Synthesis and Physico-Chemical Properties of 2-SF_5-(Aza)indoles, A New Family of SF_5-Heterocycles

Vincent Debrauwer,[a] Ivo Leito,[b] Märt Lõkov,[b] Sofja Tshepelevitsh,[b] Michael Parmentier,[c] Nicolas Blanchard*[a] and Vincent Bizet*[a]

[a]Université de Haute-Alsace, Université de Strasbourg, CNRS, LIMA, UMR 7042, 68000 Mulhouse, France
[b]Institute of Chemistry, University of Tartu, Tartu 50411, Estonia
[c]Chemical and Analytical Development, Novartis Pharma AG, CH-4056 Basel, Switzerland

n.blanchard@unistra.fr

vbizet@unistra.fr

Supporting Information

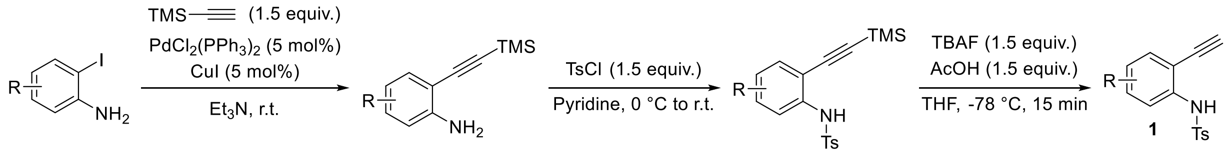
Table of Contents

1 General

NMR spectra were recorded on Brucker AV 400 or AV 500 spectrometer at 400 MHz or 500 MHz for ^{1}H NMR, at 100 or 125 MHz for ^{13}C NMR and at 471 MHz for ^{19}F NMR. The spectra were calibrated using undeuterated solvent as internal reference, unless otherwise indicated. ^{1}H and $^{13}C\{^{1}H\}$ NMR chemical shifts are given in ppm relative to $SiMe_4$, with the solvent resonance used as internal reference. $^{19}F\{^{1}H\}$ NMR chemical shifts are reported in ppm relative to $CFCl_3$. NMR yields were determined by ^{19}F NMR, using trifluorotoluene as internal standard. The following abbreviations were used to explain multiplicities: s = singlet, d = doublet, t = triplet, q = quartet, quint. = quintet, sex. = sextet, m = multiplet, and b = broad. Coupling constant (J) were reported in Hertz. High resolution mass spectra (HRMS) in positive mode were recorded using a 6520 series quadrupole time-of-flight (Q-TOF) mass spectrometer (Agilent) fitted with a multimode ion source (in mixed mode that enables both electrospray ionization, ESI, and atmospheric pressure chemical ionization, APCI). Samples were directly infused into the source using 50/50-methanol/formic acid 0.2 % in water. Infrared spectra were obtained on a *Perkin-Elmer* 1650 FT-IR spectrometer using neat samples on a diamond ATR Golden Gate sampler. Tetrahydrofuran (THF) was distilled under nitrogen from sodium-benzophenone. Reagents were purchased from Merck, Fluorochem or ABCR and used without further purification, unless otherwise noted. All non-commercially available reagents were prepared using literature procedure.[1] Yields refer to chromatographically and spectroscopically (^{1}H, ^{13}C and ^{19}F NMR) homogeneous materials, unless otherwise noted. Reactions were monitored by thin-layer chromatography (TLC) carried out on Merck TLC silica gel 60 F254 aluminum plates, using UV light or potassium permanganate as visualizing agents. All separations were performed by chromatography on Merck silica gel 60 (40-63 µm) or by preparative TLC chromatography (layer thickness of 500 µm).

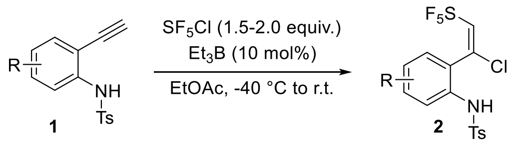
2 Experimental procedures

2.1 General procedure (GP1) for the synthesis of *N*-(2-ethynylphenyl)-4-methylbenzenesulfonamide derivatives 1



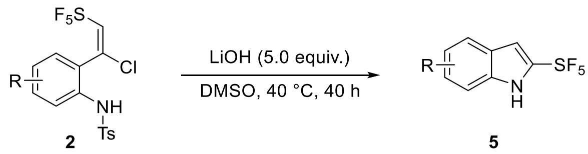
In a 100 mL round bottom flask equipped with a magnetic stir bar, the iodoaniline derivative (1 equiv.), $PdCl_2(PPh_3)_2$ (5 mol%) and CuI (5 mol%) were charged and dissolved in Et_3N (0.4 M) under N_2. Trimethylsilylacetylene (1.5 equiv.) was the added dropwise to the mixture and it was stirred at room temperature until completion of the reaction. The crude mixture was filtered on a short pad of silica gel and concentrated under reduced pressure. Without further purification it was dissolved in pyridine (0.5 M) and cooled down to 0 °C, *p*-toluenesulfonyl chloride (1.5 equiv.) was added portionwise under N_2. The reaction mixture was stirred at room temperature until full conversion was observed by TLC. The reaction was quenched with water and extracted with 3 volumes of EtOAc, the combined layers were dried over $MgSO_4$, filtered and concentrated under reduced pressure. Without further purification, the crude mixture was dissolved in THF and cooled down to - 78 °C, then AcOH (1.5 equiv.) and TBAF (1.5 equiv.) were added. The reaction was stirred at this temperature for 15 min and quenched with saturated aqueous solution of NH_4Cl and extracted with 3 volumes of EtOAc. The combined organic layers were dried over $MgSO_4$, filtered, and concentrated under reduced pressure. The crude mixture was purified by silica gel column chromatography to afford the *N*-(2-ethynylphenyl)-4-methylbenzenesulfonamide derivatives **1**.

2.2 General procedure (GP2) for the radical addition of SF_5Cl on terminal alkynes



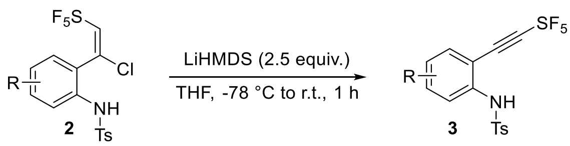
In a 10 mL pressure tube under N_2 equipped with a magnetic stir bar, the *N*-(2-ethynylphenyl)-4-methylbenzenesulfonamide **1** (1.0 equiv.) derivative was introduced and dissolved in EtOAc (0.4 M). At - 40 °C, gaseous SF_5Cl (1.5 - 2.0 equiv.) was condensed in the solution and it was stirred for 5 min at this temperature before Et_3B (10 mol%) was added dropwise followed by a catalytic amount of air. The tube was sealed, and it was stirred at room temperature for 16 h. The reaction mixture was quenched with saturated solution of $NaHCO_3$ and it was extracted with 3 volumes of EtOAc. The combined organic layers were dried over $MgSO_4$, filtered, and concentrated at reduced pressure. No further purification is needed when conversion is total, otherwise NMR yield is reported, and the corresponding product **2** was purified by chromatography on silica gel.

2.3 General procedure (GP3) for the synthesis of the 2-SF_5 indoles 5:



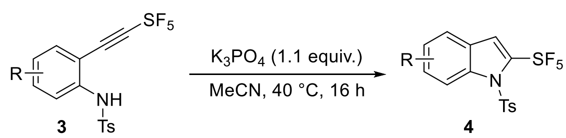
In 5 mL round bottom flask equipped with a magnetic stir bar containing the chloro pentafluorosulfanylated olefin **2** was introduced $LiOH.H_2O$ (5 equiv.) and DMSO (0.4 M). The reaction mixture was stirred at 40 °C for 40 h. The reaction was quenched with saturated solution of NH_4Cl and extracted with 3 volumes of EtOAc. The combined organic layers were dried over $MgSO_4$, filtered and concentrated under reduced pressure. The crude mixture was purified by silica gel column chromatography affording the corresponding 2-SF_5 indole **5**.

2.4 General procedure (GP4) for the synthesis of SF_5-alkynes 3:



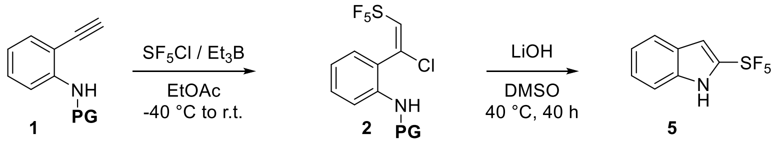
In a 5 mL Schlenk tube equipped with a magnetic stir bar, the chloro pentafluorosulfanylated olefin **2** was dissolved in THF (0.2 M) under N_2 and the mixture was cooled down to - 78 °C. LiHMDS (2.5 equiv.) was added dropwise and the reaction was stirred at rt for 1 hour. The reaction mixture was quenched with a saturated solution of NH_4Cl and extracted with 3 volumes of EtOAc. The combined organic layers were dried over $MgSO_4$, filtered, and concentrated under reduced pressure to give pure product **3**. No purification was necessary at this step.

2.5 General procedure (GP5) for the synthesis of the 2-SF_5-*N*-Ts-indoles 4:



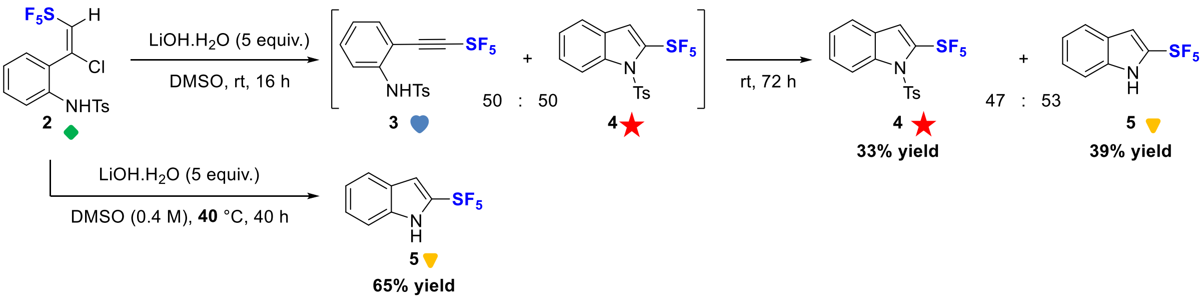
In a 10 mL Shlenck tube under N_2 equipped with a magnetic stir bar, SF_5-alkyne **3** and K_3PO_4 (1.1 equiv.) were dissolved in MeCN (0.07 M) and stirred at 40 °C for 16 hours. The mixture was concentrated and purified by silica gel column chromatography (P.E/EtOAc 90/10) affording the corresponding *N*-Ts 2-SF_5-indole **4**.

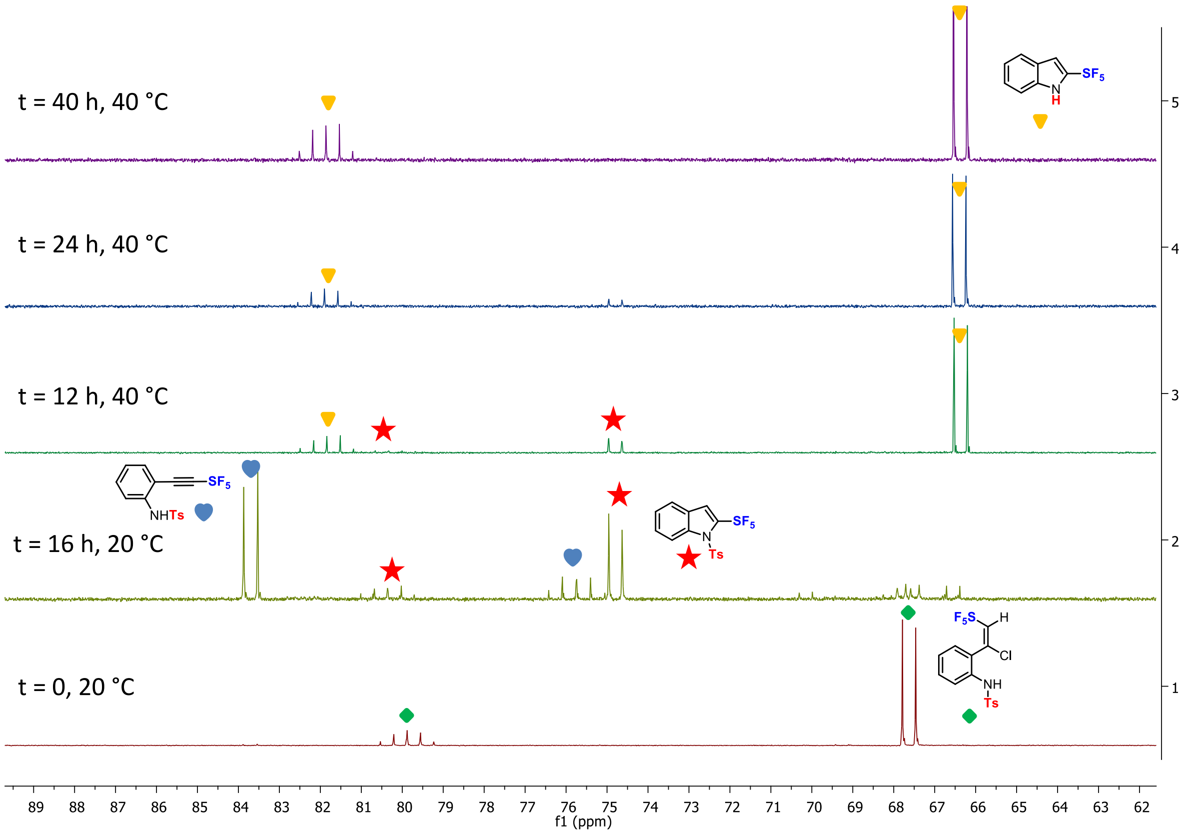
3 Evaluation of protecting groups



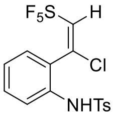
PG =	2 (^{19}F NMR yields)	5 (^{19}F NMR yields)
H	0%	-
Ts	100%	100%
Ms	9%	-
Cbz	49%	0%
Bn	0%	-
Boc	0%	-
Bz	100%	0%

4 Monitoring of the cyclization reaction by ^{19}F NMR





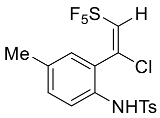
5 Characterization data



(*E*)-*N*-(2-(1-Chloro-2-(pentafluoro-λ6-sulfanyl)vinyl)phenyl)-4-toluenesulfonamide 2a

Prepared according to **GP2** from *N*-(2-ethynylphenyl)-4-toluenesulfonamide **1a** (600 mg, 2.21 mmol, 1 equiv.). No purification needed and **2a** (958 mg, 100 %) was obtained as grey powder.

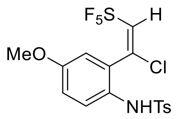
^{1}H-NMR ($CDCl_3$, 500 MHz): δ (ppm) = 2.37 (s, 3H), 6.64 (bs, 1H), 7.02 (quint., *J* = 7.5 Hz, 1H), 7.07-7.15 (m, 2H), 7.25 (d, *J* = 8.2 Hz, 2H), 7.34-7.39 (m, 1H), 7.68 (d, *J* = 8.3 Hz, 1H), 7.75 (d, *J* = 8.3 Hz, 2H); **^{13}C{^{1}H}-NMR ($CDCl_3$, 125 MHz):** δ (ppm) = 21.7, 119.7, 124.2, 125.5, 127.6, 129.1, 129.8, 131.6, 133.7, 136.2, 138.9 (quint., *J* = 6.7 Hz), 142.0 (quint., *J* = 21.5 Hz), 144.6; **^{19}F{^{1}H}-NMR ($CDCl_3$, 471 MHz):** δ (ppm) = 67.6 (d, *J* = 152.8 Hz, 4F), 79.2-80.5 (m, 1F); **IR spectrum (neat)** (cm^{-1}) = 3279, 3102, 1600, 1491, 1407, 1340, 1162, 1091, 931, 860, 844, 714, 663, 559; **HRMS (ESI)**: *m*/*z* calculated for $C_{15}H_{13}ClF_5NO_2S_2^{+\bullet}$ $[M+H]^{+\bullet}$ 434.0069, found 434.0062.



(*E*)-*N*-(2-(1-Chloro-2-(pentafluoro-λ6-sulfanyl)vinyl)-4-methylphenyl)-4-toluenesulfonamide 2b

Prepared according to **GP2** from *N*-(2-ethynyl-4-methylphenyl)-4-toluenesulfonamide **1b** (200 mg, 0.7 mmol, 1 equiv.). No purification needed and **2b** (294 mg, 94 %) was obtained as orange powder.

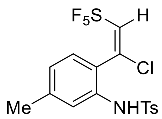
^{1}H-NMR ($CDCl_3$, 500 MHz): δ (ppm) = 2.27 (s, 3H), 2.37 (s, 3H), 6.51 (s, 1H), 6.92 (s, 1H), 6.98 (quint., *J* = 7.4 Hz, 1H), 7.17 (dd, *J* = 8.5 Hz, *J* = 2.1 Hz, 1H), 7.23 (d, *J* = 8.1 Hz, 2H), 7.56 (d, *J* = 8.5 Hz, 1H), 7.73 (d, *J* = 8.3 Hz, 2H); **^{13}C{^{1}H}-NMR ($CDCl_3$, 125 MHz):** δ (ppm) = 20.7, 21.7, 120.4, 125.9, 127.6, 129.3, 129.8, 131.0, 132.2, 134.4, 136.3, 139.1 (quint., *J* = 6.3 Hz), 141.6 (quint., *J* = 21.5 Hz), 144.4; **^{19}F{^{1}H}-NMR ($CDCl_3$, 471 MHz):** δ (ppm) 67.7 (d, *J* = 152.9 Hz, 4F), 79.4-80.7 (m, 1F); **IR spectrum (neat)** (cm^{-1}) = 3272, 1597, 1497, 1398, 1337, 1161, 1092, 961, 886, 863, 719, 662.



(*E*)-*N*-(2-(1-Chloro-2-(pentafluoro-λ^6-sulfanyl)vinyl)-4-methoxyphenyl)-4-toluenesulfonamide 2c

Prepared according to **GP2** from *N*-(2-ethynylphenyl)-4-toluenesulfonamide **1c** (200 mg, 0.66 mmol, 1 equiv.). The NMR shows 77% conv. and the reaction was purified by silica gel column chromatography (Petroleum ether/EtOAc 95/5 to 90/10) affording **2c** (83 mg, 27 %) as an orange oil.

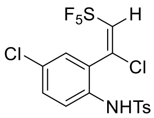
^{1}H-NMR ($CDCl_3$, 500 MHz): δ (ppm) = 2.37 (s, 3H), 3.75 (s, 3H), 6.38 (bs, 1H), 6.65 (d, *J* = 2.6 Hz, 1H), 6.91 (dd, *J* = 9.1 Hz, *J* = 3.0 Hz, 1H), 6.96 (quint., *J* = 7.4 Hz, 1H), 7.23 (d, *J* = 8.0 Hz, 2H), 7.57 (d, *J* = 9.1 Hz, 2H), 7.69 (d, *J* = 8.3 Hz, 2H); **^{13}C{^{1}H}-NMR ($CDCl_3$, 125 MHz):** δ (ppm) = 21.7, 55.7, 114.2, 116.9, 123.7, 126.2, 127.6, 128.5, 129.7, 136.5, 138.8 (quint., *J* = 6.5 Hz), 141.5 (quint., *J* = 21.8 Hz), 144.3, 156.6; **^{19}F{^{1}H}-NMR ($CDCl_3$, 471 MHz):** δ (ppm) = 67.71 (d, *J* = 152.8 Hz, 4F), 79.3-80.6 (m, 1F); **IR spectrum (neat)** (cm^{-1}) = 3264, 2842, 1599, 1494, 1338, 1158, 1091, 959, 840, 644.



(*E*)-*N*-(2-(1-Chloro-2-(pentafluoro-λ^6-sulfanyl)vinyl)-5-methylphenyl)-4-toluenesulfonamide 2d

Prepared according to **GP2** from *N*-(2-ethynyl-5-methylphenyl)-4-toluenesulfonamide **1d** (120 mg, 0.42 mmol, 1 equiv.). No purification needed and **2d** (195 mg, Quant.) was obtained as an orange/yellow solid.

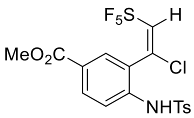
^{1}H-NMR ($CDCl_3$, 500 MHz): δ (ppm) = 2.34 (s, 3H), 2.37 (s, 3H), 6.57 (bs, 1H), 6.91 (dd, *J* = 7.9 Hz, *J* = 1.6 Hz, 1H), 6.95 - 7.02 (m, 2H), 7.25 (d, *J* = 8.1 Hz, 2H), 7.50 (d, *J* = 1.5 Hz, 1H), 7.75 (d, *J* = 8.4 Hz, 2H); **^{13}C{^{1}H}-NMR ($CDCl_3$, 125 MHz):** δ (ppm) = 21.7, 21.8, 120.3, 122.7, 125.1, 127.6, 128.9, 129.8, 133.5, 136.2, 139.2 (quint., *J* = 6.4 Hz), 141.9 (quint., *J* = 21.7 Hz), 142.2, 144.5; **^{19}F{^{1}H}-NMR ($CDCl_3$, 471 MHz):** δ (ppm) = 67.6 (d, *J* = 153.0 Hz, 4F), 79.4-80.7 (m, 1F); **IR spectrum (neat)** (cm^{-1}) = 3287, 3080, 1639, 1504, 1402, 1332, 1167, 1157, 1094, 916, 852, 714, 643.



(*E*)-*N*-(4-Chloro-2-(1-chloro-2-(pentafluoro-λ⁶-sulfanyl)vinyl)phenyl)-4-toluenesulfonamide 2e

Prepared according to **GP2** from *N*-(4-chloro-2-ethynylphenyl)-4-toluenesulfonamide **1e** (300 mg, 1.0 mmol, 1 equiv.). No purification needed and **2e** (358 mg, 78 % conv.) was obtained as orange solid.

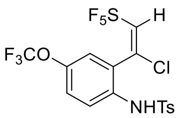
^{1}H-NMR ($CDCl_3$, 500 MHz): δ (ppm) = 2.38 (s, 3H), 6.76 (s, 1H), 7.02 (quint., *J* = 7.4 Hz, 1H), 7.11 (d, *J* = 2.1 Hz, 1H), 7.26 (d, *J* = 8.0 Hz, 2H), 7.33 (dd, *J* = 8.9 Hz, *J* = 2.4 Hz, 1H), 7.66 (d, *J* = 8.9 Hz, 1H), 7.74 (d, *J* = 8.4 Hz, 2H); **^{13}C{^{1}H}-NMR ($CDCl_3$, 125 MHz):** δ (ppm) = 21.7, 121.2, 126.9, 127.6, 128.8, 129.6, 129.9, 131.5, 132.4, 135.8, 137.1 (quint., *J* = 6.4 Hz), 142.6 (quint., *J* = 22.0 Hz), 144.9; **^{19}F{^{1}H}-NMR ($CDCl_3$, 471 MHz):** δ (ppm) = 67.7 (d, *J* = 152.8 Hz, 4F), 78.8-80.1 (m, 1F); **IR spectrum (neat)** (cm^{-1}) = 3265, 3084, 1734, 1598, 1483, 1393, 1338, 1163, 1090, 948, 893, 849, 719, 646, 545.



Methyl (*E*)-3-(1-chloro-2-(pentafluoro-λ⁶-sulfanyl)vinyl)-4-(4-toluenesulfonamido)benzoate 2f

Prepared according to **GP2** from methyl 3-ethynyl-4-(4-toluenesulfonamido)benzoate **1f** (277 mg, 1.7 mmol). The NMR shows 88% conv., the reaction was purified by silica gel column chromatography (petroleum ether/EtOAc 90:10) and **2f** (210 mg, 37 %) was obtained as white powder.

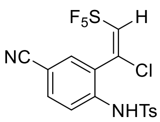
^{1}H-NMR ($CDCl_3$, 500 MHz): δ (ppm) = 2.38 (s, 3H), 3.87 (s, 3H), 6.96 (bs, 1H), 7.08 (quint., *J* = 7.3 Hz, 1H), 7.26 (d, *J* = 8.0 Hz, 2H), 7.74 (d, *J* = 8.8 Hz, 1H), 7.78 (d, *J* = 8.3 Hz, 2H), 7.82 (bs, 1H), 8.02 (dd, *J* = 8.8 Hz, *J* = 1.9 Hz, 1H); **^{13}C{^{1}H}-NMR ($CDCl_3$, 125 MHz):** δ (ppm) = 21.7, 52.5, 118.0, 124.4, 125.6, 127.7, 130.0, 130.8, 132.9, 135.6, 137.6 (quint., *J* = 6.5 Hz), 137.7,142.8 (quint., *J* = 22.0 Hz), 145.1, 165.6. **^{19}F{^{1}H}-NMR ($CDCl_3$, 471 MHz):** δ (ppm) = 67.7 (d, *J* = 152.8 Hz, 4F), 78.7-80.0 (m, 1F); **IR spectrum (neat)** (cm^{-1}) = 3279, 3102, 1600, 1491, 1407, 1340, 1162, 1091, 931, 860, 844, 714, 663, 559.



(*E*)-N-(2-(1-chloro-2-(pentafluoro-λ^6-sulfanyl)vinyl)-4-(trifluoromethoxy)phenyl)-4-methylbenzene-sulfonamide 2g

Prepared according to **GP2** from *N*-[2-ethynyl-4-(trifluoromethoxy)phenyl]-4-methylbenzene-1-sulfonamide **1g** (200 mg, 0.56 mmol, 1 equiv.). No purification needed and **2g** (290 mg, 100 % conv.) was obtained as orange sticky solid.

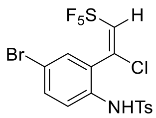
^{1}H-NMR (CDCl$_3$, 500 MHz): δ (ppm) = 2.39 (s, 3H), 6.78 (s, 1H), 7.02 (s, 1H), 7.03 (quint., *J* = 7.2 Hz, 1H), 7.23 (dd, *J* = 9.1 Hz, *J* = 2.3 Hz, 1H), 7.27 (d, *J* = 8.1 Hz, 2H), 7.72 (d, *J* = 9.1 Hz, 1H), 7.75 (d, *J* = 8.3 Hz, 2H); **^{13}C{^{1}H}-NMR (CDCl$_3$, 125 MHz):** δ (ppm) = 21.7, 120.4 (q, *J* = 258.6 Hz), 121.2, 122.0, 124.1, 126.6, 127.6, 130.0, 132.5, 135.9, 136.9 (quint., *J* = 6.3 Hz), 142.8 (quint., *J* = 22.1 Hz), 144.9 (q, *J* = 2.1 Hz), 144.9; **^{19}F{^{1}H}-NMR (CDCl$_3$, 471 MHz):** δ (ppm) = -58.4 (s, 3F), 67.6 (d, *J* = 152.6 Hz, 4F), 78.6-79.9 (m, 1F); **IR spectrum (neat)** (cm^{-1}) = 3272, 3086, 1738, 1598, 1494, 1403, 1253, 1155, 1091, 848, 647, 600, 564, 545.



(*E*)-N-(2-(1-chloro-2-(pentafluoro-λ^6-sulfanyl)vinyl)-4-cyanophenyl)-4-methylbenzenesulfonamide 2h

Prepared according to **GP2** from N-(4-cyano-2-ethynylphenyl)-4-methylbenzenesulfonamide **1h** (170 mg, 0.57 mmol, 1 equiv.). The NMR shows 78% conv., the reaction was purified by silica gel column chromatography (petroleum ether/EtOAc 95:5) and **2g** (121 mg, 46%) was obtained as white powder.

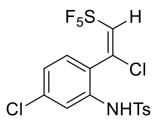
^{1}H-NMR (CDCl$_3$, 500 MHz): δ (ppm) = 2.40 (s, 3H), 7.09 (quint., *J* = 7.3 Hz, 1H), 7.30 (d, *J* = 8.0 Hz, 2H), 7.42 (s, 1H), 7.62 (dd, *J* = 8.8 Hz, *J* =2.0 Hz, 1H), 7.78 (d, *J* = 8.2 Hz, 2H), 7.79 (d, *J* = 8.7 Hz, 1H); **^{13}C{^{1}H}-NMR (CDCl$_3$, 125 MHz):** δ (ppm) = 21.8, 107.4, 117.5, 118.6, 125.2, 127.6, 130.2, 133.0, 135.2, 135.3, 136.0 (quint., *J* = 6.1 Hz), 137.9, 143.6 (quint., *J* = 22.3 Hz), 145.5; **^{19}F{^{1}H}-NMR (CDCl$_3$, 471 MHz):** δ (ppm) 67.6 (d, *J* = 152.8 Hz, 4F), 78.5-79.8 (m, 1F); **IR spectrum (neat)** (cm^{-1}) = 3216, 3039, 2242, 1649, 1603, 1490, 1402, 1170, 1155, 1090, 967, 879, 846, 814, 721, 666, 569, 547.



(*E*)-*N*-(4-Bromo-2-(1-chloro-2-(pentafluoro-λ^{6}-sulfanyl)vinyl)phenyl)-4-toluenesulfonamide 2i

Prepared according to **GP2** from *N*-(4-bromo-2-ethynylphenyl)-4-toluenesulfonamide **1i** (150 mg, 0.43 mmol, 1 equiv.). No purification needed and **2i** (220 mg, 100 %) was obtained as yellow pale solid.

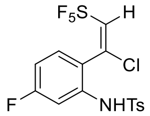
^{1}H-NMR ($CDCl_3$, 500 MHz): δ (ppm) = 2.39 (s, 3H), 6.59 (s, 1H), 7.02 (quint., *J* = 7.3 Hz, 1H), 7.25 (s, 1H), 7.26 (d, *J* = 8.0 Hz, 2H), 7.48 (dd, *J* = 8.9 Hz, *J* = 2.2 Hz, 1H), 7.60 (d, *J* = 8.9 Hz, 1H), 7.73 (d, *J* = 8.3 Hz, 2H); **^{13}C{^{1}H}-NMR ($CDCl_3$, 125 MHz):** δ (ppm) = 21.7, 116.9, 121.3, 127.0, 127.6, 130.0, 131.6, 132.9, 134.5, 135.8, 137.1 (quint., *J* = 6.2 Hz), 142.6 (quint., *J* = 22.0 Hz), 144.9; **^{19}F{^{1}H}-NMR ($CDCl_3$, 471 MHz):** δ (ppm) = 67.7 (d, *J* = 152.8 Hz, 4F), 78.7-80.0 (m, 1F); **IR spectrum (neat)** (cm^{-1}) = 3264, 2924, 1639, 1484, 1389, 1164, 1090, 942, 848, 811, 719, 646.



(*E*)-*N*-(5-Chloro-2-(1-chloro-2-(pentafluoro-λ^{6}-sulfanyl)vinyl)phenyl)-4-toluenesulfonamide 2j

Prepared according to **GP2** from *N*-(5-chloro-2-ethynylphenyl)-4-toluenesulfonamide **1j** (250 mg, 0.82 mmol, 1 equiv.) in DCM instead of EtOAc. The NMR shows 90% conv., no purification needed and **2j** (382 mg, 90 %) was obtained as an orange/yellow solid.

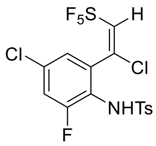
^{1}H-NMR ($CDCl_3$, 500 MHz): δ (ppm) = 2.39 (s, 3H), 6.78 (bs, 1H), 7.02 (quint., *J* = 7.4 Hz, 1H), 7.05-7.06 (m, 2H), 7.28 (d, *J* = 8.2 Hz, 2H), 7.73 (d, *J* = 1.7 Hz, 1H), 7.77 (d, *J* = 8.4 Hz, 2H); **^{13}C{^{1}H}-NMR ($CDCl_3$, 125 MHz):** δ (ppm) = 21.7, 119.6, 123.5, 124.3, 127.7, 130.0, 130.1, 135.0, 135.8, 137.7, 137.8 (quint., *J* = 6.5 Hz), 142.6 (quint., *J* = 21.9 Hz), 145.0; **^{19}F{^{1}H}-NMR ($CDCl_3$, 471 MHz):** δ (ppm) = 67.0 (d, *J* = 152.4 Hz, 4F), 79.9 (quint., *J* = 152.8 Hz, 1F); **IR spectrum (neat)** (cm^{-1}) = 3282, 3084, 1736, 1594, 1487, 1387, 1335, 1163, 1086, 940, 847, 666, 641, 541.



(*E*)-*N*-(2-(1-Chloro-2-(pentafluoro-λ^6-sulfanyl)vinyl)-5-fluorophenyl)-4-toluenesulfonamide 2k

Prepared according to **GP2** from *N*-(2-ethynyl-5-fluorophenyl)-4-toluenesulfonamide **1k** (300 mg, 1.0 mmol, 1 equiv.). The NMR shows 100% conv., no purification needed and **2k** (369 mg, 79 %) was obtained as an orange solid.

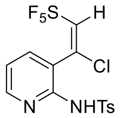
^{1}H-NMR ($CDCl_3$, 500 MHz): δ (ppm) = 2.39 (s, 3H), 6.73 (bs, 1H), 6.79 (td, *J* = 8.2 Hz, *J* = 2.4 Hz, 1H), 7.03 (quint., *J* = 7.3 Hz, 1H), 7.10 (dd, *J* = 8.4 Hz, *J* = 6.1 Hz, 1H), 7.28 (d, *J* = 8.5 Hz, 2H), 7.46 (dd, *J* = 10.6 Hz, *J* = 2.4 Hz, 1H), 7.77 (d, *J* = 8.4 Hz, 2H); **^{13}C{^{1}H}-NMR ($CDCl_3$, 125 MHz):** δ (ppm) = 21.7, 106.9 (d, *J* = 27.6 Hz), 111.2 (d, *J* = 22.6 Hz), 120.8 (d, *J* = 3.6 Hz), 127.6, 130.0, 130.8 (d, *J* = 10.0 Hz), 135.7, 135.7 (d, *J* = 11.2 Hz), 138.0 (quint., *J* = 6.4 Hz), 142.7 (quint., *J* = 22.2 Hz), 145.0, 164.2 (d, *J* = 250.9 Hz); **^{19}F{^{1}H}-NMR ($CDCl_3$, 471 MHz):** δ (ppm) = - 106.1 (s, 1F), 67.50 (d, *J* = 152.8 Hz, 4F), 79.0-80.3 (m, 1F); **IR spectrum (neat)** (cm^{-1}) = 3261, 3097, 1594, 1494, 1422, 1336, 1165, 919, 841, 717, 640, 558.



(*E*)-N-(4-chloro-2-(1-chloro-2-(pentafluoro-λ^6-sulfanyl)vinyl)-6-fluorophenyl)-4-methylbenzene-sulfonamide 2l

Prepared according to **GP2** from *N*-(4-chloro-2-ethynyl-6-fluorophenyl)-4-methylbenzene-1-sulfonamide **1l** (200 mg, 0.62 mmol, 1 equiv.). The NMR shows 16% conv., the reaction was purified by silica gel column chromatography (petroleum ether/EtOAc 90:10) and **2l** (20 mg, 7 %) was obtained as orange sticky solid.

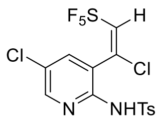
^{1}H-NMR ($CDCl_3$, 500 MHz): δ (ppm) = 2.44 (s, 3H), 6.14 (s, 1H), 7.04 (quint., *J* = 7.6 Hz, 1H), 7.12-7.16 (m, 2H), 7.30 (d, *J* = 8.0 Hz, 2H), 7.77 (d, *J* = 8.2 Hz, 2H); **^{13}C{^{1}H}-NMR ($CDCl_3$, 125 MHz):** δ (ppm) = 21.8, 119.0 (d, *J* = 24.1 Hz), 120.8 (d, *J* = 15.4 Hz), 125.3, 127.5 (d, *J* = 1.3 Hz), 129.7, 133.8 (d, *J* = 10.3 Hz), 135.8 (d, *J* = 1.8 Hz), 137.0-137.2 (m), 137.2 (d, *J* = 1.2 Hz), 141.5 (quint., *J* = 22.3 Hz), 144.4, 157.8 (d, *J* = 255.2 Hz); **^{19}F{^{1}H}-NMR ($CDCl_3$, 471 MHz):** δ (ppm) = -113.4 (s, 1F), 68.0 (d, *J* = 152.7 Hz, 4F), 79.6-80.9 (m, 1F). **IR spectrum (neat)** (cm^{-1}) = 3282, 3084, 1736, 1598, 1483, 1393, 1338, 1163, 1090, 948, 893, 847, 719, 646, 545.



(*E*)-N-(3-(1-chloro-2-(pentafluoro-λ^6-sulfanyl)vinyl)pyridin-2-yl)-4-methylbenzenesulfonamide 2o

Prepared according to **GP2** from *N*-(3-ethynylpyridin-2-yl)-4-methylbenzenesulfonamide **1o** (170 mg, 0.62 mmol, 1 equiv.) in DCM instead of EtOAc. The NMR shows 44% conv., the reaction was purified by silica gel column chromatography (petroleum ether/EtOAc 90:10) and **2o** (40 mg, 15 %) was obtained as pale-yellow sticky solid.

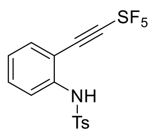
^{1}H-NMR ($CDCl_3$, 500 MHz): δ (ppm) = 2.42 (s, 3H), 7.08 (quint., *J* = 7.3 Hz, 1H), 7.30 (d, *J* = 8.2 Hz, 2H), 7.44 (d, *J* = 2.1 Hz, 1H), 7.97 (d, *J* = 8.3 Hz, 2H), 8.20 (s, 1H); **^{13}C{^{1}H}-NMR ($CDCl_3$, 125 MHz):** δ (ppm) = 21.8, 117.1, 128.5, 129.5, 135.3 (quint., *J* = 6.1 Hz), 136.6, 137.3, 142.8, 143.3 (quint., *J* = 21.5 Hz), 144.6, 145.4, 148.4; **^{19}F{^{1}H}-NMR ($CDCl_3$, 471 MHz):** δ (ppm) = 67.6 (d, *J* = 152.7 Hz), 79.5 (quint., *J* = 152.9 Hz); **IR spectrum (neat)** (cm^{-1}) = 3246, 3089, 2925, 1560, 1443, 1338, 1163, 1138, 1089, 958, 902, 841, 723, 646, 599, 560.



(*E*)-N-(5-chloro-3-(1-chloro-2-(pentafluoro-λ^6-sulfanyl)vinyl)pyridin-2-yl)-4-methylbenzene-sulfonamide 2p

Prepared according to **GP2** from *N*-(5-chloro-3-ethynylpyridin-2-yl)-4-methylbenzenesulfonamide **1p** (205.6 mg, 0.67 mmol, 1 equiv.) in DCM instead of EtOAc. The NMR shows 33% conv., the reaction was purified by silica gel column chromatography (petroleum ether/EtOAc 90:10) and **2p** (41 mg, 13 %) was obtained as pale yellow solid.

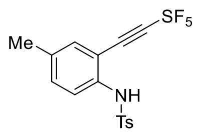
^{1}H-NMR ($CDCl_3$, 500 MHz): δ (ppm) = 2.42 (s, 3H), 7.10 (quint., *J* = 7.2 Hz, 1H), 7.30 (d, *J* = 8.1 Hz, 2H), 7.44 (d, *J* = 2.1 Hz, 1H), 7.96 (d, *J* = 8.3 Hz, 2H), 8.21 (d, *J* = 2.1 Hz, 1H); **^{13}C{^{1}H}-NMR ($CDCl_3$, 125 MHz):** δ (ppm) = 21.8, 119.0, 128.7, 129.5, 135.3 (quint., *J* = 6.4 Hz), 136.4, 137.1, 143.4 (quint., *J* = 22.8 Hz), 144.7, 145.2, 148.6, 153.2; **^{19}F{^{1}H}-NMR ($CDCl_3$, 471 MHz):** δ (ppm) = 67.6 (d, *J* = 152.7 Hz), , 79.4 (quint., *J* = 154.0 Hz); **IR spectrum (neat)** (cm^{-1}) = 3252, 1687, 1560, 1445, 1339, 1167, 1140, 1090, 962, 905, 846, 724, 645, 564.



N-(2-((Pentafluoro-λ^6-sulfanyl)ethynyl)phenyl)-4-toluenesulfonamide 3a

Prepared according to **GP4** from (*E*)-*N*-(2-(1-chloro-2-(pentafluoro-λ^6-sulfanyl)vinyl)phenyl)-4-toluenesulfonamide **2a** (91.1 mg, 0.21 mmol). No purification needed and **3a** (84 mg, quant. yield) was obtained as a yellow powder.

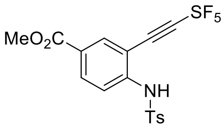
^{1}H-NMR ($CDCl_3$, 500 MHz): δ (ppm) = 2.38 (s, 3H), 6.77 (bs, 1H), 7.16 (td, *J* = 7.7 Hz, *J* = 1.1 Hz, 1H), 7.21-7.23 (m, 2H), 7.41 (dd, *J* = 7.9 Hz, *J* = 1.6 Hz, 1H), 7.48 (ddd, *J* = 8.5 Hz, *J* = 7.5 Hz, *J* = 1.6 Hz, 1H), 7.59-7.61 (m, 2H), 7.71 (dd, *J* = 8.3 Hz, *J* = 1.1 Hz, 1H); **^{13}C{^{1}H}-NMR ($CDCl_3$, 125 MHz):** δ (ppm) = 21.7, 73.4 (quint., *J* = 8.0 Hz), 95.1 (quint., *J* = 42.2 Hz), 109.8, 122.8, 125.6, 127.3, 130.0, 132.9, 133.6, 135.7, 139.1, 144.7; **^{19}F{^{1}H}-NMR ($CDCl_3$, 471 MHz):** δ (ppm) = 74.8-76.2 (m, 1F), 83.7 (d, *J* = 153.2 Hz, 4F); **IR spectrum (neat)** (cm^{-1}) = 3251, 2924, 2222, 1599, 1488, 1332, 1170, 1091, 868, 787, 758, 668; **HRMS (ESI)**: *m/z* calculated for $C_{15}H_{13}F_5NO_2S_2^{+\bullet}$ $[M+H]^{+\bullet}$ 398.0302, found 398.0281.



N-(4-Methyl-2-((pentafluoro-λ^6-sulfanyl)ethynyl)phenyl)-4-toluenesulfonamide 3b

Prepared according to **GP4** from (*E*)-*N*-(2-(1-chloro-2-(pentafluoro-λ^6-sulfanyl)vinyl)-4-methylphenyl)-4-toluenesulfonamide **2b** (100 mg, 0.22 mmol). No purification needed and **3b** (71 mg, 77 %) was obtained as a sticky brown powder.

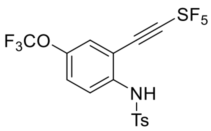
^{1}H-NMR ($CDCl_3$, 400 MHz): δ (ppm) = 2.29 (s, 3H), 2.38 (s, 3H), 6.62 (bs, 1H), 7.20-7.22 (m, 3H), 7.29 (dd, *J* = 8.4 Hz, *J* = 2.1 Hz, 1H), 7.57 (d, *J* = 8.3 Hz, 2H), 7.60 (d, *J* = 8.4 Hz, 1H); **^{13}C{^{1}H}-NMR ($CDCl_3$, 125 MHz):** δ (ppm) = 20.7, 21.7, 73.7 (quint., *J* = 7.9 Hz), 94.6 (quint., *J* = 44.1 Hz), 110.2, 123.6, 127.3, 129.9, 133.7, 133.8, 135.7, 135.9, 136.5, 144.5; **^{19}F{^{1}H}-NMR ($CDCl_3$, 471 MHz):** δ (ppm) = 75.1-76.5 (m, 1F), 93.5-83.9 (m, 4F); **IR spectrum (neat)** (cm^{-1}) = 3246, 2927, 2210, 1600, 1495, 1394, 1345, 1169, 1092, 957, 874, 677, 582, 550, 525; **HRMS (ESI)**: *m/z* calculated for $C_{16}H_{14}F_5NO_2S_2^{+\bullet}$ $[M]^{+\bullet}$ 4110381, found 411.0384.



methyl 4-((4-methylphenyl)sulfonamido)-3-((pentafluoro- λ6-sulfanyl)ethynyl)benzoate 3f

Prepared according to **GP4** from methyl (*E*)-3-(1-chloro-2-(pentafluoro-λ6-sulfanyl)vinyl)-4-((4-methylphenyl)sulfonamido)benzoate **2g** (52 mg, 0.106 mmol). No purification needed and **3g** (47 mg, 98 %) was obtained as an orange powder.

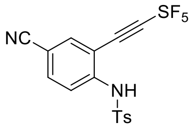
^{1}H-NMR ($CDCl_3$, 500 MHz): δ (ppm) = 2.39 (s, 3H), 3.90 (s, 3H), 7.08 (bs, 1H), 7.24-7.27 (m, 2H), 7.67 (d, *J* = 8.4 Hz, 2H), 7.74 (dd, *J* = 8.6 Hz, *J* = 0.7 H, 1H), 8.07-8.10 (m, 2H); **^{13}C{^{1}H}-NMR ($CDCl_3$, 125 MHz):** δ (ppm) = 21.7, 52.7, 72.3 (quint., *J* = 8.0 Hz), 95.8 (quint., *J* = 44.6 Hz), 108.5, 120.3, 126.8, 127.3, 130.2, 133.9, 135.3, 135.5, 142.8, 145.2, 165.1; **^{19}F{^{1}H}-NMR ($CDCl_3$, 471 MHz):** δ (ppm) = 73.9-75.4 (m, 1F), 83.6 (d, *J* = 161.2 Hz, 4F); **IR spectrum (neat)** (cm^{-1}) = 3260, 2959, 2215, 1596, 1582, 1500, 1435, 1303, 1279, 0188, 940, 870, 843, 665, 580, 549; **HRMS (ESI)**: *m/z* calculated for $C_{17}H_{14}F_5NO_4S_2^{+\bullet}$ $[M]^{+\bullet}$ 456.0357, found 456.0393.



4-methyl-N-(2-((pentafluoro-λ6-sulfanyl)ethynyl)-4-(trifluoromethoxy)phenyl)benzenesulfonamide 3g

Prepared according to **GP4** from *N*-{2-[(E)-1-chloro-2-(pentafluoro-λ6-sulfanyl)ethenyl]-4-(trifluoromethoxy)phenyl}-4-methylbenzene-1-sulfonamide **2g** (80 mg, 0.15 mmol). No purification needed and **3g** (73 mg, 100%) was obtained as brown sticky powder.

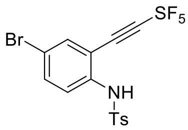
^{1}H-NMR ($CDCl_3$, 500 MHz): δ (ppm) = 2.40 (s, 3H), 6.84 (bs, 1H), 7.25 (d, *J* = 8.0 Hz, 2H), 7.26-7.28 (m, 1H), 7.34 (dd, *J* = 9.0 Hz, *J* = 2.7 Hz, 1H), 7.60 (d, *J* = 8.4 Hz, 2H), 7.74 (d, *J* = 9.1 Hz, 1H); **^{13}C{^{1}H}-NMR ($CDCl_3$, 125 MHz):** δ (ppm) = 21.7, 71.7 (quint. *J* = 8.6 Hz), 95.5 (quint. *J* = 43.5 Hz), 111.3, 120.3 (q, *J* = 258.9 Hz), 124.6, 125.6, 125.7, 127.2, 130.1, 135.5, 137.8, 145.0, 146.0 (q, *J* = 2.3 Hz); **^{19}F{^{1}H}-NMR ($CDCl_3$, 471 MHz):** δ (ppm) = -58.2 (s, 3F), 73.7-75.0 (m, 1F), 83.4 (d, *J* = 161.5 Hz); **IR spectrum (neat)** (cm^{-1}) = 3255, 2222, 1654, 1598, 1401, 1342, 1254, 1219, 1160, 988, 851, 813, 770, 663, 578, 544; **HRMS (ESI)**: *m/z* calculated for $C_{16}H_{11}F_8NO_3S_2^{+\bullet}$ $[M]^{+\bullet}$ 481.0047, found 481.0067.



N-(4-cyano-2-((pentafluoro- λ^6-sulfanyl)ethynyl)phenyl)-4-methylbenzenesulfonamide 3h

Prepared according to **GP4** from N-{2-[(E)-1-chloro-2-(pentafluoro-λ^6-sulfanyl)ethenyl]-4-cyanophenyl}-4-methylbenzene-1-sulfonamide **2h** (60 mg, 0.13 mmol). No purification needed and **3h** (57 mg, quant. yield) was obtained as brown oil.

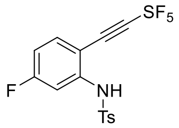
^{1}H-NMR ($CDCl_3$, 500 MHz): δ (ppm) = 2.41 (s, 3H), 7.27 (bs, 1H), 7.29 (d, *J* = 8.2 H, 2H), 7.67-7.72 (m, 3H), 7.73 (d, *J* = 1.9 Hz, 1H), 7.78 (d, *J* = 8.8 Hz, 1H); **^{13}C{^{1}H}-NMR ($CDCl_3$, 125 MHz):** δ (ppm) = 21.8, 70.8 (quint., *J* = 7.5 Hz), 96.8 (quint., *J* = 42.9 Hz), 108.7, 109.2, 116.9, 120.6, 127.3, 130.3, 135.4, 135.9, 137.4, 142.9, 145.5; **^{19}F{^{1}H}-NMR ($CDCl_3$, 471 MHz):** δ (ppm) = 73.7 (quint., *J* = 163.6 Hz, 1F), 83.5 (d, *J* = 161.5 Hz, 4F); **IR spectrum (neat)** (cm^{-1}) = 3181, 2961, 2246, 2217, 1607, 1494, 1402, 1350, 1263, 1166, 1090, 963, 880, 848, 842, 661, 545; **HRMS (ESI)**: *m/z* calculated for $C_{16}H_{11}F_5N_2O_2S_2^{+\bullet}$ $[M]^{+\bullet}$ 422.0182, found 422.189.



N-(4-bromo-2-((pentafluoro- λ^6-sulfanyl)ethynyl)phenyl)-4-methylbenzenesulfonamide 3i

Prepared according to **GP4** from N-{4-bromo-2-[(E)-1-chloro-2-(pentafluoro-λ^6-sulfanyl)ethenyl]phenyl}-4-methylbenzene-1-sulfonamide **2i** (18 mg, 0.035 mmol). No purification needed and **3i** (17 mg, quant. yield) was obtained as brown solid.

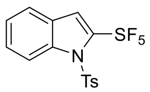
^{1}H-NMR ($CDCl_3$, 500 MHz): δ (ppm) = 2.39 (s, 3H), 6.77 (bs, 1H), 7.24 (d, *J* = 8.1 Hz, 2H), 7.54 (d, *J* = 1.6 Hz, 1H), 7.58 -7.61 (m, 4H); **^{13}C{^{1}H}-NMR ($CDCl_3$, 125 MHz):** δ (ppm) = 21.7, 71.8 (quint., *J* = 7.2 Hz), 95.6 (quint., *J* = 45.2 Hz), 111.7, 118.4, 124.4, 127.2, 130.1, 135.5, 135.8, 135.9, 138.2, 145.0; **^{19}F{^{1}H}-NMR ($CDCl_3$, 471 MHz):** δ (ppm) = 73.4-76.1 (m, 1F), 83.5 (d, *J* = 161.1 Hz, 4F); **IR spectrum (neat)** (cm^{-1}) = 2962, 2222, 1598, 1482, 1387, 1338, 1165, 1089, 872, 811, 663, 601, 579, 542; **HRMS (ESI)**: *m/z* calculated for $C_{15}H_{12}BrF_5NO_2S_2^{+\bullet}$ $[M+H]^{+\bullet}$ 475.9408, found 475.9384.



N-(5-Fluoro-2-((pentafluoro-λ^6-sulfanyl)ethynyl)phenyl)-4-toluenesulfonamide 3k

Prepared according to **GP4** from (*E*)-*N*-(2-(1-chloro-2-(pentafluoro-λ^6-sulfanyl)vinyl)-5-fluorophenyl)-4-toluenesulfonamide **2k** (100 mg, 0.22 mmol). No purification needed and **3k** (86.4 mg, 94 %) was obtained as a brown powder.

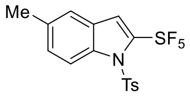
^{1}H-NMR (CDCl$_3$, 400 MHz): δ (ppm) = 2.40 (s, 3H), 6.83 (bs, 1H), 6.85 (ddd, *J* = 8.6 Hz, *J* = 7.8 Hz, *J* = 2.5 Hz, 1H), 7.26 (d, *J* = 8.1 Hz, 2H), 7.41 (dd, *J* = 8.7 Hz, *J* = 5.9 Hz, 1H), 7.45 (dd, *J* = 10.1 Hz, *J* = 2.5 Hz, 1H), 7.66 (d, *J* = 8.4 Hz, 2H); **^{13}C{^{1}H}-NMR (CDCl$_3$, 125 MHz):** δ (ppm) = 21.7, 72.7 (quint., *J* = 7.4 Hz), 95.4 (quint., *J* = 42.8 Hz), 104.9, 109.4 (d, *J* = 27.1 Hz), 113.0 (d, *J* = 22.8 Hz), 127.3, 130.2, 135.4 (d, *J* = 10.2 Hz), 135.5, 141.4 (d, *J* = 12.4 Hz), 145.1, 164.9 (d, *J* = 255.3 Hz); **^{19}F{^{1}H}-NMR (CDCl$_3$, 471 MHz):** δ (ppm) = -101.3 (1F), 74.6-75.9 (m, 1F), 83.6-84.0 (m, 4F); **IR spectrum (neat)** (cm^{-1}) = 3211, 2222, 1607, 1500, 1335, 1174, 1159, 1090, 986, 872, 795, 583; **HRMS (ESI)**: *m/z* calculated for $C_{15}H_{11}F_6NO_2S_2^{+\bullet}$ $[M]^{+\bullet}$ 415.0130, found 415.0146.



N-Tosyl-2-(pentafluoro-λ^6-sulfanyl)-1*H*-indole 4a

Prepared according to **GP5** from 4-methyl-N-(2-[2-(pentafluoro-λ^6-sulfanyl)ethynyl]phenyl)benzene-1-sulfonamide **3a** (20 mg, 0.05 mmol). The reaction afforded a mixture of *N*-Ts and *N*-H-indole in a ratio 96:4 **4a**:**5a**. It was purified by silica gel column chromatography (Petroleum ether/EtOAc, 90/10 to 80/20) affording **4a** (16 mg, 80%) as a slightly yellow solid.

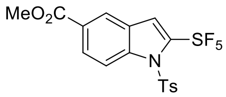
^{1}H-NMR (CDCl$_3$, 500 MHz): δ (ppm) = 2.31 (s, 3H), 7.12 (d, *J* = 8.2 Hz, 2H), 7.31-7.35 (m, 2H), 7.49-7.54 (m, 4H), 8.35 (d, *J* = 8.6 Hz, 1H); **^{13}C{^{1}H}-NMR (CDCl$_3$, 125 MHz):** δ (ppm) = 21.7, 117.9, 120.6 (quint., *J* = 6.1 Hz), 122.9, 125.3, 126.7, 127.0, 128.5, 129.7, 134.6, 138.8, 145.4, 148.2 (quint., *J* = 25.3 Hz); **^{19}F{^{1}H}-NMR (CDCl$_3$, 471 MHz):** δ (ppm) = 74.8 (d, *J* = 152.4 Hz, 4F), 79.7-81.0 (m, 1F); **IR spectrum (neat)** (cm^{-1}) = 2930, 1600, 1387, 1180, 853, 840, 761, 652, 564; **HRMS (ESI)**: *m/z* calculated for $C_{15}H_{13}F_5NO_2S_2^{+\bullet}$ $[M+H]^{+\bullet}$ 398.0302, found 398.0315.



N-Tosyl-5-methyl-2-(pentafluoro-λ⁶-sulfanyl)-1H-indole 4b

Prepared according to **GP5** from 4-methyl-*N*-(4-methyl-2-[2-(pentafluoro-λ⁶-sulfanyl)ethynyl]phenyl)benzene-1-sulfonamide **3b** (30 mg, 0.07 mmol). The reaction afforded a mixture of *N*-Ts and *N*-H-indole in a ratio 95:5 **4b**:**5b**. It was purified by preparative TLC (Petroleum ether/EtOAc 95/5) affording **4b** (21 mg, 70%) as a white powder.

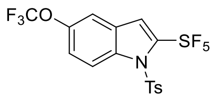
^{1}H-NMR ($CDCl_3$, 500 MHz): δ (ppm) = 2.31 (s, 3H), 2.41 (s, 3H), 7.11 (d, *J* = 8.1 Hz, 2H), 7.26 (s, 1H), 7.29 (d, *J* = 0.6 Hz, 1H), 7.31 (dd, *J* = 8.8 Hz, *J* = 1.5 Hz, 1H), 7.50 (d, *J* = 8.4 Hz, 2H), 8.21 (d, *J* = 8.7 Hz, 1H); **^{13}C{^{1}H}-NMR ($CDCl_3$, 125 MHz):** δ (ppm) = 21.3, 21.7, 117.6, 120.6 (quint., *J* = 5.0 Hz), 122.5, 126.9, 127.0, 129.6, 130.0, 134.5, 135.2, 137.0, 145.3, 148.1 (quint., *J* = 25.5 Hz); **^{19}F{^{1}H}-NMR ($CDCl_3$, 471 MHz):** 74.7 (d, *J* = 153.3 Hz, 4F), 79.9-81.2 (m, 1F); **IR spectrum (neat)** (cm^{-1}) = 2925, 2850, 1593, 1385, 1178, 1152, 1105, 1084, 976, 843, 786, 671, 575, 542, 463; **HRMS (ESI)**: *m/z* calculated for $C_{16}H_{15}F_5NO_2S_2^{+\bullet}$ $[M+H]^{+\bullet}$ 412.0459, found 412.0449.



Methyl N-tosyl-2-(pentafluoro-λ⁶-sulfanyl)-1H-indole-5-carboxylate 4f

Prepared according to **GP5** from methyl 4-(4-methylbenzenesulfonamido)-3-[2-(pentafluoro-λ⁶-sulfanyl)ethynyl]benzoate **3f** (43 mg, 0.094 mmol). The reaction afforded a mixture of *N*-Ts and *N*-indole in a ratio 71:29 **4f**:**5f**. It was purified by silica gel column chromatography affording **4f** (18 mg, 42%) as a colorless oil.

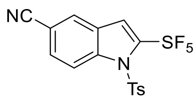
^{1}H-NMR ($CDCl_3$, 500 MHz): δ (ppm) = 2.32 (s, 3H), 3.94 (s, 3H), 7.15 (d, *J* = 8.1 Hz, 2H), 7.39 (s, 1H), 7.54 (d, *J* = 8.5 Hz, 2H), 8.17 (dd, *J* = 9.0 Hz, 1.8 Hz, 1H), 8.26 (d, *J* = 1.3 Hz, 1H), 8.41 (d, *J* = 9.0 Hz, 1H); **^{13}C{^{1}H}-NMR ($CDCl_3$, 125 MHz):** δ (ppm) = 21.8, 52.6, 117.6, 119.8 (quint., *J* = 6.5 Hz), 125.0, 126.3, 127.0, 127.3, 129.2, 129.9, 134.6, 141.0, 145.9, 148.7-149.5 (m), 166.5; **^{19}F{^{1}H}-NMR ($CDCl_3$, 471 MHz):** δ (ppm) = 74.7-75.1 (m, 4F), 78.5-80.1 (m, 1F); **IR spectrum (neat)** (cm^{-1}) = 2958, 1720, 1614, 1597, 1432, 1596, 1322, 1279, 1263, 1130, 1089, 993, 837, 785, 665, 570, 541; **HRMS (ESI)**: *m/z* calculated for $C_{17}H_{15}F_5NO_4S_2^{+\bullet}$ $[M+H]^{+\bullet}$ 456.0357, found 456.0383.



N-Tosyl-5-(trifluoromethoxy)-2-(pentafluoro-λ6-sulfanyl)-1H-indole 4g

Prepared according to **GP5** from 4-methyl-*N*-(2-((pentafluoro-λ6-sulfaneyl)ethynyl)-4-(trifluoromethoxy)phenyl)benzenesulfonamide **3g** (38.5 mg, 0.08 mmol). The reaction afforded a mixture of *N*-H and *N*-Ts-indole in a ratio 79:21 **4g**:**5g** of. It was purified by preparative TLC (Petroleum ether/EtOAc 90/10) affording **4g** (25 mg, 65%) as a white powder.

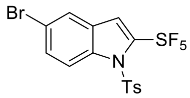
^{1}H-NMR ($CDCl_3$, 500 MHz): δ (ppm) = 2.34 (s, 3H), 7.17 (d, *J* = 8.1 Hz, 2H), 7.33 (s, 1H), 7.36 (dd, *J* = 9.3 Hz, *J* = 1.8 Hz, 1H), 7.40 (s, 1H), 7.53 (d, *J* = 8.5 Hz, 2H), 8.40 (d, *J* = 9.3 Hz, 1H); **^{13}C{^{1}H}-NMR ($CDCl_3$, 125 MHz):** δ (ppm) = 21.8, 114.6, 119.2 (quint., *J* = 6.3 Hz), 119.3, 120.6 (q, *J* = 258.0 Hz), 121.8, 127.0, 127.2, 129.9, 134.6, 136.6, 145.9, 146.4, 149.5 (quint., *J* = 24.9 Hz); **^{19}F{^{1}H}-NMR ($CDCl_3$, 471 MHz):** δ (ppm) = -58.1 (s, 3F), 74.5-74.9 (m, 4F), 78.6-79.9 (m, 1F); **IR spectrum (neat)** (cm^{-1}) = 3145, 2925, 1596, 1531, 1449, 1392, 1256, 1221, 1150, 1122, 1087, 1001, 851, 799, 781, 741, 668, 572, 542; **HRMS (ESI)**: *m/z* calculated for $C_{16}H_{12}F_8NO_3S_2^{+\bullet}$ $[M+H]^{+\bullet}$ 482.0125, found 482.0137.



N-tosyl-2-(pentafluoro-λ6-sulfanyl)-1H-indole-5-carbonitrile 4h

Prepared according to **GP5** from *N*-(4-cyano-2-((pentafluoro-λ6-sulfaneyl)ethynyl)phenyl)-4-methylbenzenesulfonamide **3h** (38 mg, 0.09 mmol). The reaction afforded a mixture of *N*-Ts and *N*-indole in a ratio 50:50 **4h**:**5h**. It was purified by silica gel column chromatography affording **4h** (8 mg, 21%) as a colorless oil.

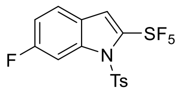
^{1}H-NMR ($CDCl_3$, 500 MHz): δ (ppm) = 2.35 (s, 3H), 7.20 (d, *J* = 8.1 Hz, 2H), 7.38 (s, 1H), 7.55 (d, *J* = 8.6 Hz, 2H), 7.74 (d, *J* = 9.0 Hz, *J* = 1.7 Hz, 1H), 7.91 (d, *J* = 1.7Hz, 1H), 8.50 (d, *J* = 8.9 Hz, 1H); **^{13}C{^{1}H}-NMR ($CDCl_3$, 125 MHz):** δ (ppm) = 21.8, 109.1, 118.1 (quint., *J* = 6.1 Hz), 118.4, 118.7, 126.4, 127.0, 127.7, 130.1, 130.7, 134.6, 140.0, 146.3, 149.3-150.3 (m); **^{19}F{^{1}H}-NMR ($CDCl_3$, 471 MHz):** δ (ppm) = 74.8-75.3 (m, 4F), 77.8-79.2 (m, 1F); **IR spectrum (neat)** (cm^{-1}) = 3133, 2919, 2850, 2230, 1597, 1391, 1194, 1117, 1084, 989, 880, 853, 828, 788, 745, 671, 573, 544; **HRMS (ESI)**: *m/z* calculated for $C_{16}H_{12}F_5N_2O_2S_2^{+\bullet}$ $[M+H]^{+\bullet}$ 423.0255, found 423.0273.



N-Tosyl-5-bromo-2-(pentafluoro-λ^6-sulfanyl)-1H-indole 4i

Prepared according to **GP5** from *N*-(4-bromo-2-((pentafluoro-λ^6-sulfaneyl)ethynyl)phenyl)-4-methylbenzenesulfonamide **3i** (12 mg, 0.025 mmol). The reaction afforded a mixture of *N*-Ts- and *N*-H indole in a ratio 74:26 **4i**:**5i**. It was purified by preparative TLC (Petroleum ether/EtOAc 90/10) affording **4i** (7 mg, 58%) as a white powder.

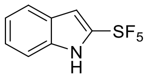
^{1}H-NMR ($CDCl_3$, 500 MHz): δ (ppm) = 2.34 (s, 3H), 7.16 (d, *J* = 7.8 Hz, 2H), 7.26 (s, 1H), 7.51 (d, *J* = 8.5 Hz, 2H), 7.59 (dd, *J* = 9.1 Hz, *J* = 2.0 Hz, 1H), 7.67 (d, *J* = 2.0 Hz, 1H), 8.24 (d, *J* = 9.1 Hz, 1H); **^{13}C{^{1}H}-NMR ($CDCl_3$, 125 MHz):** δ (ppm) = 21.8, 118.7, 118.9 (quint., *J* = 5.8 Hz), 119.4, 125.4, 127.0, 128.2, 129.9, 131.4, 134.5, 137.3, 145.8, 149.0 (quint., *J* = 26.1 Hz); **^{19}F{^{1}H}-NMR ($CDCl_3$, 471 MHz):** δ (ppm) = 74.6-75.0 (m, 4F), 78.8-80.1 (m, 1F); **IR spectrum (neat)** (cm^{-1}) = 2963, 2922, 2851, 1738, 1463, 1385, 1260, 1180, 1066, 852, 810, 787, 703, 669, 574; **HRMS (ESI)**: *m/z* calculated for $C_{15}H_{12}BrF_5N_2O_2S_2^{+\bullet}$ $[M+H]^{+\bullet}$ 475.9408, found 475.9394.



N-Tosyl-6-fluoro-2-(pentafluoro-λ^6-sulfanyl)-1H-indole 4k

Prepared according to **GP5** from N-(5-fluoro-2-[2-(pentafluoro-λ^6-sulfanyl)ethynyl]phenyl)-4-methylbenzene-1-sulfonamide **3k** (35 mg, 0.08 mmol). The reaction afforded a mixture of *N*-Ts- and *N*-H indole in a ratio 69:31 **4k**:**5k**. It was purified by preparative TLC (Petroleum ether/EtOAc 90/10) affording **4k** (23 mg, 66%) as a white powder.

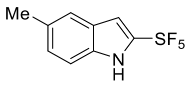
^{1}H-NMR ($CDCl_3$, 500 MHz): δ (ppm) = 2.33 (s, 3H), 7.10 (dt, *J* = 8.7 Hz, *J* = 2.3 Hz, 1H), 7.16 (d, *J* = 8.1 Hz, 2H), 7.31 (s, 1H), 7.49 (dd, *J* = 8.7 Hz, *J* = 5.5 Hz, 1H), 7.53 (d, *J* = 8.4 Hz, 2H), 8.09 (dd, *J* = 10.5 Hz, *J* = 2.3 Hz, 1H); **^{13}C{^{1}H}-NMR ($CDCl_3$, 125 MHz):** δ (ppm) = 21.7, 105.2 (d, *J* = 29.8 Hz), 114.3 (d, *J* = 24.7 Hz), 119.8 (quint., *J* = 5.7 Hz), 122.9 (d, *J* = 1.8 Hz), 124.1 (d, *J* = 10.1 Hz), 127.0, 129.9, 134.5, 139.2 (d, *J* = 12.7 Hz), 145.8, 148.2 (quint., *J* = 25.8 Hz), 162.9 (d, *J* = 246.7 Hz); **^{19}F{^{1}H}-NMR ($CDCl_3$, 471 MHz):** δ (ppm) = -109.4 (s, 1F), 74.7-75.0 (m, 4F), 79.4-80.7 (m, 1F); **IR spectrum (neat)** (cm^{-1}) = 3140, 2917, 2849, 1617, 1595, 1521, 1483, 1265, 1193, 1183, 1088, 964, 847, 806, 766, 670, 574; **HRMS (ESI)**: *m/z* calculated for $C_{15}H_{12}F_6NO_2S_2^{+\bullet}$ $[M+H]^{+\bullet}$ 416.0208, found 416.0205.



2-(Pentafluoro-λ⁶-sulfanyl)-1*H*-indole 5a

Prepared according to **GP3** from crude (*E*)-*N*-(2-(1-chloro-2-(pentafluoro-λ⁶-sulfanyl)vinyl)phenyl)-4-toluenesulfonamide **2a** (86.8 mg, 0.2 mmol). The NMR shows 100% conv., the reaction was purified by silica gel column chromatography (petroleum ether/EtOAc 90:10) affording **5a** (31 mg, 65 % over 2 steps) as yellow powder.

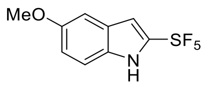
^{1}H-NMR ($CDCl_3$, 500 MHz): δ (ppm) = 6.95 (s, 1H), 7.22 (dt, *J* = 7.1 Hz, *J* = 0.9 Hz, 1H), 7.37 (t, *J* = 8.1 Hz, 1H), 7.43 (dd, *J* = 8.3, 0.7 Hz, 1H), 7.69 (d, *J* = 8.0 Hz, 1H), 8.61 (bs, 1H); **^{13}C{^{1}H}-NMR ($CDCl_3$, 125 MHz):** δ (ppm) = 103.50 (quint., *J* = 4.8 Hz), 111.8, 121.7, 122.6, 125.4, 125.6, 134.0, 143.6 (quint., *J* = 24.2 Hz); **^{19}F{^{1}H}-NMR ($CDCl_3$, 471 MHz):** δ (ppm) = 66.3 (d, *J* = 152.9 Hz, 4F), 81.0-82.3 (m, 1F); **IR spectrum (neat)** (cm^{-1}) = 3403, 2925, 2850, 1448, 1107, 955, 854, 822, 752, 571; **HRMS (ESI)**: *m/z* calculated for $C_8H_6F_5NS^{+\bullet}$ $[M]^{+\bullet}$ 243.0136, found 243.0141.



5-Methyl-2-(pentafluoro-λ⁶-sulfanyl)-1*H*-indole 5b

Prepared according to **GP3** from crude (*E*)-*N*-(2-(1-Chloro-2-(pentafluoro-λ⁶-sulfanyl)vinyl)-4-methylphenyl)-4-toluenesulfonamide **2b** (89.6 mg, 0.2 mmol). The NMR shows 76% conv., the reaction was purified by preparative TLC (petroleum ether/EtOAc 90:10) affording **5b** (19.5 mg, 38 % over 2 steps) as white powder.

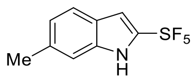
^{1}H-NMR ($CDCl_3$, 500 MHz): δ (ppm) 2.45 (s, 3H), 6.85 (s, 1H), 7.19 (d, *J* = 8.3 Hz, 1H), 7.31 (d, *J* = 8.4 Hz, 1H), 7.45 (s, 1H), 8.50 (bs, 1H); **^{13}C{^{1}H}-NMR ($CDCl_3$, 125 MHz):** δ (ppm) = 21.6, 103.0 (quint., *J* = 4.9 Hz), 111.5, 121.9, 125.6, 127.4, 131.1, 132.3, 143.6 (quint., *J* = 24.3 Hz); **^{19}F{^{1}H}-NMR ($CDCl_3$, 471 MHz):** δ (ppm) 66.23 (d, *J* = 152.9 Hz, 4F), 81.3-82.6 (m, 1F); **IR spectrum (neat)** (cm^{-1}) = 3394, 2923, 1733, 1523, 1450, 1152, 1108, 962, 882, 827, 792, 656; **HRMS (ESI)**: *m/z* calculated for $C_9H_8F_5NS^{+\bullet}$ $[M]^{+\bullet}$ 257.0292, found 257.0304.



5-Methoxy-2-(pentafluoro-λ^6-sulfanyl)-1*H*-indole 5c

Prepared according to **GP3** from (*E*)-*N*-(2-(1-chloro-2-(pentafluoro-λ^6-sulfanyl)vinyl)-4-methoxyphenyl)-4-toluenesulfonamide **2c** (92.8 mg, 0.2 mmol). The NMR shows 100% conv., the reaction was purified by preparative TLC (petroleum ether/EtOAc 90:10) affording **5c** (37 mg, 68 %) as a colorless oil.

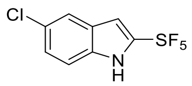
^{1}H-NMR (CDCl$_3$, 500 MHz): δ (ppm) 3.85 (s, 3H), 6.86 (d, *J* = 2.2 Hz, 1H), 7.03 (dd, *J* = 8.9 Hz, *J* = 2.5 Hz, 1H), 7.08 (d, *J* = 2.4 Hz, 1H), 7.31 (dt, *J* = 9.0 Hz, *J* = 0.8 Hz, 1H), 8.53 (bs, 1H); **^{13}C{^{1}H}-NMR (CDCl$_3$, 125 MHz):** δ (ppm) = 55.9, 103.0, 103.2 (quint., *J* = 4.9 Hz), 112.8, 116.9, 125.8, 129.0, 143.9 (quint., *J* = 25.3 Hz), 155.3; **^{19}F{^{1}H}-NMR (CDCl$_3$, 471 MHz):** δ (ppm) 66.1 (d, *J* = 152.8 Hz, 4F), 81.2-82.6 (m, 1F); **IR spectrum (neat)** (cm^{-1}) 3296, 2938, 1629, 1520, 1458, 1293, 1199, 1163, 956, 827, 789, 751, 672; **HRMS (ESI)**: *m*/*z* calculated for $C_9H_8F_5NOS^{+\bullet}$ [M]$^{+\bullet}$ 273.0241, found 273.0260.



6-Methyl-2-(pentafluoro-λ^6-sulfanyl)-1*H*-indole 5d

Prepared according to **GP3** from crude (*E*)-*N*-(2-(1-Chloro-2-(pentafluoro-λ^6-sulfanyl)vinyl)-5-methylphenyl)-4-toluenesulfonamide **2d** (67 mg, 0.15 mmol). The NMR shows 78% conv., the reaction was purified by preparative TLC (petroleum ether/EtOAc 90:10) affording **5d** (22 mg, 57 % over 2 steps) as a pale-yellow powder.

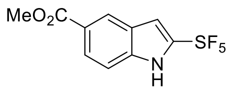
^{1}H-NMR (CDCl$_3$, 400 MHz): δ (ppm) = 2.49 (s, 3H), 6.89 (s, 1H), 7.06 (dd, *J* = 8.2, 0.7 Hz, 1H), 7.20 (s, 1H), 7.56 (d, *J* = 8.2 Hz, 1H), 8.46 (bs, 1H); **^{13}C{^{1}H}-NMR (CDCl$_3$, 125 MHz):** δ (ppm) = 22.1, 103.40 (quint., *J* = 4.9 Hz), 111.4, 122.2, 123.1, 123.7, 134.4, 135.8, 143.1 (quint., *J* = 24.0 Hz); **^{19}F{^{1}H}-NMR (CDCl$_3$, 471 MHz):** δ (ppm) = 66.4 (d, *J* = 152.9 Hz, 4F), 81.5-82.8 (m, 1F); **IR spectrum (neat)** (cm^{-1}) = 3475, 3398, 2926, 1629, 1512, 1438, 1385, 1316, 1107, 959, 832, 820, 652; **HRMS (ESI)**: *m*/*z* calculated for $C_9H_8F_5NS^{+\bullet}$ [M]$^{+\bullet}$ 257.0292, found 257.0305.



5-Chloro-2-(pentafluoro-λ^6-sulfanyl)-1*H*-indole 5e

Prepared according to **GP3** from crude (*E*)-*N*-(4-chloro-2-(1-chloro-2-(pentafluoro-λ^6-sulfanyl)vinyl)phenyl)-4-toluenesulfonamide **2e** (70 mg, 0.15 mmol). The NMR shows 90% conv., the reaction was purified by preparative TLC (petroleum ether/EtOAc 90:10) affording **5e** (22.1 mg, 53 % over 2 steps) as a white powder.

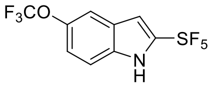
^{1}H-NMR ($CDCl_3$, 500 MHz): δ (ppm) = 6.88 (s, 1H), 7.31-7.37 (m, 2H), 7.66 (s, 1H), 8.67 (bs, 1H); **^{13}C{^{1}H}-NMR ($CDCl_3$, 125 MHz):** δ (ppm) = 103.0 (quint., *J* = 5.1 Hz), 113.1, 121.9, 126.2, 126.3, 127.4, 132.3, 144.6 (quint., *J* = 25.4 Hz); **^{19}F{^{1}H}-NMR ($CDCl_3$, 471 MHz):** δ (ppm) = 66.0 (d, *J* = 153.0 Hz, 4F), 80.2-81.5 (m, 1F); **IR spectrum (neat)** (cm^{-1}) = 3406, 2923, 1440, 1110, 1063, 956, 826, 806, 786, 658, 591, 470; **HRMS (ESI)**: *m/z* calculated for $C_8H_5ClF_5NS^{+\bullet}$ $[M]^{+\bullet}$ 276.9746, found 276.9734.



Methyl 2-(pentafluoro-λ^6-sulfanyl)-1*H*-indole-5-carboxylate 5f

Prepared according to **GP3** from methyl (*E*)-3-(1-chloro-2-(pentafluoro-λ^6-sulfanyl)vinyl)-4-(4-toluenesulfonamido)benzoate **2f** (80 mg, 0.16 mmol). The NMR shows 71% conv., the reaction was purified by silica gel column chromatography (petroleum ether/EtOAc 90:10) affording **5f** (20.0 mg, 41%) as a white powder.

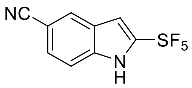
^{1}H-NMR ($CDCl_3$, 500 MHz): δ (ppm) = 3.95 (s, 3H), 7.03 (s, 1H), 7.46 (d, *J* = 8.7 Hz, 1H), 8.06 (dd, *J* = 8.7 Hz, *J* = 1.2 Hz, 1H), 8.46 (s, 1H), 8.98 (bs, 1H); **^{13}C{^{1}H}-NMR ($CDCl_3$, 125 MHz):** δ (ppm) = 52.3, 104.6 (quint., *J* = 4.9 Hz), 111.8, 124.0, 124.9, 125.7, 126.6, 136.4, 144.8 (quint., *J* = 24.3 Hz), 167.6; **^{19}F{^{1}H}-NMR ($CDCl_3$, 471 MHz):** δ (ppm) = 66.1 (d, *J* = 153.1 Hz, 4F), 80.1-81.4 (m, 1F); **IR spectrum (neat)** (cm^{-1}) = 3479, 3130, 1613, 1509, 1436, 1337, 1213, 955, 817, 788, 654; **HRMS (ESI)**: *m/z* calculated for $C_{10}H_9F_5NO_2S^{+\bullet}$ $[M+H]^{+\bullet}$ 302.0269, found 302.0268.



2-(pentafluoro-λ⁶-sulfanyl)-5-(trifluoromethoxy)-1H-indole 5g

Prepared according to **GP3** from *N*-{2-[(E)-1-chloro-2-(pentafluoro-λ⁶-sulfanyl)ethenyl]-4-(trifluoromethoxy)phenyl}-4-methylbenzene-1-sulfonamide **2g** (70 mg, 0.14 mmol). A mixture of product indole(NH) (68%) and indole(NTs) (32%) was obtained. The NMR shows only 68% conv., the reaction was purified by silica gel column chromatography (petroleum ether/EtOAc 98:2) affording **5g** (17 mg, 38% yield over 2 steps) as a colorless oil and **4g** (9 mg, 14% yield) as colorless oil.

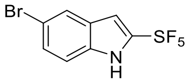
^{1}H-NMR ($CDCl_3$, 500 MHz): δ (ppm) = 6.96 (d, *J* = 1.7 Hz, 1H), 7.25 (dd, *J* = 9.2 Hz, *J* = 1.7 Hz, 1H), 7.43 (d, *J* = 8.9 Hz, 1H), 7.55 (s, 1H), 8.75 (bs, 1H); **^{13}C{^{1}H}-NMR ($CDCl_3$, 125 MHz):** δ (ppm) = 103.8 (quint., *J* = 5.0 Hz), 113.0, 114.9, 120.0, 120.8 (q, *J* = 256.3 Hz), 125.6, 132.2, 144.18 (q, *J* = 1.6 Hz), 145.0 (quint., *J* = 24.8 Hz); **^{19}F{^{1}H}-NMR ($CDCl_3$, 471 MHz):** δ (ppm) = -58.3 (s, 3F), 65.92 (d, *J* = 153.0 Hz, 4F), 79.9-81.3 (m, 1F); **IR spectrum (neat)** (cm^{-1}) = 3490, 1525, 1452, 1254, 1209, 1151, 1106, 955, 794, 771, 675, 654, 605, 460; **HRMS (ESI)**: *m/z* calculated for $C_9H_5F_8NOS^{+\bullet}$ $[M]^{+\bullet}$ 326.9959, found 329.9970.



2-(pentafluoro-λ⁶-sulfanyl)-1H-indole-5-carbonitrile 5h

Prepared according to **GP3** from *N*-{2-[(E)-1-chloro-2-(pentafluoro-λ⁶-sulfanyl)ethenyl]-4-cyanophenyl}-4-methylbenzene-1-sulfonamide **2h** (64 mg, 0.14 mmol). The NMR shows 90% conv., the reaction was purified by preparative TLC (petroleum ether/EtOAc 90:10) affording **5h** (15 mg, 40 % yield over 2 steps) as a white powder.

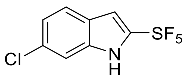
^{1}H-NMR ($CDCl_3$, 500 MHz): δ (ppm) = 7.03 (s, 1H), 7.53 (d, *J* = 8.6 Hz, 1H), 7.60 (dd, *J* = 8.6 Hz, *J* = 1.4 Hz, 1H), 8.08 (s, 1H), 9.05 (bs, 1H); **^{13}C{^{1}H}-NMR ($CDCl_3$, 125 MHz):** δ (ppm) = 101.6, 103.9 (quint., *J* = 5.0 Hz), 105.5, 113.1, 119.7, 125.4 (quint., *J* = 23.0 Hz), 128.1, 128.4, 135.5; **^{19}F{^{1}H}-NMR ($CDCl_3$, 471 MHz):** δ (ppm) 66.0 (d, *J* = 153.2 Hz, 4F), 79.1-80.4 (m, 1F); **IR spectrum (neat)** (cm^{-1}) = 3213, 3040, 3003, 2234, 1741, 1621, 1472, 1318, 1236, 1110, 956, 833, 791, 743, 675, 598, 496, 410; **HRMS (ESI)**: *m/z* calculated for $C_9H_6F_5N_2S^{+\bullet}$ $[M+H]^{+\bullet}$ 269.0166, found 269.0165.



5-Bromo-2-(pentafluoro-λ^6-sulfanyl)-1*H*-indole 5i

Prepared according to **GP3** from crude (*E*)-*N*-(4-bromo-2-(1-chloro-2-(pentafluoro-λ^6-sulfanyl)vinyl)phenyl)-4-toluenesulfonamide **2i** (77 mg, 0.15 mmol). The NMR shows 90% conv., the reaction was purified by silica gel column chromatography (petroleum ether/EtOAc 95:5) affording **5i** (28.0 mg, 53 % over 2 steps) as a white powder.

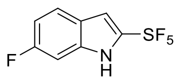
^{1}H-NMR ($CDCl_3$, 500 MHz): δ (ppm) = 6.88 (s, 1H), 7.31 (d, *J* = 8.8 Hz, 1H), 7.45 (dd, *J* = 8.8 Hz, *J* = 1.7 Hz, 1H), 7.82 (s, 1H), 8.64 (bs, 1H); **^{13}C{^{1}H}-NMR ($CDCl_3$, 125 MHz):** δ (ppm) = 102.90 (quint., *J* = 4.9 Hz), 113.4, 114.8, 125.0, 127.0, 128.7, 132.5, 144.5 (quint., *J* = 24.2 Hz); **^{19}F{^{1}H}-NMR ($CDCl_3$, 471 MHz):** δ (ppm) = 66.1 (d, *J* = 153.0 Hz, 4F), 80.1-81.4 (m, 1F); **IR spectrum (neat)** (cm^{-1}) = 3406, 1438, 1304, 1229, 1109, 956, 879, 828, 804, 789, 680, 658, 585; **HRMS (ESI)**: *m/z* calculated for $C_8H_5BrF_5NS^{+\bullet}$ $[M]^{+\bullet}$ 320.9241, found 320.9242.



6-Chloro-2-(pentafluoro-λ^6-sulfanyl)-1*H*-indole 5j

Prepared according to **GP3** from crude (*E*)-*N*-(5-chloro-2-(1-chloro-2-(pentafluoro-λ^6-sulfanyl)vinyl)phenyl)-4-toluenesulfonamide **2j** (93.6 mg, 0.2 mmol). The NMR shows 100% conv., the reaction was purified by silica gel column chromatography (petroleum ether/EtOAc 90:10) affording **5j** (36.1 mg, 65 % over 2 steps) as a white powder.

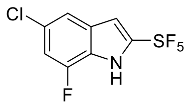
^{1}H-NMR ($CDCl_3$, 500 MHz): δ (ppm) = 6.92 (s, 1H), 7.19 (d, *J* = 8.5 Hz, 1H), 7.42 (s, 1H), 7.60 (d, *J* = 8.5 Hz, 1H), 8.61 (bs, 1H); **^{13}C{^{1}H}-NMR ($CDCl_3$, 125 MHz):** δ (ppm) = 103.6 (quint., *J* = 4.9 Hz), 111.7, 122.8, 123.6, 123.9, 131.5, 134.2, 144.1 (quint., *J* = 24.2 Hz); **^{19}F{^{1}H}-NMR ($CDCl_3$, 471 MHz):** δ (ppm) = 66.1 (d, *J* = 153.3 Hz, 4F), 80.4-81.7 (m, 1F); **IR spectrum (neat)** (cm^{-1}) = 3308, 2922, 2850, 1686, 1617, 1527, 1293, 1217, 1114, 954, 833, 763; **HRMS (ESI)**: *m/z* calculated for $C_8H_5ClF_5NS^{+\bullet}$ $[M]^{+\bullet}$ 276.9746, found 276.9748.



6-Fluoro-2-(pentafluoro-λ^6-sulfanyl)-1*H*-indole 5k

Prepared according to **GP3** from crude **(***E***)-***N*-(2-(1-Chloro-2-(pentafluoro-λ^6-sulfanyl)vinyl)-5-fluorophenyl)-4-toluenesulfonamide **2k** (68 mg, 0.15 mmol). The NMR shows 100% conv., the reaction was purified by silica gel column chromatography (petroleum ether/EtOAc 90:10 affording **5k** (27 mg, 69 % over 2 steps) as a white powder.

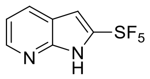
^{1}H-NMR ($CDCl_3$, 500 MHz): δ (ppm) = 6.92 (d, *J* = 1.4 Hz, 1H), 6.99 (ddd, *J* = 9.4 Hz, *J* = 8.9 Hz, *J* = 2.3 Hz, 1H), 7.10 (dd, *J* = 9.1 Hz, *J* = 2.2 Hz, 1H), 7.62 (dd, *J* = 8.8 Hz, *J* = 5.2 Hz, 1H), 8.65 (bs, 1H); **^{13}C{^{1}H}-NMR ($CDCl_3$, 125 MHz):** δ (ppm) = 98.0 (d, *J* = 26.7 Hz), 103.6 (quint., *J* = 4.8 Hz), 111.3 (d, *J* = 25.1 Hz), 121.9, 123.9 (d, *J* = 10.2 Hz), 134.0 (d, *J* = 12.7 Hz), 143.9 (quint., *J* = 24.5 Hz), 161.7 (d, *J* = 242.6 Hz); **^{19}F{^{1}H}-NMR ($CDCl_3$, 471 MHz):** δ (ppm) = -115.2 (s, 1F), 66.2 (d, *J* = 153.0 Hz, 4F), 80.8-82.1 (m, 1F); **IR spectrum (neat)** (cm^{-1}) = 3451, 3141, 2929, 1630, 1501, 1441, 1296, 1225, 1139, 963, 793, 756, 654, 602, 515; **HRMS (ESI)**: *m/z* calculated for $C_8H_5F_6NS^{+\bullet}$ $[M]^{+\bullet}$ 261.0041, found 261.0054.



5-chloro-7-fluoro-2-(pentafluoro-λ^6-sulfanyl)-1H-indole 5l

Prepared according to **GP3** from *N*-{4-chloro-2-[(E)-1-chloro-2-(pentafluoro-λ^6-sulfanyl)ethenyl]-6-fluorophenyl}-4-methylbenzene-1-sulfonamide **2l** (20 mg, 0.04 mmol). The NMR shows 100% conv., The reaction was purified by TLC preparative (petroleum ether/EtOAc 90:10) affording **5l** (8 mg, 66% yield over the cyclization step) as a white powder. The compound has been repurified several times due to instability in solution.

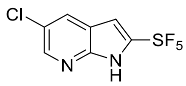
^{1}H-NMR ($CDCl_3$, 500 MHz): δ (ppm) = 6.92 (d, *J* = 2.8 Hz, 1H), 7.11 (dd, *J* = 10.4 Hz, *J* = 1.6 Hz, 1H), 7.46 (d, *J* = 1.6 Hz, 1H), 8.94 (bs, 1H); **^{13}C{^{1}H}-NMR ($CDCl_3$, 125 MHz):** δ (ppm) = 103.5-103.8 (m), 111.6 (d, *J* = 19.3 Hz), 117.8 (d, *J* = 4.2 Hz), 126.9 (d, *J* = 7.5 Hz), 128.6-128.7 (m), 129.0, 131.1, 149.0 (d, *J* = 250.1 Hz); **^{19}F{^{1}H}-NMR ($CDCl_3$, 471 MHz):** δ (ppm) = -131.0 (s, 1F), 66.05 (d, *J* = 153.3 Hz, 4F), 79.2-80-5 (m, 1F); **IR spectrum (neat)** (cm^{-1}) = 3485, 2925, 2854, 1709, 1586, 1297, 1125, 1064, 956, 902, 828, 782, 677, 604, 501; **HRMS (ESI)**: *m/z* calculated for $C_8H_4ClF_6NS^{+\bullet}$ $[M]^{+\bullet}$ 294.9652, found 294.9651.



2-(pentafluoro-λ^6-sulfanyl)-1H-pyrrolo[2,3-b]pyridine 5o

Prepared according to **GP3** from *N*-{3-[(E)-1-chloro-2-(pentafluoro-λ^6-sulfanyl)ethenyl]pyridin-2-yl}-4-methylbenzene-1-sulfonamide **2o** (27 mg, 0.06 mmol). The NMR shows 55% conv., the reaction was purified by TLC preparative (petroleum ether/EtOAc 80:20) affording **5o** (5 mg, 33% yield over the cyclization step) as a white powder as a mixture with **4o** (**4o**:**5o** 12:88). Product **5o** appears to be partially unstable in solution.

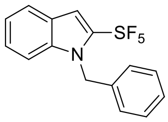
^{1}H-NMR ($CDCl_3$, 500 MHz): δ (ppm) = 6.92 (t, *J* = 2.5 Hz, 1H), 7.11 (dd, *J* = 10.4, 1.6 Hz, 1H), 7.46 (d, *J* = 1.5 Hz, 1H), 8.89 (bs, 1H); **^{13}C{^{1}H}-NMR ($CDCl_3$, 125 MHz):** δ (ppm) = 103.5-103.8 (m), 111.6 (d, *J* = 19.3 Hz) 117.8 (d, *J* = 4.2 Hz), 126.9 (d, *J* = 7.5 Hz), 128.6-128.7 (m), 129.0, 131.1, 149.0 (d, *J* = 250.1 Hz); **^{19}F{^{1}H}-NMR ($CDCl_3$, 471 MHz):** δ (ppm) = -131.0 (s, 1F), 66.05 (d, *J* = 153.5 Hz), 79.8 (quint., *J* = 154.2 Hz, 1F); **IR spectrum (neat)** (cm^{-1}) = 2958, 2924, 2852, 1727, 1597, 1464, 1381, 1279, 1197, 1121, 1074, 866, 793, 665, 571; **HRMS (ESI)**: *m/z* calculated for $C_7H_6F_5N_2S^{+\bullet}$ $[M+H]^{+\bullet}$ 245.0166 found 245.0171.



5-chloro-2-(pentafluoro-λ^6-sulfanyl)-1H-pyrrolo[2,3-b]pyridine 5p

Prepared according to **GP3** from *N*-{5-chloro-3-[(E)-1-chloro-2-(pentafluoro-λ^6-sulfanyl)ethenyl]pyridin-2-yl}-4-methylbenzene-1-sulfonamide **2p** (18 mg, 0.04 mmol). The NMR shows 71% conv., the reaction was purified by preparative TLC (petroleum ether/EtOAc 80:20) affording **5p** (7 mg, 53% yield over the cyclization step) as a white powder.

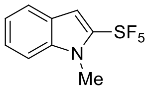
^{1}H-NMR ($CDCl_3$, 500 MHz): δ (ppm) = 6.89 (s, 1H), 8.09 (d, *J* = 2.2 Hz, 1H), 8.47 (d, *J* = 2.2 Hz, 1H), 13.04 (bs, 1H); **^{13}C{^{1}H}-NMR ($CDCl_3$, 125 MHz):** δ (ppm) = 100.7 (quint., *J* = 5.3 Hz), 119.4, 125.6, 131.1, 144.4 (m), 145.1, 146.1 (quint., *J* = 26.1 Hz); **^{19}F{^{1}H}-NMR ($CDCl_3$, 471 MHz):** δ (ppm) = 65.9 (d, *J* = 153.7 Hz, 4F), 79.4-80.7 (m, 1F); **IR spectrum (neat)** (cm^{-1}) = 3663, 2988, 2904, 1575, 1394, 1224, 1066, 947, 792, 680; **HRMS (ESI)**: *m/z* calculated for $C_7H_5ClF_5N_2S^{+\bullet}$ $[M+H]^{+\bullet}$ 278.9777 found 278.9773.



N-benzyl-2-(pentafluoro-λ⁶-sulfanyl)-1H-indole 7

In a 10 mL pressure tube under N_2 equipped with a magnetic stir bar, the *N*-(2-ethynylphenyl)-4-toluenesulfonamide **1a** (250 mg, 0.92 mmol, 1 equiv.) was introduced and dissolved in EtOAc (0.4 M). At - 40 °C, gaseous SF_5Cl (300 mg, 1.84 mmol, 2.0 equiv.) was condensed in the solution and it was stirred for 5 min at this temperature before Et_3B (10 mol%) was added dropwise. The tube was sealed, and it was stirred at room temperature for 16 h. The solvent was removed under vacuum, then $LiOH.H_2O$ (193 mg, 4.6 mmol, 5 equiv.) and DMSO (2.4 mL, 0.4 M) were added and the reaction mixture was stirred at 40 °C for 40 h. Then, Bn-Br (220 µL, 1.84 mmol, 2 equiv.) was added via a syringe and the mixture was stirred for 2 hours at 40 °C. The reaction was quenched with saturated solution of NH_4Cl and extracted with 3 volumes of EtOAc. The combined organic layers were dried over $MgSO_4$, filtered and concentrated under reduced pressure. The crude mixture was purified by silica gel column chromatography (100% Cyclohexane) affording **7** (255 mg, 83%) as a colorless solid.

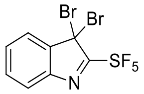
^{1}H-NMR ($CDCl_3$, 400 MHz): δ (ppm) = 5.65 (s, 2H), 6.93 (d, *J* = 6.8 Hz, 2H), 7.13 (s, 1H), ,7.16-7.32 (m, 6H), 7.71 (d, *J* = 7.9 Hz, 1H); **^{13}C{^{1}H}-NMR ($CDCl_3$, 125 MHz):** δ (ppm) = 49.5 (quint. *J* = 3.5 Hz), 105.8 (quint., *J* = 5.1 Hz), 111.4, 121.7, 122.6, 124.5, 125.5, 125.6, 127.4, 128.8, 136.2, 137.1, 146.7 (quint., *J* = 22.7 Hz); **^{19}F{^{1}H}-NMR ($CDCl_3$, 471 MHz):** δ (ppm) = 72.8 (d, *J* = 153.5 Hz, 4F), 82.8-84.2 (m, 1F); **IR spectrum (neat)** (cm^{-1}) = 3145, 2925, 1596, 1531, 1449, 1392, 1256, 1221, 1150, 1122, 1087, 1001, 851, 799, 781, 741, 668, 572, 542; **HRMS (ESI)**: *m/z* calculated for $C_{15}H_{12}F_5NS^{+\bullet}$ $[M]^{+\bullet}$ 333.0605, found 333.0595.



1-Methyl-2-(pentafluoro-λ⁶-sulfanyl)-1H-indole 8

Product **8** was prepared from **1a** (580 mg, 2.14 mmol) following the same procedure described for product **7**, expect that the alkylation was performed by addition of Me-I (267 µL, 2 equiv.) and the mixture was stirred for 0.5 hour at 25 °C. Solvent was evaporated under vacuum and the crude mixture was purified by silica gel column chromatography and purified with 100% of P.E. affording **8** (375 mg, 68%) as a white powder.

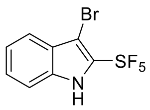
^{1}H-NMR ($CDCl_3$, 500 MHz): δ (ppm) = 3.94 (s, 1H), 7.03 (s, 1H), 7.20-7.23 (m, 1H), 7.38-7.42 (m, 2H), 7.67 (d, *J* = 7.9 Hz, 1H); **^{13}C{^{1}H}-NMR ($CDCl_3$, 125 MHz):** δ (ppm) = 32.9 (quint. *J* = 3.9 Hz), 105.1 (quint., *J* = 5.2 Hz), 110.4, 121.3, 122.5, 124.3, 125.2, 136.3, 146.1-146.9 (m); **^{19}F{^{1}H}-NMR ($CDCl_3$, 471 MHz):** δ (ppm) = 72.2 (d, *J* = 152.6 Hz, 4F), 83.1-84.4 (m, 1F); **IR spectrum (neat)** (cm^{-1}) = 3118, 1615, 1467, 1428, 1318, 1176, 1105, 1072, 936, 898, 829, 777, 750, 675, 637, 604, 528, 460; **HRMS (ESI)**: *m/z* calculated for $C_9H_8F_5NS^{+\bullet}$ $[M]^{+\bullet}$ 257.0292, found 257.0298.



3,3-dibromo-2-(pentafluoro- λ^6-sulfanyl)-3*H*-indole 9

To a Schlenk tube under nitrogen containing 2-(pentafluoro-λ^6-sulfanyl)-1*H*-indole **5a** (20 mg, 0.082 mmol) dissolved in dichloromethane (0.5 mL) was added *N*-bromosuccinimide (36.6 mg, 0.206 mmol) and the reaction was stirred at room temperature for 30 min. The crude mixture was concentrated under reduced pressure and purified by silica gel column chromatography (cyclohexane) affording **9** (31 mg, 94%) as a white solid.

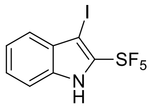
^{1}H-NMR (CDCl$_3$, 500 MHz): δ (ppm) = 7.48 (dt, *J* = 7.7 Hz, *J* = 1.2 Hz, 1H), 7.55 (dt, *J* = 7.6 Hz, *J* = 1.1 Hz, 1H), 7.66 (d, *J* = 7.6 Hz, 1H), 7.72-7.74 (m, 1H); **^{13}C{^{1}H}-NMR (CDCl$_3$, 125 MHz):** δ (ppm) = 43.3, 124.0, 124.1, 131.4, 131.6, 141.2, 142.5, 178.3 (quint., *J* = 23.2 Hz); **^{19}F{^{1}H}-NMR (CDCl$_3$, 471 MHz):** δ (ppm) = 63.6 (d, *J* = 153.5 Hz, 4F), 73.3-74.7 (m, 1F); **IR spectrum (neat)** (cm^{-1}) = 3082, 2927, 1554, 1468, 1454, 1206, 1172, 1126, 920, 838, 761, 734, 677, 577; **HRMS (ESI)**: *m/z* calculated for $C_8H_4Br_2F_5NS^{+\bullet}$ $[M]^{+\bullet}$ 398.8346, found 398.8347.



3-Bromo-2-(pentafluoro-λ^6-sulfanyl)-1*H*-indole 10

To a Schlenk tube under nitrogen containing 2-(pentafluoro-λ^6-sulfanyl)-1*H*-indole **5a** (20 mg, 0.082 mmol) dissolved in dry dichloromethane (0.5 mL) was added *N*-bromosuccinimide (17.6 mg, 0.099 mmol), triethylamine (13.7 µL, 0.099 mmol) and the reaction was stirred at room temperature for 1h. The crude mixture was concentrated under reduced pressure and purified by silica gel column chromatography (cyclohexane/EtOAc 95:5) affording **10** (15 mg, 57%) as a white solid.

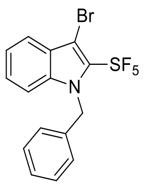
^{1}H-NMR (CDCl$_3$, 500 MHz): δ (ppm) = 7.23-7.32 (m, 1H), 7.38-7.41 (m, 2H), 7.69 (d, *J* = 7.8 Hz, 1H), 8.77 (bs, 1H); **^{13}C{^{1}H}-NMR (CDCl$_3$, 125 MHz):** δ (ppm) = 91.8 (quint., *J* = 3.4 Hz), 111.8, 121.6, 122.3, 125.8, 126.8, 132.9, 142.2 (quint., *J* = 23.7 Hz); **^{19}F{^{1}H}-NMR (CDCl$_3$, 471 MHz):** δ (ppm) = 68.9 (d, *J* = 154.8 Hz, 4F), 75.6-83.1 (m, 1F); **IR spectrum (neat)** (cm^{-1}) = 3393, 2923, 1620, 1578, 1446, 1304, 1203, 1118, 1023, 907, 836, 781, 747, 679, 649, 577, 539; **HRMS (ESI)**: *m/z* calculated for $C_8H_5BrF_5NS^{+\bullet}$ $[M]^{+\bullet}$ 320.9241, found 320.9237.



3-Iodo-2-(pentafluoro-λ[6]-sulfanyl)-1*H*-indole 11

2-(Pentafluoro-λ[6]-sulfanyl)-1*H*-indole **5a** (40 mg, 0.16 mmol, 1 equiv.) and KOH (2.5 eq., 23.069 mg, 0.41 mmol) were dissolved in DMF (0.5 mL) and the mixture was stirred at rt for 20 min. Then at rt, a solution of iodine (1 eq., 41.74 mg, 0.0085 mL, 0.16 mmol) in DMF (0.3 mL) was added and the mixture was stirred at rt for 2 hours. The reaction was quenched with NH_4Cl sat. solution and extracted with EtOAc. The combined organic layers were dried over $MgSO_4$, filtered and concentrated under reduced pressure. The crude mixture was purified by silica gel column chromatography (100% Cyclohexane) affording **11** (49 mg, 81%) as an orange solid.

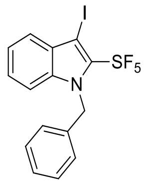
^{1}H-NMR (CDCl$_3$, 500 MHz): δ (ppm) = 7.28-7.31 (m, 1H), 7.37-7.43 (m, 2H), 7.59 (d, *J* = 8.1 Hz, 1H), 8.85 (bs, 1H); **^{13}C{^{1}H}-NMR (CDCl$_3$, 125 MHz):** δ (ppm) = 59.8 (quint., *J* = 3.9 Hz), 111.8, 122.5, 124.0, 126.8, 129.3, 133.4, 146.9 (quint., *J* = 24.1 Hz); **^{19}F{^{1}H}-NMR (CDCl$_3$, 471 MHz):** δ (ppm) = 69.1 (d, *J* = 155.2 Hz, 4F), 80.5-81.9 (m, 1F); **IR spectrum (neat)** (cm^{-1}) = 3361, 2922, 1737, 1617, 1500, 1443, 1198, 1117, 1013, 995, 904, 832, 744675, 648, 604, 535, 474; **HRMS (ESI)**: *m*/*z* calculated for $C_8H_5F_5INS^{+\bullet}$ $[M]^{+\bullet}$ 368.9102, found 368.9097.



1-Benzyl-3-dibromo-2-(pentafluoro- λ[6]-sulfanyl)-1*H*-indole 12

To a Schlenk tube under nitrogen containing 2-(pentafluoro-λ[6]-sulfanyl)-1*H*-indole **5a** (20 mg, 0.082 mmol) dissolved in DMF (1 mL) was added sodium hydride 60% in mineral oil (7.5 mg, 0.19 mmol) followed by benzyl bromide (22.3 µL, 0.19 mmol) and the reaction was stirred at 50 °C overnight. The crude ^{19}F NMR shows 88% conversion and 12% starting material left. The mixture was concentrated under reduced pressure and purified by silica gel column chromatography (cyclohexane) affording **12** (32 mg, 83%) as a colorless oil.

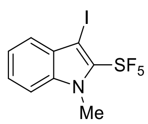
^{1}H-NMR (CDCl$_3$, 500 MHz): δ (ppm) = 5.74 (s, 2H), 6.90 (d, *J* = 8.2 Hz, 2H), 7.19 (d, *J* = 8.4 Hz, 1H), 7.25-7.32 (m, 4H), 7.34-7.39 (m, 1H), 7.76 (d, *J* = 7.4 Hz, 1H); **^{13}C{^{1}H}-NMR (CDCl$_3$, 125 MHz):** δ (ppm) = 50.5 (quint., *J* = 3.5 Hz), 93.7 (quint., *J* = 4.1 Hz), 111.6, 121.8, 122.4, 125.4, 125.5, 126.9, 127.5, 128.9, 135.2, 136.8, 145.1 (quint., *J* = 21.1 Hz); **^{19}F{^{1}H}-NMR (CDCl$_3$, 471 MHz):** δ (ppm) = 72.7 (d, *J* = 154.3 Hz, 4F), 81.6-82.9 (m, 1F); **IR spectrum (neat)** (cm^{-1}) = 3028, 1612, 1498, 1464, 1445, 1318, 1193, 1114, 1016, 942, 843, 775, 740, 728, 692, 577. **HRMS (ESI)**: *m/z* calculated for $C_{15}H_{11}BrF_5NS^{+\bullet}$ $[M]^{+\bullet}$ 410.9710, found 410.9738.



1-Benzyl-3-iodo-2-(pentafluoro-λ⁶-sulfanyl)-1*H*-indole 13

In a Schlenk tube under nitrogen were dissolved 2-(pentafluoro-λ^6-sulfanyl)-1H-indole **5a** (30 mg, 0.12 mmol) and KOH (17.3 mg, 0.26 mmol) in DMF (0.6 mL) and the mixture was stirred at room temperature for 25 min. Then a solution of iodine (31.3 mg, 0.12 mmol) in DMF (0.6 mL) was added dropwise and stirred at room temperature for 2h until full conversion. Sodium hydride (60% in mineral oil, 9.9 mg, 0.25 mmol) was added followed by benzyl bromide (30 µL, 0.25 mmol) and the reaction was stirred overnight. Quenched with saturated solution of NH_4Cl and extracted with EtOAc, dried over $MgSO_4$, filtered and concentrated under vaccum. The crude mixture was purified by silica gel column chromatography (cyclohexane) affording **13** (33 mg, 58%) as a colorless oil.

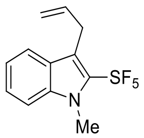
^{1}H-NMR ($CDCl_3$, 500 MHz): δ (ppm) = 5.78 (s, 2H), 6.90-6.91 (m, 2H), 7.16 (d, *J* = 8.4 Hz, 1H), 7.25-7.37 (m, 5H), 7.68 (dd, *J* = 8.4 Hz, *J* = 1.2 Hz, 1H); **$^{13}C\{^1H\}$-NMR ($CDCl_3$, 125 MHz):** δ (ppm) = 50.9 (quint., *J* = 4.1 Hz), 62.1 (quint., *J* = 4.5 Hz), 111.7, 122.6, 124.6, 125.4, 126.8, 127.5, 128.9, 129.1, 135.7, 136.9, 149.5 (quint., *J* = 21.6 Hz); **$^{19}F\{^1H\}$-NMR ($CDCl_3$, 471 MHz):** δ (ppm) = 73.2 (d, *J* = 155.1 Hz, 4F), 82.3-83.7 (m, 1F); **IR spectrum (neat)** (cm^{-1}) = 3032, 2904, 1606, 1489, 1441, 1327, 1265, 1192, 1104, 1018, 931, 837, 771, 675, 579, 458; **HRMS (ESI)**: *m/z* calculated for $C_{15}H_{11}F_5INS^{+\bullet}$ $[M]^{+\bullet}$ 458.9572, found 458.9572.



3-Iodo-1-methyl-2-(pentafluoro-λ⁶-sulfanyl)-1*H*-indole 14

In a Schlenk tube under nitrogen were dissolved 2-(pentafluoro-λ^6-sulfanyl)-1H-indole **5a** (25 mg, 0.103 mmol) and KOH (17 mg, 0.26 mmol) in DMF (0.6 mL) and the mixture was stirred at room temperature for 25 min. Then a solution of iodine (26.1 mg, 0.103 mmol) in DMF (0.6 mL) was added dropwise and stirred at room temperature for 2h until full conversion. Sodium hydride (60% in mineral oil, 8.2 mg, 0.206 mmol) was added followed by iodomethane (9.6 µL, 0.15 mmol) and the reaction was stirred overnight. Quenched with saturated solution of NH_4Cl and extracted with EtOAc, dried over $MgSO_4$, filtered and concentrated under vaccum. The crude mixture was purified by silica gel column chromatography (petroleum ether/EtOAc 90:10) affording **14** (35 mg, 89%) as a white solid.

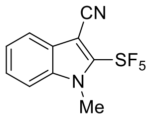
^{1}H-NMR ($CDCl_3$, 500 MHz): δ (ppm) = 4.03 (quint., *J* = 1.2Hz, 3H), 7.29 (ddd, *J* = 8.1 Hz, *J* = 7.0 Hz, *J* = 1.0 Hz, 1H), 7.35 (d, *J* = 8.5 Hz, 1H), 7.45 (ddd, *J* = 8.3 Hz, *J* = 6.9 Hz, *J* = 1.2 Hz, 1 H), 7.60 (d, *J* = 8.1 Hz, 1H); **^{13}C{^{1}H}-NMR ($CDCl_3$, 125 MHz):** δ (ppm) = 34.5 (quint., *J* = 4.5 Hz), 61.1 (quint., *J* = 5.0 Hz), 110.6, 122.3, 124.5, 126.4, 128.9, 135.9, 149.4 (quint., *J* = 19.6 Hz); **^{19}F{^{1}H}-NMR ($CDCl_3$, 471 MHz):** δ (ppm) = 72.5 (d, *J* = 154.4 Hz, 4F), 82.5-83.8 (m, 1F); **IR spectrum (neat)** (cm^{-1}) = 2958, 1462, 1343, 1234, 1163, 1110, 933, 830, 781, 761, 742, 675, 584, 549; **HRMS (ESI)**: *m/z* calculated for $C_9H_7F_5INS^{+\bullet}$ $[M]^{+\bullet}$ 382.9259, found 382.9280.



1-Methyl-2-(pentafluoro-λ^{6}-sulfanyl)-3-(prop-2-en-1-yl)-1*H*-indole 15

In 5 mL round bottom flask equipped with a magnetic stir bar, 3-iodo-1-methyl-2-(pentafluoro-λ^{6}-sulfanyl)-1H-indole **14** (10 mg, 0.026 mmol) was dissolved in THF (0.2 mL) under N2. The mixture was cooled down to - 20 °C and *i*PrMgCl (2M in THF) (14.4 µL, 1.1 equiv.) was added dropwise. The reaction was stirred at - 20 °C for 1 hour, and allyl bromide (4.5 µL, 2 equiv.) was added via a syringe. The reaction was stirred at rt for 2 hours. The crude mixture was purified by silica gel column chromatography (100% Cyclohexane) affording **15** (6 mg, 77%) as a colorless oil.

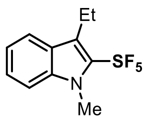
^{1}H-NMR ($CDCl_3$, 500 MHz): δ (ppm) = 3.77 (d, *J* = 5.8 Hz, 2H), 3.93 (s, 3H), 5.03 (dd, *J* = 10.1 Hz, *J* = 1.1 Hz, 1H), 5.09 (dd, *J* = 17.1 Hz, *J* = 1.4 Hz, 1H), 5.94 (ddt, *J* = 16.5 Hz, *J* = 10.1 Hz, *J* = 6.2 Hz, 1H), 7.19 (t, *J* = 7.5 Hz, 1H), 7.33-7.43 (m, 2H), 7.67 (d, *J* = 8.0 Hz, 1H); **^{13}C{^{1}H}-NMR ($CDCl_3$, 125 MHz):** δ (ppm) = 29.9, 33.3 (quint., *J* = 4.6 Hz), 110.3, 114.5 (quint., *J* = 3.7 Hz), 115.8, 120.7, 121.2, 125.2, 125.5, 136.1 (2C), 143.7-144.0 (m); **^{19}F{^{1}H}-NMR ($CDCl_3$, 471 MHz):** δ (ppm) = 73.2 (d, *J* = 151.7 Hz, 4F), 85.0-86.3 (m, 1F); **IR spectrum (neat)** (cm^{-1}) = 3083, 2980, 1640, 1613, 1531, 1466, 1351, 1327, 1249, 1169, 1147, 1017, 912, 829, 774, 738, 672, 587; **HRMS (ESI)**: *m/z* calculated for $C_{12}H_{12}F_5NS^{+\bullet}$ $[M]^{+\bullet}$ 297.0605, found 297.0590.



1-Methyl-2-(pentafluoro-λ^6-sulfanyl)-1H-indole-3-carbonitrile 16

In 5 mL round bottom flask equipped with a magnetic stir bar, 3-iodo-1-methyl-2-(pentafluoro-λ^6-sulfanyl)-1*H*-indole **14** (54 mg, 0.14 mmol) was dissolved in THF (0.5 mL) under N_2. The mixture was cooled down to - 20 °C and *i*PrMgCl (2M in THF) (77.5 µL, 1.1 equiv.) was added dropwise. The reaction was stirred at - 20 °C for 1 hour, and TsCN (51 mg, 2 equiv.) was added as solution in THF (0.5 mL) via a syringe. The reaction was stirred at rt for 16 hours. The crude mixture was purified by silica gel column chromatography (P.E:EtOAc 95:5) affording **16** (19 mg, 48%) as a white solid.

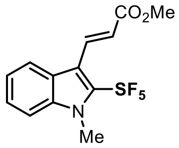
^{1}H-NMR ($CDCl_3$, 500 MHz): δ (ppm) = 4.05 (s, 3H), 7.42 (t, *J* = 7.5 Hz, 1H), 7.48-7.55 (m, 2H), 7.83 (d, *J* = 8.1 Hz, 1H); **^{13}C{^{1}H}-NMR ($CDCl_3$, 125 MHz):** δ (ppm) = 34.1 (quint. *J* = 4.0 Hz), 88.3-88.4 (m), 111.3, 113.1, 121.1, 124.1, 125.4, 127.1, 135.0, 149.6-150.4 (m); **^{19}F{^{1}H}-NMR ($CDCl_3$, 471 MHz):** δ (ppm) = 72.1 (d, *J* = 152.6 Hz, 4F), 78.2-79.5 (m, 1F); **IR spectrum (neat)** (cm^{-1}) = 2968, 2234, 1515, 1468, 1359, 1246, 1169, 1150, 1012, 850, 836, 785, 743, 681, 661, 620, 593, 575, 507; **HRMS (ESI)**: *m*/*z* calculated for $C_{10}H_7F_5N_2NaS^{+\bullet}$ $[M+Na]^{+\bullet}$ 305.0142, found 305.0146.



3-Ethyl-1-methyl-2-(pentafluoro-λ^6-sulfanyl)-1H-indole 17

In a 5 mL shlenck vial, 3-iodo-1-methyl-2-(pentafluoro-λ^6-sulfanyl)-1H-indole **14** (30 mg, 0.078 mmol) and bis(tri-*tert*-butylphosphine)palladium(0) (2 mg, 5 mol%) were dissolved in THF (0.3 mL) under N_2. At room temperature, diethylzinc (0.2 mL, 2.5 equiv.) solution in THF (1M) was added via a syringe. The black mixture was stirred at 60 °C for 16 hours. The solvent was evaporated and ^{19}F NMR showed product with 78% conversion. It was purified by chromatoghraphy on silica gel (100% P.E) affording a mixture of expected product **17** and reduced product **8** as side product of the reaction. Unfortunately, these 2 products were not separable by chromatography.

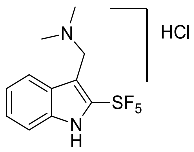
^{1}H-NMR ($CDCl_3$, 500 MHz): δ (ppm) = 1.26 (t, *J* = 7.5 Hz, 3H), 3.03 (q, *J* = 7.4 Hz, 2H), 3.91 (s, 3H), 7.17-7.23 (m, 1H), 7.33-7.42 (m, 2H), 7.68 (d, *J* = 8.0 Hz, 1H); **^{13}C{^{1}H}-NMR ($CDCl_3$, 125 MHz):** δ (ppm) = 15.4, 18.8, 33.2 (quint., *J* = 4.6 Hz), 110.3, 119.1 (quint., *J* = 3.9 Hz), 120.5, 120.9, 124.8, 125.4, 136.2, 143.0-143.6 (m); **^{19}F{^{1}H}-NMR ($CDCl_3$, 471 MHz):** δ (ppm) = 73.0 (d, *J* = 151.6 Hz, 4F), 85.3-86.6 (m, 1F).



Methyl (2E)-3-[1-methyl-2-(pentafluoro-λ⁶-sulfanyl)-1H-indol-3-yl]prop-2-enoate 18

In a 5 mL shlenck vial, 3-iodo-1-methyl-2-(pentafluoro-λ^6-sulfanyl)-1H-indole **14** (30 mg, 0.078 mmol) and palladium acetate (2.25 mg, 20 mol%) and triphenylphosphine (7.12 mg, 40 mol%) were dissolved in DMF (0.4 mL) under N_2. At room temperature, triethylamine (24 µL, 2.5 equiv.) and methyl acrylate (15 µL, 2.5 equiv.) were added via a syringe. The brown mixture was stirred at 100 °C for 12 hours. The solvent was evaporated and ^{19}F NMR showed product with 68% conversion (24% of starting material was not consumed). It was purified by TLC prep (P.E:EtOAc, 90:10) affording **18** (15.4 mg, 58%) as colorless oil.

^{1}H-NMR ($CDCl_3$, 500 MHz): δ (ppm) = 3.85 (s, 3H), 4.00 (s, 3H), 6.56 (d, *J* = 16.1 Hz, 1H), 7.31 (ddd, *J* = 8.1 Hz, *J* = 6.4 Hz, *J* = 1.7 Hz, 1H), 7.41-7.48 (m, 2H), 7.95 (d, *J* = 8.2 Hz, 1H), 8.15 (d, *J* = 16.1 Hz, 1H); **^{13}C{^{1}H}-NMR ($CDCl_3$, 125 MHz):** δ (ppm) = 33.8 (quint., *J* = 4.2 Hz), 51.9, 110.9, 111.7-111.8 (m), 121.2, 122.0, 122.8, 123.2, 126.1, 136.4 (2C), 146.1-146.7 (m), 167.5; **^{19}F{^{1}H}-NMR ($CDCl_3$, 471 MHz):** δ (ppm) = 74.0 (d, *J* = 151.9 Hz, 4F), 83.0-84.3 (m, 1F); **IR spectrum (neat)** (cm^{-1}) = 2984, 1722, 1630, 1469, 1434, 1354, 1058, 978, 851, 782, 676, 597.

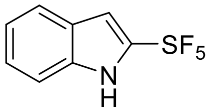
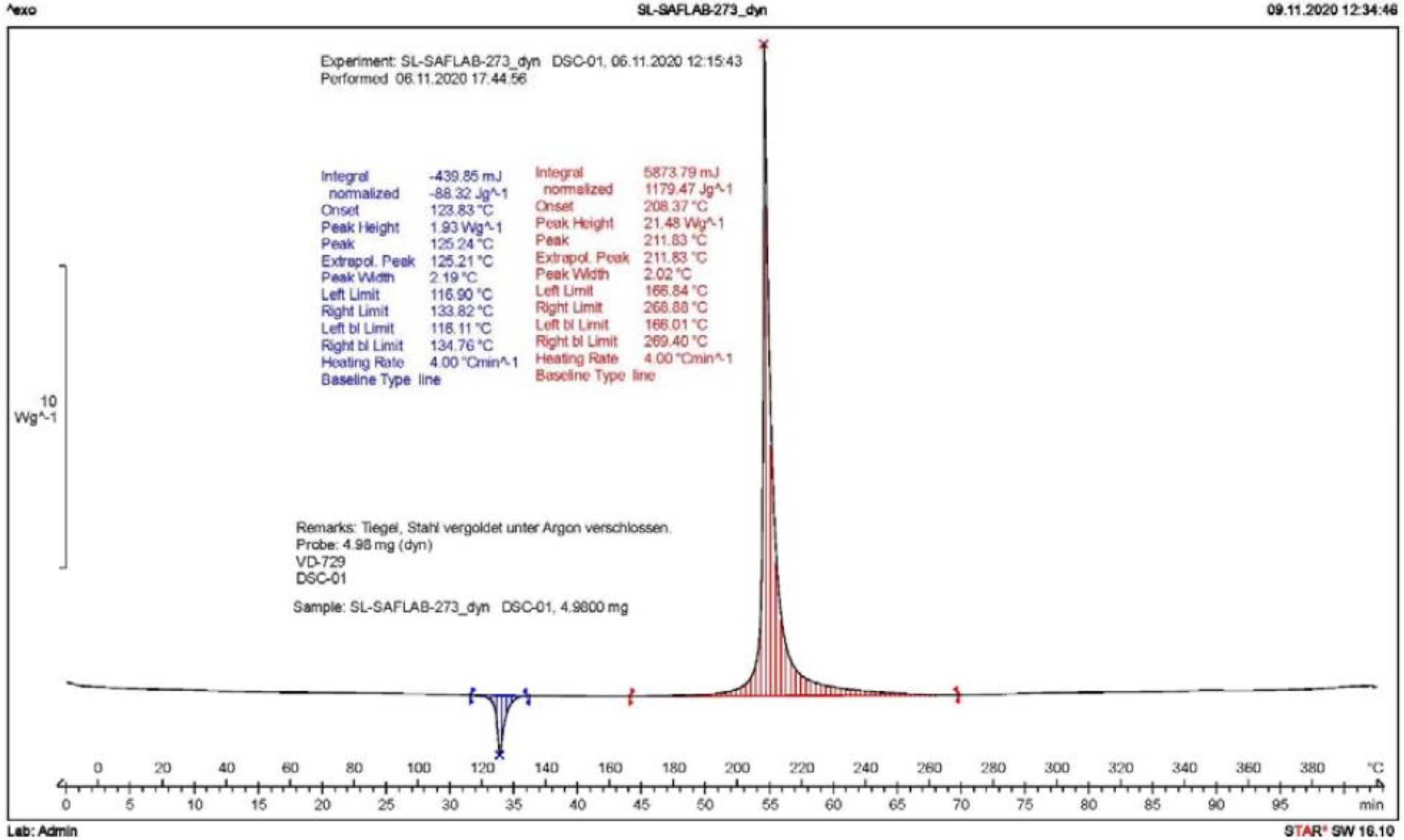


Dimethyl({[2-(pentafluoro-λ⁶-sulfanyl)-1*H*-indol-3-yl]methyl})amine hydrochloride 19

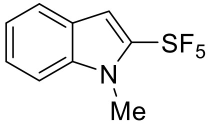
A solution of formaldehyde (10 eq., 185 µL, 2.47 mmol), in AcOH (500 µL), water (240 µL) and 1,4-dioxane (500 µL) was cooled down to 0 °C and Me_2NH (2M in THF) (10 eq., 1.2 mL, 2.47 mmol) was added dropwise to the solution. The mixture was stirred at 0 °C for 5 min and 2-(pentafluoro-λ^6-sulfanyl)-1H-indole **5a** (1 eq., 60 mg, 0.25 mmol) in 1,4-dioxane (0.5 mL) was added slowly to the solution. It was stirred at 0 °C for 2 hours then rt for 16 h. The reaction mixture was quenched with $NaHCO_3$ sat. solution and extracted with EtOAc. The combined organic layers were dried over $MgSO_4$, filtered and concentrated at reduced pressure. HCl (4M in 1,4-dioxane) (123 µL, 2 equiv.) was added dropwise, the solvent was removed, and the product was recrystallized from acetone and pentane affording **19** (47 mg, 57%) as a white powder.

^{1}H-NMR (DMSO d_6, 500 MHz): δ (ppm) = 2.82 (s, 6H), 4.69 (s, 2H), 7.28 (t, *J* = 7.5 Hz, 1H), 7.43 (t, *J* = 7.6 Hz, 1H), 7.56 (d, *J* = 8.3 Hz, 1H), 8.10 (d, *J* = 8.1 Hz, 1H), 9.79 (bs, 1H), 13.19 (s, 1H); **(DMSO d_6, 125 MHz):** δ (ppm) = 42.8, 49.9, 102.4, 112.7, 121.4, 121.5, 124.7, 125.8, 133.5, 143.1 (quint., *J* = 22.5 Hz); **^{19}F{^{1}H}-NMR (DMSO d_6, 471 MHz):** δ (ppm) = 72.4 (d, *J* = 153.5 Hz, 4F), 83.8-85.1 (m, 1F); **IR spectrum (neat)** (cm^{-1}) **=** 2972, 2902, 1714, 1535, 1478, 1435, 1388, 1346, 1307, 1232, 1101, 1018, 974, 930, 838, 771, 744, 670, 581; **HRMS (ESI):** m/z calculated for $C_{11}H_{14}F_5N_2S^{+\bullet}$ $[M+H]^{+\bullet}$ 301.0792, found 301.0815.

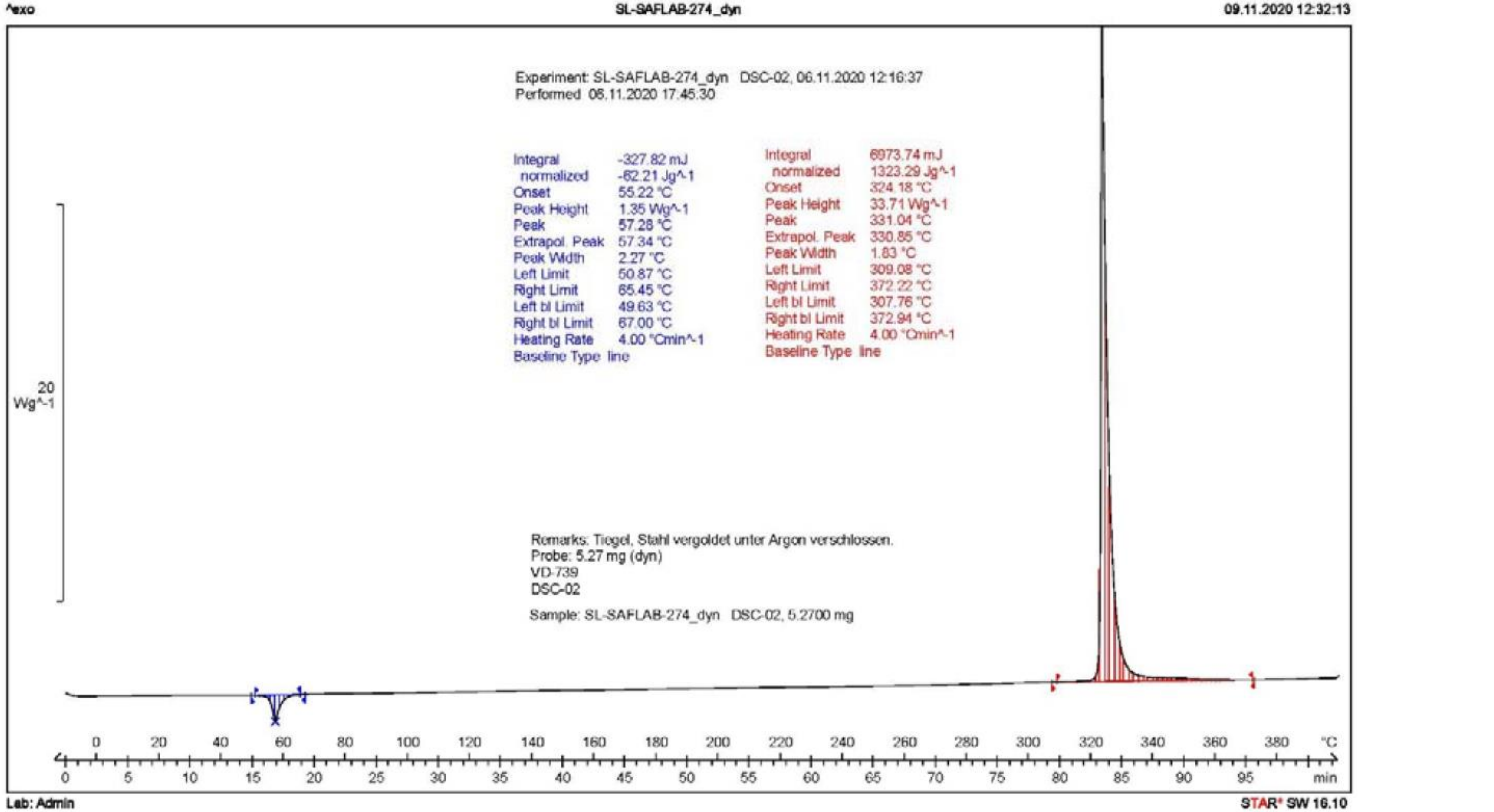
6 DSC Analysis

Substrate	DSC
 5a	

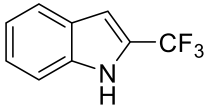
Atm.	Exo. Reaction	Spont. Reaction	Enthalpy	Endo. Reaction	Remarks
Argon	Above ca. 165°C	No	-1180 kJ/kg	From ca. 115°C	Very strong exothermy



8



Atm.	Exo. Reaction	Spont. Reaction	Enthalpy	Endo. Reaction	Remarks
Argon	Above ca. 310°C	Yes	-1324 kJ/kg	From ca. 50°C	Very strong exothermy



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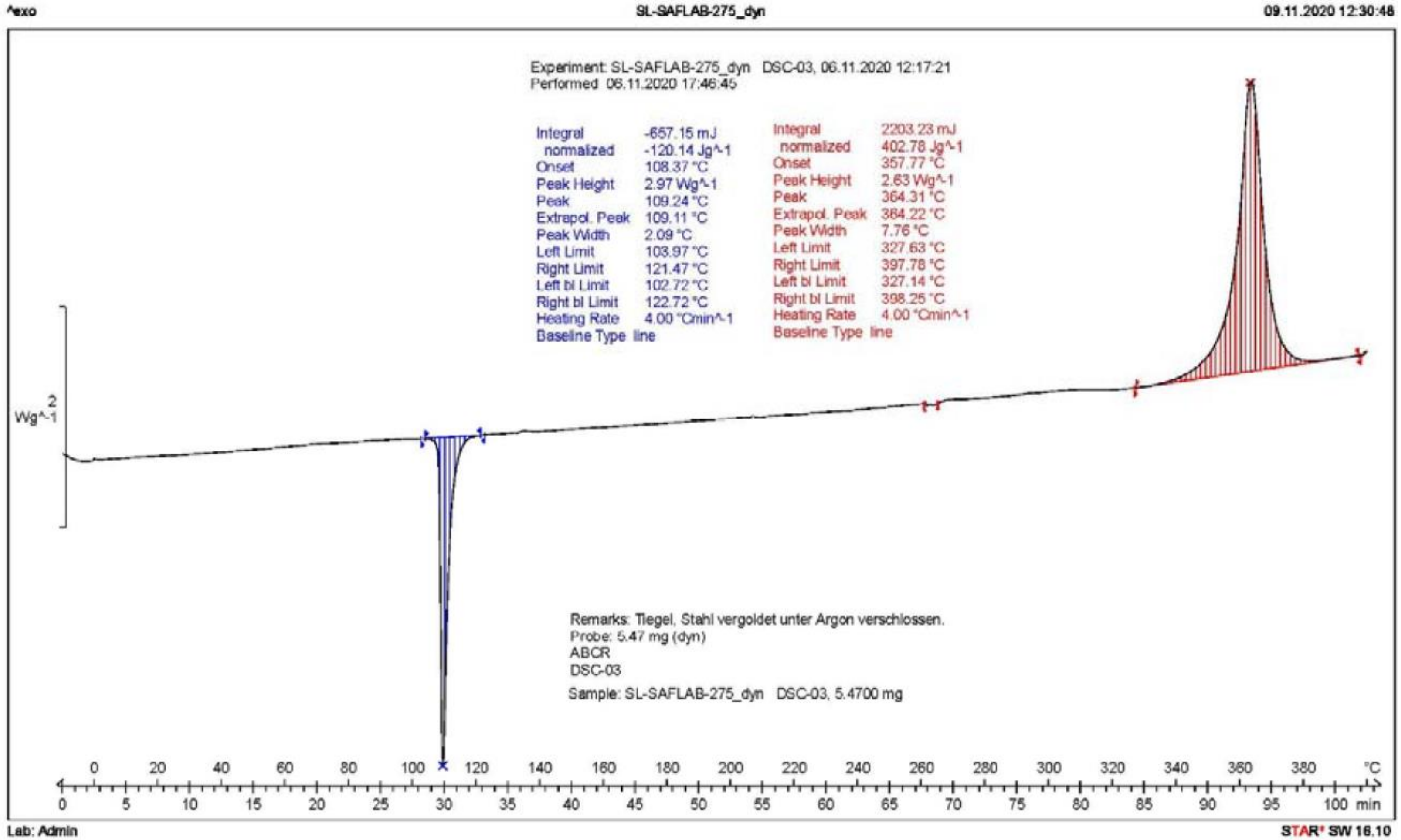
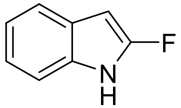


Atm.	Exo. Reaction	Spont. Reaction	Enthalpy	Endo. Reaction
Argon	Above ca. 325°C	No	-403 kJ/kg	From ca. 100°C



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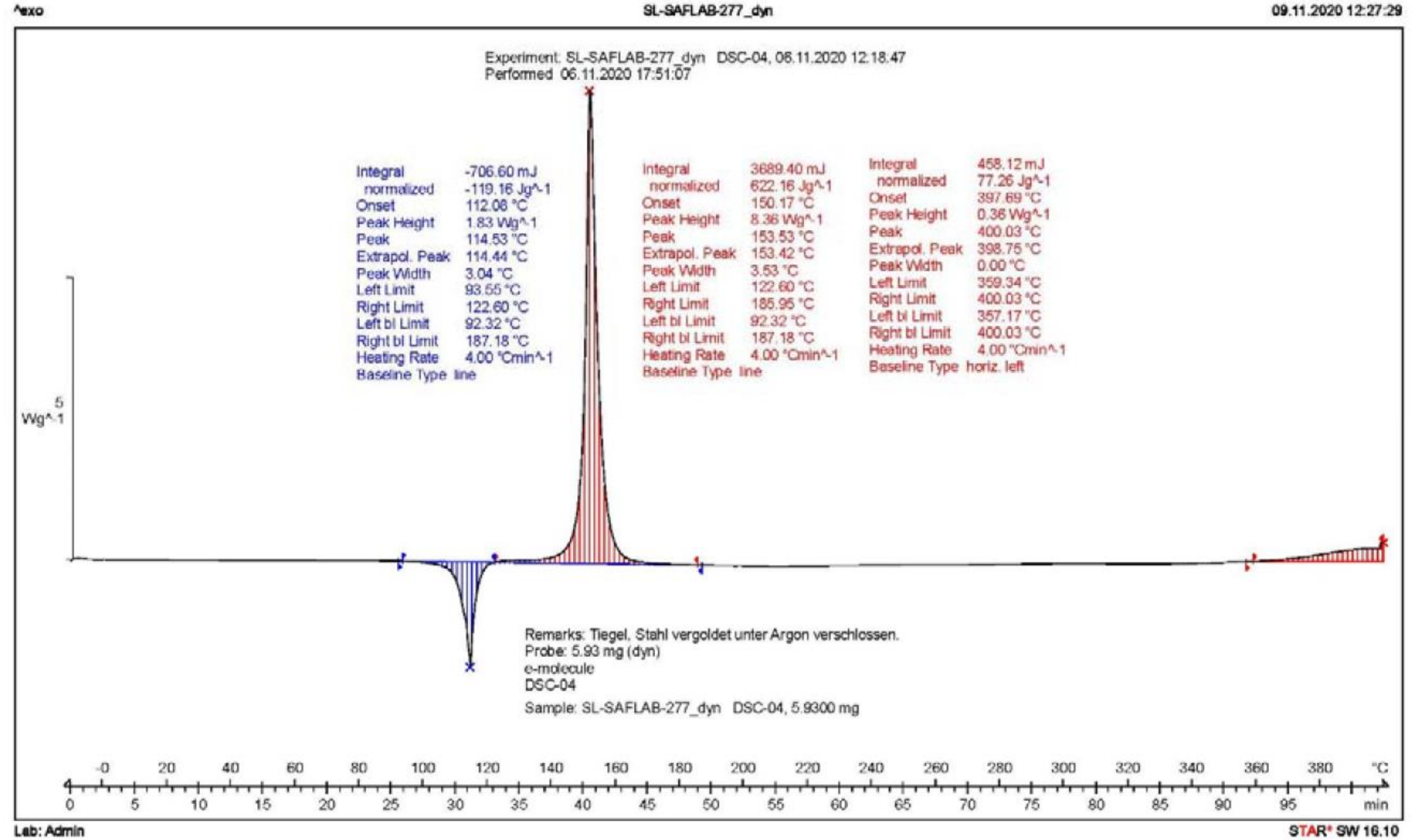
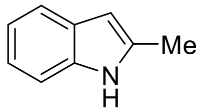


Atm.	Exo. Reaction	Spont. Reaction	Enthalpy	Endo. Reaction	Remarks
Argon	Above ca. 120°C	No	-623 kJ/kg	From ca. 90°C	First strong exothermy shortly after the melting process
Argon	Above ca. 360°C	No	at least -78 kJ/kg	-	Second exothermy



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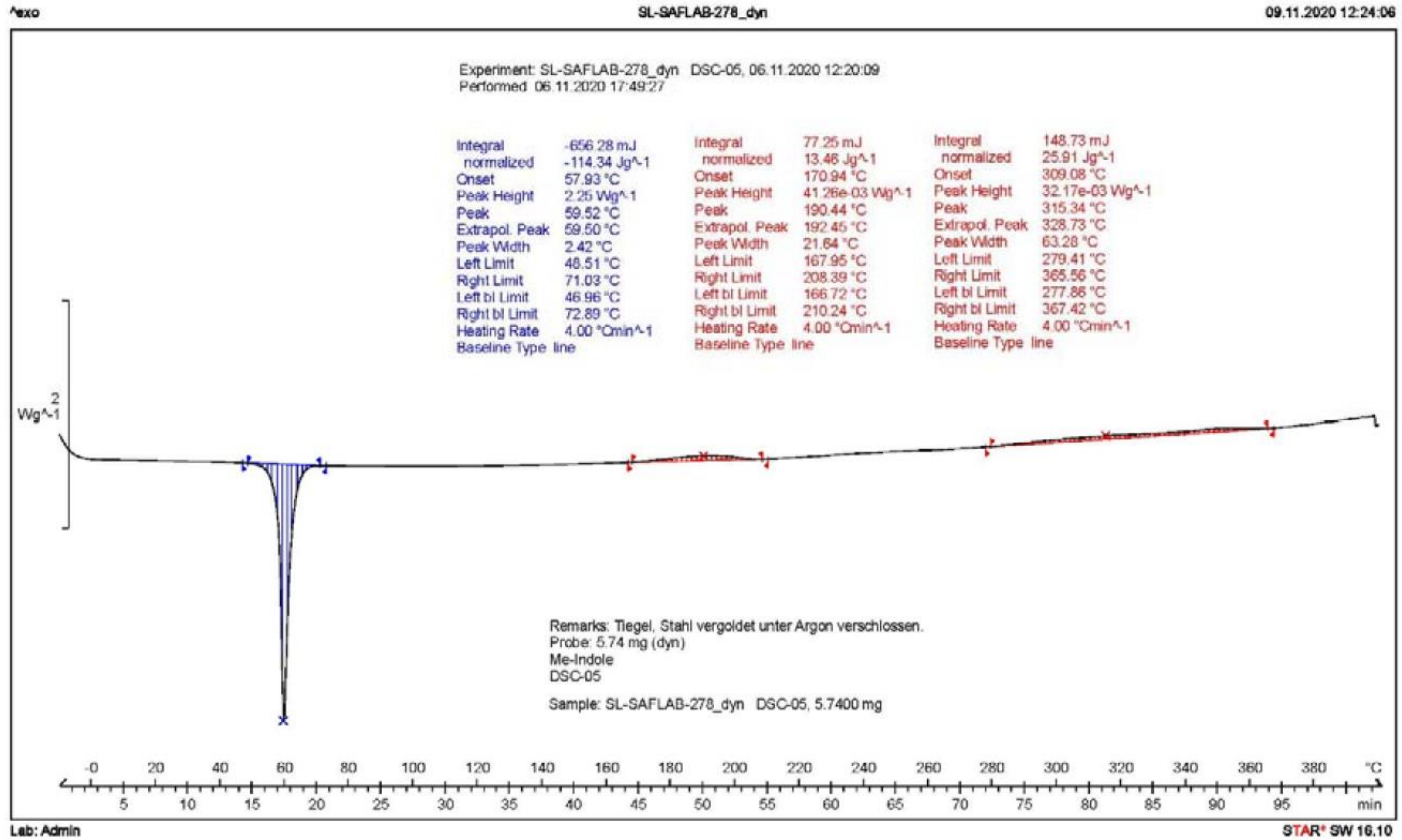
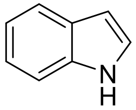


Atm.	Exo. Reaction	Spont. Reaction	Enthalpy	Endo. Reaction	Remarks
Argon	Above ca. 165°C	No	-14 kJ/kg	From ca. 45°C	First very weak exothermy
Argon	Above ca. 200°C	No	-26 kJ/kg	-	Second weak exothermy



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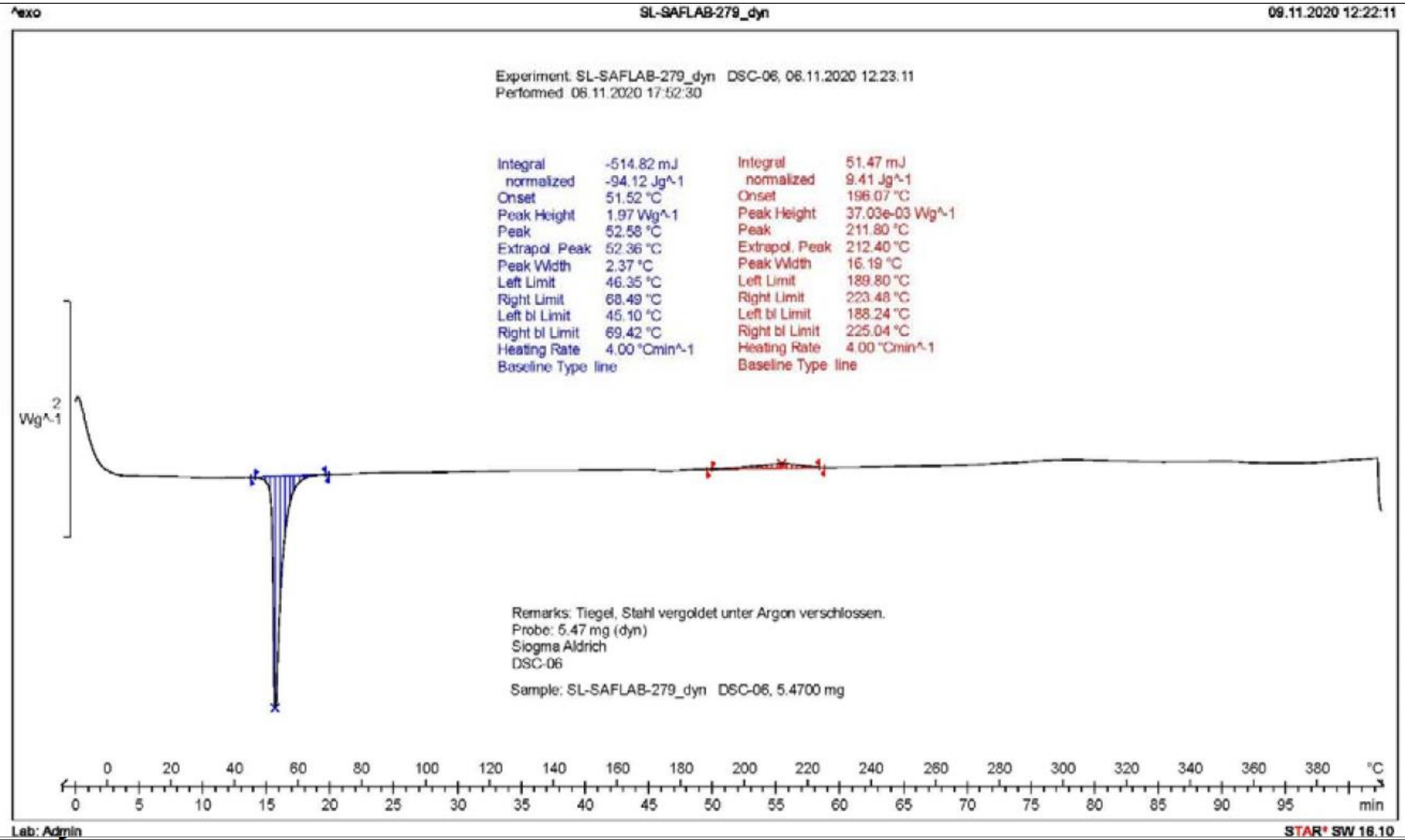


Atm.	Exo. Reaction	Spont. Reaction	Enthalpy	Endo. Reaction	Remarks
Argon	Above ca. 190°C	No	-10 kJ/kg	From ca. 45°C	Very weak exothermy

In-Silico Assessment :

Compound	**ICH M7 Class[2]**	**Summary of the results and conclusions**
2-(pentafluoro- λ^6-sulfaneyl)-1H-indole No CAS	Uncertain	No structural concern for mutagenicity detected in Derek. Outside domain in Sarah Nexus with one positive prediction hypothesis identified, which is based on indole moiety. Positive Case Ultra prediction was obtained with alerts that were located in indole moiety. Indole is considered to be non-mutagenic and therefore there is no mutagenicity concern emerging from the indole moiety itself. Uncovered fragments detected in all three systems (SF_5 moiety). Hence, due to incomplete coverage, it is recommended to perform an Ames test to evaluate potential mutagenic activity of the SF5 fragment
1-methyl-2-(pentafluoro-λ^6-sulfaneyl)-1H-indole No CAS	Uncertain	No structural concern for mutagenicity detected in Derek. Outside domain in Sarah Nexus with one positive prediction hypothesis identified that is based on indole moiety. Positive Case Ultra prediction was obtained with alerts that were located in indole moiety. Indole is considered to be non-mutagenic and therefore there is no mutagenicity concern emerging from the indole moiety. Uncovered fragments detected in all three systems (SF_5 moiety). Hence, due to incomplete coverage, it is recommended to perform an Ames test to evaluate potential mutagenic activity of the SF5 moiety
2-trifluoromethylindole CAS 51310-54-4	4	No structural concern for mutagenicity detected using Derek and Sarah Nexus. Case Ultra gave a positive prediction; however, the same positive alerts were obtained for indole, which was shown to be non-mutagenic in Ames test. 2-trifluoromethylindole can therefore be considered as non-mutagenic impurity.
2-difluoromethylindole No CAS	4	No structural concern for mutagenicity detected in Derek and Sarah. Inconclusive result obtained in Case Ultra, however, detected positive alerts were also obtained for indole, which is considered non-mutagenic. Can be considered as non-mutagenic impurity.
2-fluoroindole No CAS	4	No structural alert for mutagenicity detected in Derek. Positive Sarah prediction based on indole moiety. In addition, positive Case Ultra prediction was obtained with alerts that were also detected for indole. Considering that indole was shown to be non-mutagenic, 2-fluoroindole can be considered non-mutagenic.
2-methyl-1H-indole CAS 95-20-5	5	Not mutagenic in Ames test (EFSA, 2018)[3]
1H-indole CAS 120-72-9	5	Can be considered as a non-mutagenic compound (EFSA, 2018)[3]

Class assignments of compounds (according to Müller et al 2006)[4]

- Class 1: Known mutagenic carcinogens
- Class 2: Known mutagens with unknown carcinogenic potential
- Class 3: Alerting structure, unrelated to the structure of the drug substance
- Class 4: Alerting structure, same alert in drug substance or compounds related to the drug substance (e.g., process intermediates) which have been tested and are non-mutagenic
- Class 5: No structural alerts, or alerting structure with sufficient data to demonstrate lack of mutagenicity

Methodology & Computer systems

- Derek Nexus, v. 6.1.0, KB 2020 1.0 (Lhasa Ltd. Leeds, UK)
- Sarah Nexus v. 3.1.0 Model 2020.1 (Lhasa Ltd. Leeds, UK)
- Case Ultra v. 1.8.0.2 (MultiCASE Inc, Beachwood, Ohio, USA)

7 Physico-chemical properties

7.1 pK_a determination in acetonitrile

The experimental methodology and setup for the pK_a determination in acetonitrile (MeCN) were essentially the same as described in more detail in a previous publication.[5] A brief description of the spectrophotometric titration method will be given here.

The pK_a determination in acetonitrile is based on the determination of differences of pK_a values of two acids of which one is a reference acid with a previously published pK_a value, and the other is a compound with an unknown pK_a value. In the present paper the acid with an unknown pK_a value is a substituted indole. These indoles, as well as the reference acids are separately titrated to obtain the UV-Vis spectra of the protonated as well as their deprotonated forms. Then the same titration is done with a mixture consisting of an indole and a reference acid in the same solution. After mathematically treating the spectral data obtained from the titration of the mixture at multiple wavelengths using multilinear regression analysis the dissociation levels $\alpha = [A^-]/([A^-] + [HA])$ of both acids in all the mixtures formed during titration are calculated and are then in turn used to calculate the differences of pK_a values (ΔpK_a) of the indoles and the used reference acids according to the following equation:

$$\Delta \mathrm{p}K_\mathrm{a} = \log \frac{\alpha_1(1-\alpha_2)}{\alpha_2(1-\alpha_1)}$$

The pK_a values of **2-F-indole, 2-CF_3-indole** and **2-SF_5-indole** are calculated as a result of ΔpK_a measurements against at least three different reference acids. Compounds with previously published pK_a values in acetonitrile were used as reference acids.[6]

An Agilent Cary 60 spectrophotometer (scanning speed 600 nm/min) connected with optical fibre cables to an external cell compartment inside a MBraun Unilab glovebox filled with 99.999 % pure argon was used for the spectrophotometric titrations. This setup ensured that during all titrations the moisture and oxygen contents inside the glovebox were always under 10 ppm.

Methanesulfonic acid (Aldrich, 99+ %) was used to prepare the acidic titrant solution and t*ert*-butylimino-tris(pyrrolidino)phosphorane (Aldrich, ≥97 %) or Phosphazene base P2-Et (Aldrich, ≥98.0%) were used to prepare the basic titrant. The concentration of the acidic titrant was in the range of 5.7 - 8.2·10^{-3} mol L^{-1} and the concentration of the basic titrant was 1.7 - 3.1·10^{-3} mol L^{-1}. The concentrations of the studied indoles were between 5.4 - 8.6·10^{-5} mol L^{-1} during the titrations.

Acetonitrile (Romil 190 SpS far UV/gradient quality) was used as solvent after drying with molecular sieves (3 Å) for at least 12 hours, which ensured a water content of under 6 ppm. Water content of the solvent was monitored using coulometric Karl Fischer titration.

Table 1. pK_a measurement results in acetonitrile

Acid	Reference acid (Ref)	pK_a (Ref)	ΔpK_a	pK_a (Acid)	Assigned pK_a
2-SF$_5$-indole	$(C_6H_5)(C_6F_5)CHCN$	26.16	1.72	24.44	**24.44**
	9-$COOCH_3$-fluorene	23.54	-0.95	24.49	
	2,3,4,5,6-$(CF_3)_5$-aniline	24.57	0.18	24.39	
2-CF$_3$-indole	$(C_6H_5)(C_6F_5)CHCN$	26.16	-0.62	26.78	**26.76**
	(4-Me-C_6F_4)$(C_6H_5)CHCN$	26.98	0.26	26.72	
	$C_6F_5NHCOCH_3$	26.45	-0.33	26.78	
2-F-indole	(4-Me-C_6F_4)$(C_6H_5)CHCN$	26.98	-0.17	27.15	**27.20**
	9-C_6F_5-fluorene	28.14	0.90	27.24	
	$(C_6H_5)(C_6F_5)CHCN$	26.16	-1.05	27.21	
	$C_6F_5NHCOCH_3$	26.45	-0.68	27.13	

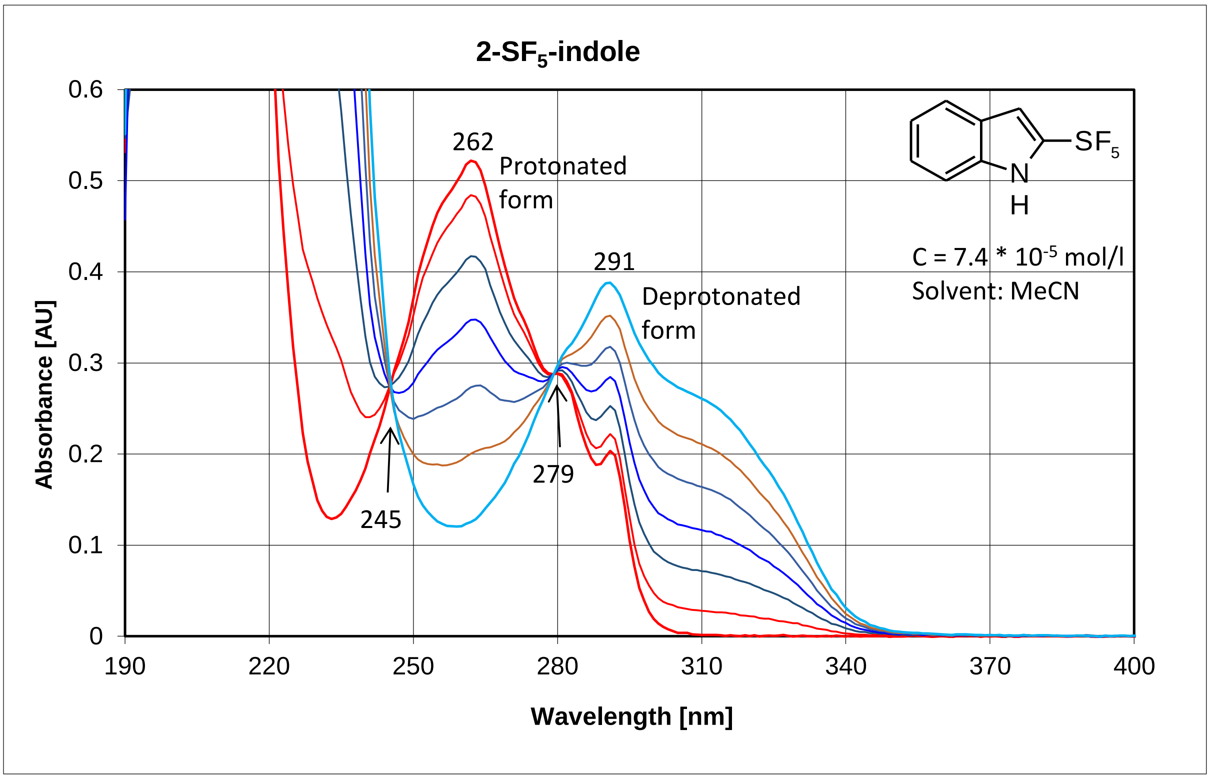


Figure 1. UV-Vis titration spectra of 2-SF$_5$-indole

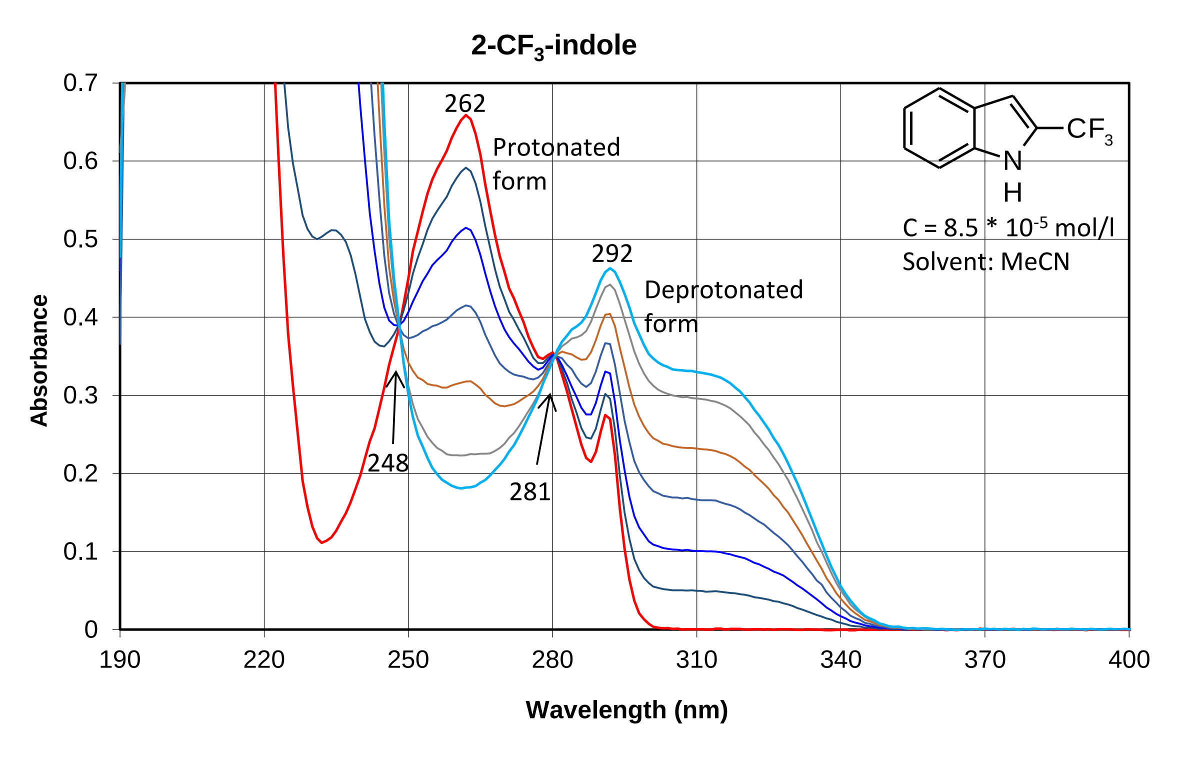


Figure 2. UV-Vis titration spectra of 2-CF_3-indole

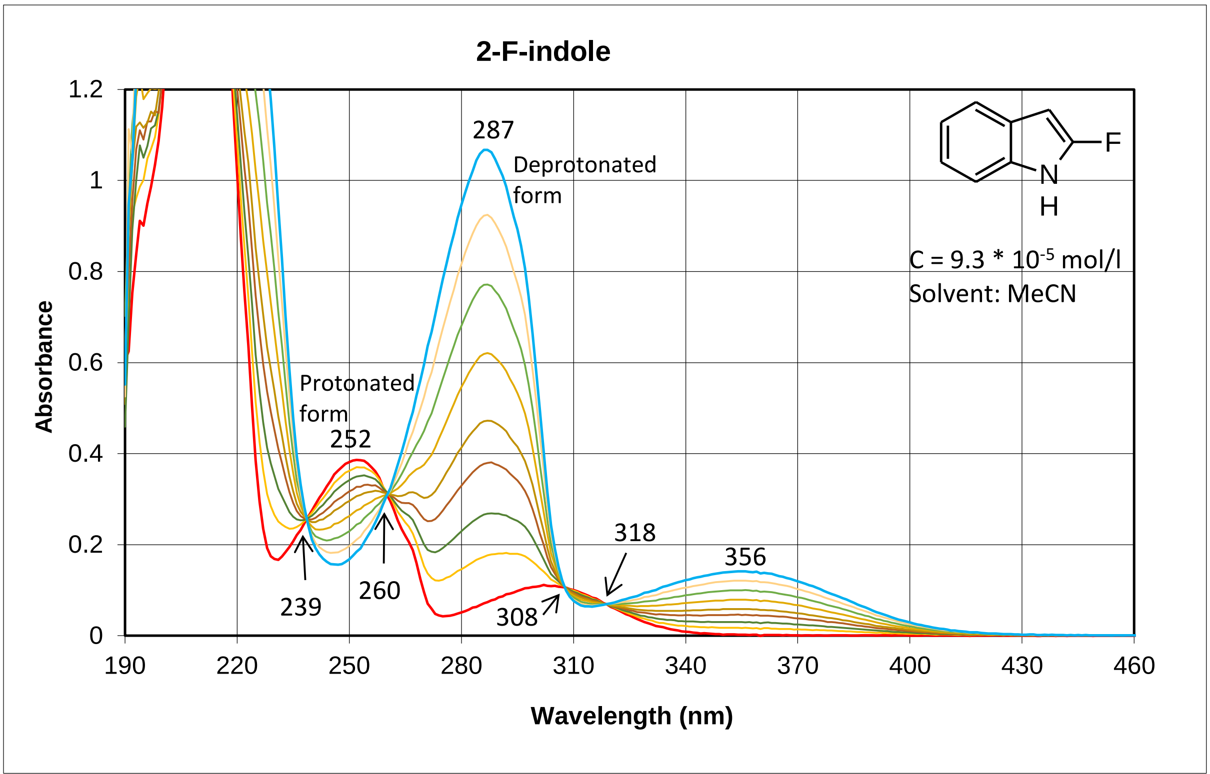


Figure 3. UV-Vis titration spectra of 2-F-indole

7.2 Log*P* measurements

The log*P* values in the 1-octanol/water system were determined using four approaches:

I. **Direct determination by shake-flask method.**[7] The preferred approach, as it does not rely on assumptions or extrapolations. However, the used methodology is not very accurate for high (>3.5) and not applicable for very high log*P* values.

0.03-1.4 mg or the studied compound was combined in a chromatographic vial with 0.5 ml of 1-octanol (Sigma-Aldrich, ≥99%) and 0.5 ml of water and shaken for 45-50 min at ambient temperature (22°C). Both liquid phases were then analysed by RP-HPLC with UV-Vis detection and log*P* values were calculated from the ratio of peak areas in two phases. Please see ref. 7 for a more detailed description. Replicate measurements were carried out on three different days. Compounds were analysed individually (i.e. only one analyte in each vial) to avoid the effect of possible analyte-analyte interactions on the results.

II. **Computationally supplemented chromatographic method**.

The retention factors of the studied compounds in C18 column at several different fractions of methanol in the eluent were measured and combined with some calculated descriptors to produce log*P* values. Please see ref 8 for details. The results are the averages of the three predictive equations derived in ref 8.

III. **Correlation between chromatographic retention factors and lipophilicities** for a group of 7 structurally related compounds. This approach is better tuned to the compounds of interest compared to a more universal approach II.

Experimental procedure were as in ref 8.

IV. Empirically corrected **COSMO-RS**[9-11] computations. COSMO-RS gives quite accurate log*P* predictions for small molecules.[12] Correlation between experimental (from lit.) and computational values for a group of similar compounds was used to confirm the accuracy and correct a minor systematic bias of calculated values.

Calculations were performed as described in ref 8.

The results are summarized in Table 1. Consensus values were assigned to compounds based on relative reliabilities of the used approaches in each case.

Table 1. Results of log*P* determination by different methods. *u* is an estimate of standard uncertainty.

Compound	**I (±*u*)**	**II**	**III**	**IV**	**Assigned log*P* (± *u*)**
2-Fluoroindole	1.29 (±0.01)	1.2	1.1	2.7	1.29 (±0.05)
2-CF_3-indole	3.64 (±0.10)	3.3	3.4	3.5	3.5 (±0.2)
2-SF_5-indole	3.75 (±0.15)	3.7	3.7	3.9	3.8 (±0.2)
2-SF_5-N-methylindole	-	4.3	4.6	4.2	4.3 (±0.3)
Method's *u*:		0.3	0.3	0.2	

log*P* values of substituted indoles

Summary

	Method:	1 (shake-flask)	2 (HPLC)	3 (HPLC)	4 (COSMO-RS)	Consensus:	u (estimate of standard uncertainty)
2-Fluoroindole		1,29	1,2	1,1	2,7	1,29	0,05
2-CF_3-indole		3,6	3,3	3,4	3,5	3,5	0,2
2-SF_5-indole		3,8	3,7	3,7	3,9	3,8	0,2
2-SF_5-N-methylindole			4,3	4,6	4,2	4,3	0,3
	Method's u:	(varies)	0,3	0,3	0,2		

Method 1: Direct determination with shake-flask method. Methodology described in details in *ACS Omega* 2017, 2, 7772 (doi.org/10.1021/acsomega.7b01445)

	Replicate determinations of log*P* * (less reliable in red)							Mean **	St.dev(all)	St.dev(reliable)	Weighed st.dev. ***
	day 1		day 2			day 3					
2-Fluoroindole	1,29		1,29	1,28		1,30		1,29	0,01	0,01	0,01
2-CF_3-indole	3,71	3,57	3,48	3,71	3,60	3,74	3,72	3,64	0,10	0,10	0,10
2-SF_5-indole	4,01	3,73	3,77	4,13		3,75	4,19	3,75	0,20	0,02	0,15

* Different values on the same day were obtained from the same solutions under different chromatographic conditions
** Mean value was calculated from more reliable (black) values
*** Weighed estimate of standard error, see ACS Omega 2017, 2, 7772 for details

Method 2: using retention data and equations from *Anal. Chim. Acta* 2020, 1132, 123 (doi.org/10.1016/j.aca.2020.07.024)

	log*k* = *f* (v% MeOH)					PaDel descriptors				Predicted log*P*			
	60	70	80	90	Slope	MLFER_E	nAtomP	nAtomLAC	McGowan_Volume	Eq.3	Eq.4	Eq.5	Mean
2-Fluoroindole	-0,39	-0,65	-0,89		-0,02	1,108	9	0	0,9641	1,2	1,4	1,1	1,2
2-CF_3-indole	0,8	0,34	-0,08		-0,04	0,934	9	0	1,1404	3,3	3,5	3,1	3,3
2-SF_5-indole	0,97	0,49	0,04	-0,41	-0,05	0,903	9	0	1,2844	3,7	3,8	3,5	3,7
2-SF_5-N-methylindole		0,82	0,33	-0,13	-0,05	0,912	9	0	1,4253	4,3	4,3	4,3	4,3

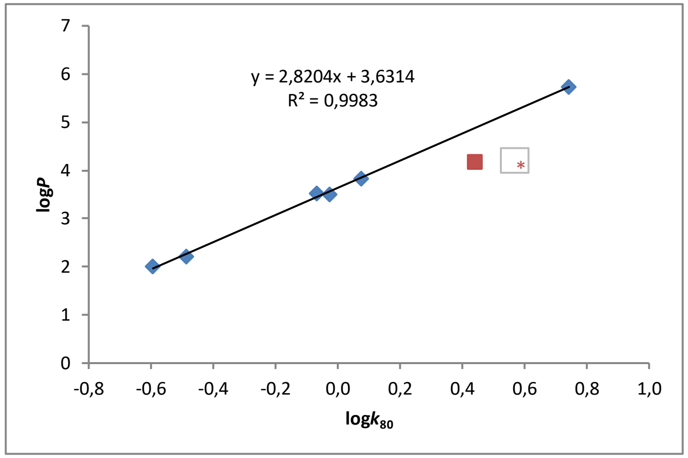
RMSE(LOO) = 0,3

Method 3: using log*P* =*f* (log*k*) correlation for similar compounds

	$\log k_{80}$	log*P* (Lit.)
Indoxyl acetate	-0,59	2,01
Indole	-0,48	2,21
Triphenylamine	0,75	5,74
1,4-Bis(trifluoromethyl)benzene	0,08	3,83
Carbazole	-0,07	3,52
Diphenylamine	-0,03	3,50
(Fluorene - excluded) *	0,44	4,18

		Predicted:
2-Fluoroindole	-0,89	1,12
2-CF_3-indole	-0,08	3,41
2-SF_5-indole	0,04	3,74
2-SF_5-N-methylindole	0,33	4,57

Expected standard uncertainty: 0,3



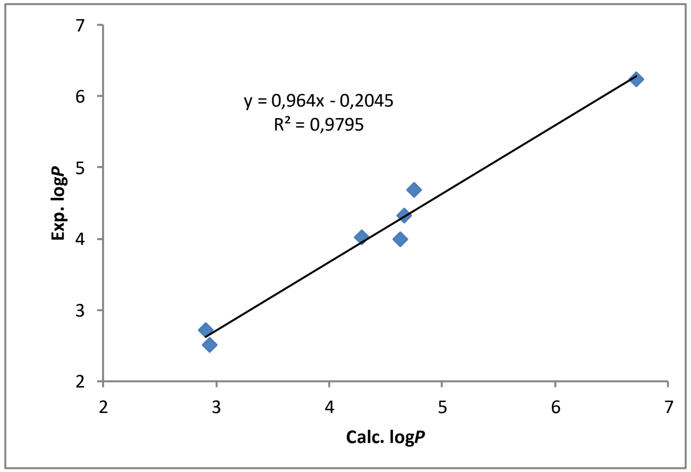
* Reason for deviation is uncertain: possibly too different structure, possibly error of the method.
Fluorene was not used for building correlation equation but taken into account when estimating uncertainty.

Method 4: empirically corrected COSMO-RS calculations

	Calc. log*P*	Exp. log*P* (Lit.)
Indoxyl acetate	2,4	2,01
Indole	2,4	2,21
Triphenylamine	6,2	5,74
1,4-Bis(trifluoromethyl)benzene	4,2	3,83
Carbazole	3,8	3,52
Diphenylamine	4,1	3,50
Fluorene	4,3	4,18

		Predicted:
2-Fluoroindole	3,0	2,7
2-CF_3-indole	3,9	3,5
2-SF_5-indole	4,2	3,9
2-SF_5-N-methylindole	4,5	4,2

Expected standard uncertainty: 0,2



8 Ames test

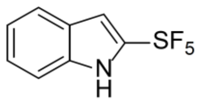
Test Item Information:

Test item: 2-(pentafluoro-λ6-sulfaneyl)-1H-indole

Vehicle: Dimethyl sulphoxide (DMSO)

Purity/Content of drug: >98%

Molecular Structure:



2-(pentafluoro-λ^6-sulfaneyl)-1*H*-indole
Chemical Formula: $C_8H_6F_5NS$
Molecular Weight: 243.20

Conclusion:

Under the testing conditions used and applying standard mutagenicity criteria, 2-(pentafluoro-λ6-sulfaneyl)-1H-indole did not show evidence of a mutagenic potential in strains TA98, TA100, TA1535, TA97a or TA102 in the absence or presence of S-9.

Results:

Concentrations tested:

- 16, 50, 160, 500, 1600 and 5000 μg/plate (using all strains +/-S-9).

Precipitation and toxicity:

No precipitation of test article was observed on any of the test plates following incubation.

Evidence of toxicity, ranging from a thinning of the background bacterial lawn with a concurrent marked reduction in revertant numbers to a complete killing of the test bacteria, was observed in all strains in both the absence and presence of S-9 at concentrations of 500 μg/plate and above.

Mutagenicity:

Data from control treatments confirmed the correct strain and assay functioning, and the data were accepted as valid.

Following treatment with 2-(pentafluoro-λ6-sulfaneyl)-1H-indole, there were no increases in the number of revertants of at least 2-fold (1.5-fold for strain TA102 or 3-fold for strain TA1535) the concurrent vehicle controls for any strains tested in the absence or presence of S-9.

Analysis of Results:

Acceptance Criteria

The assay was considered valid as all the following criteria were met:

1. Vehicle control counts fell within the normal ranges
2. The positive control chemicals induced increases in revertant numbers of ≥1.5-fold (in strain TA102), ≥2-fold (in strains TA98, TA100 and TA97a) or ≥3-fold (for strain TA1535) the concurrent vehicle controls confirming discrimination between different strains, and an active S-9 preparation.

Evaluation Criteria

For valid data, the test item was considered mutagenic in this assay if:

A concentration related increase in revertant numbers of ≥1.5-fold (in strain TA102), ≥2-fold (in strains TA98, TA100 or TA97a) or ≥3-fold (for strain TA1535) the concurrent vehicle control values was observed.

The test item was regarded positive in this assay if the above criterion was met.

The test item was regarded negative in this assay if the above criterion was not met.

Methods:

Strains of *Salmonella typhimurium* Used: TA98, TA100, TA1535, TA97a and TA102.

Metabolic Activation System: Liver S-9 mix from male rats, β-Naphthoflavone/Phenobarbital pretreated. Per plate, 0.5 mL of 10% S-9 mix was added.

Controls:

Vehicle control treatments comprised additions at the same volume per plate (0.1 mL) as the test item solutions. Positive control treatments comprised 0.05 mL volume additions. Negative controls comprised treatments with the chosen vehicle.

The positive control chemicals were supplied and used as shown in the following table:

Chemical*	Stock** concentration (μg/mL)	Final concentration (μg/plate)	Use	
			Strain(s)	S-9
2-nitrofluorene (2NF)	100	5	TA98	–
Sodium azide (NaN_3)	40	2	TA100, TA1535	–
9-Aminoacridine (AAC)	2000	100	TA97a	–
Mitomycin C (MMC)	4	0.2	TA102	–
Benzo[a]pyrene (B[a]P)	200	10	TA98	+
2-aminoanthracene (AAN)	100	5	TA100, TA1535, TA97a	+
	400	20	TA102	+

* Obtained from Sigma-Aldrich.

** Stock solutions were formulated in water (NaN_3 and MMC), or in DMSO (2NF, AAC, AAN and B[a]P). Unless used on the day of preparation, all stock solutions were stored in aliquots protected from light at 2-8°C, with the exception of B[a]P and MMC which were stored in aliquots at <-50ºC.

Raw Plate Counts, Toxicity Data and Calculated Mutagenicity Data

Table 1 **2-(pentafluoro-λ6-sulfaneyl)-1H-indole Raw Plate Counts, Toxicity Data and Calculated Mutagenicity Data, –S-9**

Strain	Test Item	Conc. Level (µg/plate)	Mean	Fold Increase	Revertant Numbers Per Plate
TA98	DMSO	-	26.0	-	28, 21, 29
	2-(pentafluoro-λ6-sulfaneyl)-1H-indole	16	29.0	1.1	27, 32, 28
		50	27.3	1.1	24, 22, 36
		160	26.3	1.0	24, 30, 25
		500	-	-	- T, - T, - T
		1600	-	-	- T, - T, - T
		5000	-	-	- T, - T, - T
	2NF	5	897.0	34.5	947, 865, 879
TA100	DMSO	-	115.7	-	114, 115, 118
	2-(pentafluoro-λ6-sulfaneyl)-1H-indole	16	116.3	1.0	117, 111, 121
		50	128.3	1.1	122, 129, 134
		160	129.7	1.1	139, 122, 128
		500	-	-	- T, - T, - T
		1600	-	-	- T, - T, - T
		5000	-	-	- T, - T, - T
	NaN_3	2	1458.3	12.6	1477, 1466, 1432
TA1535	DMSO	-	25.7	-	23, 24, 30
	2-(pentafluoro-λ6-sulfaneyl)-1H-indole	16	23.7	0.9	29, 17, 25
		50	25.0	1.0	29, 26, 20
		160	27.3	1.1	25, 26, 31
		500	-	-	- T, - T, - T
		1600	-	-	- T, - T, - T
		5000	-	-	- T, - T, - T
	NaN_3	2	1283.0	50.0	1287, 1346, 1216
TA97a	DMSO	-	98.7	-	89, 103, 104
	2-(pentafluoro-λ6-sulfaneyl)-1H-indole	16	106.3	1.1	108, 97, 114
		50	91.0	0.9	87, 76, 110
		160	88.3	0.9	83, 90, 92
		500	-	-	- T, - T, - T
		1600	-	-	- T, - T, - T
		5000	-	-	- T, - T, - T
	AAC	100	1812.7	18.4	1801, 1877, 1760

Table continued overleaf

Table 1 Continued 2-(pentafluoro-λ6-sulfaneyl)-1H-indole Raw Plate Counts, Toxicity Data and Calculated Mutagenicity Data, –S-9

Strain	Test Item	Conc. Level (µg/plate)	Mean	Fold Increase	Revertant Numbers Per Plate
TA102	DMSO	-	236.0	-	217, 261, 230
	2-(pentafluoro-λ6-sulfaneyl)-1H-indole	16	258.3	1.1	260, 264, 251
		50	272.7	1.2	267, 262, 289
		160	247.7	1.0	256, 255, 232
		500	-	-	- T, - T, - T
		1600	-	-	- T, - T, - T
		5000	-	-	- T, - T, - T
	MMC	0.2	1511.7	6.4	1485, 1402, 1648

Positive Controls		Postfixes	
2NF	2-nitrofluorene	T	Toxic, no revertant colonies
NaN_3	Sodium azide		
AAC	9-Aminoacridine		
MMC	Mitomycin C		

Table 2 2-(pentafluoro-λ6-sulfaneyl)-1H-indole Raw Plate Counts, Toxicity Data and Calculated Mutagenicity Data, +S-9

Strain	Test Item	Conc. Level (µg/plate)	Mean	Fold Increase	Revertant Numbers Per Plate
TA98	DMSO	-	31.7	-	39, 29, 27
	2-(pentafluoro-λ6-sulfaneyl)-1H-indole	16	27.0	0.9	23, 33, 25
		50	25.3	0.8	29, 20, 27
		160	31.0	1.0	26, 28, 39
		500	16.7	0.5	16 M S, 25 M S, 9 M S
		1600	-	-	- T, - T, - T
		5000	-	-	- T, - T, - T
	B[a]P	10	210.0	6.6	208, 215, 207
TA100	DMSO	-	99.0	-	97, 95, 105
	2-(pentafluoro-λ6-sulfaneyl)-1H-indole	16	110.0	1.1	101, 97, 132
		50	109.7	1.1	90, 120, 119
		160	117.3	1.2	124, 106, 122
		500	38.7	0.4	37 M S, 32 M S, 47 M S
		1600	-	-	- T, - T, - T
		5000	-	-	- T, - T, - T
	AAN	5	2713.3	27.4	2666, 3067, 2407
TA1535	DMSO	-	13.7	-	12, 13, 16
	2-(pentafluoro-λ6-sulfaneyl)-1H-indole	16	18.7	1.4	18, 12, 26
		50	16.7	1.2	18, 19, 13
		160	17.3	1.3	21, 7, 24
		500	5.0	0.4	6 M S, 6 M S, 3 M S
		1600	-	-	- T, - T, - T
		5000	-	-	- T, - T, - T
	AAN	5	43.7	3.2	51, 39, 41
TA97a	DMSO	-	114.7	-	118, 124, 102
	2-(pentafluoro-λ6-sulfaneyl)-1H-indole	16	108.3	0.9	103, 88, 134
		50	109.7	1.0	117, 115, 97
		160	103.0	0.9	98, 96, 115
		500	-	-	- T, - T, - T
		1600	-	-	- T, - T, - T
		5000	-	-	- T, - T, - T
	AAN	5	650.0	5.7	632, 745, 573

Table continued overleaf

Table 2 Continued 2-(pentafluoro-λ6-sulfaneyl)-1H-indole Raw Plate Counts, Toxicity Data and Calculated Mutagenicity Data, +S-9

Strain	Test Item	Conc. Level (µg/plate)	Mean	Fold Increase	Revertant Numbers Per Plate
TA102	DMSO	-	349.3	-	352, 340, 356
	2-(pentafluoro-λ6-sulfaneyl)-1H-indole	16	338.7	1.0	363, 350, 303
		50	331.7	0.9	313, 344, 338
		160	278.0	0.8	250, 320, 264
		500	-	-	- T, - T, - T
		1600	-	-	- T, - T, - T
		5000	-	-	- T, - T, - T
	AAN	20	3795.7	10.9	4163, 3245, 3979

Positive Controls		Postfixes	
B[a]P	Benzo[a]pyrene	M	Plate counted manually
AAN	2-aminoanthracene	S	Slight thinning of background bacterial lawn
		T	Toxic, no revertant colonies

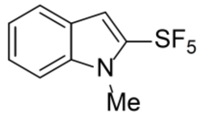
Test Item Information:

Test item: 1-methyl-2-(pentafluoro-λ6-sulfaneyl)-1H-indole

Vehicle: Dimethyl sulphoxide (DMSO)

Purity/Content of drug: >98%

Molecular Structure:



1-methyl-2-(pentafluoro-λ^6-sulfaneyl)-1*H*-indole
Chemical Formula: $C_9H_8F_5NS$
Molecular Weight: 257.22

Conclusion:

Under the testing conditions used and applying standard mutagenicity criteria, 1-methyl-2-(pentafluoro-λ6-sulfaneyl)-1H-indole did not show evidence of a mutagenic potential in strains TA98, TA100, TA1535, TA97a or TA102 in either the absence or presence of S-9.

Results:

Concentrations tested:

- 16, 50, 160, 500, 1600 and 5000 μg/plate (using all strains +/-S-9).

Precipitation and toxicity:

The test article was completely soluble in the aqueous assay system at all concentrations tested.

Evidence of toxicity in the form of a thinning of the background bacterial lawn, with or without a concurrent marked reduction in revertant numbers, was observed in all strains in the absence and presence of S-9, and occurred on all plates treated at 1600 μg/plate and above, and in some cases also on plates treated at 500 μg/plate.

Mutagenicity:

Data from control treatments confirmed the correct strain and assay functioning, and the data were accepted as valid.

Following treatment with 1-methyl-2-(pentafluoro-λ6-sulfaneyl)-1H-indole, there were no increases in the number of revertants of at least 2-fold (1.5-fold for strain TA102 or 3-fold for strain TA1535) the concurrent vehicle controls for any strains tested in the absence or presence of S-9.

Analysis of Results:

Acceptance Criteria

The assay was considered valid as all the following criteria were met:

1. Vehicle control counts fell within the normal ranges
2. The positive control chemicals induced increases in revertant numbers of ≥1.5-fold (in strain TA102), ≥2-fold (in strains TA98, TA100 and TA97a) or ≥3-fold (for strain TA1535) the concurrent vehicle controls confirming discrimination between different strains, and an active S-9 preparation.

Evaluation Criteria

For valid data, the test item was considered mutagenic in this assay if:

A concentration related increase in revertant numbers of ≥1.5-fold (in strain TA102), ≥2-fold (in strains TA98, TA100 or TA97a) or ≥3-fold (for strain TA1535) the concurrent vehicle control values was observed.

The test item was regarded positive in this assay if the above criterion was met.

The test item was regarded negative in this assay if the above criterion was not met.

Methods:

Strains of *Salmonella typhimurium* Used: TA98, TA100, TA1535, TA97a and TA102.

Metabolic Activation System: Liver S-9 mix from male rats, β-Naphthoflavone/Phenobarbital pretreated. Per plate, 0.5 mL of 10% S-9 mix was added.

Controls:

Vehicle control treatments comprised additions at the same volume per plate (0.1 mL) as the test item solutions. Positive control treatments comprised 0.05 mL volume additions. Negative controls comprised treatments with the chosen vehicle.

The positive control chemicals were supplied and used as shown in the following table:

Chemical*	Stock** concentration (μg/mL)	Final concentration (μg/plate)	Use	
			Strain(s)	S-9
2-nitrofluorene (2NF)	100	5	TA98	–
Sodium azide (NaN_3)	40	2	TA100, TA1535	–
9-Aminoacridine (AAC)	2000	100	TA97a	–
Mitomycin C (MMC)	4	0.2	TA102	–
Benzo[a]pyrene (B[a]P)	200	10	TA98	+
2-aminoanthracene (AAN)	100	5	TA100, TA1535, TA97a	+
	400	20	TA102	+

* Obtained from Sigma-Aldrich.

** Stock solutions were formulated in water (NaN_3 and MMC), or in DMSO (2NF, AAC, AAN and B[a]P). Unless used on the day of preparation, all stock solutions were stored in aliquots protected from light at 2-8°C, with the exception of B[a]P and MMC which were stored in aliquots at <-50ºC.

Raw Plate Counts, Toxicity Data and Calculated Mutagenicity Data

Table 1 1-methyl-2-(pentafluoro-λ6-sulfaneyl)-1H-indole Raw Plate Counts, Toxicity Data and Calculated Mutagenicity Data, –S-9

Strain	Test Item	Conc. Level (µg/plate)	Mean	Fold Increase	Revertant Numbers Per Plate
TA98	DMSO	-	15.0	-	19 M B, 11, 15
	1-methyl-2-(pentafluoro-λ6-sulfaneyl)-1H-indole	16	18.3	1.2	20, 20 M B, 15
		50	20.0	1.3	24, 24, 12
		160	19.0	1.3	22, 19, 16
		500	20.0	1.3	23, 17, 20
		1600	20.0	1.3	25 S, 15 S, 20 S
		5000	18.0	1.2	18 M B S, 18 S, 18 S
	2NF	5	944.7	63.0	927, 943, 964
TA100	DMSO	-	119.0	-	129, 102, 126
	1-methyl-2-(pentafluoro-λ6-sulfaneyl)-1H-indole	16	103.0	0.9	91, 112, 106
		50	93.0	0.8	101, 92, 86
		160	106.3	0.9	105, 117, 97
		500	92.0	0.8	90, 98, 88
		1600	87.7	0.7	97 S, 85 S, 81 S
		5000	69.7	0.6	61 S, 63 S, 85 S
	NaN_3	2	1088.7	9.1	1110, 1036, 1120
TA1535	DMSO	-	11.7	-	10, 17, 8
	1-methyl-2-(pentafluoro-λ6-sulfaneyl)-1H-indole	16	12.7	1.1	15, 15, 8
		50	11.7	1.0	10, 17, 8
		160	10.7	0.9	7, 17, 8
		500	15.0	1.3	8 S, 17 S, 20 S
		1600	10.0	0.9	13 S, 8 S, 9 S
		5000	8.3	0.7	8 S, 9 S, 8 S
	NaN_3	2	831.7	71.3	818, 833, 844
TA97a	DMSO	-	93.3	-	81, 92, 107
	1-methyl-2-(pentafluoro-λ6-sulfaneyl)-1H-indole	16	101.0	1.1	105, 91, 107
		50	105.0	1.1	86, 108, 121
		160	101.3	1.1	113, 100, 91
		500	81.0	0.9	93, 82, 68
		1600	86.7	0.9	89 S, 78 S, 93 S
		5000	84.3	0.9	86 S, 77 S, 90 S
	AAC	100	761.7	8.2	866, 605, 814

Table continued overleaf

Table 1 Continued 1-methyl-2-(pentafluoro-λ6-sulfaneyl)-1H-indole Raw Plate Counts, Toxicity Data and Calculated Mutagenicity Data, –S-9

Strain	Test Item	Conc. Level (µg/plate)	Mean	Fold Increase	Revertant Numbers Per Plate
TA102	DMSO	-	250.0	-	252, 236, 262
	1-methyl-2-(pentafluoro-λ6-sulfaneyl)-1H-indole	16	266.0	1.1	279, 264, 255
		50	232.0	0.9	235, 224, 237
		160	202.0	0.8	187, 195, 224
		500	206.7	0.8	209, 210, 201
		1600	161.3	0.6	163 S, 150 S, 171 S
		5000	162.3	0.6	177 S, 146 S, 164 S
	MMC	0.2	1093.7	4.4	1134, 1180, 967

Positive Controls		Postfixes	
2NF	2-nitrofluorene	M	Plate counted manually
NaN_3	Sodium azide	B	Bubbles or split in agar
AAC	9-Aminoacridine	S	Slight thinning of background bacterial lawn
MMC	Mitomycin C		

Table 2 1-methyl-2-(pentafluoro-λ6-sulfaneyl)-1H-indole Raw Plate Counts, Toxicity Data and Calculated Mutagenicity Data, +S-9

Strain	Test Item	Conc. Level (µg/plate)	Mean	Fold Increase	Revertant Numbers Per Plate
TA98	DMSO	-	31.0	-	27, 41, 25
	1-methyl-2-(pentafluoro-λ6-sulfaneyl)-1H-indole	16	24.0	0.8	23, 19, 30
		50	33.3	1.1	40, 30, 30
		160	20.3	0.7	20, 22, 19
		500	31.0	1.0	41, 22, 30
		1600	27.3	0.9	25 S, 25 S, 32 S
		5000	24.7	0.8	24 S, 32 S, 18 S
	B[a]P	10	237.0	7.6	223, 253, 235
TA100	DMSO	-	112.3	-	120, 131, 86
	1-methyl-2-(pentafluoro-λ6-sulfaneyl)-1H-indole	16	151.7	1.4	131, 148, 176
		50	116.3	1.0	116, 119, 114
		160	127.7	1.1	125, 133, 125
		500	103.0	0.9	97, 107, 105
		1600	-	-	- U, - U, - U
		5000	70.0	0.6	76 S, 73 S, 61 S
	AAN	5	2338.0	20.8	2108, 2564, 2342
TA1535	DMSO	-	10.0	-	8, 12, 10
	1-methyl-2-(pentafluoro-λ6-sulfaneyl)-1H-indole	16	16.3	1.6	19, 19, 11
		50	13.0	1.3	15, 12, 12
		160	13.3	1.3	11, 13, 16
		500	7.0	0.7	5 S, 7 S, 9 S
		1600	12.7	1.3	10 S, 15 S, 13 S
		5000	16.7	1.7	10 S, 16 S, 24 S
	AAN	5	65.7	6.6	63, 54, 80
TA97a	DMSO	-	162.7	-	117, 237, 134
	1-methyl-2-(pentafluoro-λ6-sulfaneyl)-1H-indole	16	116.0	0.7	109, 118, 121
		50	102.3	0.6	110, 100, 97
		160	95.3	0.6	110, 95, 81
		500	115.3	0.7	128, 117, 101
		1600	100.3	0.6	95 S, 106 S, 100 S
		5000	107.0	0.7	116 S, 111 S, 94 S
	AAN	5	578.7	3.6	591, 554, 591

Table continued overleaf

Table 2 Continued 1-methyl-2-(pentafluoro-λ6-sulfaneyl)-1H-indole Raw Plate Counts, Toxicity Data and Calculated Mutagenicity Data, +S-9

Strain	Test Item	Conc. Level (µg/plate)	Mean	Fold Increase	Revertant Numbers Per Plate
TA102	DMSO	-	306.0	-	299, 288, 331
	1-methyl-2-(pentafluoro-λ6-sulfaneyl)-1H-indole	16	324.3	1.1	322, 307, 344
		50	317.3	1.0	303, 314, 335
		160	290.7	0.9	334, 285, 253
		500	248.0	0.8	235 S, 255 S, 254 S
		1600	234.0	0.8	246 S, 237 S, 219 S
		5000	220.7	0.7	229 S, 217 S, 216 S
	AAN	20	2768.0	9.0	2819, 2625, 2860

Positive Controls		Postfixes	
B[a]P	Benzo[a]pyrene	S	Slight thinning of background bacterial lawn
AAN	2-aminoanthracene	U	No data obtained

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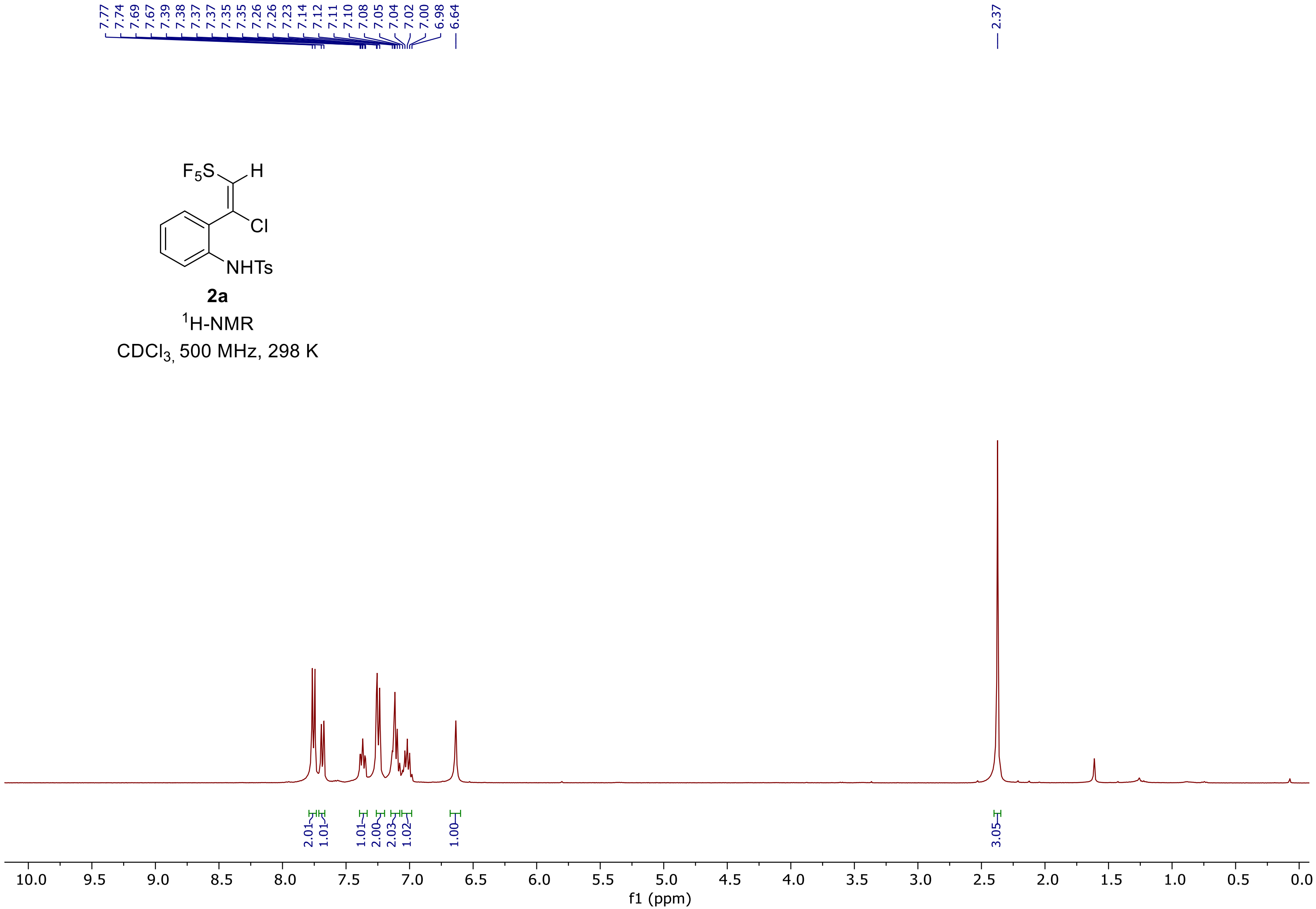
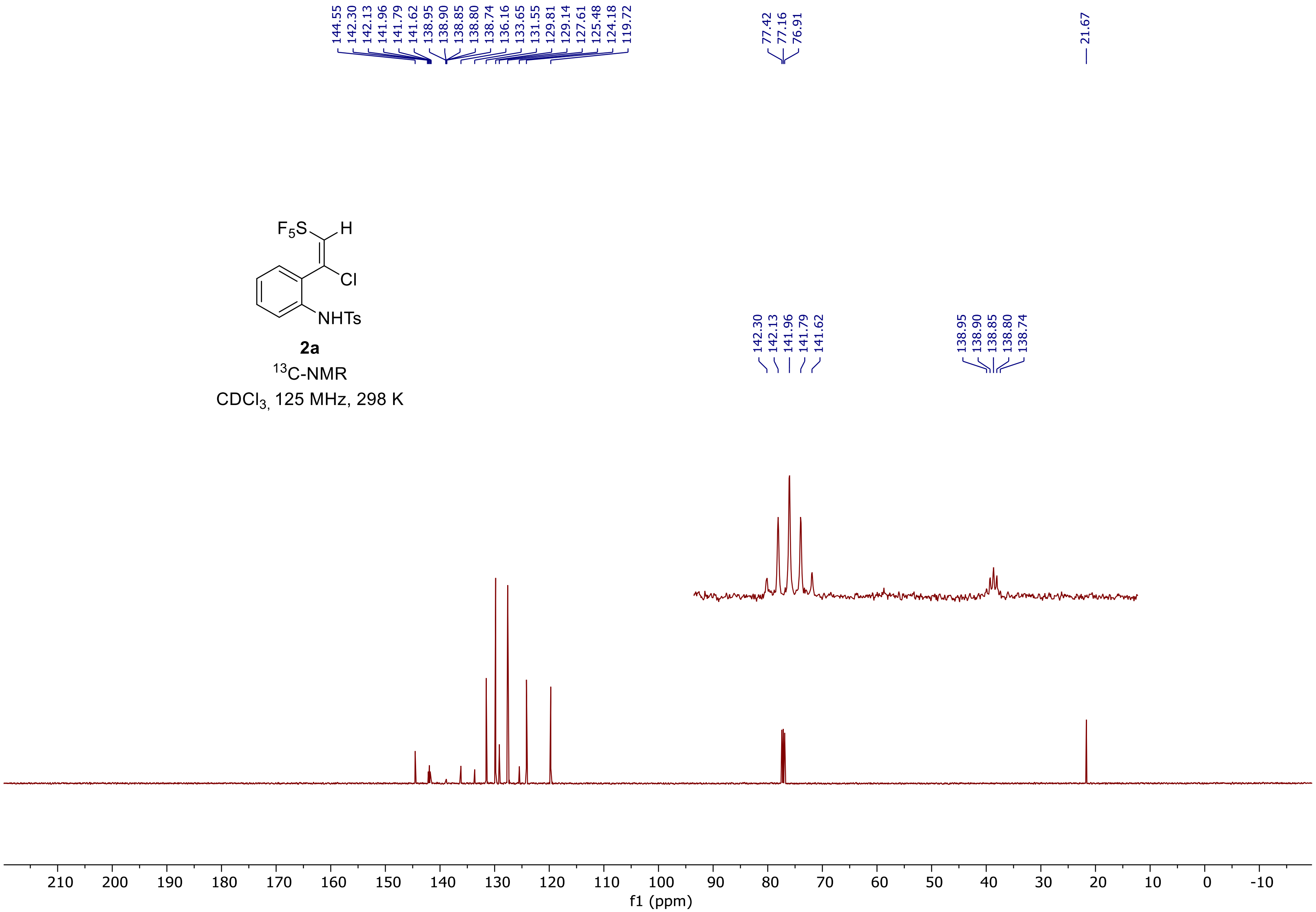
10 NMR spectra





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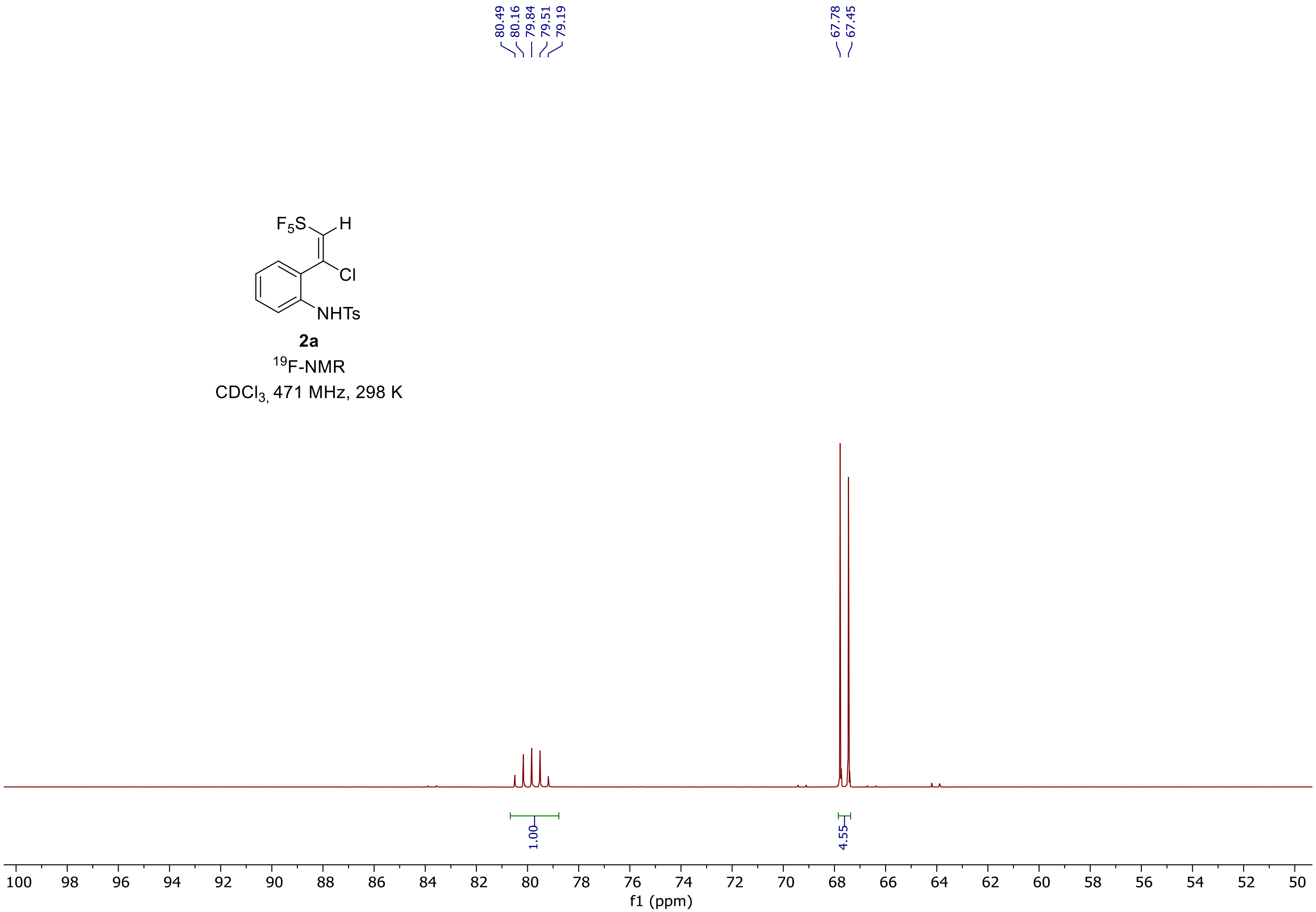
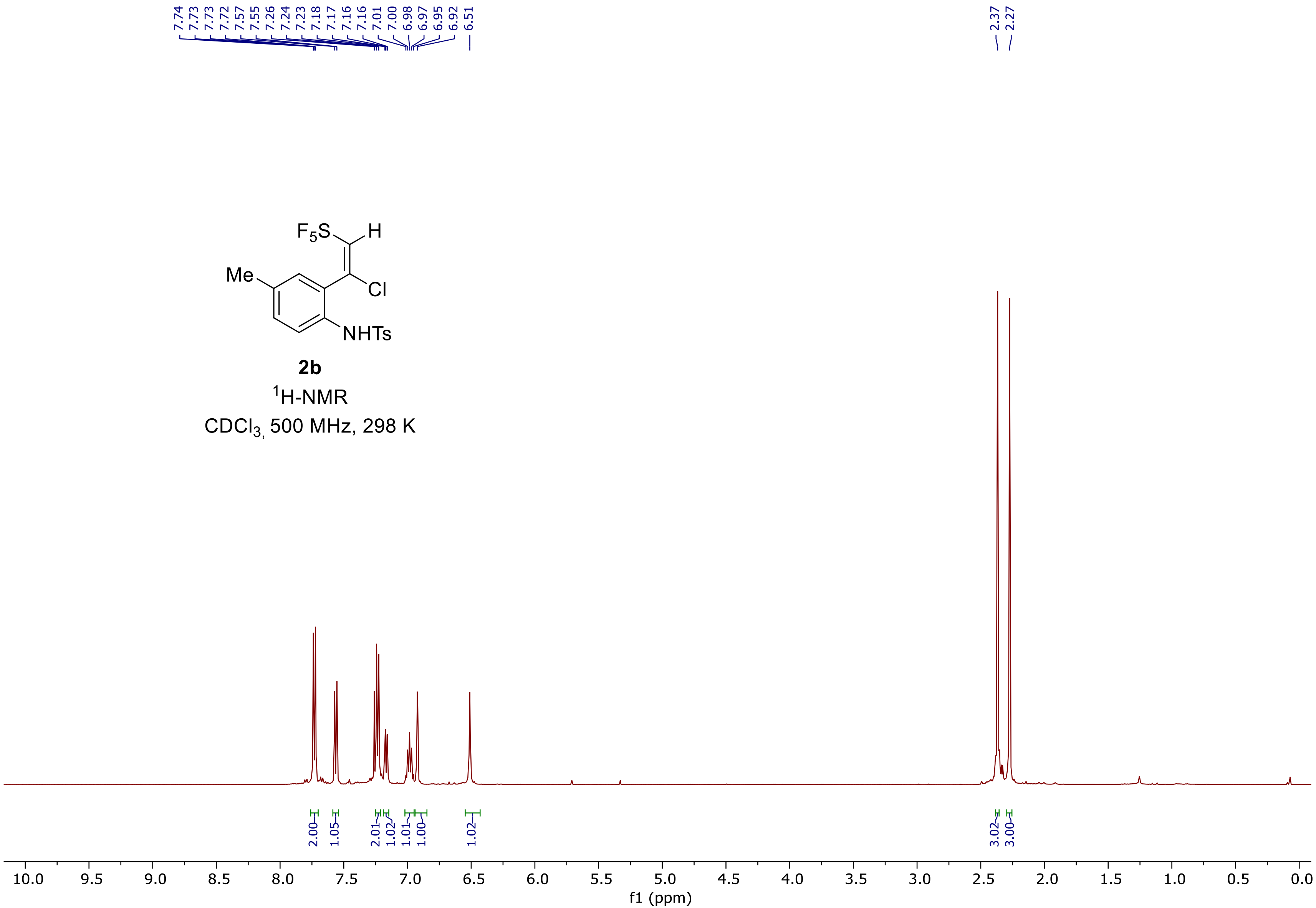


2a

^{19}F-NMR

$CDCl_3$, 471 MHz, 298 K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7.00
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6.51
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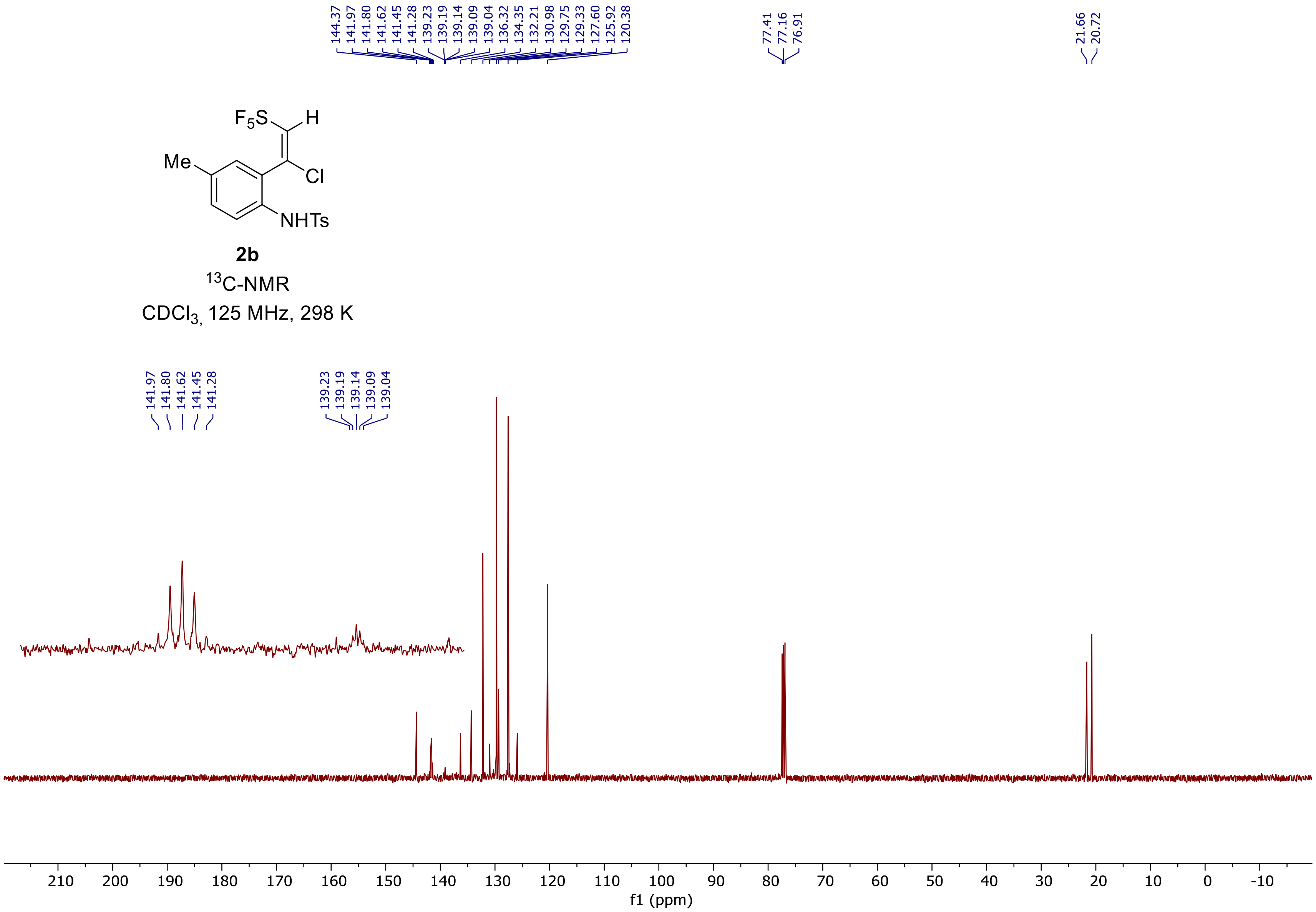

2b

^{13}C-NMR

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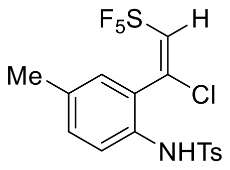
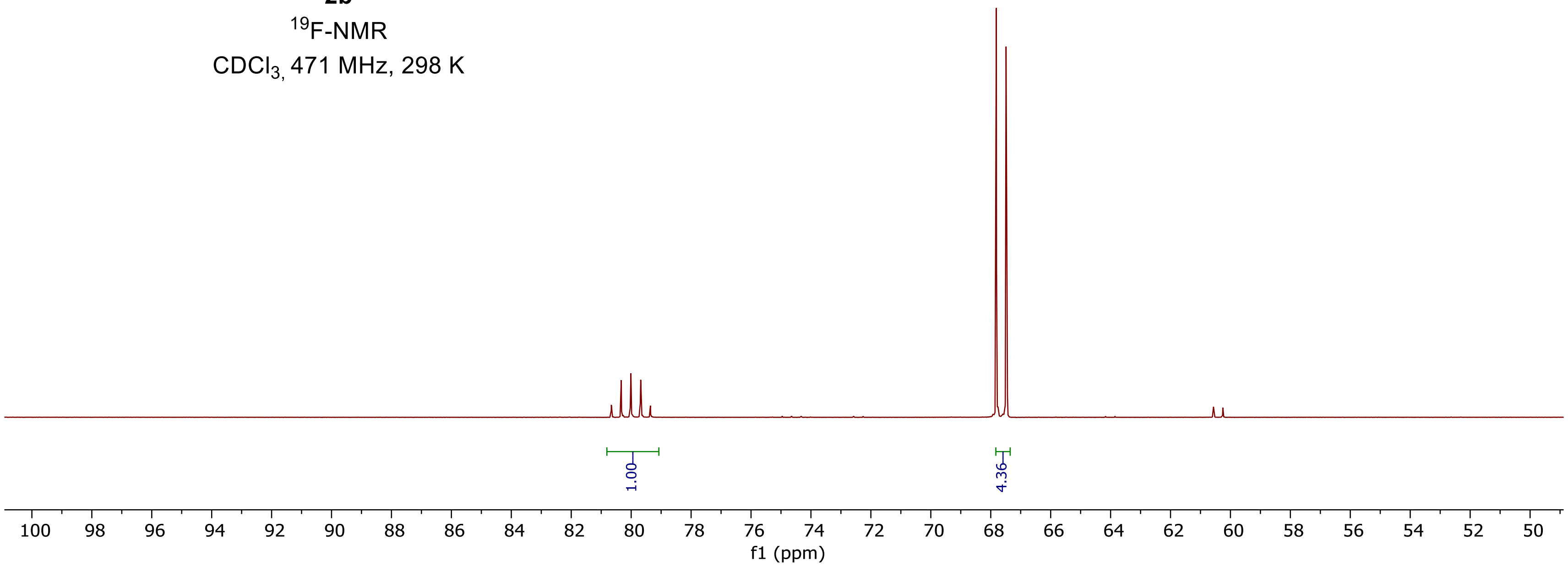
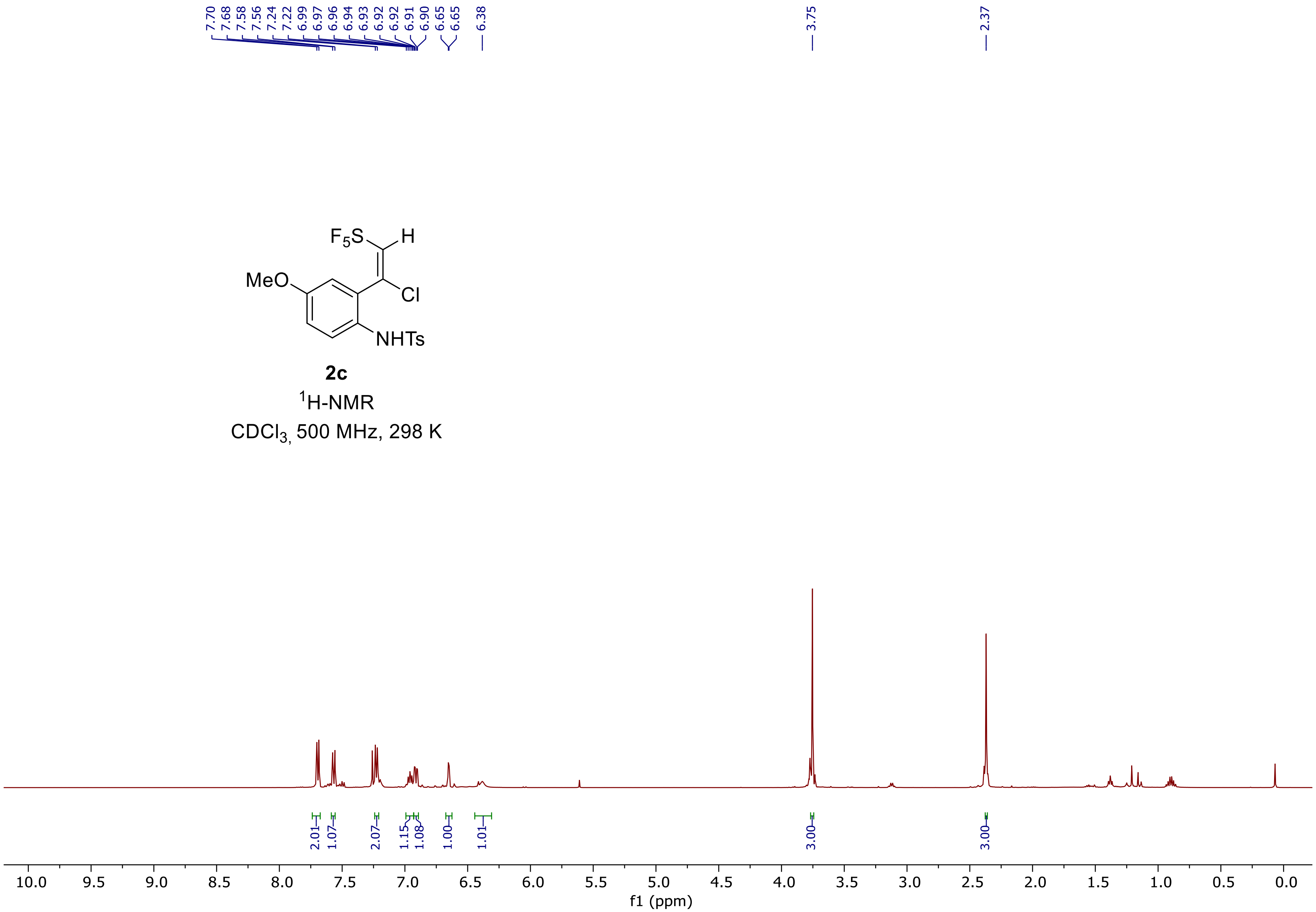


2b

^{19}F-NMR

$CDCl_3$, 471 MHz, 298 K





2c

^{1}H-NMR

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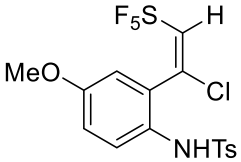

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^{13}C-NMR

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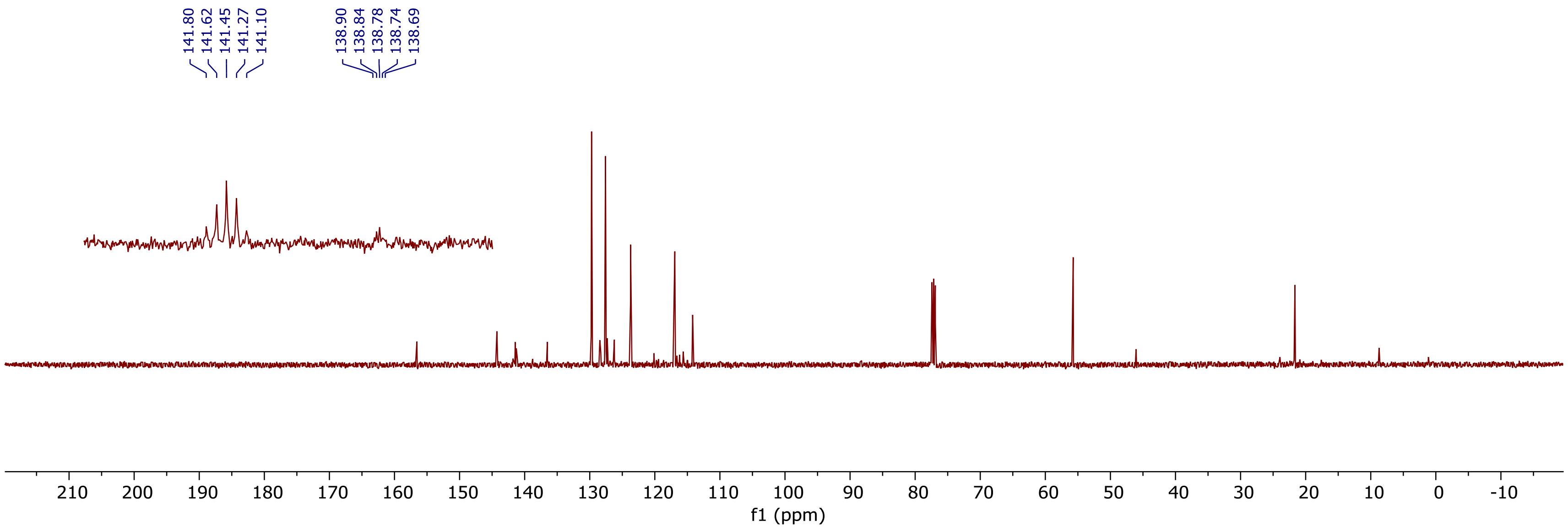

2c
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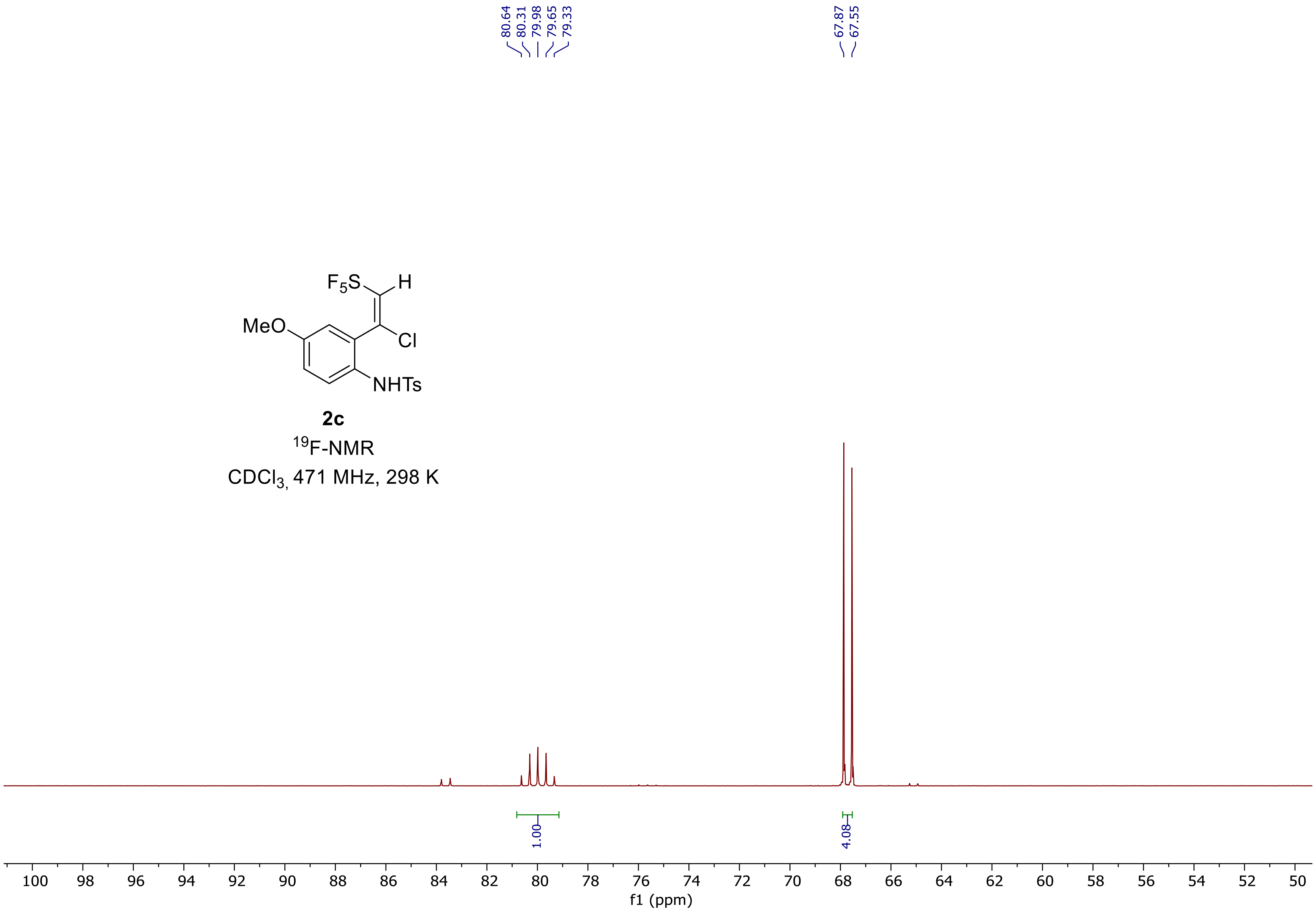
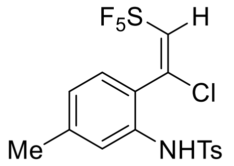
$CDCl_3$, 471 MHz, 298 K

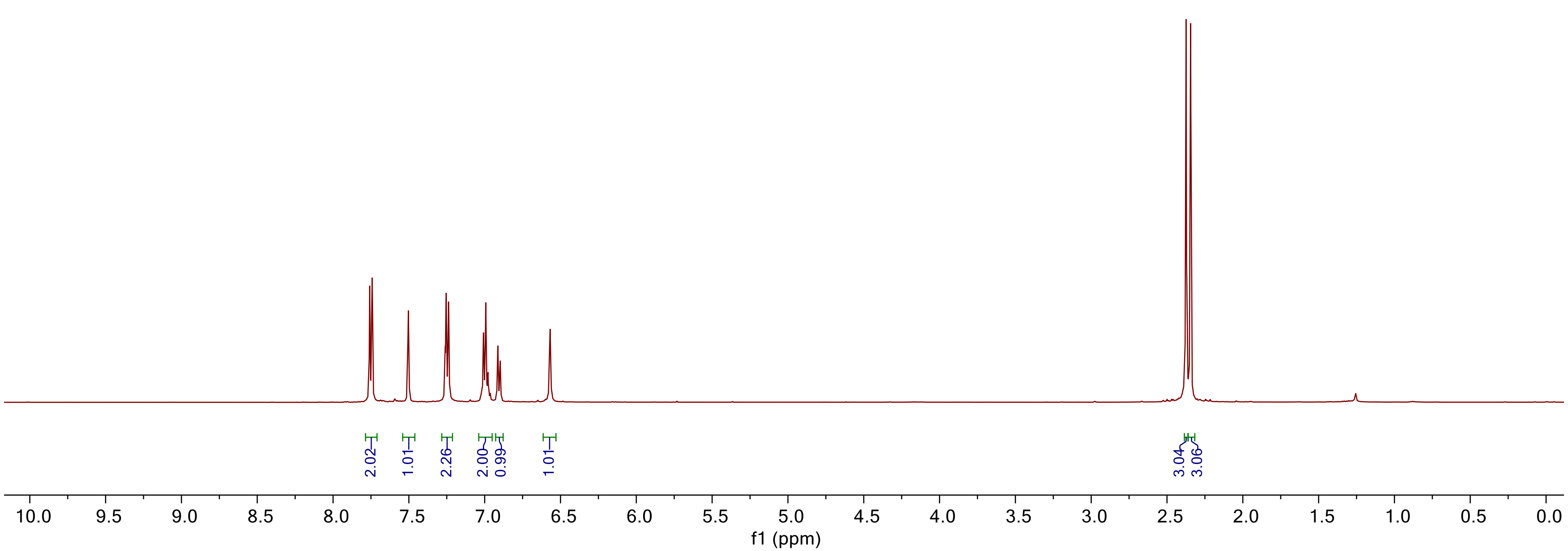


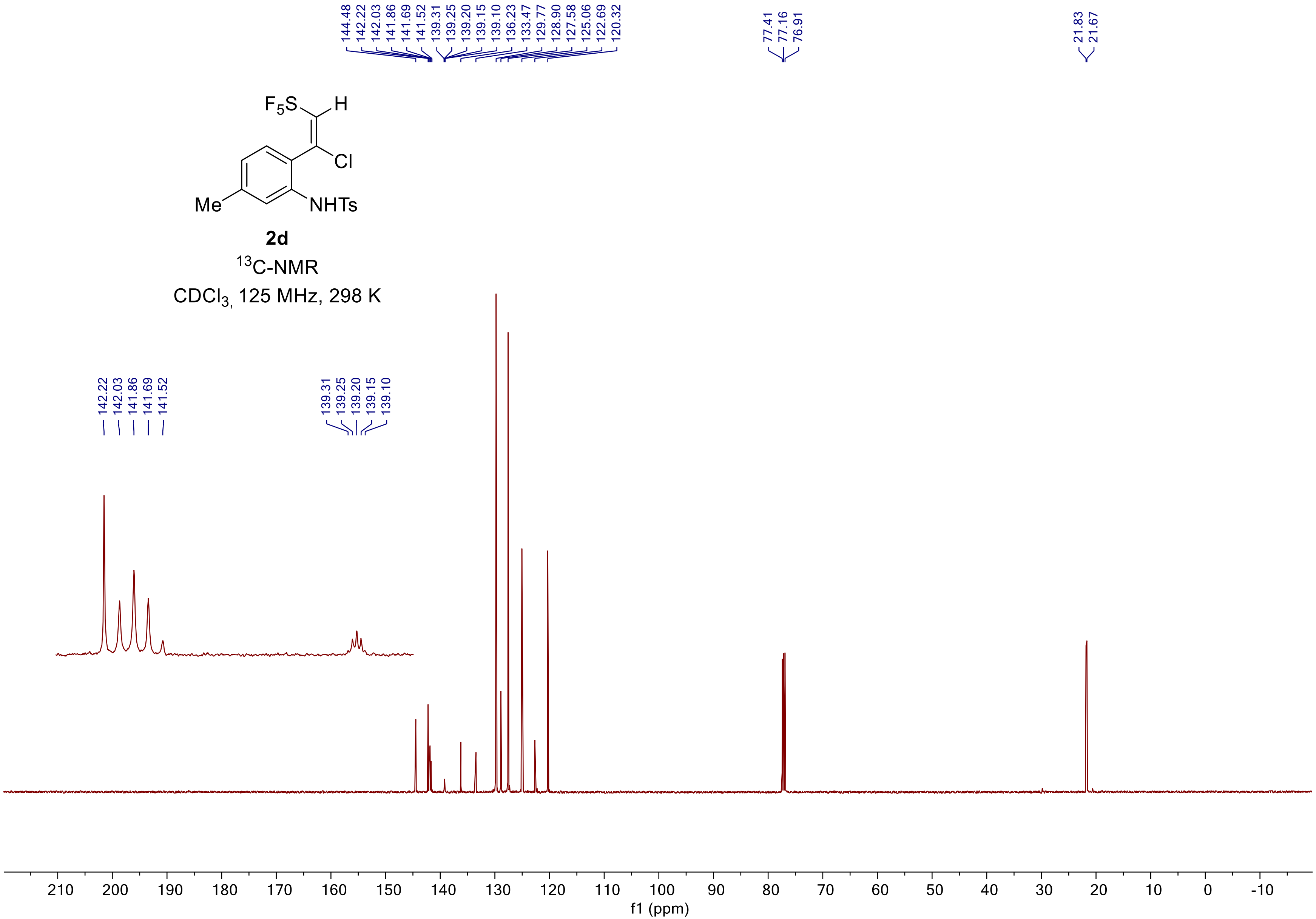


2d

^{1}H-NMR

$CDCl_3$, 500 MHz, 298 K

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2d
13C-NMR
CDCl3, 125 MHz, 298 K
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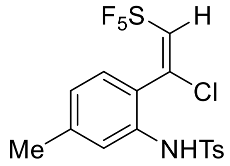
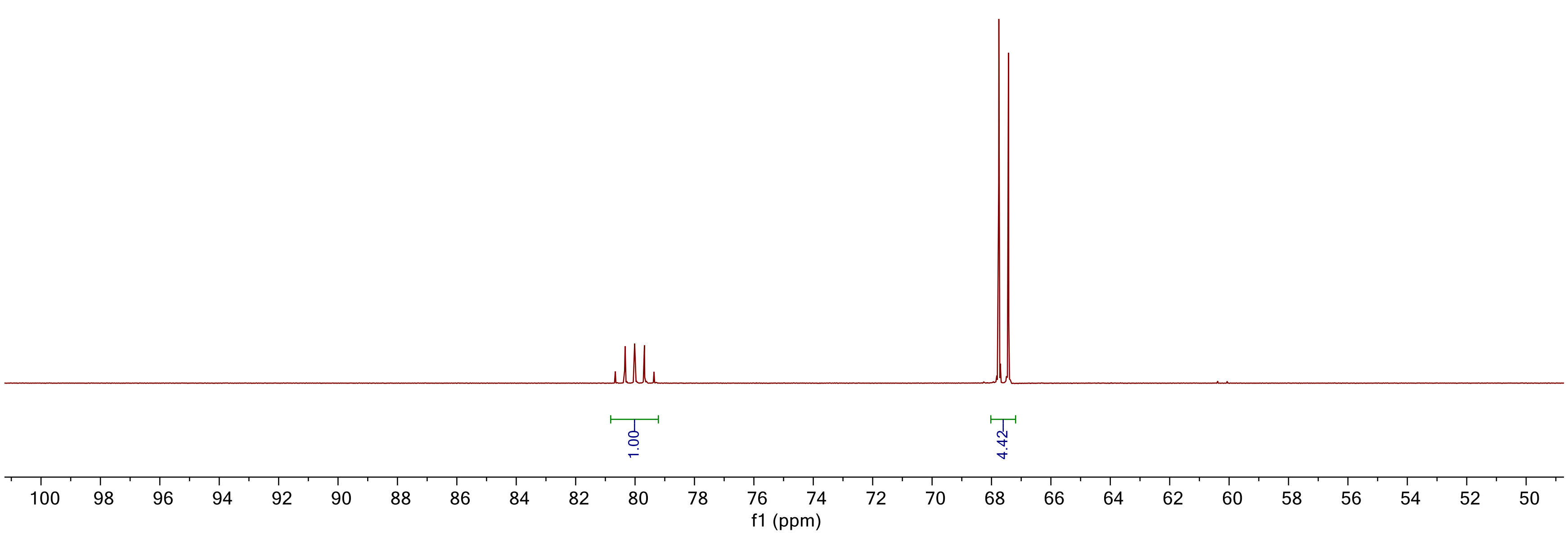
f1 (ppm)

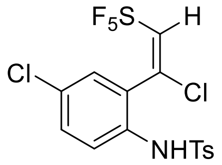


2d

^{19}F-NMR

$CDCl_3$, 471 MHz, 298 K

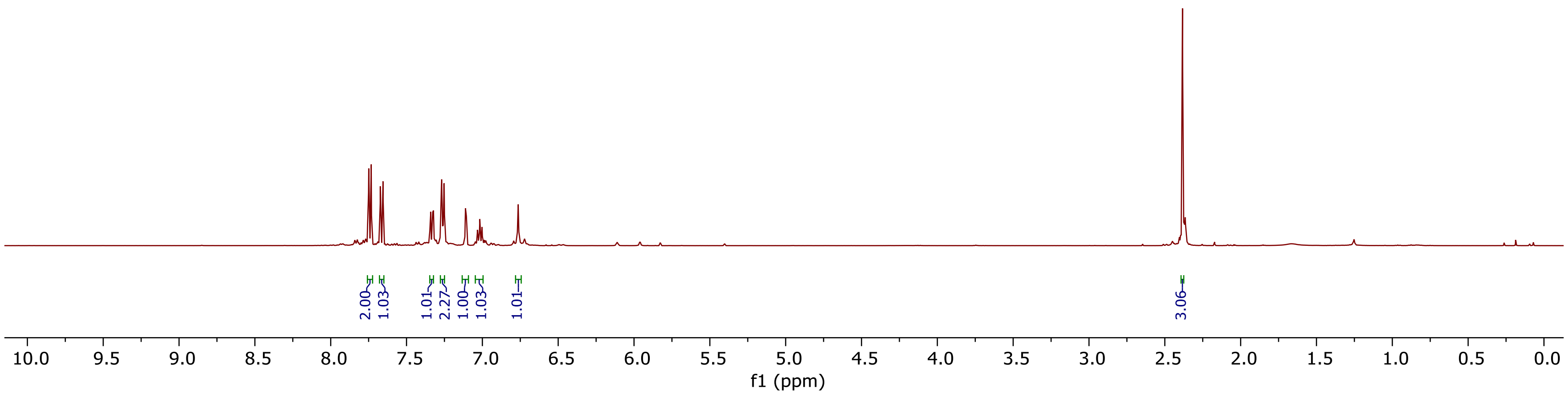


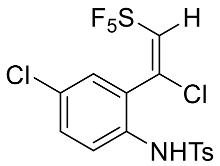


2e

^{1}H-NMR

$CDCl_3$, 500 MHz, 298 K

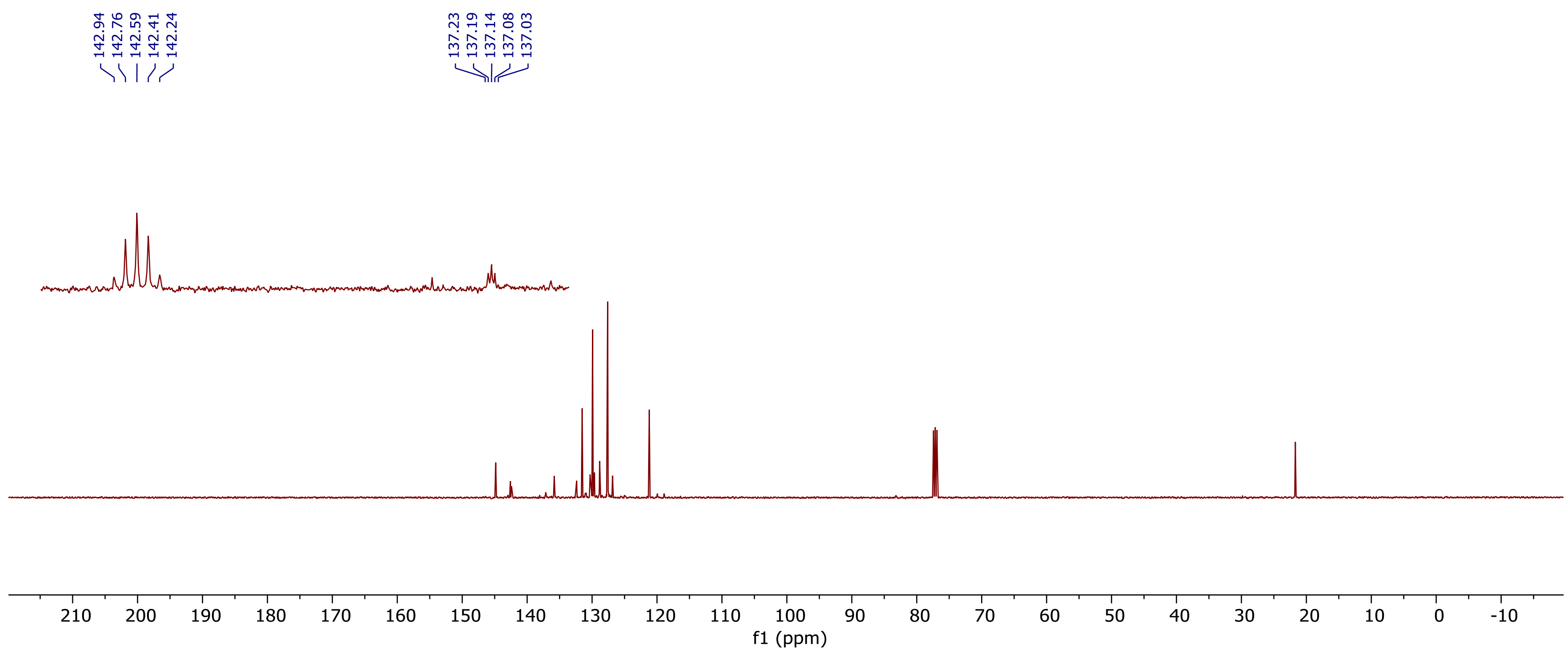


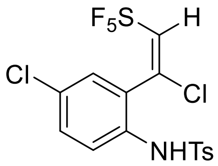


2e

^{13}C-NMR

$CDCl_3$, 125 MHz, 298 K

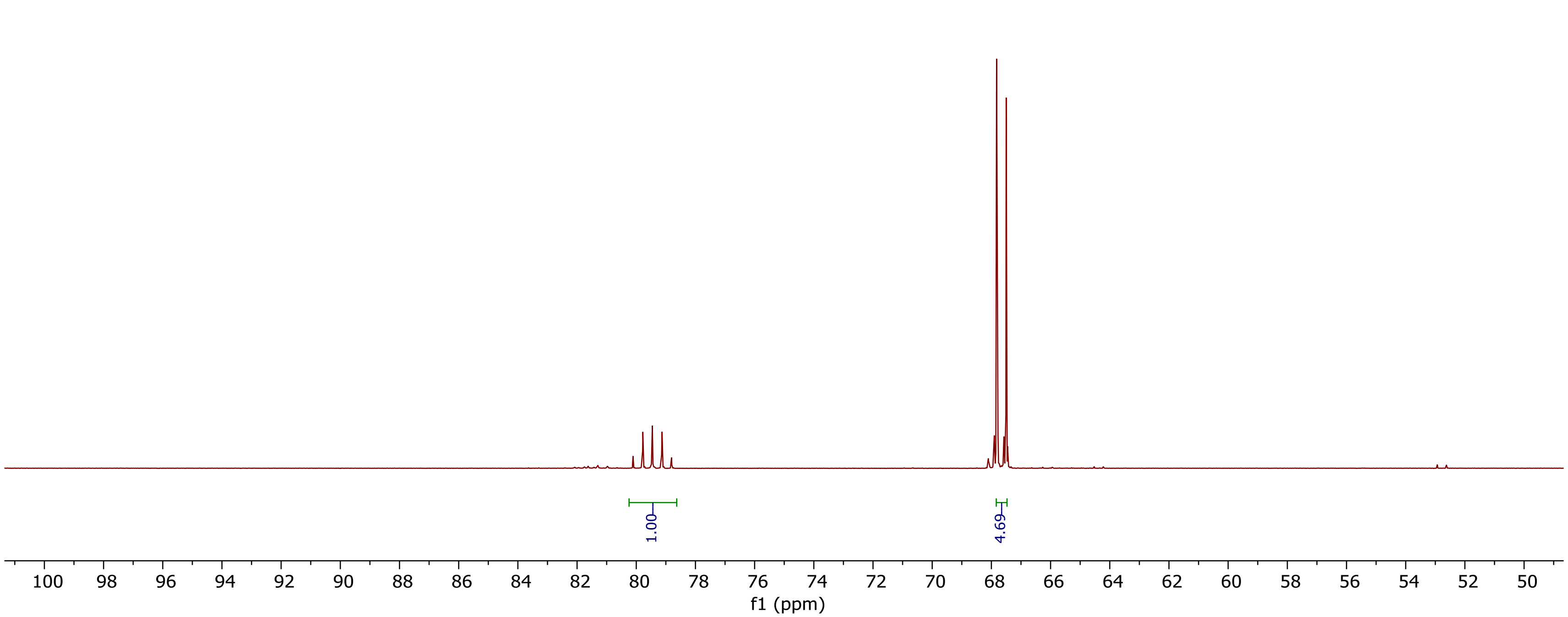


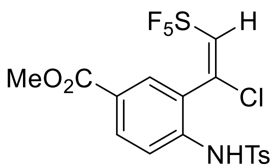


2e

^{19}F-NMR

$CDCl_3$, 471 MHz, 298 K

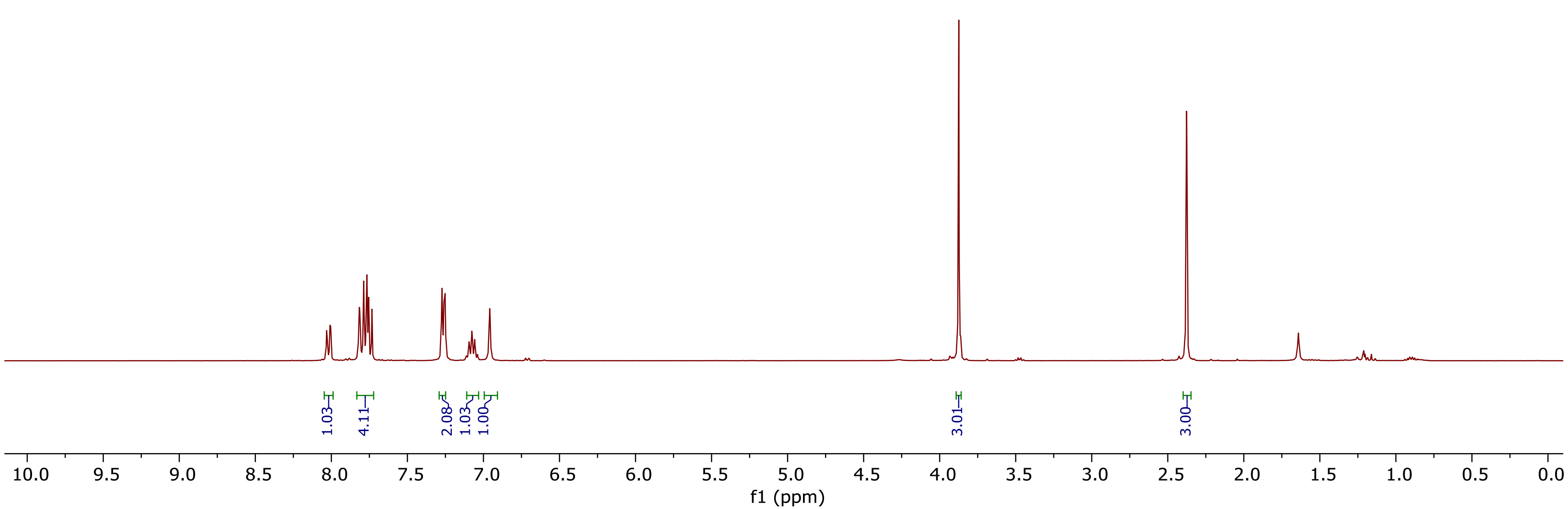


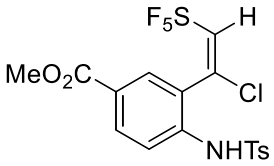


2f

^{1}H-NMR

$CDCl_3$, 500 MHz, 298 K

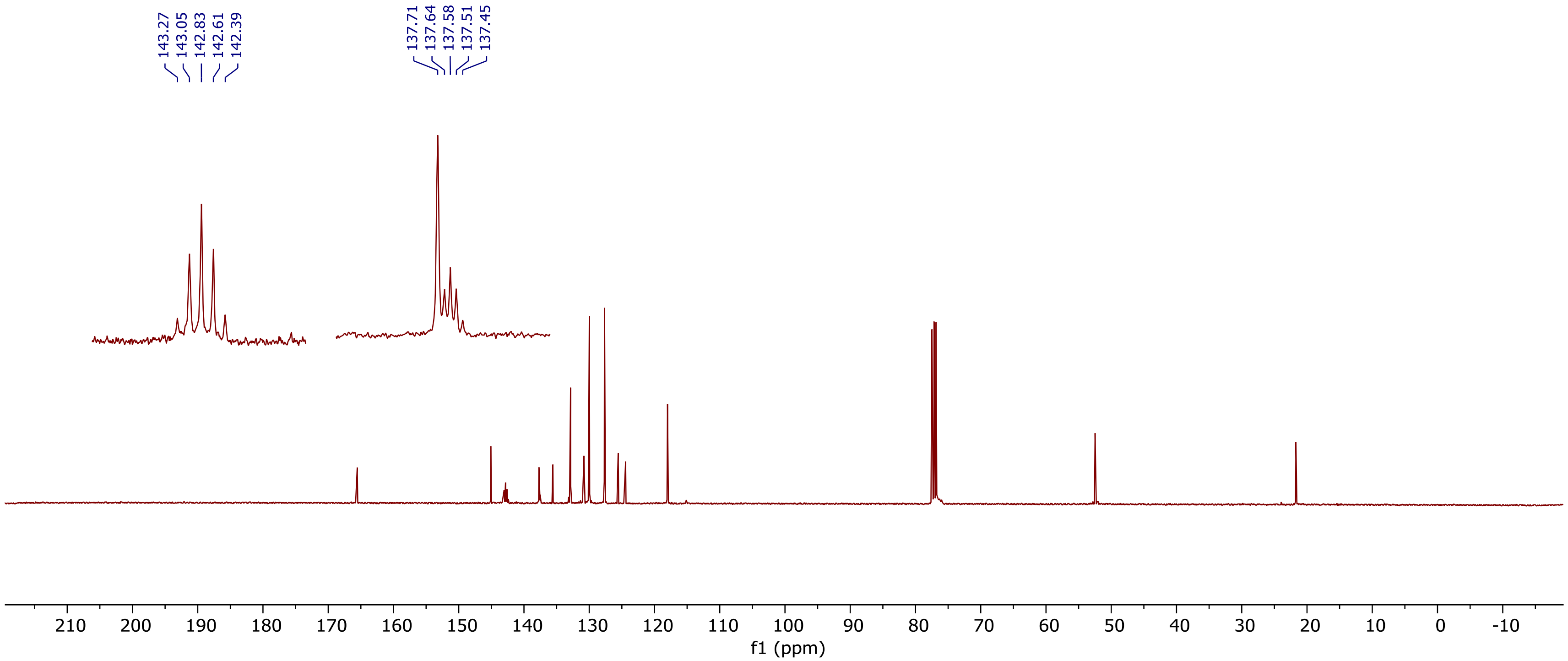


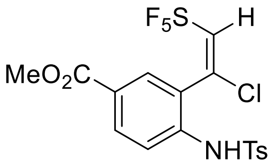


2f

^{13}C-NMR

$CDCl_3$, 125 MHz, 298 K

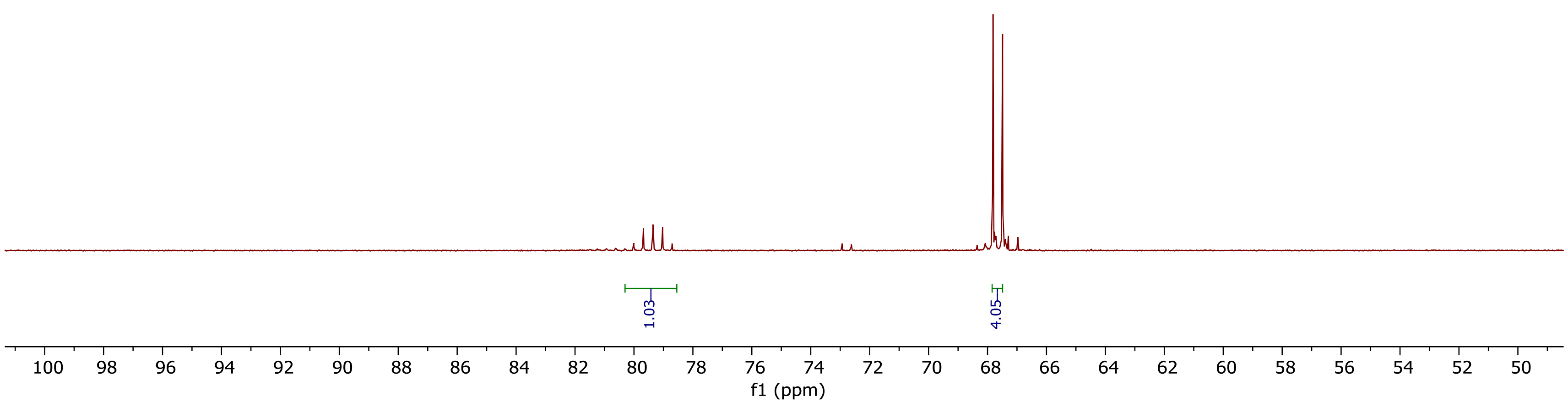


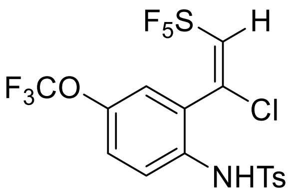


2f

^{19}F-NMR

$CDCl_3$, 471 MHz, 298 K

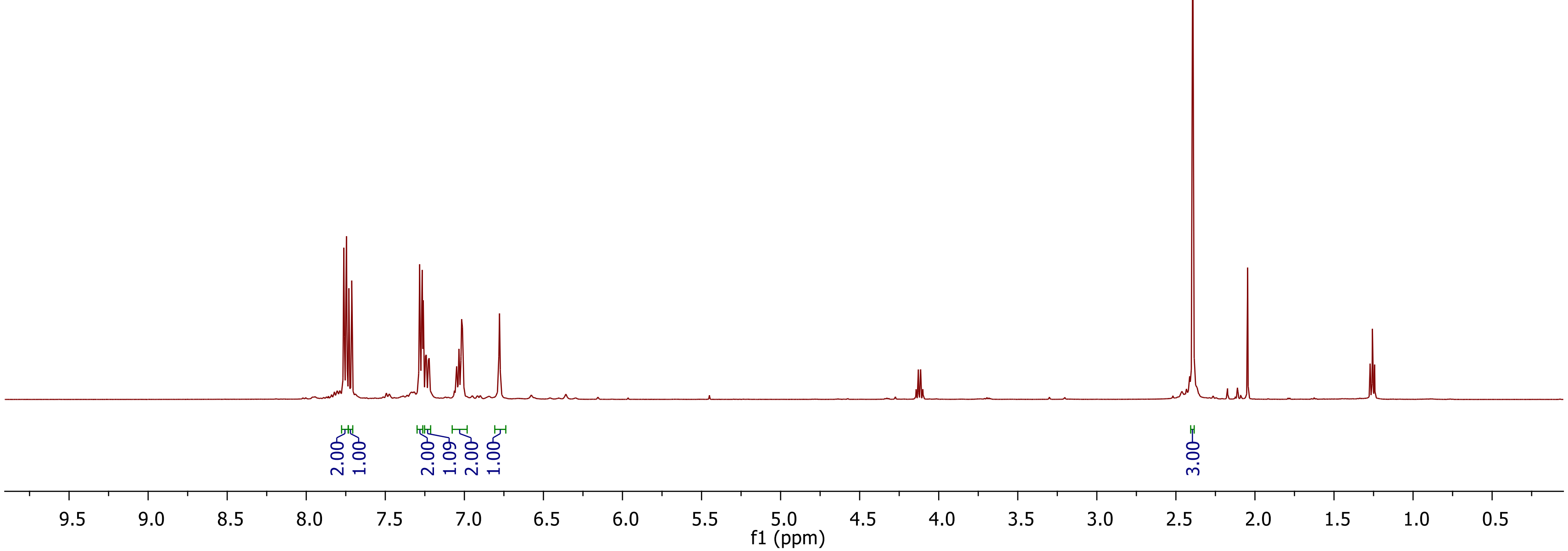


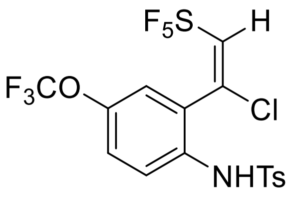


2g

^{1}H-NMR

$CDCl_3$, 500 MHz, 298 K

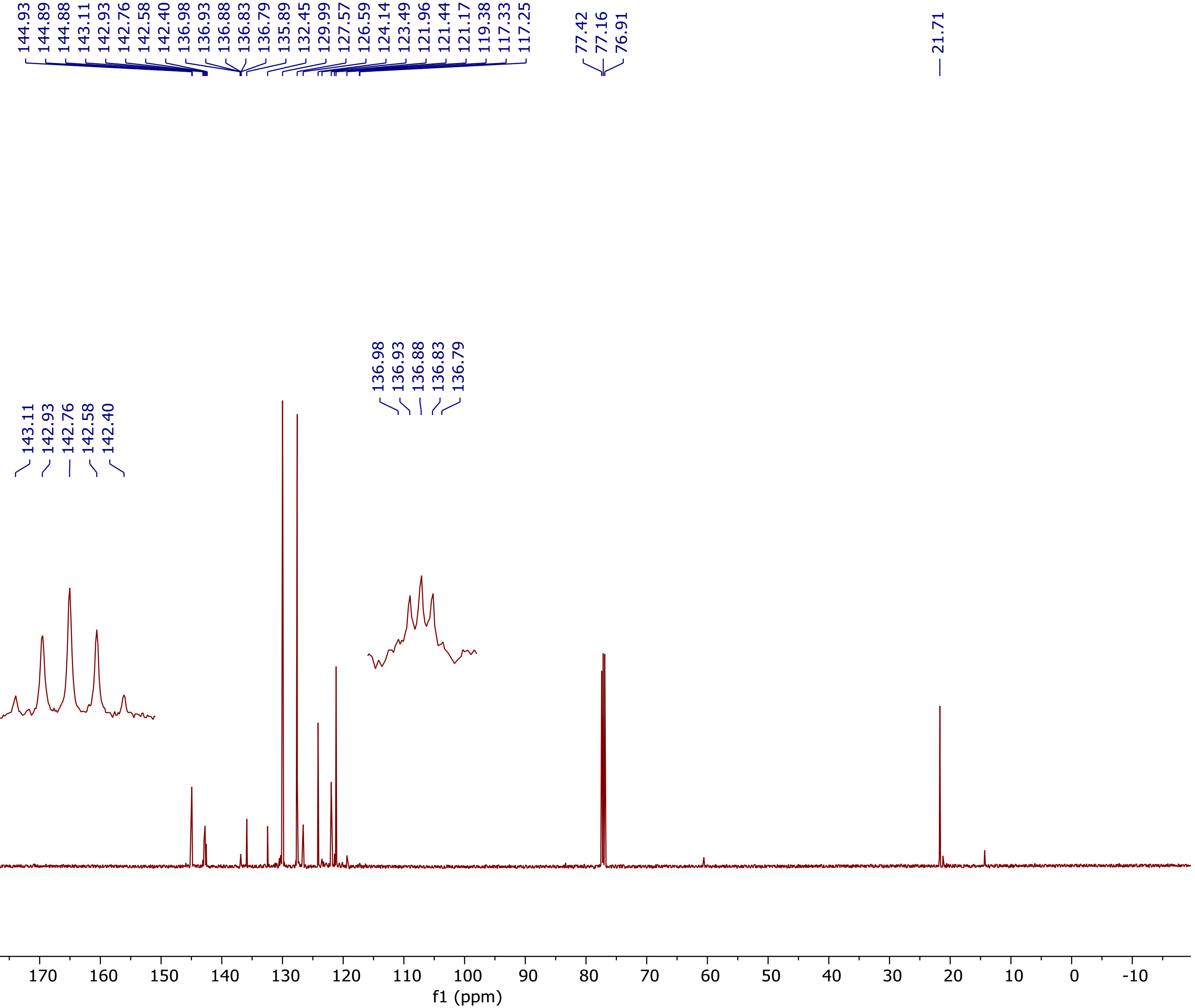


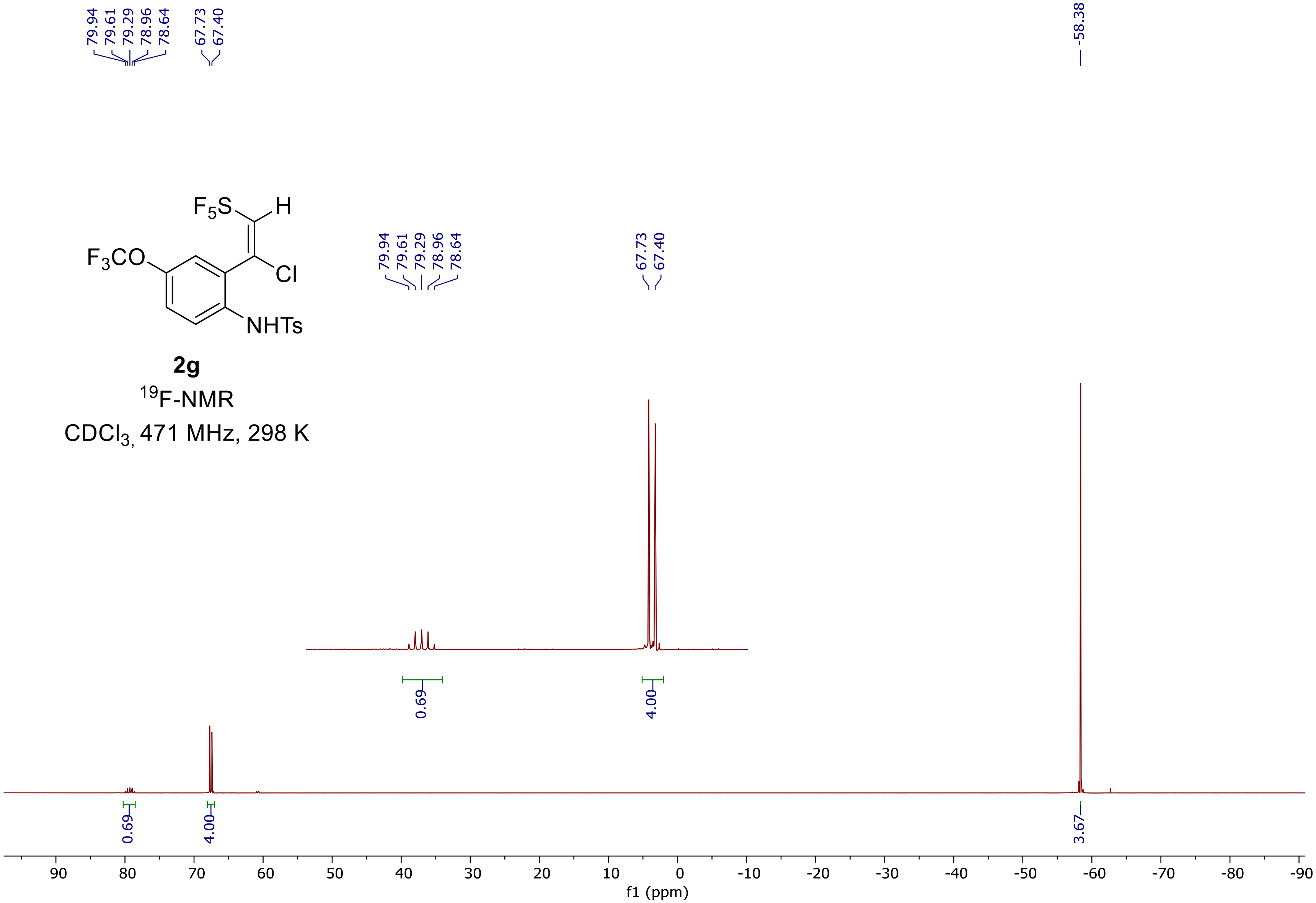


2g

^{13}C-NMR

$CDCl_3$, 125 MHz, 298 K

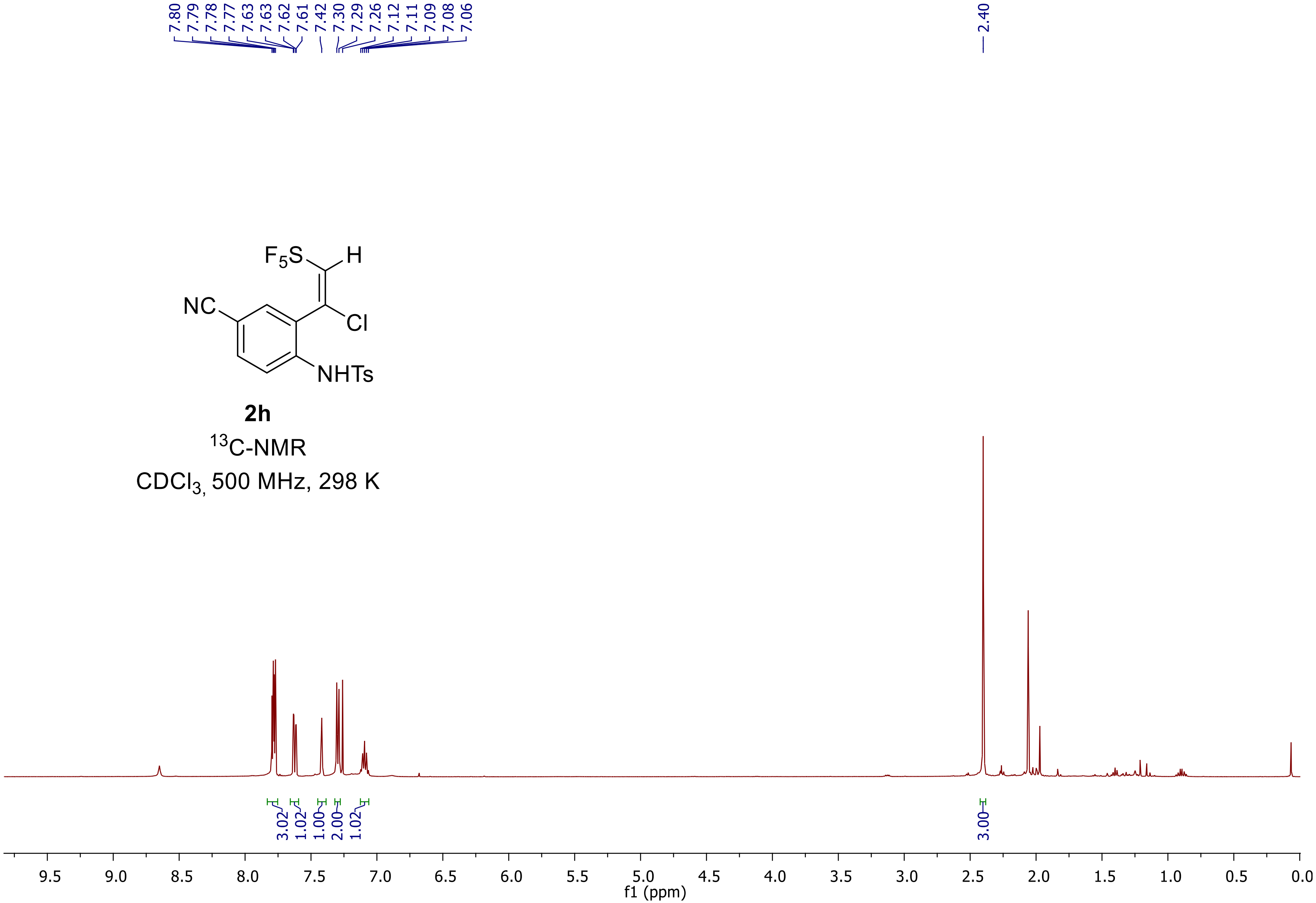




2g

^{19}F-NMR

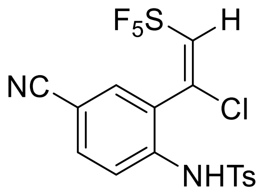
$CDCl_3$, 471 MHz, 298 K



2h

^{13}C-NMR

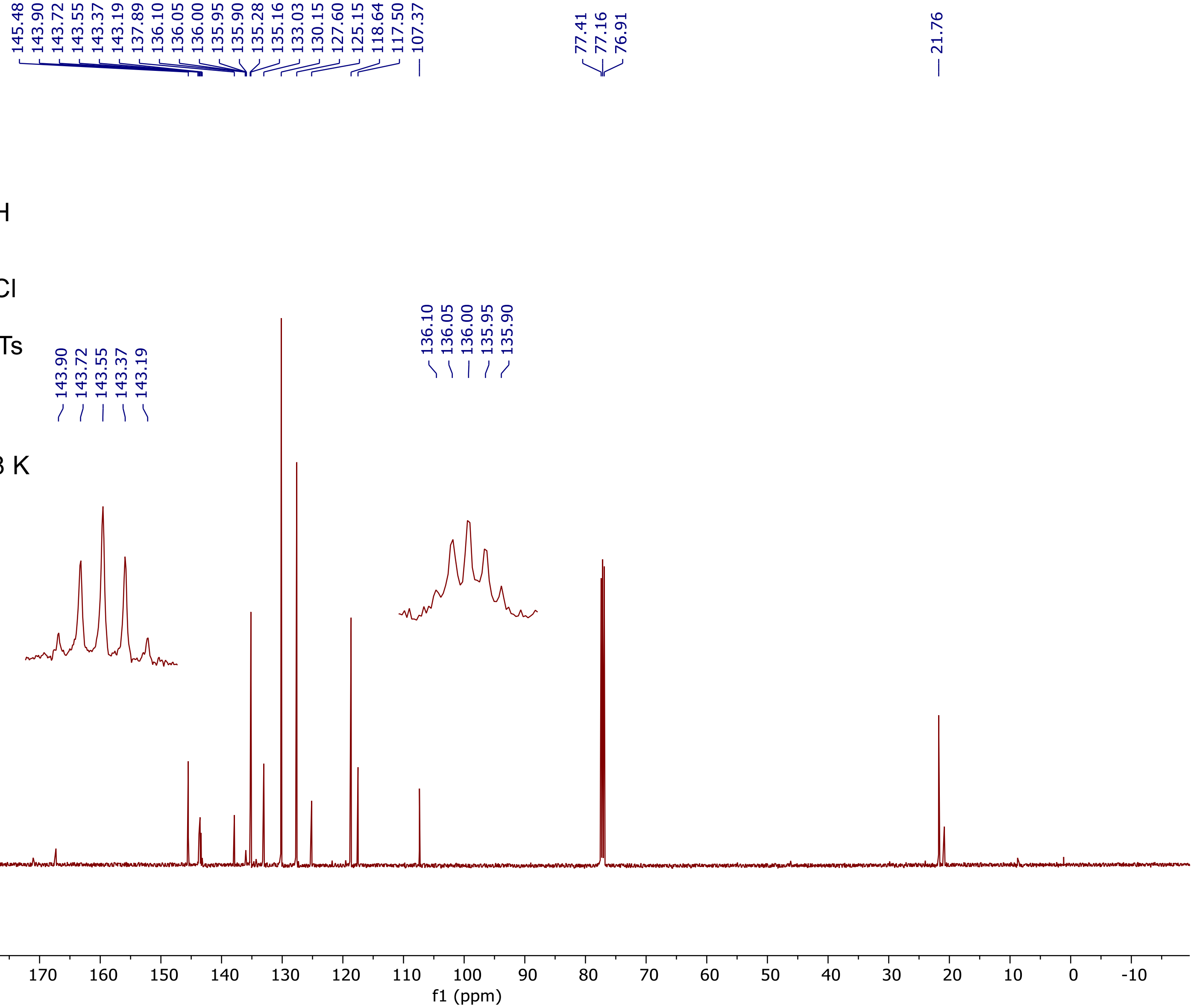
$CDCl_3$, 500 MHz, 298 K

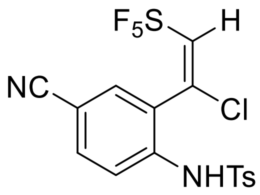


2h

^{13}C-NMR

$CDCl_3$, 125 MHz, 298 K

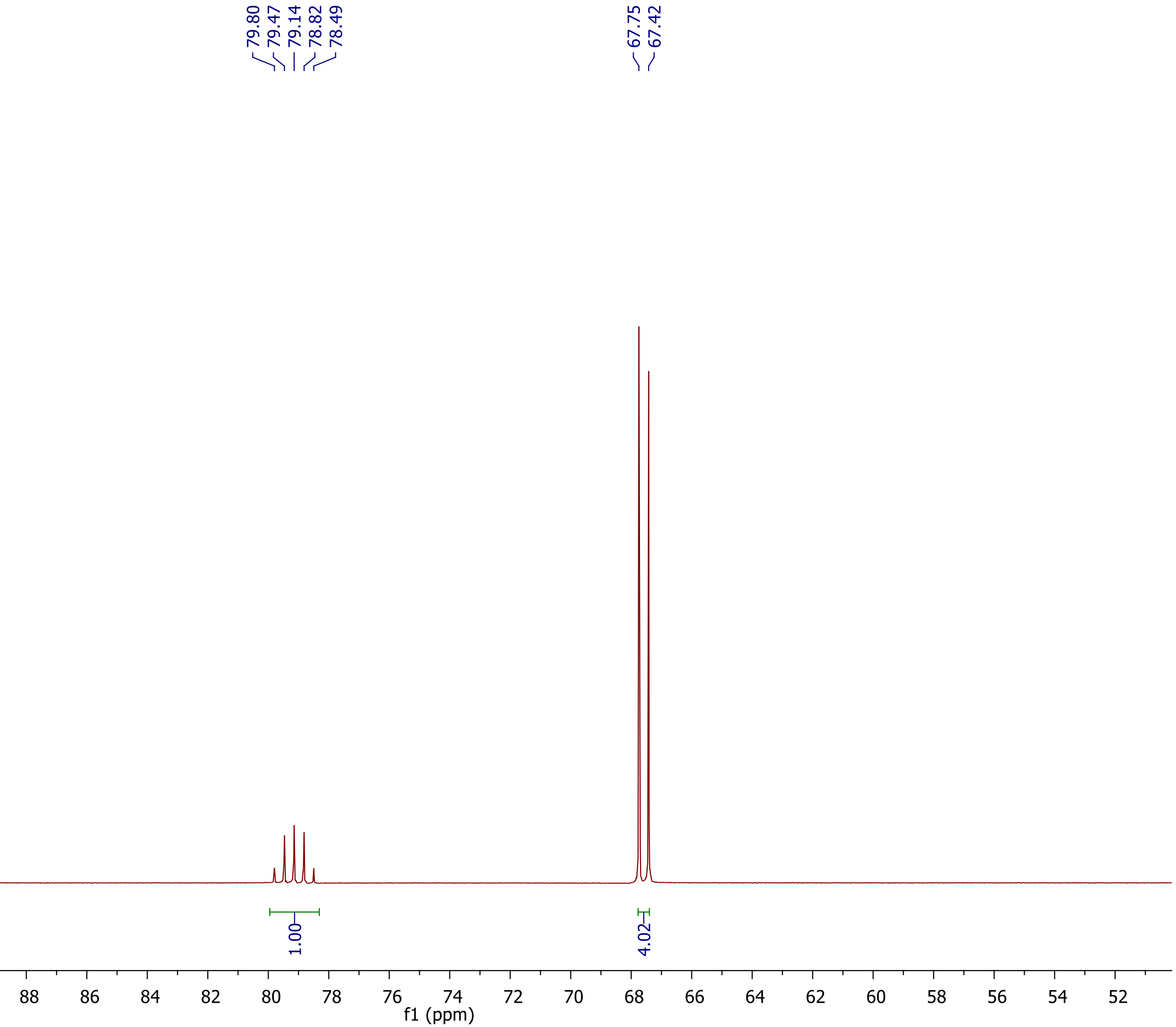


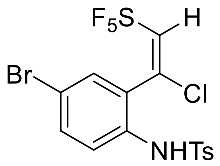


2h

^{19}F-NMR

$CDCl_3$, 471 MHz, 298 K

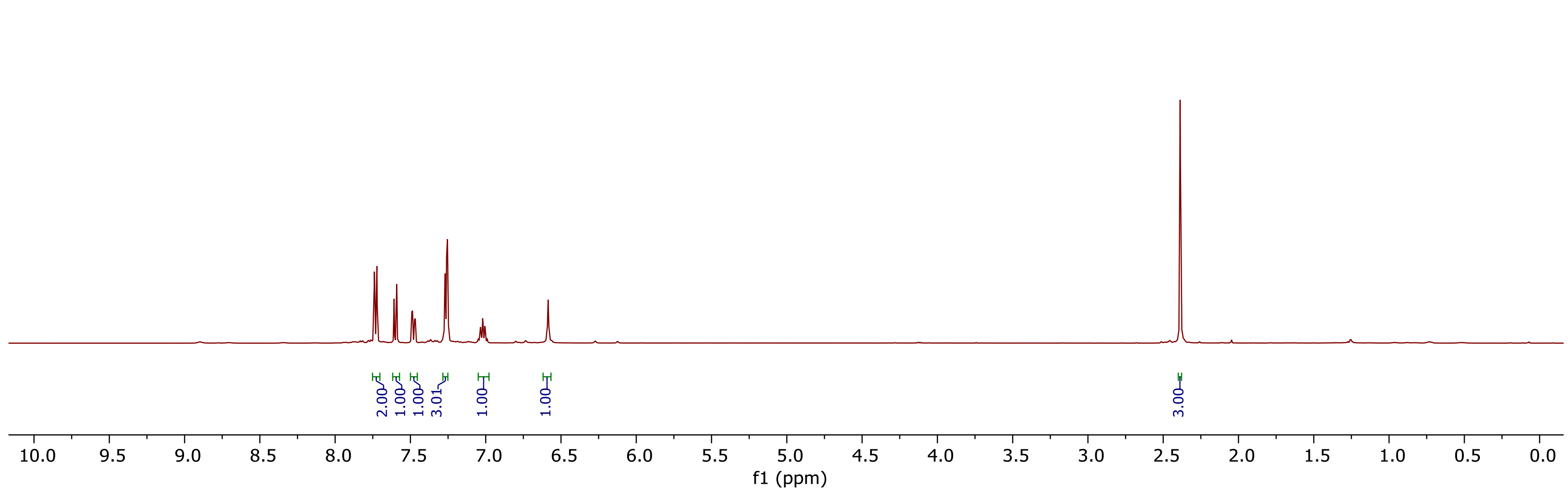


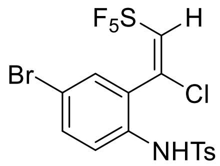


2i

[1]H-NMR

$CDCl_3$, 500 MHz, 298 K

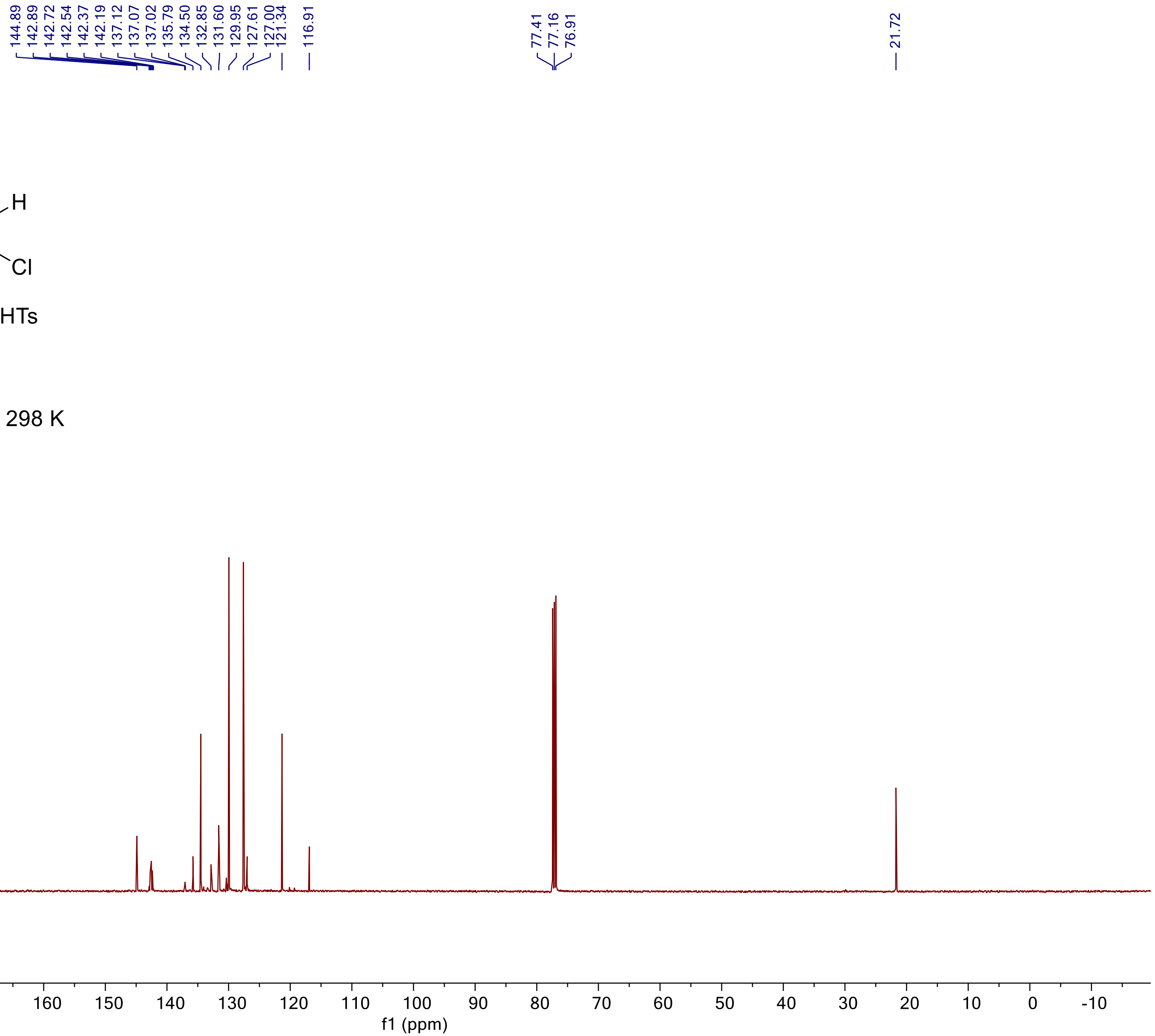


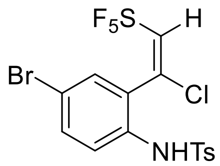


2i

^{13}C-NMR

$CDCl_3$, 125 MHz, 298 K

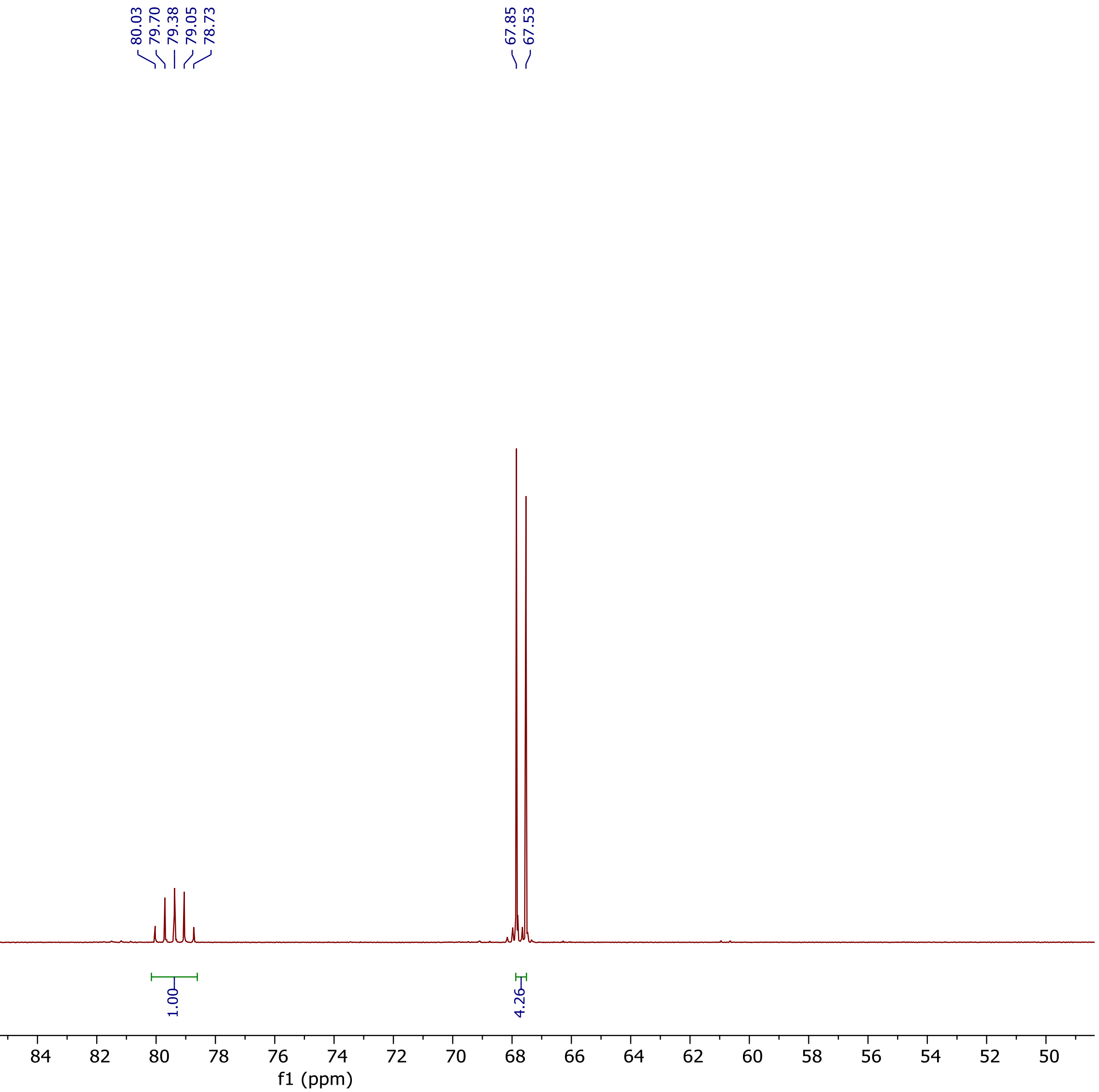


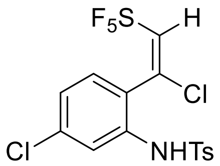


2i

^{19}F-NMR

$CDCl_3$, 471 MHz, 298 K

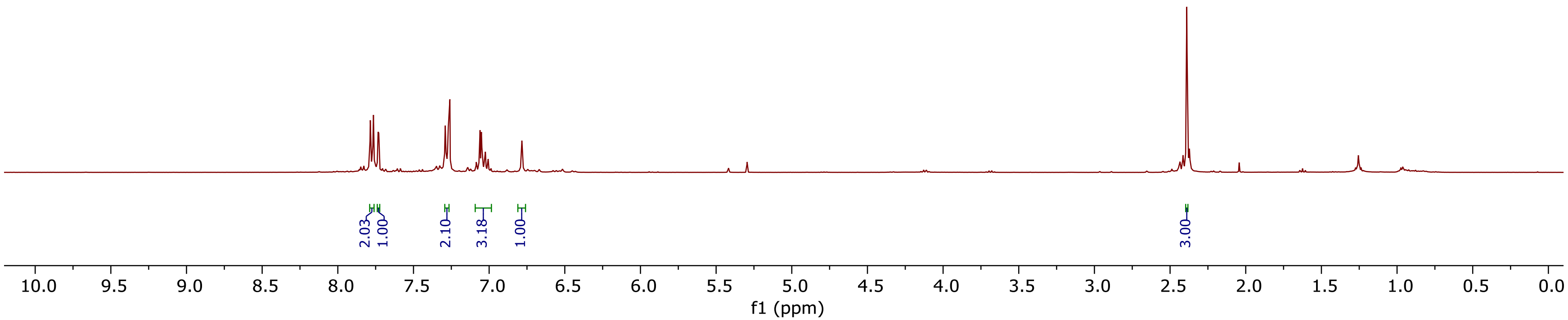


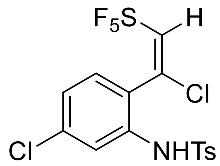


2j

^{1}H-NMR

$CDCl_3$, 500 MHz, 298 K

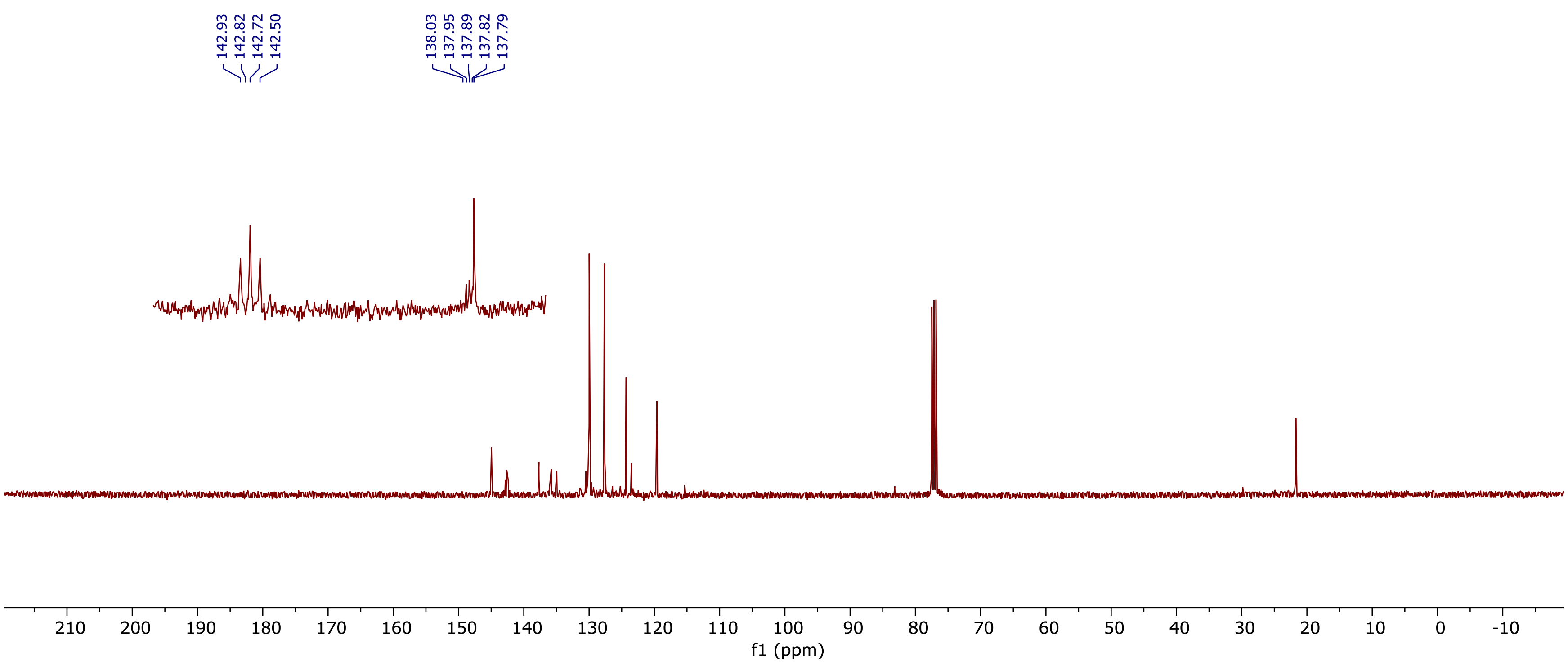


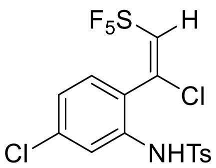


2j

^{13}C-NMR

$CDCl_3$, 125 MHz, 298 K

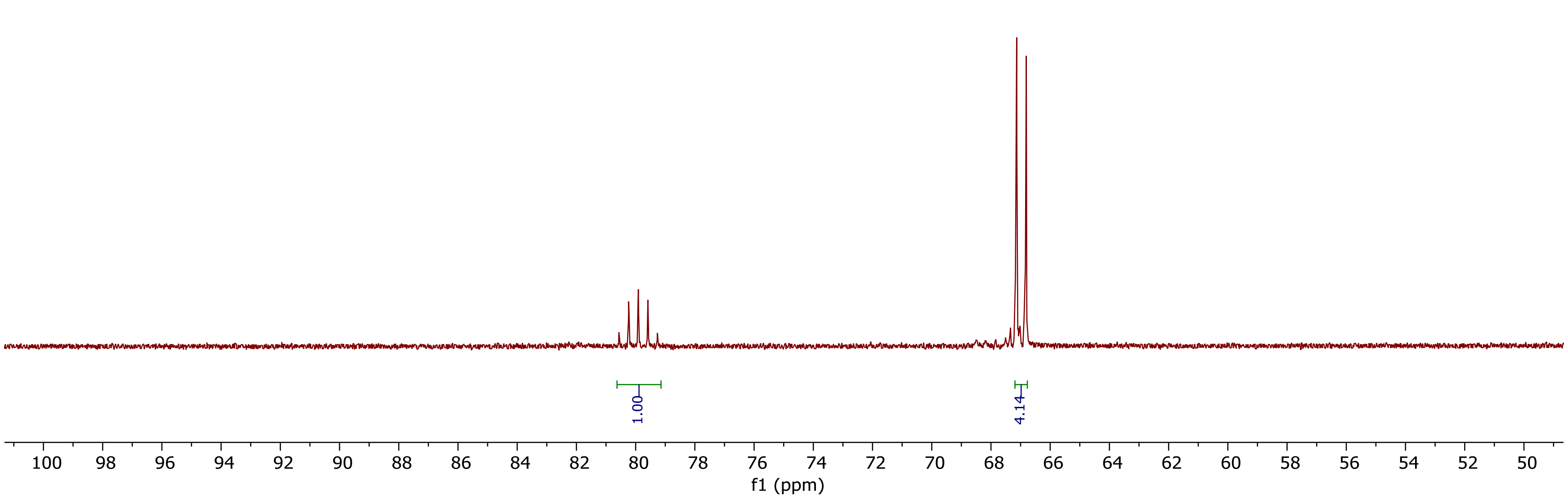


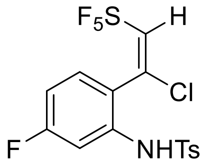


2j

^{19}F-NMR

$CDCl_3$, 471 MHz, 298 K

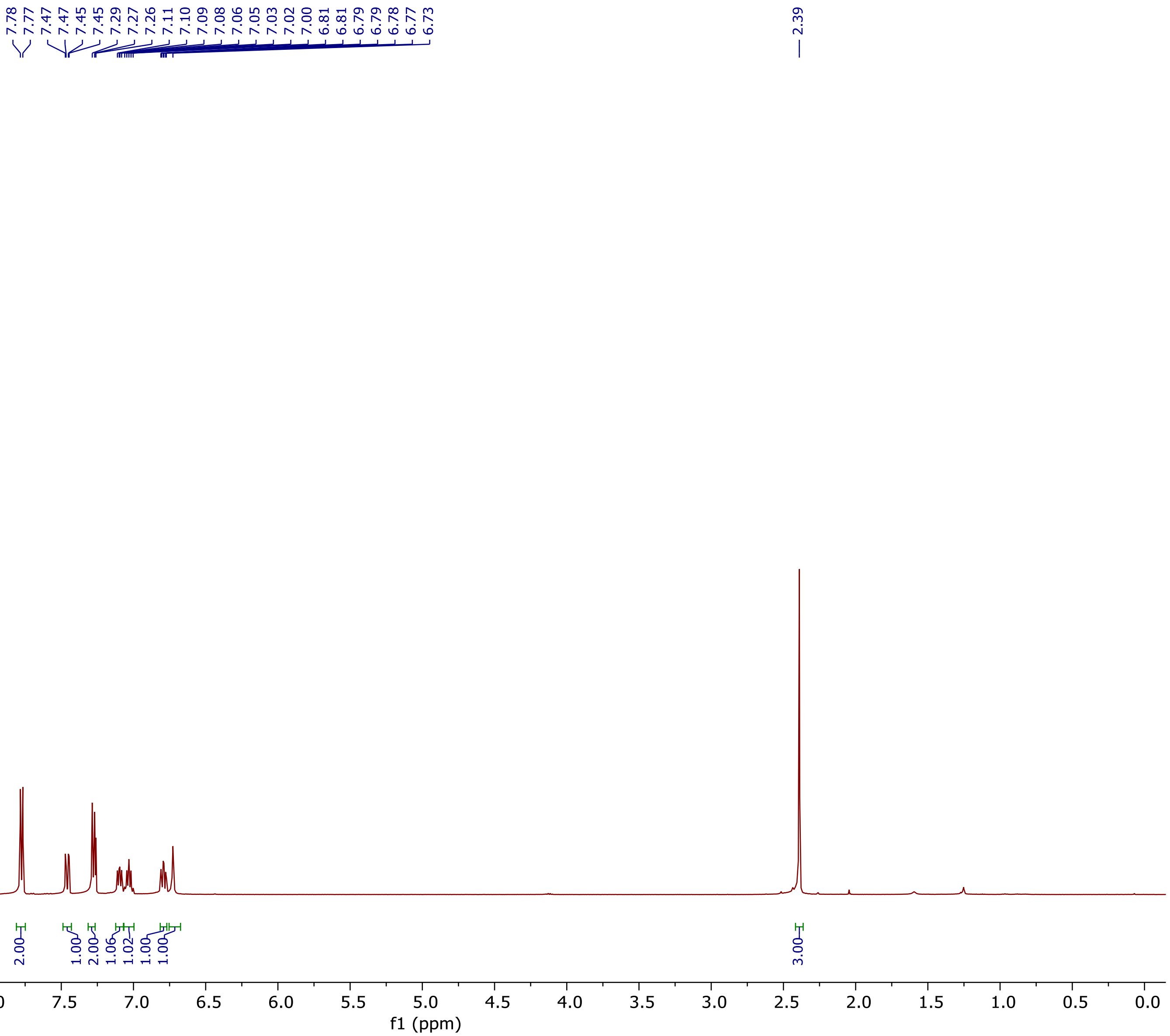


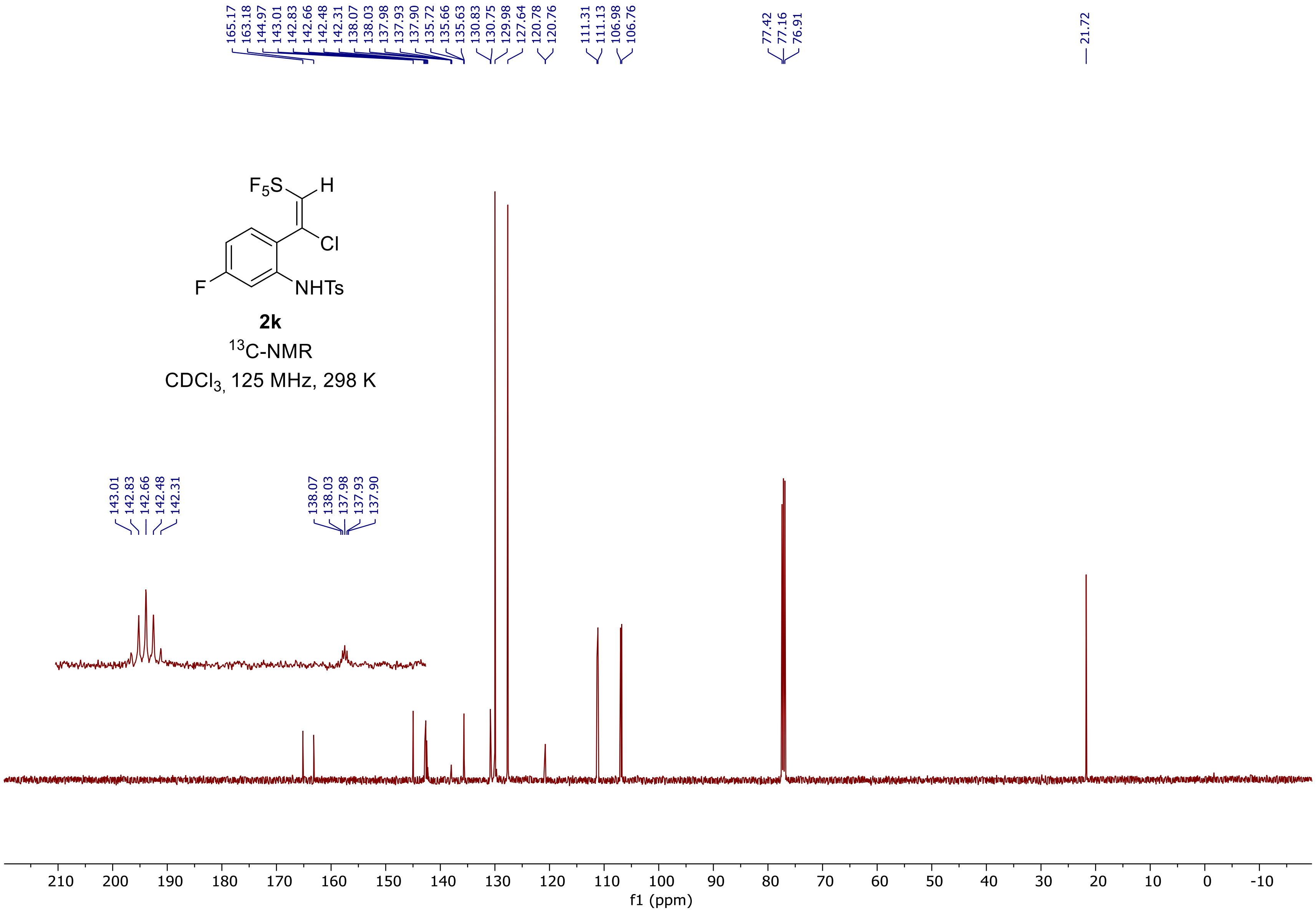


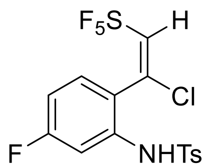
2k

^{1}H-NMR

$CDCl_3$, 500 MHz, 298 K



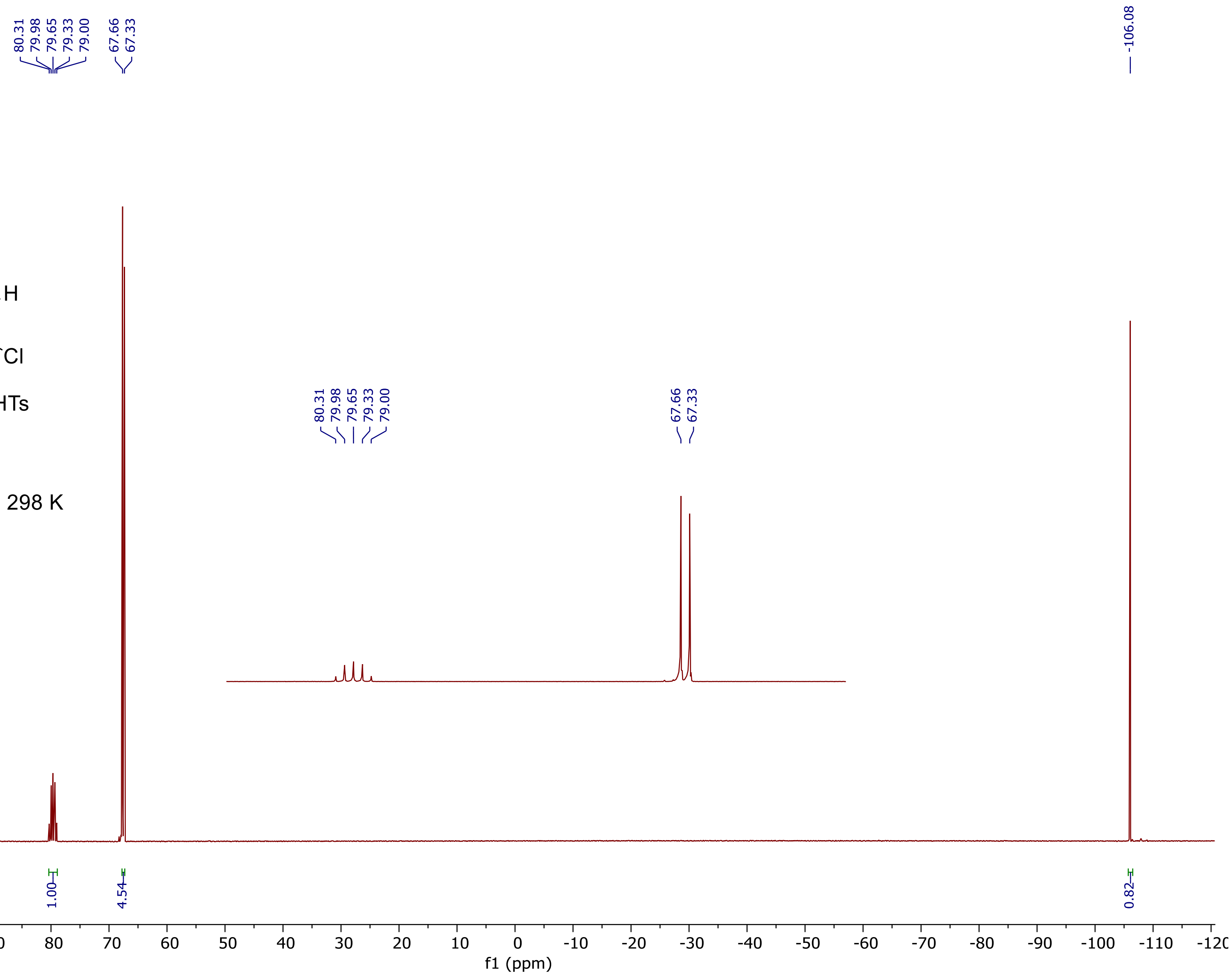

165.17
163.18
144.97
143.01
142.83
142.66
142.48
142.31
138.07
138.03
137.98
137.93
137.90
135.72
135.66
135.63
130.83
130.75
129.98
127.64
120.78
120.76
111.31
111.13
106.98
106.76
77.42
77.16
76.91
21.72
F_5S
H
Cl
F
NHTs
2k
^{13}C-NMR
$CDCl_3$, 125 MHz, 298 K
143.01
142.83
142.66
142.48
142.31
138.07
138.03
137.98
137.93
137.90
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

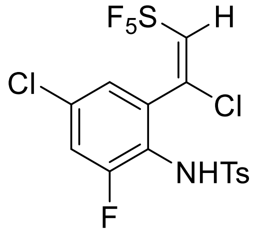


2k

^{19}F-NMR

$CDCl_3$, 471 MHz, 298 K

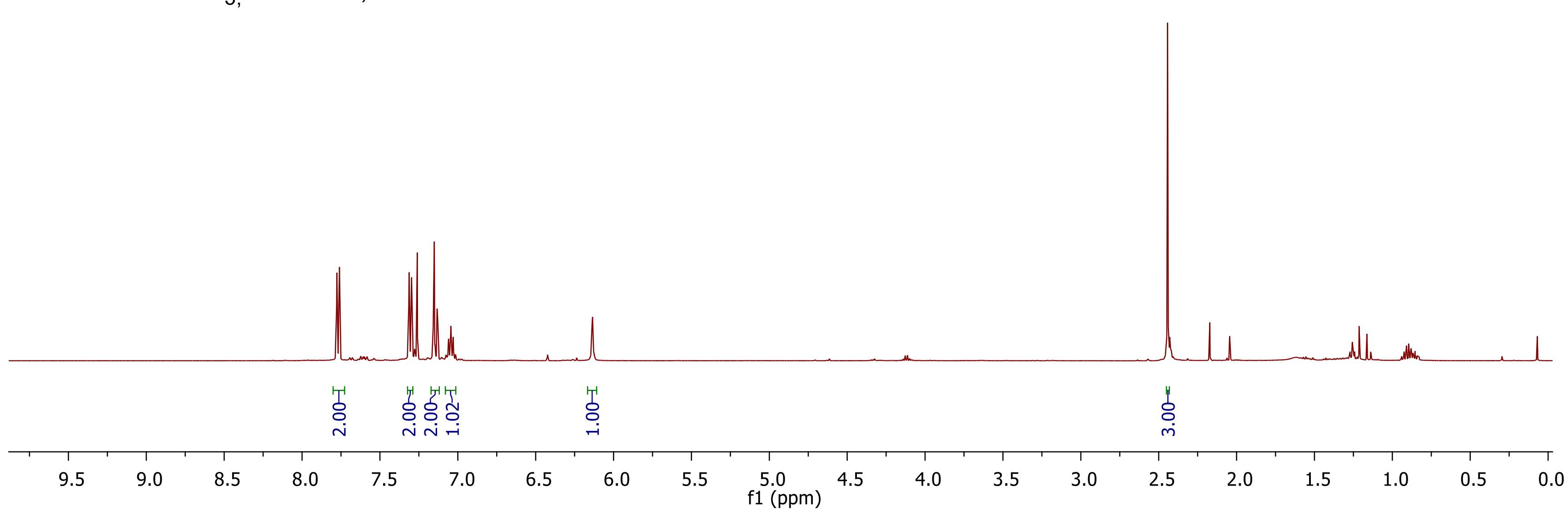


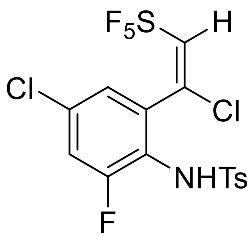


2l

^{1}H-NMR

$CDCl_3$, 500 MHz, 298 K

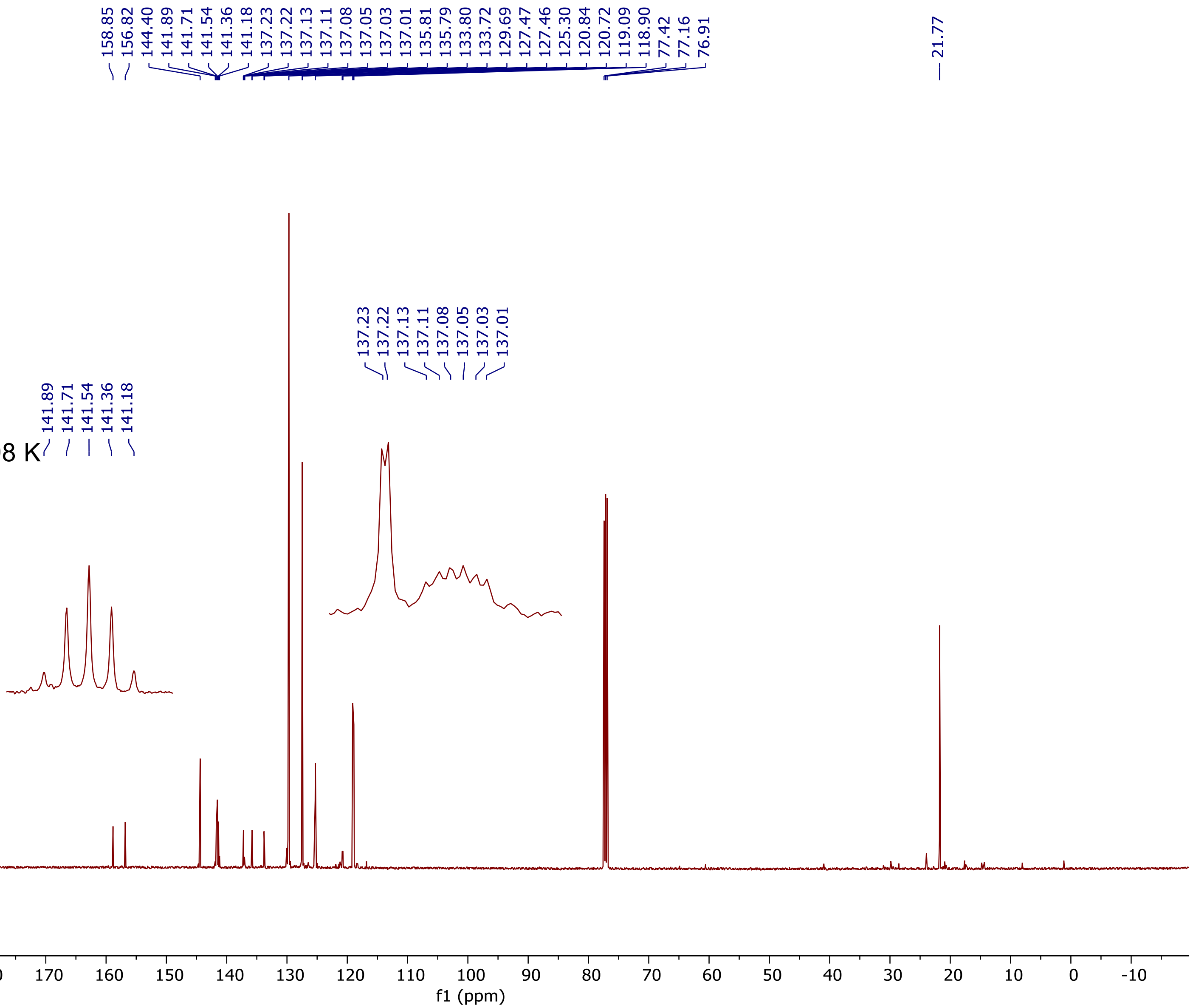


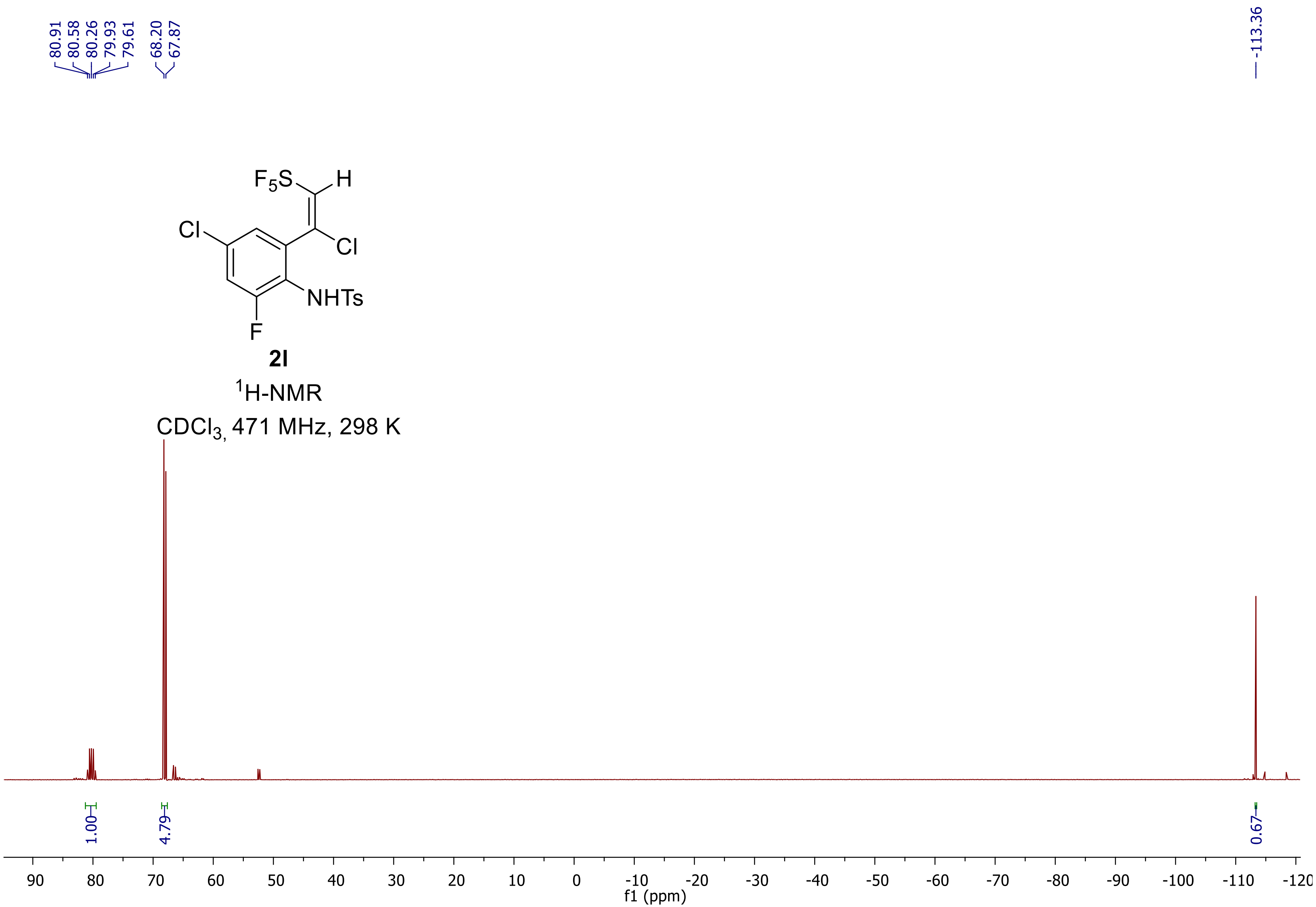


2l

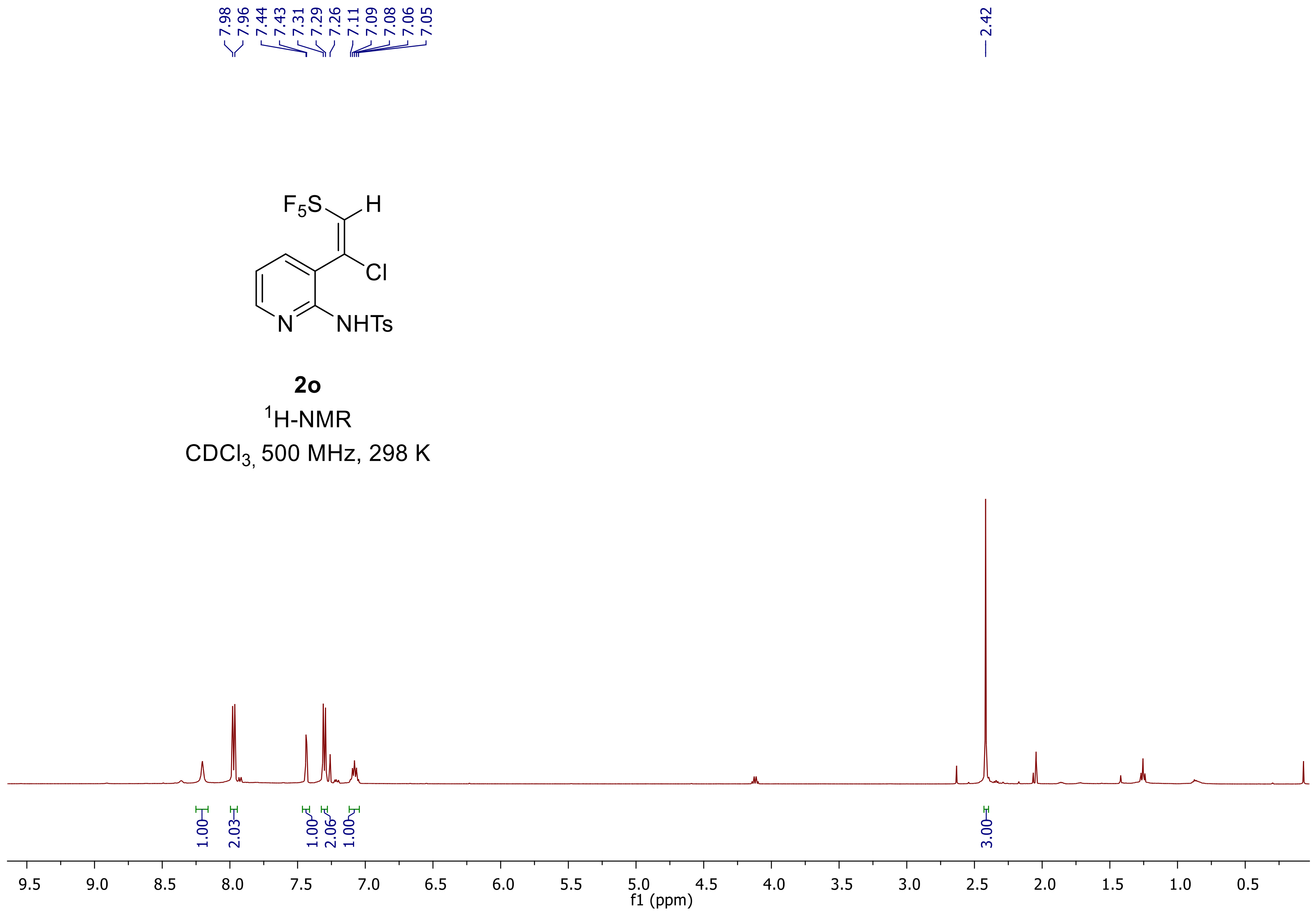
^{1}H-NMR

$CDCl_3$, 125 MHz, 298 K





80.91
80.58
80.26
79.93
79.61
68.20
67.87
-113.36
F5S
H
Cl
Cl
NHTs
F
2l
1H-NMR
CDCl3, 471 MHz, 298 K
1.00
4.79
0.67
90 80 70 60 50 40 30 20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120
f1 (ppm)



2o

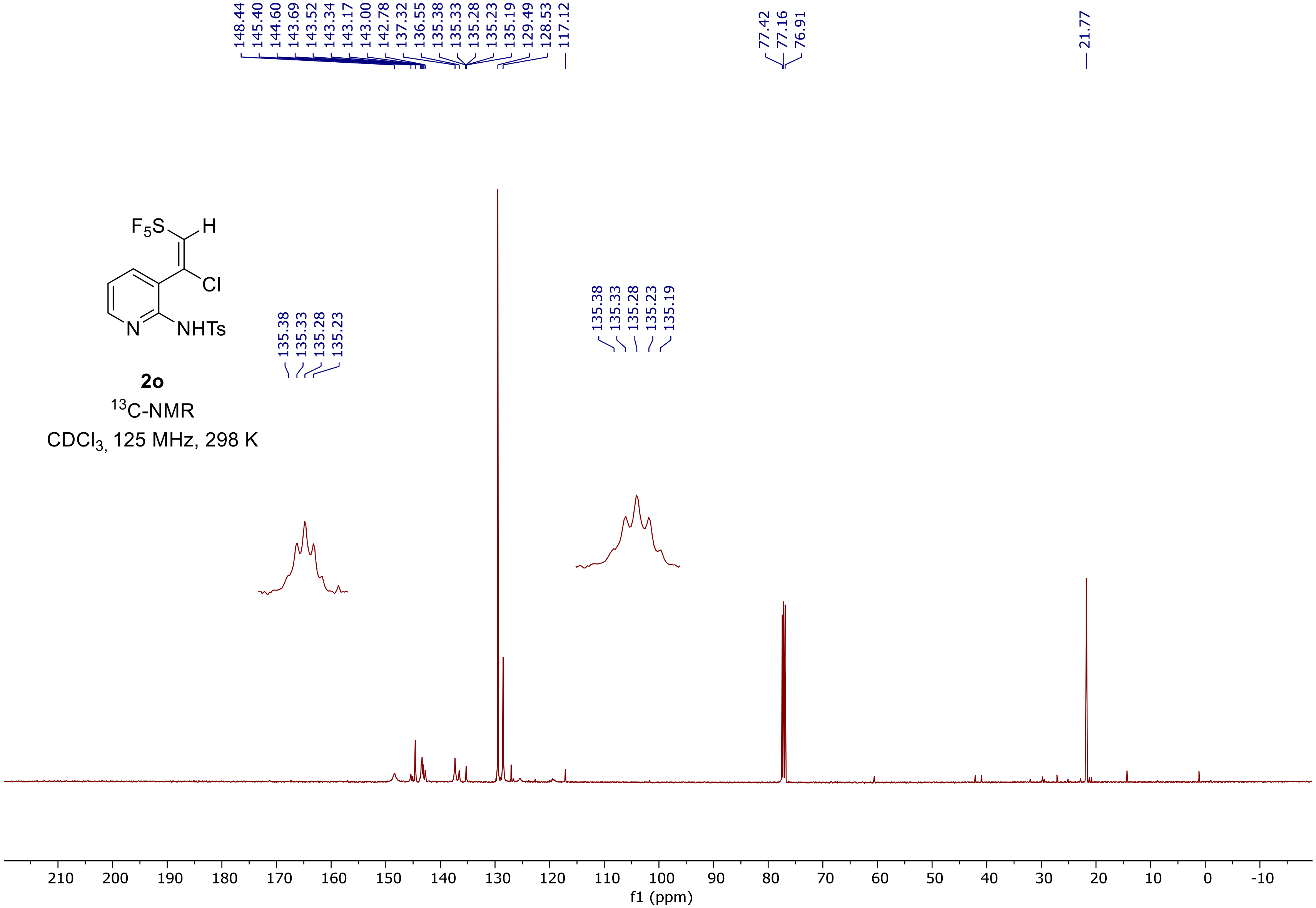
^{1}H-NMR

$CDCl_3$, 500 MHz, 298 K

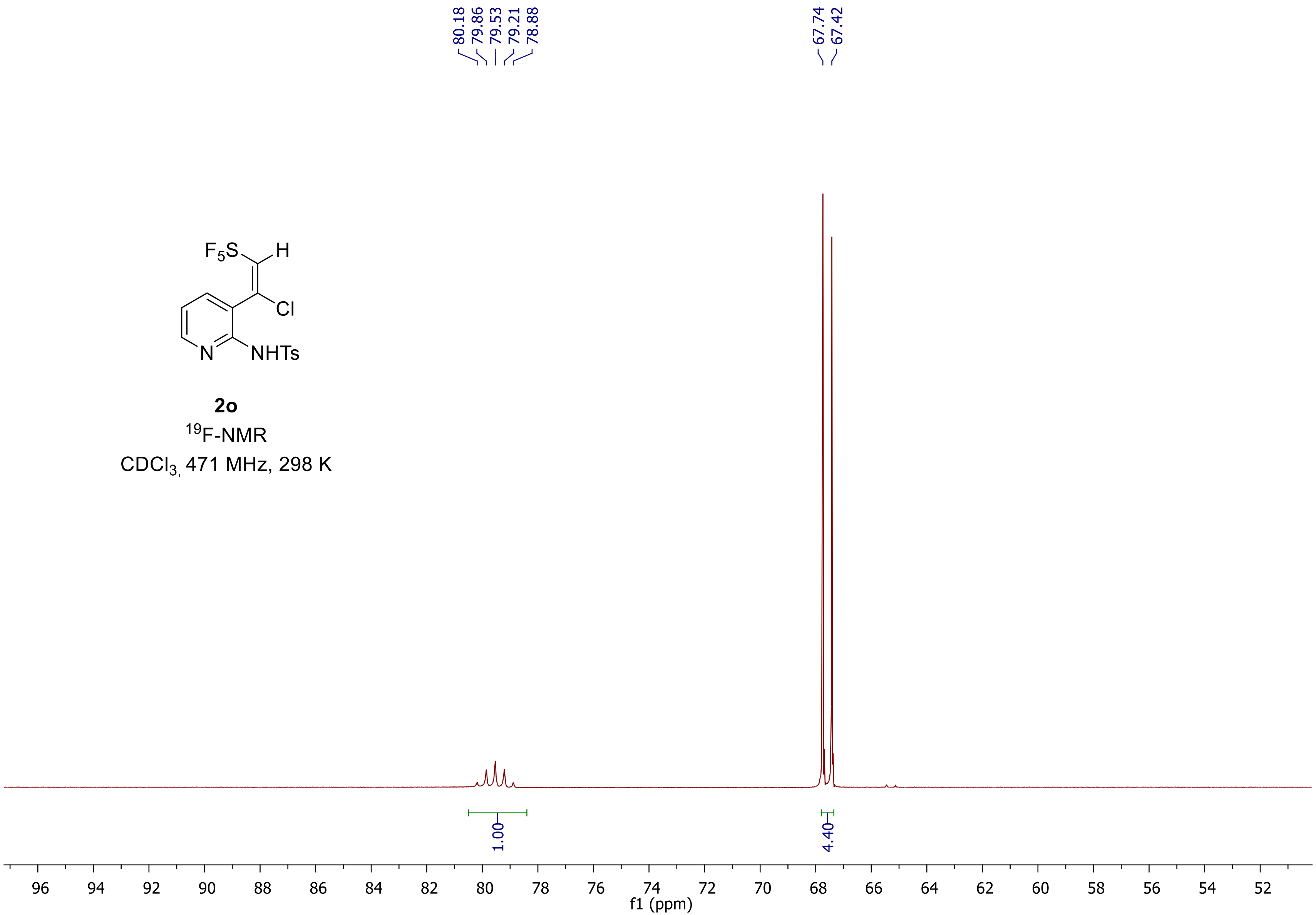
2o

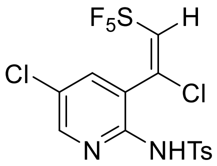
^{13}C-NMR

$CDCl_3$, 125 MHz, 298 K

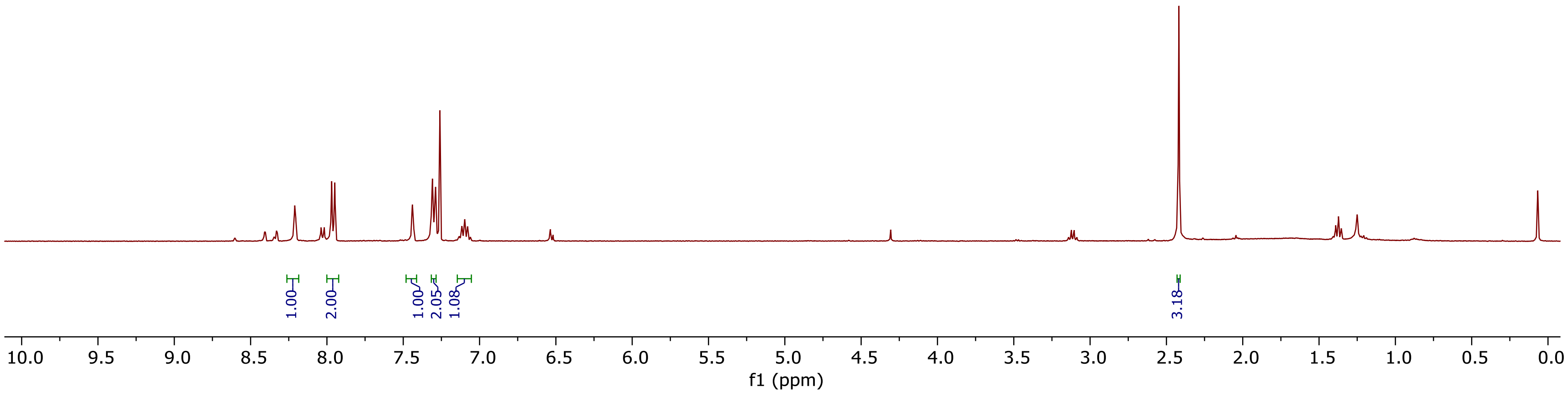


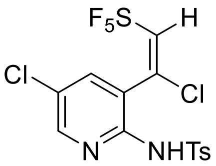
2o
^{19}F-NMR
$CDCl_3$, 471 MHz, 298 K





2p
^{1}H-NMR
$CDCl_3$, 500 MHz, 298 K

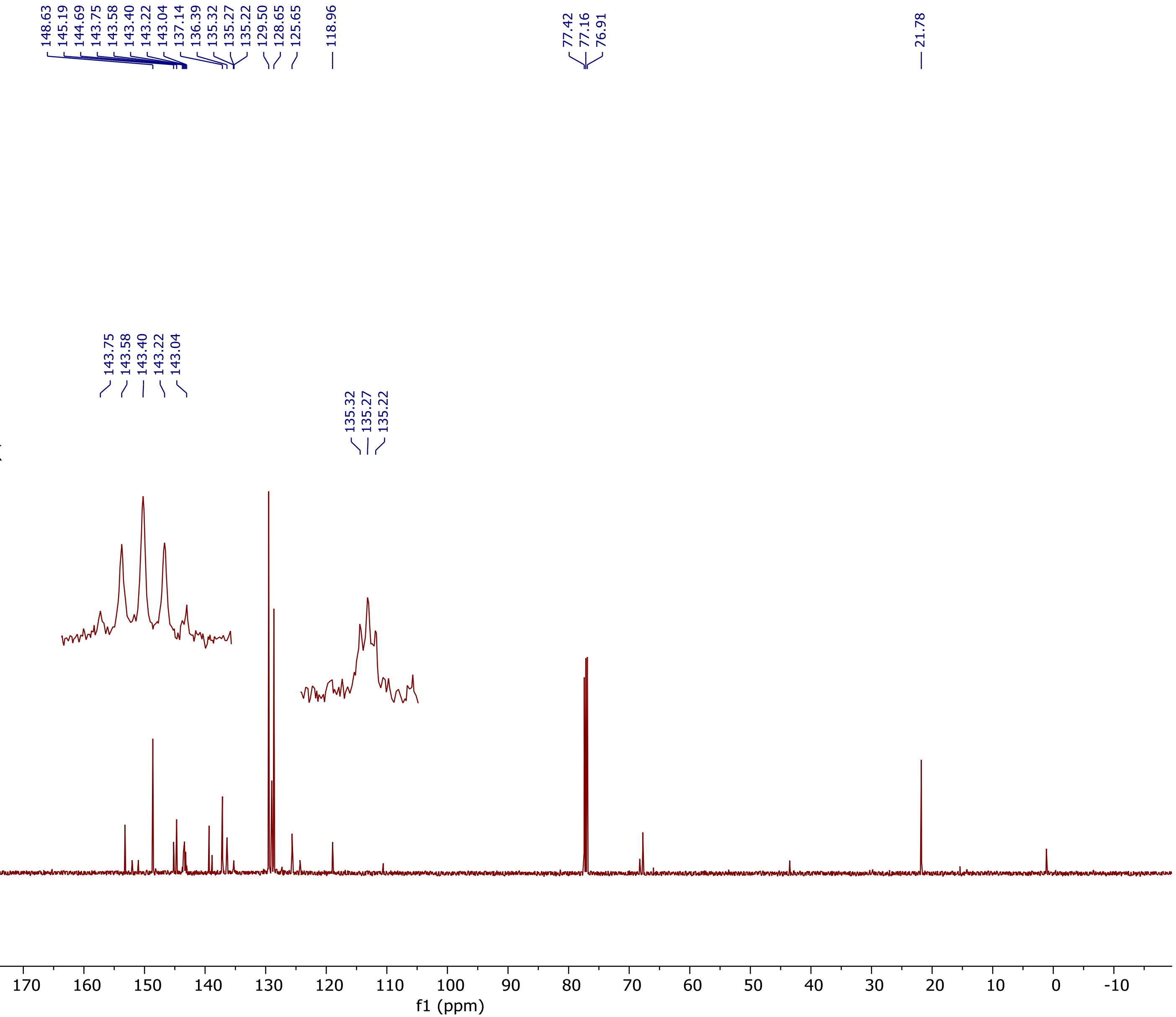


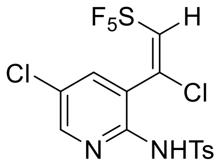


2p

^{13}C-NMR

$CDCl_3$, 125 MHz, 298 K

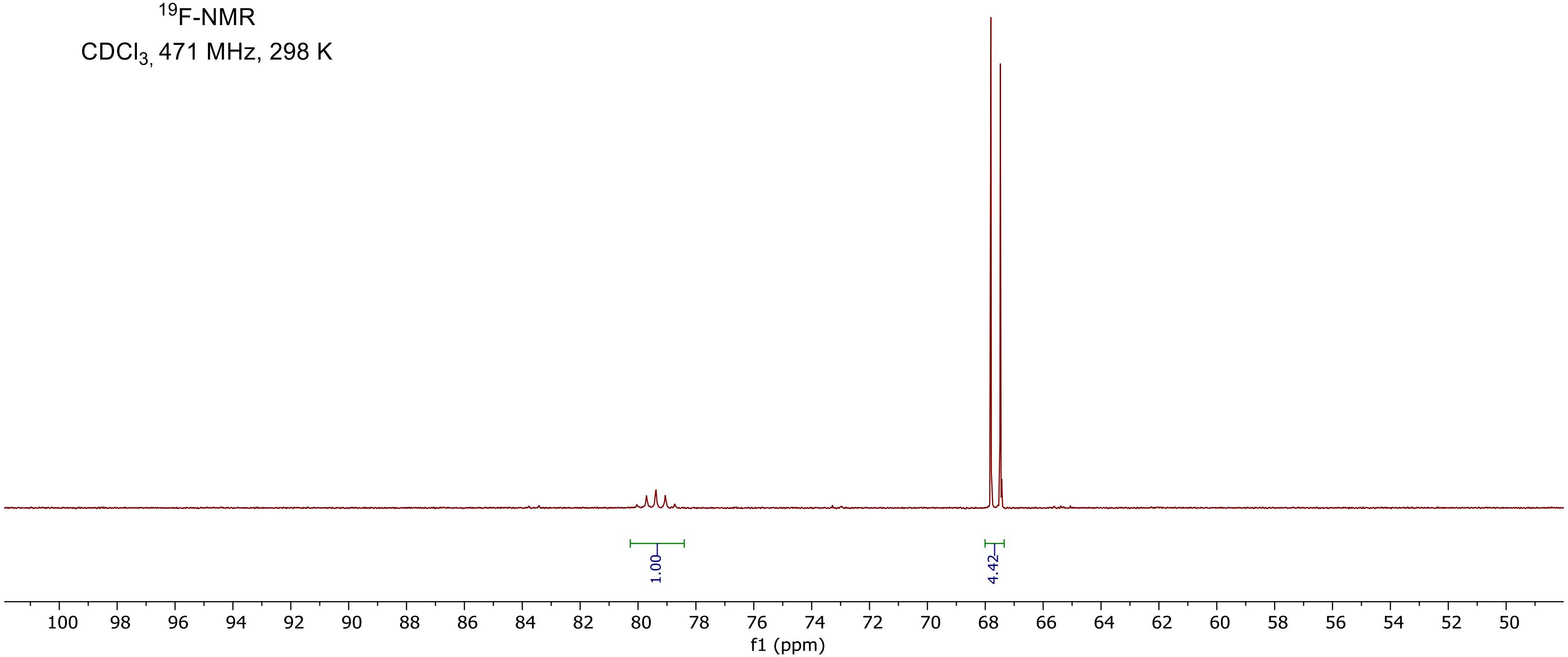


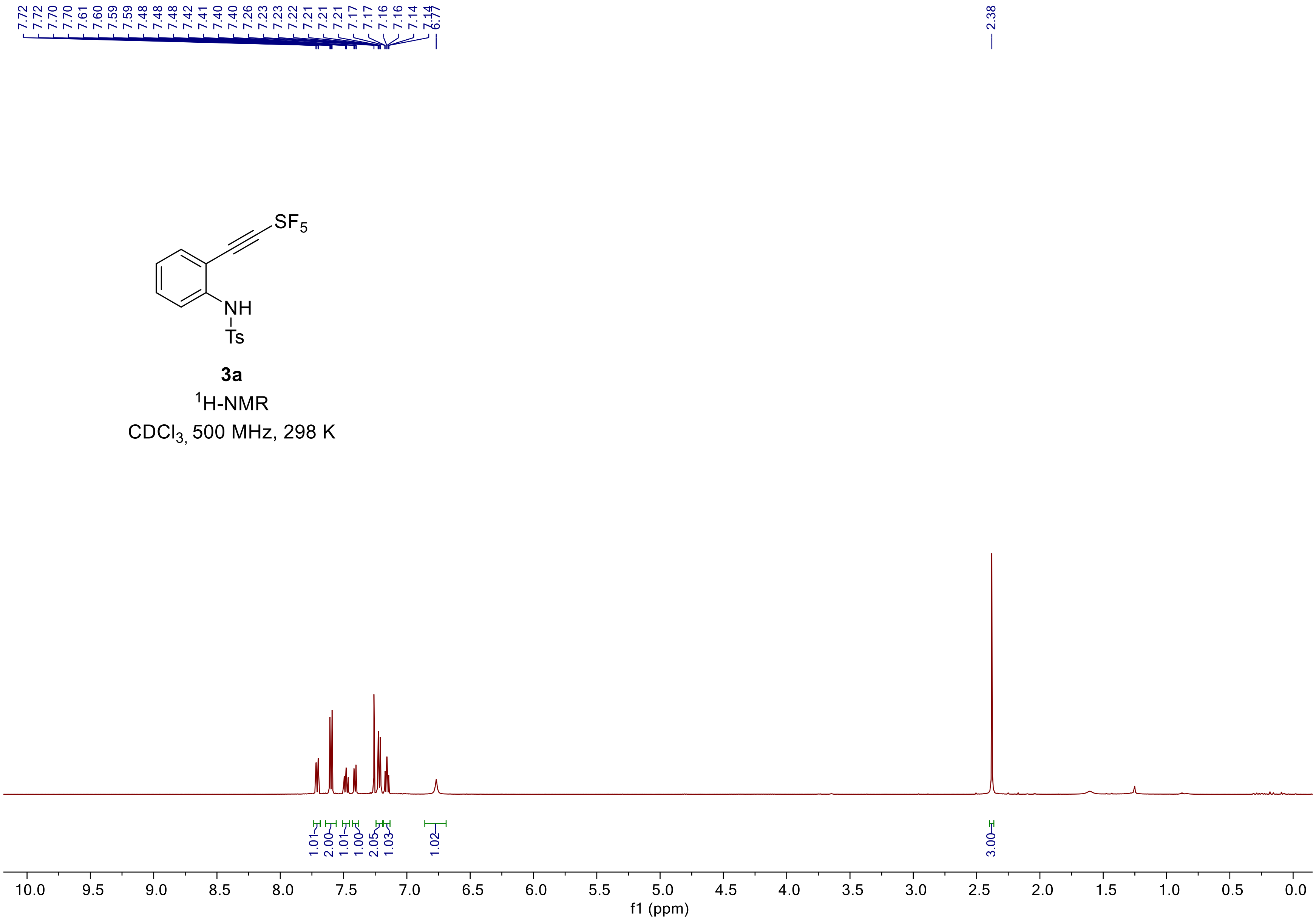


2p

^{19}F-NMR

$CDCl_3$, 471 MHz, 298 K

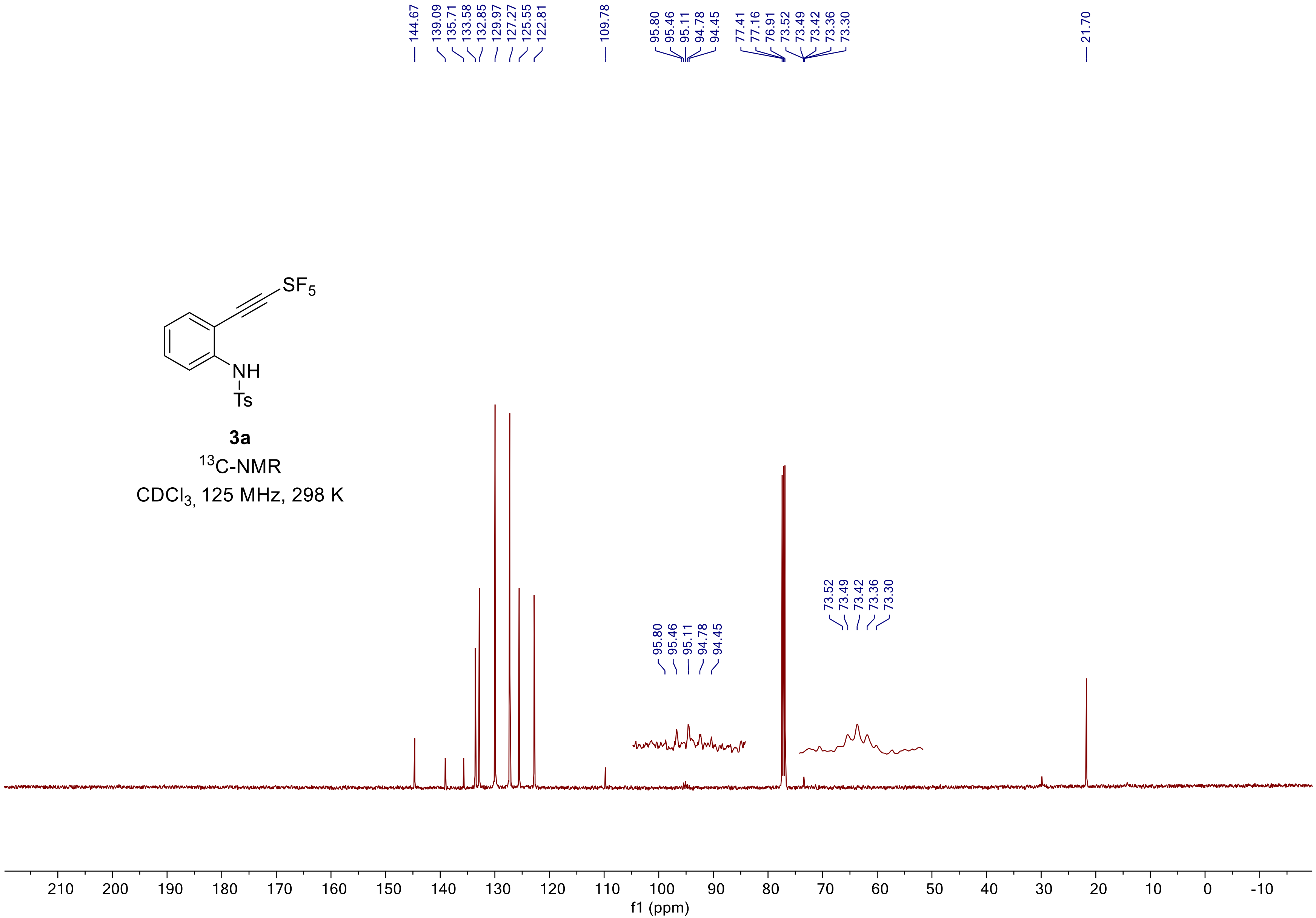




3a

^{1}H-NMR

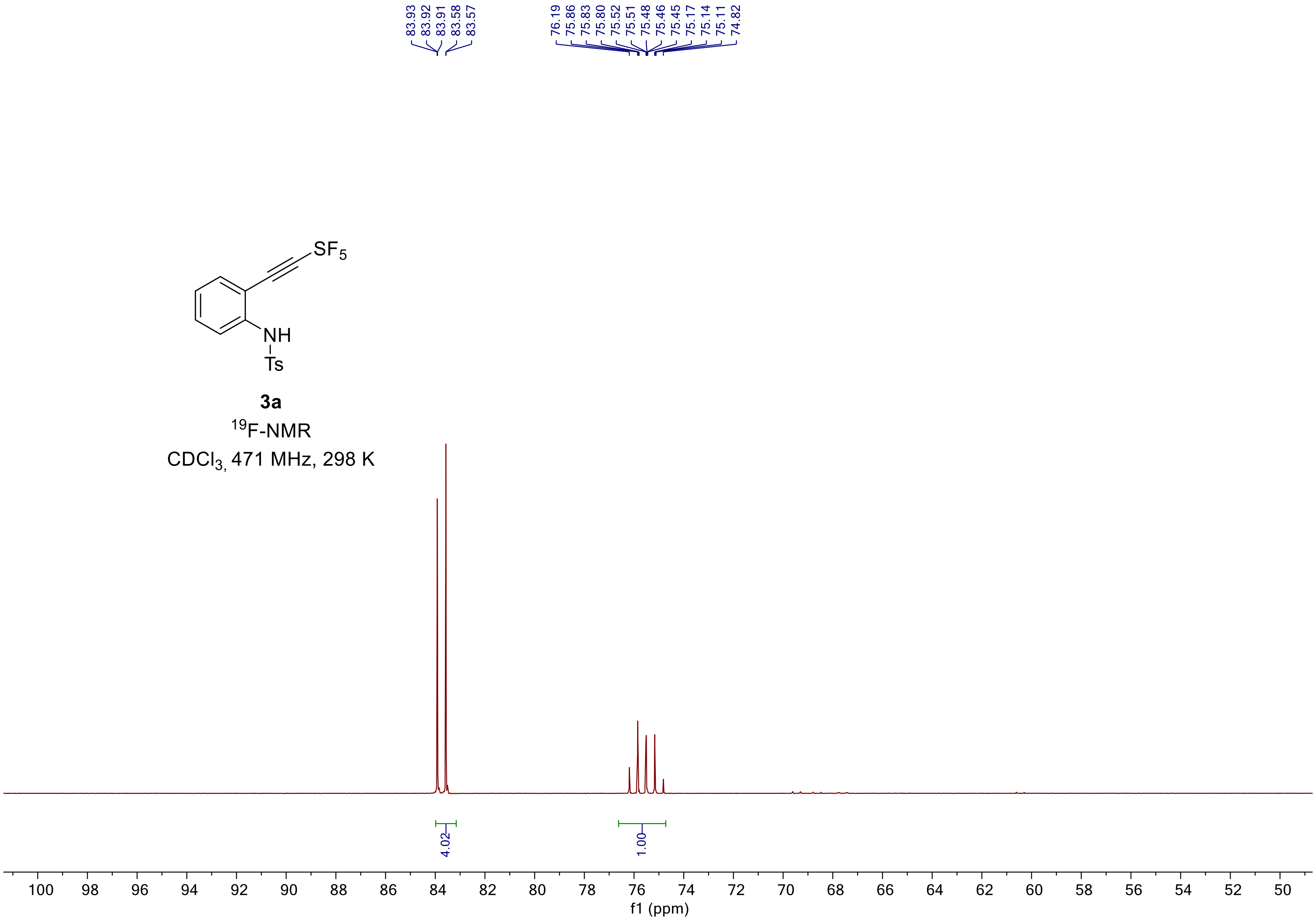
$CDCl_3$, 500 MHz, 298 K

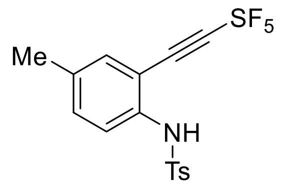


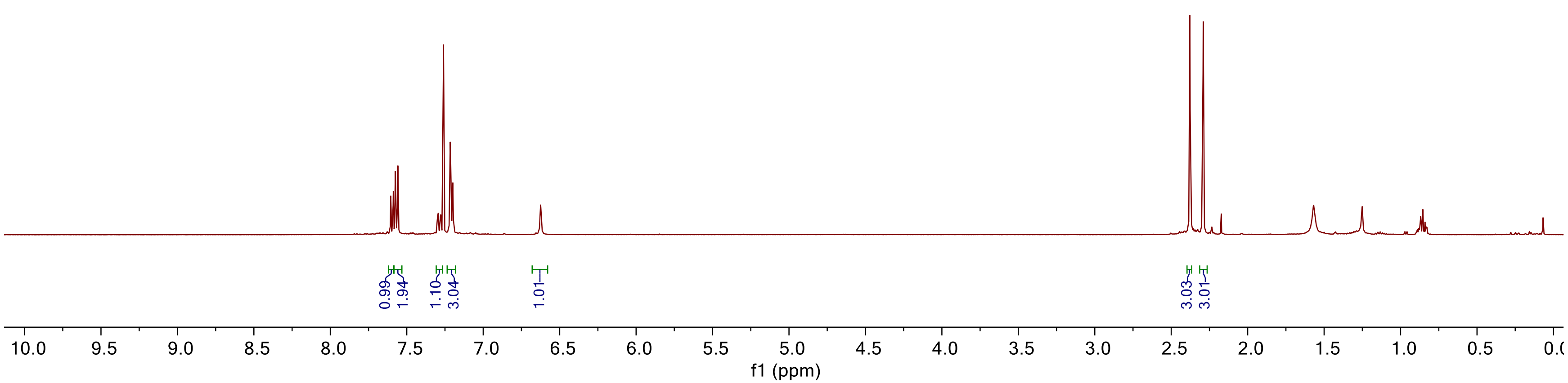
3a

^{13}C-NMR

$CDCl_3$, 125 MHz, 298 K


83.93
83.92
83.91
83.58
83.57
76.19
75.86
75.83
75.80
75.52
75.51
75.48
75.46
75.45
75.17
75.14
75.11
74.82
SF5
NH
Ts
3a
19F-NMR
CDCl3, 471 MHz, 298 K
4.02
1.00
100 98 96 94 92 90 88 86 84 82 80 78 76 74 72 70 68 66 64 62 60 58 56 54 52 50
f1 (ppm)

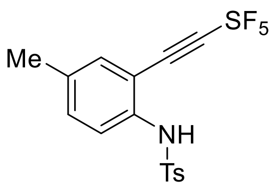




3b

^{1}H-NMR

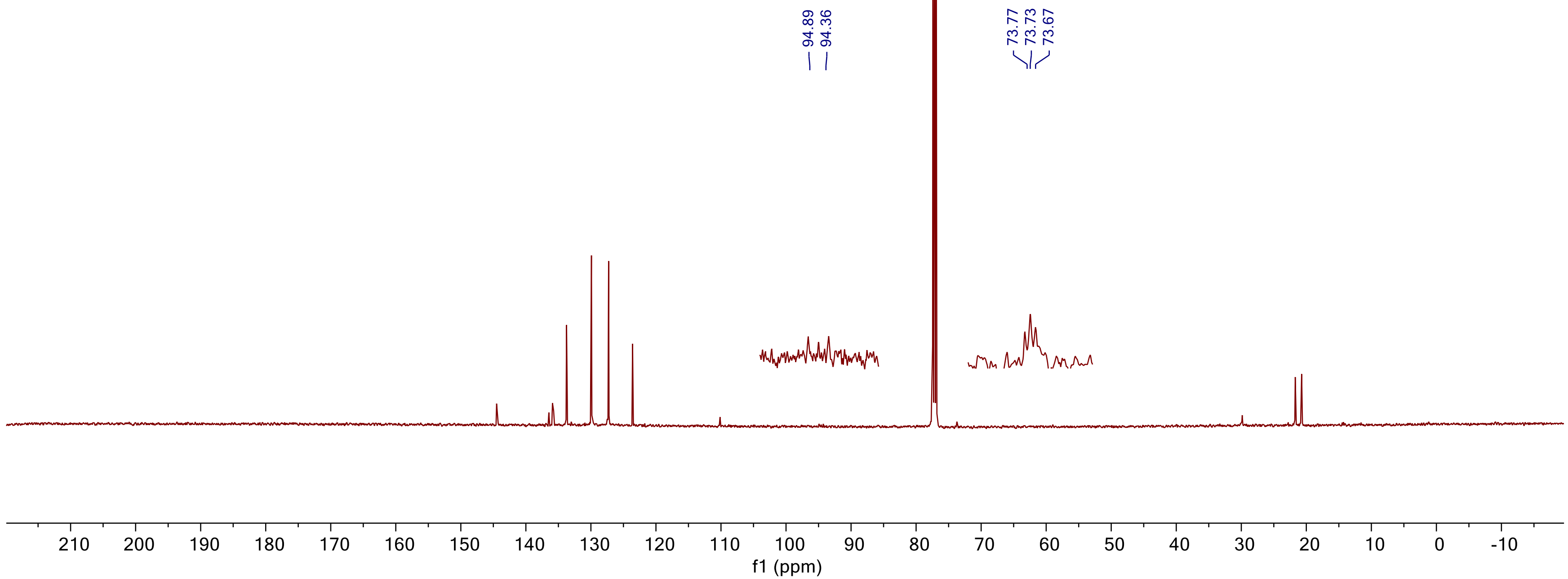
$CDCl_3$, 500 MHz, 298 K

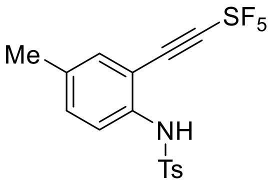


3b

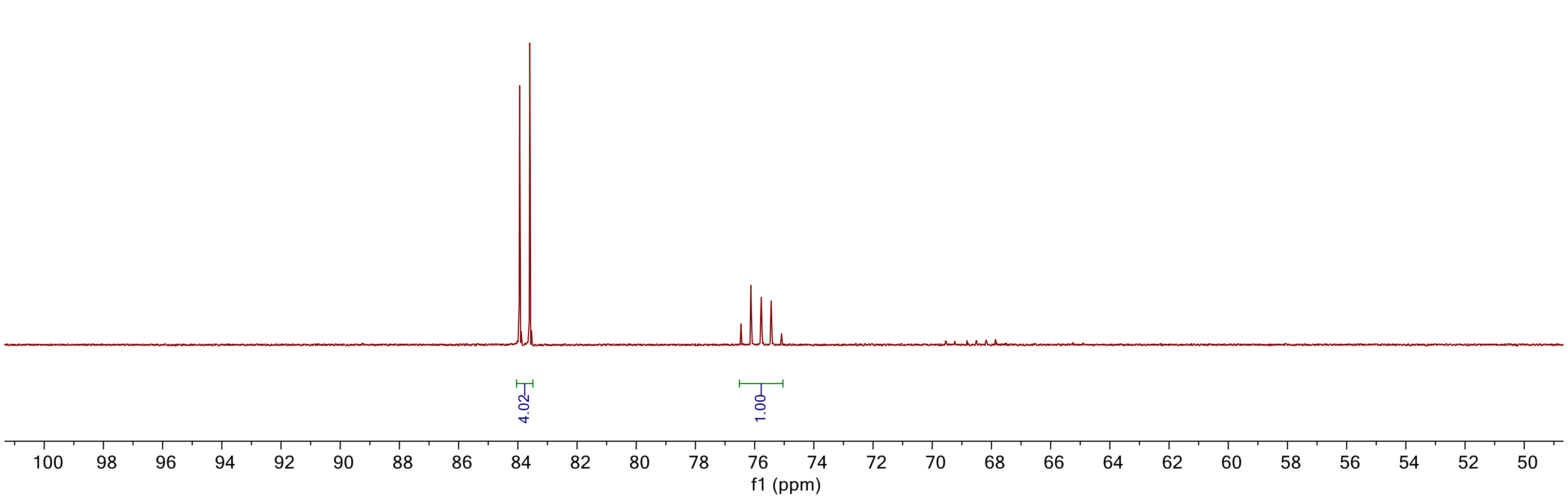
^{13}C-NMR

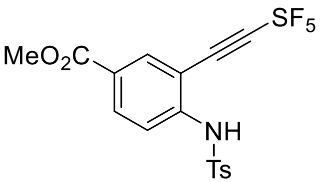
$CDCl_3$, 125 MHz, 298 K





3b
^{19}F-NMR
$CDCl_3$, 471 MHz, 298 K

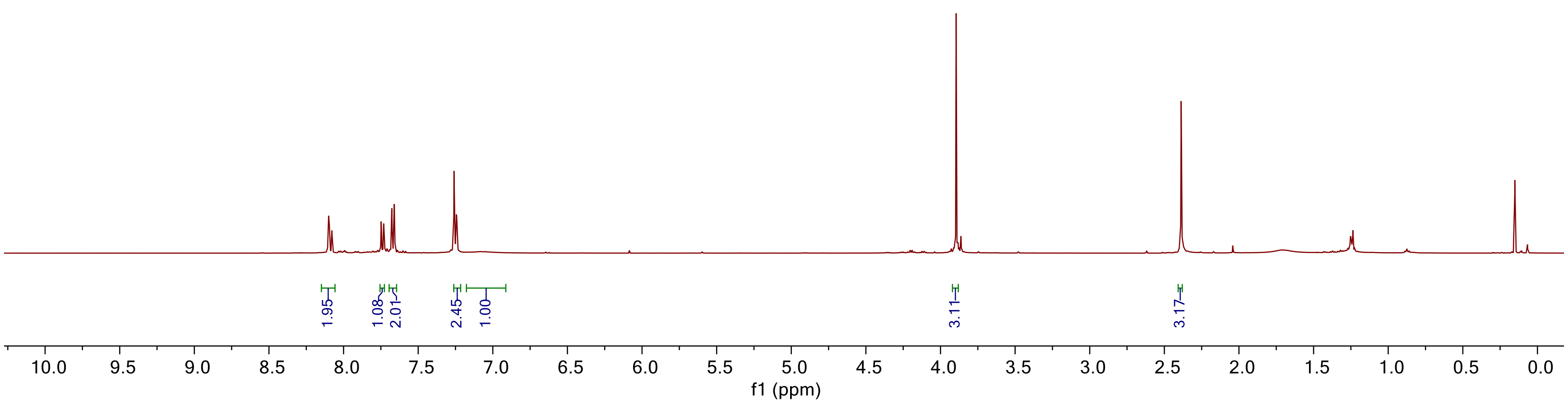


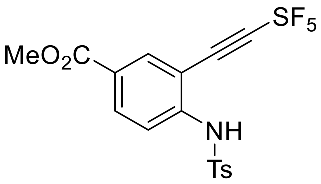


3f

^{1}H-NMR

$CDCl_3$, 500 MHz, 298 K

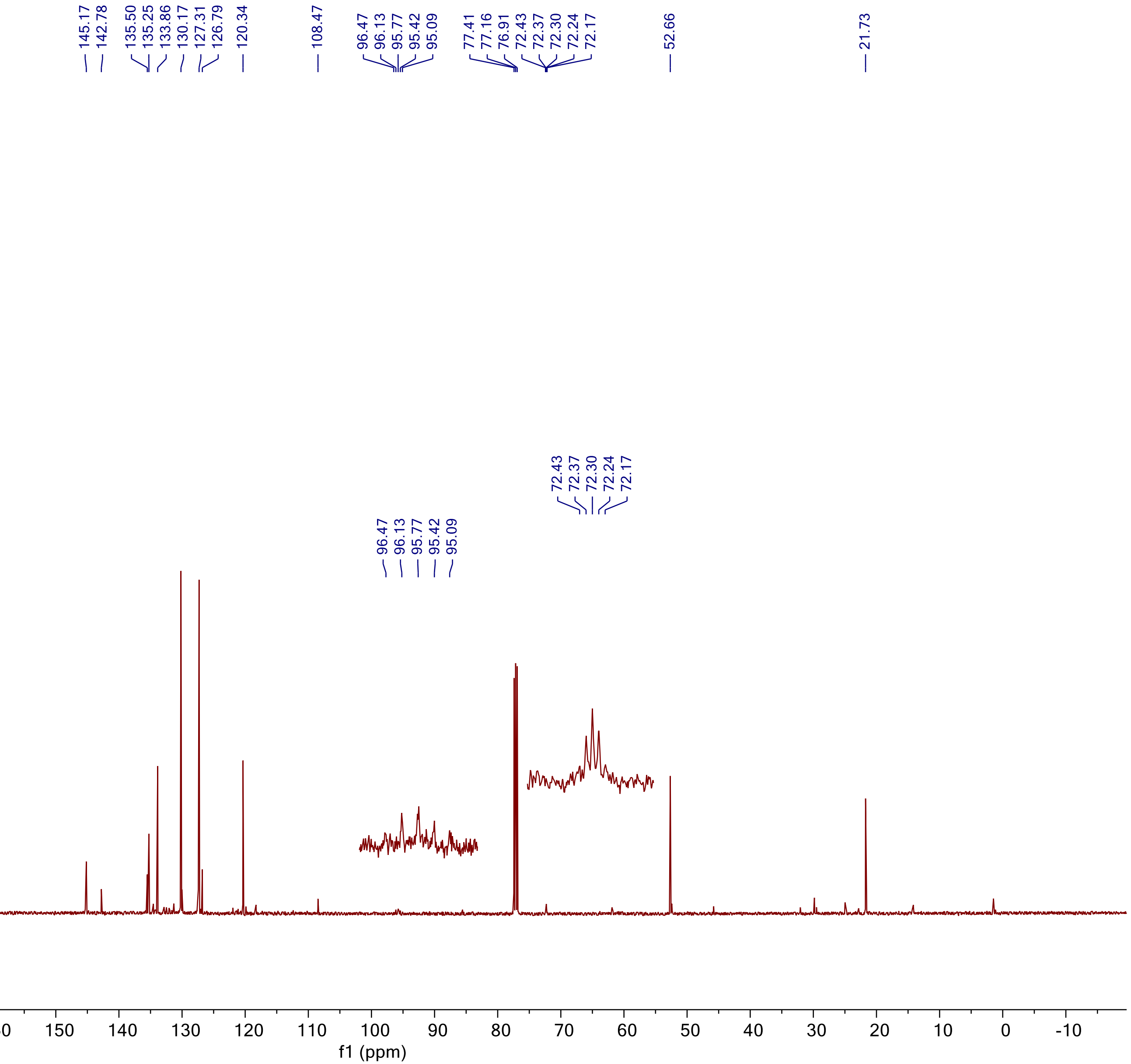


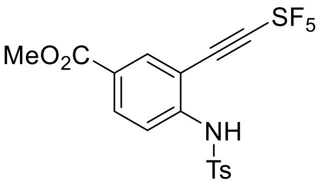


3f

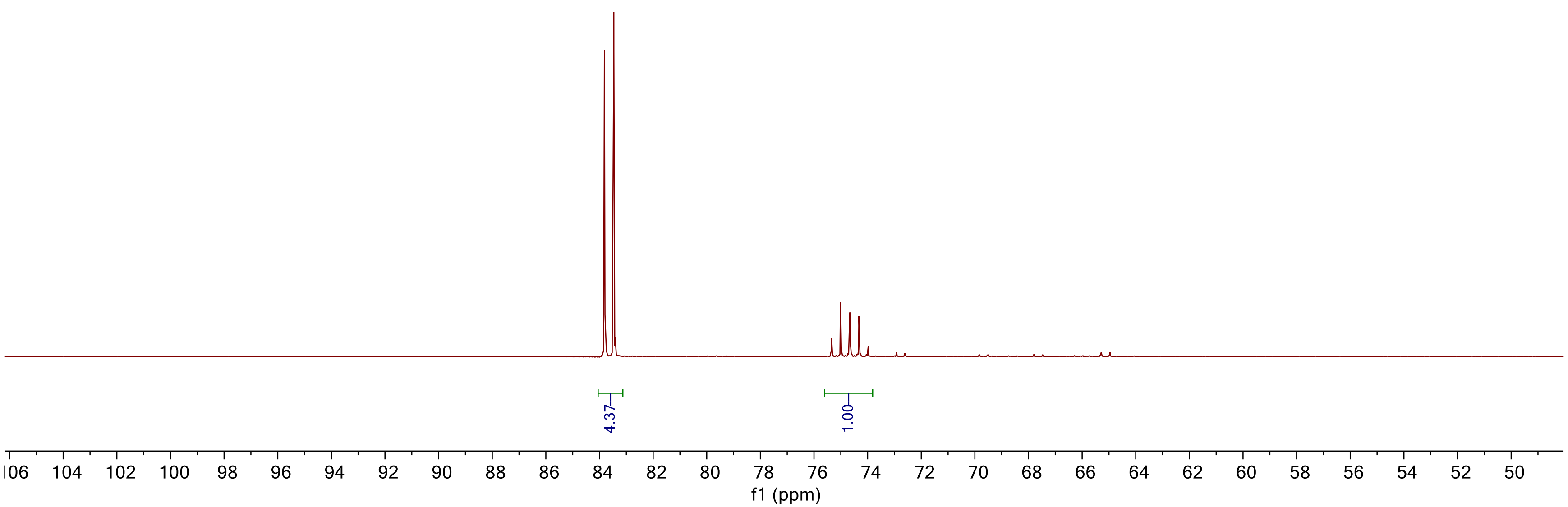
^{13}C-NMR

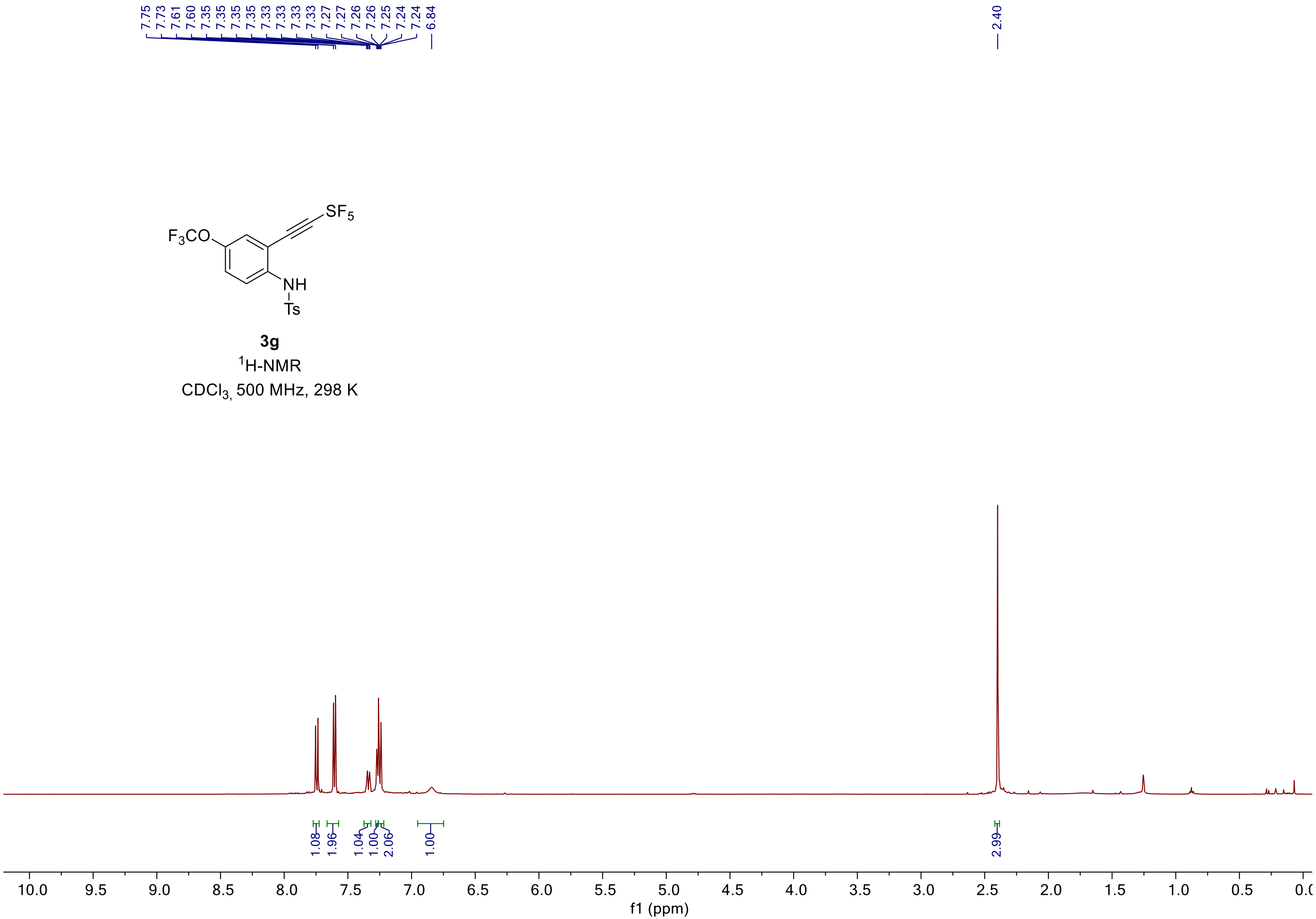
$CDCl_3$, 125 MHz, 298 K



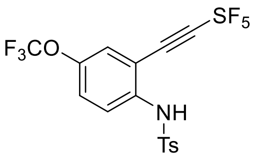


3f
^{19}F-NMR
$CDCl_3$, 471 MHz, 298 K





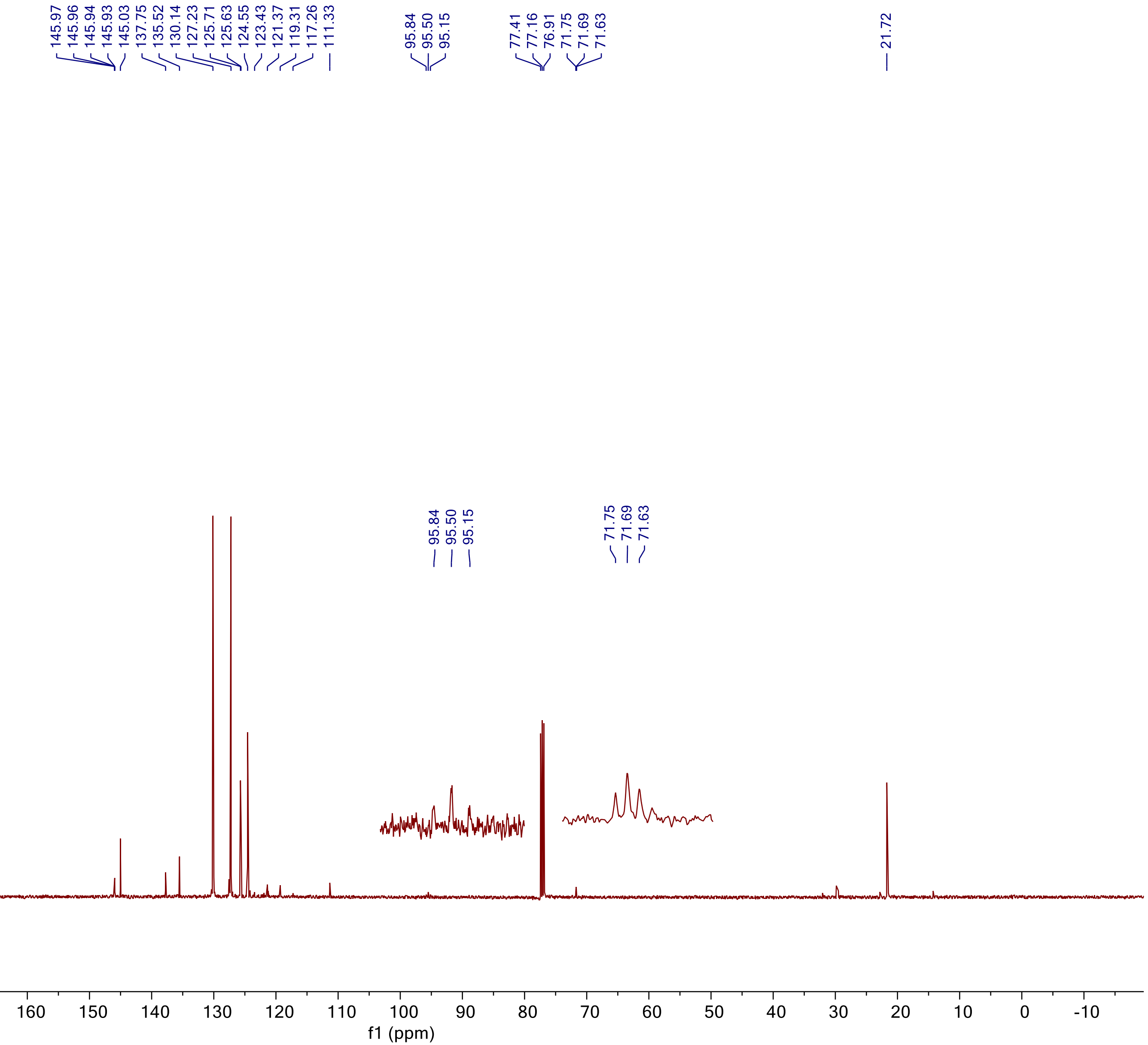
3g
^{1}H-NMR
$CDCl_3$, 500 MHz, 298 K

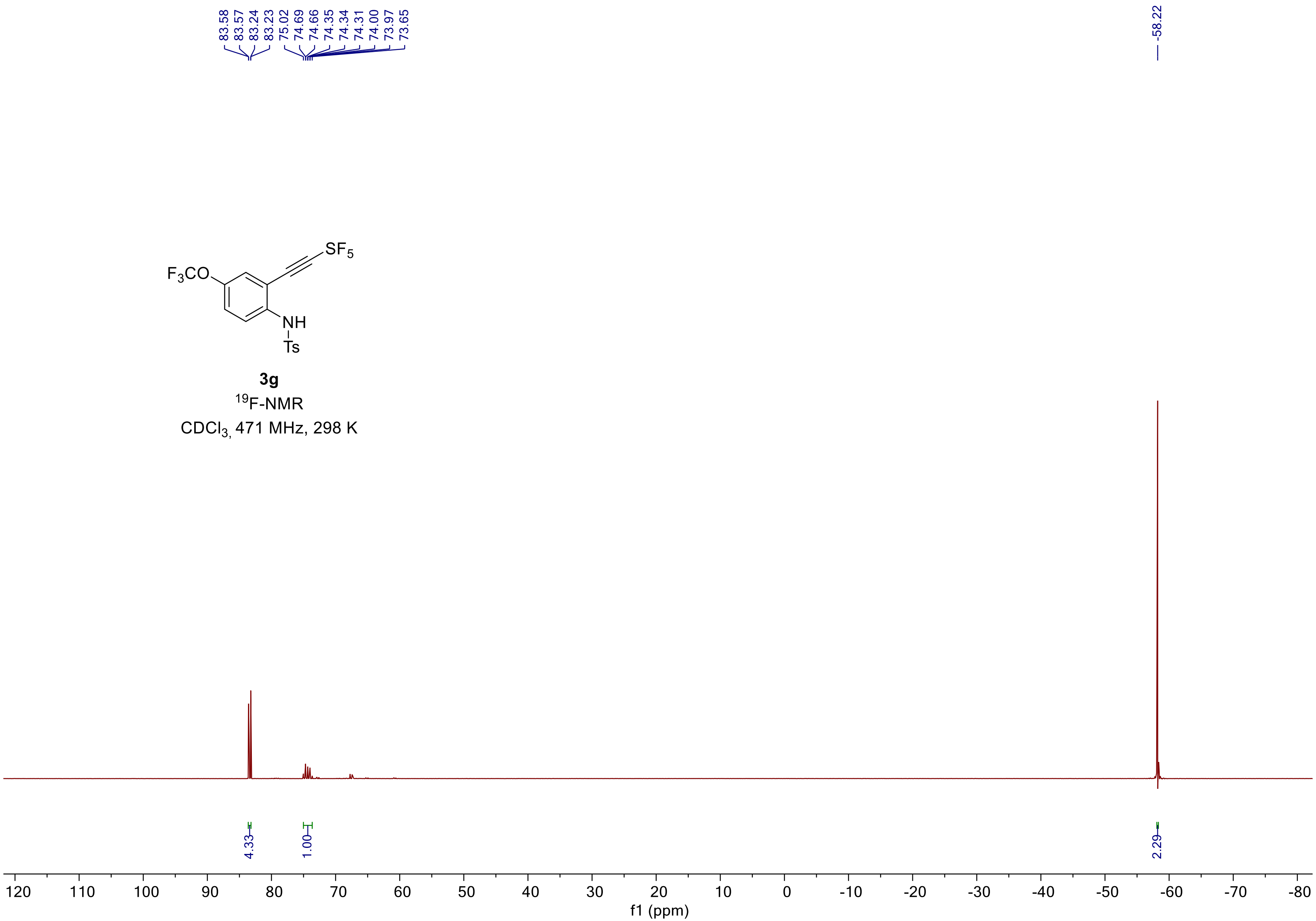


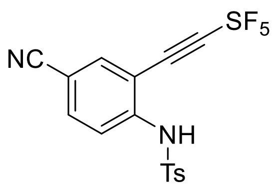
3g

^{13}C-NMR

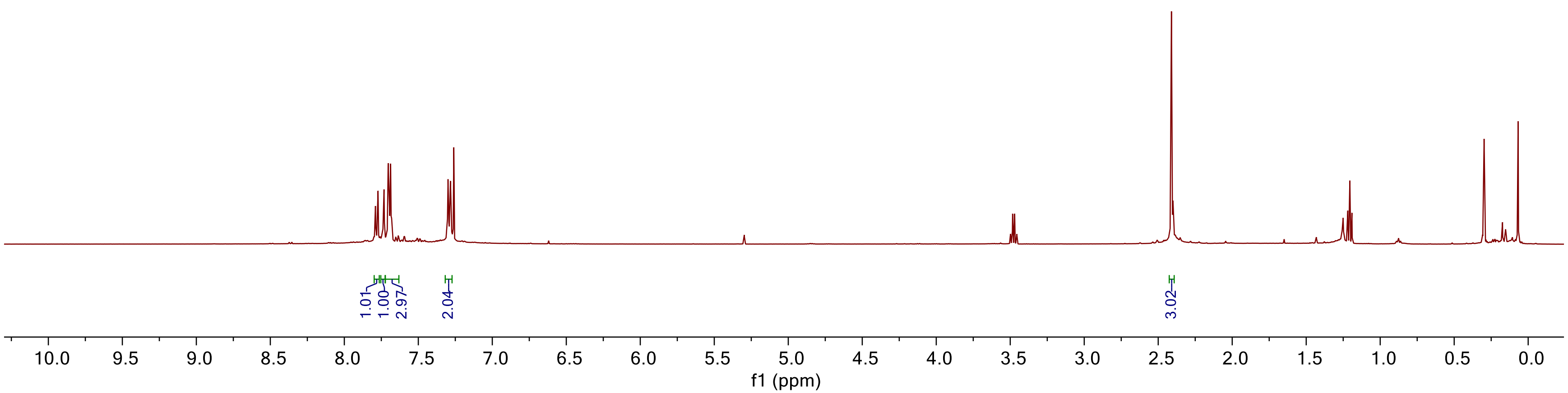
$CDCl_3$, 125 MHz, 298 K

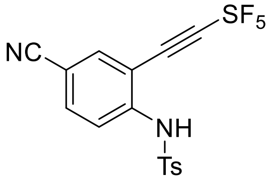



83.58
83.57
83.24
83.23
75.02
74.69
74.66
74.35
74.34
74.31
74.00
73.97
73.65
-58.22
SF5
F3CO
NH
Ts
3g
19F-NMR
CDCl3, 471 MHz, 298 K
4.33
1.00
2.29
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
-20
-30
-40
-50
-60
-70
-80
f1 (ppm)



3h
^{1}H-NMR
$CDCl_3$, 500 MHz, 298 K

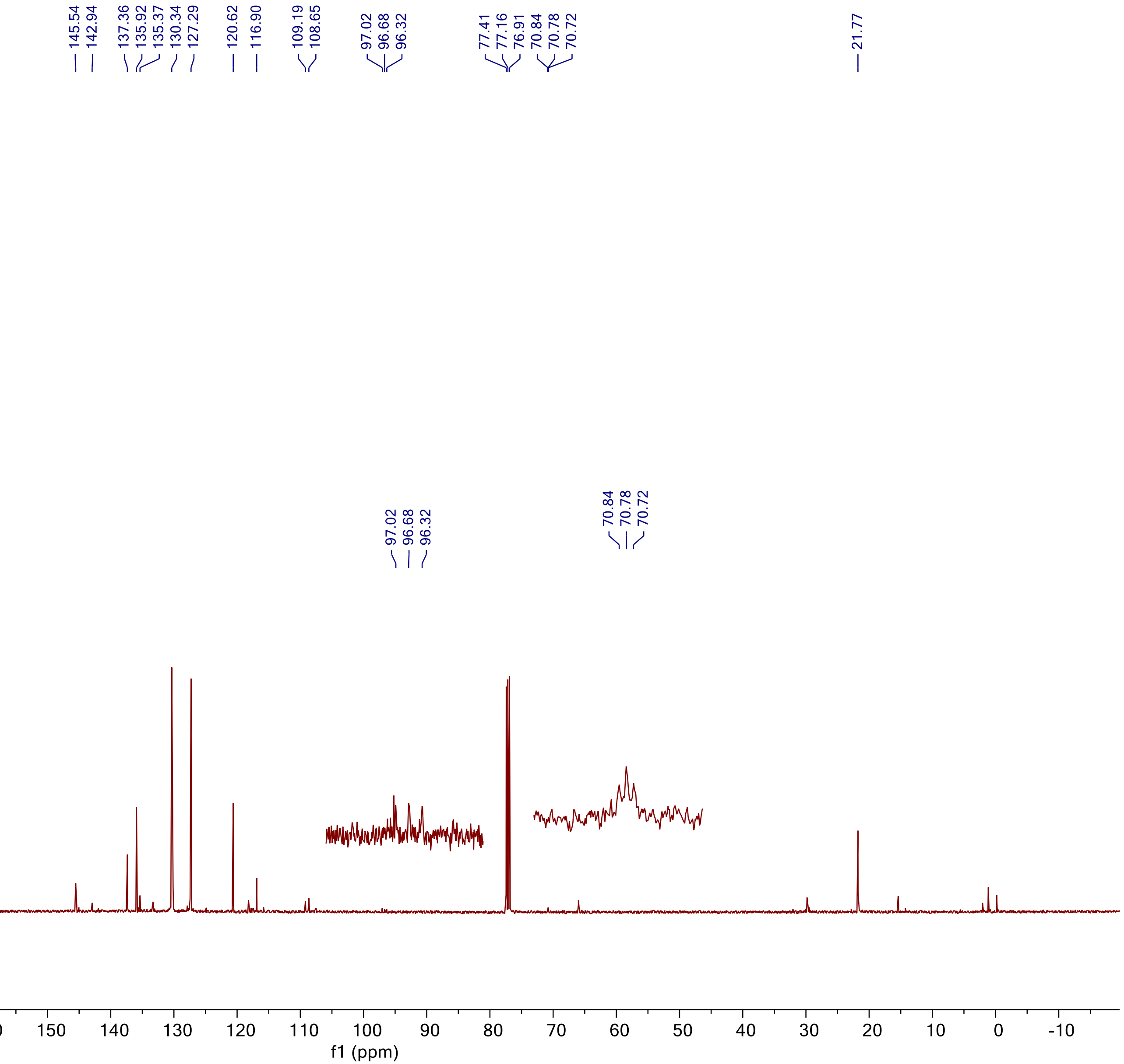


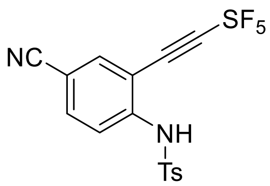


3h

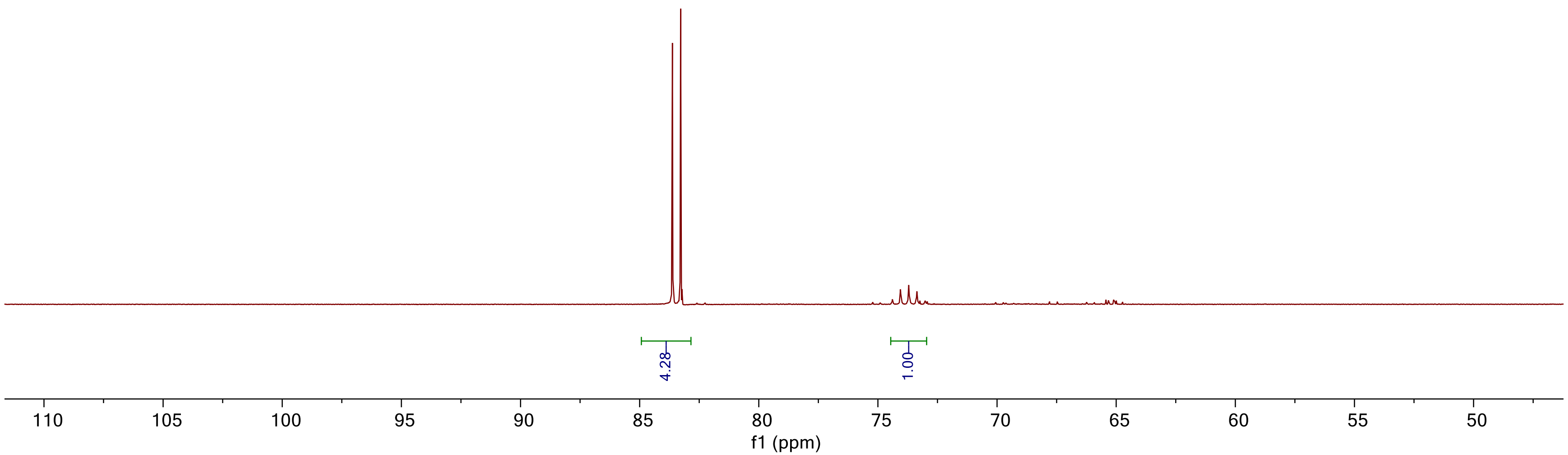
^{13}C-NMR

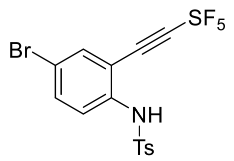
$CDCl_3$, 125 MHz, 298 K





3h
^{19}F-NMR
$CDCl_3$, 471 MHz, 298 K

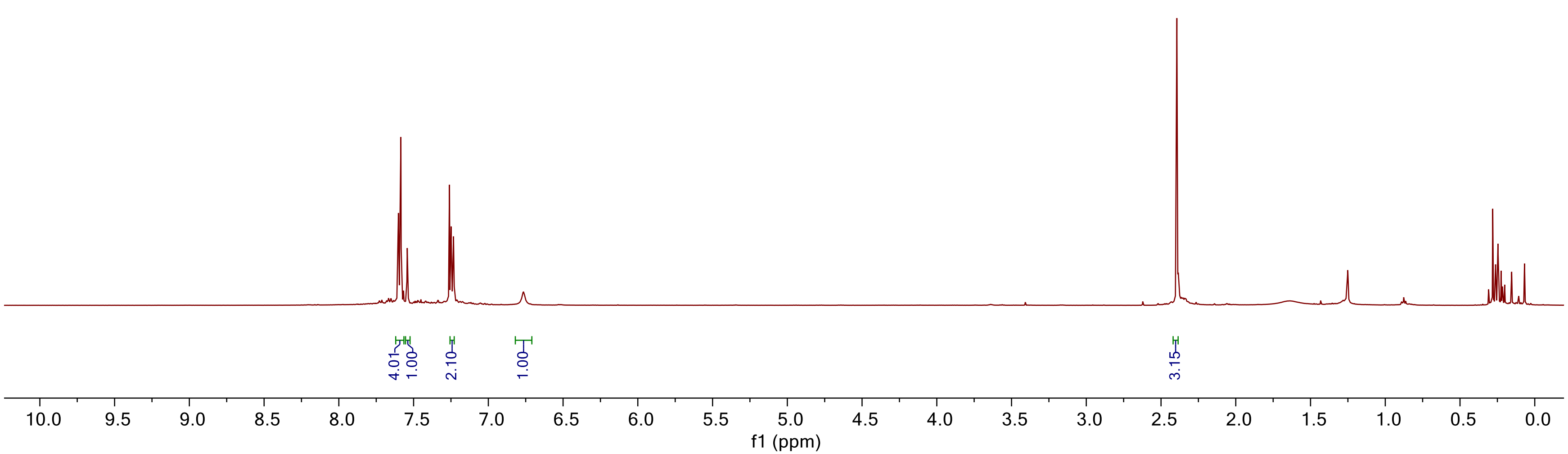


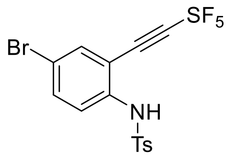


3i

^{1}H-NMR

$CDCl_3$, 500 MHz, 298 K

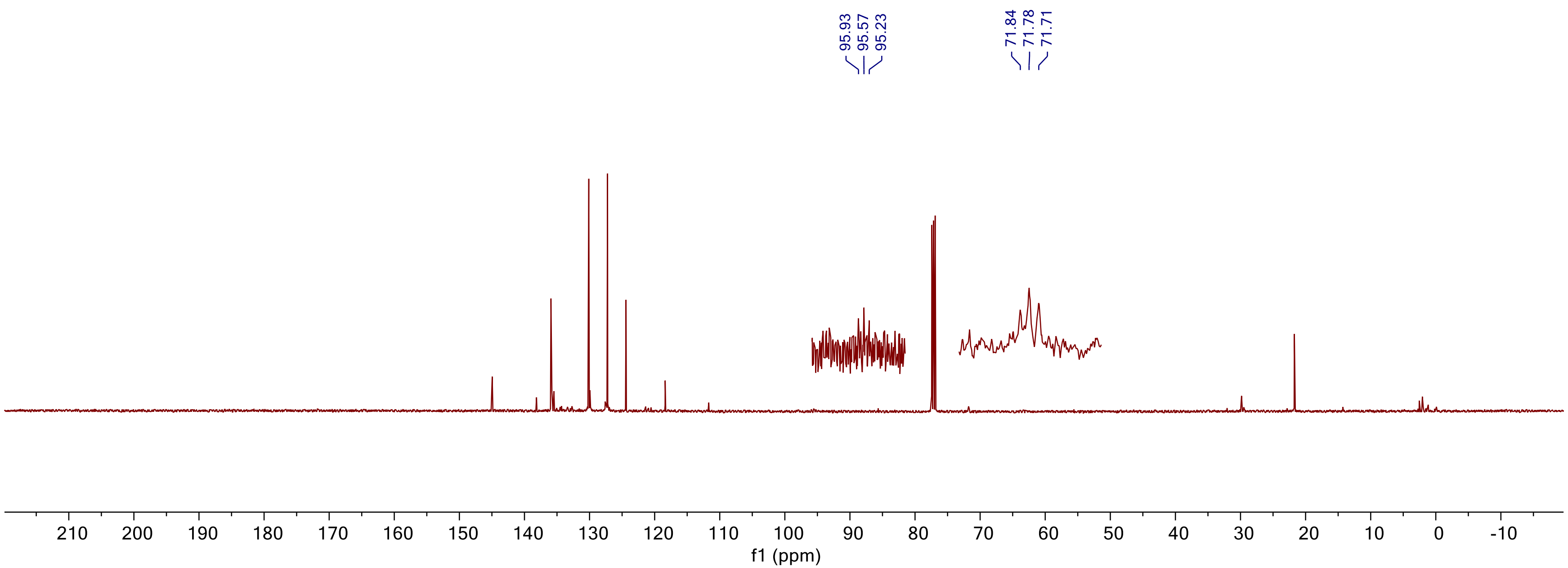


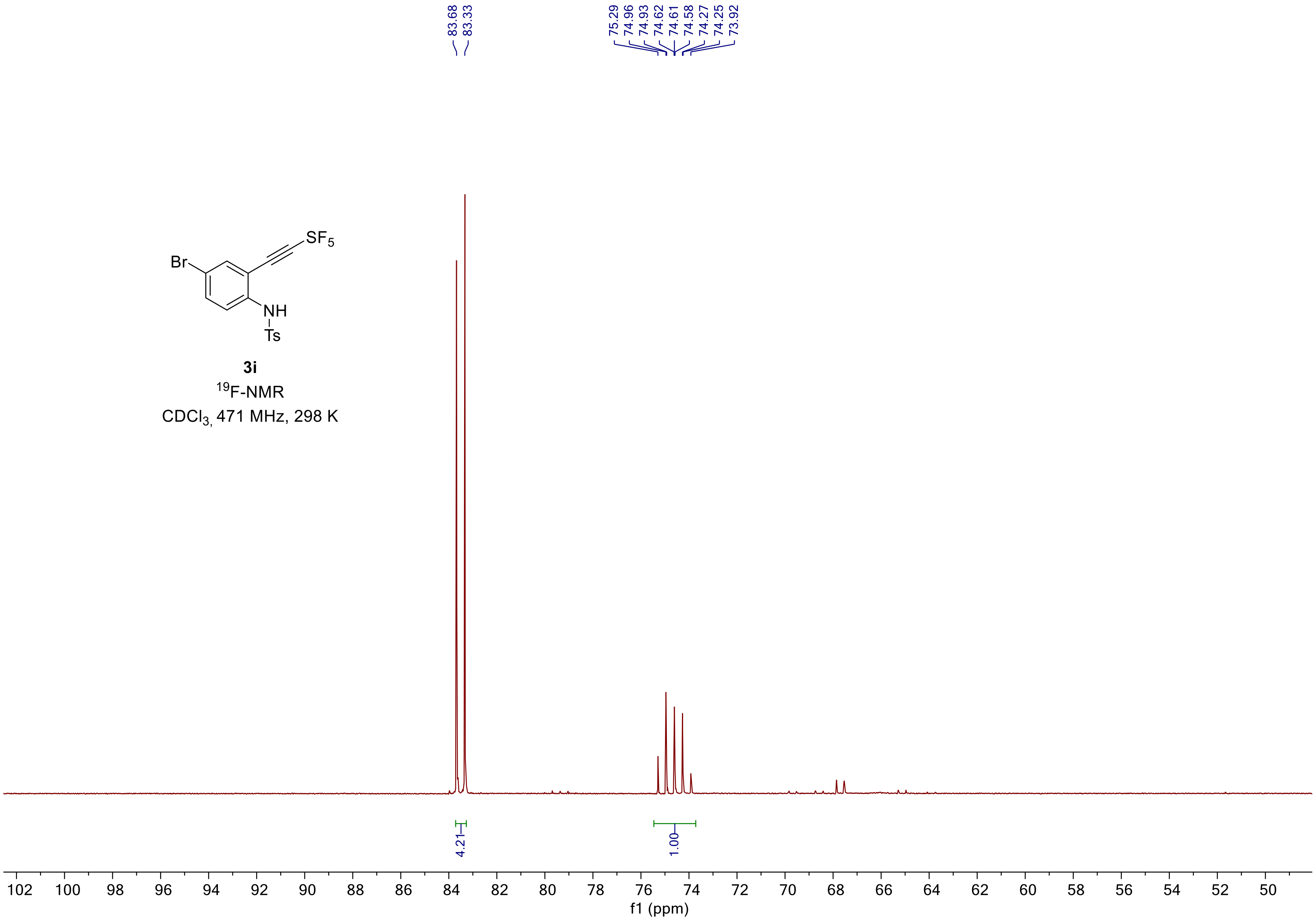


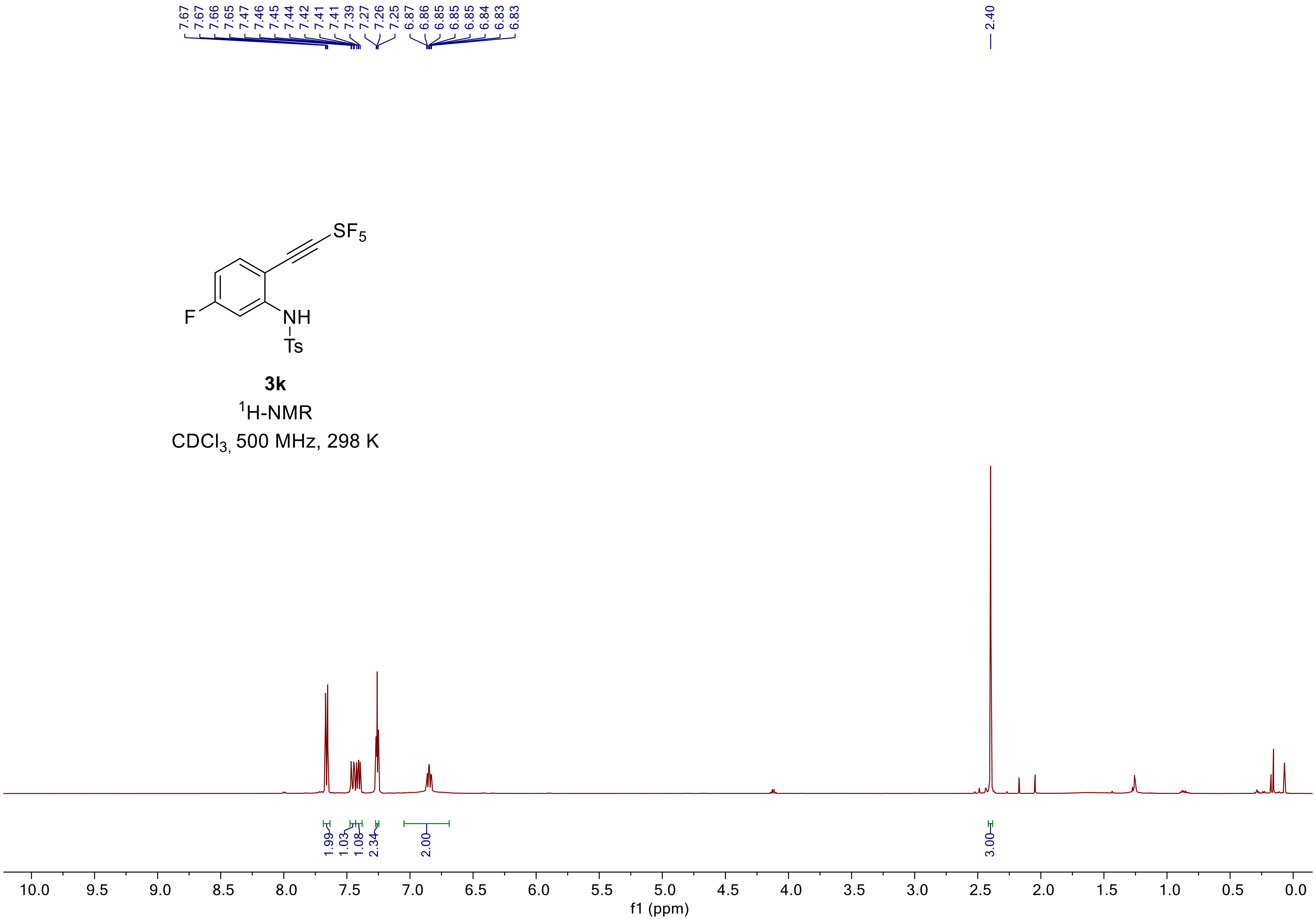
3i

^{13}C-NMR

$CDCl_3$, 125 MHz, 298 K



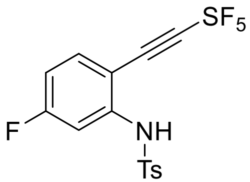

83.68
83.33
75.29
74.96
74.93
74.62
74.61
74.58
74.27
74.25
73.92
SF5
Br
NH
Ts
3i
19F-NMR
CDCl3, 471 MHz, 298 K
4.21
1.00
102 100 98 96 94 92 90 88 86 84 82 80 78 76 74 72 70 68 66 64 62 60 58 56 54 52 50
f1 (ppm)



3k

^{1}H-NMR

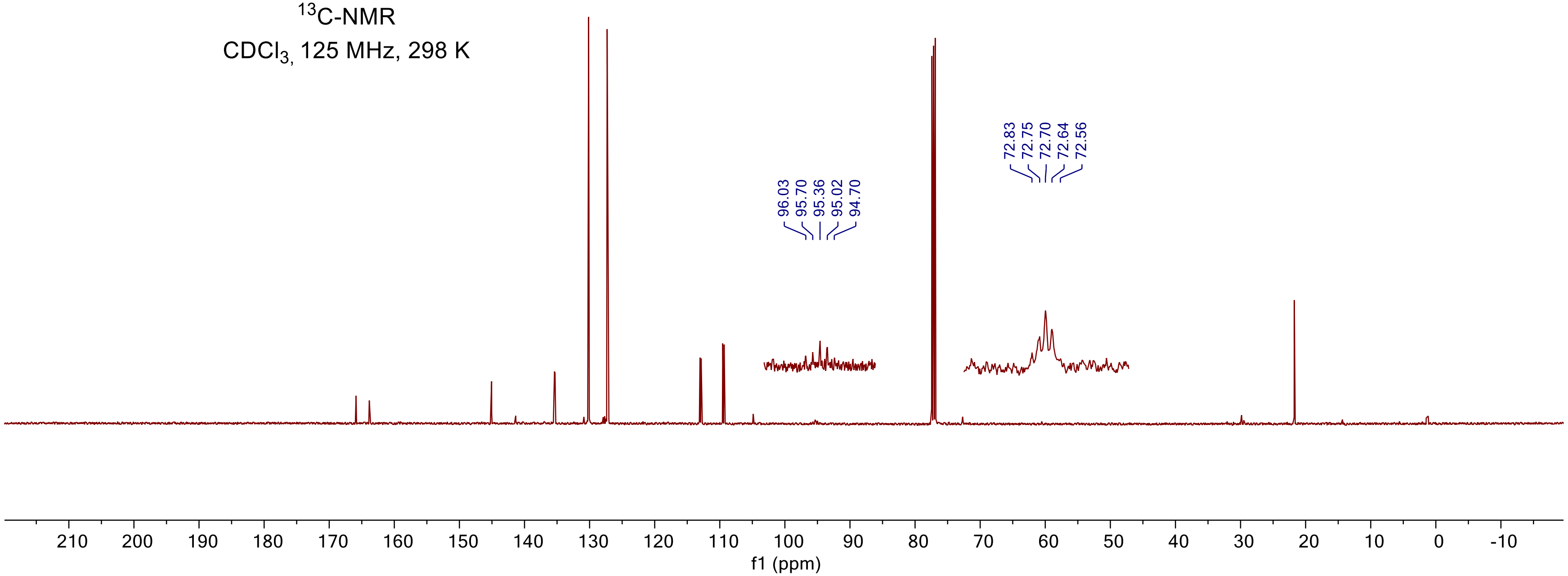
$CDCl_3$, 500 MHz, 298 K

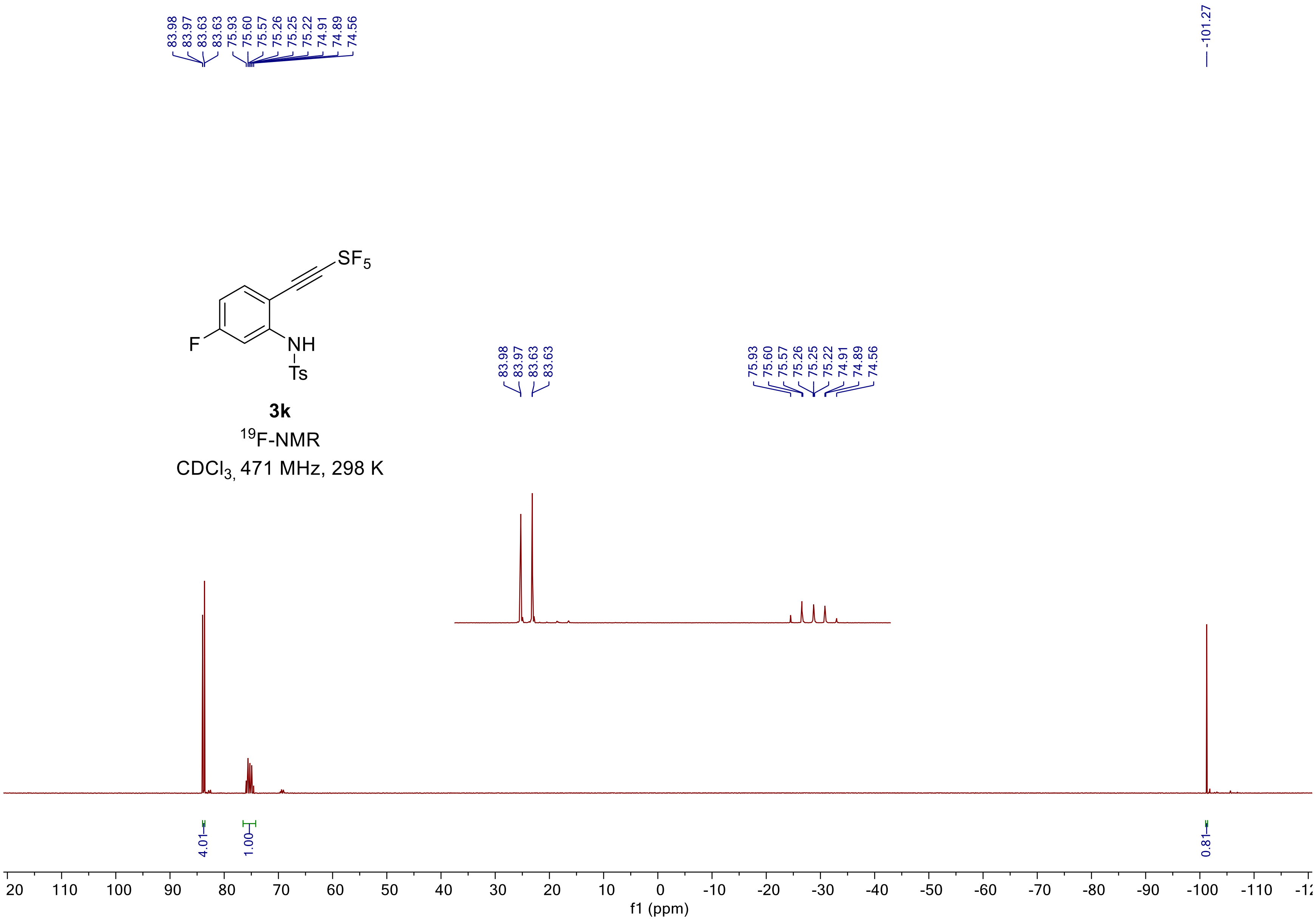


3k

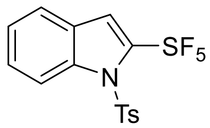
^{13}C-NMR

$CDCl_3$, 125 MHz, 298 K





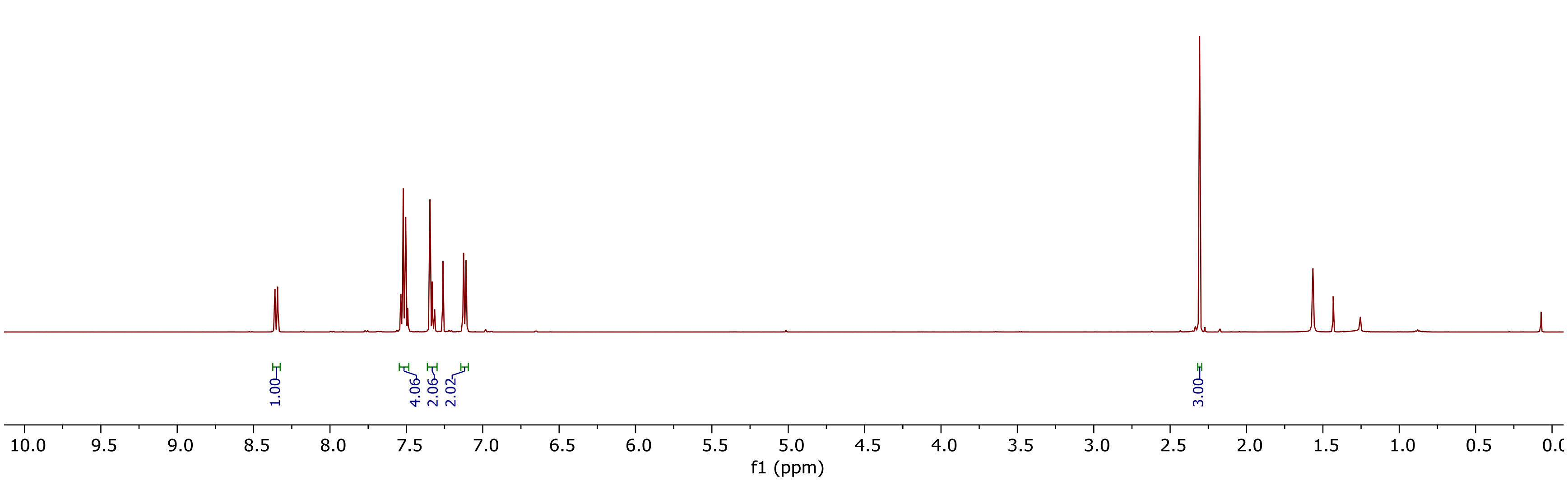
83.98
83.97
83.63
83.63
75.93
75.60
75.57
75.26
75.25
75.22
74.91
74.89
74.56
-101.27
SF5
F
NH
Ts
3k
19F-NMR
CDCl3, 471 MHz, 298 K
4.01
1.00
0.81
f1 (ppm)

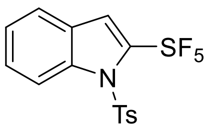


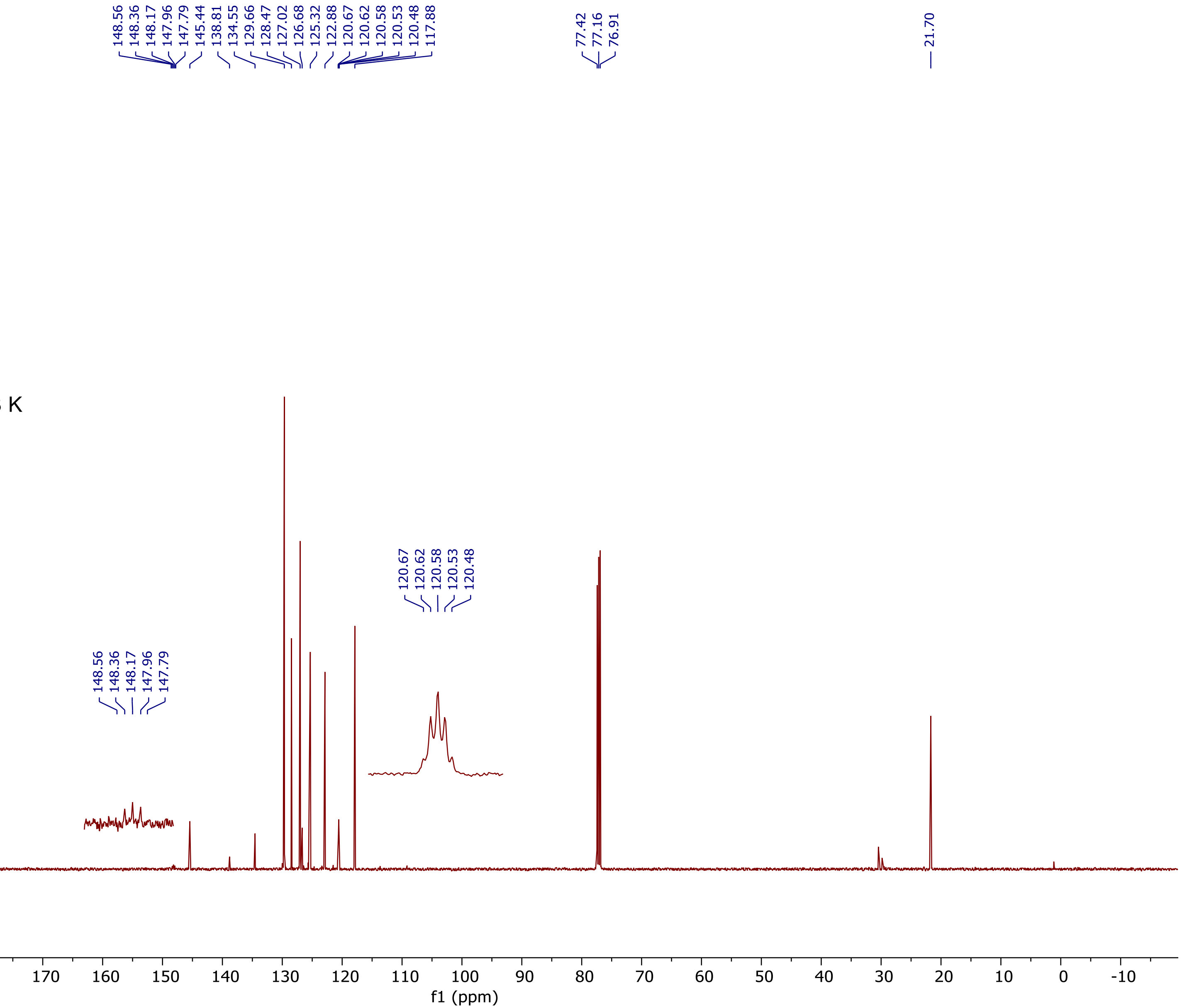
4a

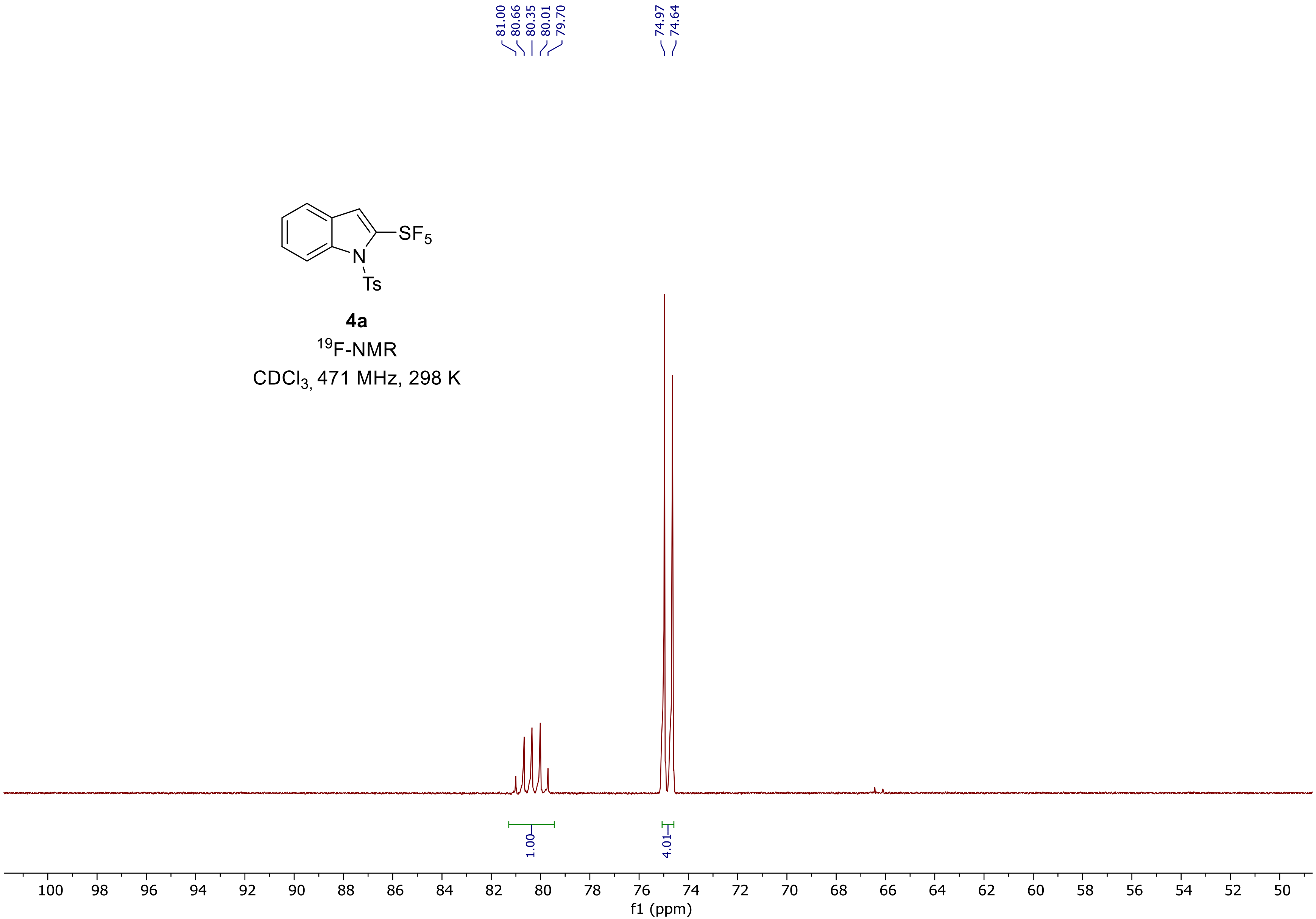
^{1}H-NMR

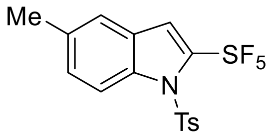
$CDCl_3$, 500 MHz, 298 K




4a
^{13}C-NMR
$CDCl_3$, 125 MHz, 298 K



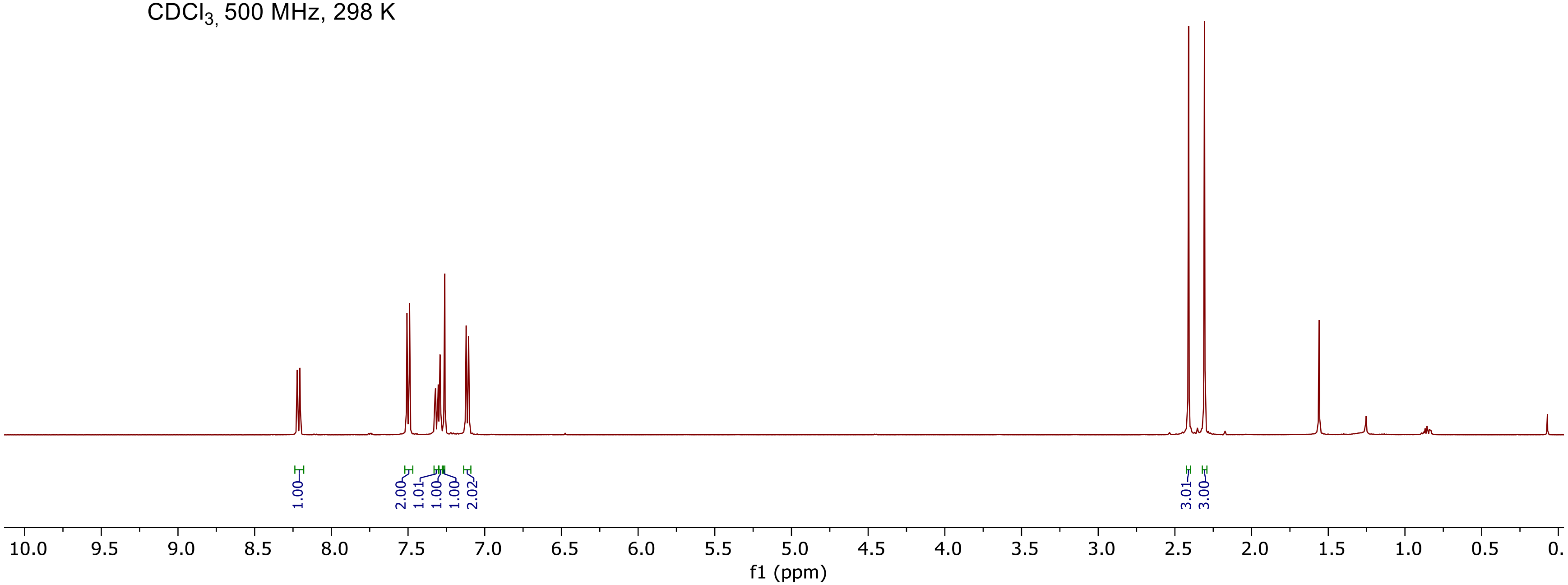

81.00
80.66
80.35
80.01
79.70
74.97
74.64
SF5
N
Ts
4a
19F-NMR
CDCl3, 471 MHz, 298 K
1.00
4.01
100 98 96 94 92 90 88 86 84 82 80 78 76 74 72 70 68 66 64 62 60 58 56 54 52 50
f1 (ppm)

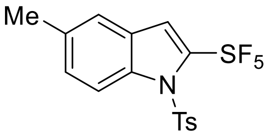


4b

^{1}H-NMR

$CDCl_3$, 500 MHz, 298 K

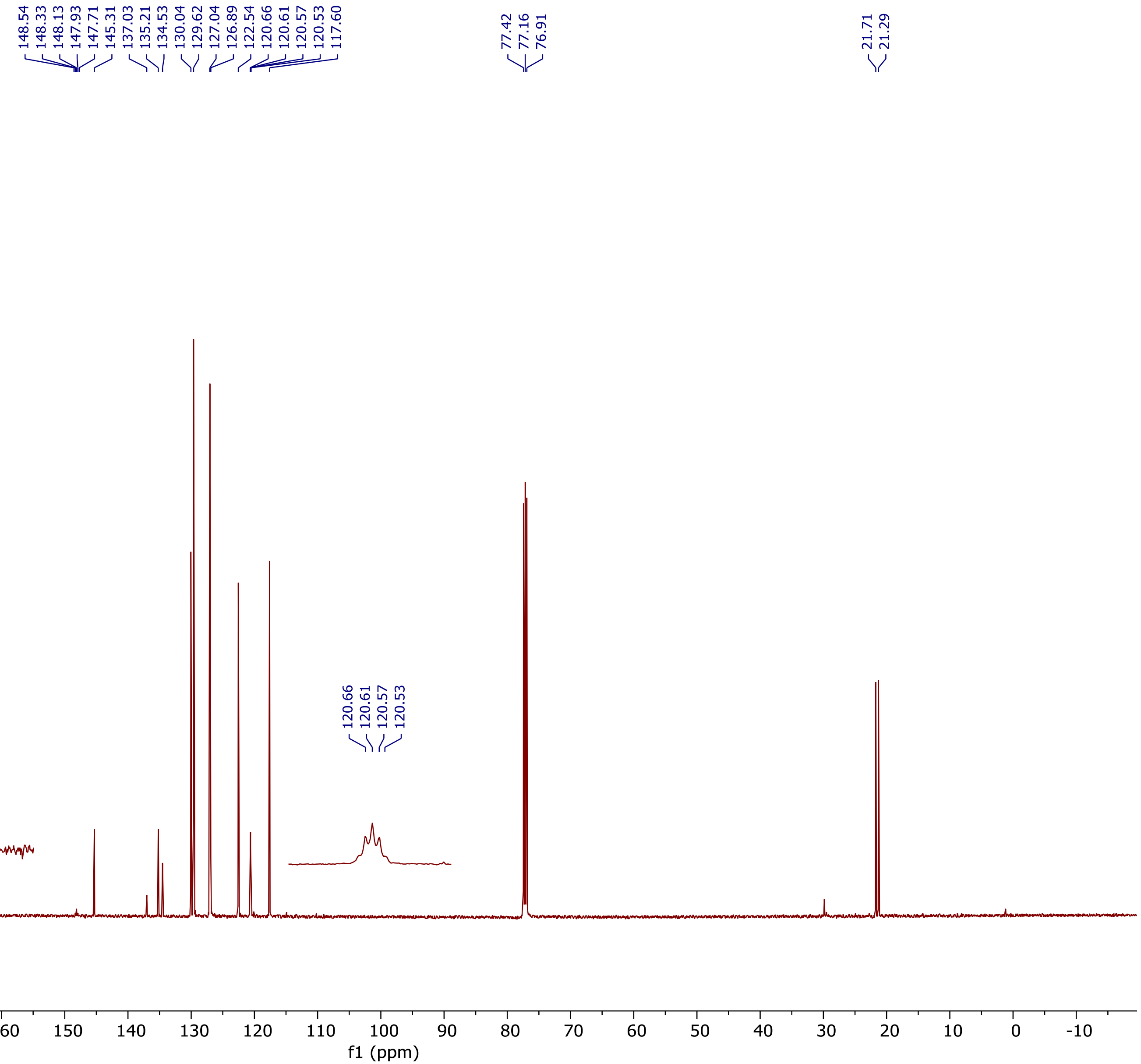


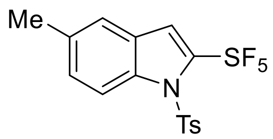


4b

^{13}C-NMR

$CDCl_3$, 125 MHz, 298 K

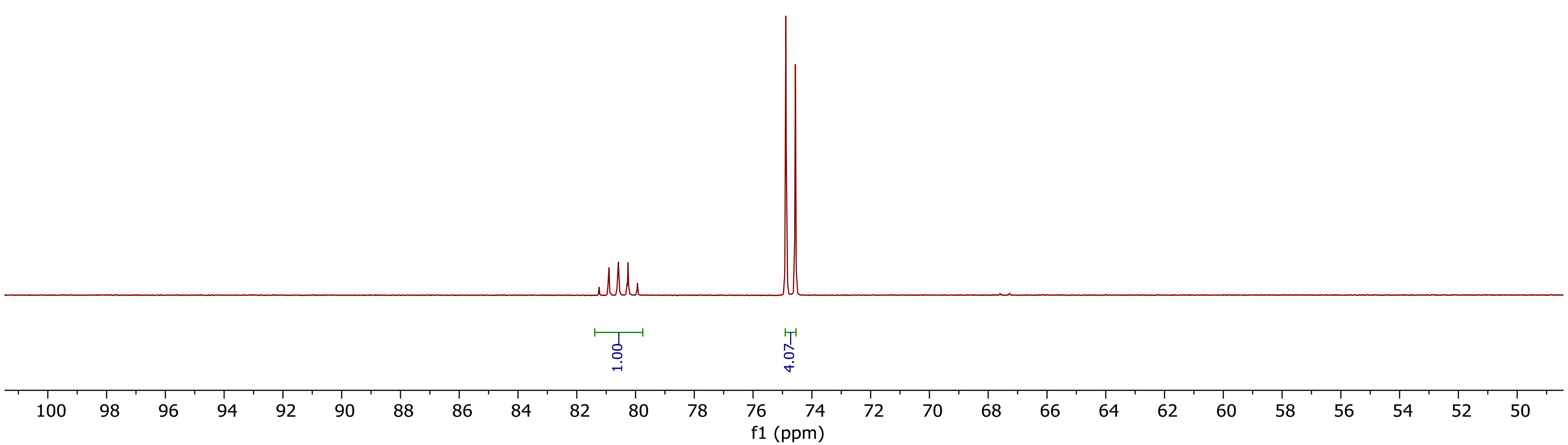


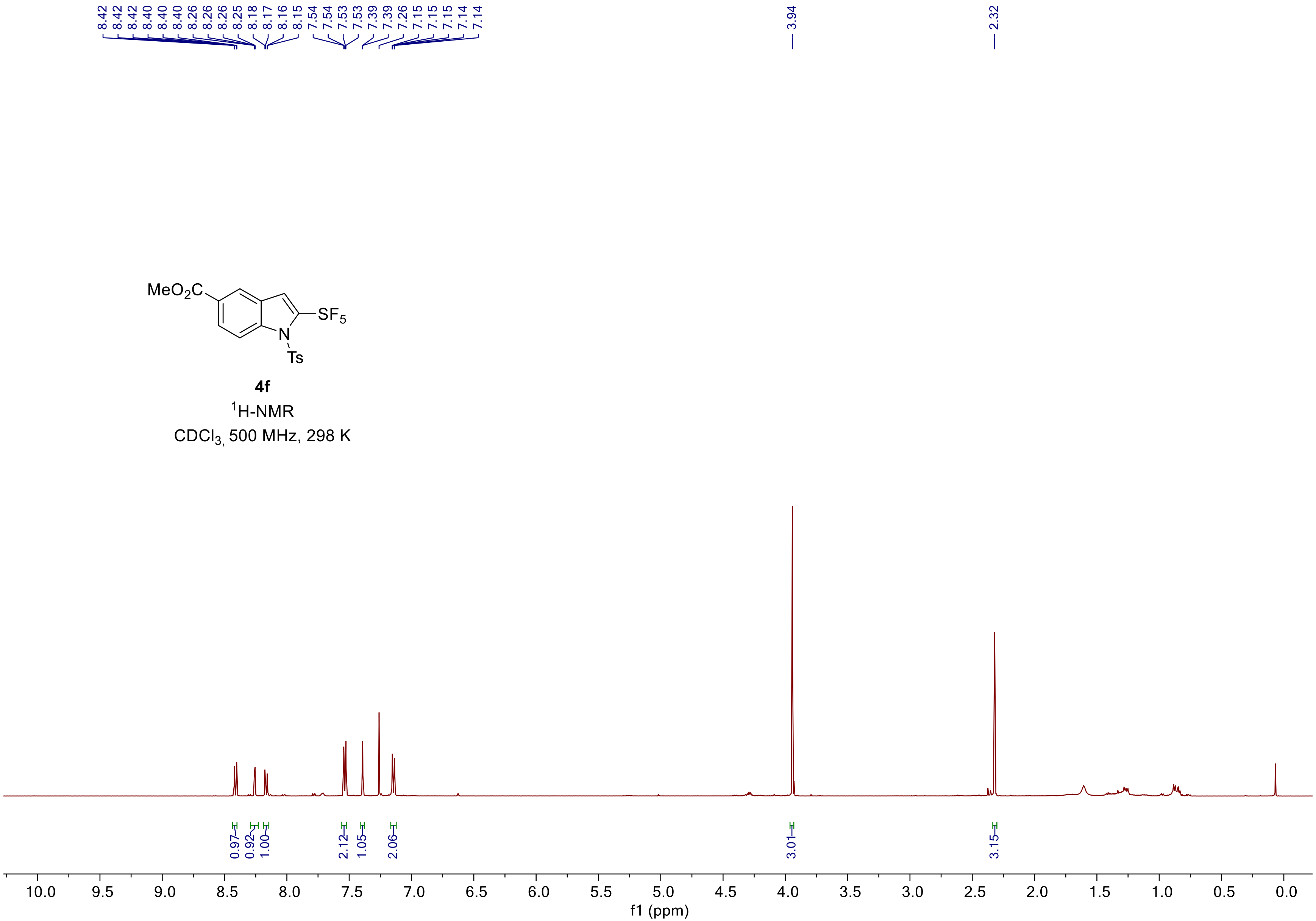


4b

^{19}F-NMR

$CDCl_3$, 471 MHz, 298 K

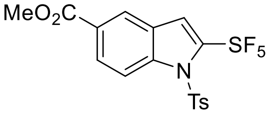




4f

^{1}H-NMR

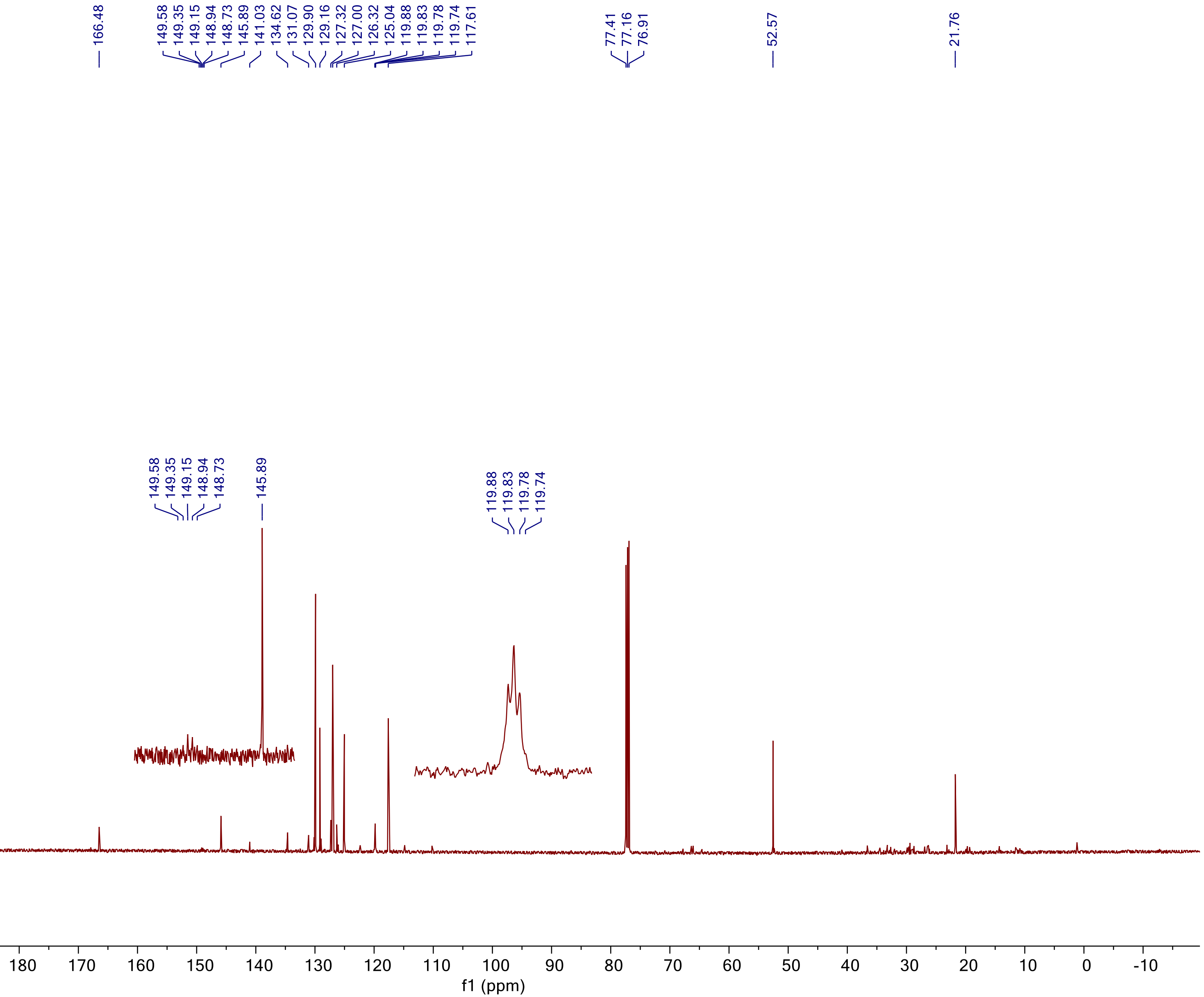
$CDCl_3$, 500 MHz, 298 K

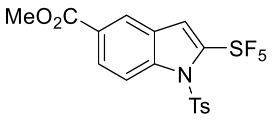


4f

^{13}C-NMR

$CDCl_3$, 125 MHz, 298 K

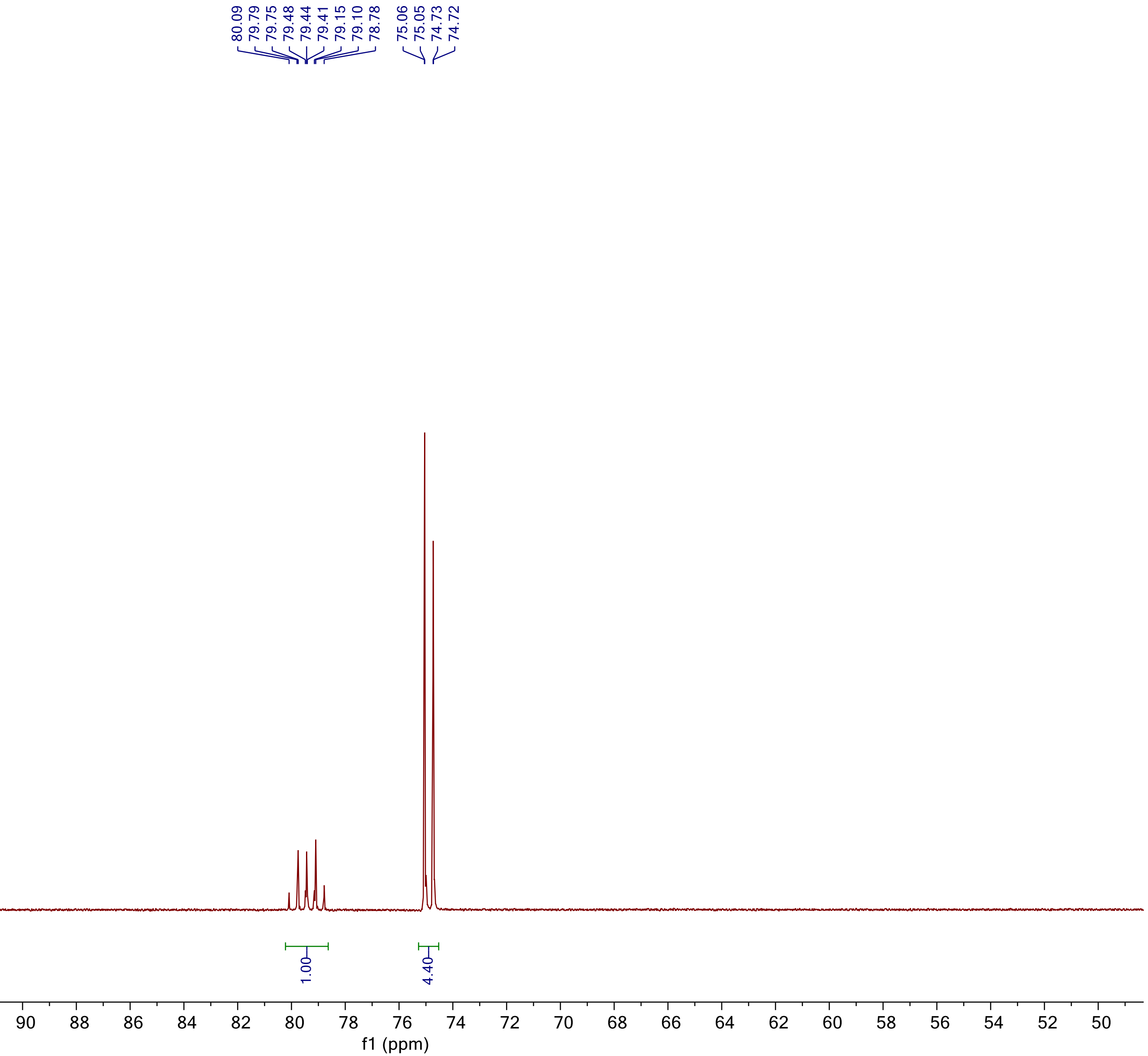


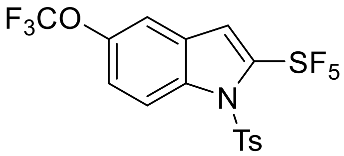


4f

^{19}F-NMR

$CDCl_3$, 471 MHz, 298 K

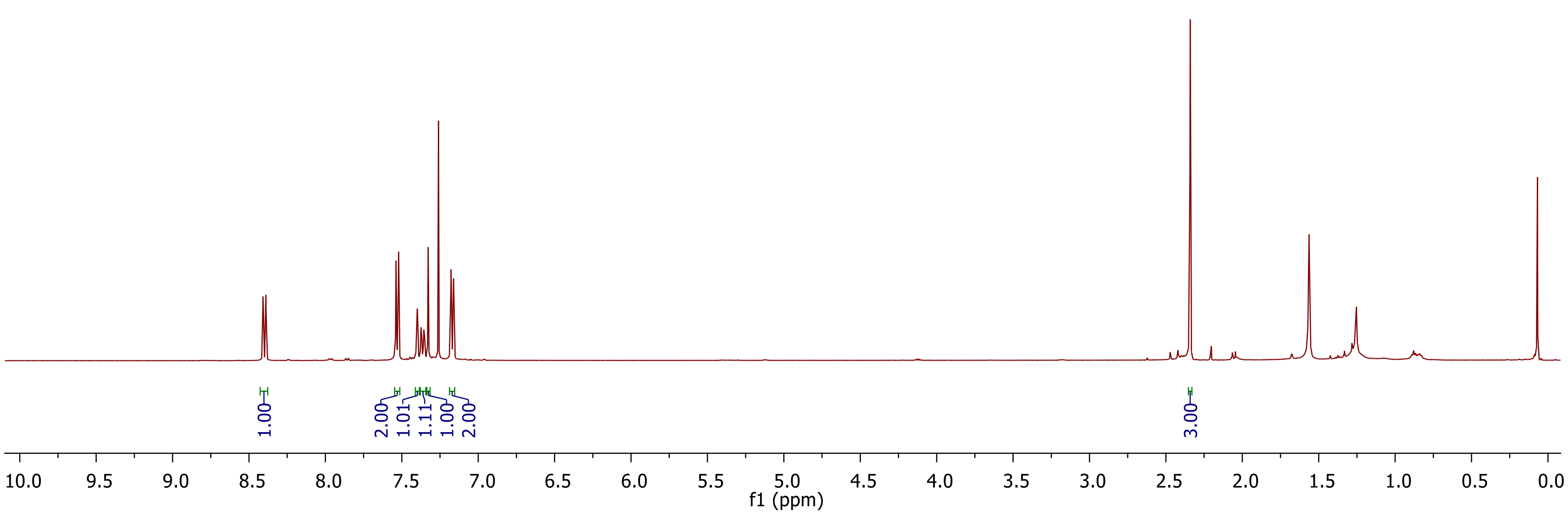


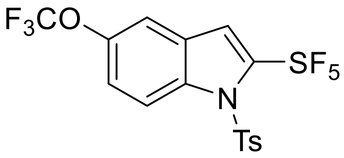


4g

^{1}H-NMR

$CDCl_3$, 500 MHz, 298 K

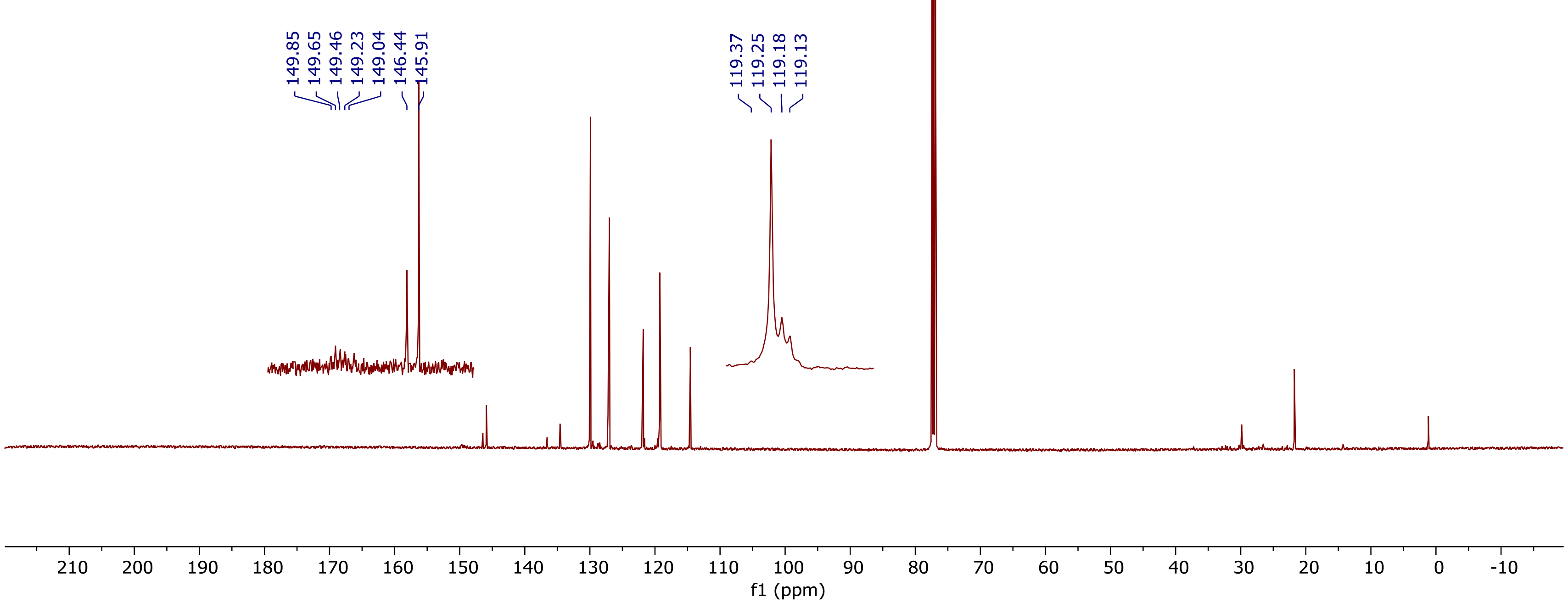


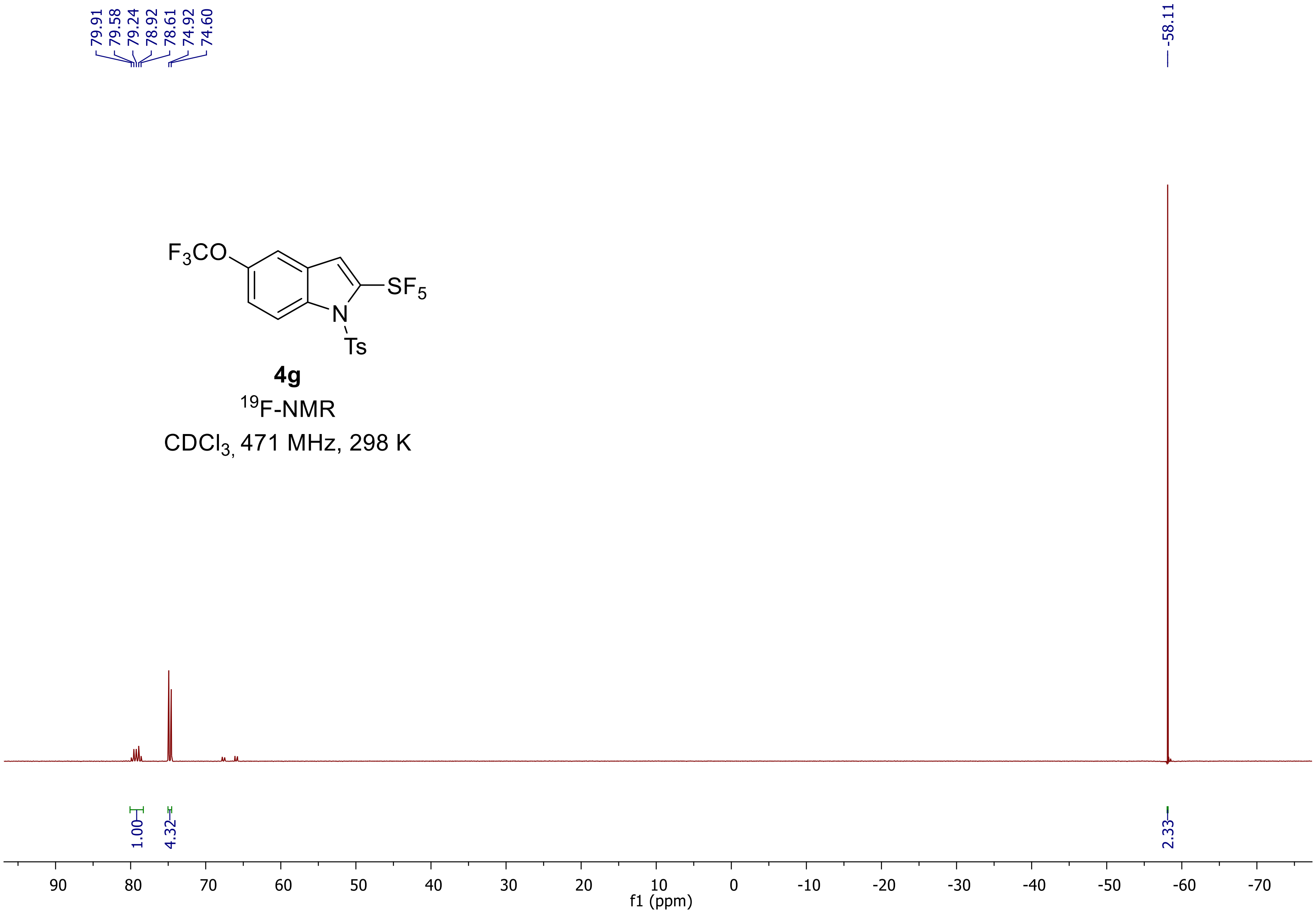


4g

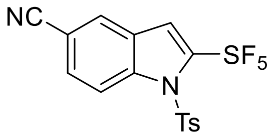
^{13}C-NMR

$CDCl_3$, 125 MHz, 298 K





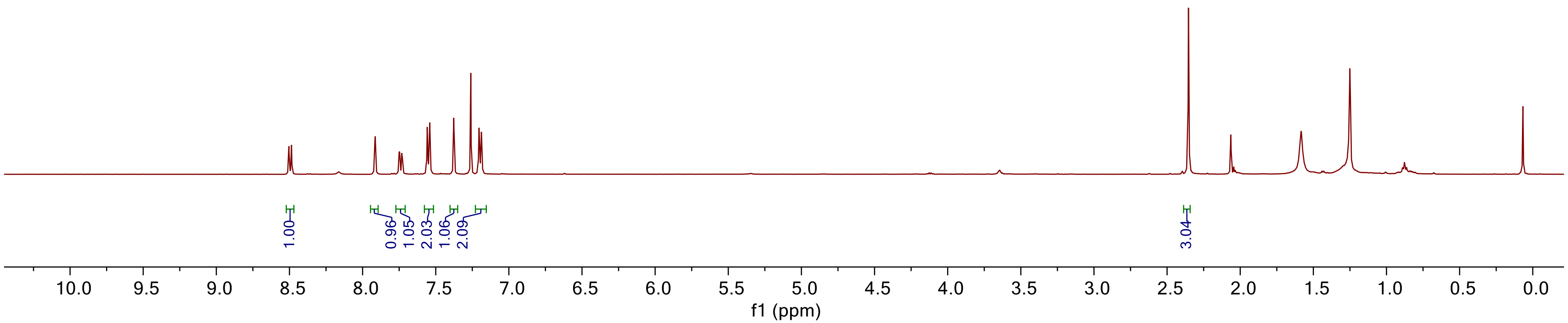
79.91
79.58
79.24
78.92
78.61
74.92
74.60
-58.11
F3CO
SF5
N
Ts
4g
19F-NMR
CDCl3, 471 MHz, 298 K
1.00
4.32
2.33
90
80
70
60
50
40
30
20
10
0
-10
-20
-30
-40
-50
-60
-70
f1 (ppm)

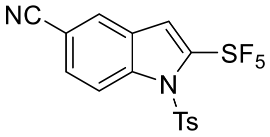


4h

^{1}H-NMR

$CDCl_3$, 500 MHz, 298 K

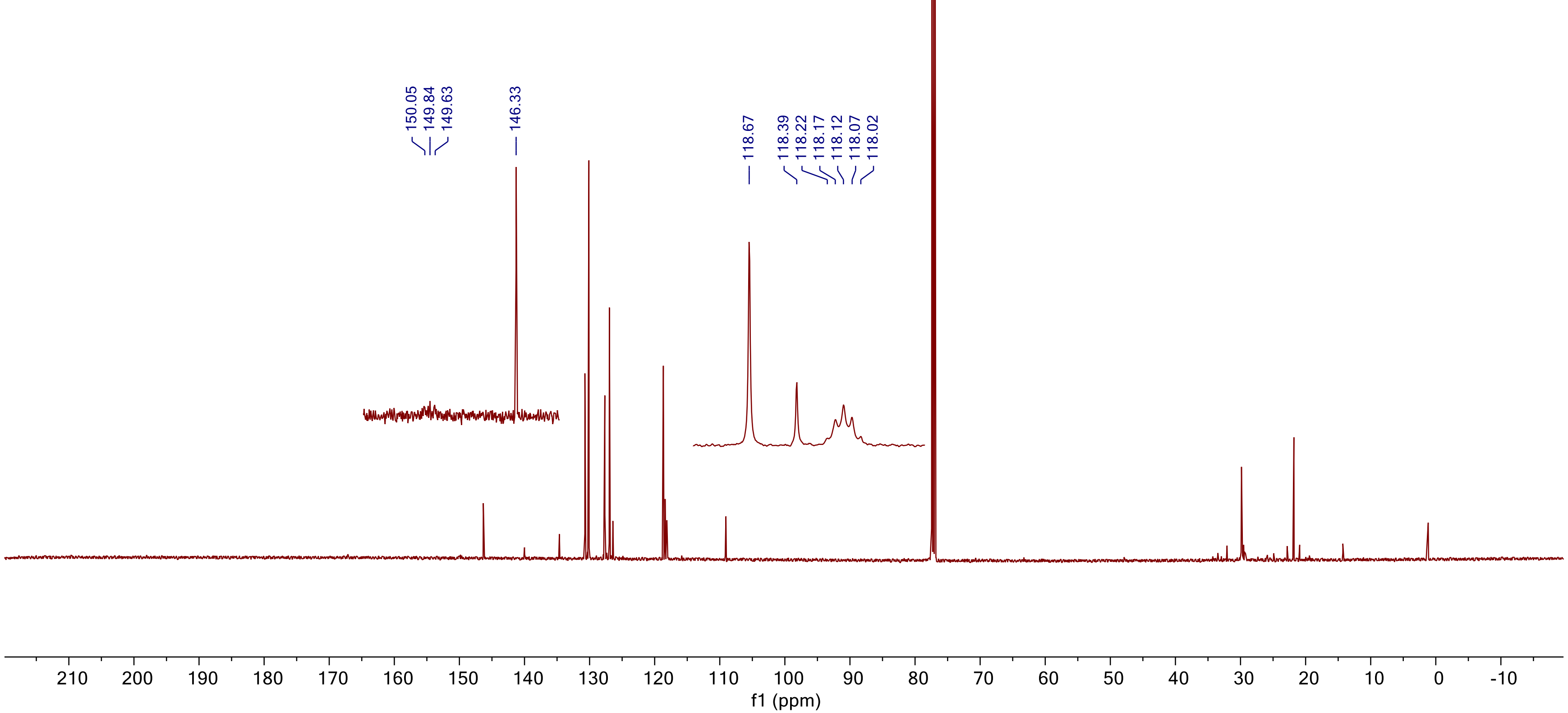


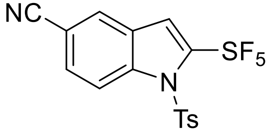


4h

^{13}C-NMR

$CDCl_3$, 125 MHz, 298 K

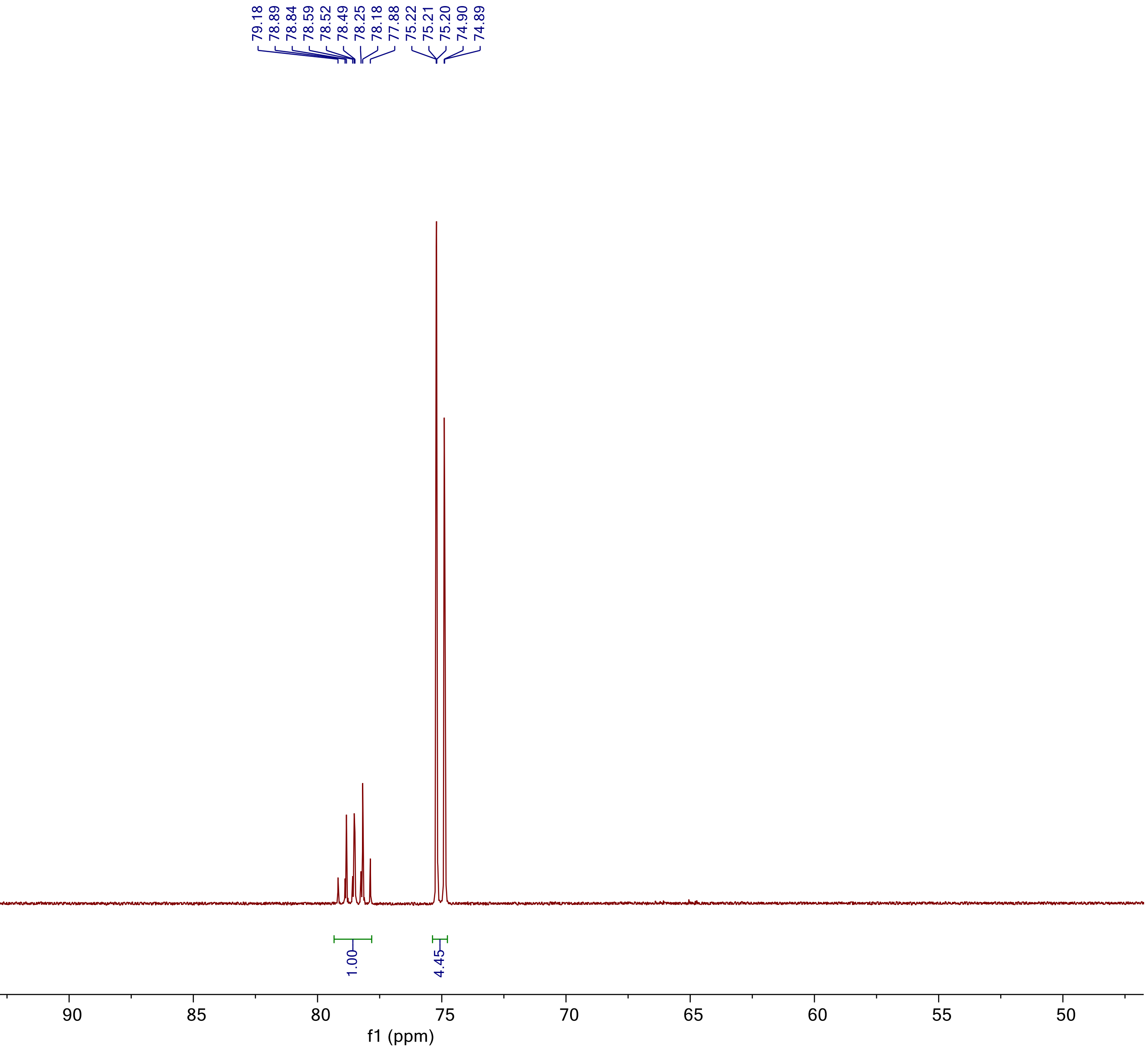


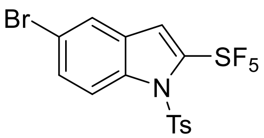


4h

^{19}F-NMR

$CDCl_3$, 471 MHz, 298 K

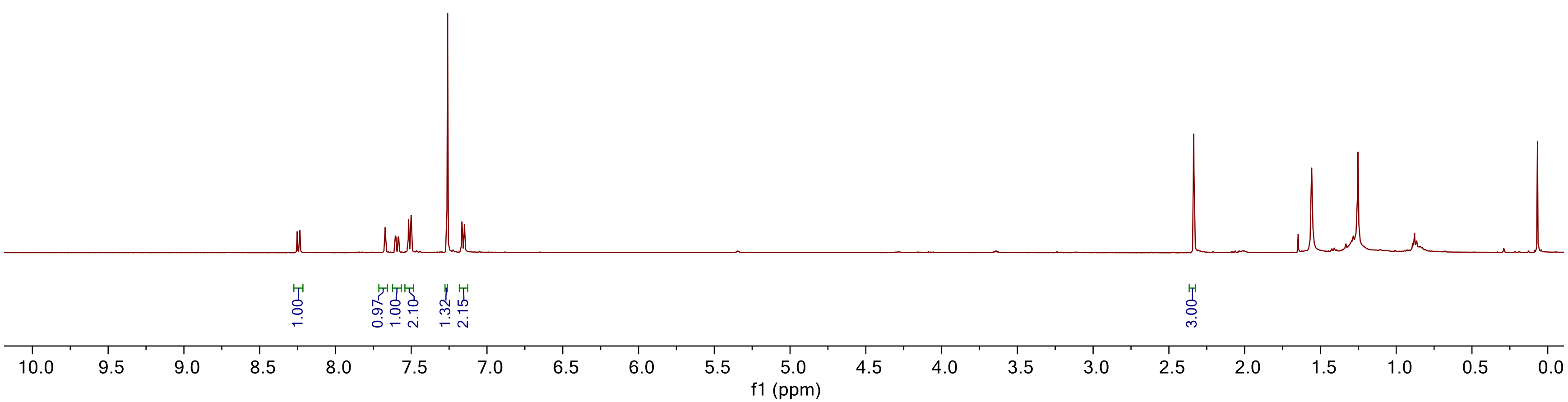


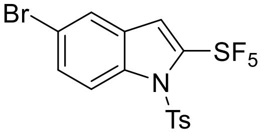


4i

^{1}H-NMR

CDCl$_3$, 500 MHz, 298 K

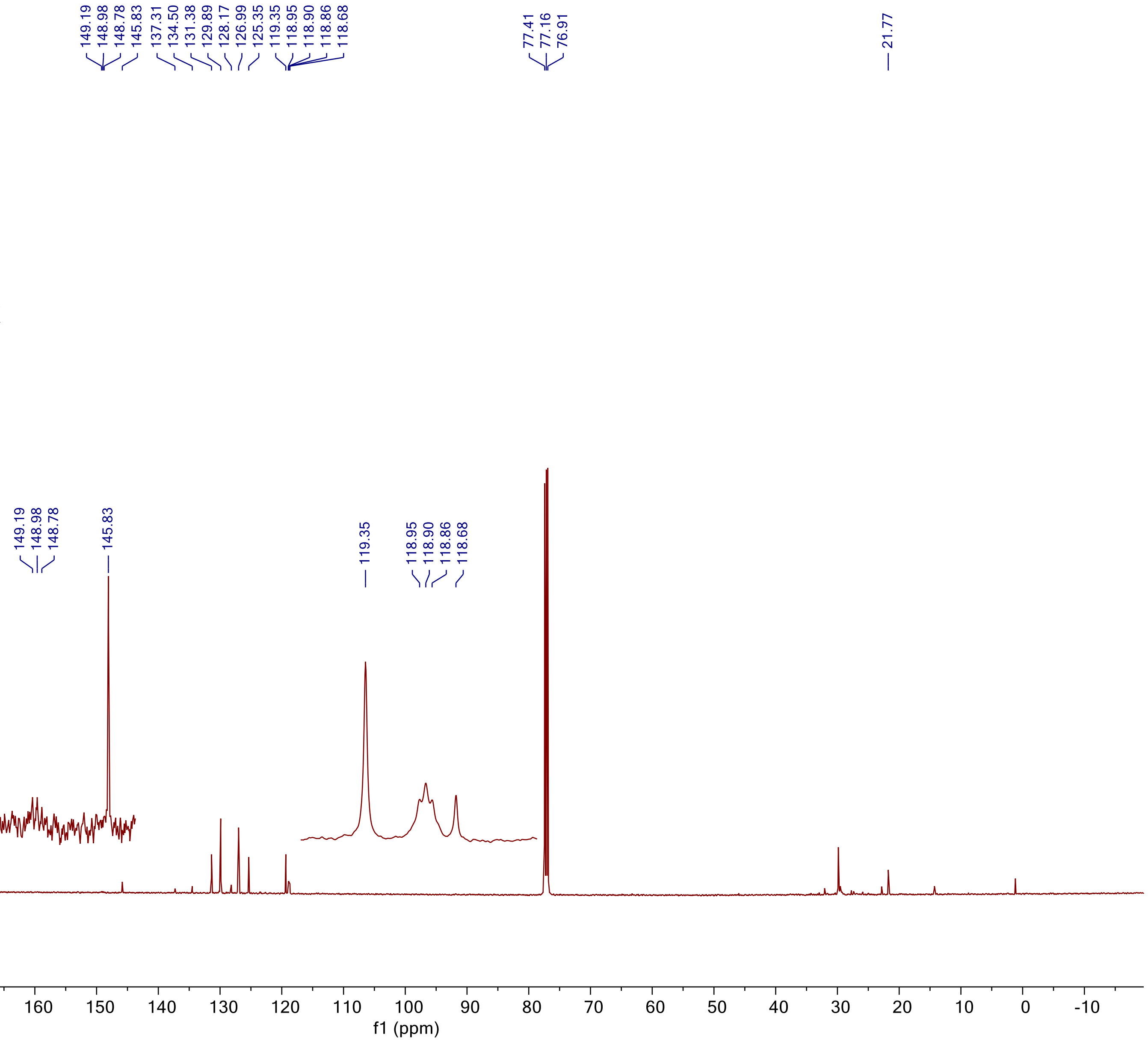


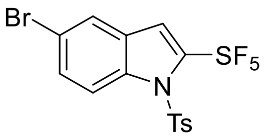


4i

^{13}C-NMR

$CDCl_3$, 125 MHz, 298 K

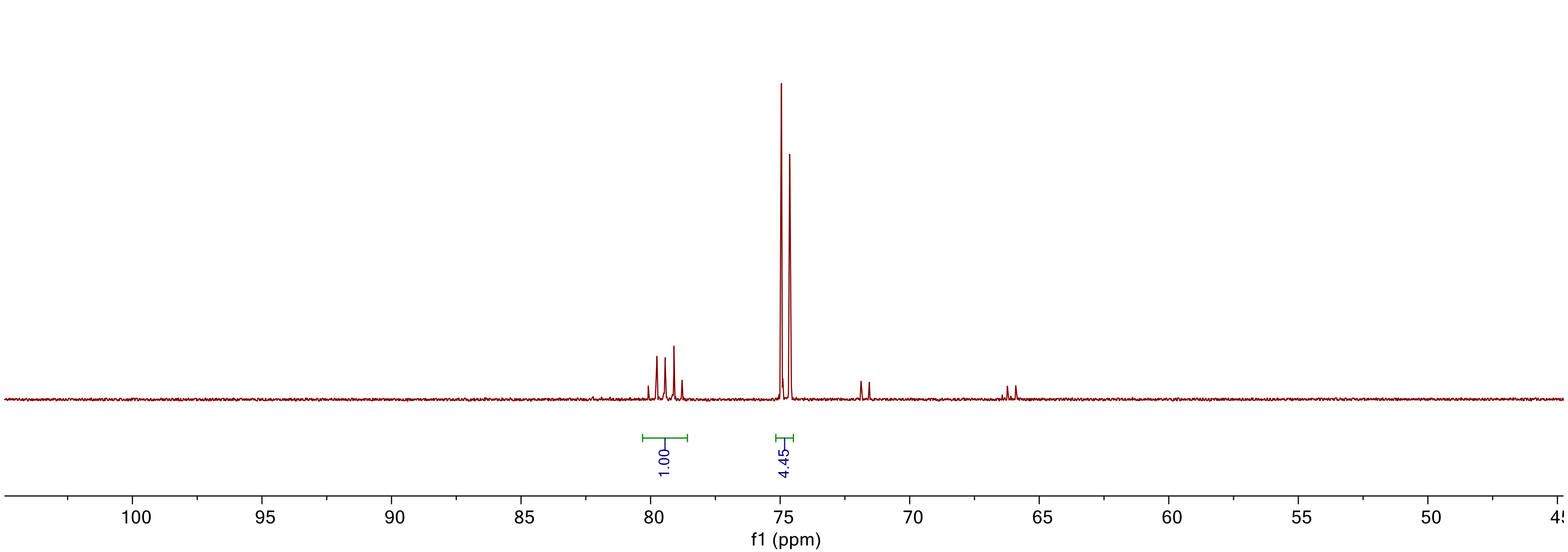


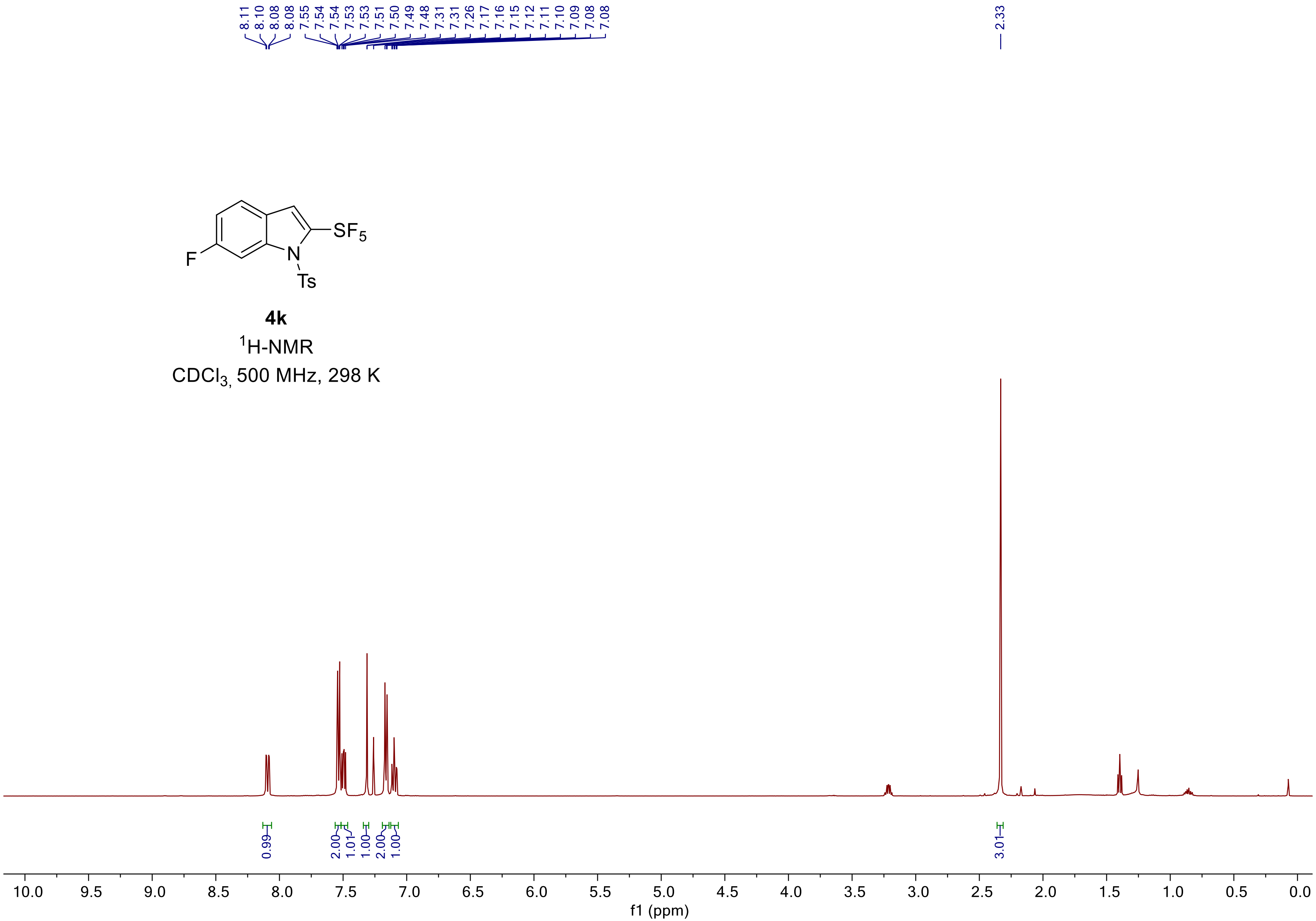


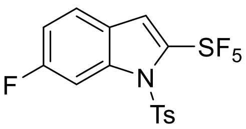
4i

^{19}F-NMR

$CDCl_3$, 471 MHz, 298 K



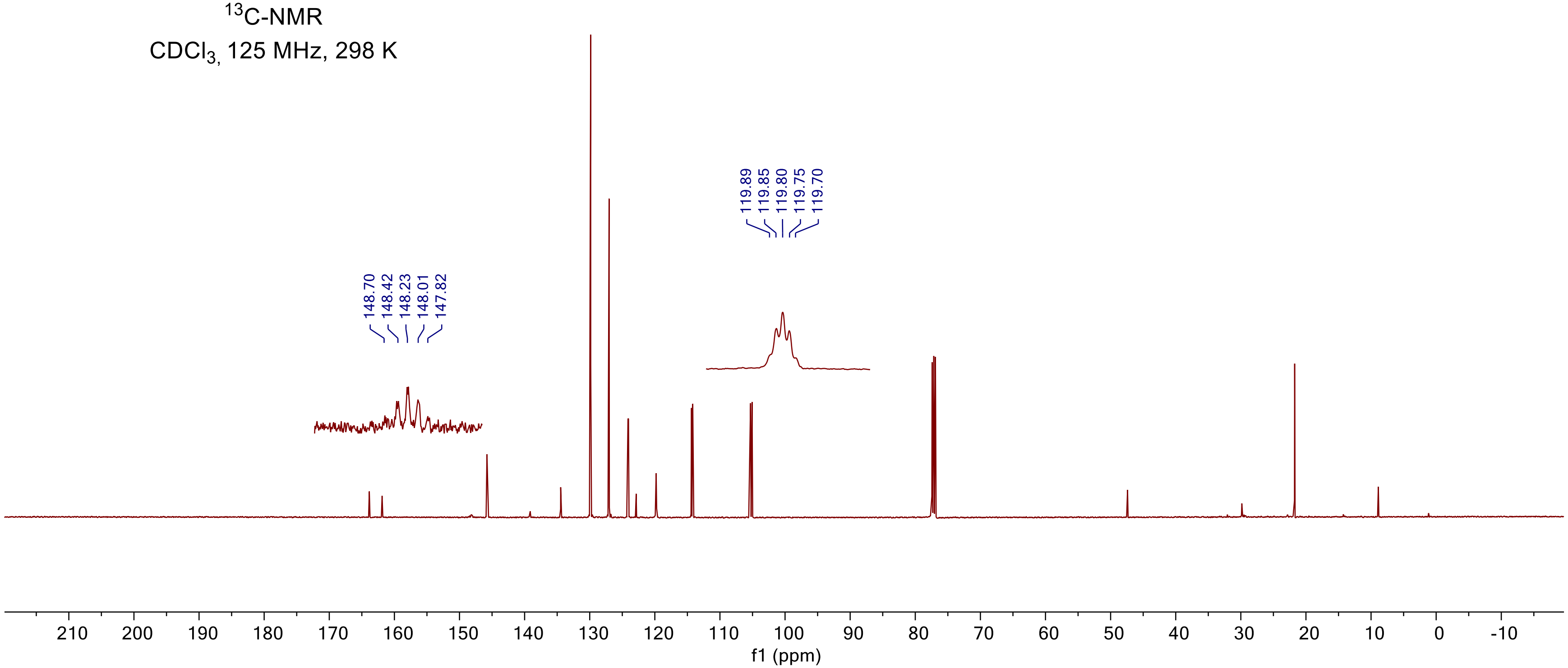

8.11
8.10
8.08
8.08
7.55
7.54
7.54
7.53
7.53
7.51
7.50
7.49
7.48
7.31
7.31
7.26
7.17
7.16
7.15
7.12
7.11
7.10
7.09
7.08
7.08
2.33
SF5
F
N
Ts
4k
1H-NMR
CDCl3, 500 MHz, 298 K
0.99
2.00
1.01
1.00
2.00
1.00
3.01
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

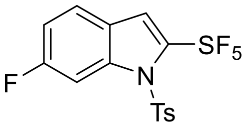


4k

^{13}C-NMR

$CDCl_3$, 125 MHz, 298 K

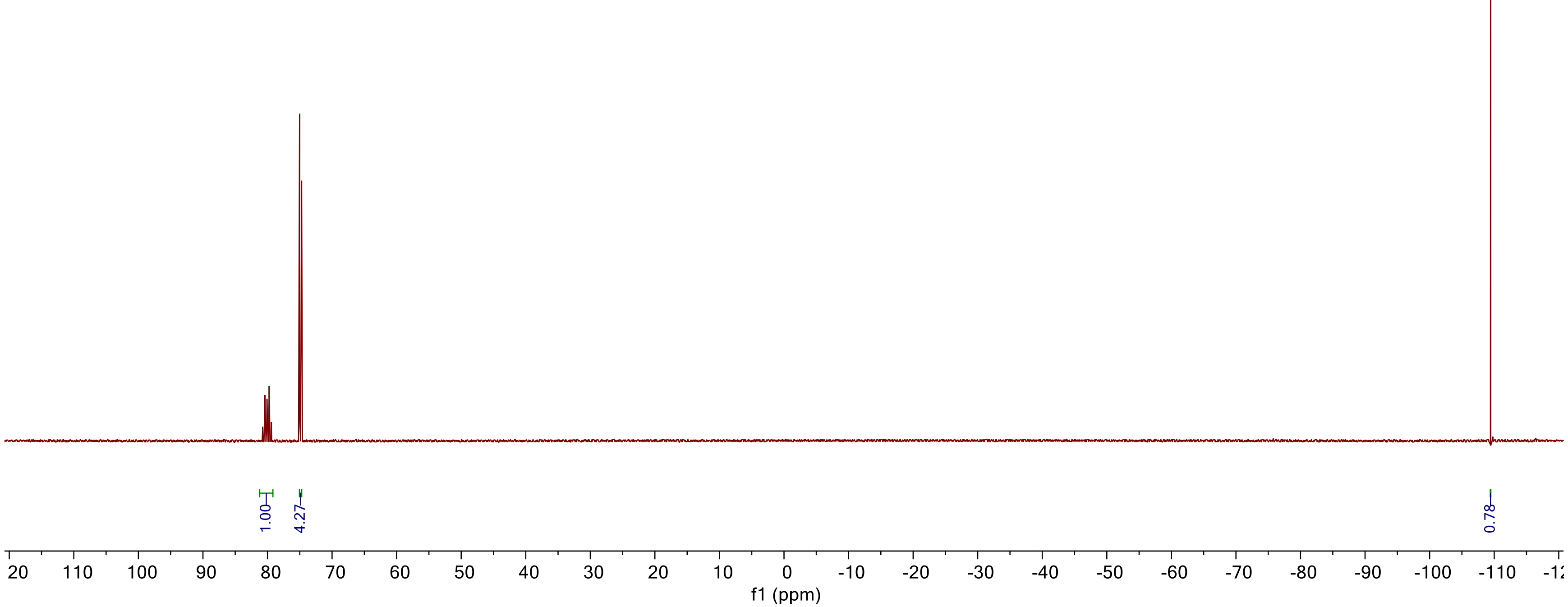


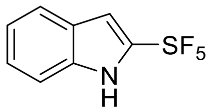


4k

^{19}F-NMR

$CDCl_3$, 471 MHz, 298 K

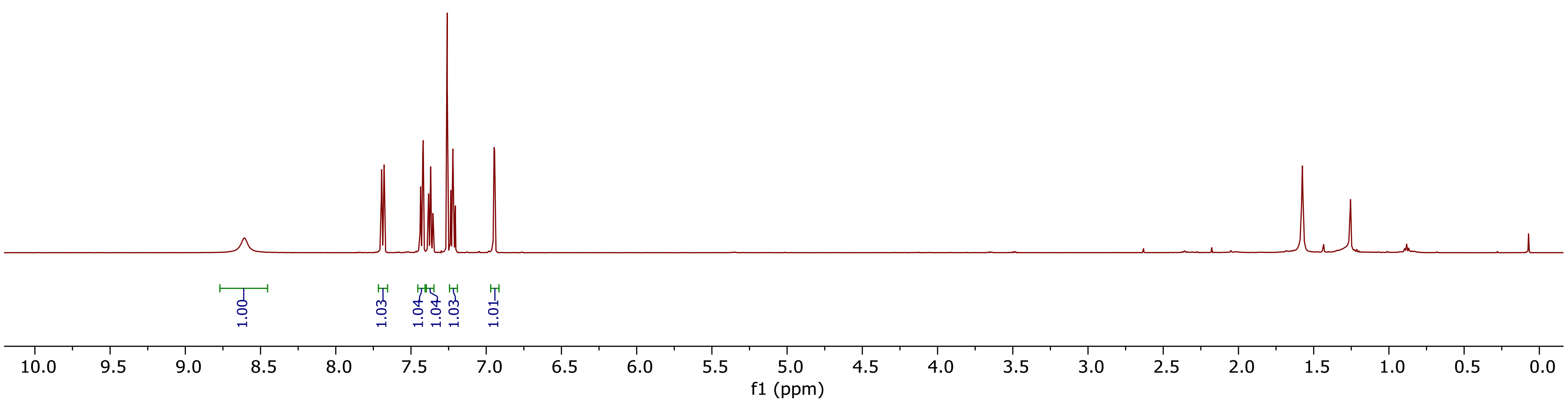


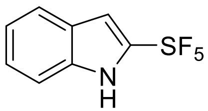


5a

^{1}H-NMR

$CDCl_3$, 500 MHz, 298 K

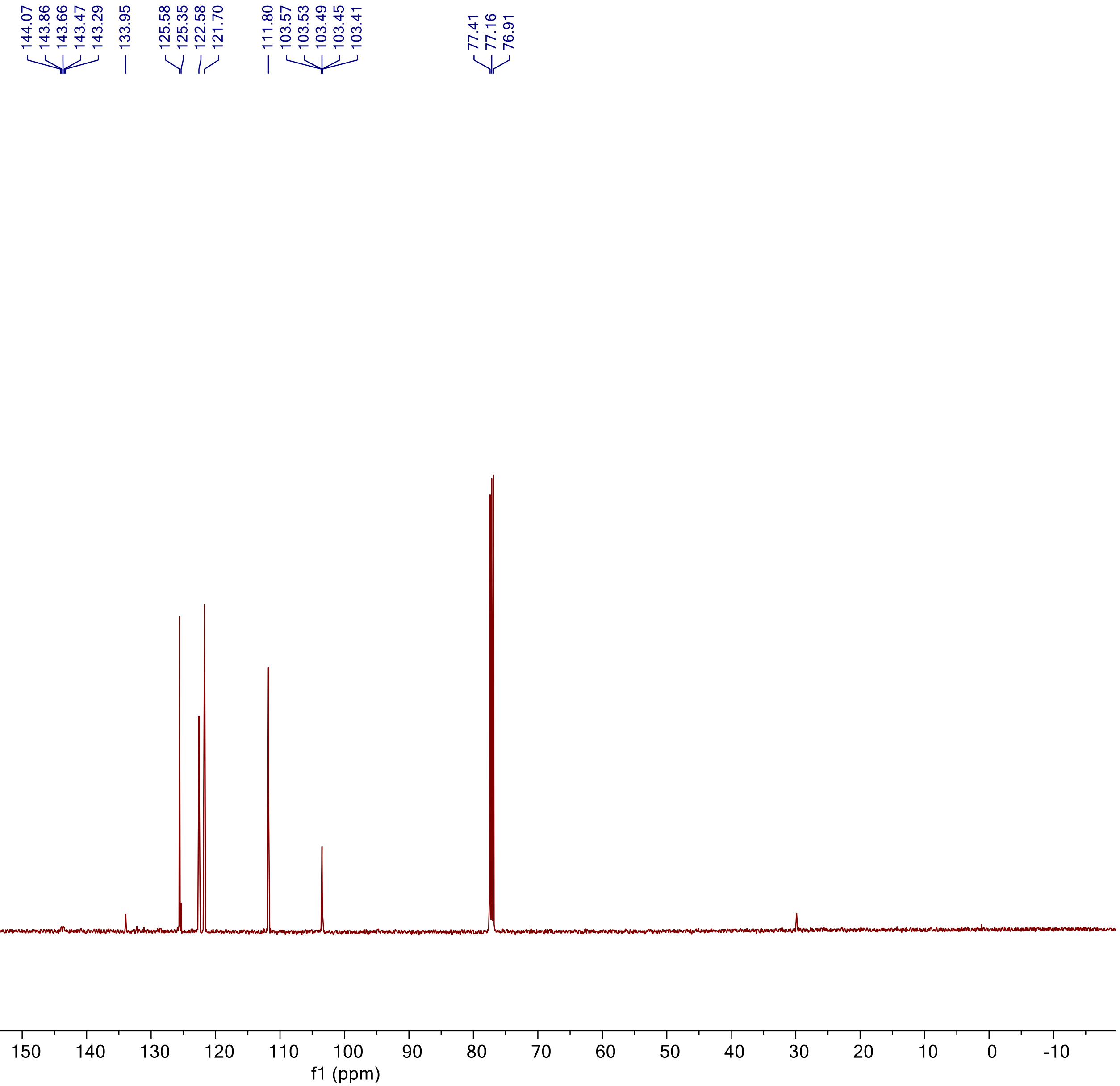


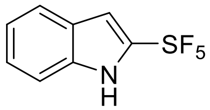


5a

^{13}C-NMR

$CDCl_3$, 125 MHz, 298 K

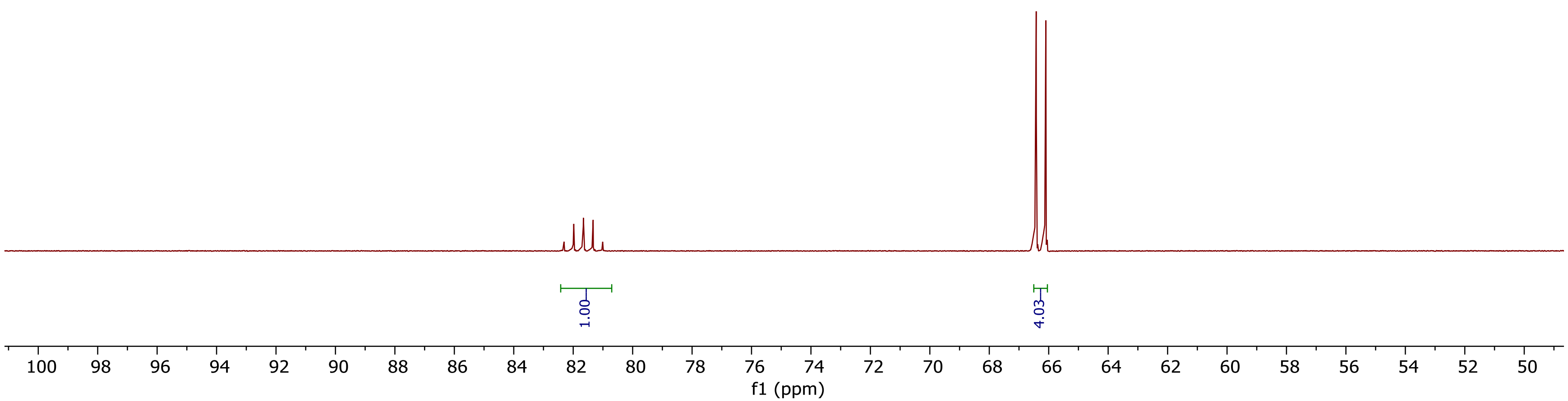


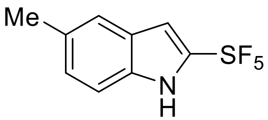


5a

^{19}F-NMR

$CDCl_3$, 471 MHz, 298 K

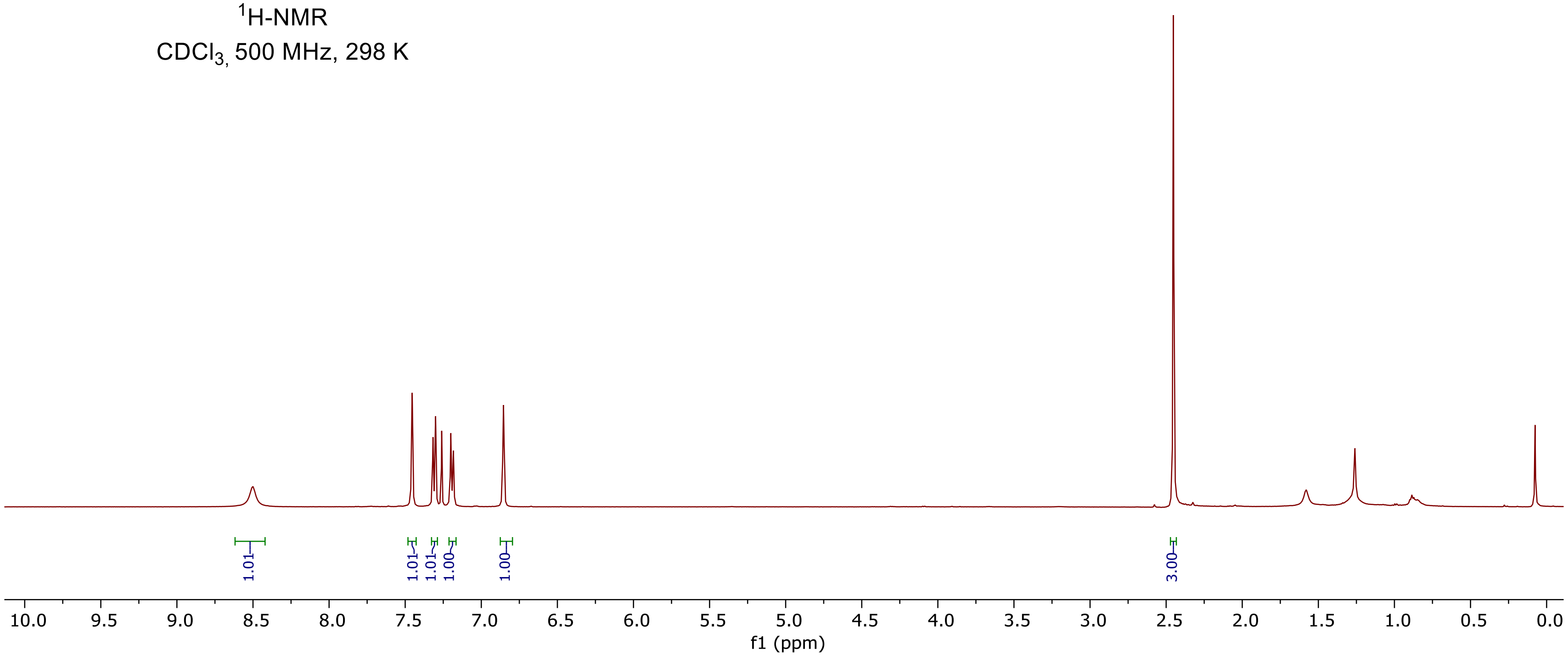


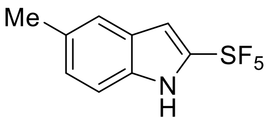


5b

^{1}H-NMR

$CDCl_3$, 500 MHz, 298 K

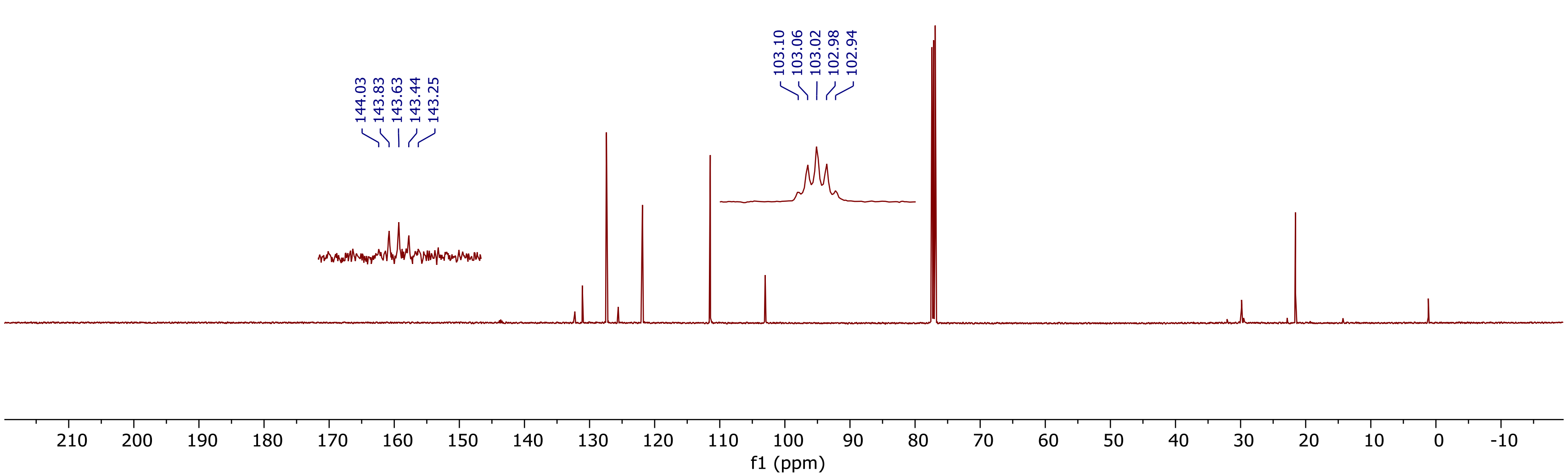


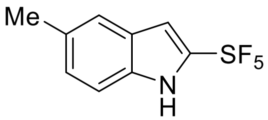


5b

^{13}C-NMR

$CDCl_3$, 125 MHz, 298 K

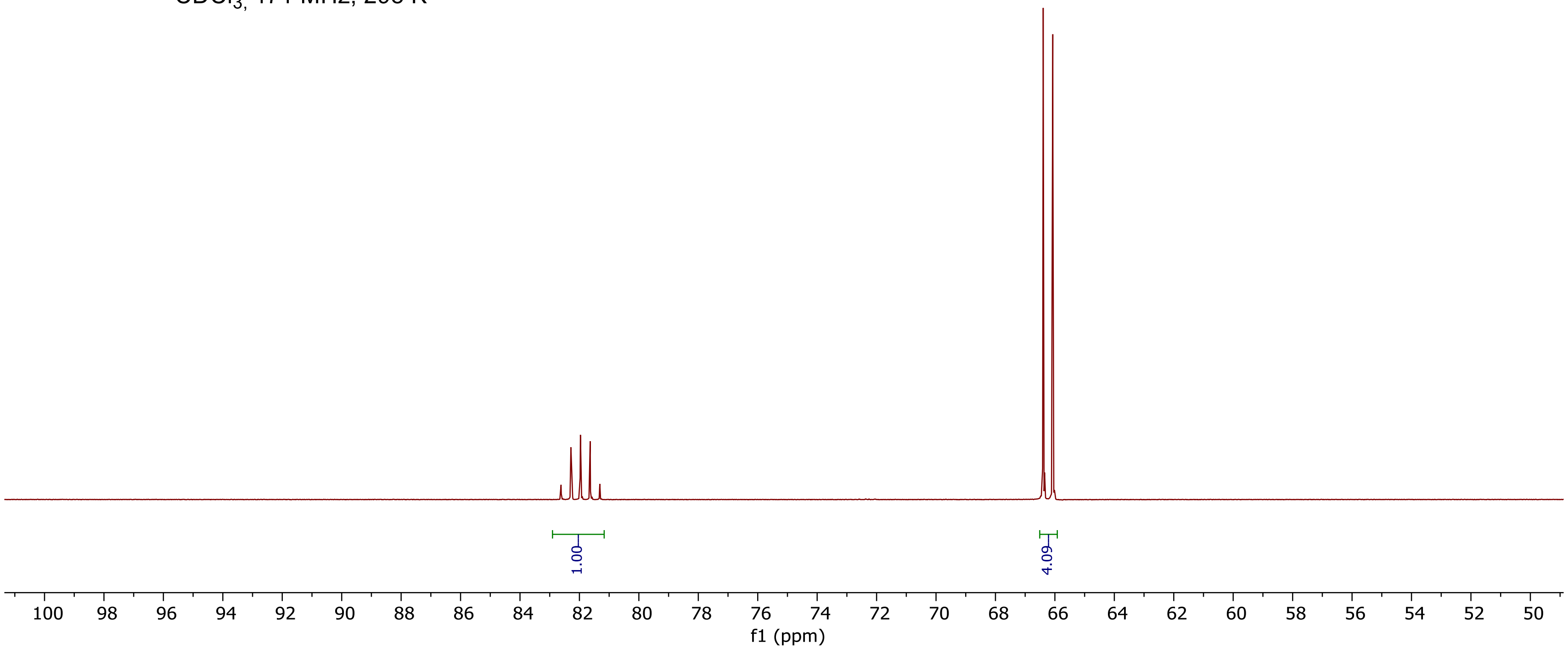


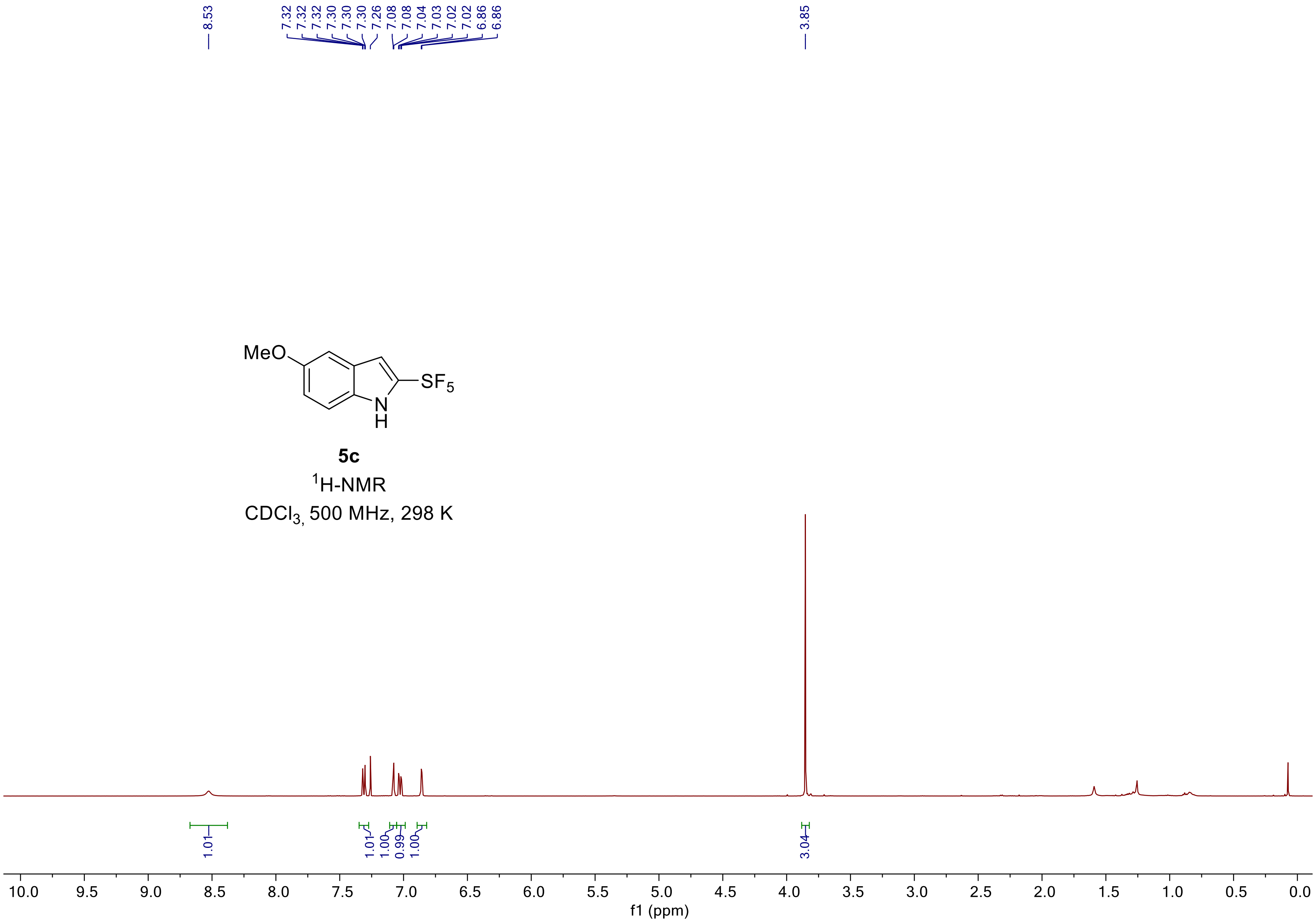


5b

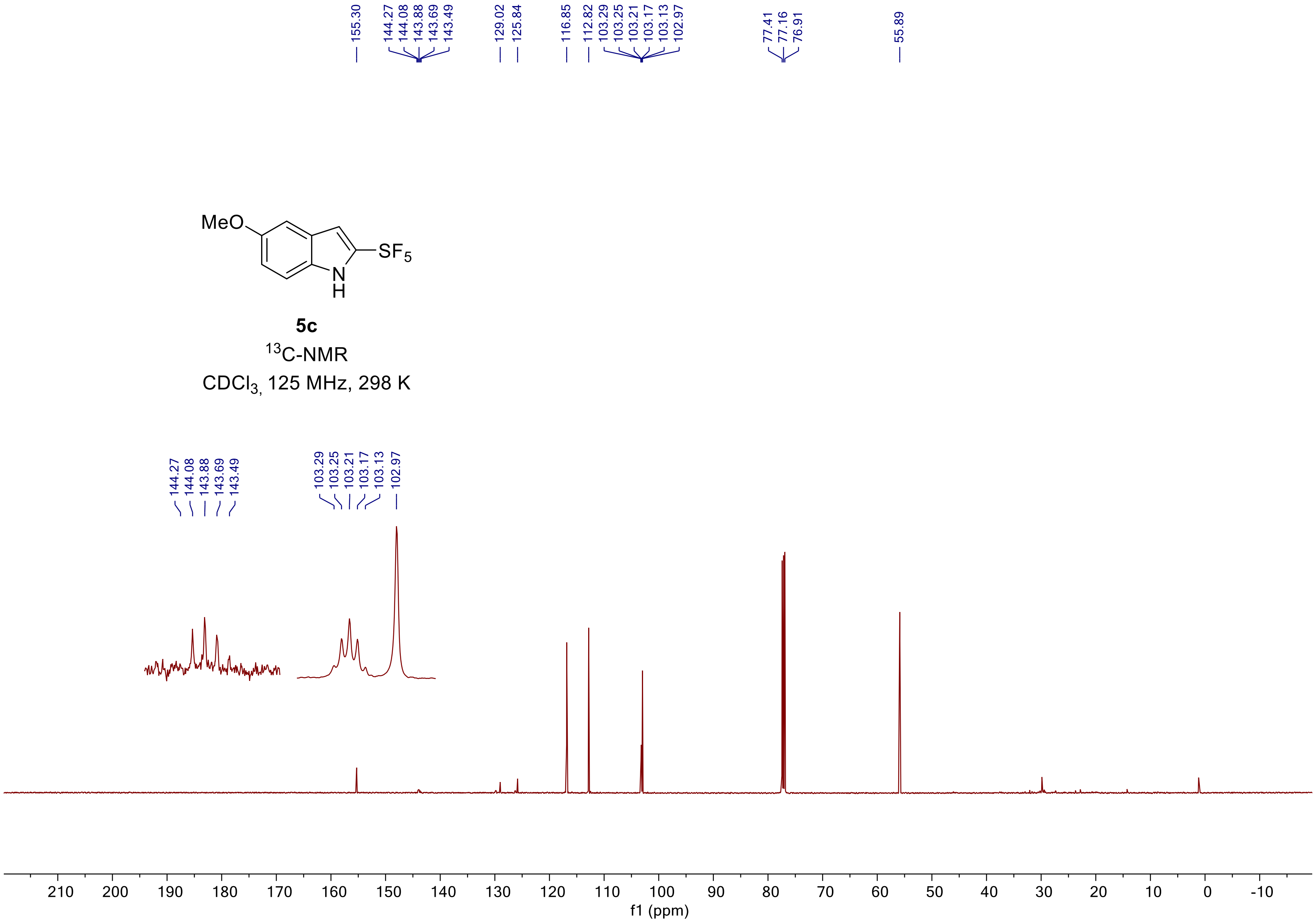
^{19}F-NMR

$CDCl_3$, 471 MHz, 298 K





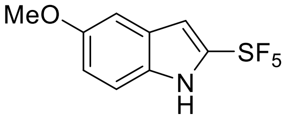
8.53
7.32
7.32
7.32
7.30
7.30
7.30
7.26
7.08
7.08
7.04
7.03
7.02
7.02
6.86
6.86
3.85
MeO
SF5
N
H
5c
1H-NMR
CDCl3, 500 MHz, 298 K
1.01
1.01
1.00
0.99
1.00
3.04
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)



5c

^{13}C-NMR

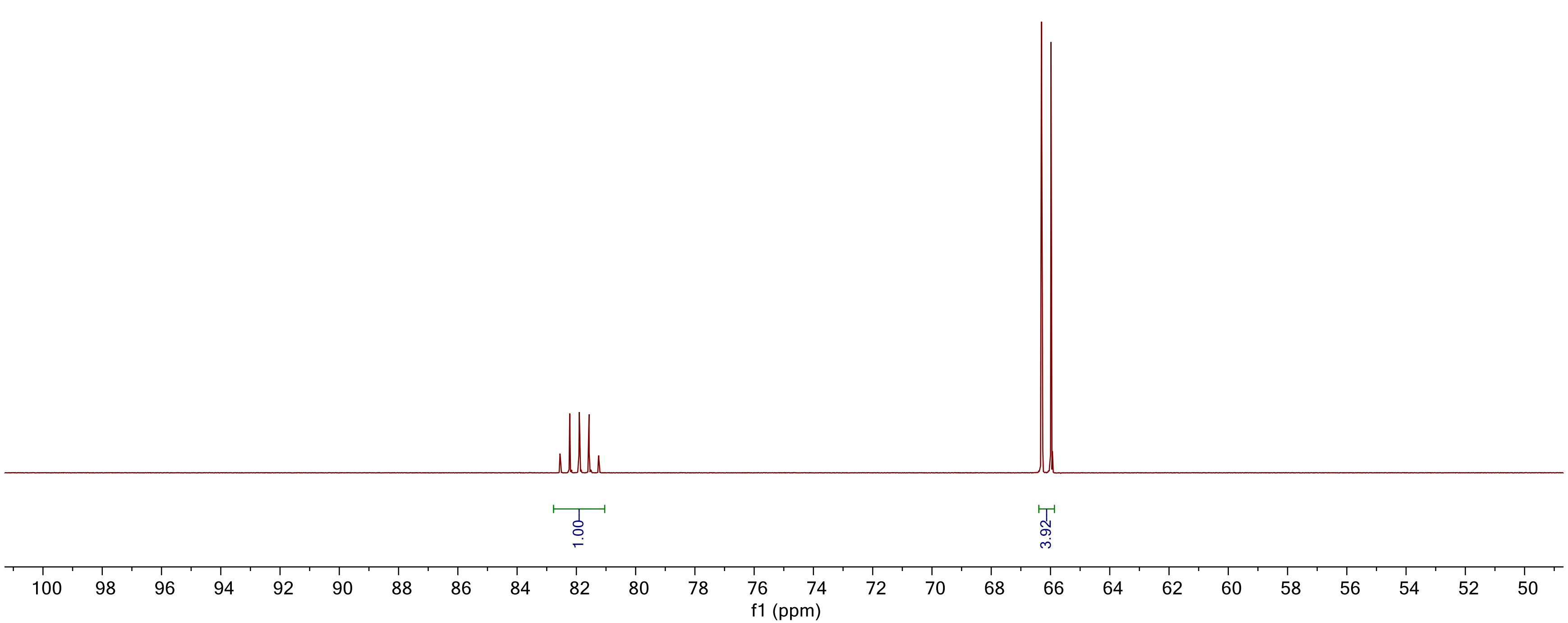
$CDCl_3$, 125 MHz, 298 K

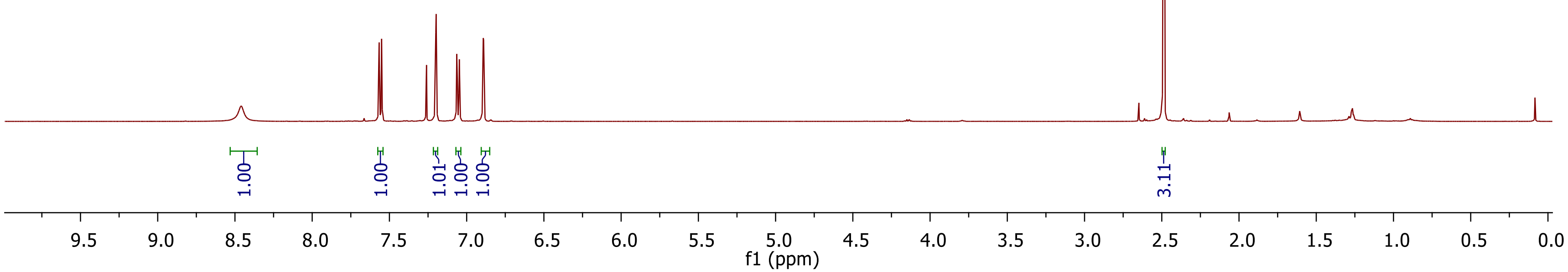


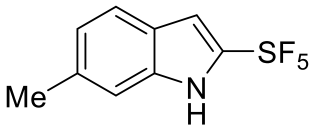
5c

^{19}F-NMR

$CDCl_3$, 471 MHz, 298 K



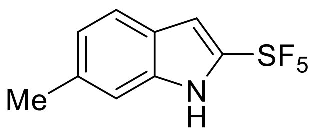




5d

^{1}H-NMR

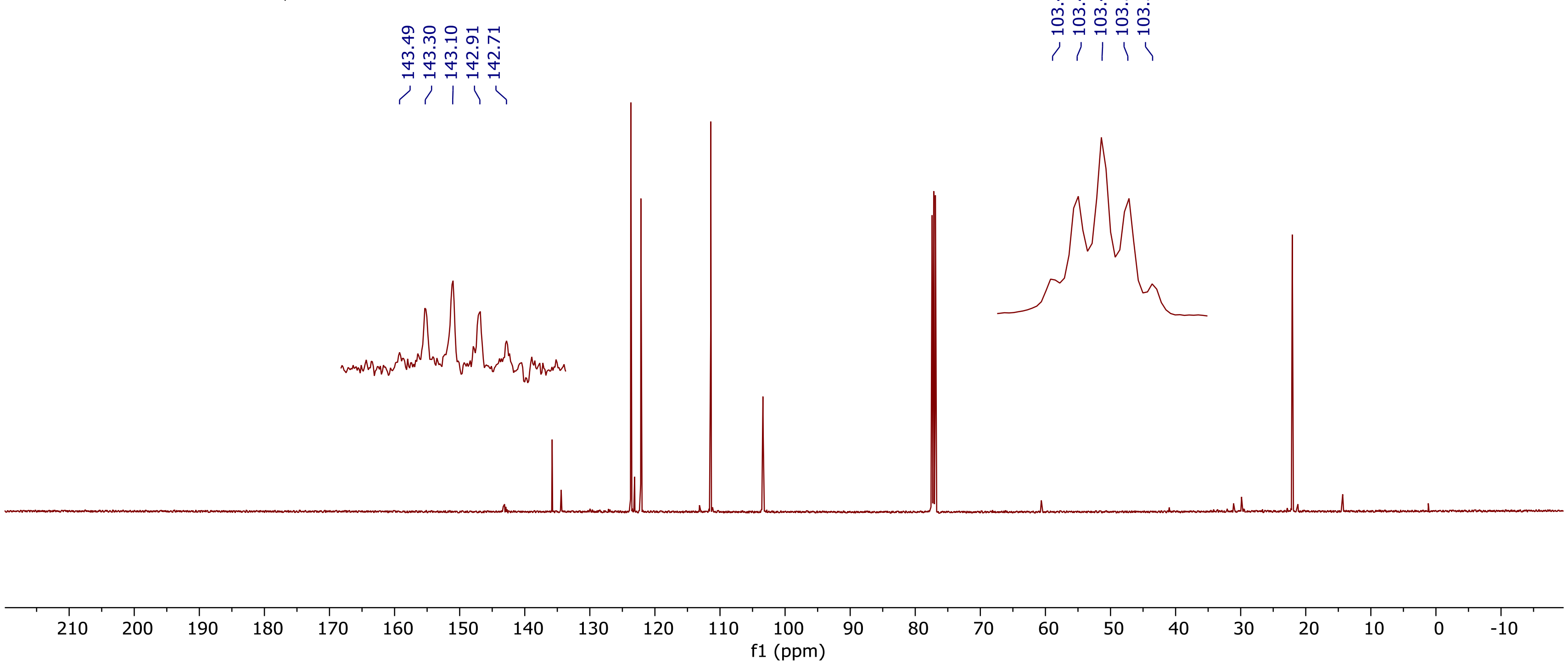
$CDCl_3$, 500 MHz, 298 K

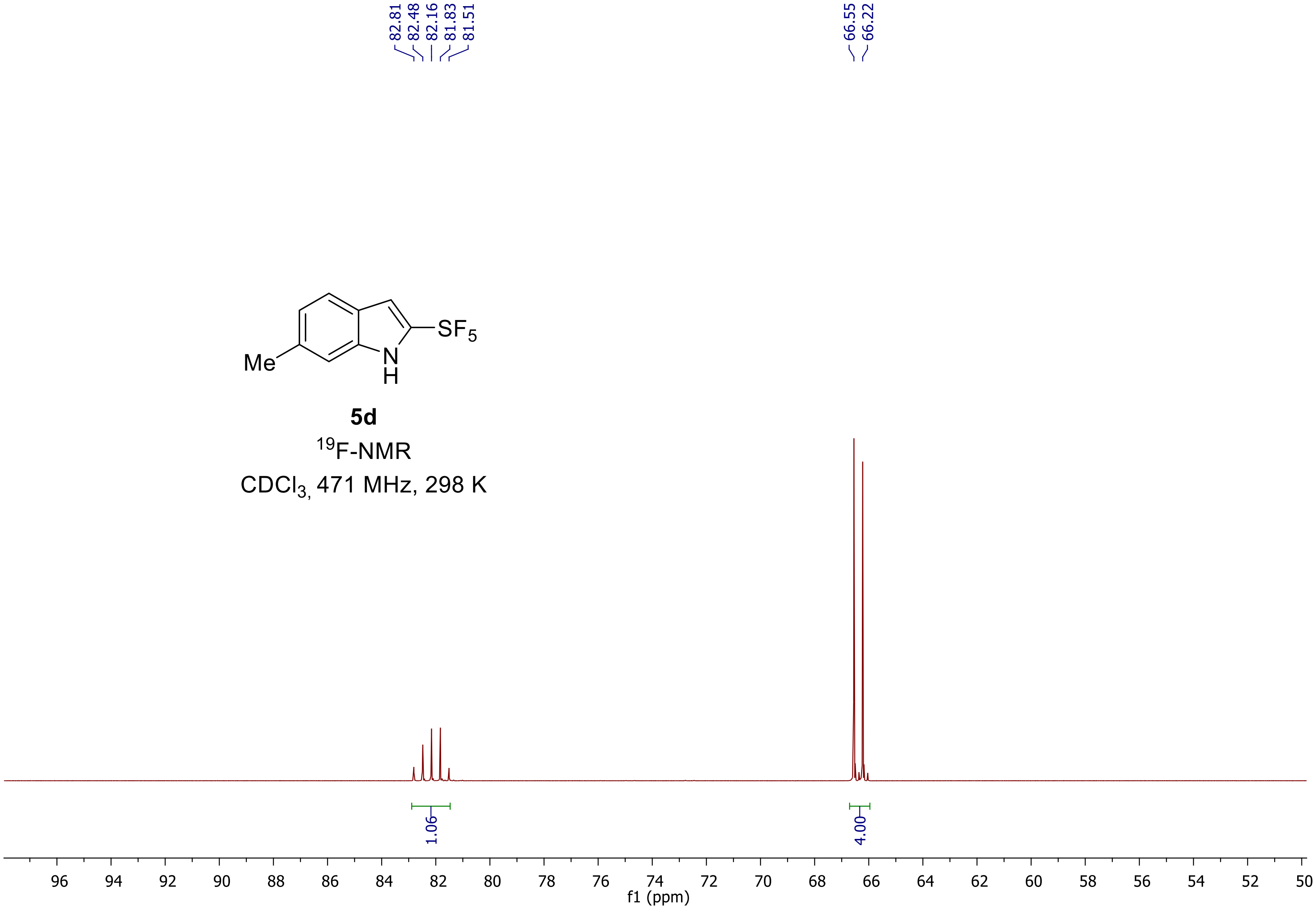


5d

^{13}C-NMR

$CDCl_3$, 125 MHz, 298 K

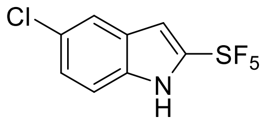




5d

^{19}F-NMR

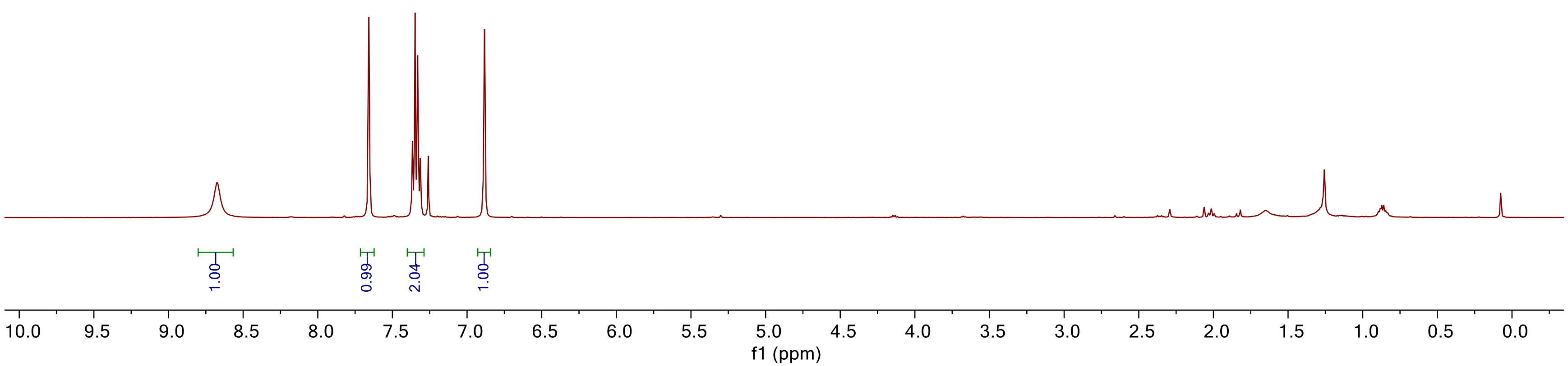
$CDCl_3$, 471 MHz, 298 K



5e

^{1}H-NMR

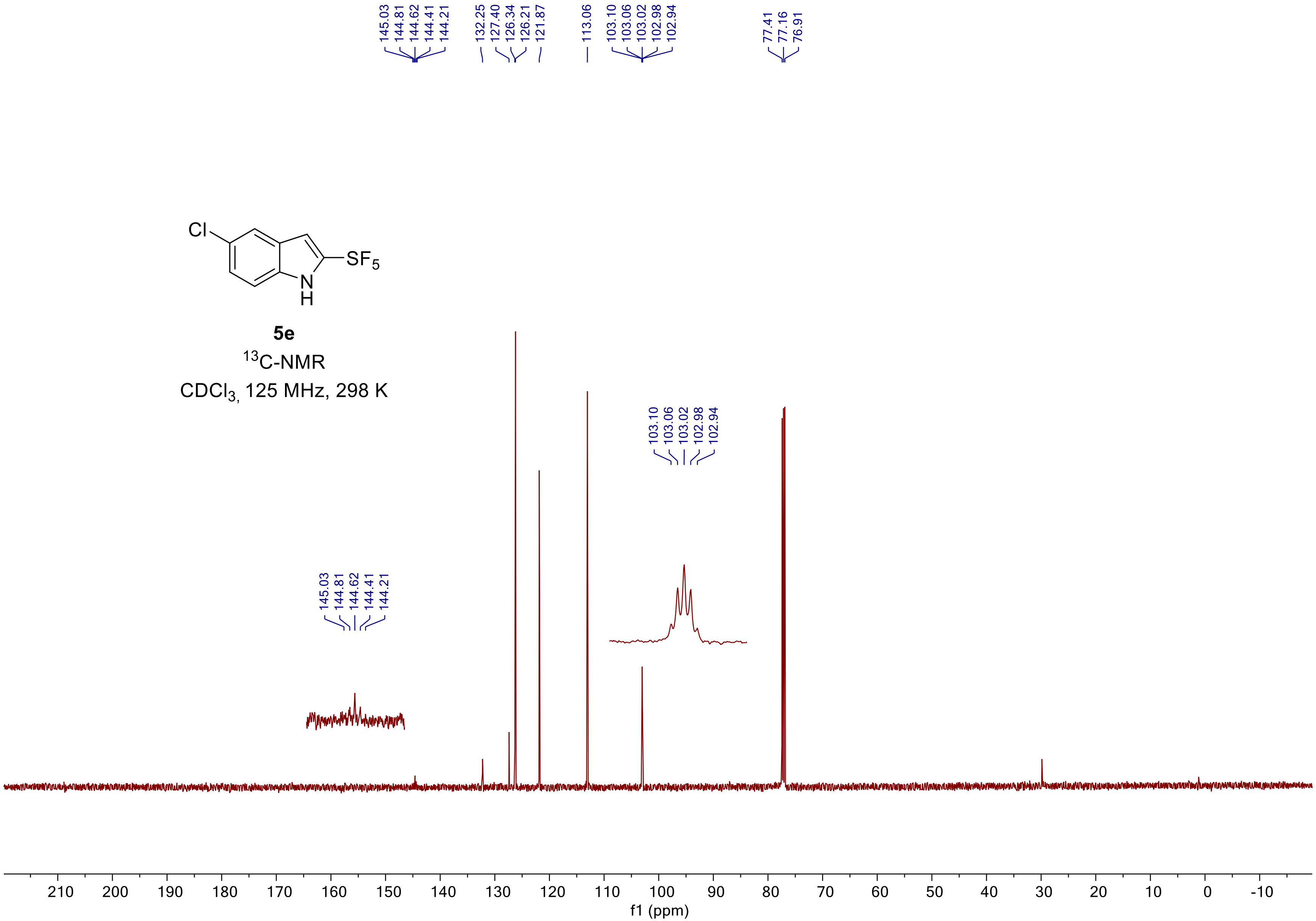
$CDCl_3$, 500 MHz, 298 K

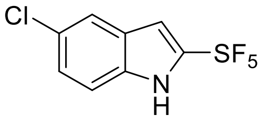


5e

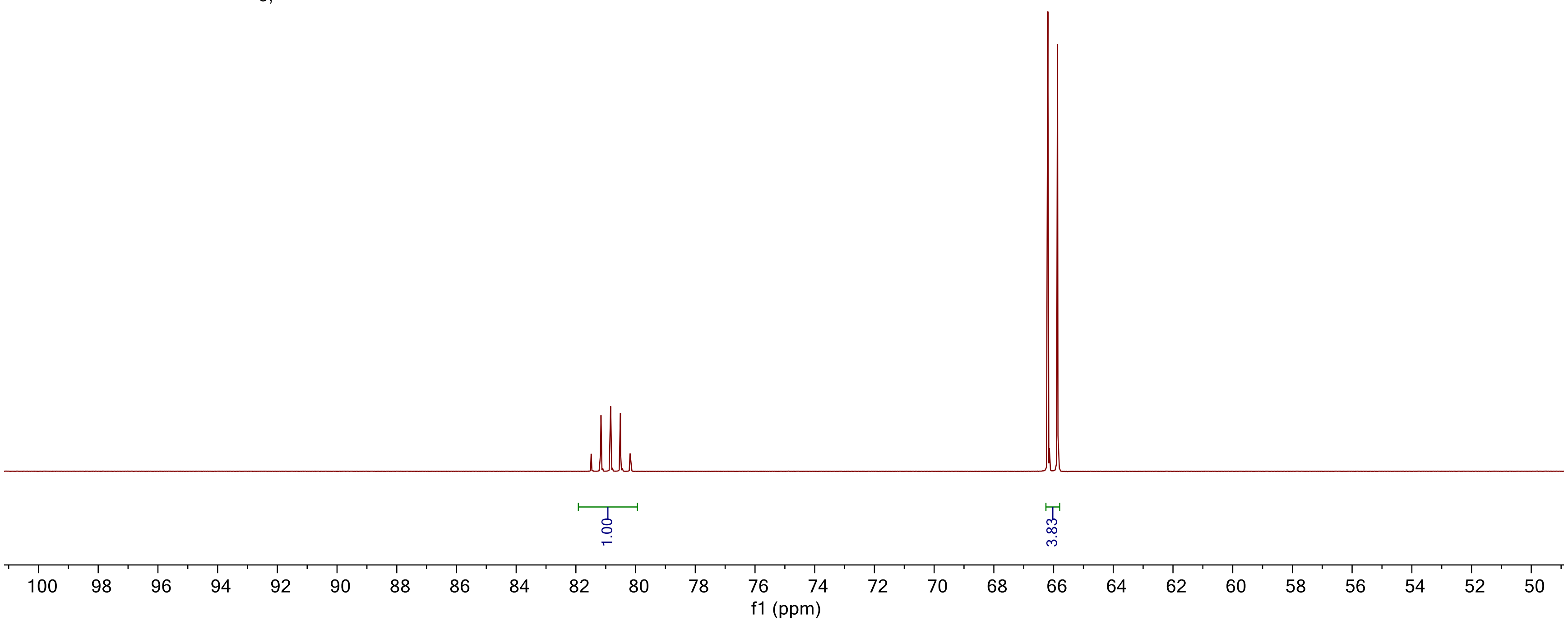
^{13}C-NMR

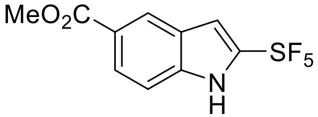
$CDCl_3$, 125 MHz, 298 K





5e
^{19}F-NMR
$CDCl_3$, 471 MHz, 298 K

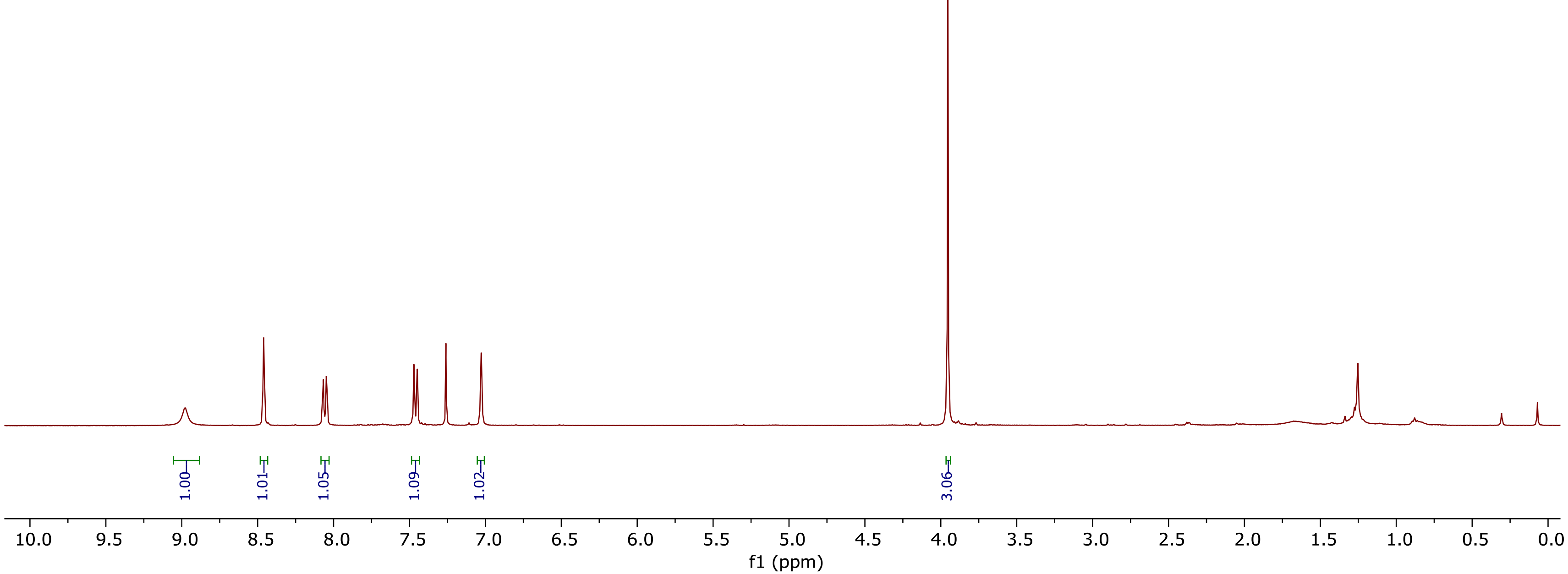


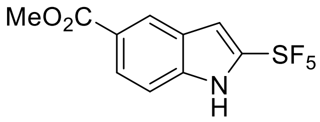


5f

^{1}H-NMR

$CDCl_3$, 500 MHz, 298 K

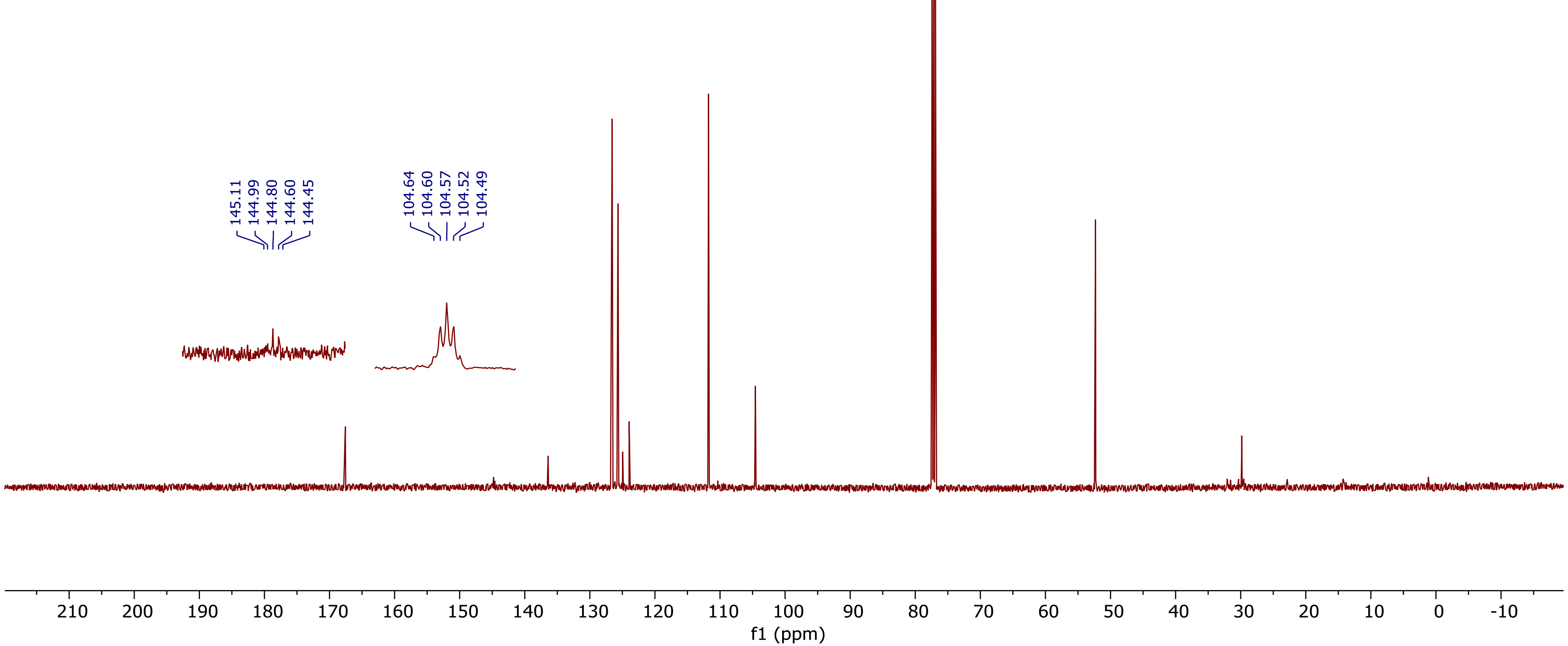


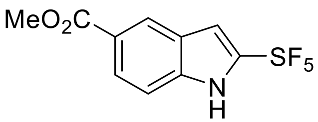


5f

^{13}C-NMR

$CDCl_3$, 125 MHz, 298 K

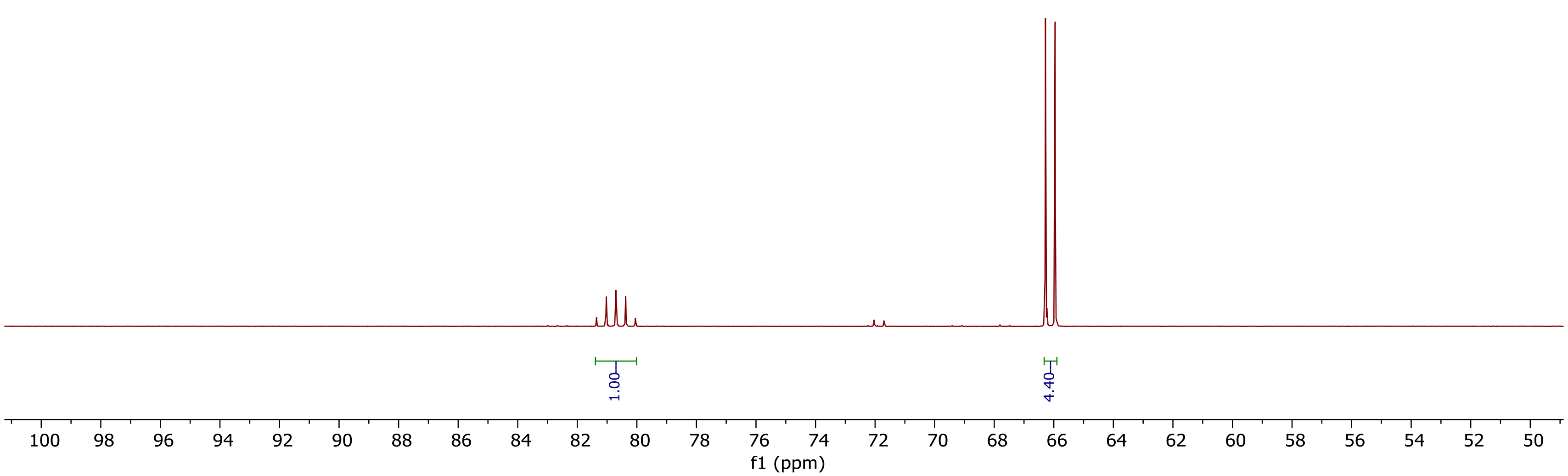


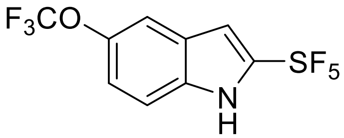


5f

^{19}F-NMR

$CDCl_3$, 471 MHz, 298 K

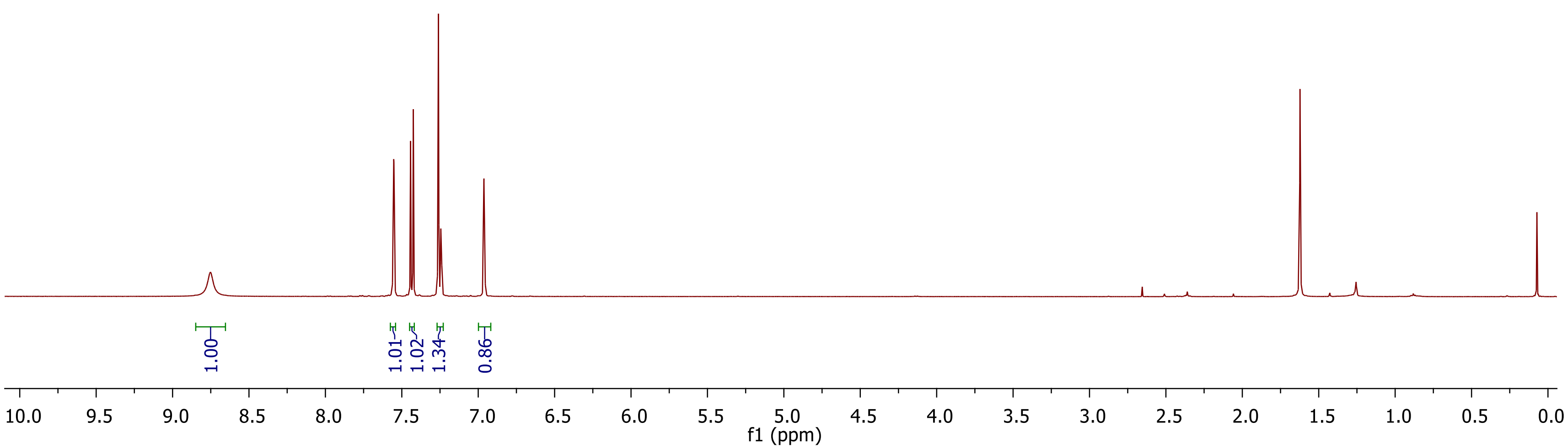


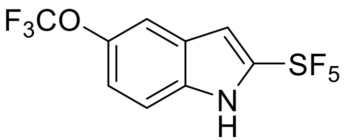


5g

^{1}H-NMR

$CDCl_3$, 500 MHz, 298 K

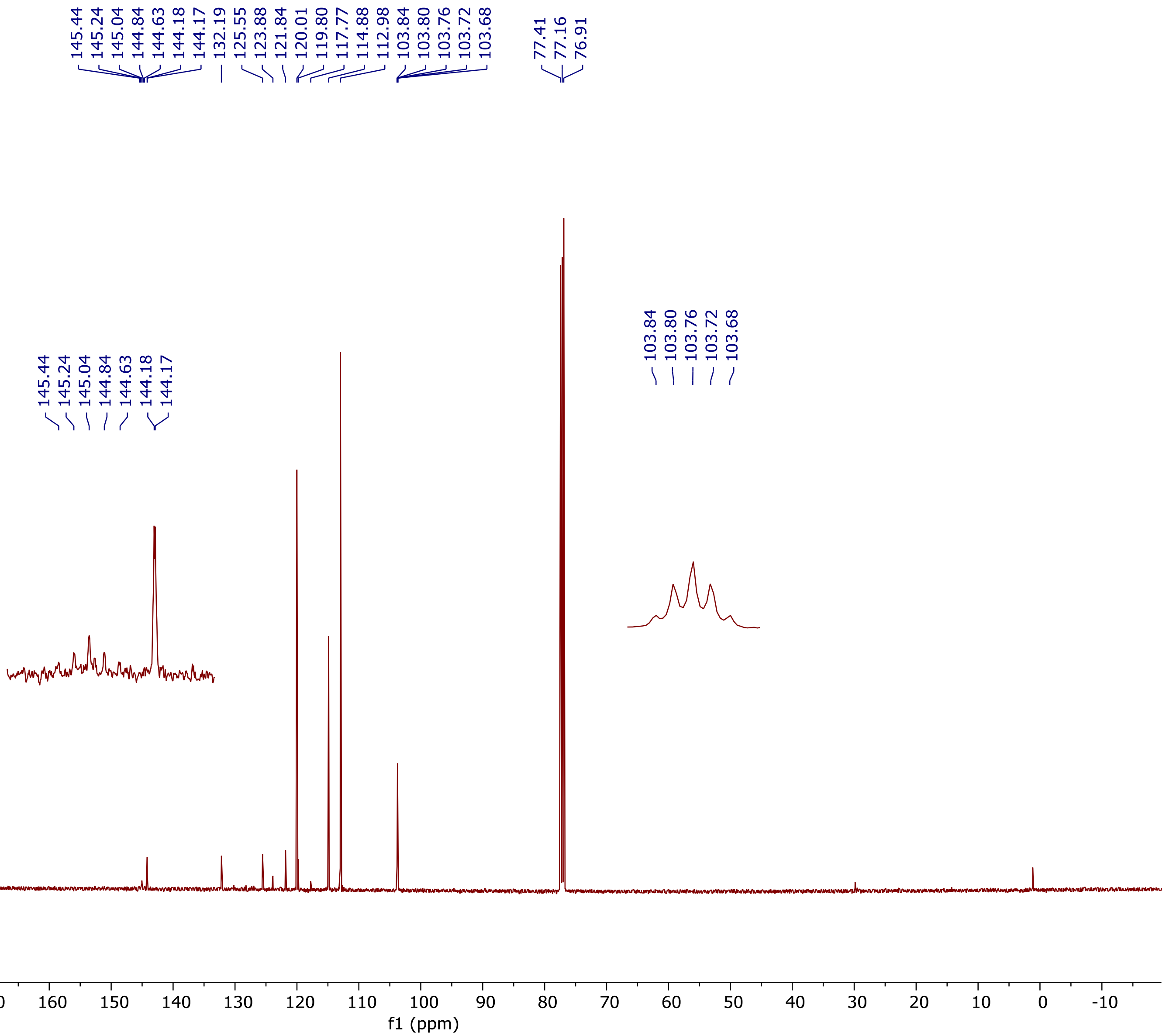


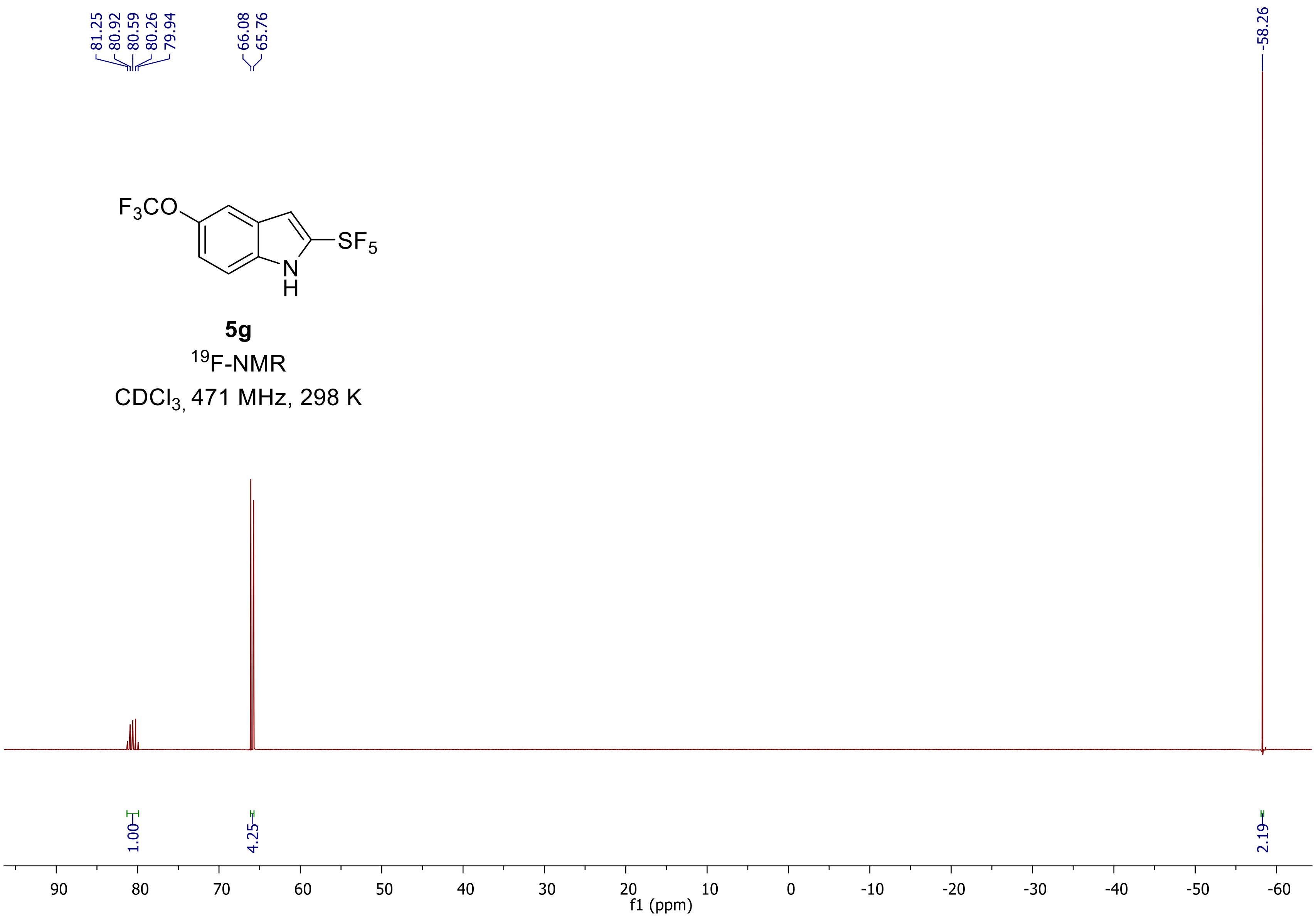


5g

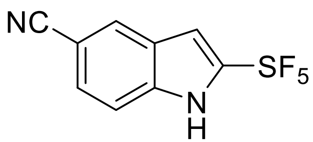
^{13}C-NMR

$CDCl_3$, 125 MHz, 298 K





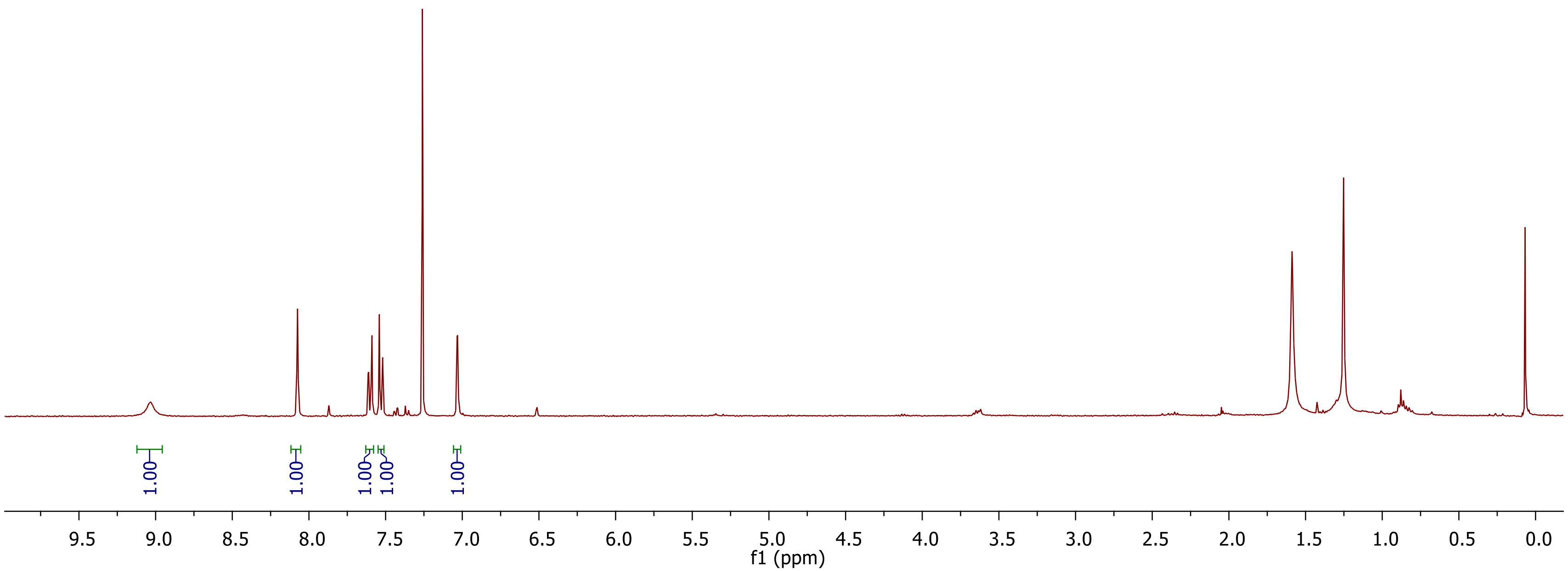
81.25
80.92
80.59
80.26
79.94
66.08
65.76
-58.26
F3CO
SF5
N
H
5g
19F-NMR
CDCl3, 471 MHz, 298 K
1.00
4.25
2.19
90
80
70
60
50
40
30
20
10
0
-10
-20
-30
-40
-50
-60
f1 (ppm)

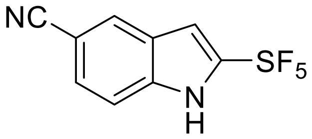


5h

^{1}H-NMR

$CDCl_3$, 400 MHz, 298 K

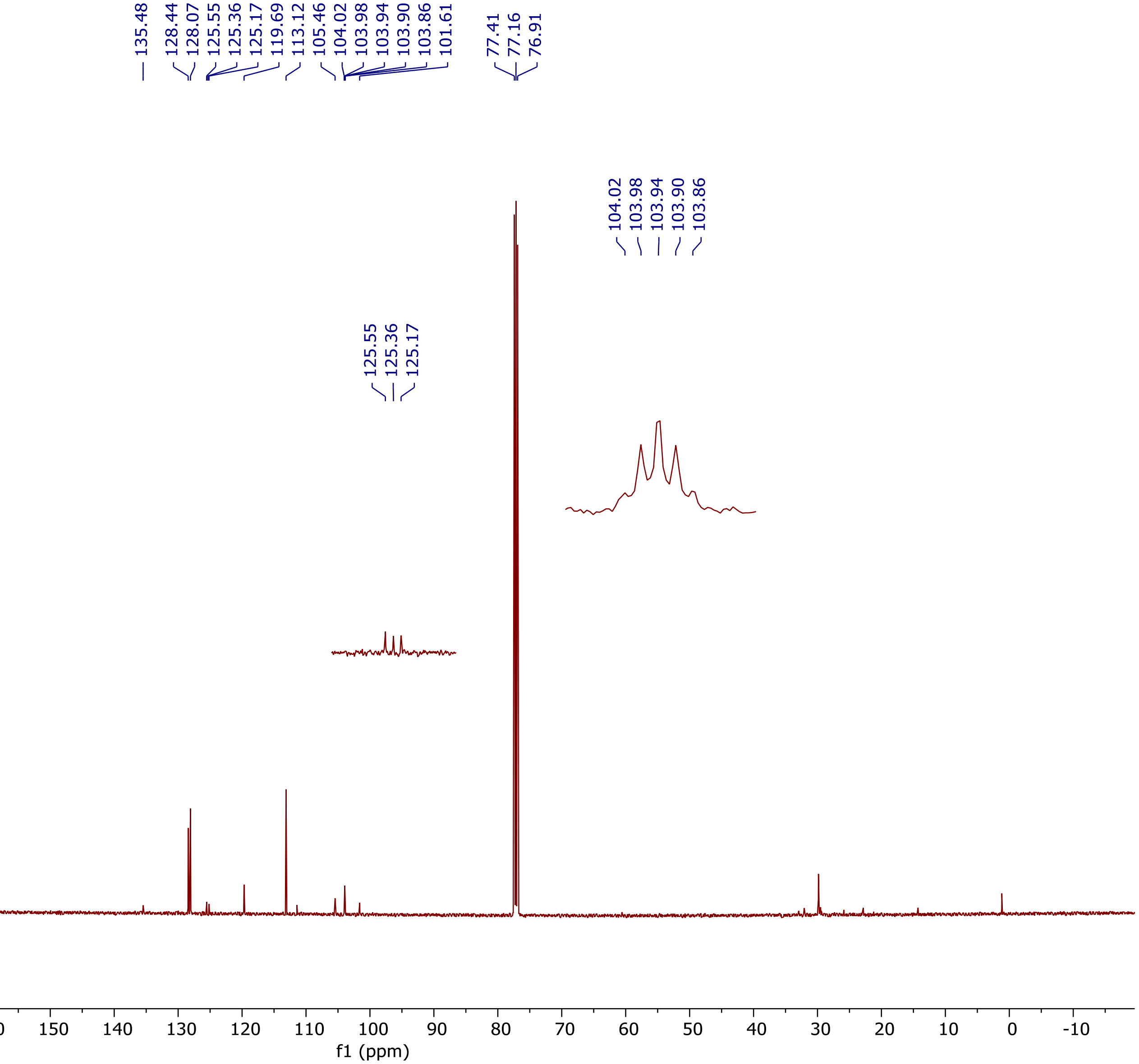


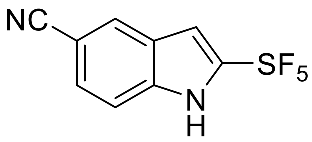


5h

^{13}C-NMR

$CDCl_3$, 125 MHz, 298 K

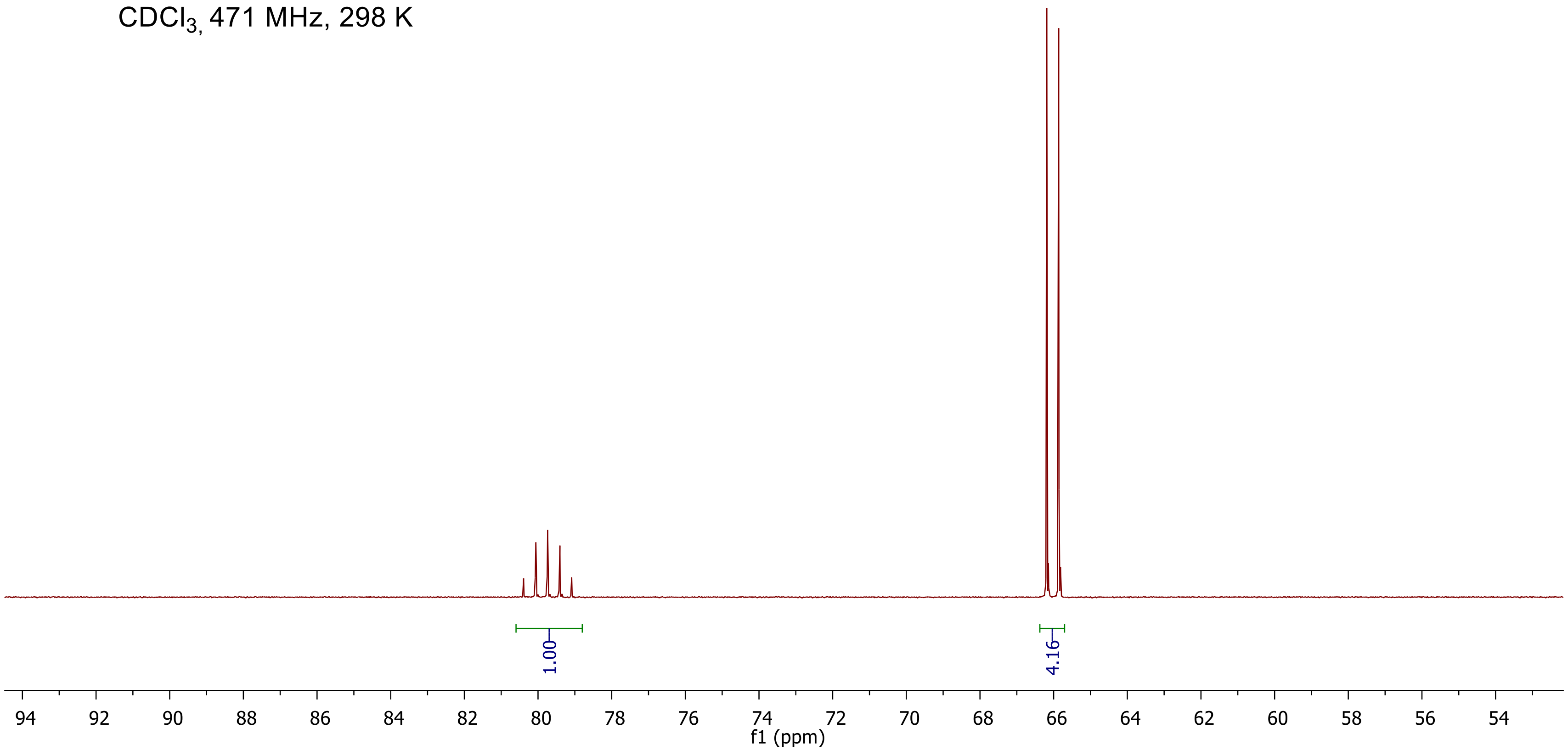


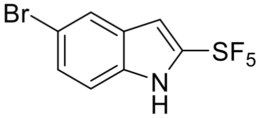


5h

^{19}F-NMR

$CDCl_3$, 471 MHz, 298 K

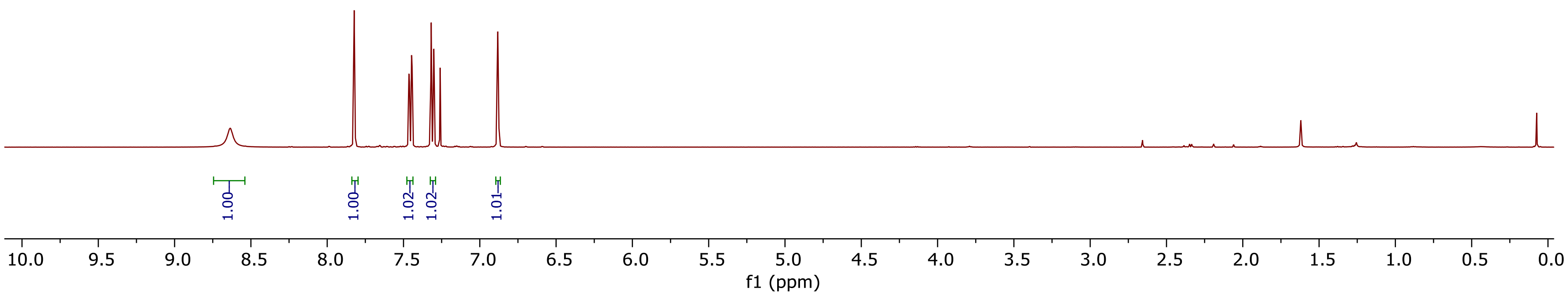


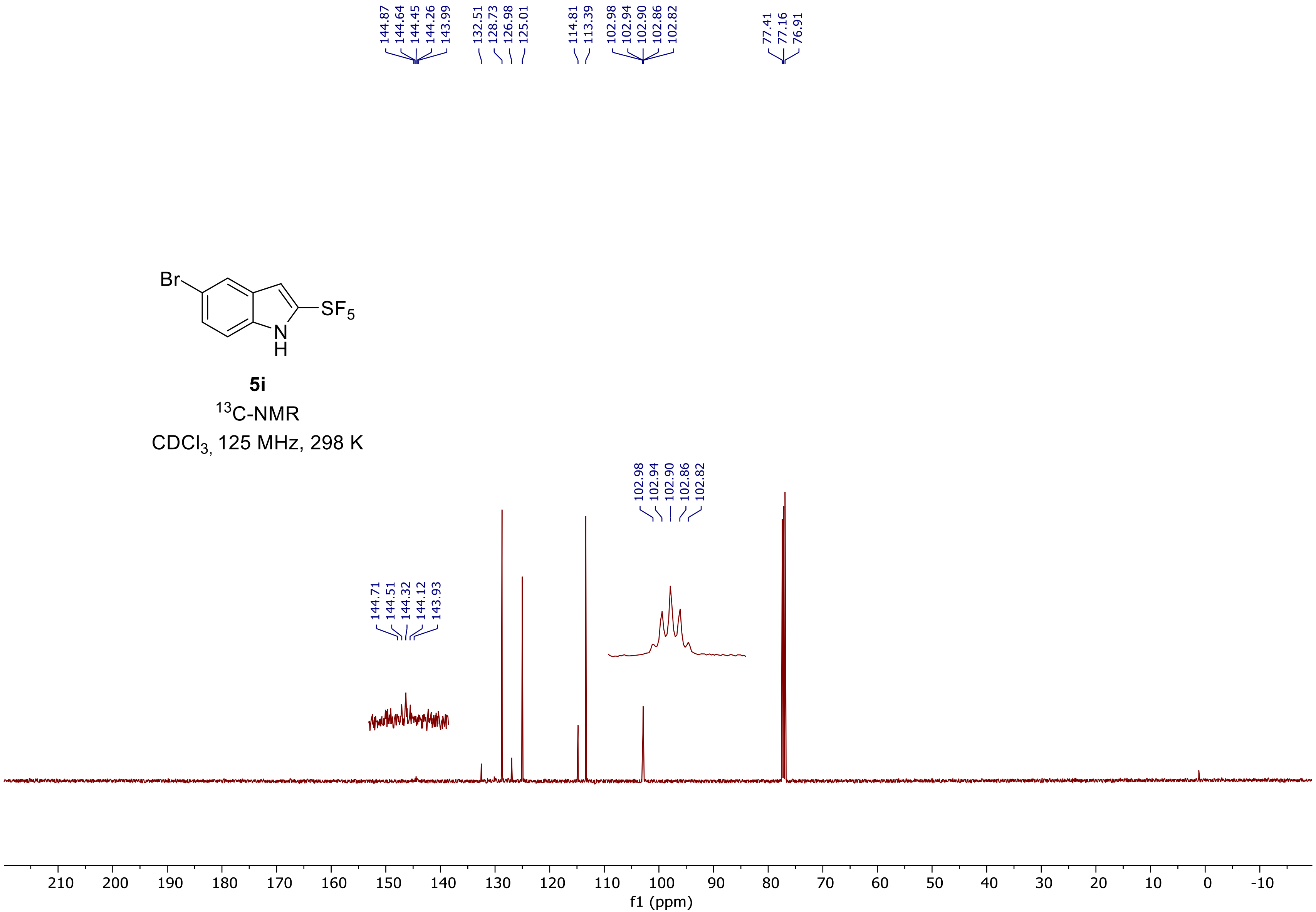


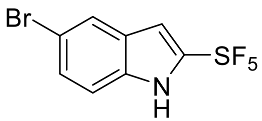
5i

^{1}H-NMR

$CDCl_3$, 500 MHz, 298 K



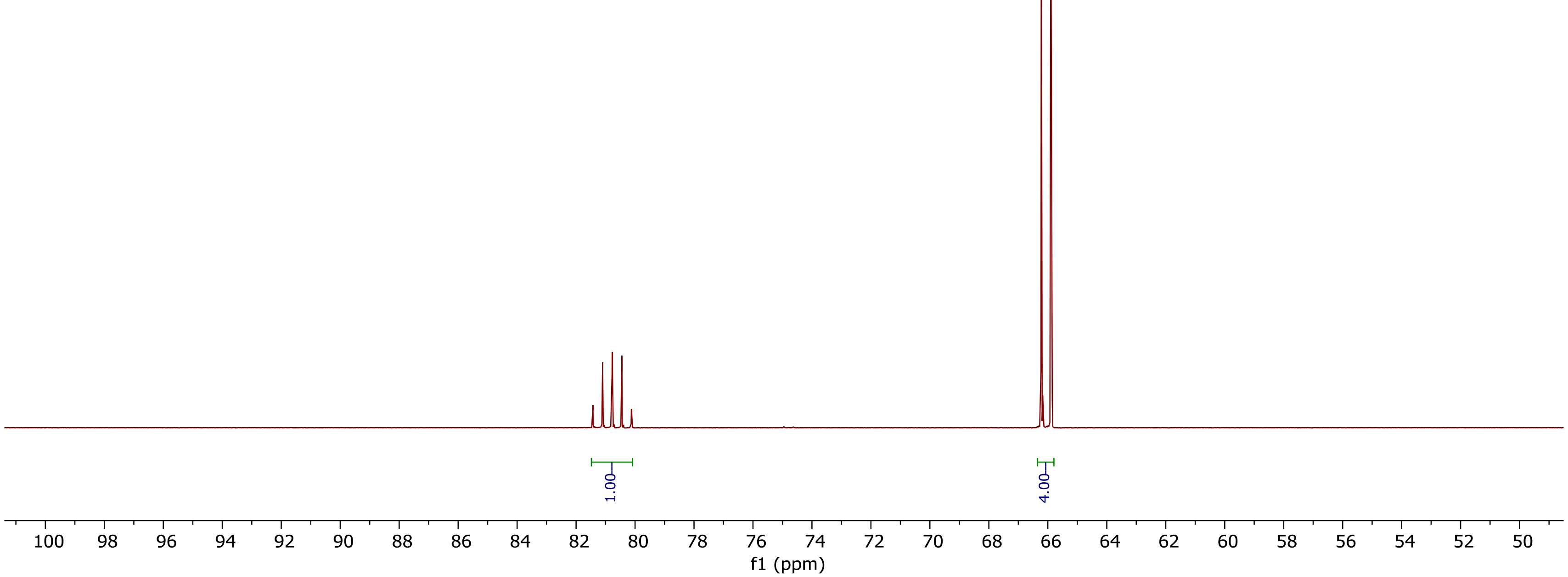

144.87
144.64
144.45
144.26
143.99
132.51
128.73
126.98
125.01
114.81
113.39
102.98
102.94
102.90
102.86
102.82
77.41
77.16
76.91
Br
SF5
N
H
5i
13C-NMR
CDCl3, 125 MHz, 298 K
144.71
144.51
144.32
144.12
143.93
102.98
102.94
102.90
102.86
102.82
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

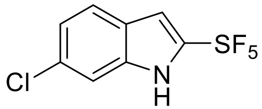


5i

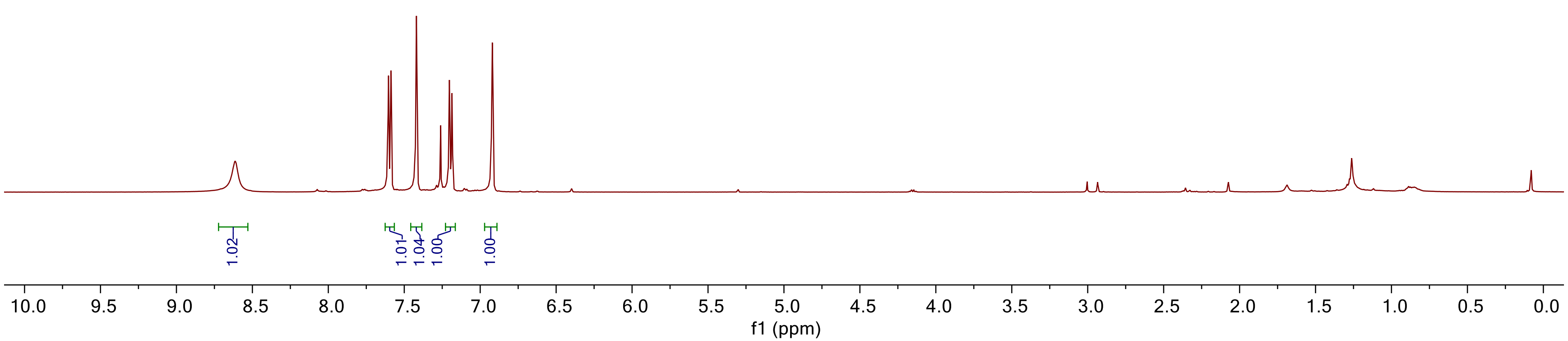
^{19}F-NMR

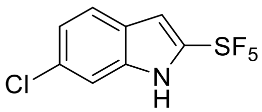
$CDCl_3$, 471 MHz, 298 K





5j
^{1}H-NMR
$CDCl_3$, 500 MHz, 298 K

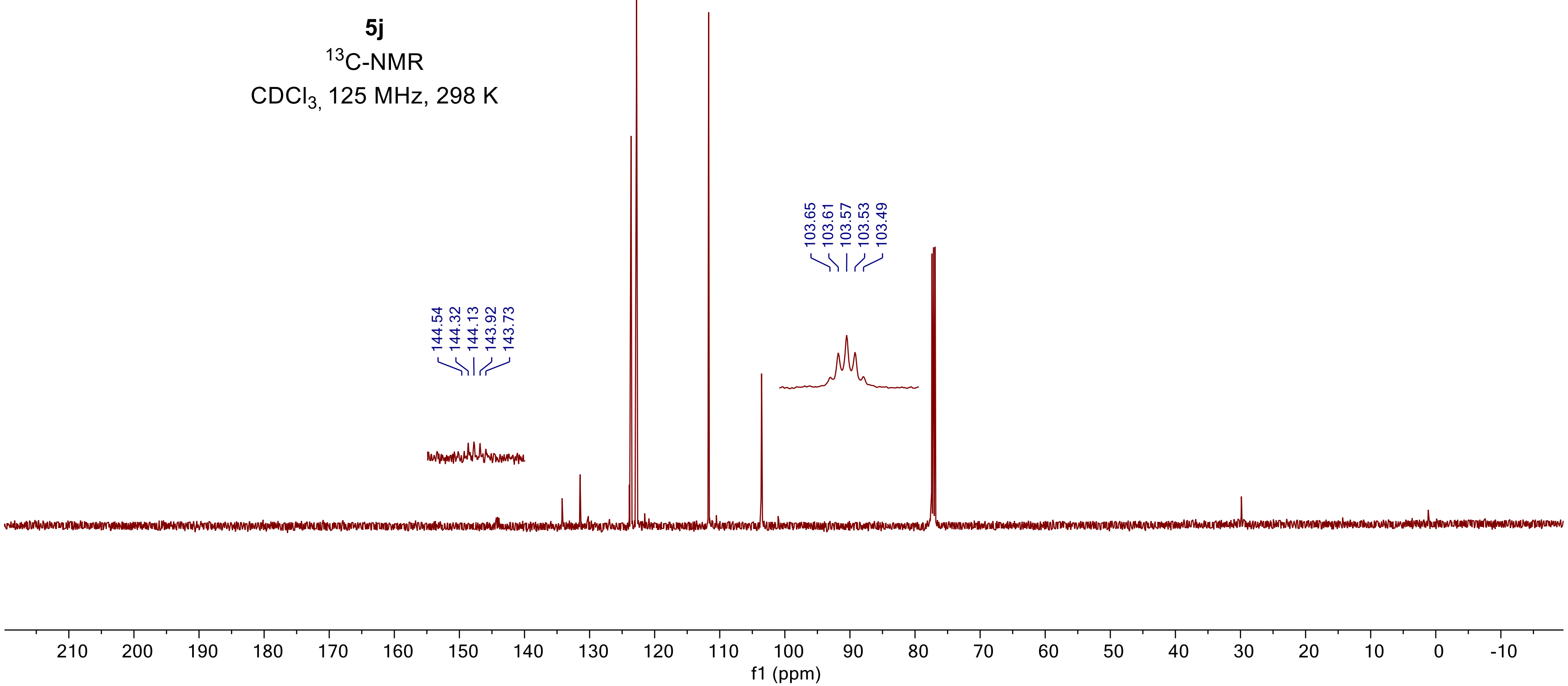


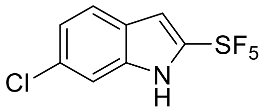


5j

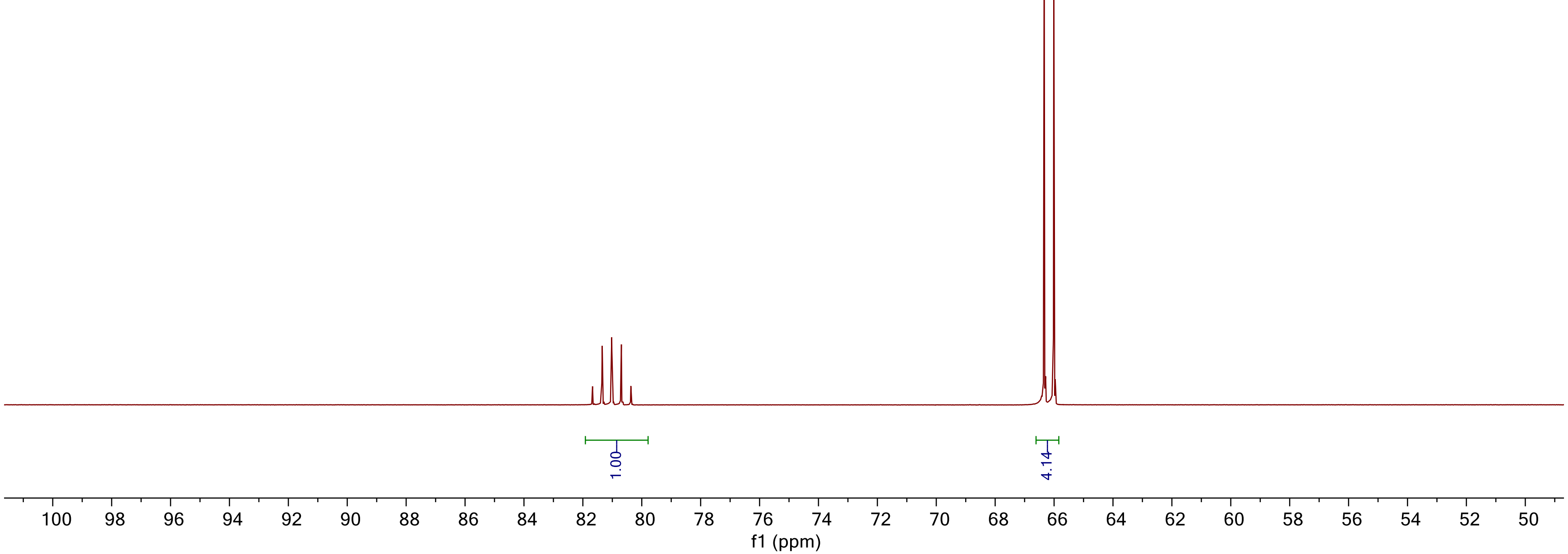
^{13}C-NMR

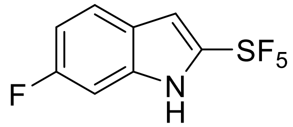
$CDCl_3$, 125 MHz, 298 K





5j
^{19}F-NMR
$CDCl_3$, 471 MHz, 298 K

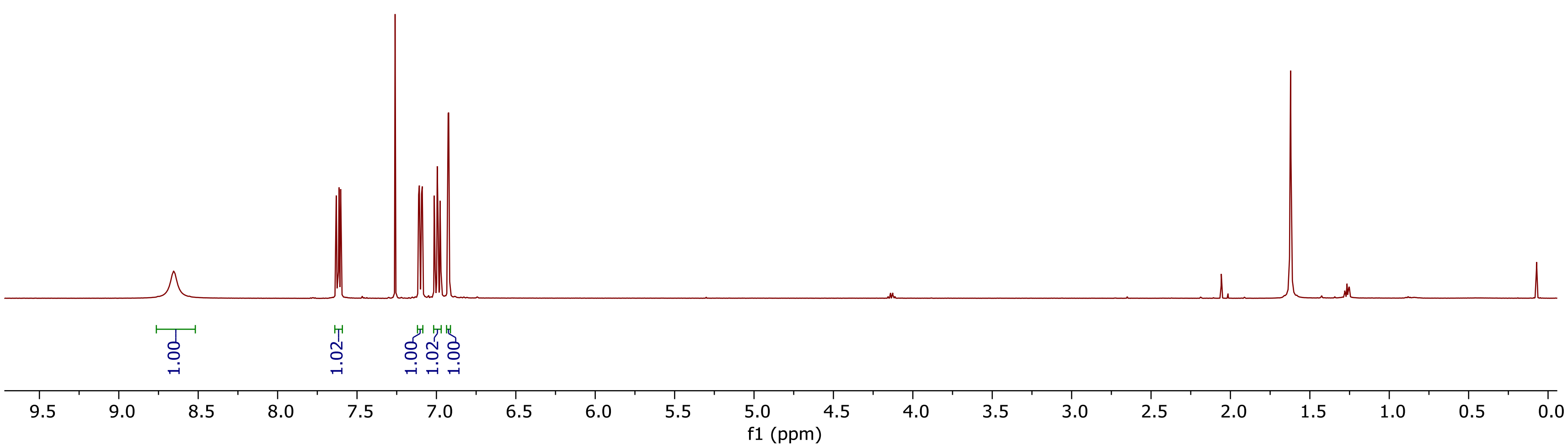


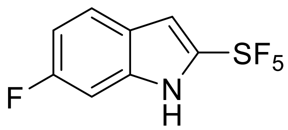


5k

^{1}H-NMR

$CDCl_3$, 500 MHz, 298 K

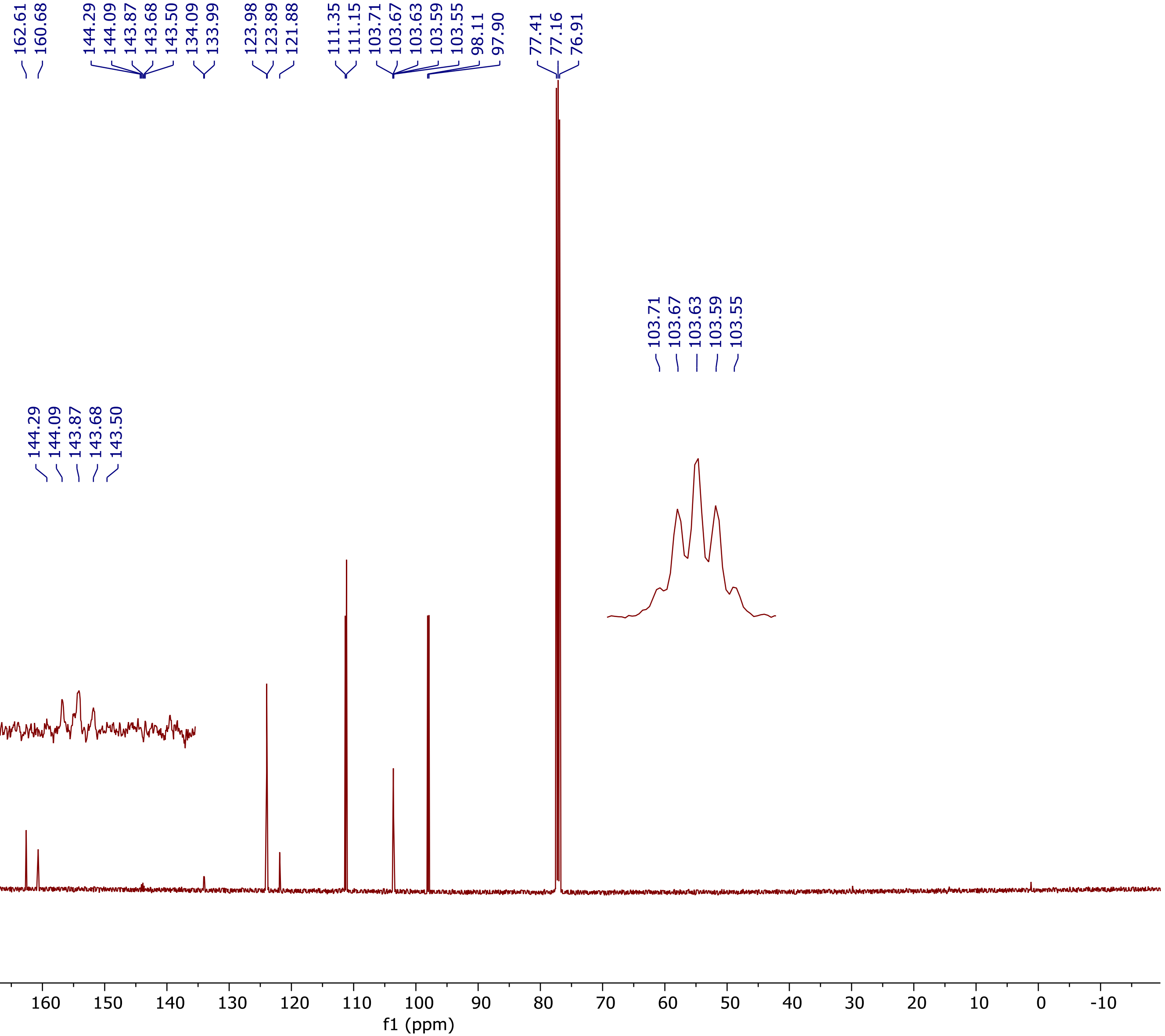


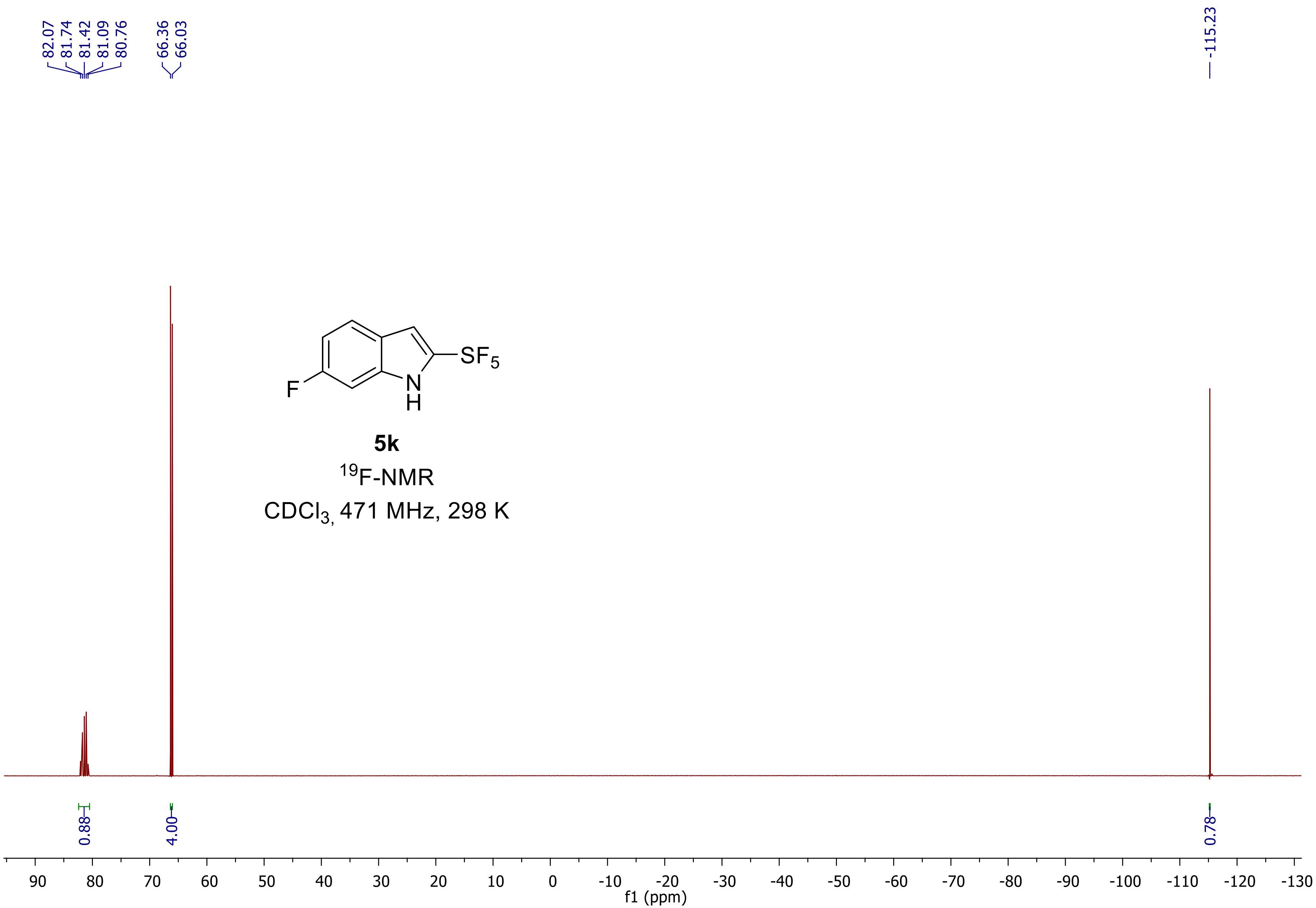


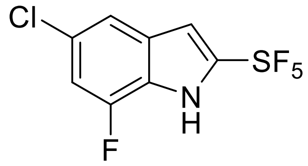
5k

^{13}C-NMR

$CDCl_3$, 125 MHz, 298 K



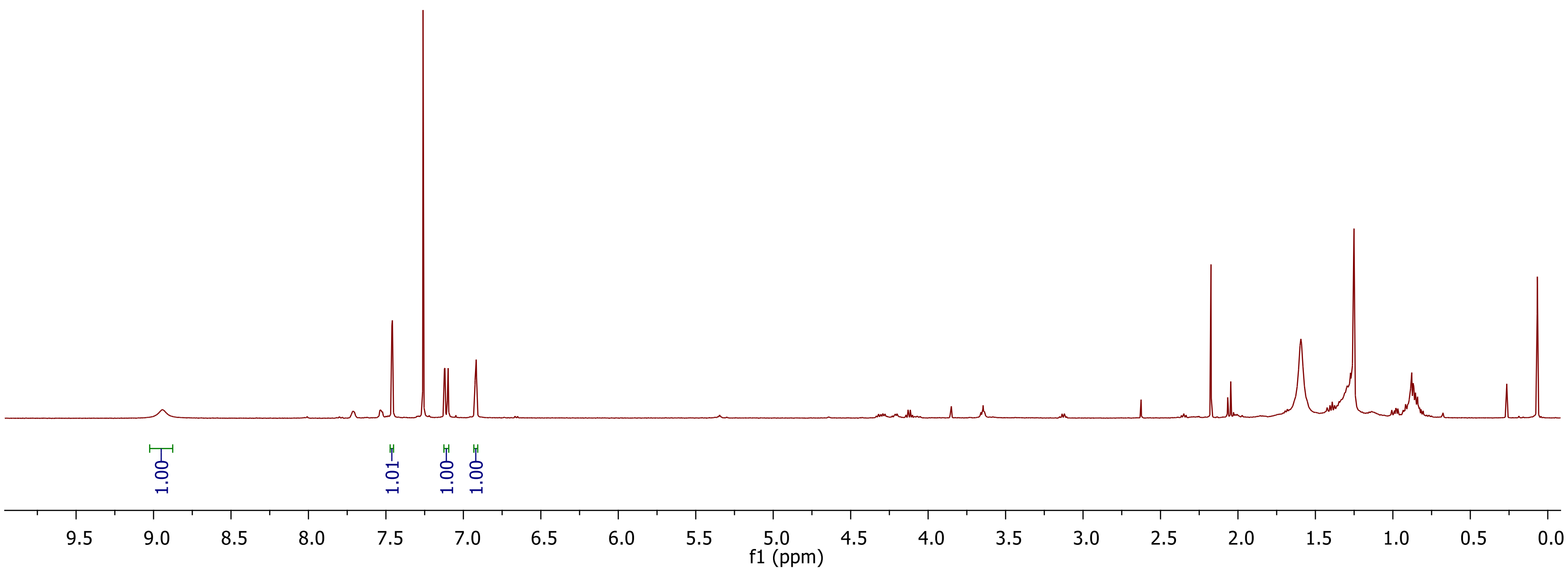

82.07
81.74
81.42
81.09
80.76
66.36
66.03
-115.23
SF5
F
N
H
5k
19F-NMR
CDCl3, 471 MHz, 298 K
0.88
4.00
0.78
90 80 70 60 50 40 30 20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130
f1 (ppm)

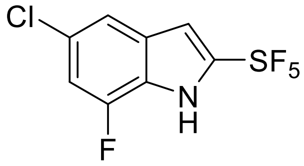


5l

^{1}H-NMR

$CDCl_3$, 500 MHz, 298 K

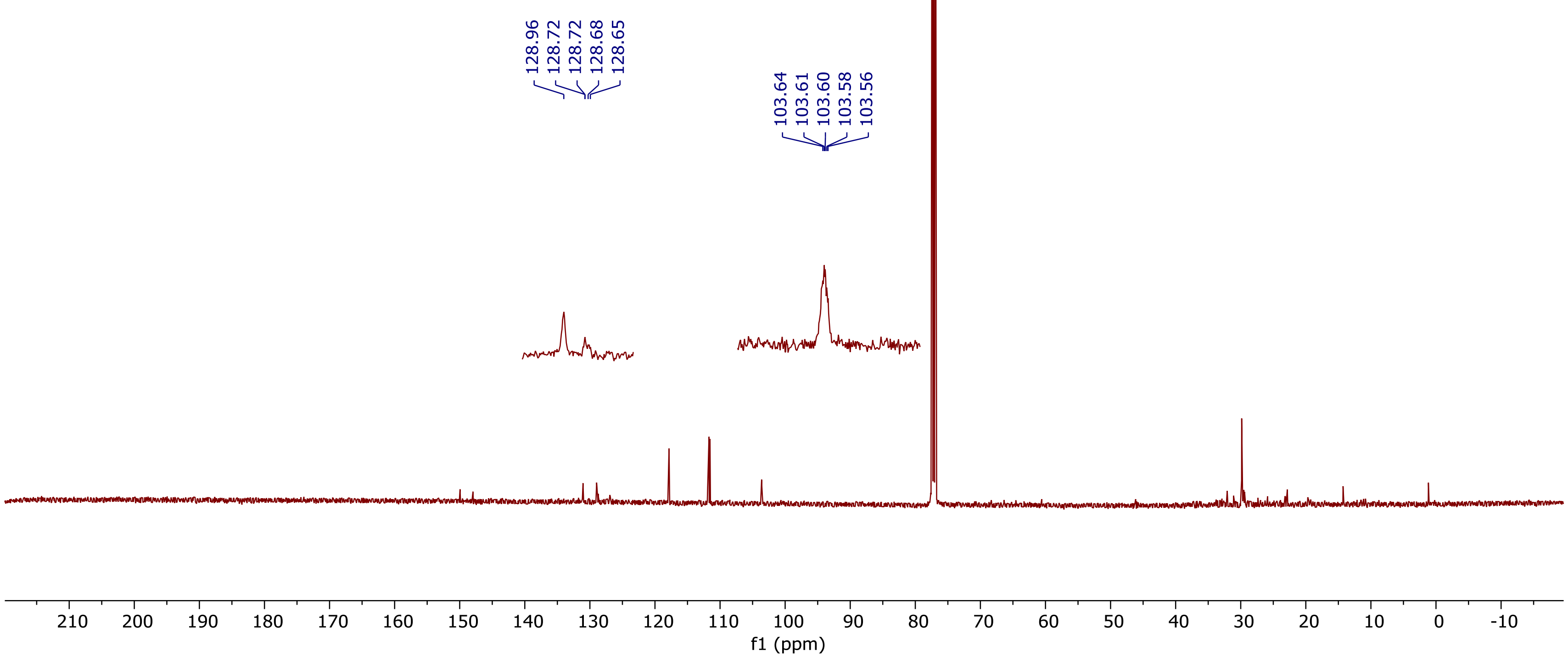


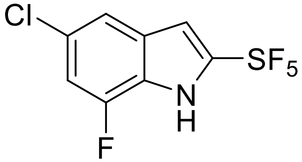


5l

^{13}C-NMR

$CDCl_3$, 125 MHz, 298 K

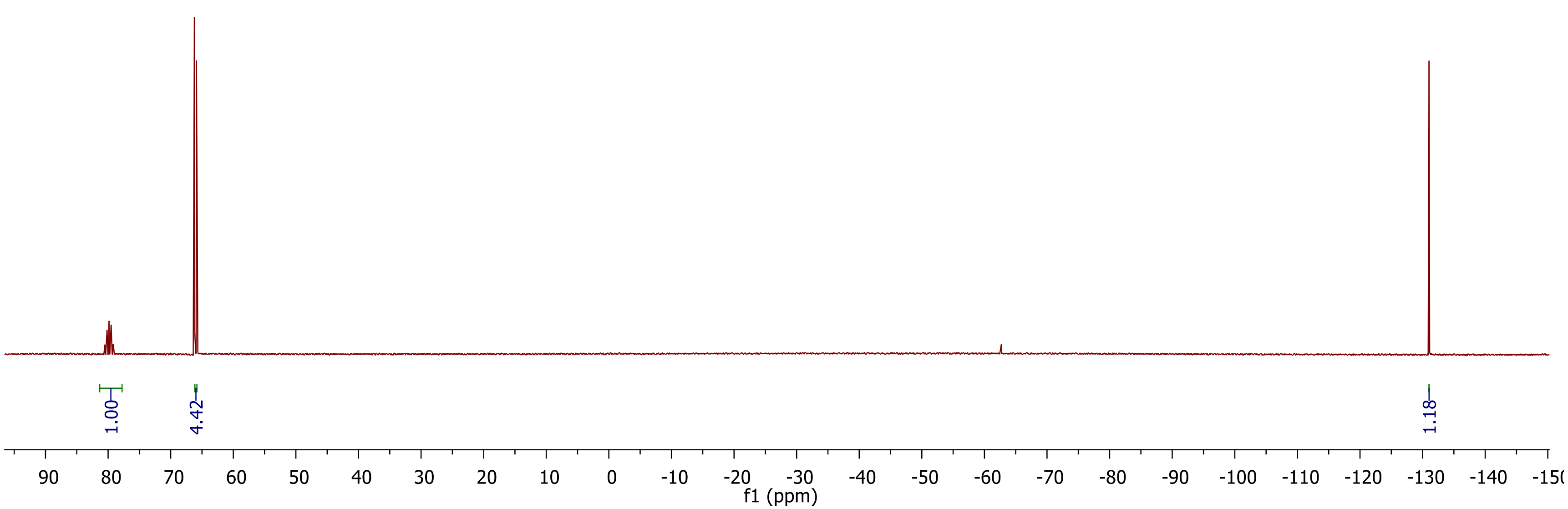


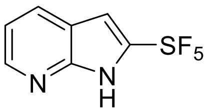


5l

^{19}F-NMR

$CDCl_3$, 471 MHz, 298 K

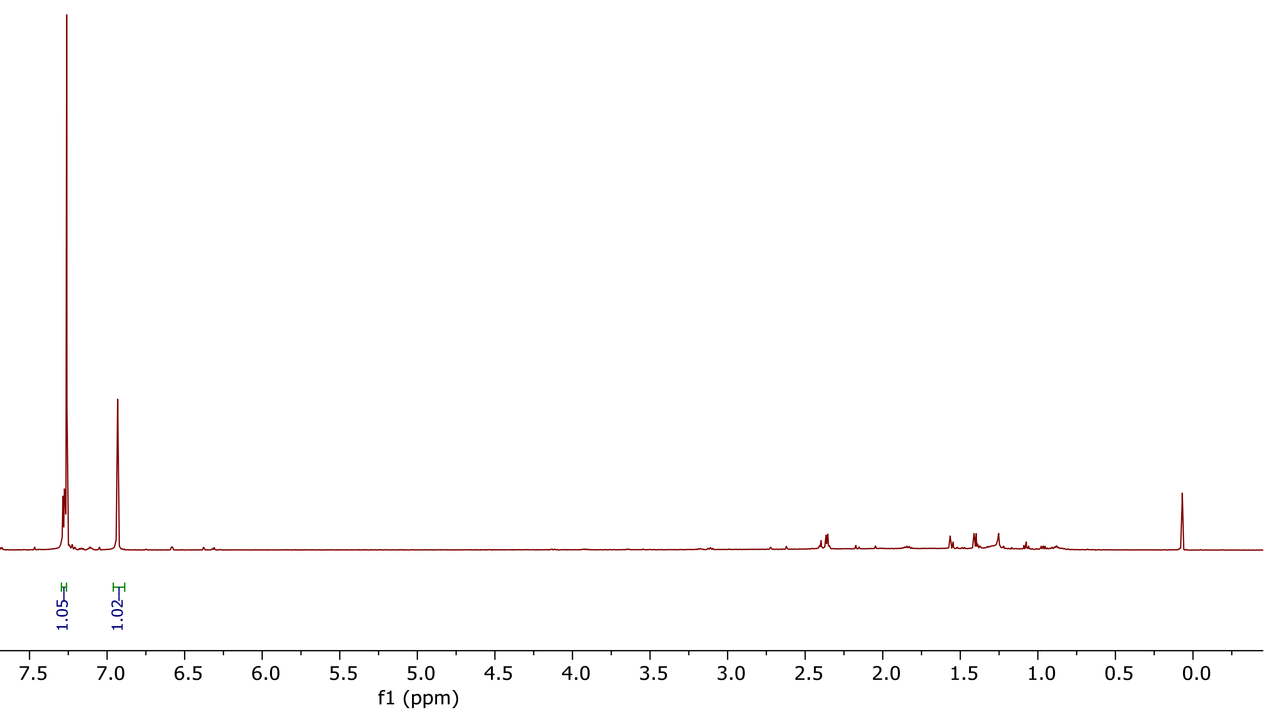




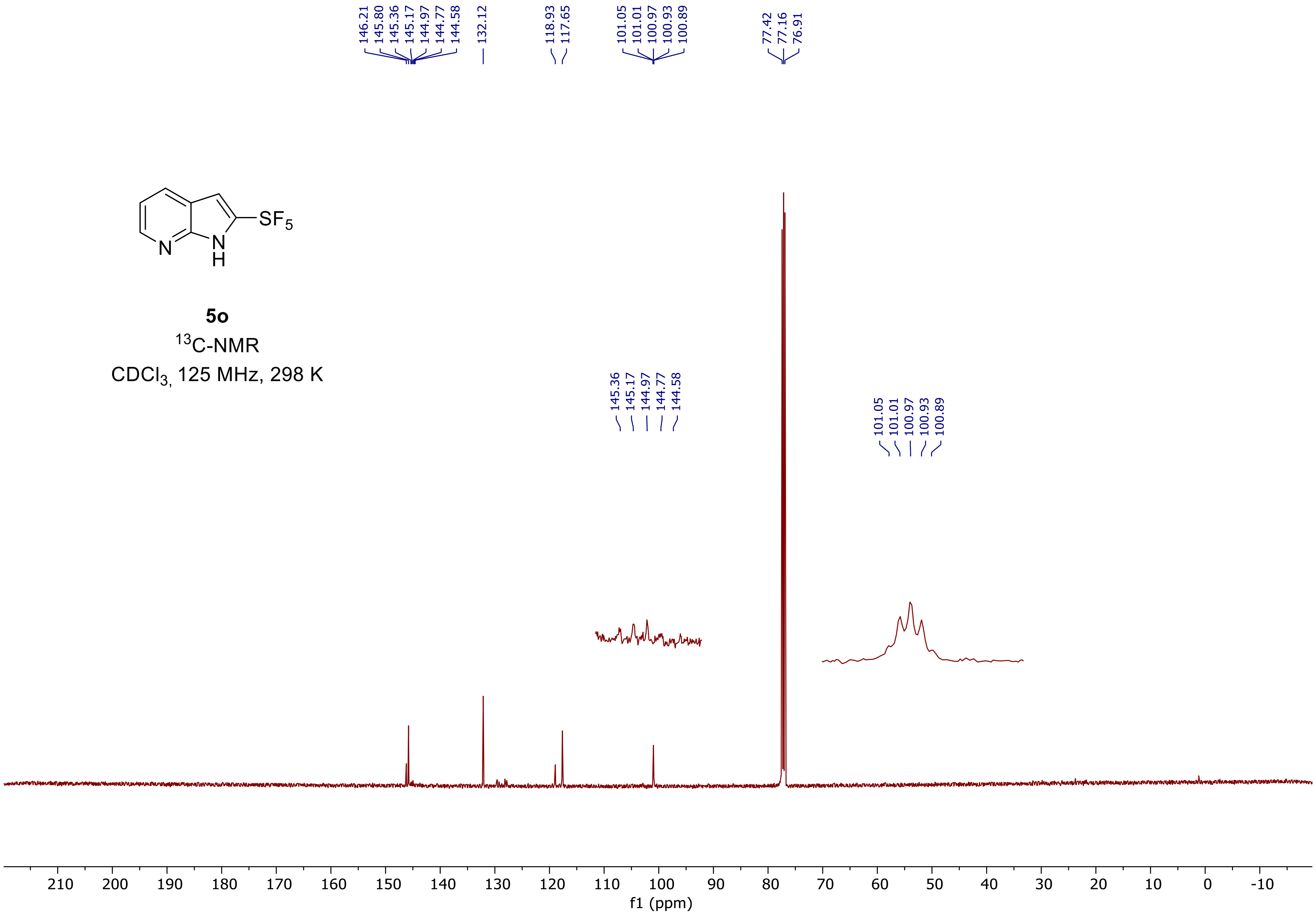
5o

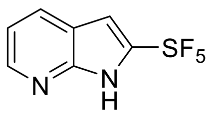
^{1}H-NMR

$CDCl_3$, 500 MHz, 298 K



5o
^{13}C-NMR
$CDCl_3$, 125 MHz, 298 K

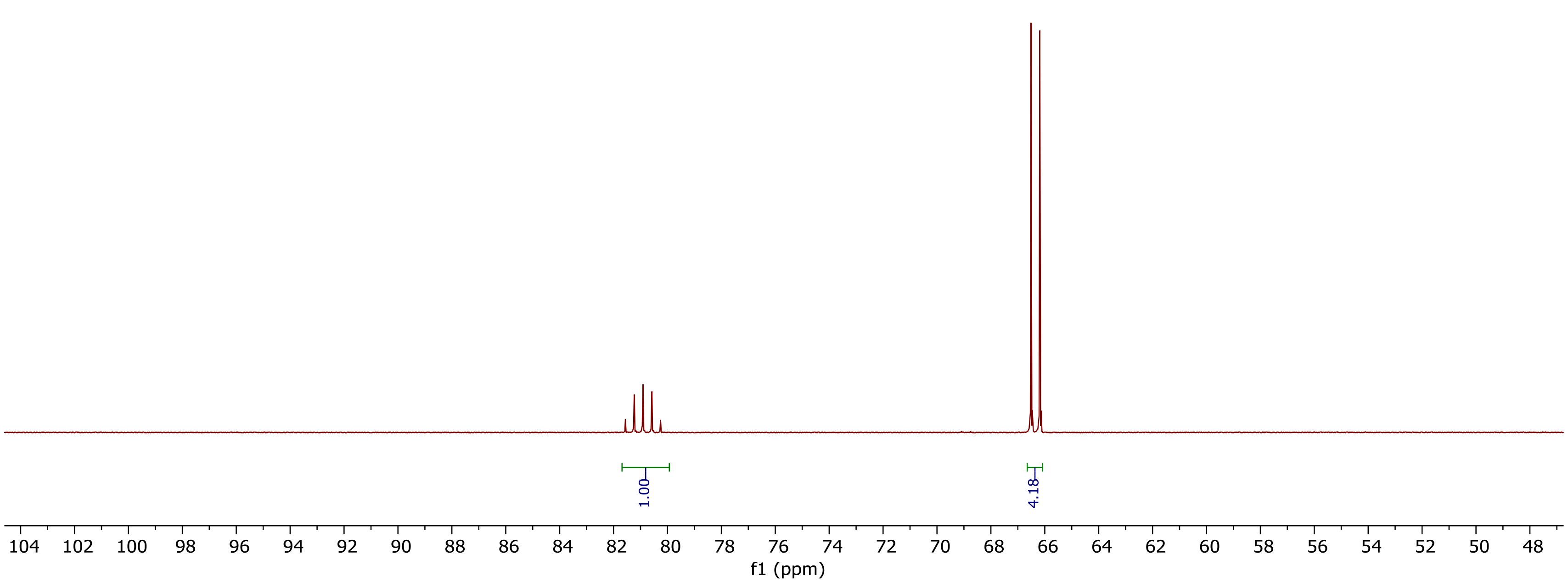


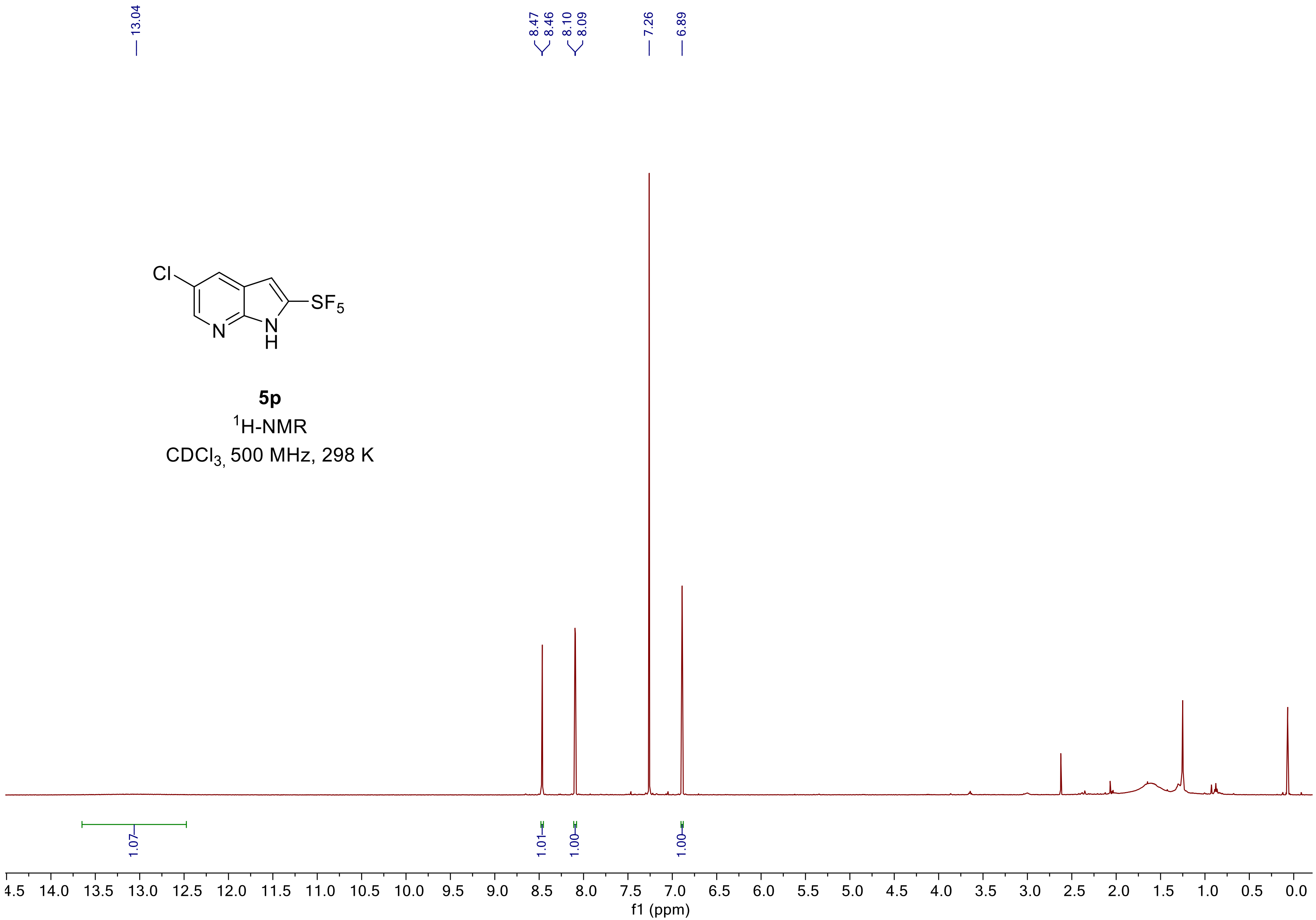


5o

^{19}F-NMR

$CDCl_3$, 471 MHz, 298 K

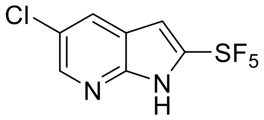




5p

^{1}H-NMR

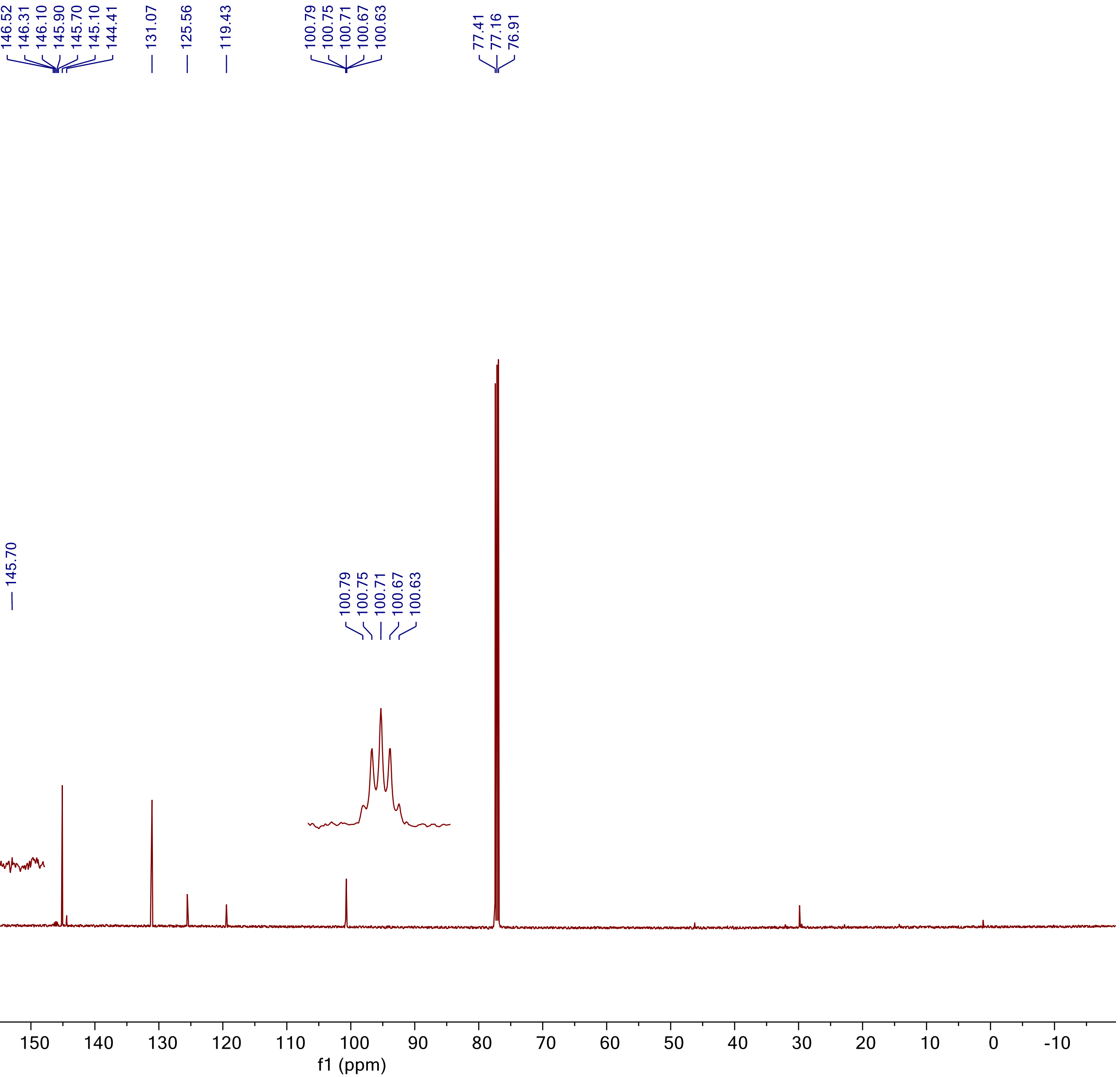
$CDCl_3$, 500 MHz, 298 K

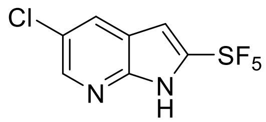


5p

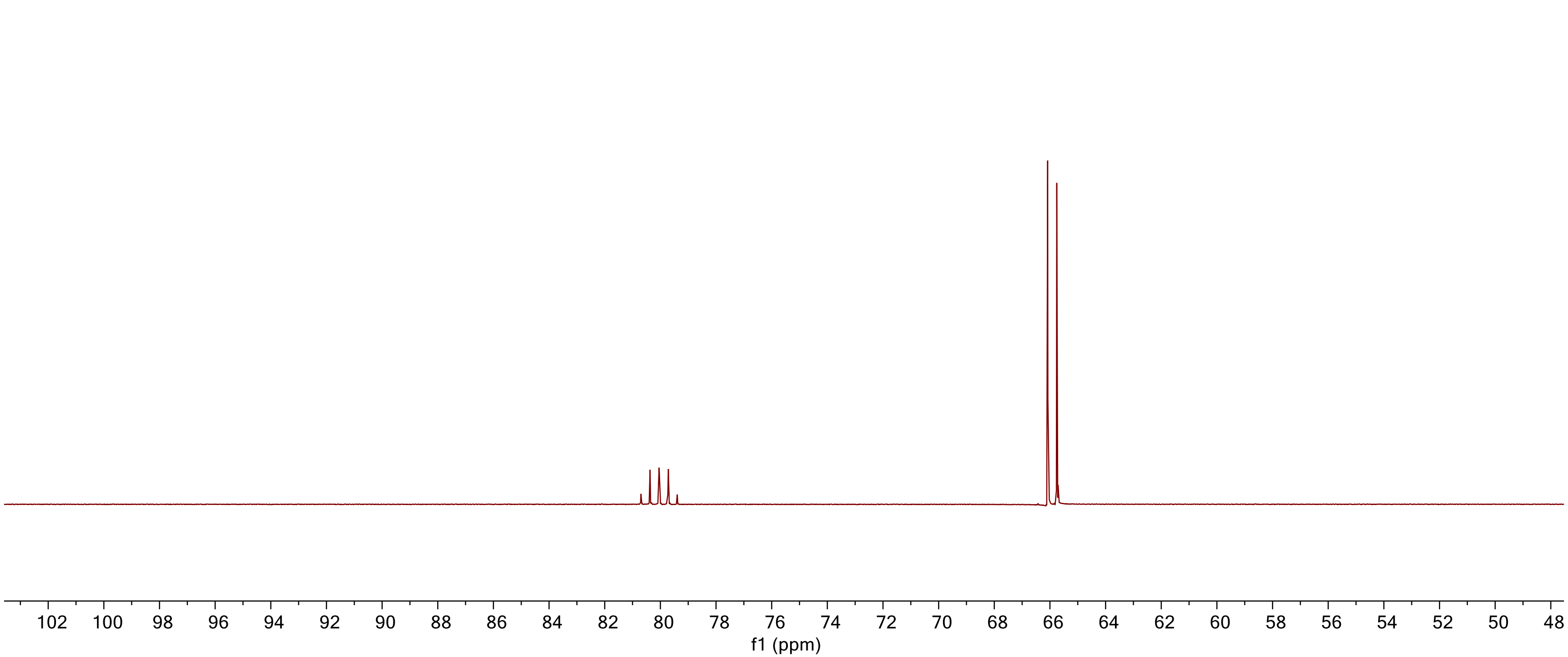
^{13}C-NMR

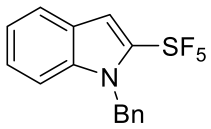
$CDCl_3$, 125 MHz, 298 K





5p
^{19}F-NMR
$CDCl_3$, 471 MHz, 298 K

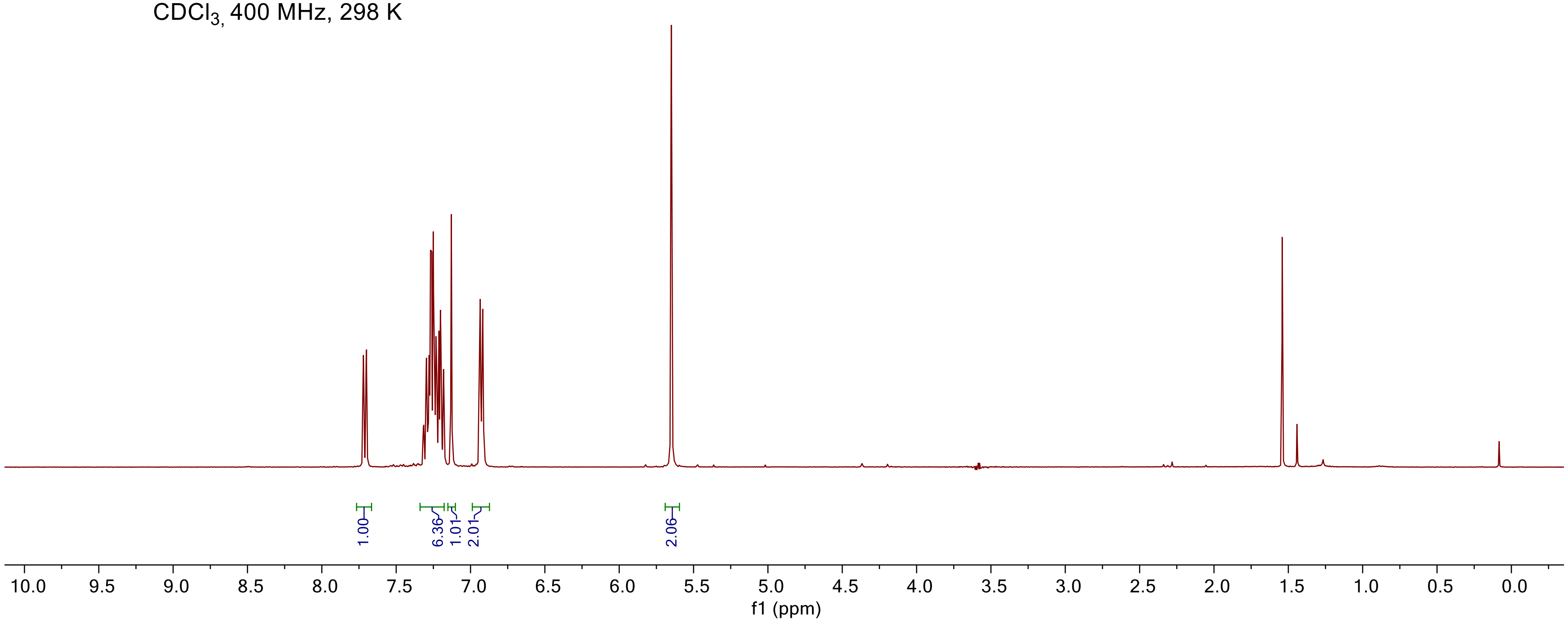


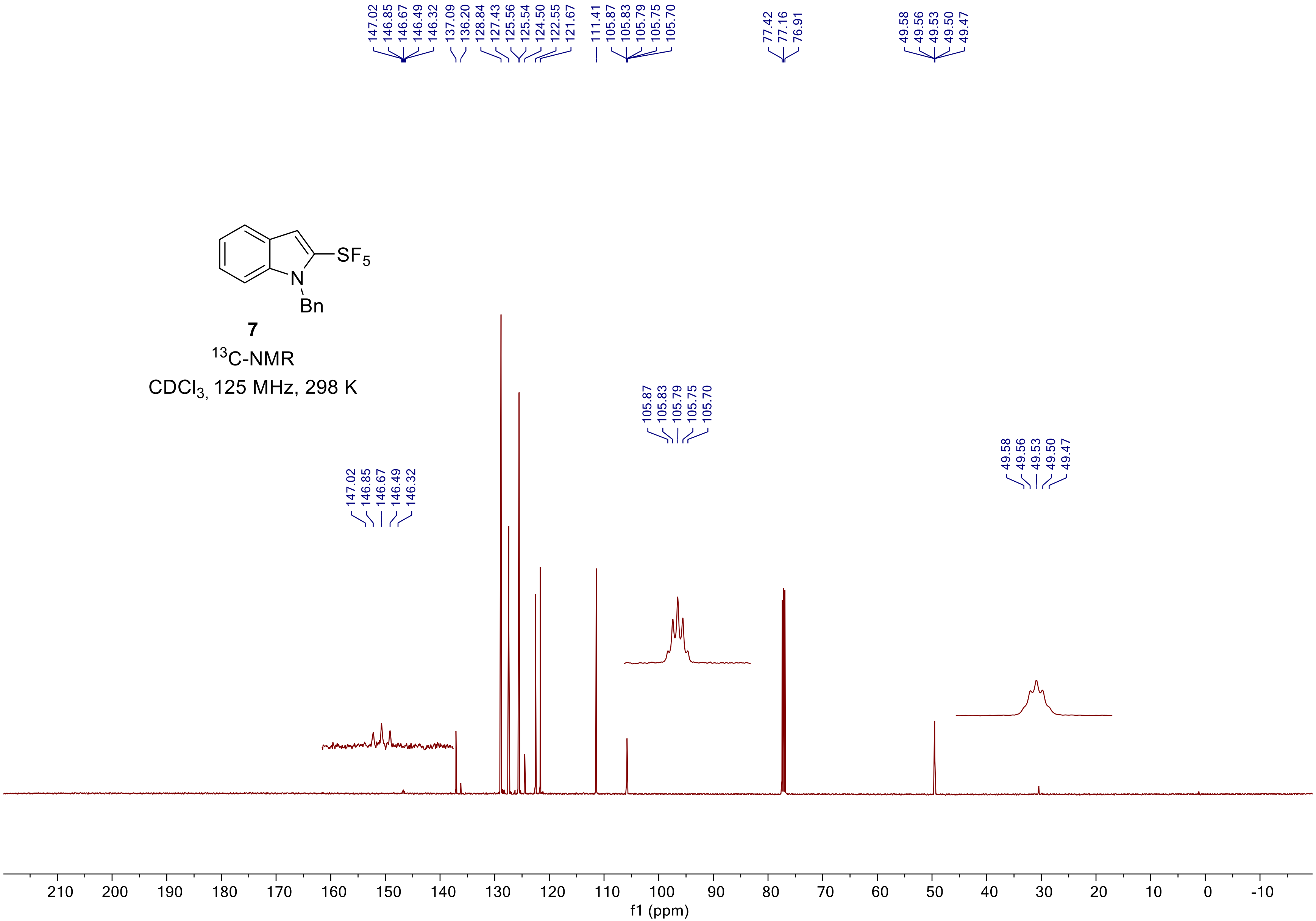


7

^{1}H-NMR

$CDCl_3$, 400 MHz, 298 K

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146.85
146.67
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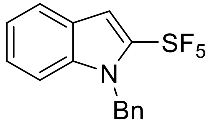
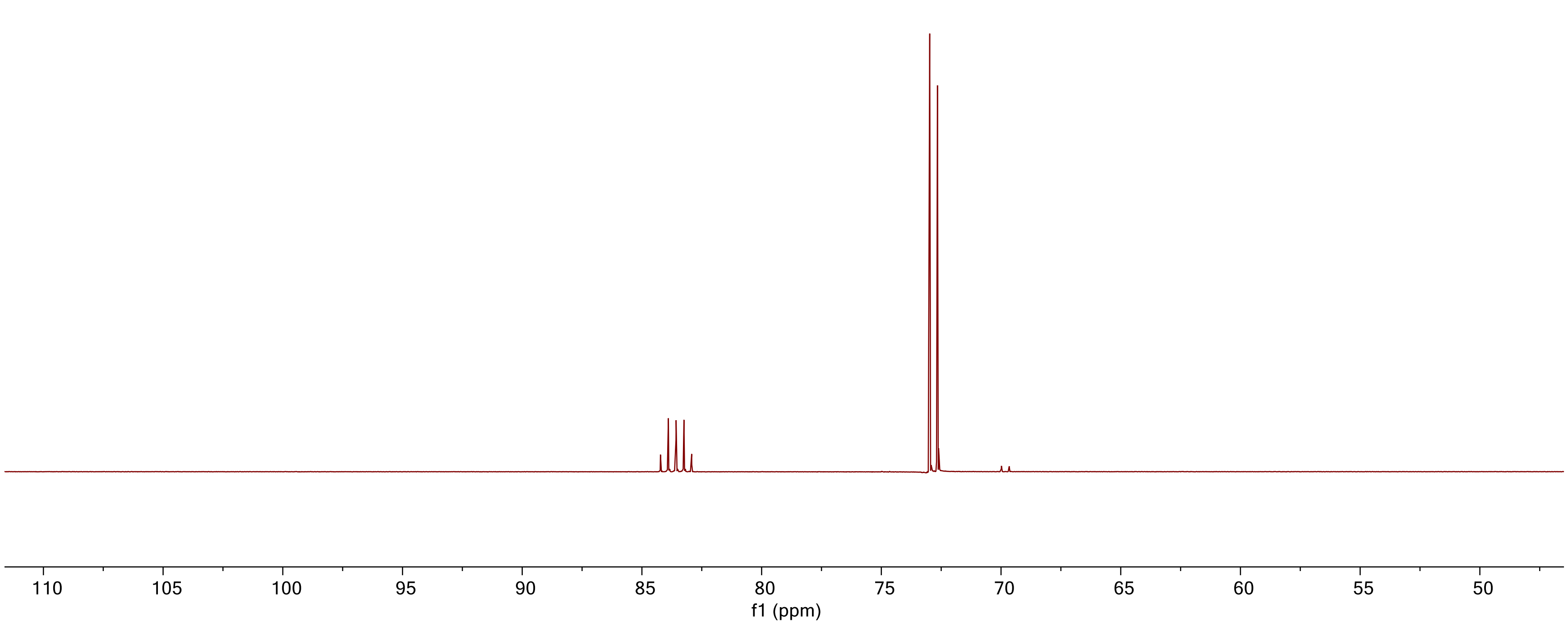
146.32
137.09
136.20
128.84
127.43
125.56
125.54
124.50
122.55
121.67
111.41
105.87
105.83
105.79
105.75
105.70
77.42
77.16
76.91
49.58
49.56
49.53
49.50
49.47
SF5
N
Bn
7
13C-NMR
CDCl3, 125 MHz, 298 K
f1 (ppm)

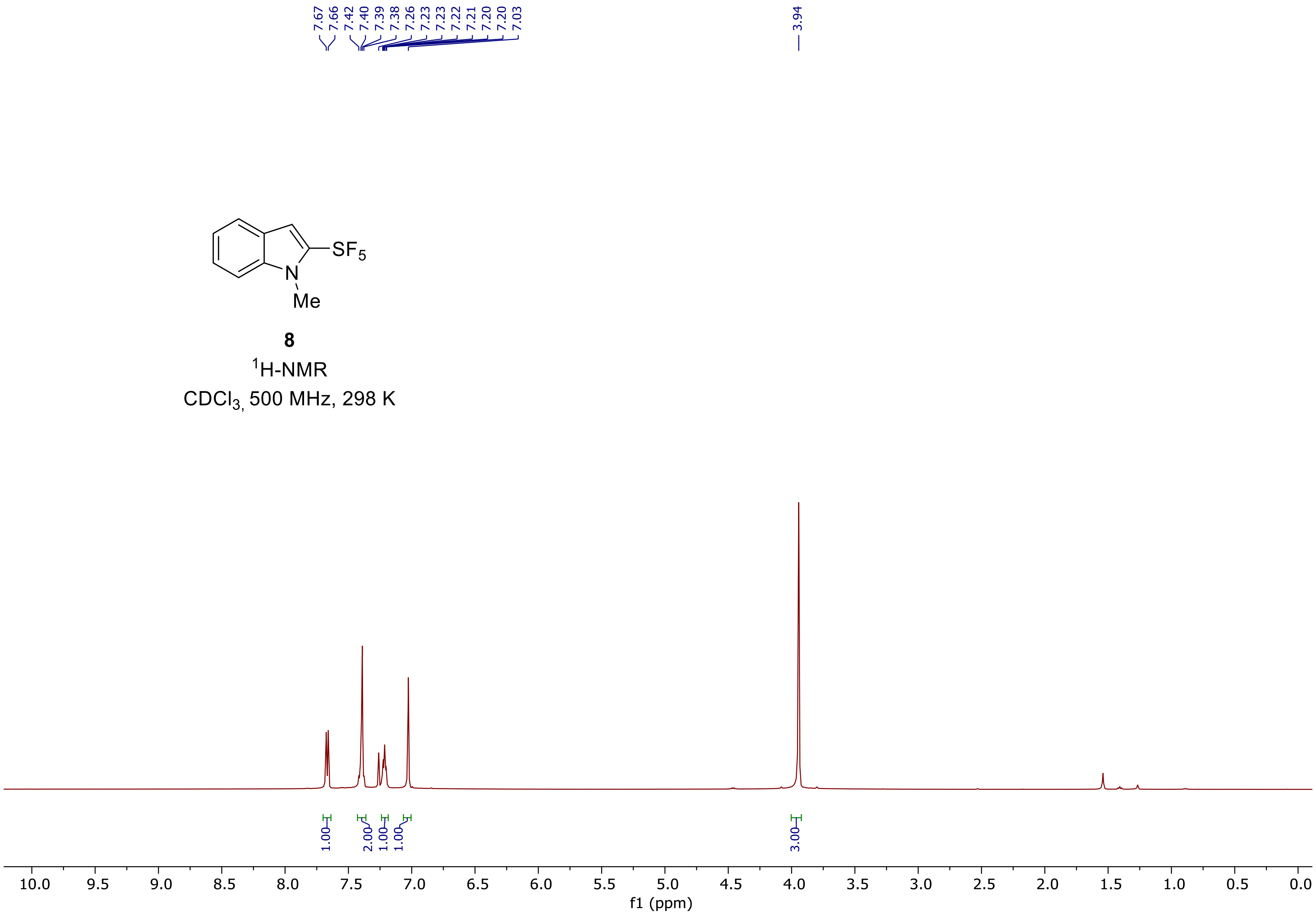


7

^{19}F-NMR

$CDCl_3$, 471 MHz, 298 K

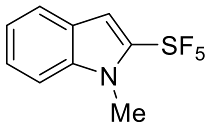




8

^{1}H-NMR

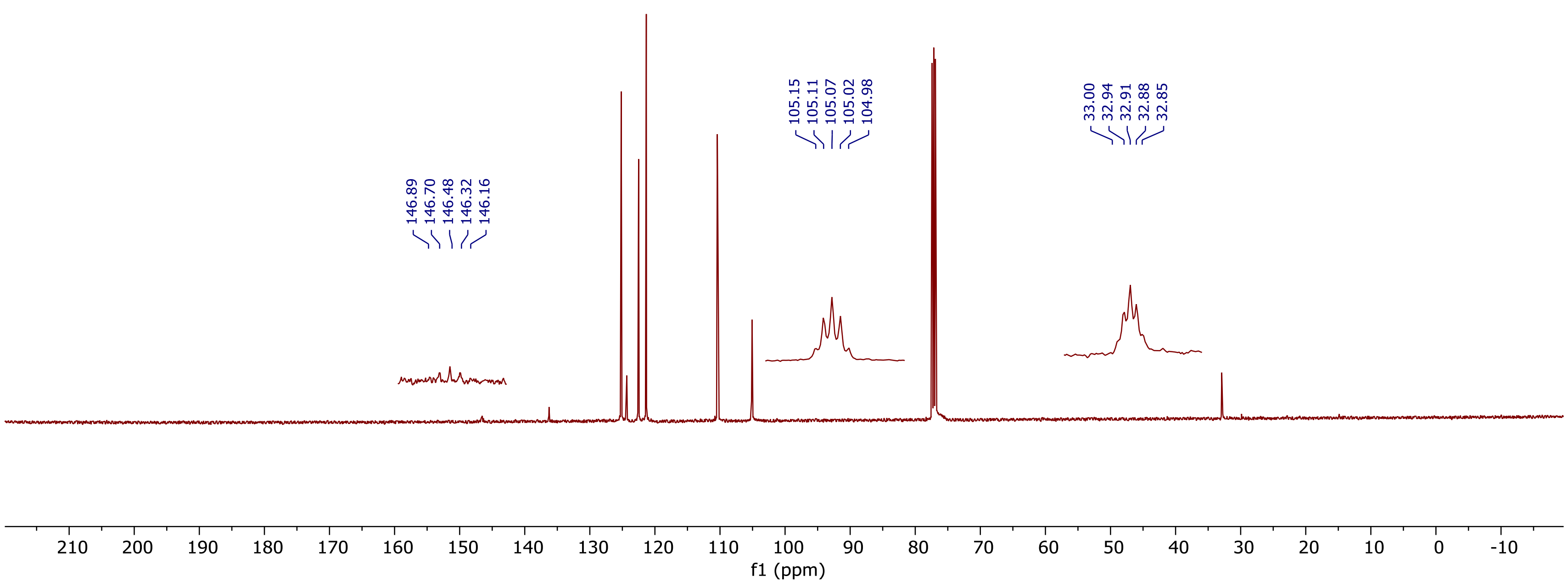
$CDCl_3$, 500 MHz, 298 K

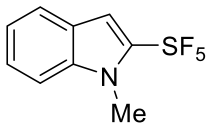


8

^{13}C-NMR

$CDCl_3$, 125 MHz, 298 K

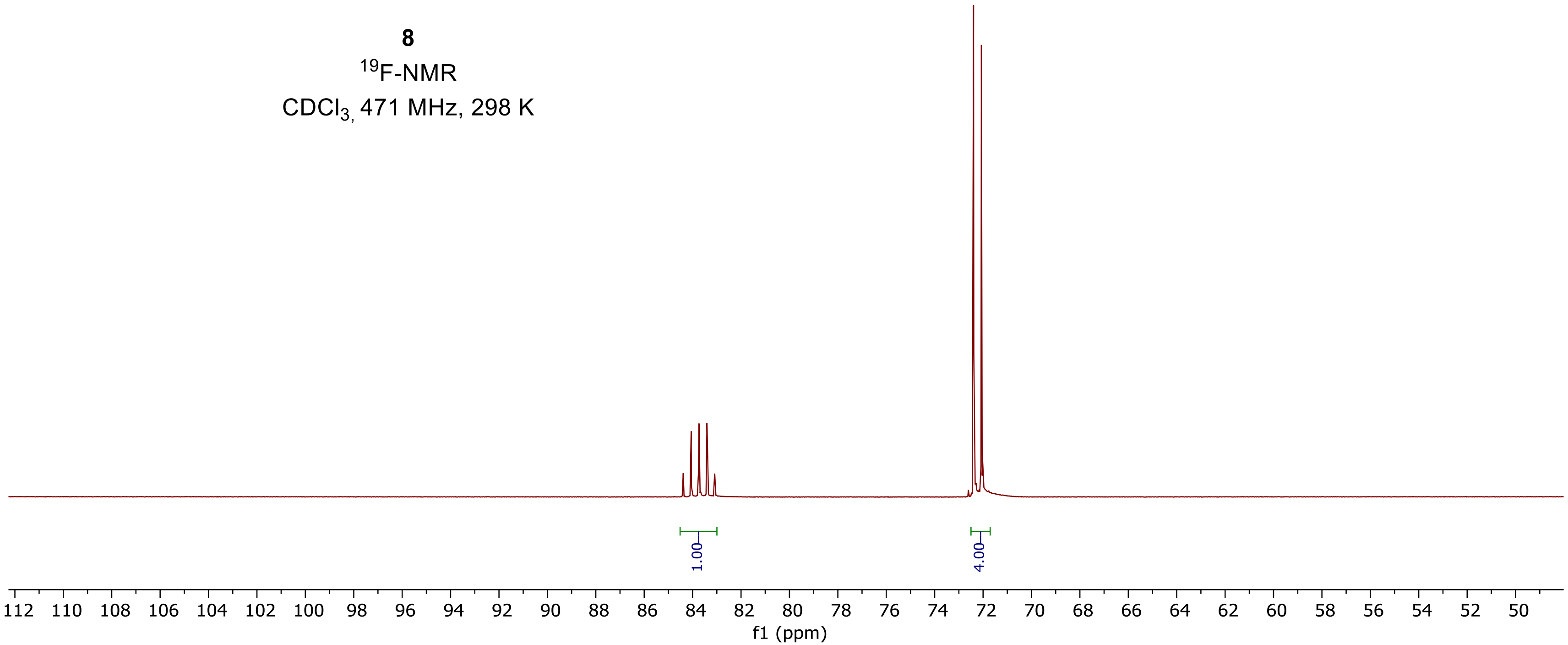


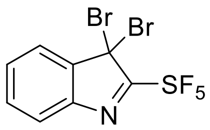


8

^{19}F-NMR

$CDCl_3$, 471 MHz, 298 K

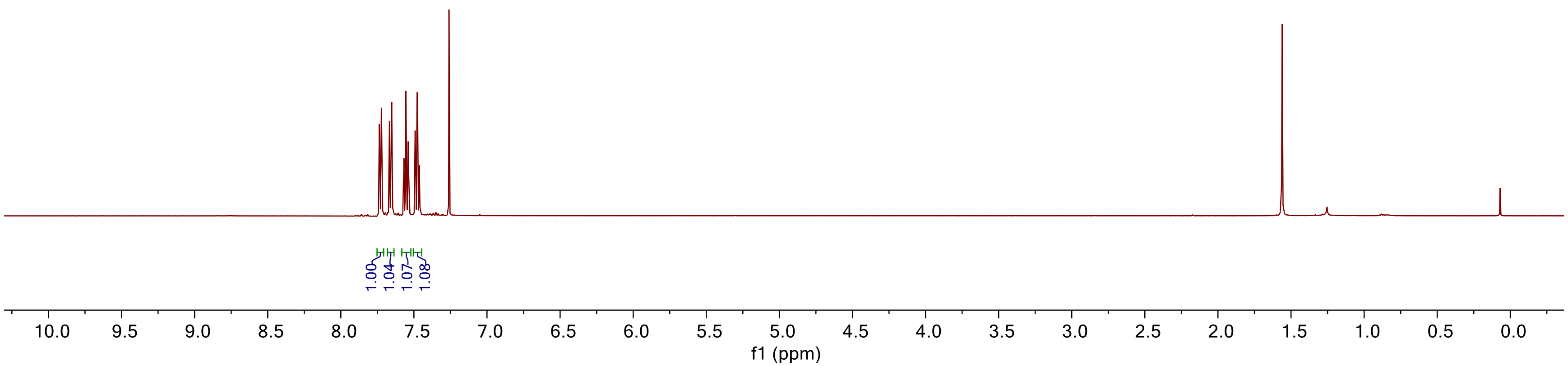


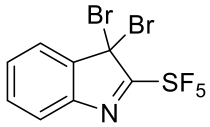


9

^{1}H-NMR

$CDCl_3$, 500 MHz, 298 K

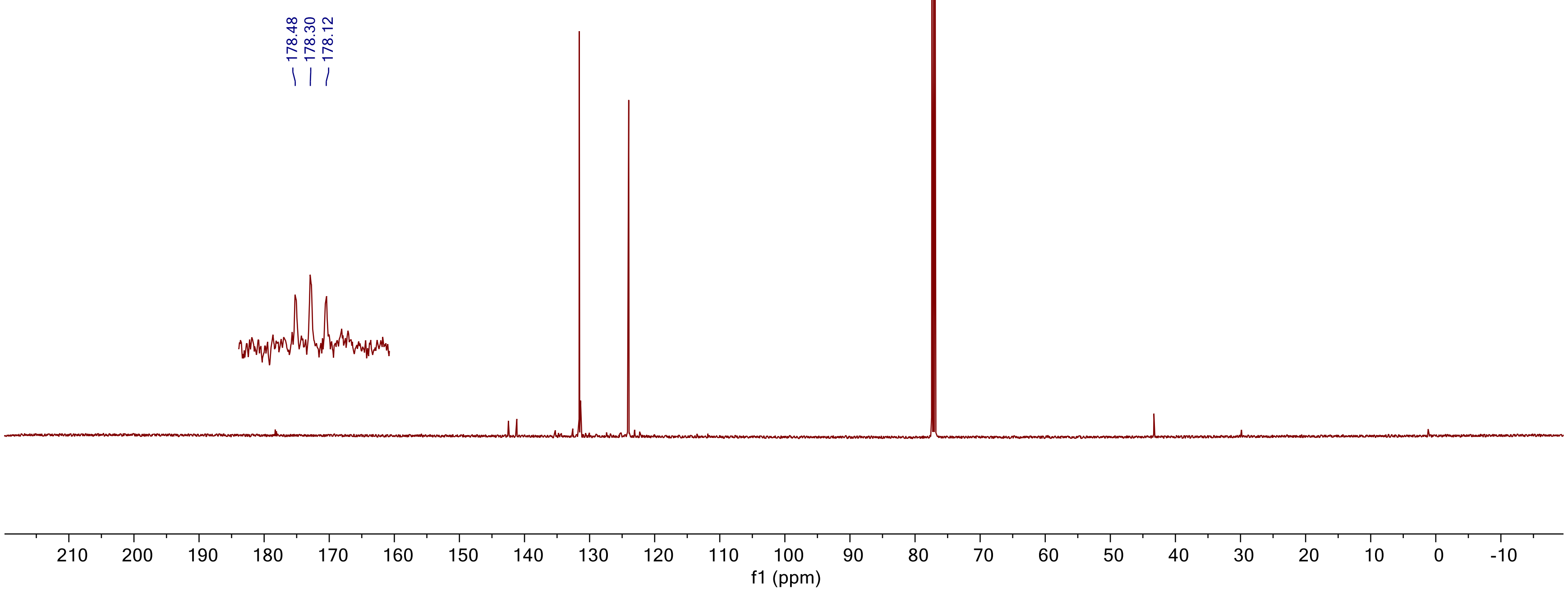


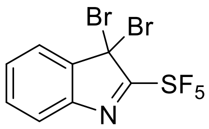


9

^{13}C-NMR

$CDCl_3$, 125 MHz, 298 K

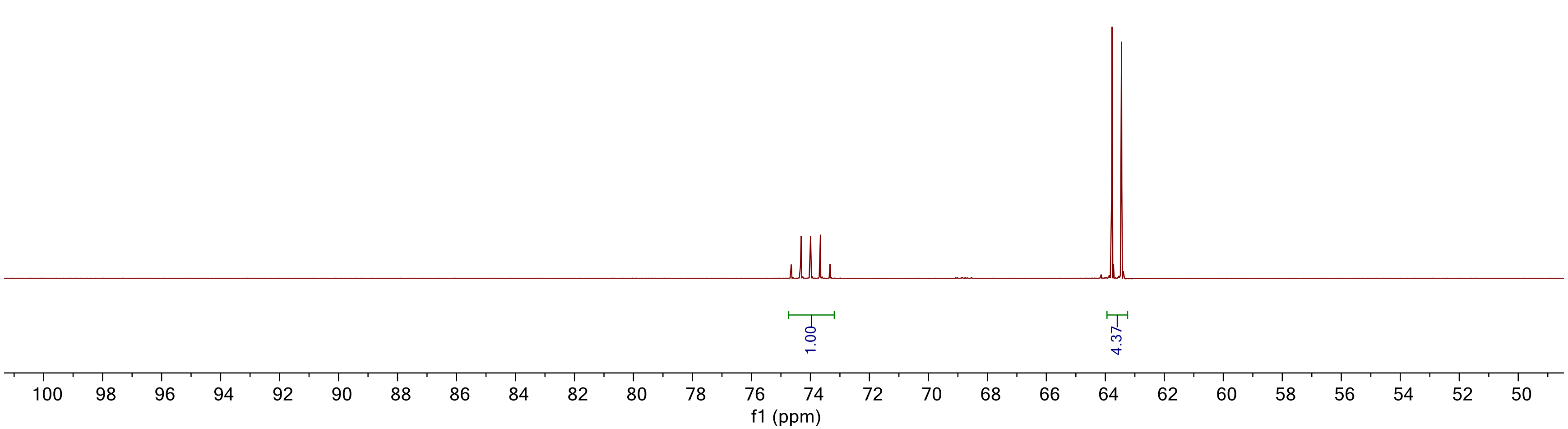


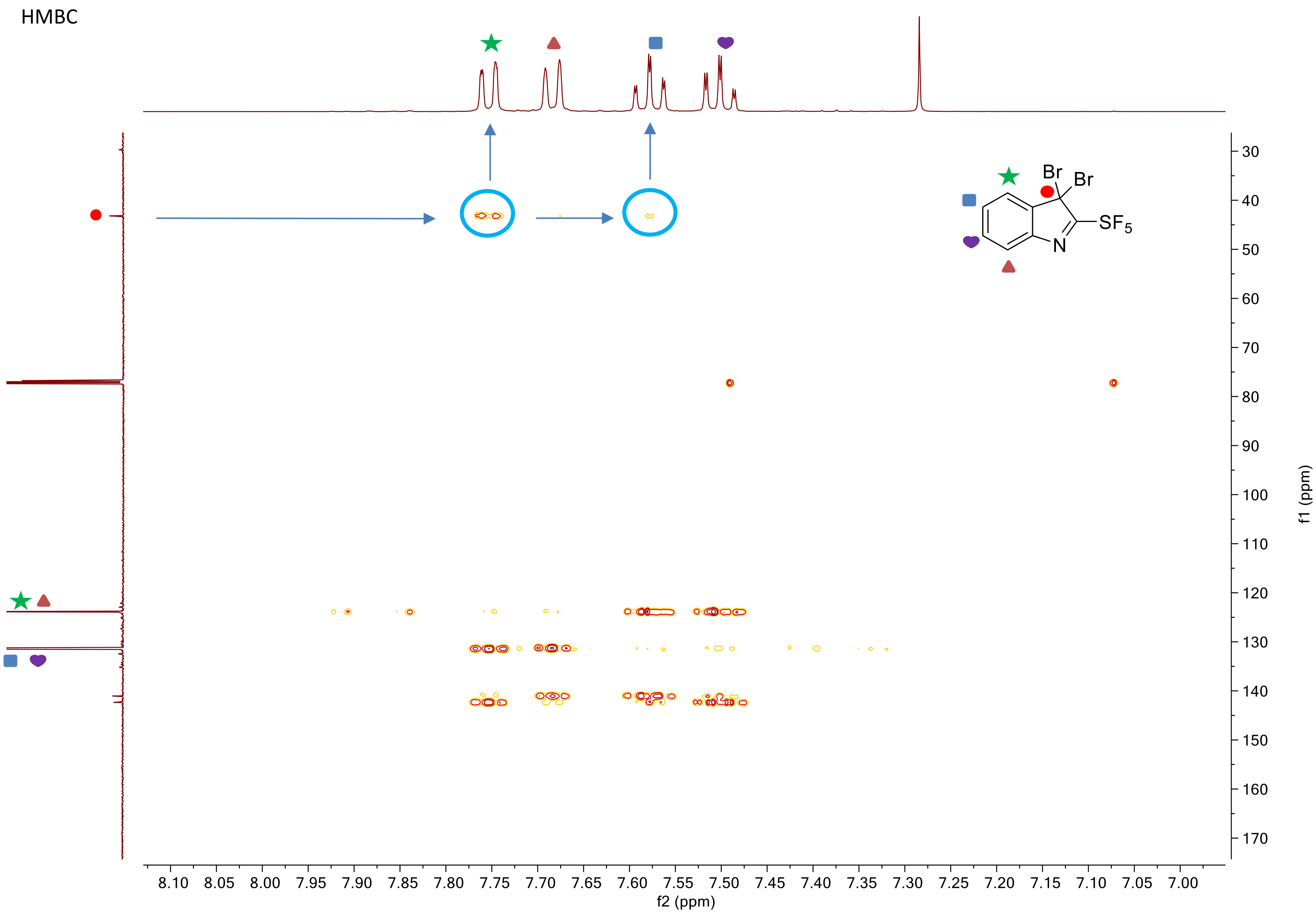


9

^{19}F-NMR

$CDCl_3$, 471 MHz, 298 K





HMBC
Br
Br
SF_5
N
30
40
50
60
70
80
90
100
110
120
130
140
150
160
170
f1 (ppm)
8.10
8.05
8.00
7.95
7.90
7.85
7.80
7.75
7.70
7.65
7.60
7.55
7.50
7.45
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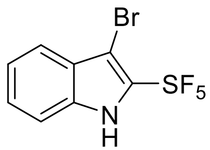
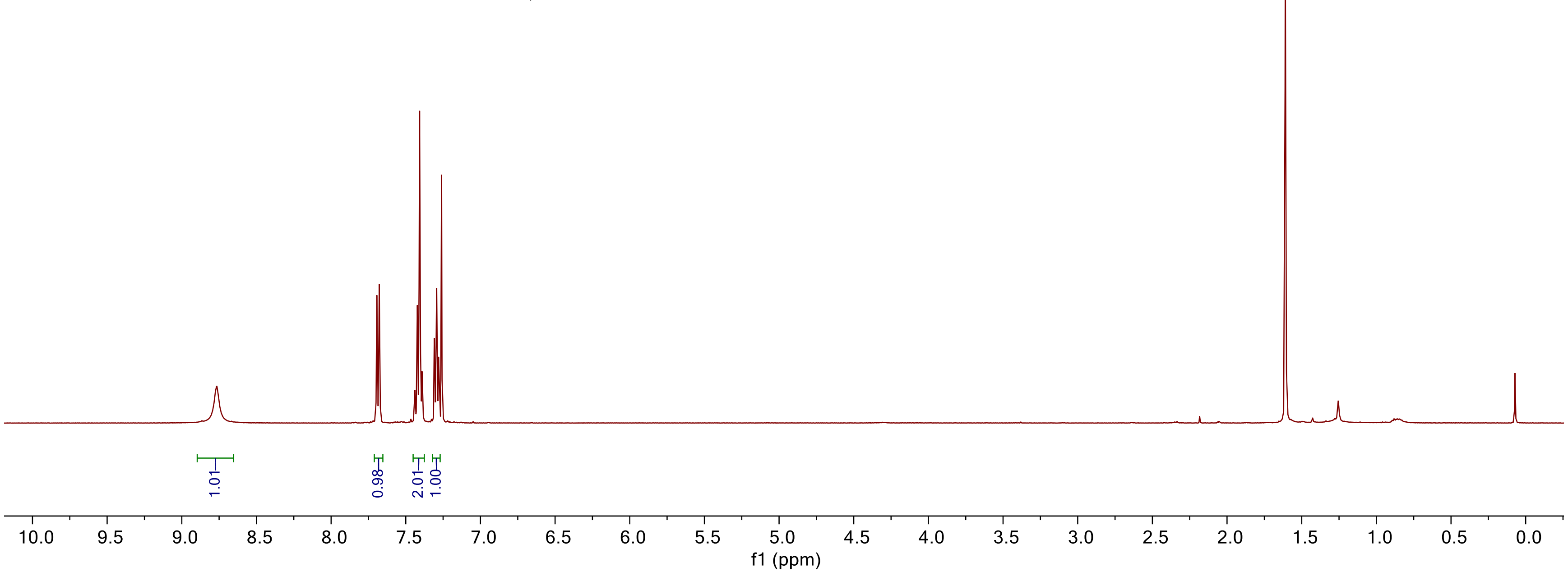
7.35
7.30
7.25
7.20
7.15
7.10
7.05
7.00
f2 (ppm)

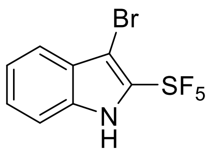


10

^{1}H-NMR

$CDCl_3$, 500 MHz, 298 K

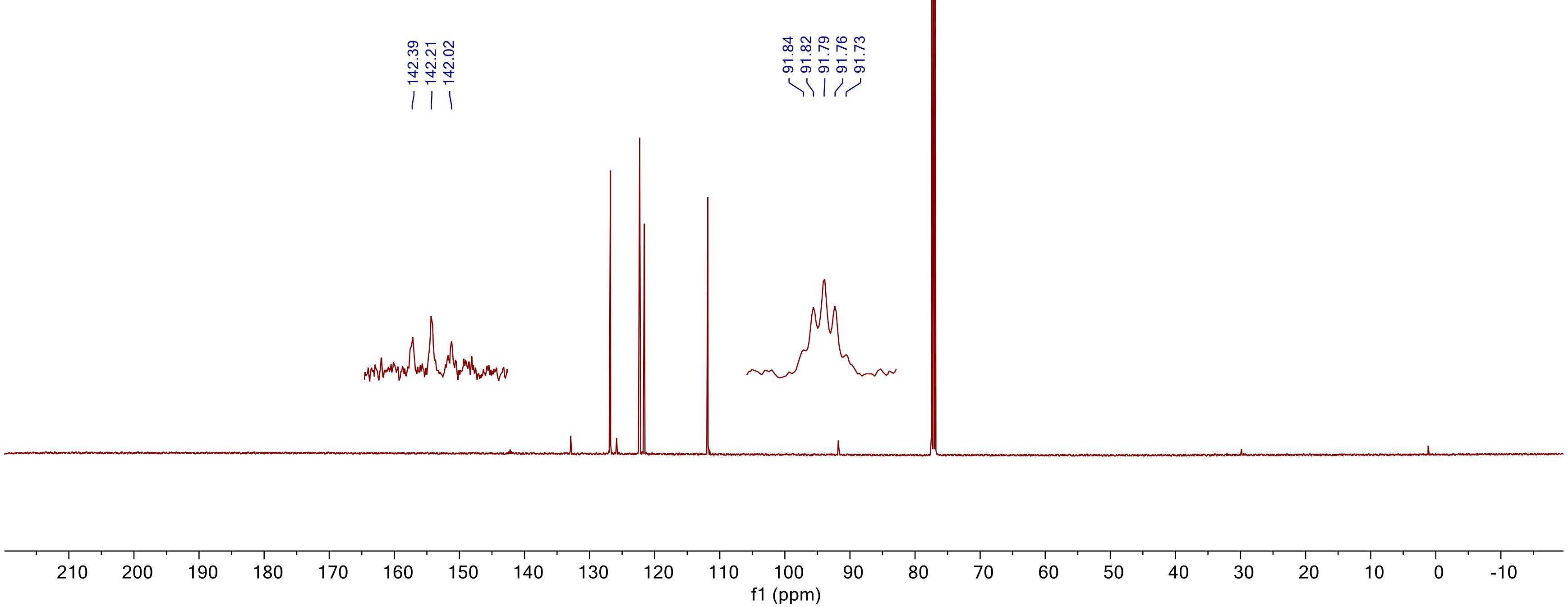


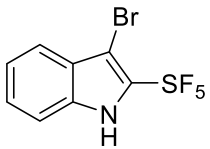


10

^{13}C-NMR

$CDCl_3$, 125 MHz, 298 K

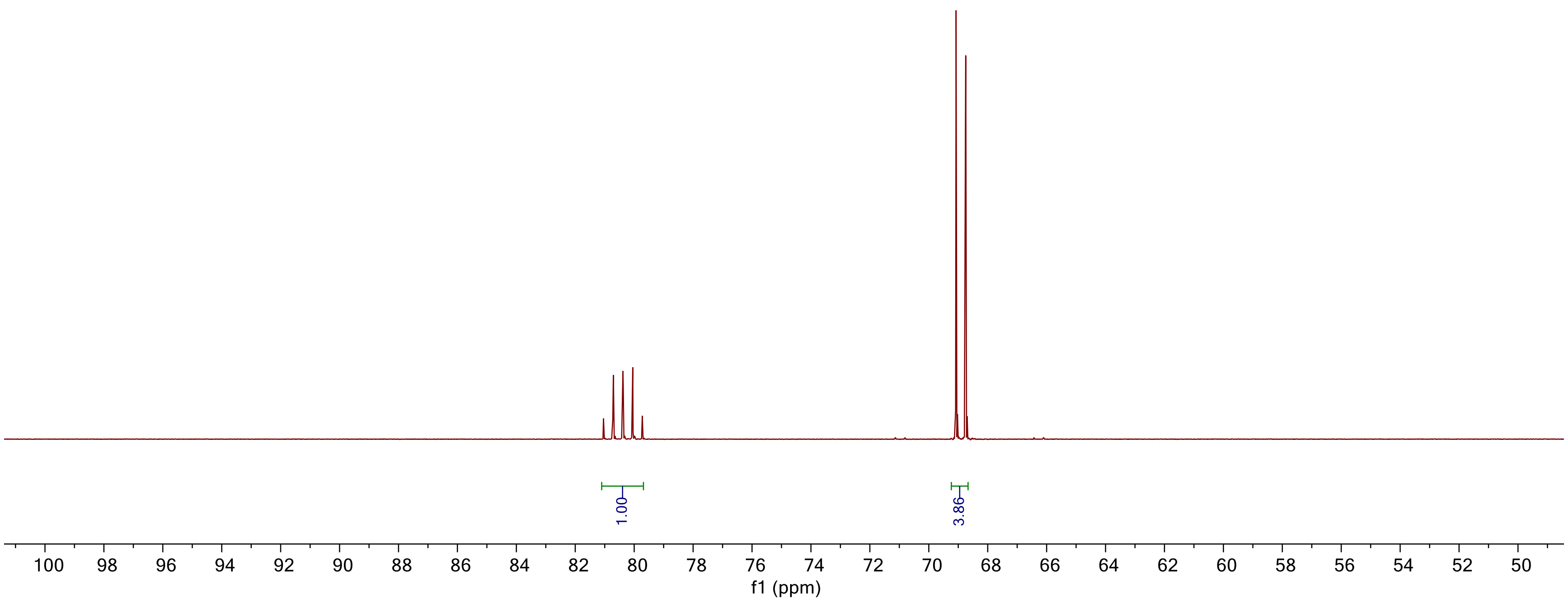


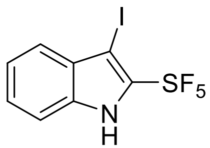


10

^{19}F-NMR

$CDCl_3$, 471 MHz, 298 K

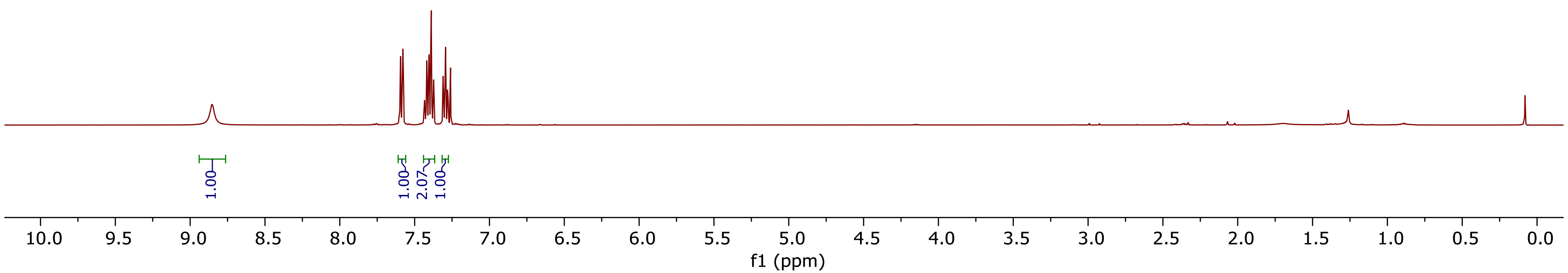


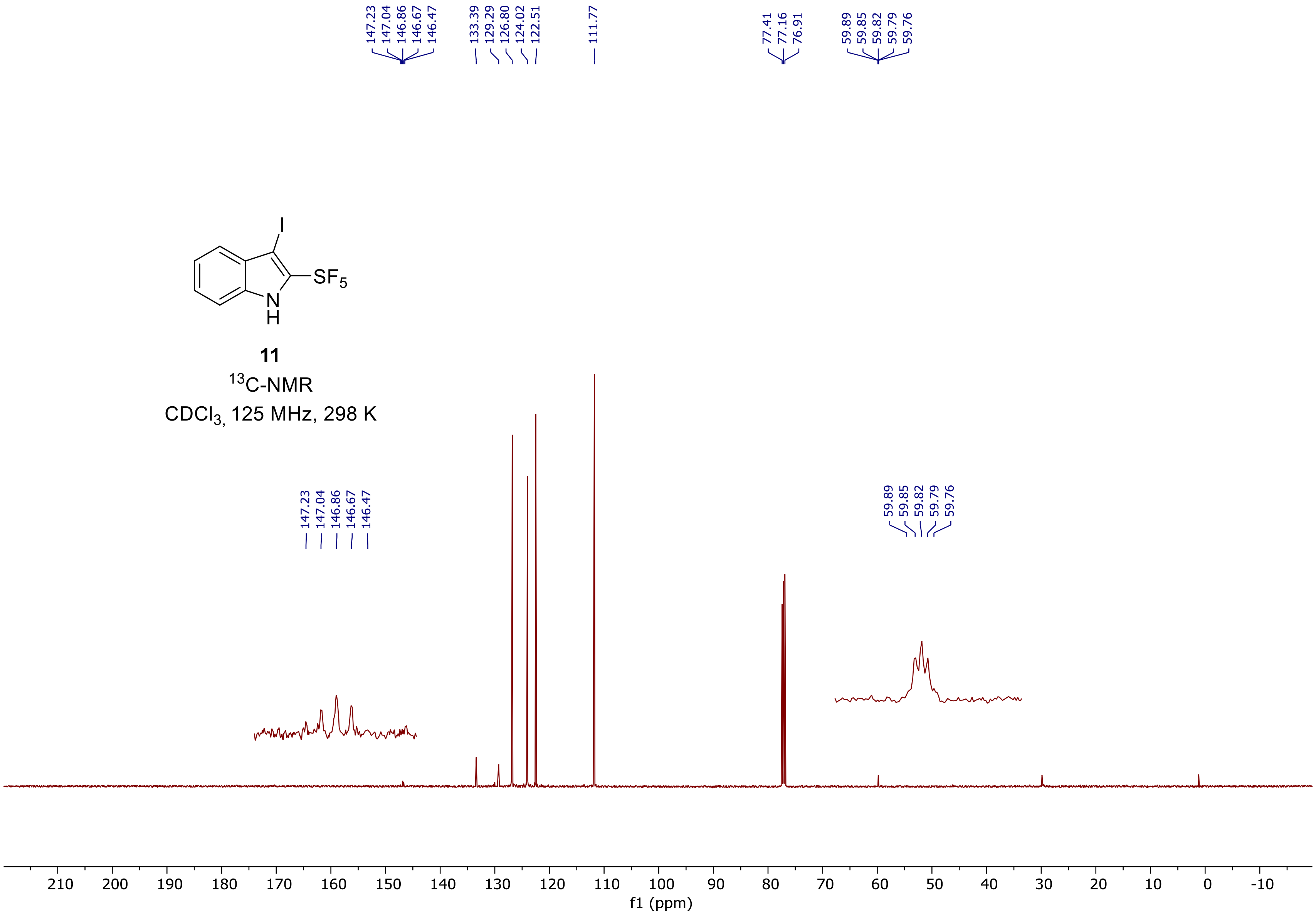


11

^{1}H-NMR

$CDCl_3$, 500 MHz, 298 K





147.23
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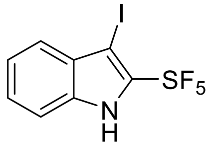
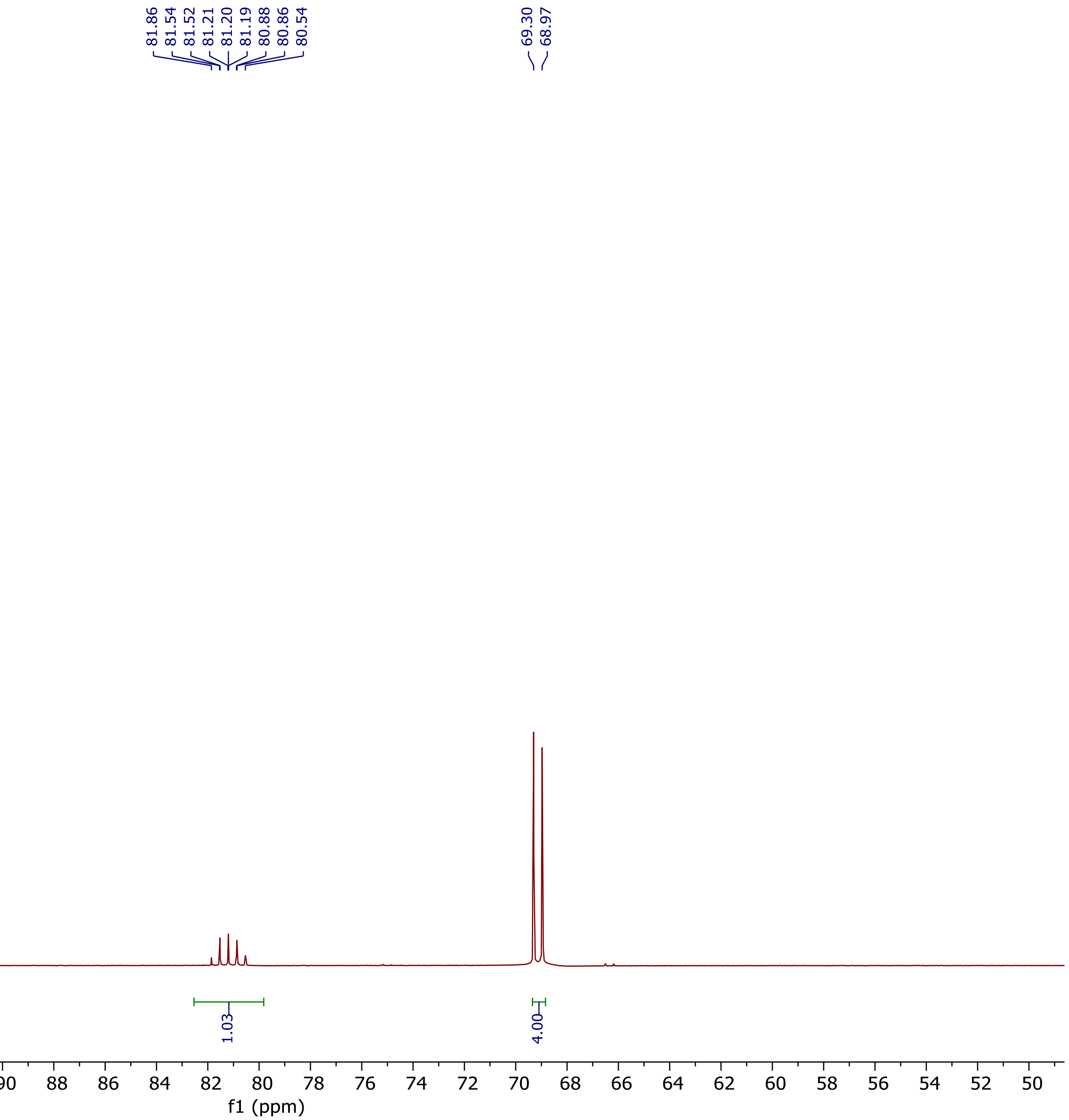
133.39
129.29
126.80
124.02
122.51
111.77
77.41
77.16
76.91
59.89
59.85
59.82
59.79
59.76
I
SF5
N
H
11
13C-NMR
CDCl3, 125 MHz, 298 K
f1 (ppm)

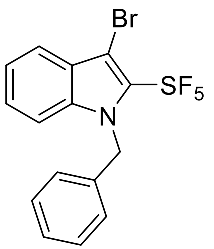


11

^{19}F-NMR

$CDCl_3$, 471 MHz, 298 K

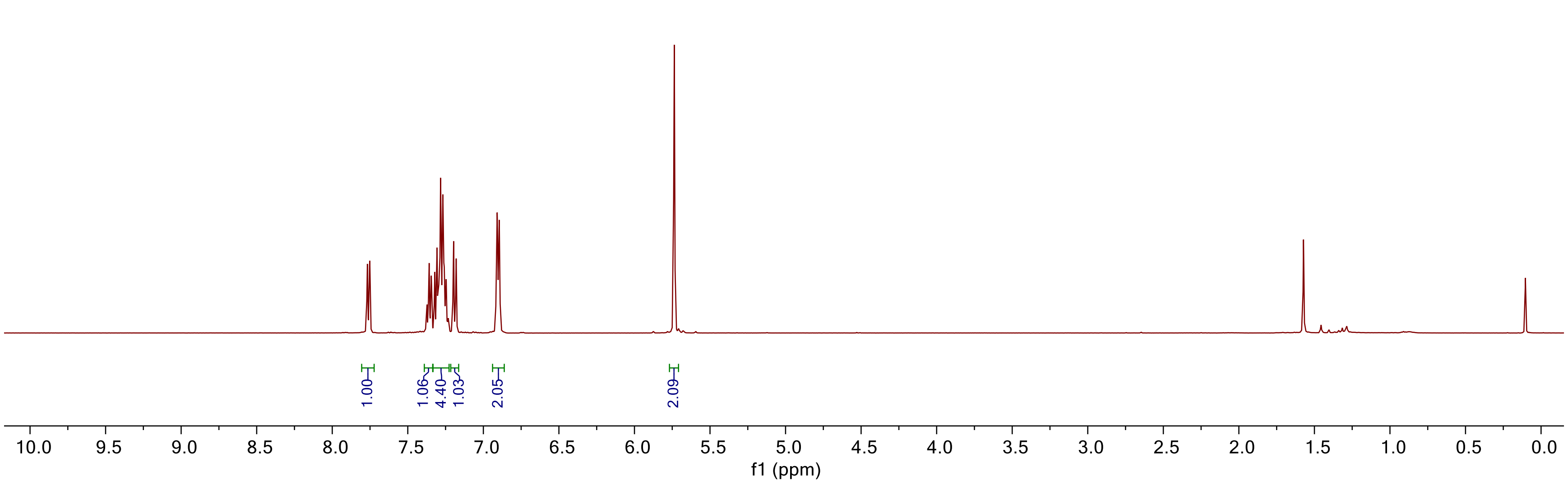


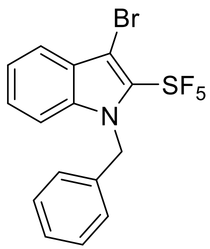


12

^{1}H-NMR

$CDCl_3$, 500 MHz, 298 K

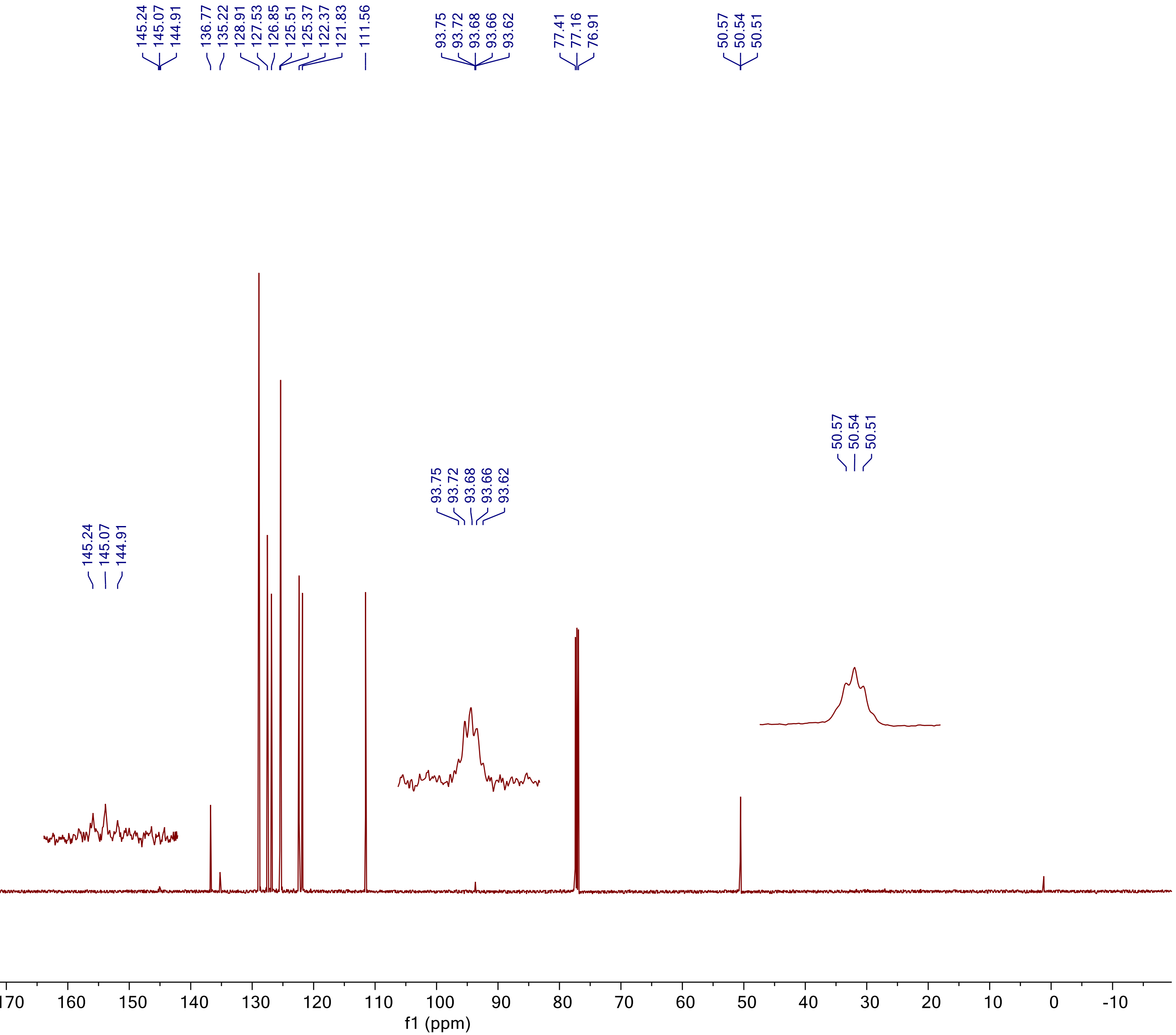


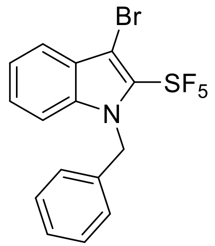


12

^{13}C-NMR

$CDCl_3$, 125 MHz, 298 K

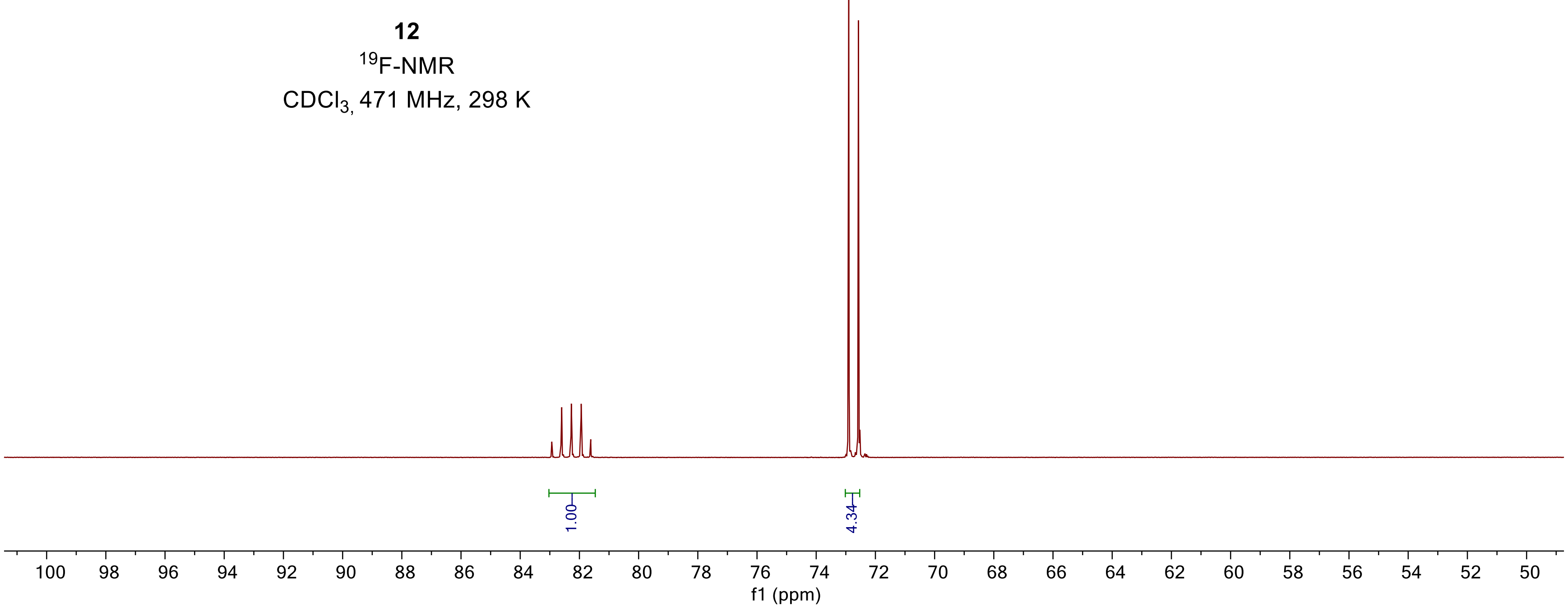


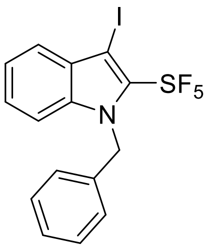


12

^{19}F-NMR

$CDCl_3$, 471 MHz, 298 K

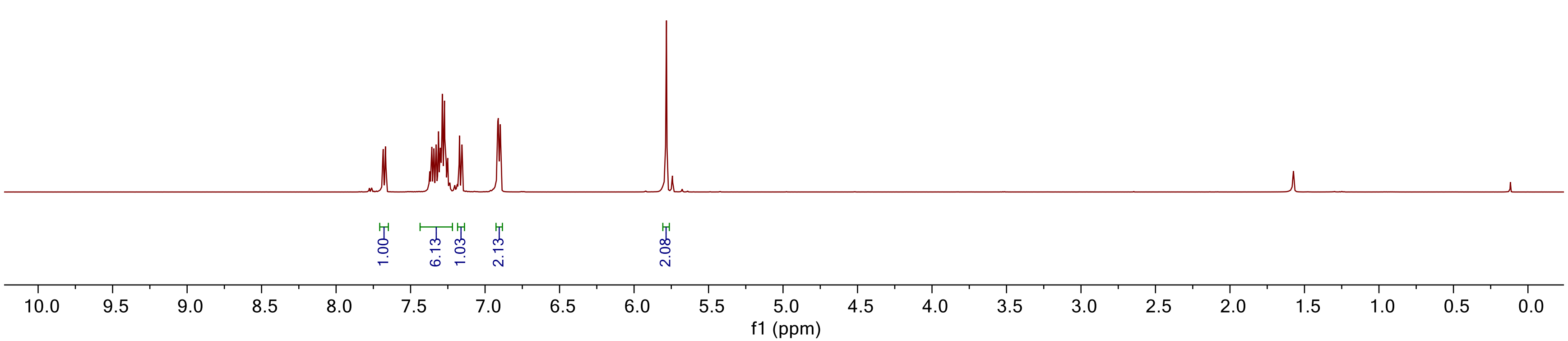


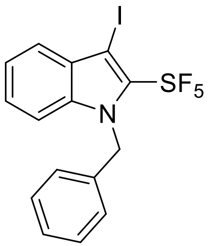


13

^{1}H-NMR

$CDCl_3$, 500 MHz, 298 K

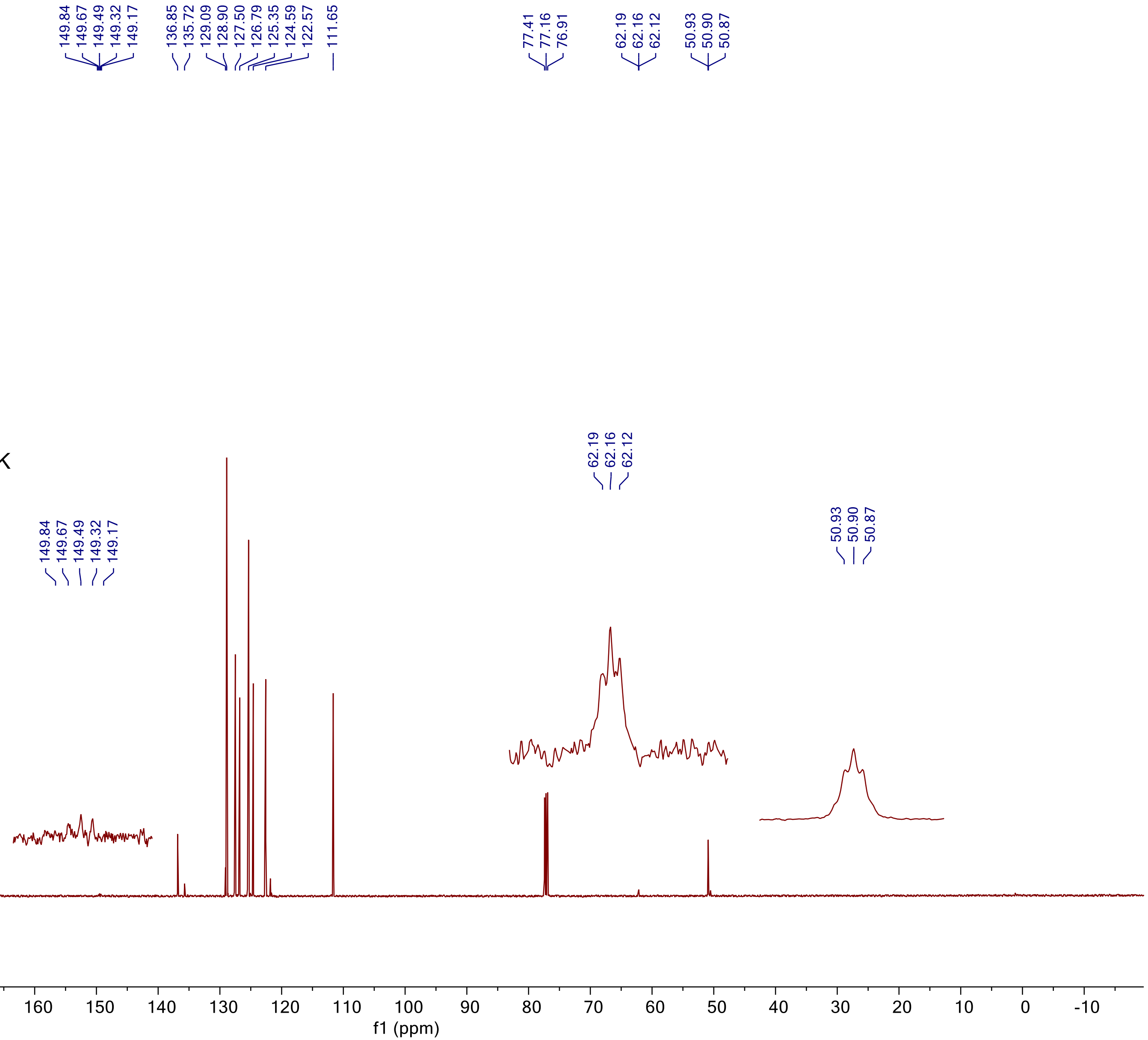


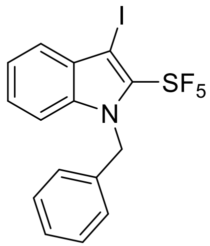


13

^{13}C-NMR

$CDCl_3$, 125 MHz, 298 K

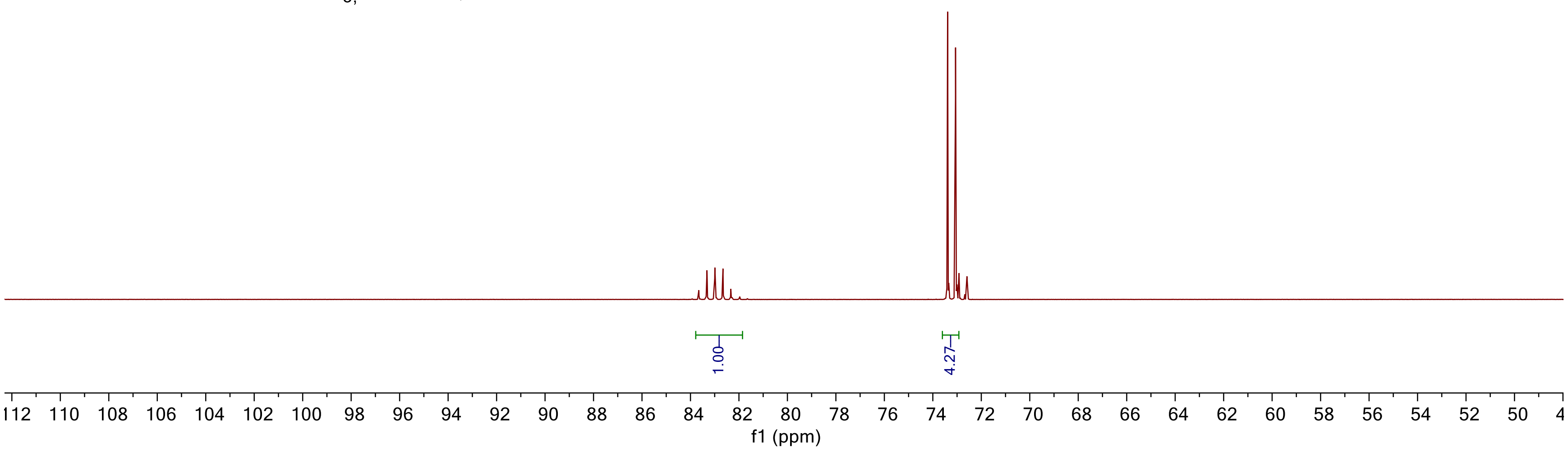


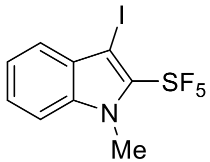


13

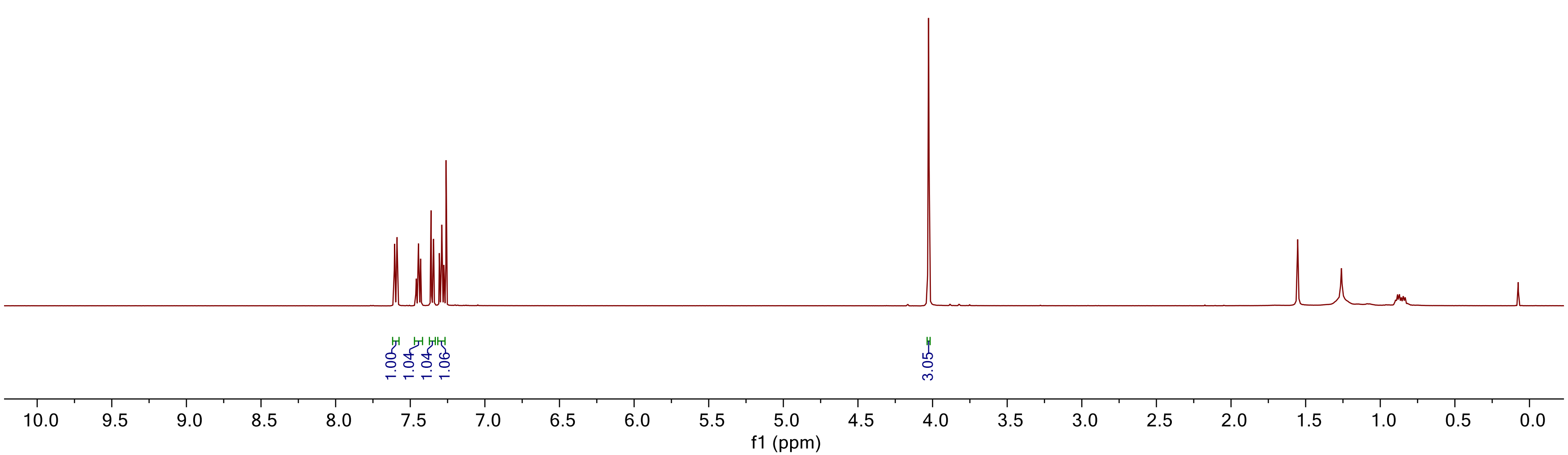
^{19}F-NMR

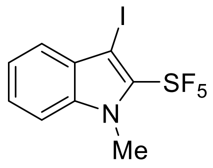
$CDCl_3$, 471 MHz, 298 K





14
^{1}H-NMR
$CDCl_3$, 500 MHz, 298 K

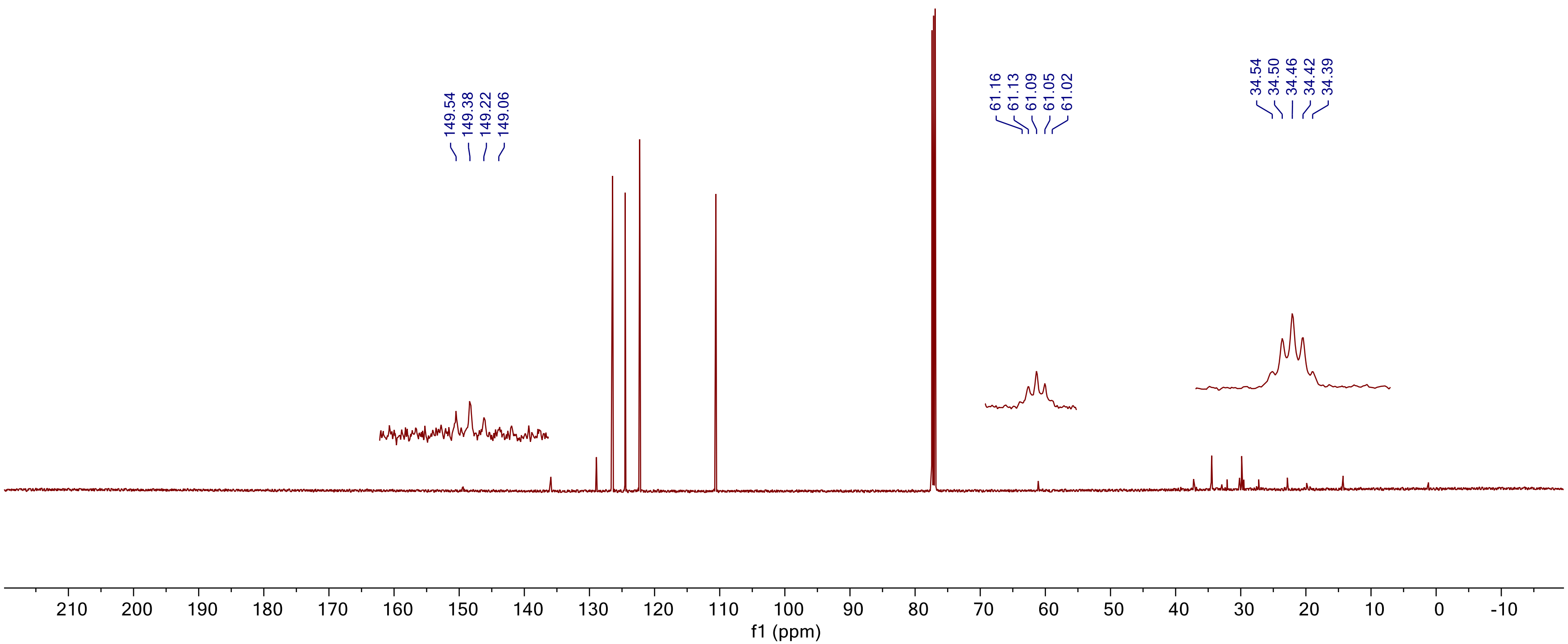


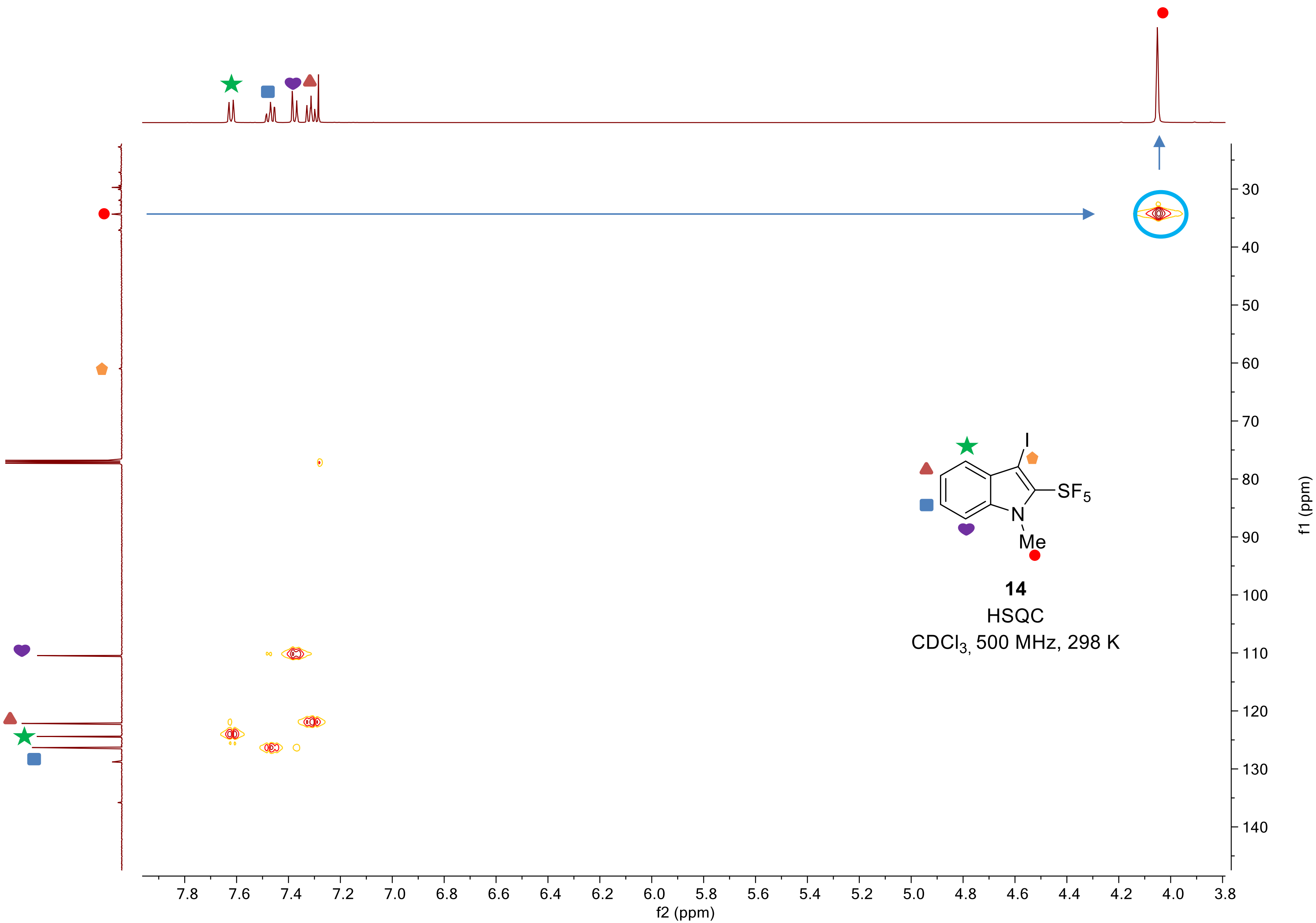


14

^{13}C-NMR

$CDCl_3$, 125 MHz, 298 K




I
SF5
N
Me
14
HSQC
CDCl3, 500 MHz, 298 K
f2 (ppm)
f1 (ppm)
7.8
7.6
7.4
7.2
7.0
6.8
6.6
6.4
6.2
6.0
5.8
5.6
5.4
5.2
5.0
4.8
4.6
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4.0
3.8
30
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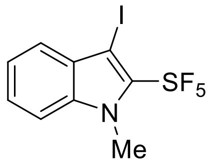
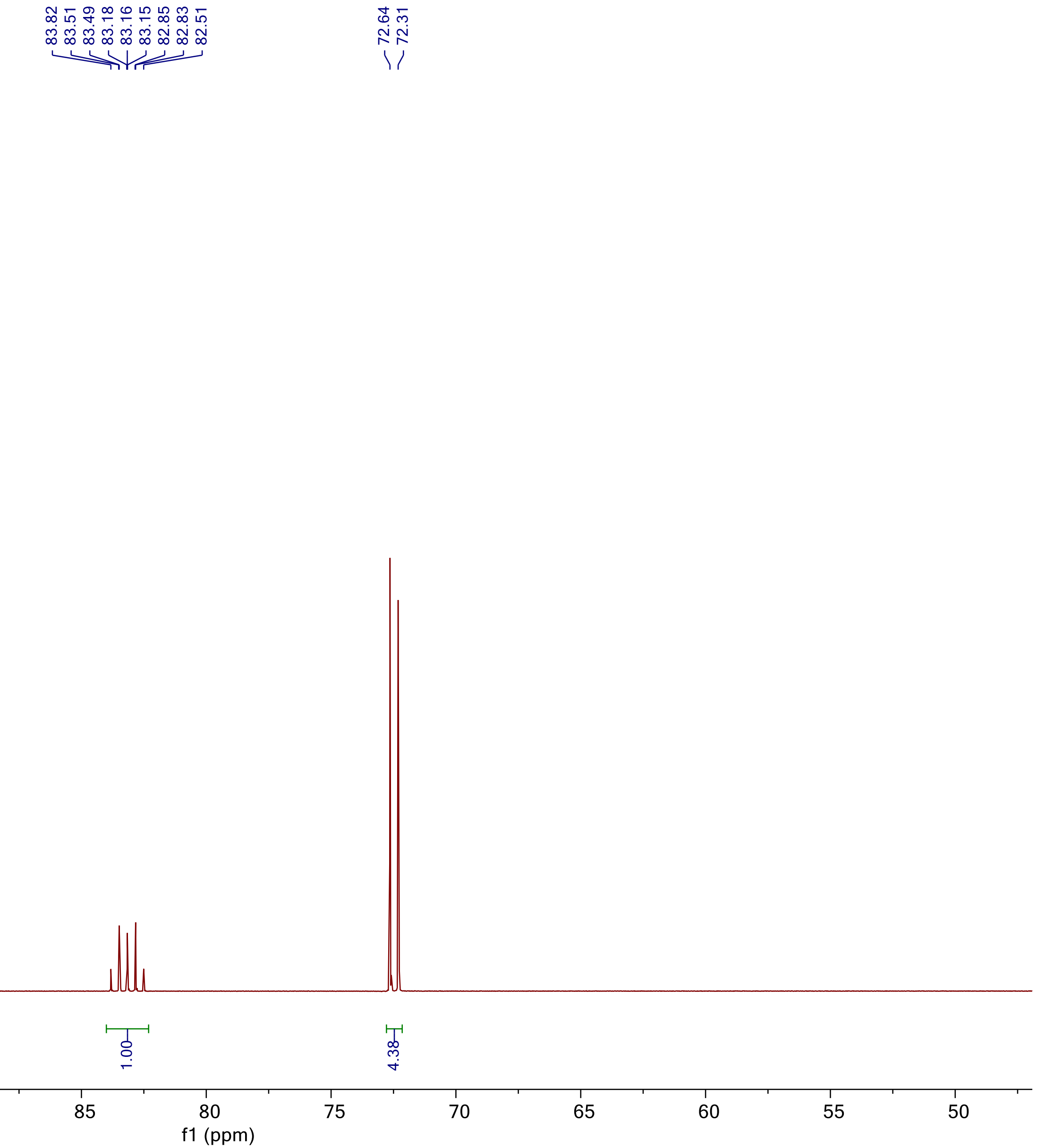
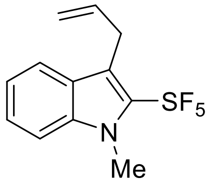


14

^{19}F-NMR

$CDCl_3$, 471 MHz, 298 K

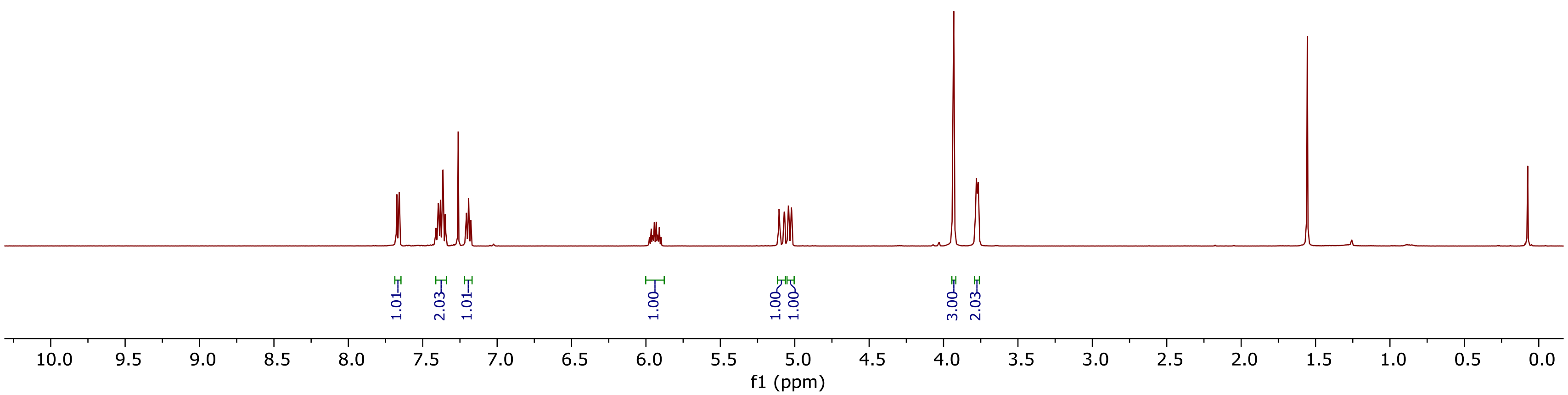


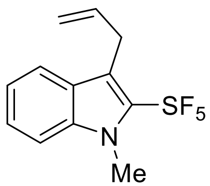


15

^{1}H-NMR

$CDCl_3$, 500 MHz, 298 K

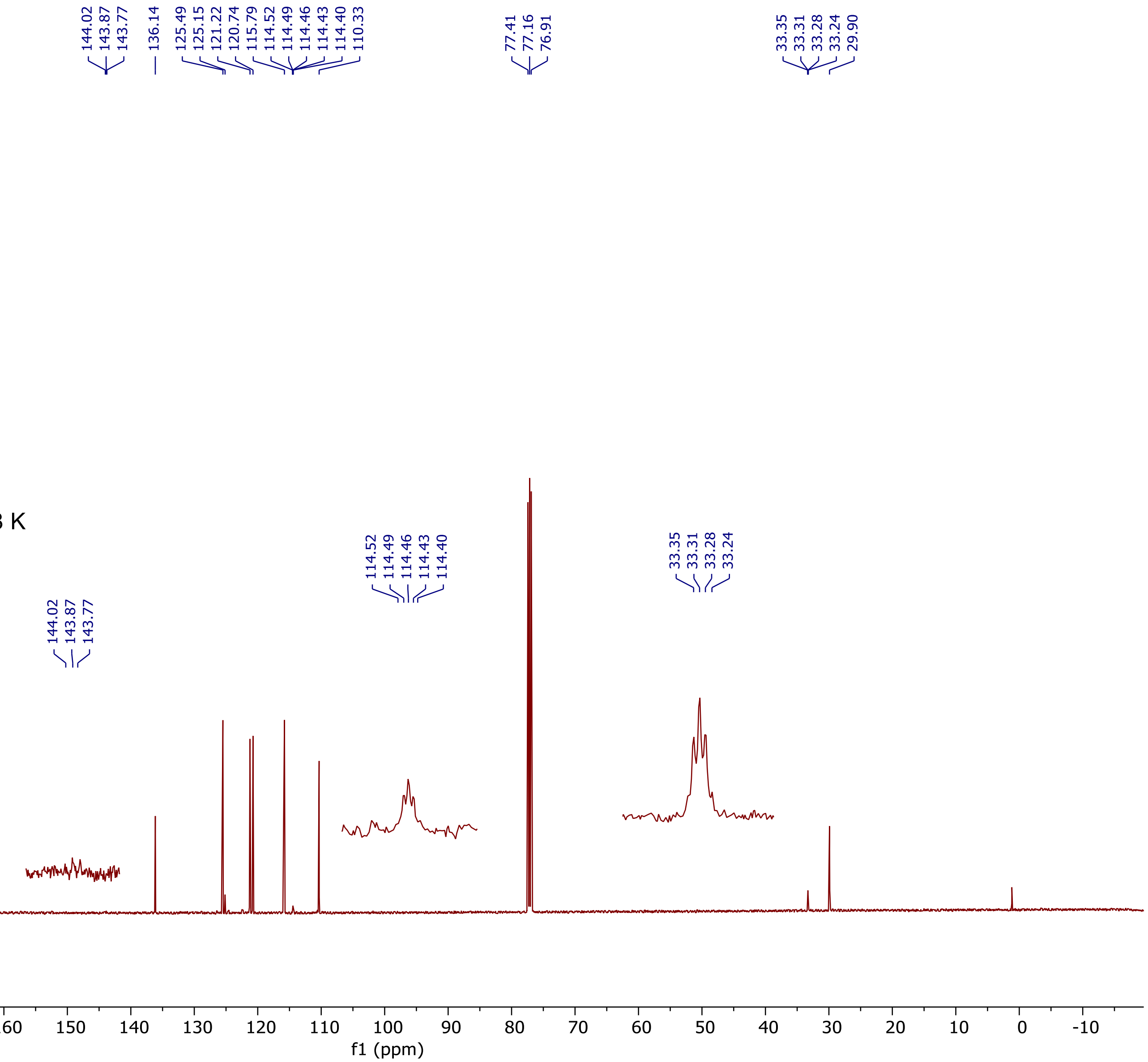


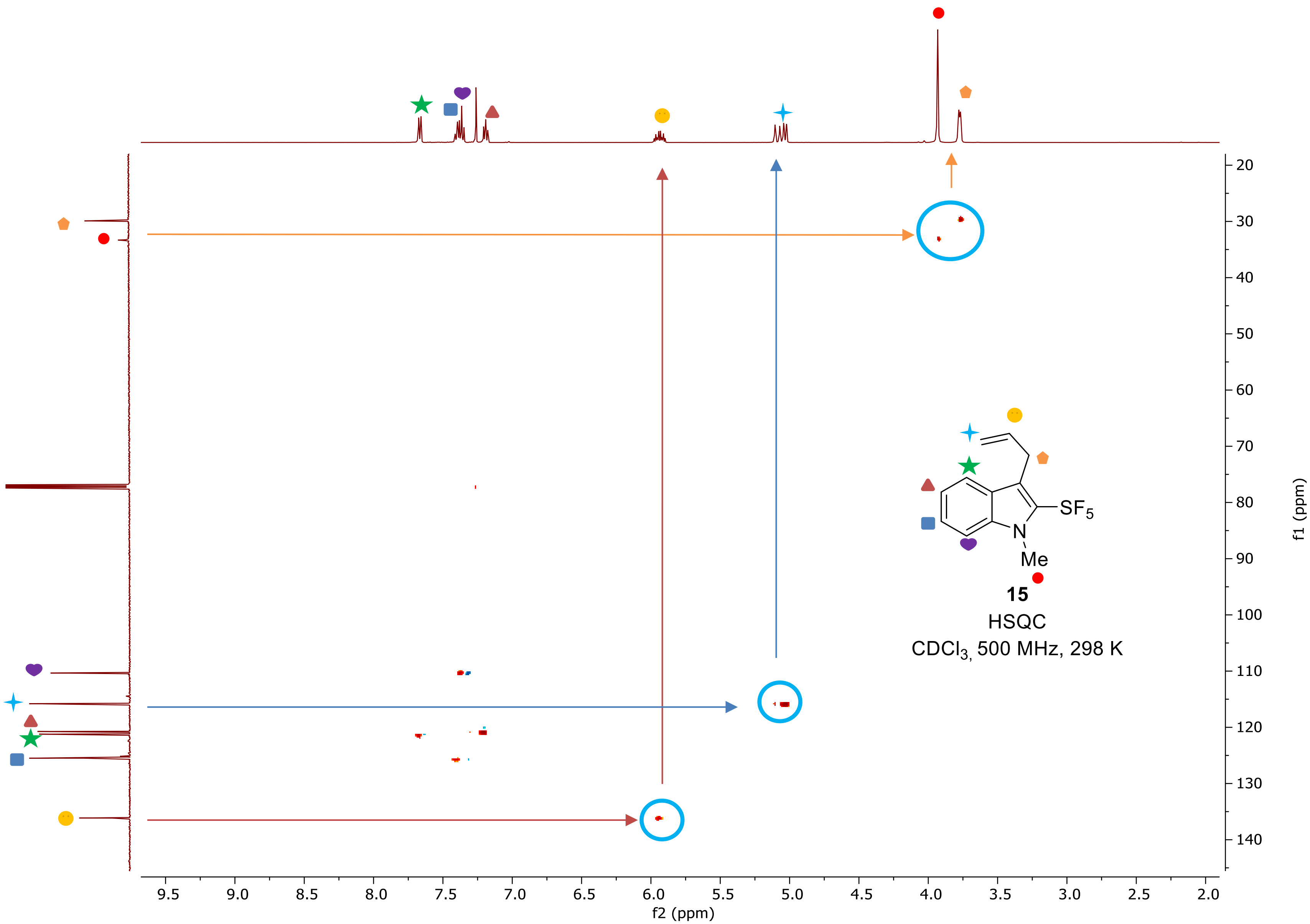


15

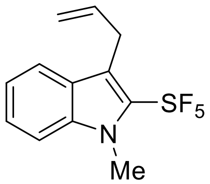
^{13}C-NMR

$CDCl_3$, 125 MHz, 298 K





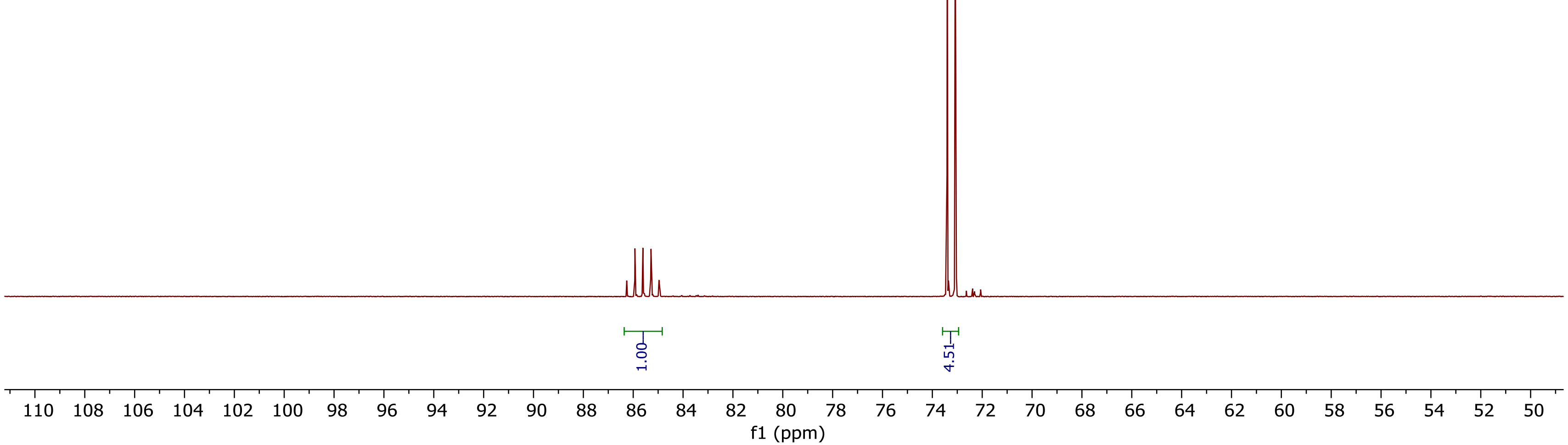
SF5
N
Me
15
HSQC
CDCl3, 500 MHz, 298 K
f2 (ppm)
f1 (ppm)

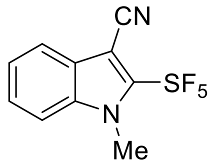


15

^{19}F-NMR

$CDCl_3$, 471 MHz, 298 K

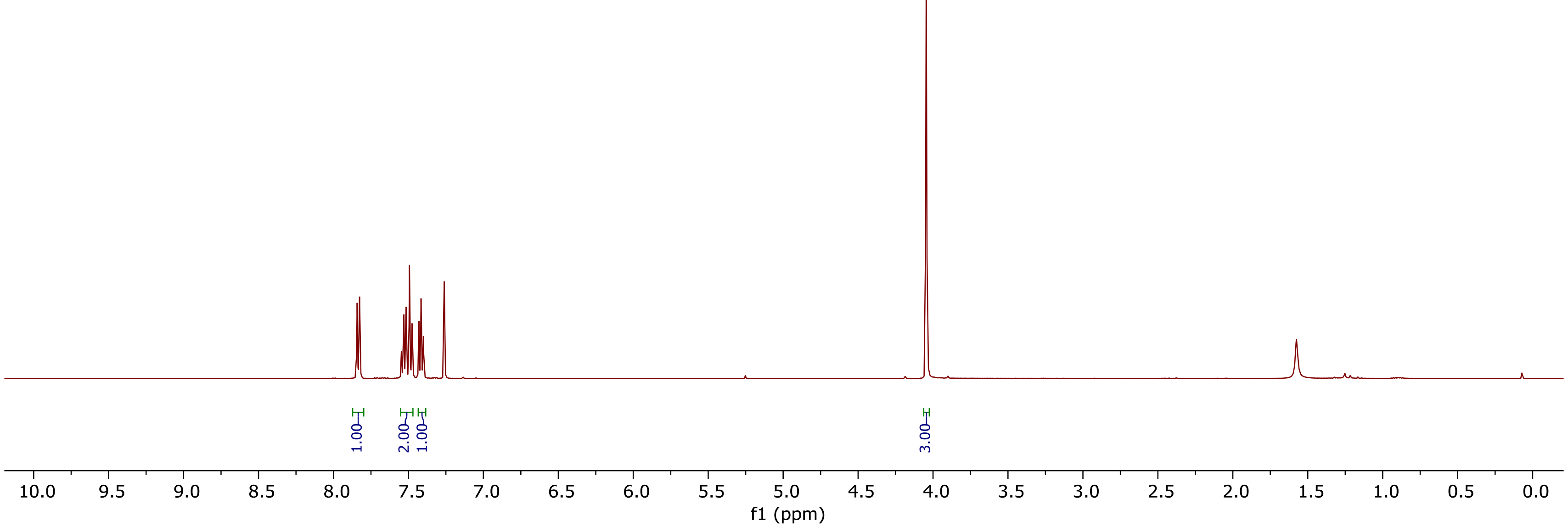


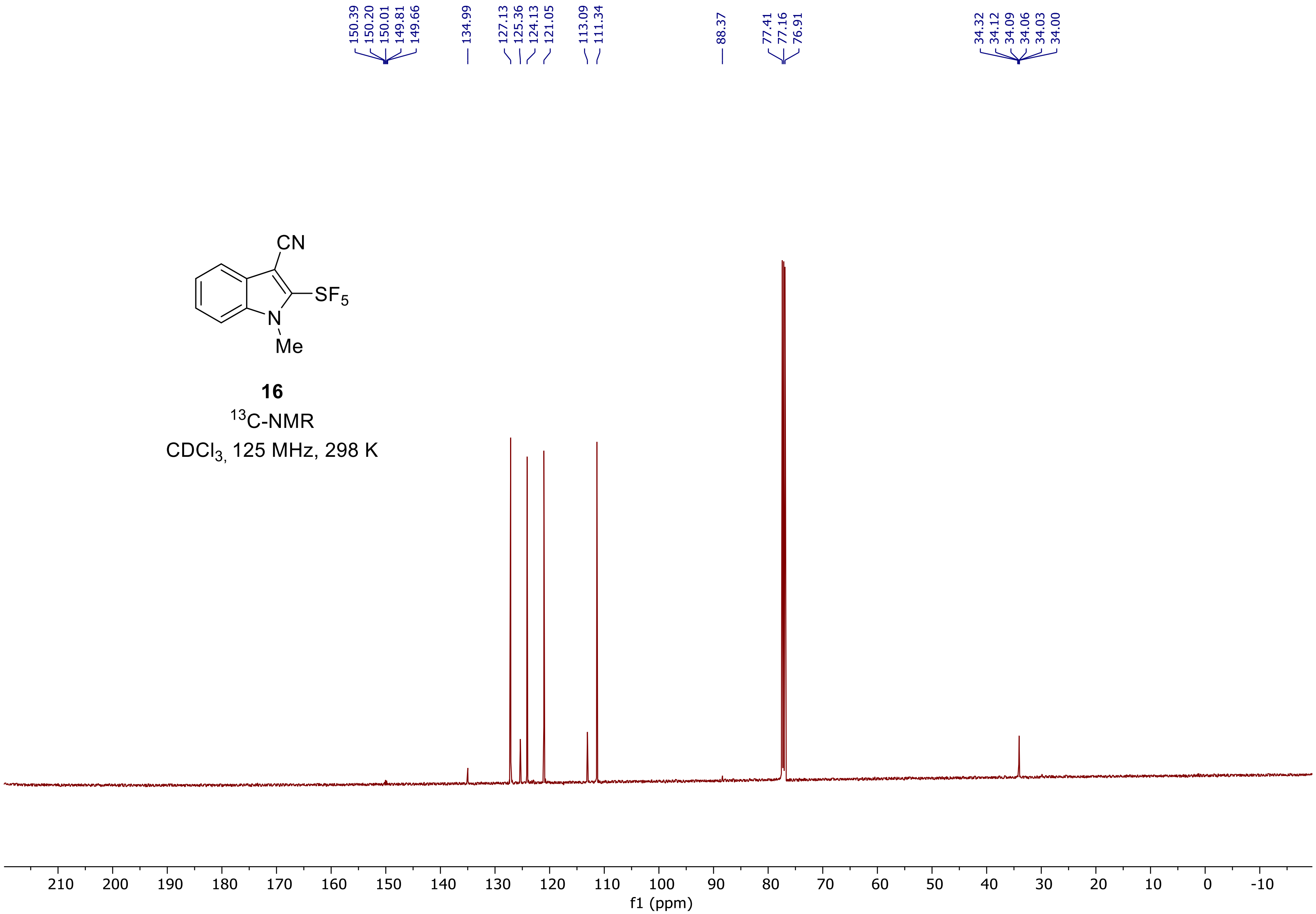


16

^{1}H-NMR

$CDCl_3$, 500 MHz, 298 K

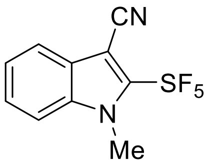




16

^{13}C-NMR

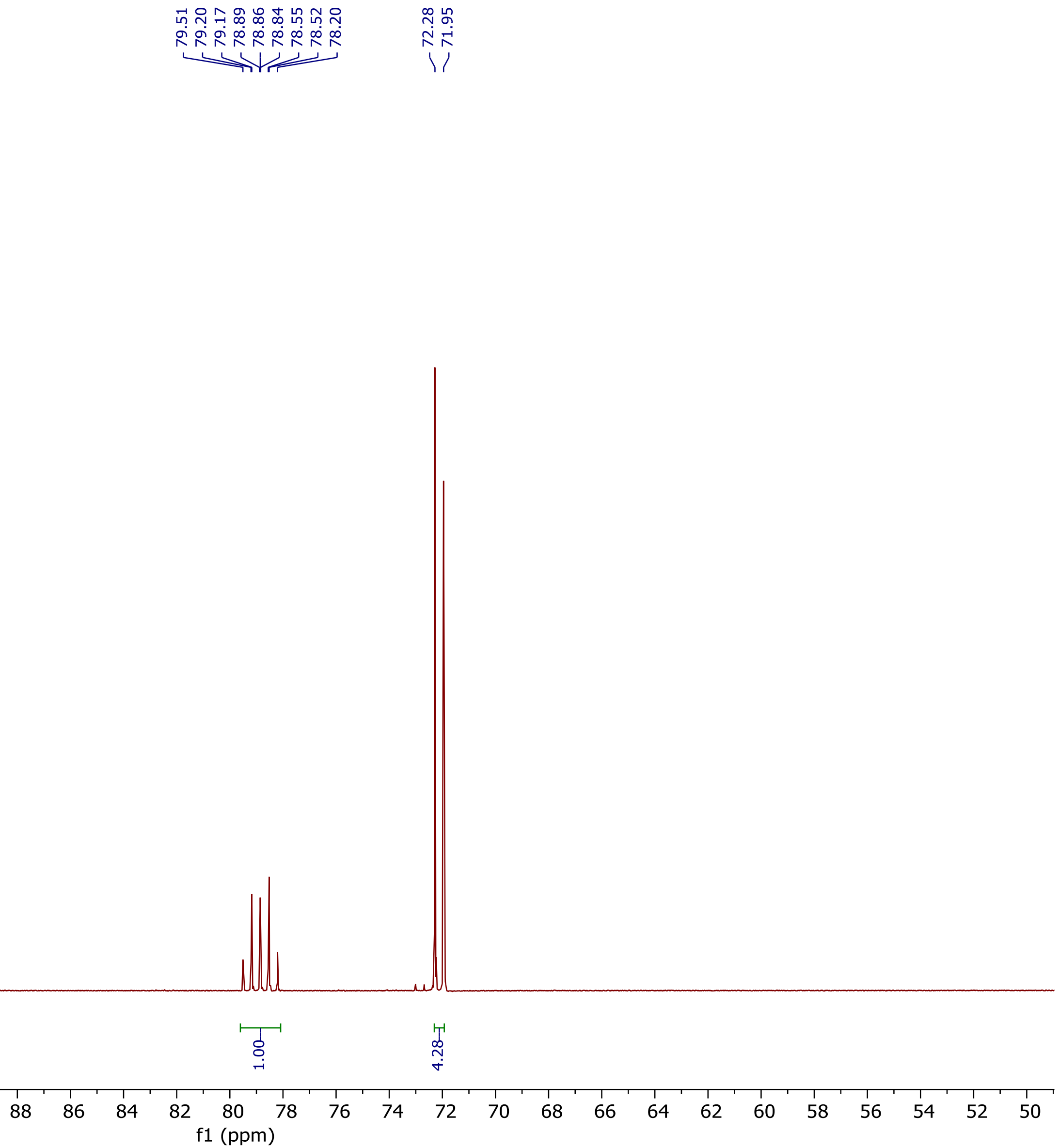
$CDCl_3$, 125 MHz, 298 K

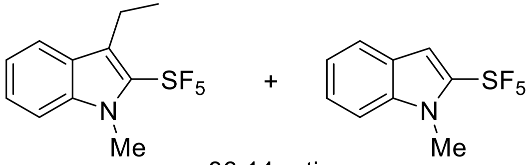


16

^{19}F-NMR

$CDCl_3$, 471 MHz, 298 K





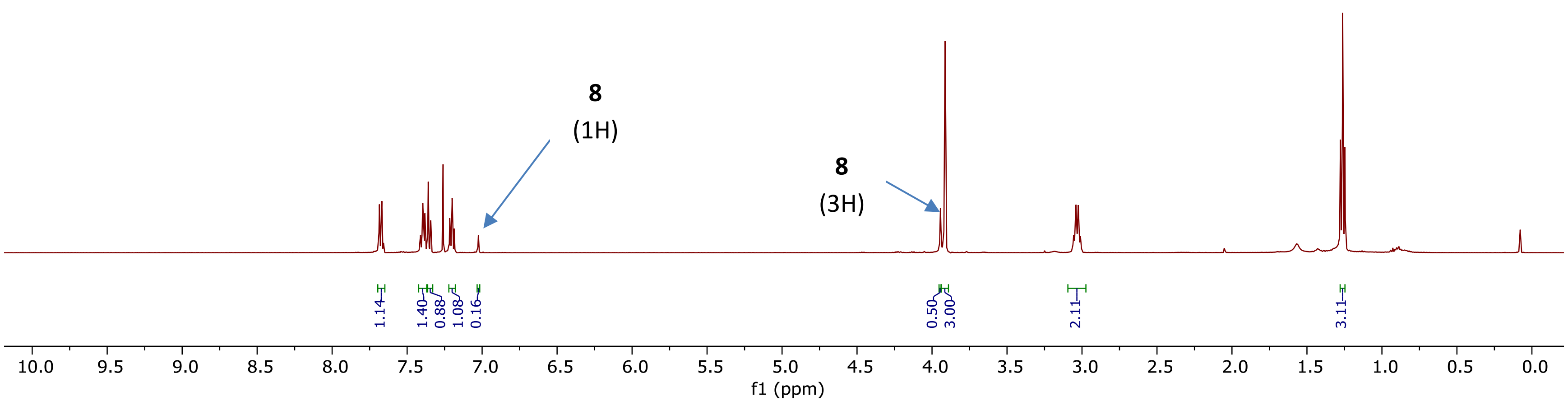
17

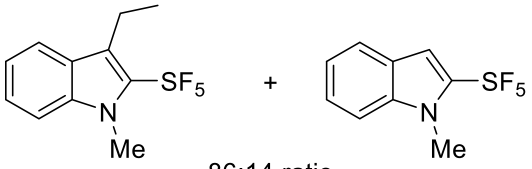
86:14 ratio

8

^{1}H-NMR

$CDCl_3$, 500 MHz, 298 K

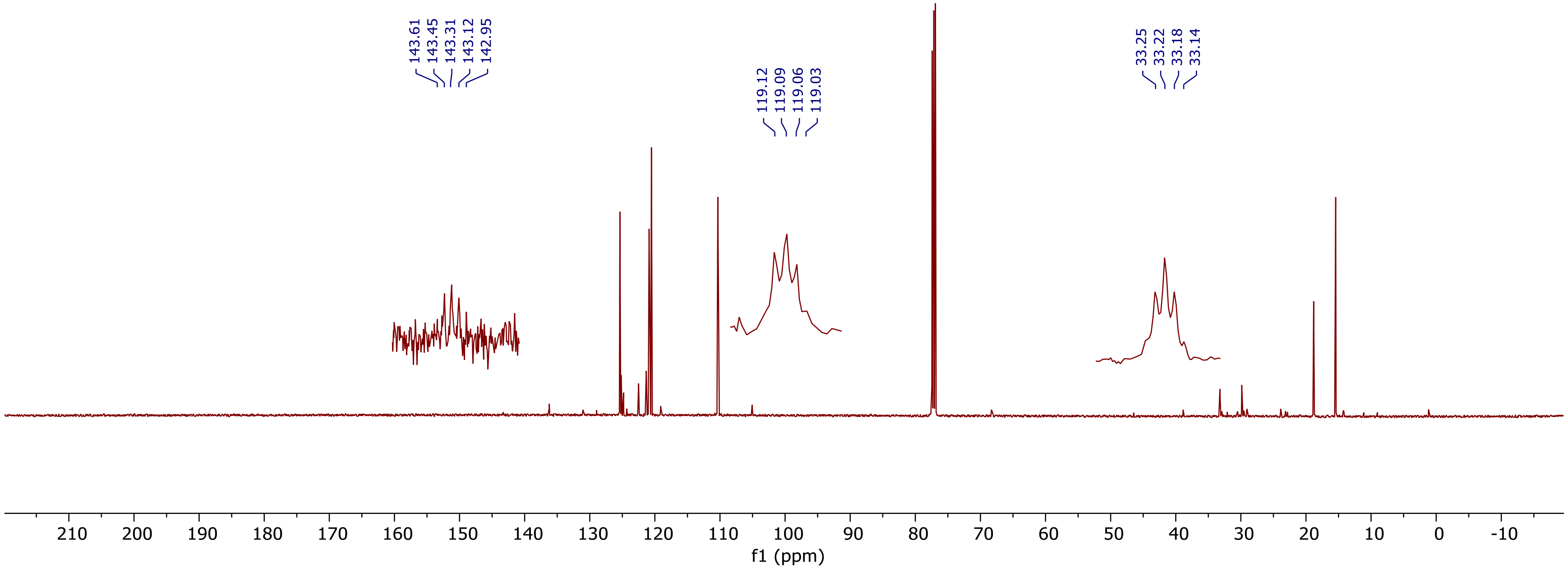


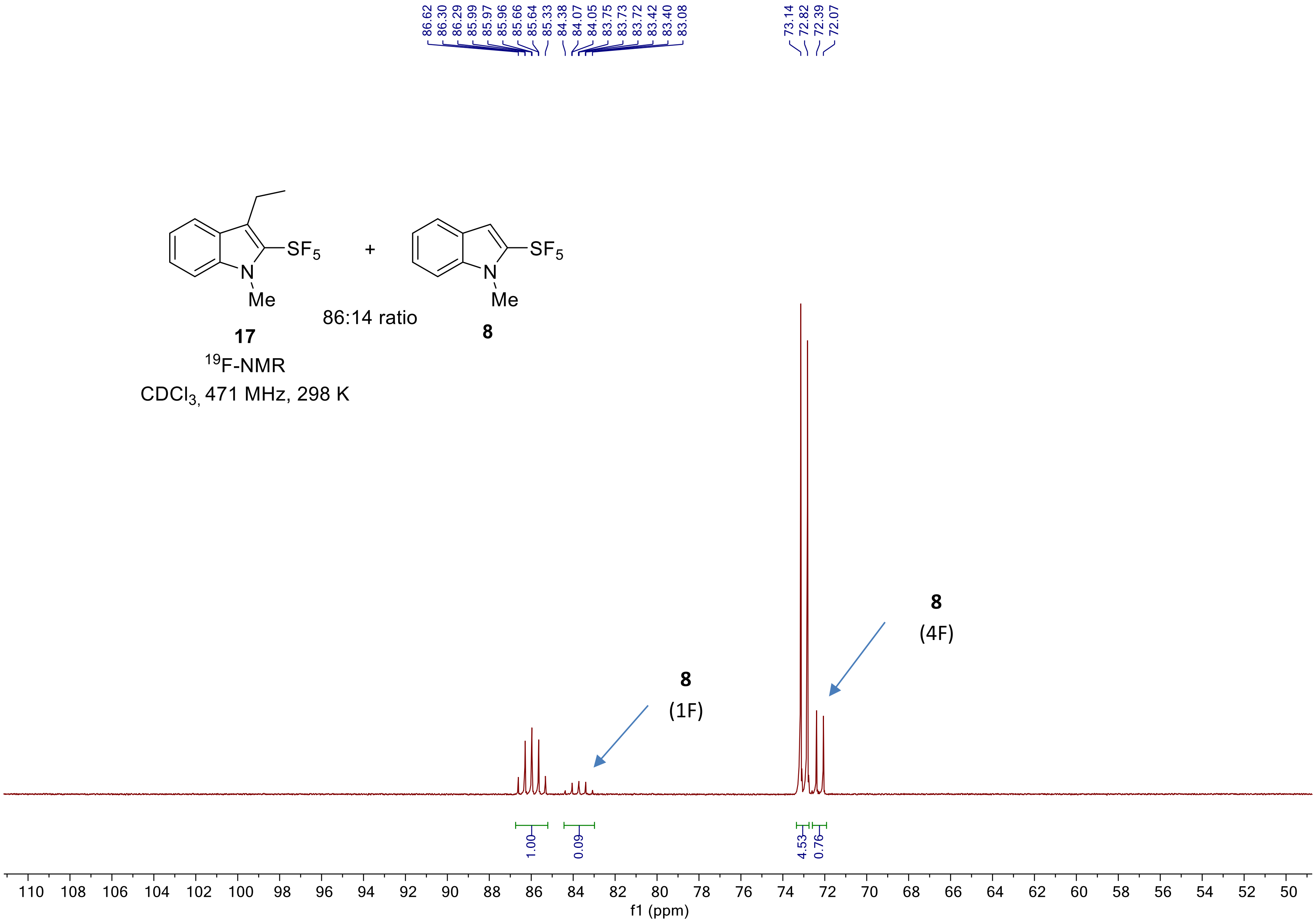


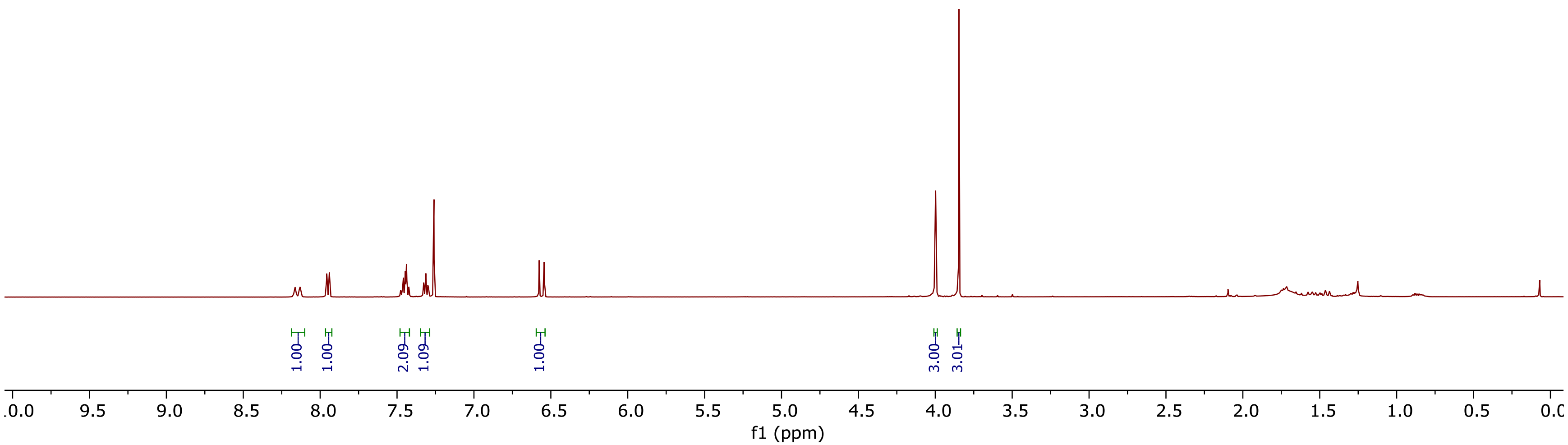
17 86:14 ratio **8**

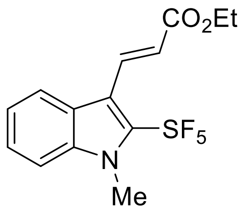
^{13}C-NMR

$CDCl_{3,}$ 100 MHz, 298 K




86.62
86.30
86.29
85.99
85.97
85.96
85.66
85.64
85.33
84.38
84.07
84.05
83.75
83.73
83.72
83.42
83.40
83.08
73.14
72.82
72.39
72.07
SF5
N
Me
+
SF5
N
Me
17
86:14 ratio
8
19F-NMR
CDCl3, 471 MHz, 298 K
8
(1F)
8
(4F)
1.00
0.09
4.53
0.76
f1 (ppm)

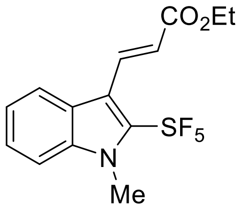




18

^{1}H-NMR

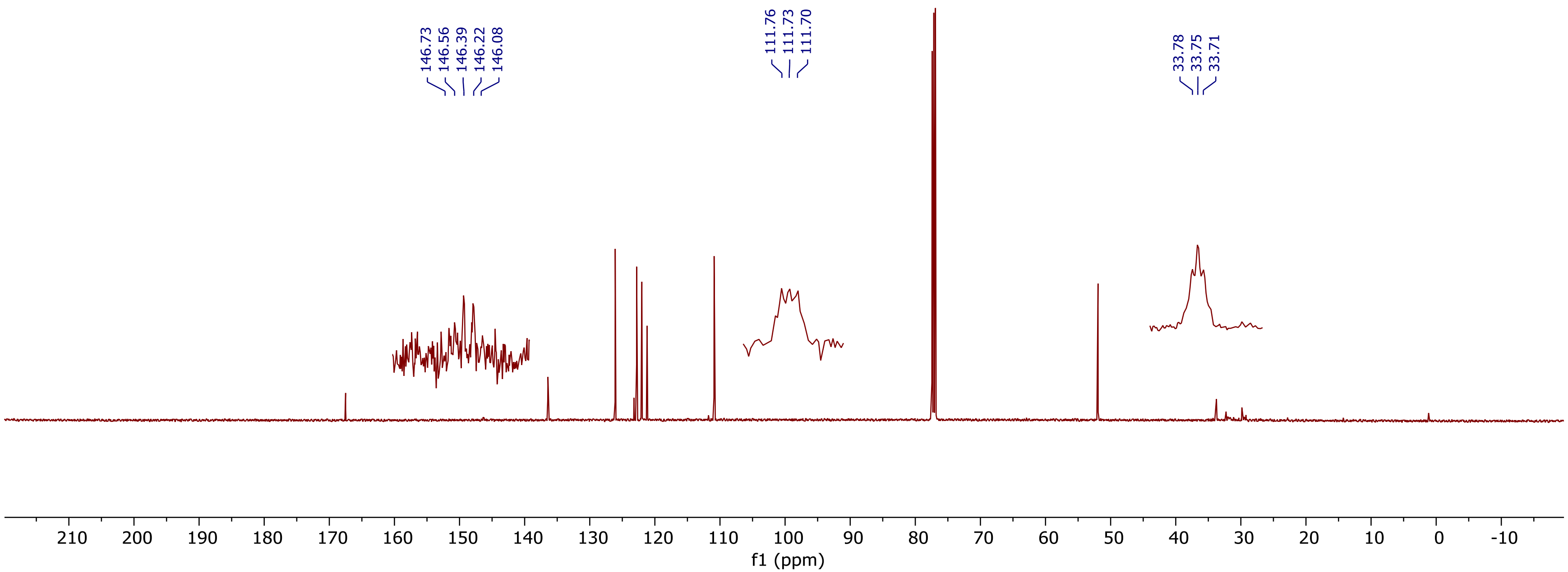
$CDCl_3$, 500 MHz, 298 K

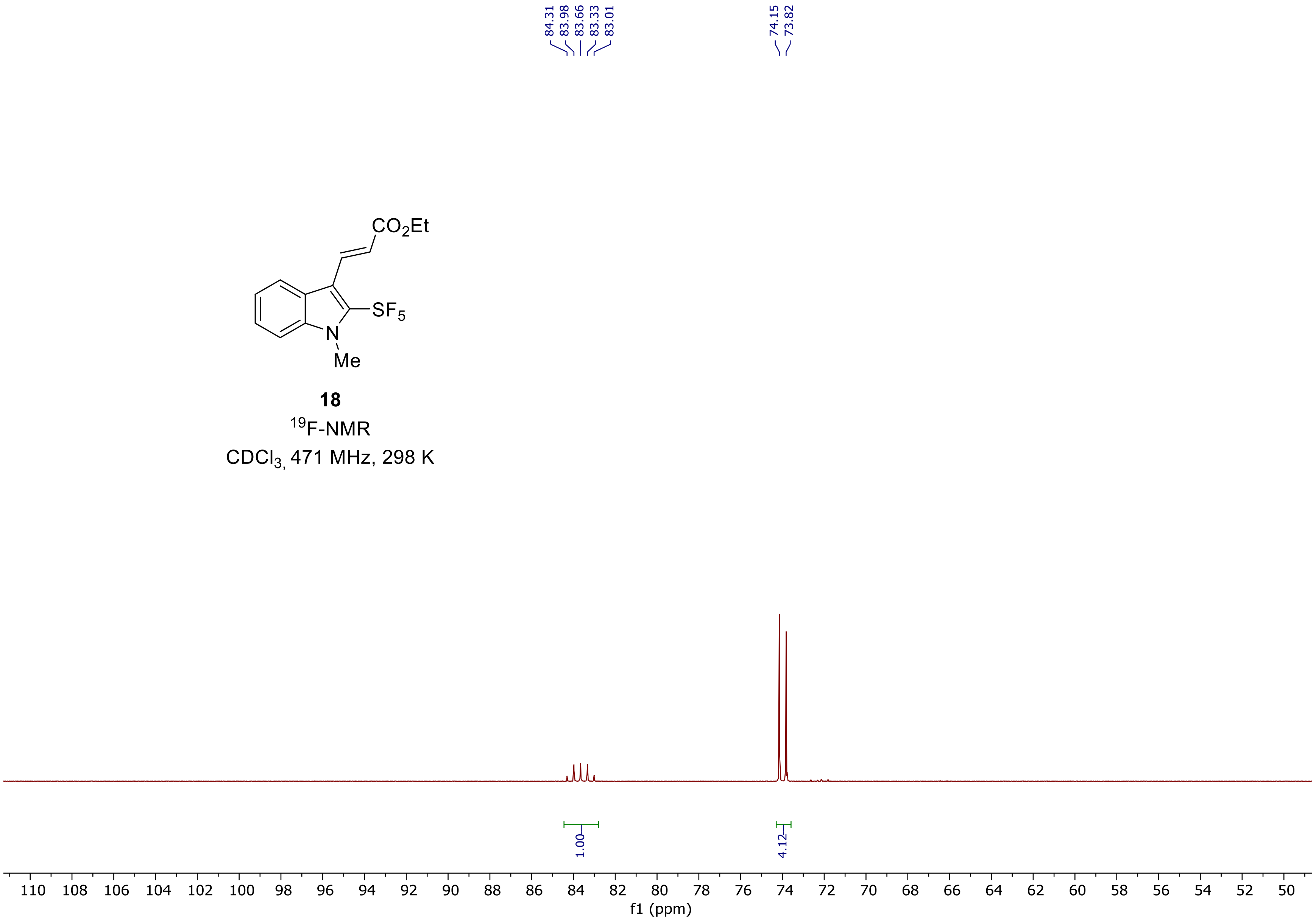


18

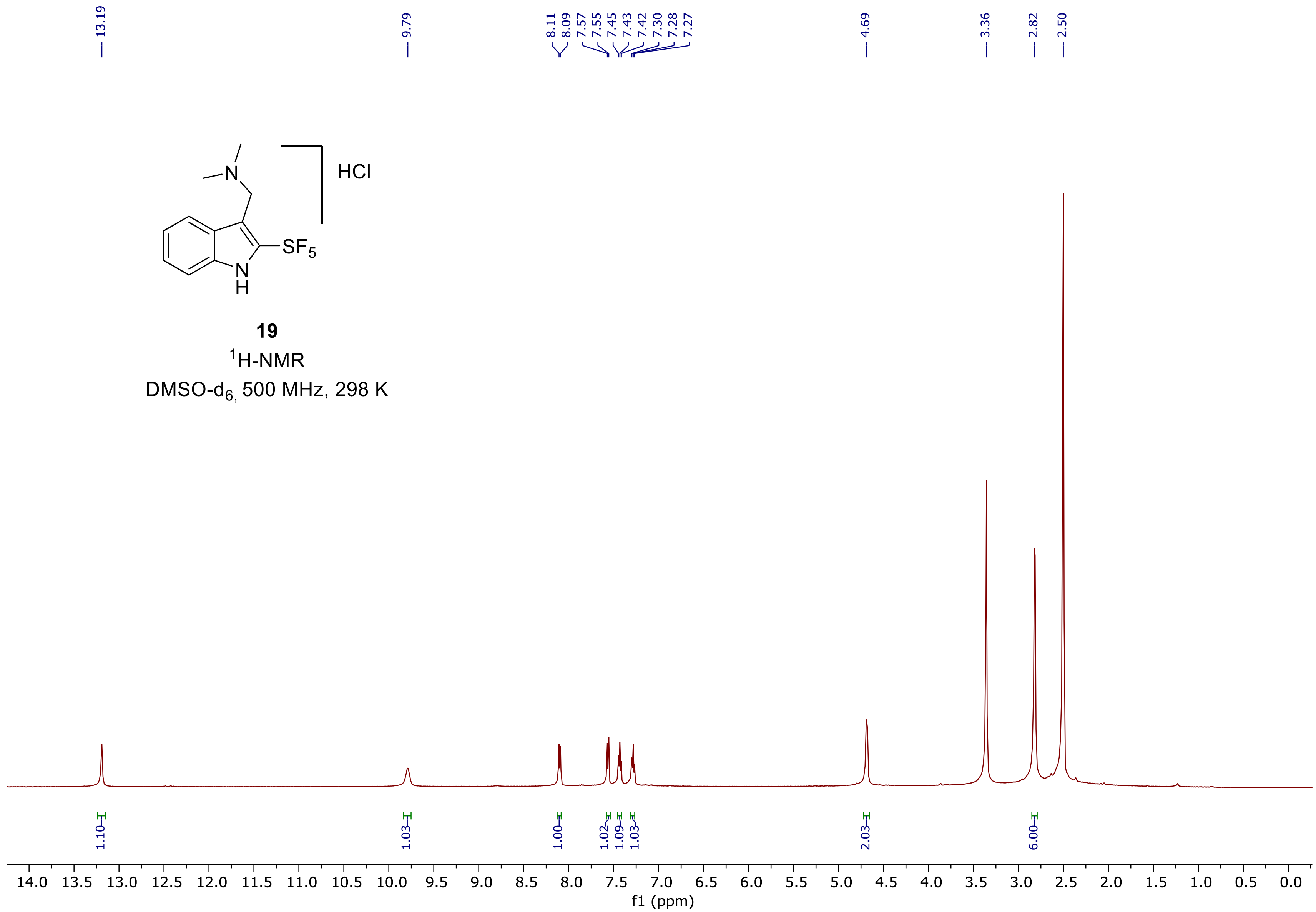
^{13}C-NMR

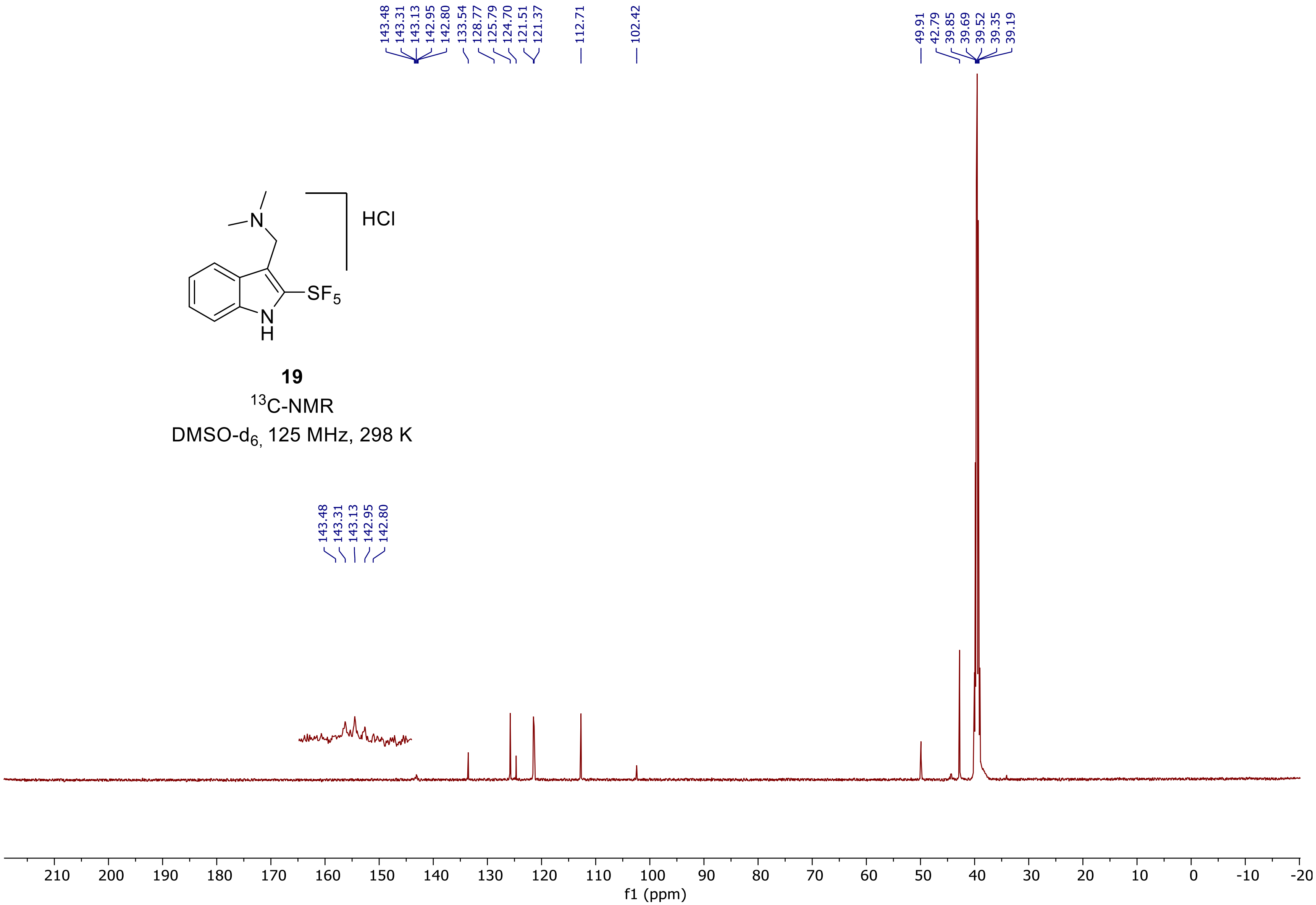
$CDCl_3$, 400 MHz, 298 K





18
^{19}F-NMR
$CDCl_3$, 471 MHz, 298 K

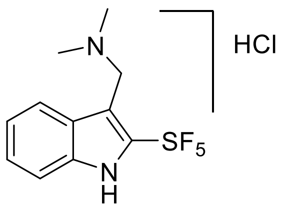

HCl
SF_5
N
H
19
^{1}H-NMR
DMSO-d_6, 500 MHz, 298 K
13.19
9.79
8.11
8.09
7.57
7.55
7.45
7.43
7.42
7.30
7.28
7.27
4.69
3.36
2.82
2.50
1.10
1.03
1.00
1.02
1.09
1.03
2.03
6.00
14.0 13.5 13.0 12.5 12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)



19

^{13}C-NMR

DMSO-d_6, 125 MHz, 298 K



19

^{19}F-NMR

DMSO-d_6, 471 MHz, 298 K