Supporting Information

Hydroboration of vinylsilanes providing diversity-oriented hydrophobic building blocks for biofunctional molecules

Nao Namba, Shinya Fujii

Institute of Biomaterials and Bioengineering, Tokyo Medical and Dental University,

2-3-10 Kanda-Surugadai, Chiyoda-ku, Tokyo 101-0062, Japan

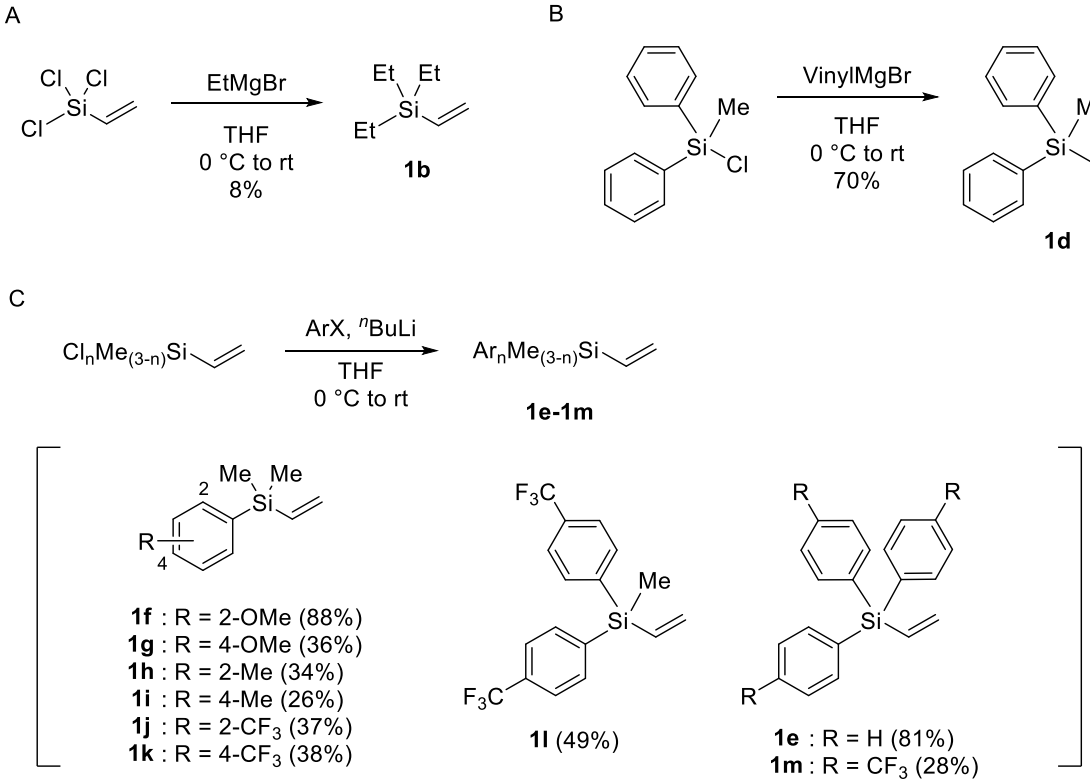
Table of Contents

1. Supplementary Figures
   - Scheme S1 2
   - Table S1 3

2. Experimental Procedure of Synthesis
   - 2.1. General remarks 4
   - 2.2. Synthesis of vinylsilanes **1b, 1d, 1e-m** 4
   - 2.3. Hydroboration of vinylsilanes 8
   - 2.4. Synthesis of silylethoxy derivatives **4a-e, 5a-e** 12
   - 2.5. References 15

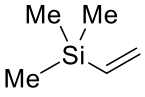
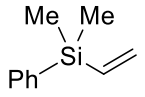
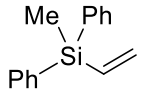
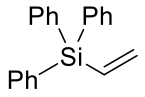
3. NMR spectra 16

1. Supplementary Scheme



Scheme. S1. Synthesis of vinylsilane substrates **1b,1d-1m**. A) Synthesis of triethyl(vinyl)silane **1b** using Ethylmagnesium bromide. B) Synthesis of Methyldiphenyl(vinyl)silane **1d** using vinylmagnesium bromide. C) Synthesis of arylvinylsilane **1e-1m** via lithiation of aryl halide.

Table S2. Calculation of transit state energy of **1a, c-e** using B3LYP/6-31G* basis.

		M-addition	AM-addition
 **1a**	E [au]	-513.901049	-513.902327
	H^0 [au]	-513.712465	-513.713090
	S^0 [J/mol]	433.14	426.80
	G^0 [au]	-513.761652	-513.761556
 **1c**	E [au]	-705.637937	-705.636334
	H^0 [au]	-705.395197	-705.393818
	S^0 [J/mol]	506.49	514.95
	G^0 [au]	-705.452713	-705.452296
 **1d**	E [au]	-897.373320	-897.371199
	H^0 [au]	-897.076345	-897.074217
	S^0 [J/mol]	582.59	587.88
	G^0 [au]	-897.142503	-897.140976
 **1e**	E [au]	-1077.34866	-1077.34411
	H^0 [au]	-1076.95618	-1076.95224
	S^0 [J/mol]	599.46	602.50
	G^0 [au]	-1077.02425	-1077.02065

2. Experimental Procedure of Synthesis

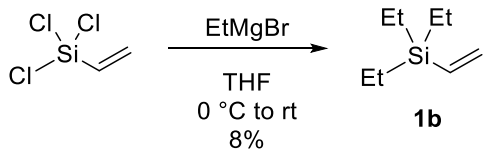
2.1. General remarks

All reagents were purchased from TCI Chemicals, Fujifilm Wako Pure Chemical Industries, or Kanto Kagaku Co. Inc., and used without further purification: Thin-layer chromatography (TLC) was performed using silica gel coated with a fluorescent indicator F254 (Merck, #1.05715.0001). Silica gel column chromatography was performed using neutral silica gel (60 Å, 40–50 μm) purchased from Kanto Kagaku Co. Inc. NMR spectra were recorded on Bruker Avance 400 (^{1}H: 400 MHz and ^{13}C: 101 MHz), Bruker Avance 500 (^{1}H: 500 MHz and ^{13}C: 126 MHz), and JEOL JNM-GX500 (^{1}H: 500 MHz, ^{13}C: 126 MHz) spectrometers. Chemical shift values for protons are referenced to the signal of the residual signal chloroform-d (δ 7.26) or acetone-d_6 (δ 2.05), and chemical shift values for carbons are referenced to the carbon resonance of chloroform-d (δ 77.16) or acetone-d_6 (δ 29.84). High-resolution mass (HRMS) spectra were taken on a Bruker Daltonics micrOTOF-2 using the electron spray ionization time-of-flight (ESI-TOF) method.

Due to their very low polarity, measurement of mass spectrometry was not possible for several compounds (**1h**, **1j**, **1l**, **1m**).

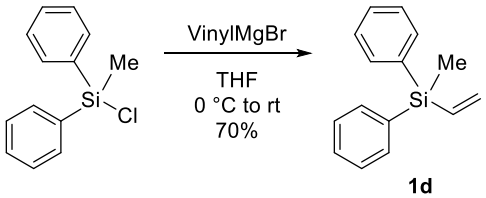
2.2. Synthesis of vinylsilanes **1b, 1d, 1e-m**

2.2.1. Preparation of triethyl(vinyl)silane **(1b)**



To a mixture of trichlorovinylsilane (0.63 mL, 5.0 mmol) and dry THF (15 mL) was added ethylmagnesium bromide (1.0 M THF solution, 15 mL, 15 mmol) dropwise under Ar atmosphere at 0 °C. The mixture was stirred at rt for 4 h. The reaction mixture was quenched with sat. NH_4Cl, and the whole was extracted with diethyl ether. The extract was successively washed with water and brine, and then dried over $MgSO_4$. The solvent was evaporated, and the residue was purified by means of silica gel column chromatography (Hexane) to give **1b** (57 mg, 8% yield) as colorless oil. The NMR spectra was identical to the reported data.[1]

2.2.2. Preparation of methyldiphenyl(vinyl)silane **(1d)**

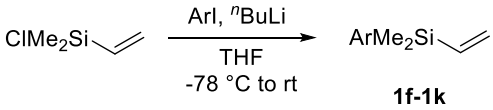


1d

To a mixture of diphenylmethylchlorovinyl silane (1.1 mL, 5.0 mmol) and dry THF (15 mL) was added vinylmagnesium bromide (1.0 M THF solution, 10 mL, 10 mmol) dropwise under Ar atmosphere at 0 ℃. The mixture was stirred at reflux condition for 5 h. The reaction mixture was quenched with sat. NH_4Cl, and the whole was extracted with ethyl acetate three times. The extract was successively washed with water and brine, and then dried over Na_2SO_4. The solvent was evaporated, and the residue was purified by means of silica gel column chromatography (Hex-EtOAc, EA = 0-5% gradient) to give **1d** (789 mg, 70% yield) as colorless oil. The NMR spectra was identical to the reported data.[2]

2.2.3. Synthesis of vinylsilanes via lithiation of aryl halides

2.2.3.1. *General Procedure A*



1f-1k

To a mixture of aryl iodide (1.00 mmol) and dry THF (5.0 mL) was added *n*-BuLi in *n*-Hexane (1.6 M hexane solution, 0.75 mL, 1.20 mmol) dropwise under Ar atmosphere at -78 ℃. The mixture was stirred at -78 ℃ for 1 h. dimethylchlorovinylsilane (0.28 mL, 2.0 mmol) was added and stirring at rt for 2 h. The reaction mixture was quenched with satulated NH_4Cl.aq, and the whole was extracted with EtOAc three times. The extract was successively washed with water and brine, and then dried over Na_2SO_4. The solvent was evaporated, and the residue was purified by means of silica gel column chromatography (Hex-EtOAc, EA=0-16% gradient) to give the target vinyl product.

2.2.3.2. (2-Methoxyphenyl)dimethyl(vinyl)silane (**1f**)

Following the general procedure A, **1f** was obtained as colorless oil in 88% yield as colorless oil. The NMR spectra was identical to the reported data.[3]

2.2.3.3. (4-Methoxyphenyl)dimethyl(vinyl)silane (**1g**)

Following the general procedure A, **1g** was obtained as colorless oil in 36% yield as colorless oil. The NMR spectra was identical to the reported data.[4]

2.2.3.4. Dimethyl(*o*-tolyl)(vinyl)silane (**1h**)

Following the general procedure A, **1h** was obtained as colorless oil in 34% yield as colorless oil. ^{1}H-NMR (400 MHz, $CDCl_3$) δ 7.48 (d, *J* = 7.2 Hz, 1H), 7.29 (t, *J* = 7.2 Hz, 1H), 7.19-7.15 (m, 2H), 6.35 (dd, *J* = 20.4 Hz, 14.4 Hz, 1H), 6.04 (dd, *J* = 14.4 Hz, 3.6 Hz, , 1H), 5.75 (dd, *J* = 20.4 Hz, 3.6 Hz, 1H), 2.44 (s, 3H), 0.40 (d, 6H, *J* = 0.8 Hz), ^{13}C-NMR (126 MHz, $CDCl_3$) δ 144.0, 138.8, 136.6, 135.0, 132.5, 129.9, 129.5, 125.1, 23.2, -1.9.

2.2.3.5. Dimethyl(*p*-tolyl)(vinyl)silane (**1i**)

Following the general procedure A, **1i** was obtained as colorless oil in 26% yield as colorless oil. The NMR spectra was identical to the reported data.[4]

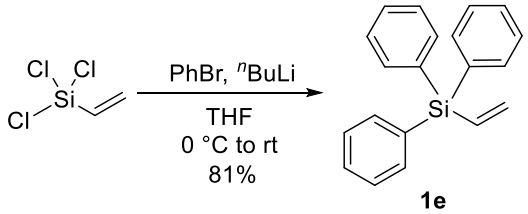
2.2.3.6. Dimethyl(2-(trifluoromethyl)phenyl)(vinyl)silane (**1j**)

Following the general procedure A, **1j** was obtained as colorless oil in 37% yield as colorless oil. ^{1}H-NMR (500 MHz, $CDCl_3$) δ 7.73-7.72 (m, 1H), 7.69-7.68 (m, 1H), 7.51-7.45 (m, 2H), 6.36 (dd, *J* = 20.3, 14.6 Hz, 1H), 6.06 (dd, *J* = 14.3, 3.4 Hz, 1H), 5.76 (dd, *J* = 20.3, 3.7 Hz, 1H), 0.42 (s, 6H), ^{13}C-NMR (126 MHz, $CDCl_3$) δ 138.4, 136.9, 136.7, 135.2 (q, *J* = 31 Hz) , 132.7, 130.8, 129.3, 128.4, 125.2 (q, *J* = 4.8 Hz) , 125.2 (q, *J* = 272 Hz), -1.5.

2.2.3.7. Dimethyl(4-(trifluoromethyl)phenyl)(vinyl)silane (**1k**)

Following the general procedure A, **1k** was obtained as colorless oil in 38% yield as colorless oil. The NMR spectra was identical to the reported data.[4]

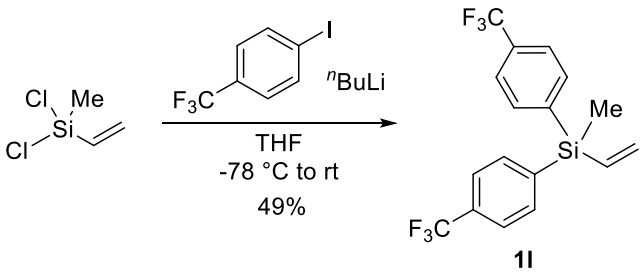
2.2.4. Synthesis of (triphenyl)dimethyl(vinyl)silane (**1e**)



1e

To a mixture of bromobenzene (2.1 mL, 20 mmol) and dry THF (25 mL) was added *n*-BuLi (1.6 M hexane solution, 13 mL, 20 mmol) dropwise under Ar atmosphere at -78 ℃. The mixture was stirred at -78 ℃ for 1 h. trichlorovinylsilane (0.6 mL, 5.0 mmol) was added and stirring at rt for 2 h. The reaction mixture was quenched with sat. NH_4Cl.aq, and the whole was extracted three times with EtOAc. The extract was successively washed with brine, and then dried over Na_2SO_4. The solvent was evaporated, and the residue was purified by means of silica gel column chromatography (Hex-EtOAc, EA = 4-9% gradient) to give **1e** as white solid (1.2 g, 81% isolated yield). The NMR spectra was identical to the reported data.[5]

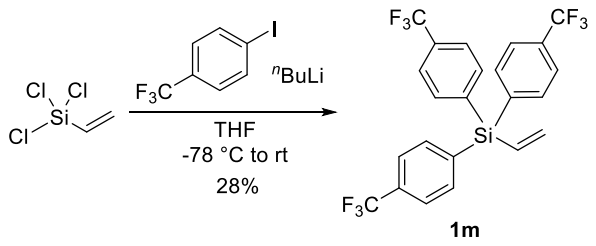
2.2.5. Synthesis of methylbis(4-(trifluoromethyl)phenyl)(vinyl)silane (**1l**)



1l

To a mixture of 1-iodo-4-(trifluoromethyl)benzene (0.44 mL, 3.0 mmol) and dry THF (15 mL) was added *n*-BuLi (2.6 M hexane solution, 1.4 mL, 3.6 mmol) dropwise under Ar atmosphere at -78 ℃. The mixture was stirred at -78 ℃ for 1 h. dichloromethylvinylsilane (0.2 mL, 1.8 mmol) was added and stirring at rt for 12 h. The reaction mixture was quenched with water, and the whole was extracted three times with EtOAc. The extract was successively washed with brine, and then dried over Na_2SO_4. The solvent was evaporated, and the residue was purified by means of silica gel column chromatography (Hex-EtOAc, EA = 4%) to give **1l** as colorless oil (528 mg, 49% isolated yield). ^{1}H-NMR (500 MHz, $CDCl_3$) δ 7.62 (s, 8H), 6.45 (dd, *J* = 20.0, 14.9 Hz, 1H), 6.27 (dd, *J* = 14.9, 3.4 Hz, 1H), 5.82 (dd, *J* = 20.0, 3.4 Hz, 1H), 0.68 (s, 3H), ^{13}C-NMR (126 MHz, $CDCl_3$) δ 140.5, 136.7, 135.2, 134.0, 131.8 (q, *J* = 33 Hz), 124.6 (q, *J* = 12 Hz), 126.2 (q, *J* = 271 Hz), -4.3.

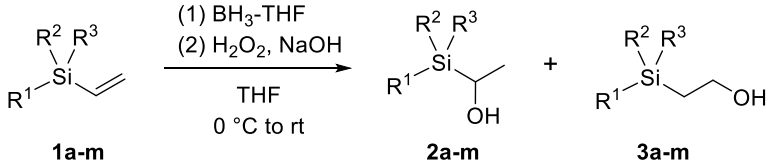
2.2.6. Synthesis of tris(4-(trifluoromethyl)phenyl)(vinyl)silane (**1m**)



1m

To a mixture of 4-trifluoromethyl iodobenzene (0.74 mL, 5.0 mmol) and dry THF (25 mL) was added *n*-BuLi (1.6 M hexane solution, 3.8 mL, 6.0 mmol) dropwise under Ar atmosphere at -78 ℃. The mixture was stirred at -78 ℃ for 1 h. trichlorovinylsilane (1.3 mL, 1.7 mmol) was added and stirring at rt for 12 h. The reaction mixture was quenched with sat. NH_4Cl, and the whole was extracted with EtOAc three times. The extract was successively washed with brine, and then dried over Na_2SO4. The solvent was evaporated, and the residue was purified by means of silica gel column chromatography (Hex-EtOAc, EA = 9%) to give the mixture contained **1m** as white needle-like crystal (273 mg, 28% NMR yield). The mixture was further purified by recrystallization (EtOH). mp 88.9-92.5 ℃; ^{1}H-NMR (400 MHz, $CDCl_3$) δ 7.65 (d, *J* = 8.4 Hz, 6H), 7.61 (d, *J* = 8.0 Hz, 6H), 6.67(dd, *J* = 20.4 Hz, 14.8 Hz, 1H), 6.44(dd, *J* = 14.8 Hz, 3.2 Hz, 1H), 5.84(dd, *J* = 20.4 Hz, 3.2 Hz, 1H), ^{13}C-NMR (126 MHz, $CDCl_3$) δ 139.3, 137.5, 136.3, 132.8, 132.4 (q, *J* = 32 Hz), 125.0, 124.1 (q, *J* = 272 Hz).

2.3. General procedures of hydroboration of vinylsilanes



BH_3 (0.9 M THF solution, 2.0 eq.) was added to a mixture of **1** (1.0 eq) and THF (0.2 M) under 0 ℃ and stirred for 10 min at the same temperature, then stirred at rt for 1 h. NaOH.aq (2 mol/L ca. 10 mL), H_2O_2.aq (30%, ca.10 mL) was dropped slowly under 0 ℃ and stirred for 10 min at the same temperature, then stirred at rt for 1 h. The reaction mixture was quenched by sat. NaCl. aq.

Extraction method B: The resulted mixture was extracted with diethylether for three times. The organic layer was successively washed with brine, and then dried over $MgSO_4$. The solvent was evaporated to obtain the crude product. The crude product was purified by means of silica gel column chromatography (Hex-EtOAc, EA=14%) to give **2** and **3** separately.

Extraction method C: The resulted mixture was extracted with ethyl acetate for three times. The extract was successively washed with brine, and then dried over Na_2SO_4. The solvent was evaporated to obtain the crude product. The crude product was purified by means of silica gel column chromatography (Hex-EtOAc, EA=14%) to give **2** and **3** separately.

1-Silylethanols **2a-m** were generally less polar (Rf = ca. 0.4 in the condition of Hex-EtOAc, EA=14%) than the corresponding 2-silylethanols **3a-m** (Rf = ca. 0.2 in the condition of Hex-EtOAc, EA=14%), and therefore these isomers can be easily separated by column chromatography.

2.3.1. 1-(Trimethylsilyl)ethan-1-ol (**2a**) and 2-(trimethylsilyl)ethan-1-ol (**3a**)

By using extraction method C, **2a**, **3a** were obtained in 30% NMR yield (**2a**), 30% NMR yield (**3a**), respectively. The NMR spectra was identical to the reported data.[6]

2.3.2. 1-(Triethylsilyl)ethan-1-ol (**2b**) and 2-(triethylsilyl)ethan-1-ol (**3b**)

By using extraction method C, **2b**, **3b** were obtained in 18% NMR yield (**2b**), 15% NMR yield (**3b**), respectively.

1-(Triethylsilyl)ethan-1-ol (**2b**): colorless oil; ^{1}H-NMR (500 MHz, $CDCl_3$) δ 3.64 (q, *J* = 7.6 Hz, 1H), 1.31 (d, *J* = 8.0 Hz, 3H), 0.99 (t, *J* = 8.0 Hz, 9H), 0.60 (qd, *J* = 7.9, 2.7 Hz, 6H); ^{13}C-NMR (126 MHz, $CDCl_3$) δ 60.3, 20.4, 7.6, 1.6; HRMS(ESI): Calculated for $C_8H_{20}KOSi$ $[M+K]^+$ 199.0915, found 199.0913.

2-(Triethylsilyl)ethan-1-ol (**3b**): colorless oil; 1H-NMR (500 MHz, $CDCl_3$) δ 3.74-3.71 (m, 2H), 1.00-0.97 (m, 2H), 0.93 (t, J = 8.6 Hz, 9H), 0.52 (q, J = 7.8 Hz, 6H); 13C-NMR (126 MHz, $CDCl_3$) δ 60.2, 17.6, 7.5, 3.6; HRMS(ESI): Calculated for $C_{16}H_{40}NaO_2Si_2$ $[2M+Na]^+$ 343.2459, found 343.2460.

2.3.3. 1-(Dimethyl(phenyl)silyl)ethan-1-ol (**2c**) and 2-(dimethyl(phenyl)silyl)ethan-1-ol (**3c**)

By using extraction method D, **2c**, **3c** were obtained in 65% NMR yield (**2c**), 33% NMR yield (**3c**), respectively. The NMR spectra was identical to the reported data.[7]

2.3.4. 1-(Methyldiphenylsilyl)ethan-1-ol (**2d**) and 2-(methyldiphenylsilyl)ethan-1-ol (**3d**)

By using extraction method D, **2d**, **3d** were obtained in 53% NMR yield (**2d**), 27% NMR yield (**3d**), respectively. The NMR spectra of **3d** was identical to the reported data.[8]

1-(Methyldiphenylsilyl)ethan-1-ol (**2d**): colorless oil, ^{1}H-NMR (500 MHz, $CDCl_3$) δ 7.64-7.62 (m, 2H), 7.60-7.58 (m, 2H), 7.44-7.36 (m, 6H), 4.08 (qd, *J* = 7.3, 2.9 Hz, 1H), 1.37 (d, *J* = 7.4 Hz, 3H), 1.11 (d, *J* = 3.4 Hz, 1H), 0.60 (s, 3H); ^{13}C-NMR (126 MHz, $CDCl_3$) δ 136.3, 133.0, 130.0, 128.2, 60.4, 20.2; HRMS(ESI): Calculated for $C_{15}H_{18}NaOSi$ $[M+Na]^+$ 265.1019, found 265.1012

2.3.5. 1-(Triphenylsilyl)ethan-1-ol (**2e**) nad 2-(triphenylsilyl)ethan-1-ol (**3e**)

By using extraction method D, **2e**, **3e** were obtained in 50% NMR yield (**2e**), 18% NMR yield (**3e**), respectively. The NMR spectra of **3e** was identical to the reported data.[8]

2-(Triphenylsilyl)ethan-1-ol (**2e**) : white solid; mp 99.7-102.5 °C; ^{1}H-NMR (500 MHz, $CDCl_3$) δ 7.65-7.61 (m, 7H), 7.46-7.43 (m, 3H), 7.40-7.37 (m, 7H), 4.39 (qd, *J* = 7.5, 4.7 Hz, 1H), 1.50 (d, *J* = 7.4 Hz, 3H), 1.25 (d, *J* = 5.2 Hz, 1H); ^{13}C-NMR (126 MHz, $CDCl_3$) δ 136.3, 133.0, 130.0, 128.2, 60.4, 20.2; HRMS(ESI): Calculated for $C_{20}H_{20}NaOSi$ $[M+Na]^+$ 327.1176, found 327.1168

2.3.6. 1-((2-Methoxyphenyl)dimethylsilyl)ethan-1-ol (**2f**) and 2-((2-methoxyphenyl)dimethylsilyl)ethan-1-ol (**3f**)

By using extraction method D, **2f**, **3f** were obtained in 42% NMR yield (**2f**), 17% NMR yield (**3f**), respectively.

1-((2-Methoxyphenyl)dimethyllsilyl)ethan-1-ol (**2f**): colorless oil; ^{1}H-NMR (500 MHz, acetone-d_6) δ 7.42 (dd, *J* = 7.4, 1.7 Hz, 1H), 7.35 (td, *J* = 7.7, 1.5 Hz, 1H), 6.95-6.92 (m, 2H), 3.82 (s, 3H), 3.81-3.74 (m, 1H), 3.03 (d, *J* = 5.2 Hz, 1H), 1.18 (d, *J* = 7.4 Hz, 3H), 0.27 (s, 3H), 0.25 (s, 3H); ^{13}C-NMR (126 MHz, acetone-d_6) δ 165.2, 136.4, 131.8, 126.0, 121.3, 110.6, 60.1, 55.5, 20.1, -4.7, -5.4; HRMS(ESI): Calculated for $C_{11}H_{19}O_2Si$ $[M+H]^+$ 211.1149, found 211.1154

2-((2-Methoxyphenyl)dimethylsilyl)ethan-1-ol (**3f**): colorless oil; ^{1}H-NMR (500 MHz, acetone-d_6) δ 7.36-7.33 (m, 2H), 6.94-6.91 (m, 2H), 3.82 (s, 3H), 3.64-3.60 (m, 2H), 3.37 (t, *J* = 4.9 Hz, 1H), 1.20-1.17 (m, 2H), 0.26 (s, 6H); ^{13}C-NMR (126 MHz, acetone-d_6) δ 164.5, 135.0, 131.0, 126.2, 120.5, 109.7, 58.8, 54.6, 20.8, -2.9; HRMS(ESI): Calculated for $C_{11}H_{18}NaO_2Si$ $[M+Na]^+$ 233.0968, found 233.0966

2.3.7. 1-((4-Methoxyphenyl)dimethylsilyl)ethan-1-ol (**2g**) and 2-((4-methoxyphenyl)dimethylsilyl)ethan-1-ol (**3g**)

By using extraction method D, **2g**, **3g** were obtained in 44% NMR yield (**2g**), 23% NMR yield (**3g**), respectively.

1-((4-Mmethoxyphenyl)dimethylsilyl)ethan-1-ol (**2g**): colorless oil; ^{1}H-NMR (400 MHz, acetone-d_6) δ 7.51 (d, *J* = 8.4 Hz, 2H), 6.92 (d, *J* = 8.8 Hz, 2H), 3.79 (s, 3H), 3.64-3.57 (m, 1H), 3.16 (d, *J* = 4.8 Hz, 1H), 1.20 (d, *J* = 7.6 Hz,

3H), 0.26 (s, 3H), 0.25 (s, 3H); ^{13}C-NMR (126 MHz, acetone-d_6) δ 161.5, 136.4, 128.9, 114.2, 60.4, 55.2, 20.0, -5.1, -5.4; HRMS(ESI): Calculated for $C_{11}H_{18}NaO_2Si$ $[M+Na]^+$ 233.0968, found 233.0967

2-((4-methoxyphenyl)dimethylsilyl)ethan-1-ol (**3g**) The NMR spectra was identical to the reported data.[9]

2.3.8. 1-(Dimethyl(*o*-tolyl)silyl)ethan-1-ol (**2h**) and 2-(dimethyl(*o*-tolyl)silyl)ethan-1-ol (**3h**)

By using extraction method D, **2h**, **3h** were obtained in 60% NMR yield (**2h**), 23% NMR yield (**3h**), respectively.

1-(Dimethyl(o-tolyl)silyl)ethan-1-ol (**2h**): colorless oil; ^{1}H-NMR (400 MHz, $CDCl_3$) δ 7.52-7.49 (m, 1H), 7.31-7.27 (m, 1H), 7.20-7.16 (m, 2H), 3.86 (q, *J* = 7.6 Hz, 1H), 2.47 (s, 3H), 1.29 (d, *J* = 7.6 Hz, 3H), 0.40 (s, 3H), 0.36 (s, 3H); 13C-NMR (126 MHz, $CDCl_3$) δ 144.0, 135.4, 135.0, 130.1, 129.7, 125.2, 61.1, 23.6, 19.7; HRMS(ESI): Calculated for $C_{11}H_{18}NaOSi$ $[M+Na]^+$ 217.1019, found 217.1022

2-(Dimethyl(o-tolyl)silyl)ethan-1-ol (**3h**): colorless oil; ^{1}H-NMR (400 MHz, $CDCl_3$) δ 7.46-7.43 (m, 1H), 7.30-7.28 (m, 1H), 7.19-7.15(m, 2H), 3.75-3.71 (m, 2H), 2.46 (s, 3H), 1.30-1.26 (m, 2H), 0.36 (s, 6H); ^{13}C-NMR (126 MHz, $CDCl_3$) δ 143.7, 136.7, 134.6, 130.1, 129.6, 125.2, 60.3, 23.2, 21.5, -1.4; HRMS(ESI): Calculated for $C_{11}H_{18}NaOSi$ $[M+Na]^+$ 217.1019, found 217.1016

2.3.9. 1-(Dimethyl(*p*-tolyl)silyl)ethan-1-ol (**2i**) and 2-(dimethyl(*p*-tolyl)silyl)ethan-1-ol (**3i**)

By using extraction method D, **2i**, **3i** were obtained in 46% NMR yield (**2i**), 22% NMR yield (**3i**), respectively.

1-(Dimethyl(*p*-tolyl)silyl)ethan-1-ol (**2i**): colorless oil; ^{1}H-NMR (400 MHz, $CDCl_3$) δ 7.46 (d, *J* = 8.0 Hz, 2H), 7.20 (d, *J* =7.6 Hz, 2H), 3.66 (q, *J* = 7.2 Hz, 1H), 2.36 (s, 3H), 1.28 (d, *J* = 7.6 Hz, 3H), 0.32 (s, 3H), 0.31 (s, 3H); ^{13}C-NMR (126 MHz, $CDCl_3$) δ 139.4, 134.3, 132.8, 128.9, 61.3, 21.6, 19.5, -5.5, -5.9; HRMS(ESI): Calculated for $C_{11}H_{18}NaOSi$ $[M+Na]^+$ 217.1019, found 217.1025

2-(Dimethyl(*p*-tolyl)silyl)ethan-1-ol (**3i**): The NMR spectra was identical to the reported data.[10]

2.3.10. 1-(Dimethyl(2-(trifluoromethyl)phenyl)silyl)ethan-1-ol (**2j**) and
2-(dimethyl(2-(trifluoromethyl)phenyl)silyl)ethan-1-ol (**3j**)

By using extraction method D, **2j**, **3j** were obtained in 50% NMR yield (**2j**), 24% NMR yield (**3j**), respectively.

1-(Dimethyl(2-(trifluoromethyl)phenyl)silyl)ethan-1-ol (**2j**): colorless oil; ^{1}H-NMR (400 MHz, $CDCl_3$) δ 7.81 (d, *J* = 7.2 Hz, 1H), 7.71 (d, *J* = 7.6 Hz, 1H), 7.55-7.47 (m, 2H), 3.89 (qd, *J* = 7.6 Hz, 0.8Hz, 1H), 1.27 (d, *J* = 7.6 Hz, 3H), 0.42 (d, *J* = 1.2 Hz, 3H), 0.38 (d, *J* = 1.2Hz, 3H); ^{13}C-NMR (126 MHz, $CDCl_3$) δ 136.8, 135.2 (q, *J* = 30 Hz), 130.9, 129.5, 126.3 (q, *J* = 5.9 Hz), 125.0 (q, *J* = 274 Hz), 61.0, 19.8, -4.0, -4.2; HRMS(ESI): Calculated for $C_{11}H_{15}ClF_3OSi$ $[M+Cl]^-$ 283.0538, found 283.0532

2-(Dmethyl(2-(trifluoromethyl)phenyl)silyl)ethan-1-ol (**3j**): colorless oil; ^{1}H-NMR (400 MHz, $CDCl_3$) δ 7.70 (d, *J* = 7.6 Hz, 2H), 7.54-7.46 (m, 2H), 3.72-3.68 (m, 2H), 1.30-1.26 (m, 2H), 0.39 (d, *J* = 1.2 Hz, 6H); ^{13}C-NMR (126 MHz, $CDCl_3$) δ 136.7, 136.2, 135.0 (q, *J* = 31 Hz), 130.9, 129.4,126.3 (q, *J* = 4.8 Hz), 125.1 (q, *J* = 274 Hz), 60.1, 21.8, -0.9; HRMS(ESI): Calculated for $C_{11}H_{15}F_3NaOSi$ $[M+Na]^+$ 271.0736, found 271.0727

2.3.11. 1-(Dimethyl(4-(trifluoromethyl)phenyl)silyl)ethan-1-ol (**2k**) and 2-(dimethyl(4-(trifluoromethyl)phenyl)silyl)ethan-1-ol (**3k**)

By using extraction method D, **2k**, **3k** were obtained in 52% NMR yield (**2k**), 19% NMR yield (**3k**), respectively.

1-(Dimethyl(4-(trifluoromethyl)phenyl)silyl)ethan-1-ol (**2k**): colorless oil; ^{1}H-NMR (400 MHz, $CDCl_3$) δ 7.69 (d, *J* = 7.6 Hz, 2H), 7.61 (d, *J* = 7.6 Hz, 2H), 3.71 (q, *J* = 7.2 Hz, 1H), 1.29 (d, *J* = 7.6 Hz, 3H), 0.36 (s, 3H), 0.35 (s, 3H); ^{13}C-NMR (126 MHz, $CDCl_3$) δ 141.8, 134.6, 131.4 (q, *J* = 32 Hz), 126.5 (q, *J* = 3.7 Hz), 124.3 (q, *J* = 271 Hz), 123.2, 121.1, 61.0, 19.7, -5.6; HRMS(ESI): Calculated for $C_{11}H_{15}F_3NaOSi$ $[M+Na]^+$ 271.0736, found 271.0739

2-(Dimethyl (4-(trifluoromethyl)phenyl)silyl)ethan-1-ol (**3k**): colorless oil; ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.63 (d, *J* = 8.0 Hz, 2H), 7.60 (d, *J* = 8.4 Hz, 2H), 3.76-3.72 (m, 2H), 1.26-1.19 (m, 2H), 0.33 (s, 3H); ^{13}C-NMR (126 MHz, $CDCl_3$) δ 143.8, 133.9,131.2 (q, *J* = 31 Hz),124.5 (q, *J* = 3.5 Hz), 124.3 (q, *J* = 273 Hz), 59.9, 20.9, -2.7; HRMS(ESI): Calculated for $C_{11}H_{15}F_3NaOSi$ $[M+Na]^+$ 271.0736, found 271.0737

2.3.12. 1-(Methylbis(4-(trifluoromethyl)phenyl)silyl)ethan-1-ol (**2l**) and 2-(methylbis(4-(trifluoromethyl)phenyl)silyl)ethan-1-ol (**3l**)

By using extraction method D, **2l**, **3l** were obtained in 55% NMR yield (**2l**), 18% NMR yield (**3l**), respectively.

1-(Methylbis(4-(trifluoromethyl)phenyl)silyl)ethan-1-ol (**2l**): colorless oil; ^{1}H-NMR (400 MHz, $CDCl_3$) δ 7.75 (d, *J* = 7.6 Hz, 2H), 7.70 (d, *J* = 7.6 Hz, 2H),7.64-7.62(m, 4H), 4.12 (q, *J* = 7.6 Hz, 1H), 1.37 (d, *J* = 7.6 Hz, 3H), 0.65(s, 3H); ^{13}C-NMR (126 MHz, $CDCl_3$) δ 139.4, 138.9, 135.6, 135.3, 132.5 (q, *J* = 32 Hz), 131.9 (q, *J* = 33 Hz), 124.8, 124.2 (q, *J* = 273 Hz), 60.2, 20.1, -6.9; HRMS(ESI): Calculated for $C_{17}H_{16}F_6NaOSi$ $[M+Na]^+$ 401.0767, found 401.0782

2-(Methylbis(4-(trifluoromethyl)phenyl)silyl)ethan-1-ol (**3l**): brown oil; ^{1}H-NMR (500 MHz, $CDCl_3$) δ 7.62 (s, 8H), 3.82-3.79 (m, 2H), 1.57-1.54 (m, 2H), 0.66 (s, 3H); ^{13}C-NMR (126 MHz, $CDCl_3$) δ 140.9, 134.8, 131.8 (q, *J* = 33 Hz),124.8 (q, *J* = 3.6 Hz), 124.2 (q, *J* = 273 Hz), 59.5, 19.0, -4.0; HRMS(ESI): Calculated for $C_{17}H_{16}F_6NaOSi$ $[M+Na]^+$ 401.0767, found 401.0774

2.3.13. 1-(Tris(4-(trifluoromethyl)phenyl)silyl)ethan-1-ol (**2m**) and 2-(tris(4-(trifluoromethyl)phenyl)silyl)ethan-1-ol (**3m**)

By using extraction method D, **2m**, **3m** were obtained in 43% NMR yield (**2m**), 16% NMR yield (**3m**), respectively.

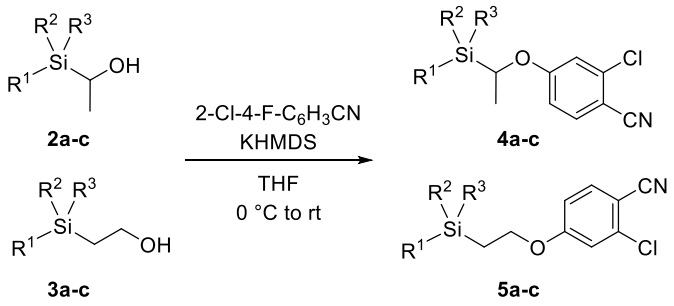
1-(Tris(4-(trifluoromethyl)phenyl)silyl)ethan-1-ol (**2m**): white solid; mp 124.8-127.2 °C; ^{1}H-NMR (400 MHz, $CDCl_3$) δ 7.73 (d, *J* = 8.0 Hz, 6H), 7.66 (d, *J* = 8.0 Hz, 1H), 4.47 (q, *J* = 7.6 Hz, 1H), 1.51 (d, *J* = 7.6 Hz, 3H); ^{13}C-NMR (126 MHz, $CDCl_3$) δ 136.6, 136.5, 132.5 (q, *J* = 33 Hz), 125.1 (q, *J* = 20 Hz), 124.1 (q, *J* = 273 Hz), 59.9, 20.6; HRMS(ESI): Calculated for $C_{23}H_{17}F_9NaOSi$ $[M+Na]^+$ 531.0797, found 531.0797

2-(Tris(4-(trifluoromethyl)phenyl)silyl)ethan-1-ol (**3m**): white solid; mp 124.4-125.9 °C; ^{1}H-NMR (500 MHz, $CDCl_3$) δ 7.65 (d, *J* = 8.6 Hz, 6H), 7.63 (d, *J* = 8.0 Hz, 7H), 3.90-3.86 (m, 2H), 1.90-1.87 (m, 2H); ^{13}C-NMR (126

MHz, $CDCl_3$) δ 138.1, 135.9, 132.7, 132.5, 132.2, 132.0, 127.3, 125.1, 125.0, 125.0, 123.0, 120.8, 59.1, 17.8; HRMS(ESI): Calculated for $C_{23}H_{17}F_9NaOSi$ $[M+Na]^+$ 531.0797, found 531.0785

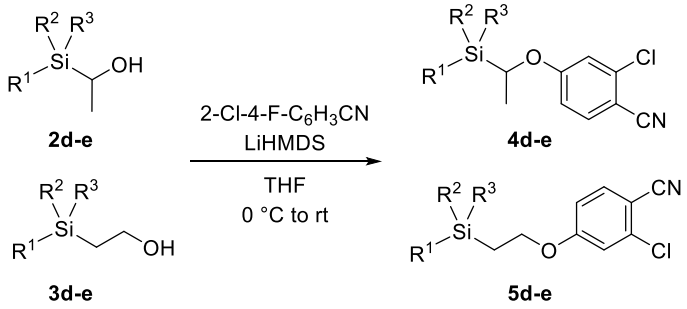
2.4. Synthesis of silylethoxy derivatives **4a-e, 5a-e**

General procedure D



To a mixture of 2-chloro-4-fluorobenzonitrile (0.6 mmol), silylethenol (0.2 mmol), and THF (2 mL) was added KHMDS (0.5 M toluene solution, 0.8 mL, 0.40 mmol) under 0 ℃. After stirred for 4 h under rt, the reaction mixture was added 1M $KHSO_4$. aq. The whole was extracted three times with ethyl acetate. The extract was successively washed with water and brine, and then dried over Na_2SO_4. The solvent was evaporated, and the residue was purified by means of silica gel column chromatography (Hex-EtOAc, EA=5-40% gradient) to give the mixture contained target product and substrate fluorobenzene. This mixture was purified by GPC (3-4 cycle) and get pure silylethoxy product.

General procedure E



To a mixture of 2-chloro-4-fluorobenzonitrile (117 mg, 0.75 mmol), silylethenol (0.50 mmol), and THF (5 mL) was added LiHMDS (1.3 M THF solution, 0.8 mL, 1.0 mmol) under 0 ℃. After stirred for 17 h under rt, the reaction mixture was added 1M $KHSO_4$. aq. The whole was extracted three times with ethyl acetate. The extract was successively washed with water and brine, and then dried over Na_2SO_4. The solvent was evaporated, and the residue was purified by means of silica gel column chromatography (Hex-EtOAc, EA=5-30% gradient) to give the mixture contained target product and substrate fluorobenzene. This mixture was further purified by GPC (3-4 cycle) and get pure silylethoxy product.

2.4.1. 2-Cchloro-4-(1-(trimethylsilyl)ethoxy)benzonitrile (**4a**)

Following the general procedure D, **4a** was obtained as colorless oil in 24% yield. ^{1}H-NMR (500 MHz, $CDCl_3$) δ 7.53 (d, *J* = 8.6 Hz, 1H), 7.00 (d, *J* = 2.9 Hz, 1H), 6.84 (dd, *J* = 9.2, 2.3 Hz, 1H), 4.11 (q, *J* = 7.3 Hz, 1H), 1.33 (d, *J* = 6.9 Hz, 3H), 0.09 (s, 9H); ^{13}C-NMR (126 MHz, $CDCl_3$) δ 163.8, 138.4, 135.1, 116.8, 116.7, 114.5, 104.2, 68.9, 14.9, -3.9; HRMS(ESI) : Calculated for $C_{12}H_{17}ClNOSi$ $[M+H]^+$ 254.0762, found 254.0756

2.4.2. 2-Chloro-4-(2-(trimethylsilyl)ethoxy)benzonitrile (**5a**)

Following the general procedure D, **5a** was obtained as white solid in 36% yield. mp 53.7-54.4 ℃; ^{1}H-NMR (500 MHz, $CDCl_3$) δ 7.55 (d, *J* = 8.6 Hz, 1H), 6.97 (d, *J* = 2.6 Hz, 1H), 6.83 (dd, *J* = 8.6, 2.3 Hz, 1H), 4.13-4.09 (m, 2H), 1.16-1.13 (m, 2H), 0.09 (s, 9H); ^{13}C-NMR (126 MHz, $CDCl_3$) δ 163.6, 138.4, 135.2, 116.8, 116.6, 114.4, 104.2, 67.5, 15.4, 7.5, 1.7; HRMS(ESI) : Calculated for $C_{12}H_{16}ClNNaOSi$ $[M+Na]^+$ 276.0582, found 276.0577

2.4.3. 2-Chloro-4-(1-(triethylsilyl)ethoxy)benzonitrile (**4b**)

Following the general procedure D, **4b** was obtained as colorless oil in 31% yield. ^{1}H-NMR (500 MHz, $CDCl_3$) δ 7.54 (d, *J* = 8.6 Hz, 1H), 7.00 (d, *J* = 2.3 Hz, 1H), 6.85 (dd, *J* = 8.9, 2.6 Hz, 1H), 4.26 (q, *J* = 7.3 Hz, 1H), 1.37 (d, *J* = 7.4 Hz, 3H), 0.99 (t, *J* = 8.0 Hz, 9H), 0.72-0.62 (m, 6H); ^{13}C-NMR (126 MHz, $CDCl_3$) δ 163.6, 138.4, 135.2, 116.8, 116.6, 114.4, 104.2, 67.5, 15.4, 7.5, 1.7; HRMS(ESI) : Calculated for $C_{15}H_{22}ClNNaOSi$ $[M+Na]^+$ 318.1051, found 318.1044

2.3.4. 2-Chloro-4-(2-(triethylsilyl)ethoxy)benzonitrile (**5b**)

Following the general procedure D, **5b** was obtained as colorless oil in 17% yield. ^{1}H-NMR (500 MHz, $CDCl_3$) δ 7.55 (d, *J* = 9.2 Hz, 1H), 6.96 (d, *J* = 2.3 Hz, 1H), 6.82 (dd, *J* = 8.6, 2.3 Hz, 1H), 4.12-4.08 (m, 2H), 1.18-1.15 (m, 2H), 0.97 (t, *J* = 7.7 Hz, 9H), 0.59 (q, *J* = 8.0 Hz, 6H); ^{13}C-NMR (126 MHz, $CDCl_3$) δ 162.9, 138.4, 135.1, 116.7, 116.1, 114.1, 104.8, 66.8, 12.8, 7.5, 3.6; HRMS (ESI) : Calculated for $C_{15}H_{22}ClNNaOSi$ $[M+Na]^+$ 318.1051, found 318.1048

2.3.5. 2-Chloro-4-(1-(dimethyl(phenyl)silyl)ethoxy)benzonitrile (**4c**)

Following the general procedure D, **4c** was obtained as colorless oil in 22% yield. ^{1}H-NMR (500 MHz, $CDCl_3$) δ 7.55-7.53 (m, 2H), 7.51 (d, *J* = 8.6 Hz, 1H), 7.42-7.35 (m, 3H), 6.98 (d, *J* = 2.3 Hz, 1H), 6.83 (dd, *J* = 8.9, 2.6 Hz, 1H), 4.30 (q, *J* = 7.3 Hz, 1H), 1.33 (d, *J* = 6.9 Hz, 3H), 0.40 (s, 3H), 0.39 (s, 3H); ^{13}C-NMR (126 MHz, $CDCl_3$) δ 163.5, 138.3, 135.5, 135.1, 134.2, 129.9, 128.1, 116.8, 114.5, 104.4, 68.7, 15.2, -5.5, -5.6; HRMS(ESI) : Calculated for $C_{17}H_{18}ClNNaOSi$ $[M+Na]^+$ 338.0738, found 338.0734

2.3.6. 2-Chloro-4-(2-(dimethyl(phenyl)silyl)ethoxy)benzonitrile (**5c**)

Following the general procedure D, **5c** was obtained as white solid in 20% yield. mp 40.2-41.1 ℃; ^{1}H-NMR (500

MHz, $CDCl_3$) δ 7.53-7.51 (m, 3H), 7.40-7.36 (m, 3H), 6.89 (d, *J* = 2.3 Hz, 1H), 6.75 (dd, *J* = 8.6, 2.3 Hz, 1H), 4.09-4.06 (m, 2H), 1.39-1.36 (m, 2H), 0.37 (s, 6H); ^{13}C-NMR (126 MHz, $CDCl_3$) δ 162.8, 138.4, 137.8, 135.1, 133.6, 129.5, 128.2, 116.6, 116.1, 114.0, 104.8, 66.6, 16.9, -2.6; HRMS(ESI) : Calculated for $C_{17}H_{18}ClNNaOSi$ $[M+Na]^+$ 338.0738, found 338.0729

2.3.7. 2-Chloro-4-(1-(methyldiphenylsilyl)ethoxy)benzonitrile (**4d**)

Following the general procedure E, **4d** was obtained as colorless oil in 62% yield. ^{1}H-NMR (500 MHz, $CDCl_3$) δ 7.59-7.55 (m, 4H), 7.52 (d, *J* = 8.6 Hz, 1H), 7.44-7.35 (m, 6H), 7.01 (d, *J* = 2.3 Hz, 1H), 6.86 (dd, *J* = 8.6, 2.3 Hz, 1H), 4.65 (q, *J* = 7.3 Hz, 1H), 1.40 (d, *J* = 7.4 Hz, 3H), 0.68 (s, 3H); ^{13}C-NMR (126 MHz, $CDCl_3$) δ 163.2, 138.4, 135.1, 135.0, 133.8, 133.7, 130.1, 128.3, 128.2, 116.8, 116.7, 114.6, 104.6, 68.0, 15.4, -6.5; HRMS(ESI) : Calculated for $C_{22}H_{20}ClNNaOSi$ $[M+Na]^+$ 400.0895, found 400.0892

2.3.8. 2-Chloro-4-(2-(methyldiphenylsilyl)ethoxy)benzonitrile (**5d**)

Following the general procedure E, **5d** was obtained as white solid in 27% yield. mp 54.8-56.1 ℃; ^{1}H-NMR (500 MHz, $CDCl_3$) δ 7.54-7.49 (m, 5H), 7.43-7.36 (m, 6H), 6.84 (d, *J* = 2.3 Hz, 1H), 6.70 (dd, *J* = 8.6, 2.3 Hz, 1H), 4.14-4.11 (m, 2H), 1.71-1.68 (m, 2H), 0.65 (s, 3H); ^{13}C-NMR (126 MHz, $CDCl_3$) δ 162.7, 138.3, 135.8, 135.1, 134.5, 129.8, 128.2, 116.6, 116.1, 114.0, 104.9, 66.4, 15.6, -3.7; HRMS(ESI) : Calculated for $C_{22}H_{21}ClNOSi$ $[M+H]^+$ 378.1075, found 378.1081

2.3.9. 2-Chloro-4-(1-(triphenylsilyl)ethoxy)benzonitrile (**4e**)

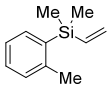
Following the general procedure E, **4e** was obtained as white solid in 48% yield. mp 122.2-123.0 ℃; ^{1}H-NMR (500 MHz, acetone-d_6) δ 7.76 (d, *J* = 8.6 Hz, 1H), 7.66 (dd, *J* = 8.0, 1.7 Hz, 6H), 7.50-7.47 (m, 3H), 7.43 (t, *J* = 7.4 Hz, 6H), 7.40 (d, *J* = 2.3 Hz, 1H), 7.21 (dd, *J* = 8.6, 2.3 Hz, 1H), 5.44 (q, *J* = 7.3 Hz, 1H), 1.54 (d, *J* = 7.4 Hz, 3H); ^{13}C-NMR (126 MHz, $CDCl_3$) δ 163.1, 138.5, 136.2, 135.2, 132.1, 130.3, 128.3, 116.8, 116.7, 114.6, 104.8, 67.9, 15.7; HRMS(ESI) : Calculated for $C_{27}H_{22}ClNNaOSi$ $[M+Na]^+$ 462.1051, found 462.1057

2.3.10. 2-Chloro-4-(2-(triphenylsilyl)ethoxy)benzonitrile (**5e**)

Following the general procedure E, **5e** was obtained as white solid in 14% yield. mp 135.0-136.4 ℃; ^{1}H-NMR (500 MHz, $CDCl_3$) δ 7.55-7.53 (m, 6H), 7.48-7.43 (m, 4H), 7.40-7.37 (m, 6H), 6.78 (d, *J* = 2.3 Hz, 1H), 6.64 (dd, *J* = 8.9, 2.6 Hz, 1H), 4.21-4.18 (m, 2H), 2.01-1.98 (m, 2H); ^{13}C-NMR (126 MHz, $CDCl_3$) δ 162.6, 138.3, 135.6, 135.0, 133.8, 130.1, 128.3, 116.6, 116.1, 114.0, 104.8, 66.2, 14.7; HRMS(ESI) : Calculated for $C_{27}H_{23}ClNOSi$ $[M+H]^+$ 440.1232, found 440.1242

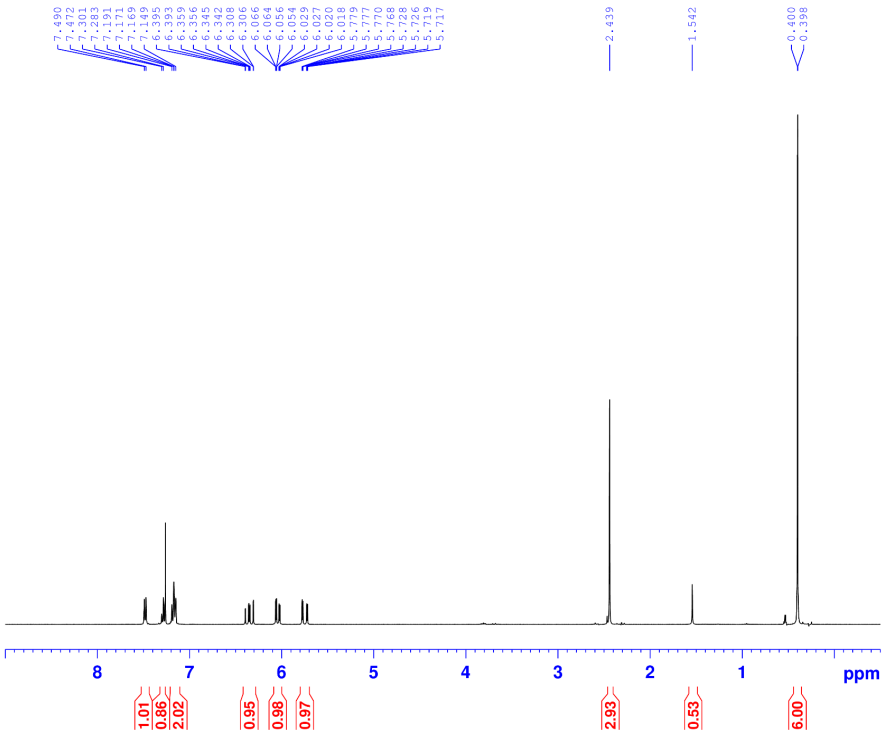
References for Supporting Information

1. J. A. Soderquist, I. Rivera and A. Negron, *J. Org. Chem.*, **1989**, *54*, 4051–4055.
2. C.-H. Jun and R. H. Crabtree, *J. Organomet. Chem.*, **1993**, *447*, 177–187.
3. D. Brösamlen and M. Oestreich, *Org. Lett.*, **2023**, *25*, 5319–5323.
4. T. Kratz, P. Steinbach, S. Breitenlechner, G. Storch, C. Bannwarth and T. Bach, *J. Am. Chem. Soc.*, **2022**, *144*, 10133–10138.
5. A. K. Sahoo, T. Oda, Y. Nakao and T. Hiyama, *Adv. Synth. Catal.*, **2004**, *346*, 1715–1727.
6. J. A. Soderquist and S.-J. H. Lee, *Tetrahedron*, **1988**, *44*, 4033–4042.
7. R. Tacke, S. A. Wagner, S. Brakmann, F. Wuttke, U. Eilert, L. Fischer and C. Syldatk, *J. Organomet. Chem.*, **1993**, *458*, 13–17.
8. J. E. Celebuski, C. Chan and R. A. Jones, *J. Org. Chem.*, **1992**, *57*, 5535–5538.
9. M. Fujio, M. Uchida, A. Okada, M. A. Alam, R. Fujiyama, H. U. Siehl and Y. Tsuno, *Bull. Chem. Soc. Jpn.*, **2005**, *78*, 1834–1842.
10. J. Vencl, J. Hetflejš, P. Kučera, J. Čermák and V. Chvalovský, *Collect. Czechoslov. Chem. Commun.*, **1973**, *38*, 1248–1255.



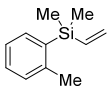
1f

o-Me col 5-7 GPC1



IBB-nmr Analysis

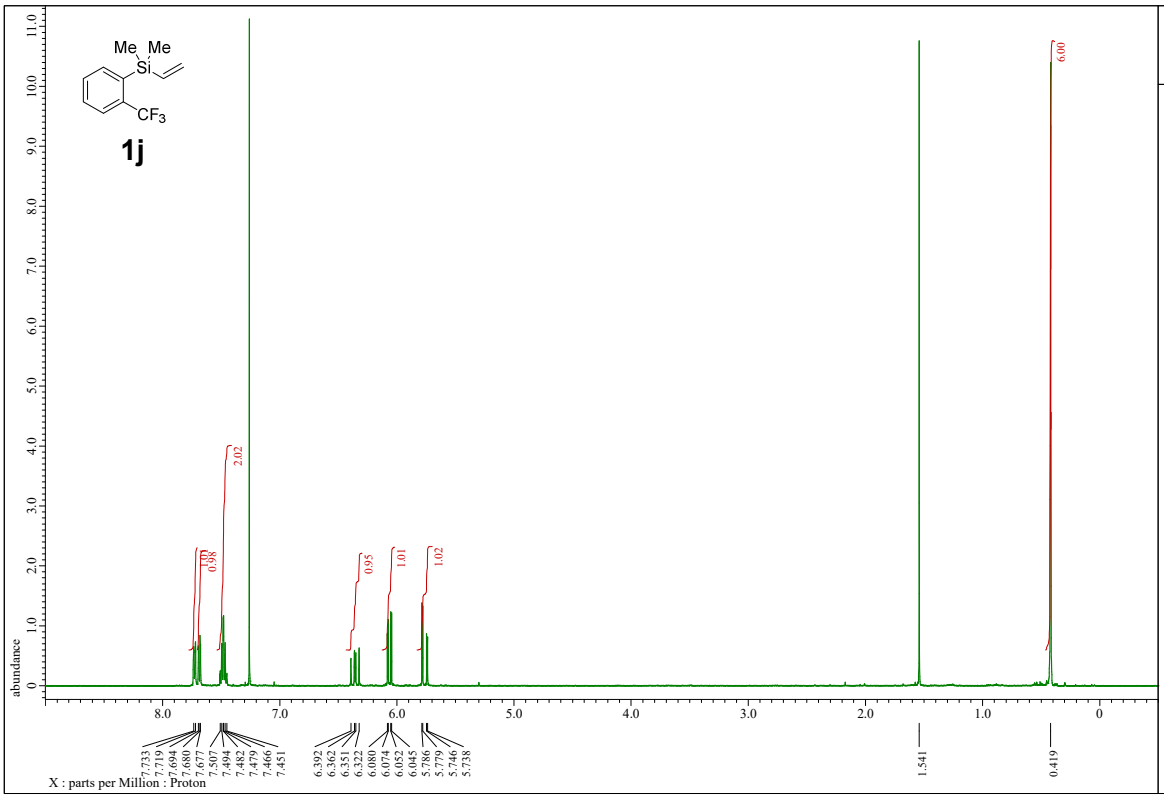
NAME	NN248-042
EXPNO	3
PROCNO	1
Date_	20220430
Time	20.05
INSTRUM	av400
PROBHD	5 mm PABBO BB-
PULPROG	zg30
TD	65536
SOLVENT	CDCl3
NS	16
DS	2
SWH	8223.685 Hz
FIDRES	0.125483 Hz
AQ	3.9846387 sec
RG	203
DW	60.800 usec
DE	6.50 usec
TE	296.5 K
D1	1.00000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	1H
P1	14.00 usec
PL1	-1.80 dB
PL1W	14.82738590 W
SFO1	400.1324710 MHz
SI	32768
SF	400.1300096 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00



1f

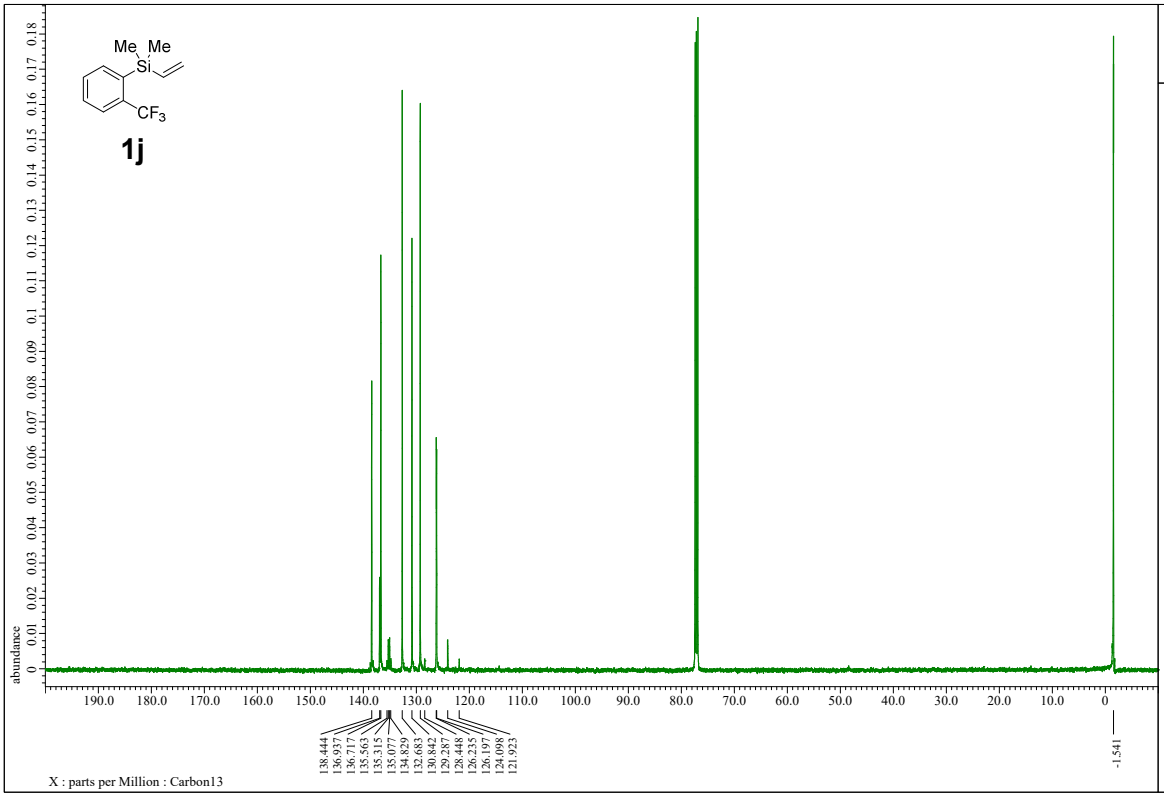
JEOL

Filename	= 042col4-7_gpc1_Carbon-1-3
Author	= delta
Experiment	= carbon.jxp
Sample_Id	= 042col4-7_gpc1
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 30-APR-2022 21:53:13
Revision_Time	= 20-FEB-2024 13:53:33
Comment	= single pulse decoupled ga
Data_Format	= 1D COMPLEX
Dim_Size	= 26214
X_Domain	= Carbon
Dim_Title	= Carbon13
Dim_Units	= [ppm]
Dimensions	= X
Site	= JNM-ECA500
Spectrometer	= DELTA2_NMR
Field_Strength	= 11.7473579[T] (500[MHz])
X_Acq_Duration	= 0.83361792[s]
X_Domain	= 13C
X_Freq	= 125.76529768[MHz]
X_Offset	= 100[ppm]
X_Points	= 32768
X_Prescans	= 4
X_Resolution	= 1.19959034[Hz]
X_Sweep	= 39.3081761[kHz]
X_Sweep_Clipped	= 31.44654088[kHz]
Irr_Domain	= Proton
Irr_Freq	= 500.15991521[MHz]
Irr_Offset	= 5.0[ppm]
Clipped	= FALSE
Scans	= 2048
Total_Scans	= 2048
Relaxation_Delay	= 2[s]
Recvr_Gain	= 50
Temp_Get	= 22.3[dC]
X_90_Width	= 12.65[us]
X_Acq_Time	= 0.83361792[s]
X_Angle	= 30[deg]
X_Atn	= 7[dB]
X_Pulse	= 4.21666667[us]
Irr_Atn_Dec	= 25.254[dB]
Irr_Atn_Noe	= 25.254[dB]
Irr_Noise	= WALTZ
Irr_Pwidth	= 92[us]
Decoupling	= TRUE
Initial_Wait	= 1[s]
Noe	= TRUE
Noe_Time	= 2[s]
Repetition_Time	= 2.83361792[s]



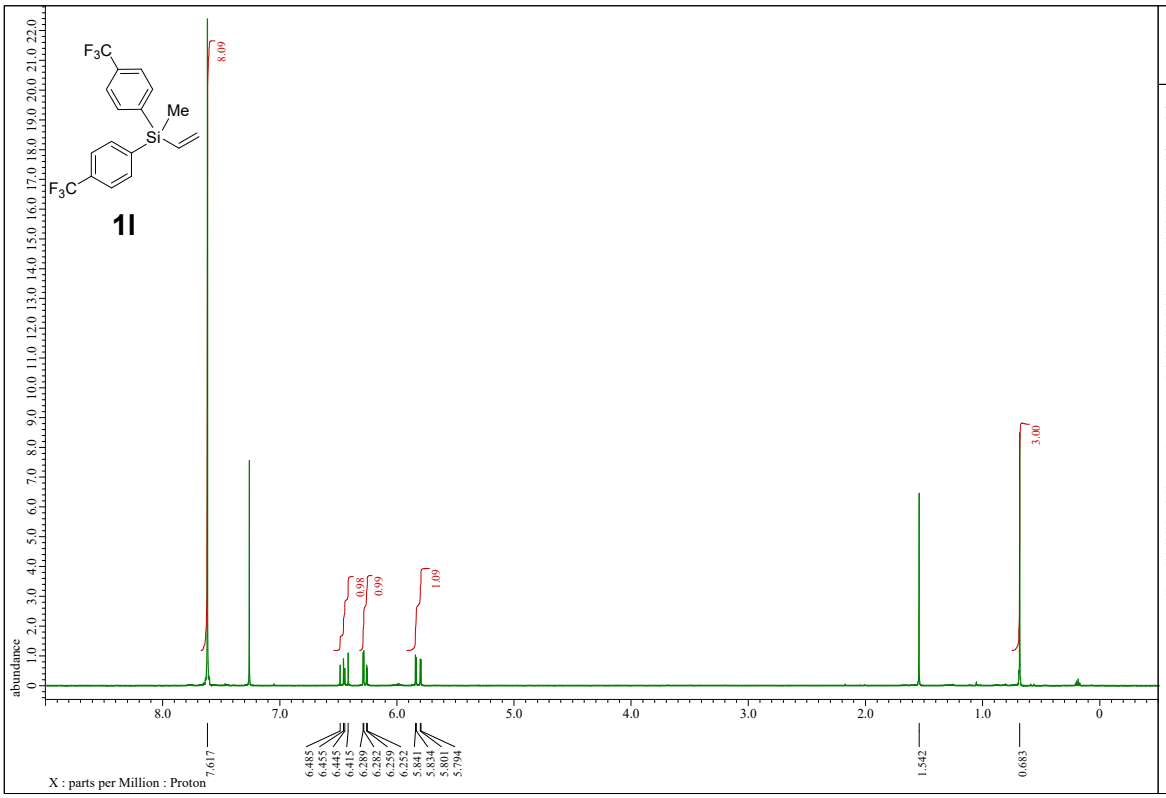
JEOL

```
Filename          = 248-041_oCF3_vinyl_Proton
Author            = delta
Experiment        = proton.jxp
Sample_Id         = 248-041_oCF3_vinyl
Solvent           = CHLOROFORM-D
Actual_Start_Time = 21-SEP-2023 23:31:24
Revision_Time     = 20-FEB-2024 15:29:54

Comment           = single_pulse
Data_Format       = 1D COMPLEX
Dim_Size          = 13107
X_Domain          = Proton
Dim_Title         = Proton
Dim_Units         = [ppm]
Dimensions        = X
Site              = JNM-ECA500
Spectrometer      = DELTA2_NMR

Field_Strength    = 11.7473579[T] (500[MHz])
X_Acq_Duration    = 1.74587904[s]
X_Domain          = 1H
X_Freq            = 500.15991521[MHz]
X_Offset          = 5.0[ppm]
X_Points          = 16384
X_Prescans        = 1
X_Resolution      = 0.57277737[Hz]
X_Sweep           = 9.38438438[kHz]
X_Sweep_Clipped   = 7.50750751[kHz]
Irr_Domain        = Proton
Irr_Freq          = 500.15991521[MHz]
Irr_Offset        = 5.0[ppm]
Tri_Domain        = Proton
Tri_Freq          = 500.15991521[MHz]
Tri_Offset        = 5.0[ppm]
Clipped           = FALSE
Scans             = 8
Total_Scans       = 8

Relaxation_Delay  = 5[s]
Recvr_Gain        = 58
Temp_Get          = 22.7[dC]
X_90_Width        = 6.7[us]
X_Acq_Time        = 1.74587904[s]
X_Angle           = 45[deg]
X_Atn             = 2.5[dB]
X_Pulse           = 3.35[us]
Irr_Mode          = Off
Tri_Mode          = Off
Dante_Presat      = FALSE
Initial_Wait      = 1[s]
Repetition_Time   = 6.74587904[s]
```



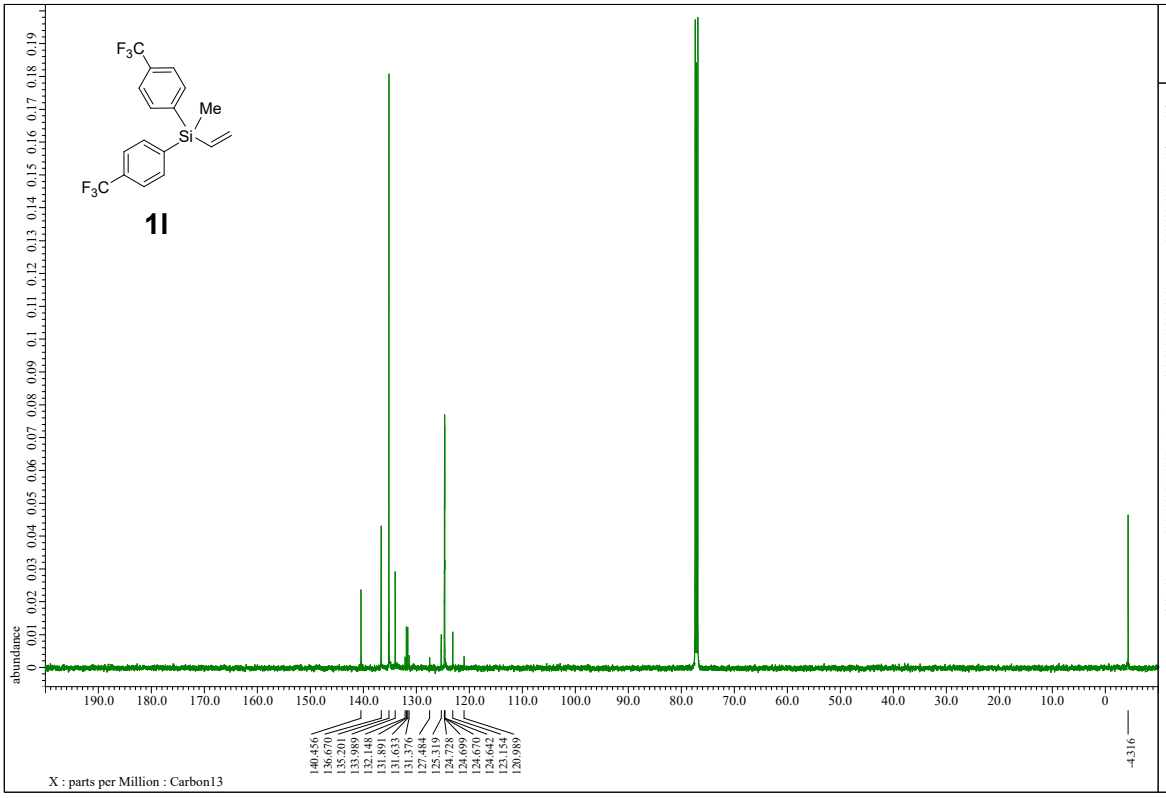
JEOL

```
Filename          = 041-co17_Carbon-1-2.jdf
Author            = delta
Experiment        = carbon.jxp
Sample_Id         = 041-co17
Solvent           = CHLOROFORM-D
Actual_Start_Time = 27-APR-2022 23:44:31
Revision_Time     = 20-FEB-2024 13:58:50

Comment           = single pulse decoupled ga
Data_Format       = 1D COMPLEX
Dim_Size          = 26214
X_Domain          = Carbon
Dim_Title         = Carbon13
Dim_Units         = [ppm]
Dimensions        = X
Site              = JNM-ECA500
Spectrometer      = DELTA2_NMR

Field_Strength    = 11.7473579[T] (500[MHz])
X_Acq_Duration    = 0.83361792[s]
X_Domain          = 13C
X_Freq            = 125.76529768[MHz]
X_Offset          = 100[ppm]
X_Points          = 32768
X_Prescans        = 4
X_Resolution      = 1.19959034[Hz]
X_Sweep           = 39.3081761[kHz]
X_Sweep_Clipped   = 31.44654088[kHz]
Irr_Domain        = Proton
Irr_Freq          = 500.15991521[MHz]
Irr_Offset        = 5.0[ppm]
Clipped           = FALSE
Scans             = 2048
Total_Scans       = 2048

Relaxation_Delay  = 2[s]
Recvr_Gain        = 50
Temp_Get          = 22.5[dC]
X_90_Width        = 12.65[us]
X_Acq_Time        = 0.83361792[s]
X_Angle           = 30[deg]
X_Atn             = 7[dB]
X_Pulse           = 4.21666667[us]
Irr_Atn_Dec       = 25.254[dB]
Irr_Atn_Noe       = 25.254[dB]
Irr_Noise         = WALTZ
Irr_Pwidth        = 92[us]
Decoupling        = TRUE
Initial_Wait      = 1[s]
Noe               = TRUE
Noe_Time          = 2[s]
Repetition_Time   = 2.83361792[s]
```



JEOL

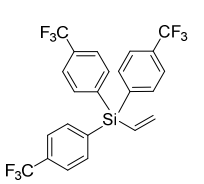
```
Filename          = 248-063_(pCF3)2Me_Vinyl_P
Author            = delta
Experiment        = proton.jxp
Sample_Id         = 248-063_(pCF3)2Me_Vinyl
Solvent           = CHLOROFORM-D
Actual_Start_Time = 21-SEP-2023 23:39:48
Revision_Time     = 20-FEB-2024 15:41:05

Comment           = single_pulse
Data_Format       = 1D COMPLEX
Dim_Size          = 13107
X_Domain          = Proton
Dim_Title         = Proton
Dim_Units         = [ppm]
Dimensions        = X
Site              = JNM-ECA500
Spectrometer      = DELTA2_NMR

Field_Strength    = 11.7473579[T] (500[MHz])
X_Acq_Duration    = 1.74587904[s]
X_Domain          = 1H
X_Freq            = 500.15991521[MHz]
X_Offset          = 5.0[ppm]
X_Points          = 16384
X_Prescans        = 1
X_Resolution      = 0.57277737[Hz]
X_Sweep           = 9.38438438[kHz]
X_Sweep_Clipped   = 7.50750751[kHz]
Irr_Domain        = Proton
Irr_Freq          = 500.15991521[MHz]
Irr_Offset        = 5.0[ppm]
Tri_Domain        = Proton
Tri_Freq          = 500.15991521[MHz]
Tri_Offset        = 5.0[ppm]
Clipped           = FALSE
Scans             = 8
Total_Scans       = 8

Relaxation_Delay  = 5[s]
Recvr_Gain        = 58
Temp_Get          = 22.6[dC]
X_90_Width        = 6.7[us]
X_Acq_Time        = 1.74587904[s]
X_Angle           = 45[deg]
X_Atn             = 2.5[dB]
X_Pulse           = 3.35[us]
Irr_Mode          = Off
Tri_Mode          = Off
Dante_Presat      = FALSE
Initial_Wait      = 1[s]
Repetition_Time   = 6.74587904[s]
```



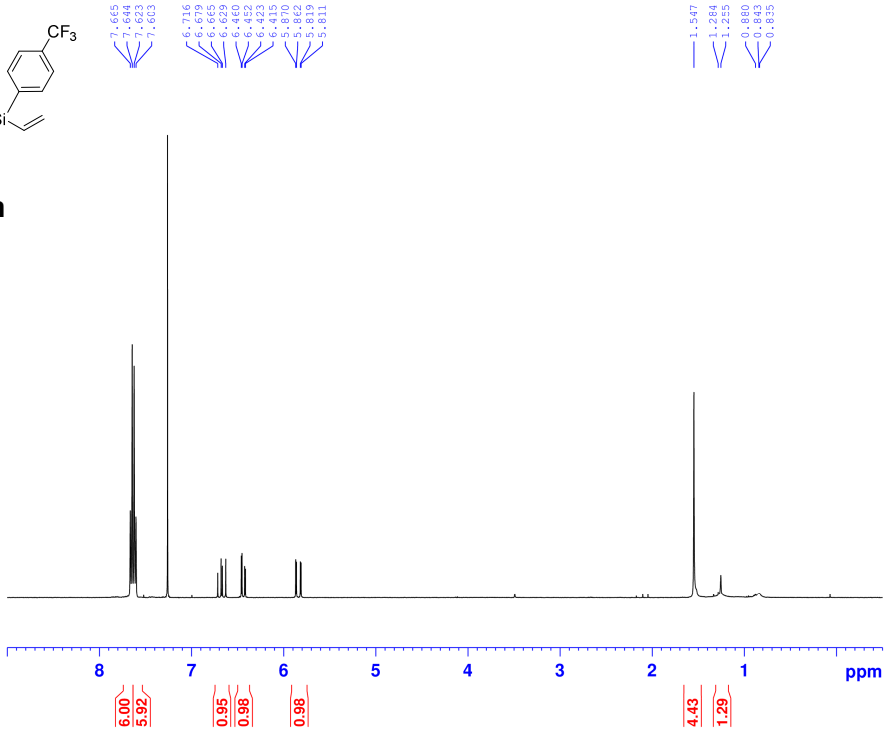
JEOL

```
Filename          = 063-GPC111-116_Carbon-1-2
Author            = delta
Experiment        = carbon.jxp
Sample_Id         = 063-GPC111-116
Solvent           = CHLOROFORM-D
Actual_Start_Time =  7-JUL-2022 11:51:58
Revision_Time     = 20-FEB-2024 14:10:00

Comment           = single pulse decoupled ga
Data_Format       = 1D COMPLEX
Dim_Size          = 26214
X_Domain          = Carbon
Dim_Title         = Carbon13
Dim_Units         = [ppm]
Dimensions        = X
Site              = JNM-ECA500
Spectrometer      = DELTA2_NMR

Field_Strength    = 11.7473579[T] (500[MHz])
X_Acq_Duration    = 0.83361792[s]
X_Domain          = 13C
X_Freq            = 125.76529768[MHz]
X_Offset          = 100[ppm]
X_Points          = 32768
X_Prescans        = 4
X_Resolution      = 1.19959034[Hz]
X_Sweep           = 39.3081761[kHz]
X_Sweep_Clipped   = 31.44654088[kHz]
Irr_Domain        = Proton
Irr_Freq          = 500.15991521[MHz]
Irr_Offset        = 5.0[ppm]
Clipped           = FALSE
Scans             = 1024
Total_Scans       = 1024

Relaxation_Delay  = 2[s]
Recvr_Gain        = 50
Temp_Get          = 22[dC]
X_90_Width        = 12.65[us]
X_Acq_Time        = 0.83361792[s]
X_Angle           = 30[deg]
X_Atn             = 7[dB]
X_Pulse           = 4.21666667[us]
Irr_Atn_Dec       = 25.254[dB]
Irr_Atn_Noe       = 25.254[dB]
Irr_Noise         = WALTZ
Irr_Pwidth        = 92[us]
Decoupling        = TRUE
Initial_Wait      = 1[s]
Noe               = TRUE
Noe_Time          = 2[s]
Repetition_Time   = 2.83361792[s]
```

(p-CF3)3 vinyl col4-8 recry

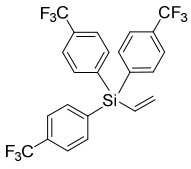


1m



IBB-nmr Analysis

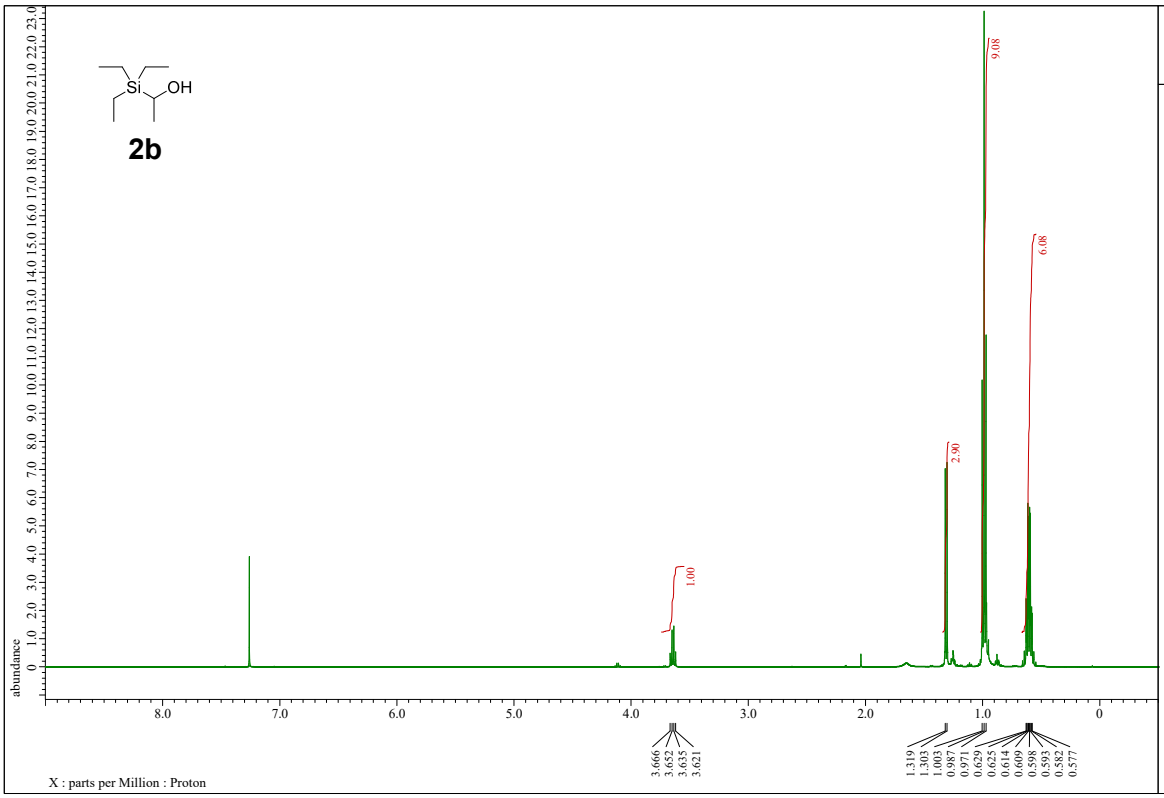
NAME	NN248-052
EXPNO	2
PROCNO	1
Date_	20220606
Time	21.25
INSTRUM	av400
PROBHD	5 mm PABBO BB-
PULPROG	zg30
TD	65536
SOLVENT	CDC13
NS	16
DS	2
SWH	8223.685 Hz
FIDRES	0.125483 Hz
AQ	3.9846387 sec
RG	203
DW	60.800 usec
DE	6.50 usec
TE	296.9 K
D1	1.00000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	1H
P1	14.00 usec
PL1	-1.80 dB
PL1W	14.82738590 W
SFO1	400.1324710 MHz
SI	32768
SF	400.1300096 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00



1m

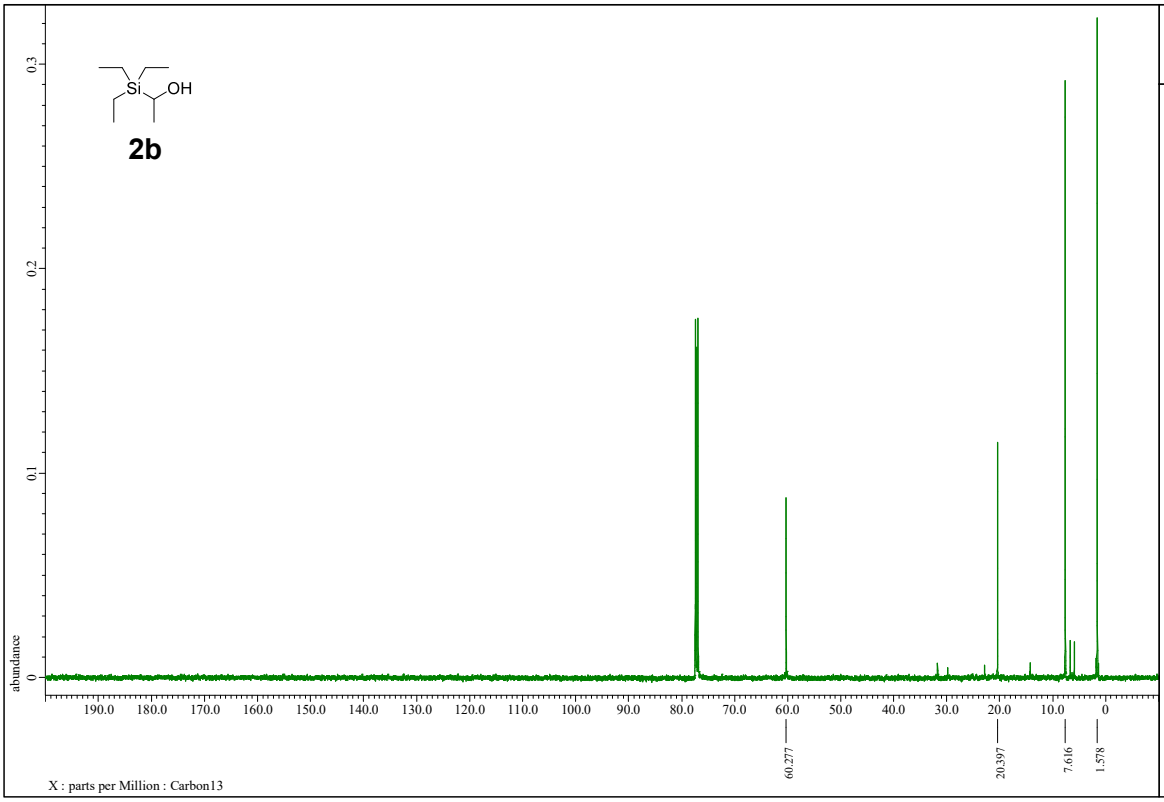
JEOL

Filename	= 048-col2-3-recry_Carbon-1
Author	= delta
Experiment	= carbon.jxp
Sample_Id	= 048-col2-3-recry
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 3-JUN-2022 18:20:48
Revision_Time	= 20-FEB-2024 14:29:07
Comment	= single pulse decoupled ga
Data_Format	= 1D COMPLEX
Dim_Size	= 26214
X_Domain	= Carbon
Dim_Title	= Carbon13
Dim_Units	= [ppm]
Dimensions	= X
Site	= JNM-ECA500
Spectrometer	= DELTA2_NMR
Field_Strength	= 11.7473579[T] (500[MHz])
X_Acq_Duration	= 0.83361792[s]
X_Domain	= 13C
X_Freq	= 125.76529768[MHz]
X_Offset	= 100[ppm]
X_Points	= 32768
X_Prescans	= 4
X_Resolution	= 1.19959034[Hz]
X_Sweep	= 39.3081761[kHz]
X_Sweep_Clipped	= 31.44654088[kHz]
Irr_Domain	= Proton
Irr_Freq	= 500.15991521[MHz]
Irr_Offset	= 5.0[ppm]
Clipped	= FALSE
Scans	= 2048
Total_Scans	= 2048
Relaxation_Delay	= 2[s]
Recvr_Gain	= 50
Temp_Get	= 22.9[dC]
X_90_Width	= 12.65[us]
X_Acq_Time	= 0.83361792[s]
X_Angle	= 30[deg]
X_Atn	= 7[dB]
X_Pulse	= 4.21666667[us]
Irr_Atn_Dec	= 25.254[dB]
Irr_Atn_Noe	= 25.254[dB]
Irr_Noise	= WALTZ
Irr_Pwidth	= 92[us]
Decoupling	= TRUE
Initial_Wait	= 1[s]
Noe	= TRUE
Noe_Time	= 2[s]
Repetition_Time	= 2.83361792[s]



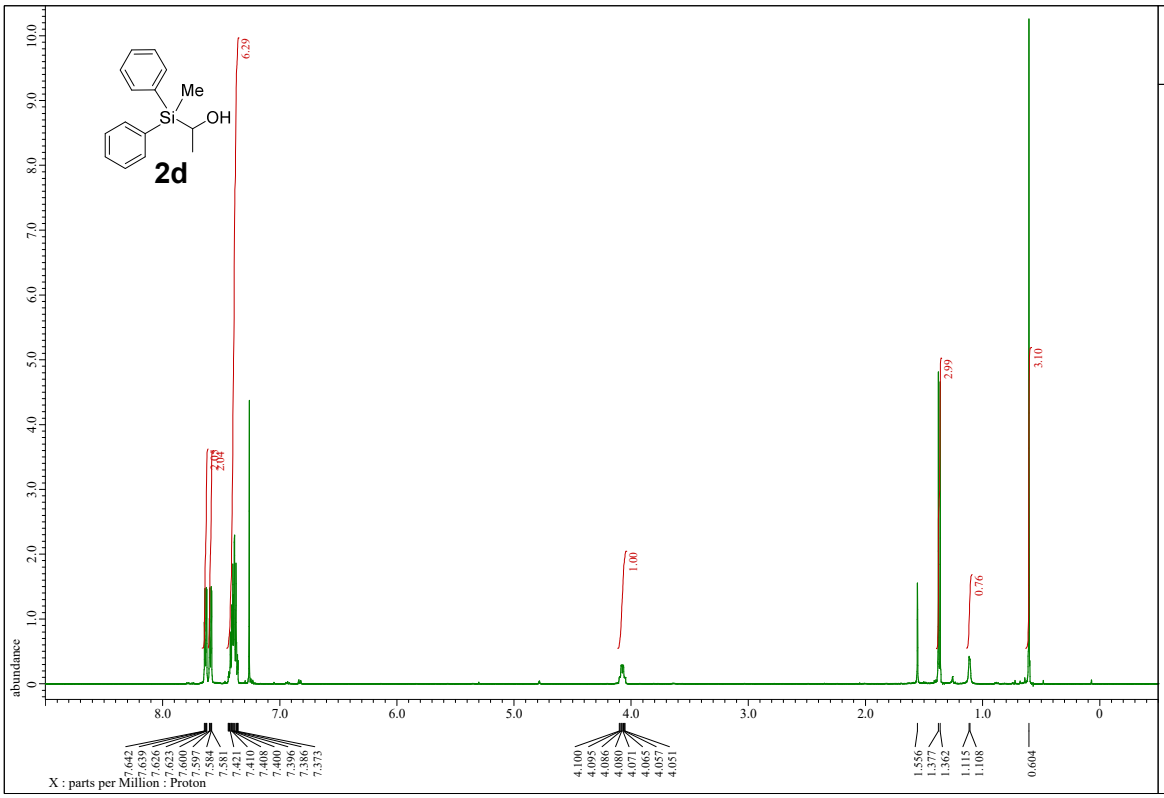
JEOL

```
Filename          = 270-042-3_col11-16_dist_P
Author            = delta
Experiment        = proton.jxp
Sample_Id         = 270-042-3_col11-16_dist
Solvent           = CHLOROFORM-D
Actual_Start_Time = 11-SEP-2023 15:54:49
Revision_Time     = 20-FEB-2024 16:51:13

Comment           = single_pulse
Data_Format       = 1D COMPLEX
Dim_Size          = 13107
X_Domain          = Proton
Dim_Title         = Proton
Dim_Units         = [ppm]
Dimensions        = X
Site              = JNM-ECA500
Spectrometer      = DELTA2_NMR

Field_Strength    = 11.7473579[T] (500[MHz])
X_Acq_Duration    = 1.74587904[s]
X_Domain          = 1H
X_Freq            = 500.15991521[MHz]
X_Offset          = 5.0[ppm]
X_Points          = 16384
X_Prescans        = 1
X_Resolution      = 0.57277737[Hz]
X_Sweep           = 9.38438438[kHz]
X_Sweep_Clipped   = 7.50750751[kHz]
Irr_Domain        = Proton
Irr_Freq          = 500.15991521[MHz]
Irr_Offset        = 5.0[ppm]
Tri_Domain        = Proton
Tri_Freq          = 500.15991521[MHz]
Tri_Offset        = 5.0[ppm]
Clipped           = FALSE
Scans             = 16
Total_Scans       = 16

Relaxation_Delay  = 5[s]
Recvr_Gain        = 42
Temp_Get          = 22.8[dC]
X_90_Width        = 6.7[us]
X_Acq_Time        = 1.74587904[s]
X_Angle           = 45[deg]
X_Atn             = 2.5[dB]
X_Pulse           = 3.35[us]
Irr_Mode          = Off
Tri_Mode          = Off
Dante_Presat      = FALSE
Initial_Wait      = 1[s]
Repetition_Time   = 6.74587904[s]
```



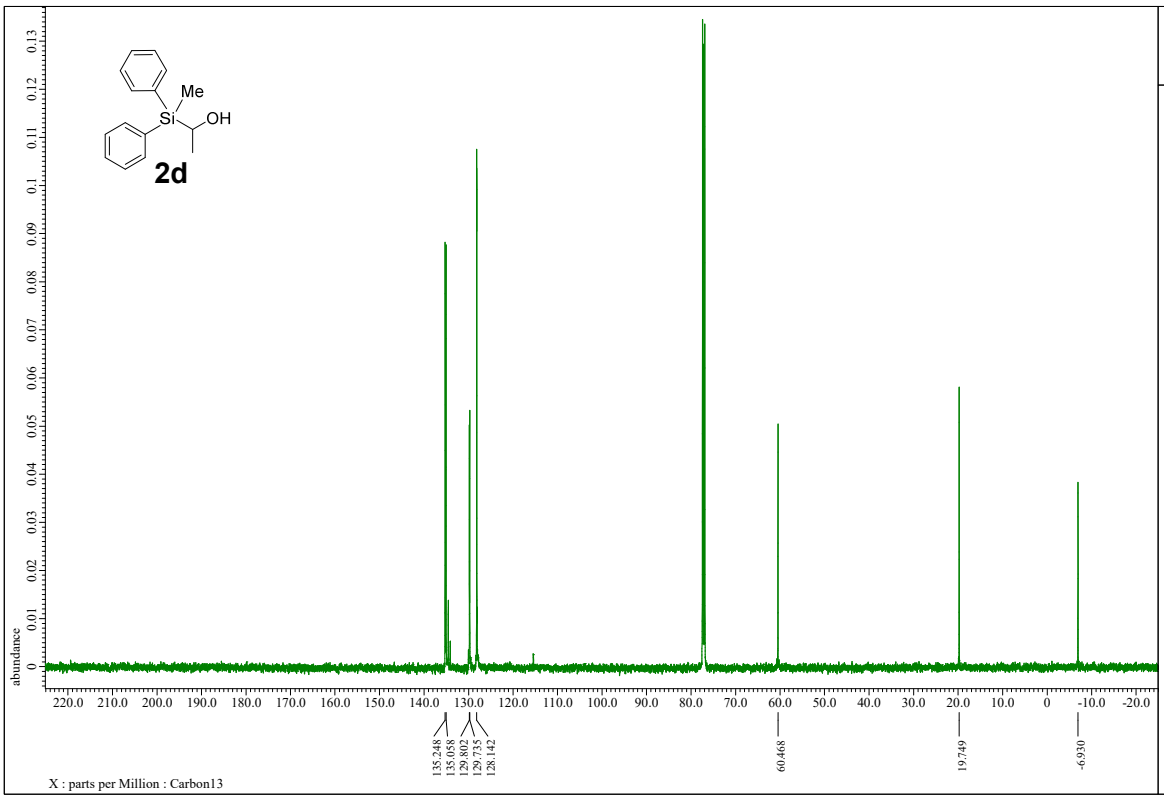
JEOL

```
Filename          = 270-042-3_col11-16_dist_C
Author            = delta
Experiment        = carbon.jxp
Sample_Id         = 270-042-3_col11-16_dist
Solvent           = CHLOROFORM-D
Actual_Start_Time = 11-SEP-2023 16:55:11
Revision_Time     = 20-FEB-2024 16:56:01

Comment           = single pulse decoupled ga
Data_Format       = 1D COMPLEX
Dim_Size          = 26214
X_Domain          = Carbon
Dim_Title         = Carbon13
Dim_Units         = [ppm]
Dimensions        = X
Site              = JNM-ECA500
Spectrometer      = DELTA2_NMR

Field_Strength    = 11.7473579[T] (500[MHz])
X_Acq_Duration    = 0.83361792[s]
X_Domain          = 13C
X_Freq            = 125.76529768[MHz]
X_Offset          = 100[ppm]
X_Points          = 32768
X_Prescans        = 4
X_Resolution      = 1.19959034[Hz]
X_Sweep           = 39.3081761[kHz]
X_Sweep_Clipped   = 31.44654088[kHz]
Irr_Domain        = Proton
Irr_Freq          = 500.15991521[MHz]
Irr_Offset        = 5.0[ppm]
Clipped           = FALSE
Scans             = 512
Total_Scans       = 512

Relaxation_Delay  = 2[s]
Recvr_Gain        = 50
Temp_Get          = 22.6[dC]
X_90_Width        = 12.65[us]
X_Acq_Time        = 0.83361792[s]
X_Angle           = 30[deg]
X_Atn             = 7[dB]
X_Pulse           = 4.21666667[us]
Irr_Atn_Dec       = 25.254[dB]
Irr_Atn_Noe       = 25.254[dB]
Irr_Noise         = WALTZ
Irr_Pwidth        = 92[us]
Decoupling        = TRUE
Initial_Wait      = 1[s]
Noe               = TRUE
Noe_Time          = 2[s]
Repetition_Time   = 2.83361792[s]
```



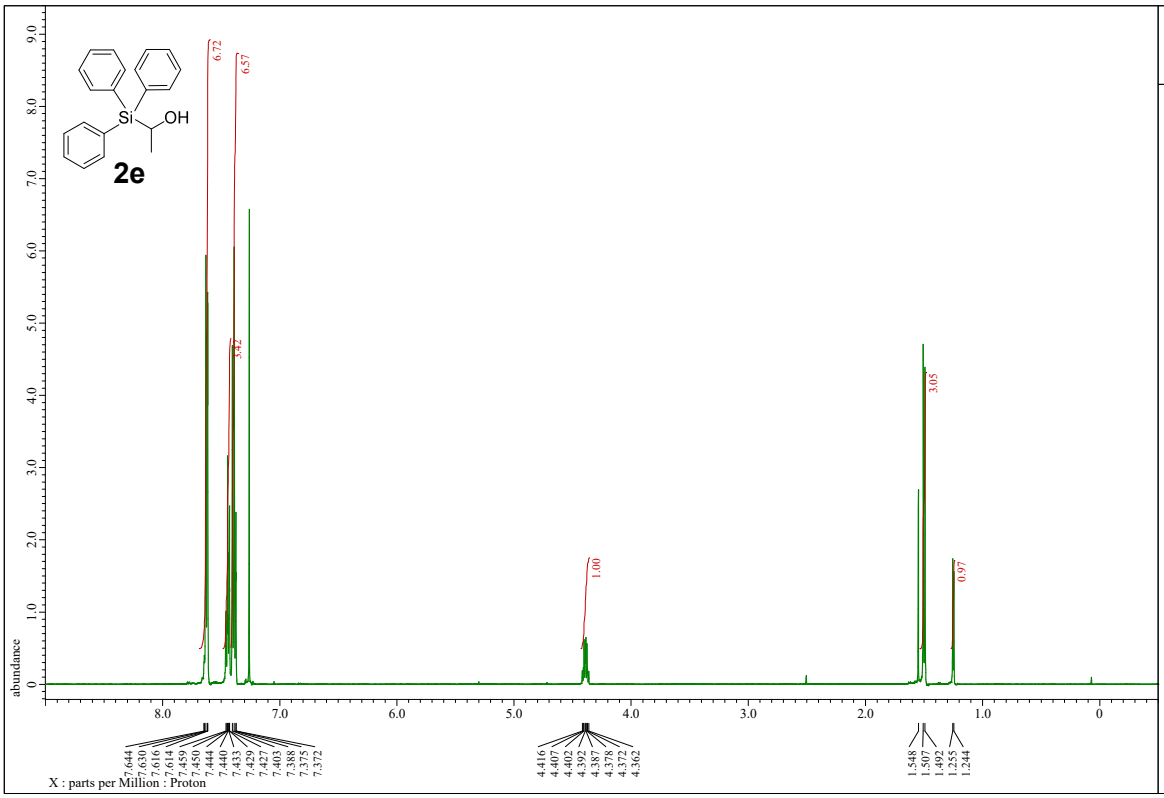
JEOL

```
Filename          = 270-017-8_col2_11_Proton-
Author            = delta
Experiment        = proton.jxp
Sample_Id         = 270-017-8_col2_11
Solvent           = CHLOROFORM-D
Actual_Start_Time = 23-MAR-2024 22:36:32
Revision_Time     = 25-MAR-2024 16:55:06

Comment           = single_pulse
Data_Format       = 1D COMPLEX
Dim_Size          = 13107
X_Domain          = Proton
Dim_Title         = Proton
Dim_Units         = [ppm]
Dimensions        = X
Site              = JNM-ECA500
Spectrometer      = DELTA2_NMR

Field_Strength    = 11.7473579[T] (500[MHz])
X_Acq_Duration    = 1.74587904[s]
X_Domain          = 1H
X_Freq            = 500.15991521[MHz]
X_Offset          = 5.0[ppm]
X_Points          = 16384
X_Prescans        = 1
X_Resolution      = 0.57277737[Hz]
X_Sweep           = 9.38438438[kHz]
X_Sweep_Clipped   = 7.50750751[kHz]
Irr_Domain        = Proton
Irr_Freq          = 500.15991521[MHz]
Irr_Offset        = 5.0[ppm]
Tri_Domain        = Proton
Tri_Freq          = 500.15991521[MHz]
Tri_Offset        = 5.0[ppm]
Clipped           = FALSE
Scans             = 16
Total_Scans       = 16

Relaxation_Delay  = 5[s]
Recvr_Gain        = 54
Temp_Get          = 19.4[dC]
X_90_Width        = 6.7[us]
X_Acq_Time        = 1.74587904[s]
X_Angle           = 45[deg]
X_Atn             = 2.5[dB]
X_Pulse           = 3.35[us]
Irr_Mode          = Off
Tri_Mode          = Off
Dante_Presat      = FALSE
Initial_Wait      = 1[s]
Repetition_Time   = 6.74587904[s]
```



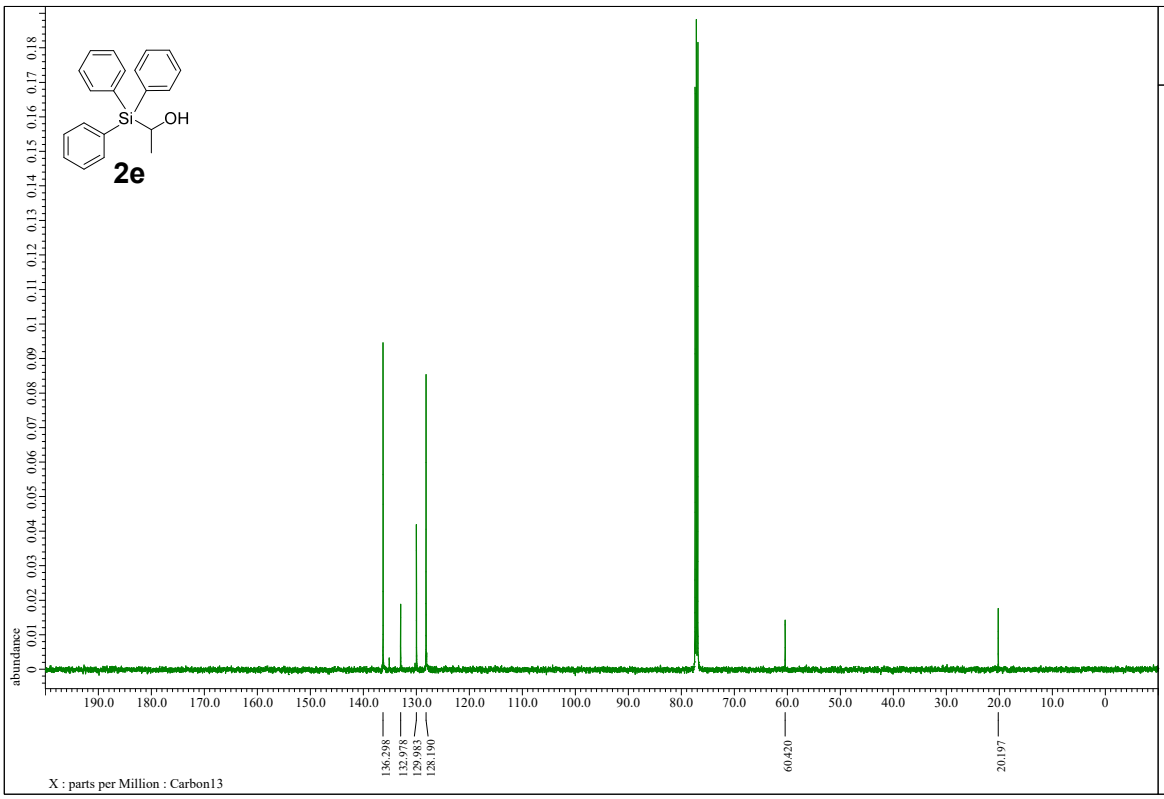
JEOL

```
Filename          = 270-017-8_col3_14_Carbon-
Author            = delta
Experiment        = carbon.jxp
Sample_Id         = 270-017-8_col3_14
Solvent           = CHLOROFORM-D
Actual_Start_Time = 25-MAR-2024 20:25:22
Revision_Time     = 25-MAR-2024 23:14:39

Comment           = single pulse decoupled ga
Data_Format       = 1D COMPLEX
Dim_Size          = 26214
X_Domain          = Carbon
Dim_Title         = Carbon13
Dim_Units         = [ppm]
Dimensions        = X
Site              = JNM-ECA500
Spectrometer      = DELTA2_NMR

Field_Strength    = 11.7473579[T] (500[MHz])
X_Acq_Duration    = 0.83361792[s]
X_Domain          = 13C
X_Freq            = 125.76529768[MHz]
X_Offset          = 100[ppm]
X_Points          = 32768
X_Prescans        = 4
X_Resolution      = 1.19959034[Hz]
X_Sweep           = 39.3081761[kHz]
X_Sweep_Clipped   = 31.44654088[kHz]
Irr_Domain        = Proton
Irr_Freq          = 500.15991521[MHz]
Irr_Offset        = 5.0[ppm]
Clipped           = FALSE
Scans             = 1024
Total_Scans       = 1024

Relaxation_Delay  = 2[s]
Recvr_Gain        = 50
Temp_Get          = 20.3[dC]
X_90_Width        = 12.65[us]
X_Acq_Time        = 0.83361792[s]
X_Angle           = 30[deg]
X_Atn             = 7[dB]
X_Pulse           = 4.21666667[us]
Irr_Atn_Dec       = 25.254[dB]
Irr_Atn_Noe       = 25.254[dB]
Irr_Noise         = WALTZ
Irr_Pwidth        = 92[us]
Decoupling        = TRUE
Initial_Wait      = 1[s]
Noe               = TRUE
Noe_Time          = 2[s]
Repetition_Time   = 2.83361792[s]
```



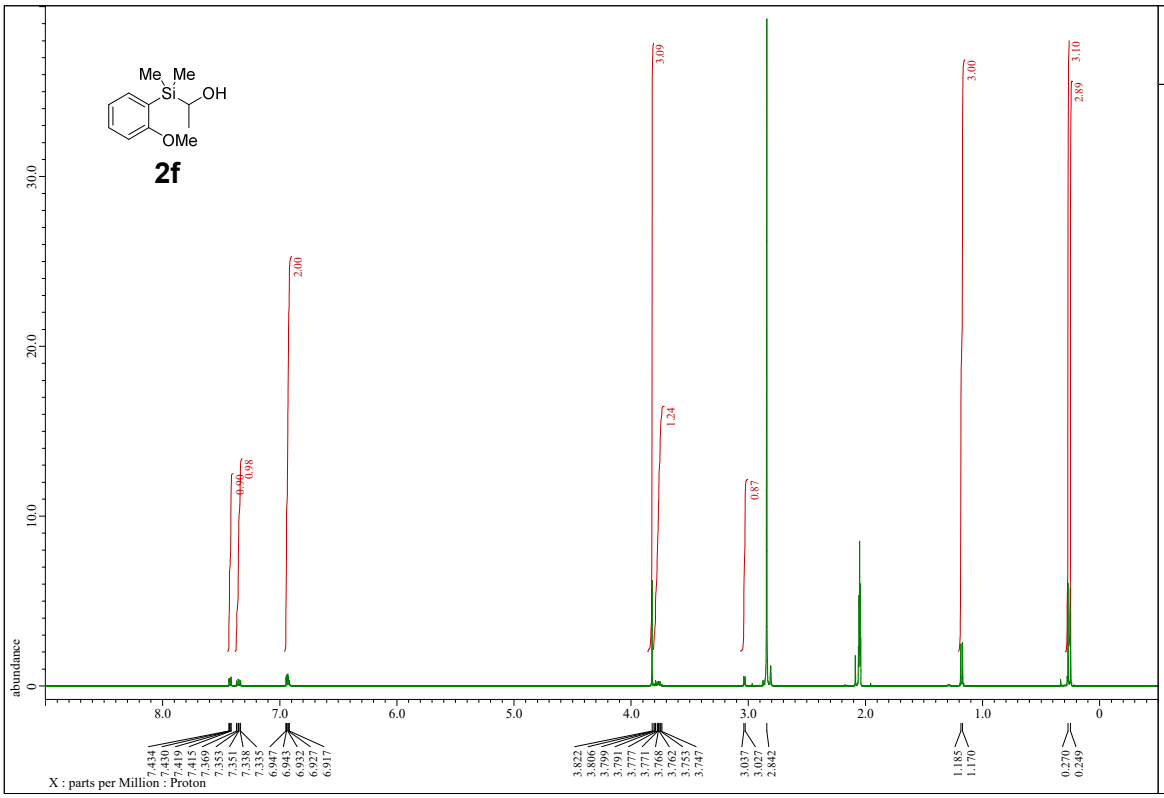
JEOL

```
Filename          = 270-050-7_col2_14-15_Prot
Author            = delta
Experiment        = proton.jxp
Sample_Id         = 270-050-7_col2_14-15
Solvent           = CHLOROFORM-D
Actual_Start_Time = 22-MAR-2024 22:27:18
Revision_Time     = 25-MAR-2024 16:49:33

Comment           = single_pulse
Data_Format       = 1D COMPLEX
Dim_Size          = 13107
X_Domain          = Proton
Dim_Title         = Proton
Dim_Units         = [ppm]
Dimensions        = X
Site              = JNM-ECA500
Spectrometer      = DELTA2_NMR

Field_Strength    = 11.7473579[T] (500[MHz])
X_Acq_Duration    = 1.74587904[s]
X_Domain          = 1H
X_Freq            = 500.15991521[MHz]
X_Offset          = 5.0[ppm]
X_Points          = 16384
X_Prescans        = 1
X_Resolution      = 0.57277737[Hz]
X_Sweep           = 9.38438438[kHz]
X_Sweep_Clipped   = 7.50750751[kHz]
Irr_Domain        = Proton
Irr_Freq          = 500.15991521[MHz]
Irr_Offset        = 5.0[ppm]
Tri_Domain        = Proton
Tri_Freq          = 500.15991521[MHz]
Tri_Offset        = 5.0[ppm]
Clipped           = FALSE
Scans             = 16
Total_Scans       = 16

Relaxation_Delay  = 5[s]
Recvr_Gain        = 58
Temp_Get          = 18.9[dC]
X_90_Width        = 6.7[us]
X_Acq_Time        = 1.74587904[s]
X_Angle           = 45[deg]
X_Atn             = 2.5[dB]
X_Pulse           = 3.35[us]
Irr_Mode          = Off
Tri_Mode          = Off
Dante_Presat      = FALSE
Initial_Wait      = 1[s]
Repetition_Time   = 6.74587904[s]
```



JEOL

```
Filename          = 270-050-7_col2_14-15_Carb
Author            = delta
Experiment        = carbon.jxp
Sample_Id         = 270-050-7_col2_14-15
Solvent           = CHLOROFORM-D
Actual_Start_Time = 23-MAR-2024 22:46:07
Revision_Time     = 25-MAR-2024 16:46:06

Comment           = single pulse decoupled ga
Data_Format       = 1D COMPLEX
Dim_Size          = 26214
X_Domain          = Carbon
Dim_Title         = Carbon13
Dim_Units         = [ppm]
Dimensions        = X
Site              = JNM-ECA500
Spectrometer      = DELTA2_NMR

Field_Strength    = 11.7473579[T] (500[MHz])
X_Acq_Duration    = 0.83361792[s]
X_Domain          = 13C
X_Freq            = 125.76529768[MHz]
X_Offset          = 100[ppm]
X_Points          = 32768
X_Prescans        = 4
X_Resolution      = 1.19959034[Hz]
X_Sweep           = 39.3081761[kHz]
X_Sweep_Clipped   = 31.44654088[kHz]
Irr_Domain        = Proton
Irr_Freq          = 500.15991521[MHz]
Irr_Offset        = 5.0[ppm]
Clipped           = FALSE
Scans             = 1024
Total_Scans       = 1024

Relaxation_Delay  = 2[s]
Recvr_Gain        = 50
Temp_Get          = 18.6[dC]
X_90_Width        = 12.65[us]
X_Acq_Time        = 0.83361792[s]
X_Angle           = 30[deg]
X_Atn             = 7[dB]
X_Pulse           = 4.21666667[us]
Irr_Atn_Dec       = 25.254[dB]
Irr_Atn_Noe       = 25.254[dB]
Irr_Noise         = WALTZ
Irr_Pwidth        = 92[us]
Decoupling        = TRUE
Initial_Wait      = 1[s]
Noe               = TRUE
Noe_Time          = 2[s]
Repetition_Time   = 2.83361792[s]
```

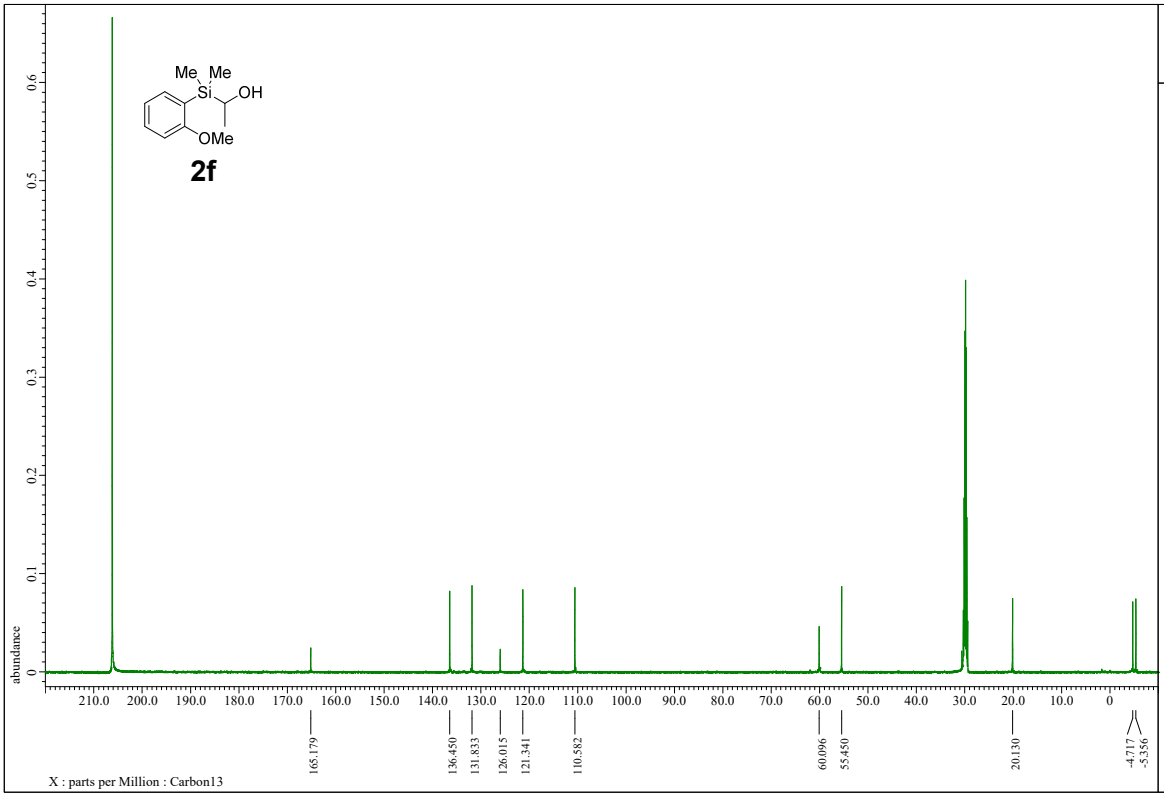


Filename = 248-032_(o-OMe)Me2_1-OH_P
Author = delta
Experiment = proton.jxp
Sample_Id = 248-032_(o-OMe)Me2_1-OH
Solvent = ACETONE-D6
Actual_Start_Time = 4-OCT-2023 18:26:56
Revision_Time = 20-FEB-2024 17:04:10

Comment = single_pulse
Data_Format = 1D COMPLEX
Dim_Size = 13107
X_Domain = Proton
Dim_Title = Proton
Dim_Units = [ppm]
Dimensions = X
Site = JNM-ECA500
Spectrometer = DELTA2_NMR

Field_Strength = 11.7473579[T] (500[MHz])
X_Acq_Duration = 1.74587904[s]
X_Domain = 1H
X_Freq = 500.15991521[MHz]
X_Offset = 5.0[ppm]
X_Points = 16384
X_Prescans = 1
X_Resolution = 0.57277737[Hz]
X_Sweep = 9.38438438[kHz]
X_Sweep_Clipped = 7.50750751[kHz]
Irr_Domain = Proton
Irr_Freq = 500.15991521[MHz]
Irr_Offset = 5.0[ppm]
Tri_Domain = Proton
Tri_Freq = 500.15991521[MHz]
Tri_Offset = 5.0[ppm]
Clipped = FALSE
Scans = 8
Total_Scans = 8

Relaxation_Delay = 5[s]
Recvr_Gain = 54
Temp_Get = 22.3[dC]
X_90_Width = 6.7[us]
X_Acq_Time = 1.74587904[s]
X_Angle = 45[deg]
X_Atn = 2.5[dB]
X_Pulse = 3.35[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Presat = FALSE
Initial_Wait = 1[s]
Repetition_Time = 6.74587904[s]



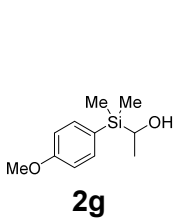
Filename = 032-co113-16_Carbon-1-3.j
Author = delta
Experiment = carbon.jxp
Sample_Id = 032-co113-16
Solvent = ACETONE-D6
Actual_Start_Time = 13-JUL-2022 16:23:23
Revision_Time = 20-FEB-2024 16:07:52

Comment = single pulse decoupled ga
Data_Format = 1D COMPLEX
Dim_Size = 26214
X_Domain = Carbon
Dim_Title = Carbon13
Dim_Units = [ppm]
Dimensions = X
Site = JNM-ECA500
Spectrometer = DELTA2_NMR

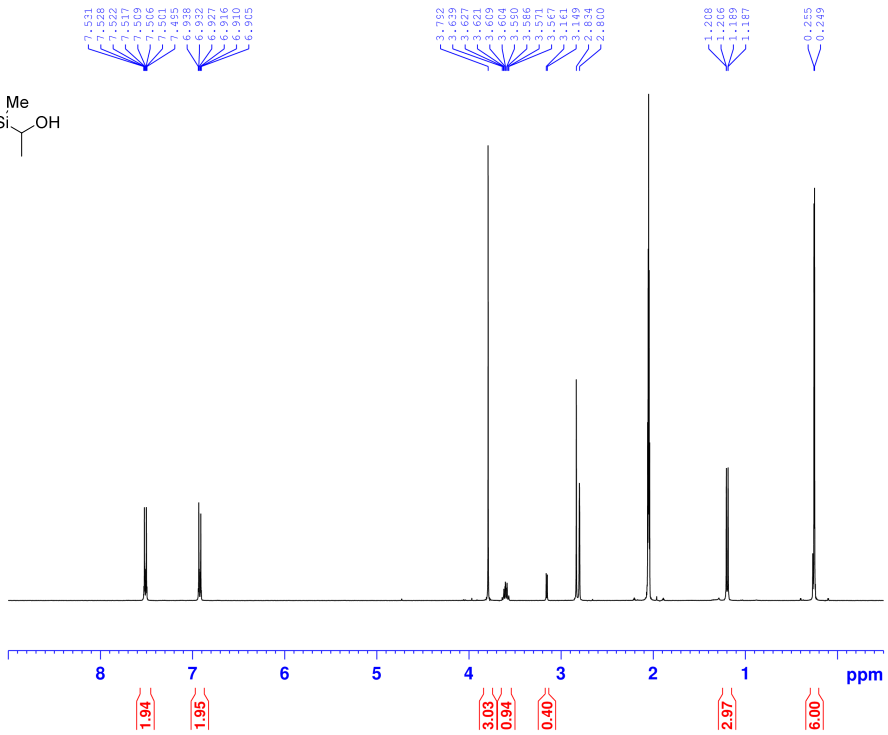
Field_Strength = 11.7473579[T] (500[MHz])
X_Acq_Duration = 0.83361792[s]
X_Domain = 13C
X_Freq = 125.76529768[MHz]
X_Offset = 100[ppm]
X_Points = 32768
X_Prescans = 4
X_Resolution = 1.19959034[Hz]
X_Sweep = 39.3081761[kHz]
X_Sweep_Clipped = 31.44654088[kHz]
Irr_Domain = Proton
Irr_Freq = 500.15991521[MHz]
Irr_Offset = 5.0[ppm]
Clipped = FALSE
Scans = 1024
Total_Scans = 1024

Relaxation_Delay = 2[s]
Recvr_Gain = 50
Temp_Get = 22[dC]
X_90_Width = 12.65[us]
X_Acq_Time = 0.83361792[s]
X_Angle = 30[deg]
X_Atn = 7[dB]
X_Pulse = 4.21666667[us]
Irr_Atn_Dec = 25.254[dB]
Irr_Atn_Noe = 25.254[dB]
Irr_Noise = WALTZ
Irr_Pwidth = 92[us]
Decoupling = TRUE
Initial_Wait = 1[s]
Noe = TRUE
Noe_Time = 2[s]
Repetition_Time = 2.83361792[s]

p-OMe HB col126-29 acetone 4/30

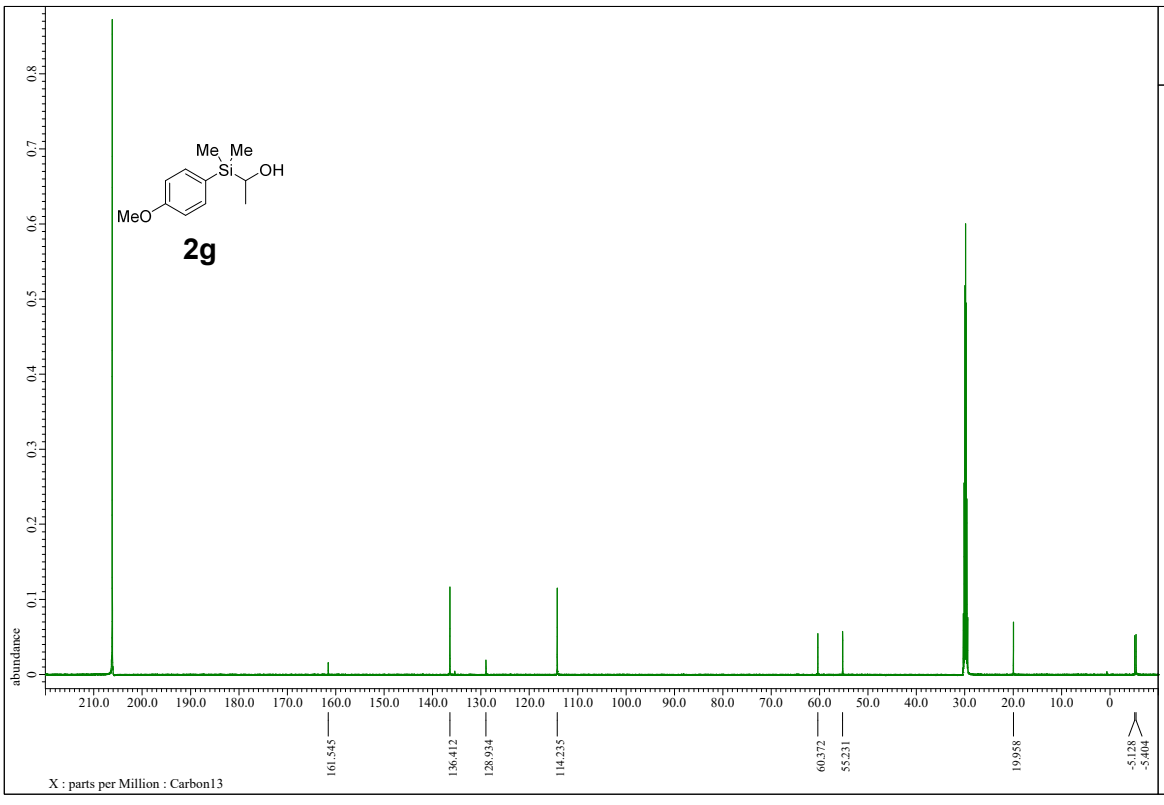


2g



IBB-nmr Analysis

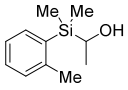
NAME	NN248-039
EXPNO	8
PROCNO	1
Date_	20220430
Time	20.20
INSTRUM	av400
PROBHD	5 mm PABBO BB-
PULPROG	zg30
TD	65536
SOLVENT	Acetone
NS	16
DS	2
SWH	8223.685 Hz
FIDRES	0.125483 Hz
AQ	3.9846387 sec
RG	203
DW	60.800 usec
DE	6.50 usec
TE	296.5 K
D1	1.00000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	1H
P1	14.00 usec
PL1	-1.80 dB
PL1W	14.82738590 W
SFO1	400.1324710 MHz
SI	32768
SF	400.1300067 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00



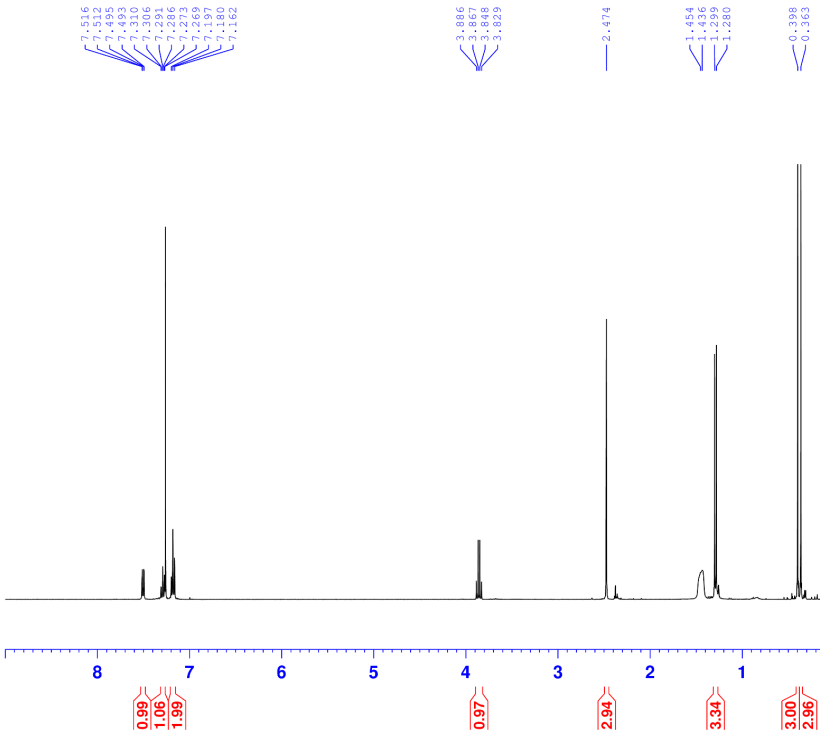
JEOL

Filename	= 039-co126-29_Carbon-1-3.j
Author	= delta
Experiment	= carbon.jxp
Sample_Id	= 039-co126-29
Solvent	= ACETONE-D6
Actual_Start_Time	= 2-MAY-2022 15:30:31
Revision_Time	= 20-FEB-2024 15:47:48
Comment	= single pulse decoupled ga
Data_Format	= 1D COMPLEX
Dim_Size	= 26214
X_Domain	= Carbon
Dim_Title	= Carbon13
Dim_Units	= [ppm]
Dimensions	= X
Site	= JNM-ECA500
Spectrometer	= DELTA2_NMR
Field_Strength	= 11.7473579[T] (500[MHz])
X_Acq_Duration	= 0.83361792[s]
X_Domain	= 13C
X_Freq	= 125.76529768[MHz]
X_Offset	= 100[ppm]
X_Points	= 32768
X_Prescans	= 4
X_Resolution	= 1.19959034[Hz]
X_Sweep	= 39.3081761[kHz]
X_Sweep_Clipped	= 31.44654088[kHz]
Irr_Domain	= Proton
Irr_Freq	= 500.15991521[MHz]
Irr_Offset	= 5.0[ppm]
Clipped	= FALSE
Scans	= 2048
Total_Scans	= 2048
Relaxation_Delay	= 2[s]
Recvr_Gain	= 50
Temp_Get	= 22.1[dC]
X_90_Width	= 12.65[us]
X_Acq_Time	= 0.83361792[s]
X_Angle	= 30[deg]
X_Atn	= 7[dB]
X_Pulse	= 4.21666667[us]
Irr_Atn_Dec	= 25.254[dB]
Irr_Atn_Noe	= 25.254[dB]
Irr_Noise	= WALTZ
Irr_Pwidth	= 92[us]
Decoupling	= TRUE
Initial_Wait	= 1[s]
Noe	= TRUE
Noe_Time	= 2[s]
Repetition_Time	= 2.83361792[s]

o-Me HB col11-13 dry

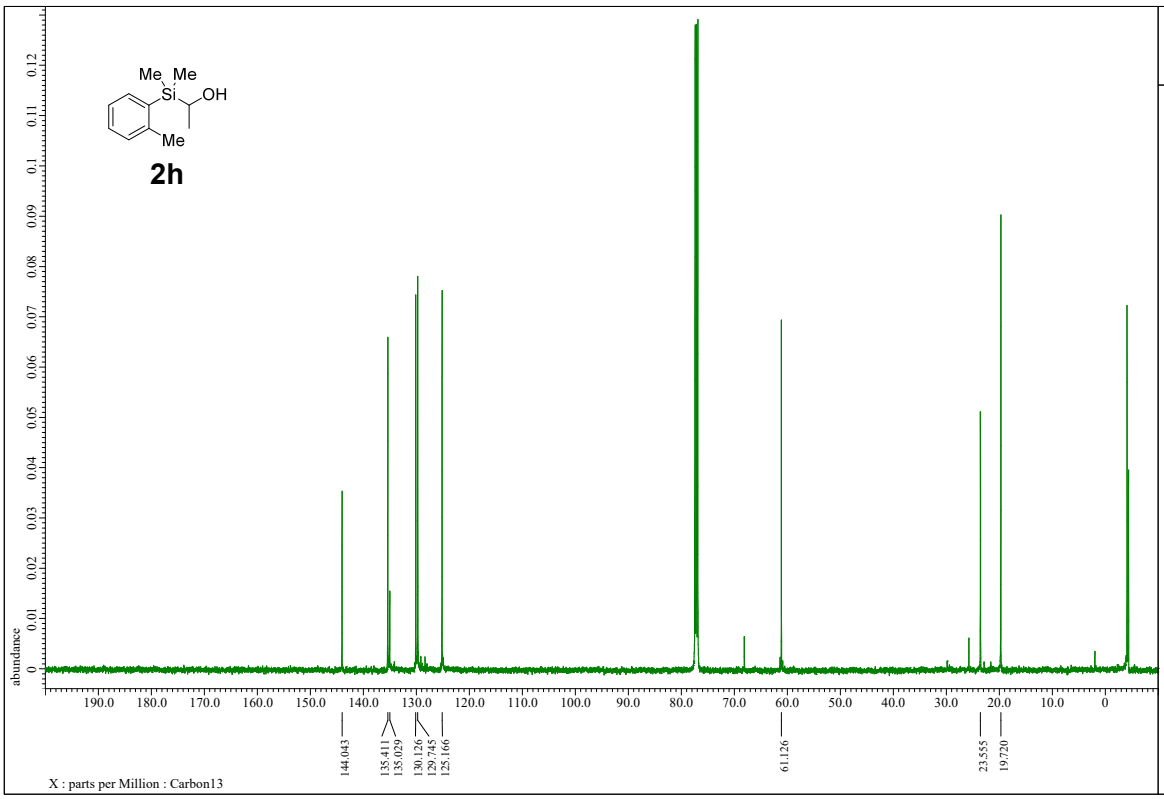


2h



IBB-nmr Analysis

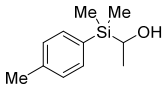
```
NAME            NN248-046
EXPNO                   5
PROCNO                  1
Date_            20220517
Time                21.14
INSTRUM             av400
PROBHD    5 mm PABBO BB-
PULPROG              zg30
TD                  65536
SOLVENT             CDCl3
NS                     16
DS                      2
SWH              8223.685 Hz
FIDRES           0.125483 Hz
AQ               3.9846387 sec
RG                    203
DW                60.800 usec
DE                 6.50 usec
TE                297.0 K
D1             1.00000000 sec
TD0                     1

======== CHANNEL f1 ========
NUC1                   1H
P1                 14.00 usec
PL1                -1.80 dB
PL1W         14.82738590 W
SFO1         400.1324710 MHz
SI                  32768
SF           400.1300096 MHz
WDW                    EM
SSB                     0
LB                 0.30 Hz
GB                      0
PC                 1.00
```



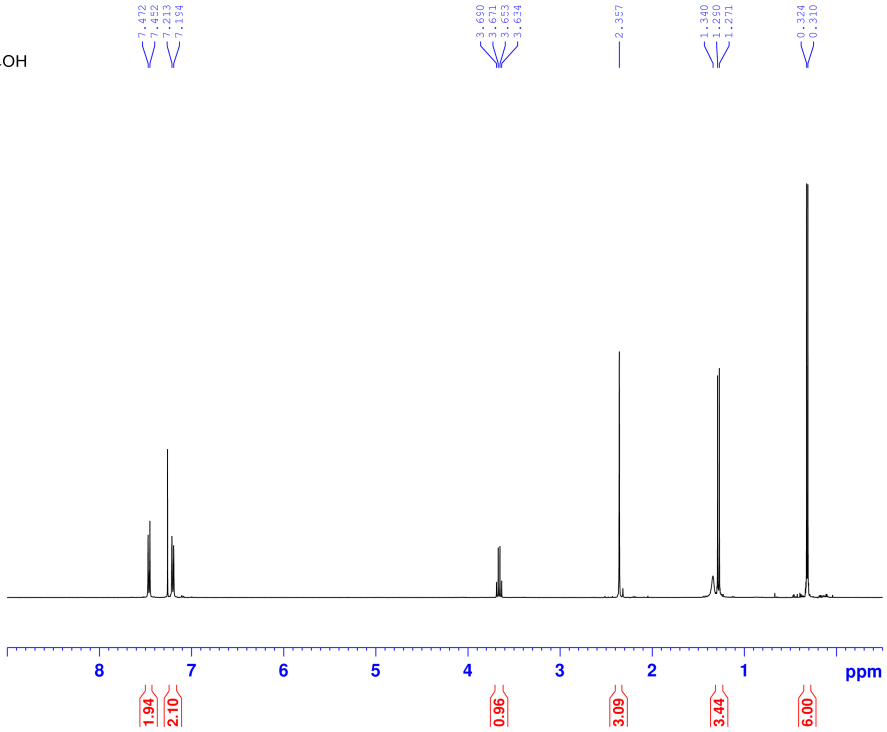
JEOL

```
Filename          = 045-col11-13_Carbon-1-2.j
Author            = delta
Experiment        = carbon.jxp
Sample_Id         = 045-col11-13
Solvent           = CHLOROFORM-D
Actual_Start_Time = 27-MAY-2022 17:37:06
Revision_Time     = 20-FEB-2024 16:22:43

Comment           = single pulse decoupled ga
Data_Format       = 1D COMPLEX
Dim_Size          = 26214
X_Domain          = Carbon
Dim_Title         = Carbon13
Dim_Units         = [ppm]
Dimensions        = X
Site              = JNM-ECA500
Spectrometer      = DELTA2_NMR

Field_Strength    = 11.7473579[T] (500[MHz])
X_Acq_Duration    = 0.83361792[s]
X_Domain          = 13C
X_Freq            = 125.76529768[MHz]
X_Offset          = 100[ppm]
X_Points          = 32768
X_Prescans        = 4
X_Resolution      = 1.19959034[Hz]
X_Sweep           = 39.3081761[kHz]
X_Sweep_Clipped   = 31.44654088[kHz]
Irr_Domain        = Proton
Irr_Freq          = 500.15991521[MHz]
Irr_Offset        = 5.0[ppm]
Clipped           = FALSE
Scans             = 2048
Total_Scans       = 2048

Relaxation_Delay  = 2[s]
Recvr_Gain        = 50
Temp_Get          = 22.4[dC]
X_90_Width        = 12.65[us]
X_Acq_Time        = 0.83361792[s]
X_Angle           = 30[deg]
X_Atn             = 7[dB]
X_Pulse           = 4.21666667[us]
Irr_Atn_Dec       = 25.254[dB]
Irr_Atn_Noe       = 25.254[dB]
Irr_Noise         = WALTZ
Irr_Pwidth        = 92[us]
Decoupling        = TRUE
Initial_Wait      = 1[s]
Noe               = TRUE
Noe_Time          = 2[s]
Repetition_Time   = 2.83361792[s]
```

p-Me HB col11-13

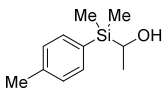


2i



IBB-nmr Analysis

```
NAME            NN248-037
EXPNO                   2
PROCNO                  1
Date_            20220422
Time                20.52
INSTRUM             av400
PROBHD    5 mm PABBO BB-
PULPROG              zg30
TD                  65536
SOLVENT             CDCl3
NS                     16
DS                      2
SWH              8223.685 Hz
FIDRES           0.125483 Hz
AQ               3.9846387 sec
RG                    203
DW                60.800 usec
DE                 6.50 usec
TE                296.9 K
D1             1.00000000 sec
TD0                     1

======== CHANNEL f1 ========
NUC1                   1H
P1                 14.00 usec
PL1                -1.80 dB
PL1W         14.82738590 W
SFO1         400.1324710 MHz
SI                  32768
SF           400.1300096 MHz
WDW                    EM
SSB                     0
LB                 0.30 Hz
GB                      0
PC                 1.00
```

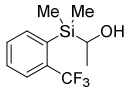


2i

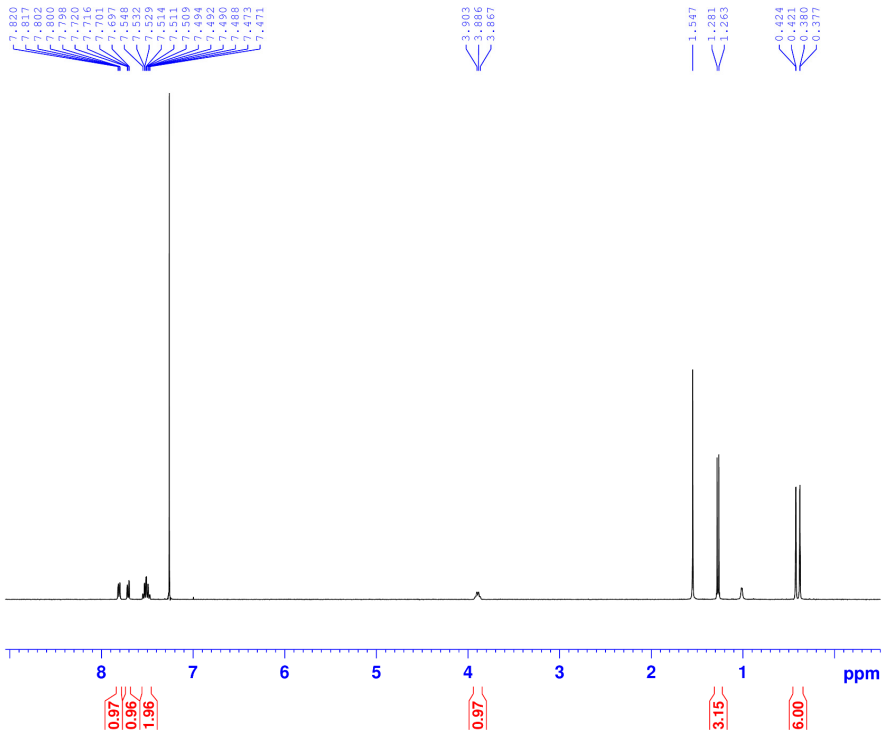
JEOL

```
Filename          = 037-col11-13_Carbon-1-2.j
Author            = delta
Experiment        = carbon.jxp
Sample_Id         = 037-col11-13
Solvent           = CHLOROFORM-D
Actual_Start_Time = 28-APR-2022 16:25:08
Revision_Time     = 20-FEB-2024 16:01:49

Comment           = single pulse decoupled ga
Data_Format       = 1D COMPLEX
Dim_Size          = 26214
X_Domain          = Carbon
Dim_Title         = Carbon13
Dim_Units         = [ppm]
Dimensions        = X
Site              = JNM-ECA500
Spectrometer      = DELTA2_NMR

Field_Strength    = 11.7473579[T] (500[MHz])
X_Acq_Duration    = 0.83361792[s]
X_Domain          = 13C
X_Freq            = 125.76529768[MHz]
X_Offset          = 100[ppm]
X_Points          = 32768
X_Prescans        = 4
X_Resolution      = 1.19959034[Hz]
X_Sweep           = 39.3081761[kHz]
X_Sweep_Clipped   = 31.44654088[kHz]
Irr_Domain        = Proton
Irr_Freq          = 500.15991521[MHz]
Irr_Offset        = 5.0[ppm]
Clipped           = TRUE
Scans             = 2048
Total_Scans       = 2048

Relaxation_Delay  = 2[s]
Recvr_Gain        = 50
Temp_Get          = 22.5[dC]
X_90_Width        = 12.65[us]
X_Acq_Time        = 0.83361792[s]
X_Angle           = 30[deg]
X_Atn             = 7[dB]
X_Pulse           = 4.21666667[us]
Irr_Atn_Dec       = 25.254[dB]
Irr_Atn_Noe       = 25.254[dB]
Irr_Noise         = WALTZ
Irr_Pwidth        = 92[us]
Decoupling        = TRUE
Initial_Wait      = 1[s]
Noe               = TRUE
Noe_Time          = 2[s]
Repetition_Time   = 2.83361792[s]
```

o-CF3 HB col12-13 GPC 121-127min 7/11

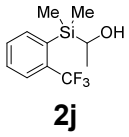


2j



IBB-nmr Analysis

```
NAME            NN248-049
EXPNO                   7
PROCNO                  1
Date_            20220711
Time                21.31
INSTRUM           av400
PROBHD    5 mm PABBO BB-
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                      4
DS                      2
SWH             8223.685 Hz
FIDRES          0.125483 Hz
AQ              3.9846387 sec
RG                    203
DW                60.800 usec
DE                 6.50 usec
TE                297.4 K
D1             1.00000000 sec
TD0                     1

======== CHANNEL f1 ========
NUC1                  1H
P1                14.00 usec
PL1               -1.80 dB
PL1W         14.82738590 W
SFO1         400.1324710 MHz
SI                  32768
SF           400.1300096 MHz
WDW                   EM
SSB                    0
LB                  0.30 Hz
GB                     0
PC                  1.00
```

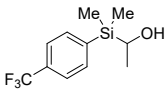


2j

JEOL

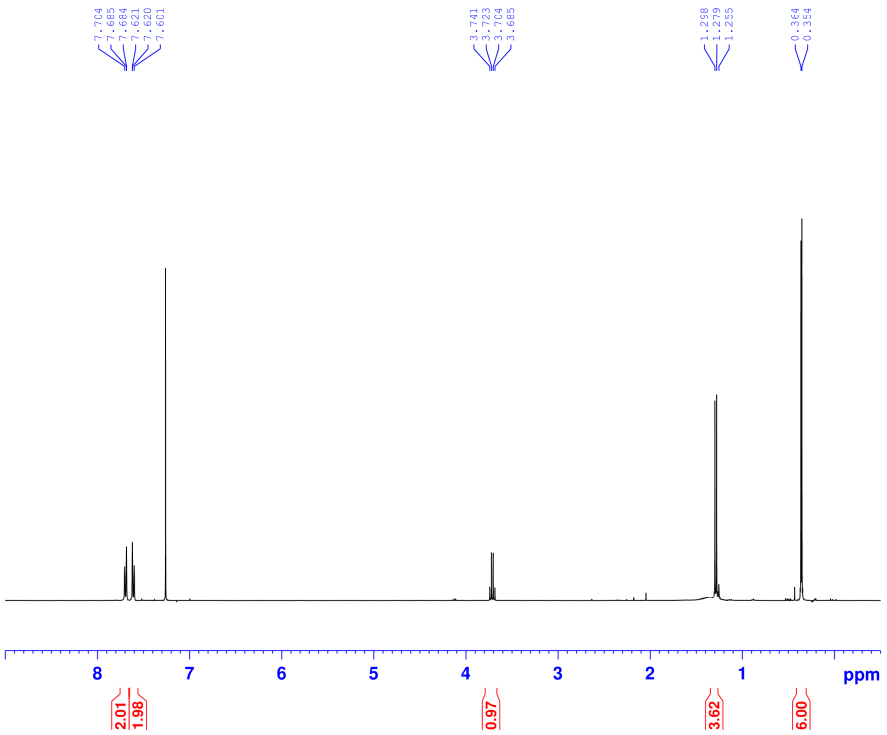
```
Filename          = o-CF3_Me2_1OH_13C-2.jdf
Author            = delta
Experiment        = carbon.jxp
Sample_Id         = 049-col12-13-GPC
Solvent           = CHLOROFORM-D
Actual_Start_Time = 11-JUL-2022 22:47:38
Revision_Time     = 20-FEB-2024 16:20:00

Comment           = single pulse decoupled ga
Data_Format       = 1D COMPLEX
Dim_Size          = 26214
X_Domain          = Carbon
Dim_Title         = Carbon13
Dim_Units         = [ppm]
Dimensions        = X
Site              = JNM-ECA500
Spectrometer      = DELTA2_NMR

Field_Strength    = 11.7473579[T] (500[MHz])
X_Acq_Duration    = 0.83361792[s]
X_Domain          = 13C
X_Freq            = 125.76529768[MHz]
X_Offset          = 100[ppm]
X_Points          = 32768
X_Prescans        = 4
X_Resolution      = 1.19959034[Hz]
X_Sweep           = 39.3081761[kHz]
X_Sweep_Clipped   = 31.44654088[kHz]
Irr_Domain        = Proton
Irr_Freq          = 500.15991521[MHz]
Irr_Offset        = 5.0[ppm]
Clipped           = TRUE
Scans             = 4096
Total_Scans       = 4096

Relaxation_Delay  = 2[s]
Recvr_Gain        = 50
Temp_Get          = 22.2[dC]
X_90_Width        = 12.65[us]
X_Acq_Time        = 0.83361792[s]
X_Angle           = 30[deg]
X_Atn             = 7[dB]
X_Pulse           = 4.21666667[us]
Irr_Atn_Dec       = 25.254[dB]
Irr_Atn_Noe       = 25.254[dB]
Irr_Noise         = WALTZ
Irr_Pwidth        = 92[us]
Decoupling        = TRUE
Initial_Wait      = 1[s]
Noe               = TRUE
Noe_Time          = 2[s]
Repetition_Time   = 2.83361792[s]
```

p-CF3 HB col25-28

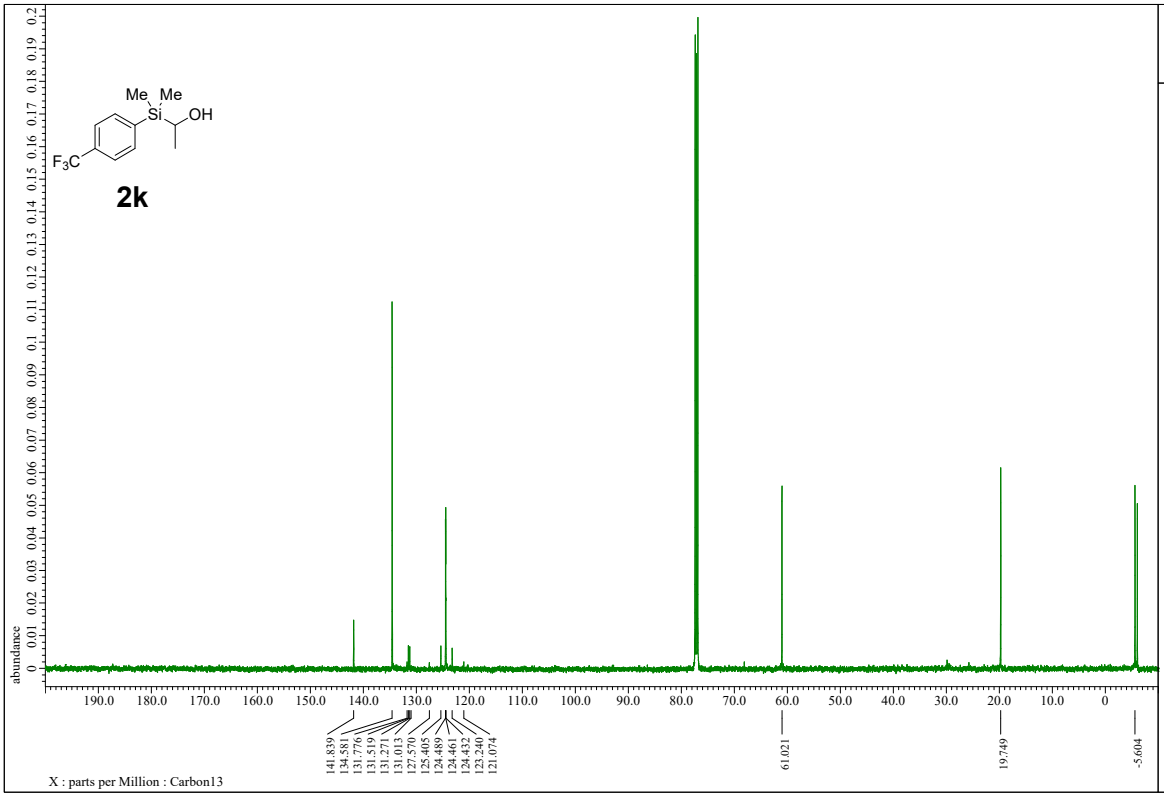


2k

IBB-nmr Analysis




```
NAME            NN248-030
EXPNO                   2
PROCNO                  1
Date_            20220329
Time                23.19
INSTRUM             av400
PROBHD    5 mm PABBO BB-
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                    16
DS                     2
SWH             8223.685 Hz
FIDRES          0.125483 Hz
AQ              3.9846387 sec
RG                   203
DW                60.800 usec
DE                 6.50 usec
TE                296.2 K
D1             1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  1H
P1                 14.00 usec
PL1                -1.80 dB
PL1W         14.82738590 W
SFO1         400.1324710 MHz
SI                 32768
SF           400.1300096 MHz
WDW                   EM
SSB                    0
LB                  0.30 Hz
GB                     0
PC                  1.00
```

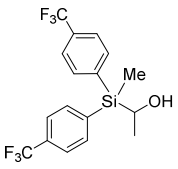


2k

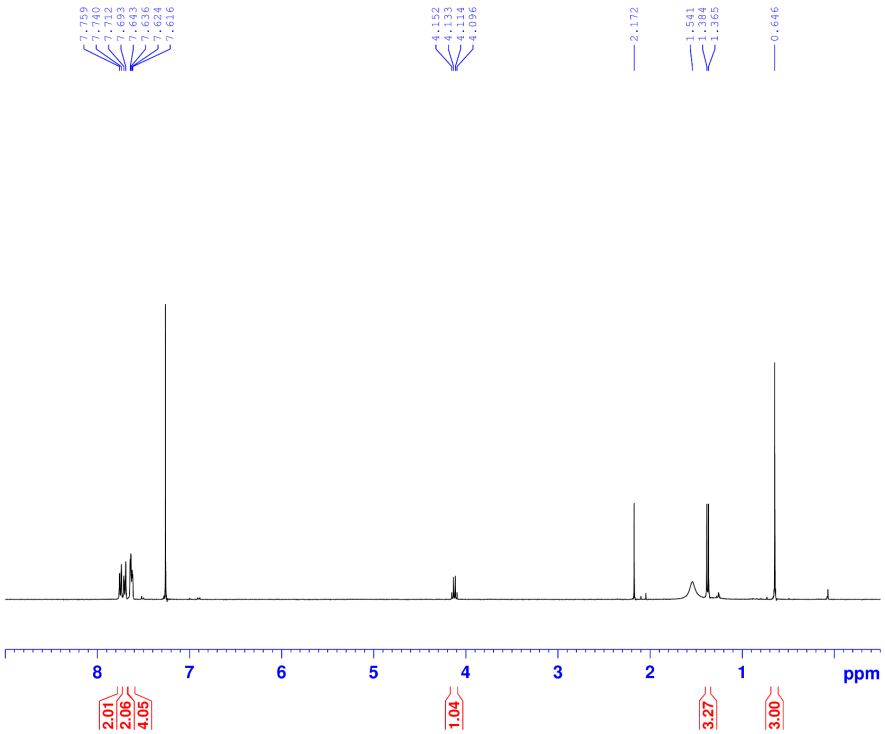
JEOL

```
Filename          = 030-col2528_Carbon-1-2.jd
Author            = delta
Experiment        = carbon.jxp
Sample_Id         = 030-col2528
Solvent           = CHLOROFORM-D
Actual_Start_Time = 30-MAR-2022 15:13:13
Revision_Time     = 20-FEB-2024 15:52:48

Comment           = single pulse decoupled ga
Data_Format       = 1D COMPLEX
Dim_Size          = 26214
X_Domain          = Carbon
Dim_Title         = Carbon13
Dim_Units         = [ppm]
Dimensions        = X
Site              = JNM-ECA500
Spectrometer      = DELTA2_NMR

Field_Strength    = 11.7473579[T] (500[MHz])
X_Acq_Duration    = 0.83361792[s]
X_Domain          = 13C
X_Freq            = 125.76529768[MHz]
X_Offset          = 100[ppm]
X_Points          = 32768
X_Prescans        = 4
X_Resolution      = 1.19959034[Hz]
X_Sweep           = 39.3081761[kHz]
X_Sweep_Clipped   = 31.44654088[kHz]
Irr_Domain        = Proton
Irr_Freq          = 500.15991521[MHz]
Irr_Offset        = 5.0[ppm]
Clipped           = FALSE
Scans             = 1024
Total_Scans       = 1024

Relaxation_Delay  = 2[s]
Recvr_Gain        = 50
Temp_Get          = 21.3[dC]
X_90_Width        = 12.65[us]
X_Acq_Time        = 0.83361792[s]
X_Angle           = 30[deg]
X_Atn             = 7[dB]
X_Pulse           = 4.21666667[us]
Irr_Atn_Dec       = 25.254[dB]
Irr_Atn_Noe       = 25.254[dB]
Irr_Noise         = WALTZ
Irr_Pwidth        = 92[us]
Decoupling        = TRUE
Initial_Wait      = 1[s]
Noe               = TRUE
Noe_Time          = 2[s]
Repetition_Time   = 2.83361792[s]
```

(p-CF3)2Me HB col11-14 6/24

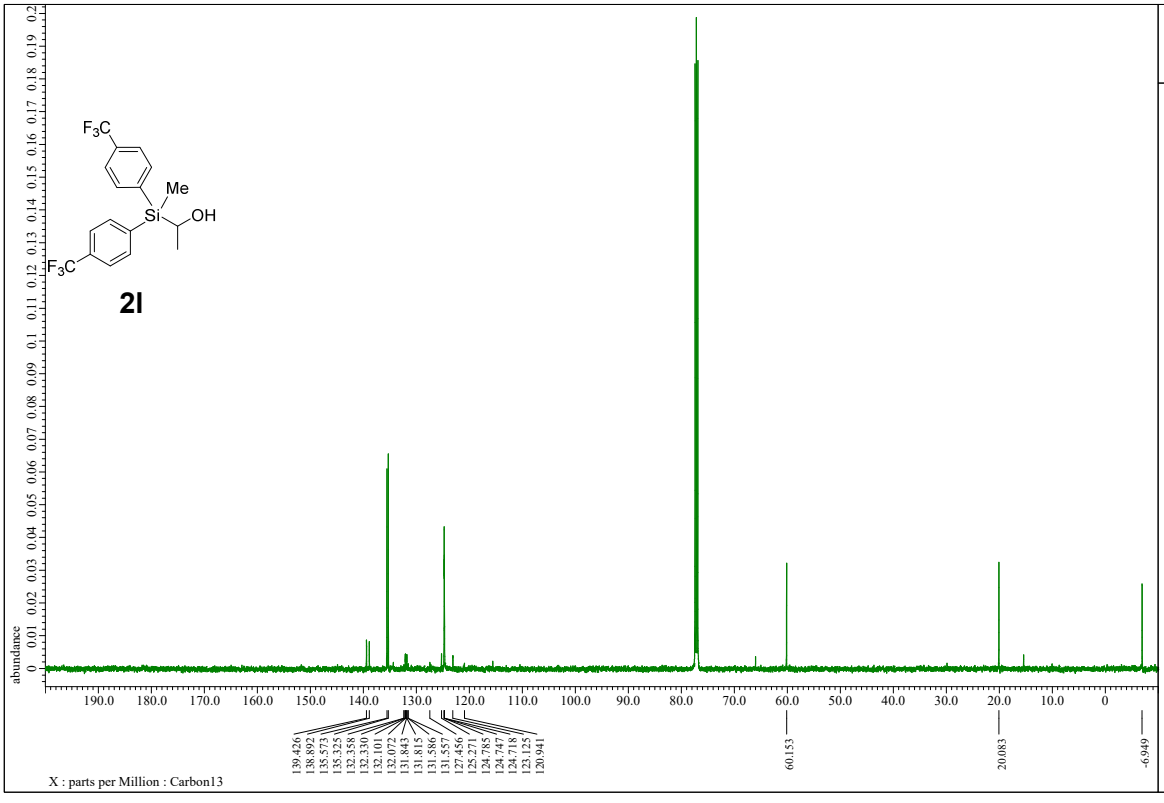


2l



IBB-nmr Analysis

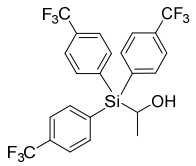
NAME	NN248-066
EXPNO	4
PROCNO	1
Date_	20220624
Time	14.38
INSTRUM	av400
PROBHD	5 mm PABBO BB-
PULPROG	zg30
TD	65536
SOLVENT	CDCl3
NS	4
DS	2
SWH	8223.685 Hz
FIDRES	0.125483 Hz
AQ	3.9846387 sec
RG	203
DW	60.800 usec
DE	6.50 usec
TE	297.2 K
D1	1.00000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	1H
P1	14.00 usec
PL1	-1.80 dB
PL1W	14.82738590 W
SFO1	400.1324710 MHz
SI	32768
SF	400.1300096 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00



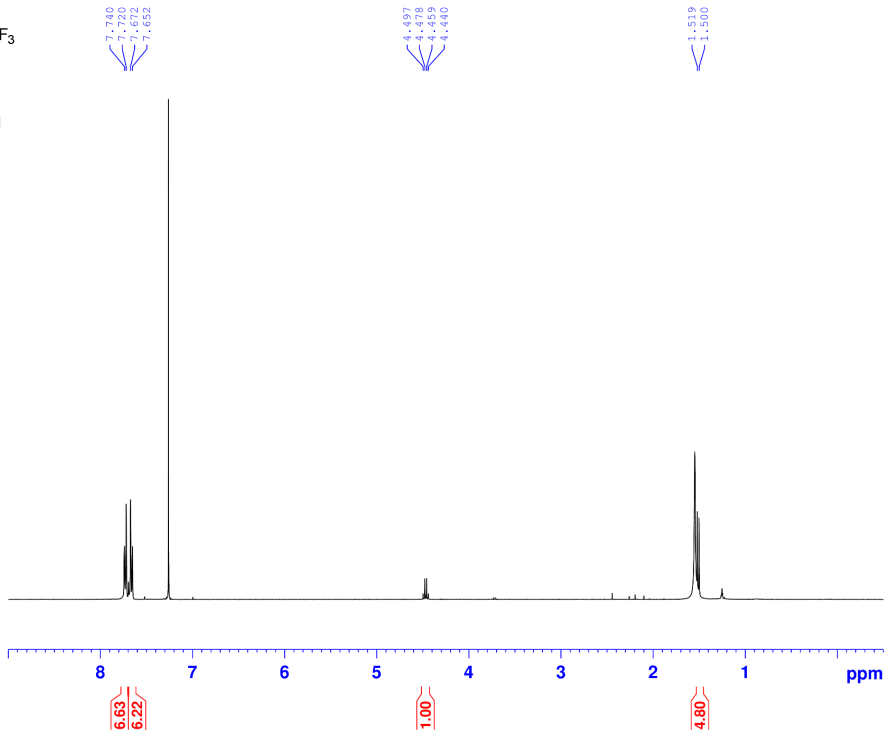
JEOL

Filename	= 066-col11-14_Carbon-1-2.j
Author	= delta
Experiment	= carbon.jxp
Sample_Id	= 066-col11-14
Solvent	= CHLOROFORM-D
Actual_Start_Time	= 7-JUL-2022 12:49:13
Revision_Time	= 20-FEB-2024 16:27:45
Comment	= single pulse decoupled ga
Data_Format	= 1D COMPLEX
Dim_Size	= 26214
X_Domain	= Carbon
Dim_Title	= Carbon13
Dim_Units	= [ppm]
Dimensions	= X
Site	= JNM-ECA500
Spectrometer	= DELTA2_NMR
Field_Strength	= 11.7473579[T] (500[MHz])
X_Acq_Duration	= 0.83361792[s]
X_Domain	= 13C
X_Freq	= 125.76529768[MHz]
X_Offset	= 100[ppm]
X_Points	= 32768
X_Prescans	= 4
X_Resolution	= 1.19959034[Hz]
X_Sweep	= 39.3081761[kHz]
X_Sweep_Clipped	= 31.44654088[kHz]
Irr_Domain	= Proton
Irr_Freq	= 500.15991521[MHz]
Irr_Offset	= 5.0[ppm]
Clipped	= FALSE
Scans	= 1024
Total_Scans	= 1024
Relaxation_Delay	= 2[s]
Recvr_Gain	= 50
Temp_Get	= 22.1[dC]
X_90_Width	= 12.65[us]
X_Acq_Time	= 0.83361792[s]
X_Angle	= 30[deg]
X_Atn	= 7[dB]
X_Pulse	= 4.21666667[us]
Irr_Atn_Dec	= 25.254[dB]
Irr_Atn_Noe	= 25.254[dB]
Irr_Noise	= WALTZ
Irr_Pwidth	= 92[us]
Decoupling	= TRUE
Initial_Wait	= 1[s]
Noe	= TRUE
Noe_Time	= 2[s]
Repetition_Time	= 2.83361792[s]

(p-CF3)3 HB col16-30 recry

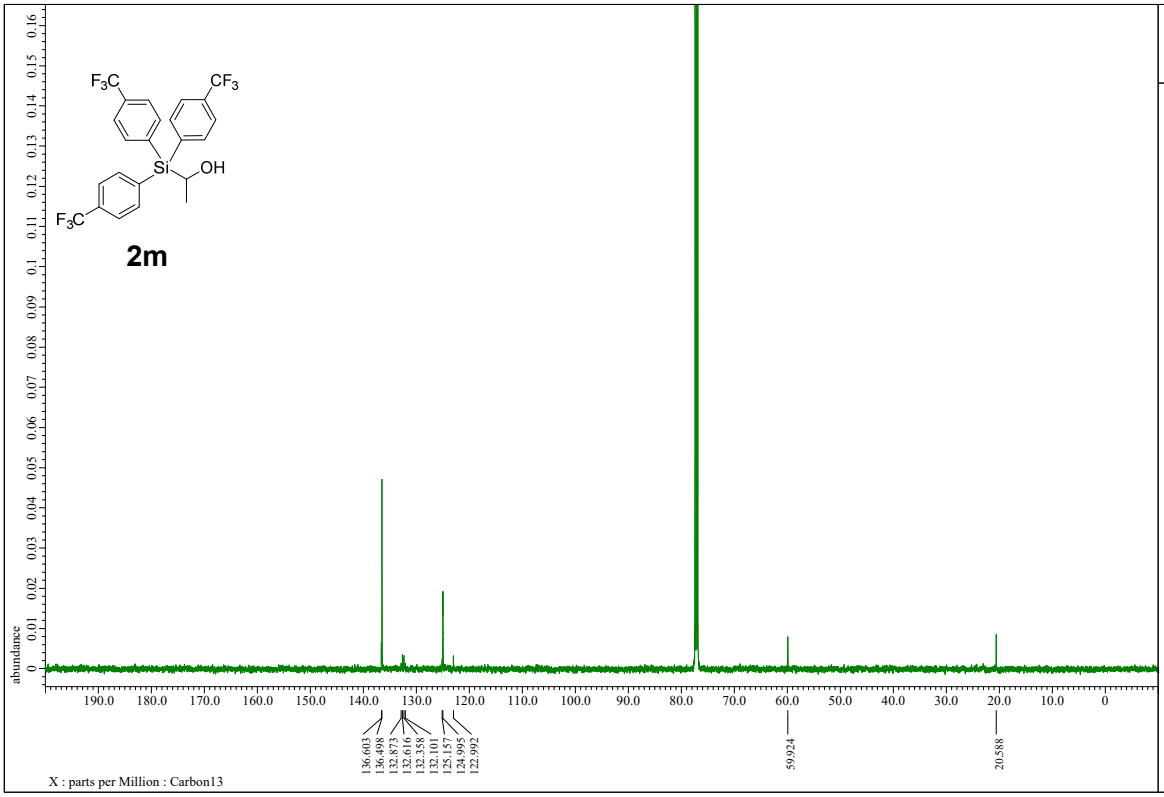


2m

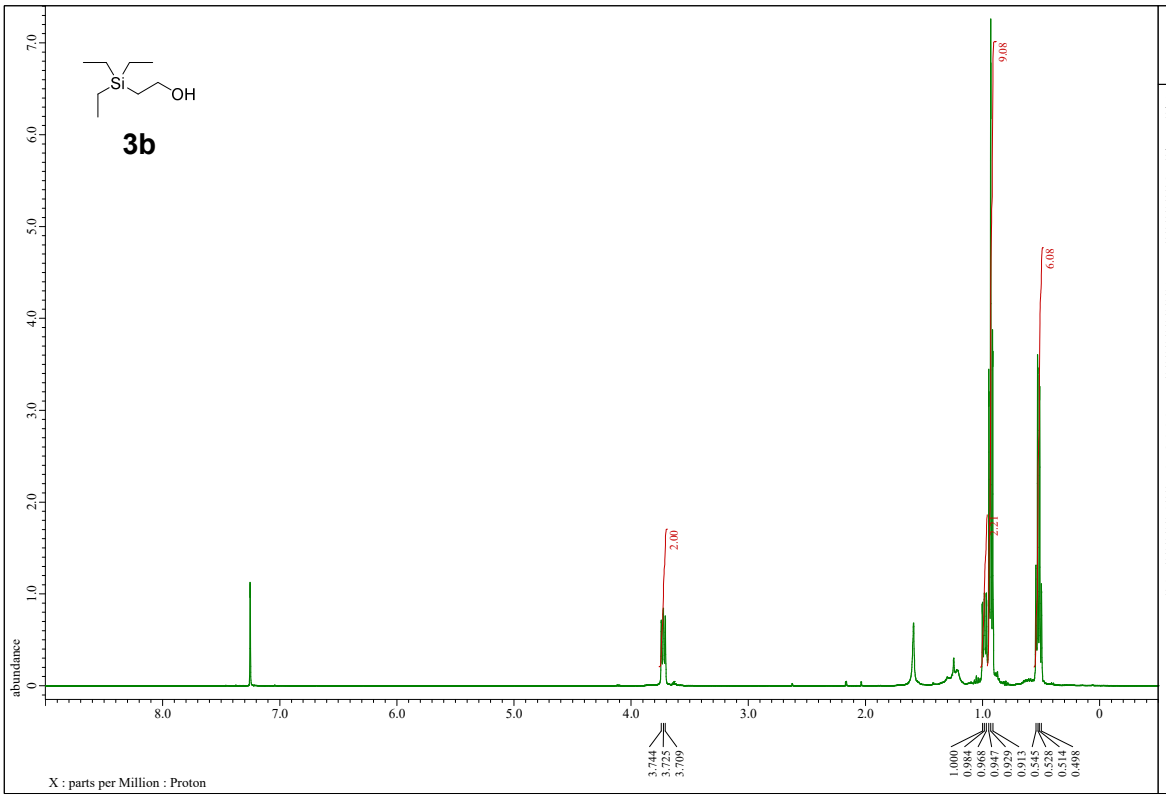


IBB-nmr Analysis

```
NAME            NN248-054
EXPNO                   3
PROCNO                  1
Date_            20220610
Time                19.00
INSTRUM             av400
PROBHD    5 mm PABBO BB-
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                    16
DS                     2
SWH             8223.685 Hz
FIDRES          0.125483 Hz
AQ              3.9846387 sec
RG                   203
DW                60.800 usec
DE                 6.50 usec
TE                297.1 K
D1             1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  1H
P1                14.00 usec
PL1               -1.80 dB
PL1W         14.82738590 W
SFO1         400.1324710 MHz
SI                 32768
SF           400.1300096 MHz
WDW                   EM
SSB                    0
LB                  0.30 Hz
GB                     0
PC                  1.00
```

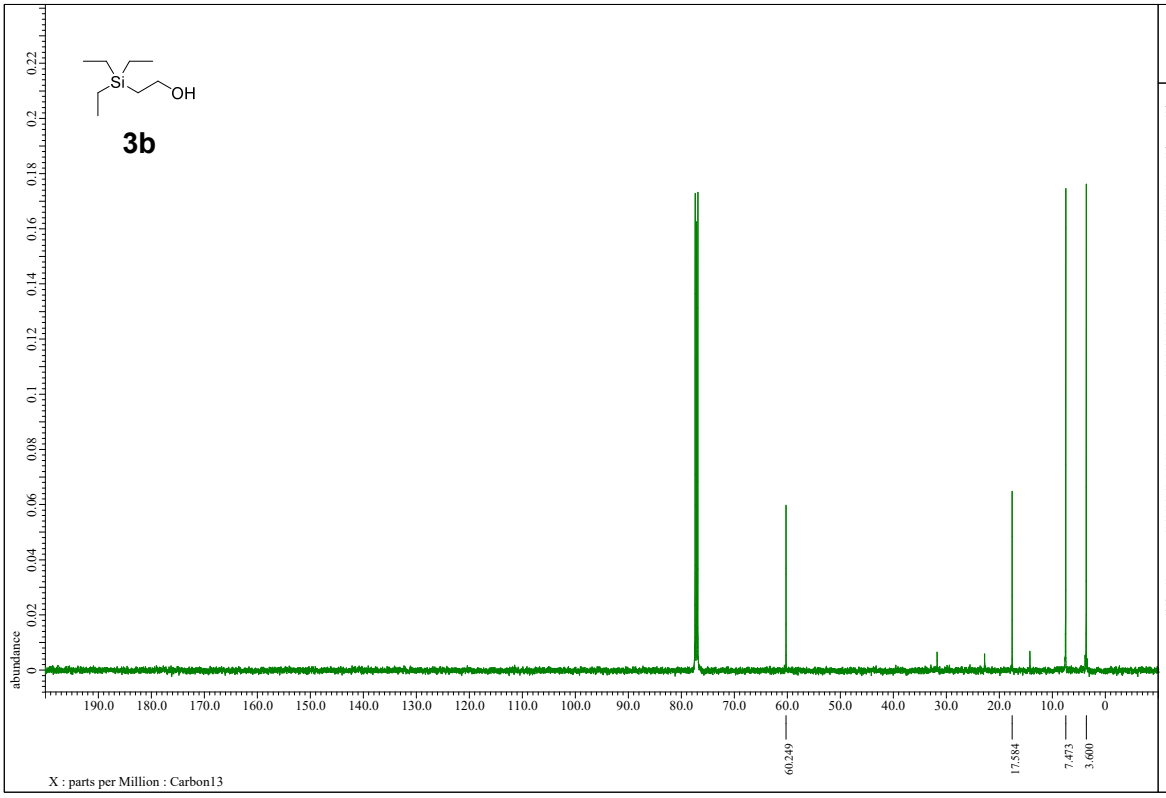



```
Filename          = 054-col6-10-recry_Carbon-
Author            = delta
Experiment        = carbon.jxp
Sample_Id         = 054-col6-10-recry
Solvent           = CHLOROFORM-D
Actual_Start_Time = 13-JUL-2022 17:35:08
Revision_Time     = 20-FEB-2024 16:29:50

Comment           = single pulse decoupled ga
Data_Format       = 1D COMPLEX
Dim_Size          = 26214
X_Domain          = Carbon
Dim_Title         = Carbon13
Dim_Units         = [ppm]
Dimensions        = X
Site              = JNM-ECA500
Spectrometer      = DELTA2_NMR

Field_Strength    = 11.7473579[T] (500[MHz])
X_Acq_Duration    = 0.83361792[s]
X_Domain          = 13C
X_Freq            = 125.76529768[MHz]
X_Offset          = 100[ppm]
X_Points          = 32768
X_Prescans        = 4
X_Resolution      = 1.19959034[Hz]
X_Sweep           = 39.3081761[kHz]
X_Sweep_Clipped   = 31.44654088[kHz]
Irr_Domain        = Proton
Irr_Freq          = 500.15991521[MHz]
Irr_Offset        = 5.0[ppm]
Clipped           = TRUE
Scans             = 1024
Total_Scans       = 1024

Relaxation_Delay  = 2[s]
Recvr_Gain        = 50
Temp_Get          = 22.1[dC]
X_90_Width        = 12.65[us]
X_Acq_Time        = 0.83361792[s]
X_Angle           = 30[deg]
X_Atn             = 7[dB]
X_Pulse           = 4.21666667[us]
Irr_Atn_Dec       = 25.254[dB]
Irr_Atn_Noe       = 25.254[dB]
Irr_Noise         = WALTZ
Irr_Pwidth        = 92[us]
Decoupling        = TRUE
Initial_Wait      = 1[s]
Noe               = TRUE
Noe_Time          = 2[s]
Repetition_Time   = 2.83361792[s]
```



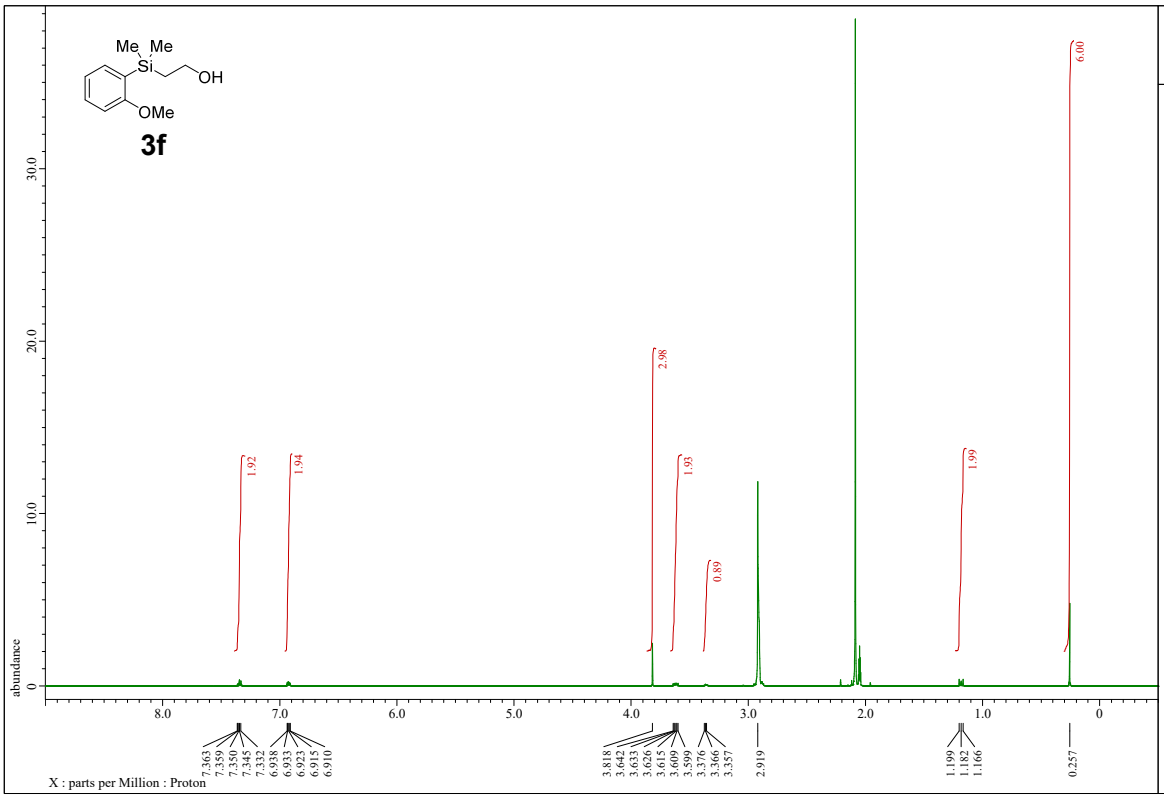
JEOL

```
Filename          = 270-042-4_col20-22_dist_P
Author            = delta
Experiment        = proton.jxp
Sample_Id         = 270-042-4_col20-22_dist
Solvent           = CHLOROFORM-D
Actual_Start_Time = 11-SEP-2023 16:06:02
Revision_Time     = 20-FEB-2024 19:21:23

Comment           = single_pulse
Data_Format       = 1D COMPLEX
Dim_Size          = 13107
X_Domain          = Proton
Dim_Title         = Proton
Dim_Units         = [ppm]
Dimensions        = X
Site              = JNM-ECA500
Spectrometer      = DELTA2_NMR

Field_Strength    = 11.7473579[T] (500[MHz])
X_Acq_Duration    = 1.74587904[s]
X_Domain          = 1H
X_Freq            = 500.15991521[MHz]
X_Offset          = 5.0[ppm]
X_Points          = 16384
X_Prescans        = 1
X_Resolution      = 0.57277737[Hz]
X_Sweep           = 9.38438438[kHz]
X_Sweep_Clipped   = 7.50750751[kHz]
Irr_Domain        = Proton
Irr_Freq          = 500.15991521[MHz]
Irr_Offset        = 5.0[ppm]
Tri_Domain        = Proton
Tri_Freq          = 500.15991521[MHz]
Tri_Offset        = 5.0[ppm]
Clipped           = FALSE
Scans             = 16
Total_Scans       = 16

Relaxation_Delay  = 5[s]
Recvr_Gain        = 48
Temp_Get          = 22.8[dC]
X_90_Width        = 6.7[us]
X_Acq_Time        = 1.74587904[s]
X_Angle           = 45[deg]
X_Atn             = 2.5[dB]
X_Pulse           = 3.35[us]
Irr_Mode          = Off
Tri_Mode          = Off
Dante_Presat      = FALSE
Initial_Wait      = 1[s]
Repetition_Time   = 6.74587904[s]
```

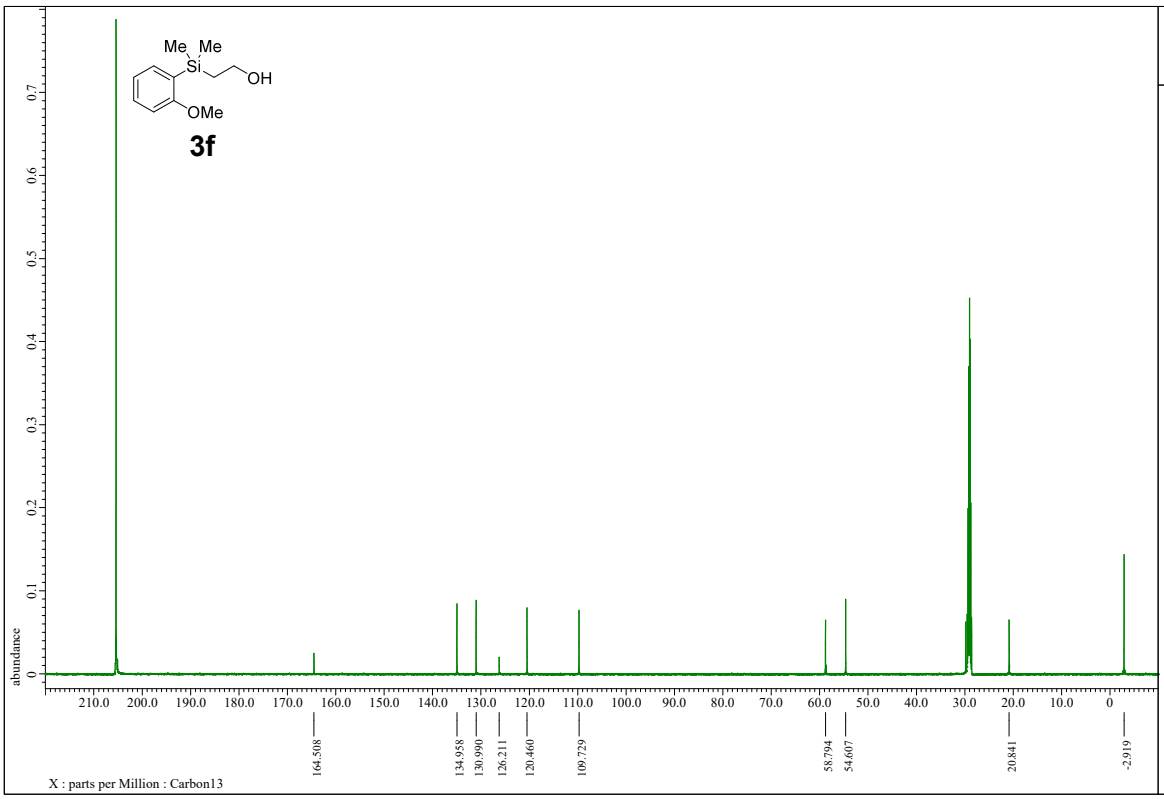


JEOL

```
Filename          = 270-042-4_col20-23_dist_C
Author            = delta
Experiment        = carbon.jxp
Sample_Id         = 270-042-4_col20-23_dist
Solvent           = CHLOROFORM-D
Actual_Start_Time = 11-SEP-2023 17:27:26
Revision_Time     = 20-FEB-2024 19:18:55

Comment           = single pulse decoupled ga
Data_Format       = 1D COMPLEX
Dim_Size          = 26214
X_Domain          = Carbon
Dim_Title         = Carbon13
Dim_Units         = [ppm]
Dimensions        = X
Site              = JNM-ECA500
Spectrometer      = DELTA2_NMR

Field_Strength    = 11.7473579[T] (500[MHz])
X_Acq_Duration    = 0.83361792[s]
X_Domain          = 13C
X_Freq            = 125.76529768[MHz]
X_Offset          = 100[ppm]
X_Points          = 32768
X_Prescans        = 4
X_Resolution      = 1.19959034[Hz]
X_Sweep           = 39.3081761[kHz]
X_Sweep_Clipped   = 31.44654088[kHz]
Irr_Domain        = Proton
Irr_Freq          = 500.15991521[MHz]
Irr_Offset        = 5.0[ppm]
Clipped           = FALSE
Scans             = 512
Total_Scans       = 512

Relaxation_Delay  = 2[s]
Recvr_Gain        = 50
Temp_Get          = 22.8[dC]
X_90_Width        = 12.65[us]
X_Acq_Time        = 0.83361792[s]
X_Angle           = 30[deg]
X_Atn             = 7[dB]
X_Pulse           = 4.21666667[us]
Irr_Atn_Dec       = 25.254[dB]
Irr_Atn_Noe       = 25.254[dB]
Irr_Noise         = WALTZ
Irr_Pwidth        = 92[us]
Decoupling        = TRUE
Initial_Wait      = 1[s]
Noe               = TRUE
Noe_Time          = 2[s]
Repetition_Time   = 2.83361792[s]
```

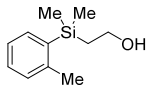



```
Filename          = 248-032_(o-OMe)Me2_2-OH_P
Author            = delta
Experiment        = proton.jxp
Sample_Id         = 248-032_(o-OMe)Me2_2-OH
Solvent           = ACETONE-D6
Actual_Start_Time =  4-OCT-2023 15:23:14
Revision_Time     = 20-FEB-2024 19:34:59

Comment           = single_pulse
Data_Format       = 1D COMPLEX
Dim_Size          = 13107
X_Domain          = Proton
Dim_Title         = Proton
Dim_Units         = [ppm]
Dimensions        = X
Site              = JNM-ECA500
Spectrometer      = DELTA2_NMR

Field_Strength    = 11.7473579[T] (500[MHz])
X_Acq_Duration    = 1.74587904[s]
X_Domain          = 1H
X_Freq            = 500.15991521[MHz]
X_Offset          = 5.0[ppm]
X_Points          = 16384
X_Prescans        = 1
X_Resolution      = 0.57277737[Hz]
X_Sweep           = 9.38438438[kHz]
X_Sweep_Clipped   = 7.50750751[kHz]
Irr_Domain        = Proton
Irr_Freq          = 500.15991521[MHz]
Irr_Offset        = 5.0[ppm]
Tri_Domain        = Proton
Tri_Freq          = 500.15991521[MHz]
Tri_Offset        = 5.0[ppm]
Clipped           = FALSE
Scans             = 8
Total_Scans       = 8

Relaxation_Delay  = 5[s]
Recvr_Gain        = 42
Temp_Get          = 22.4[dC]
X_90_Width        = 6.7[us]
X_Acq_Time        = 1.74587904[s]
X_Angle           = 45[deg]
X_Atn             = 2.5[dB]
X_Pulse           = 3.35[us]
Irr_Mode          = Off
Tri_Mode          = Off
Dante_Presat      = FALSE
Initial_Wait      = 1[s]
Repetition_Time   = 6.74587904[s]
```




```
Filename          = 032-co118-20-recol20-22_C
Author            = delta
Experiment        = carbon.jxp
Sample_Id         = 032-co118-20-recol20-22
Solvent           = ACETONE-D6
Actual_Start_Time = 13-JUL-2022 15:26:55
Revision_Time     = 20-FEB-2024 18:19:59

Comment           = single pulse decoupled ga
Data_Format       = 1D COMPLEX
Dim_Size          = 26214
X_Domain          = Carbon
Dim_Title         = Carbon13
Dim_Units         = [ppm]
Dimensions        = X
Site              = JNM-ECA500
Spectrometer      = DELTA2_NMR

Field_Strength    = 11.7473579[T] (500[MHz])
X_Acq_Duration    = 0.83361792[s]
X_Domain          = 13C
X_Freq            = 125.76529768[MHz]
X_Offset          = 100[ppm]
X_Points          = 32768
X_Prescans        = 4
X_Resolution      = 1.19959034[Hz]
X_Sweep           = 39.3081761[kHz]
X_Sweep_Clipped   = 31.44654088[kHz]
Irr_Domain        = Proton
Irr_Freq          = 500.15991521[MHz]
Irr_Offset        = 5.0[ppm]
Clipped           = FALSE
Scans             = 1024
Total_Scans       = 1024

Relaxation_Delay  = 2[s]
Recvr_Gain        = 50
Temp_Get          = 22[dC]
X_90_Width        = 12.65[us]
X_Acq_Time        = 0.83361792[s]
X_Angle           = 30[deg]
X_Atn             = 7[dB]
X_Pulse           = 4.21666667[us]
Irr_Atn_Dec       = 25.254[dB]
Irr_Atn_Noe       = 25.254[dB]
Irr_Noise         = WALTZ
Irr_Pwidth        = 92[us]
Decoupling        = TRUE
Initial_Wait      = 1[s]
Noe               = TRUE
Noe_Time          = 2[s]
Repetition_Time   = 2.83361792[s]
```

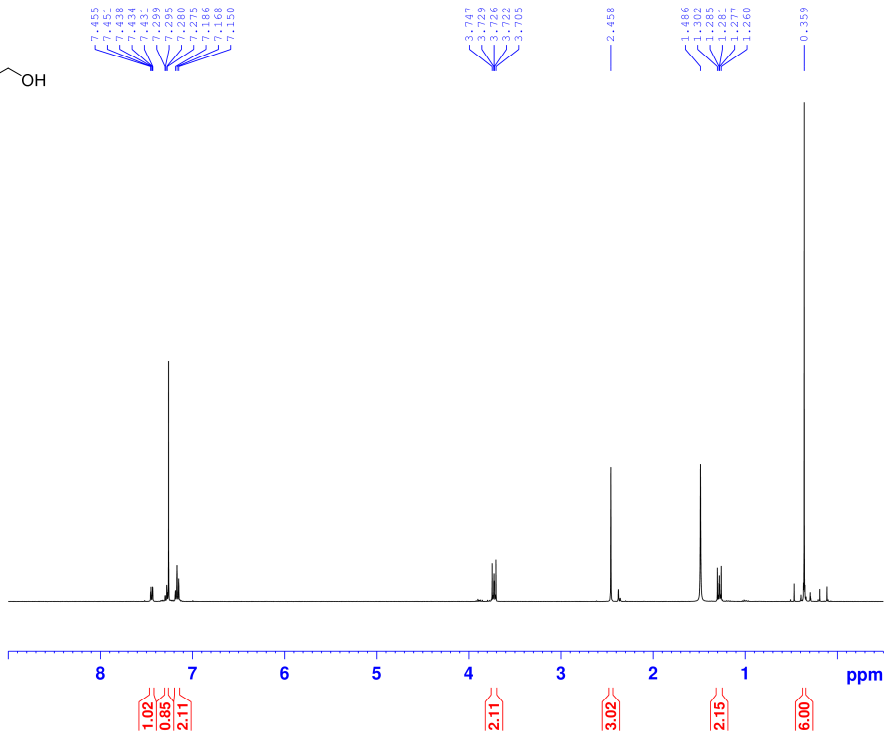
o-Me HB col15 GPC

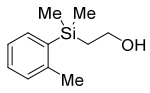


3h

IBB-nmr Analysis

```
NAME            NN248-046
EXPNO                   4
PROCNO                  1
Date_            20220517
Time                21.08
INSTRUM             av400
PROBHD    5 mm PABBO BB-
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                    16
DS                     2
SWH             8223.685 Hz
FIDRES          0.125483 Hz
AQ              3.9846387 sec
RG                   203
DW                60.800 usec
DE                 6.50 usec
TE                296.9 K
D1             1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  1H
P1                 14.00 usec
PL1                -1.80 dB
PL1W         14.82738590 W
SFO1         400.1324710 MHz
SI                 32768
SF           400.1300096 MHz
WDW                   EM
SSB                    0
LB                  0.30 Hz
GB                     0
PC                  1.00
```



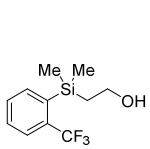


3h

JEOL

```
Filename          = 045-col15-GPC_Carbon-1-3.
Author            = delta
Experiment        = carbon.jxp
Sample_Id         = 045-col15-GPC
Solvent           = CHLOROFORM-D
Actual_Start_Time = 27-MAY-2022 19:20:43
Revision_Time     = 20-FEB-2024 18:31:30

Comment           = single pulse decoupled ga
Data_Format       = 1D COMPLEX
Dim_Size          = 26214
X_Domain          = Carbon
Dim_Title         = Carbon13
Dim_Units         = [ppm]
Dimensions        = X
Site              = JNM-ECA500
Spectrometer      = DELTA2_NMR

Field_Strength    = 11.7473579[T] (500[MHz])
X_Acq_Duration    = 0.83361792[s]
X_Domain          = 13C
X_Freq            = 125.76529768[MHz]
X_Offset          = 100[ppm]
X_Points          = 32768
X_Prescans        = 4
X_Resolution      = 1.19959034[Hz]
X_Sweep           = 39.3081761[kHz]
X_Sweep_Clipped   = 31.44654088[kHz]
Irr_Domain        = Proton
Irr_Freq          = 500.15991521[MHz]
Irr_Offset        = 5.0[ppm]
Clipped           = TRUE
Scans             = 2048
Total_Scans       = 2048

Relaxation_Delay  = 2[s]
Recvr_Gain        = 50
Temp_Get          = 22.7[dC]
X_90_Width        = 12.65[us]
X_Acq_Time        = 0.83361792[s]
X_Angle           = 30[deg]
X_Atn             = 7[dB]
X_Pulse           = 4.21666667[us]
Irr_Atn_Dec       = 25.254[dB]
Irr_Atn_Noe       = 25.254[dB]
Irr_Noise         = WALTZ
Irr_Pwidth        = 92[us]
Decoupling        = TRUE
Initial_Wait      = 1[s]
Noe               = TRUE
Noe_Time          = 2[s]
Repetition_Time   = 2.83361792[s]
```

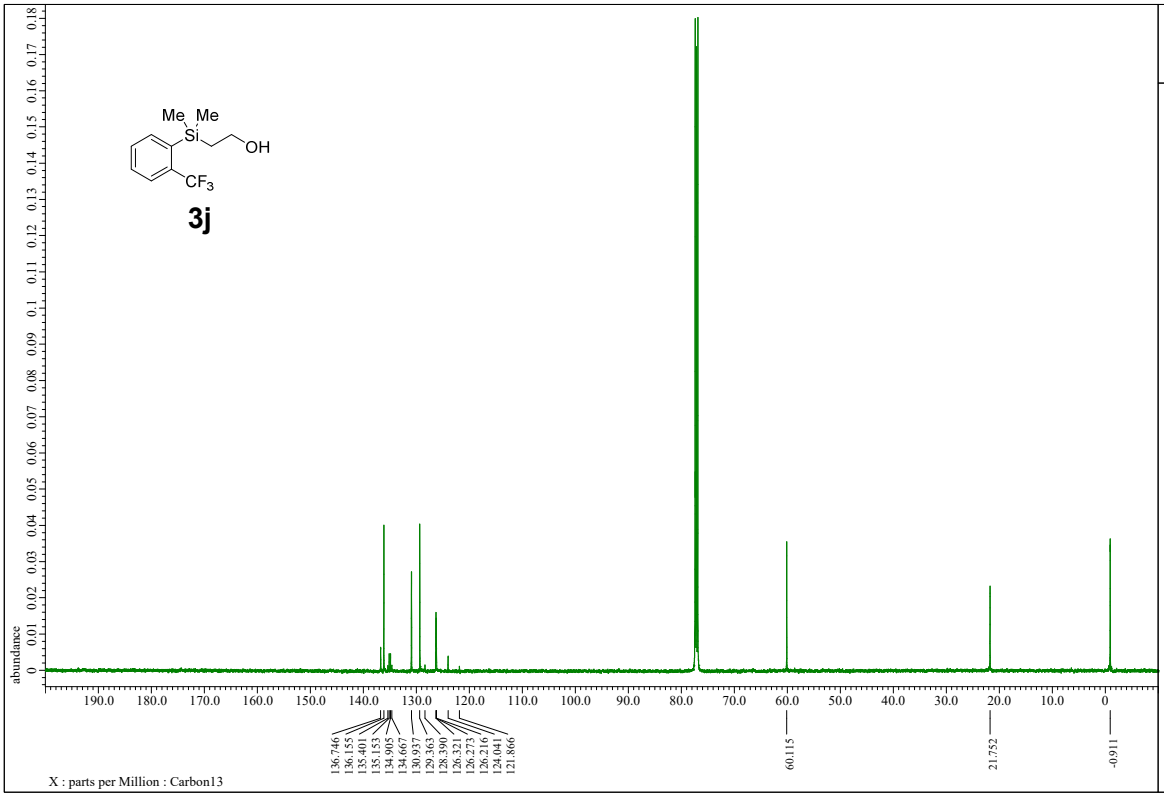
o-CF3 HB col16



3j

IBB-nmr Analysis

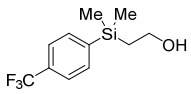
```
NAME            NN248-049
EXPNO                   4
PROCNO                  1
Date_            20220601
Time                22.25
INSTRUM             av400
PROBHD    5 mm PABBO BB-
PULPROG              zg30
TD                  65536
SOLVENT             CDCl3
NS                     16
DS                      2
SWH              8223.685 Hz
FIDRES           0.125483 Hz
AQ               3.9846387 sec
RG                    203
DW                60.800 usec
DE                 6.50 usec
TE                297.1 K
D1             1.00000000 sec
TD0                     1

======== CHANNEL f1 ========
NUC1                   1H
P1                 14.00 usec
PL1                -1.80 dB
PL1W         14.82738590 W
SFO1         400.1324710 MHz
SI                  32768
SF           400.1300096 MHz
WDW                    EM
SSB                     0
LB                 0.30 Hz
GB                      0
PC                 1.00
```

JEOL

```
Filename          = 049-col16_Carbon-2-2.jdf
Author            = delta
Experiment        = carbon.jxp
Sample_Id         = 049-col16
Solvent           = CHLOROFORM-D
Actual_Start_Time = 12-JUL-2022 02:10:24
Revision_Time     = 20-FEB-2024 18:26:57

Comment           = single pulse decoupled ga
Data_Format       = 1D COMPLEX
Dim_Size          = 26214
X_Domain          = Carbon
Dim_Title         = Carbon13
Dim_Units         = [ppm]
Dimensions        = X
Site              = JNM-ECA500
Spectrometer      = DELTA2_NMR

Field_Strength    = 11.7473579[T] (500[MHz])
X_Acq_Duration    = 0.83361792[s]
X_Domain          = 13C
X_Freq            = 125.76529768[MHz]
X_Offset          = 100[ppm]
X_Points          = 32768
X_Prescans        = 4
X_Resolution      = 1.19959034[Hz]
X_Sweep           = 39.3081761[kHz]
X_Sweep_Clipped   = 31.44654088[kHz]
Irr_Domain        = Proton
Irr_Freq          = 500.15991521[MHz]
Irr_Offset        = 5.0[ppm]
Clipped           = FALSE
Scans             = 4096
Total_Scans       = 4096

Relaxation_Delay  = 2[s]
Recvr_Gain        = 50
Temp_Get          = 22.2[dC]
X_90_Width        = 12.65[us]
X_Acq_Time        = 0.83361792[s]
X_Angle           = 30[deg]
X_Atn             = 7[dB]
X_Pulse           = 4.21666667[us]
Irr_Atn_Dec       = 25.254[dB]
Irr_Atn_Noe       = 25.254[dB]
Irr_Noise         = WALTZ
Irr_Pwidth        = 92[us]
Decoupling        = TRUE
Initial_Wait      = 1[s]
Noe               = TRUE
Noe_Time          = 2[s]
Repetition_Time   = 2.83361792[s]
```

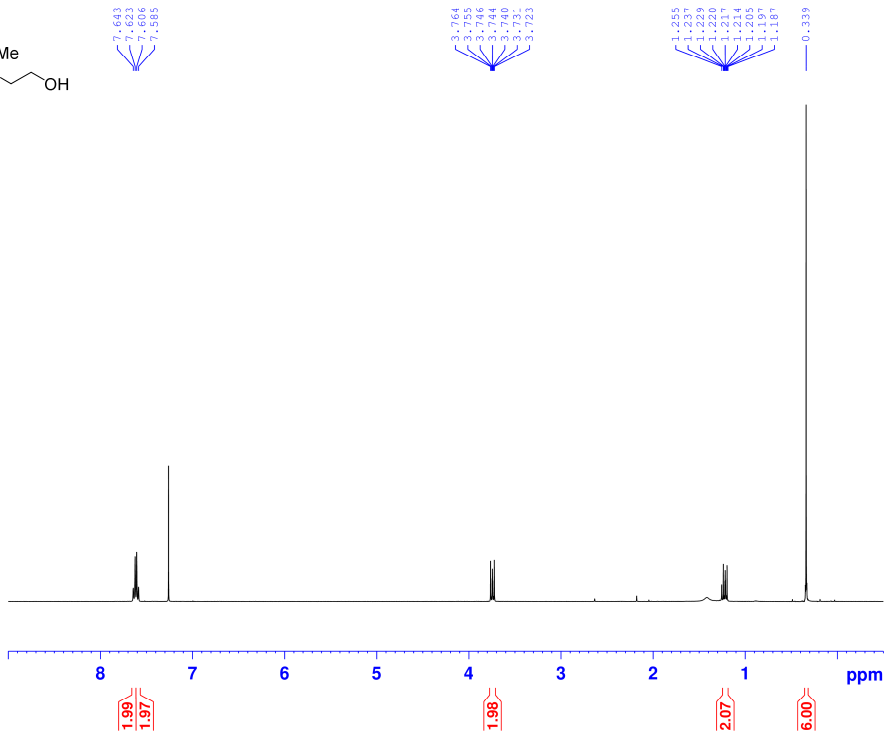
p-CF3 HB col32-35

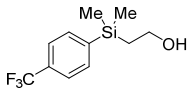


3k

IBB-nmr Analysis

```
NAME            NN248-030
EXPNO                   3
PROCNO                  1
Date_            20220329
Time                23.25
INSTRUM             av400
PROBHD    5 mm PABBO BB-
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                    16
DS                     2
SWH             8223.685 Hz
FIDRES          0.125483 Hz
AQ              3.9846387 sec
RG                   203
DW                60.800 usec
DE                 6.50 usec
TE                296.0 K
D1             1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  1H
P1                14.00 usec
PL1                -1.80 dB
PL1W         14.82738590 W
SFO1         400.1324710 MHz
SI                 32768
SF           400.1300096 MHz
WDW                   EM
SSB                    0
LB                  0.30 Hz
GB                     0
PC                  1.00
```

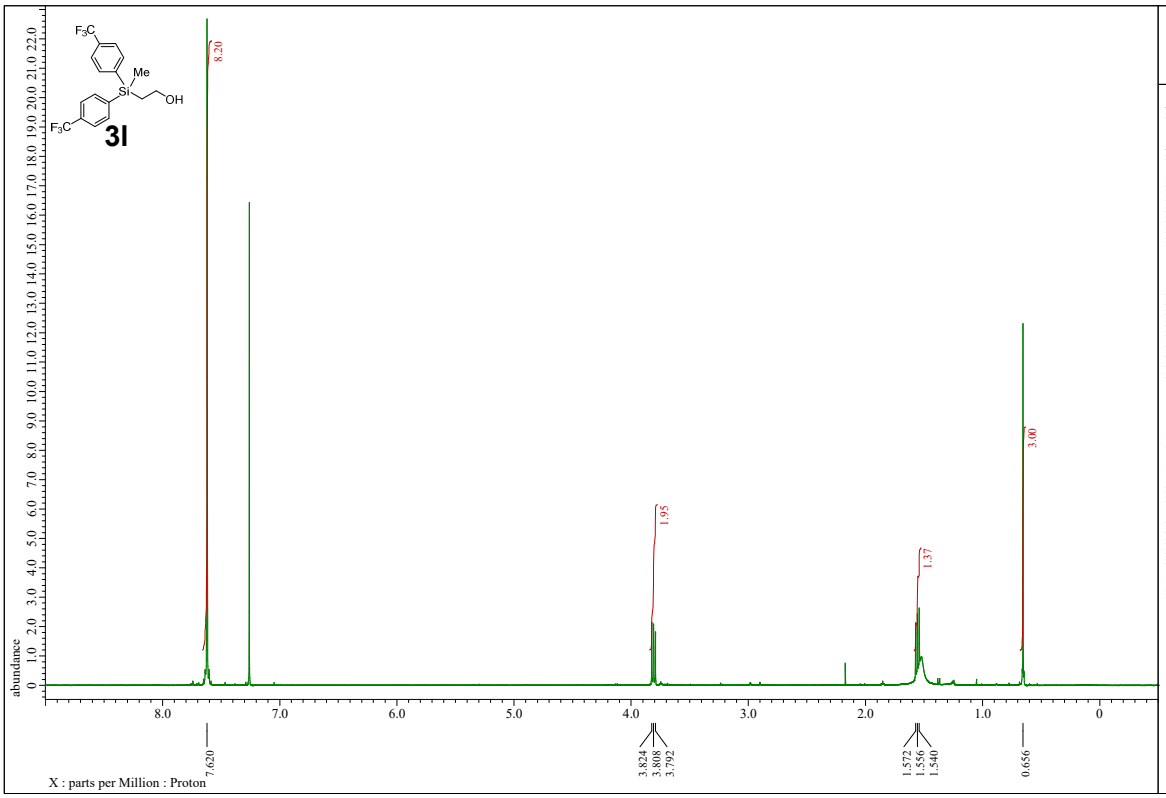




3k

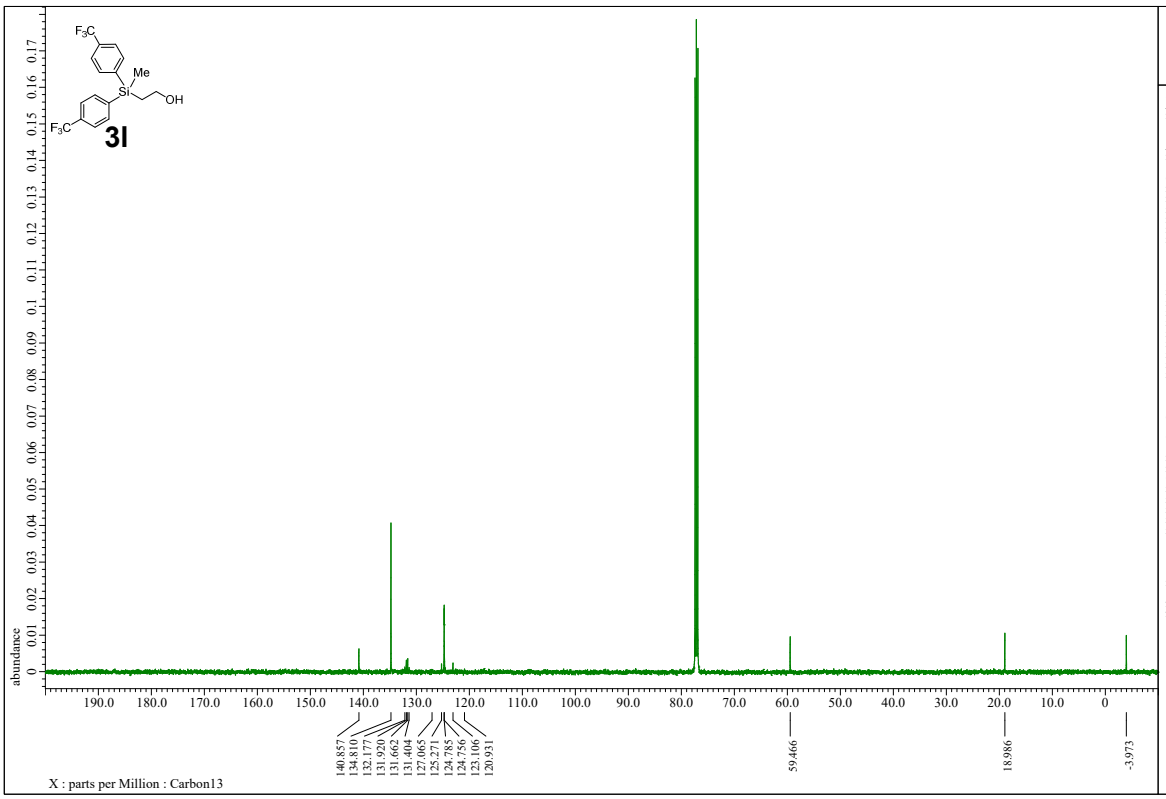
JEOL

```
Filename          = 030-col3235_Carbon-1-2.jd
Author            = delta
Experiment        = carbon.jxp
Sample_Id         = 030-col3235
Solvent           = CHLOROFORM-D
Actual_Start_Time = 30-MAR-2022 16:09:19
Revision_Time     = 20-FEB-2024 18:01:21

Comment           = single pulse decoupled ga
Data_Format       = 1D COMPLEX
Dim_Size          = 26214
X_Domain          = Carbon
Dim_Title         = Carbon13
Dim_Units         = [ppm]
Dimensions        = X
Site              = JNM-ECA500
Spectrometer      = DELTA2_NMR

Field_Strength    = 11.7473579[T] (500[MHz])
X_Acq_Duration    = 0.83361792[s]
X_Domain          = 13C
X_Freq            = 125.76529768[MHz]
X_Offset          = 100[ppm]
X_Points          = 32768
X_Prescans        = 4
X_Resolution      = 1.19959034[Hz]
X_Sweep           = 39.3081761[kHz]
X_Sweep_Clipped   = 31.44654088[kHz]
Irr_Domain        = Proton
Irr_Freq          = 500.15991521[MHz]
Irr_Offset        = 5.0[ppm]
Clipped           = FALSE
Scans             = 1024
Total_Scans       = 1024

Relaxation_Delay  = 2[s]
Recvr_Gain        = 50
Temp_Get          = 21[dC]
X_90_Width        = 12.65[us]
X_Acq_Time        = 0.83361792[s]
X_Angle           = 30[deg]
X_Atn             = 7[dB]
X_Pulse           = 4.21666667[us]
Irr_Atn_Dec       = 25.254[dB]
Irr_Atn_Noe       = 25.254[dB]
Irr_Noise         = WALTZ
Irr_Pwidth        = 92[us]
Decoupling        = TRUE
Initial_Wait      = 1[s]
Noe               = TRUE
Noe_Time          = 2[s]
Repetition_Time   = 2.83361792[s]
```



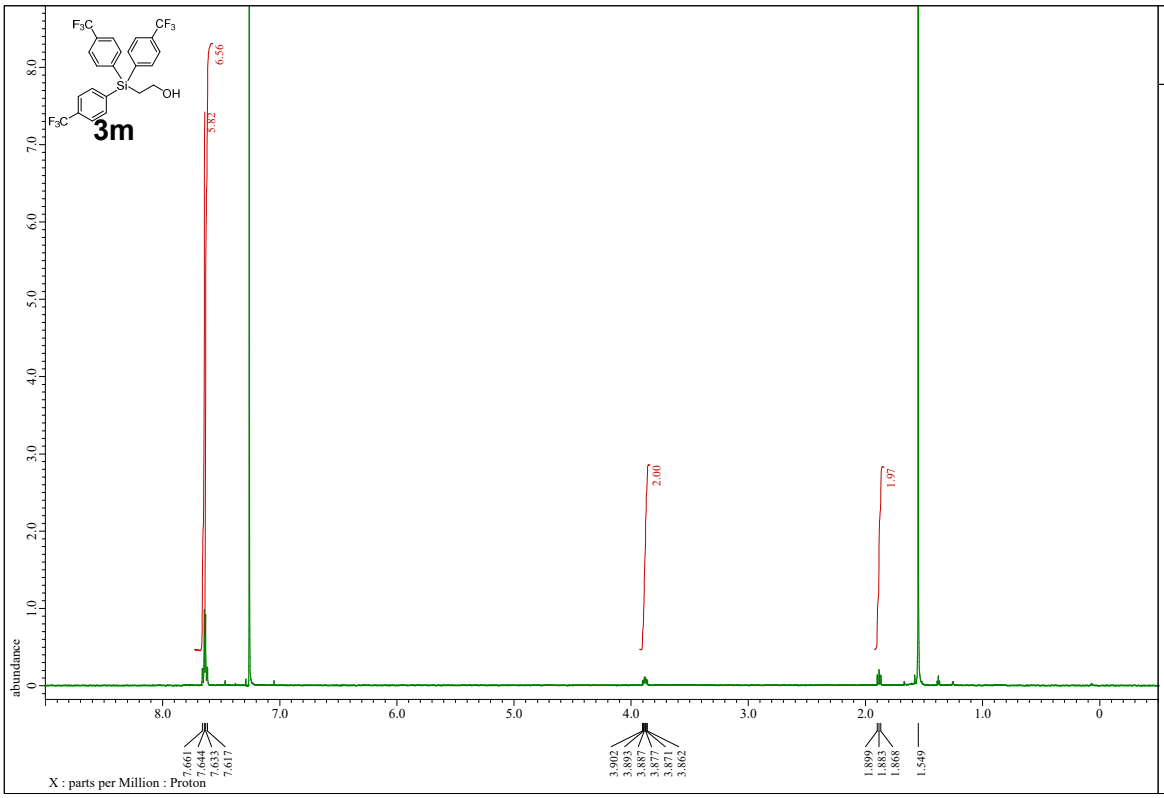
JEOL

```
Filename          = 248-066_(p-CF3)2Me_2-OH_P
Author            = delta
Experiment        = proton.jxp
Sample_Id         = 248-066_(p-CF3)2Me_2-OH
Solvent           = CHLOROFORM-D
Actual_Start_Time =  4-OCT-2023 15:14:04
Revision_Time     = 20-FEB-2024 18:34:35

Comment           = single_pulse
Data_Format       = 1D COMPLEX
Dim_Size          = 13107
X_Domain          = Proton
Dim_Title         = Proton
Dim_Units         = [ppm]
Dimensions        = X
Site              = JNM-ECA500
Spectrometer      = DELTA2_NMR

Field_Strength    = 11.7473579[T] (500[MHz])
X_Acq_Duration    = 1.74587904[s]
X_Domain          = 1H
X_Freq            = 500.15991521[MHz]
X_Offset          = 5.0[ppm]
X_Points          = 16384
X_Prescans        = 1
X_Resolution      = 0.57277737[Hz]
X_Sweep           = 9.38438438[kHz]
X_Sweep_Clipped   = 7.50750751[kHz]
Irr_Domain        = Proton
Irr_Freq          = 500.15991521[MHz]
Irr_Offset        = 5.0[ppm]
Tri_Domain        = Proton
Tri_Freq          = 500.15991521[MHz]
Tri_Offset        = 5.0[ppm]
Clipped           = FALSE
Scans             = 8
Total_Scans       = 8

Relaxation_Delay  = 5[s]
Recvr_Gain        = 60
Temp_Get          = 22.6[dC]
X_90_Width        = 6.7[us]
X_Acq_Time        = 1.74587904[s]
X_Angle           = 45[deg]
X_Atn             = 2.5[dB]
X_Pulse           = 3.35[us]
Irr_Mode          = Off
Tri_Mode          = Off
Dante_Presat      = FALSE
Initial_Wait      = 1[s]
Repetition_Time   = 6.74587904[s]
```



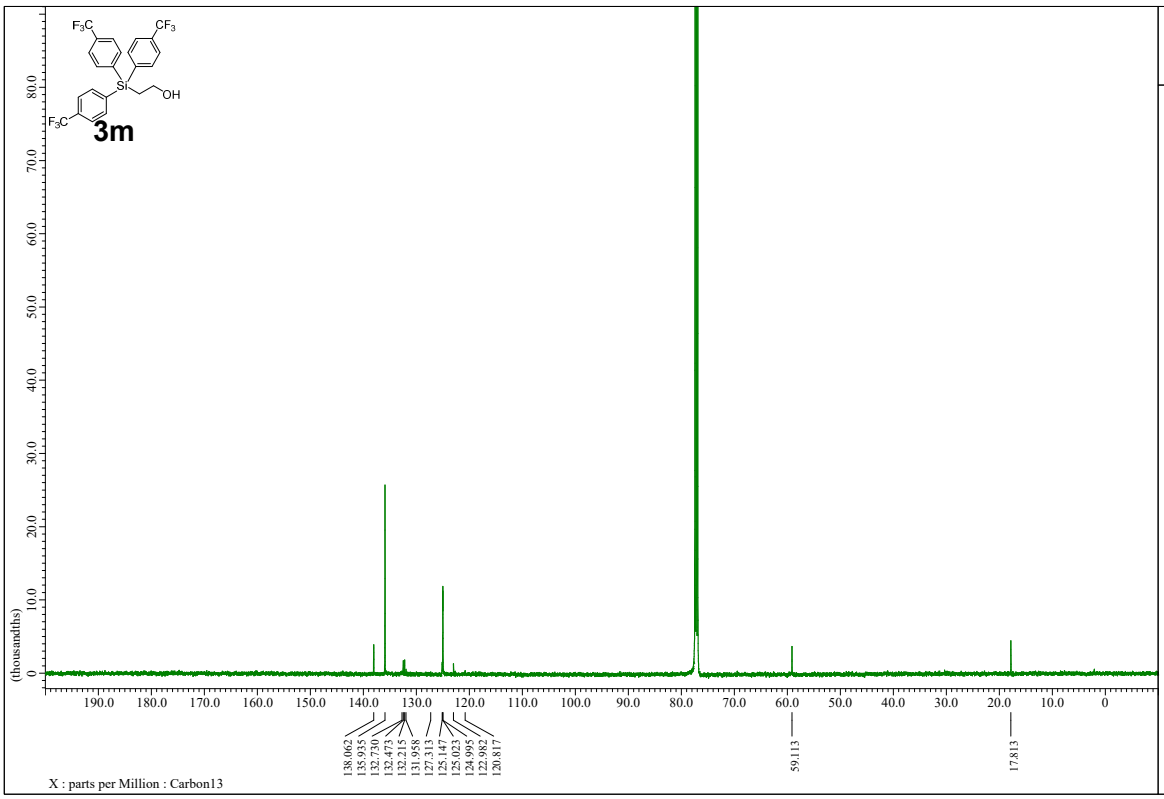
JEOL

```
Filename          = 248-066_(p-CF3)2Me_2-OH_C
Author            = delta
Experiment        = carbon.jxp
Sample_Id         = 248-066_(p-CF3)2Me_2-OH
Solvent           = CHLOROFORM-D
Actual_Start_Time =  5-OCT-2023 11:51:38
Revision_Time     = 20-FEB-2024 18:37:38

Comment           = single pulse decoupled ga
Data_Format       = 1D COMPLEX
Dim_Size          = 26214
X_Domain          = Carbon
Dim_Title         = Carbon13
Dim_Units         = [ppm]
Dimensions        = X
Site              = JNM-ECA500
Spectrometer      = DELTA2_NMR

Field_Strength    = 11.7473579[T] (500[MHz])
X_Acq_Duration    = 0.83361792[s]
X_Domain          = 13C
X_Freq            = 125.76529768[MHz]
X_Offset          = 100[ppm]
X_Points          = 32768
X_Prescans        = 4
X_Resolution      = 1.19959034[Hz]
X_Sweep           = 39.3081761[kHz]
X_Sweep_Clipped   = 31.44654088[kHz]
Irr_Domain        = Proton
Irr_Freq          = 500.15991521[MHz]
Irr_Offset        = 5.0[ppm]
Clipped           = FALSE
Scans             = 2048
Total_Scans       = 2048

Relaxation_Delay  = 2[s]
Recvr_Gain        = 50
Temp_Get          = 22.3[dC]
X_90_Width        = 12.65[us]
X_Acq_Time        = 0.83361792[s]
X_Angle           = 30[deg]
X_Atn             = 7[dB]
X_Pulse           = 4.21666667[us]
Irr_Atn_Dec       = 25.254[dB]
Irr_Atn_Noe       = 25.254[dB]
Irr_Noise         = WALTZ
Irr_Pwidth        = 92[us]
Decoupling        = TRUE
Initial_Wait      = 1[s]
Noe               = TRUE
Noe_Time          = 2[s]
Repetition_Time   = 2.83361792[s]
```



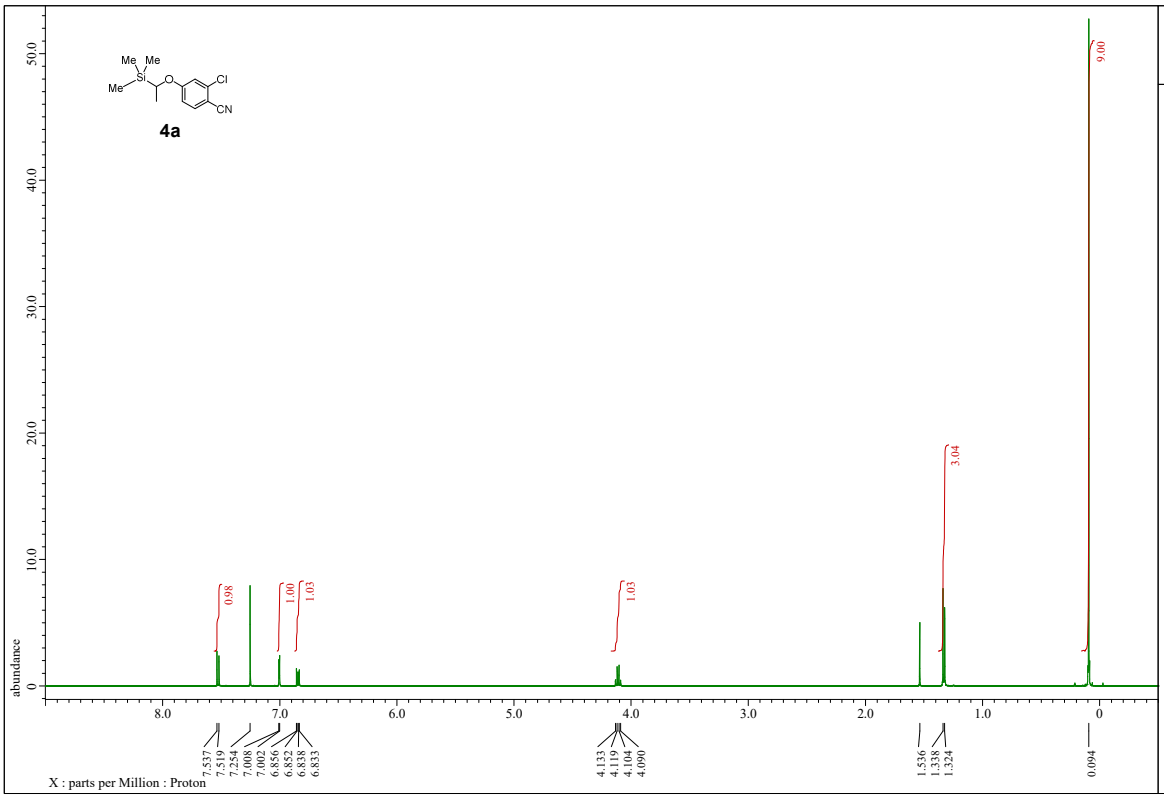
JEOL

```
Filename          = 248-054_(pCF3)3_2-OH_3_Pr
Author            = delta
Experiment        = proton.jxp
Sample_Id         = 248-054_(pCF3)3_2-OH_3
Solvent           = CHLOROFORM-D
Actual_Start_Time =  5-OCT-2023 17:33:21
Revision_Time     = 20-FEB-2024 19:39:29

Comment           = single_pulse
Data_Format       = 1D COMPLEX
Dim_Size          = 13107
X_Domain          = Proton
Dim_Title         = Proton
Dim_Units         = [ppm]
Dimensions        = X
Site              = JNM-ECA500
Spectrometer      = DELTA2_NMR

Field_Strength    = 11.7473579[T] (500[MHz])
X_Acq_Duration    = 1.74587904[s]
X_Domain          = 1H
X_Freq            = 500.15991521[MHz]
X_Offset          = 5.0[ppm]
X_Points          = 16384
X_Prescans        = 1
X_Resolution      = 0.57277737[Hz]
X_Sweep           = 9.38438438[kHz]
X_Sweep_Clipped   = 7.50750751[kHz]
Irr_Domain        = Proton
Irr_Freq          = 500.15991521[MHz]
Irr_Offset        = 5.0[ppm]
Tri_Domain        = Proton
Tri_Freq          = 500.15991521[MHz]
Tri_Offset        = 5.0[ppm]
Clipped           = FALSE
Scans             = 64
Total_Scans       = 64

Relaxation_Delay  = 5[s]
Recvr_Gain        = 64
Temp_Get          = 22.8[dC]
X_90_Width        = 6.7[us]
X_Acq_Time        = 1.74587904[s]
X_Angle           = 45[deg]
X_Atn             = 2.5[dB]
X_Pulse           = 3.35[us]
Irr_Mode          = Off
Tri_Mode          = Off
Dante_Presat      = FALSE
Initial_Wait      = 1[s]
Repetition_Time   = 6.74587904[s]
```



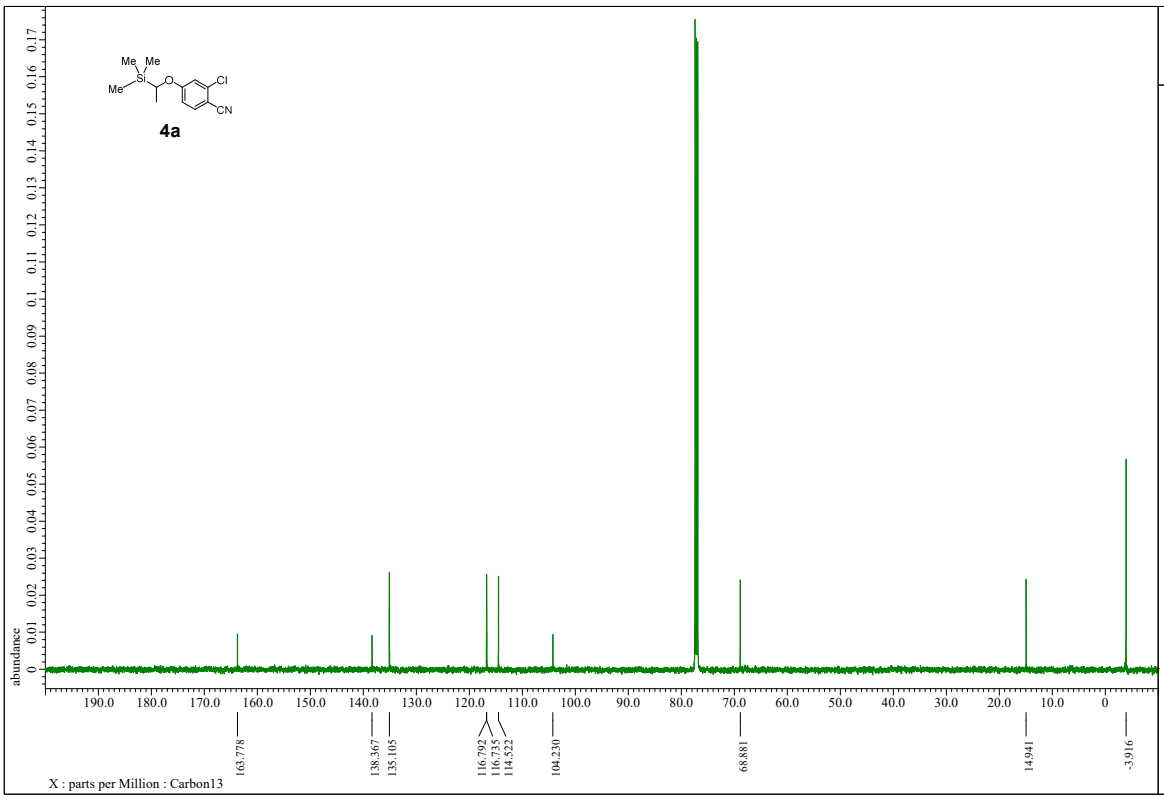
JEOL

```
Filename          = 054col18-24-recry_Carbon-
Author            = delta
Experiment        = carbon.jxp
Sample_Id         = 054col18-24-recry
Solvent           = CHLOROFORM-D
Actual_Start_Time = 15-JUL-2022 00:07:53
Revision_Time     = 20-FEB-2024 19:16:34

Comment           = single pulse decoupled ga
Data_Format       = 1D COMPLEX
Dim_Size          = 26214
X_Domain          = Carbon
Dim_Title         = Carbon13
Dim_Units         = [ppm]
Dimensions        = X
Site              = JNM-ECA500
Spectrometer      = DELTA2_NMR

Field_Strength    = 11.7473579[T] (500[MHz])
X_Acq_Duration    = 0.83361792[s]
X_Domain          = 13C
X_Freq            = 125.76529768[MHz]
X_Offset          = 100[ppm]
X_Points          = 32768
X_Prescans        = 4
X_Resolution      = 1.19959034[Hz]
X_Sweep           = 39.3081761[kHz]
X_Sweep_Clipped   = 31.44654088[kHz]
Irr_Domain        = Proton
Irr_Freq          = 500.15991521[MHz]
Irr_Offset        = 5.0[ppm]
Clipped           = FALSE
Scans             = 10000
Total_Scans       = 10000

Relaxation_Delay  = 2[s]
Recvr_Gain        = 50
Temp_Get          = 22.1[dC]
X_90_Width        = 12.65[us]
X_Acq_Time        = 0.83361792[s]
X_Angle           = 30[deg]
X_Atn             = 7[dB]
X_Pulse           = 4.21666667[us]
Irr_Atn_Dec       = 25.254[dB]
Irr_Atn_Noe       = 25.254[dB]
Irr_Noise         = WALTZ
Irr_Pwidth        = 92[us]
Decoupling        = TRUE
Initial_Wait      = 1[s]
Noe               = TRUE
Noe_Time          = 2[s]
Repetition_Time   = 2.83361792[s]
```



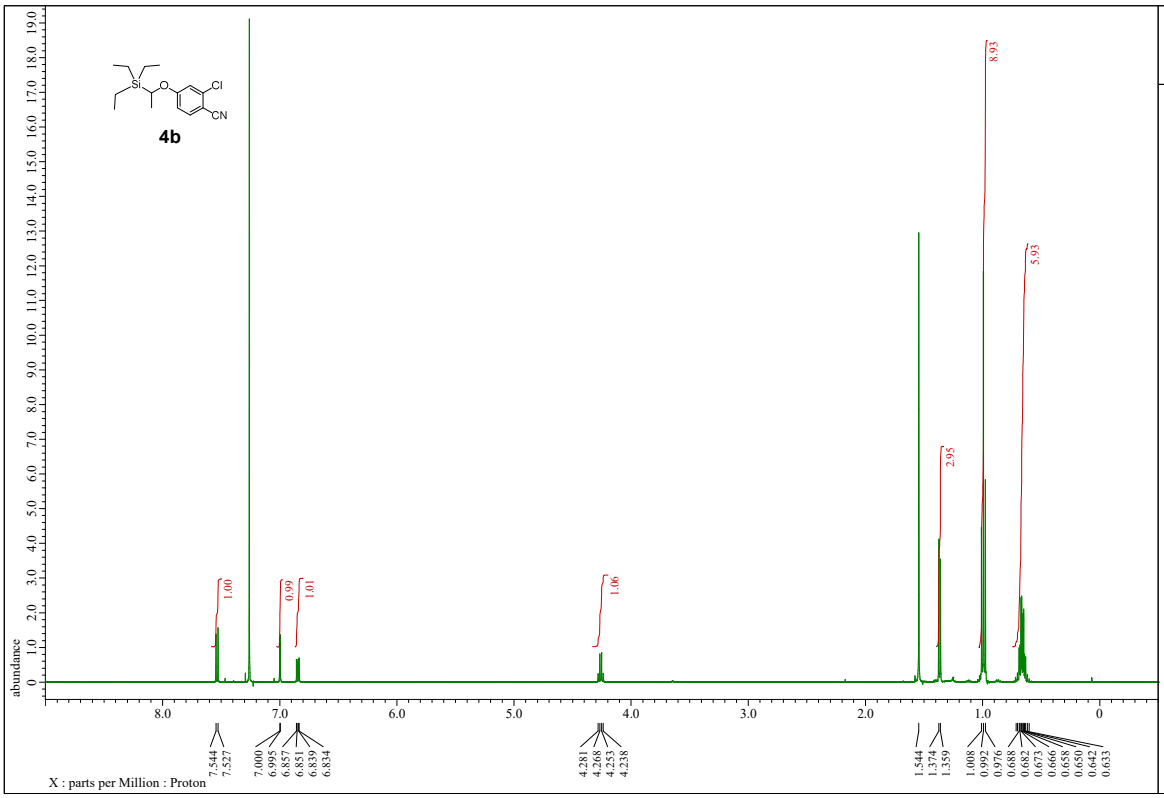
JEOL

```
Filename          = NAN43-2.jdf
Author            = delta
Experiment        = proton.jxp
Sample_Id         = 270-021-3_GPC225-234
Solvent           = CHLOROFORM-D
Actual_Start_Time = 13-JUL-2023 19:22:06
Revision_Time     = 20-FEB-2024 11:57:37

Comment           = single_pulse
Data_Format       = 1D COMPLEX
Dim_Size          = 13107
X_Domain          = Proton
Dim_Title         = Proton
Dim_Units         = [ppm]
Dimensions        = X
Site              = JNM-ECA500
Spectrometer      = DELTA2_NMR

Field_Strength    = 11.7473579[T] (500[MHz])
X_Acq_Duration    = 1.74587904[s]
X_Domain          = 1H
X_Freq            = 500.15991521[MHz]
X_Offset          = 5.0[ppm]
X_Points          = 16384
X_Prescans        = 1
X_Resolution      = 0.57277737[Hz]
X_Sweep           = 9.38438438[kHz]
X_Sweep_Clipped   = 7.50750751[kHz]
Irr_Domain        = Proton
Irr_Freq          = 500.15991521[MHz]
Irr_Offset        = 5.0[ppm]
Tri_Domain        = Proton
Tri_Freq          = 500.15991521[MHz]
Tri_Offset        = 5.0[ppm]
Clipped           = FALSE
Scans             = 16
Total_Scans       = 16

Relaxation_Delay  = 5[s]
Recvr_Gain        = 58
Temp_Get          = 22.7[dC]
X_90_Width        = 6.7[us]
X_Acq_Time        = 1.74587904[s]
X_Angle           = 45[deg]
X_Atn             = 2.5[dB]
X_Pulse           = 3.35[us]
Irr_Mode          = Off
Tri_Mode          = Off
Dante_Presat      = FALSE
Initial_Wait      = 1[s]
Repetition_Time   = 6.74587904[s]
```



JEOL

```
Filename          = NAN043_Carbon-1-4.jdf
Author            = delta
Experiment        = carbon.jxp
Sample_Id         = NAN043
Solvent           = CHLOROFORM-D
Actual_Start_Time =  1-AUG-2023 22:39:35
Revision_Time     = 20-FEB-2024 11:58:59

Comment           = single pulse decoupled ga
Data_Format       = 1D COMPLEX
Dim_Size          = 26214
X_Domain          = Carbon
Dim_Title         = Carbon13
Dim_Units         = [ppm]
Dimensions        = X
Site              = JNM-ECA500
Spectrometer      = DELTA2_NMR

Field_Strength    = 11.7473579[T] (500[MHz])
X_Acq_Duration    = 0.83361792[s]
X_Domain          = 13C
X_Freq            = 125.76529768[MHz]
X_Offset          = 100[ppm]
X_Points          = 32768
X_Prescans        = 4
X_Resolution      = 1.19959034[Hz]
X_Sweep           = 39.3081761[kHz]
X_Sweep_Clipped   = 31.44654088[kHz]
Irr_Domain        = Proton
Irr_Freq          = 500.15991521[MHz]
Irr_Offset        = 5.0[ppm]
Clipped           = FALSE
Scans             = 1024
Total_Scans       = 1024

Relaxation_Delay  = 2[s]
Recvr_Gain        = 50
Temp_Get          = 22.8[dC]
X_90_Width        = 12.65[us]
X_Acq_Time        = 0.83361792[s]
X_Angle           = 30[deg]
X_Atn             = 7[dB]
X_Pulse           = 4.21666667[us]
Irr_Atn_Dec       = 25.254[dB]
Irr_Atn_Noe       = 25.254[dB]
Irr_Noise         = WALTZ
Irr_Pwidth        = 92[us]
Decoupling        = TRUE
Initial_Wait      = 1[s]
Noe               = TRUE
Noe_Time          = 2[s]
Repetition_Time   = 2.83361792[s]
```

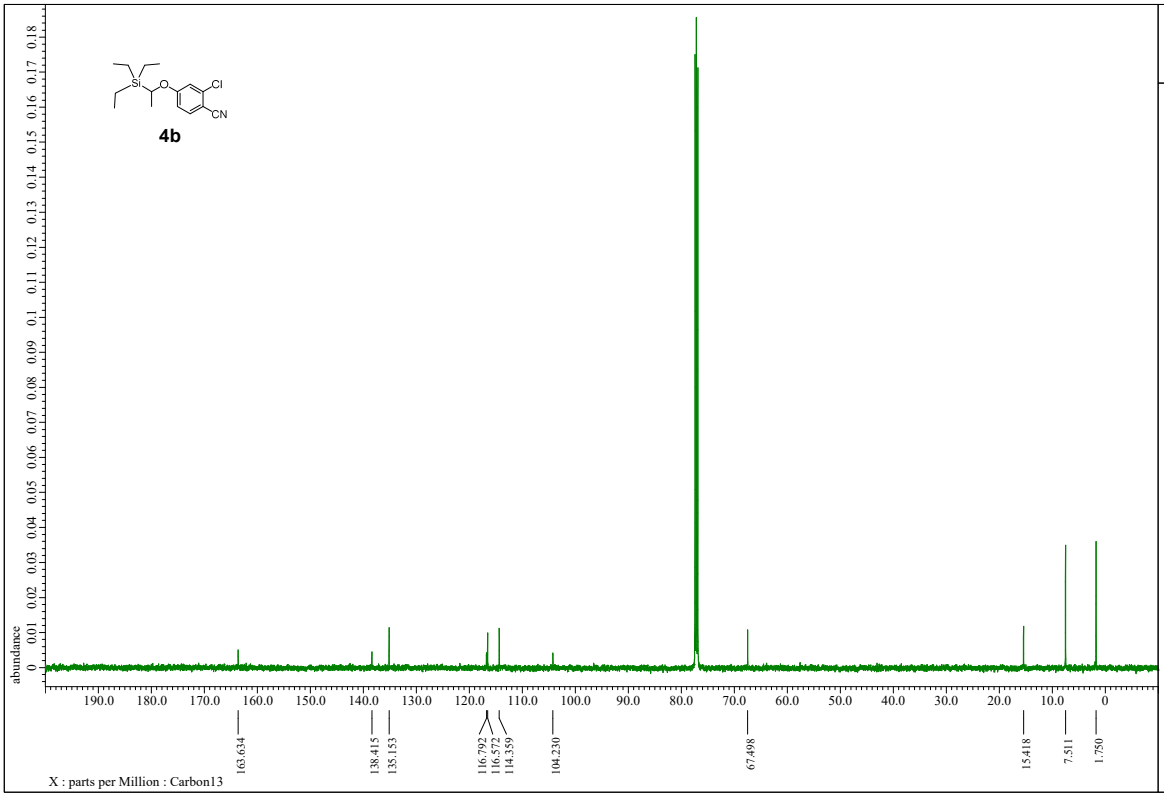


Filename = 270-014-4_col11-15_GPC_Pr
Author = delta
Experiment = proton.jxp
Sample_Id = 270-014-4_col11-15_GPC
Solvent = CHLOROFORM-D
Actual_Start_Time = 27-JUN-2023 13:16:10
Revision_Time = 20-FEB-2024 12:07:51

Comment = single_pulse
Data_Format = 1D COMPLEX
Dim_Size = 13107
X_Domain = Proton
Dim_Title = Proton
Dim_Units = [ppm]
Dimensions = X
Site = JNM-ECA500
Spectrometer = DELTA2_NMR

Field_Strength = 11.7473579[T] (500[MHz])
X_Acq_Duration = 1.74587904[s]
X_Domain = 1H
X_Freq = 500.15991521[MHz]
X_Offset = 5.0[ppm]
X_Points = 16384
X_Prescans = 1
X_Resolution = 0.57277737[Hz]
X_Sweep = 9.38438438[kHz]
X_Sweep_Clipped = 7.50750751[kHz]
Irr_Domain = Proton
Irr_Freq = 500.15991521[MHz]
Irr_Offset = 5.0[ppm]
Tri_Domain = Proton
Tri_Freq = 500.15991521[MHz]
Tri_Offset = 5.0[ppm]
Clipped = FALSE
Scans = 16
Total_Scans = 16

Relaxation_Delay = 5[s]
Recvr_Gain = 58
Temp_Get = 22[dC]
X_90_Width = 6.7[us]
X_Acq_Time = 1.74587904[s]
X_Angle = 45[deg]
X_Atn = 2.5[dB]
X_Pulse = 3.35[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Presat = FALSE
Initial_Wait = 1[s]
Repetition_Time = 6.74587904[s]

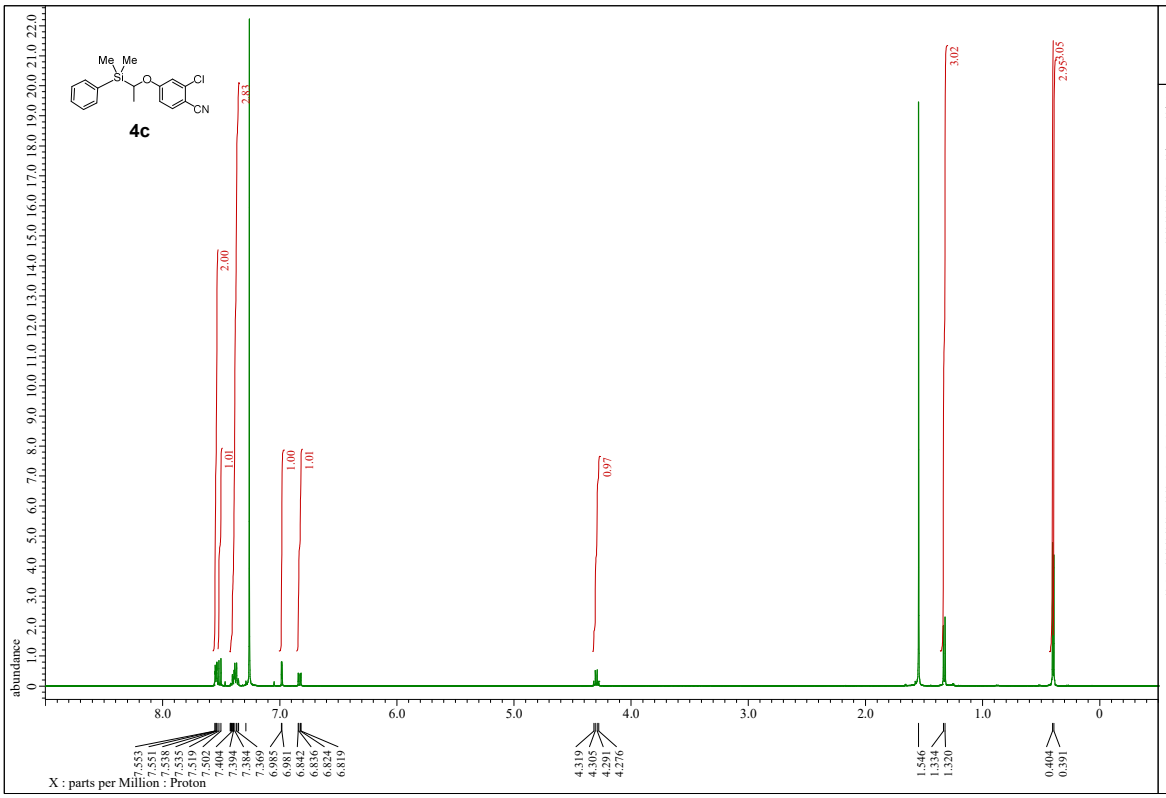


Filename = NAN045(true)_Carbon-2-4.j
Author = delta
Experiment = carbon.jxp
Sample_Id = NAN045
Solvent = CHLOROFORM-D
Actual_Start_Time = 3-AUG-2023 17:25:55
Revision_Time = 20-FEB-2024 12:11:22

Comment = single pulse decoupled ga
Data_Format = 1D COMPLEX
Dim_Size = 26214
X_Domain = Carbon
Dim_Title = Carbon13
Dim_Units = [ppm]
Dimensions = X
Site = JNM-ECA500
Spectrometer = DELTA2_NMR

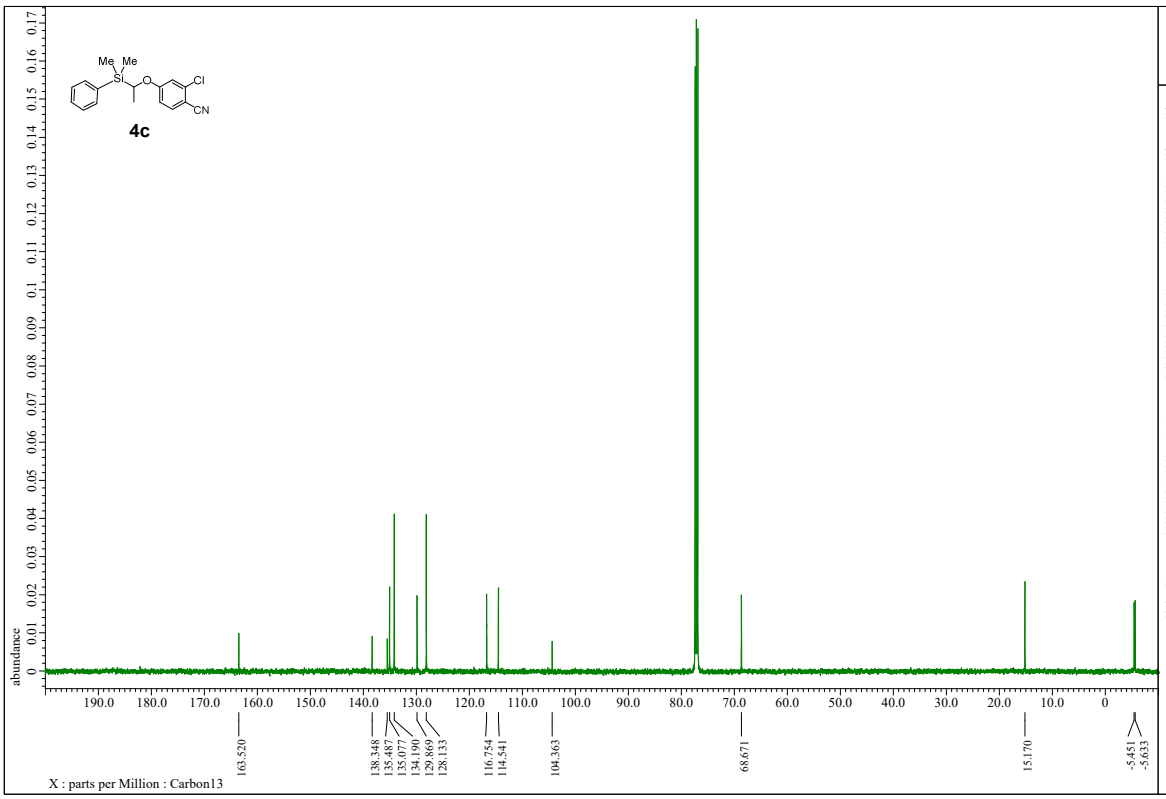
Field_Strength = 11.7473579[T] (500[MHz])
X_Acq_Duration = 0.83361792[s]
X_Domain = 13C
X_Freq = 125.76529768[MHz]
X_Offset = 100[ppm]
X_Points = 32768
X_Prescans = 4
X_Resolution = 1.19959034[Hz]
X_Sweep = 39.3081761[kHz]
X_Sweep_Clipped = 31.44654088[kHz]
Irr_Domain = Proton
Irr_Freq = 500.15991521[MHz]
Irr_Offset = 5.0[ppm]
Clipped = FALSE
Scans = 1024
Total_Scans = 1024

Relaxation_Delay = 2[s]
Recvr_Gain = 50
Temp_Get = 22.7[dC]
X_90_Width = 12.65[us]
X_Acq_Time = 0.83361792[s]
X_Angle = 30[deg]
X_Atn = 7[dB]
X_Pulse = 4.21666667[us]
Irr_Atn_Dec = 25.254[dB]
Irr_Atn_Noe = 25.254[dB]
Irr_Noise = WALTZ
Irr_Pwidth = 92[us]
Decoupling = TRUE
Initial_Wait = 1[s]
Noe = TRUE
Noe_Time = 2[s]
Repetition_Time = 2.83361792[s]



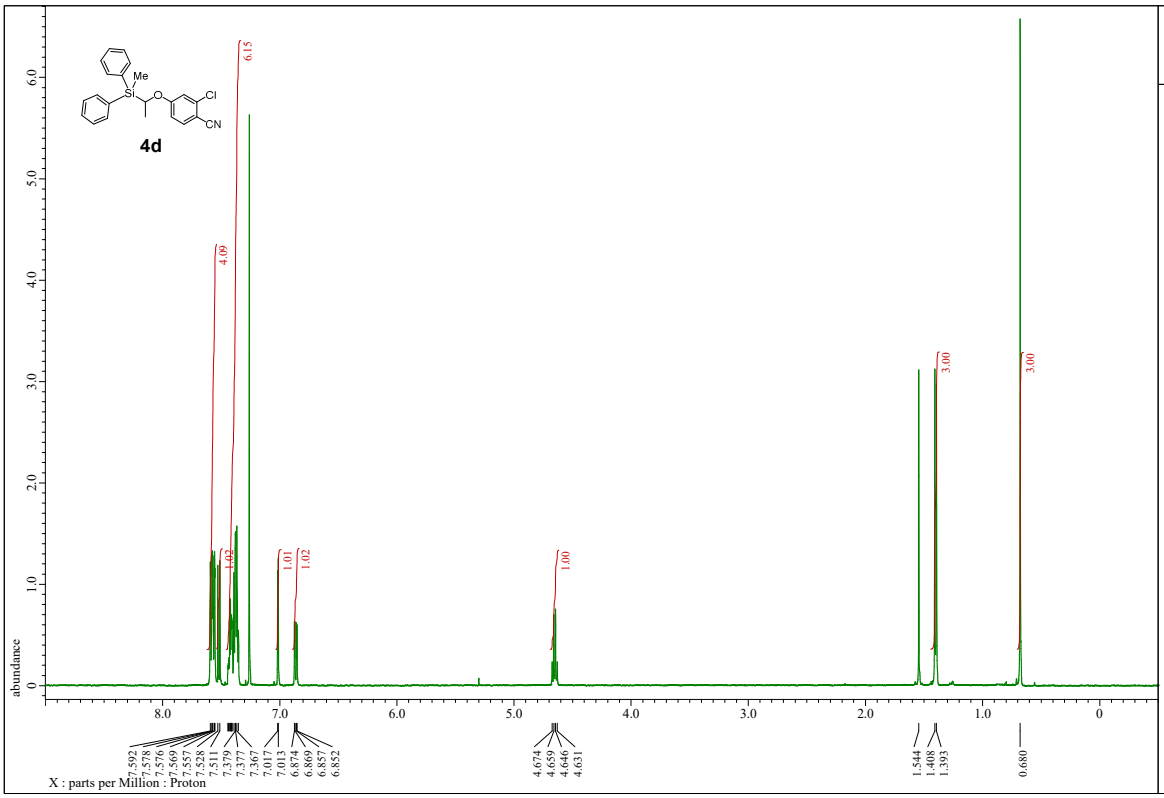
JEOL

```
Filename          = 190col20-25_GPC_Proton-2-
Author            = delta
Experiment        = proton.jxp
Sample_Id         = 190col20-25_GPC
Solvent           = CHLOROFORM-D
Actual_Start_Time = 26-APR-2023 21:02:29
Revision_Time     = 20-FEB-2024 12:26:36

Comment           = single_pulse
Data_Format       = 1D COMPLEX
Dim_Size          = 13107
X_Domain          = Proton
Dim_Title         = Proton
Dim_Units         = [ppm]
Dimensions        = X
Site              = JNM-ECA500
Spectrometer      = DELTA2_NMR

Field_Strength    = 11.7473579[T] (500[MHz])
X_Acq_Duration    = 1.74587904[s]
X_Domain          = 1H
X_Freq            = 500.15991521[MHz]
X_Offset          = 5.0[ppm]
X_Points          = 16384
X_Prescans        = 1
X_Resolution      = 0.57277737[Hz]
X_Sweep           = 9.38438438[kHz]
X_Sweep_Clipped   = 7.50750751[kHz]
Irr_Domain        = Proton
Irr_Freq          = 500.15991521[MHz]
Irr_Offset        = 5.0[ppm]
Tri_Domain        = Proton
Tri_Freq          = 500.15991521[MHz]
Tri_Offset        = 5.0[ppm]
Clipped           = FALSE
Scans             = 256
Total_Scans       = 256

Relaxation_Delay  = 5[s]
Recvr_Gain        = 66
Temp_Get          = 21.3[dC]
X_90_Width        = 6.7[us]
X_Acq_Time        = 1.74587904[s]
X_Angle           = 45[deg]
X_Atn             = 2.5[dB]
X_Pulse           = 3.35[us]
Irr_Mode          = Off
Tri_Mode          = Off
Dante_Presat      = FALSE
Initial_Wait      = 1[s]
Repetition_Time   = 6.74587904[s]
```



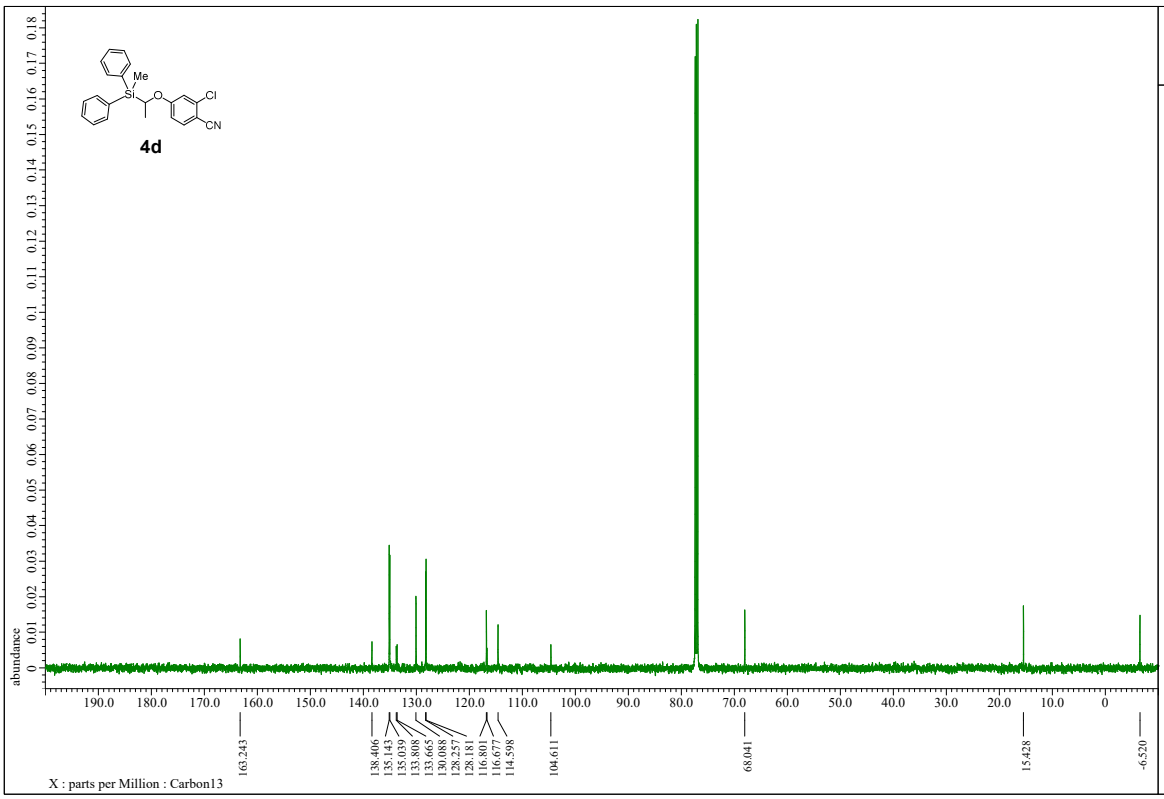
JEOL

```
Filename          = NAN037_Carbon-1-3.jdf
Author            = delta
Experiment        = carbon.jxp
Sample_Id         = NAN037
Solvent           = CHLOROFORM-D
Actual_Start_Time =  3-AUG-2023 14:04:04
Revision_Time     = 20-FEB-2024 12:28:17

Comment           = single pulse decoupled ga
Data_Format       = 1D COMPLEX
Dim_Size          = 26214
X_Domain          = Carbon
Dim_Title         = Carbon13
Dim_Units         = [ppm]
Dimensions        = X
Site              = JNM-ECA500
Spectrometer      = DELTA2_NMR

Field_Strength    = 11.7473579[T] (500[MHz])
X_Acq_Duration    = 0.83361792[s]
X_Domain          = 13C
X_Freq            = 125.76529768[MHz]
X_Offset          = 100[ppm]
X_Points          = 32768
X_Prescans        = 4
X_Resolution      = 1.19959034[Hz]
X_Sweep           = 39.3081761[kHz]
X_Sweep_Clipped   = 31.44654088[kHz]
Irr_Domain        = Proton
Irr_Freq          = 500.15991521[MHz]
Irr_Offset        = 5.0[ppm]
Clipped           = FALSE
Scans             = 2048
Total_Scans       = 2048

Relaxation_Delay  = 2[s]
Recvr_Gain        = 50
Temp_Get          = 22.9[dC]
X_90_Width        = 12.65[us]
X_Acq_Time        = 0.83361792[s]
X_Angle           = 30[deg]
X_Atn             = 7[dB]
X_Pulse           = 4.21666667[us]
Irr_Atn_Dec       = 25.254[dB]
Irr_Atn_Noe       = 25.254[dB]
Irr_Noise         = WALTZ
Irr_Pwidth        = 92[us]
Decoupling        = TRUE
Initial_Wait      = 1[s]
Noe               = TRUE
Noe_Time          = 2[s]
Repetition_Time   = 2.83361792[s]
```



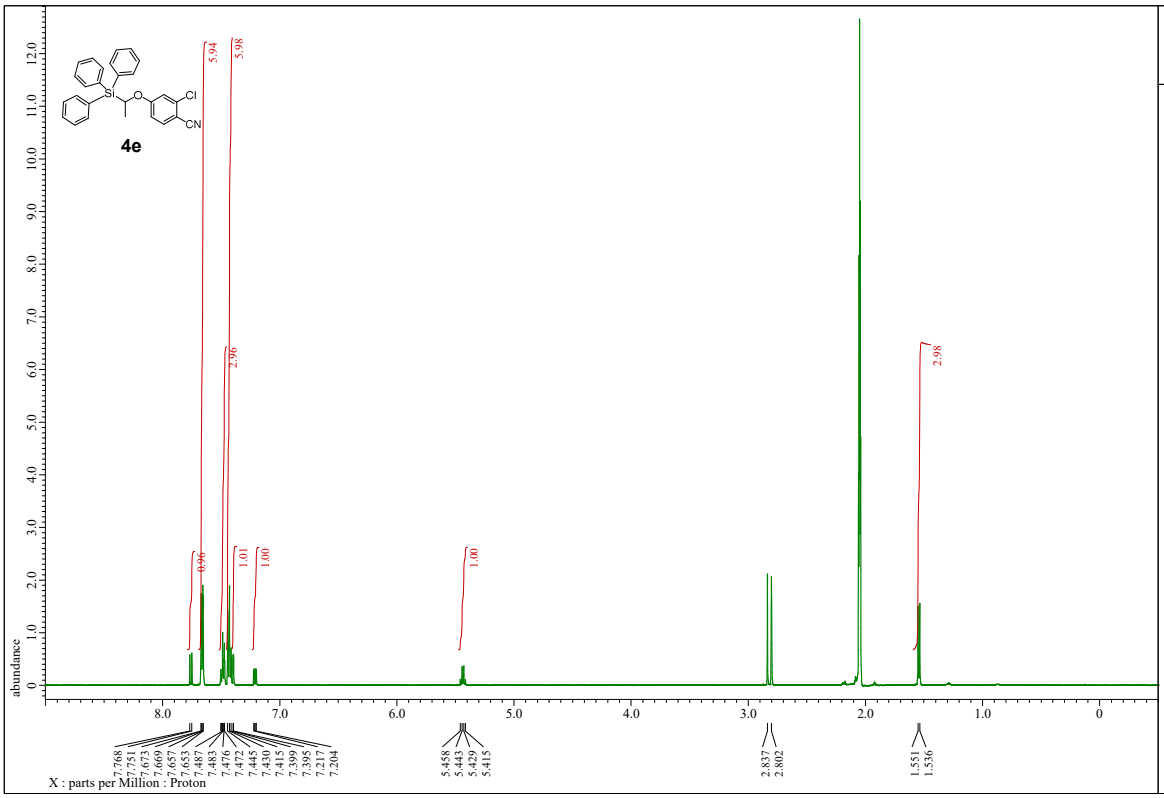
JEOL

```
Filename          = NAN39_240219_Proton-1-3.j
Author            = delta
Experiment        = proton.jxp
Sample_Id         = NAN39_240219
Solvent           = CHLOROFORM-D
Actual_Start_Time = 19-FEB-2024 22:38:11
Revision_Time     = 20-FEB-2024 12:30:54

Comment           = single_pulse
Data_Format       = 1D COMPLEX
Dim_Size          = 13107
X_Domain          = Proton
Dim_Title         = Proton
Dim_Units         = [ppm]
Dimensions        = X
Site              = JNM-ECA500
Spectrometer      = DELTA2_NMR

Field_Strength    = 11.7473579[T] (500[MHz])
X_Acq_Duration    = 1.74587904[s]
X_Domain          = 1H
X_Freq            = 500.15991521[MHz]
X_Offset          = 5.0[ppm]
X_Points          = 16384
X_Prescans        = 1
X_Resolution      = 0.57277737[Hz]
X_Sweep           = 9.38438438[kHz]
X_Sweep_Clipped   = 7.50750751[kHz]
Irr_Domain        = Proton
Irr_Freq          = 500.15991521[MHz]
Irr_Offset        = 5.0[ppm]
Tri_Domain        = Proton
Tri_Freq          = 500.15991521[MHz]
Tri_Offset        = 5.0[ppm]
Clipped           = FALSE
Scans             = 16
Total_Scans       = 16

Relaxation_Delay  = 5[s]
Recvr_Gain        = 58
Temp_Get          = 21.1[dC]
X_90_Width        = 6.7[us]
X_Acq_Time        = 1.74587904[s]
X_Angle           = 45[deg]
X_Atn             = 2.5[dB]
X_Pulse           = 3.35[us]
Irr_Mode          = Off
Tri_Mode          = Off
Dante_Presat      = FALSE
Initial_Wait      = 1[s]
Repetition_Time   = 6.74587904[s]
```



JEOL

```
Filename          = NAN039_Carbon-1-3.jdf
Author            = delta
Experiment        = carbon.jxp
Sample_Id         = NAN039
Solvent           = CHLOROFORM-D
Actual_Start_Time =  3-AUG-2023 18:23:44
Revision_Time     = 20-FEB-2024 12:32:13

Comment           = single pulse decoupled ga
Data_Format       = 1D COMPLEX
Dim_Size          = 26214
X_Domain          = Carbon
Dim_Title         = Carbon13
Dim_Units         = [ppm]
Dimensions        = X
Site              = JNM-ECA500
Spectrometer      = DELTA2_NMR

Field_Strength    = 11.7473579[T] (500[MHz])
X_Acq_Duration    = 0.83361792[s]
X_Domain          = 13C
X_Freq            = 125.76529768[MHz]
X_Offset          = 100[ppm]
X_Points          = 32768
X_Prescans        = 4
X_Resolution      = 1.19959034[Hz]
X_Sweep           = 39.3081761[kHz]
X_Sweep_Clipped   = 31.44654088[kHz]
Irr_Domain        = Proton
Irr_Freq          = 500.15991521[MHz]
Irr_Offset        = 5.0[ppm]
Clipped           = FALSE
Scans             = 512
Total_Scans       = 512

Relaxation_Delay  = 2[s]
Recvr_Gain        = 50
Temp_Get          = 22.9[dC]
X_90_Width        = 12.65[us]
X_Acq_Time        = 0.83361792[s]
X_Angle           = 30[deg]
X_Atn             = 7[dB]
X_Pulse           = 4.21666667[us]
Irr_Atn_Dec       = 25.254[dB]
Irr_Atn_Noe       = 25.254[dB]
Irr_Noise         = WALTZ
Irr_Pwidth        = 92[us]
Decoupling        = TRUE
Initial_Wait      = 1[s]
Noe               = TRUE
Noe_Time          = 2[s]
Repetition_Time   = 2.83361792[s]
```

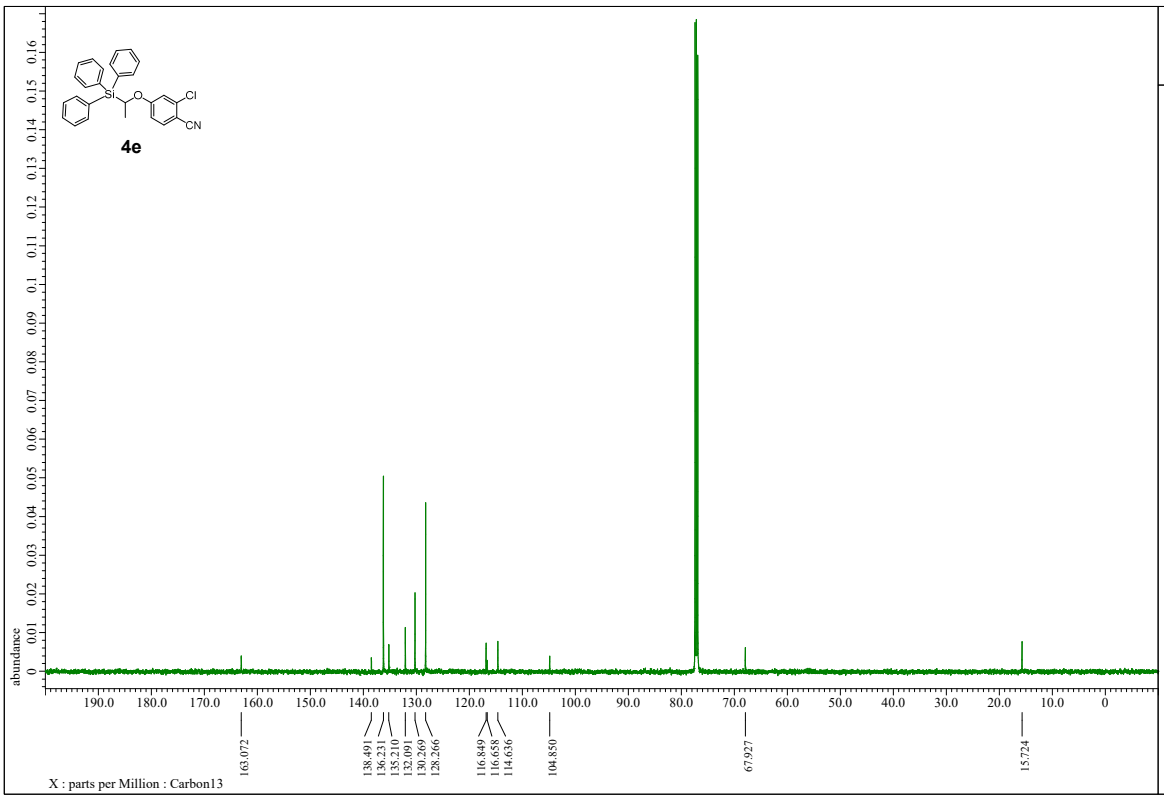


Filename = NAN43_240221_Proton-1-3.j
Author = delta
Experiment = proton.jxp
Sample_Id = NAN43_240221
Solvent = ACETONE-D6
Actual_Start_Time = 21-FEB-2024 12:39:45
Revision_Time = 21-FEB-2024 13:55:50

Comment = single_pulse
Data_Format = 1D COMPLEX
Dim_Size = 13107
X_Domain = Proton
Dim_Title = Proton
Dim_Units = [ppm]
Dimensions = X
Site = JNM-ECA500
Spectrometer = DELTA2_NMR

Field_Strength = 11.7473579[T] (500[MHz])
X_Acq_Duration = 1.74587904[s]
X_Domain = 1H
X_Freq = 500.15991521[MHz]
X_Offset = 5.0[ppm]
X_Points = 16384
X_Prescans = 1
X_Resolution = 0.57277737[Hz]
X_Sweep = 9.38438438[kHz]
X_Sweep_Clipped = 7.50750751[kHz]
Irr_Domain = Proton
Irr_Freq = 500.15991521[MHz]
Irr_Offset = 5.0[ppm]
Tri_Domain = Proton
Tri_Freq = 500.15991521[MHz]
Tri_Offset = 5.0[ppm]
Clipped = FALSE
Scans = 16
Total_Scans = 16

Relaxation_Delay = 5[s]
Recvr_Gain = 60
Temp_Get = 19.7[dC]
X_90_Width = 6.7[us]
X_Acq_Time = 1.74587904[s]
X_Angle = 45[deg]
X_Atn = 2.5[dB]
X_Pulse = 3.35[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Presat = FALSE
Initial_Wait = 1[s]
Repetition_Time = 6.74587904[s]

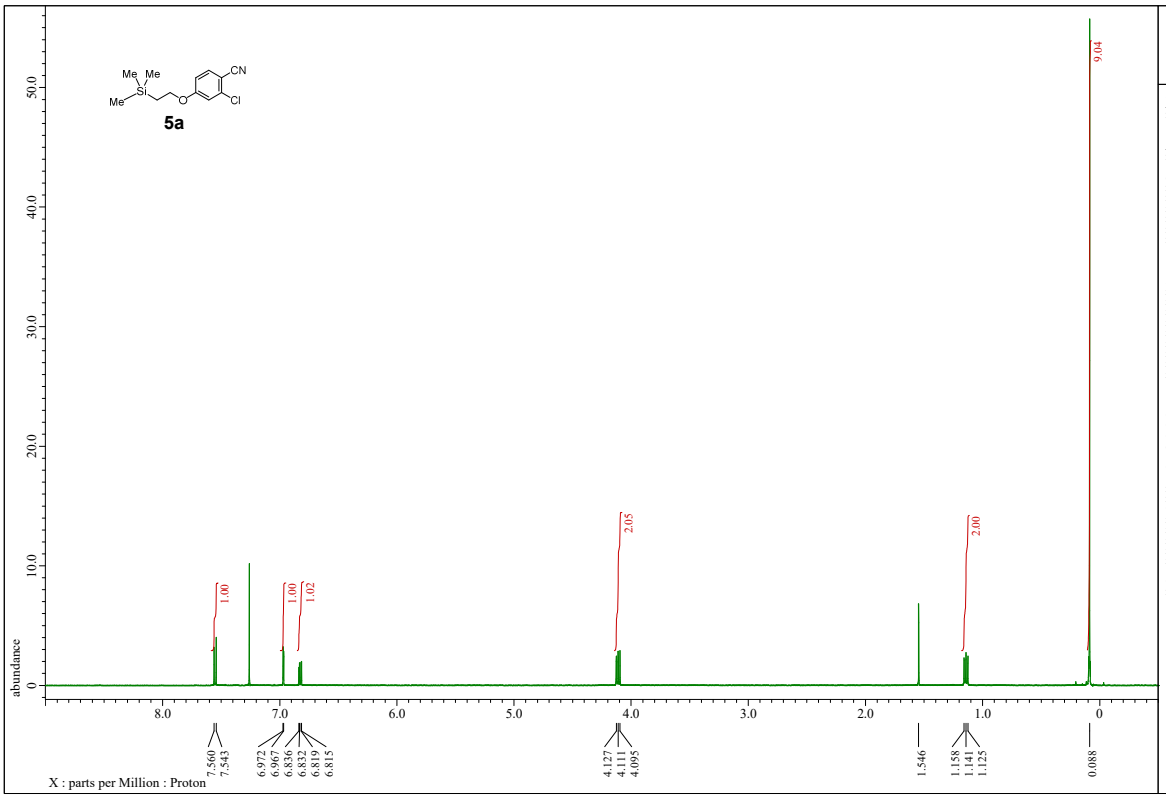


Filename = NAN041_Carbon-1-3.jdf
Author = delta
Experiment = carbon.jxp
Sample_Id = NAN041
Solvent = CHLOROFORM-D
Actual_Start_Time = 1-AUG-2023 20:53:47
Revision_Time = 20-FEB-2024 12:46:44

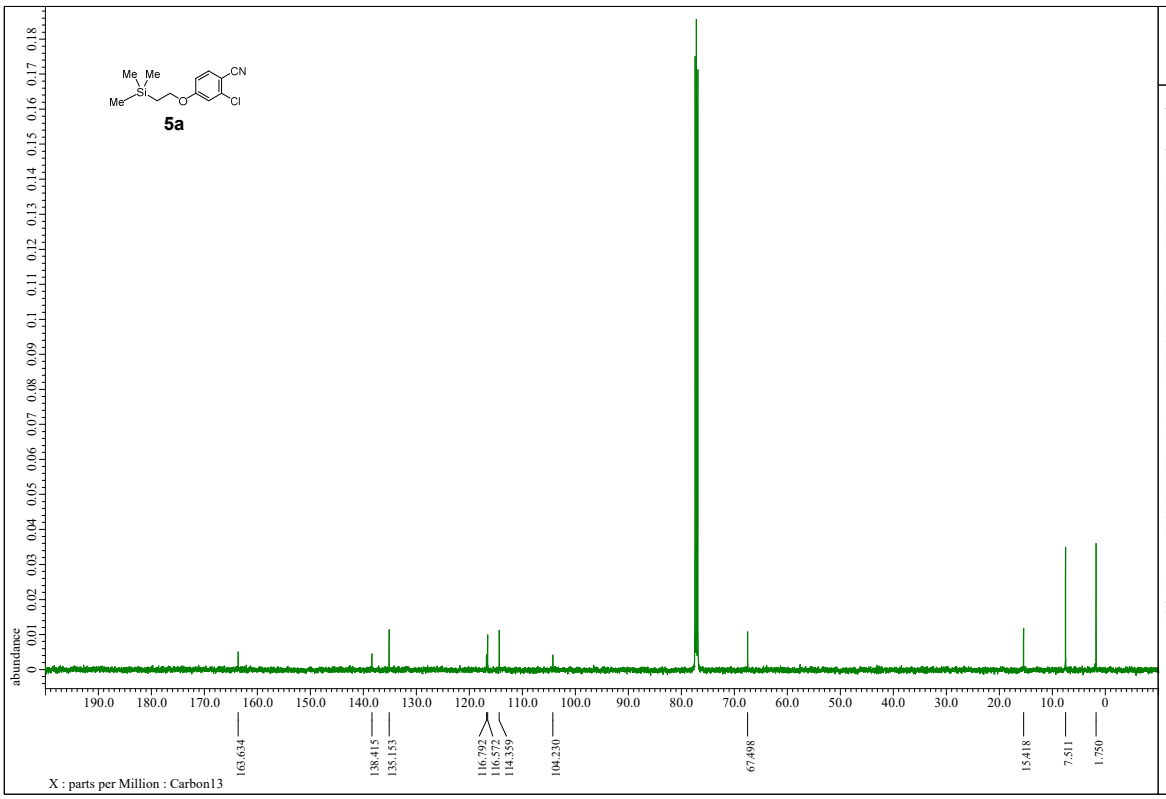
Comment = single pulse decoupled ga
Data_Format = 1D COMPLEX
Dim_Size = 26214
X_Domain = Carbon
Dim_Title = Carbon13
Dim_Units = [ppm]
Dimensions = X
Site = JNM-ECA500
Spectrometer = DELTA2_NMR

Field_Strength = 11.7473579[T] (500[MHz])
X_Acq_Duration = 0.83361792[s]
X_Domain = 13C
X_Freq = 125.76529768[MHz]
X_Offset = 100[ppm]
X_Points = 32768
X_Prescans = 4
X_Resolution = 1.19959034[Hz]
X_Sweep = 39.3081761[kHz]
X_Sweep_Clipped = 31.44654088[kHz]
Irr_Domain = Proton
Irr_Freq = 500.15991521[MHz]
Irr_Offset = 5.0[ppm]
Clipped = FALSE
Scans = 2048
Total_Scans = 2048

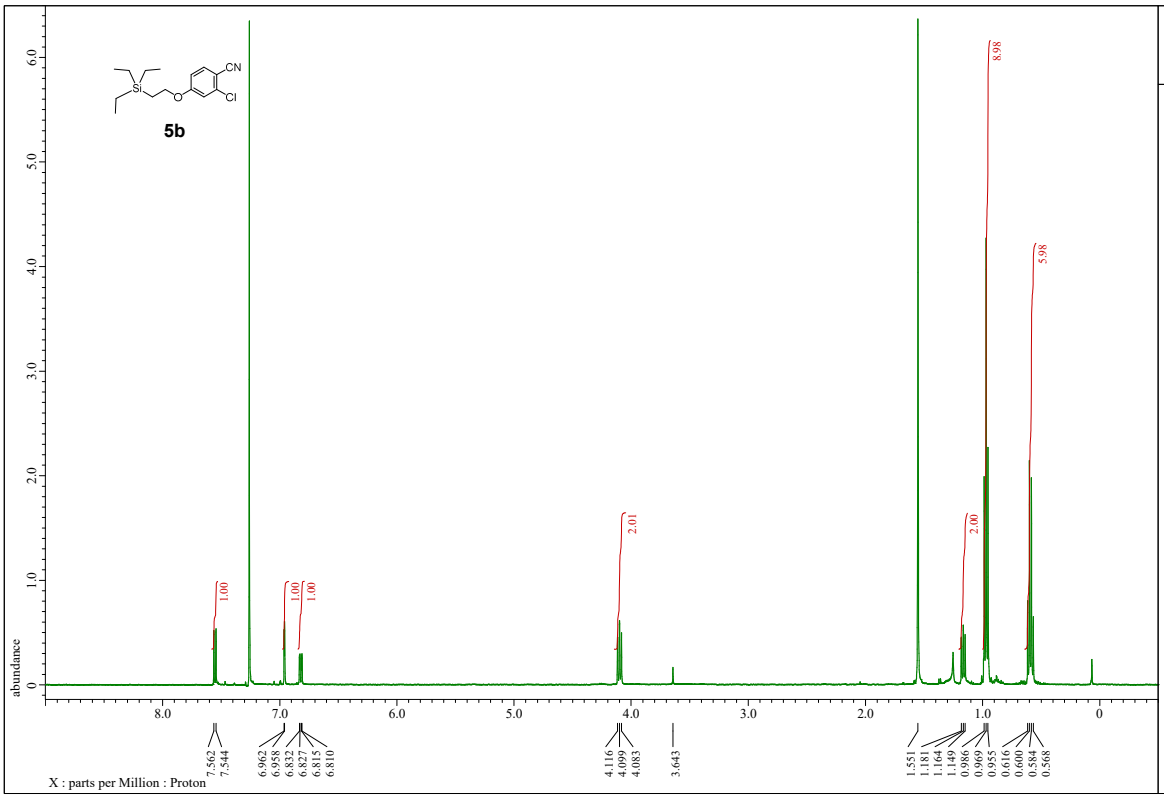
Relaxation_Delay = 2[s]
Recvr_Gain = 50
Temp_Get = 22.9[dC]
X_90_Width = 12.65[us]
X_Acq_Time = 0.83361792[s]
X_Angle = 30[deg]
X_Atn = 7[dB]
X_Pulse = 4.21666667[us]
Irr_Atn_Dec = 25.254[dB]
Irr_Atn_Noe = 25.254[dB]
Irr_Noise = WALTZ
Irr_Pwidth = 92[us]
Decoupling = TRUE
Initial_Wait = 1[s]
Noe = TRUE
Noe_Time = 2[s]
Repetition_Time = 2.83361792[s]



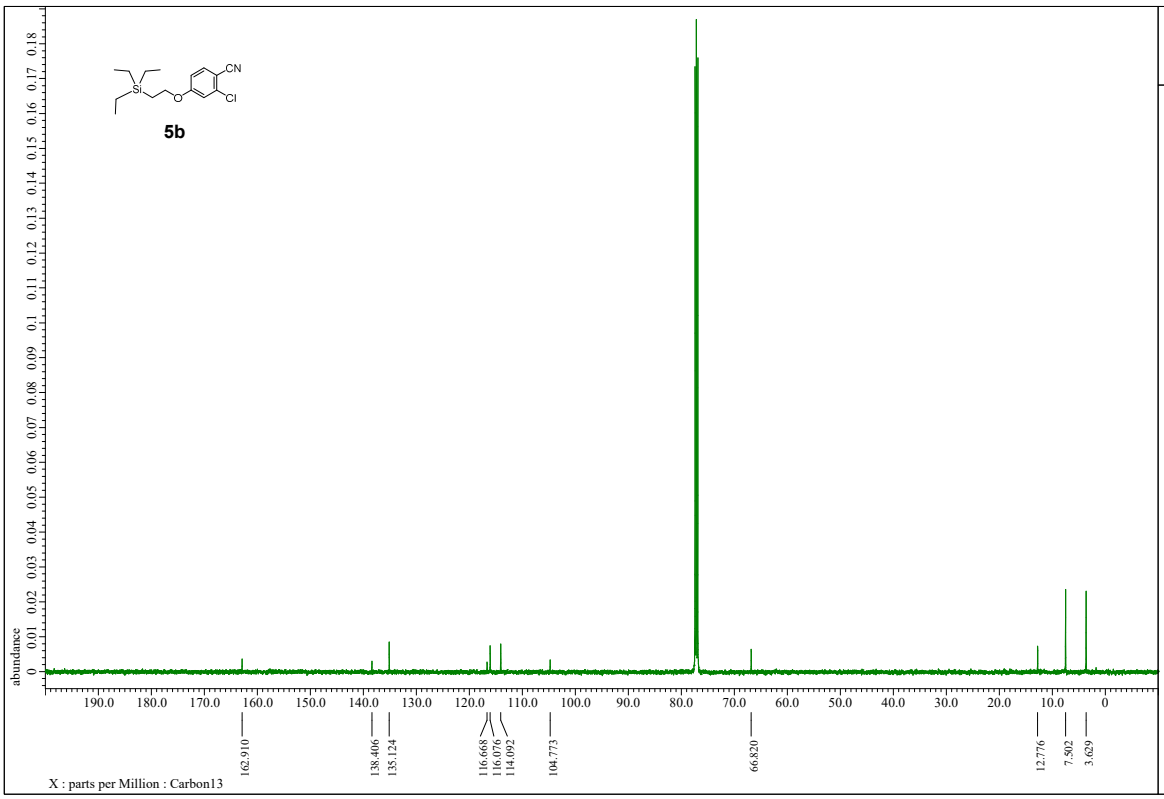

```
Filename          = 270-023-3_GPC287-292_Prot
Author            = delta
Experiment        = proton.jxp
Sample_Id         = 270-023-3_GPC287-292
Solvent           = CHLOROFORM-D
Actual_Start_Time = 18-JUL-2023 20:56:21
Revision_Time     = 20-FEB-2024 12:51:05

Comment           = single_pulse
Data_Format       = 1D COMPLEX
Dim_Size          = 13107
X_Domain          = Proton
Dim_Title         = Proton
Dim_Units         = [ppm]
Dimensions        = X
Site              = JNM-ECA500
Spectrometer      = DELTA2_NMR

Field_Strength    = 11.7473579[T] (500[MHz])
X_Acq_Duration    = 1.74587904[s]
X_Domain          = 1H
X_Freq            = 500.15991521[MHz]
X_Offset          = 5.0[ppm]
X_Points          = 16384
X_Prescans        = 1
X_Resolution      = 0.57277737[Hz]
X_Sweep           = 9.38438438[kHz]
X_Sweep_Clipped   = 7.50750751[kHz]
Irr_Domain        = Proton
Irr_Freq          = 500.15991521[MHz]
Irr_Offset        = 5.0[ppm]
Tri_Domain        = Proton
Tri_Freq          = 500.15991521[MHz]
Tri_Offset        = 5.0[ppm]
Clipped           = FALSE
Scans             = 16
Total_Scans       = 16

Relaxation_Delay  = 5[s]
Recvr_Gain        = 58
Temp_Get          = 22.7[dC]
X_90_Width        = 6.7[us]
X_Acq_Time        = 1.74587904[s]
X_Angle           = 45[deg]
X_Atn             = 2.5[dB]
X_Pulse           = 3.35[us]
Irr_Mode          = Off
Tri_Mode          = Off
Dante_Presat      = FALSE
Initial_Wait      = 1[s]
Repetition_Time   = 6.74587904[s]
```



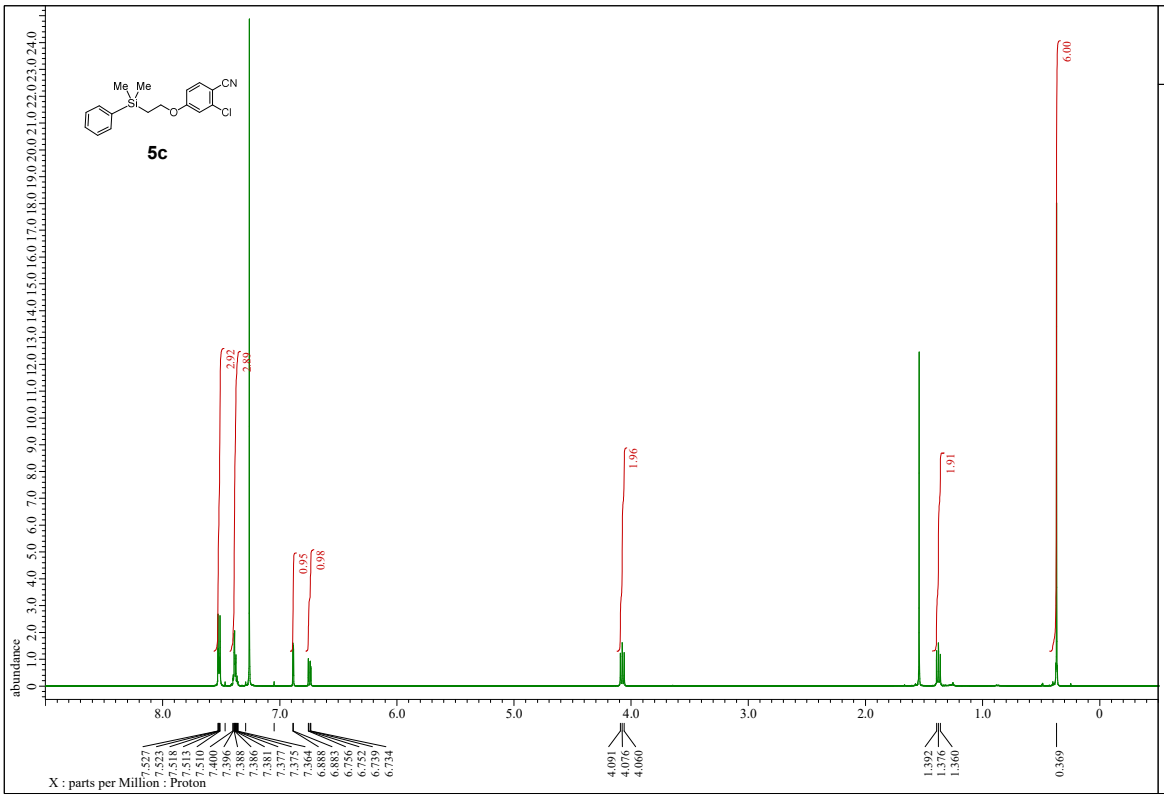

```
Filename          = NAN045(true)_Carbon-2-5.j
Author            = delta
Experiment        = carbon.jxp
Sample_Id         = NAN045
Solvent           = CHLOROFORM-D
Actual_Start_Time =  3-AUG-2023 17:25:55
Revision_Time     = 20-FEB-2024 12:52:25

Comment           = single pulse decoupled ga
Data_Format       = 1D COMPLEX
Dim_Size          = 26214
X_Domain          = Carbon
Dim_Title         = Carbon13
Dim_Units         = [ppm]
Dimensions        = X
Site              = JNM-ECA500
Spectrometer      = DELTA2_NMR

Field_Strength    = 11.7473579[T] (500[MHz])
X_Acq_Duration    = 0.83361792[s]
X_Domain          = 13C
X_Freq            = 125.76529768[MHz]
X_Offset          = 100[ppm]
X_Points          = 32768
X_Prescans        = 4
X_Resolution      = 1.19959034[Hz]
X_Sweep           = 39.3081761[kHz]
X_Sweep_Clipped   = 31.44654088[kHz]
Irr_Domain        = Proton
Irr_Freq          = 500.15991521[MHz]
Irr_Offset        = 5.0[ppm]
Clipped           = FALSE
Scans             = 1024
Total_Scans       = 1024

Relaxation_Delay  = 2[s]
Recvr_Gain        = 50
Temp_Get          = 22.7[dC]
X_90_Width        = 12.65[us]
X_Acq_Time        = 0.83361792[s]
X_Angle           = 30[deg]
X_Atn             = 7[dB]
X_Pulse           = 4.21666667[us]
Irr_Atn_Dec       = 25.254[dB]
Irr_Atn_Noe       = 25.254[dB]
Irr_Noise         = WALTZ
Irr_Pwidth        = 92[us]
Decoupling        = TRUE
Initial_Wait      = 1[s]
Noe               = TRUE
Noe_Time          = 2[s]
Repetition_Time   = 2.83361792[s]
```




```
Filename          = NAN46_col13_Proton-2-2.jd
Author            = delta
Experiment        = proton.jxp
Sample_Id         = NAN46_col13
Solvent           = CHLOROFORM-D
Actual_Start_Time = 20-FEB-2024 22:46:10
Revision_Time     = 21-FEB-2024 11:48:35

Comment           = single_pulse
Data_Format       = 1D COMPLEX
Dim_Size          = 13107
X_Domain          = Proton
Dim_Title         = Proton
Dim_Units         = [ppm]
Dimensions        = X
Site              = JNM-ECA500
Spectrometer      = DELTA2_NMR

Field_Strength    = 11.7473579[T] (500[MHz])
X_Acq_Duration    = 1.74587904[s]
X_Domain          = 1H
X_Freq            = 500.15991521[MHz]
X_Offset          = 5.0[ppm]
X_Points          = 16384
X_Prescans        = 1
X_Resolution      = 0.57277737[Hz]
X_Sweep           = 9.38438438[kHz]
X_Sweep_Clipped   = 7.50750751[kHz]
Irr_Domain        = Proton
Irr_Freq          = 500.15991521[MHz]
Irr_Offset        = 5.0[ppm]
Tri_Domain        = Proton
Tri_Freq          = 500.15991521[MHz]
Tri_Offset        = 5.0[ppm]
Clipped           = FALSE
Scans             = 64
Total_Scans       = 64

Relaxation_Delay  = 5[s]
Recvr_Gain        = 60
Temp_Get          = 20.9[dC]
X_90_Width        = 6.7[us]
X_Acq_Time        = 1.74587904[s]
X_Angle           = 45[deg]
X_Atn             = 2.5[dB]
X_Pulse           = 3.35[us]
Irr_Mode          = Off
Tri_Mode          = Off
Dante_Presat      = FALSE
Initial_Wait      = 1[s]
Repetition_Time   = 6.74587904[s]
```

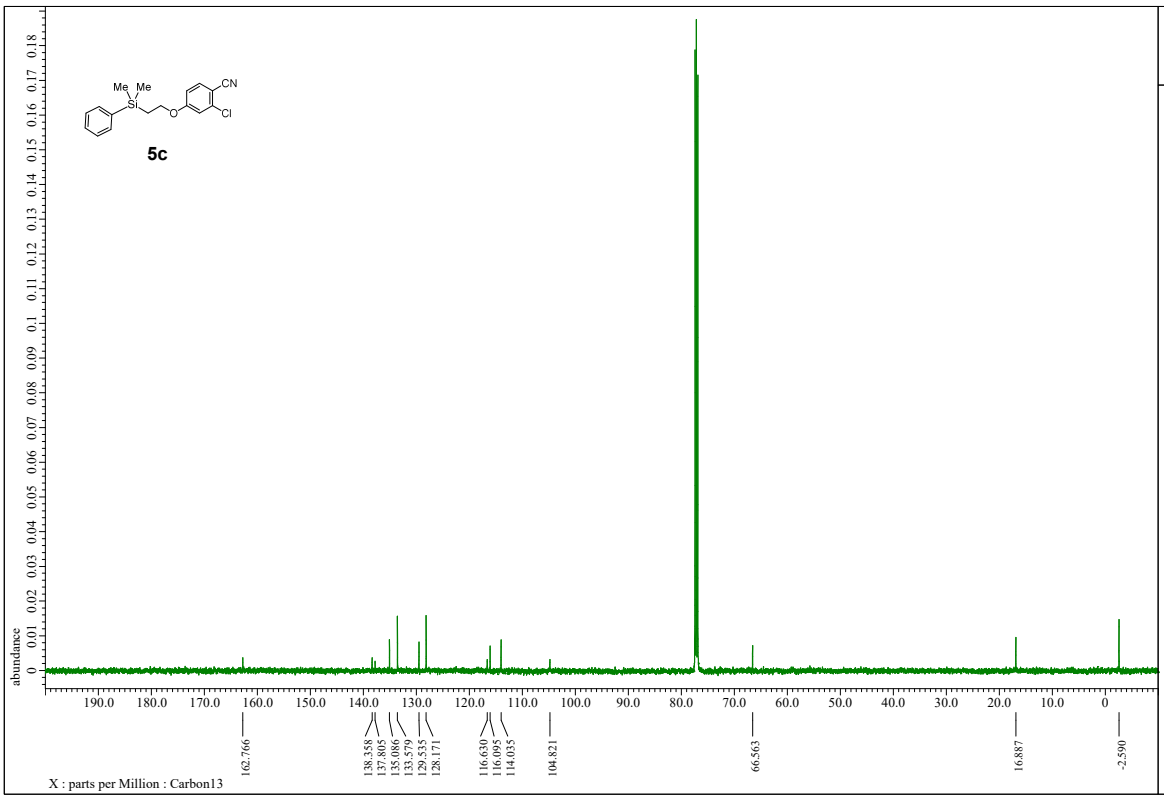



```
Filename          = NAN046_Carbon-1-2.jdf
Author            = delta
Experiment        = carbon.jxp
Sample_Id         = NAN046
Solvent           = CHLOROFORM-D
Actual_Start_Time = 11-SEP-2023 21:09:17
Revision_Time     = 20-FEB-2024 13:02:42

Comment           = single pulse decoupled ga
Data_Format       = 1D COMPLEX
Dim_Size          = 26214
X_Domain          = Carbon
Dim_Title         = Carbon13
Dim_Units         = [ppm]
Dimensions        = X
Site              = JNM-ECA500
Spectrometer      = DELTA2_NMR

Field_Strength    = 11.7473579[T] (500[MHz])
X_Acq_Duration    = 0.83361792[s]
X_Domain          = 13C
X_Freq            = 125.76529768[MHz]
X_Offset          = 100[ppm]
X_Points          = 32768
X_Prescans        = 4
X_Resolution      = 1.19959034[Hz]
X_Sweep           = 39.3081761[kHz]
X_Sweep_Clipped   = 31.44654088[kHz]
Irr_Domain        = Proton
Irr_Freq          = 500.15991521[MHz]
Irr_Offset        = 5.0[ppm]
Clipped           = FALSE
Scans             = 2048
Total_Scans       = 2048

Relaxation_Delay  = 2[s]
Recvr_Gain        = 50
Temp_Get          = 22.8[dC]
X_90_Width        = 12.65[us]
X_Acq_Time        = 0.83361792[s]
X_Angle           = 30[deg]
X_Atn             = 7[dB]
X_Pulse           = 4.21666667[us]
Irr_Atn_Dec       = 25.254[dB]
Irr_Atn_Noe       = 25.254[dB]
Irr_Noise         = WALTZ
Irr_Pwidth        = 92[us]
Decoupling        = TRUE
Initial_Wait      = 1[s]
Noe               = TRUE
Noe_Time          = 2[s]
Repetition_Time   = 2.83361792[s]
```



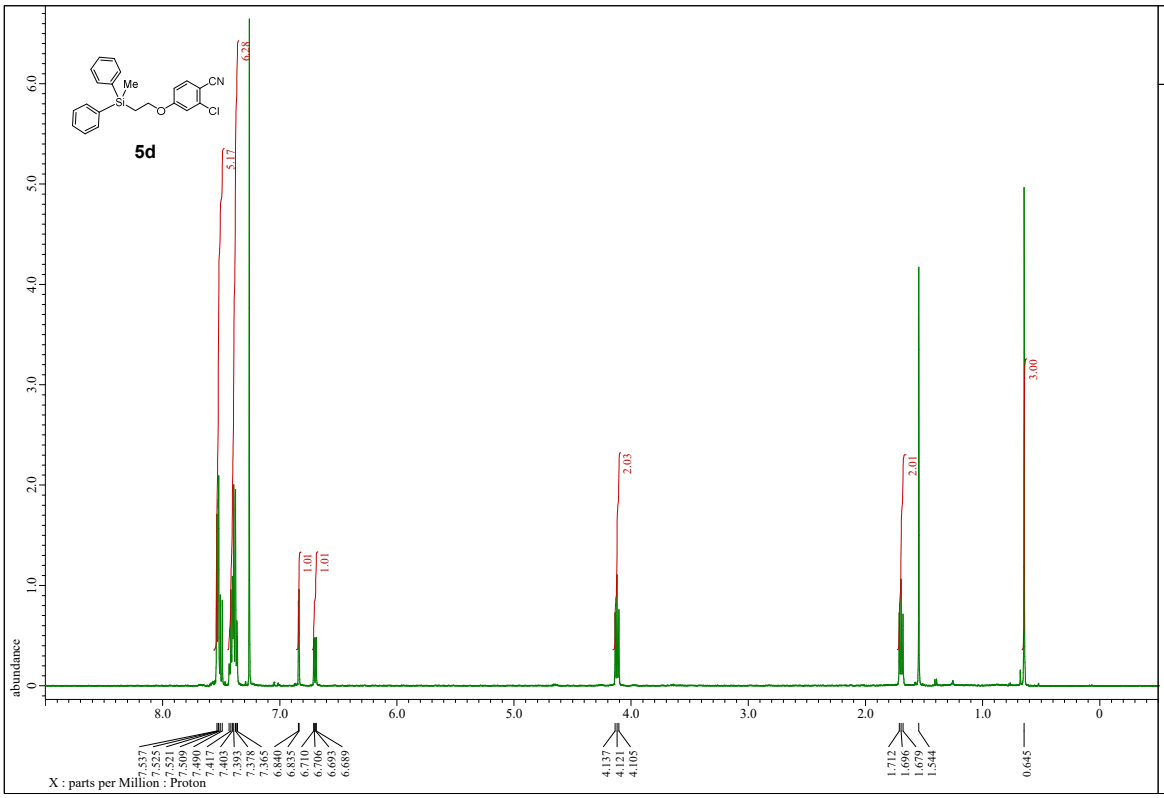
JEOL

```
Filename          = 189col215-18_GPC_Proton-1
Author            = delta
Experiment        = proton.jxp
Sample_Id         = 189col215-18_GPC
Solvent           = CHLOROFORM-D
Actual_Start_Time = 26-APR-2023 15:01:59
Revision_Time     = 20-FEB-2024 13:06:45

Comment           = single_pulse
Data_Format       = 1D COMPLEX
Dim_Size          = 13107
X_Domain          = Proton
Dim_Title         = Proton
Dim_Units         = [ppm]
Dimensions        = X
Site              = JNM-ECA500
Spectrometer      = DELTA2_NMR

Field_Strength    = 11.7473579[T] (500[MHz])
X_Acq_Duration    = 1.74587904[s]
X_Domain          = 1H
X_Freq            = 500.15991521[MHz]
X_Offset          = 5.0[ppm]
X_Points          = 16384
X_Prescans        = 1
X_Resolution      = 0.57277737[Hz]
X_Sweep           = 9.38438438[kHz]
X_Sweep_Clipped   = 7.50750751[kHz]
Irr_Domain        = Proton
Irr_Freq          = 500.15991521[MHz]
Irr_Offset        = 5.0[ppm]
Tri_Domain        = Proton
Tri_Freq          = 500.15991521[MHz]
Tri_Offset        = 5.0[ppm]
Clipped           = FALSE
Scans             = 256
Total_Scans       = 256

Relaxation_Delay  = 5[s]
Recvr_Gain        = 64
Temp_Get          = 21.6[dC]
X_90_Width        = 6.7[us]
X_Acq_Time        = 1.74587904[s]
X_Angle           = 45[deg]
X_Atn             = 2.5[dB]
X_Pulse           = 3.35[us]
Irr_Mode          = Off
Tri_Mode          = Off
Dante_Presat      = FALSE
Initial_Wait      = 1[s]
Repetition_Time   = 6.74587904[s]
```

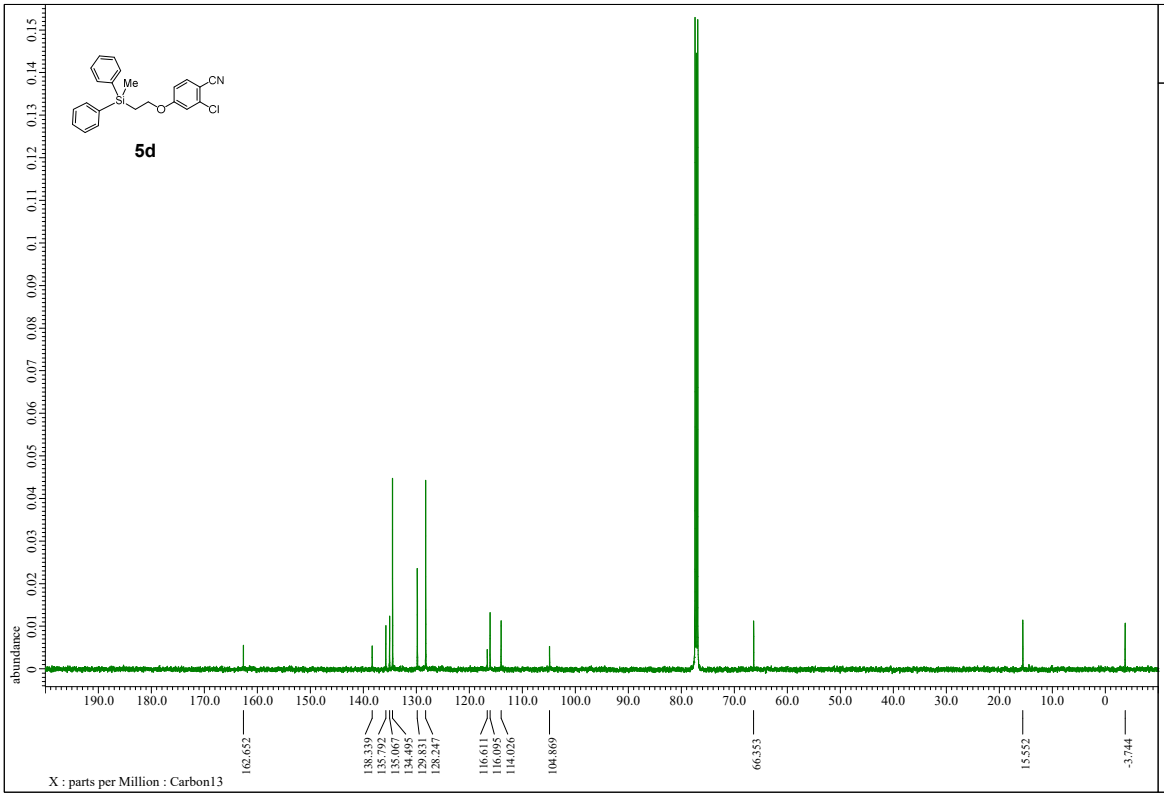


JEOL

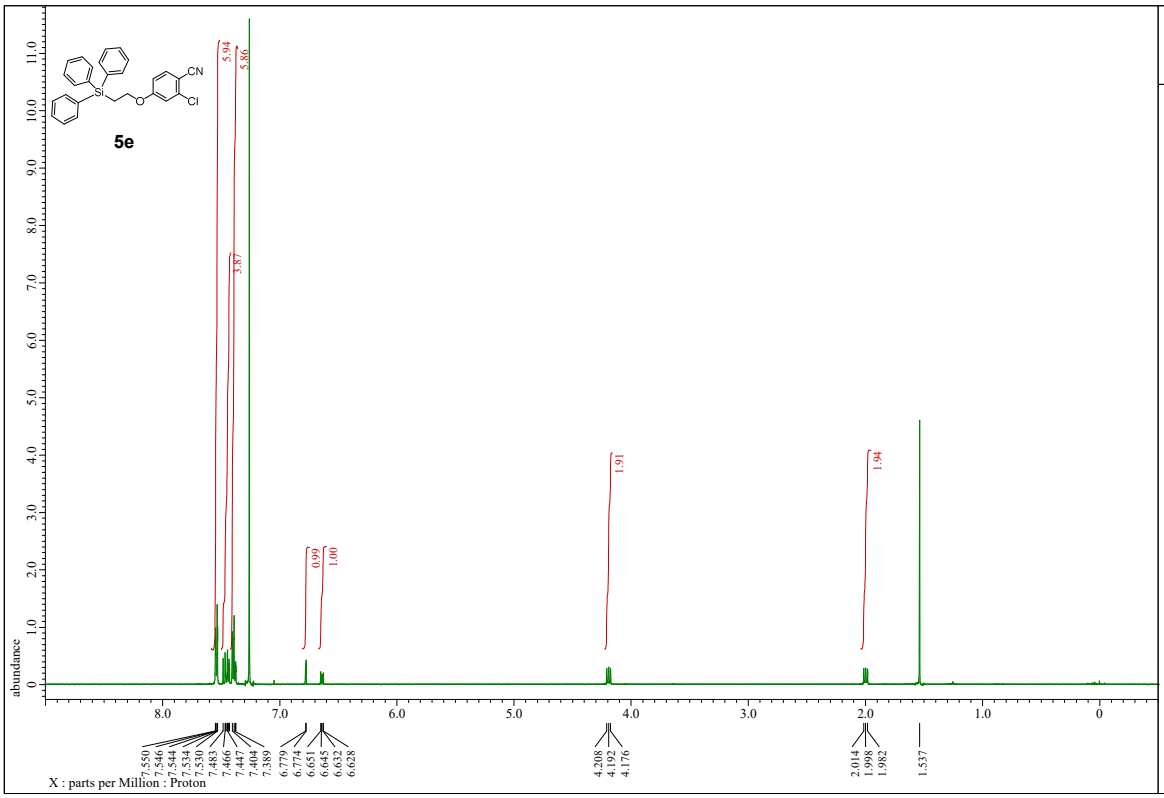
```
Filename          = NAN038_Carbon-1-7.jdf
Author            = delta
Experiment        = carbon.jxp
Sample_Id         = NAN038
Solvent           = CHLOROFORM-D
Actual_Start_Time =  3-AUG-2023 12:28:15
Revision_Time     = 20-FEB-2024 13:08:14

Comment           = single pulse decoupled ga
Data_Format       = 1D COMPLEX
Dim_Size          = 26214
X_Domain          = Carbon
Dim_Title         = Carbon13
Dim_Units         = [ppm]
Dimensions        = X
Site              = JNM-ECA500
Spectrometer      = DELTA2_NMR

Field_Strength    = 11.7473579[T] (500[MHz])
X_Acq_Duration    = 0.83361792[s]
X_Domain          = 13C
X_Freq            = 125.76529768[MHz]
X_Offset          = 100[ppm]
X_Points          = 32768
X_Prescans        = 3
X_Resolution      = 1.19959034[Hz]
X_Sweep           = 39.3081761[kHz]
X_Sweep_Clipped   = 31.44654088[kHz]
Irr_Domain        = Proton
Irr_Freq          = 500.15991521[MHz]
Irr_Offset        = 5.0[ppm]
Clipped           = FALSE
Scans             = 1024
Total_Scans       = 1024

Relaxation_Delay  = 2[s]
Recvr_Gain        = 50
Temp_Get          = 22.9[dC]
X_90_Width        = 12.65[us]
X_Acq_Time        = 0.83361792[s]
X_Angle           = 30[deg]
X_Atn             = 7[dB]
X_Pulse           = 4.21666667[us]
Irr_Atn_Dec       = 25.254[dB]
Irr_Atn_Noe       = 25.254[dB]
Irr_Noise         = WALTZ
Irr_Pwidth        = 92[us]
Decoupling        = TRUE
Initial_Wait      = 1[s]
Noe               = TRUE
Noe_Time          = 2[s]
Repetition_Time   = 2.83361792[s]
```




```
Filename          = NAN40_240219_Proton-1-3.j
Author            = delta
Experiment        = proton.jxp
Sample_Id         = NAN40_240219
Solvent           = CHLOROFORM-D
Actual_Start_Time = 19-FEB-2024 20:53:23
Revision_Time     = 20-FEB-2024 13:10:56

Comment           = single_pulse
Data_Format       = 1D COMPLEX
Dim_Size          = 13107
X_Domain          = Proton
Dim_Title         = Proton
Dim_Units         = [ppm]
Dimensions        = X
Site              = JNM-ECA500
Spectrometer      = DELTA2_NMR

Field_Strength    = 11.7473579[T] (500[MHz])
X_Acq_Duration    = 1.74587904[s]
X_Domain          = 1H
X_Freq            = 500.15991521[MHz]
X_Offset          = 5.0[ppm]
X_Points          = 16384
X_Prescans        = 1
X_Resolution      = 0.57277737[Hz]
X_Sweep           = 9.38438438[kHz]
X_Sweep_Clipped   = 7.50750751[kHz]
Irr_Domain        = Proton
Irr_Freq          = 500.15991521[MHz]
Irr_Offset        = 5.0[ppm]
Tri_Domain        = Proton
Tri_Freq          = 500.15991521[MHz]
Tri_Offset        = 5.0[ppm]
Clipped           = FALSE
Scans             = 32
Total_Scans       = 32

Relaxation_Delay  = 5[s]
Recvr_Gain        = 60
Temp_Get          = 20.5[dC]
X_90_Width        = 6.7[us]
X_Acq_Time        = 1.74587904[s]
X_Angle           = 45[deg]
X_Atn             = 2.5[dB]
X_Pulse           = 3.35[us]
Irr_Mode          = Off
Tri_Mode          = Off
Dante_Presat      = FALSE
Initial_Wait      = 1[s]
Repetition_Time   = 6.74587904[s]
```

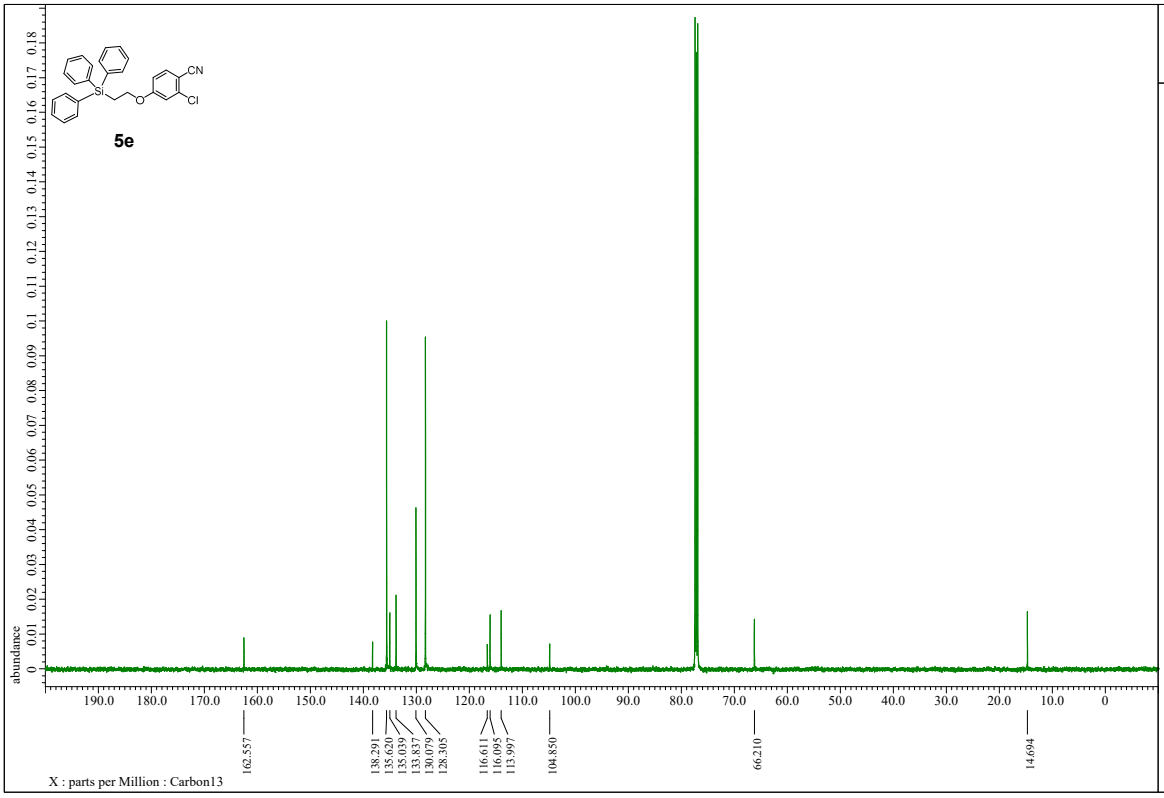



```
Filename          = NAN040_Carbon-1-3.jdf
Author            = delta
Experiment        = carbon.jxp
Sample_Id         = NAN040
Solvent           = CHLOROFORM-D
Actual_Start_Time = 28-AUG-2023 19:35:22
Revision_Time     = 20-FEB-2024 13:12:43

Comment           = single pulse decoupled ga
Data_Format       = 1D COMPLEX
Dim_Size          = 26214
X_Domain          = Carbon
Dim_Title         = Carbon13
Dim_Units         = [ppm]
Dimensions        = X
Site              = JNM-ECA500
Spectrometer      = DELTA2_NMR

Field_Strength    = 11.7473579[T] (500[MHz])
X_Acq_Duration    = 0.83361792[s]
X_Domain          = 13C
X_Freq            = 125.76529768[MHz]
X_Offset          = 100[ppm]
X_Points          = 32768
X_Prescans        = 4
X_Resolution      = 1.19959034[Hz]
X_Sweep           = 39.3081761[kHz]
X_Sweep_Clipped   = 31.44654088[kHz]
Irr_Domain        = Proton
Irr_Freq          = 500.15991521[MHz]
Irr_Offset        = 5.0[ppm]
Clipped           = FALSE
Scans             = 2048
Total_Scans       = 2048

Relaxation_Delay  = 2[s]
Recvr_Gain        = 50
Temp_Get          = 22.9[dC]
X_90_Width        = 12.65[us]
X_Acq_Time        = 0.83361792[s]
X_Angle           = 30[deg]
X_Atn             = 7[dB]
X_Pulse           = 4.21666667[us]
Irr_Atn_Dec       = 25.254[dB]
Irr_Atn_Noe       = 25.254[dB]
Irr_Noise         = WALTZ
Irr_Pwidth        = 92[us]
Decoupling        = TRUE
Initial_Wait      = 1[s]
Noe               = TRUE
Noe_Time          = 2[s]
Repetition_Time   = 2.83361792[s]
```



JEOL

```
Filename          = 270-051-5_GPC161-169_Prot
Author            = delta
Experiment        = proton.jxp
Sample_Id         = 270-051-5_GPC161-169
Solvent           = CHLOROFORM-D
Actual_Start_Time =  9-NOV-2023 17:32:31
Revision_Time     = 20-FEB-2024 13:14:19

Comment           = single_pulse
Data_Format       = 1D COMPLEX
Dim_Size          = 13107
X_Domain          = Proton
Dim_Title         = Proton
Dim_Units         = [ppm]
Dimensions        = X
Site              = JNM-ECA500
Spectrometer      = DELTA2_NMR

Field_Strength    = 11.7473579[T] (500[MHz])
X_Acq_Duration    = 1.74587904[s]
X_Domain          = 1H
X_Freq            = 500.15991521[MHz]
X_Offset          = 5.0[ppm]
X_Points          = 16384
X_Prescans        = 1
X_Resolution      = 0.57277737[Hz]
X_Sweep           = 9.38438438[kHz]
X_Sweep_Clipped   = 7.50750751[kHz]
Irr_Domain        = Proton
Irr_Freq          = 500.15991521[MHz]
Irr_Offset        = 5.0[ppm]
Tri_Domain        = Proton
Tri_Freq          = 500.15991521[MHz]
Tri_Offset        = 5.0[ppm]
Clipped           = FALSE
Scans             = 16
Total_Scans       = 16

Relaxation_Delay  = 5[s]
Recvr_Gain        = 60
Temp_Get          = 21.9[dC]
X_90_Width        = 6.7[us]
X_Acq_Time        = 1.74587904[s]
X_Angle           = 45[deg]
X_Atn             = 2.5[dB]
X_Pulse           = 3.35[us]
Irr_Mode          = Off
Tri_Mode          = Off
Dante_Presat      = FALSE
Initial_Wait      = 1[s]
Repetition_Time   = 6.74587904[s]
```



JEOL

```
Filename          = NAN042_Carbon-1-2.jdf
Author            = delta
Experiment        = carbon.jxp
Sample_Id         = 270-051-6_GPC_retake
Solvent           = CHLOROFORM-D
Actual_Start_Time = 10-NOV-2023 22:51:24
Revision_Time     = 20-FEB-2024 13:16:15

Comment           = single pulse decoupled ga
Data_Format       = 1D COMPLEX
Dim_Size          = 26214
X_Domain          = Carbon
Dim_Title         = Carbon13
Dim_Units         = [ppm]
Dimensions        = X
Site              = JNM-ECA500
Spectrometer      = DELTA2_NMR

Field_Strength    = 11.7473579[T] (500[MHz])
X_Acq_Duration    = 0.83361792[s]
X_Domain          = 13C
X_Freq            = 125.76529768[MHz]
X_Offset          = 100[ppm]
X_Points          = 32768
X_Prescans        = 4
X_Resolution      = 1.19959034[Hz]
X_Sweep           = 39.3081761[kHz]
X_Sweep_Clipped   = 31.44654088[kHz]
Irr_Domain        = Proton
Irr_Freq          = 500.15991521[MHz]
Irr_Offset        = 5.0[ppm]
Clipped           = FALSE
Scans             = 2048
Total_Scans       = 2048

Relaxation_Delay  = 2[s]
Recvr_Gain        = 50
Temp_Get          = 21.9[dC]
X_90_Width        = 12.65[us]
X_Acq_Time        = 0.83361792[s]
X_Angle           = 30[deg]
X_Atn             = 7[dB]
X_Pulse           = 4.21666667[us]
Irr_Atn_Dec       = 25.254[dB]
Irr_Atn_Noe       = 25.254[dB]
Irr_Noise         = WALTZ
Irr_Pwidth        = 92[us]
Decoupling        = TRUE
Initial_Wait      = 1[s]
Noe               = TRUE
Noe_Time          = 2[s]
Repetition_Time   = 2.83361792[s]
```