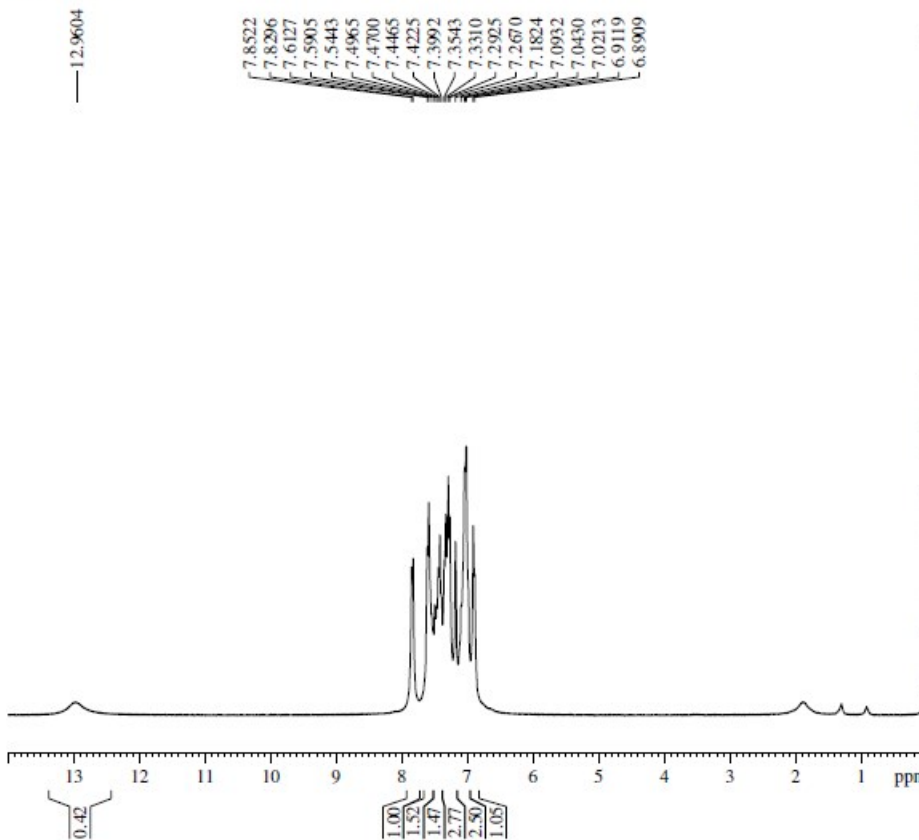
F2 - Acquisition Parameters
 Date_ 20191101
 Time 11.07
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 2048
 DS 4
 SWH 24038.461 Hz
 FIDRES 0.366798 Hz
 AQ 1.3631488 sec
 RG 201.48
 DW 20.800 usec
 DE 6.50 usec
 TE 300.0 K
 D1 2.0000000 sec
 D11 0.0300000 sec
 TD0 1

==== CHANNEL f1 ====
 SFO1 100.6304993 MHz
 NUC1 13C
 P1 9.90 usec
 PLW1 53.0000000 W
 ==== CHANNEL f2 ====
 SFO2 400.1621006 MHz
 NUC2 1H
 CPDPRG2 waltz16
 PCPD2 90.00 usec
 PLW2 13.0000000 W
 PLW12 0.27963999 W
 PLW13 0.22651000 W

F2 - Processing parameters
 SI 32768
 SF 100.6204380 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

S56: ¹³C NMR spectrum of 3p

NRLD-400



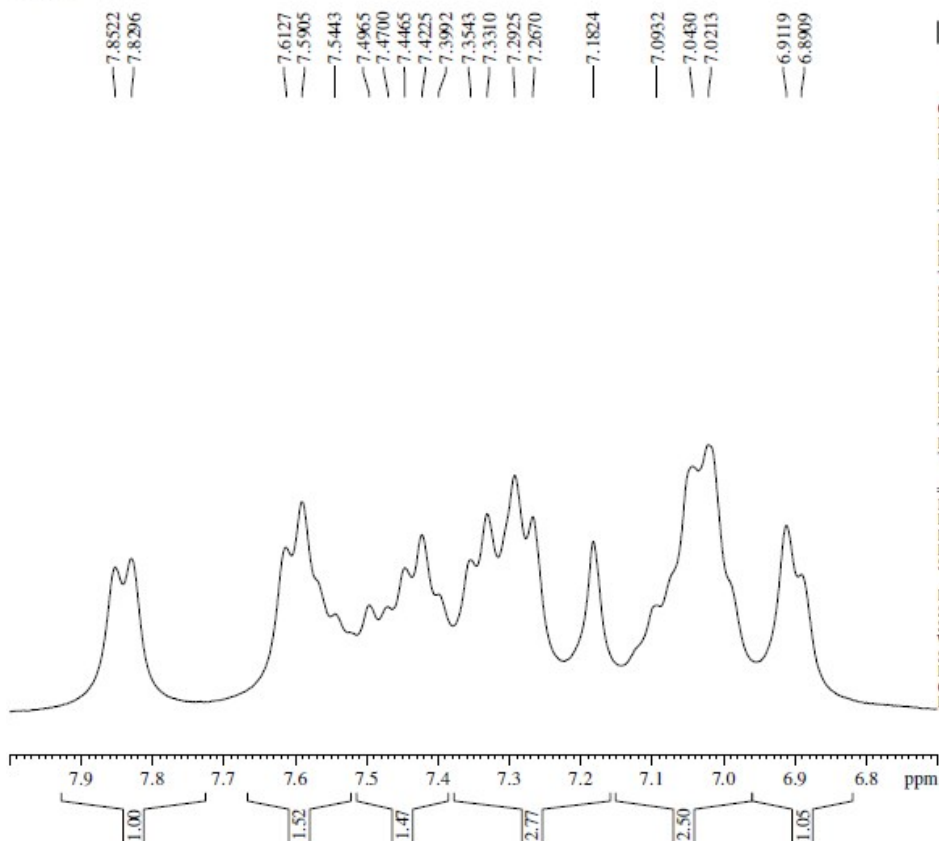
Current Data Parameters
 NAME 23-Jan-FN-2020
 EXPNO 600
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20200123
 Time 12.29
 INSTRUM spect
 PROBHD 5 mm QNP 1H/13
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 16
 DS 2
 SWH 6188.119 Hz
 FIDRES 0.094423 Hz
 AQ 5.2953086 sec
 RG 181
 DW 80.800 usec
 DE 6.50 usec
 TE 300.0 K
 D1 1.0000000 sec
 TD0 1

==== CHANNEL f1 ====
 NUC1 1H
 P1 13.95 usec
 PL1 -1.00 dB
 PL1W 15.02081871 W
 SFO1 300.2598542 MHz
 F2 - Processing parameters
 SI 32768
 SF 300.2579983 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

S57: ¹H NMR spectrum of 3q

NRLD-400



S58: ¹H NMR spectrum of 3q (expansion)



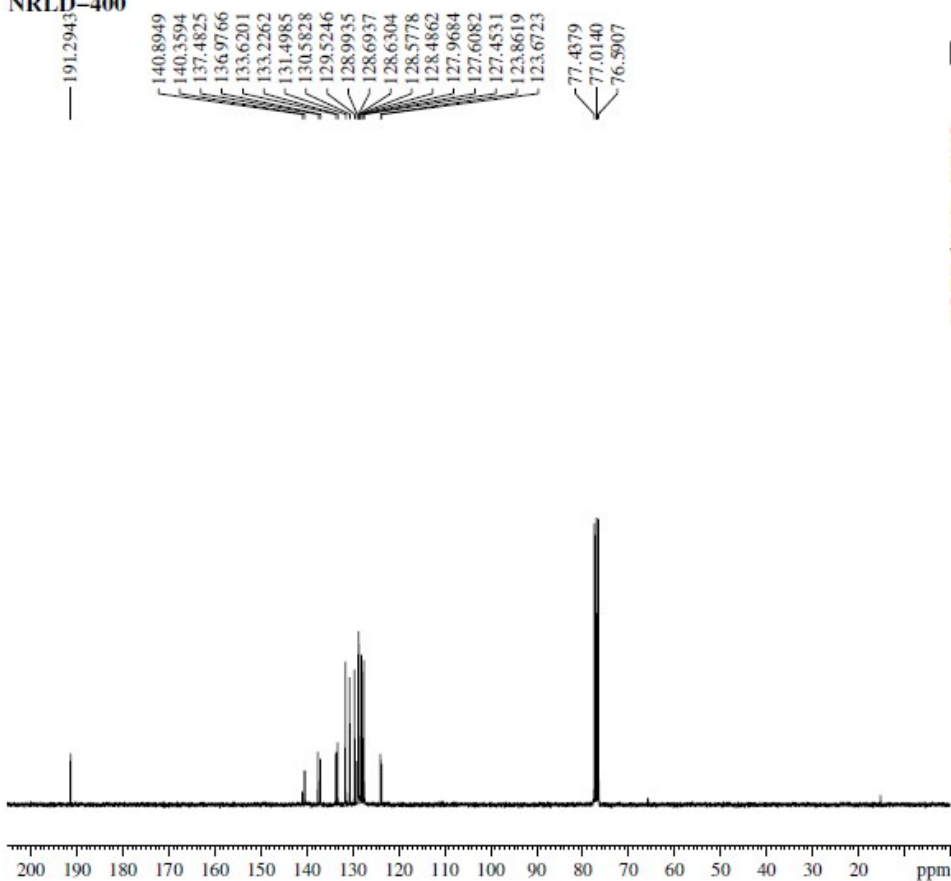
Current Data Parameters
NAME 23-Jan-FN-2020
EXPNO 600
PROCNO 1

F2 - Acquisition Parameters
Date_ 20200123
Time 12.29
INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 6188.119 Hz
FIDRES 0.094423 Hz
AQ 5.2953086 sec
RG 181
DW 80.800 usec
DE 6.50 usec
TE 300.0 K
D1 1.0000000 sec
TD0 1

==== CHANNEL f1 ====
NUC1 1H
P1 13.95 usec
PL1 -1.00 dB
PL1W 15.02081871 W
SFO1 300.2598542 MHz

F2 - Processing parameters
SI 32768
SF 300.2579983 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

NRLD-400



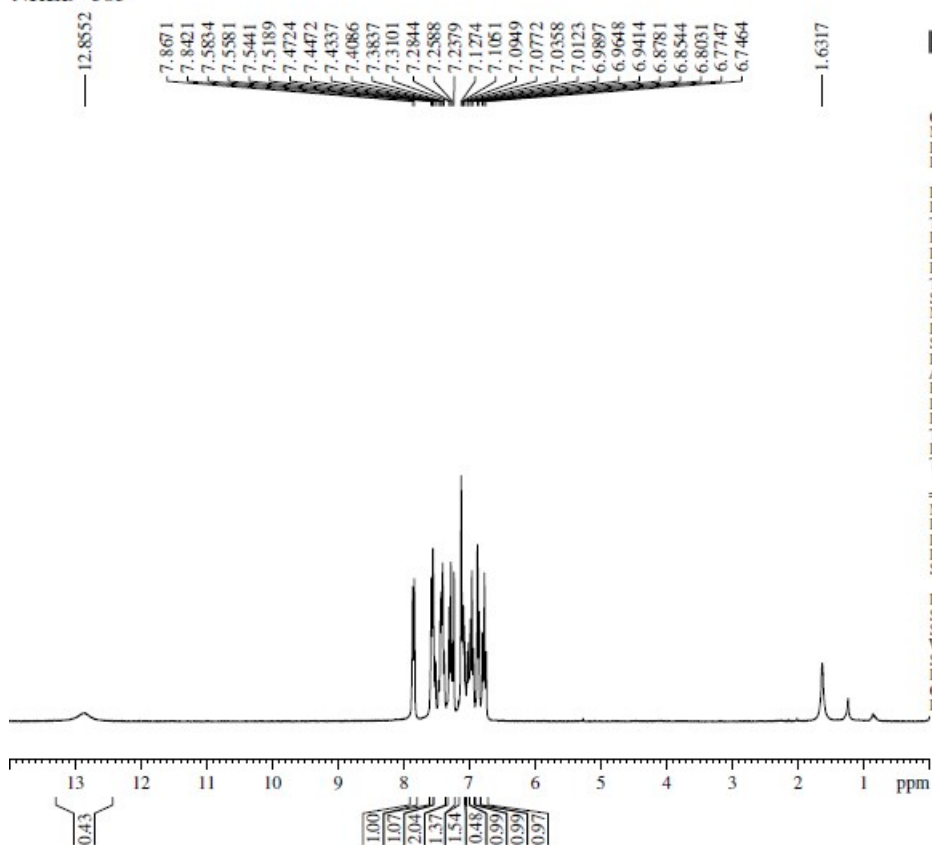
S59: ¹³C NMR spectrum of 3q



Current Data Parameters
NAME 17-Jan-AN-2020
EXPNO 330
PROCNO 1

F2 - Processing parameters
SI 32768
SF 75.4999390 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

NRLD-383



Current Data Parameters
NAME 29-Jan-FN-2020
EXPNO 440
PROCNO 1

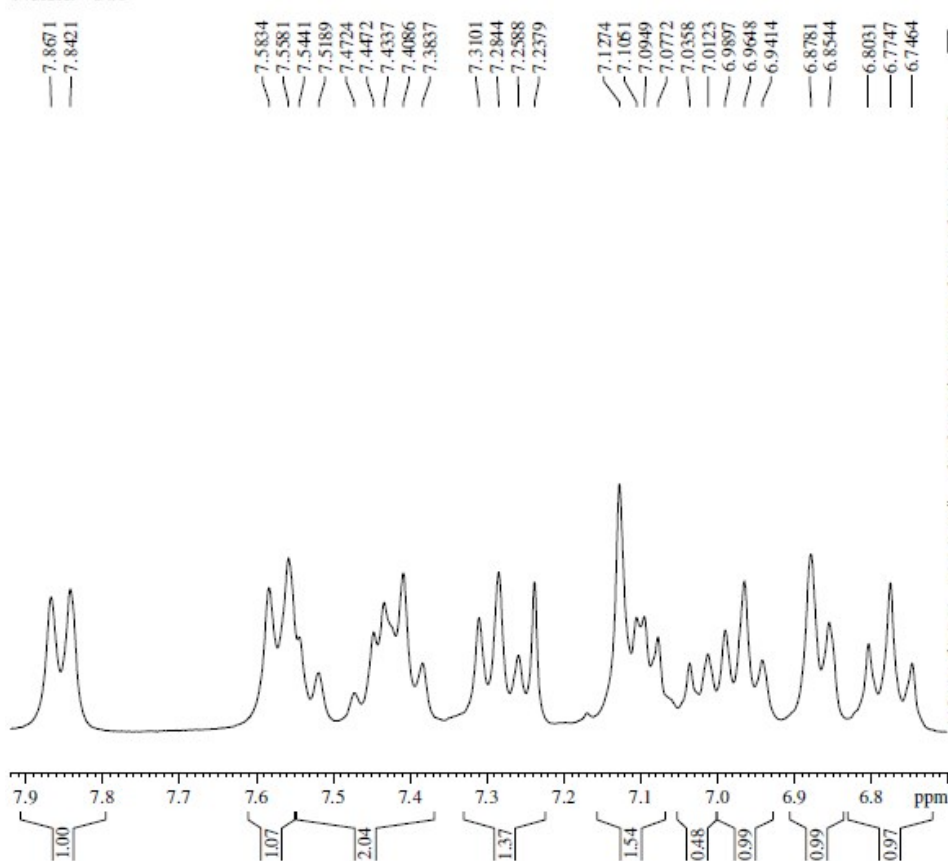
F2 - Acquisition Parameters
Date_ 20200129
Time 10.53
INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 6188.119 Hz
FIDRES 0.094423 Hz
AQ 5.2953086 sec
RG 256
DW 80.800 usec
DE 6.50 usec
TE 300.0 K
D1 1.00000000 sec
TD0 1

==== CHANNEL f1 ====
NUC1 1H
P1 13.95 usec
PL1 -1.00 dB
PL1W 15.02081871 W
SFO1 300.2598542 MHz

F2 - Processing parameters
SI 32768
SF 300.2580139 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

S60: ¹H NMR spectrum of 3r

NRLD-383



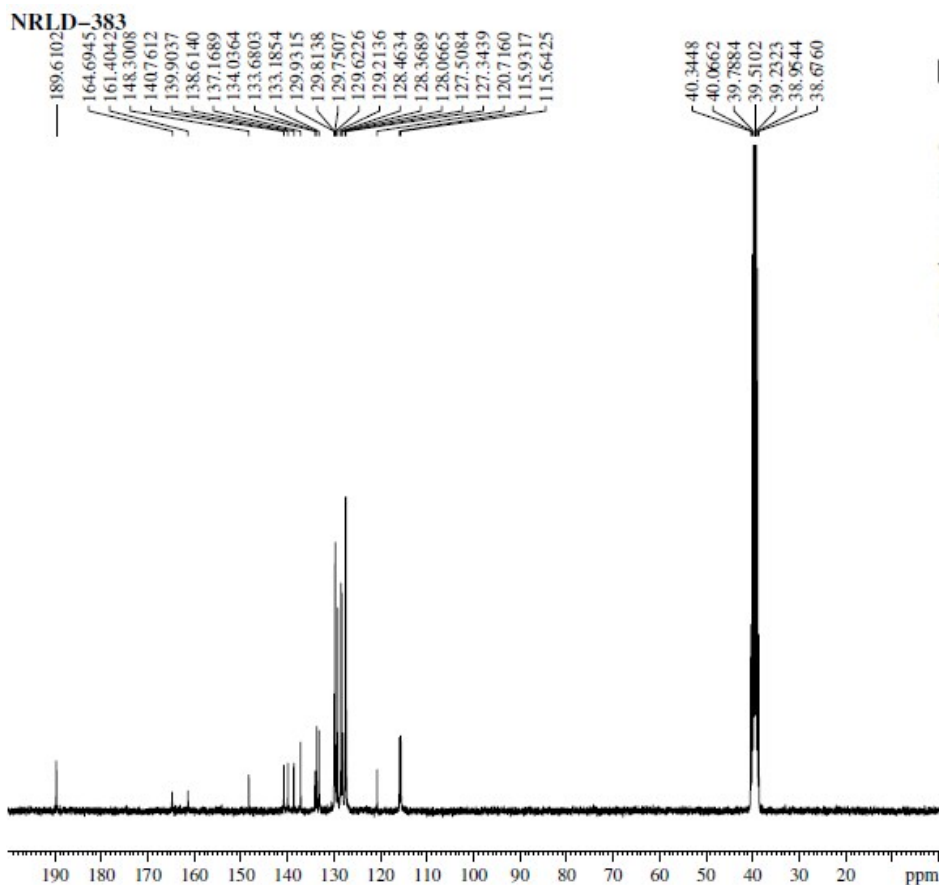
Current Data Parameters
NAME 29-Jan-FN-2020
EXPNO 440
PROCNO 1

F2 - Acquisition Parameters
Date_ 20200129
Time 10.53
INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 6188.119 Hz
FIDRES 0.094423 Hz
AQ 5.2953086 sec
RG 256
DW 80.800 usec
DE 6.50 usec
TE 300.0 K
D1 1.00000000 sec
TD0 1

==== CHANNEL f1 ====
NUC1 1H
P1 13.95 usec
PL1 -1.00 dB
PL1W 15.02081871 W
SFO1 300.2598542 MHz

F2 - Processing parameters
SI 32768
SF 300.2580139 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

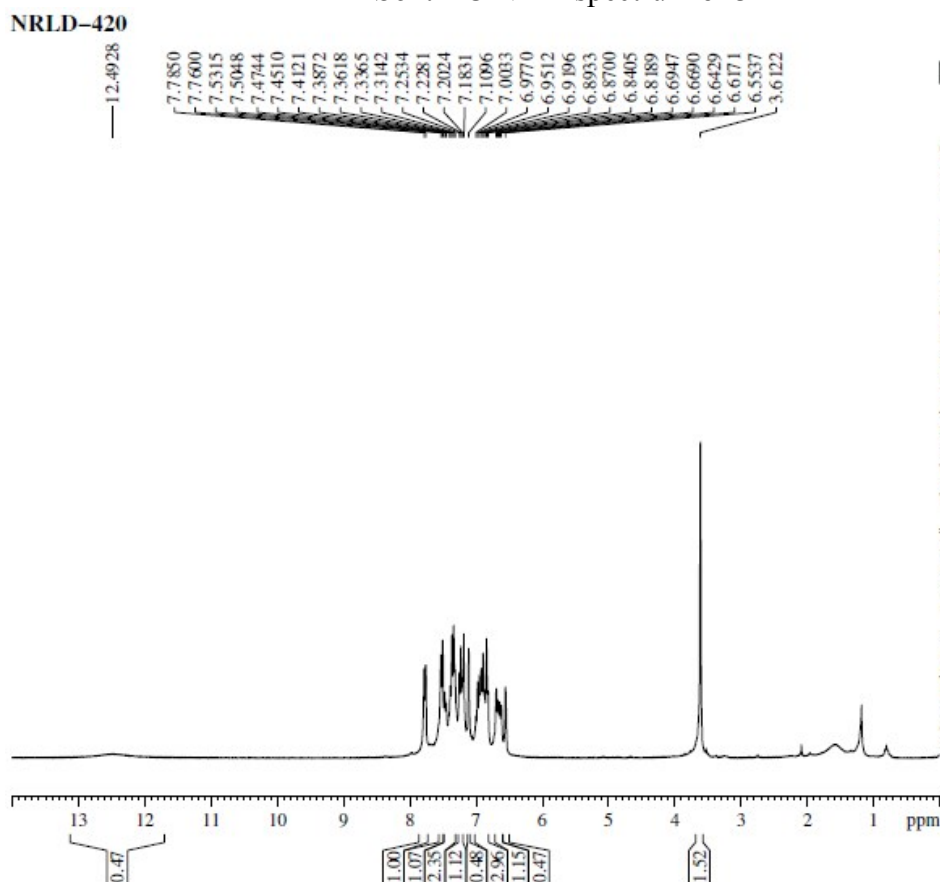
S61: ¹H NMR spectrum of 3r (expansion)



Current Data Parameters
NAME 31-Jan-AN-2020
EXPNO 570
PROCNO 1

F2 - Processing parameters
SI 32768
SF 75.4999686 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

S62: ¹³C NMR spectrum of 3r



Current Data Parameters
NAME 17-FEB-FN-2020
EXPNO 420
PROCNO 1

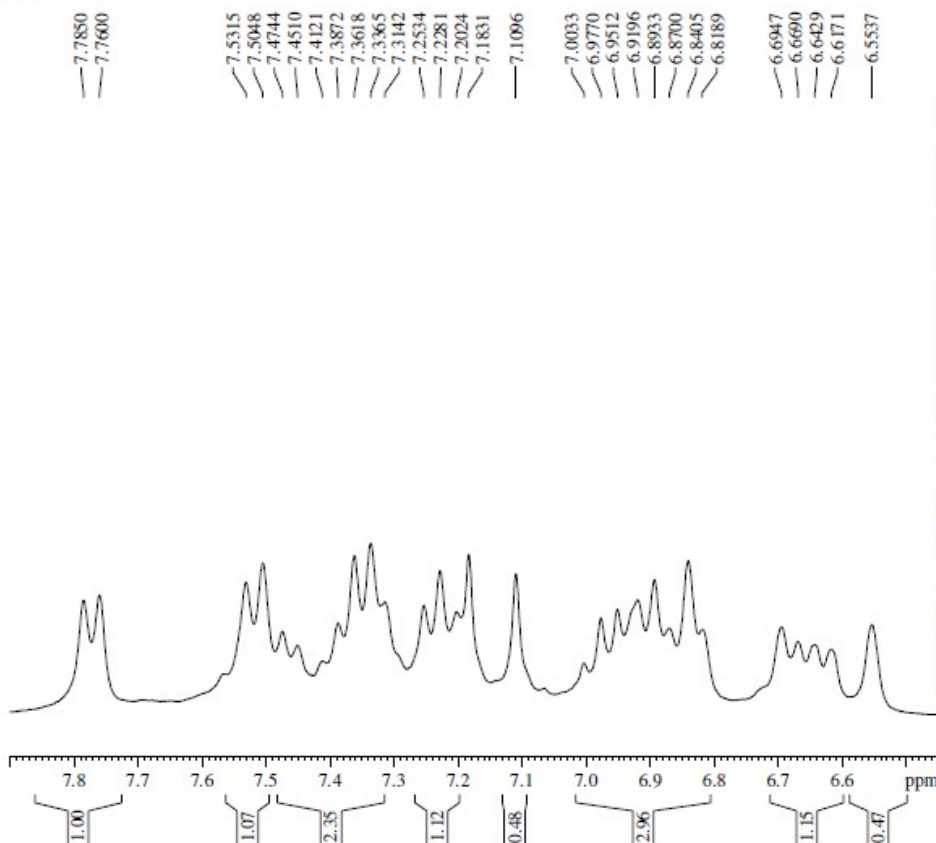
F2 - Acquisition Parameters
Date_ 20200217
Time 22.48
INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 64
DS 2
SWH 6188.119 Hz
FIDRES 0.094423 Hz
AQ 5.2953086 sec
RG 228
DW 80.800 usec
DE 6.50 usec
TE 300.0 K
D1 1.00000000 sec
TD0 1

==== CHANNEL f1 ====
NUC1 1H
P1 13.95 usec
PL1 -1.00 dB
PL1W 15.02081871 W
SFO1 300.2598542 MHz

F2 - Processing parameters
SI 32768
SF 300.2580304 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

S63: ¹H NMR spectrum of 3s

NRLD-420



Current Data Parameters
NAME 17-FEB-FN-2020
EXPNO 420
PROCNO 1

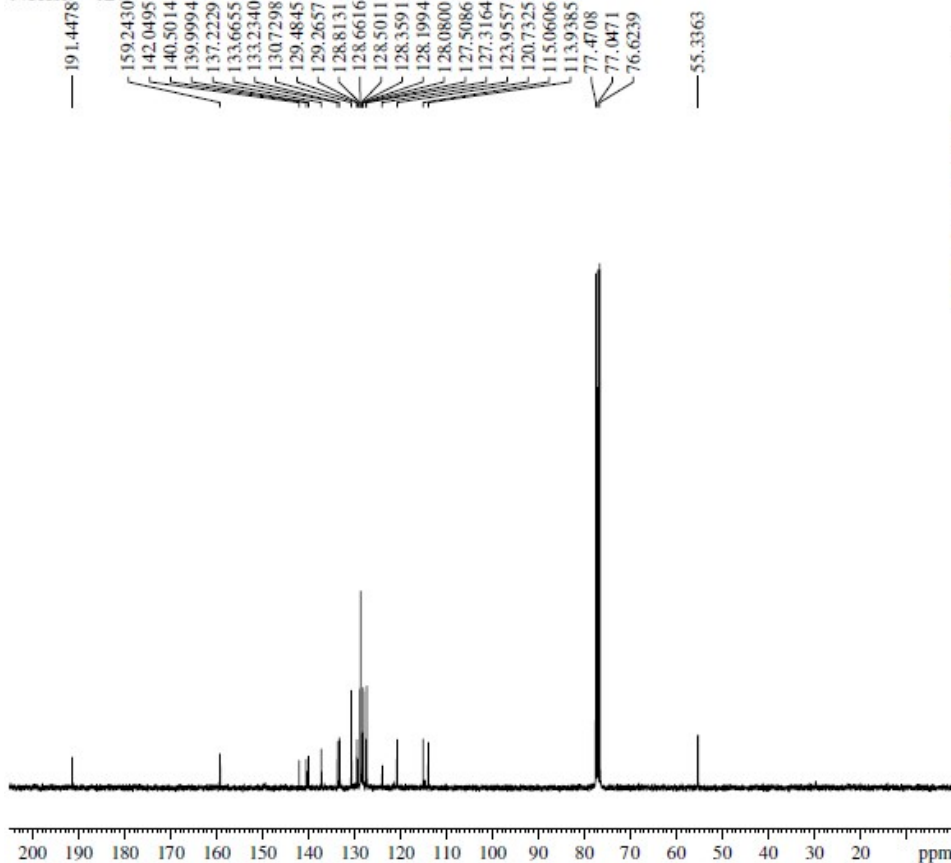
F2 - Acquisition Parameters
Date_ 20200217
Time 22.48
INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 64
DS 2
SWH 6188.119 Hz
FIDRES 0.094423 Hz
AQ 5.2953086 sec
RG 228
DW 80.800 usec
DE 6.50 usec
TE 300.0 K
D1 1.0000000 sec
TD0 1

==== CHANNEL f1 ====
NUC1 1H
P1 13.95 usec
PL1 -1.00 dB
PL1W 15.02081871 W
SFO1 300.2598542 MHz

F2 - Processing parameters
SI 32768
SF 300.2580304 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

S64: ¹H NMR spectrum of 3s (expansion)

NRLD-420

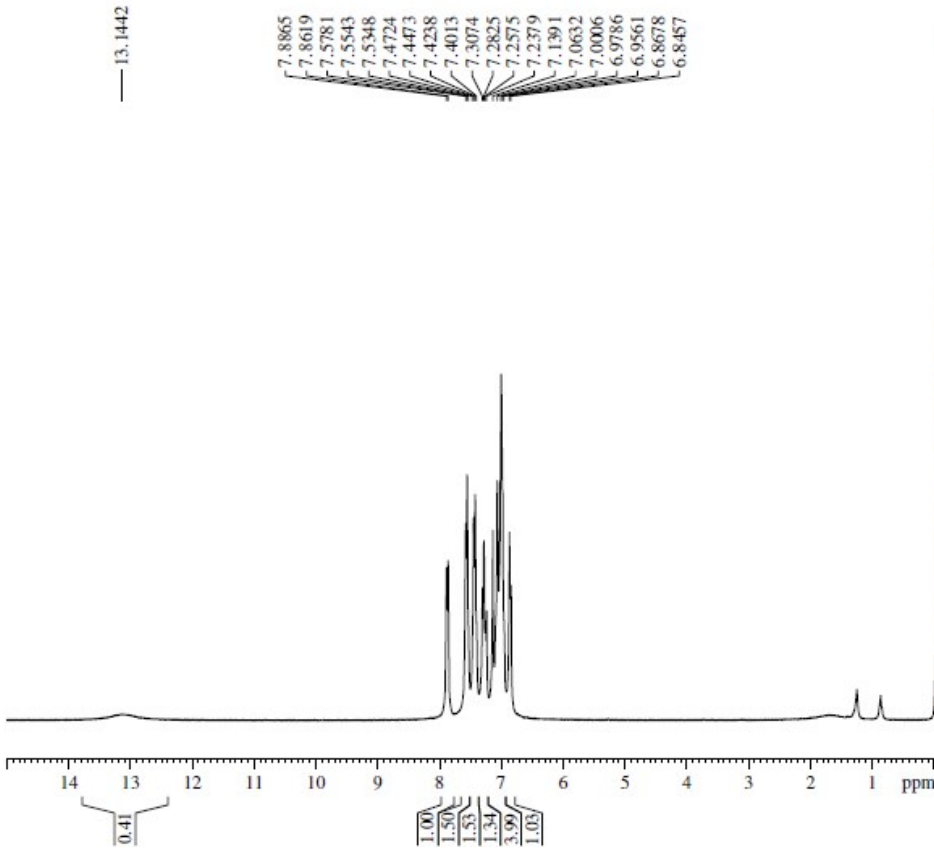


Current Data Parameters
NAME 20-Feb-FN-2020
EXPNO 460
PROCNO 1

F2 - Processing parameters
SI 32768
SF 75.4999337 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

S65: ¹³C NMR spectrum of 3s

NRLD-371



S66: ¹H NMR spectrum of 3t



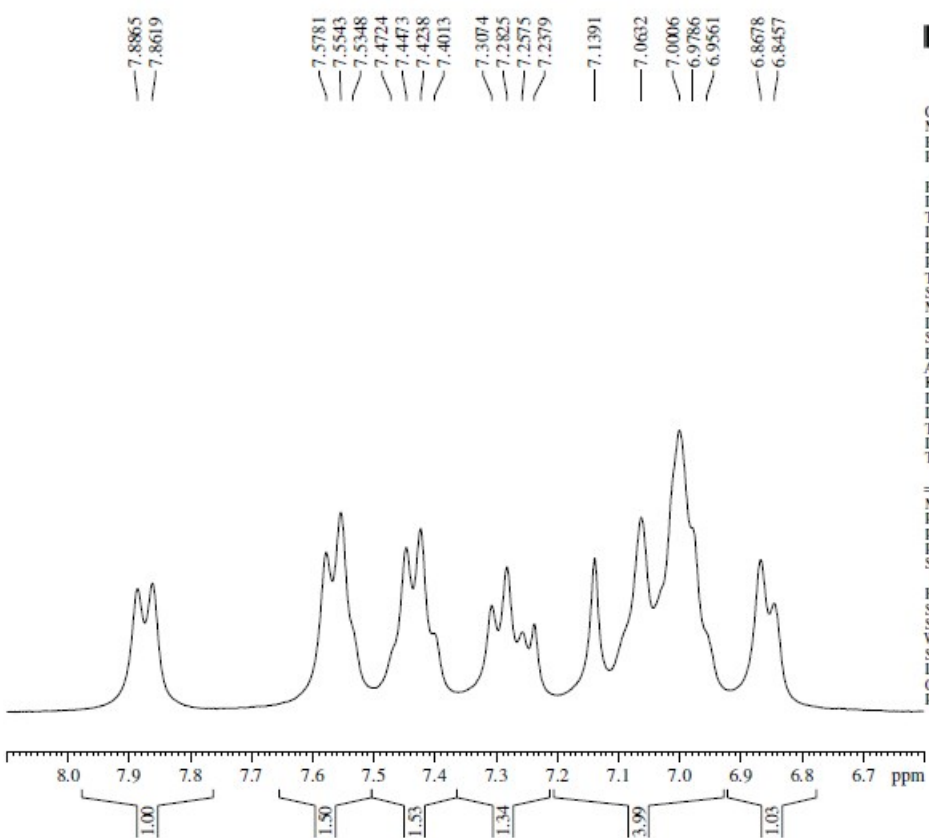
Current Data Parameters
 NAME 11-FEB-AN-2020
 EXPNO 530
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20200211
 Time 11.53
 INSTRUM spect
 PROBHD 5 mm QNP 1H/13
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 16
 DS 2
 SWH 6188.119 Hz
 FIDRES 0.094423 Hz
 AQ 5.2953086 sec
 RG 228
 DW 80.800 usec
 DE 6.50 usec
 TE 300.0 K
 D1 1.00000000 sec
 TDO 1

==== CHANNEL f1 ====
 NUC1 1H
 P1 13.95 usec
 PL1 -1.00 dB
 PL1W 15.02081871 W
 SFO1 300.2598542 MHz

F2 - Processing parameters
 SI 32768
 SF 300.2580139 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

NRLD-371



S67: ¹H NMR spectrum of 3t (expansion)



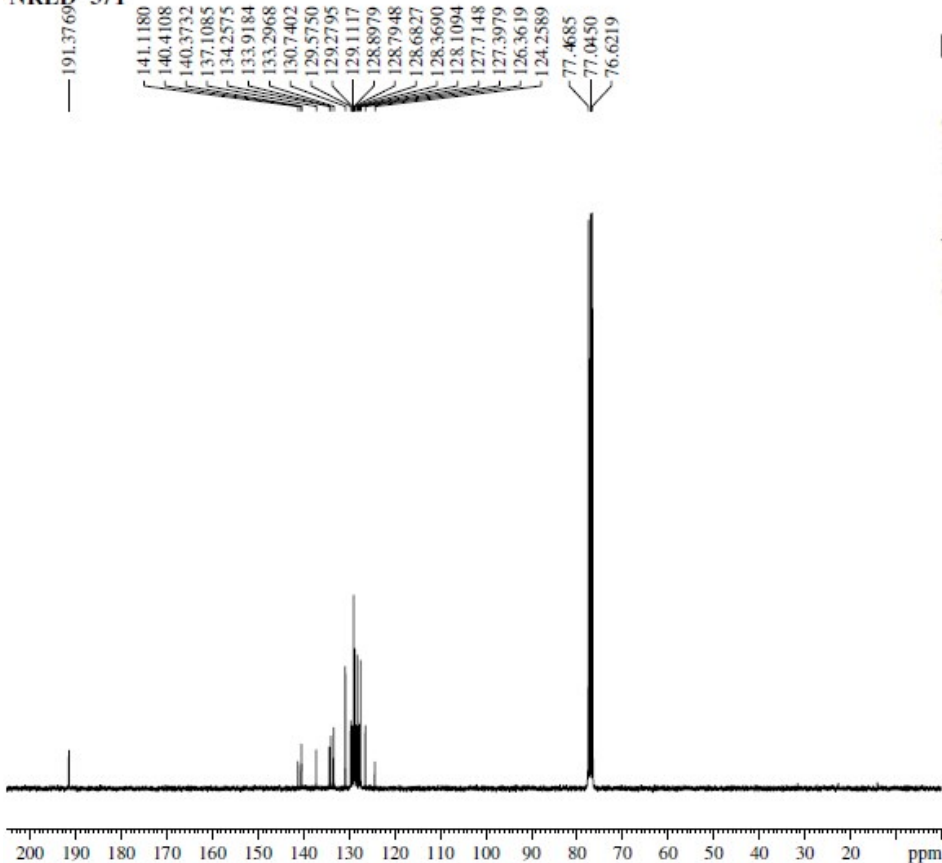
Current Data Parameters
 NAME 11-FEB-AN-2020
 EXPNO 530
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20200211
 Time 11.53
 INSTRUM spect
 PROBHD 5 mm QNP 1H/13
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 16
 DS 2
 SWH 6188.119 Hz
 FIDRES 0.094423 Hz
 AQ 5.2953086 sec
 RG 228
 DW 80.800 usec
 DE 6.50 usec
 TE 300.0 K
 D1 1.00000000 sec
 TDO 1

==== CHANNEL f1 ====
 NUC1 1H
 P1 13.95 usec
 PL1 -1.00 dB
 PL1W 15.02081871 W
 SFO1 300.2598542 MHz

F2 - Processing parameters
 SI 32768
 SF 300.2580139 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

NRLD-371

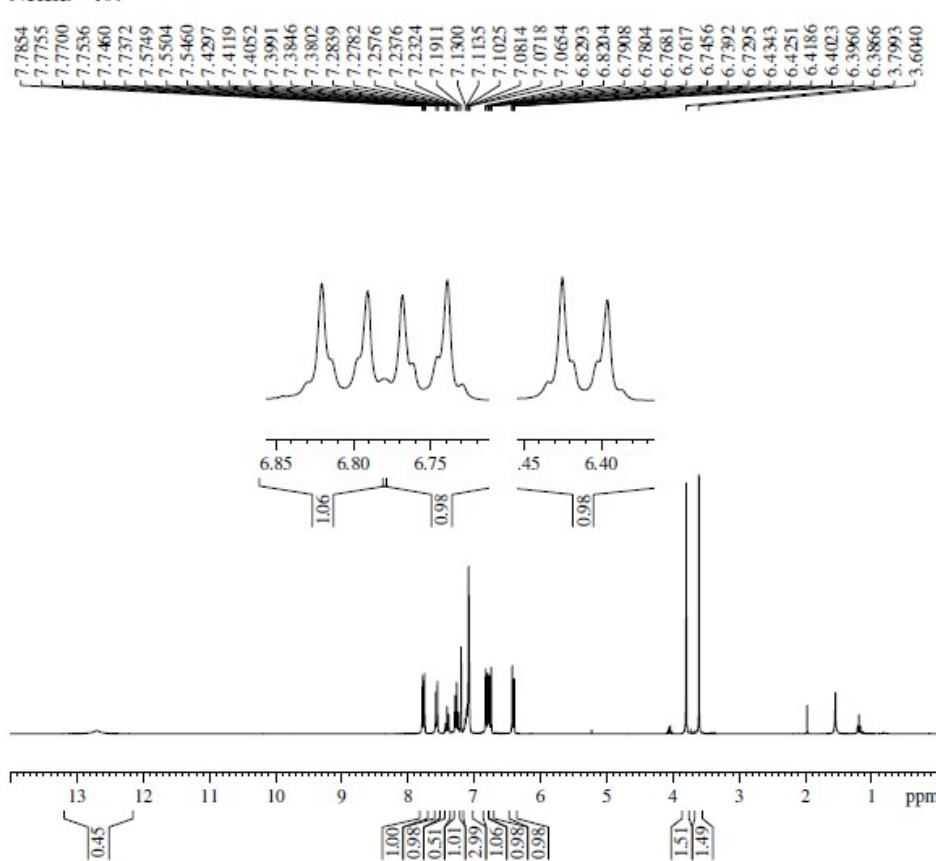


Current Data Parameters
 NAME 11-FEB-AN-2020
 EXPNO 470
 PROCNO 1

F2 - Processing parameters
 SI 32768
 SF 75.4999332 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

S68: ¹³C NMR spectrum of 3t

NRLD-407



Current Data Parameters
 NAME 30-Jan-FN-2020
 EXPNO 530
 PROCNO 1

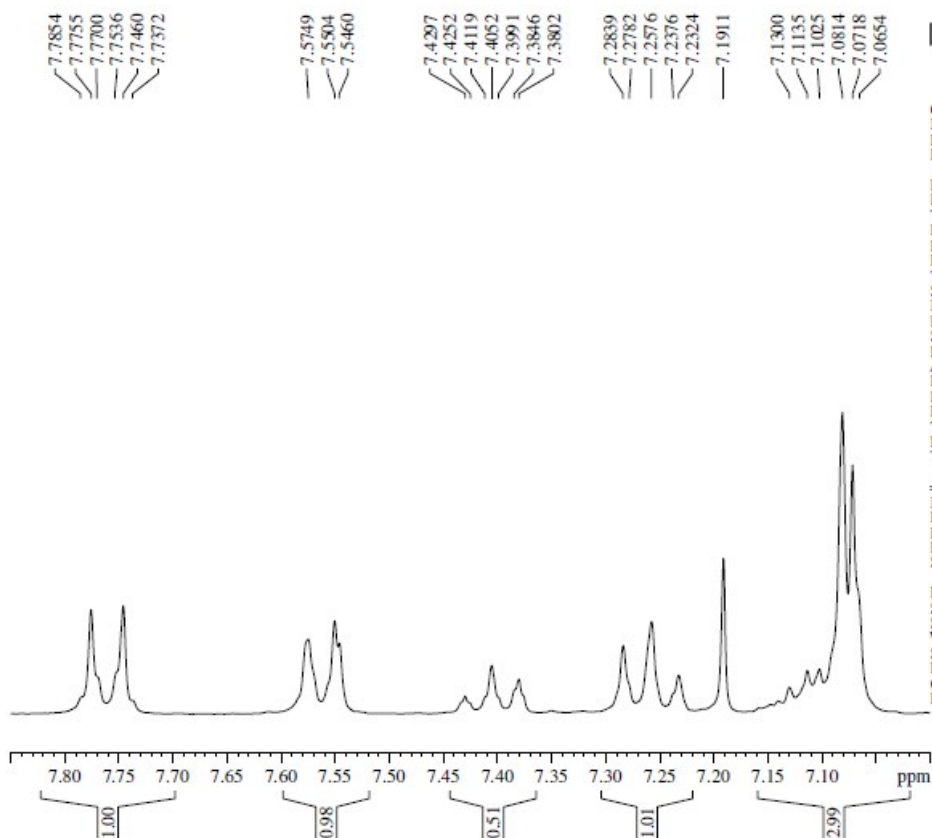
F2 - Acquisition Parameters
 Date_ 20200130
 Time 11.40
 INSTRUM spect
 PROBHD 5 mm QNP 1H/13
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 16
 DS 2
 SWH 6188.119 Hz
 FIDRES 0.094423 Hz
 AQ 5.2953086 sec
 RG 203
 DW 80.800 usec
 DE 6.50 usec
 TE 300.0 K
 DI 1.00000000 sec
 TDO 1

==== CHANNEL f1 ====
 NUC1 1H
 P1 13.95 usec
 PL1 -1.00 dB
 PL1W 15.02081871 W
 SFO1 300.2598542 MHz

F2 - Processing parameters
 SI 32768
 SF 300.2580280 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

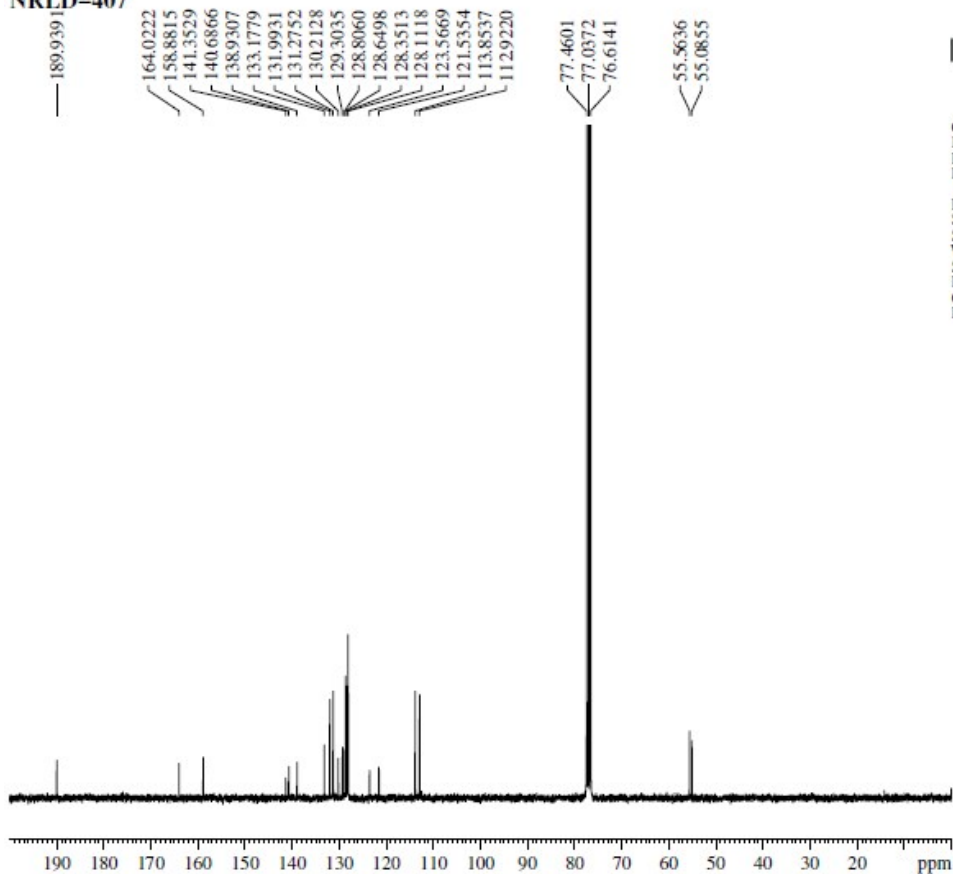
S69: ¹H NMR spectrum of 3u

NRLD-407



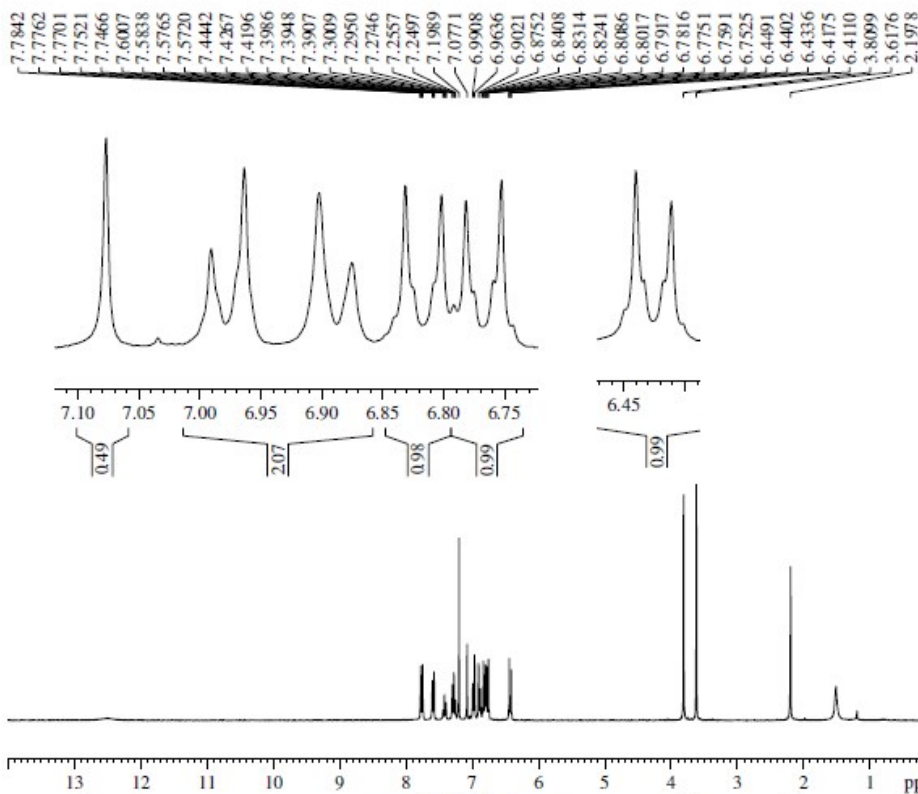
S70: ¹H NMR spectrum of **3u** (expansion)

NRLD-407



S71: ¹³C NMR spectrum of **3u**

NRLD-418



Current Data Parameters
 NAME 13-FEB-FN-2020
 EXPNO 450
 PROCNO 1

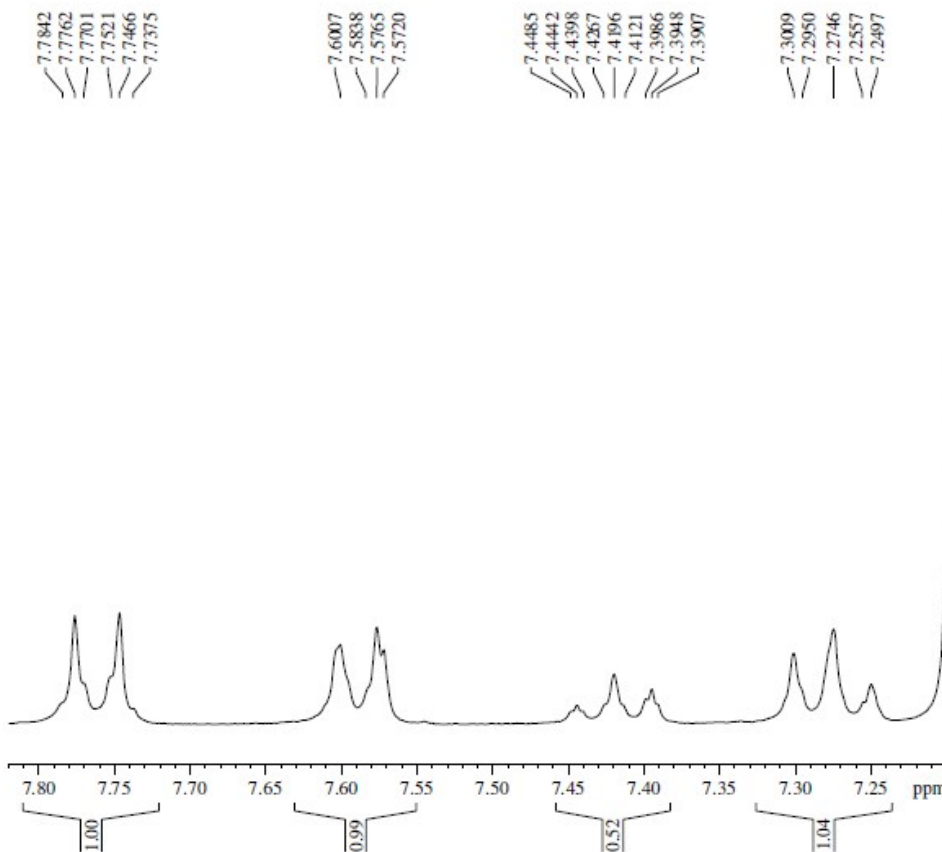
F2 - Acquisition Parameters
 Date_ 20200213
 Time 10.43
 INSTRUM spect
 PROBHD 5 mm QNP 1H/13
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 16
 DS 2
 SWH 6188.119 Hz
 FIDRES 0.094423 Hz
 AQ 5.2953086 sec
 RG 322
 DW 80.800 usec
 DE 6.50 usec
 TE 300.0 K
 D1 1.00000000 sec
 TD0 1

==== CHANNEL f1 ====
 NUC1 1H
 P1 13.95 usec
 PL1 -1.00 dB
 PL1W 15.02081871 W
 SFO1 300.2598542 MHz

F2 - Processing parameters
 SI 32768
 SF 300.2580257 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

S72: ¹H NMR spectrum of 3v

NRLD-418



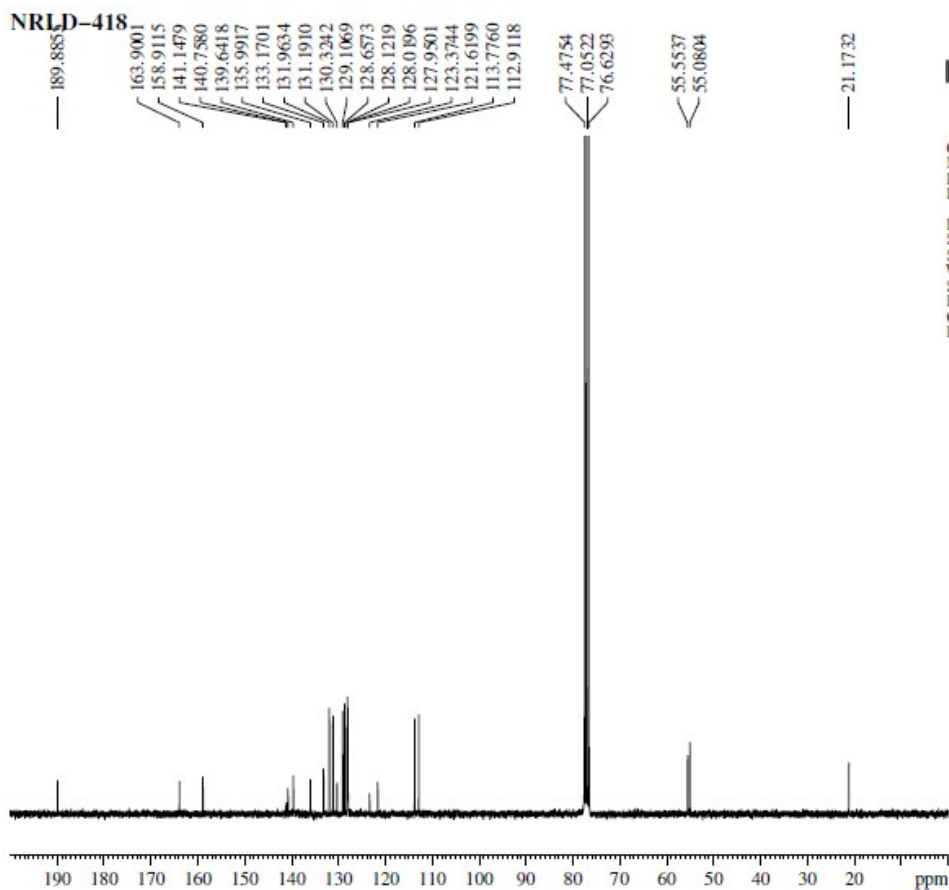
Current Data Parameters
 NAME 13-FEB-FN-2020
 EXPNO 450
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20200213
 Time 10.43
 INSTRUM spect
 PROBHD 5 mm QNP 1H/13
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 16
 DS 2
 SWH 6188.119 Hz
 FIDRES 0.094423 Hz
 AQ 5.2953086 sec
 RG 322
 DW 80.800 usec
 DE 6.50 usec
 TE 300.0 K
 D1 1.00000000 sec
 TD0 1

==== CHANNEL f1 ====
 NUC1 1H
 P1 13.95 usec
 PL1 -1.00 dB
 PL1W 15.02081871 W
 SFO1 300.2598542 MHz

F2 - Processing parameters
 SI 32768
 SF 300.2580257 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

S73: ¹H NMR spectrum of 3v (expansion)

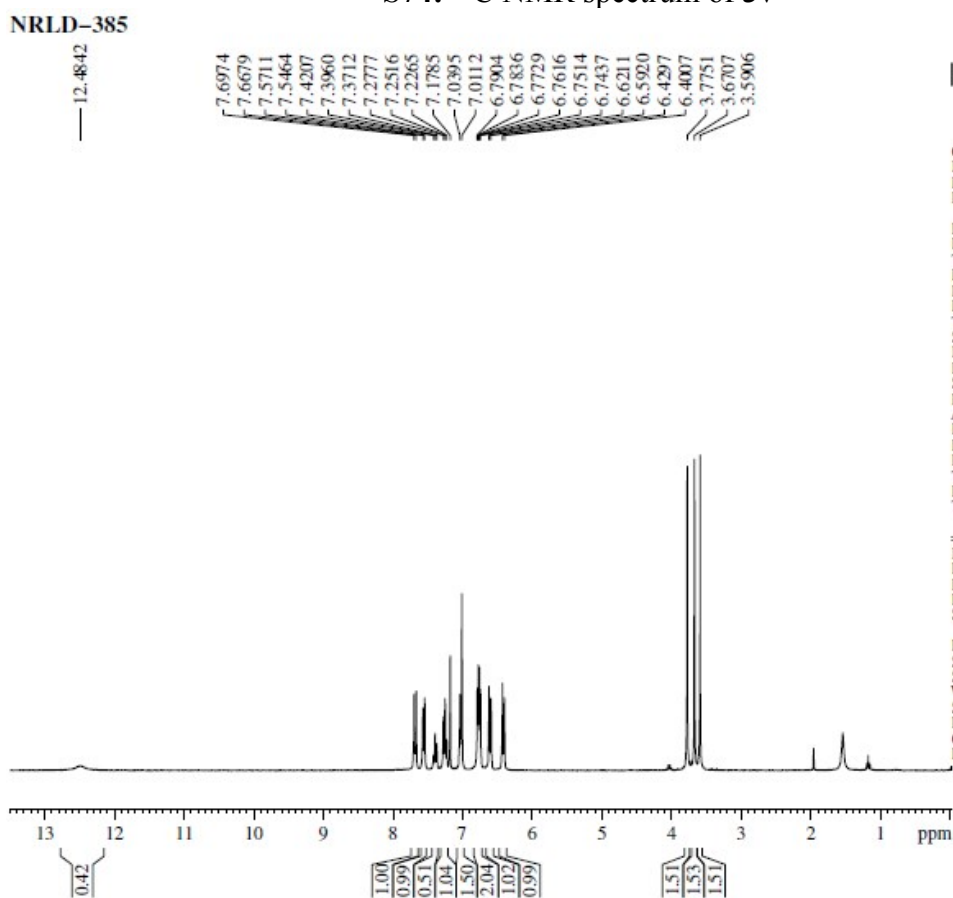


S74: ^{13}C NMR spectrum of **3v**



Current Data Parameters
NAME 12-FEB-AN-2020
EXPNO 350
PROCNO 1

F2 - Processing parameters
SI 32768
SF 75.4999320 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



S75: ^1H NMR spectrum of **3w**



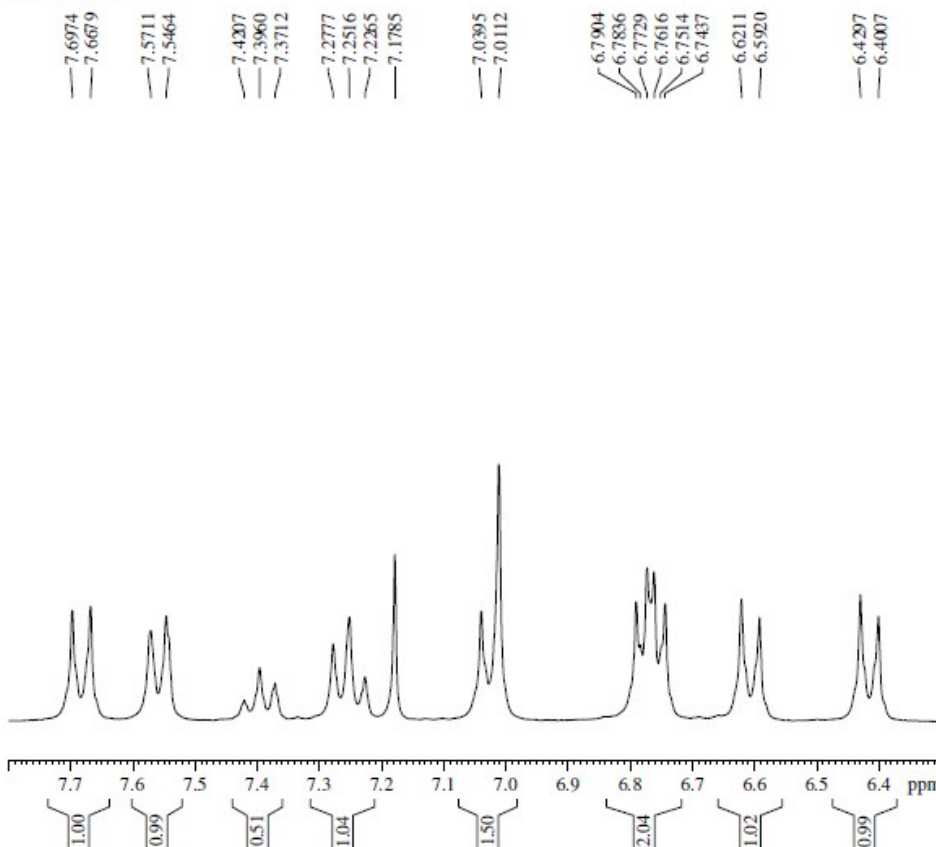
Current Data Parameters
NAME 17-JAN-FN-2020
EXPNO 550
PROCNO 1

F2 - Acquisition Parameters
Date_ 20200117
Time 11.16
INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 6188.119 Hz
FIDRES 0.094423 Hz
AQ 5.2953086 sec
RG 287
DW 80.800 usec
DE 6.50 usec
TE 300.0 K
D1 1.0000000 sec
TD0 1

==== CHANNEL f1 ====
NUC1 1H
P1 13.95 usec
PL1 -1.00 dB
PL1W 15.02081871 W
SFO1 300.2598542 MHz

F2 - Processing parameters
SI 32768
SF 300.2580318 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

NRLD-385



Current Data Parameters
 NAME 17-JAN-FN-2020
 EXPNO 550
 PROCNO 1

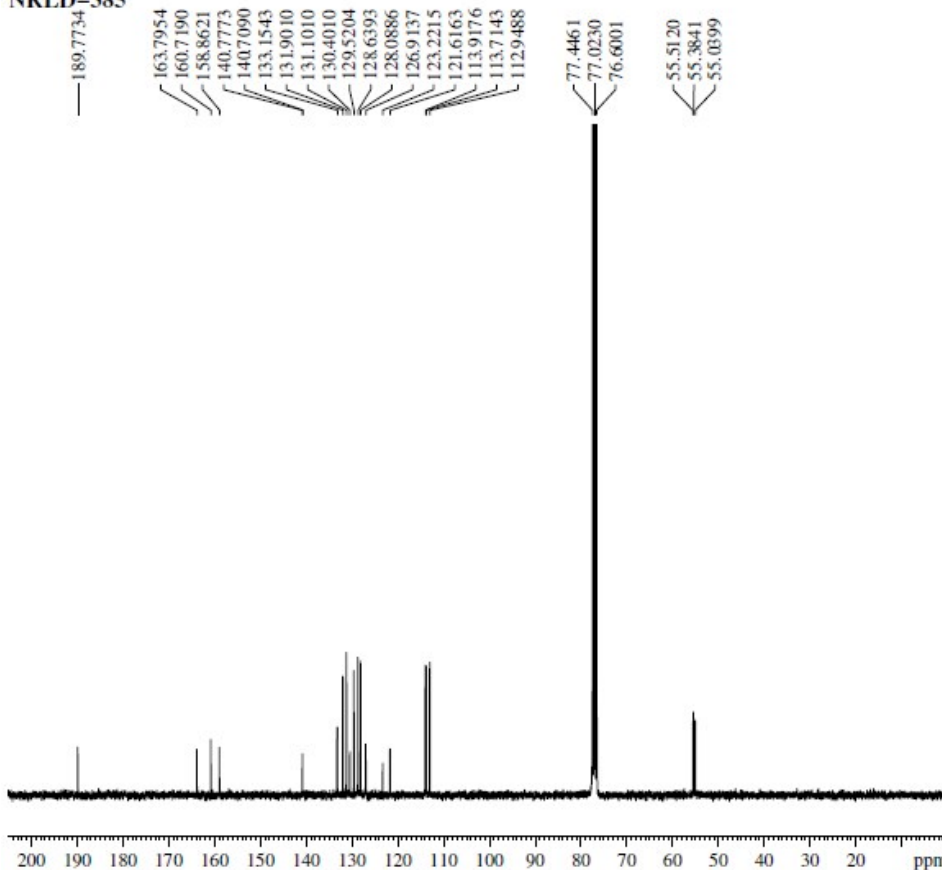
F2 - Acquisition Parameters
 Date_ 20200117
 Time 11.16
 INSTRUM spect
 PROBHD 5 mm QNP 1H/13
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 16
 DS 2
 SWH 6188.119 Hz
 FIDRES 0.094423 Hz
 AQ 5.2953086 sec
 RG 287
 DW 80.800 usec
 DE 6.50 usec
 TE 300.0 K
 D1 1.0000000 sec
 TD0 1

==== CHANNEL f1 ====
 NUC1 1H
 P1 13.95 usec
 PL1 -1.00 dB
 PL1W 15.02081871 W
 SFO1 300.2598542 MHz

F2 - Processing parameters
 SI 32768
 SF 300.2580318 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

S76: ¹H NMR spectrum of 3w (expansion)

NRLD-385

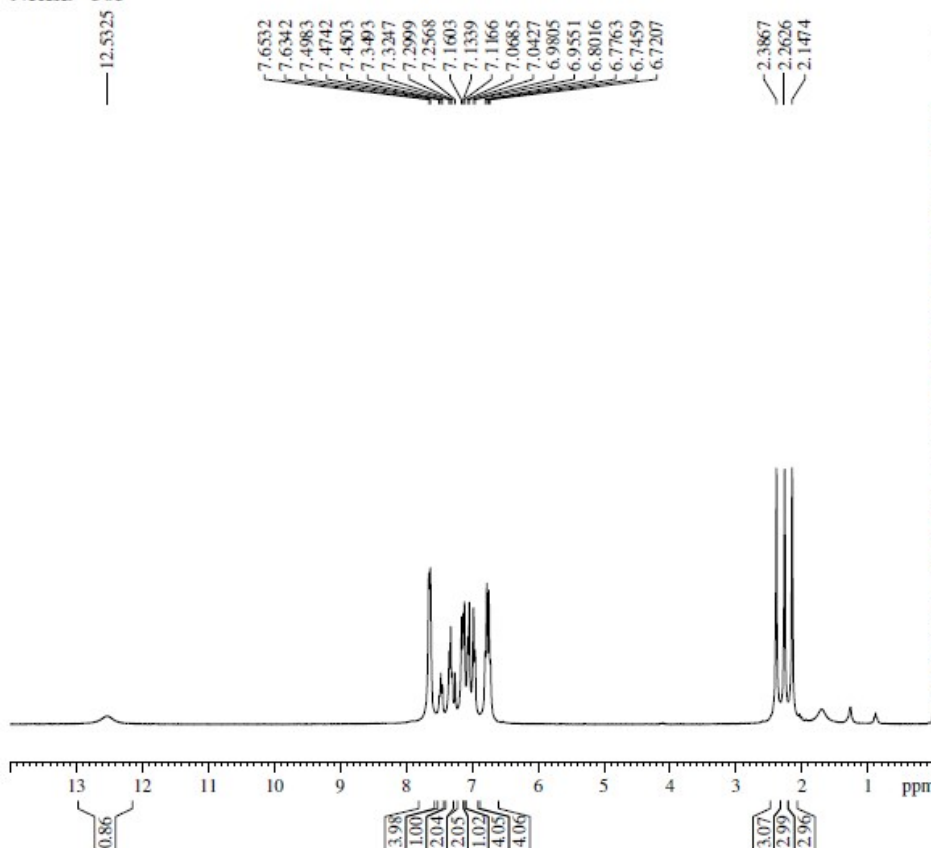


Current Data Parameters
 NAME 17-Jan-AN-2020
 EXPNO 340
 PROCNO 1

F2 - Processing parameters
 SI 32768
 SF 75.4999341 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

S77: ¹³C NMR spectrum of 3w

NRLD-365



S78: ¹H NMR spectrum of 3x



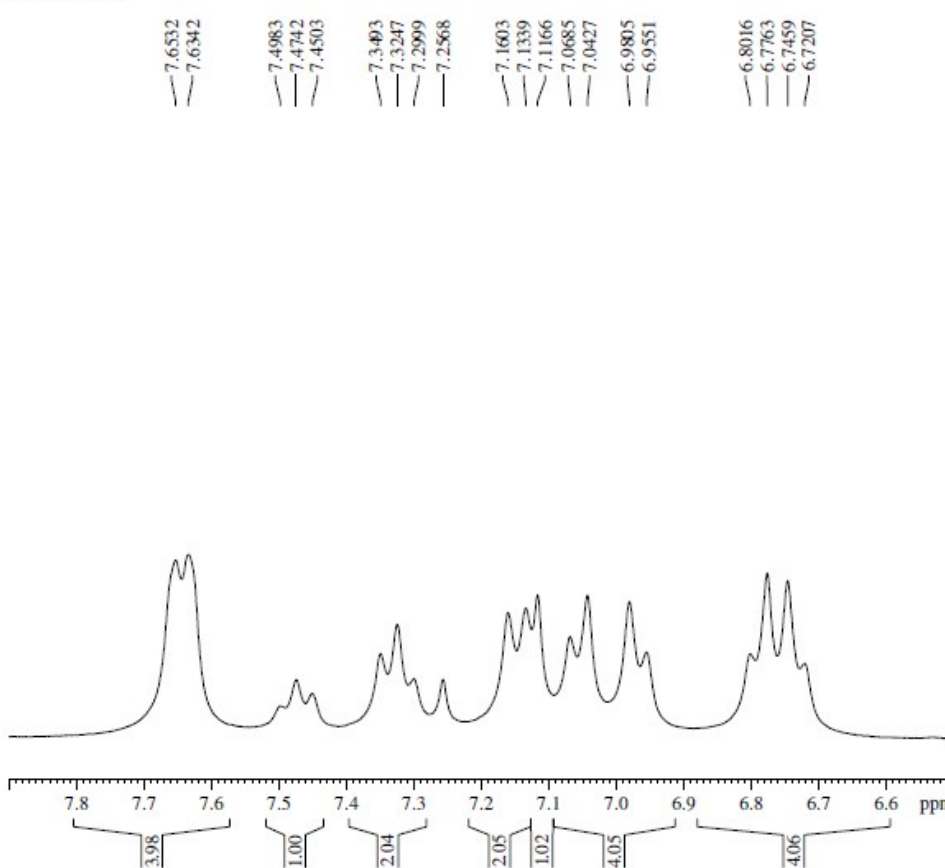
Current Data Parameters
 NAME 13-Mar-FN-2020
 EXPNO 410
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20200313
 Time 11.15
 INSTRUM spect
 PROBHD 5 mm QNP 1H/13
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 16
 DS 2
 SWH 6188.119 Hz
 FIDRES 0.094423 Hz
 AQ 5.2953086 sec
 RG 181
 DW 80.800 usec
 DE 6.50 usec
 TE 300.0 K
 D1 1.00000000 sec
 TD0 1

==== CHANNEL f1 ====
 NUC1 1H
 P1 13.95 usec
 PL1 -1.00 dB
 PL1W 15.02081871 W
 SFO1 300.2598542 MHz

F2 - Processing parameters
 SI 32768
 SF 300.2580083 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

NRLD-365



S79: ¹H NMR spectrum of 3x (expansion)



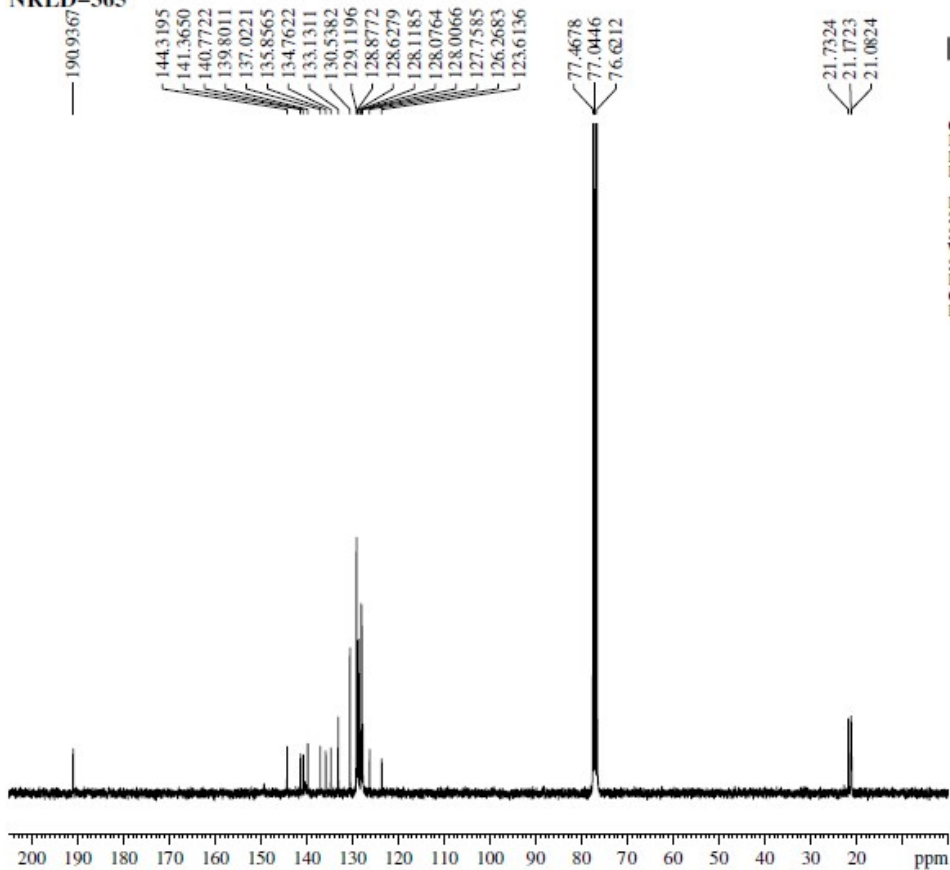
Current Data Parameters
 NAME 13-Mar-FN-2020
 EXPNO 410
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20200313
 Time 11.15
 INSTRUM spect
 PROBHD 5 mm QNP 1H/13
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 16
 DS 2
 SWH 6188.119 Hz
 FIDRES 0.094423 Hz
 AQ 5.2953086 sec
 RG 181
 DW 80.800 usec
 DE 6.50 usec
 TE 300.0 K
 D1 1.00000000 sec
 TD0 1

==== CHANNEL f1 ====
 NUC1 1H
 P1 13.95 usec
 PL1 -1.00 dB
 PL1W 15.02081871 W
 SFO1 300.2598542 MHz

F2 - Processing parameters
 SI 32768
 SF 300.2580083 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

NRLD-365

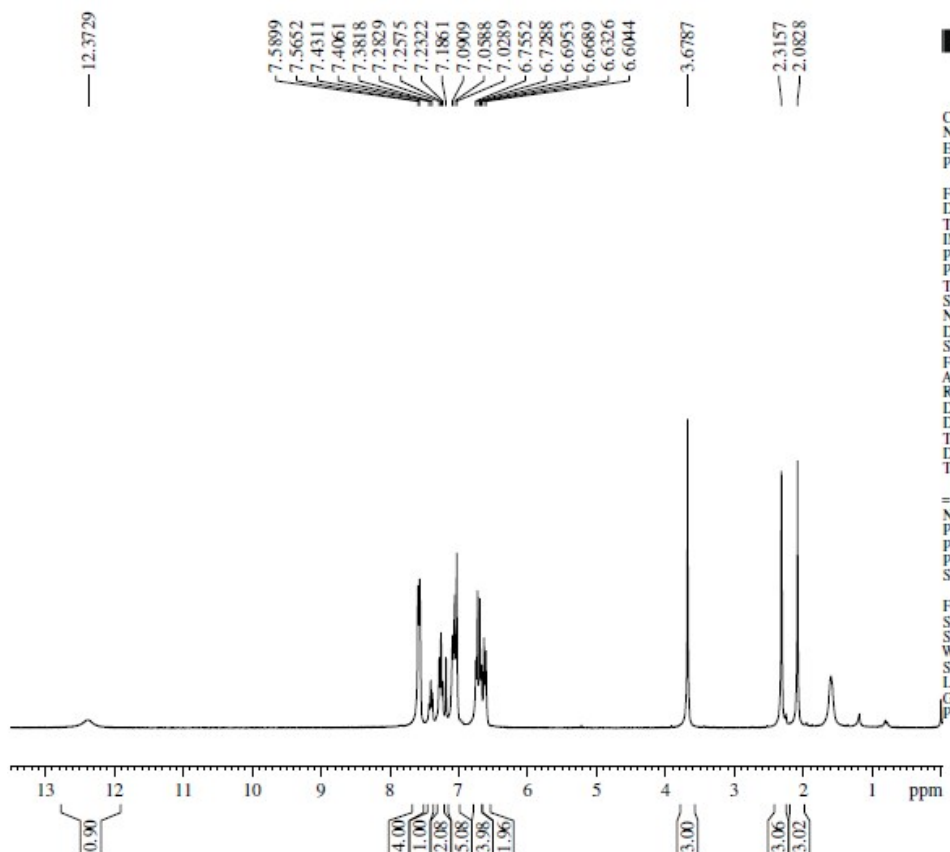


Current Data Parameters
 NAME 13-Mar-FN-2020
 EXPNO 420
 PROCNO 1

F2 - Processing parameters
 SI 32768
 SF 75.4999338 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

S80: ¹³C NMR spectrum of 3x

NRLD-366



Current Data Parameters
 NAME 27-Sept-FN-2019
 EXPNO 490
 PROCNO 1

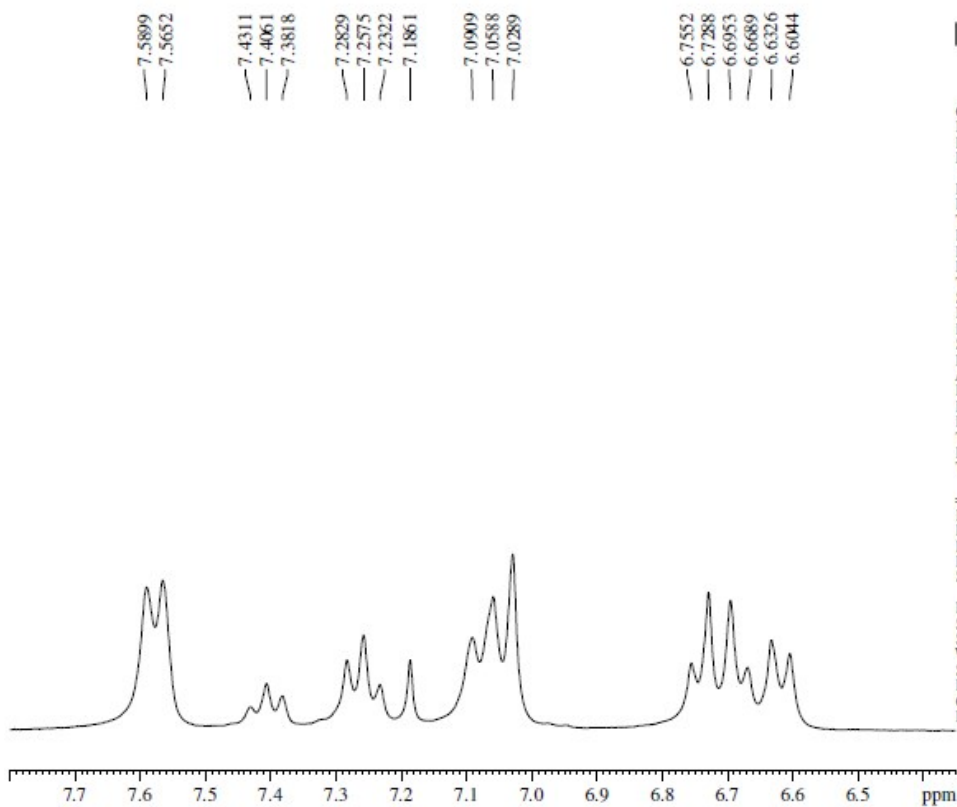
F2 - Acquisition Parameters
 Date_ 20190927
 Time 11.34
 INSTRUM spect
 PROBHD 5 mm QNP 1H/13
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 16
 DS 2
 SWH 6188.119 Hz
 FIDRES 0.094423 Hz
 AQ 5.2953086 sec
 RG 256
 DW 80.800 usec
 DE 6.50 usec
 TE 300.0 K
 D1 1.00000000 sec
 TD0 1

==== CHANNEL f1 ====
 NUC1 1H
 P1 13.95 usec
 PL1 -1.00 dB
 PL1W 15.02081871 W
 SFO1 300.2598542 MHz

F2 - Processing parameters
 SI 32768
 SF 300.2580296 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

S81: ¹H NMR spectrum of 3y

NRLD-366



Current Data Parameters
NAME 27-Sept-FN-2019
EXPNO 490
PROCNO 1

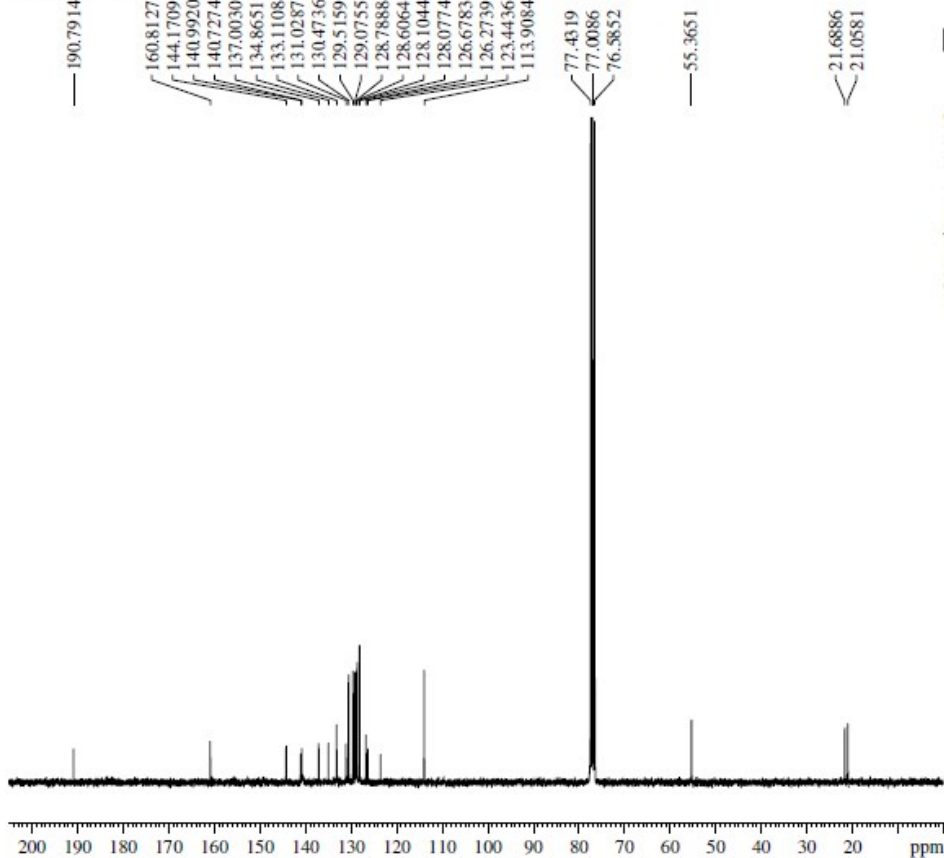
F2 - Acquisition Parameters
Date_ 20190927
Time 11.34
INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 6188.119 Hz
FIDRES 0.094423 Hz
AQ 5.2953086 sec
RG 256
DW 80.800 usec
DE 6.50 usec
TE 300.0 K
D1 1.00000000 sec
TD0 1

==== CHANNEL f1 ====
NUC1 1H
P1 13.95 usec
PL1 -1.00 dB
PL1W 15.02081871 W
SFO1 300.2598542 MHz

F2 - Processing parameters
SI 32768
SF 300.2580296 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

S82: ¹H NMR spectrum of 3y (expansion)

NRLD-366

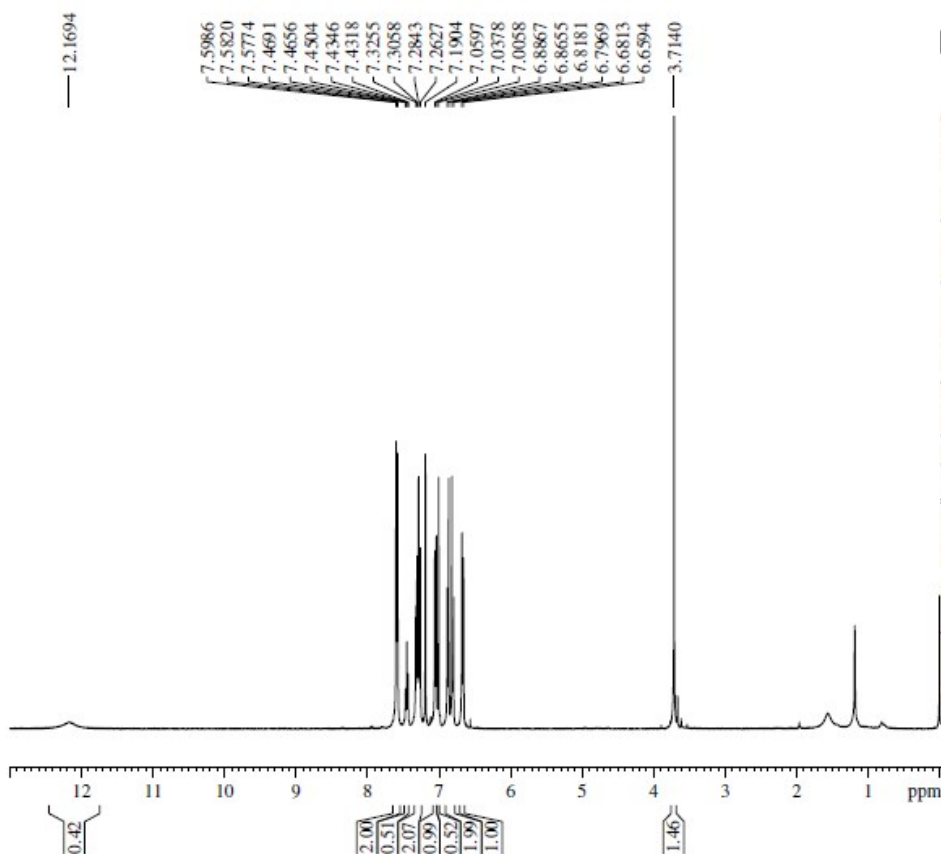


Current Data Parameters
NAME 30-Sept-FN-2019
EXPNO 460
PROCNO 1

F2 - Processing parameters
SI 32768
SF 75.4999361 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

S83: ¹³C NMR spectrum of 3y

NRLD-369



Current Data Parameters
 NAME 24-Dec-AN-2019
 EXPNO 340
 PROCNO 1

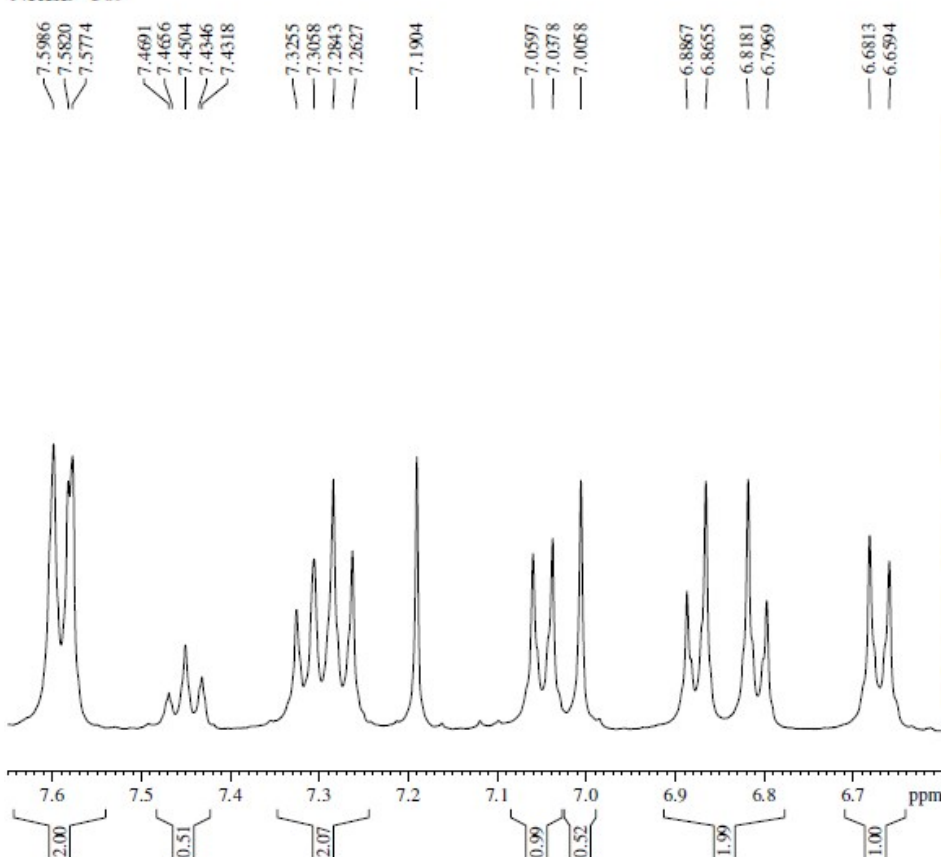
F2 - Acquisition Parameters
 Date_ 20191224
 Time 22.13
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 8
 DS 0
 SWH 9615.385 Hz
 FIDRES 0.146719 Hz
 AQ 3.4078720 sec
 RG 145.29
 DW 52.000 usec
 DE 6.50 usec
 TE 303.0 K
 D1 1.00000000 sec
 TD0 1

==== CHANNEL f1 ====
 SFO1 400.1629712 MHz
 NUC1 1H
 P1 13.20 usec
 PLW1 13.00000000 W

F2 - Processing parameters
 SI 65536
 SF 400.1605373 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

S84: ¹H NMR spectrum of 3z

NRLD-369



Current Data Parameters
 NAME 24-Dec-AN-2019
 EXPNO 340
 PROCNO 1

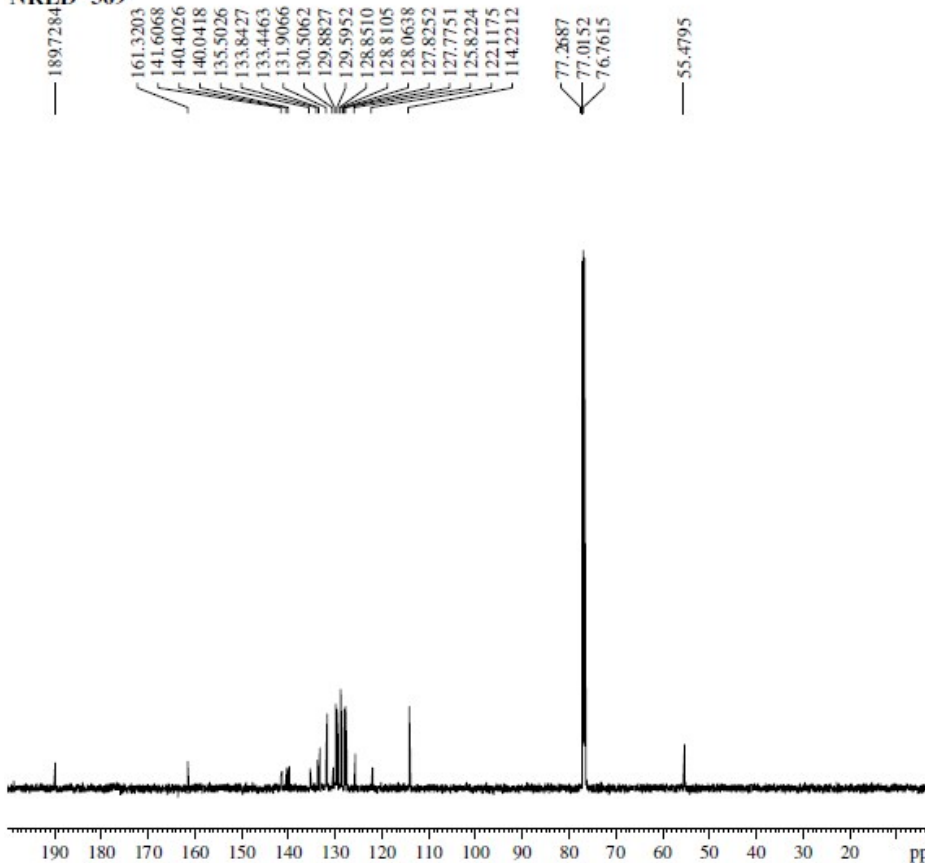
F2 - Acquisition Parameters
 Date_ 20191224
 Time 22.13
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 8
 DS 0
 SWH 9615.385 Hz
 FIDRES 0.146719 Hz
 AQ 3.4078720 sec
 RG 145.29
 DW 52.000 usec
 DE 6.50 usec
 TE 303.0 K
 D1 1.00000000 sec
 TD0 1

==== CHANNEL f1 ====
 SFO1 400.1629712 MHz
 NUC1 1H
 P1 13.20 usec
 PLW1 13.00000000 W

F2 - Processing parameters
 SI 65536
 SF 400.1605373 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

S85: ¹H NMR spectrum of 3z (expansion)

NRLD-369



Current Data Parameters
 NAME 14-NOV-FN-2019
 EXPNO 590
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20191114
 Time 11.03
 INSTRUM spect
 PROBHID 5 mm PATXI 1H
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 4096
 DS 0
 SWH 29761.904 Hz
 FIDRES 0.454131 Hz
 AQ 1.1010048 sec
 RG 87.95
 DW 16.800 usec
 DE 6.50 usec
 TE 303.0 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 TD0 1

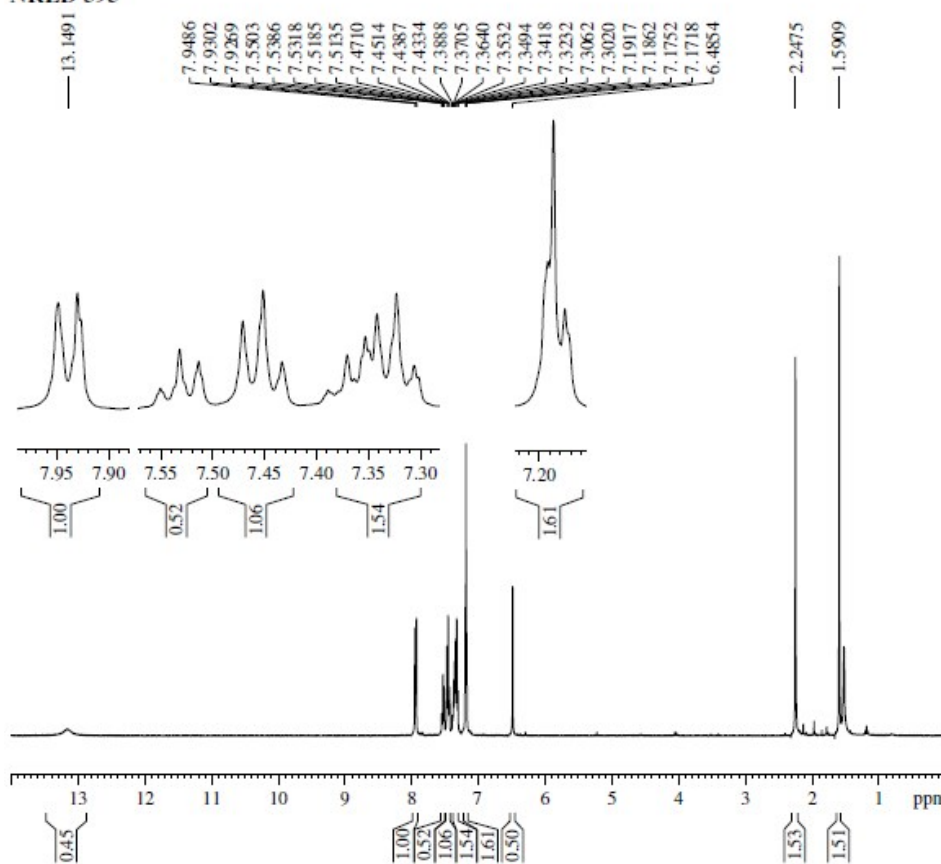
==== CHANNEL f1 ====
 SFO1 125.9077573 MHz
 NUC1 13C
 P1 9.23 usec
 PLW1 244.0000000 W

==== CHANNEL f2 ====
 SFO2 500.6783527 MHz
 NUC2 1H
 CPDPRG2 waltz16
 PCPD2 80.00 usec
 PLW2 13.60000038 W
 PLW12 0.08840500 W
 PLW13 0.05657900 W

F2 - Processing parameters
 SI 32768
 SF 125.8951680 MHz
 WDW EM
 SSB 0
 LB 3.00 Hz
 GB 0
 PC 1.40

S86: ¹³C NMR spectrum of 3z

NRLD 395



Current Data Parameters
 NAME 08-Jan-FN-2020
 EXPNO 530
 PROCNO 1

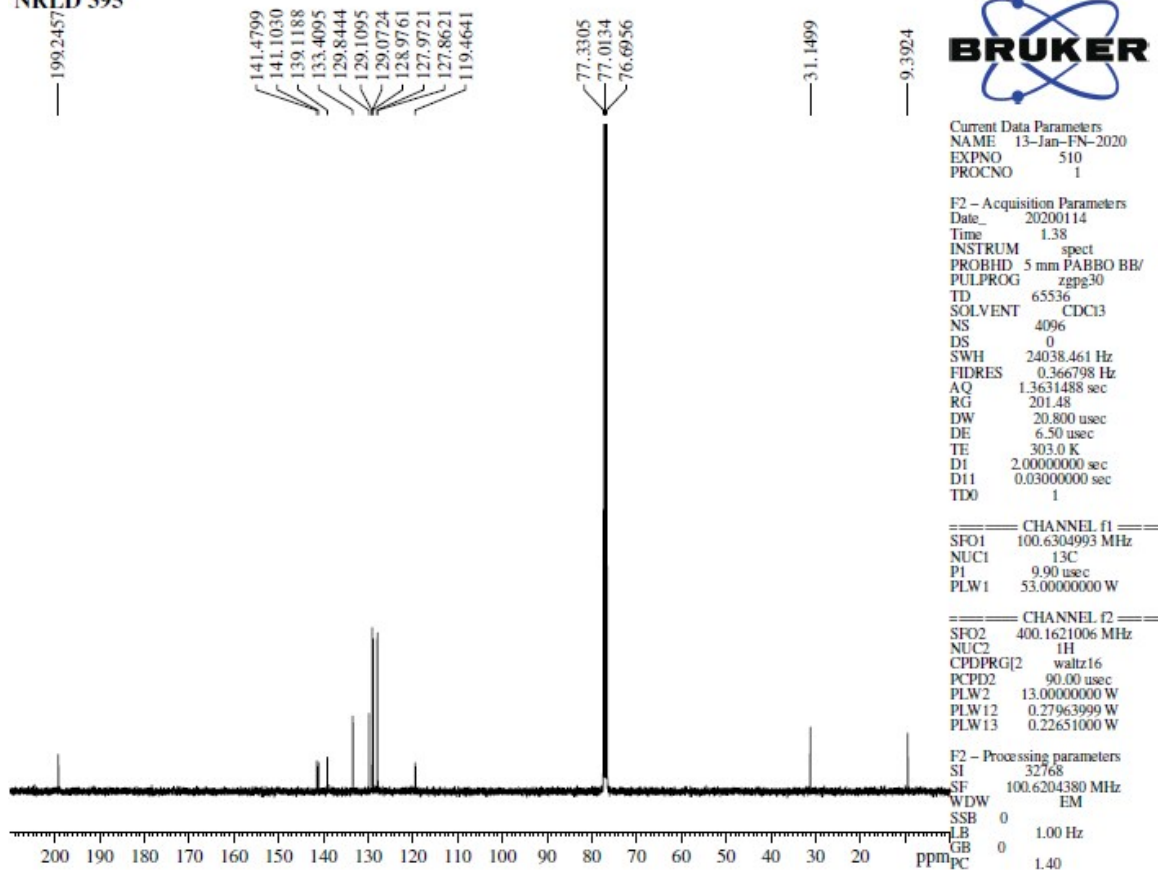
F2 - Acquisition Parameters
 Date_ 20200108
 Time 18.29
 INSTRUM spect
 PROBHID 5 mm PABBO BB/
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 8
 DS 0
 SWH 9615.385 Hz
 FIDRES 0.146719 Hz
 AQ 3.4078720 sec
 RG 159.22
 DW 52.000 usec
 DE 6.50 usec
 TE 297.3 K
 D1 1.00000000 sec
 TD0 1

==== CHANNEL f1 ====
 SFO1 400.1629712 MHz
 NUC1 1H
 P1 13.20 usec
 PLW1 13.00000000 W

F2 - Processing parameters
 SI 65536
 SF 400.1605391 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

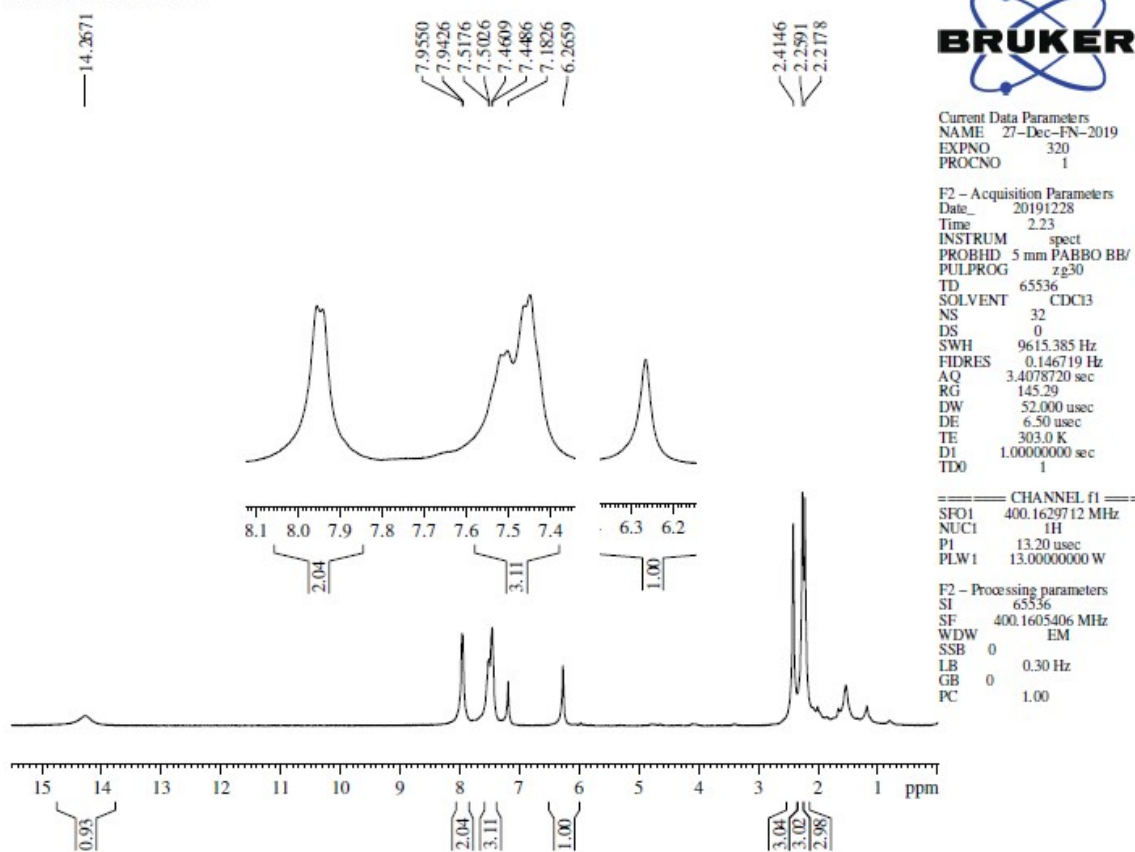
S87: ¹H NMR spectrum of 3za

NRLD 395



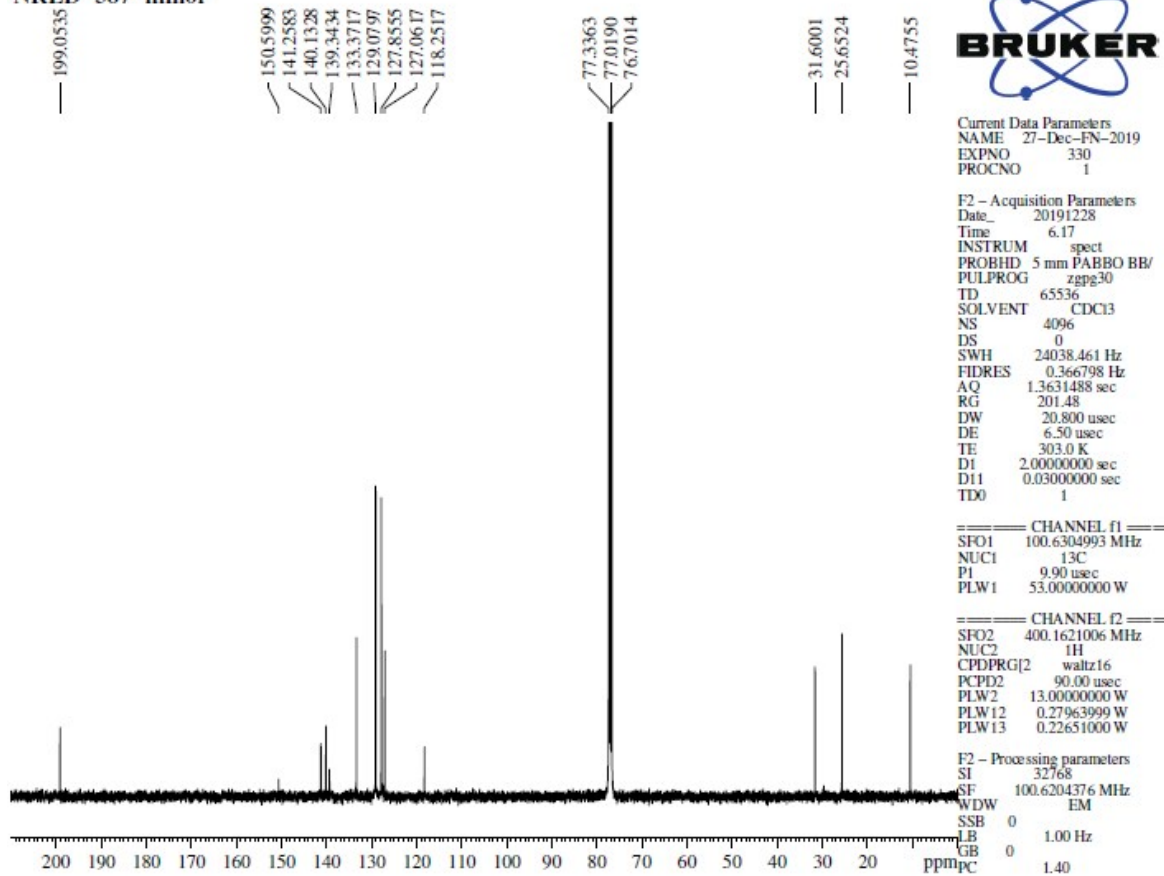
S88: ¹³C NMR spectrum of 3za

NRLD-387-minor



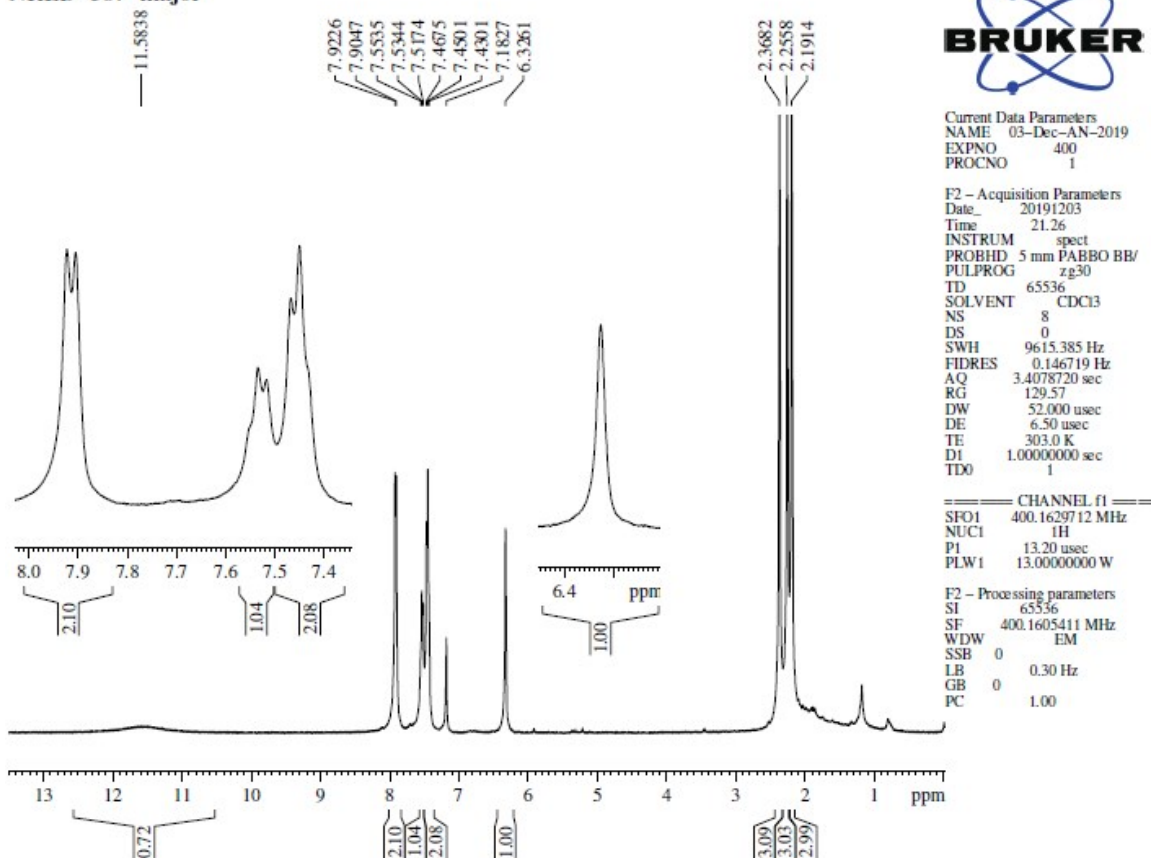
S89: ¹H NMR spectrum of 3zb (minor isomer)

NRLD-387-minor



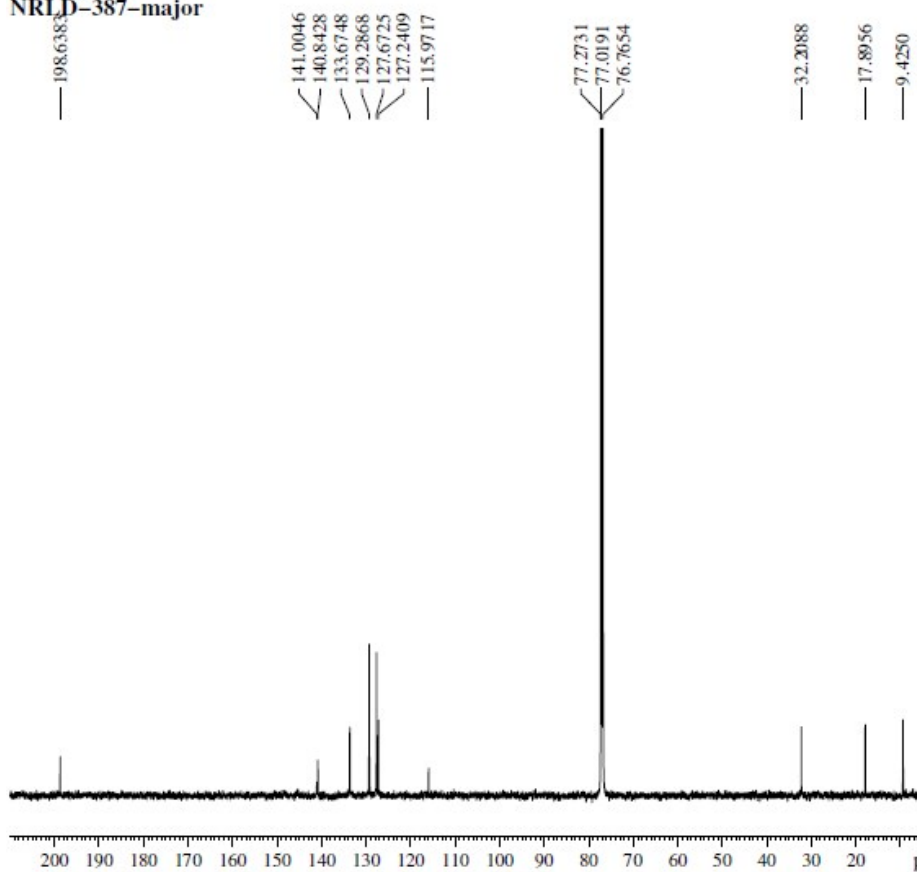
S90: ¹³C NMR spectrum of 3zb (minor isomer)

NRLD-387-major



S91: ¹H NMR spectrum of 3zb (major isomer)

NRLD-387-major



Current Data Parameters
 NAME 04-Dec-FN-2019
 EXPNO 350
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20191204
 Time 11.38
 INSTRUM spect
 PROBHD 5 mm PATXI 1H
 PULPROG zgpg30
 TD 65536
 SOLVENT CDC13
 NS 4096
 DS 4
 SWH 29761.904 Hz
 FIDRES 0.454131 Hz
 AQ 1.1010048 sec
 RG 81.53
 DW 16.800 usec
 DE 6.50 usec
 TE 303.0 K
 D1 2.0000000 sec
 D11 0.0300000 sec
 TD0 1

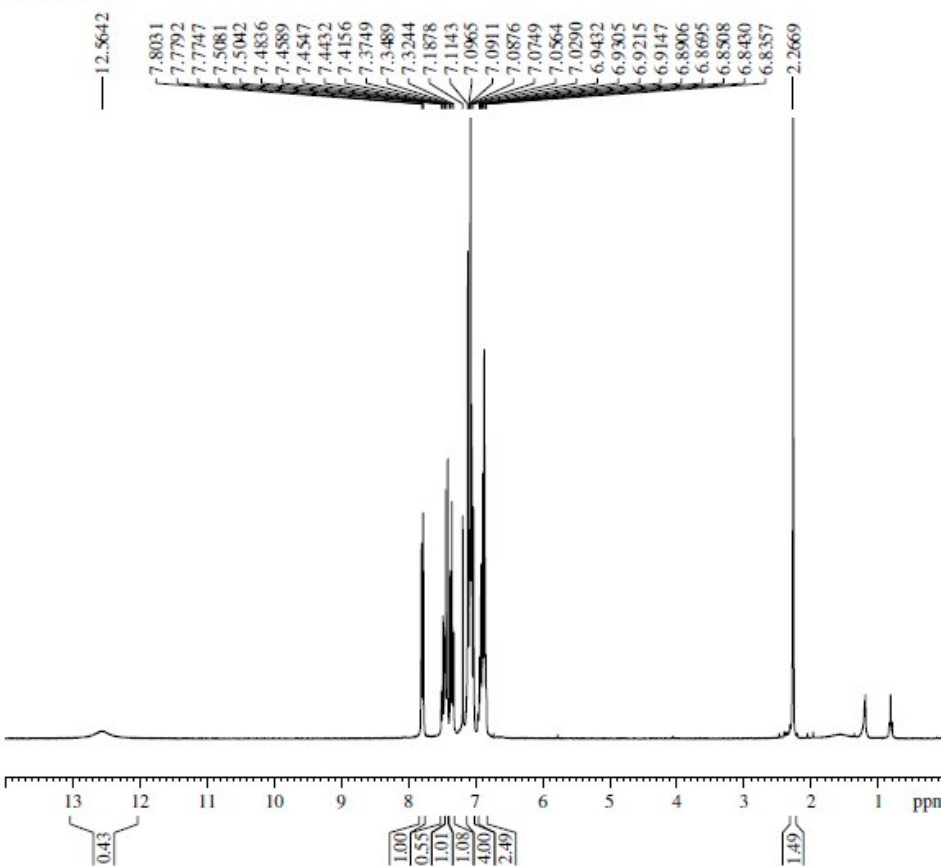
==== CHANNEL f1 ====
 SFO1 125.9077573 MHz
 NUC1 13C
 P1 9.23 usec
 PLW1 244.0000000 W

==== CHANNEL f2 ====
 SFO2 500.6783527 MHz
 NUC2 1H
 CPDPRG2 waltz16
 PCPD2 80.00 usec
 PLW2 13.6000038 W
 PLW12 0.08840500 W
 PLW13 0.05657900 W

F2 - Processing parameters
 SI 32768
 SF 125.8951680 MHz
 WDW EM
 SSB 0
 LB 3.00 Hz
 GB 0
 PC 1.40

S92: 13C NMR spectrum of 3zb (major isomer)

NRLD-425



Current Data Parameters
 NAME 26-Feb-AN-2020
 EXPNO 560
 PROCNO 1

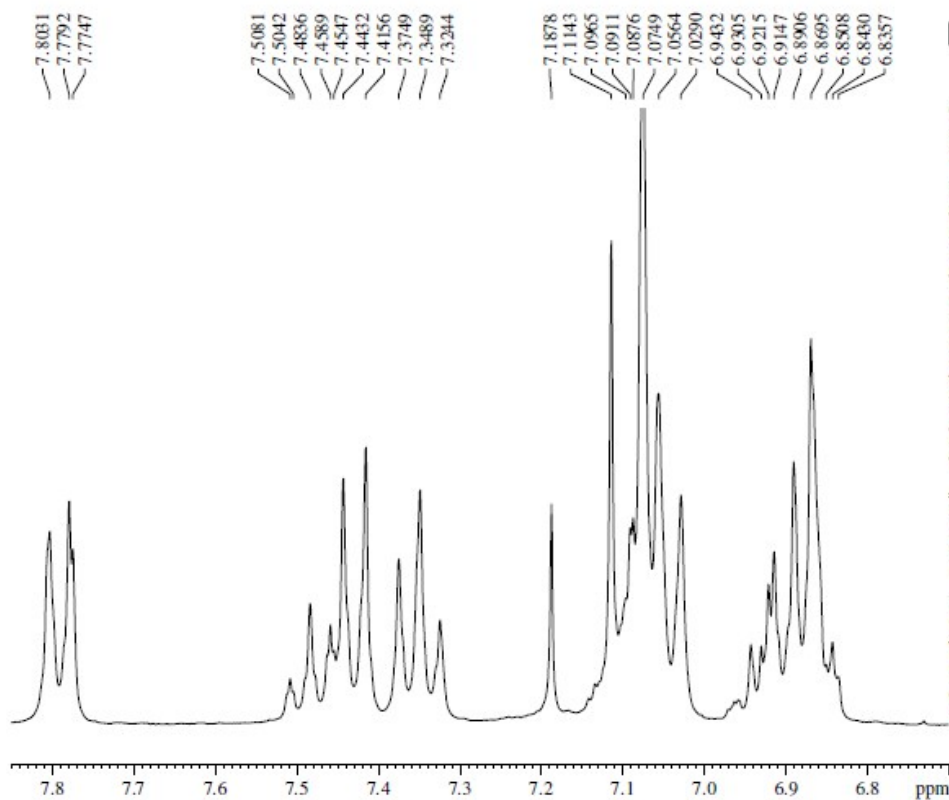
F2 - Acquisition Parameters
 Date_ 20200226
 Time 16.30
 INSTRUM spect
 PROBHD 5 mm QNP 1H/13
 PULPROG zg30
 TD 65536
 SOLVENT CDC13
 NS 16
 DS 2
 SWH 6188.119 Hz
 FIDRES 0.094423 Hz
 AQ 5.2953086 sec
 RG 256
 DW 80.800 usec
 DE 6.50 usec
 TE 300.0 K
 D1 1.0000000 sec
 TD0 1

==== CHANNEL f1 ====
 NUC1 1H
 P1 13.95 usec
 PL1 -1.00 dB
 PL1W 15.02081871 W
 SFO1 300.2598542 MHz

F2 - Processing parameters
 SI 32768
 SF 300.2580291 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

S93: 1H NMR spectrum of 3zc

NRLD-425



Current Data Parameters
 NAME 26-Feb-AN-2020
 EXPNO 560
 PROCNO 1

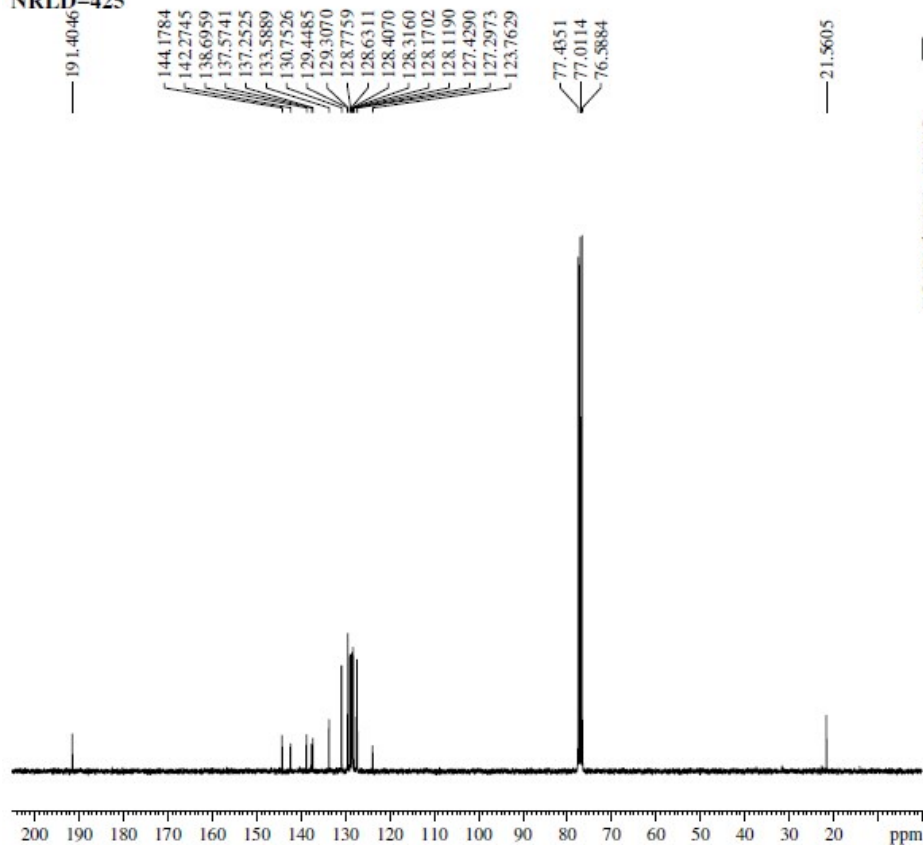
F2 - Acquisition Parameters
 Date_ 20200226
 Time 16.30
 INSTRUM spect
 PROBHD 5 mm QNP 1H/13
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 16
 DS 2
 SWH 6188.119 Hz
 FIDRES 0.094423 Hz
 AQ 5.2953086 sec
 RG 256
 DW 80.800 usec
 DE 6.50 usec
 TE 300.0 K
 D1 1.00000000 sec
 TDO 1

==== CHANNEL f1 ====
 NUC1 1H
 P1 13.95 usec
 PL1 -1.00 dB
 PL1W 15.02081871 W
 SFO1 300.2598542 MHz

F2 - Processing parameters
 SI 32768
 SF 300.2580291 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

S94: ¹H NMR spectrum of 3zc (expansion)

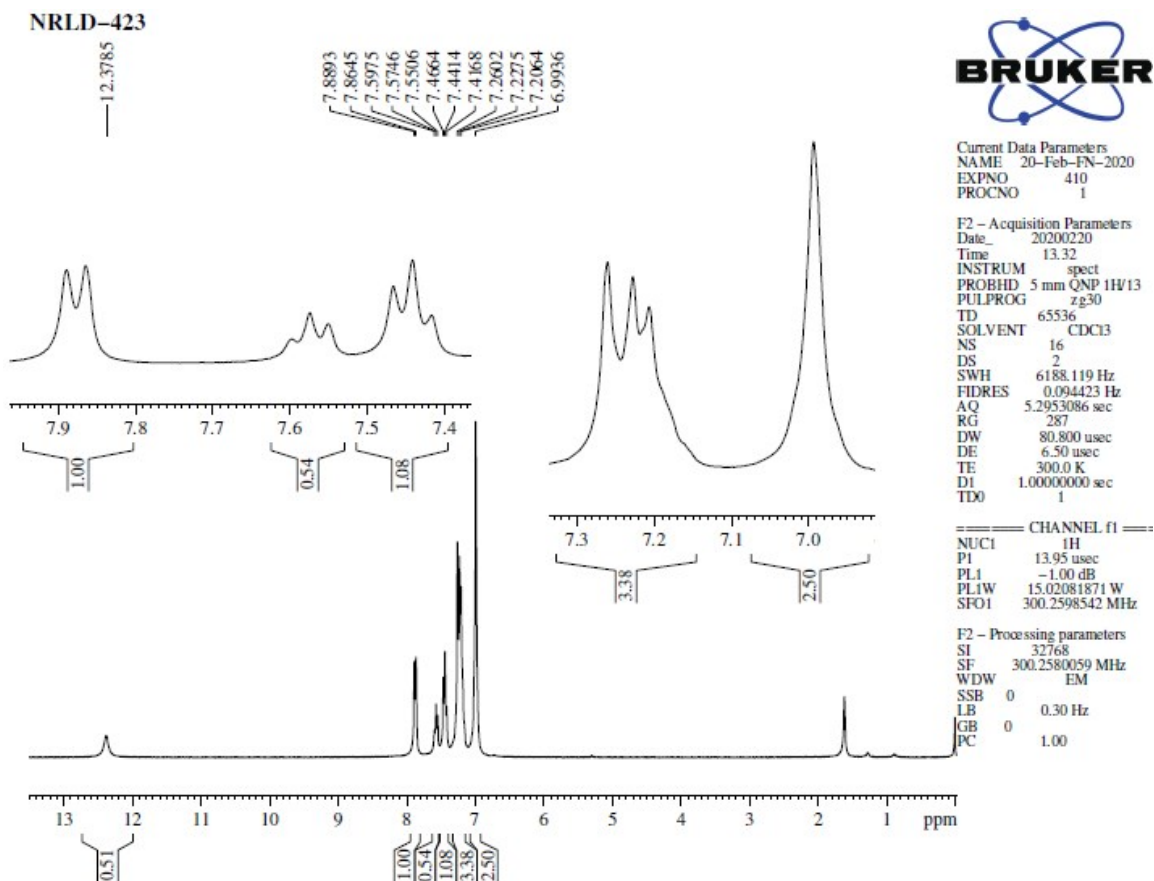
NRLD-425



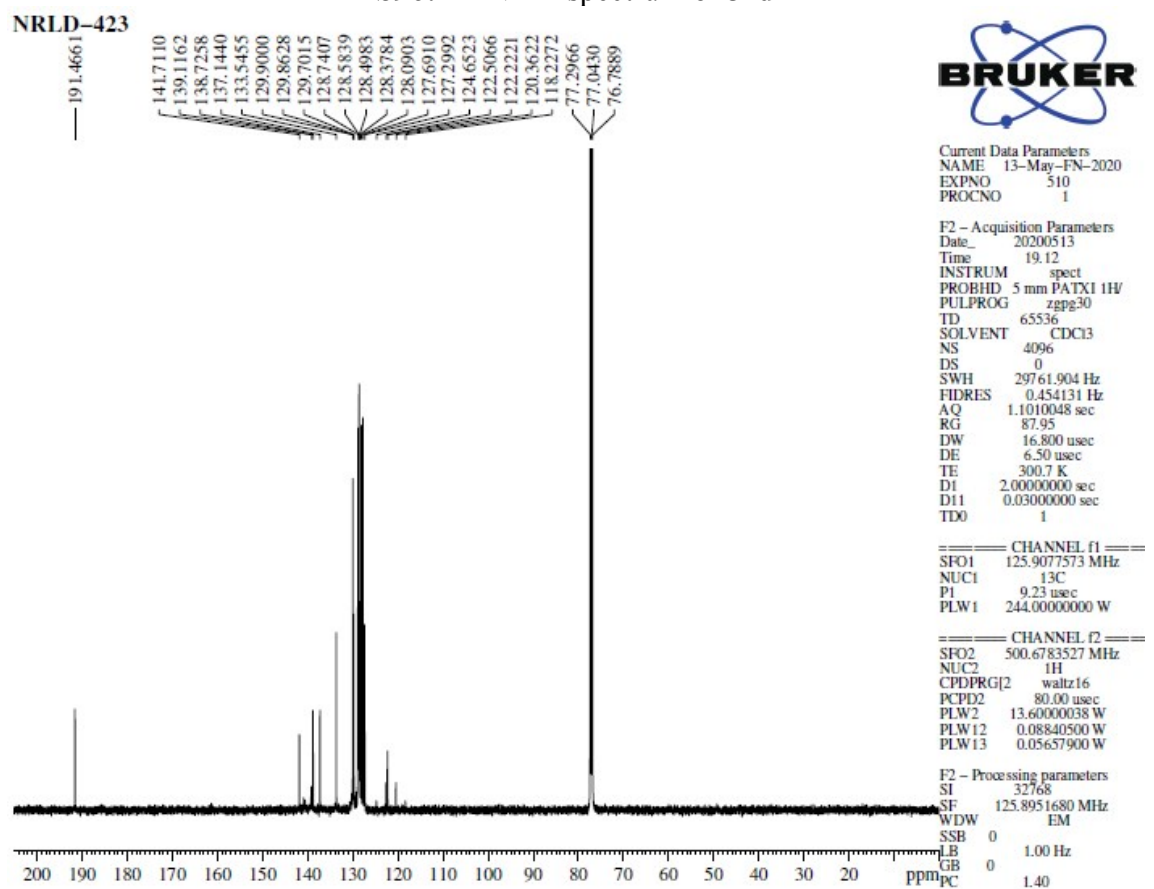
Current Data Parameters
 NAME 27-FEB-FN-2020
 EXPNO 370
 PROCNO 1

F2 - Processing parameters
 SI 32768
 SF 75.4999357 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

S95: ¹³C NMR spectrum of 3zc

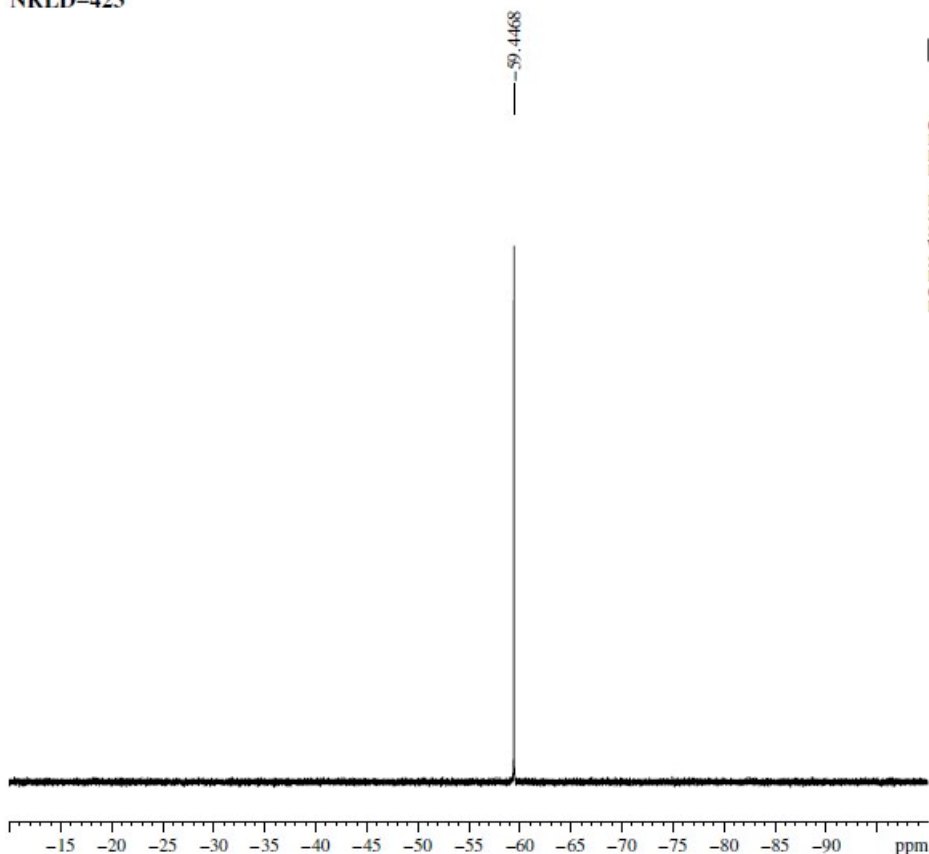


S96: ¹H NMR spectrum of 3zd



S97: ¹³C NMR spectrum of 3zd

NRLD-423

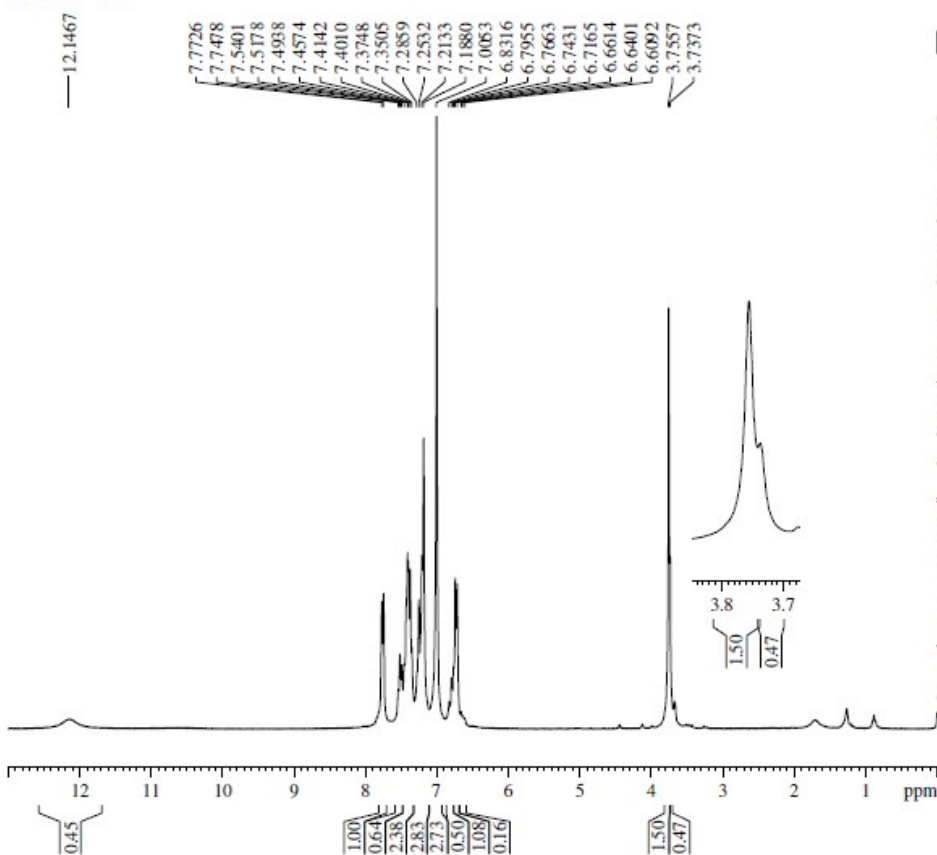


Current Data Parameters
NAME 20-Feb-FN-2020
EXPNO 420
PROCNO 1

F2 - Processing parameters
SI 65536
SF 282.5247960 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

S98: ¹⁹F NMR spectrum of 3zd

NRLD-436



Current Data Parameters
NAME 27-May-FN-2020
EXPNO 590
PROCNO 1

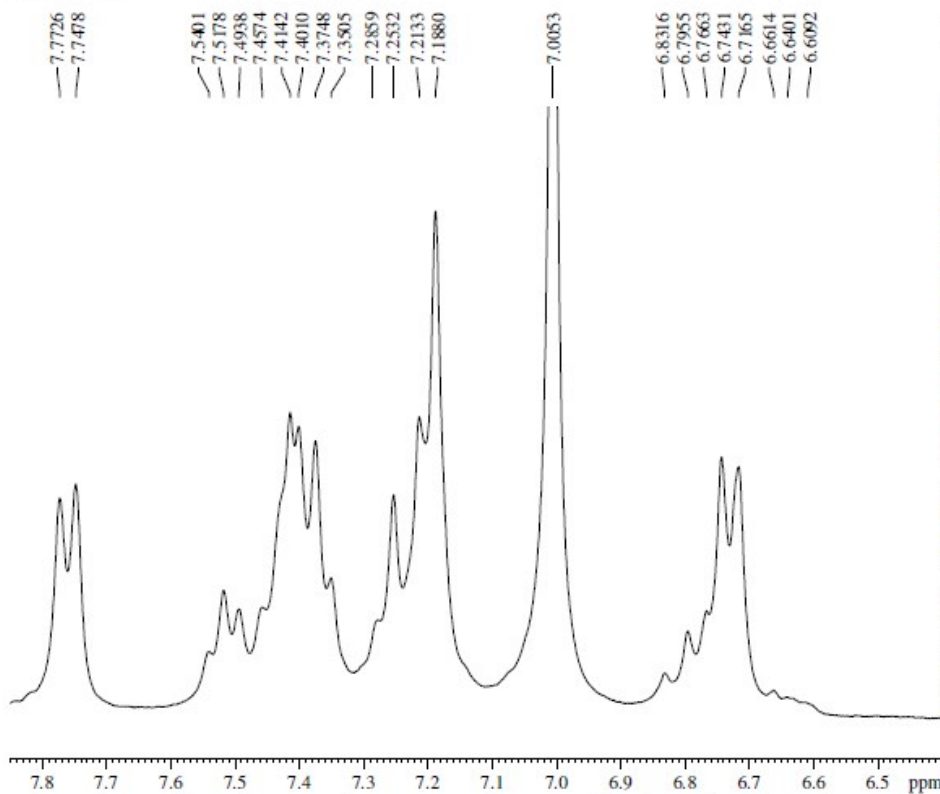
F2 - Acquisition Parameters
Date_ 20200527
Time 15.07
INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 6188.119 Hz
FIDRES 0.094423 Hz
AQ 5.2953086 sec
RG 181
DW 80.800 usec
DE 6.50 usec
TE 300.0 K
D1 1.00000000 sec
TD0 1

==== CHANNEL f1 ====
NUC1 1H
P1 13.95 usec
PL1 -1.00 dB
PL1W 15.02081871 W
SFO1 300.2598542 MHz

F2 - Processing parameters
SI 32768
SF 300.2580096 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

S99: ¹H NMR spectrum of 3ze

NRLD-436



S100: ¹H NMR spectrum of 3ze (expansion)



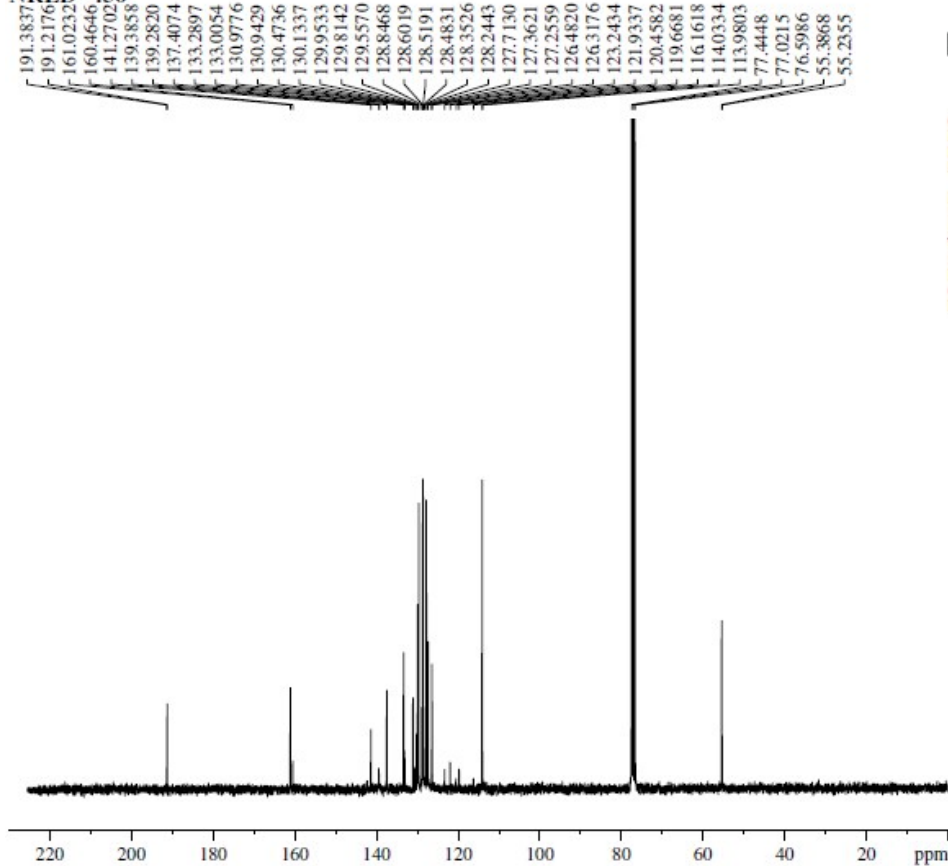
Current Data Parameters
 NAME 27-May-FN-2020
 EXPNO 590
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20200527
 Time 15.07
 INSTRUM spect
 PROBHD 5 mm QNP 1H/13
 PULPROG zg30
 TD 65536
 SOLVENT CDC13
 NS 16
 DS 2
 SWH 6188.119 Hz
 FIDRES 0.094423 Hz
 AQ 5.2953086 sec
 RG 181
 DW 80.800 usec
 DE 6.50 usec
 TE 300.0 K
 DT 1.00000000 sec
 TDO 1

==== CHANNEL f1 ====
 NUC1 1H
 P1 13.95 usec
 PL1 -1.00 dB
 PL1W 15.02081871 W
 SFO1 300.2598542 MHz

F2 - Processing parameters
 SI 32768
 SF 300.2580096 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

NRLD-436



S101: ¹³C NMR spectrum of 3ze



Current Data Parameters
 NAME 27-May-FN-2020
 EXPNO 600
 PROCNO 1

F2 - Processing parameters
 SI 32768
 SF 75.4999349 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40



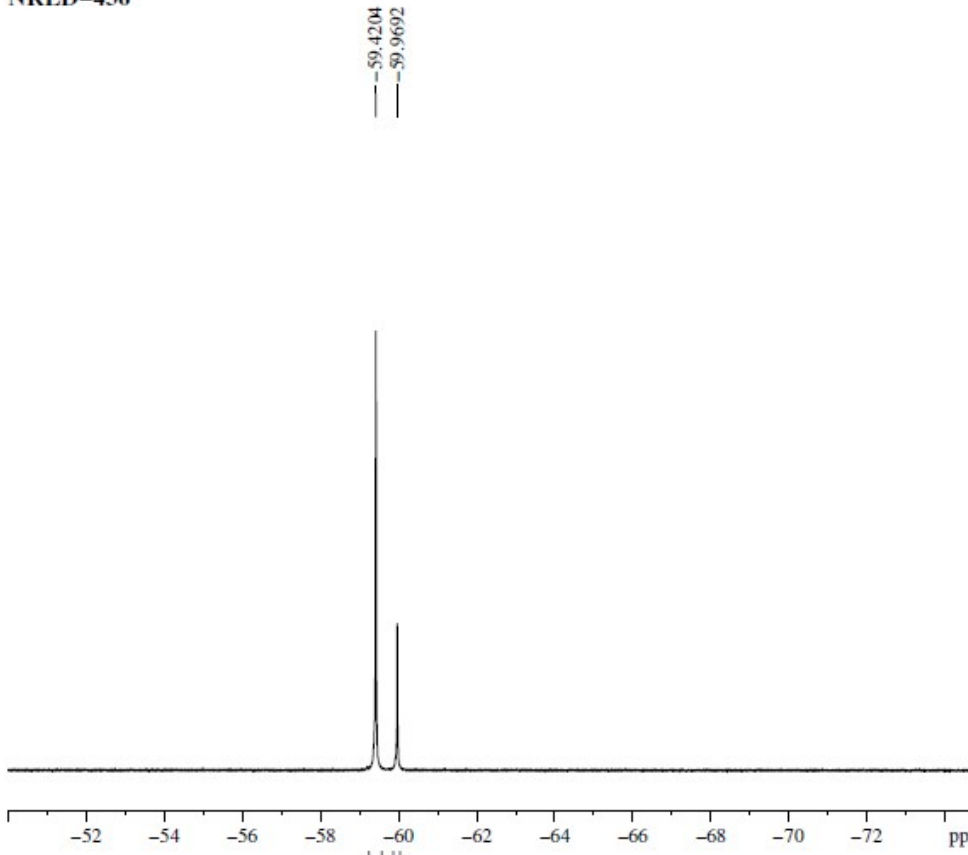
Current Data Parameters
 NAME 02-JUNE-FN-2020
 EXPNO 500
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20200602
 Time 17.16
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zgpg30
 TD 131072
 SOLVENT CDCl3
 NS 16
 DS 4
 SWH 89285.711 Hz
 FIDRES 0.681196 Hz
 AQ 0.7340032 sec
 RG 201.48
 DW 5.600 usec
 DE 6.50 usec
 TE 300.0 K
 D1 1.00000000 sec
 D11 0.03000000 sec
 D12 0.00002000 sec
 TD0 1

==== CHANNEL f1 ====
 SFO1 376.4894122 MHz
 NUC1 19F
 P1 15.00 usec
 PLW1 21.00000000 W

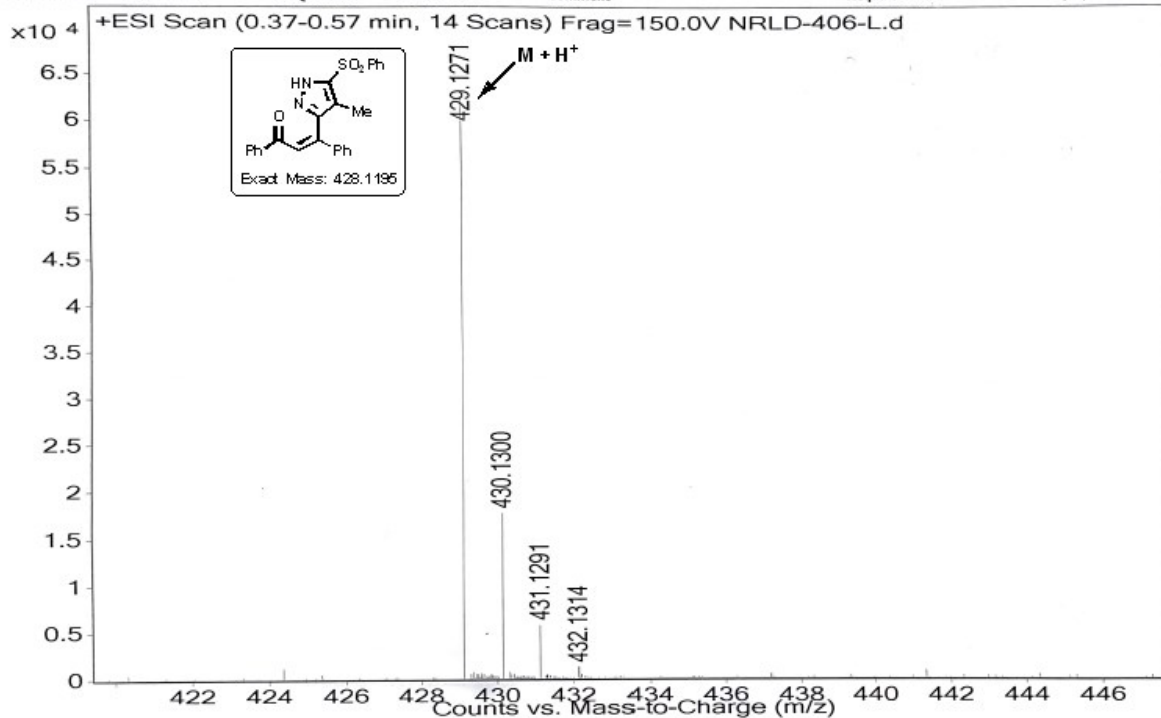
==== CHANNEL f2 ====
 SFO2 400.1621006 MHz
 NUC2 1H
 CPDPRG2 waltz16
 PCPD2 90.00 usec
 PLW2 13.00000000 W
 PLW12 0.27963999 W

F2 - Processing parameters
 SI 65556
 SF 376.5270650 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

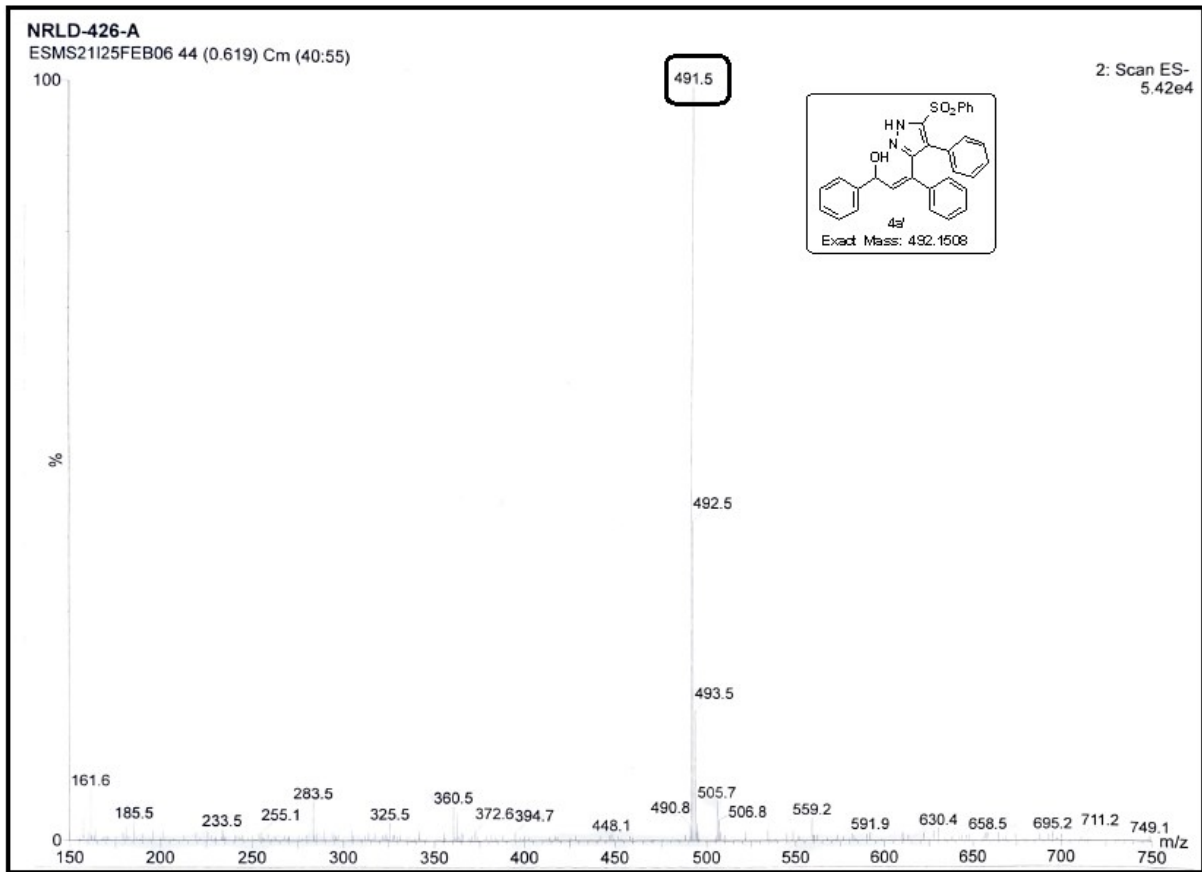


S102: ¹⁹F NMR spectrum of 3ze

Sample Name	HRMS20124JAN08	Position	Vial 8	Instrument Name	Instrument 1	User Name	
Inj Vol	2	InjPosition		SampleType	Sample	IRM Calibration Status	Success
Data Filename	NRLD-406-L.d	ACQ Method	ISOCRATIC.m	Comment		Acquired Time	1/24/2020 4:47:25 PM

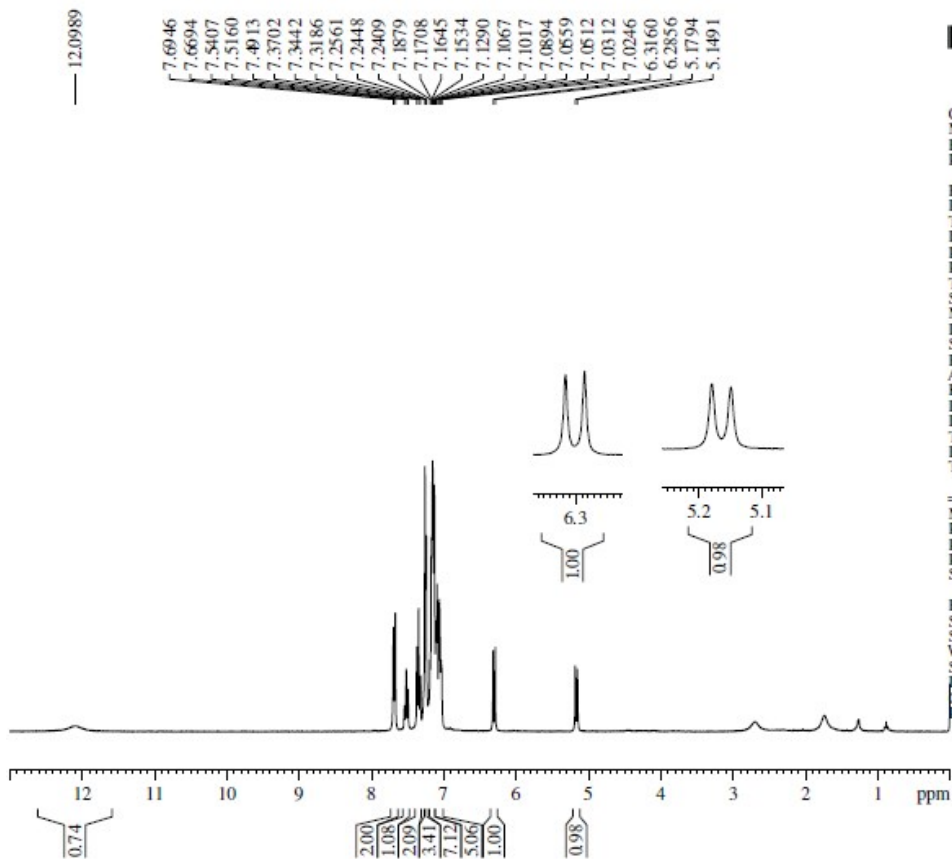


S103: HRMS of 3zf



S104: ESMS of 4a'

NRLD-426



Current Data Parameters
NAME 27-May-FN-2020
EXPNO 330
PROCNO 1

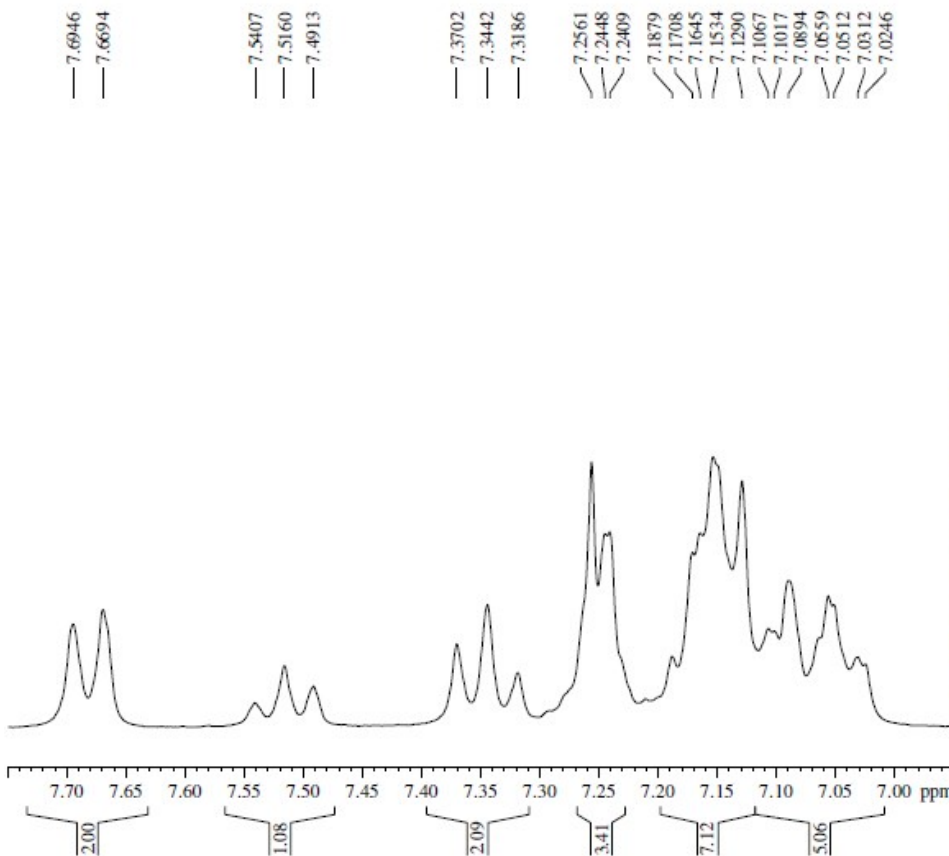
F2 - Acquisition Parameters
Date_ 20200527
Time 14.37
INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 6188.119 Hz
FIDRES 0.094423 Hz
AQ 5.2953086 sec
RG 256
DW 80.800 usec
DE 6.50 usec
TE 300.0 K
D1 1.0000000 sec
TD0 1

==== CHANNEL f1 ====
NUC1 1H
P1 13.95 usec
PL1 -1.00 dB
PL1W 15.02081871 W
SFO1 300.2598542 MHz

F2 - Processing parameters
SI 32768
SF 300.2580086 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

S105: ¹H NMR spectrum of 4a

NRLD-426



S106: ^1H NMR spectrum of 4a (expansion)



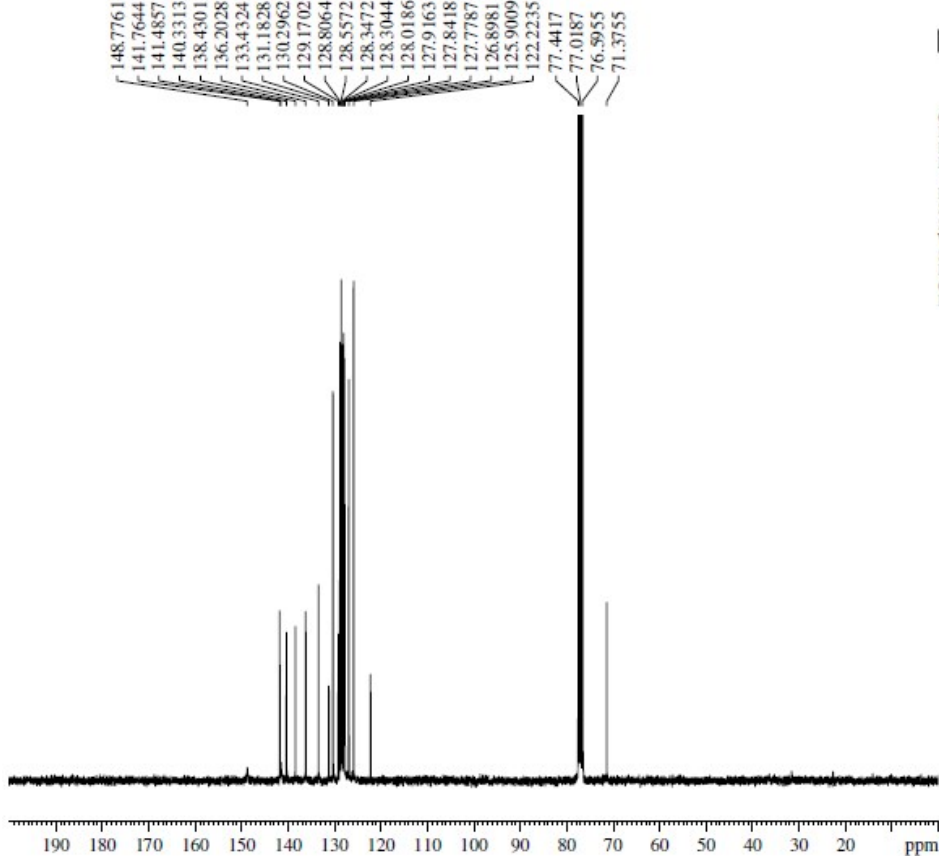
Current Data Parameters
NAME 27-May-FN-2020
EXPNO 330
PROCNO 1

F2 - Acquisition Parameters
Date_ 20200527
Time 14.37
INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 6188.119 Hz
FIDRES 0.094423 Hz
AQ 5.2953086 sec
RG 256
DW 80.800 usec
DE 6.50 usec
TE 300.0 K
D1 1.00000000 sec
TD0 1

==== CHANNEL f1 ====
NUC1 1H
P1 13.95 usec
PL1 -1.00 dB
PL1W 15.02081871 W
SFO1 300.2598542 MHz

F2 - Processing parameters
SI 32768
SF 300.2580086 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

NRLD-426



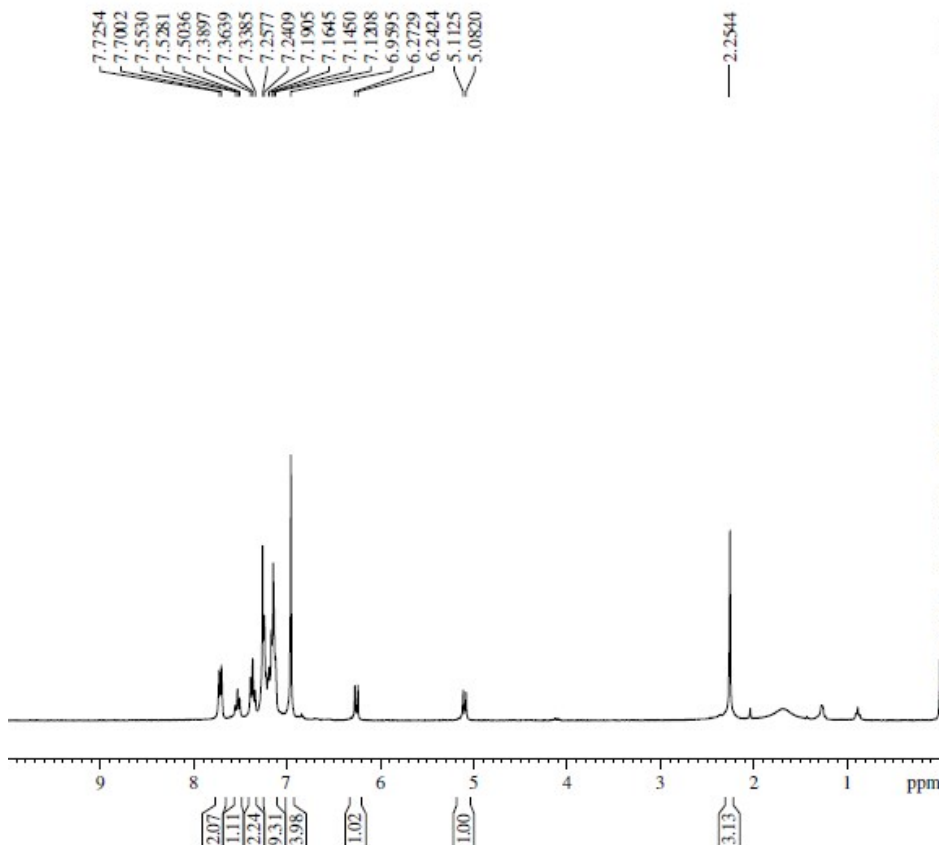
S107: ^{13}C NMR spectrum of 4a



Current Data Parameters
NAME 28-May-FN-2020
EXPNO 350
PROCNO 1

F2 - Processing parameters
SI 32768
SF 75.4999361 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

NRLD-438



S108: ^1H NMR spectrum of **4b**



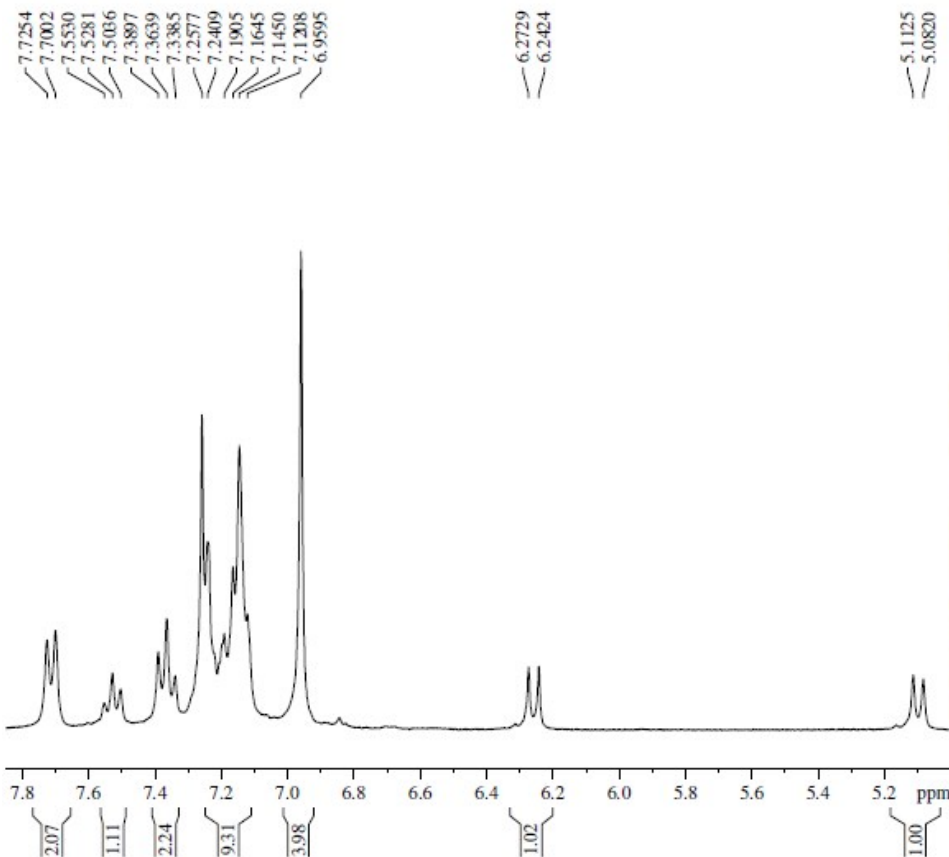
Current Data Parameters
NAME 03-June-FN-2020
EXPNO 390
PROCNO 1

F2 - Acquisition Parameters
Date_ 20200603
Time 11.53
INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 6188.119 Hz
FIDRES 0.094423 Hz
AQ 5.2953086 sec
RG 287
DW 80.800 usec
DE 6.50 usec
TE 300.0 K
D1 1.00000000 sec
TD0 1

==== CHANNEL f1 ====
NUC1 1H
P1 13.95 usec
PL1 -1.00 dB
PL1W 15.02081871 W
SFO1 300.2598542 MHz

F2 - Processing parameters
SI 32768
SF 300.2580081 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

NRLD-438



S109: ^1H NMR spectrum of **4b** (expansion)



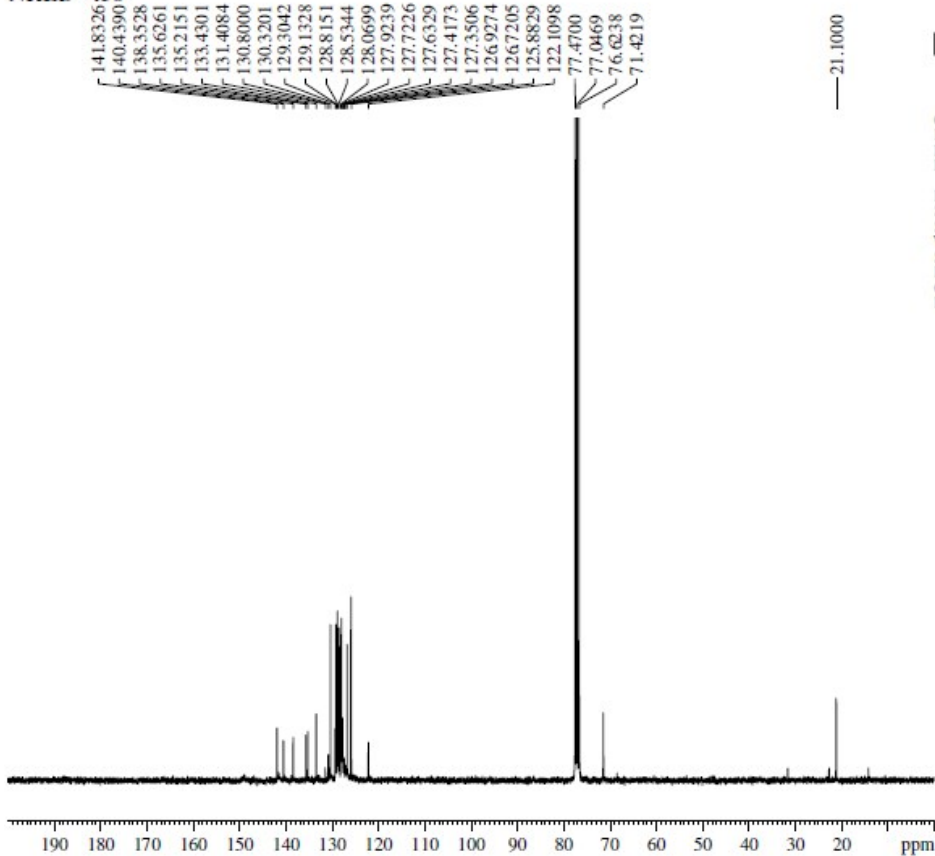
Current Data Parameters
NAME 03-June-FN-2020
EXPNO 390
PROCNO 1

F2 - Acquisition Parameters
Date_ 20200603
Time 11.53
INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 6188.119 Hz
FIDRES 0.094423 Hz
AQ 5.2953086 sec
RG 287
DW 80.800 usec
DE 6.50 usec
TE 300.0 K
D1 1.00000000 sec
TD0 1

==== CHANNEL f1 ====
NUC1 1H
P1 13.95 usec
PL1 -1.00 dB
PL1W 15.02081871 W
SFO1 300.2598542 MHz

F2 - Processing parameters
SI 32768
SF 300.2580081 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

NRLD-438

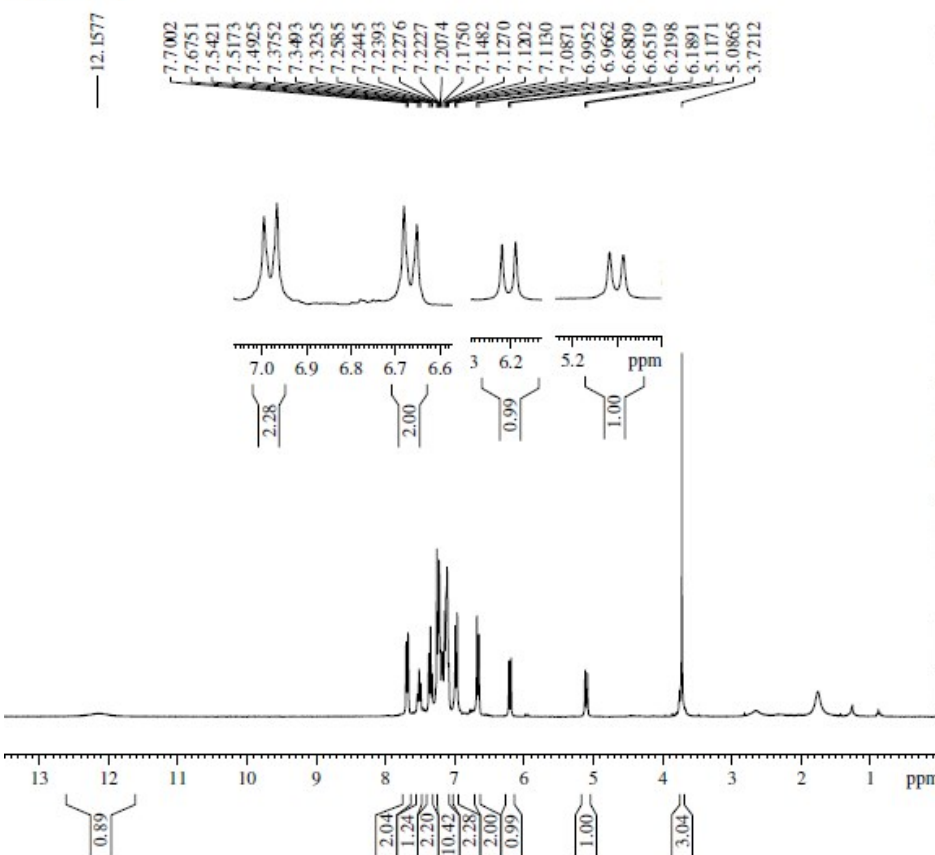


Current Data Parameters
NAME 04-JUNE-AN-2020
EXPNO 350
PROCNO 1

F2 - Processing parameters
SI 32768
SF 75.4999340 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

S110: ¹³C NMR spectrum of 4b

NRLD-394



Current Data Parameters
NAME 17-Jan-AN-2020
EXPNO 560
PROCNO 1

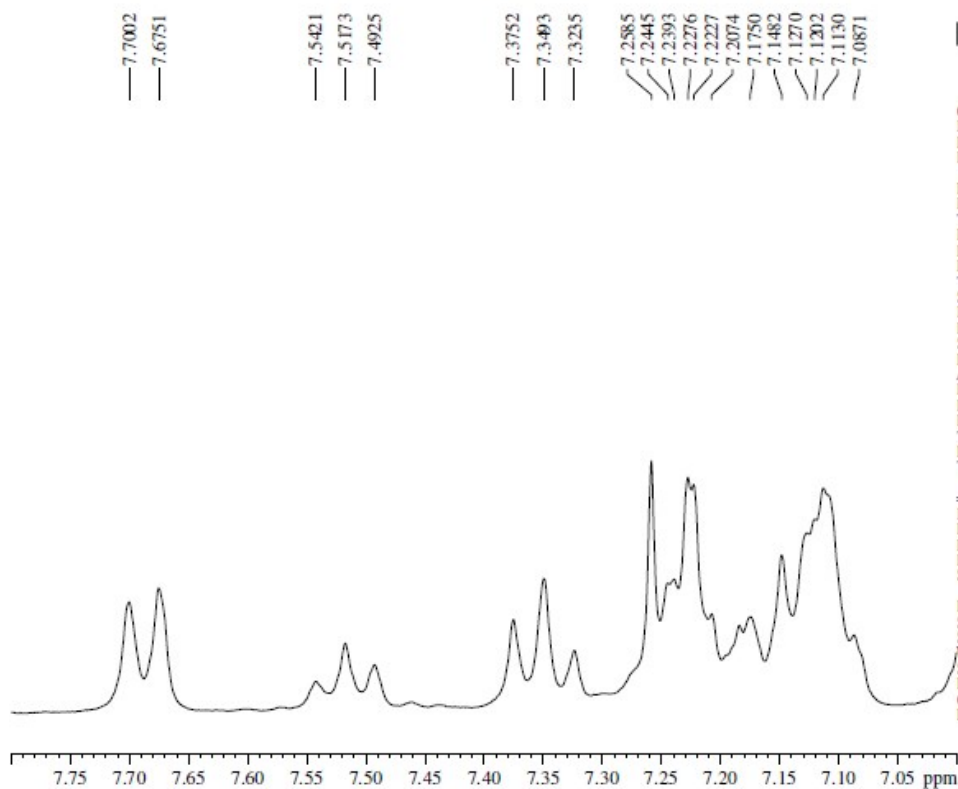
F2 - Acquisition Parameters
Date_ 20200117
Time 11.10
INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 6188.119 Hz
FIDRES 0.094423 Hz
AQ 5.2953086 sec
RG 287
DW 80.800 usec
DE 6.50 usec
TE 300.0 K
D1 1.00000000 sec
TD0 1

==== CHANNEL f1 ====
NUC1 1H
P1 13.95 usec
PL1 -1.00 dB
PL1W 15.02081871 W
SFO1 300.2598542 MHz

F2 - Processing parameters
SI 32768
SF 300.2580079 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

S111: ¹H NMR spectrum of 4c

NRLD-394



S112: ¹H NMR spectrum of 4c (expansion)



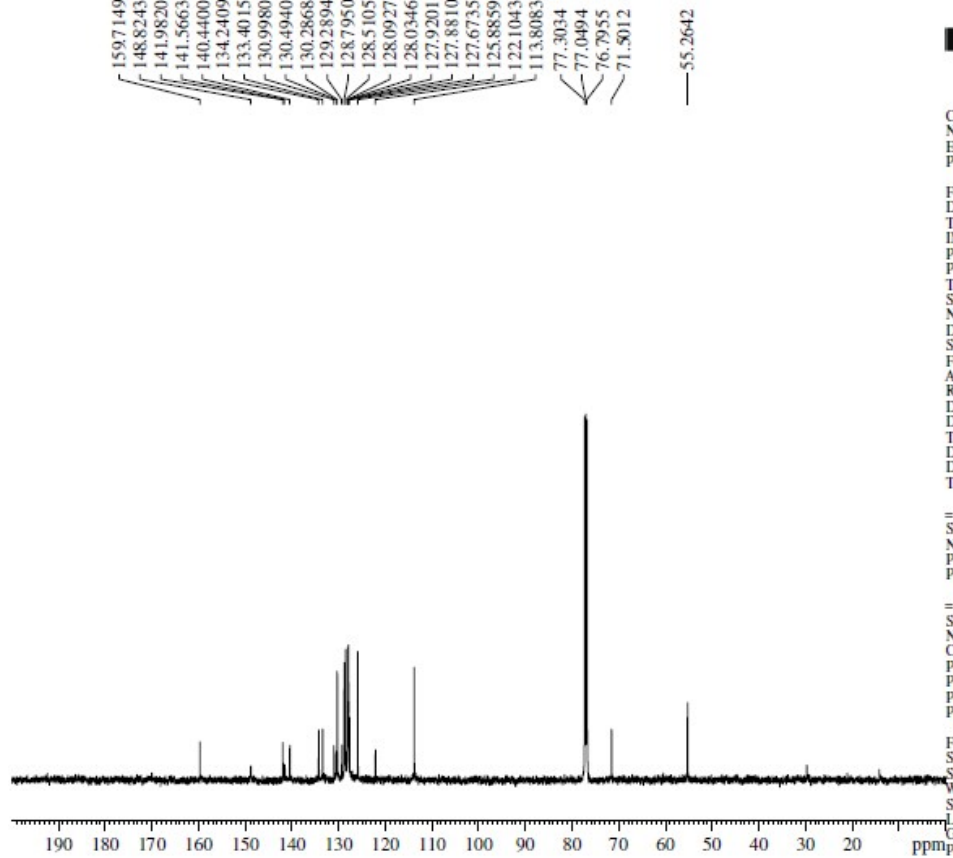
Current Data Parameters
NAME 17-Jan-AN-2020
EXPNO 560
PROCNO 1

F2 - Acquisition Parameters
Date_ 20200117
Time 11.10
INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG zg30
TD 65536
SOLVENT CDC13
NS 16
DS 2
SWH 6188.119 Hz
FIDRES 0.094423 Hz
AQ 5.2953086 sec
RG 287
DW 80.800 usec
DE 6.50 usec
TE 300.0 K
D1 1.00000000 sec
TD0 1

==== CHANNEL f1 ====
NUC1 1H
P1 13.95 usec
PL1 -1.00 dB
PL1W 15.02081871 W
SFO1 300.2598542 MHz

F2 - Processing parameters
SI 32768
SF 300.2580079 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

NRLD-394



S113: ¹³C NMR spectrum of 4c



Current Data Parameters
NAME 27-July-FN-2020
EXPNO 560
PROCNO 1

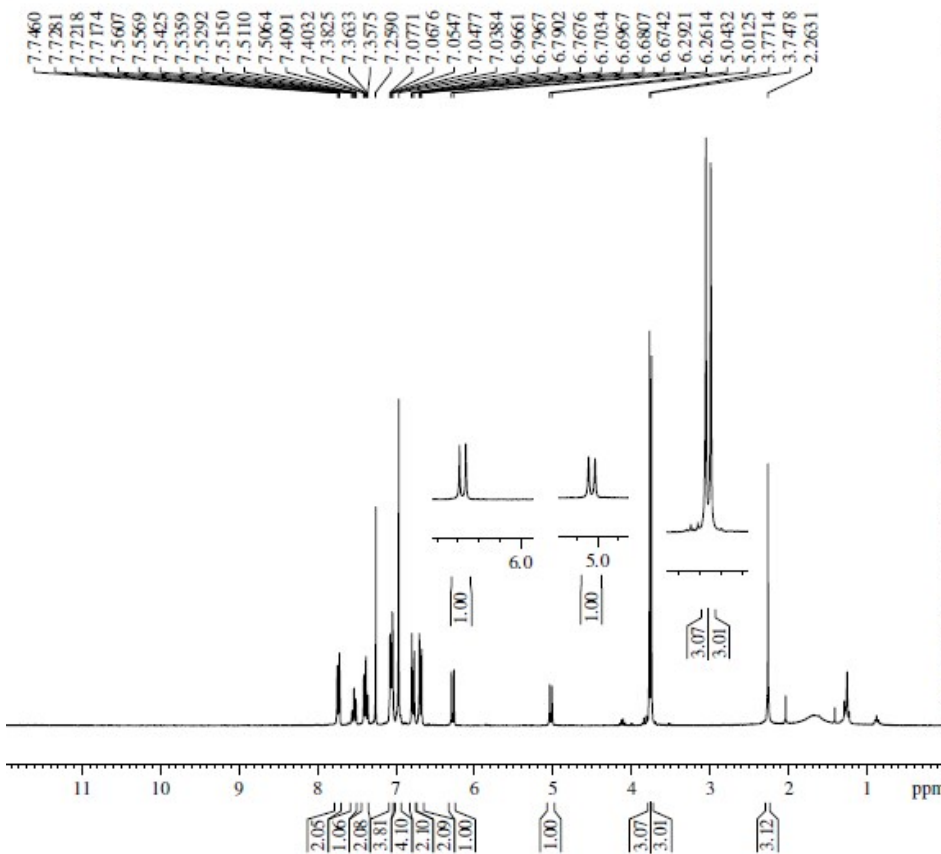
F2 - Acquisition Parameters
Date_ 20200727
Time 8.01
INSTRUM spect
PROBHD 5 mm PATX1 1H/
PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 4096
DS 0
SWH 29761.904 Hz
FIDRES 0.454131 Hz
AQ 1.1010048 sec
RG 56.22
DW 16.800 usec
DE 6.50 usec
TE 303.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

==== CHANNEL f1 ====
SFO1 125.9077573 MHz
NUC1 13C
P1 9.23 usec
PLW1 244.00000000 W

==== CHANNEL f2 ====
SFO2 500.6783527 MHz
NUC2 1H
CPDPRG[2] waltz16
PCPD2 80.00 usec
PLW2 13.60000038 W
PLW12 0.08840500 W
PLW13 0.05657900 W

F2 - Processing parameters
SI 32768
SF 125.8951680 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.40

NRLD-428



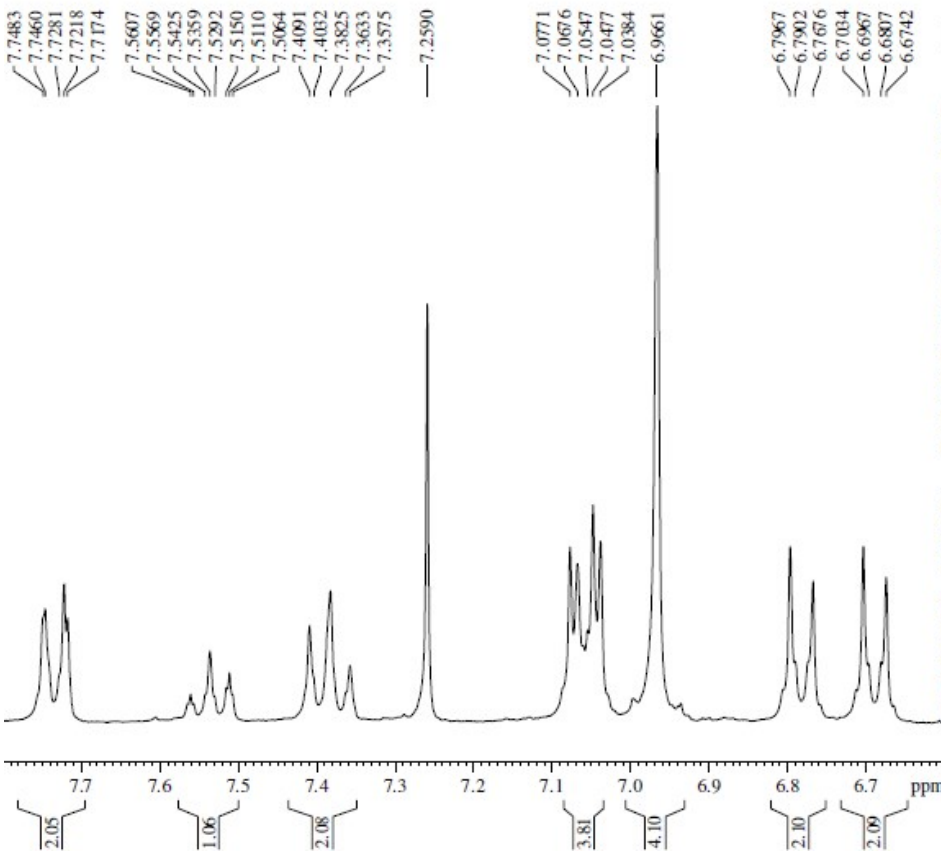
Current Data Parameters
 NAME 08-JUNE-AN-2020
 EXPNO 310
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20200608
 Time 15.42
 INSTRUM spect
 PROBHD 5 mm QNP 1H/13
 PULPROG zg30
 TD 65536
 SOLVENT CDC13
 NS 16
 DS 2
 SWH 6188.119 Hz
 FIDRES 0.094423 Hz
 AQ 5.2953086 sec
 RG 322
 DW 80.800 usec
 DE 6.50 usec
 TE 300.0 K
 D1 1.00000000 sec
 TDO 1

==== CHANNEL f1 ====
 NUC1 1H
 P1 13.95 usec
 PL1 -1.00 dB
 PL1W 15.02081871 W
 SFO1 300.2598542 MHz
 F2 - Processing parameters
 SI 32768
 SF 300.2580078 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

S114: ¹H NMR spectrum of 4d

NRLD-428



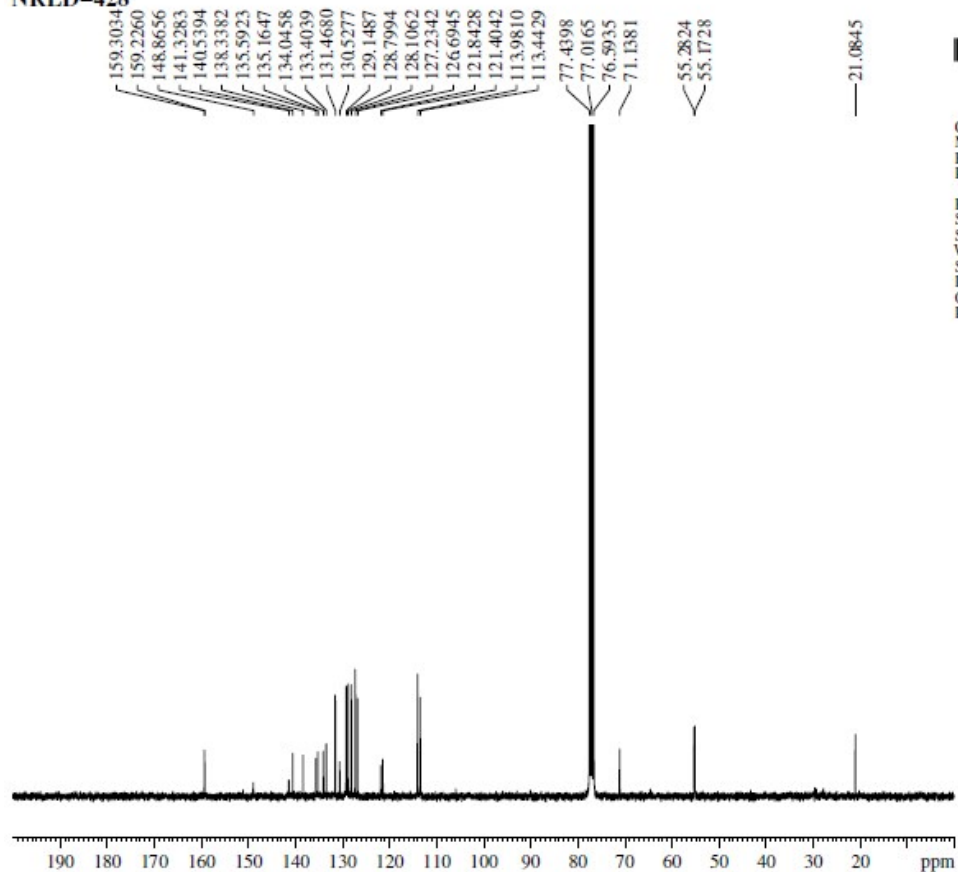
Current Data Parameters
 NAME 08-JUNE-AN-2020
 EXPNO 310
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20200608
 Time 15.42
 INSTRUM spect
 PROBHD 5 mm QNP 1H/13
 PULPROG zg30
 TD 65536
 SOLVENT CDC13
 NS 16
 DS 2
 SWH 6188.119 Hz
 FIDRES 0.094423 Hz
 AQ 5.2953086 sec
 RG 322
 DW 80.800 usec
 DE 6.50 usec
 TE 300.0 K
 D1 1.00000000 sec
 TDO 1

==== CHANNEL f1 ====
 NUC1 1H
 P1 13.95 usec
 PL1 -1.00 dB
 PL1W 15.02081871 W
 SFO1 300.2598542 MHz
 F2 - Processing parameters
 SI 32768
 SF 300.2580078 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

S115: ¹H NMR spectrum of 4d (expansion)

NRLD-428



Current Data Parameters
NAME 08-JUNE-AN-2020
EXPNO 320
PROCNO 1

F2 - Processing parameters
SI 32768
SF 75.4999347 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

S116: ¹³C NMR spectrum of 4d