Supplementary Information (SI) for Chemical Science.
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Isothiourea Catalysed Enantioselective Generation of Point and Axially Chiral Iminothia- and Iminoselenazinanones

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1. General Information

All reagents and solvents were obtained from commercial suppliers and were used without further purification unless otherwise stated. Reactions involving moisture sensitive reagents were carried out in flame-dried glassware under an inert atmosphere (N_2 or Ar) using standard vacuum line techniques. Anhydrous solvents (Et_2O, CH_2Cl_2, THF, DMF and toluene) were obtained after passing through an alumina column (Mbraun SPS-800).

Reactions were carried out in flame-dried glassware or oven-dried vials under an inert atmosphere (N_2) using standard vacuum line techniques. Room temperature (RT) refers to 20–25 °C. Temperatures of 0 °C were obtained using an ice/saltwater bath in an insulated container. Reactions involving heating were performed using either DrySyn blocks or an oil bath and a contact thermocouple. Under reduced pressure refers to the use of either a Büchi Rotavapor R-200 with a Büchi V-491 heating bath and Büchi V-800 vacuum controller, a Büchi Rotavapor R-210 with a Büchi V-491 heating bath and Büchi V-850 vacuum controller, a Heidolph Laborota 4001 with vacuum controller, an IKA RV10 rotary evaporator with a IKA HB10 heating bath and ILMVAC vacuum controller, or an IKA RV10 rotary evaporator with a IKA HB10 heating bath and Vacuubrand CVC3000 vacuum controller. Rotary evaporator condensers are fitted to Julabo FL601 Recirculating Coolers filled with ethylene glycol and set to –5 °C.

Analytical thin layer chromatography was performed on pre-coated aluminium plates (Kieselgel 60 F254 silica) and visualisation was achieved using ultraviolet light (254 nm) and/or staining with aqueous $KMnO_4$ solution followed by heating. Manual column chromatography was performed in glass columns fitted with porosity 3 sintered discs over Kieselgel 60 silica using the solvent system stated. Automated chromatography was performed on a Biotage Selekt with a UV/Vis detector using the solvent system stated and cartridges filled with Kieselgel 60 silica.

Melting points were recorded on an Electrothermal 9100 melting point apparatus, (dec) refers to decomposition.

Optical rotations were measured on a Perkin Elmer Precisely/Model-341 polarimeter operating at the sodium D line with a 100 mm path cell at 20 °C. Concentrations (*c*) are stated in g/100 mL.

HPLC analyses were obtained on either a Shimadzu HPLC consisting of a DGU-20A5 degassing unit, LC-20AT liquid chromatography pump, SIL-20AHT autosampler, CMB-20A communications bus module, SPD-M20A diode array detector and a CTO-20A column oven or a Shimadzu HPLC consisting of a DGU-20A5R degassing unit, LC-20AD liquid chromatography pump, SIL-20AHT autosampler, SPD-20A UV/Vis detector and a CTO-20A column oven. Separation was achieved using either DAICEL CHIRALCEL OD-H and OJ-H columns or DAICEL CHIRALPAK AD-H, AS-H, IA, IB, IC and ID columns using the method stated. HPLC traces of enantiomerically enriched compounds were compared with authentic racemic spectra.

Infrared (IR) spectra were recorded on a Shimadzu IRAffinity-1 Fourier transform IR spectrophotometer fitted with a Specac Quest ATR accessory (diamond puck). Spectra were recorded of either thin films or solids, with characteristic absorption wavenumbers (ν_{max}) reported in cm^{-1}.

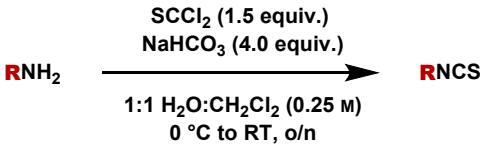
^{1}H, **^{13}C{^{1}H}**, **^{19}F{^{1}H}**, and **^{77}Se{^{1}H} NMR** spectra were acquired on either a Bruker AV400 with a BBFO probe (^{1}H 400 MHz; ^{19}F{^{1}H} 377 MHz), a Bruker AVII 400 with a BBFO probe (^{1}H 400 MHz; ^{19}F{^{1}H} 376 MHz), a Bruker AVIII-HD 500 with a SmartProbe BBFO+ probe (^{1}H 500 MHz, ^{19}F{^{1}H} 470 MHz), a Bruker AVIII 500 with a CryoProbe Prodigy BBO probe (^{1}H 500 MHz, ^{13}C{^{1}H} 126 MHz, ^{77}Se{^{1}H} 95 MHz), or a Bruker AVIII-HD 700 with a CryoProbe Prodigy TCI probe (^{13}C{^{1}H} 176 MHz) in the deuterated solvent stated. All chemical shifts are quoted in parts per million (ppm) relative to the residual solvent peak. All coupling constants, J, are quoted in Hz. Multiplicities are indicated as s (singlet), d (doublet), t (triplet), q (quartet), m (multiplet), and multiples thereof. The abbreviation Ar denotes aromatic. NMR peak assignments were confirmed using 2D ^{1}H correlated spectroscopy (COSY), 2D ^{1}H–^{13}C or ^{1}H–^{15}N heteronuclear multiple-bond correlation spectroscopy (HMBC), and 2D ^{1}H–^{13}C heteronuclear single quantum coherence (HSQC) where necessary.

Mass spectrometry (HRMS) data were acquired by either electrospray ionisation (ESI), electron impact (EI), or matrix-assisted laser desorption/ionisation with no matrix (MALDI (no matrix)) at either the University of St Andrews Mass Spectrometry Facility or SIRCAMS at University of Edinburgh.

X-ray diffraction data were collected and processed by the University of St Andrews Single Crystal X-ray Diffraction Service.

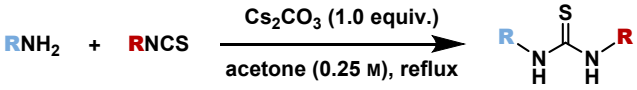
2. General Procedures

General Procedure A: Preparation of isothiocyanates



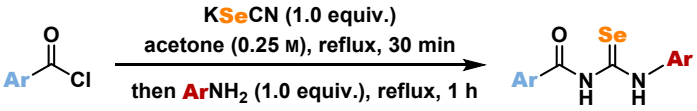
The appropriate amine (1.0 equiv.) and $NaHCO_3$ (4.0 equiv.) were dissolved in 1:1 CH_2Cl_2:H_2O (0.25 M) and the reaction mixture cooled to 0 °C. Thiophosgene (1.5 equiv.) was added dropwise then the reaction mixture warmed to RT to stir o/n. Once complete, the reaction mixture was diluted with H_2O and extracted with CH_2Cl_2 (× 2). The combined organics were dried over $MgSO_4$ then the solvent removed under reduced pressure to give the crude product which was used without further purification.

General Procedure B: Preparation of thioureas



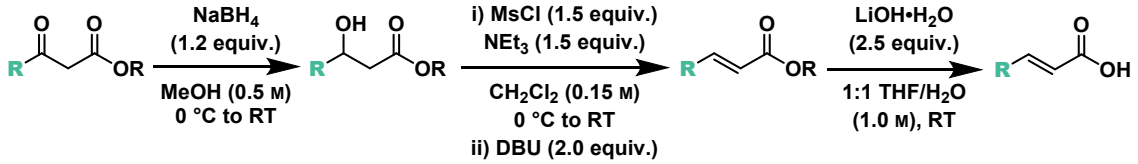
The appropriate amine (1.0 equiv.), isothiocyanate (1.0 equiv.), and Cs_2CO_3 (1.0 equiv.) were dissolved in acetone (0.25 M) and heated to reflux. Once complete, the mixture was cooled, diluted with H_2O, and acidified to pH 1 with 2 M HCl. The aqueous mixture was extracted with EtOAc (× 3), dried over $MgSO_4$ and the solvent removed under reduced pressure to give the crude product which was purified as specified.

General Procedure C: Preparation of selenoureas



The appropriate acid chloride (1.0 equiv.) was added to a solution of KSeCN (1.0 equiv.) in acetone (0.25 M) and heated to reflux for 30 min. The requisite aniline (1.0 equiv.) was then added, and the reaction mixture heated at reflux for a further 1 h. Once complete, the reaction mixture was poured into ice water with stirring. The resulting precipitate was collected by vacuum filtration to give the crude product which was purified as specified.

General Procedure D: Preparation of α,β-unsaturated acids

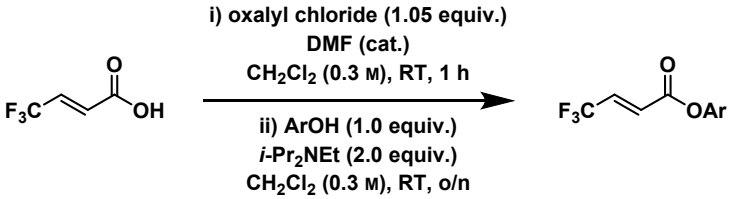


The appropriate β-ketoester (1.0 equiv.) was dissolved in MeOH (0.5 M) and cooled to 0 °C. $NaBH_4$ (1.2 equiv.) was added, and the reaction mixture warmed to RT. Once complete, the reaction mixture was quenched with 1 M HCl and extracted with EtOAc (× 2). The combined organics were then washed with sat. $NaHCO_3$ then brine, dried over $MgSO_4$ and the solvent removed under reduced pressure to afford the crude alcohol.

The crude alcohol (1.0 equiv.) and NEt_3 (1.5 equiv.) were dissolved in anhydrous CH_2Cl_2 (0.3 M), and the reaction mixture cooled to 0 °C. A solution of MsCl (1.5 equiv.) in CH_2Cl_2 (0.3 M) was then added slowly. The reaction mixture was then warmed to RT to stir for 2 h before DBU (2.0 equiv.) was added. Once complete, the reaction mixture was diluted with H_2O then washed with 1 M HCl then sat. $NaHCO_3$, dried over $MgSO_4$ and the solvent removed under reduced pressure. The resulting crude material was triturated with Et_2O, the filtrates combined, and the solvent removed under reduced pressure to give the crude α,β-unsaturated ester.

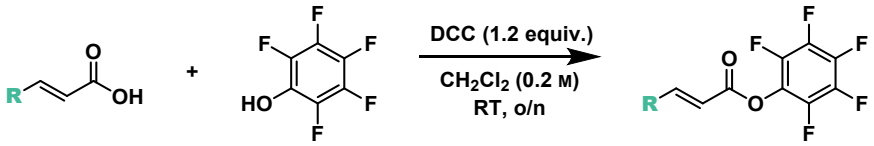
$LiOH{\cdot}H_2O$ (2.5 equiv.) was added to a solution of the crude α,β-unsaturated ester (1.0 equiv.) in 1:1 THF:H_2O (1.0 M) and the reaction mixture stirred at RT. Once complete, the majority of the THF was removed under reduced pressure then the reaction mixture acidified to pH 1 with 1 M HCl. The mixture was extracted with CH_2Cl_2 (× 3) then the combined organics dried over $MgSO_4$, and the solvent removed under reduced pressure to give the crude acid.

General Procedure E: Preparation of α,β-unsaturated esters *via* acid chloride



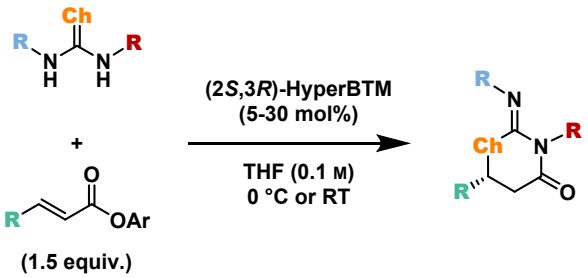
(*E*)-4,4,4-Trifluorobut-2-enoic acid (1.0 equiv.) and oxalyl chloride (1.05 equiv.) were dissolved in anhydrous CH_2Cl_2 (0.3 M). A few drops of DMF were added and the reaction mixture stirred at RT for 1 h. A solution of the requisite phenol (1.0 equiv.) and *i*-Pr_2NEt (2.0 equiv.) in anhydrous CH_2Cl_2 (0.3 M) was added slowly then the reaction mixture stirred at RT o/n. Once complete, the solvent was removed under reduced pressure and the solid triturated with Et_2O. The combined filtrates were then concentrated to give the crude product which was purified as specified.

General Procedure F: Preparation of α,β-unsaturated PFP esters



The requisite carboxylic acid (1.0 equiv.) and DCC (1.2 equiv.) were dissolved in anhydrous CH_2Cl_2 (0.2 M) with stirring at RT. After 30 min, perfluorophenol (1.0 equiv.) was added and the reaction mixture stirred o/n. Once complete, the solvent was removed under reduced pressure and the crude product purified as specified.

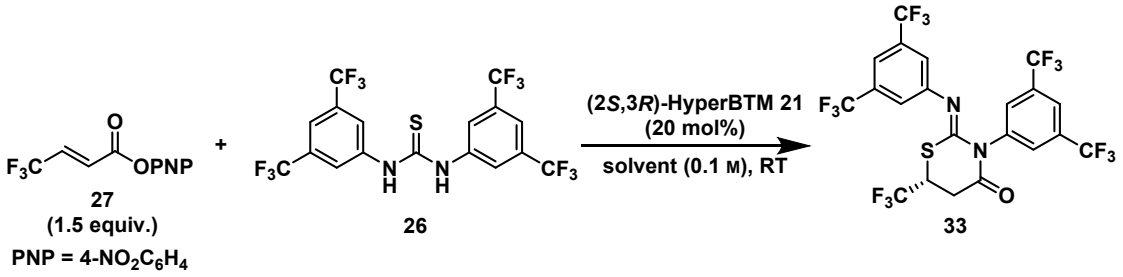
General Procedure G: Isothiourea-catalysed Michael addition of chalcogenoureas to α,β-unsaturated esters



The requisite chalcogenourea (1.0 equiv.), α,β-unsaturated ester (1.5 equiv.) and the specified loading of (2*S*,3*R*)-HyperBTM were dissolved in anhydrous THF (0.1 M) then the reaction mixture stirred at the specified temperature and time. Once complete, the reaction mixture was diluted with EtOAc then washed with either sat. Na_2CO_3 (× 3) (when PNP ester used) or sat. $NaHCO_3$ (× 3) (when PFP ester used). The combined organics were dried over $MgSO_4$ then the solvent removed under reduced pressure to give the crude product which was purified as specified.

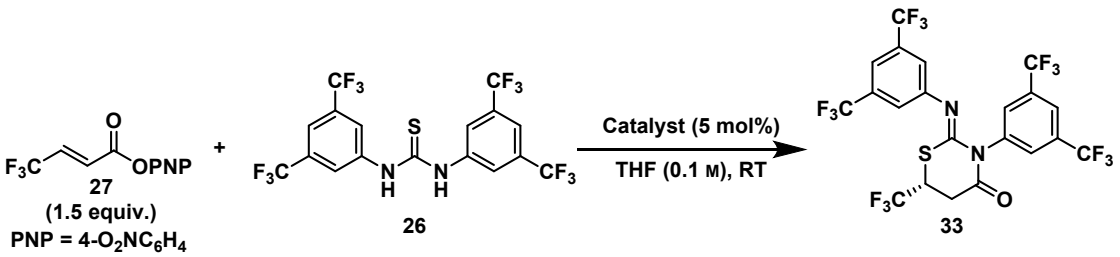
3. Reaction Optimisation

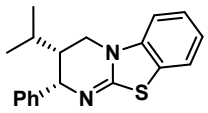
All optimisation reactions were performed on a 0.1 mmol scale.



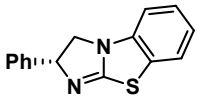
Entry	Solvent	er[a]	Yield[b] (%)
1	MeCN	78:22	quant.
2	CH_2Cl_2	66:34	quant.
3	EtOAc	90:10	quant.
4	DMF	84:16	quant.
5	THF	91:9	quant.
6	PhMe	73:27	quant.
7	MeOH	-	18
8	$CHCl_3$	69:31	quant.
9	Dioxane	84:16	98
10	Et_2O	85:15	98
11	Acetone	85:15	98
12	2-Me THF	91:9	quant.
13	*i*-PrOAc	90:10	98
14	Cyclohexanone	90:10	98
15	DMC	90:10	98
16	MTBE	86:14	95

Table S1 Solvent screen. [a] Determined by HPLC analysis on a chiral stationary phase. [b] Yield determined by ^{1}H NMR analysis relative to internal standard 1,3,5-trimethoxybenzene.

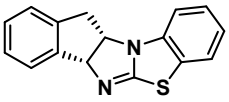




(2*S*,3*R*)-HyperBTM 21

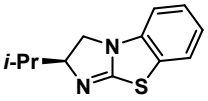


(*R*)-BTM 8

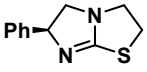


(4b*R*,11a*S*)-fused-BTM 34

(2*S*,3*R*)-HyperSe S1



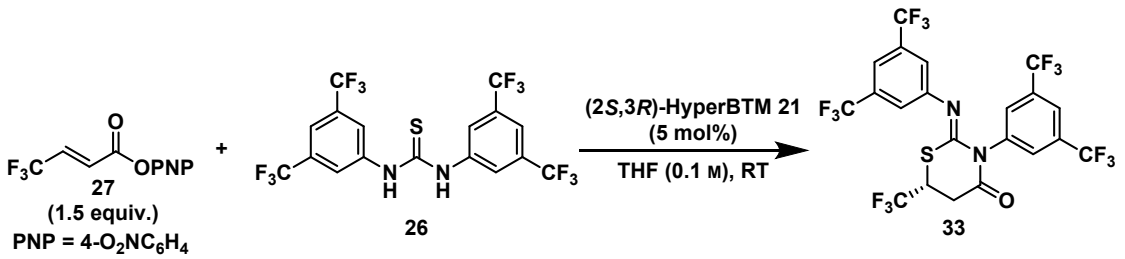
(*S*)-*i*-Pr-BTM S2



(*S*)-TM S3

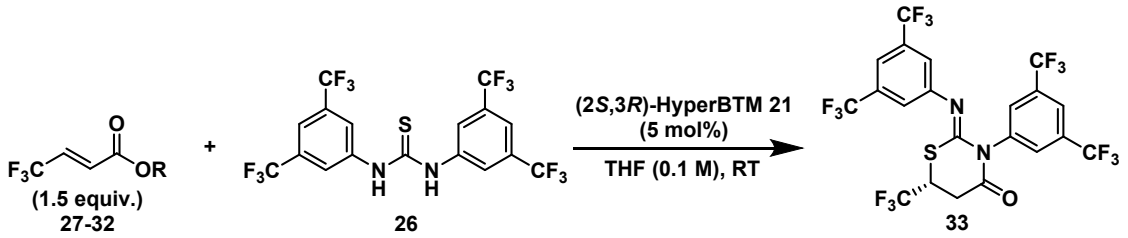
Entry	Catalyst	er[a]	Yield[b] (%)
1	**21**	91:9	quant.
2	**21**·HCl	91:9	93
3	**8**	84:16	96
4	**34**	33:67	98
5	**S1**	90:10	95
6	**S2**	27:73	90
7	**S3**	18:82	92

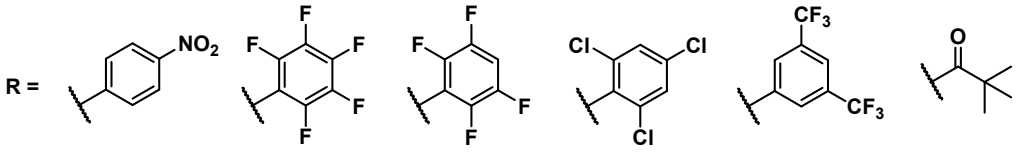
Table S2 Catalyst screen. [a] Determined by HPLC analysis on a chiral stationary phase. [b] Yield determined by ^{1}H NMR analysis relative to internal standard 1,3,5-trimethoxybenzene.



Entry	Conditions	er[a]	Yield[b] (%)
1	Concentration 0.5 M	87:13	92
2	Concentration 0.01 M	90:10	87
3	Stoichiometry reversed	91:9	quant.
4	**27** added over 1 h	90:10	98
5	**26** added over 1 h	91:9	84

Table S3 Optimisation of reaction conditions. [a] Determined by HPLC analysis on a chiral stationary phase. [b] Yield determined by ^{1}H NMR analysis relative to internal standard 1,3,5-trimethoxybenzene.



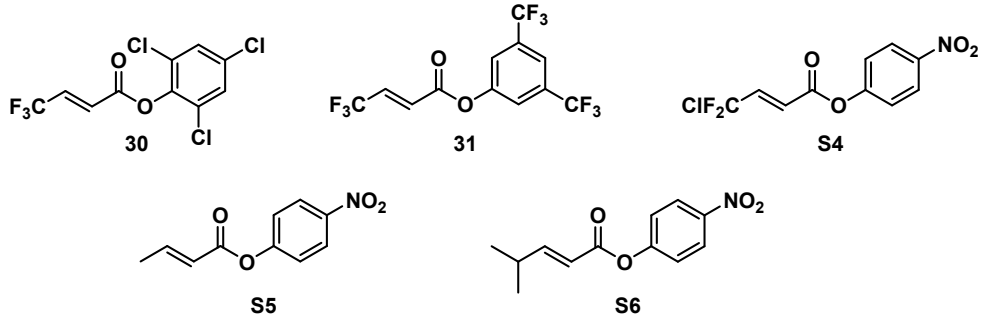


Entry	Precursor	Phenol pK_a[a]	er[b]	Yield[c] (%)
1	**27**	7.16	91:9	quant.
2	**28**	5.53	93:7	90
3	**29**	6.00	92:8	quant.
4	**30**	5.99	92:8	96
5	**31**	8.26	90:10	95
6[d]	**32**	-	90:10	83
7[e]	**28**	5.53	95:5	quant.

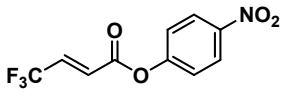
Table S4 Screen of α,β-unsaturated acyl ammonium precursors. [a] pK_a in H_2O[1-3] [b] Determined by HPLC analysis on a chiral stationary phase. [c] Yield determined by ^{1}H NMR analysis relative to internal standard 1,3,5-trimethoxybenzene. [d] Formed *in situ* from (*E*)-4,4,4-trifluorobut-2-enoic acid (1.5 equiv.), pivaloyl chloride (1.5 equiv.), and i-Pr_2NEt (1.5 equiv.). [e] Reaction temperature was 0 °C.

4. Preparation of α,β-Unsaturated Esters

The following esters were available in the laboratory, previously prepared in accordance with literature: **30**,[4] **31**,[4] **S4**,[5] **S5**,[6] and **S6**.[7]



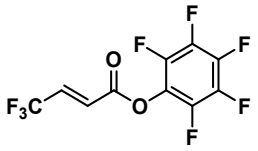
4-Nitrophenyl (*E*)-4,4,4-trifluorobut-2-enoate (27)



27

Following General Procedure E, (*E*)-4,4,4-trifluorobut-2-enoic acid (2.33 g, 16.6 mmol, 1.0 equiv.), oxalyl chloride (1.47 mL, 17.4 mmol, 1.05 equiv.), then 4-nitrophenol (2.31 g, 16.6 mmol, 1.0 equiv.) and *i*-Pr_2NEt (5.68 mL, 33.2 mmol, 2.0 equiv.) in CH_2Cl_2 (0.17 M) gave crude product that was purified by flash silica column chromatography (CH_2Cl_2, R_F 0.81), then recrystallised from hexane to give the title compound as colourless crystals (3.75 g, 86%). **mp** 70 – 72 °C {lit[4] 93 – 95 °C}; **^{1}H NMR** (400 MHz, $CDCl_3$) δ_H: 6.72 (1H, dq, *J* 15.8, 1.9, C(2)*H*), 7.02 (1H, dq, *J* 15.8, 6.4, C(3)*H*), 7.34 – 7.39 (2H, m, ArC(2,6)*H*), 8.28 – 8.35 (2H, m, ArC(3,5)*H*); **^{19}F{^{1}H} NMR** (377 MHz, $CDCl_3$) δ_F: –65.7 (s, C*F*$_3$). Spectroscopic data in accordance with the literature.[4]

Perfluorophenyl (*E*)-4,4,4-trifluorobut-2-enoate (28)



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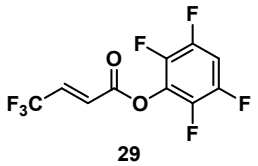
Following General Procedure F, (*E*)-4,4,4-trifluorobut-2-enoic acid (6.00 g, 42.8 mmol, 1.0 equiv.), pentafluorophenol (7.88 g, 42.8 mmol, 1.0 equiv.) and DCC (10.6 g, 51.4 mmol, 1.2 equiv.) in anhydrous CH_2Cl_2 (0.2 M) gave crude product that was purified by flash silica column chromatography (hexane:CH_2Cl_2 100:0 to 70:30, R_F 0.95 at 70:30) to give the title compound as a colourless oil (6.57 g, 50%). **^{1}H NMR** (400 MHz, $CDCl_3$) δ_H: 6.76 (1H, dq, *J* 15.8, 1.9, C(2)*H*), 7.06 (1H, dq, *J* 15.8, 6.3, C(3)*H*); **^{19}F{^{1}H} NMR** (377 MHz, $CDCl_3$) δ_F: –161.6 – –161.4 (m, ArC*F*), –156.6 – –156.4 (m, ArC*F*), –152.3 – –152.2 (m, ArC*F*), –66.0 (s, C*F*$_3$); **IR** ν_{max} (film) 1778, 1518, 1323, 1300, 1271, 1215, 1119, 993, 968, 937, 862. Spectroscopic data in accordance with the literature.[8]

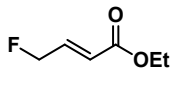
2,3,5,6-Tetrafluorophenyl (*E*)-4,4,4-trifluorobut-2-enoate (29)



29

Following General Procedure E, (*E*)-4,4,4-trifluorobut-2-enoic acid (0.42 g, 3.0 mmol, 1.0 equiv.), oxalyl chloride (0.27 mL, 3.2 mmol, 1.05 equiv.), then 2,3,5,6-tetrafluorophenol (0.50 g, 3.0 mmol, 1.0 equiv.) and *i*-Pr_2NEt (1.03 mL, 6.0 mmol, 2.0 equiv.) in CH_2Cl_2 (0.17 M) gave crude product that was purified by flash silica column chromatography (hexane:CH_2Cl_2 80:20, R_F 0.57) to give the title compound as a colourless low-melting solid (0.62 g, 72%). **^{1}H NMR** (500 MHz, $CDCl_3$) δ_H: 6.76 (1H, dq, *J* 15.8, 1.9, C(2)*H*), 7.02 – 7.12 (2H, m, C(3)*H* and ArC(4)*H*); **^{19}F{^{1}H} NMR** (377 MHz, $CDCl_3$) δ_F: –152.5 – –152.4 (m, ArC*F*), –138.3 – –138.1 (m, ArC*F*), –65.9 (s, CF_3); **^{13}C{^{1}H} NMR** (126 MHz, $CDCl_3$) δ_C: 104.1 (t, *J* 22.8, Ar*C*(4)H), 121.6 (q, *J* 270.9, *C*F_3), 126.0 (q, *J* 6.2, *C*(2)H), 129.0 (tt, *J* 14.0, 4.0, Ar*C*(1)), 135.3 (q, *J* 36.3, *C*(3)H), 139.4 – 141.8 (m, Ar*C*F), 145.1 – 147.4 (m, Ar*C*F), 159.9 (*C*(1)); **IR** ν_{max} (film) 3094, 1776, 1524, 1487, 1308, 1275, 1213, 1121, 1063, 1051, 955, 843, 785; **HRMS** (ESI^-) $C_{10}H_2O_2F_7$ $[M-H]^-$ found 286.9952, requires 286.9949 (+1.0 ppm).

Ethyl (*E*)-4-fluorobut-2-enoate (S7)

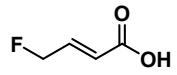


S7

Ethyl (*E*)-4-bromobut-2-eoate (3.86 g, 20.0 mmol, 1.0 equiv.) and silver(I) fluoride (7.61 g, 60.0 mmol, 30 equiv.) were dissolved in MeCN (0.5 M) and stirred at RT in the absence of light. Once complete, the reaction mixture was filtered through Celite® washing with THF then concentrated to give the crude product as a brown oil. Purification by flash silica column chromatography (hexane:EtOAc 98:2 to 90:10, R_F 0.22 at 90:10) gave the title compound as a colourless oil (1.56 g, 59%). **^{1}H NMR** (500 MHz, $CDCl_3$) δ_H: 1.30 (3H, t, *J* 7.1, CH_2CH_3), 4.22 (2H, q, *J* 7.1, CH_2CH_3), 5.05 (2H, ddd, *J* 46.1, 3.8, 2.0, CH_2F), 6.11 (1H, ddt, *J* 15.8, 2.0, 2.0, C(2)*H*), 6.96 (1H, ddt, *J* 23.1, 15.8, 3.8, C(3)*H*); **^{19}F{^{1}H} NMR** (377 MHz, $CDCl_3$) δ_F: –223.3 (s, CH_2F); **^{13}C{^{1}H} NMR** (126 MHz, $CDCl_3$) δ_C: 14.4 (CH_3), 60.8 (CH_2CH_3), 81.2 (d, *J* 171.3, CH_2F), 121.5 (d, *J* 11.0, *C*(2)H), 141.5 (d, *J*

16.0, *C*(3)H), 165.9 (*C*(1)); **IR** ν_{max} (film) 2959, 1724, 1308, 1275, 1179; **HRMS** (ESI^+) $C_6H_{10}O_2F$ $[M+H]^+$ found 133.0658, requires 133.0659 (–0.8 ppm).

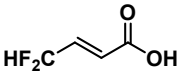
(*E*)-4-Fluorobut-2-enoic acid (S8)



S8

Following General Procedure D, ethyl (*E*)-4-fluorobut-2-enoate **S7** (1.39 g, 10.5 mmol, 1.0 equiv.) and $LiOH{\cdot}H_2O$ (490 mg, 11.6 mmol, 1.1 equiv.) in H_2O:THF 1:1 (10 mL) after 5 h gave the title compound as a colourless solid (1.09 g, 62%), which was used without further purification. **mp** 100 – 102 °C; **^{1}H NMR** (500 MHz, $CDCl_3$) δ_H: 5.10 (2H, ddd, *J* 46.1, 3.5, 2.2, CH_2F), 6.14 (1H, dtd, *J* 15.8, 2.2, 1.4, C(2)*H*), 7.08 (1H, ddt, *J* 23.7, 15.8, 3.5, C(3)*H*); **^{19}F{^{1}H} NMR** (377 MHz, $CDCl_3$) δ_F: –224.1 (s, CH_2F); **^{13}C{^{1}H} NMR** (126 MHz, $CDCl_3$) δ_C: 81.0 (d, *J* 172.8, *C*H_2F), 120.5 (d, *J* 11.4, *C*(2)H), 144.5 (d, *J* 15.8, *C*(3)H), 171.4 (*C*(1)); **IR** ν_{max} (film) 2947, 1645, 1425, 1312, 1285, 1213, 1065, 1022, 964, 907; **HRMS** (ESI^-) $C_4H_4O_2F$ $[M-H]^-$ found 103.0196, requires 103.0201 (–4.9 ppm).

(*E*)-4,4-Difluorobut-2-enoic acid (S9)



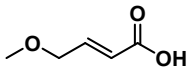
S9

Following General Procedure D, ethyl 4,4-difluoroacetoacetate (4.05 mL, 30.0 mmol, 1.0 equiv.) and $NaBH_4$ (1.36 g, 36.0 mmol, 1.2 equiv.) in MeOH (0.5 M) gave the crude alcohol. The crude alcohol (3.00 g, 17.8 mmol, 1.0 equiv.), NEt_3 (3.72 mL, 26.7 mmol, 1.5 equiv.), MsCl (2.07 mL, 26.7 mmol, 1.5 equiv.), then DBU (5.31 mL, 35.6 mmol, 2.0 equiv.) in CH_2Cl_2 (0.15 M) gave the crude α,β-unsaturated ethyl ester. The crude α,β-unsaturated ethyl ester (2.46 g, 16.4 mmol, 1.0 equiv.) and $LiOH{\cdot}H_2O$ (1.72 g, 41.0 mmol, 2.5 equiv.) in 1:1 THF:H_2O (1.0 M) gave the crude title compound (82:18 (*E*):(*Z*)) as a brown oil (1.42 g, 39%) which was used without further purification.

An analytical sample was obtained by sublimation to give the title compound as colourless crystals. **mp** 51 – 53 °C; **^{1}H NMR** (400 MHz, $CDCl_3$) δ_H: 6.27 (1H, tdd, *J* 54.6, 4.0, 1.0, CF_2H), 6.31 (1H, dtd, *J* 15.9, 3.0, 1.0, C(2)*H*), 6.92 (1H, dtd, *J* 15.9, 10.2, 4.0, C(3)*H*);

^{19}F{^{1}H} NMR (377 MHz, $CDCl_3$) δ_F: –116.8 (s, C*F*$_2$H); **^{13}C{^{1}H} NMR** (126 MHz, $CDCl_3$) δ_C: 112.2 (t, *J* 237.8, *C*F$_2$H), 126.5 (t, *J* 10.4, *C*(2)H), 139.1 (t, *J* 24.2, *C*(3)H), 170.1 (*C*(1)); **IR** ν_{max} (film) 2880, 2664, 2575, 1697, 1657, 1423, 1385, 1346, 1279, 1250, 1225, 1047, 980, 876; **HRMS** (ESI$^-$) $C_4H_3O_2F_2$ [M-H]$^-$ found 121.0106, requires 121.0107 (–0.8 ppm).

(*E*)-4-Methoxybut-2-enoic acid (S10)

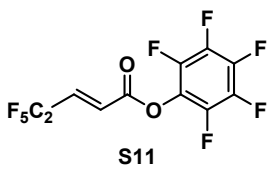


S10

Following General Procedure D, methyl 4-methoxyacetoacetate (3.88 mL, 30.0 mmol, 1.0 equiv.) and $NaBH_4$ (1.36 g, 36.0 mmol, 1.2 equiv.) in MeOH (0.5 M) gave the crude alcohol. The crude alcohol (2.03 g, 13.7 mmol, 1.0 equiv.), NEt_3 (2.09 mL, 20.6 mmol, 1.5 equiv.), MsCl (1.60 mL, 20.6 mmol, 1.5 equiv.), then DBU (4.10 mL, 27.4 mmol, 2.0 equiv.) in CH_2Cl_2 (0.15 M) gave the crude α,β-unsaturated methyl ester. The crude α,β-unsaturated ethyl ester (1.82 g, 14.0 mmol, 1.0 equiv.) and $LiOH{\cdot}H_2O$ (1.47 g, 35.0 mmol, 2.5 equiv.) in 1:1 THF:H_2O (1.0 M) gave the crude title compound (95:5 (*E*):(*Z*)) as a colourless solid (1.07 g, 31%) which was used without further purification. **mp** 48 – 50 °C; **^{1}H NMR** (400 MHz, $CDCl_3$) δ_H: 3.40 (3H, s, OC*H*$_3$), 4.11 (2H, dd, *J* 4.1, 2.1, C(4)*H*$_2$), 6.07 (1H, dd, *J* 15.7, 2.1, C(2)*H*), 7.05 (1H, dd, *J* 15.7, 4.1, C(3)*H*); **^{13}C{^{1}H} NMR** (126 MHz, $CDCl_3$) δ_C: 58.9 (OCH_3), 71.1 (*C*(4)H_2), 120.6 (*C*(2)H), 147.0 (*C*(3)H), 171.7 (*C*(1)); **IR** ν_{max} (film) 2934, 2596, 1686, 1655, 1643, 1449, 1425, 1387, 1308, 1217, 1186, 1125, 1022, 962, 920, 841.

Spectroscopic data in accordance with literature.[9]

Perfluorophenyl (*E*)-4,4,5,5,5-pentafluoropent-2-enoate (S11)

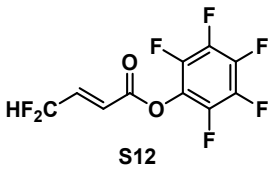


S11

Following General Procedure F, (*E*)-4,4,5,5,5-pentafluoropent-2-enoic acid (0.76 g, 4.0 mmol, 1.0 equiv.), pentafluorophenol (0.74 g, 4.0 mmol, 1.0 equiv.) and DCC (0.99 g, 4.8 mmol, 1.2 equiv.) in anhydrous CH_2Cl_2 (0.2 M) gave crude product that was

purified by flash silica column chromatography (hexane:Et_2O 100:0 to 95:5, R_F 0.82 at 95:5) to give the title compound as a colourless oil (0.26 g, 18%). **^{1}H NMR** (400 MHz, $CDCl_3$) δ_H: 6.81 (1H, dt, *J* 15.9, 2.1, C(2)*H*), 7.09 (1H, dt, *J* 15.9, 11.4, C(3)*H*); **^{19}F{^{1}H} NMR** (377 MHz, $CDCl_3$) δ_F: –162.0 – –161.8 (m, ArC*F*), –156.9 (t, *J* 21.4, ArC*F*), –152.6 – –152.5 (m, ArC*F*), –117.8 (q, *J* 2.2, CF_2CF_3), –84.6 (t, *J* 2.2, CF_2CF_3); **^{13}C{^{1}H} NMR** (126 MHz, $CDCl_3$) δ_C: 111.1 (tq, *J* 252.8, 39.7, *C*F_2CF_3), 118.3 (qt, *J* 285.6, 36.0, CF_2CF_3), 124.1 – 124.5 (m, Ar*C*(1)), 127.5 (t, *J* 8.5, *C*(2)H), 134.6 (t, *J* 24.3, *C*(3)H), 136.7 – 139.2 (m, ArCF), 138.7 – 141.3 (m, ArCF), 139.8 – 142.1 (m, Ar*C*F), 159.5 (*C*(1)); **IR** ν_{max} (film) 1780, 1518, 1281, 1200, 1148, 1121, 1043, 995, 972, 939; **HRMS** (EI^+) $C_{11}H_2O_2F_{10}$ $[M]^+$ found 355.9897, requires 355.9890 (+2.0 ppm).

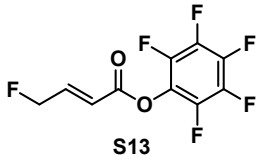
Perfluorophenyl (*E*)-4,4-difluorobut-2-enoate (S12)



S12

Following General Procedure F, (*E*)-4,4-difluorobut-2-enoic acid **S9** (0.92 g, 7.5 mmol, 1.0 equiv.), pentafluorophenol (1.38 g, 7.5 mmol, 1.0 equiv.) and DCC (1.86 g, 9.0 mmol, 1.2 equiv.) in anhydrous CH_2Cl_2 (0.2 M) gave crude product that was purified by flash silica column chromatography (hexane:EtOAc 100:0 to 90:10, R_F 0.57 at 90:10) to give the title compound as a colourless oil (0.64 g, 30%). **^{1}H NMR** (400 MHz, $CDCl_3$) δ_H: 6.34 (1H, tdd, *J* 54.4, 3.7, 1.1, CF_2H), 6.55 (1H, dtd, *J* 15.9, 2.9, 1.1, C(2)*H*), 7.10 (1H, dtd, *J* 15.9, 10.3, 3.7, C(3)*H*); **^{19}F{^{1}H} NMR** (377 MHz, $CDCl_3$) δ_F: –162.0 – –161.9 (m, ArC*F*), –157.2 (t, *J* 21.7, ArC*F*), –152.5 – –152.4 (m, ArC*F*), –117.6 (s, CF_2H); **^{13}C{^{1}H} NMR** (126 MHz, $CDCl_3$) δ_C: 111.8 (t, *J* 238.6, *C*F_2H), 124.0 (t, *J* 10.4, *C*(2)H), 124.5 – 124.9 (m, Ar*C*(1)), 136.9 – 139.3 (m, ArCF), 138.8 – 141.2 (ArCF), 140.1 – 142.4 (m, ArCF), 140.9 (t, *J* 24.2, *C*(3)H), 160.6 (*C*(1)); **IR** ν_{max} (film) 2988, 1773, 1516, 1385, 1267, 1254, 1219, 1123, 1045, 993, 934, 864; **HRMS** (EI^+) $C_{10}H_3O_2F_7$ $[M]^+$ found 288.0013, requires 288.0016 (–1.0 ppm).

Perfluorophenyl (*E*)-4-fluorobut-2-enoate (S13)

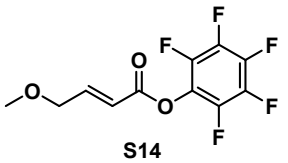


S13

Following General Procedure F, (*E*)-4-fluorobut-2-enoic acid **S8** (0.19 g, 1.8 mmol, 1.0 equiv.), pentafluorophenol (0.33 g, 1.8 mmol, 1.0 equiv.) and DCC (0.45 g, 2.2 mmol, 1.2 equiv.) in anhydrous CH_2Cl_2 (0.2 M) gave crude product that was purified by flash silica column chromatography (hexane:Et_2O 100:0 to 90:10, R_F 0.33 at 95:5) to give the title compound as a colourless solid (0.34 g, 70%). **mp** 44 – 46 °C; **^{1}H NMR** (400 MHz, $CDCl_3$) δ_H: 5.17 (2H, ddd, *J* 46.0, 3.2, 2.2, C(4)H_2F), 6.39 (1H, dtd, *J* 15.8, 2.2, 1.1, C(2)*H*), 7.27 (1H, ddt, *J* 24.2, 15.8, 3.2, C(3)*H*); **^{19}F{^{1}H} NMR** (377 MHz, $CDCl_3$) δ_F: –224.9 (s, C(4)H_2*F*),

–162.6 – –162.4 (m, ArC*F*), –158.1 (t, *J* 21.5, ArC*F*), –152.8 – –152.7 (m, ArC*F*); **^{13}C{^{1}H} NMR** (126 MHz, $CDCl_3$) δ_C: 80.9 (d, *J* 174.7, *C*(4)H_2F), 117.6 (d, *J* 12.0, *C*(2)H), 124.9 – 125.3 (m, Ar*C*(1)), 136.9 – 139.3 (m, Ar*C*F), 138.5 – 140.9 (m, Ar*C*F), 140.2 – 142.5 (m, Ar*C*F), 147.1 (d, *J* 15.5, *C*(3)H), 161.5 (*C*(1)); **IR** ν_{max} (film) 2930, 1755, 1663, 1514, 1470, 1445, 1298, 1275, 1148, 1125, 1078, 991, 959, 937, 916, 824; **HRMS** (EI^+) $C_{10}H_4O_2F_6$ $[M]^+$ found 270.0118, requires 270.0110 (+3.0 ppm).

Perfluorophenyl (*E*)-4-methoxybut-2-enoate (S14)



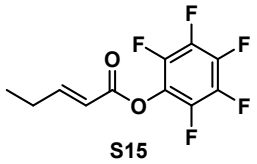
S14

Following General Procedure F, (*E*)-4-methoxybut-2-enoic acid **S10** (0.99 g, 8.5 mmol, 1.0 equiv.), pentafluorophenol (1.56 g, 8.5 mmol, 1.0 equiv.) and DCC (2.10 g, 10.2 mmol, 1.2 equiv.) in anhydrous CH_2Cl_2 (0.2 M) gave crude product that was purified by flash silica column chromatography (hexane:Et_2O 100:0 to 85:15, R_F 0.39 at 90:10) to give the title compound as a colourless oil (0.66 g, 28%). **^{1}H NMR** (400 MHz, $CDCl_3$) δ_H: 3.45 (3H, s, OCH_3), 4.19 (2H, dd, *J* 3.8, 2.2, C(4)H_2), 6.34 (1H, dt, *J* 15.7, 2.2, C(2)*H*), 7.26 (1H, dt, *J* 15.7, 3.8, C(3)*H*); **^{19}F{^{1}H} NMR** (376 MHz, $CDCl_3$) δ_F: –162.7 – –162.6 (m, ArC*F*),

–158.4 (t, *J* 21.8, ArC*F*), –152.8 – –152.7 (m, ArC*F*); **^{13}C{^{1}H} NMR** (126 MHz, $CDCl_3$) δ_C: 59.1

(OCH_3), 71.1 (*C*(4)H_2), 117.5 (*C*(2)H), 125.0 – 125.4 (m, Ar*C*(1)), 136.8 – 139.2 (m, Ar*C*F), 138.4 – 140.7 (m, Ar*C*F), 140.2 – 142.6 (m, Ar*C*F), 150.1 (*C*(3)H), 162.0 (*C*(1)); **IR** ν_{max} (film) 2934, 2830, 1759, 1659, 1516, 1472, 1281, 1192, 1111, 991, 928; **HRMS** (EI^+) $C_{11}H_7O_3F_5$ $[M]^+$ found 282.0308, requires 282.0310 (–0.7 ppm).

Perfluorophenyl (*E*)-pent-2-enoate (S15)

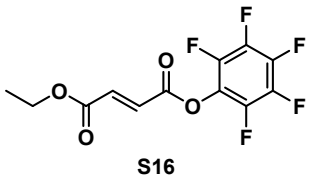


S15

(*E*)-Pent-2-enoic acid (0.51 mL, 5.0 mmol, 1.0 equiv.) and oxalyl chloride (0.44 mL, 5.25 mmol, 1.05 equiv.) were dissolved in anhydrous CH_2Cl_2 (0.3 M). A few drops of DMF were added and the reaction mixture stirred at RT for 1 h. A solution of pentafluorophenol (0.92 g, 5.0 mmol, 1.0 equiv.) and *i*-Pr_2NEt (1.71 mL, 10.0 mmol, 2.0 equiv.) in anhydrous CH_2Cl_2 (0.3 M) was then added dropwise and the reaction mixture stirred at RT o/n. Once complete, the solvent was removed under reduced pressure to give the crude product which was purified by flash silica column chromatography (hexane:CH_2Cl_2 80:20 to 50:50, R_F 0.84 at 50:50) to give the title compound as a colourless oil (0.84 g, 63%). **^{1}H NMR** (400 MHz, $CDCl_3$) δ_H: 1.15 (3H, t, *J* 7.4, C(5)H_3), 2.32 – 2.41 (2H, m, C(4)H_2), 6.06 (1H, dt, *J* 15.7, 1.8, C(2)*H*), 7.36 (1H, dt, *J* 15.7, 6.3, C(3)*H*); **^{19}F{^{1}H} NMR** (377 MHz, $CDCl_3$) δ_F: –162.8 – –162.6 (m, ArC*F*), –158.6 (t, *J* 21.7, ArC*F*), –152.9 – –152.7 (m, ArC*F*); **IR** ν_{max} (film) 2974, 1759, 1651, 1514, 1283, 1209, 1123, 1101, 1024, 991, 891, 854.

Spectroscopic data in accordance with the literature.[8]

Ethyl perfluorophenyl fumarate (S16)

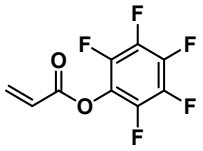


S16

(*E*)-4-Ethoxy-4-oxobut-2-enoic acid (2.88 g, 20.0 mmol, 2.0 equiv.) and EDCI·HCl (2.88 g, 15.0 mmol, 1.5 equiv.) were dissolved in anhydrous CH_2Cl_2 (0.3 M) and stirred at RT for 15 min. Pentafluorophenol (1.84 g, 10.0 mmol, 1.0 equiv.) was then added and the reaction mixture stirred at RT o/n. Once complete, the mixture was diluted with CH_2Cl_2 and washed with sat. $NaHCO_3$ (× 3), dried over $MgSO_4$, and the solvent removed under reduced pressure to give the crude product. Purification by flash silica column chromatography (hexane:CH_2Cl_2 80:20 to 0:100, R_F 0.44 at 50:50) gave the title compound as a colourless low-melting solid (1.83 g, 59%). **^{1}H NMR** (400 MHz, $CDCl_3$) δ_H: 1.35 (3H, t, *J* 7.1, C*H*$_3$), 4.32 (2H, q, *J* 7.1, C*H*$_2$), 7.06 (1H, d, 15.8, C*H*=CH), 7.12 (1H, d, 15.8, CH=C*H*); **^{19}F{^{1}H} NMR** (376 MHz, $CDCl_3$) δ_F: –162.0 – –161.8 (m, ArC*F*), –157.1 (t, *J* 21.6, ArC*F*), –152.4 – –152.3 (m, ArC*F*); **IR** ν_{max} (film) 2990, 1767, 1726, 1516, 1283, 1117, 993, 982, 926, 764.

Spectroscopic data in accordance with the literature.[8]

Perfluorophenyl acrylate (75)



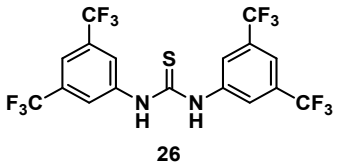
75

Following General Procedure F, acrylic acid (1.37 mL, 20.0 mmol, 1.0 equiv.), pentafluorophenol (3.68 g, 20.0 mmol, 1.0 equiv.) and DCC (4.95 g, 24.0 mmol, 1.2 equiv.) in anhydrous CH_2Cl_2 (0.2 M) gave crude product that was purified by flash silica column chromatography (hexane:Et_2O 100:0 to 90:10, R_F 0.66 at 90:10) to give the title compound as a colourless volatile oil (2.67 g, 56%). **^{1}H NMR** (400 MHz, $CDCl_3$) δ_H: 6.18 (1H, dd, *J* 10.5, 1.0, CHC*H*^{A}H^B), 6.37 (1H, dd, *J* 17.3, 10.5, C*H*CH$_2$), 6.72 (1H, dd, *J* 17.3, 1.0, CHCH^{A}C*H*^{B}); **^{19}F{^{1}H} NMR** (377 MHz, $CDCl_3$) δ_F: –162.5 – –162.3 (m, ArC*F*), –158.0 (t, *J* 21.7, ArC*F*), –152.7 – –152.6 (m, ArC*F*); **IR** ν_{max} (film) 1771, 1514, 1406, 1217, 1111, 991, 978, 870, 797.

Spectroscopic data in accordance with the literature.[10]

5. Preparation of Thioureas

1,3-Bis(3,5-bis(trifluoromethyl)phenyl)thiourea (26)

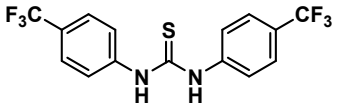


26

3,5-Bis(trifluoromethyl)phenyl isothiocyanate (1.83 mL, 10 mmol, 1.0 equiv.) and 3,5-bis(trifluoromethyl)aniline (1.56 mL, 10 mmol, 1.0 equiv.) were dissolved in anhydrous CH_2Cl_2 (0.2 M) and the reaction mixture stirred at RT for 5 h. Once complete the solvent was removed to give the crude product as a white solid. Recrystallisation from $CHCl_3$/EtOAc gave the title compound as colourless crystals (4.39 g, 88%). **mp** 143 – 145 °C {lit[11] 170 – 172}; **^{1}H NMR** (400 MHz, $CDCl_3$) δ_H: 7.78 (2H, s, ArC(4)*H*), 7.89 (4H, s, ArC(2,6)*H*), 7.92 (2H, s, N*H*); **^{19}F{^{1}H} NMR** (377 MHz, $CDCl_3$) δ_F: –63.0 (s, CF_3).

Spectroscopic data in accordance with literature.[11]

1,3-Bis(4-(trifluoromethyl)phenyl)thiourea (S17)



S17

4-Trifluoromethylphenyl isothiocyanate (2.03 g, 10 mmol, 1.0 equiv.) and 4-trifluoromethylaniline (1.26 mL, 10 mmol, 1.0 equiv.) were dissolved in anhydrous CH_2Cl_2 (0.2 M) and the reaction mixture stirred at RT for 6 h. Once complete the solvent was removed to give the crude product as a yellow solid. Recrystallisation from $CHCl_3$/EtOAc gave the title compound as colourless crystals (2.87 g, 79%). **mp** 131 – 133 °C {lit[11] 161 – 163 °C}; **^{1}H NMR** (400 MHz, $CDCl_3$) δ_H: 7.53 – 7.60 (4H, m, ArC(2,6)*H*), 7.68 – 7.75 (4H, m, ArC(3,5)*H*), 7.89 (2H, br s, N*H*); **^{19}F{^{1}H} NMR** (377 MHz, $CDCl_3$) δ_F: –62.5 (s, CF_3).

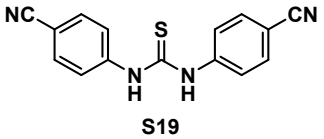
Spectroscopic data in accordance with literature.[11]

1,3-Bis(4-nitrophenyl)thiourea (S18)

S18

4-Nitrophenylisothiocyanate (2.70 g, 15 mmol, 1.0 equiv.) and 4-nitroaniline (2.07 g, 15 mmol, 1.0 equiv.) were dissolved in anhydrous CH_2Cl_2 (0.2 M). Pyridine (1.21 mL, 15 mmol, 1.0 equiv.) was added and the reaction mixture stirred at RT. Once complete, the solvent was removed, and the crude product recrystallised from acetone to give the title compound as golden crystals (3.64 g, 76%). **mp** 163 – 165 °C; **^{1}H NMR** (400 MHz, $(CD_3)_2SO$) δ_H: 7.81 – 7.87 (4H, m, ArC(2,6)*H*), 8.21 – 8.27 (4H, m, ArC(3,5)*H*), 10.77 (2H, br s, N*H*); **^{13}C{^{1}H} NMR** (126 MHz, $(CD_3)_2SO$) δ_C: 122.5 (Ar*C*(2,6)H), 125.0 (Ar*C*(3,5)H), 143.2 (Ar*C*(1)), 146.3(Ar*C*(4)), 179.6 (*C*S); **IR** ν_{max} (film) 3318, 1589, 1580, 1539, 1493, 1317, 1292, 1242, 1233, 1173, 1105, 860, 843, 804; **HRMS** (ESI^-) $C_{13}H_9O_4N_4S$ $[M-H]^-$ found 317.0348, requires 317.0350 (–0.6 ppm).

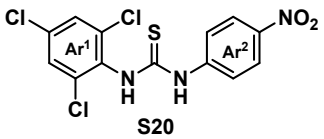
1,3-Bis(4-cyanophenyl)thiourea (S19)



S19

4-Cyanophenylisothiocyanate (1.60 g, 10 mmol, 1.0 equiv.) and 4-aminobenzonitrile (1.18 g, 10 mmol, 1.0 equiv.) were dissolved in anhydrous Et_2O (0.2 M). Pyridine (0.81 mL, 10 mmol, 1.0 equiv.) was added and the reaction mixture stirred at RT. Once complete, the precipitate was filtered off washing with CH_2Cl_2 to afford the title compound as a white solid (2.09 g, 75%). **mp** 144 – 146 °C; **^{1}H NMR** (400 MHz, $(CD_3)_2SO$) δ_H: 7.74 – 7.83 (8H, m, ArC(2,6)*H* and ArC(3,5)*H*), 10.52 (2H, br s, N*H*); **^{13}C{^{1}H} NMR** (126 MHz, $(CD_3)_2SO$) δ_C: 106.3 (*C*N), 119.4 (Ar*C*(4)), 123.1 (Ar*C*(2,6)H), 133.3 (Ar*C*(3,5)H), 144.1 (Ar*C*(1)), 179.6 (*C*S); **IR** ν_{max} (film) 3291, 2218, 1589, 1526, 1506, 1327, 1290, 1254, 1229, 1198, 1173, 827; **HRMS** (ESI^+) $C_{15}H_{10}N_4NaS$ $[M+Na]^+$ found 301.0514, requires 301.0518 (–1.3 ppm).

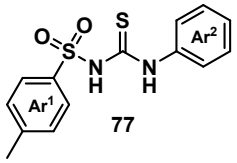
1-(4-Nitrophenyl)-3-(2,4,6-trichlorophenyl)thiourea (S20)



S20

2,4,6-Trichlorophenylisothiocyanate (1.19 g, 5.0 mmol, 1.0 equiv.) and 4-nitroaniline (0.69 g, 5.0 mmol, 1.0 equiv.) were dissolved in anhydrous CH_2Cl_2 (0.2 M). Pyridine (0.40 mL, 5.0 mmol, 1.0 equiv.) was added and the reaction mixture stirred at RT. Once complete, the solvent was removed under reduced pressure to afford the crude product which was recrystallised from acetone to give the title compound as yellow crystals (0.81 g, 43%). **mp** 140 – 142 °C; **^{1}H NMR** (500 MHz, $(CD_3)_2SO$) δ_H: 7.78 (2H, s, Ar^{1}C(3,5)*H*), 7.86 – 7.96 (2H, m, Ar^{2}C(2,6)*H*), 8.20 – 8.26 (2H, m, Ar^{2}C(3,5)*H*), 9.86 (1H, br s, N*H*), 10.79 (1H, br s, N*H*); **^{13}C{^{1}H} NMR** (126 MHz, $(CD_3)_2SO$) δ_C: 121.7 (Ar^2*C*(2,6)H), 124.4 (Ar^2*C*(3,5)H), 128.3 (Ar^1*C*(3,5)H), 132.8 (Ar^1*C*(4)), 133.8 (Ar^1*C*(1)), 135.6 (Ar^1*C*(2,6)), 142.7 (Ar^2*C*(1)), 145.8 (Ar^1*C*(4)), 180.4 (*C*S); **IR** ν_{max} (film) 3374, 3281, 3051, 1589, 1495, 1479, 1325, 1302, 1265, 1186, 1107, 853, 831, 818, 800; **HRMS** (ESI^-) $C_{13}H_7O_2N_3{}^{35}Cl_3S$ $[M-H]^-$ found 373.9337, requires 373.9330 (+1.9 ppm).

4-Methyl-*N*-(phenylcarbamothioyl)benzenesulfonamide (77)

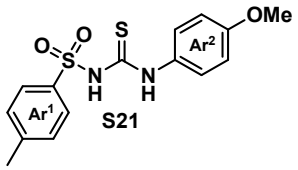


77

Following General Procedure B, *p*-toluenesulfonamide (0.86 g, 5.0 mmol, 1.0 equiv.), phenyl isothiocyanate (0.60 mL, 5.0 mmol, 1.0 equiv.) and Cs_2CO_3 (1.63 g, 5.0 mmol, 1.0 equiv.) in acetone (0.25 M) gave the title compound as a white solid (0.69 g, 45%). **mp** 105 – 107 °C {lit[12] 145 – 148 °C}; **^{1}H NMR** (400 MHz, $(CD_3)_2SO$) δ_H: 2.50 (3H, s, C*H*$_3$), 7.27 – 7.34 (1H, m, Ar^{2}C(4)*H*), 7.42 – 7.50 (2H, m, Ar^{2}C(3,5)*H*), 7.51 – 7.61 (4H, m, Ar^{1}C(3,5)*H* and Ar^{2}C(2,6)*H*), 7.97 – 8.04 (2H, m, Ar^{1}C(2,6)*H*), 10.36 (1H, s, N*H*), 11.66 (1H, br s, N*H*).

Spectroscopic data in accordance with literature.[12]

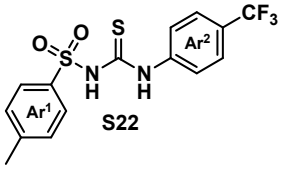
***N*-((4-Methoxyphenyl)carbamothioyl)-4-methylbenzenesulfonamide (S21)**



Following General Procedures A and B, *p*-anisidine (0.62 g, 5.0 mmol, 1.0 equiv.), thiophosgene (0.57 mL, 7.5 mmol, 1.5 equiv.) and $NaHCO_3$ (1.68 g, 20.0 mmol, 4.0 equiv.) in 1:1 H_2O:CH_2Cl_2 (0.25 M) followed by *p*-toluenesulfonamide (0.86 g, 5.0 mmol, 1.0 equiv.) and Cs_2CO_3 (1.63 g, 5.0 mmol, 1.0 equiv.) in acetone (0.25 M) gave the crude product as a pale-brown solid. The crude product was recrystallised from EtOH to afford the title compound as pale-brown crystals (0.90 g, 54%). **mp** 108 – 110 °C {lit[13] 144 °C}; **^{1}H NMR** (400 MHz, ($CDCl_3$) δ_H: 2.45 (3H, s, C*H*$_3$), 3.79 (3H, s, OC*H*$_3$), 6.85 – 6.92 (2H, m, Ar^{2}C(3,5)*H*), 7.23 – 7.29 (2H, m, Ar^{1}C(3,5)*H*), 7.33 – 7.39 (2H, m, Ar^{2}C(2,6)*H*), 7.77 – 7.84 (2H, m, Ar^{1}C(2,6)*H*), 8.55 (1H, br s, N*H*), 9.60 (1H, br s, N*H*).

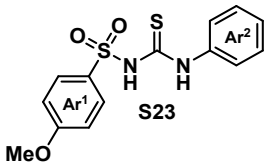
Spectroscopic data in accordance with the literature.[13]

4-Methyl-*N*-((4-(trifluoromethyl)phenyl)carbamothioyl)benzenesulfonamide (S22)



Following General Procedure B, *p*-toluenesulfonamide (0.86 g, 5.0 mmol, 1.0 equiv.), 4-(trifluoromethyl)phenyl isothiocyanate (1.02 g, 5.0 mmol, 1.0 equiv.) and Cs_2CO_3 (1.63 g, 5.0 mmol, 1.0 equiv.) in acetone (0.25 M) gave the title compound as a white solid (1.73 g, 93%). **mp** 131 – 133 °C; **^{1}H NMR** (400 MHz, $CDCl_3$) δ_H: 2.47 (3H, s, C*H*$_3$), 7.35 – 7.41 (2H, m, Ar^{1}C(3,5)*H*), 7.61 – 7.71 (4H, m, Ar^{2}C(2,3,5,6)*H*), 7.78 – 7.84 (2H, m, Ar^{1}C(2,6)*H*), 8.24 (1H, br s, N*H*), 9.90 (1H, s, N*H*); **^{19}F{^{1}H} NMR** (377 MHz, $CDCl_3$) δ_F: –62.5 (s, C*F*$_3$); **^{13}C{^{1}H} NMR** (126 MHz, $CDCl_3$) δ_C: 21.9 (*C*H$_3$), 123.9 (q, *J* 272.1, *C*F$_3$), 124.0 (Ar^2*C*(2,6)H), 126.4 (q, *J* 3.8, Ar^2*C*(3,5)H), 127.2 (Ar^1*C*(2,6)H), 129.0 (q, *J* 33.0, Ar^2*C*(4)), 130.6 (Ar^1*C*(3,5)H), 135.3 (Ar^1*C*(1)), 140.5 (Ar^2*C*(1)), 146.3 (Ar^1*C*(4)), 176.8 (*C*S); **IR** ν_{max} (film) 3291, 3049, 2907, 1618, 1595, 1530, 1476, 1377, 1319, 1146, 1105, 1080, 1063, 1016, 920, 843, 812; **HRMS** (ESI^-) $C_{15}H_{12}O_2N_2F_3S_2$ $[M-H]^-$ found 373.0296, requires 373.0298 (–0.5 ppm).

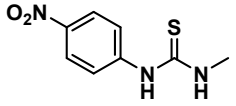
4-Methoxy-*N*-(phenylcarbamothioyl)benzenesulfonamide (S23)



S23

Following General Procedures A and B, 4-methoxybenzenesulfonamide (0.56 g, 3.0 mmol, 1.0 equiv.), phenyl isothiocyanate (0.36 mL, 3.0 mmol, 1.0 equiv.) and Cs_2CO_3 (0.98 g, 3.0 mmol, 1.0 equiv.) in acetone (0.25 M) gave the title compound, after trituration with Et_2O, as a white solid (0.74 g, 76%). **mp** 102 – 104 °C; **^{1}H NMR** (500 MHz, $(CD_3)_2SO$) δ_H: 3.85 (3H, s, CH_3), 7.11 – 7.23 (3H, m, Ar^{1}C(3,5)*H* and Ar^{2}C(4)*H*), 7.31 – 7.38 (2H, m, Ar^{2}C(3,5)*H*), 7.40 – 7.46 (2H, m, Ar^{2}C(2,6)*H*), 7.89 – 7.94 (2H, m, Ar^{1}C(2,6)*H*), 10.18 (1H, s, N*H*), 11.45 (1H, br s, N*H*); **^{13}C{^{1}H} NMR** (126 MHz, $(CD_3)_2SO$) δ_C: 55.8 (*C*H$_3$), 114.2 (Ar^1*C*(3,5)H), 124.1 (Ar^2*C*(2,6)H), 125.8 (Ar^2*C*(4)H), 130.8 (Ar^1*C*(1)), 128.6 (Ar^2*C*(3,5)H), 130.1 (Ar^1*C*(2,6)H), 138.2 (Ar^2*C*(1)), 163.0 (Ar^1*C*(4)), 177.6 (*C*S); **IR** ν_{max} (film) 3292, 3007, 2901, 2841, 2747, 1591, 1508, 1495, 1379, 1265, 1173, 1140, 1082, 1022, 907, 845, 827, 800; **HRMS** (ESI^-) $C_{14}H_{13}O_3N_2S_2$ $[M-H]^-$ found 321.0369, requires 321.0373 (–1.2 ppm).

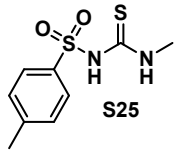
1-Methyl-3-(4-nitrophenyl)thiourea (S24)



S24

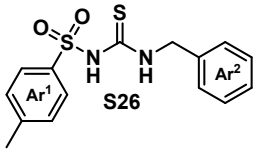
Methylamine (2 M in THF) (1.1 mL, 2.2 mmol, 1.0 equiv.) was added to a solution of 4-nitrophenylisothiocyanate (0.40 g, 2.2 mmol, 1.0 equiv.) in anhydrous Et_2O (0.2 M). The reaction mixture was stirred at RT for 30 min. The resulting precipitate was filtered under vacuum, washing with Et_2O to afford the title compound as an off-white solid (0.29 g, 63%). **mp** 151 – 153 °C; **^{1}H NMR** (400 MHz, $(CD_3)_2SO$) δ_H: 2.93 (3H, d, *J* 4.4, CH_3), 7.74 – 7.83 (2H, m, ArC(2,6)*H*), 8.14 – 8.20 (2H, m, ArC(3,5)*H*), 8.25 (1H, br s, N*H*), 10.19 (1H, s, N*H*); **^{13}C{^{1}H} NMR** (126 MHz, $(CD_3)_2SO$) δ_C: 31.2 (*C*H$_3$), 120.3 (Ar*C*(2,6)H), 124.6 (Ar*C*(3,5)H), 141.7 (Ar*C*(1)), 146.4 (Ar*C*(4)), 180.8 (*C*S); **IR** ν_{max} (film) 3262, 3215, 3098, 3049, 1580, 1557, 1506, 1495, 1435, 1329, 1277, 1242, 1179, 1111, 1055, 849; **HRMS** (ESI^+) $C_8H_9O_2N_3NaS$ $[M+Na]^+$ found 234.0310, requires 234.0308 (+0.9 ppm).

4-Methyl-*N*-(methylcarbamothioyl)benzenesulfonamide (S25)



Following General Procedure B, *p*-toluenesulfonamide (0.34 g, 2.0 mmol, 1.0 equiv.), methyl isothiocyanate (0.13 mL, 2.0 mmol, 1.0 equiv.) and Cs_2CO_3 (0.65 g, 2.0 mmol, 1.0 equiv.) in acetone (0.25 M) gave the crude product as a brown solid. Trituration with Et_2O gave the title compound as a colourless solid (0.20 g, 41%). **mp** 132 – 134 °C; **^{1}H NMR** (400 MHz, $(CD_3)_2SO$) δ_H: 2.39 (3H, s, C*H*$_3$), 2.88 (3H, d, *J* 4.5, NC*H*$_3$), 7.40 – 7.46 (2H, m, ArC(3,5)*H*), 7.78 – 7.83 (2H, m, ArC(2,6)*H*), 8.48 (1H, q, *J* 4.5, N*H*), 11.55 (1H, br s, N*H*); **^{13}C{^{1}H} NMR** (126 MHz, $(CD_3)_2SO$) δ_C: 21.1 (*C*H$_3$), 32.2 (NCH$_3$), 127.2 (Ar*C*(2,6)H), 129.6 (Ar*C*(3,5)H), 136.5 (Ar*C*(1)), 144.2 (Ar*C*(4)), 178.8 (*C*S); **IR** ν_{max} (film) 3337, 3294, 3211, 3038, 1570, 1543, 1483, 1464, 1416, 1364, 1159, 1152, 1123, 1084, 1036, 858, 810; **HRMS** (ESI^-) $C_9H_{11}O_2N_2S_2$ $[M-H]^-$ found 243.0268, requires 243.0267 (+0.4 ppm).

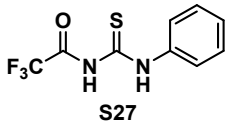
4-Methyl-*N*-(benzylcarbamothioyl)benzenesulfonamide (S26)



Following General Procedures A and B, benzylamine (1.09 mL, 10.0 mmol, 1.0 equiv.), thiophosgene (1.15 mL, 15.0 mmol, 1.5 equiv.) and $NaHCO_3$ (3.36 g, 40.0 mmol, 4.0 equiv.) in 1:1 H_2O:CH_2Cl_2 (0.25 M) followed by *p*-toluenesulfonamide (1.71 g, 10.0 mmol, 1.0 equiv.) and Cs_2CO_3 (3.26 g, 10.0 mmol, 1.0 equiv.) in acetone (0.25 M) gave the crude product as a pale-brown solid. The crude product was triturated with Et_2O to afford the title compound as an off-white solid (1.67 g, 52%). **mp** 125 – 127 °C; **^{1}H NMR** (400 MHz, $(CD_3)_2SO$) δ_H: 2.41 (3H, s, C*H*$_3$), 4.68 (2H, d, *J* 5.7, C*H*$_2$), 7.09 – 7.16 (2H, m, Ar^{2}C(2,6)*H*), 7.19 – 7.31 (3H, m, Ar^{2}C(3,4,5)*H*), 7.38 – 7.45 (2H, m, Ar^{1}C(3,5)*H*), 7.77 – 7.82 (2H, m, Ar^{1}C(2,6)*H*), 8.89 (1H, t, *J* 5.7, N*H*), 11.62 (1H, s, N*H*); **^{13}C{^{1}H} NMR** (126 MHz, $(CD_3)_2SO$) δ_C: 21.1 (*C*H$_3$), 47.7 (*C*H$_2$), 127.0 (Ar^2*C*(4)H), 127.3 (Ar^1*C*(2,6)H), 127.3 (Ar^2*C*(2,6)H), 128.2 (Ar^2*C*(3,5(H), 129.7 (Ar^1*C*(3,5)H), 136.3 (Ar^1*C*(1)), 137.4 (Ar^2*C*(1)), 144.3 (Ar^1*C*(4)), 178.6 (*C*S); **IR** ν_{max} (film) 3321, 2980, 1543, 1489, 1435, 1383, 1344, 1256, 1171, 1134, 1084, 1065,

937, 856, 810; **HRMS** (ESI^-) $C_{15}H_{15}O_2N_2S_2$ $[M-H]^-$ found 319.0581, requires 319.0580 (+0.3 ppm).

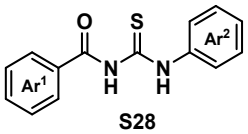
2,2,2-Trifluoro-*N*-(phenylcarbamothioyl)acetamide (S27)



S27

Following General Procedure B, trifluoroacetamide (0.57 g, 5.0 mmol, 1.0 equiv.), phenyl isothiocyanate (0.60 mL, 5.0 mmol, 1.0 equiv.) and Cs_2CO_3 (1.63 g, 5.0 mmol, 1.0 equiv.) in acetone (0.25 M) gave the crude product as a yellow solid. Purification by flash silica column chromatography (hexane:CH_2Cl_2 25:75 to 0:100, R_F 0.29 at 0:100) gave the title compound as a white solid (0.48 g, 39%). **mp** 70 – 72 °C; **^{1}H NMR** (400 MHz, $(CD_3)_2SO$) δ_H: 7.26 – 7.33 (1H, m, ArC(4)*H*), 7.40 – 7.47 (2H, m, ArC(3,5)*H*), 7.63 – 7.71 (2H, m, ArC(2,6)*H*), 11.61 (1H, br s, N*H*), 12.47 (1H, br s, N*H*); **^{19}F{^{1}H} NMR** (377 MHz, $(CD_3)_2SO$) δ_F: –73.8 (s, C*F*$_3$); **^{13}C{^{1}H} NMR** (126 MHz, $(CD_3)_2SO$) δ_C: 115.3 (q, *J* 288.5, *C*F$_3$), 123.9 (Ar*C*(2,6)H), 126.7 (Ar*C*(4)H), 128.8 (Ar*C*(3,5)H), 137.9 (Ar*C*(1)), 154.6 (q, *J* 39.2, *C*OCF$_3$), 176.4 (*C*S); **IR** ν_{max} (film) 3262, 3211, 3044, 1715, 1595, 1533, 1452, 1302, 1207, 1152, 1107, 1070, 941, 858; **HRMS** (ESI^-) $C_9H_6ON_2F_3S$ $[M-H]^-$ found 247.0159, requires 247.0158 (+0.4 ppm).

***N*-(Phenylcarbamothioyl)benzamide (S28)**

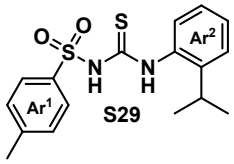


S28

Benzoyl chloride (1.16 mL, 10.0 mmol, 1.0 equiv.) was added slowly to a solution of NH_4SCN (0.84 g, 11.0 mmol, 1.1 equiv.) in acetone (0.25 M) then heated to reflux for 15 min. Aniline (0.91 mL, 10.0 mmol, 1.0 equiv.) was then added and the reaction mixture heated to reflux for a further 30 min. Once complete, the reaction mixture was poured into ice water with stirring. The resulting precipitate was filtered off under vacuum washing with H_2O to give the crude product as an off-white solid. Recrystallisation from EtOH (0.2 M) gave the title compound as colourless needles (2.01 g, 79%). **mp** 115 – 117

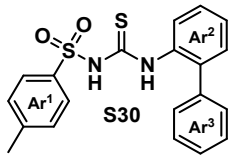
°C; **^{1}H NMR** (500 MHz, $(CD_3)_2SO$) δ_H: 7.24 – 7.31 (1H, m, $Ar^2C(4)H$), 7.40 – 7.46 (2H, m, $Ar^2C(3,5)H$), 7.51 – 7.57 (2H, m, $Ar^1C(3,5)H$), 7.63 – 7.68 (1H, m, $Ar^1C(4)H$), 7.69 – 7.73 (2H, m, $Ar^2C(2,6)H$), 7.96 – 8.02 (2H, m, $Ar^1C(2,6)H$), 11.57 (1H, s, N*H*), 12.64 (1H, s, N*H*); **^{13}C{^{1}H} NMR** (126 MHz, $(CD_3)_2SO$) δ_C: 124.3 ($Ar^2C(2,6)H$), 126.3 ($Ar^2C(4)H$), 128.4 ($Ar^2C(3,5)H$), 128.7 ($Ar^1C(3,5)H$), 128.7 ($Ar^1C(2,6)H$), 132.1 ($Ar^1C(1)$), 133.1 ($Ar^1C(4)H$), 138.0 ($Ar^2C(1)$), 168.3 (*C*S), 179.1 (*C*O); **IR** ν_{max} (film) 3258, 2986, 1670, 1599, 1558, 1526, 1483, 1447, 1356, 1254, 1142, 1070, 1026, 905, 793; **HRMS** (ESI^+) $C_{14}H_{12}ON_2NaS$ $[M+Na]^+$ found 279.0568, requires 279.0563 (+1.8 ppm).

_N_-((2-_iso_-Propylphenyl)carbamothioyl)-4-methylbenzenesulfonamide (S29)



Following General Procedures A and B, 2-*iso*-propylaniline (1.42 mL, 10.0 mmol, 1.0 equiv.), thiophosgene (1.15 mL, 15.0 mmol, 1.5 equiv.) and $NaHCO_3$ (3.36 g, 40.0 mmol, 4.0 equiv.) in 1:1 H_2O:CH_2Cl_2 (0.25 M) followed by *p*-toluenesulfonamide (1.71 g, 10.0 mmol, 1.0 equiv.) and Cs_2CO_3 (3.26 g, 10.0 mmol, 1.0 equiv.) in acetone (0.25 M) gave the crude product as a pale-brown solid. The crude product was recrystallised from EtOH to afford the title compound as colourless crystals (1.85 g, 53%). **mp** 146 – 148 °C; **^{1}H NMR** (400 MHz, $(CD_3)_2SO$) δ_H: 1.03 (6H, d, *J* 6.8, $CH(CH_3)_2$), 2.42 (3H, s, CH_3), 2.71 (1H, hept, *J* 6.8, $CH(CH_3)_2$), 7.01 – 7.06 (1H, m, $Ar^2C(6)H$), 7.13 – 7.20 (1H, m, $Ar^2C(5)H$), 7.23 – 7.32 (2H, m, $Ar^2C(3)H$ and $Ar^2C(4)H$), 7.43 – 7.49 (2H, m, $Ar^1C(3,5)H$), 7.87 – 7.93 (2H, m, $Ar^1C(2,6)H$), 9.76 (1H, br s, N*H*), 11.78 (1H, br s, N*H*); **^{13}C{^{1}H} NMR** (126 MHz, $(CD_3)_2SO$) δ_C: 21.1 (CH_3), 23.1 ($CH(CH_3)_2$), 27.5 ($CH(CH_3)_2$), 125.8 ($Ar^2C(3)H$), 125.9 ($Ar^2C(6)H$), 127.5 ($Ar^1C(2,6)H$), 127.9 ($Ar^2C(5)H$), 128.5 ($Ar^2C(4)H$), 129.6 ($Ar^1C(3,5)H$), 135.7 ($Ar^2C(1)$), 136.4 ($Ar^1C(1)$), 144.2 ($Ar^1C(4)$), 144.9 ($Ar^2C(2)$), 179.3 (*C*S); **IR** ν_{max} (film) 3281, 2961, 2911, 1516, 1474, 1456, 1373, 1244, 1177, 1134, 1080, 918, 849, 835, 812, 766; **HRMS** (ESI^+) $C_{17}H_{20}O_2N_2NaS_2$ $[M+Na]^+$ found 371.0867, requires 371.0858 (+2.4 ppm).

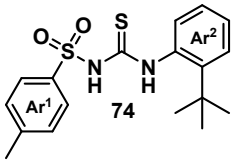
***N*-([1,1'-Biphenyl]-2-ylcarbamothioyl)-4-methylbenzenesulfonamide (S30)**



Following General Procedures A and B, 2-aminobiphenyl (1.69 g, 10.0 mmol, 1.0 equiv.), thiophosgene (1.15 mL, 15.0 mmol, 1.5 equiv.) and $NaHCO_3$ (3.36 g, 40.0 mmol, 4.0 equiv.) in 1:1 H_2O:CH_2Cl_2 (0.25 M) followed by *p*-toluenesulfonamide (1.71 g, 10.0 mmol, 1.0 equiv.) and Cs_2CO_3 (3.26 g, 10.0 mmol, 1.0 equiv.) in acetone (0.25 M) gave the crude product as a pale-brown solid. The crude product was triturated with Et_2O to afford the title compound as a white solid (2.20 g, 58%). **mp** 129 – 131 °C; **^{1}H NMR** (500 MHz, $(CD_3)_2SO$) δ_H: 2.43 (3H, s, C*H*$_3$), 7.27 – 7.39 (9H, m, Ar^{2}C(3,4,5,6)*H* and Ar^{3}C(2,3,4,5,6)*H*), 7.40 – 7.44 (2H, m, Ar^{1}C(3,5)*H*), 7.69 – 7.74 (2H, m, Ar^{1}C(2,6)*H*), 9.66 (1H, br s, N*H*), 11.56 (1H, br s, N*H*); **^{13}C{^{1}H} NMR** (126 MHz, $(CD_3)_2SO$) δ_C: 21.1 (*C*H$_3$), 127.5 (Ar^1*C*(2,6)H), 127.5 (ArCH), 127.6 (ArCH), 127.7 (ArCH), 128.3 (ArCH), 128.6 (ArCH), 129.0 (ArCH), 129.5 (Ar^1*C*(3,5)H), 130.2 (ArCH), 135.2 (Ar*C*), 136.4 (Ar^1*C*(1)), 138.2 (Ar*C*), 138.3 (Ar*C*), 144.1 (Ar^1*C*(4)), 178.7 (*C*S); **IR** ν_{max} (film) 3283, 3028, 2901, 1593, 1524, 1476, 1389, 1173, 1136, 1080, 924, 831, 812, 762; **HRMS** (ESI^-) $C_{20}H_{17}O_2N_2S_2$ $[M-H]^-$ found 381.0731, requires 381.0737 (–1.6 ppm).

Note: the biphenyl carbon signals could not be unambiguously assigned, even with 2D NMR.

***N*-((2-(*tert*-Butyl)phenyl)carbamothioyl)-4-methylbenzenesulfonamide (74)**

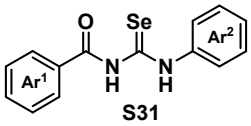


Following General Procedures A and B, 2-*tert*-butylaniline (1.56 mL, 10.0 mmol, 1.0 equiv.), thiophosgene (1.15 mL, 15.0 mmol, 1.5 equiv.) and $NaHCO_3$ (3.36 g, 40.0 mmol, 4.0 equiv.) in 1:1 H_2O:CH_2Cl_2 (0.25 M) followed by *p*-toluenesulfonamide (1.71 g, 10.0 mmol, 1.0 equiv.) and Cs_2CO_3 (3.26 g, 10.0 mmol, 1.0 equiv.) in acetone (0.25 M) gave the crude product as a pale-brown solid. The crude product was triturated with Et_2O to afford the title compound as a white solid (2.02 g, 56%). **mp** 150 – 152 °C; **^{1}H NMR** (400 MHz, $(CD_3)_2SO$) δ_H: 1.24 (9H, s, C(C*H*$_3$)$_3$), 2.41 (3H, s, C*H*$_3$), 6.91 – 6.96 (1H, m,

$Ar^2C(6)H$), 7.14 – 7.28 (2H, m, $Ar^2C(4)H$ and $Ar^2C(5)H$), 7.37 – 7.42 (1H, m, $Ar^2C(3)H$), 7.42 – 7.48 (2H, m, $Ar^1C(3,5)H$), 7.83 – 7.90 (2H, m, $Ar^1C(2,6)H$), 9.56 (1H, s, N*H*), 11.86 (1H, br s, N*H*); **$^{13}C\{^1H\}$ NMR** (126 MHz, $(CD_3)_2SO$) δ_C: 21.1 (CH_3), 30.5 ($C(CH_3)_3$), 34.6 ($C(CH_3)_3$), 126.3 ($Ar^2C(3)H$), 126.9 ($Ar^2C(6)H$), 127.6 ($Ar^1C(2,6)H$), 127.7 ($Ar^2C(5)H$), 129.6 ($Ar^1C(3,5)H$), 131.6 ($Ar^2C(4)H$), 136.2 ($Ar^2C(1)$), 136.5 ($Ar^1C(1)$), 144.2 ($Ar^1C(4)$), 145.8 ($Ar^2C(2)$), 178.9 (*C*S); **IR** ν_{max} (film) 3292, 2986, 2901, 2750, 1508, 1489, 1381, 1177, 1136, 1082, 918, 851, 835, 812, 760; **HRMS** (ESI^-) $C_{18}H_{21}O_2N_2S_2$ $[M-H]^-$ found 361.1047, requires 361.1050 (–0.8 ppm).

6. Preparation of Selenoureas

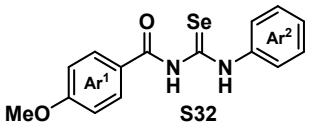
N-(Phenylcarbamoselenoyl)benzamide (S31)



S31

Following General Procedure C, benzoyl chloride (0.58 mL, 5.0 mmol, 1.0 equiv.), potassium selenocyanate (0.72 g, 5.0 mmol, 1.0 equiv.) and aniline (0.46 mL, 5.0 mmol, 1.0 equiv.) in acetone (0.25 M) gave the crude product as an orange solid. Purification by flash silica column chromatography (hexane:EtOAc 90:10 to 50:50, R_F 0.30 at 80:20) gave the title compound as a yellow solid (0.49 g, 32%). **mp** 99 – 101 °C; **^1H NMR** (400 MHz, $(CD_3)_2SO$) δ_H: 7.29 – 7.36 (1H, m, $Ar^2C(4)H$), 7.39 – 7.49 (2H, m, $Ar^2C(3,5)H$), 7.51 – 7.58 (2H, m, $Ar^1C(3,5)H$), 7.63 – 7.72 (3H, m, $Ar^1C(4)H$ and $Ar^2C(2,6)H$), 7.94 – 8.02 (2H, m, $Ar^1C(2,6)H$), 11.81 (1H, s, N*H*), 12.98 (1H, s, N*H*); **$^{13}C\{^1H\}$ NMR** (126 MHz, $(CD_3)_2SO$) δ_C: 125.1 ($Ar^2C(2,6)H$), 126.9 ($Ar^2C(4)H$), 128.4 ($Ar^1C(3,5)H$), 128.7 ($Ar^2C(3,5)H$), 128.8 ($Ar^1C(2,6)H$), 131.9 ($Ar^1C(1)$), 133.2 ($Ar^1C(4)H$), 139.0 ($Ar^2C(1)$), 168.1 (*C*Se), 180.5 (*C*O); **$^{77}Se\{^1H\}$ NMR** (95 MHz, $CDCl_3$) δ_{Se}: 415.6 (s, C*Se*); **IR** ν_{max} (film) 3237, 2957, 1668, 1597, 1558, 1520, 1497, 1483, 1447, 1356, 1260, 1130, 1076, 1061, 1024, 905, 835, 795; **HRMS** (ESI^+) $C_{14}H_{12}ON_2Na^{80}Se$ $[M+Na]^+$ found 327.0011, requires 327.0007 (+1.2 ppm).

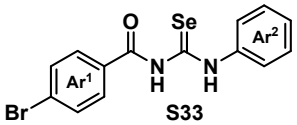
4-Methoxy-*N*-(phenylcarbamoselenoyl)benzamide (S32)



S32

Following General Procedure C, 4-methoxybenzoyl chloride (0.41 mL, 3.0 mmol, 1.0 equiv.), potassium selenocyanate (0.43 g, 3.0 mmol, 1.0 equiv.) and aniline (0.27 mL, 3.0 mmol, 1.0 equiv.) in acetone (0.25 M) gave the crude product as a brown solid. Purification by flash silica column chromatography (hexane:CH_2Cl_2 80:20 to 0:100, R_F 0.50 at 0:100) gave the title compound as a yellow solid (0.81 g, 81%). **mp** 118 – 120 °C; **^{1}H NMR** (400 MHz, $CDCl_3$) δ_H: 3.88 (3H, s, C*H*$_3$), 6.96 – 7.03 (2H, m, Ar^{1}C(3,5)*H*), 7.29 – 7.36 (1H, m, Ar^{2}C(4)*H*), 7.39 – 7.46 (2H, m, Ar^{2}C(3,5)*H*), 7.68 – 7.73 (2H, m, Ar^{2}C(2,6)*H*), 7.83 – 7.89 (2H, m, Ar^{1}C(2,6)*H*), 9.39 (1H, s, N*H*), 13.08 (1H, s, N*H*); **^{13}C{^{1}H} NMR** (126 MHz, $CDCl_3$) δ_C: 55.8 (*C*H$_3$), 114.6 (Ar^1*C*(3,5)H), 123.1 (Ar^1*C*(1)), 124.8 (Ar^2*C*(2,6)H), 127.6 (Ar^2*C*(4)H), 129.0 (Ar^2*C*(3,5)H), 129.9 (Ar^1*C*(2,6)H), 138.6 (Ar^2*C*(1)), 164.3 (Ar^1*C*(4)), 166.4 (*C*Se), 180.1 (*C*O); **^{77}Se{^{1}H} NMR** (95 MHz, $CDCl_3$) δ_{Se}: 394.3 (s, C*Se*); **IR** ν_{max} (film) 3264, 2940, 1657, 1589, 1522, 1491, 1447, 1312, 1256, 1177, 1157, 1136, 1115, 1026, 843, 804; **HRMS** (ESI^+) $C_{15}H_{14}O_2N_2Na^{80}Se$ $[M+Na]^+$ found 357.0113, requires 357.0113 (±0.0 ppm).

4-Bromo-*N*-(phenylcarbamoselenoyl)benzamide (S33)



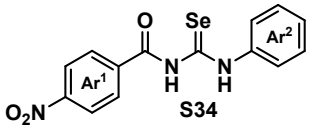
S33

Following General Procedure C, 4-bromobenzoyl chloride (0.66 g, 3.0 mmol, 1.0 equiv.), potassium selenocyanate (0.43 g, 3.0 mmol, 1.0 equiv.) and aniline (0.27 mL, 3.0 mmol, 1.0 equiv.) in acetone (0.25 M) gave the crude product as a beige solid. Purification by flash silica column chromatography (hexane:CH_2Cl_2 80:20 to 0:100, R_F 0.59 at 25:75) gave the title compound as a yellow solid (0.53 g, 46%). **mp** 115 – 117 °C; **^{1}H NMR** (400 MHz, $CDCl_3$) δ_H: 7.32 – 7.38 (1H, m, Ar^{2}C(4)*H*), 7.41 – 7.48 (2H, m, Ar^{2}C(3,5)*H*), 7.67 – 7.73 (4H, m, Ar^{1}C(3,5)*H* and Ar^{2}C(2,6)*H*), 7.75 – 7.80 (2H, m, Ar^{1}C(2,6)*H*), 9.38 (1H, s, N*H*), 12.92 (1H, s, N*H*); **^{13}C{^{1}H} NMR** (126 MHz, $CDCl_3$) δ_C: 124.8 (Ar^2*C*(2,6)H), 127.8 (Ar^2*C*(4)H), 129.2 (Ar^1*C*(3,5)H), 129.2 (Ar^2*C*(3,5)H), 129.4 (Ar^1*C*(4)), 132.8 (Ar^1*C*(2,6)H), 130.2 (Ar^1*C*(1)),

138.5 (Ar^2*C*(1)), 166.1 (*C*Se), 180.0 (*C*O); **^{77}Se{^{1}H} NMR** (95 MHz, $CDCl_3$) δ_{Se}: 414.3 (s, C*Se*);

IR ν_{max} (film) 3358, 2972, 1672, 1589, 1508, 1394, 1327, 1256, 1146, 1130, 1109, 1072, 1009, 910, 837; **HRMS** (ESI^+) $C_{14}H_{11}ON_2{}^{79}BrNa^{80}Se$ $[M+Na]^+$ found 404.9107, requires 404.9112 (–1.2 ppm).

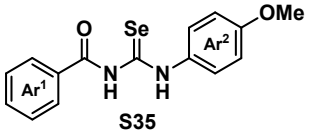
4-Nitro-*N*-(phenylcarbamoselenoyl)benzamide (S34)



S34

Following General Procedure C, 4-nitrobenzoyl chloride (0.56 g, 3.0 mmol, 1.0 equiv.), potassium selenocyanate (0.43 g, 3.0 mmol, 1.0 equiv.) and aniline (0.27 mL, 3.0 mmol, 1.0 equiv.) in acetone (0.25 M) gave the crude product as an orange solid. Purification by flash silica column chromatography (CH_2Cl_2:Et_2O 100:0 to 90:10, R_F 0.48 at 100:0) gave the title compound as a yellow solid (0.57 g, 55%). **mp** 123 – 125 °C; **^{1}H NMR** (400 MHz, $CDCl_3$) δ_H: 7.34 – 7.40 (1H, m, Ar^{2}C(4)*H*), 7.42 – 7.49 (2H, m, Ar^{2}C(3,5)*H*), 7.67 – 7.73 (2H, m, Ar^{2}C(2,6)*H*), 8.07 – 8.14 (2H, m, Ar^{1}C(2,6)*H*), 8.36 – 8.42 (2H, m, Ar^{1}C(3,5)*H*), 9.62 (1H, s, N*H*), 12.81 (1H, s, N*H*); **^{13}C{^{1}H} NMR** (126 MHz, $CDCl_3$) δ_C: 124.5 (Ar^1*C*(3,5)H), 124.8 (Ar^2*C*(2,6)H), 128.0 (Ar^2*C*(4)H), 129.1 (Ar^2*C*(3,5)H), 129.3 (Ar^1*C*(2,6)H), 136.9 (Ar^1*C*(1)), 138.3 (Ar^2*C*(1)), 150.9 (Ar^1*C*(4)), 165.1 (*C*Se), 179.8 (*C*O); **^{77}Se{^{1}H} NMR** (95 MHz, $CDCl_3$) δ_{Se}: 430.8 (s, C*Se*); **IR** ν_{max} (film) 3227, 2988, 1668, 1593, 1553, 1516, 1447, 1339, 1321, 1261, 1132, 1113, 1013, 868, 831, 795, 764; **HRMS** (ESI^+) $C_{14}H_{11}O_3N_3Na^{80}Se$ $[M+Na]^+$ found 371.9858, requires 371.9858 (±0.0 ppm).

***N*-((4-Methoxyphenyl)carbamoselenoyl)benzamide (S35)**

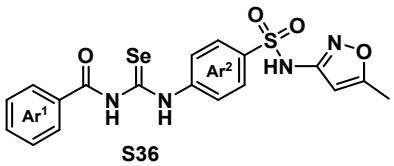


S35

Following General Procedure C, benzoyl chloride (0.35 mL, 3.0 mmol, 1.0 equiv.), potassium selenocyanate (0.43 g, 3.0 mmol, 1.0 equiv.) and *p*-anisidine (0.43 g, 3.0 mmol, 1.0 equiv.) in acetone (0.25 M) gave the crude product as an orange solid. Purification by

flash silica column chromatography (hexane:CH_2Cl_2 50:50 to 0:100, R_F 0.43 at 0:100) gave the title compound as a yellow solid (0.64 g, 64%). **mp** 110 – 112 °C; **^{1}H NMR** (500 MHz, $CDCl_3$) δ_H: 3.84 (3H, s, OCH_3), 6.94 – 6.98 (2H, m, Ar^{2}C(3,5)*H*), 7.53 – 7.60 (4H, m, Ar^{1}C(3,5)*H* and Ar^{2}C(2,6)*H*), 7.65 – 7.69 (1H, m, Ar^{1}C(4)*H*), 7.88 – 7.92 (2H, m, Ar^{1}C(2,6)*H*), 9.42 (1H, br s, N*H*), 12.84 (1H, br s, N*H*); **^{13}C{^{1}H} NMR** (126 MHz, $CDCl_3$) δ_C: 55.6 (OCH_3), 114.3 (Ar^2*C*(3,5)H), 126.4 (Ar^1*C*(3,5)H), 127.7 (Ar^1*C*(2,6)H), 129.4 (Ar^2*C*(2,6)H), 131.4 (Ar^1*C*(1)), 131.5 (Ar^2*C*(1)), 134.0 (Ar^1*C*(4)), 158.8 (Ar^2*C*(4)), 167.0 (*C*Se), 180.3 (*C*O); **^{77}Se{^{1}H} NMR** (95 MHz, $CDCl_3$) δ_{Se}: 391.1 (s, C*Se*); **IR** ν_{max} (film) 3136, 1668, 1599, 1506, 1487, 1460, 1445, 1331, 1298, 1246, 1161, 1138, 1103, 1024, 826; **HRMS** (ESI^+) $C_{15}H_{14}O_2N_2Na^{80}Se$ $[M+Na]^+$ found 357.0110, requires 357.0113 (–0.8 ppm).

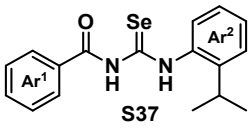
***N*-((4-(*N*-(5-Methylisoxazol-3-yl)sulfamoyl)phenyl)carbamoselenoyl)benzamide (S36)**



S36

Following General Procedure C, benzoyl chloride (0.35 mL, 3.0 mmol, 1.0 equiv.), potassium selenocyanate (0.43 g, 3.0 mmol, 1.0 equiv.) and sulfamethoxazole (0.76 g, 3.0 mmol, 1.0 equiv.) in acetone (0.25 M) gave the crude product as an orange solid. Recrystallisation from EtOH gave the title compound as a green solid (0.41 g, 29%). **mp** 146 – 148 °C; **^{1}H NMR** (400 MHz, $(CD_3)_2SO$) δ_H: 2.31 (3H, s, CH_3), 6.18 (1H, s, C*H*), 7.51 – 7.59 (2H, m, Ar^{1}C(3,5)*H*), 7.64 – 7.71 (1H, m, Ar^{1}C(4)*H*), 7.86 – 7.92 (2H, m, Ar^{2}C(3,5)*H*), 7.93 – 7.99 (4H, m, Ar^{1}C(2,6)*H* and Ar^{2}C(2,6)*H*), 11.51 (1H, br s, N*H*), 11.96 (1H, br s, N*H*), 13.02 (1H, br s, N*H*); **^{13}C{^{1}H} NMR** (126 MHz, $(CD_3)_2SO$) δ_C: 12.1 (*C*H_3), 95.4 (*C*H), 125.6 (Ar^2*C*(2,6)H), 127.4 (Ar^2*C*(3,5)H), 128.4 (Ar^1*C*(3,5)H), 128.9 (Ar^1*C*(2,6)H), 131.8 (Ar^1*C*(1)), 133.3 (Ar^1*C*(4)H), 137.0 (Ar^2*C*(4)), 143.3 (Ar^2*C*(1)), 157.5 (*C*=N), 167.9 (*C*Se), 170.4 (*C*-O), 181.0 (*C*O); **^{77}Se{^{1}H} NMR** (95 MHz, $CDCl_3$) δ_{Se}: 444.1 (s, C*Se*); **IR** ν_{max} (film) 3231, 3154, 2974, 1682, 1609, 1516, 1506, 1472, 1387, 1317, 1250, 1163, 1090, 1065, 930, 905, 858, 791; **HRMS** (ESI^+) $C_{18}H_{16}O_4N_4NaS^{80}Se$ $[M+Na]^+$ found 486.9949, requires 486.9950 (–0.2 ppm).

***N*-((2-*iso*-Propylphenyl)carbamoselenoyl)benzamide (S37)**

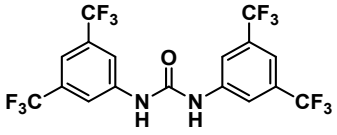


S37

Following General Procedure C, benzoyl chloride (0.35 mL, 3.0 mmol, 1.0 equiv.), potassium selenocyanate (0.43 g, 3.0 mmol, 1.0 equiv.) and 2-*iso*-propylaniline (0.42 mL, 3.0 mmol, 1.0 equiv.) in acetone (0.25 M) gave the crude product as a brown solid. Purification by flash silica column chromatography (hexane:CH_2Cl_2 80:20 to 0:100, R_F 0.53 at 25:75) gave the title compound as a yellow solid (0.61 g, 59%). **mp** 109 – 111 °C; **^{1}H NMR** (400 MHz, $CDCl_3$) δ_H: 1.29 (6H, d, *J* 6.9, CH(CH_3)$_2$), 3.14 (1H, h, *J* 6.9, CH(CH$_3$)$_2$), 7.27 – 7.32 (1H, m, Ar^{2}C(5)H), 7.36 – 7.42 (2H, m, Ar^{2}C(3,4)H), 7.54 – 7.60 (3H, m, Ar^{1}C(3,5)H and Ar^{2}C(6)H), 7.66 – 7.70 (1H, m, Ar^{1}C(4)H), 7.91 – 7.96 (2H, m, Ar^{1}C(2,6)H), 9.52 (1H, s, NH), 12.66 (1H, s, NH); **^{13}C{^{1}H} NMR** (126 MHz, $CDCl_3$) δ_C: 23.4 (CH(*C*H$_3$)$_2$), 28.7 (*C*H(CH$_3$)$_2$), 126.4 (Ar^2*C*(3)H), 126.5 (Ar^2*C*(5)H), 127.7 (Ar^2*C*(6)H), 127.8 (Ar^1*C*(2,6)H), 128.9 (Ar^2*C*(4)H), 129.4 (Ar^1*C*(3,5)H), 131.4 (Ar^1*C*(1)), 134.1 (Ar^1*C*(4)H), 136.5 (Ar^2*C*(1)), 144.0 (Ar^2*C*(2)), 167.1 (*C*Se), 182.2 (*C*O); **^{77}Se{^{1}H} NMR** (95 MHz, $CDCl_3$) δ_{Se}: 397.6 (s, C*Se*); **IR** ν_{max} (film) 3181, 2953, 1659, 1533, 1508, 1483, 1317, 1248, 1198, 1140, 1082, 1026, 756; **HRMS** (ESI^+) $C_{17}H_{18}ON_2Na^{80}Se$ $[M+Na]^+$ found 369.0475, requires 369.0477 (–0.5 ppm).

7. Preparation of Ureas

1,3-Bis(3,5-bis(trifluoromethyl)phenyl)urea (S38)

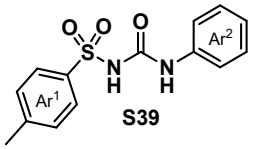


S38

3,5-Bis(trifluoromethyl)phenyl isocyanate (0.52 mL, 3.0 mmol, 1.0 equiv.), 3,5-bis(trifluoromethyl)aniline (0.56 mL, 3.6 mmol, 1.2 equiv.), and NEt_3 (0.84 mL, 6.0 mmol, 2.0 equiv.) were dissolved in CH_2Cl_2 (0.1 M) and stirred at RT for 4 h. Once complete, the precipitate was collected by vacuum filtration washing with CH_2Cl_2 to give the title compound as a white solid (0.63 g, 43%). **mp** 193 – 195 °C {lit[11] 236 – 238}; **^{1}H NMR** (400 MHz, CD_3CN) δ_H: 7.65 (2H, s, ArC(4)*H*), 7.99 (2H, br s, N*H*), 8.08 (4H, s, ArC(2,6)*H*); **^{19}F{^{1}H} NMR** (376 MHz, CD_3CN) δ_F: –63.6 (s, CF_3).

Spectroscopic data in accordance with literature.[11]

4-Methyl-*N*-(phenylcarbamoyl)benzenesulfonamide (S39)



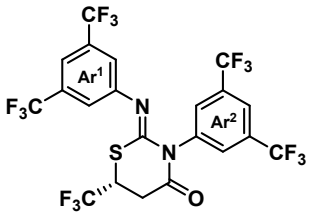
S39

p-Toluenesulfonamide (0.86 g, 5.0 mmol, 1.0 equiv.), phenyl isocyanate (0.54 mL, 5.0 mmol, 1.0 equiv.), and Cs_2CO_3 (1.63 g, 5.0 mmol, 1.0 equiv.) were dissolved in acetone (0.25 M) and heated to reflux for 4 h. Once complete, the reaction mixture was cooled to RT, diluted with H_2O and acidified to pH 1. The reaction mixture was extracted with EtOAc (× 3), the combined organics dried over $MgSO_4$, and the solvent removed under reduced pressure to give the crude product as an off-white solid. Recrystallisation from heptane/EtOAc gave the title compound as white crystals (0.20 g, 14%). **mp** 128 – 130 °C; **^{1}H NMR** (400 MHz, $CDCl_3$) δ_H: 2.43 (3H, s, CH_3), 7.10 – 7.17 (1H, m, Ar^{2}C(4)*H*), 7.29 – 7.41 (7H, m, Ar^{1}C(3,5)*H*, Ar^{2}C(2,3,5,6)*H* and N*H*), 7.80 – 7.85 (2H, m, Ar^{1}C(2,6)*H*), 8.44 (1H, br s, N*H*).

Spectroscopic data in accordance with literature.[14]

8. Isothiourea Catalysis Products

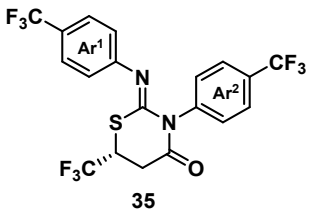
(*R*,*Z*)-3-(3,5-Bis(trifluoromethyl)phenyl)-2-((3,5-bis(trifluoromethyl)phenyl)imino)-6-(trifluoromethyl)-1,3-thiazinan-4-one (33)



33

Following General Procedure G, perfluorophenyl (*E*)-4,4,4-trifluorobut-2-enoate **28** (138 mg, 0.45 mmol, 1.5 equiv.), 1,3-bis(3,5-bis(trifluoromethyl)phenyl)thiourea **26** (150 mg, 0.30 mmol, 1.0 equiv.) and (2*S*,3*R*)-HyperBTM **21** (4.6 mg, 0.015 mmol, 5 mol%) in anhydrous THF (0.1 M) for 24 h at 0 °C gave crude product that was purified by flash silica column chromatography (hexane:CH_2Cl_2 90:10 to 25:75) to give the title compound as a white solid (178 mg, 95%). **mp** 140 – 142 °C; $[\alpha]_D^{20}$ +2.8 (*c* 1.0 in $CHCl_3$); **Chiral HPLC analysis,** Chiralcel OD-H (90:10 *n*-hexane : IPA, flow rate 1.0 mLmin^{-1}, 254 nm, 30 °C) t_R (*S*) 4.7 min, t_R (*R*) 5.3 min, 95:5 er; **IR** ν_{max} (film) 2976, 1715, 1607, 1460, 1373, 1277, 1169, 1132, 1123, 1105, 1005, 908, 880; **^{1}H NMR** (400 MHz, $CDCl_3$) δ_H: 3.46 (1H, dd, *J* 17.2, 5.4, C(5)*H*^{A}H^B), 3.55 (1H, dd, *J* 17.2, 4.2, C(5)H^A*H*^{B}), 3.92 (1H, qdd, *J* 7.8, 5.4, 4.2, C(6)*H*), 7.23 (2H, s, Ar^{1}C(2,6)*H*), 7.66 (1H, s, Ar^{1}C(4)*H*), 7.69 (2H, s, Ar^{2}C(2,6)*H*), 7.97 (1H, s, Ar^{2}C(4)*H*); **^{19}F{^{1}H} NMR** (376 MHz, $CDCl_3$) δ_F: –71.4 (s, C*F*$_3$), –63.0 (s, C*F*$_3$), –62.8 (s, C*F*$_3$); **^{13}C{^{1}H} NMR** (126 MHz, $CDCl_3$) δ_C: 33.7 (*C*(5)H$_2$), 39.4 (q, *J* 32.8, *C*(6)H), 118.5 – 118.7 (m, Ar^1*C*(4)H), 120.8 – 121.0 (m, Ar^1*C*(2,6)H), 122.7 (q, *J* 273.0, *C*F$_3$), 122.9 (q, *J* 272.9, *C*F$_3$), 122.9 – 123.2 (m, Ar^2*C*(4)H), 124.5 (q, *J* 280.0, *C*F$_3$), 129.3 – 129.5 (m, Ar^2*C*(2,6)H), 132.3 – 133.5 (m, Ar^1*C*(3,5) and Ar^2*C*(3,5)), 138.2 (Ar^2*C*(1)), 147.4 (Ar^1*C*(1)), 150.2 (*C*(2)), 165.6 (*C*(4)); **HRMS** (ESI^+) $C_{21}H_{10}ON_2F_{15}S$ $[M+H]^+$ found 623.0274, requires 623.0269 (+0.8 ppm).

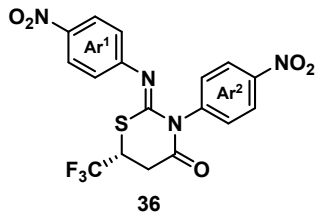
(*R*,*Z*)-6-(Trifluoromethyl)-3-(4-(trifluoromethyl)phenyl)-2-((4-(trifluoromethyl)phenyl)imino)-1,3-thiazinan-4-one (35)



35

Following General Procedure G, perfluorophenyl (*E*)-4,4,4-trifluorobut-2-enoate **28** (138 mg, 0.45 mmol, 1.5 equiv.), 1,3-bis(4-(trifluoromethyl)phenyl)thiourea **S17** (109 mg, 0.30 mmol, 1.0 equiv.) and (2*S*,3*R*)-HyperBTM **21** (18.5 mg, 0.06 mmol, 20 mol%) in anhydrous THF (0.1 M) for 24 h at RT gave crude product that was purified by flash silica column chromatography (hexane:CH_2Cl_2 80:20 to 0:100, R_F 0.68 at 0:100) to give the title compound as white solid (115 mg, 79%). **mp** 99 – 101 °C; $[\alpha]_D^{20}$ +29.2 (*c* 1.0 in $CHCl_3$); **Chiral HPLC analysis,** Chiralpak AD-H (97:3 *n*-hexane : IPA, flow rate 2.0 mLmin^{-1}, 220 nm, 40 °C) t_R (*R*) 9.1 min, t_R (*S*) 14.5 min, 95:5 er; **IR** ν_{max} (film) 2359, 1705, 1603, 1364, 1323, 1163, 1119, 1105, 1065, 1015, 891, 841; **^{1}H NMR** (400 MHz, $CDCl_3$) δ_H: 3.41 (1H, dd, *J* 17.0, 5.4, C(5)*H*^{A}H^B), 3.49 (1H, dd, *J* 17.0, 4.3, C(5)H^A*H*^{B}), 3.92 (1H, qdd, *J* 7.9, 5.4, 4.3, C(6)*H*), 6.84 – 6.91 (2H, m, Ar^{1}C(2,6)*H*), 7.35 – 7.42 (2H, m, Ar^{2}C(2,6)*H*), 7.55 – 763 (2H, m, Ar^{1}C(3,5)*H*), 7.74 – 7.81 (2H, m, Ar^{2}C(3,5)*H*); **^{19}F{^{1}H} NMR** (376 MHz, $CDCl_3$) δ_F: –71.4 (s, C*F*$_3$), –62.7 (s, C*F*$_3$), –62.1 (s, C*F*$_3$); **^{13}C{^{1}H} NMR** (126 MHz, $CDCl_3$) δ_C: 33.9 (*C*(5)H$_2$), 39.4 (q, *J* 32.4, *C*(6)H), 120.5 (Ar^1*C*(2,6)H), 123.7 (q, *J* 272.4, *C*F$_3$), 124.1 (q, *J* 271.7, *C*F$_3$), 124.7 (q, *J* 279.9, *C*F$_3$), 126.5 (q, *J* 4.1 Ar^1*C*(3,5)H), 126.6 (q, *J* 4.1 Ar^2*C*(3,5)H), 126.9 (q, *J* 32.7, Ar^1*C*(4)), 129.2 (Ar^2*C*(2,6)H), 130.8 (q, *J* 32.8, Ar^2*C*(4)), 140.4 (Ar^2*C*(1)), 148.7 (*C*(2)), 149.7 (Ar^1*C*(1)), 165.8 (*C*(4)); **HRMS** (ESI^-) $C_{19}H_{10}ON_2F_9S$ $[M-H]^-$ found 485.0369, requires 485.0376 (–1.4 ppm).

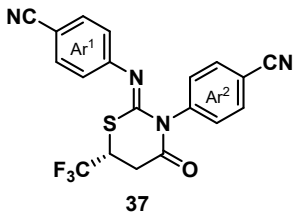
(*R*,*Z*)-3-(4-Nitrophenyl)-2-((4-nitrophenyl)imino)-6-(trifluoromethyl)-1,3-thiazinan-4-one (36)



36

Following General Procedure G, perfluorophenyl (*E*)-4,4,4-trifluorobut-2-enoate **28** (138 mg, 0.45 mmol, 1.5 equiv.), 1,3-bis(4-nitrophenyl)thiourea **S18** (95.5 mg, 0.30 mmol, 1.0 equiv.) and (2*S*,3*R*)-HyperBTM **21** (4.6 mg, 0.015 mmol, 5 mol%) in anhydrous THF (0.1 M) for 24 h at 0 °C gave crude product that was purified by flash silica column chromatography (CH_2Cl_2:Et_2O 100:0 to 90:10, R_F 0.71 at 90:10) to give the title compound as a pale yellow solid (125 mg, 95%). **mp** 72 – 74 °C; $[\alpha]_D^{20}$ +66.4 (*c* 1.1 in $CHCl_3$); **Chiral HPLC analysis,** Chiralpak AD-H (70:30 *n*-hexane : IPA, flow rate 1.0 mLmin^{-1}, 211 nm, 30 °C) t_R (*R*) 13.1 min, t_R (*S*) 24.7 min, 98:2 er; **IR** ν_{max} (film) 3078, 2953, 1709, 1612, 1582, 1510, 1337, 1296, 1225, 1157, 1109, 893, 856, 843; **^{1}H NMR** (400 MHz, $CDCl_3$) δ_H: 3.47 (1H, dd, *J* 17.2, 5.3, C(5)*H*^{A}H^B), 3.53 (1H, dd, *J* 17.2, 4.4, C(5)H^A*H*^{B}), 4.00 (1H, qdd, *J* 7.9, 5.3, 4.4, C(6)*H*), 6.87 – 6.92 (2H, m, Ar^{1}C(2,6)*H*), 7.41 – 7.46 (2H, m, Ar^{2}C(2,6)*H*), 8.18 – 8.23 (2H, m, Ar^{1}C(3,5)*H*), 8.34 – 8.39 (2H, m, Ar^{2}C(3,5)*H*); **^{19}F{^{1}H} NMR** (377 MHz, $CDCl_3$) δ_F: –71.4 (s, C*F*$_3$); **^{13}C{^{1}H} NMR** (126 MHz, $CDCl_3$) δ_C: 33.7 (*C*(5)H$_2$), 39.5 (q, *J* 32.7, *C*(6)H), 120.9 (Ar^1*C*(2,6)H), 124.6 (q, *J* 280.1, *C*F$_3$), 124.9 (Ar^2*C*(3,5)H), 125.3 (Ar^1*C*(3,5)H), 129.9 (Ar^2*C*(2,6)H), 142.8 (Ar^2*C*(1)), 144.8 (Ar^1*C*(4)), 147.7 (Ar^2*C*(4)), 149.1 (*C*(2)), 152.2 (Ar^1*C*(1)), 165.6 (*C*(4)); **HRMS** (ESI^+) $C_{17}H_{11}O_5N_4F_3NaS$ $[M+Na]^+$ found 463.0290, requires 463.0294 (–0.9 ppm).

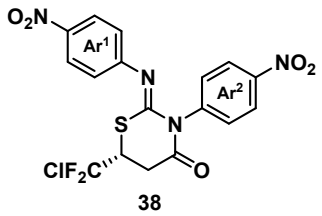
(*R*,*Z*)-4-((3-(4-Cyanophenyl)-4-oxo-6-(trifluoromethyl)-1,3-thiazinan-2-ylidene)amino)benzonitrile (37)



37

Following General Procedure G, perfluorophenyl (*E*)-4,4,4-trifluorobut-2-enoate **28** (138 mg, 0.45 mmol, 1.5 equiv.), 1,3-bis(4-cyanophenyl)thiourea **S19** (83.5 mg, 0.3 mmol, 1.0 equiv.) and (2*S*,3*R*)-HyperBTM **21** (4.6 mg, 0.015 mmol, 5 mol%) in anhydrous THF (0.1 M) for 24 h at 0 °C gave crude product that was purified by flash silica column chromatography (hexane:EtOAc 100:0 to 50:50, R_F 0.32 at 50:50) to give the title compound as a white solid (100 mg, 83%). **mp** 149 – 151 °C; $[\alpha]_D^{20}$ +64.7 (*c* 1.0 in $CHCl_3$); **Chiral HPLC analysis,** Chiralpak AD-H (70:30 *n*-hexane : IPA, flow rate 1.0 mLmin^{-1}, 211 nm, 30 °C) t_R (*R*) 9.8 min, t_R (*S*) 16.5 min, 97:3 er; **IR** ν_{max} (film) 2951, 2228, 1709, 1618, 1593, 1499, 1364, 1227, 1179, 1161, 1119, 889, 841; **^{1}H NMR** (400 MHz, $CDCl_3$) δ_H: 3.42 (1H, dd, *J* 17.1, 5.4, C(5)*H*^{A}H^B), 3.49 (1H, dd, *J* 17.1, 4.2, C(5)H^A*H*^{B}), 3.96 (1H, qdd, *J* 7.9, 5.4, 4.2, C(6)*H*), 6.82 – 6.88 (2H, m, Ar^{1}C(2,6)*H*), 7.34 – 7.38 (2H, m, Ar^{2}C(2,6)*H*), 7.58 – 763 (2H, m, Ar^{1}C(3,5)*H*), 7.76 – 7.81 (2H, m, Ar^{2}C(3,5)*H*); **^{19}F{^{1}H} NMR** (376 MHz, $CDCl_3$) δ_F: –71.4 (s, C*F*$_3$); **^{13}C{^{1}H} NMR** (126 MHz, $CDCl_3$) δ_C: 33.8 (*C*(5)H$_2$), 39.4 (q, *J* 32.6, *C*(6)H), 108.4 (Ar^1*C*(4)), 112.9 (Ar^2*C*(4)), 118.0 (Ar^2*C*N), 118.8 (Ar^{1}CN), 121.2 (Ar^1*C*(2,6)H), 124.6 (q, *J* 280.0, *C*F$_3$), 129.8 (Ar^2*C*(2,6)H), 133.3 (Ar^2*C*(3,5)H), 133.5 (Ar^1*C*(3,5)H), 141.2 (Ar^2*C*(1)), 148.9 (*C*(2)), 150.4 (Ar^1*C*(1)), 165.6 (*C*(4)); **HRMS** (ESI^+) $C_{19}H_{11}ON_4F_3NaS$ $[M+Na]^+$ found 423.0489, requires 423.0498 (–2.1 ppm).

(*R*,*Z*)-6-(Chlorodifluoromethyl)-3-(4-nitrophenyl)-2-((4-nitrophenyl)imino)-1,3-thiazinan-4-one (38)

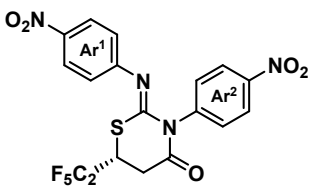


38

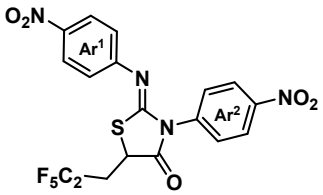
Following General Procedure G, 4-nitrophenyl (*E*)-4-chloro-4,4-difluorobut-2-enoate **S4** (125 mg, 0.45 mmol, 1.5 equiv.), 1,3-bis(4-nitrophenyl)thiourea **S18** (95.5 mg, 0.30 mmol, 1.0 equiv.) and (2*S*,3*R*)-HyperBTM **21** (4.6 mg, 0.015 mmol, 5 mol%) in anhydrous THF (0.1 M) at 0 °C for 48 h, without workup, gave crude product that was purified by flash silica column chromatography (CH_2Cl_2:hexane 50:50 to 100:0, R_F 0.43 at 100:0 then EtOAc:hexane 30:70 to 70:30, R_F 0.38 at 50:50) to give the title compound as a pale yellow solid (107 mg, 78%). *Note: a workup was not performed to avoid elimination of HCl.*

mp 55 – 57 °C; $[\alpha]_D^{20}$ +104.5 (*c* 1.0 in $CHCl_3$); **Chiral HPLC analysis,** Chiralpak AD-H (70:30 *n*-hexane : IPA, flow rate 1.0 mLmin^{-1}, 211 nm, 30 °C) t_R (*R*) 15.3 min, t_R (*S*) 23.5 min, 98:2 er; **IR** ν_{max} (film) 1711, 1616, 1584, 1516, 1342, 1300, 1157, 1109, 858; **^{1}H NMR** (500 MHz, $CDCl_3$) δ_H: 3.48 (1H, dd, *J* 17.2, 5.5, C(5)H^AH^B), 3.59 (1H, dd, *J* 17.2, 4.4, C(5)H^AH^B), 4.05 – 4.15 (1H, m, C(6)*H*), 6.83 – 6.92 (2H, m, Ar^{1}C(2,6)*H*), 7.36 – 7.46 (2H, m, Ar^{2}C(2,6)*H*), 8.16 – 8.22 (2H, m, Ar^{1}C(3,5)*H*), 8.30 – 8.39 (2H, m, Ar^{2}C(3,5)*H*); **^{19}F{^{1}H} NMR** (377 MHz, $CDCl_3$) δ_F: –58.1 (d, *J* 167.1, CF^AF^BCl), –56.2 (d, *J* 167.1, CF^AF^BCl); **^{13}C{^{1}H} NMR** (126 MHz, $CDCl_3$) δ_C: 34.8 (*C*(5)H_2), 39.5 (t, *J* 27.7, *C*(6)H), 121.0 (Ar^1*C*(2,6)H), 124.9 (Ar^2*C*(3,5)H), 125.4 (Ar^1*C*(3,5)H), 128.0 (t, *J* 294.7, *C*F_2Cl), 130.0 (Ar^2*C*(2,6)H), 142.9 (Ar^2*C*(1)), 144.8 (Ar^1*C*(4)), 147.8 (Ar^2*C*(4)), 149.3 (*C*(2)), 152.3 (Ar^1*C*(1)), 165.8 (*C*(4)); **HRMS** (ESI^+) $C_{17}H_{11}O_5N_4{}^{35}ClF_2NaS$ $[M+Na]^+$ found 478.9987, requires 478.9999 (–2.5 ppm).

(*R*,*Z*)-3-(4-Nitrophenyl)-2-((4-nitrophenyl)imino)-6-(perfluoroethyl)-1,3-thiazinan-4-one (39) and (*Z*)-3-(4-nitrophenyl)-2-((4-nitrophenyl)imino)-5-(2,2,3,3,3-pentafluoropropyl)thiazolidin-4-one (S40)



39



S40

Following General Procedure G, perfluorophenyl (*E*)-4,4,5,5,5-pentafluoropent-2-enoate **S11** (160 mg, 0.45 mmol, 1.5 equiv.), 1,3-bis(4-nitrophenyl)thiourea **S18** (95.5 mg, 0.30 mmol, 1.0 equiv.) and (2*S*,3*R*)-HyperBTM **21** (4.6 mg, 0.015 mmol, 5 mol%) in anhydrous THF (0.1 M) for 48 h at 0 °C gave crude product that was purified by flash silica column chromatography (CH_2Cl_2:hexane 30:70 to 100:0) to give:

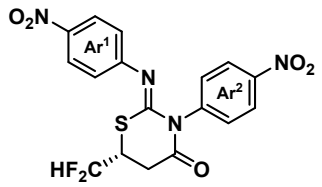
39: (86 mg, 59%) as a white solid. **mp** 93 – 95 °C; $[\alpha]_D^{20}$ +79.4 (*c* 1.0 in $CHCl_3$); **Chiral HPLC analysis,** Chiralpak AD-H (80:20 *n*-hexane : IPA, flow rate 1.0 mLmin^{-1}, 211 nm, 30 °C) t_R (*R*) 16.9 min, t_R (*S*) 25.2 min, 98:2 er; **IR** ν_{max} (film) 3082, 2953, 1713, 1612, 1582, 1510, 1491, 1337, 1296, 1198, 1153, 1107, 1030, 856, 843; **^{1}H NMR** (500 MHz, $CDCl_3$) δ_H: 3.50 (1H, dd, *J* 17.2, 5.1, C(5)H^AH^B), 3.54 (1H, dd, *J* 17.2, 4.6, C(5)H^AH^B), 3.98 – 4.09 (1H, m, C(6)*H*), 6.84 – 6.90 (2H, m, Ar^{1}C(2,6)*H*), 7.39 – 7.46 (2H, m, Ar^{2}C(2,6)*H*), 8.16 – 8.21 (2H, m, Ar^{1}C(3,5)*H*), 8.32 – 8.37 (2H, m, Ar^{2}C(3,5)*H*); **^{19}F{^{1}H} NMR** (377 MHz, $CDCl_3$) δ_F: –118.2 (d, *J* 271.7, C*F*^{A}F^{B}CF$_3$), –115.6 (d, *J* 271.7, CF^A*F*^{B}CF$_3$), –81.0 (s, C*F*$_3$); **^{13}C{^{1}H} NMR** (126 MHz, $CDCl_3$) δ_C: 33.9 (*C*(5)H$_2$), 37.9 (t, *J* 24.4, *C*(6)H), 113.8 (tq, *J* 258.4, 37.7, *C*F$_2$CF$_3$), 118.5 (qt, *J* 287.3, 35.7, CF$_2$*C*F$_3$), 120.9 (Ar^1*C*(2,6)H), 124.9 (Ar^2*C*(3,5)H), 125.3 (Ar^1*C*(3,5)H), 129.9 (Ar^2*C*(2,6)H), 142.7 (Ar^2*C*(1)), 144.8 (Ar^1*C*(4)), 147.7 (Ar^2*C*(4)), 149.0 (*C*(2)), 152.2 (Ar^1*C*(1)), 165.6 (*C*(4)); **HRMS** (ESI^+) $C_{18}H_{12}O_5N_4F_5S$ $[M+H]^+$ found 491.0437, requires 491.0443 (–1.2 ppm).

S40: (15 mg, 10%) as a white solid. **mp** 88 – 90 °C; **Chiral HPLC analysis,** Chiralpak AD-H (70:30 *n*-hexane : IPA, flow rate 1.0 mLmin^{-1}, 211 nm, 30 °C) t_R 10.2 min, t_R 16.2 min, 50:50 er; **IR** ν_{max} (film) 2359, 1734, 1638, 1585, 1516, 1341, 1194, 1155, 1069, 858; **^{1}H NMR** (500 MHz, $CDCl_3$) δ_H: 2.61 – 2.76 (1H, m, CH^AH^B), 3.20 – 3.35 (1H, m, CH$^AH^B$), 4.61 (1H, dd, *J* 11.0, 2.2, C(5)*H*), 7.01 – 7.07 (2H, m, Ar^{1}C(2,6)*H*), 7.60 – 7.65 (2H, m, Ar^{2}C(2,6)*H*), 8.22 – 8.27 (2H, m, Ar^{1}C(3,5)*H*), 8.38 – 8.44 (2H, m, Ar^{2}C(3,5)*H*); **^{19}F{^{1}H} NMR** (376 MHz, $CDCl_3$)

δ_F: –118.0 (d, *J* 265.5, C*F*^{A}F^{B}CF$_3$), –116.1 (d, *J* 265.5, CF^A*F*^{B}CF$_3$), –85.4 (s, C*F*$_3$); **^{13}C{^{1}H} NMR** (126 MHz, $CDCl_3$) δ_C: 34.9 (t, *J* 20.7, *C*H$_2$C$_2$F$_5$), 40.7 (*C*(5)), 121.4 (Ar^1*C*(2,6)H), 124.8 (Ar^2*C*(3,5)H), 125.4 (Ar^1*C*(3,5)H), 129.0 (Ar^2*C*(2,6)H), 139.1 (Ar^2*C*(1)), 145.1 (Ar^1*C*(4)), 147.8 (Ar^2*C*(4)), 152.7 (*C*(2)), 153.7 (Ar^1*C*(1)), 171.2 (*C*(4)); **HRMS** (ESI^-) $C_{18}H_{10}O_5N_4F_5S$ $[M-H]^-$ found 489.0294, requires 489.0298 (–0.7 ppm).

Note: the C_2F_5 $^{13}C\{^1H\}$ NMR multiplets can be seen on the baseline but are not fully resolved.

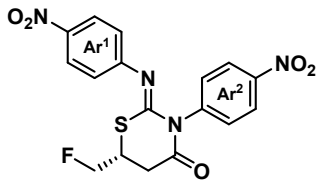
(*R*,*Z*)-6-(Difluoromethyl)-3-(4-nitrophenyl)-2-((4-nitrophenyl)imino)-1,3-thiazinan-4-one (40)



40

Following General Procedure G, perfluorophenyl (*E*)-4,4-difluorobut-2-enoate **S12** (130 mg, 0.45 mmol, 1.5 equiv.), 1,3-bis(4-nitrophenyl)thiourea **S18** (95.5 mg, 0.30 mmol, 1.0 equiv.) and (2*S*,3*R*)-HyperBTM **21** (4.6 mg, 0.015 mmol, 5 mol%) in anhydrous THF (0.1 M) for 24 h at 0 °C gave crude product that was purified twice by flash silica column chromatography (CH_2Cl_2:Et_2O 100:0 to 95:5, R_F 0.49 at 95:5 then hexane:EtOAc 100:0 to 0:100, R_F 0.28 at 50:50) to give the title compound as a pale yellow solid (96 mg, 76%). **mp** 133 – 135 °C; $[\alpha]_D^{20}$ +52.0 (*c* 1.0 in $CHCl_3$); **Chiral HPLC analysis,** Chiralpak AD-H (70:30 *n*-hexane : IPA, flow rate 1.0 mLmin^{-1}, 211 nm, 30 °C) t_R (*R*) 24.4 min, t_R (*S*) 34.1 min, 80:20 er; **IR** ν_{max} (film) 1707, 1614, 1584, 1342, 1219, 1159, 1109, 860; **^{1}H NMR** (500 MHz, $CDCl_3$) δ_H: 3.39 (1H, dd, *J* 17.0, 5.4, C(5)*H*^{A}H^B), 3.45 (1H, dd, *J* 17.0, 4.4, C(5)H^A*H*^{B}), 3.70 – 3.82 (1H, m, C(6)*H*), 6.10 (1H, td, *J* 55.2, 2.2, CF_2H), 6.86 – 6.92 (2H, m, Ar^{1}C(2,6)*H*), 7.41 – 7.47 (2H, m, Ar^{2}C(2,6)*H*), 8.17 – 8.22 (2H, m, Ar^{1}C(3,5)*H*), 8.33 – 8.39 (2H, m, Ar^{2}C(3,5)*H*); **^{19}F{^{1}H} NMR** (376 MHz, $CDCl_3$) δ_F: –123.0 (d, *J* 283.2, C*F*^{A}F^{B}H), –118.8 (d, *J* 283.2, CF^A*F*^{B}H); **^{13}C{^{1}H} NMR** (126 MHz, $CDCl_3$) δ_C: 33.1 (*C*(5)H_2), 39.2 (t, *J* 23.6, *C*(6)H), 114.7 (t, *J* 247.6, *C*F_2H), 121.0 (Ar^1*C*(2,6)H), 124.8 (Ar^2*C*(3,5)H), 125.2 (Ar^1*C*(3,5)H), 130.0 (Ar^2*C*(2,6)H), 143.2 (Ar^2*C*(1)), 144.6 (Ar^1*C*(4)), 147.6 (Ar^2*C*(4)), 150.2 (*C*(2)), 152.7 (Ar^1*C*(1)), 166.7 (*C*(4)); **HRMS** (ESI^+) $C_{17}H_{13}O_5N_4F_2S$ $[M+H]^+$ found 423.0560, requires 423.0569 (–2.2 ppm).

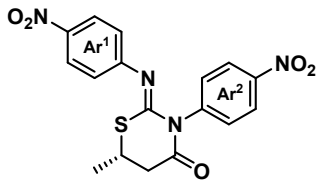
(*R*,*Z*)-6-(Fluoromethyl)-3-(4-nitrophenyl)-2-((4-nitrophenyl)imino)-1,3-thiazinan-4-one (41)



41

Following General Procedure G, perfluorophenyl (*E*)-4-fluorobut-2-enoate **S13** (122 mg, 0.45 mmol, 1.5 equiv.), 1,3-bis(4-nitrophenyl)thiourea **S18** (95.5 mg, 0.30 mmol, 1.0 equiv.) and (2*S*,3*R*)-HyperBTM **21** (9.3 mg, 0.03 mmol, 10 mol%) in anhydrous THF (0.1 M) for 48 h at 0 °C gave crude product that was purified by flash silica column chromatography (hexane:EtOAc 100:0 to 0:100, R_F 0.19 at 50:50) to give the title compound as a pale yellow solid (118 mg, 98%). **mp** 150 – 152 °C; $[\alpha]_D^{20}$ +39.0 (*c* 0.1 in MeCN); **Chiral HPLC analysis,** Chiralcel OJ-H (50:50 *n*-hexane : IPA, flow rate 0.7 mLmin^{-1}, 211 nm, 40 °C) t_R (*S*) 37.1 min, t_R (*R*) 44.5 min, 83:17 er; **IR** ν_{max} (film) 2920, 1705, 1612, 1578, 1526, 1508, 1491, 1337, 1285, 1213, 1153, 1103, 1016, 856, 839; **^{1}H NMR** (400 MHz, $(CD_3)_2CO$) δ_H: 3.24 (1H, dd, *J* 16.5, 6.9, C(5)*H*^{A}H^B), 3.41 (1H, dd, *J* 16.5, 4.4, C(5)H^A*H*^{B}), 4.03 – 4.16 (1H, m, C(6)*H*), 4.67 – 4.77 (1H, m, C*H*^{A}H^{B}F), 4.79 – 4.88 (1H, m, CH^A*H*^{B}F), 6.92 – 6.97 (2H, m, Ar^{1}C(2,6)*H*), 7.60 – 7.65 (2H, m, Ar^{2}C(2,6)*H*), 8.13 – 8.18 (2H, m, Ar^{1}C(3,5)*H*), 8.27 – 8.32 (2H, m, Ar^{2}C(3,5)*H*); **^{19}F{^{1}H} NMR** (376 MHz, $(CD_3)_2CO$) δ_F: –222.0 (s, CH_2*F*); **^{13}C{^{1}H} NMR** (126 MHz, $(CD_3)_2CO$) δ_C: 37.1 (d, *J* 3.6, *C*(5)H_2), 38.1 (d, *J* 20.1, *C*(6)H), 85.4 (d, *J* 173.3, *C*H_2F), 122.0 (Ar^1*C*(2,6)H), 124.8 (Ar^2*C*(3,5)H), 125.7 (Ar^1*C*(3,5)H), 131.4 (Ar^2*C*(2,6)H), 144.9 (Ar^2*C*(1)), 145.4 (Ar^1*C*(4)), 148.1 (Ar^2*C*(4)), 153.7 (*C*(2)), 154.8 (Ar^1*C*(1)), 168.9 (*C*(4)); **HRMS** (ESI^+) $C_{17}H_{14}O_5N_4FS$ $[M+H]^+$ found 405.0655, requires 405.0663 (–2.0 ppm).

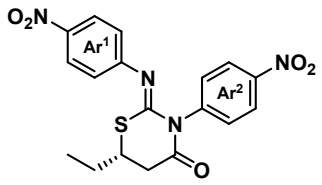
(*S*,*Z*)-6-Methyl-3-(4-nitrophenyl)-2-((4-nitrophenyl)imino)-1,3-thiazinan-4-one (42)



42

Following General Procedure G, 4-nitrophenyl (*E*)-but-2-enoate **S5** (93.2 mg, 0.45 mmol, 1.5 equiv.), 1,3-bis(4-nitrophenyl)thiourea **S18** (95.5 mg, 0.30 mmol, 1.0 equiv.) and (2*S*,3*R*)-HyperBTM **21** (18.5 mg, 0.06 mmol, 20 mol%) in anhydrous THF (0.1 M) for 48 h at RT gave crude product that was purified by flash silica column chromatography (hexane:CH_2Cl_2 30:70 to 0:100, R_F 0.34 at 0:100) to give the title compound as a pale yellow solid (101 mg, 87%). **mp** 186 – 188 °C; $[\alpha]_D^{20}$ –21.5 (*c* 0.2 in MeCN); **Chiral HPLC analysis,** Chiralpak IB (80:20 *n*-hexane : IPA, flow rate 1.5 mLmin^{-1}, 211 nm, 30 °C) t_R (*R*) 19.3 min, t_R (*S*) 21.7 min, 86:14 er; **IR** ν_{max} (film) 3107, 3080, 2978, 1699, 1612, 1582, 1528, 1508, 1491, 1327, 1283, 1217, 1152, 1105, 856, 839; **^{1}H NMR** (500 MHz, CD_3CN) δ_H: 1.40 (3H, d, *J* 6.8, CH_3), 2.95 (1H, dd, *J* 16.4, 10.1, C(5)H^AH^B), 3.18 (1H, dd, *J* 16.4, 3.3, C(5)H^AH^B), 3.78 (1H, dqd, *J* 10.1, 6.8, 3.3, C(6)*H*), 6.85 – 6.92 (2H, m, Ar^{1}C(2,6)*H*), 7.54 – 7.59 (2H, m, Ar^{2}C(2,6)*H*), 8.12 – 8.19 (2H, m, Ar^{1}C(3,5)*H*), 8.27 – 8.33 (2H, m, Ar^{2}C(3,5)*H*); **^{13}C{^{1}H} NMR** (126 MHz, CD_3CN) δ_C: 20.4 (*C*H$_3$), 33.6 (*C*(5)H$_2$), 43.4 (*C*(6)H), 122.0 (Ar^1*C*(2,6)H), 125.2 (Ar^2*C*(3,5)H), 126.0 (Ar^1*C*(3,5)H), 131.6 (Ar^2*C*(2,6)H), 143.9 (Ar^2*C*(1)), 145.1 (Ar^1*C*(4)), 145.7 (Ar^2*C*(4)), 148.3 (*C*(2)), 155.1 (Ar^1*C*(1)), 170.4 (*C*(4)); **HRMS** (ESI^+) $C_{17}H_{14}O_5N_4NaS$ $[M+Na]^+$ found 409.0573, requires 409.0577 (–1.0 ppm).

(*S*,*Z*)-6-Ethyl-3-(4-nitrophenyl)-2-((4-nitrophenyl)imino)-1,3-thiazinan-4-one (43)

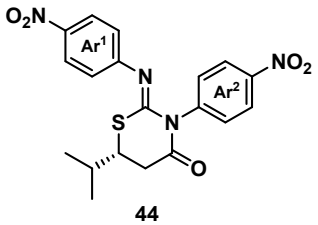


43

Following General Procedure G, perfluorophenyl (*E*)-pent-2-enoate **S15** (120 mg, 0.45 mmol, 1.5 equiv.), 1,3-bis(4-nitrophenyl)thiourea **S18** (95.5 mg, 0.30 mmol, 1.0 equiv.) and (2*S*,3*R*)-HyperBTM **21** (18.5 mg, 0.06 mmol, 20 mol%) in anhydrous THF (0.1 M) for

48 h at RT gave crude product that was purified by flash silica column chromatography (hexane:EtOAc 100:0 to 50:50, R_F 0.44 at 50:50) to give the title compound as a pale yellow solid (97 mg, 81%). **mp** 147 – 149 °C; $[\alpha]_D^{20}$ –38.9 (*c* 1.0 in $CHCl_3$); **Chiral HPLC analysis,** Chiralcel OD-H (70:30 *n*-hexane : IPA, flow rate 1.0 mLmin^{-1}, 211 nm, 30 °C) t_R (*R*) 18.1 min, t_R (*S*) 20.7 min, 89:11 er; **IR** ν_{max} (film) 2968, 1705, 1609, 1580, 1508, 1339, 1302, 1217, 1155, 1109, 858; **^{1}H NMR** (500 MHz, $CDCl_3$) δ_H: 1.08 (3H, t, *J* 7.4, CH_2CH_3), 1.73 – 1.91 (2H, m, $CH^AH^BCH_3$ and $CH^AH^BCH_3$), 3.04 (1H, dd, *J* 16.2, 10.0, C(5)H^AH^B), 3.30 (1H, dd, *J* 16.2, 3.2, C(5)H^AH^B), 3.46 – 3.54 (1H, m, C(6)*H*), 6.84 – 6.90 (2H, m, Ar^{1}C(2,6)*H*), 7.41 – 7.48 (2H, m, Ar^{2}C(2,6)*H*), 8.16 – 8.23 (2H, m, Ar^{1}C(3,5)*H*), 8.33 – 8.40 (2H, m, Ar^{2}C(3,5)*H*); **^{13}C{^{1}H} NMR** (126 MHz, $CDCl_3$) δ_C: 11.2 (CH_2CH_3), 27.9 (CH_2CH_3), 39.6 (*C*(5)H_2), 41.2 (*C*(6)H), 121.1 (Ar^1*C*(2,6)H), 124.7 (Ar^2*C*(3,5)H), 125.1 (Ar^1*C*(3,5)H), 130.1 (Ar^2*C*(2,6)H), 143.6 (Ar^2*C*(1)), 144.4 (Ar^1*C*(4)), 147.5 (Ar^2*C*(4)), 153.1 (*C*(2)), 153.3 (Ar^1*C*(1)), 169.0 (*C*(4)); **HRMS** (ESI^+) $C_{18}H_{16}O_5N_4NaS$ $[M+Na]^+$ found 423.0722, requires 423.0734 (–2.8 ppm).

(*R*,*Z*)-6-*iso*-Propyl-3-(4-nitrophenyl)-2-((4-nitrophenyl)imino)-1,3-thiazinan-4-one (44)

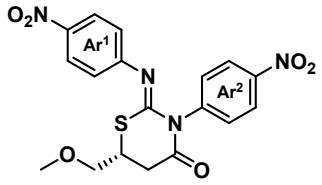


44

Following General Procedure G, 4-nitrophenyl (*E*)-4-methylpent-2-enoate **S6** (106 mg, 0.45 mmol, 1.5 equiv.), 1,3-bis(4-nitrophenyl)thiourea **S18** (95.5 mg, 0.30 mmol, 1.0 equiv.) and (2*S*,3*R*)-HyperBTM **21** (27.8 mg, 0.09 mmol, 30 mol%) in anhydrous THF (0.1 M) for 72 h at RT gave crude product that was purified twice by flash silica column chromatography (hexane:EtOAc 100:0 to 50:50, R_F 0.69 at 50:50 then hexane:CH_2Cl_2 50:50 to 0:100, R_F 0.49 at 0:100) to give the title compound as a pale yellow solid (95 mg, 77%). **mp** 54 – 56 °C; $[\alpha]_D^{20}$ –55.7 (*c* 1.0 in $CHCl_3$); **Chiral HPLC analysis,** Chiralpak AD-H (60:40 *n*-hexane : IPA, flow rate 1.0 mLmin^{-1}, 211 nm, 30 °C) t_R (*R*) 18.3 min, t_R (*S*) 22.5 min, 94:6 er; **IR** ν_{max} (film) 2967, 1705, 1612, 1582, 1510, 1339, 1281, 1219, 1155, 1109, 858; **^{1}H NMR** (500 MHz, $CDCl_3$) δ_H: 1.06 (6H, d, *J* 6.8, CH(CH_3)$_2$), 1.98 (1H, septd, *J* 6.8, 6.4, C*H*(CH_3)$_2$), 3.05 (1H, dd, *J* 16.2, 10.7, C(5)H^AH^B), 3.25 (1H, dd, *J* 16.2, 3.1, C(5)H^AH^B), 3.44

(1H, ddd, *J* 10.7, 6.4, 3.1, C(6)*H*), 6.82 – 6.87 (2H, m, Ar^{1}C(2,6)*H*), 7.40 – 7.45 (2H, m, Ar^{2}C(2,6)*H*), 8.14 – 8.19 (2H, m, Ar^{1}C(3,5)*H*), 8.31 – 8.36 (2H, m, Ar^{2}C(3,5)*H*); **^{13}C{^{1}H} NMR** (126 MHz, $CDCl_3$) δ_C: 19.6 ($CH(CH_3)_2$), 32.2 ($CH(CH_3)_2$), 39.3 ($C(5)H_2$), 44.9 ($C(6)H$), 121.2 (Ar^1*C*(2,6)H), 124.8 (Ar^2*C*(3,5)H), 125.2 (Ar^1*C*(3,5)H), 130.2 (Ar^2*C*(2,6)H), 143.8 (Ar^2*C*(1)), 144.4 (Ar^1*C*(4)), 147.5 (Ar^2*C*(4)), 153.4 (*C*(2)), 153.5 (Ar^1*C*(1)), 169.5 (*C*(4)); **HRMS** (ESI^+) $C_{19}H_{19}O_5N_4S$ $[M+H]^+$ found 415.1061, requires 415.1071 (–2.3 ppm).

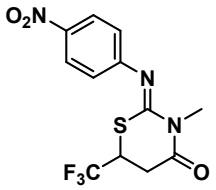
(*R*,*Z*)-6-(Methoxymethyl)-3-(4-nitrophenyl)-2-((4-nitrophenyl)imino)-1,3-thiazinan-4-one (45)



45

Following General Procedure G, perfluorophenyl (*E*)-4-methoxybut-2-enoate **S14** (127 mg, 0.45 mmol, 1.5 equiv.), 1,3-bis(4-nitrophenyl)thiourea **S18** (95.5 mg, 0.30 mmol, 1.0 equiv.) and (2*S*,3*R*)-HyperBTM **21** (18.5 mg, 0.06 mmol, 20 mol%) in anhydrous THF (0.1 M) for 24 h at RT gave crude product that was purified by flash silica column chromatography (CH_2Cl_2:Et_2O 100:0 to 95:5, R_F 0.58 at 95:5) to give the title compound as a pale yellow solid (110 mg, 88%). **mp** 67 – 69 °C; $[\alpha]_D^{20}$ +47.7 (*c* 1.0 in $CHCl_3$); **Chiral HPLC analysis,** Chiralpak AD-H (70:30 *n*-hexane : IPA, flow rate 1.0 mLmin^{-1}, 211 nm, 30 °C) t_R (*S*) 28.8 min, t_R (*R*) 35.2 min, 86:14 er; **IR** ν_{max} (film) 2930, 1705, 1612, 1582, 1516, 1508, 1341, 1298, 1219, 1157, 1111, 860; **^{1}H NMR** (500 MHz, $CDCl_3$) δ_H: 3.15 (1H, dd, *J* 16.4, 7.1, C(5)H^AH^B), 3.26 (1H, dd, *J* 16.4, 4.1, C(5)H^AH^B), 3.41 (3H, s, OCH_3), 3.61 – 3.73 (3H, m, C(6)*H* and CH_2O), 6.81 – 6.89 (2H, m, Ar^{1}C(2,6)*H*), 7.39 – 7.46 (2H, m, Ar^{2}C(2,6)*H*), 8.11 – 8.18 (2H, m, Ar^{1}C(3,5)*H*), 8.29 – 8.36 (2H, m, Ar^{2}C(3,5)*H*); **^{13}C{^{1}H} NMR** (126 MHz, $CDCl_3$) δ_C: 37.8 ($C(5)H_2$), 38.0 ($C(6)H$), 59.6 (OCH_3), 74.6 (CH_2O), 121.2 (Ar^1*C*(2,6)H), 124.7 (Ar^2*C*(3,5)H), 125.1 (Ar^1*C*(3,5)H), 130.1 (Ar^2*C*(2,6)H), 144.0 (Ar^2*C*(1)), 144.3 (Ar^1*C*(4)), 147.4 (Ar^2*C*(4)), 153.1 (*C*(2)), 153.5 (Ar^1*C*(1)), 168.6 (*C*(4)); **HRMS** (ESI^+) $C_{18}H_{17}O_6N_4S$ $[M+H]^+$ found 417.0858, requires 417.0863 (–1.2 ppm).

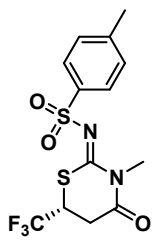
(*Z*)-3-Methyl-2-((4-nitrophenyl)imino)-6-(trifluoromethyl)-1,3-thiazinan-4-one (46)



46

Following General Procedure G, perfluorophenyl (*E*)-4,4,4-trifluorobut-2-enoate **28** (138 mg, 0.45 mmol, 1.5 equiv.), 1-methyl-3-(4-nitrophenyl)thiourea **S24** (63.4 mg, 0.30 mmol, 1.0 equiv.) and (2*S*,3*R*)-HyperBTM **21** (18.5 mg, 0.06 mmol, 20 mol%) in anhydrous THF (0.1 M) for 48 h at RT gave crude product that was purified by flash silica column chromatography (hexane:CH_2Cl_2 90:10 to 0:100, R_F 0.34 at 0:100) to give the title compound as a white solid (77 mg, 77%). **mp** 97 – 99 °C; **Chiral HPLC analysis,** Chiralcel OD-H (90:10 *n*-hexane : IPA, flow rate 1.0 mLmin^{-1}, 211 nm, 30 °C) t_R 19.0 min, t_R 24.9 min, 50:50 er; **IR** ν_{max} (film) 2934, 1686, 1611, 1584, 1508, 1337, 1215, 1200, 1165, 1126, 1107, 1049, 962, 854; **^{1}H NMR** (400 MHz, $CDCl_3$) δ_H: 3.20 (1H, dd, *J* 17.0, 5.3, C(5)H^AH^B), 3.28 (1H, dd, *J* 17.0, 5.2, C(5)H^AH^B), 3.49 (3H, s, CH_3), 3.75 – 3.85 (1H, m, C(6)*H*), 6.93 – 7.00 (2H, m, ArC(2,6)*H*), 8.19 – 8.26 (2H, m, ArC(3,5)*H*); **^{19}F{^{1}H} NMR** (377 MHz, $CDCl_3$) δ_F: –71.7 (s, CF_3); **^{13}C{^{1}H} NMR** (126 MHz, $CDCl_3$) δ_C: 31.4 (CH_3), 33.4 (*C*(5)H_2), 39.2 (q, *J* 32.6, *C*(6)H), 121.3 (Ar*C*(3,5)H), 124.5 (q, *J* 279.8, *C*F_3), 125.4 (Ar*C*(2,6)H), 144.7 (Ar*C*(1)), 148.4 (Ar*C*(4)), 153.2 (*C*(2)), 166.1 (*C*(4)); **HRMS** (ESI^+) $C_{12}H_{10}O_3N_3F_3NaS$ $[M+Na]^+$ found 356.0289, requires 356.0287 (+0.6 ppm).

(*R*,*Z*)-4-Methyl-*N*-(3-methyl-4-oxo-6-(trifluoromethyl)-1,3-thiazinan-2-ylidene)benzenesulfonamide (47)

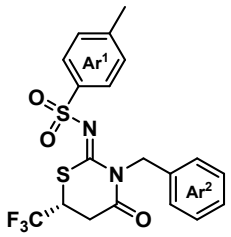


47

Following General Procedure G, perfluorophenyl (*E*)-4,4,4-trifluorobut-2-enoate **28** (138 mg, 0.45 mmol, 1.5 equiv.), 4-methyl-*N*-(methylcarbamothioyl)benzenesulfonamide

S25 (73.3 mg, 0.30 mmol, 1.0 equiv.), and (2*S*,3*R*)-HyperBTM **21** (4.6 mg, 0.015 mmol, 5 mol%) in anhydrous THF (0.1 M) for 24 h at 0 °C gave crude product that was purified by flash silica column chromatography (CH_2Cl_2:Et_2O 100:0 to 90:10, R_F 0.50 at 95:5) to give the title compound as a white solid (97 mg, 88%). **mp** 113 – 115 °C; $[\alpha]_D^{20}$ –2.5 (*c* 1.0 in $CHCl_3$); **Chiral HPLC analysis,** Chiralpak IB (80:20 *n*-hexane : IPA, flow rate 1.5 mLmin^{-1}, 254 nm, 30 °C) t_R (*S*) 11.6 min, t_R (*R*) 23.6 min, 67:33 er; **IR** ν_{max} (film) 2957, 1717, 1599, 1510, 1414, 1315, 1155, 1125, 1088, 1051, 962, 926, 820, 775; **^{1}H NMR** (400 MHz, $CDCl_3$) δ_H: 2.42 (3H, s, CH_3), 3.25 – 3.28 (2H, m, C(5)H_2), 3.30 (3H, s, NCH_3), 3.94 (1H, qt, *J* 7.7, 5.3, C(6)*H*), 7.28 – 7.34 (2H, m, ArC(3,5)*H*), 7.80 – 7.86 (2H, m, ArC(2,6)*H*); **^{19}F{^{1}H} NMR** (377 MHz, $CDCl_3$) δ_F: –71.3 (s, CF_3); **^{13}C{^{1}H} NMR** (126 MHz, $CDCl_3$) δ_C: 21.7 (*C*H_3), 32.2 (NCH_3), 32.8 (*C*(5)H_2), 39.6 (q, *J* 32.5, *C*(6)H), 124.3 (q, *J* 280.2, *C*F_3), 127.1 (Ar*C*(2,6)H), 129.7 (Ar*C*(3,5)H), 137.6 (Ar*C*(1)), 144.3 (Ar*C*(4)), 160.1 (*C*(2)), 166.0 (*C*(4)); **HRMS** (ESI^+) $C_{13}H_{13}O_3N_2F_3NaS_2$ $[M+Na]^+$ found 389.0214, requires 389.0212 (+0.5 ppm).

(*R*,*Z*)-*N*-(3-Benzyl-4-oxo-6-(trifluoromethyl)-1,3-thiazinan-2-ylidene)-4-methylbenzenesulfonamide (48)

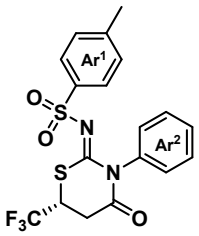


48

Following General Procedure G, perfluorophenyl (*E*)-4,4,4-trifluorobut-2-enoate **28** (138 mg, 0.45 mmol, 1.5 equiv.), 4-methyl-*N*-(benzylcarbamothioyl)benzenesulfonamide **S26** (96.1 mg, 0.30 mmol, 1.0 equiv.), and (2*S*,3*R*)-HyperBTM **21** (4.6 mg, 0.015 mmol, 5 mol%) in anhydrous THF (0.1 M) for 24 h at 0 °C gave crude product that was purified by flash silica column chromatography (hexane:CH_2Cl_2 100:0 to 0:100, R_F 0.17 at 0:100) to give the title compound as a colourless oil (130 mg, 98%). $[\alpha]_D^{20}$ +12.8 (*c* 0.5 in CH_2Cl_2); **Chiral HPLC analysis,** Chiralcel OD-H (70:30 *n*-hexane : IPA, flow rate 1.0 mLmin^{-1}, 211 nm, 30 °C) t_R (*S*) 13.4 min, t_R (*R*) 27.4 min, 78:22 er; **IR** ν_{max} (film) 2953, 1717, 1508, 1429, 1373, 1352, 1317, 1304, 1215, 1173, 1152, 1121, 1088, 1020, 961, 889, 816, 779; **^{1}H NMR** (400 MHz, $CDCl_3$) δ_H: 2.43 (3H, s, CH_3), 3.27 (1H, dd, *J* 17.0, 5.5, C(5)H^AH^B), 3.33 (1H, dd, *J* 17.0,

4.9, C(5)H^{A}*H*^{B}), 3.90 (1H, qdd, *J* 7.9, 5.5, 4.9, C(6)*H*), 5.09 (1H, d, *J* 14.1, NC*H*^{A}H^{B}), 5.22 (1H, d, *J* 14.1, NCH^{A}*H*^{B}), 7.05 – 7.10 (2H, m, Ar^{2}C(2,6)*H*), 7.11 – 7.22 (3H, m, Ar^{2}C(3,4,5)*H*), 7.23 – 7.28 (2H, m, Ar^{1}C(3,5)*H*), 7.64 – 7.69 (2H, m, Ar^{1}C(2,6)*H*); **^{19}F{^{1}H} NMR** (377 MHz, $CDCl_3$) δ_F: –71.3 (s, C*F*$_3$); **^{13}C{^{1}H} NMR** (126 MHz, $CDCl_3$) δ_C: 21.7 (*C*H$_3$), 32.8 (*C*(5)H$_2$), 39.5 (q, *J* 32.6, *C*(6)H), 47.7 (NC*H*$_2$), 124.3 (q, *J* 280.3, *C*F$_3$), 127.1 (Ar^{1}*C*(2,6)H), 127.7 (Ar^{2}*C*(4)H), 128.4 (Ar^{2}*C*(3,5)H), 128.8 (Ar^{2}*C*(2,6)H), 129.5 (Ar^{1}*C*(3,5)H), 135.6 (Ar^{2}*C*(1)), 137.3 (Ar^{1}*C*(1)), 144.1 (Ar^{1}*C*(4)), 159.2 (*C*(2)), 166.0 (*C*(4)); **HRMS** (ESI^+) $C_{19}H_{17}O_3N_2F_3NaS_2$ $[M+Na]^+$ found 465.0519, requires 465.00525 (–1.3 ppm).

(*R*,*Z*)-4-Methyl-*N*-(4-oxo-3-phenyl-6-(trifluoromethyl)-1,3-thiazinan-2-ylidene)benzenesulfonamide (49)



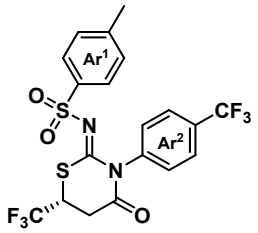
49

Following General Procedure G, perfluorophenyl (*E*)-4,4,4-trifluorobut-2-enoate **28** (138 mg, 0.45 mmol, 1.5 equiv.), 4-methyl-*N*-(phenylcarbamothioyl)benzenesulfonamide **77** (91.9 mg, 0.30 mmol, 1.0 equiv.), and (2*S*,3*R*)-HyperBTM **21** (4.6 mg, 0.015 mmol, 5 mol%) in anhydrous THF (0.1 M) for 24 h at 0 °C gave crude product that was purified by flash silica column chromatography (CH_2Cl_2:Et_2O 100:0 to 90:10, R_F 0.35 at 95:5) to give the title compound as a white solid (117 mg, 91%). **mp** 157 – 159 °C; $[\alpha]_D^{20}$ +66.6 (*c* 0.5 in CH_3CN); **Chiral HPLC analysis,** Chiralpak IA (80:20 *n*-hexane : IPA, flow rate 1.0 mLmin^{-1}, 211 nm, 30 °C) t_R (*S*) 13.7 min, t_R (*R*) 15.5 min, 91:9 er; **IR** ν_{max} (film) 2970, 1722, 1533, 1279, 1167, 1142, 1121, 1088, 1005, 959, 837, 816; **^{1}H NMR** (400 MHz, CD_3CN) δ_H: 2.38 (3H, s, C*H*$_3$), 3.33 (1H, dd, *J* 17.4, 4.2, C(5)*H*^{A}H^{B}), 3.58 (1H, dd, *J* 17.4, 5.5, C(5)H^{A}*H*^{B}), 4.37 (1H, qdd, *J* 8.4, 5.5, 4.2, C(6)*H*), 7.05 (2H, br s, Ar^{2}C(2,6)*H*), 7.25 – 7.32 (2H, m, Ar^{1}C(3,5)*H*), 7.38 – 7.53 (5H, m, Ar^{1}C(2,6)*H* and Ar^{2}C(3,4,5)*H*); **^{19}F{^{1}H} NMR** (377 MHz, CD_3CN)

δ_F: –71.9 (s, C*F*$_3$); **^{13}C{^{1}H} NMR** (126 MHz, CD_3CN) δ_C: 21.5 (*C*H$_3$), 33.6 (*C*(5)H$_2$), 40.3 (q, *J* 32.0, *C*(6)H), 126.1 (q, *J* 279.5, *C*F$_3$), 127.3 (Ar^{1}*C*(2,6)H), 129.0 (Ar^{2}*C*(2,6)H), 129.7

(Ar^2*C*(3,5)H), 130.3 (Ar^2*C*(4)H), 130.4 (Ar^1*C*(3,5)H), 138.3 (Ar^2*C*(1)), 138.6 (Ar^1*C*(1)), 145.1 (Ar^1*C*(4)), 163.5 (*C*(2)), 167.7 (*C*(4)); **HRMS** ($^{ESI+}$) $C_{18}H_{15}O_3N_2F_3NaS_2$ $[M+Na]^+$ found 451.0372, requires 451.0368 (+0.9 ppm).

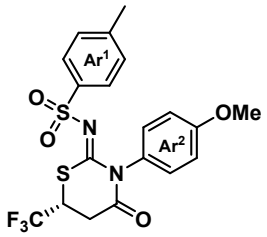
(*R*,*Z*)-4-Methyl-*N*-(4-oxo-6-(trifluoromethyl)-3-(4-(trifluoromethyl)phenyl)-1,3-thiazinan-2-ylidene)benzenesulfonamide (50)



50

Following General Procedure G, perfluorophenyl (*E*)-4,4,4-trifluorobut-2-enoate **28** (138 mg, 0.45 mmol, 1.5 equiv.), 4-methyl-*N*-((4-(trifluoromethyl)phenyl)carbamothioyl) benzenesulfonamide **S22** (112 mg, 0.30 mmol, 1.0 equiv.), and (2*S*,3*R*)-HyperBTM **21** (4.6 mg, 0.015 mmol, 5 mol%) in anhydrous THF (0.1 M) for 24 h at 0 °C gave crude product that was purified by flash silica column chromatography (CH_2Cl_2:Et_2O 100:0 to 95:5, R_F 0.37 at 95:5) to give the title compound as a white solid (118 mg, 79%). **mp** 182 – 184 °C; $[\alpha]_D^{20}$ +56.8 (*c* 0.5 in CH_3CN); **Chiral HPLC analysis,** Chiralpak ID (93:7 *n*-hexane : IPA, flow rate 1.0 mLmin^{-1}, 254 nm, 40 °C) t_R (*S*) 22.9 min, t_R (*R*) 25.8 min, 88:12 er; **IR** ν_{max} (film) 2968, 2359, 1732, 1520, 1373, 1331, 1281, 1167, 1125, 1090, 1069, 1003, 961, 851, 818; **^{1}H NMR** (400 MHz, CD_3CN) δ_H: 2.38 (3H, s, CH_3), 3.35 (1H, dd, *J* 17.4, 4.3, C(5)H^AH^B), 3.59 (1H, dd, *J* 17.4, 5.5, C(5)H^A*H*^{B}), 4.41 (1H, qdd, *J* 8.4, 5.5, 4.3, C(6)*H*), 7.20 – 7.31 (4H, m, Ar^{1}C(3,5)*H* and Ar^{2}C(2,6)*H*), 7.46 – 7.52 (2H, m, Ar^{1}C(2,6)*H*), 7.73 – 7.78 (2H, m, Ar^{2}C(3,5)*H*); **^{19}F{^{1}H} NMR** (377 MHz, CD_3CN) δ_F: –71.9 (s, CF_3), -63.2 (s, CF_3); **^{13}C{^{1}H} NMR** (126 MHz, CD_3CN) δ_C: 21.5 (*C*H_3), 33.5 (*C*(5)H_2), 40.4 (q, *J* 31.9, *C*(6)H), 125.0 (q, *J* 271.6, *C*F_3), 126.0 (q, *J* 279.5, *C*F_3), 127.4 (Ar^1*C*(2,6)H), 127.4 – 127.5 (m, Ar^2*C*(3,5)H), 130.2 (Ar^2*C*(2,6)H), 130.4 (Ar^1*C*(3,5)H), 131.1 (q, *J* 32.5, Ar^2*C*(4)), 138.4 (Ar^1*C*(1)), 141.9 (Ar^2*C*(1)), 145.4 (Ar^1*C*(4)), 163.3 (*C*(2)), 167.7 (*C*(4)); **HRMS** ($^{ESI+}$) $C_{19}H_{14}O_3N_2F_6NaS_2$ $[M+Na]^+$ found 519.0244, requires 519.0242 (+0.4 ppm).

(*R*,*Z*)-*N*-(3-(4-Methoxyphenyl)-4-oxo-6-(trifluoromethyl)-1,3-thiazinan-2-ylidene)-4-methylbenzenesulfonamide (51)

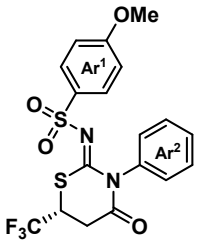


51

Following General Procedure G, perfluorophenyl (*E*)-4,4,4-trifluorobut-2-enoate **28** (138 mg, 0.45 mmol, 1.5 equiv.), *N*-((4-methoxyphenyl)carbamothioyl)-4-methylbenzenesulfonamide **S21** (101 mg, 0.30 mmol, 1.0 equiv.), and (2*S*,3*R*)-HyperBTM **21** (4.6 mg, 0.015 mmol, 5 mol%) in anhydrous THF (0.1 M) for 24 h at 0 °C gave crude product that was purified by flash silica column chromatography (CH_2Cl_2:Et_2O 100:0 to 95:5, R_F 0.33 at 95:5) to give the title compound as a mixture of regioisomers (90:10) as a white solid (122 mg, 88%). **mp** 131 – 133 °C; $[\alpha]_D^{20}$ +79.8 (*c* 0.5 in CH_3CN); **Chiral HPLC analysis,** Chiralpak AD-H (80:20 *n*-hexane : IPA, flow rate 1.0 mLmin^{-1}, 254 nm, 30 °C) t_R (*S*) 18.0 min, t_R (*R*) 22.1 min, 90:10 er; **IR** ν_{max} (film) 2959, 1724, 1607, 1518, 1508, 1371, 1279, 1248, 1163, 1142, 1123, 1086, 1028, 1001, 957, 885, 845, 816; **^{1}H NMR** (400 MHz, CD_3CN) δ_H: 2.39 (3H, s, CH_3), 3.32 (1H, dd, *J* 17.3, 4.2, C(5)H^AH^B), 3.56 (1H, dd, *J* 17.3, 5.5, C(5)H^AH^B), 3.81 (3H, s, OCH_3), 4.35 (1H, qdd, *J* 8.4, 5.5, 4.2, C(6)*H*), 6.93 – 6.99 (4H, m, Ar^{2}C(2,3,5,6)*H*), 7.26 – 7.32 (2H, m, Ar^{1}C(3,5)*H*), 7.50 – 7.55 (2H, m, Ar^{2}C(2,6)*H*); **^{19}F{^{1}H} NMR** (376 MHz, CD_3CN) δ_F: –71.9 (s, CF_3); **^{13}C{^{1}H} NMR** (126 MHz, CD_3CN) δ_C: 21.5 (*C*H_3), 33.7 (*C*(5)H_2), 40.2 (q, *J* 31.9, *C*(6)H), 56.2 (O*C*H_3),115.4 (Ar^2*C*(3,5)H), 126.1 (q, *J* 279.5, *C*F_3), 127.3 (Ar^1*C*(2,6)H), 130.0 (br, Ar^2*C*(2,6)H), 130.4 (Ar^1*C*(3,5)H), 130.5 (Ar^2*C*(1)), 138.7 (Ar^1*C*(1)), 145.1 (Ar^1*C*(4)), 160.6 (Ar^1*C*(4)), 163.8 (*C*(2)), 167.8 (*C*(4));

HRMS (ESI^+) $C_{19}H_{17}O_4N_2F_3NaS_2$ $[M+Na]^+$ found 481.0473, requires 481.0474 (–0.2 ppm).

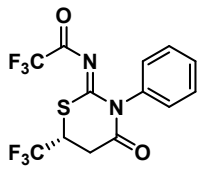
(*R*,*Z*)-4-Methoxy-*N*-(4-oxo-3-phenyl-6-(trifluoromethyl)-1,3-thiazinan-2-ylidene) benzenesulfonamide (52)



52

Following General Procedure G, perfluorophenyl (*E*)-4,4,4-trifluorobut-2-enoate **28** (138 mg, 0.45 mmol, 1.5 equiv.), 4-methoxy-*N*-(phenylcarbamothioyl)benzenesulfonamide **S23** (96.7 mg, 0.30 mmol, 1.0 equiv.), and (2*S*,3*R*)-HyperBTM **21** (4.6 mg, 0.015 mmol, 5 mol%) in anhydrous THF (0.1 M) for 24 h at 0 °C gave crude product that was purified by flash silica column chromatography (CH_2Cl_2:Et_2O 100:0 to 95:5, R_F 0.30 at 95:5) to give the title compound as a white solid (128 mg, 96%). **mp** 128 – 130 °C; $[\alpha]_D^{20}$ +77.0 (*c* 0.5 in CH_3CN); **Chiral HPLC analysis,** Chiralpak IA (80:20 *n*-hexane : IPA, flow rate 1.0 mLmin^{-1}, 211 nm, 30 °C) t_R (*S*) 17.2 min, t_R (*R*) 21.2 min, 91:9 er; **IR** ν_{max} (film) 2968, 1719, 1593, 1518, 1491, 1323, 1260, 1167, 1138, 1117, 1088, 1007, 959, 883, 833, 766; **^{1}H NMR** (400 MHz, CD_3CN) δ_H: 3.33 (1H, dd, *J* 17.4, 4.2, C(5)*H*^{A}H^B), 3.56 (1H, dd, *J* 17.4, 5.5, C(5)H^A*H*^{B}), 3.83 (3H, s, OC*H*$_3$), 4.37 (1H, qdd, *J* 8.4, 5.5, 4.2, C(6)*H*), 6.94 – 6.99 (2H, m, Ar^{1}C(3,5)*H*), 7.04 (2H, br s, Ar^{2}C(2,6)*H*), 7.39 – 7.48 (3H, m, Ar^{2}C(3,4,5)*H*), 7.54 – 7.59 (2H, m, Ar^{1}C(2,6)*H*); **^{19}F{^{1}H} NMR** (377 MHz, CD_3CN) δ_F: –71.8 (s, C*F*$_3$); **^{13}C{^{1}H} NMR** (126 MHz, CD_3CN) δ_C: 33.6 (*C*(5)H$_2$), 40.3 (q, *J* 31.9, *C*(6)H), 56.5 (OCH$_3$), 115.0 (Ar^1*C*(3,5)H), 126.1 (q, *J* 279.5, *C*F$_3$), 129.1 (Ar^2*C*(2,6)H), 129.6 (Ar^1*C*(2,6)H), 129.7 (Ar^2*C*(4)H), 130.3 (Ar^2*C*(3,5)H), 133.1 (Ar^1*C*(1)), 138.3 (Ar^2*C*(1)), 163.2 (Ar^1*C*(4)), 164.2 (*C*(2)), 167.7 (*C*(4)); **HRMS** (ESI^+) $C_{18}H_{15}O_4N_2F_3NaS_2$ $[M+Na]^+$ found 467.0315, requires 467.0318 (–0.6 ppm).

(*R*,*Z*)-2,2,2-Trifluoro-*N*-(4-oxo-3-phenyl-6-(trifluoromethyl)-1,3-thiazinan-2-ylidene)acetamide (53)

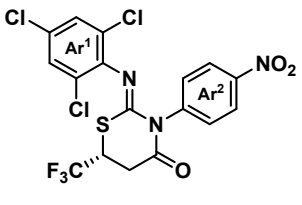


53

Following General Procedure G, perfluorophenyl (*E*)-4,4,4-trifluorobut-2-enoate **28** (138 mg, 0.45 mmol, 1.5 equiv.), 2,2,2-trifluoro-*N*-(phenylcarbamothioyl)acetamide **S27** (74.5 mg, 0.30 mmol, 1.0 equiv.), and (2*S*,3*R*)-HyperBTM **21** (4.6 mg, 0.015 mmol, 5 mol%) in anhydrous THF (0.1 M) for 24 h at 0 °C gave crude product that was purified by flash silica column chromatography (hexane:CH_2Cl_2 80:20 to 0:100, R_F 0.45 at 0:100) to give the title compound as a colourless glass (63 mg, 57%). $[\alpha]_D^{20}$ +11.0 (*c* 0.6 in $CHCl_3$); **Chiral HPLC analysis,** Chiralcel OD-H (90:10 *n*-hexane : IPA, flow rate 2.0 mLmin^{-1}, 211 nm, 40 °C) t_R (*S*) 7.0 min, t_R (*R*) 16.5 min, 96:4 er; **IR** ν_{max} (film) 2949, 1655, 1595, 1491, 1360, 1315, 1231, 1167, 1115, 1043, 978, 910, 835, 797, 756; **^{1}H NMR** (400 MHz, $CDCl_3$) δ_H: 3.45 (1H, dd, *J* 17.3, 5.4, C(5)H^AH^B), 3.52 (1H, dd, *J* 17.3, 4.4, C(5)H^AH^B), 3.97 (1H, qdd, *J* 7.9, 5.4, 4.4, C(6)*H*), 7.03 – 7.10 (2H, m, ArC(2,6)*H*), 7.41 – 7.51 (3H, m, ArC(3,4,5)*H*); **^{19}F{^{1}H} NMR** (377 MHz, $CDCl_3$) δ_F: –76.8 (s, CF_3), –71.1 (s, CF_3); **^{13}C{^{1}H} NMR** (126 MHz, $CDCl_3$) δ_C: 33.2 (*C*(5)H_2), 39.8 (q, *J* 32.5, *C*(6)H), 115.5 (q, *J* 287.0, *C*F_3), 124.6 (q, *J* 280.3, *C*F_3), 127.7 (Ar^2*C*(2,6)H), 129.4 (Ar^2*C*(4)H), 129.6 (Ar^2*C*(3,5)H), 136.5 (Ar*C*(1)), 165.9 (*C*(2)), 166.3

(q, *J* 39.1, *C*(O)CF_3), 167.5 (*C*(4)); **HRMS** (ESI^-) $C_{13}H_7O_2N_2F_6S$ $[M-H]^-$ found 369.0142, requires 369.0138 (+1.1 ppm).

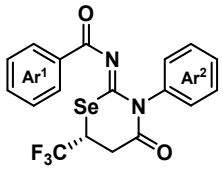
(*R*,*Z*)-3-(4-Nitrophenyl)-2-((2,4,6-trichlorophenyl)imino)-6-(trifluoromethyl)-1,3-thiazinan-4-one (54)



54

Following General Procedure G, perfluorophenyl (*E*)-4,4,4-trifluorobut-2-enoate **28** (138 mg, 0.45 mmol, 1.5 equiv.), 1-(4-nitrophenyl)-3-(2,4,6-trichlorophenyl)thiourea **S20** (113 mg, 0.30 mmol, 1.0 equiv.) and (2*S*,3*R*)-HyperBTM **21** (9.3 mg, 0.015 mmol, 5 mol%) in anhydrous THF (0.1 M) for 48 h at 0 °C gave crude product that was purified by flash silica column chromatography (hexane:EtOAc 95:5 to 70:30, R_F 0.23 at 75:25) to give the title compound as a yellow solid (138 mg, 92%). **mp** 157 – 159 °C; $[\alpha]_D^{20}$ +41.7 (*c* 1.0 in $CHCl_3$); **Chiral HPLC analysis,** Chiralpak AD-H (90:10 *n*-hexane : IPA, flow rate 1.0 mLmin^{-1}, 211 nm, 30 °C) t_R (*R*) 14.0 min, t_R (*S*) 17.9 min, 98:2 er; **IR** ν_{max} (film) 1713, 1614, 1524, 1348, 1298, 1227, 1177, 1121, 853, 841; **^{1}H NMR** (500 MHz, $CDCl_3$) δ_H: 3.46 (1H, dd, *J* 17.3, 5.4, C(5)H^AH^B), 3.51 (1H, dd, *J* 17.3, 4.0, C(5)H^AH^B), 3.86 – 3.95 (1H, m, C(6)*H*), 7.30 (1H, d, *J* 2.2, Ar^{1}C(3)*H*), 7.32 (1H, d, *J* 2.2, Ar^{1}C(5)*H*), 7.44 – 7.49 (2H, m, Ar^{2}C(2,6)*H*), 8.33 – 8.38 (2H, m, Ar^{2}C(3,5)*H*); **^{19}F{^{1}H} NMR** (376 MHz, $CDCl_3$) δ_F: –71.3 (s, CF_3); **^{13}C{^{1}H} NMR** (126 MHz, $CDCl_3$) δ_C: 33.7 (*C*(5)H_2), 39.5 (q, *J* 32.8, *C*(6)H), 124.7 (q, *J* 280.2, *C*F_3), 124.9 (Ar^2*C*(3,5)H), 126.6 (Ar^1*C*(2)), 127.0 (Ar^1*C*(6)), 128.3 (Ar^1*C*(5)H), 128.7 (Ar^1*C*(3)H), 130.1 (Ar^2*C*(2,6)H), 130.2 (Ar^1*C*(4)), 140.1 (Ar^1*C*(1)), 142.7 (Ar^2*C*(1)), 147.9 (Ar^2*C*(4)), 152.3 (*C*(2)), 165.6 (*C*(4)); **HRMS** (ESI^+) $C_{17}H_{10}O_3N_3F_3{}^{35}Cl_3S$ $[M+H]^+$ found 497.9442, requires 497.9455 (–2.6 ppm).

(*R*,*Z*)-*N*-(4-Oxo-3-phenyl-6-(trifluoromethyl)-1,3-selenazinan-2-ylidene)benzamide (55)

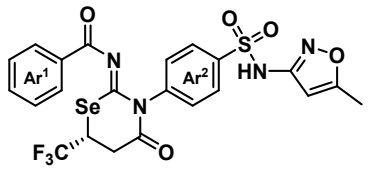


55

Following General Procedure G, perfluorophenyl (*E*)-4,4,4-trifluorobut-2-enoate **28** (138 mg, 0.45 mmol, 1.5 equiv.), *N*-(phenylcarbamoselenoyl)benzamide **S31** (91.0 mg, 0.30 mmol, 1.0 equiv.), and (2*S*,3*R*)-HyperBTM **21** (9.3 mg, 0.03 mmol, 10 mol%) in anhydrous THF (0.1 M) for 24 h at 0 °C gave crude product that was purified by flash silica column chromatography (hexane:CH_2Cl_2 60:40 to 0:100, R_F 0.47 at 0:100) to give the title compound as a colourless solid (124 mg, 97%). **mp** 117 – 119 °C; $[\alpha]_D^{20}$ +21.3 (*c* 0.8 in $CHCl_3$); **Chiral HPLC analysis,** Chiralpak IA (80:20 *n*-hexane : IPA, flow rate 1.0 mLmin^{-1}, 254 nm, 30 °C) t_R (*S*) 8.0 min, t_R (*R*) 10.2 min, 99:1 er; **IR** ν_{max} (film) 2965, 1717,

1634, 1497, 1476, 1362, 1325, 1233, 1169, 1153, 1103, 1086, 1024, 887; **^{1}H NMR** (500 MHz, $CDCl_3$) δ_H: 3.56 (1H, dd, *J* 16.7, 5.0, C(5)H^AH^B), 3.66 (1H, dd, *J* 16.7, 5.2, C(5)H^AH^B), 3.79 (1H, qdd, *J* 9.0, 5.2, 5.0, C(6)*H*), 7.16 – 7.20 (2H, m, Ar^{2}C(2,6)*H*), 7.28 – 7.34 (2H, m, Ar^{1}C(3,5)*H*), 7.45 – 7.50 (2H, m, Ar^{1}C(4)*H* and Ar^{2}C(4)*H*), 7.51 – 7.56 (2H, m, Ar^{2}C(3,5)*H*), 7.72 – 7.76 (2H, m, Ar^{1}C(2,6)*H*); **^{19}F{^{1}H} NMR** (470 MHz, $CDCl_3$) δ_F: –69.1 (s, CF_3); **^{13}C{^{1}H} NMR** (126 MHz, $CDCl_3$) δ_C: 32.8 (q, *J* 31.5, *C*(6)H), 35.5 (*C*(5)H_2), 126.0 (q, *J* 278.1, *C*F_3), 128.0 (Ar^2*C*(2,6)H), 128.5 (Ar^1*C*(3,5)H), 128.6 (Ar^2*C*(4)H), 129.4 (Ar^2*C*(3,5)H), 130.3 (Ar^1*C*(2,6)H), 133.6 (Ar^1*C*(4)), 134.6 (Ar^1*C*(1)), 139.6 (Ar^2*C*(1)), 164.8 (*C*(2)), 168.2 (*C*(4)), 177.1 (*C*O); **^{77}Se{^{1}H} NMR** (95 MHz, $CDCl_3$) δ_{Se}: 498.9 (s, C*Se*); **HRMS** (ESI^+) $C_{18}H_{13}O_2N_2F_3Na^{80}Se$ $[M+Na]^+$ found 448.9988, requires 448.9987 (+0.2 ppm).

(*R*,*Z*)-*N*-(3-(4-(*N*-(5-Methylisoxazol-3-yl)sulfamoyl)phenyl)-4-oxo-6-(trifluoromethyl)-1,3-selenazinan-2-ylidene)benzamide (56)

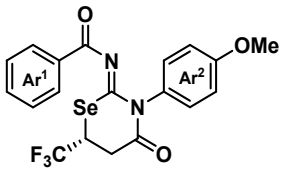


56

Following General Procedure G, perfluorophenyl (*E*)-4,4,4-trifluorobut-2-enoate **28** (138 mg, 0.45 mmol, 1.5 equiv.), *N*-((4-(*N*-(5-methylisoxazol-3-yl)sulfamoyl) phenyl)carbamoselenoyl)benzamide **S36** (139 mg, 0.30 mmol, 1.0 equiv.), and (2*S*,3*R*)-HyperBTM **21** (9.3 mg, 0.03 mmol, 10 mol%) in anhydrous THF (0.1 M) for 24 h at 0 °C gave crude product that was purified by flash silica column chromatography (hexane:EtOAc 90:10 to 0:100, R_F 0.42 at 50:50) to give the title compound as a white solid (108 mg, 61%). **mp** 140 °C (dec.); $[\alpha]_D^{20}$ +49.0 (*c* 0.2 in CH_3CN); **Chiral HPLC analysis,** Chiralpak AD-H (60:40 *n*-hexane : IPA, flow rate 1.0 mLmin^{-1}, 254 nm, 30 °C) t_R (*S*) 8.8 min, t_R (*R*) 12.0 min, 98:2 er; **IR** ν_{max} (film) 3273, 1718, 1616, 1458, 1387, 1323, 1248, 1219, 1161, 1090, 1067, 993, 926, 891; **^{1}H NMR** (500 MHz, CD_3CN) δ_H: 2.29 (3H, s, CH_3), 3.53 (1H, dd, *J* 17.0, 4.8, C(5)H^AH^B), 3.69 (1H, dd, *J* 17.0, 5.1, C(5)H^AH^B), 3.79 (1H, qdd, *J* 9.5, 5.1, 4.8, C(6)*H*), 6.21 (1H, s, C*H*), 7.30 – 7.36 (2H, m, Ar^{1}C(3,5)*H*), 7.39 – 7.45 (2H, m, Ar^{2}C(2,6)*H*), 7.52 – 7.58 (1H, m, Ar^{1}C(4)*H*), 7.58 – 7.63 (2H, m, Ar^{2}C(3,5)*H*), 8.01 – 8.06 (2H, m, Ar^{1}C(2,6)*H*); **^{19}F{^{1}H} NMR** (470 MHz, CD_3CN) δ_F: –69.8 (s, CF_3); **^{13}C{^{1}H} NMR** (126 MHz,

CD_3CN) δ_C: 12.6 (CH_3), 33.3 (q, *J* 31.0, *C*(6)H), 35.8 (*C*(5)H_2), 96.5 (*C*H), 127.5 (q, *J* 277.4, *C*F_3), 129.1 (Ar^2*C*(2,6)H), 129.5 (Ar^1*C*(3,5)H), 130.3 (Ar^2*C*(3,5)H), 130.6 (Ar^1*C*(2,6)H), 134.5 (Ar^1*C*(4)H), 135.3 (Ar^1*C*(1)), 140.0 (Ar^2*C*(4)), 145.7 (Ar^2*C*(1)), 158.4 (*C*=N), 166.8 (*C*(2)), 169.7 (*C*(4)), 172.2 (*C*-O), 177.5 (*C*O); **^{77}Se{^{1}H} NMR** (95 MHz, CD_3CN) δ_{Se}: 495.0 (s, C*Se*); **HRMS** (ESI^-) $C_{22}H_{16}O_5N_4F_3S^{80}Se$ $[M-H]^-$ found 584.9960, requires 584.9964 (–0.7 ppm).

(*R*,*Z*)-*N*-(3-(4-Methoxyphenyl)-4-oxo-6-(trifluoromethyl)-1,3-selenazinan-2-ylidene)benzamide (57)

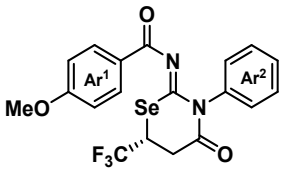


57

Following General Procedure G, perfluorophenyl (*E*)-4,4,4-trifluorobut-2-enoate **28** (138 mg, 0.45 mmol, 1.5 equiv.), *N*-((4-methoxyphenyl)carbamoselenoyl)benzamide **S35** (100 mg, 0.30 mmol, 1.0 equiv.), and (2*S*,3*R*)-HyperBTM **21** (9.3 mg, 0.03 mmol, 10 mol%) in anhydrous THF (0.1 M) for 24 h at 0 °C gave crude product that was purified by flash silica column chromatography (hexane:CH_2Cl_2 60:40 to 0:100, R_F 0.38 at 0:100) to give the title compound as a colourless solid (133 mg, 97%). **mp** 100 – 102 °C; $[\alpha]_D^{20}$ +27.5 (*c* 1.0 in $CHCl_3$); **Chiral HPLC analysis,** Chiralpak IA (80:20 *n*-hexane : IPA, flow rate 1.0 mLmin^{-1}, 220 nm, 30 °C) t_R (*S*) 10.8 min, t_R (*R*) 12.1 min, 98:2 er; **IR** ν_{max} (film) 2959, 1715, 1632, 1508, 1476, 1364, 1325, 1248, 1233, 1153, 1103, 1086, 1045, 1024, 889, 791; **^{1}H NMR** (500 MHz, $CDCl_3$) δ_H: 3.54 (1H, dd, *J* 16.7, 5.0, C(5)*H*^{A}H^B), 3.64 (1H, dd, *J* 16.7, 5.3, C(5)H^A*H*^{B}), 3.77 (1H, qdd, *J* 9.0, 5.3, 5.0, C(6)*H*), 3.88 (3H, s, OCH_3), 7.02 – 7.06 (2H, m, Ar^{2}C(3,5)*H*), 7.07 – 7.12 (2H, m, Ar^{2}C(2,6)*H*), 7.31 – 7.37 (2H, m, Ar^{1}C(3,5)*H*), 7.46 – 7.52 (1H, m, Ar^{1}C(4)*H*), 7.78 – 7.83 (2H, m, Ar^{1}C(2,6)*H*); **^{19}F{^{1}H} NMR** (376 MHz, $CDCl_3$) δ_F: –69.1 (s, CF_3); **^{13}C{^{1}H} NMR** (126 MHz, $CDCl_3$) δ_C: 32.7 (q, *J* 31.6, *C*(6)H), 35.5 (*C*(5)H_2), 55.6 (OCH_3), 114.6 (Ar^2*C*(3,5)H), 126.0 (q, *J* 278.1, *C*F_3), 128.5 (Ar^1*C*(3,5)H), 129.0 (Ar^2*C*(2,6)H), 130.3 (Ar^1*C*(2,6)H), 132.1 (Ar^2*C*(1)), 133.6 (Ar^1*C*(4)H), 134.6 (Ar^1*C*(1)), 159.4 (Ar^2*C*(4)), 165.0 (*C*(2)), 168.4 (*C*(4)), 177.2 (*C*O); **^{77}Se{^{1}H} NMR** (95 MHz, $CDCl_3$) δ_{Se}: 500.0

(s, C*Se*); **HRMS** (ESI^+) $C_{19}H_{15}O_3N_2F_3Na^{80}Se$ $[M+Na]^+$ found 479.0093, requires 479.0092 (+0.2 ppm).

(*R*,*Z*)-4-Methoxy-*N*-(4-oxo-3-phenyl-6-(trifluoromethyl)-1,3-selenazinan-2-ylidene)benzamide (58)

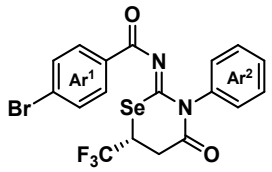


58

Following General Procedure G**,** perfluorophenyl (*E*)-4,4,4-trifluorobut-2-enoate **28** (138 mg, 0.45 mmol, 1.5 equiv.), 4-methoxy-*N*-(phenylcarbamoselenoyl)benzamide **S32** (100 mg, 0.30 mmol, 1.0 equiv.), and (2*S*,3*R*)-HyperBTM **21** (9.3 mg, 0.03 mmol, 10 mol%) in anhydrous THF (0.1 M) for 24 h at 0 °C gave crude product that was purified by flash silica column chromatography (hexane:CH_2Cl_2 80:20 to 0:100, R_F 0.34 at 0:100) to give the title compound as a colourless solid (110 mg, 80%). **mp** 156 – 158 °C; $[\alpha]_D^{20}$ +20.0 (*c* 0.5 in $CHCl_3$); **Chiral HPLC analysis,** Chiralpak IB (90:10 *n*-hexane : IPA, flow rate 1.0 mLmin^{-1}, 211 nm, 30 °C) t_R (*S*) 30.6 min, t_R (*R*) 37.3 min, 99:1 er; **IR** ν_{max} (film) 2359, 1717, 1597, 1510, 1489, 1312, 1260, 1236, 1152, 1101, 1084, 849; **^{1}H NMR** (400 MHz, $CDCl_3$)

δ_H: 3.55 (1H, dd, *J* 16.6, 5.0, C(5)H^AH^B), 3.65 (1H, dd, *J* 16.6, 5.3, C(5)H^AH^B), 3.71 – 3.84 (4H, m, C(6)*H* and OCH_3), 6.75 – 6.81 (2H, m, Ar^{1}C(3,5)*H*), 7.14 – 7.20 (2H, m, Ar^{2}C(2,6)*H*), 7.43 – 7.56 (3H, m, Ar^{2}C(3,5)*H* and Ar^{2}C(4)*H*), 7.66 – 7.72 (2H, m, Ar^{1}C(2,6)*H*); **^{19}F{^{1}H} NMR** (377 MHz, $CDCl_3$) δ_F: –69.0 (s, CF_3); **^{13}C{^{1}H} NMR** (126 MHz, $CDCl_3$) δ_C: 32.8 (q, *J* 31.5, *C*(6)H), 35.6 (*C*(5)H_2), 55.6 (OCH_3), 113.8 (Ar^1*C*(3,5)H), 126.1 (q, *J* 278.1, *C*F_3), 127.4 (Ar^1*C*(1)), 128.1 (Ar^2*C*(2,6)H), 128.5 (Ar^2*C*(4)H), 129.4 (Ar^2*C*(3,5)H), 132.6 (Ar^1*C*(2,6)H), 139.8 (Ar^2*C*(1)), 163.7 (*C*(2)), 164.1 (Ar^1*C*(4)), 168.2 (*C*(4)), 176.3 (*C*O); **^{77}Se{^{1}H} NMR** (95 MHz, $CDCl_3$) δ_{Se}: 496.9 (s, C*Se*); **HRMS** (ESI^+) $C_{19}H_{15}O_3N_2F_3Na^{80}Se$ $[M+Na]^+$ found 479.0091, requires 479.0092 (–0.2 ppm).

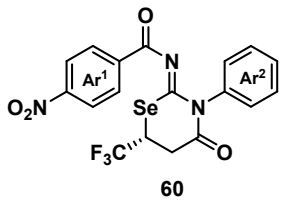
(*R*,*Z*)-4-Bromo-*N*-(4-oxo-3-phenyl-6-(trifluoromethyl)-1,3-selenazinan-2-ylidene)benzamide (59)



59

Following General Procedure G, perfluorophenyl (*E*)-4,4,4-trifluorobut-2-enoate **28** (138 mg, 0.45 mmol, 1.5 equiv.), 4-bromo-*N*-(phenylcarbamoselenoyl)benzamide **S33** (115 mg, 0.30 mmol, 1.0 equiv.), and (2*S*,3*R*)-HyperBTM **21** (9.3 mg, 0.03 mmol, 10 mol%) in anhydrous THF (0.1 M) for 24 h at 0 °C gave crude product that was purified by flash silica column chromatography (hexane:CH_2Cl_2 100:0 to 0:100, R_F 0.63 at 0:100) to give the title compound as a colourless glass (139 mg, 92%). $[\alpha]_D^{20}$ +17.9 (*c* 0.7 in $CHCl_3$); **Chiral HPLC analysis,** Chiralpak IA (80:20 *n*-hexane : IPA, flow rate 1.0 mLmin^{-1}, 254 nm, 30 °C) t_R (*S*) 11.1 min, t_R (*R*) 12.5 min, 98:2 er; **IR** ν_{max} (film) 1715, 1630, 1587, 1489, 1474, 1362, 1325, 1231, 1165, 1153, 1103, 1084, 1045, 1010, 762; **^{1}H NMR** (400 MHz, $CDCl_3$) δ_H: 3.55 (1H, dd, *J* 16.7, 5.1, C(5)*H*^{A}H^B), 3.66 (1H, dd, *J* 16.7, 5.1, C(5)H^A*H*^{B}), 3.80 (1H, qdd, *J* 8.8, 5.1, 5.1, C(6)*H*), 7.13 – 7.18 (2H, m, Ar^{2}C(2,6)*H*), 7.41 – 7.60 (7H, m, Ar^{1}C(2,6)*H*, Ar^{1}C(3,5)*H*, Ar^{2}C(3,5)*H* and Ar^{2}C(4)*H*); **^{19}F{^{1}H} NMR** (377 MHz, $CDCl_3$) δ_F: –69.1 (s, C*F*$_3$); **^{13}C{^{1}H} NMR** (126 MHz, $CDCl_3$) δ_C: 32.8 (q, *J* 31.5, *C*(6)H), 35.4 (*C*(5)H$_2$), 126.0 (q, *J* 278.3, *C*F$_3$), 127.9 (Ar^2*C*(2,6)H), 128.6 (Ar^2*C*(4)H), 128.8 (Ar^1*C*(4)), 129.4 (Ar^2*C*(3,5)H), 131.7 (Ar^1*C*(2,6)H), 131.8 (Ar^1*C*(3,5)H), 133.5 (Ar^1*C*(1)), 139.5 (Ar^2*C*(1)), 165.6 (*C*(2)), 168.1 (*C*(4)), 176.2 (*C*O); **^{77}Se{^{1}H} NMR** (95 MHz, $CDCl_3$) δ_{Se}: 500.7 (s, C*Se*); **HRMS** (ESI^+) $C_{18}H_{12}O_2N_2{}^{79}BrF_3Na^{80}Se$ $[M+Na]^+$ found 526.9088, requires 526.9092 (–0.8 ppm).

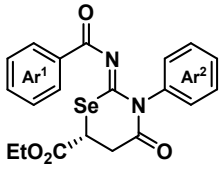
(*R*,*Z*)-4-Nitro-*N*-(4-oxo-3-phenyl-6-(trifluoromethyl)-1,3-selenazinan-2-ylidene)benzamide (60)



60

Following General Procedure G, perfluorophenyl (*E*)-4,4,4-trifluorobut-2-enoate **28** (138 mg, 0.45 mmol, 1.5 equiv.), 4-nitro-*N*-(phenylcarbamoselenoyl)benzamide **S34** (104 mg, 0.30 mmol, 1.0 equiv.), and (2*S*,3*R*)-HyperBTM **21** (9.3 mg, 0.03 mmol, 10 mol%) in anhydrous THF (0.1 M) for 24 h at 0 °C gave crude product that was purified by flash silica column chromatography (hexane:CH_2Cl_2 70:30 to 0:100, R_F 0.51 at 0:100) to give the title compound as a pale yellow solid (118 mg, 84%). **mp** 86 – 88 °C; $[\alpha]_D^{20}$ +23.4 (*c* 0.5 in $CHCl_3$); **Chiral HPLC analysis,** Chiralpak IA (80:20 *n*-hexane : IPA, flow rate 1.0 mLmin^{-1}, 211 nm, 30 °C) t_R (*S*) 13.8 min, t_R (*R*) 15.8 min, 97:3 er; **IR** ν_{max} (film) 2359, 1717, 1636, 1597, 1522, 1458, 1362, 1329, 1231, 1153, 1103, 1088, 1045, 854; **^{1}H NMR** (400 MHz, $CDCl_3$) δ_H: 3.58 (1H, dd, *J* 16.8, 5.1, C(5)H^AH^B), 3.69 (1H, dd, *J* 16.8, 5.1, C(5)H^AH^B), 3.85 (1H, qdd, *J* 8.8, 5.1, 5.1, C(6)*H*), 7.13 – 7.19 (2H, m, Ar^{2}C(2,6)*H*), 7.47 – 7.57 (3H, m, Ar^{2}C(3,5)*H* and Ar^{2}C(4)*H*), 7.80 – 7.86 (2H, m, Ar^{1}C(2,6)*H*), 8.09 – 8.15 (2H, m, Ar^{1}C(3,5)*H*); **^{19}F{^{1}H} NMR** (377 MHz, $CDCl_3$) δ_F: –69.1 (s, CF_3); **^{13}C{^{1}H} NMR** (126 MHz, $CDCl_3$) δ_C: 33.0 (q, *J* 31.8, *C*(6)H), 35.3 (*C*(5)H_2), 123.6 (Ar^1*C*(3,5)H), 125.9 (q, *J* 278.3, *C*F_3), 127.9 (Ar^2*C*(2,6)H), 128.9 (Ar^2*C*(4)H), 129.6 (Ar^2*C*(3,5)H), 131.1 (Ar^1*C*(2,6)H), 139.4 (Ar^1*C*(1)), 139.8 (Ar^2*C*(1)), 150.5 (Ar^1*C*(4)), 167.6 (*C*(2)), 167.9 (*C*(4)), 175.0 (*C*O); **^{77}Se{^{1}H} NMR** (95 MHz, $CDCl_3$) δ_{Se}: 504.4 (s, C*Se*); **HRMS** (ESI^+) $C_{18}H_{12}O_4N_3F_3Na^{80}Se$ $[M+Na]^+$ found 493.9837, requires 493.9837 (±0.0 ppm).

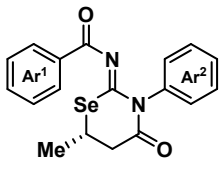
Ethyl (*R*,*Z*)-2-(benzoylimino)-4-oxo-3-phenyl-1,3-selenazinane-6-carboxylate (61)



61

Following General Procedure G, ethyl perfluorophenyl fumarate **S16** (140 mg, 0.45 mmol, 1.5 equiv.), *N*-(phenylcarbamoselenoyl)benzamide **S31** (91.0 mg, 0.30 mmol, 1.0 equiv.), and (2*S*,3*R*)-HyperBTM **21** (9.3 mg, 0.03 mmol, 10 mol%) in anhydrous THF (0.1 M) for 24 h at RT gave crude product that was purified by flash silica column chromatography (hexane:EtOAc 100:0 to 50:50, R_F 0.48 at 60:40) to give the title compound as a colourless solid (92 mg, 71%). **mp** 88 – 90 °C; $[\alpha]_D^{20}$ –46.2 (*c* 0.5 in CH_2Cl_2); **Chiral HPLC analysis,** Chiralpak IA (80:20 *n*-hexane : IPA, flow rate 1.0 mLmin^{-1}, 211 nm, 30 °C) t_R (*S*) 12.1 min, t_R (*R*) 18.8 min, 93:7 er; **IR** ν_{max} (film) 2980, 1721, 1628, 1614, 1597, 1576, 1493, 1470, 1452, 1371, 1331, 1308, 1233, 1209, 1190, 1169, 1090, 1049, 1022, 991, 858, 806, 779; **^{1}H NMR** (500 MHz, $CDCl_3$) δ_H: 1.30 (3H, t, *J* 7.1, CH_3), 3.48 (1H, dd, *J* 16.5, 4.1, C(5)H^AH^B), 3.61 (1H, dd, *J* 16.5, 5.6, C(5)H$^A H^B$), 3.95 (1H, dd, *J* 5.6, 4.1, C(6)*H*), 4.26 (2H, q, *J* 7.1, CH_2CH$_3$), 7.21 – 7.25 (2H, m, Ar^{2}C(2,6)*H*), 7.27 – 7.32 (2H, m, Ar^{1}C(3,5)*H*), 7.43 – 7.48 (2H, m, Ar^{1}C(4)*H* and Ar^{2}C(4)*H*), 7.50 – 7.55 (2H, m, Ar^{2}C(3,5)*H*), 7.71 – 7.75 (2H, m, Ar^{1}C(2,6)*H*); **^{13}C{^{1}H} NMR** (126 MHz, $CDCl_3$) δ_C: 14.2 (*C*H$_3$), 31.2 (*C*(6)H), 37.9 (*C*(5)H$_2$), 62.4 (*C*H$_2$CH$_3$), 128.2 (Ar^2*C*(2,6)H), 128.3 (Ar^2*C*(4)H), 128.4 (Ar^1*C*(3,5)H), 129.2 (Ar^2*C*(3,5)H), 130.2 (Ar^1*C*(2,6)H), 133.3 (Ar^1*C*(4)), 134.9 (Ar^1*C*(1)), 140.0 (Ar^2*C*(1)), 166.0 (*C*(2)), 169.7 (*C*(4)), 171.4 (*C*(O)O), 177.0 (NCO); **^{77}Se{^{1}H} NMR** (95 MHz, $CDCl_3$) δ_{Se}: 560.2 (s, C*Se*); **HRMS** (ESI^+) $C_{20}H_{18}O_4N_2Na^{80}Se$ $[M+Na]^+$ found 453.0320, requires 453.0324 (–0.9 ppm).

(*S*,*Z*)-*N*-(6-Methyl-4-oxo-3-phenyl-1,3-selenazinan-2-ylidene)benzamide (62)

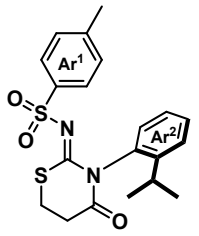


62

Following General Procedure G, 4-nitrophenyl (*E*)-but-2-enoate **S5** (93.2 mg, 0.45 mmol, 1.5 equiv.), *N*-(phenylcarbamoselenoyl)benzamide **S31** (91.0 mg, 0.30 mmol, 1.0 equiv.),

and (2*S*,3*R*)-HyperBTM **21** (27.8 mg, 0.09 mmol, 30 mol%) in anhydrous THF (0.1 M) for 48 h at RT gave crude product that was purified, directly without aqueous workup, by flash silica column chromatography (hexane:EtOAc 100:0 to 50:50, R_F 0.35 at 70:30) to give the title compound as a colourless solid (32 mg, 29%). **mp** 115 – 117 °C; $[\alpha]_D^{20}$ –70.0 (*c* 0.5 in $CHCl_3$); **Chiral HPLC analysis,** Chiralpak IA (90:10 *n*-hexane : IPA, flow rate 1.0 mLmin^{-1}, 211 nm, 30 °C) t_R (*R*) 16.0 min, t_R (*S*) 17.5 min, 87:13 er; **IR** ν_{max} (film) 3063, 2957, 2922, 1705, 1632, 1472, 1352, 1314, 1219, 1165, 1059, 1013, 716, 694; **^{1}H NMR** (500 MHz, $CDCl_3$) δ_H: 1.61 (3H, d, *J* 6.9, CH_3), 3.23 (1H, dd, *J* 16.0, 10.2, C(5)H^AH^B), 3.48 (1H, dd, *J* 16.0, 3.2, C(5)H^AH^B), 3.62 (1H, dqd, *J* 10.2, 6.9, 3.2, C(6)*H*), 7.17 – 7.22 (2H, m, Ar^{2}C(2,6)*H*), 7.26 – 7.32 (2H, m, Ar^{1}C(3,5)*H*), 7.42 – 7.48 (2H, m, Ar^{1}C(4)*H* and Ar^{2}C(4)*H*), 7.50 – 7.55 (2H, m, Ar^{2}C(3,5)*H*), 7.70 – 7.75 (2H, m, Ar^{1}C(2,6)*H*); **^{13}C{^{1}H} NMR** (126 MHz, $CDCl_3$) δ_C: 20.8 (CH_3), 26.4 (*C*(6)H), 44.8 (*C*(5)H_2), 128.3 (Ar^2*C*(4)H), 128.4 (Ar^1*C*(3,5)H and Ar^2*C*(2,6)H), 129.3 (Ar^2*C*(3,5)H), 130.1 (Ar^1*C*(2,6)H), 133.1 (Ar^1*C*(4)), 135.2 (Ar^1*C*(1)), 140.0 (Ar^2*C*(1)), 165.7 (*C*(2)), 171.2 (*C*(4)), 176.8 (*C*O); **^{77}Se{^{1}H} NMR** (95 MHz, $CDCl_3$) δ_{Se}: 543.3 (s, C*Se*); **HRMS** (ESI^+) $C_{18}H_{16}O_2N_2Na^{80}Se$ $[M+Na]^+$ found 395.0269, requires 395.0269 (±0.0 ppm).

(R_a,*Z*)-*N*-(3-(2-*iso*-Propylphenyl)-4-oxo-1,3-thiazinan-2-ylidene)-4-methylbenzenesulfonamide (63)

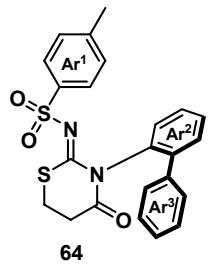


63

Following General Procedure G, perfluorophenyl acrylate **75** (107 mg, 0.45 mmol, 1.5 equiv.), *N*-((2-*iso*-propylphenyl)carbamothioyl)-4-methylbenzenesulfonamide **S29** (105 mg, 0.30 mmol, 1.0 equiv.), and (2*S*,3*R*)-HyperBTM **21** (4.6 mg, 0.015 mmol, 5 mol%) in anhydrous THF (0.1 M) for 24 h at 0 °C gave crude product that was purified by flash silica column chromatography (CH_2Cl_2:Et_2O 100:0 to 90:10, R_F 0.32 at 90:10) to give the title compound as a colourless solid (101 mg, 83%). **mp** 151 – 153 °C; $[\alpha]_D^{20}$ +51.2 (*c* 0.5 in $CHCl_3$); **Chiral HPLC analysis,** Chiralpak IB (80:20 *n*-hexane : IPA, flow rate 1.0

mLmin^{-1}, 211 nm, 30 °C) t_R (R_a) 26.0 min, t_R (S_a) 31.5 min, 87:13 er; **IR** ν_{max} (film) 2965, 1717, 1491, 1341, 1314, 1291, 1256, 1150, 1088, 993, 908, 835, 787; **^{1}H NMR** (400 MHz, $CDCl_3$) δ_H: 0.97 (3H, d, *J* 6.8, CH(CH_3)^A(CH$_3$)^B), 1.10 (3H, d, *J* 6.8, CH(CH$_3$)^A(CH_3)^B), 2.33 (3H, s, CH_3), 2.55 (1H, h, *J* 6.8, C*H*(CH$_3$)$_2$), 3.15 – 3.34 (4H, m, C(5)H_2 and C(6)H_2), 6.87 – 6.95 (1H, m, Ar^{2}C(6)*H*), 7.07 – 7.13 (2H, m, Ar^{1}C(3,5)*H*), 7.17 – 7.24 (1H, m, Ar^{2}C(5)*H*), 7.30 – 7.42 (4H, m, Ar^{2}C(3)*H*, Ar^{2}C(4)*H* and Ar^{1}C(2,6)*H*); **^{13}C{^{1}H} NMR** (126 MHz, $CDCl_3$) δ_C: 21.5 (*C*H$_3$), 23.1 (CH(*C*H$_3$)^A(CH$_3$)^B), 23.3 (CH(CH$_3$)^A(*C*H$_3$)^B), 23.8 (*C*(6)H$_2$), 28.6 (*C*H(CH$_3$)$_2$), 34.4 (*C*(5)H$_2$), 126.5 (Ar^1*C*(2,6)H), 126.7 (Ar^2*C*(3)H), 126.7 (Ar^2*C*(6)H), 128.1 (Ar^2*C*(5)H), 129.1 (Ar^1*C*(3,5)H), 129.4 (Ar^2*C*(4)H), 134.7 (Ar^2*C*(1)), 138.2 (Ar^1*C*(1)), 143.2 (Ar^1*C*(4)), 145.6 (Ar^2*C*(2)), 164.3 (*C*(2)), 169.1 (*C*(4)); **HRMS** (ESI^+) $C_{20}H_{22}O_3N_2NaS_2$ $[M+Na]^+$ found 425.0967, requires 425.0964 (+0.7 ppm).

(R_a,*Z*)-*N*-(3-([1,1'-Biphenyl]-2-yl)-4-oxo-1,3-thiazinan-2-ylidene)-4-methylbenzenesulfonamide (64)

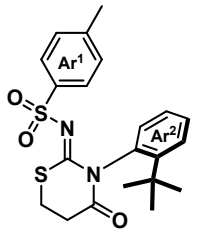


64

Following General Procedure G, perfluorophenyl acrylate **75** (107 mg, 0.45 mmol, 1.5 equiv.), *N*-([1,1'-biphenyl]-2-ylcarbamothioyl)-4-methylbenzenesulfonamide **S30** (115 mg, 0.30 mmol, 1.0 equiv.), and (2*S*,3*R*)-HyperBTM **21** (4.6 mg, 0.015 mmol, 5 mol%) in anhydrous THF (0.1 M) for 24 h at 0 °C gave crude product that was purified by flash silica column chromatography (hexane:EtOAc 100:0 to 0:100, R_F 0.23 at 50:50) to give the title compound as a colourless glass (128 mg, 98%). $[\alpha]_D^{20}$ +3.2 (*c* 0.5 in $CHCl_3$); **Chiral HPLC analysis,** Chiralpak IB (80:20 *n*-hexane : IPA, flow rate 1.0 mLmin^{-1}, 211 nm, 30 °C) t_R (R_a) 31.9 min, t_R (S_a) 41.2 min, 73:27 er; **IR** ν_{max} (film) 1717, 1597, 1497, 1435, 1342, 1315, 1288, 1150, 1088, 993, 907, 837, 787; **^{1}H NMR** (400 MHz, $CDCl_3$) δ_H: 2.41 (3H, s, CH_3), 2.49 – 2.61 (1H, m, C(6)H^AH^B), 2.81 – 3.02 (3H, m, C(5)H_2 and C(6)H^AH^B), 6.93 – 6.99 (2H, m, Ar^{3}C(2,6)*H*), 7.13 – 7.35 (7H, m, Ar^{1}C(3,5)*H*, Ar^{2}C(3,6)*H*, and Ar^{3}C(3,4,5)*H*), 7.39 – 7.49 (2H, m, Ar^{2}C(4,5)*H*), 7.49 – 7.55 (2H, m, Ar^{1}C(2,6)*H*); **^{13}C{^{1}H} NMR** (126 MHz, $CDCl_3$) δ_C: 21.6

(CH_3), 22.9 (C(6)H_2), 34.3 (C(5)H_2), 126.8 (Ar^1C(2,6)H), 127.8 (Ar^3C(4)H), 128.2 (Ar^3C(3,5)H), 128.2 (Ar^3C(2,6)H), 128.4 (Ar^2C(5)H), 129.0 (Ar^2C(4)H), 129.2 (Ar^1C(3,5)H), 129.4 (Ar^2C(6)H), 130.5 (Ar^2C(3)H), 135.1 (Ar^2C(1)), 138.1 (Ar^1C(1)), 138.4 (Ar^3C(1)), 139.9 (Ar^2C(2)), 143.4 (Ar^1C(4)), 165.1 (C(2)), 169.0 (C(4)); **HRMS** (ESI^+) $C_{23}H_{20}O_3N_2NaS_2$ $[M+Na]^+$ found 459.0807, requires 459.0808 (–0.2 ppm).

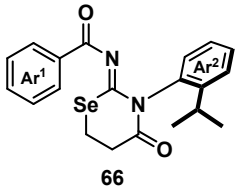
(R_a,*Z*)-*N*-(3-(2-(*tert*-Butyl)phenyl)-4-oxo-1,3-thiazinan-2-ylidene)-4-methylbenzenesulfonamide (65)



65

Following General Procedure G, perfluorophenyl acrylate **75** (107 mg, 0.45 mmol, 1.5 equiv.), *N*-((2-(*tert*-butyl)phenyl)carbamothioyl)-4-methylbenzenesulfonamide **74** (109 mg, 0.30 mmol, 1.0 equiv.), and (2*S*,3*R*)-HyperBTM **21** (18.5 mg, 0.06 mmol, 20 mol%) in anhydrous THF (0.1 M) for 48 h at RT gave crude product that was purified by flash silica column chromatography (hexane:EtOAc 100:0 to 0:100, R_F 0.23 at 60:40) to give the title compound as a colourless glass (91 mg, 73%). $[\alpha]_D^{20}$ –34.0 (c 0.5 in CH_2Cl_2); **Chiral HPLC analysis,** Chiralpak IB (60:40 *n*-hexane : IPA, flow rate 1.0 mLmin^{-1}, 211 nm, 30 °C) t_R (R_a) 12.1 min, t_R (S_a) 15.2 min, 80:20 er; **IR** ν_{max} (film) 2965, 1719, 1516, 1495, 1437, 1341, 1288, 1250, 1171, 1150, 1088, 991, 905, 827, 787; **^{1}H NMR** (400 MHz, $CDCl_3$) δ_H: 1.20 (9H, s, C(CH_3)$_3$), 2.34 (3H, s, CH_3), 3.11 – 3.25 (3H, m, C(5)H^AH^B and C(6)H_2), 3.27 – 3.38 (1H, m, C(5)H^AH^B), 6.80 (1H, dd, *J* 7.8, 1.5, Ar^{2}C(6)*H*), 7.07 – 7.13 (2H, m, Ar^{1}C(3,5)*H*), 7.21 (1H, ddd, *J* 7.8, 7.2, 1.5, Ar^{2}C(5)*H*), 7.33 (1H, ddd, *J* 8.1, 7.2, 1.5, Ar^{2}C(4)*H*), 7.36 – 7.40 (2H, m, Ar^{1}C(2,6)*H*), 7.49 (1H, dd, *J* 8.1, 1.5, Ar^{2}C(3)*H*); **^{13}C{^{1}H} NMR** (126 MHz, $CDCl_3$) δ_C: 21.6 (CH_3), 22.7 (C(6)H_2), 31.6 (C(CH_3)$_3$), 34.7 (C(5)H_2), 35.9 (C(CH$_3$)$_3$), 126.5 (Ar^1C(2,6)H), 127.1 (Ar^2C(5)H), 128.9 (Ar^2C(4)H), 129.1 (Ar^1C(3,5)H), 129.1 (Ar^2C(6)H), 131.3 (Ar^2C(3)H), 134.8 (Ar^2C(1)), 138.4 (Ar^1C(1)), 143.2 (Ar^1C(4)), 145.8 (Ar^2C(2)), 164.8 (C(2)), 169.7 (C(4)); **HRMS** (ESI^+) $C_{21}H_{24}O_3N_2NaS_2$ $[M+Na]^+$ found 439.1117, requires 439.1121 (–0.9 ppm).

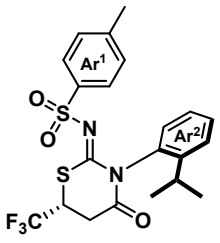
(R_a,*Z*)-*N*-(3-(2-*iso*-Propylphenyl)-4-oxo-1,3-selenazinan-2-ylidene)benzamide (66)



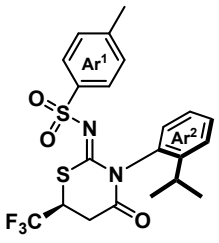
66

Following General Procedure G, perfluorophenyl acrylate **75** (107 mg, 0.45 mmol, 1.5 equiv.), *N*-((2-*iso*-propylphenyl)carbamoselenoyl)benzamide **S37** (104 mg, 0.30 mmol, 1.0 equiv.), and (2*S*,3*R*)-HyperBTM **21** (18.5 mg, 0.06 mmol, 20 mol%) in anhydrous THF (0.1 M) for 48 h at RT gave crude product that was purified by flash silica column chromatography (hexane:CH_2Cl_2 100:0 to 0:100, R_F 0.25 at 25:75) to give the title compound as a colourless solid (85 mg, 71%). **mp** 129 – 131 °C; $[\alpha]_D^{20}$ +35.0 (*c* 0.2 in $CHCl_3$); **Chiral HPLC analysis,** Chiralpak IB (80:20 *n*-hexane : IPA, flow rate 1.0 mLmin^{-1}, 254 nm, 30 °C) t_R (R_a) 8.3 min, t_R (S_a) 9.7 min, 77:23 er; **IR** ν_{max} (film) 2961, 1705, 1630, 1576, 1472, 1323, 1306, 1229, 1153, 1080, 1065, 1020, 762; **^{1}H NMR** (500 MHz, $CDCl_3$) δ_H: 1.11 (3H, d, *J* 6.9, CH(CH_3)^A(CH_3)^B), 1.18 (3H, d, *J* 6.9, CH(CH_3)^A(CH_3)^B), 2.73 (1H, h, *J* 6.9, C*H*(CH_3)$_2$), 3.02 – 3.17 (2H, m, C(6)H_2), 3.40 – 3.48 (2H, m, C(5)H_2), 7.03 – 7.08 (1H, m, Ar^{2}C(6)*H*), 7.24 – 7.34 (3H, m, Ar^{1}C(3,5)*H* and Ar^{2}C(5)*H*), 7.40 – 7.49 (3H, m, Ar^{1}C(4)*H* and Ar^{2}C(3,4)*H*), 7.67 – 7.72 (2H, m, Ar^{1}C(2,6)*H*); **^{13}C{^{1}H} NMR** (126 MHz, $CDCl_3$) δ_C: 15.1 (*C*(6)H_2), 23.5 (CH(*C*H_3)^A(CH_3)^B), 23.9 (CH(CH_3)^A(*C*H_3)^B), 28.8 (*C*H(CH_3)$_2$), 36.7 (*C*(5)H_2), 126.6 (Ar^2*C*(4)H), 126.7 (Ar^2*C*(5)H), 128.0 (Ar^2*C*(6)H), 128.3 (Ar^1*C*(3,5)H), 129.0 (Ar^2*C*(3)H), 130.1 (Ar^1*C*(2,6)H), 133.1 (Ar^1*C*(4)H), 135.2 (Ar^1*C*(1)), 137.8 (Ar^2*C*(1)), 145.3 (Ar^2*C*(2)), 166.3 (*C*(2)), 171.3 (*C*(4)), 176.7 (*C*O); **^{77}Se{^{1}H} NMR** (95 MHz, $CDCl_3$) δ_{Se}: 464.9 (s, C*Se*); **HRMS** (ESI^+) $C_{20}H_{20}O_2N_2Na^{80}Se$ $[M+Na]^+$ found 423.0581, requires 423.0582 (–0.2 ppm).

(*R*,R_a,*Z*)-*N*-(3-(2-*iso*-Propylphenyl)-4-oxo-6-(trifluoromethyl)-1,3-thiazinan-2-ylidene)-4-methylbenzenesulfonamide (67) and (*S*,R_a,*Z*)-*N*-(3-(2-*iso*-propylphenyl)-4-oxo-6-(trifluoromethyl)-1,3-thiazinan-2-ylidene)-4-methylbenzenesulfonamide (S41)



67



S41

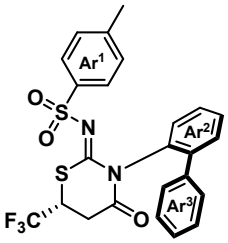
Following General Procedure G, perfluorophenyl (*E*)-4,4,4-trifluorobut-2-enoate **28** (138 mg, 0.45 mmol, 1.5 equiv.), *N*-((2-*iso*-propylphenyl)carbamothioyl)-4-methylbenzenesulfonamide **S29** (105 mg, 0.30 mmol, 1.0 equiv.), and (2*S*,3*R*)-HyperBTM **21** (4.6 mg, 0.015 mmol, 5 mol%) in anhydrous THF (0.1 M) for 24 h at 0 °C gave crude product that was purified by flash silica column chromatography (hexane:CH_2Cl_2 50:50 to 0:100, R_F 0.23 at 0:100) to give the title compound (92:8 dr) as a colourless solid (133 mg, 94%). **mp** 45 – 47 °C; $[\alpha]_D^{20}$ +94.5 (*c* 1.0 in $CHCl_3$); **IR** ν_{max} (film) 2967, 1719, 1518, 1508, 1362, 1319, 1277, 1229, 1152, 1119, 1088, 999, 826, 772; **HRMS** (ESI^+) $C_{21}H_{21}O_3N_2F_3NaS_2$ $[M+Na]^+$ found 493.0840, requires 493.0838 (+0.4 ppm).

Data for major diastereoisomer (*R*,R_a,*Z*)-**67**: **Chiral HPLC analysis,** Chiralpak AD-H (80:20 *n*-hexane : IPA, flow rate 1.0 mLmin^{-1}, 254 nm, 30 °C) t_R (*R*,R_a) 7.8 min, t_R (*S*,S_a) 17.5 min, 98:2 er; **^{1}H NMR** (400 MHz, $CDCl_3$) δ_H: 1.00 (3H, d, *J* 6.8, CH(CH_3)^A(CH_3)^B), 1.11 (3H, d, *J* 6.8, CH(CH_3)^A(CH_3)^B), 2.38 (3H, s, CH_3), 2.55 (1H, h, *J* 6.8, C*H*(CH_3)$_2$), 3.45 (2H, d, *J* 4.8, C(5)H_2), 4.05 (1H, qt, *J* 8.0, 4.8, C(6)*H*), 6.79 – 6.84 (1H, m, Ar^{2}C(6)*H*), 7.13 – 7.19 (2H, m, Ar^{1}C(3,5)*H*), 7.20 – 7.25 (1H, m, Ar^{2}C(5)*H*), 7.34 – 7.41 (2H, m, Ar^{2}C(3)*H* and Ar^{2}C(4)*H*), 7.42 – 7.46 (2H, m, Ar^{1}C(2,6)*H*); **^{19}F{^{1}H} NMR** (377 MHz, $CDCl_3$) δ_F: –71.0 (s, CF_3); **^{13}C{^{1}H} NMR** (126 MHz, $CDCl_3$) δ_C: 21.5 (*C*H_3), 23.2 (CH(*C*H_3)^A(CH_3)^B), 23.7 (CH(CH_3)^A(*C*H_3)^B), 28.7 (*C*H(CH_3)$_2$), 33.0 (*C*(5)H_2), 39.9 (q, *J* 32.5, *C*(6)H), 124.6 (q, *J* 280.4, *C*F_3), 126.6 (Ar^1*C*(2,6)H), 126.7 (Ar^2*C*(3)H), 126.9 (Ar^2*C*(6)H), 127.0 (Ar^2*C*(5)H), 129.2 (Ar^1*C*(3,5)H), 129.6 (Ar^2*C*(4)H), 134.3 (Ar^2*C*(1)), 137.5 (Ar^1*C*(1)), 143.7 (Ar^1*C*(4)), 146.1 (Ar^2*C*(2)), 159.7 (*C*(2)), 165.6 (*C*(4)).

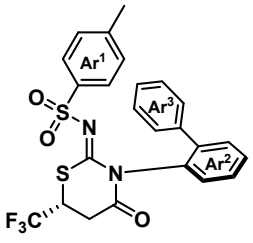
Data for minor diastereoisomer (*S*,R_a,*Z*)-**S41**: **Chiral HPLC analysis,** er not determined; **^{1}H NMR** (400 MHz, $CDCl_3$) (*selected*) δ_H: 0.93 (3H, d, *J* 6.9, CH(CH_3)^A(CH_3)^B), 1.09 (3H, d,

J 6.9, CH(CH$_3$)^A(C*H*$_3$)^B), 4.10 – 4.17 (1H, m, C(6)*H*), 6.89 – 6.93 (1H, m, Ar^{2}C(5)*H*); **^{19}F{^{1}H} NMR** (377 MHz, $CDCl_3$) δ_F: –71.4 (s, C*F*$_3$); **^{13}C{^{1}H} NMR** (126 MHz, $CDCl_3$) (*selected*) δ_C: 22.6 (CH(*C*H$_3$)^A(CH$_3$)^B), 23.7 (CH(CH$_3$)^A(*C*H$_3$)^B), 28.1 (*C*H(CH$_3$)$_2$), 32.7 (*C*(5)H$_2$), 128.0 (Ar^2*C*(5)H), 134.3 (Ar^2*C*(1)), 137.6 (Ar^1*C*(1)), 145.8 (Ar^2*C*(2)), 159.5 (*C*(2)), 165.9 (*C*(4)).

(*R*,*R*$_a$,*Z*)-*N*-(3-([1,1'-Biphenyl]-2-yl)-4-oxo-6-(trifluoromethyl)-1,3-thiazinan-2-ylidene)-4-methylbenzenesulfonamide (68) and (*R*,*S*$_a$,*Z*)-*N*-(3-([1,1'-biphenyl]-2-yl)-4-oxo-6-(trifluoromethyl)-1,3-thiazinan-2-ylidene)-4-methylbenzenesulfonamide (S42)



68



S42

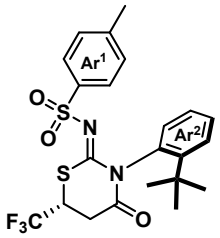
Following General Procedure G, perfluorophenyl (*E*)-4,4,4-trifluorobut-2-enoate **28** (138 mg, 0.45 mmol, 1.5 equiv.), *N*-([1,1'-biphenyl]-2-ylcarbamothioyl)-4-methylbenzenesulfonamide **S30** (115 mg, 0.30 mmol, 1.0 equiv.), and (2*S*,3*R*)-HyperBTM **21** (4.6 mg, 0.015 mmol, 5 mol%) in anhydrous THF (0.1 M) for 24 h at 0 °C gave crude product (90:10 dr) that was purified by flash silica column chromatography (hexane:CH_2Cl_2 100:0 to 0:100, R_F 0.30 at 0:100) to give the title compound as an inseparable mixture of diastereoisomers (88:12 dr) as a colourless glass (140 mg, 93%). $[\alpha]_D^{20}$ +57.8 (*c* 0.5 in $CHCl_3$); **IR** ν_{max} (film) 2955, 1724, 1520, 1362, 1321, 1279, 1227, 1153, 1121, 1088, 1001, 957, 887, 826, 773; **HRMS** (ESI^+) $C_{24}H_{19}O_3N_2F_3NaS_2$ $[M+Na]^+$ found 527.0679, requires 527.0681 (–0.4 ppm).

Data for major diastereoisomer (*R*,*R*$_a$,*Z*)-**68**: **Chiral HPLC analysis,** Chiralcel OD-H (70:30 *n*-hexane : IPA, flow rate 1.0 mLmin^{-1}, 211 nm, 30 °C) t_R (*S*,*S*$_a$) 7.8 min, t_R (*R*,*R*$_a$) 18.5 min, 95:5 er; **^{1}H NMR** (400 MHz, $CDCl_3$) δ_H: 2.43 (3H, s, C*H*$_3$), 2.91 (1H, dd, *J* 16.7, 4.8, C(5)*H*^{A}H^B), 3.19 (1H, dd, *J* 16.7, 6.3, C(5)H^A*H*^{B}), 3.53 – 3.65 (1H, m, C(6)*H*), 6.96 – 7.01 (2H, m, Ar^{3}C(2,6)*H*), 7.20 – 7.37 (7H, m, Ar^{1}C(3,5)*H*, Ar^{2}C(3,6)*H*, and Ar^{3}C(3,4,5)*H*), 7.39 – 7.50 (2H, m, Ar^{2}C(4,5)*H*), 7.52 – 7.58 (2H, m, Ar^{1}C(2,6)*H*); **^{19}F{^{1}H} NMR** (377 MHz, $CDCl_3$) δ_F: –71.0 (s, C*F*$_3$); **^{13}C{^{1}H} NMR** (126 MHz, $CDCl_3$) δ_C: 21.6 (*C*H$_3$), 33.2 (*C*(5)H$_2$), 40.0 (q, *J* 32.4, *C*(6)H), 124.2 (q, *J* 280.1, *C*F$_3$), 126.9 (Ar^1*C*(2,6)H), 127.9 (Ar^3*C*(4)H), 128.1

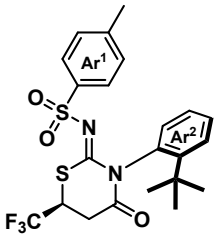
(Ar^3*C*(3,5)H), 128.3 (Ar^3*C*(2,6)H), 128.4 (Ar^2*C*(5)H), 128.7 (Ar^2*C*(4)H), 129.4 (Ar^1*C*(3,5)H), 129.4 (Ar^2*C*(6)H), 130.6 (Ar^2*C*(3)H), 134.8 (Ar^2*C*(1)), 137.5 (Ar^1*C*(1)), 138.3 (Ar^3*C*(1)), 140.3 (Ar^2*C*(2)), 144.0 (Ar^1*C*(4)), 160.1 (*C*(2)), 165.8 (*C*(4)).

Data for minor diastereoisomer (*R*,S_a,*Z*)-**S42**: **Chiral HPLC analysis,** Chiralcel OD-H (70:30 *n*-hexane : IPA, flow rate 1.0 mLmin^{-1}, 211 nm, 30 °C) t_R (*S*,R_a) 14.0 min, t_R (*R*,S_a) 33.2 min, 63:37 er; **^{1}H NMR** (400 MHz, $CDCl_3$) (*selected*) δ_H: 3.02 (1H, dd, *J* 16.6, 6.4, C(5)H^AH^B), 3.93 – 4.05 (1H, m, C(6)*H*), 7.04 – 7.08 (2H, m, Ar^{3}C(2,6)*H*); **^{19}F{^{1}H} NMR** (377 MHz, $CDCl_3$) δ_F: –71.6 (s, CF_3); **^{13}C{^{1}H} NMR** (126 MHz, $CDCl_3$) (*selected*) δ_C: 32.6 (*C*(5)H_2), 127.8 (Ar^3*C*(4)H), 128.1 (Ar^3*C*(3,5)H), 128.6 (Ar^2*C*(4)H), 129.2 (Ar^2*C*(6)H), 131.2 (Ar^2*C*(3)H), 137.6 (Ar^1*C*(1)), 137.9 (Ar^3*C*(1)), 141.0 (Ar^2*C*(2)), 143.9 (Ar^1*C*(4)), 160.0 (*C*(2)), 166.0 (*C*(4)).

(*R*,R_a,*Z*)-*N*-(3-(2-(*tert*-Butyl)phenyl)-4-oxo-6-(trifluoromethyl)-1,3-thiazinan-2-ylidene)-4-methylbenzenesulfonamide (69) and (*S*,R_a,*Z*)-*N*-(3-(2-(*tert*-butyl)phenyl)-4-oxo-6-(trifluoromethyl)-1,3-thiazinan-2-ylidene)-4-methylbenzenesulfonamide (S43)



69



S43

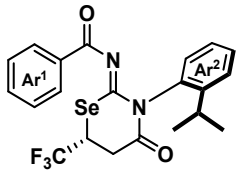
Following General Procedure G, perfluorophenyl (*E*)-4,4,4-trifluorobut-2-enoate **28** (138 mg, 0.45 mmol, 1.5 equiv.), *N*-((2-(*tert*-butyl)phenyl)carbamothioyl)-4-methylbenzenesulfonamide **74** (109 mg, 0.30 mmol, 1.0 equiv.), and (2*S*,3*R*)-HyperBTM **21** (4.6 mg, 0.015 mmol, 5 mol%) in anhydrous THF (0.1 M) for 48 h at RT gave crude product that was purified by flash silica column chromatography (hexane:EtOAc 100:0 to 50:50, R_F 0.60 at 60:40) to give the title compound as an inseparable mixture of diastereoisomers (88:12 dr) as a colourless glass (80 mg, 55%). $[\alpha]_D^{20}$ +48.6 (*c* 0.5 in $CHCl_3$); **IR** ν_{max} (film) 2961, 1722, 1522, 1508, 1362, 1319, 1281, 1227, 1153, 1119, 1088, 999, 957, 887, 826, 770; **HRMS** (ESI^+) $C_{22}H_{23}O_3N_2F_3NaS_2$ $[M+Na]^+$ found 507.0993, requires 507.0994 (–0.2 ppm).

Data for major diastereoisomer (*R*,R_a,*Z*)-**69**: **Chiral HPLC analysis,** Chiralpak IB (90:10 *n*-hexane : IPA, flow rate 1.0 mLmin^{-1}, 211 nm, 30 °C) t_R (*R*,R_a) 15.8 min, t_R (*S*,S_a) 20.3 min,

97:3 er; **^{1}H NMR** (500 MHz, $CDCl_3$) δ_H: 1.19 (9H, s, C(CH_3)$_3$), 2.36 (3H, s, CH_3), 3.31 (1H, dd, *J* 16.9, 5.2, C(5)H^AH^B), 3.42 (1H, dd, *J* 16.9, 5.1, C(5)H^AH^B), 4.01 (1H, qdd, *J* 7.7, 5.2, 5.1, C(6)*H*), 6.67 (1H, dd, *J* 7.9, 1.4, Ar^{2}C(6)*H*), 7.12 – 7.16 (2H, m, Ar^{1}C(3,5)*H*), 7.19 (1H, ddd, *J* 7.9, 7.2, 1.5, Ar^{2}C(5)*H*), 7.33 (1H, ddd, *J* 8.3, 7.2, 1.5, Ar^{2}C(4)*H*), 7.40 – 7.44 (2H, m, Ar^{1}C(2,6)*H*), 7.50 (1H, dd, *J* 8.3, 1.5, Ar^{2}C(3)*H*); **^{19}F{^{1}H} NMR** (377 MHz, $CDCl_3$) δ_F: –71.1 (s, CF_3); **^{13}C{^{1}H} NMR** (126 MHz, $CDCl_3$) δ_C: 21.6 (CH_3), 31.6 (C(CH_3)$_3$), 33.6 (*C*(5)H_2), 36.2 (*C*(CH_3)$_3$), 40.0 (q, *J* 32.5, *C*(6)H), 124.5 (q, *J* 280.3, *C*F_3), 126.7 (Ar^1*C*(2,6)H), 127.4 (Ar^2*C*(5)H), 129.2 (Ar^2*C*(4)H), 129.3 (Ar^1*C*(3,5)H), 129.5 (Ar^2*C*(6)H), 129.9 (Ar^2*C*(3)H), 134.0 (Ar^2*C*(1)), 137.7 (Ar^1*C*(1)), 143.7 (Ar^1*C*(4)), 146.4 (Ar^2*C*(2)), 160.2 (*C*(2)), 166.5 (*C*(4)).

Data for minor diastereoisomer (*S*,R_a,*Z*)-**S43**: **Chiral HPLC analysis,** Chiralpak IB (90:10 *n*-hexane : IPA, flow rate 1.0 mLmin^{-1}, 211 nm, 30 °C) t_R (*S*,R_a) 26.1 min, t_R (*R*,S_a) 40.6 min, 53:47 er; **^{1}H NMR** (500 MHz, $CDCl_3$) (*selected*) δ_H: 1.15 (9H, s, C(CH_3)$_3$), 4.16 – 4.26 (1H, m, C(6)*H*), 7.36 – 7.39 (2H, m, Ar^{1}C(2,6)*H*); **^{19}F{^{1}H} NMR** (377 MHz, $CDCl_3$) δ_F: –70.7 (s, CF_3); **^{13}C{^{1}H} NMR** (126 MHz, $CDCl_3$) (*selected*) δ_C: 31.2 (C(CH_3)$_3$), 35.9 (*C*(CH_3)$_3$), 126.6 (Ar^1*C*(2,6)H), 129.2 (Ar^1*C*(3,5)H), 130.2 (Ar^2*C*(3)H), 134.8 (Ar^2*C*(1)), 137.8 (Ar^1*C*(1)), 147.0 (Ar^2*C*(2)), 159.9 (*C*(2)), 166.9 (*C*(4)).

(*R*,R_a,*Z*)-*N*-(3-(2-*iso*-Propylphenyl)-4-oxo-6-(trifluoromethyl)-1,3-selenazinan-2-ylidene)benzamide (70)

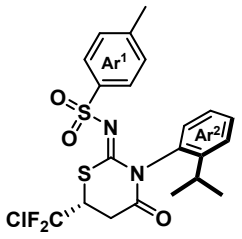


70

Following General Procedure G, perfluorophenyl (*E*)-4,4,4-trifluorobut-2-enoate **28** (138 mg, 0.45 mmol, 1.5 equiv.), *N*-((2-*iso*-propylphenyl)carbamoselenoyl)benzamide **S37** (104 mg, 0.30 mmol, 1.0 equiv.), and (2*S*,3*R*)-HyperBTM **21** (9.3 mg, 0.03 mmol, 10 mol%) in anhydrous THF (0.1 M) for 48 h at RT gave crude product that was purified by flash silica column chromatography (hexane:CH_2Cl_2 100:0 to 0:100, R_F 0.30 at 25:75) to give the title compound (>95:5 dr) as a colourless glass (120 mg, 86%). $[\alpha]_D^{20}$ +75.7 (*c* 1.0 in $CHCl_3$); **Chiral HPLC analysis,** Chiralpak IB (98:2 *n*-hexane : IPA, flow rate 2.0 mLmin^{-1}, 220 nm, 30 °C) t_R (*S*,S_a) 8.6 min, t_R (*R*,R_a) 12.4 min, 98:2 er; **IR** ν_{max} (film) 2967, 1713, 1632, 1495, 1477,

1362, 1323, 1312, 1263, 1233, 1155, 1103, 1045, 1024, 758; **^{1}H NMR** (400 MHz, $CDCl_3$) δ_H: 1.12 (3H, d, *J* 6.9, CH(CH_3)^A(CH_3)^B), 1.18 (3H, d, *J* 6.9, CH(CH_3)^A(CH_3)^B), 2.69 (1H, h, *J* 6.9, C*H*(CH_3)$_2$), 3.57 (1H, dd, *J* 16.7, 5.1, C(5)H^AH^B), 3.67 (1H, dd, *J* 16.7, 4.9, C(5)H^AH^B), 3.79 (1H, qdd, *J* 8.8, 5.1, 4.9, C(6)*H*), 6.98 – 7.03 (1H, m, Ar^{2}C(6)*H*), 7.27 – 7.35 (3H, m, Ar^{1}C(3,5)*H* and Ar^{2}C(5)*H*), 7.44 – 7.51 (3H, m, Ar^{1}C(4)*H* and Ar^{2}C(3,4)*H*), 7.69 – 7.74 (2H, m, Ar^{1}C(2,6)*H*); **^{19}F{^{1}H} NMR** (377 MHz, $CDCl_3$) δ_F: –69.0 (s, CF_3); **^{13}C{^{1}H} NMR** (126 MHz, $CDCl_3$) δ_C: 23.6 (CH(*C*H_3)^A(CH_3)^B), 23.9 (CH(CH_3)^A(*C*H_3)^B), 28.8 (*C*H(CH_3)$_2$), 32.7 (q, *J* 31.6, *C*(6)H), 35.4 (*C*(5)H_2), 126.1 (q, *J* 278.2, *C*F_3), 126.6 (Ar^2*C*(4)H), 127.0 (Ar^2*C*(5)H), 127.0 (Ar^2*C*(6)H), 128.5 (Ar^1*C*(3,5)H), 129.3 (Ar^2*C*(3)H), 130.3 (Ar^1*C*(2,6)H), 133.6 (Ar^1*C*(4)H), 134.5 (Ar^1*C*(1)), 137.5 (Ar^2*C*(1)), 145.7 (Ar^2*C*(2)), 164.6 (*C*(2)), 168.1 (*C*(4)), 177.1 (*C*O); **^{77}Se{^{1}H} NMR** (95 MHz, $CDCl_3$) δ_{Se}: 496.5 (s, C*Se*); **HRMS** ($^{ESI^+}$) $C_{21}H_{19}O_2N_2F_3Na^{80}Se$ $[M+Na]^+$ found 491.0459, requires 491.0456 (+0.6 ppm).

(*R*,R_a,*Z*)-*N*-(6-(Chlorodifluoromethyl)-3-(2-*iso*-propylphenyl)-4-oxo-1,3-thiazinan-2-ylidene)-4-methylbenzenesulfonamide (71)



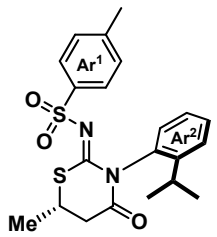
71

Following General Procedure G, 4-nitrophenyl (*E*)-4-chloro-4,4-difluorobut-2-enoate **S4** (125 mg, 0.45 mmol, 1.5 equiv.), *N*-((2-*iso*-propylphenyl)carbamothioyl)-4-methylbenzenesulfonamide **S29** (105 mg, 0.30 mmol, 1.0 equiv.), and (2*S*,3*R*)-HyperBTM **21** (4.6 mg, 0.015 mmol, 5 mol%) in anhydrous THF (0.1 M) for 24 h at 0 °C gave crude product (>95:5 dr) that was purified by flash silica column chromatography (hexane:Et_2O 80:20 until elution of PNPOH then hexane:CH_2Cl_2 50:50 to 0:100, R_F 0.30 at 0:100) to give the title compound (>95:5 dr) as a colourless solid (130 mg, 89%). *Note: a workup was not performed to avoid elimination of HCl.*

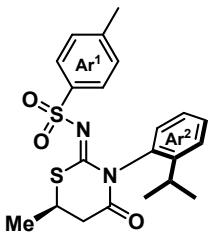
mp 53 – 55 °C; $[\alpha]_D^{20}$ +92.6 (*c* 0.5 in $CHCl_3$); **Chiral HPLC analysis,** Chiralpak AD-H (80:20 *n*-hexane : IPA, flow rate 1.0 mLmin^{-1}, 211 nm, 30 °C) t_R (*R*,R_a) 8.7 min, t_R (*S*,S_a) 20.3 min, 98:2 er; **IR** ν_{max} (film) 2967, 1722, 1520, 1506, 1354, 1319, 1283, 1206, 1152, 1088, 970, 928,

826, 812, 768; **^{1}H NMR** (400 MHz, $CDCl_3$) δ_H: 0.98 (3H, d, *J* 6.8, CH(CH_3)^A(CH_3)^B), 1.09 (3H, d, *J* 6.8, CH(CH_3)^A(CH_3)^B), 2.35 (3H, s, CH_3), 2.52 (1H, h, *J* 6.8, C*H*(CH_3)$_2$), 3.54 (1H, dd, *J* 17.1, 5.6, C(5)H^AH^B), 3.54 (1H, dd, *J* 17.1, 4.3, C(5)H^AH^B), 4.14 (1H, dddd, *J* 12.1, 9.5, 5.6, 4.3, C(6)*H*), 6.77 – 6.82 (1H, m, Ar^{2}C(6)*H*), 7.11 – 7.16 (2H, m, Ar^{1}C(3,5)*H*), 7.17 – 7.22 (1H, m, Ar^{2}C(5)*H*), 7.31 – 7.40 (2H, m, Ar^{2}C(3)*H* and Ar^{2}C(4)*H*), 7.40 – 7.45 (2H, m, Ar^{1}C(2,6)*H*); **^{19}F{^{1}H} NMR** (377 MHz, $CDCl_3$) δ_F: –57.9 (d, *J* 167.1, CF^AF^{B}Cl), –56.1 (d, *J* 167.1, CF^AF^BCl); **^{13}C{^{1}H} NMR** (126 MHz, $CDCl_3$) δ_C: 21.6 (CH_3), 23.2 (CH(CH_3)^A(CH_3)^B), 23.8 (CH(CH_3)^A(CH_3)^B), 28.7 (*C*H(CH_3)$_2$), 34.0 (*C*(5)H_2), 46.5 (t, *J* 27.7, *C*(6)H), 126.6 (Ar^1*C*(2,6)H), 126.7 (Ar^2*C*(3)H), 127.0 (Ar^2*C*(6)H), 127.0 (Ar^2*C*(5)H), 127.9 (t, *J* 295.0, *C*F_2Cl), 129.3 (Ar^1*C*(3,5)H), 129.7 (Ar^2*C*(4)H), 134.3 (Ar^2*C*(1)), 137.6 (Ar^1*C*(1)), 143.7 (Ar^1*C*(4)), 146.1 (Ar^2*C*(2)), 160.0 (*C*(2)), 165.7 (*C*(4)); **HRMS** (ESI^+) $C_{21}H_{21}O_3N_2F_2{}^{35}ClNaS_2$ $[M+Na]^+$ found 509.0540, requires 509.0542 (–0.4 ppm).

(*S*,R_a,*Z*)-*N*-(3-(2-*iso*-Propylphenyl)-6-methyl-4-oxo-1,3-thiazinan-2-ylidene)-4-methylbenzenesulfonamide (72) and (*R*,R_a,*Z*)-*N*-(3-(2-*iso*-propylphenyl)-6-methyl-4-oxo-1,3-thiazinan-2-ylidene)-4-methylbenzenesulfonamide (S44)



72



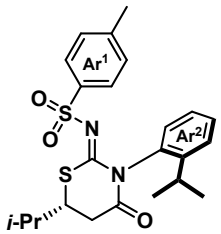
S44

Following General Procedure G, 4-nitrophenyl (*E*)-but-2-enoate **S5** (93.2 mg, 0.45 mmol, 1.5 equiv.), *N*-((2-*iso*-propylphenyl)carbamothioyl)-4-methylbenzenesulfonamide **S29** (105 mg, 0.30 mmol, 1.0 equiv.), and (2*S*,3*R*)-HyperBTM **21** (18.5 mg, 0.06 mmol, 20 mol%) in anhydrous THF (0.1 M) for 24 h at RT gave crude product (88:12 dr) that was purified by flash silica column chromatography (hexane:CH_2Cl_2 100:0 to 0:100, R_F 0.17 at 0:100) to give the title compound as an inseparable mixture of diastereoisomers (88:12 dr) as a colourless oil (102 mg, 82%). $[\alpha]_D^{20}$ –21.2 (*c* 0.5 in $CHCl_3$); **IR** ν_{max} (film) 2965, 1717, 1597, 1506, 1491, 1449, 1348, 1319, 1300, 1150, 1088, 1034, 974, 864, 826, 791; **HRMS** (ESI^+) $C_{21}H_{24}O_3N_2NaS_2$ $[M+Na]^+$ found 439.1118, requires 439.1121 (–0.7 ppm).

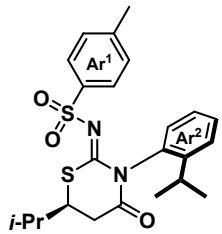
Data for major diastereoisomer (*S*,R_a,*Z*)-**72**: **Chiral HPLC analysis,** Chiralpak IA (95:5 *n*-hexane : IPA, flow rate 1.0 mLmin^{-1}, 211 nm, 40 °C) t_R (*S*,R_a) 47.0 min, t_R (*R*,S_a) 58.5 min, 92:8 er; **^{1}H NMR** (400 MHz, $CDCl_3$) δ_H: 0.98 (3H, d, *J* 6.8, CH(CH_3)^A(CH_3)^B), 1.10 (3H, d, *J* 6.8, CH(CH_3)^A(CH_3)^B), 1.54 (3H, d, *J* 6.8, C(6)HCH_3), 2.33 (3H, s, CH_3), 2.58 (1H, h, *J* 6.8, C*H*(CH_3)$_2$), 3.00 (1H, dd, *J* 16.3, 10.6, C(5)*H*^{A}H^B), 3.24 (1H, dd, *J* 16.3, 3.2, C(5)H^A*H*^{B}), 3.72 (1H, dqd, *J* 10.6, 6.8, 3.2, C(6)*H*), 6.90 – 6.95 (1H, m, Ar^{2}C(6)*H*), 7.07 – 7.12 (2H, m, Ar^{1}C(3,5)*H*), 7.19 – 7.24 (1H, m, Ar^{2}C(5)*H*), 7.31 – 7.41 (4H, m, Ar^{2}C(3,4)*H* and Ar^{1}C(2,6)*H*); **^{13}C{^{1}H} NMR** (126 MHz, $CDCl_3$) δ_C: 19.9 (C(6)HCH_3), 21.5 (*C*H_3), 23.0 (CH(*C*H_3)^A(CH_3)^B), 23.8 (CH(CH_3)^A(*C*H_3)^B), 28.6 (*C*H(CH_3)$_2$), 33.6 (*C*(5)H_2), 42.4 (*C*(6)H), 126.4 (Ar^1*C*(2,6)H), 126.6 (Ar^2*C*(3)H), 126.7 (Ar^2*C*(6)H), 128.6 (Ar^2*C*(5)H), 129.1 (Ar^1*C*(3,5)H), 129.4 (Ar^2*C*(4)H), 134.7 (Ar^2*C*(1)), 138.3 (Ar^1*C*(1)), 143.1 (Ar^1*C*(4)), 145.1 (Ar^2*C*(2)), 163.9 (*C*(2)), 168.9 (*C*(4)).

Data for minor diastereoisomer (*R*,R_a,*Z*)-**S44**: **Chiral HPLC analysis,** Chiralpak IA (95:5 *n*-hexane : IPA, flow rate 1.0 mLmin^{-1}, 211 nm, 40 °C) t_R (*S*,S_a) 53.4 min, t_R (*R*,R_a) 76.0 min, 88:12 er; **^{1}H NMR** (400 MHz, $CDCl_3$) (*selected*) δ_H: 3.00 (1H, dd, *J* 16.3, 10.9, C(5)*H*^{A}H^B), 3.22 (1H, dd, *J* 16.3, 3.2, C(5)H^A*H*^{B}), 6.85 – 6.89 (1H, m, Ar^{2}C(6)*H*); **^{13}C{^{1}H} NMR** (126 MHz, $CDCl_3$) (*selected*) δ_C: 23.1 (CH(*C*H_3)^A(CH_3)^B), 28.7 (*C*H(CH_3)$_2$), 42.3 (*C*(6)H), 126.5 (Ar^1*C*(2,6)H), 126.8 (Ar^2*C*(3)H), 127.6 (Ar^2*C*(6)H), 134.8 (Ar^2*C*(1)), 146.2 (Ar^2*C*(2)), 163.8 (*C*(2)).

(*R*,R_a,*Z*)-*N*-(6-*iso*-Propyl-3-(2-*iso*-propylphenyl)-4-oxo-1,3-thiazinan-2-ylidene)-4-methylbenzenesulfonamide (73) and (*S*,R_a,*Z*)-*N*-(6-*iso*-propyl-3-(2-*iso*-propylphenyl)-4-oxo-1,3-thiazinan-2-ylidene)-4-methylbenzenesulfonamide (S45)



73



S45

Following General Procedure G, 4-nitrophenyl (*E*)-4-methylpent-2-enoate **S6** (106 mg, 0.45 mmol, 1.5 equiv.), *N*-((2-*iso*-propylphenyl)carbamothioyl)-4-methylbenzenesulfonamide **S29** (105 mg, 0.30 mmol, 1.0 equiv.), and (2*S*,3*R*)-HyperBTM **21** (18.5 mg, 0.06 mmol, 20 mol%) in anhydrous THF (0.1 M) for 24 h at RT gave crude

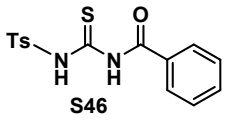
product (92:8 dr) that was purified by flash silica column chromatography (hexane:CH_2Cl_2 80:20 to 0:100, R_F 0.25 at 0:100) to give the title compound as an inseparable mixture of diastereoisomers (92:8 dr) as a colourless oil (115 mg, 86%). $[\alpha]_D^{20}$ –36.2 (*c* 0.5 in $CHCl_3$); **IR** ν_{max} (film) 2965, 1717, 1516, 1508, 1491, 1339, 1314, 1265, 1150, 1088, 876, 816, 791, 758; **HRMS** (ESI^+) $C_{23}H_{28}O_3N_2NaS_2$ $[M+Na]^+$ found 467.1431, requires 467.1434 (–0.6 ppm).

Data for major diastereoisomer (*R*,R_a,*Z*)-**73**: **Chiral HPLC analysis,** Chiralpak AD-H (90:10 *n*-hexane : IPA, flow rate 1.0 mLmin^{-1}, 211 nm, 30 °C) t_R (*R*,R_a) 33.1 min, t_R (*S*,S_a) 47.1 min, 95:5 er; **^{1}H NMR** (400 MHz, $CDCl_3$) δ_H: 1.00 (3H, d, *J* 6.8, CH(CH_3)^A(CH_3)^B), 1.11 (3H, d, *J* 6.8, CH(CH_3)^A(CH_3)^B), 1.12 (3H, d, *J* 6.8, CH(CH_3)^A(CH_3)^B), 1.14 (3H, d, *J* 6.8, CH(CH_3)^A(CH_3)^B), 2.05 (1H, h, *J* 6.8, C*H*(CH_3)$_2$), 2.33 (3H, s, CH_3), 2.59 (1H, h, *J* 6.8, C*H*(CH_3)$_2$), 3.06 (1H, dd, *J* 16.1, 10.8, C(5)H^AH^B), 3.24 (1H, dd, *J* 16.1, 3.2, C(5)H^AH^B), 3.44 (1HH, ddd, *J* 10.8, 6.5, 3.2, C(6)*H*), 6.88 – 6.93 (1H, m, Ar^{2}C(6)*H*), 7.06 – 7.11 (2H, m, Ar^{1}C(3,5)*H*), 7.18 – 7.24 (1H, m, Ar^{2}C(5)*H*), 7.31 – 7.40 (4H, m, Ar^{2}C(3,4)*H* and Ar^{1}C(2,6)*H*); **^{13}C{^{1}H} NMR** (126 MHz, $CDCl_3$) δ_C: 19.4 (CH(*C*H_3)^A(CH_3)^B), 19.7 (CH(CH_3)^A(*C*H_3)^B), 21.5 (*C*H_3), 23.0 (CH(*C*H_3)^A(CH_3)^B), 23.9 (CH(CH_3)^A(*C*H_3)^B), 28.5 (*C*H(CH_3)$_2$), 31.9 (*C*H(CH_3)$_2$), 38.3 (*C*(5)H_2), 45.2 (*C*(6)H), 126.4 (Ar^1*C*(2,6)H), 126.6 (Ar^2*C*(3)H), 126.7 (Ar^2*C*(6)H), 128.4 (Ar^2*C*(5)H), 129.0 (Ar^1*C*(3,5)H), 129.3 (Ar^2*C*(4)H), 134.8 (Ar^2*C*(1)), 138.4 (Ar^1*C*(1)), 143.0 (Ar^1*C*(4)), 145.1 (Ar^2*C*(2)), 164.0 (*C*(2)), 169.4 (*C*(4)).

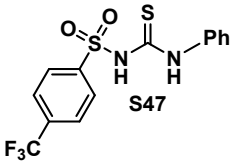
Data for minor diastereoisomer (*S*,R_a,*Z*)-**S45**: **Chiral HPLC analysis,** Chiralpak AD-H (90:10 *n*-hexane : IPA, flow rate 1.0 mLmin^{-1}, 211 nm, 30 °C) t_R (*R*,S_a) 29.1 min, t_R (*S*,R_a) 54.7 min, 68:32 er; **^{1}H NMR** (400 MHz, $CDCl_3$) (*selected*) δ_H: 0.96 (3H, d, *J* 6.8, CH(CH_3)^A(CH_3)^B), 3.52 (1H, ddd, *J* 12.0, 6.4, 2.9, C(6)*H*), 6.85 – 6.89 (1H, m, Ar^{2}C(6)*H*); **^{13}C{^{1}H} NMR** (126 MHz, $CDCl_3$) (*selected*) δ_C: 19.3 (CH(*C*H_3)^A(CH_3)^B), 19.6 (CH(CH_3)^A(*C*H_3)^B), 23.2 (CH(*C*H_3)^A(CH_3)^B), 23.8 (CH(CH_3)^A(*C*H_3)^B), 28.7 (*C*H(CH_3)$_2$), 31.6 (*C*H(CH_3)$_2$), 45.3 (*C*(6)H), 126.5 (Ar^1*C*(2,6)H), 126.8 (Ar^2*C*(3)H), 127.4 (Ar^2*C*(6)H), 134.9 (Ar^2*C*(1)), 138.4 (Ar^1*C*(1)), 146.3 (Ar^2*C*(2)), 164.0 (*C*(2)), 169.5 (*C*(4)).

9. Unsuccessful Substrates

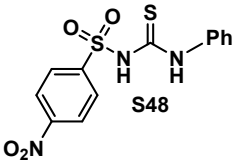
Substrates **S46 – S49** could not be synthesised using the methods detailed in Sections 5 and 6.



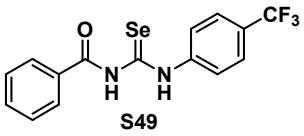
S46



S47

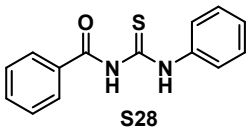


S48

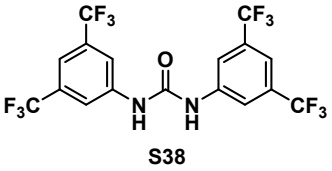


S49

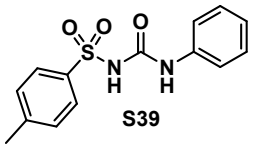
Substrates **S28, S38 and S39** were unreactive under the optimised reaction conditions, returning only starting materials.



S28



S38



S39

10. Structure Elucidation of Minor Regioisomer

The structure of regioisomeric product **S40** has been elucidated by NMR spectroscopy (Figure S1). Large coupling constants consistent with $^{2}J_{C\text{-}F}$ and $^{3}J_{H\text{-}F}$ coupling indicate that the carbon bearing diastereotopic CH_2 protons (•) is adjacent to the perfluoroethyl group. This can only be true for a 5-membered heterocycle with an exocyclic $CH_2C_2F_5$. The ^{13}C chemical shift of ring carbon (• 40.7 ppm) and quaternary carbon (• 152.7 ppm) of **S40** was compared to literature known compounds **S50** (• 42.8 ppm and • 154.2 ppm)[15] and **S51** (• 61.2 ppm and • 179.8 ppm).[16] There was no literature data available for the third possible class of regioisomers **S52**. Good agreement with the ^{13}C chemical shifts of **S50** led to unambiguous assignment of the structure of **S40**.

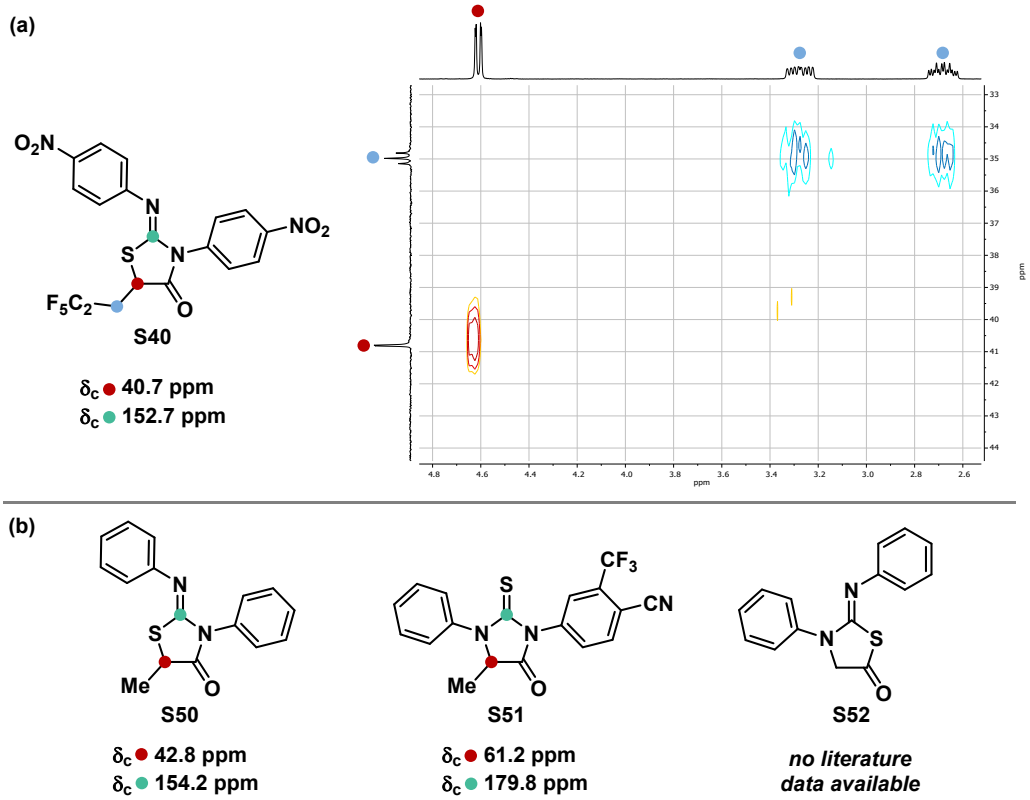


Figure S1 (a) Structural assignment of regioisomeric product **S40** by ^{1}H–^{13}C HSQC NMR and (b) comparison of ^{13}C chemical shifts to known compounds. All chemical shifts were measured in $CDCl_3$.

11. Conformation of Structure by ^{1}H–^{15}N HMBC

The structures of both **46** and **54** were confirmed by ^{1}H–^{15}N HMBC (Figure S2). In each case the diastereotopic protons (•) showed only one cross peak corresponding to the ring nitrogen (•). Any other proton signals that showed a cross peak with the ring nitrogen (•) would then be the substituent on this nitrogen. The methyl protons (•) in **46** showed a cross peak with the ring nitrogen (•), confirming the structure of **46**. Similarly, the *ortho* protons of the 4-nitrophenyl ring (•) in **54** showed a cross peak with the ring nitrogen (•), confirming the structure of **54**.

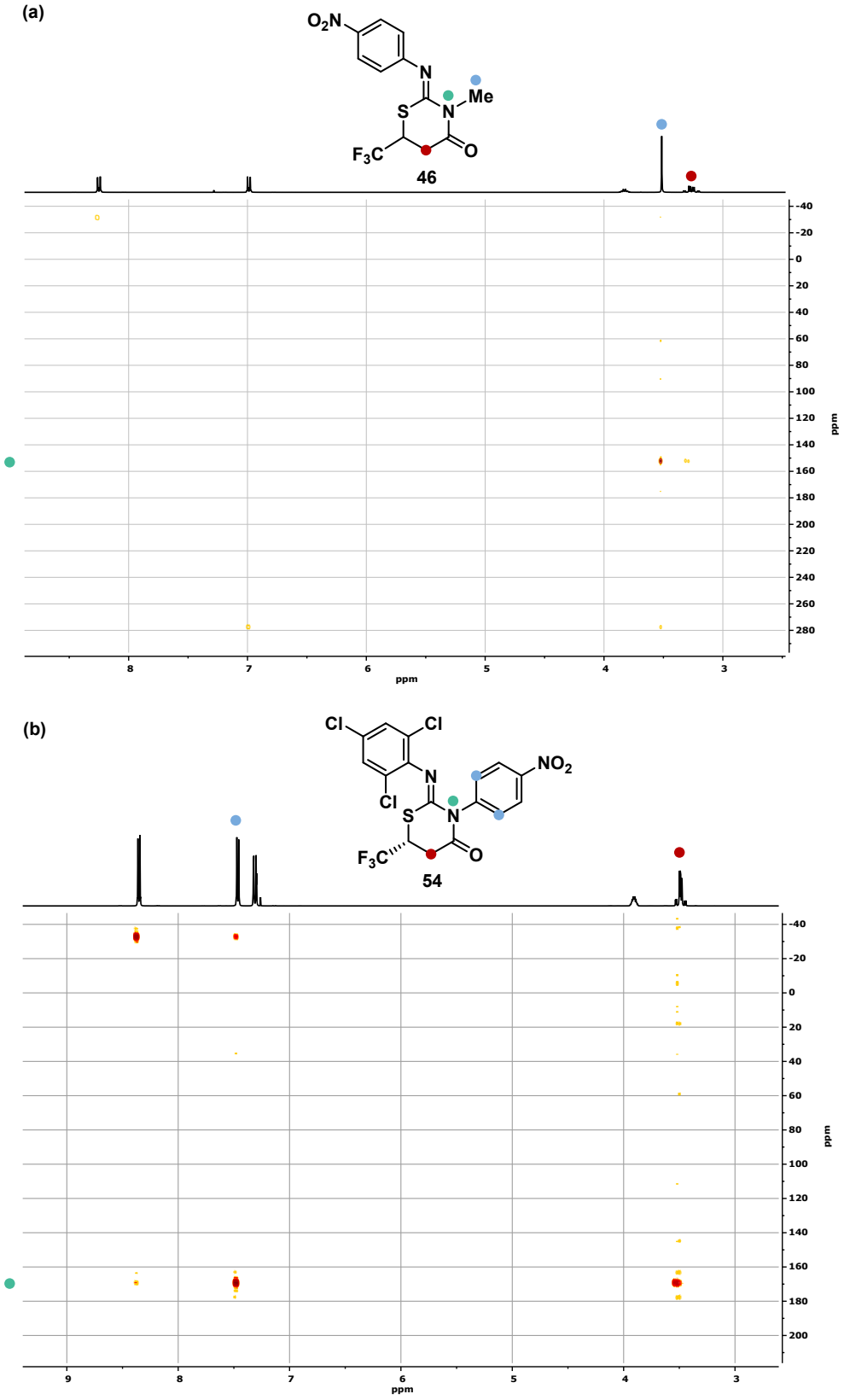
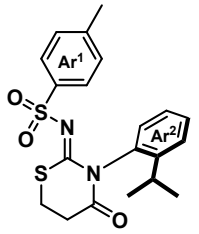


Figure S2 (a) ^{1}H–^{15}N HMBC spectrum of **46** and (b) ^{1}H–^{15}N HMBC spectrum of **54**.

12. Calculation of Configurational Stability

Following the procedure of Armstrong,[17] **63** (20 mg) was dissolved in MeCN (10 mL) and heated to 50 °C. Aliquots (0.3 mL) were taken at defined time points and the er determined by HPLC analysis on a chiral stationary phase (Table S5).



63

Time (s)	ee	ln(1/ee)
0	0.74724	0.291370
1800	0.73276	0.310937
3600	0.71728	0.332289
5400	0.69818	0.359278
7200	0.69006	0.370977
9000	0.67914	0.386928
12600	0.64948	0.431583
19800	0.59322	0.522190
27000	0.55182	0.594533
34200	0.50880	0.675700
86400	0.27864	1.277835

Table S5 Racemisation of **63** at 50 °C in MeCN.

According to Equation S1, a plot of ln(1/ee) vs time afforded a straight line with gradient equal to the rate constant for racemisation (k_{rac}) at this temperature.

$$\ln\left(\frac{1}{ee}\right) = k_{rac}t + \ln\left(\frac{1}{ee_{t=0}}\right)$$

Equation S1 Kinetic analysis for racemisation.

The graph plotted from the data in Table S5 for the racemisation of **63** is shown in Figure S3.

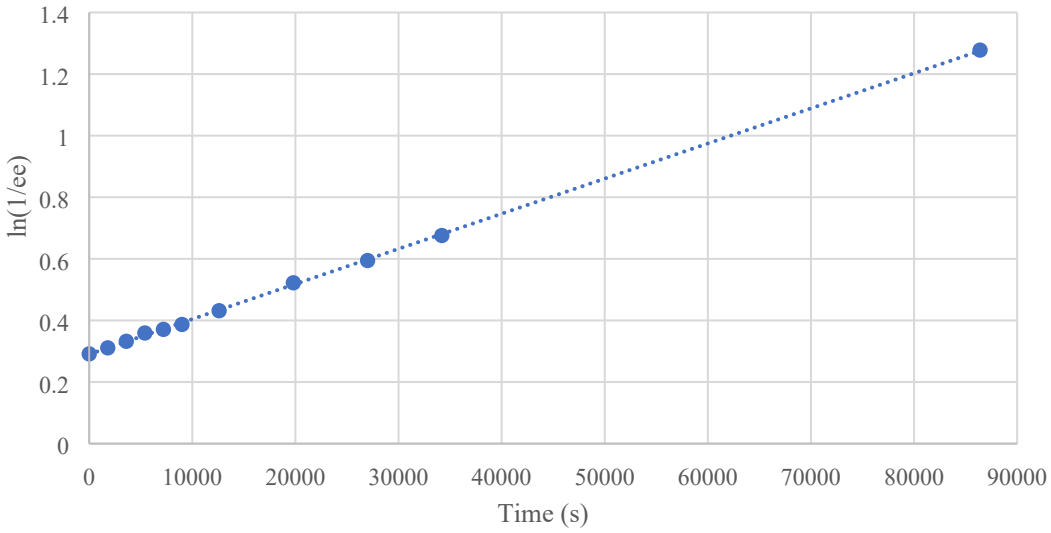


Figure S3 Plot of ln(1/ee) vs time for racemisation of **63**.

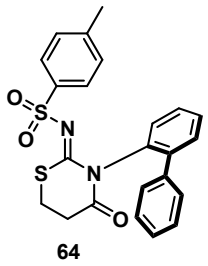
From Figure S3: $k_{rac} = gradient = 1.1406 \times 10^{-5}\, s^{-1}$

$$k_{ent} = \frac{k_{rac}}{2} = \frac{1.1406 \times 10^{-5}}{2} = 5.703 \times 10^{-6}\, s^{-1}$$

$$\Delta G^{\ddagger}_{323} = RT\ln\left(\frac{k_B T}{k_{ent} h}\right) = 8.314 \times 323.15 \times \ln\left(\frac{1.381 \times 10^{-23} \times 323.15}{5.703 \times 10^{-6} \times 6.626 \times 10^{-34}}\right)$$

$$\Delta G^{\ddagger}_{323} = 1.118 \times 10^{5}\, J\, mol^{-1} = 26.7 \pm 0.1\, kcal\, mol^{-1}$$

Following the procedure of Armstrong,[17] **64** (20 mg) was dissolved in MeCN (10 mL) and heated to 50 °C. Aliquots (0.3 mL) were taken at defined time points and the er determined by HPLC analysis on a chiral stationary phase (Table S6).



64

Time (s)	ee	ln(1/ee)
0	0.21488	1.537676
1800	0.10596	2.244694
3600	0.05192	2.958051
5400	0.02722	3.603803
7200	0.01340	4.312501
9000	0.00732	4.917145
10800	0.00400	5.521461

Table S6 Racemisation of **64** at 50 °C in MeCN.

The graph plotted from the data in Table S6 for the racemisation of **64** is shown in Figure S4.

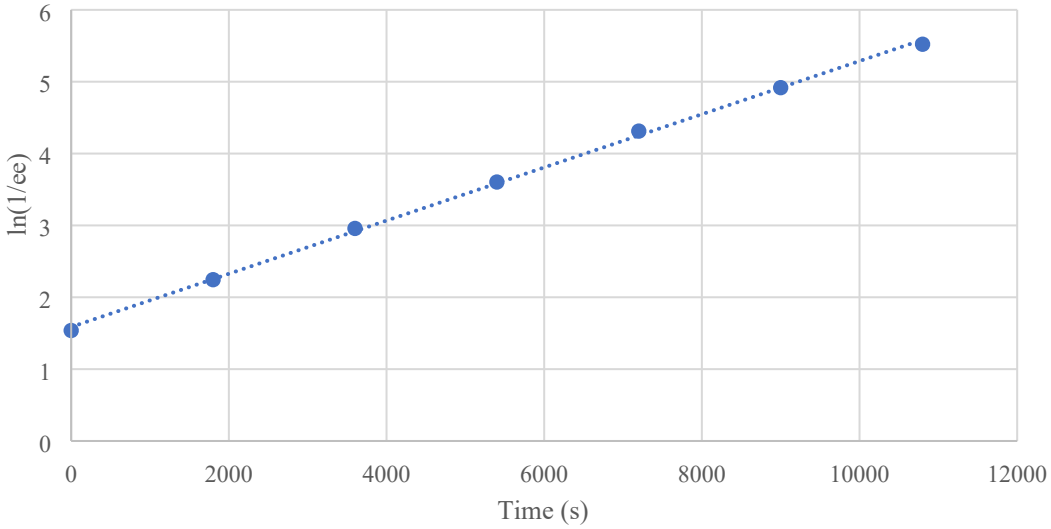


Figure S4 Plot of ln(1/ee) vs time for racemisation of **64**.

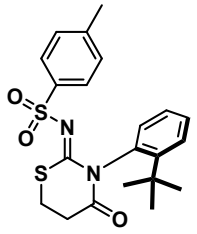
From Figure S4: $k_{rac} = gradient = 3.7005 \times 10^{-4}\, s^{-1}$

$$k_{ent} = \frac{k_{rac}}{2} = \frac{3.7005 \times 10^{-4}}{2} = 1.850 \times 10^{-4}\, s^{-1}$$

$$\Delta G^{\ddagger}_{323} = RT\ln\left(\frac{k_B T}{k_{ent} h}\right) = 8.314 \times 323.15 \times \ln\left(\frac{1.381 \times 10^{-23} \times 323.15}{1.850 \times 10^{-4} \times 6.626 \times 10^{-34}}\right)$$

$$\Delta G^{\ddagger}_{323} = 1.025 \times 10^{5}\, J\, mol^{-1} = 24.5 \pm 0.1\, kcal\, mol^{-1}$$

Following the procedure of Armstrong,[17] **65** (20 mg) was dissolved in mesitylene (10 mL) and heated to 120 °C. Aliquots (0.3 mL) were taken at defined time points and the er determined by HPLC analysis on a chiral stationary phase (Table S7).



65

Time (s)	ee	ln(1/ee)
0	0.58250	0.540426
1800	0.57108	0.560226
3600	0.56300	0.574476
5400	0.55304	0.592325
9000	0.52972	0.635407
16200	0.50322	0.686728
23400	0.47508	0.744272
30600	0.44534	0.808917
86400	0.25960	1.348613

Table S7 Racemisation of **65** at 120 °C in mesitylene.

The graph plotted from the data in Table S7 for the racemisation of **65** is shown in Figure S5.

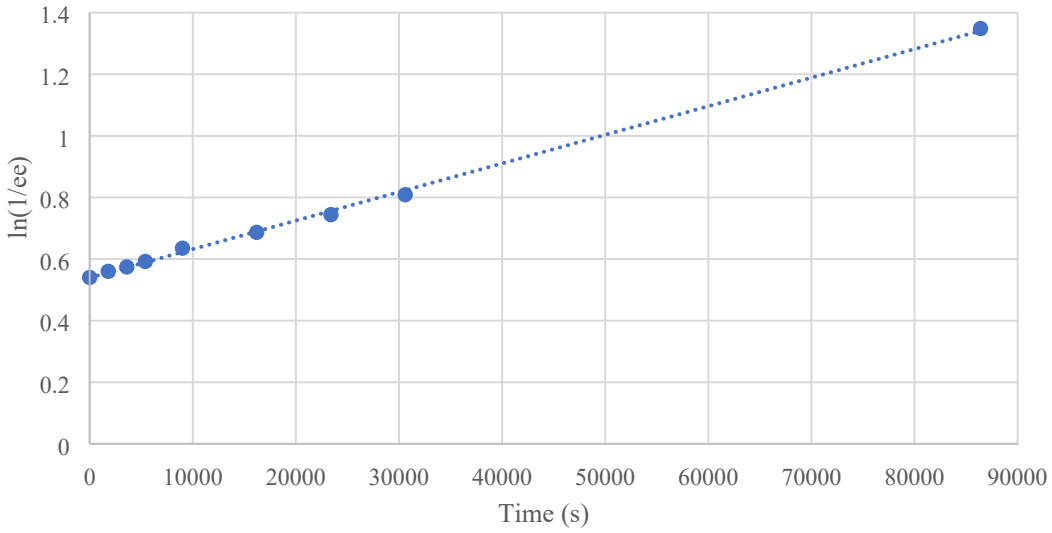


Figure S5 Plot of ln(1/ee) vs time for racemisation of **65**.

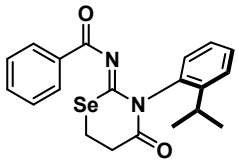
From Figure S5: $k_{rac} = gradient = 9.2813 \times 10^{-6}\ s^{-1}$

$$k_{ent} = \frac{k_{rac}}{2} = \frac{9.2813 \times 10^{-6}}{2} = 4.641 \times 10^{-6}\ s^{-1}$$

$$\Delta G^{\ddagger}_{393} = RT\ln\left(\frac{k_B T}{k_{ent} h}\right) = 8.314 \times 393.15 \times \ln\left(\frac{1.381 \times 10^{-23} \times 393.15}{4.641 \times 10^{-6} \times 6.626 \times 10^{-34}}\right)$$

$$\Delta G^{\ddagger}_{393} = 1.373 \times 10^{5}\ J\ mol^{-1} = 32.8 \pm 0.1\ kcal\ mol^{-1}$$

Following the procedure of Armstrong,[17] **66** (20 mg) was dissolved in MeCN (10 mL) and heated to 50 °C. Aliquots (0.3 mL) were taken at defined time points and the er determined by HPLC analysis on a chiral stationary phase (Table S8).



66

Time (s)	ee	ln(1/ee)
0	0.44606	0.807302
1800	0.40798	0.896537
3600	0.37000	0.994252
5400	0.34116	1.075404
7200	0.31204	1.164624
9000	0.28442	1.257303
12600	0.23702	1.439611
16200	0.19638	1.627704
19800	0.16160	1.822631
27000	0.10966	2.210371
34200	0.07418	2.601261

Table S8 Racemisation of **66** at 50 °C in MeCN.

The graph plotted from the data in Table S8 for the racemisation of **66** is shown in Figure S6.

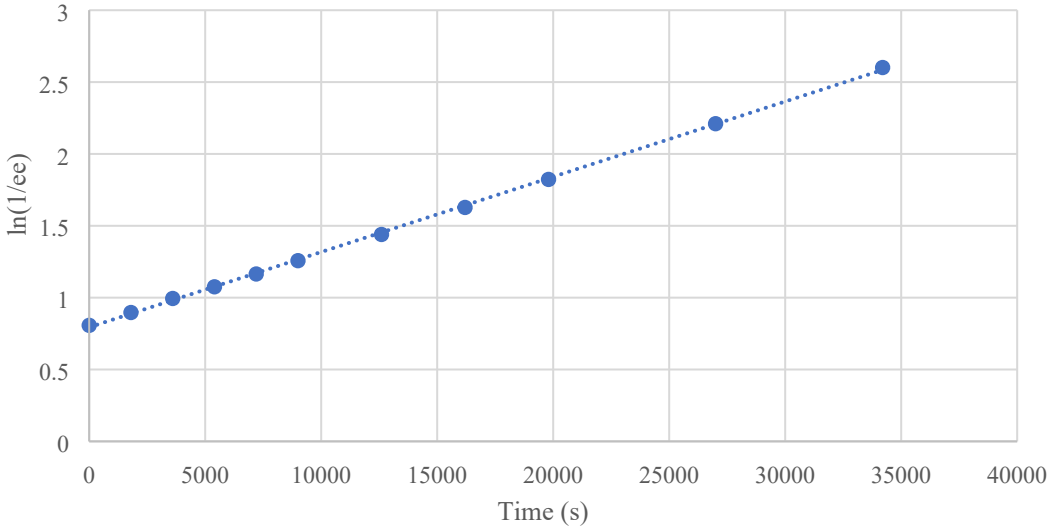


Figure S6 Plot of ln(1/ee) vs time for racemisation of **66**.

From Figure S6: $k_{rac} = gradient = 5.2356 \times 10^{-5}\ s^{-1}$

$$k_{ent} = \frac{k_{rac}}{2} = \frac{5.2356 \times 10^{-5}}{2} = 2.618 \times 10^{-5}\ s^{-1}$$

$$\Delta G_{323}^{\ddagger} = RT\ln\left(\frac{k_B T}{k_{ent} h}\right) = 8.314 \times 323.15 \times \ln\left(\frac{1.381 \times 10^{-23} \times 323.15}{2.618 \times 10^{-5} \times 6.626 \times 10^{-34}}\right)$$

$$\Delta G_{323}^{\ddagger} = 1.077 \times 10^{5}\ J\ mol^{-1} = 25.7 \pm 0.1\ kcal\ mol^{-1}$$

13. Configuration of Major Diastereoisomer Determined by ^{1}H NOESY

The absolute configuration of (6*R*,R_a,*Z*)-**67** was supported by single crystal X-ray crystallography. However, since the crystal used to obtain the X-ray structure was grown from a mixture of diastereoisomers, it was not known if the structure of the major or minor diastereoisomer was obtained. Unfortunately, HPLC analysis of the crystal from which the X-ray structure was obtained did not yield a UV trace and so was unsuccessful. The relative configuration of the major diastereoisomer of atropisomeric product **72** was determined by ^{1}H NOESY NMR.The coincident methyl peak for both diastereoisomers was irradiated and a response for the C(6) aromatic proton from only the major diastereoisomer was obtained. A reciprocal NOE was also obtained when the C(6) proton of the major diastereoisomer was irradiated. Assuming the stereoselectivity of the reaction does not change, the crystal structure obtained was of the major diastereoisomer of **67**.

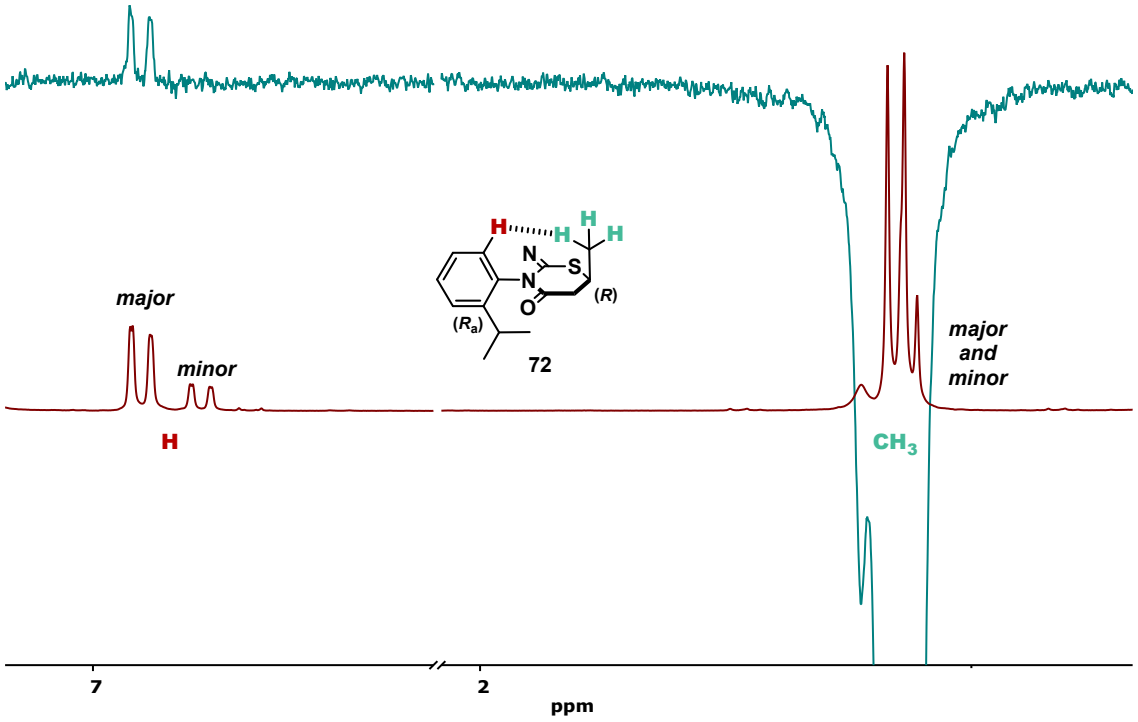
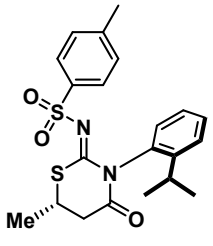


Figure S7 Top: ^{1}H NOESY NMR of **72** and bottom: ^{1}H NMR of **72**. Tosyl substituent omitted for clarity.

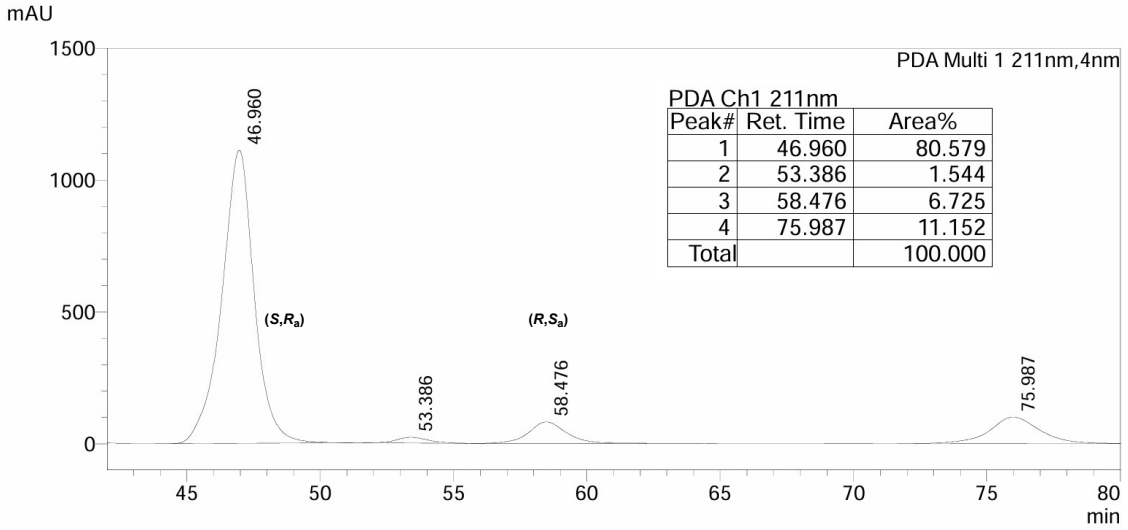
14. Determining the Configuration of Minor Diastereoisomers

The configuration of the major enantiomer within the minor diastereoisomer of the atropisomeric products was determined by HPLC analysis on a chiral stationary phase. A sample of known dr and er was heated to facilitate epimerisation via rotation around the hindered axis. It cannot be guaranteed that a diastereomeric ratio can be accurately determined by HPLC. However, for the following samples the initial dr determined by HPLC was consistent with that obtained by ^{1}H NMR analysis.



(*S*,*R*$_a$)-72

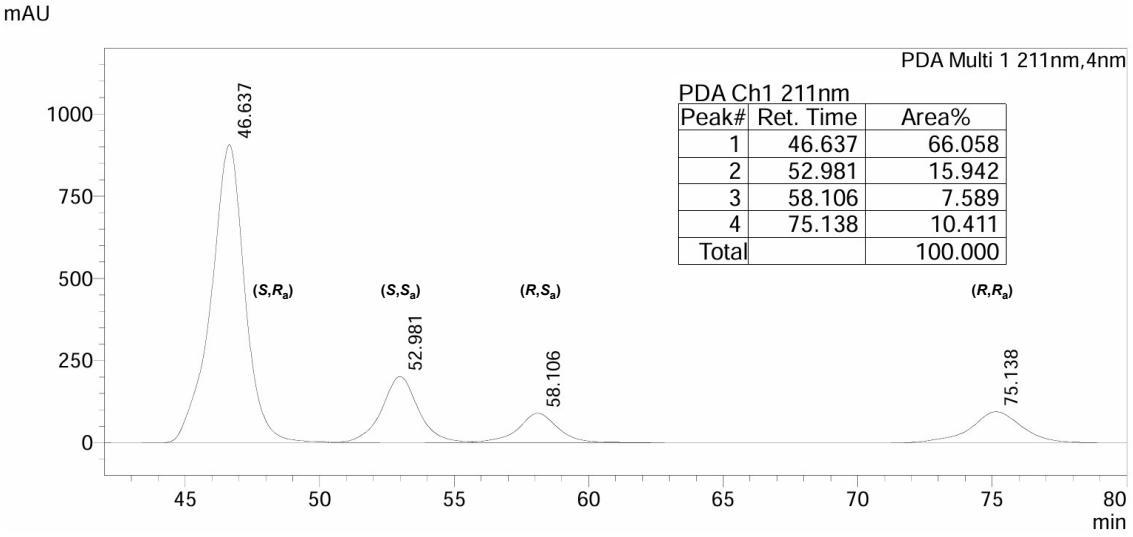
A sample of (S,R_a)-**72** with 87:13 dr, 92:8 er_{major}, and 88:12 er_{minor} (Figure S8) was heated at 70 °C for 1.5 h. Once complete, the sample now had 74:26 dr, 90:10 er_{major}, and 40:60 er_{minor} (Figure S9). The reduction in dr was expected due to epimerisation. The major enantiomer within the minor diastereoisomer was changed and thus assigned as (S,S_a), coming from the epimerisation of (S,R_a). The major enantiomer within the minor diastereoisomer in the initial mixture was therefore assigned (R,R_a).



PDA Ch1 211nm

Peak#	Ret. Time	Area%
1	46.960	80.579
2	53.386	1.544
3	58.476	6.725
4	75.987	11.152
Total		100.000

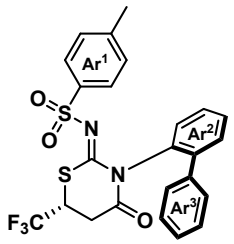
Figure S8 HPLC of **72** before heating.



PDA Ch1 211nm

Peak#	Ret. Time	Area%
1	46.637	66.058
2	52.981	15.942
3	58.106	7.589
4	75.138	10.411
Total		100.000

Figure S9 HPLC of **72** after heating.



(*R*,*R*$_a$)-**68**

A sample of (*R*,*R*$_a$)-**68** with 87:13 dr, 95:5 er$_{major}$, and 63:37 er$_{minor}$ (Figure S10) was heated at 50 °C for 30 min. Once complete, the sample now had 65:35 dr, 91:9 er$_{major}$, and 90:10 er$_{minor}$ (Figure S11). Again, the reduction in dr was expected due to epimerisation. The er within the minor diastereoisomer had increased and the major enantiomer was assigned (*R*,*S*$_a$), coming from the epimerisation of (*R*,*R*$_a$). The minor enantiomer within the minor diastereoisomer was therefore assigned (*S*,*R*$_a$). In this case, epimerisation either during the reaction or during product isolation was the main source of the minor diastereoisomer, and hence the opposite enantioselectivity observed.

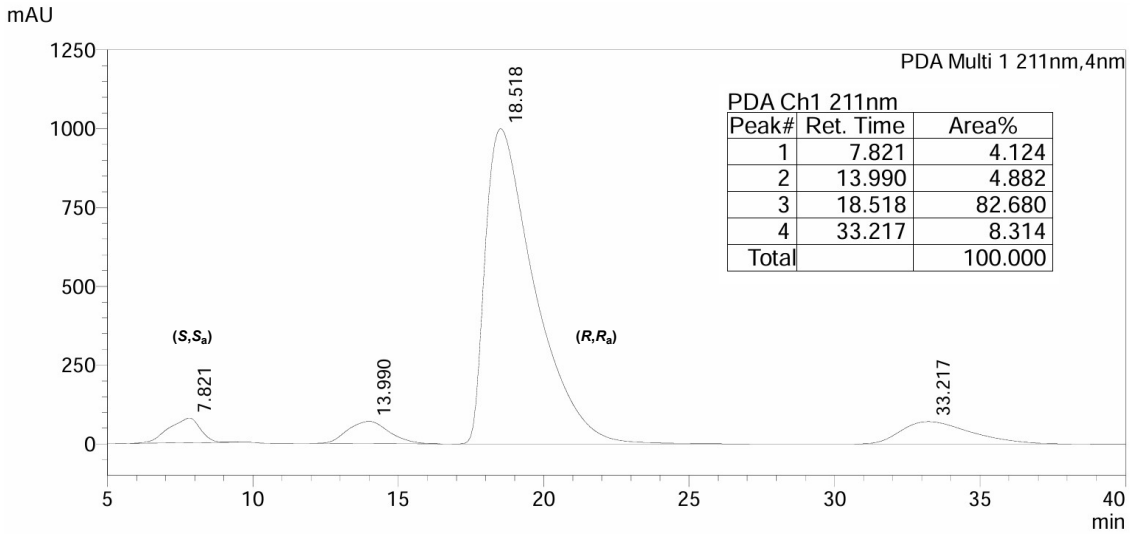


Figure S10 HPLC of **68** before heating.

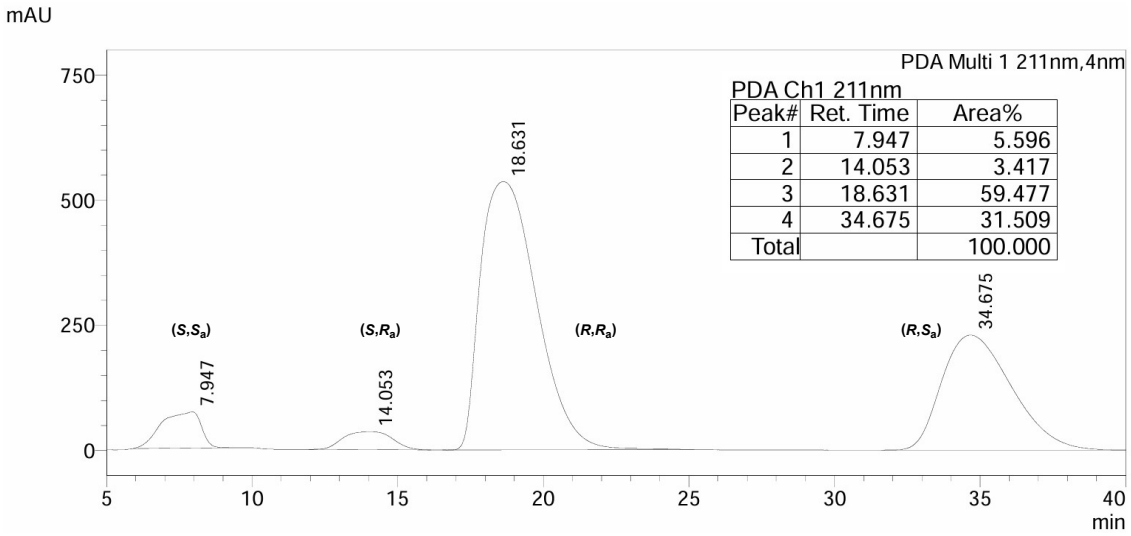


Figure S11 HPLC of **68** after heating.

15. Mechanistic Studies

Procedure for NMR titration of Schreiner's thiourea 26 with NBu_4OPNP (Scheme 5A)

Schreiner's thiourea **26** (37.5 mg, 0.075 mmol, 1.0 equiv.) was dissolved in d_8-THF (0.1 M) and a reference ^1H NMR taken. NBu_4OPNP (5.7 mg, 0.015 mmol, 20 mol%) was added to the solution and another ^1H NMR taken. This was repeated for 40 mol%, 60 mol%, 80 mol%, and 100 mol% of NBu_4OPNP.

Procedure for background reaction with NBu_4OPNP (Scheme 5B)

Schreiner's thiourea **26** (50.0 mg, 0.10 mmol, 1.0 equiv.), 4-nitrophenyl (*E*)-4,4,4-trifluorobut-2-enoate **27** (39.2 mg, 0.15 mmol, 1.5 equiv.), and NBu_4OPNP (3.8 mg, 0.01 mmol, 10 mol%) were dissolved in anhydrous THF (0.1 M) and stirred at RT for 24 h. Once complete, the solvent was removed under reduced pressure, 1,3,5-trimethoxybenzene (0.1 M in $CDCl_3$, 0.5 mL, 0.05 mmol) was then added and ^1H NMR obtained.

Procedure for NMR titration of PNP ester S5 with Schreiner's thiourea 26 (Figure S12)

4-Nitrophenyl crotonate **S5** (23.3 mg, 0.11 mmol, 1.5 equiv.) was dissolved in d_8-THF (0.1 M) and a reference ^1H NMR taken. Schreiner's thiourea **26** (7.5 mg, 0.015 mmol, 20 mol%) was added to the solution and another ^1H NMR taken. This was repeated for 40 mol%, 60 mol%, 80 mol%, 100 mol%, and 150 mol% of Schreiner's thiourea **26**.

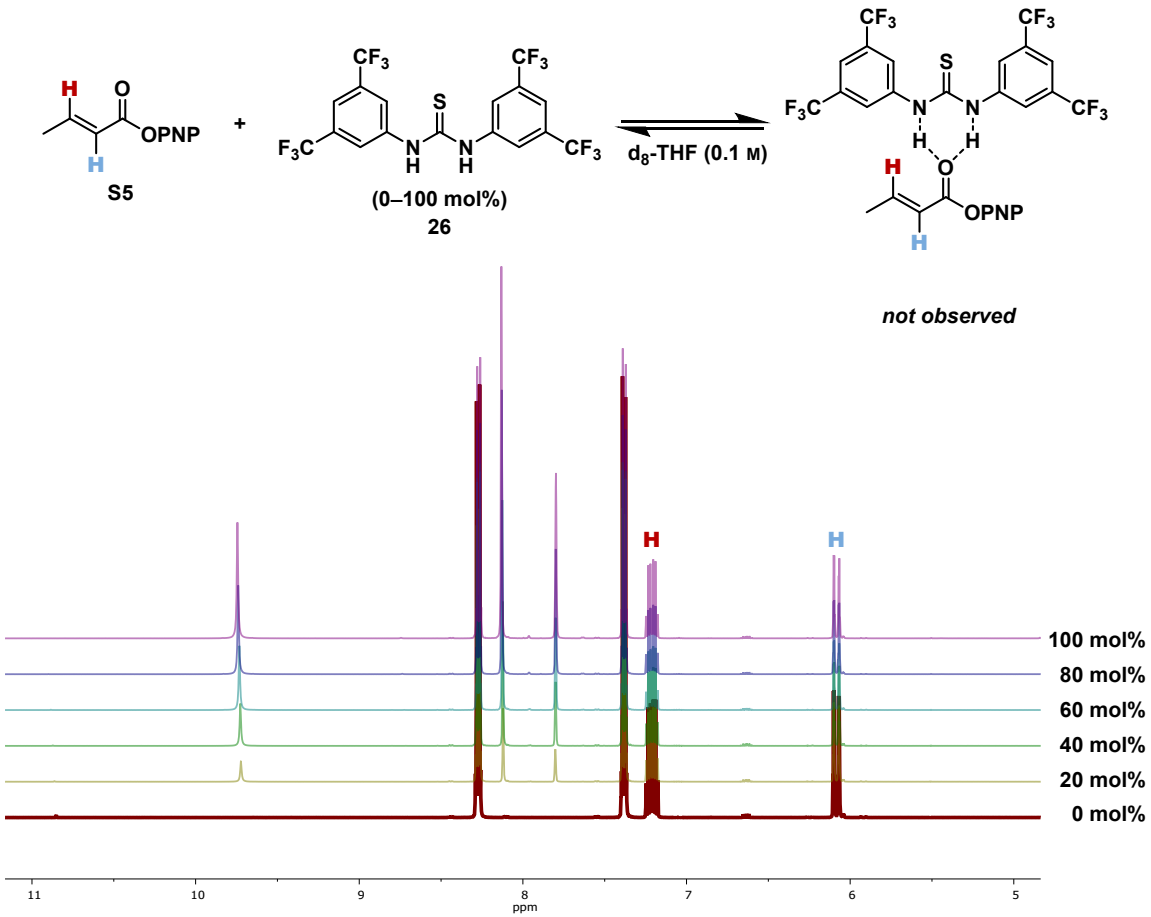
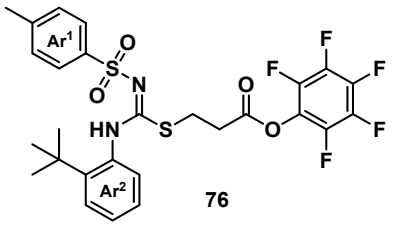


Figure S12 NMR titration of PNP ester **S5** with Schreiner's thiourea **26**.

Perfluorophenyl 3-((*N*-(2-(*tert*-butyl)phenyl)-*N*'-tosylcarbamimidoyl)thio)propanoate (76)



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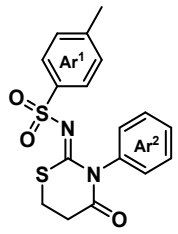
Perfluorophenyl acrylate **75** (360 mg, 1.5 mmol, 1.5 equiv.), *N*-((2-(*tert*-butyl)phenyl)carbamothioyl)-4-methylbenzenesulfonamide **74** (360 mg, 1.0 mmol, 1.0 equiv.) and (±)-HyperBTM **21** (15.4 mg, 0.05 mmol, 5 mol%) were dissolved in anhydrous THF (0.1 M) and stirred at 0 °C for 5 h. After removal of the solvent under reduced pressure, the crude reaction mixture was purified directly by flash silica column chromatography (hexane:EtOAc 100:0 to 0:100, R_F 0.23 at 50:50) to give the title compound as a white solid (330 mg, 55%). **mp** 99 – 101 °C; **^{1}H NMR** (500 MHz, $CDCl_3$) δ_H: 1.40 (9H, s, C(C*H*$_3$)$_3$), 2.44 (3H, s, C*H*$_3$), 2.94 (2H, t, *J* 6.9, C(3)*H*$_2$), 3.21 (2H, t, *J* 6.9, C(2)*H*$_2$), 7.15 (1H, dd, *J* 7.8, 1.5, Ar^{2}C(6)*H*), 7.20 – 7.25 (1H, m, Ar^{2}C(5)*H*), 7.30 – 7.37 (3H, m, Ar^{1}C(3,5)*H* and Ar^{2}C(4)*H*), 7.48 (1H, dd, *J* 8.0, 1.5, Ar^{2}C(3)*H*), 7.87 – 7.91 (2H, m, Ar^{1}C(2,6)*H*), 9.83 (1H, br s, N*H*); **^{19}F{^{1}H} NMR** (470 MHz, $CDCl_3$) δ_F: –162.2 – –162.0 (m, ArC*F*), –157.6 (t, *J* 21.7, ArC*F*), –152.6 – –152.5 (m, ArC*F*); **^{13}C{^{1}H} NMR** (126 MHz, $CDCl_3$) δ_C: 21.7 (*C*H$_3$), 26.3 (*C*(2)H$_2$), 30.6 (C(*C*H$_3$)$_3$), 33.6 (*C*(3)H$_2$), 35.3 (*C*(CH$_3$)$_3$), 124.7 – 125.0 (Ar*C*(1)), 126.5 (Ar^1*C*(2,6)H), 127.0 (Ar^2*C*(5)H), 127.8 (Ar^2*C*(3)H), 129.6 (Ar^2*C*(4)H), 129.7 (Ar^1*C*(3,5)H), 131.3 (Ar^2*C*(6)H), 134.0 (Ar^2*C*(1)), 136.7 – 139.2 (m, ArCF), 138.5 – 140.8 (ArCF), 139.5 (Ar^1*C*(1)), 139.9 – 142.4 (m, ArCF), 143.4 (Ar^1*C*(4)), 147.2 (Ar^2*C*(2)), 167.6 (*C*N), 168.1 (*C*O); **IR** ν_{max} (film) 3269, 2972, 1790, 1562, 1516, 1402, 1321, 1269, 1138, 1092, 1084, 1038, 982, 856, 829; **HRMS** (ESI^+) $C_{27}H_{25}O_4N_2F_5S_2Na$ $[M+Na]^+$ found 623.1067, requires 623.1068 (–0.2 ppm).

(*Z*)-4-Methyl-*N*-(4-oxo-3-phenyl-1,3-thiazinan-2-ylidene)benzenesulfonamide (78)



78

Perfluorophenyl 3-((*N*-(2-(*tert*-butyl)phenyl)-*N*'-tosylcarbamimidoyl)thio)propanoate **76** (120 mg, 0.20 mmol, 1.0 equiv.), 4-methyl-*N*-(phenylcarbamothioyl)benzenesulfonamide **77** (61.3 mg, 0.20 mmol, 1.0 equiv.), and (±)-HyperBTM **21** (6.2 mg, 0.020 mmol, 10 mol%) were dissolved in anhydrous THF (0.1 M) and stirred for 24 h at RT. Once complete, the reaction mixture was diluted with EtOAc and washed with sat. $NaHCO_3$ ($\times$ 3), dried over $MgSO_4$, then the solvent removed under reduced pressure to afford the crude product. The crude product was purified by flash silica column chromatography (CH_2Cl_2:Et_2O 100:0 to 90:10, R_F 0.32 at 95:5) to give the title compound as a white solid (37 mg, 51%). **mp** 164 – 166 °C; **IR** ν_{max} (film) 2920, 1713, 1514, 1344, 1279, 1140, 1088, 993, 841, 694, 671; **^{1}H NMR** (400 MHz, $CDCl_3$) δ_H: 2.36 (3H, s, CH_3), 3.17 – 3.23 (2H, m, C(5)H_2), 3.24 – 3.30 (2H, m, C(6)H_2), 7.01 – 7.06 (2H, m, Ar^{2}C(2,6)*H*), 7.10 – 7.15 (2H, m, Ar^{1}C(3,5)*H*), 7.35 – 7.45 (5H, m, Ar^{1}C(2,6)*H* and Ar^{2}C(3,4,5)*H*); **^{13}C{^{1}H} NMR** (126 MHz, $CDCl_3$) δ_C: 21.6 (*C*H_3), 23.4 (*C*(5)H_2), 34.5 (*C*(5)H_2), 126.5 (Ar^1*C*(2,6)H), 128.4 (Ar^2*C*(2,6)H), 128.7 (Ar^2*C*(4)H), 129.2 (Ar^2*C*(3,5)H), 129.4 (Ar^1*C*(3,5)H), 137.1 (Ar^2*C*(1)), 138.3 (Ar^1*C*(1)), 143.3 (Ar^1*C*(4)), 164.7 (*C*(2)), 169.1 (*C*(4)); **HRMS** (ESI^+) $C_{17}H_{16}O_3N_2NaS_2$ $[M+Na]^+$ found 383.0493, requires 383.0495 (–0.5 ppm).

16. Computational Studies

Geometry optimisations were performed with the *meta*-hybrid M06-2X functional[18] using the double-ζ, def2-SVP basis set from the redefinition of the Ahlrichs family of basis sets.[19-22] Implicit solvation was considered through the use of the SMD model employing the parameters of THF (ε = 7.4257).[23] An ultrafine integration grid (99 radial shells with 590 angular points per shell) was used for all calculations and all species were formally treated as closed-shell systems with restricted Kohn-Sham DFT used throughout. The nature of minima and transition states located were verified by the computation of harmonic frequencies at the same level of theory. Single-point energies (E_{sp}) were also evaluated using the M06-2X functional[18] with a larger, triple-ζ, def2-TZVP basis. Implicit solvation was also included at this level of theory using the same ultrafine integration grid (99,590). Additional empirical dispersion corrections were not included as the functional implicitly accounts for dispersion due to the nature of its construction. Thermochemistry was evaluated at 1 atm and 298.15 K using thermodynamic calculations at the level of geometry optimisation (thermal corrections to enthalpy, $\delta H_{298.15}$, and entropies $S_{298.15}$) in combination with energetics obtained from single-point calculations. Gibbs free energies were calculated at 273 K (and 323 K for atropisomeric rotational barriers to correspond with experiment) using Equation **S2**, with additional Martin Hay Pratt empirical entropic corrections included (S_{MHP} = 3.05 kcal/mol per particle, evaluated at 276 atm to mimic bulk THF, Equations **S3-S4**).[24] Conformational flexibility of minima species was evaluated using CREST,[25] retaining the lowest lying GFN2-xTB conformation of the minima. The key enantiodetermining transition state **TS1** was subject to a more rigorous conformational treatment, with DFT evaluation of different staggered conformations around the forming S-C bond with *cis-cis*, *trans-cis* and *trans-trans* conformations of the thiourea nucleophile (see Figures **S13-S14**). All computations were performed using the Gaussian16, C.01 programme[26] with visualisation of structures using PyMol.[27] This and similar levels of DFT have previously been used successfully to rationalise reactivities and selectivities of organocatalytic reactions with isothioureas.[5, 28]

$$G_{298.15} = E_{sp} + \delta H_{298.15} - TS_{298.15} + S_{MHP}$$

Equation S2 Calculation of Gibbs free energies.

$$p = \rho RT/M = 276.340 \text{ atm}$$

Equation S3 Evaluation of pressure for S_{MHP} correction.[24] Where p = pressure of THF, ρ = density of THF (0.889 g/cm^3), M = molar mass of THF (72.107 g/mol).

$$S_{MHP} = RT \ln(p/p^0) = 3.05 \text{ kcal/mol per particle,}$$

Equation S4 Evaluation of S_{MHP} correction.[24] Where R = ideal gas constant, T = temperature (273.15 K).

Conformational Screening of Michael addition TS

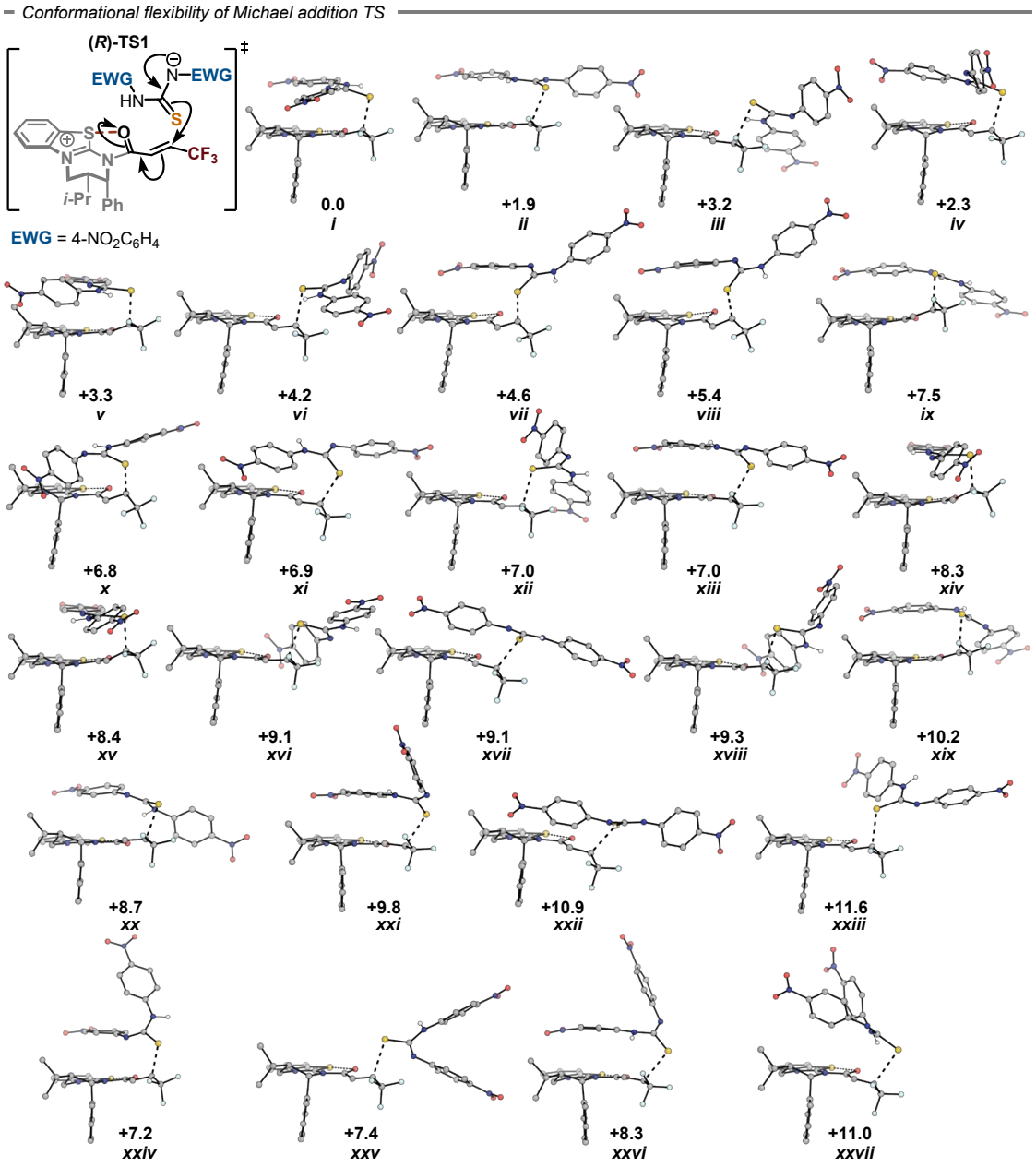


Figure S13 Conformational screening of (*R*)-TS1. Gibbs free energies are shown in kcal/mol.

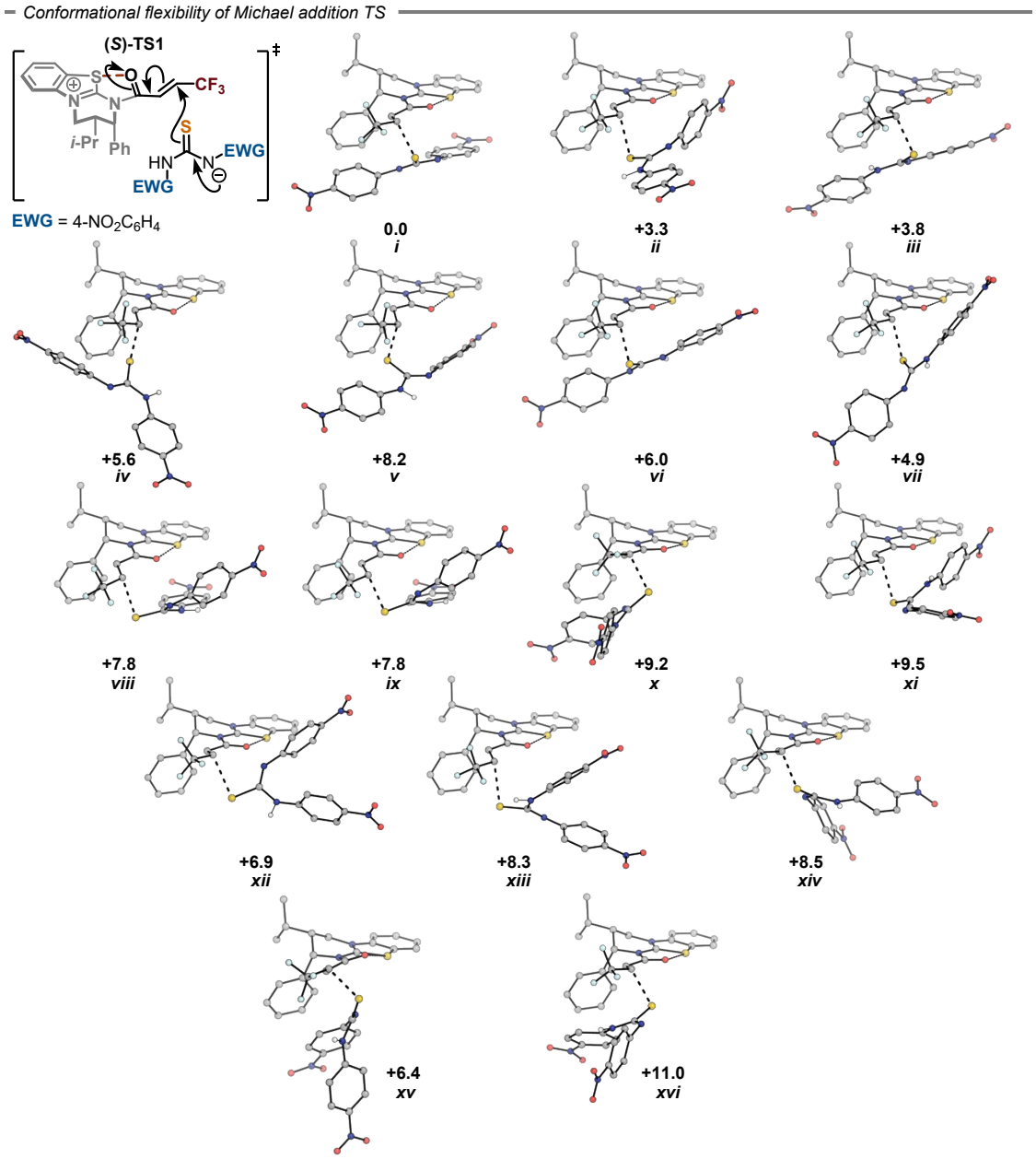


Figure S14 Conformational screening of (*S*)-TS1. Gibbs free energies are shown in kcal/mol.

Stability of Michael Adduct Species

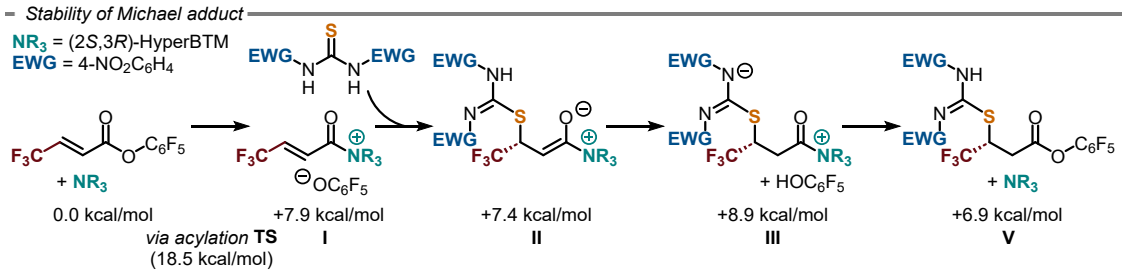


Figure S15 Computed stability of different Michael addition adducts. Gibbs free energies (ΔG_{273}) are shown in kcal/mol.

Variation of Michael Acceptor

By changing the CF_3 of the Michael acceptor to a methyl group, there is a reduction in driving force alongside an increase in barrier heights for **TS1-3**, indicating that the reaction may be slightly slower with the more donating methyl group. The barrier for catalyst acylation is also increased from 18.5 kcal/mol to 22.2 kcal/mol. The presence of an electron withdrawing group increases the electrophilicity of this component, facilitating the Michael addition and subsequent reactivity. The er of this substrate (**42**) is computed to remain high through the lactamisation (99:1 (*R*) er computed, 86:14 (*R*) er experimental), though the selectivity of the Michael addition step is significantly reduced, and we would predict an almost racemic mixture of the products based on the kinetic selectivity of the Michael addition alone.

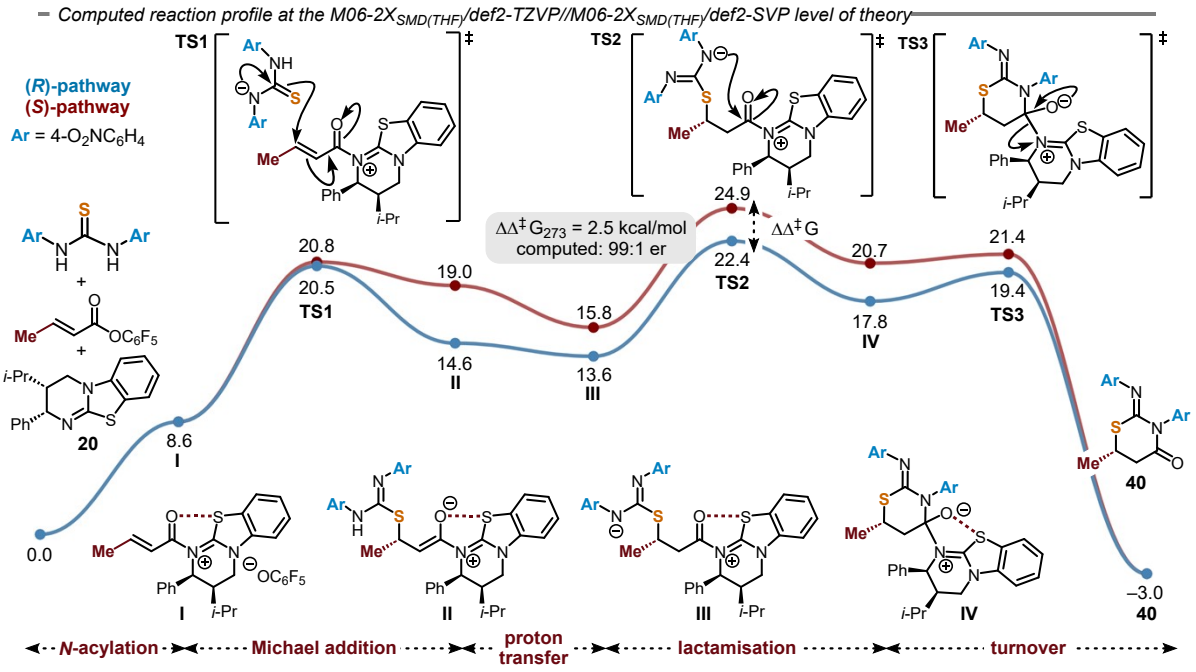


Figure S16 Computed reaction profile of methyl analogue **42** at the M06-2X$_{SMD(THF)}$/def2-TZVP//M06-2X$_{SMD(THF)}$/def2-SVP level of theory. Gibbs free energies (ΔG_{273}) are shown in kcal/mol. Lactamisation in the (*S*)-pathway is facilitated by rotation of the acyl component (same as **36**).

Atropisomerism Rotational Barriers

Rotational barriers were computed for rotation of the ortho-alkyl or -aryl moiety past the C=N-R group (see TS in Figure S17) for consistency as this was computed to be lower in energy than rotation of the *i*-Pr moiety past the C=O group for product **67** ($\Delta\Delta^{\ddagger}G$ = 0.5 kcal/mol). Calculations appear to overestimate the barrier height compared to experiment but reflect the trends with the introduction of more bulk.

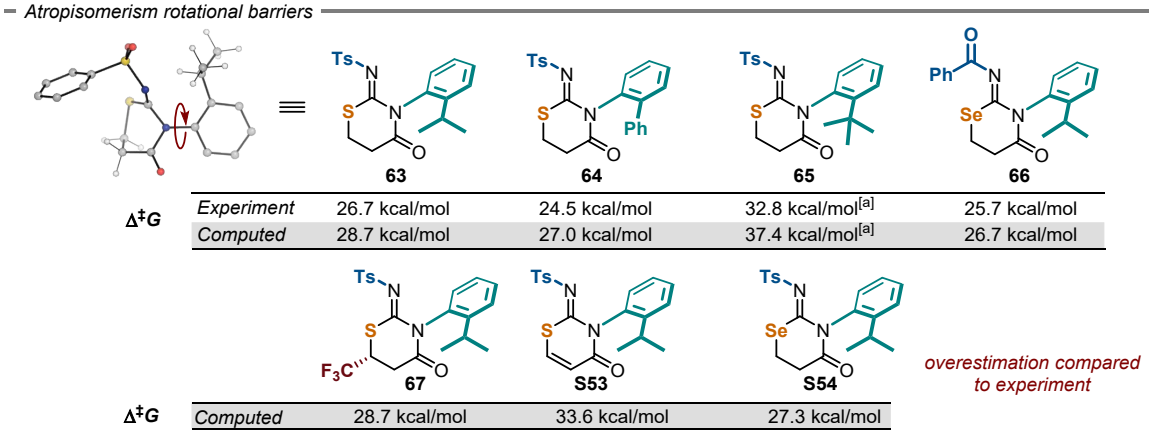


Figure S17 Computed and experimental rotational barrier heights of atropisomeric products evaluated at 323 K. Gibbs free energies (ΔG_{323}) are shown in kcal/mol. [a] evaluated at 393 K.

17. Single Crystal X-ray Diffraction Data

X-ray diffraction data for compounds **37**, **55**, and **67** were collected using a Rigaku MM-007HF High Brilliance RA generator/confocal optics with either XtaLAB P100 or P200 diffractometers [Cu Kα radiation (λ = 1.54187 Å)]. Data for all compounds analysed were collected (using a calculated strategy) and processed (including correction for Lorentz, polarization and absorption) using CrysAlisPro.[29] Structures were solved by dual-space methods (SHELXT)[30] and refined by full-matrix least-squares against F^2 (SHELXL-2019/3).[31] Non-hydrogen atoms were refined anisotropically, and hydrogen atoms were refined using a riding model. All calculations were performed using the Olex2[32] interface. Selected crystallographic data are presented in Tables S9 – S11.

CCDC 2410987-2410989 contains the supplementary crystallographic data for this paper. These data can be obtained free of charge from The Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/structures.

Table S9: X-ray data for 37

	(6*R*,*Z*)-37
CCDC	2410987
empirical formula	$C_{19.33}H_{11.33}ClF_3N_4OS$
fw	440.17
crystal description	colourless prism
crystal size [mm]	0.30×0.21×0.18
space group	R3
a [Å]	21.67271(16)
b [Å]	21.67271(16)
c [Å]	10.76754(10)
vol [Å]^3	4379.99(8)
Z	9
p (calc) [g/cm^3]	1.502
μ [mm^{-1}]	3.174
F(000)	2010
reflections collected	41954
independent reflections ($\boldsymbol{R}_{int}$)	3444(0.0239)
parameters/restraints	265/1
GOF on F^2	1.058
R_1 [I > 2σ(l)]	0.0215
wR_2 (all data)	0.0560
largest diff. peak/hole [e/Å^3]	0.17, -0.28
Flack parameter	0.005(4)

Table S10: X-ray data for 55

	(6*R*,*Z*)-55
CCDC	2410988
empirical formula	$C_{18}H_{13}F_3N_2O_2Se$
fw	425.26
crystal description	colourless prism
crystal size [mm]	0.09×0.07×0.01
space group	$P2_1$
a [Å]	9.51115(5)
b [Å]	16.17558(9)
c [Å]	10.71507(5)
vol [Å]^3	1647.968(15)
Z	4
p (calc) [g/cm^3]	1.714
μ [mm^{-1}]	3.538
F(000)	848.0
reflections collected	61612
independent reflections ($\boldsymbol{R}_{int}$)	6656(0.0709)
parameters/restraints	469/1
GOF on F^2	1.070
R_1 [I > 2σ(l)]	0.0280
wR_2 (all data)	0.0755
largest diff. peak/hole [e/Å^3]	0.44, -0.50
Flack parameter	-0.046(10)

Table S11: X-ray data for 67

	(6*R*,R_a,*Z*)-67
CCDC	2410989
empirical formula	$C_{21}H_{21}F_3N_2O_3S_2$
fw	470.52
crystal description	colourless prism
crystal size [mm]	0.500×0.025×0.007
space group	$P2_12_12_1$
a [Å]	8.07483(6)
b [Å]	15.56758(15)
c [Å]	17.59729(15)
vol [Å]^3	2212.08(3)
Z	4
p (calc) [g/cm^3]	1.413
μ [mm^{-1}]	2.639
F(000)	976.0
reflections collected	43774
independent reflections ($\boldsymbol{R}_{int}$)	4547(0.0938)
parameters/restraints	283/0
GOF on F^2	1.043
R_1 [I > 2σ(l)]	0.0386
wR_2 (all data)	0.1033
largest diff. peak/hole [e/Å^3]	0.69, -0.20
Flack parameter	-0.008(10)

18. References

[1] A. Kütt, V. Movchun, T. Rodima, T. Dansauer, E. B. Rusanov, I. Leito, I. Kaljurand, J. Koppel, V. Pihl, I. Koppel, G. Ovsjannikov, L. Toom, M. Mishima, M. Medebielle, E. Lork, G.-V. Röschenthaler, I. A. Koppel and A. A. Kolomeitsev, *J. Org. Chem.*, 2008, **73**, 2607-2620.

[2] S. Espinosa, E. Bosch and M. Roses, *J. Chromatogr. A*, 2002, **964**, 55-66.

[3] J. Han and F. M. Tao, *J. Phys. Chem. A*, 2006, **110**, 257-263.

[4] M. D. Greenhalgh, S. Qu, A. M. Z. Slawin and A. D. Smith, *Chem. Sci.*, 2018, **9**, 4909-4918.

[5] J. Wu, C. M. Young, A. A. Watts, A. M. Z. Slawin, G. R. Boyce, M. Bühl and A. D. Smith, *Org. Lett.*, 2022, **24**, 4040-4045.

[6] A. Matviitsuk, M. D. Greenhalgh, D.-J. B. Antúnez, A. M. Z. Slawin and A. D. Smith, *Angew. Chem. Int. Ed.*, 2017, **56**, 12282-12287.

[7] H. Liu, A. M. Z. Slawin and A. D. Smith, *Org. Lett.*, 2020, **22**, 1301-1305.

[8] B. Kim, Y. Song and S. Y. Lee, *Chem. Commun.*, 2021, **57**, 11052-11055.

[9] Z. Wang, L. Hu, N. Chekshin, Z. Zhuang, S. Qian, J. X. Qiao and J.-Q. Yu, *Science*, 2021, **374**, 1281-1285.

[10] J.-C. Blazejewski, J. W. Hofstraat, C. Lequesne, C. Wakselman and U. E. Wiersum, *J. Fluorine Chem.*, 1998, **91**, 175-177.

[11] N. Busschaert, I. L. Kirby, S. Young, S. J. Coles, P. N. Horton, M. E. Light and P. A. Gale, *Angew. Chem. Int. Ed.*, 2012, **51**, 4426-4430.

[12] M. C. Risi, G. C. Saunders and W. Henderson, *Inorg. Chim. Acta*, 2021, **526**, 120506.

[13] F. Lacan, M. Varache-Lembège, J. Vercauteren, J.-M. Léger, B. Masereel, J.-M. Dogné and A. Nuhrich, *Eur. J. Med. Chem.*, 1999, **34**, 311-328.

[14] D. Tan, V. Štrukil, C. Mottillo and T. Friščić, *Chem. Commun.*, 2014, **50**, 5248-5250.

[15] B. Haouas, N. Sbei, H. Ayari, M. L. Benkhoud and B. Batanero, *New J. Chem.*, 2018, **42**, 11776-11781.

[16] L. Ma, Y. Zhou, D. Yang, M.-W. Wang, W. Lu and J. Jin, *Molecules*, 2022, **27**, 5867.

[17] J.-P. Heeb, J. Clayden, M. D. Smith and R. J. Armstrong, *Nat. Protoc.*, 2023, **18**, 2745-2771.

[18] Y. Zhao and D. G. Truhlar, *Theor. Chem. Acc.*, 2008, **120**, 215-241.

[19] F. Weigend and R. Ahlrichs, *Phys. Chem. Chem. Phys.*, 2005, **7**, 3297-3305.

[20] F. Weigend, *Phys. Chem. Chem. Phys.*, 2006, **8**, 1057-1065.

[21] A. Schäfer, H. Horn and R. Ahlrichs, *J. Chem. Phys.*, 1992, **97**, 2571-2577.

[22] A. Schäfer, C. Huber and R. Ahlrichs, *J. Chem. Phys.*, 1994, **100**, 5829-5835.

[23] A. V. Marenich, C. J. Cramer and D. G. Truhlar, *J. Phys. Chem. B*, 2009, **113**, 6378-6396.

[24] R. L. Martin, P. J. Hay and L. R. Pratt, *J. Phys. Chem. A*, 1998, **102**, 3565-3573.

[25] P. Pracht, F. Bohle and S. Grimme, *Phys. Chem. Chem. Phys.*, 2020, **22**, 7169–7192.

[26] G. W. T. M. J. Frisch, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, G. A. Petersson, H. Nakatsuji, X. Li, M. Caricato, A. V Marenich, J. Bloino, B. G. Janesko, R. Gomperts, B. Mennucci, H. P. Hratchian, J. V. Ortiz, A. F. Izmaylov, J. L. Sonnenberg, D. Williams-Young, F. Ding, F. Lipparini, F. Egidi, J. Goings, B. Peng, A. Petrone, T. Henderson, D. Ranasinghe, V. G. Zakrzewski, J. Gao, N. Rega, G. Zheng, W. Liang, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H.

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[27] The PyMOL Molecular Graphics System, Version 2.4.1, Schrödinger, LLC.

[28] C. Wang, S.-J. Li, Q.-C. Zhang, D. Wei and L. Ding, *Catal. Sci. Technol.*, 2020, **10**, 3664-3669.

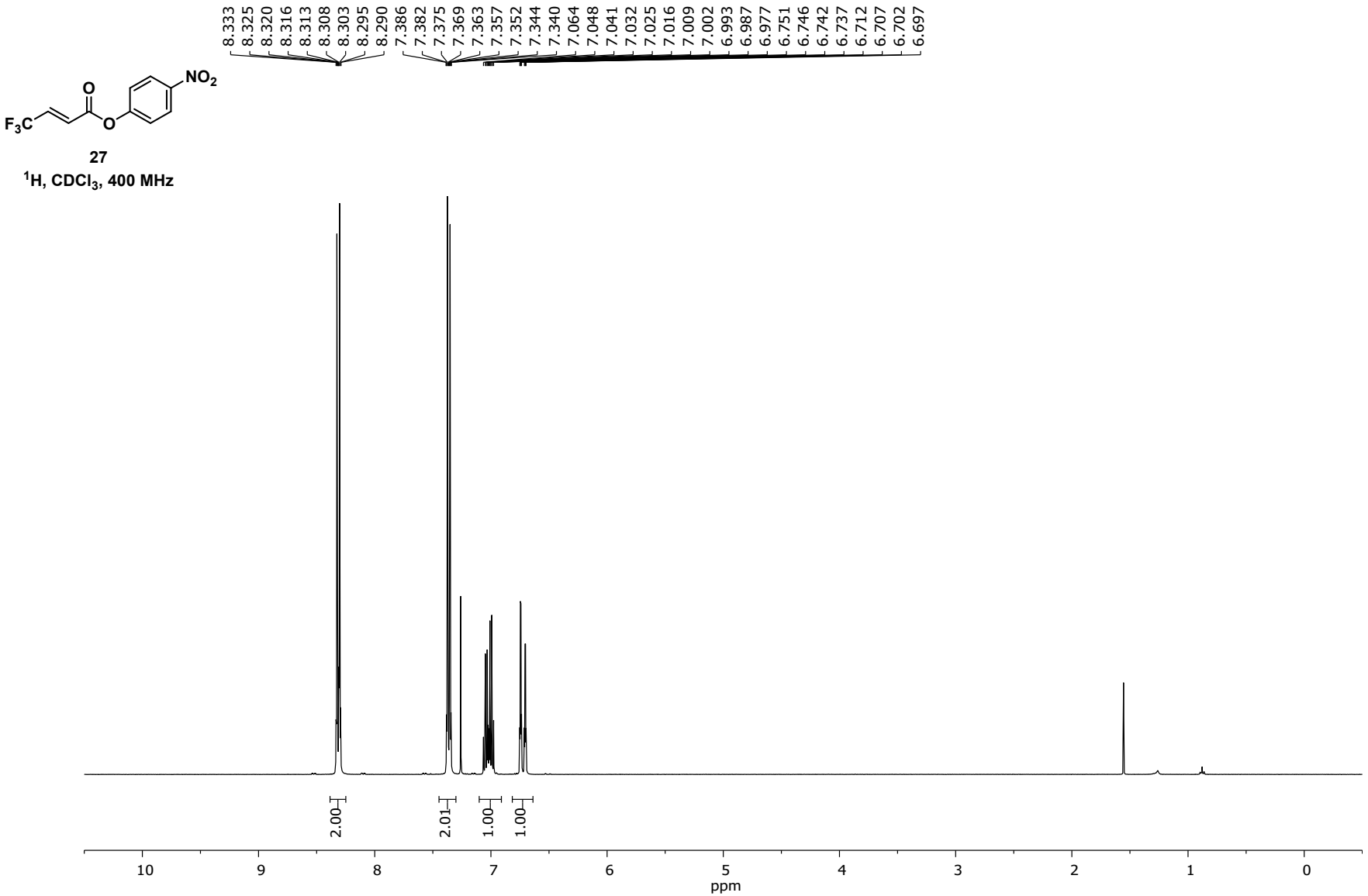
[29] *CrysAlisPro* v1.171.42.82a, 94a. and 43.109a Rigaku Oxford Diffraction, Rigaku Corporation, Tokyo, Japan, 2023.

[30] G. M. Sheldrick, *Acta Crystallogr., Sect. A: Found. Adv.*, 2015, **71**, 3-8.

[31] G. M. Sheldrick, *Acta Crystallogr., Sect. C: Struct. Chem.*, 2015, **71**, 3-8.

[32] O. V. Dolomanov, L. J. Bourhis, R. J. Gildea, J. A. K. Howard and H. Puschmann, *J. Appl. Crystallogr.*, 2009, **42**, 339-341.

Appendix I: ^{1}H, $^{19}F\{^{1}H\}$, $^{13}C\{^{1}H\}$, and $^{77}Se\{^{1}H\}$ NMR Spectra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7.002
6.993
6.987
6.977
6.751
6.746
6.742
6.737
6.712
6.707
6.702
6.697
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NO2
F3C
O
27
1H, CDCl3, 400 MHz
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1.00
1.00
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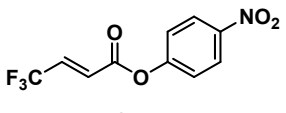
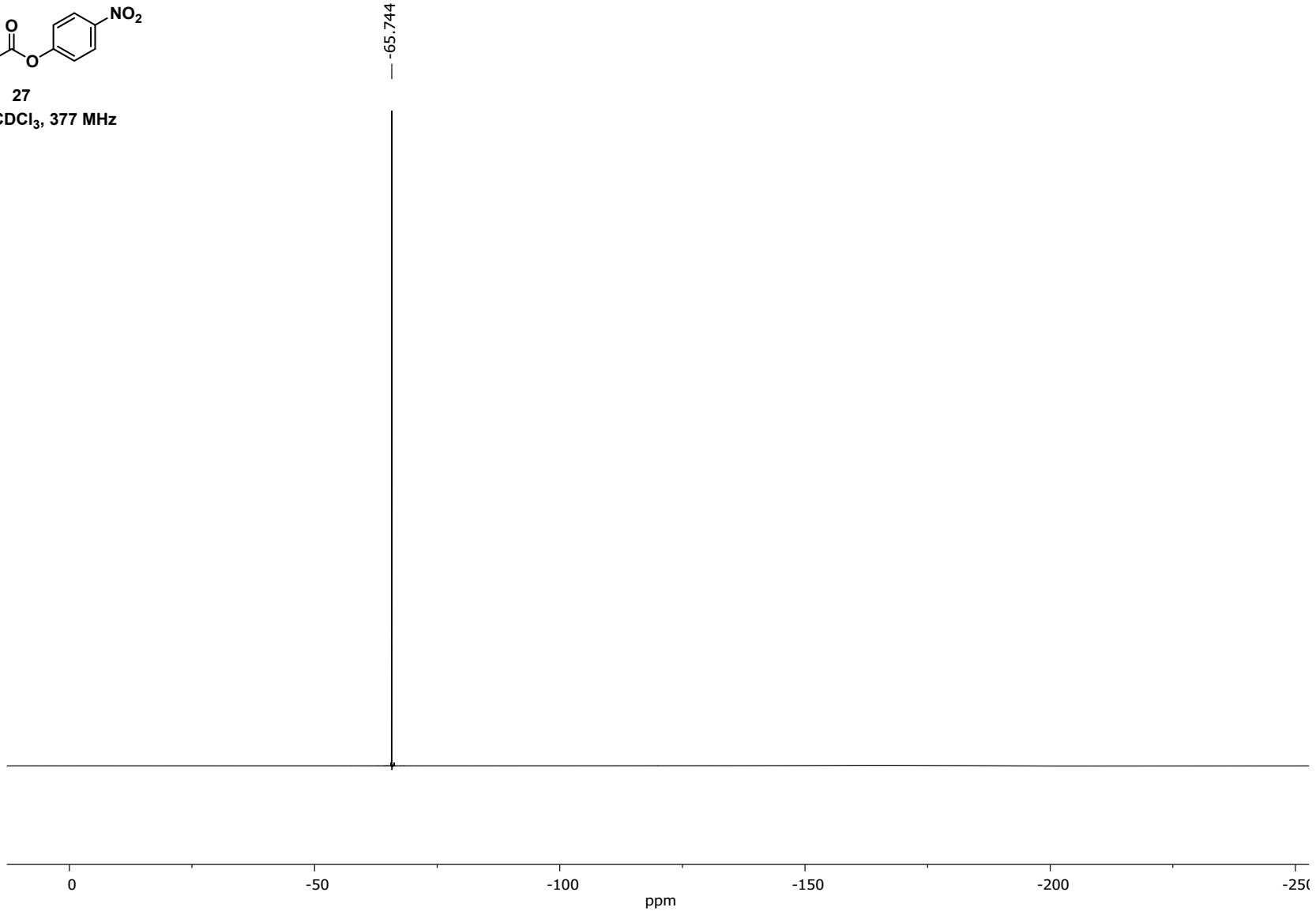
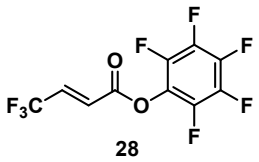
8
7
6
5
4
3
2
1
0
ppm



27

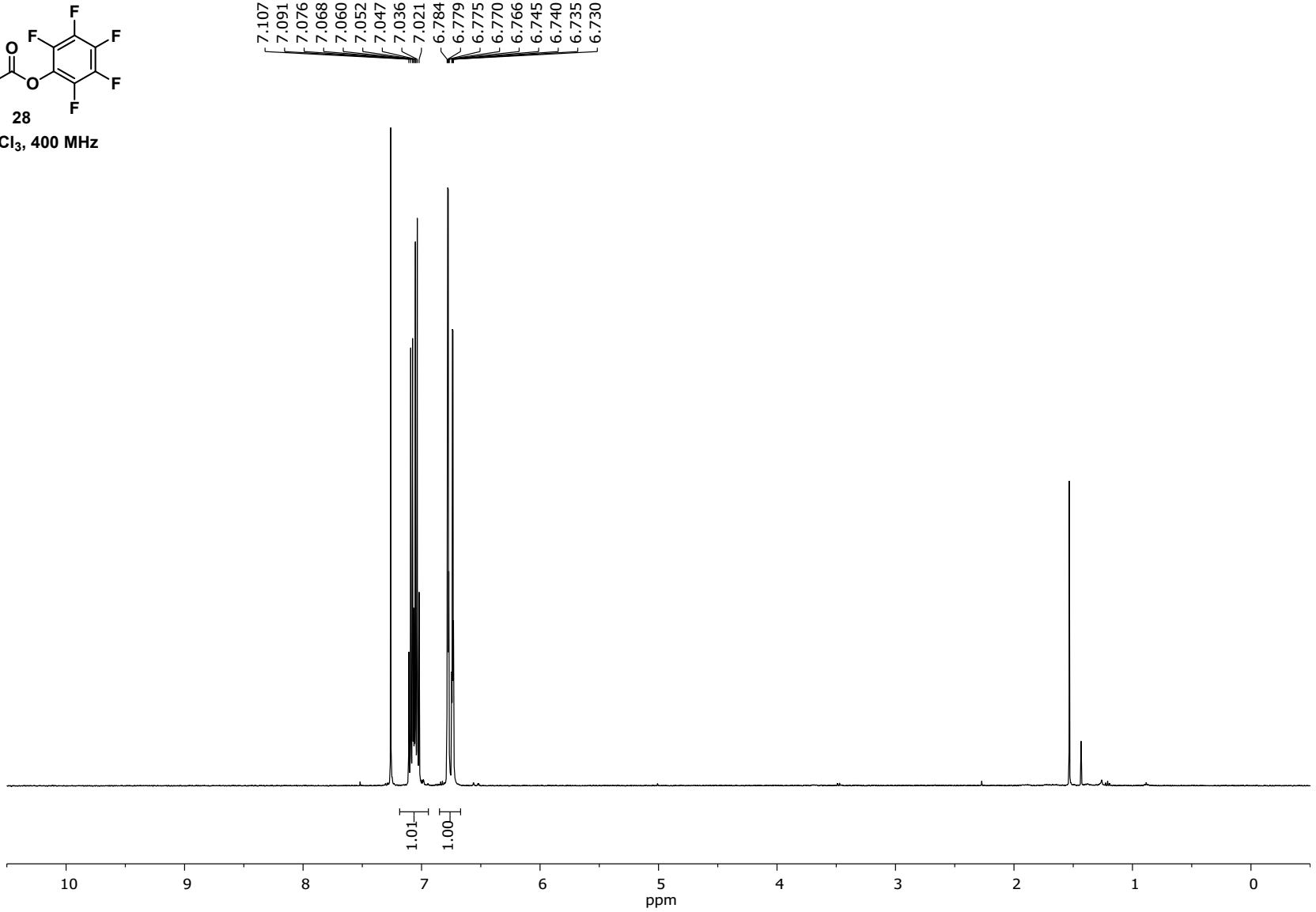
$^{19}F\{^{1}H\}$, $CDCl_3$, 377 MHz

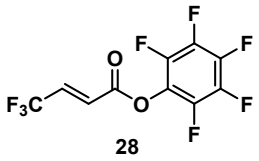




28

^{1}H, $CDCl_3$, 400 MHz





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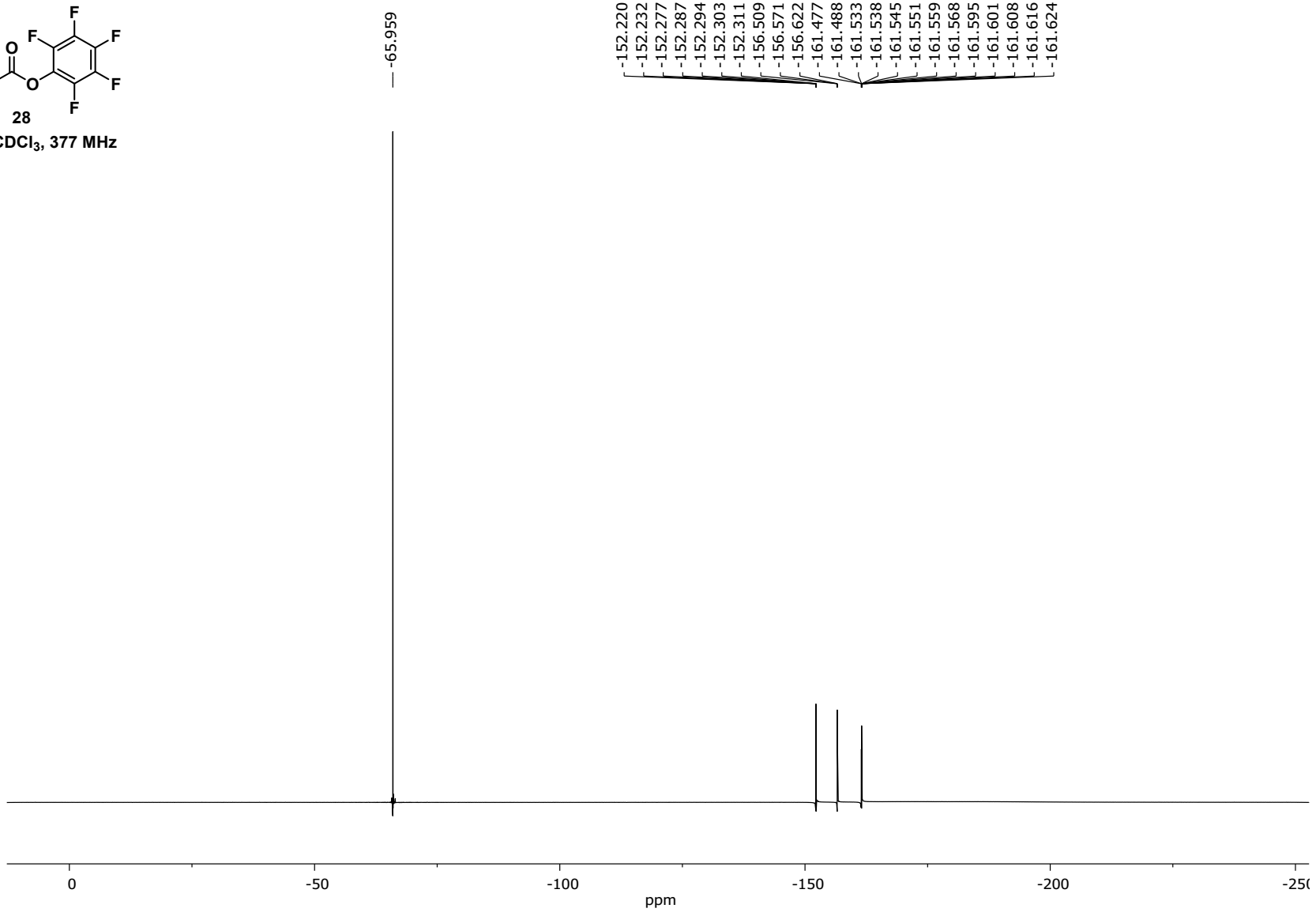
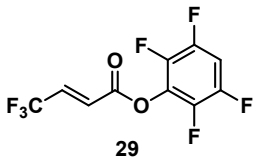
$^{19}F\{^{1}H\}$, $CDCl_3$, 377 MHz





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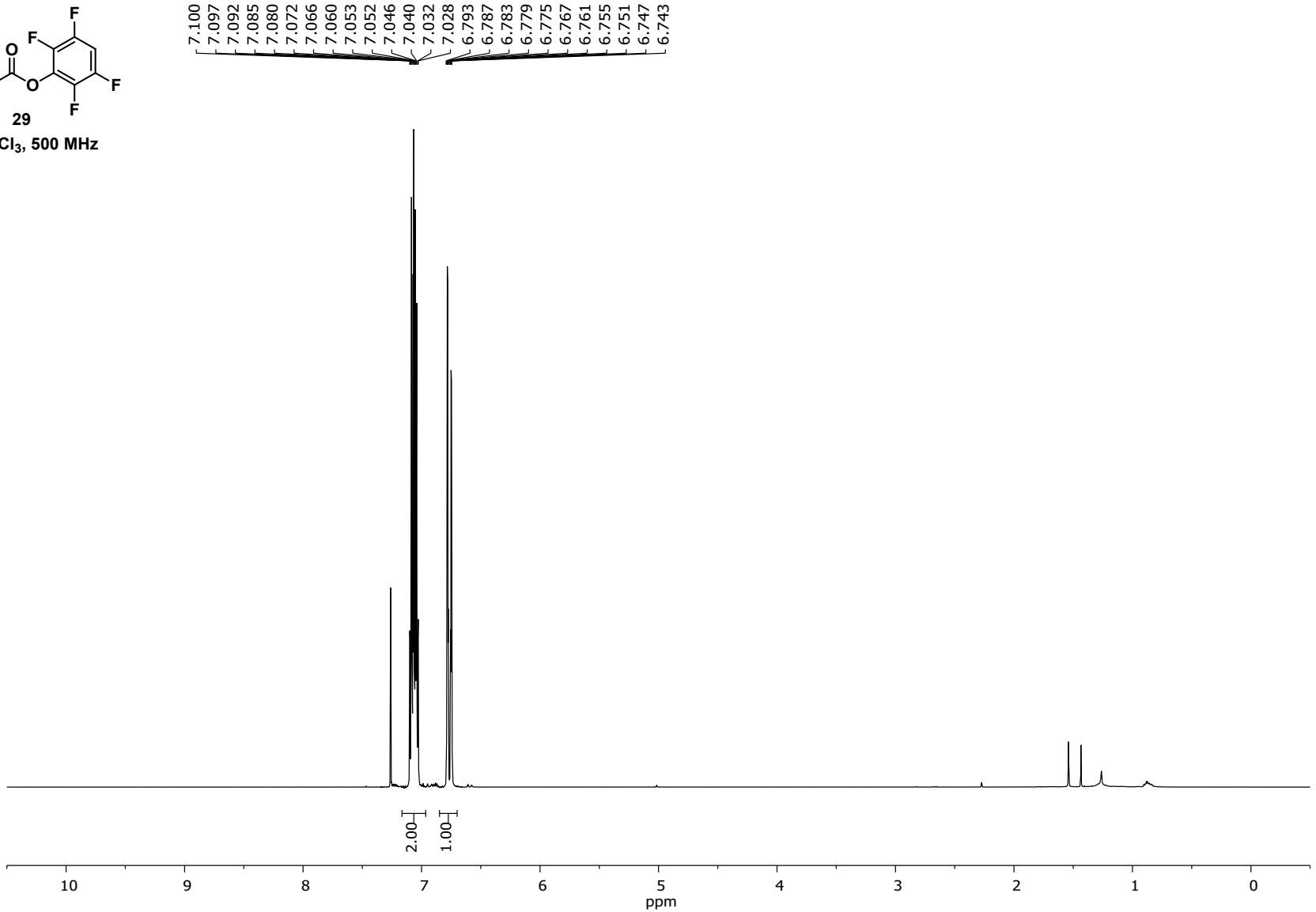
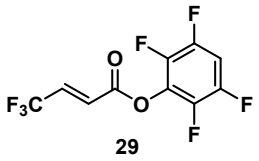
^{1}H, $CDCl_3$, 500 MHz





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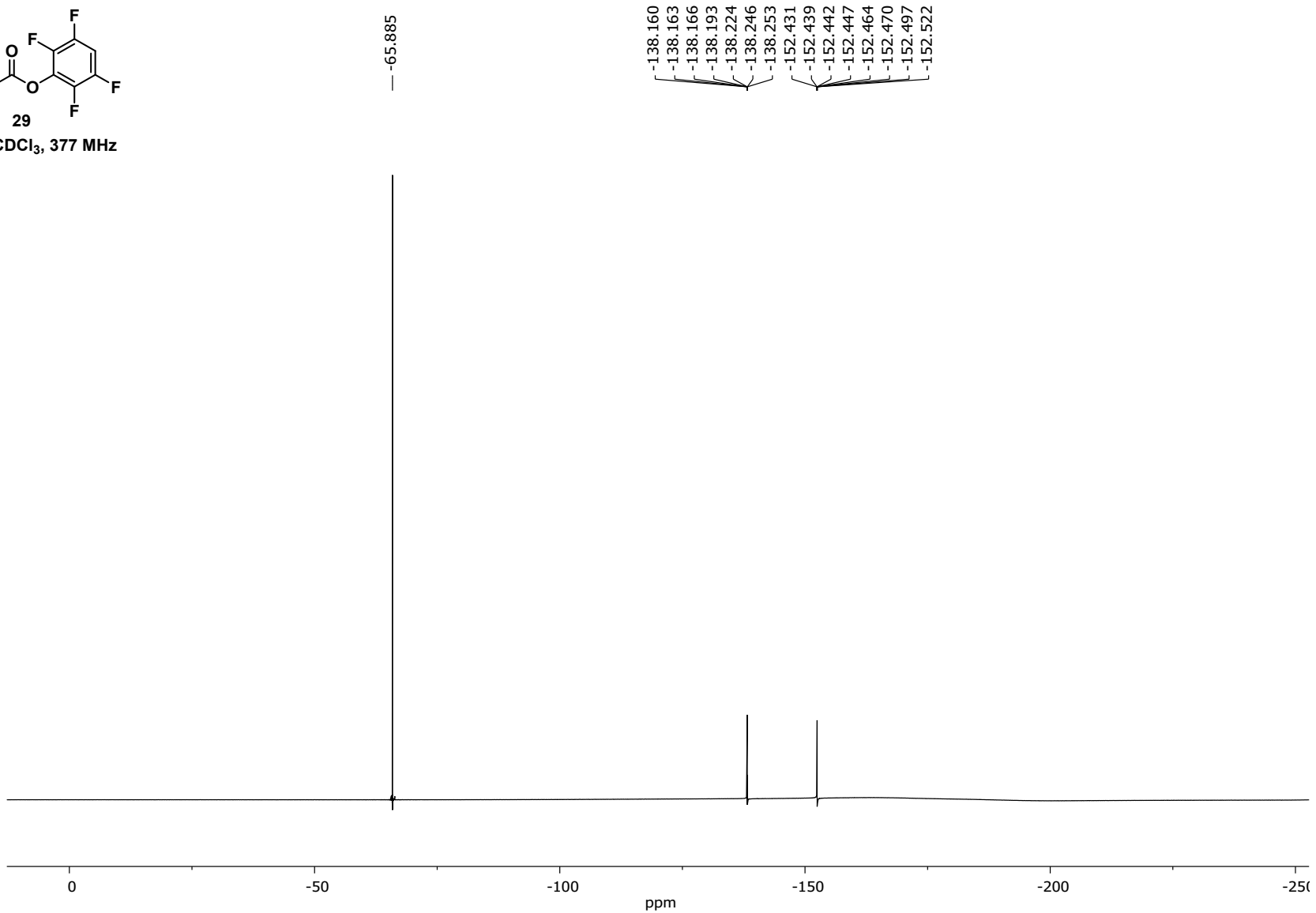
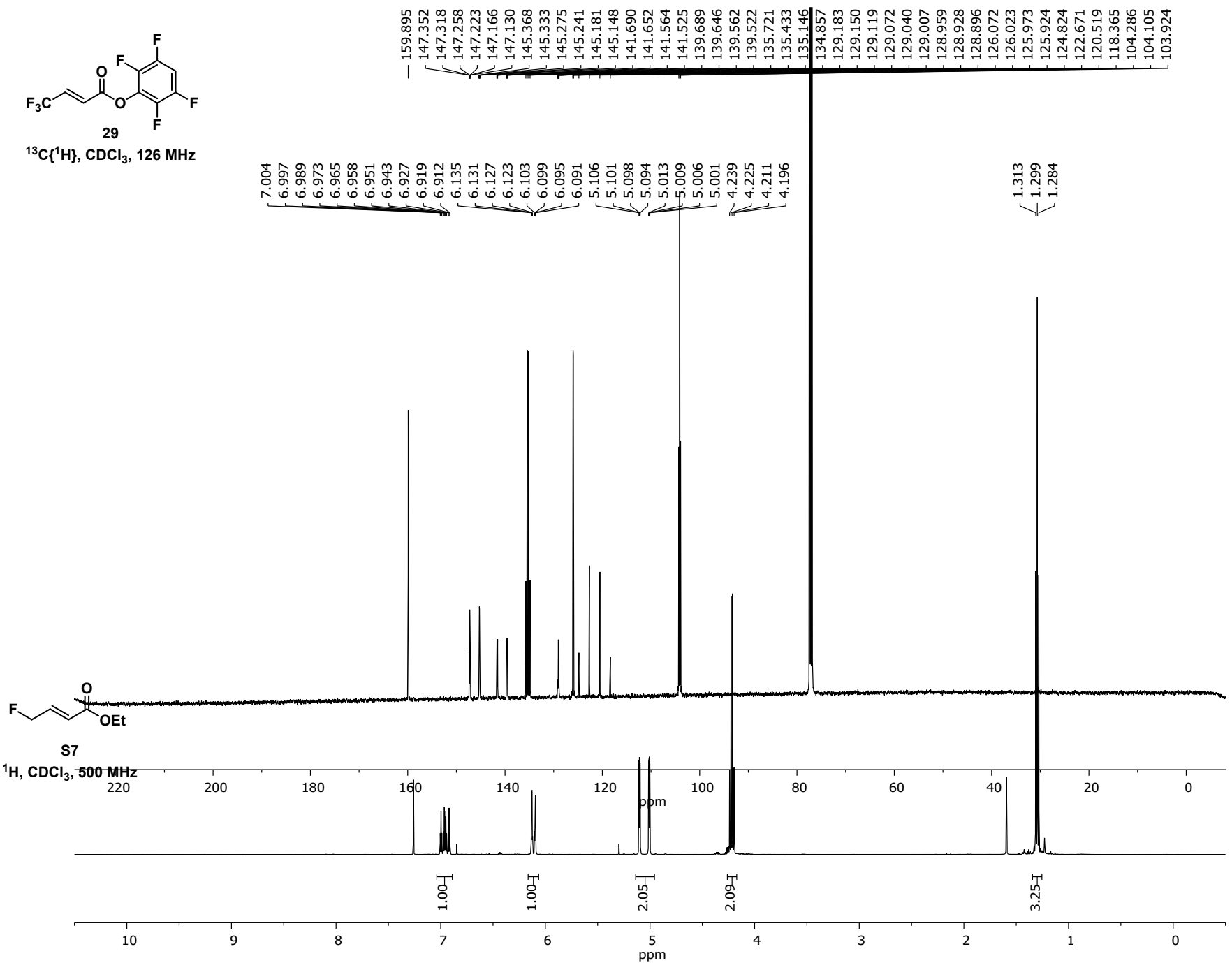
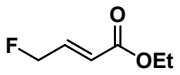
$^{19}F\{^{1}H\}$, $CDCl_3$, 377 MHz

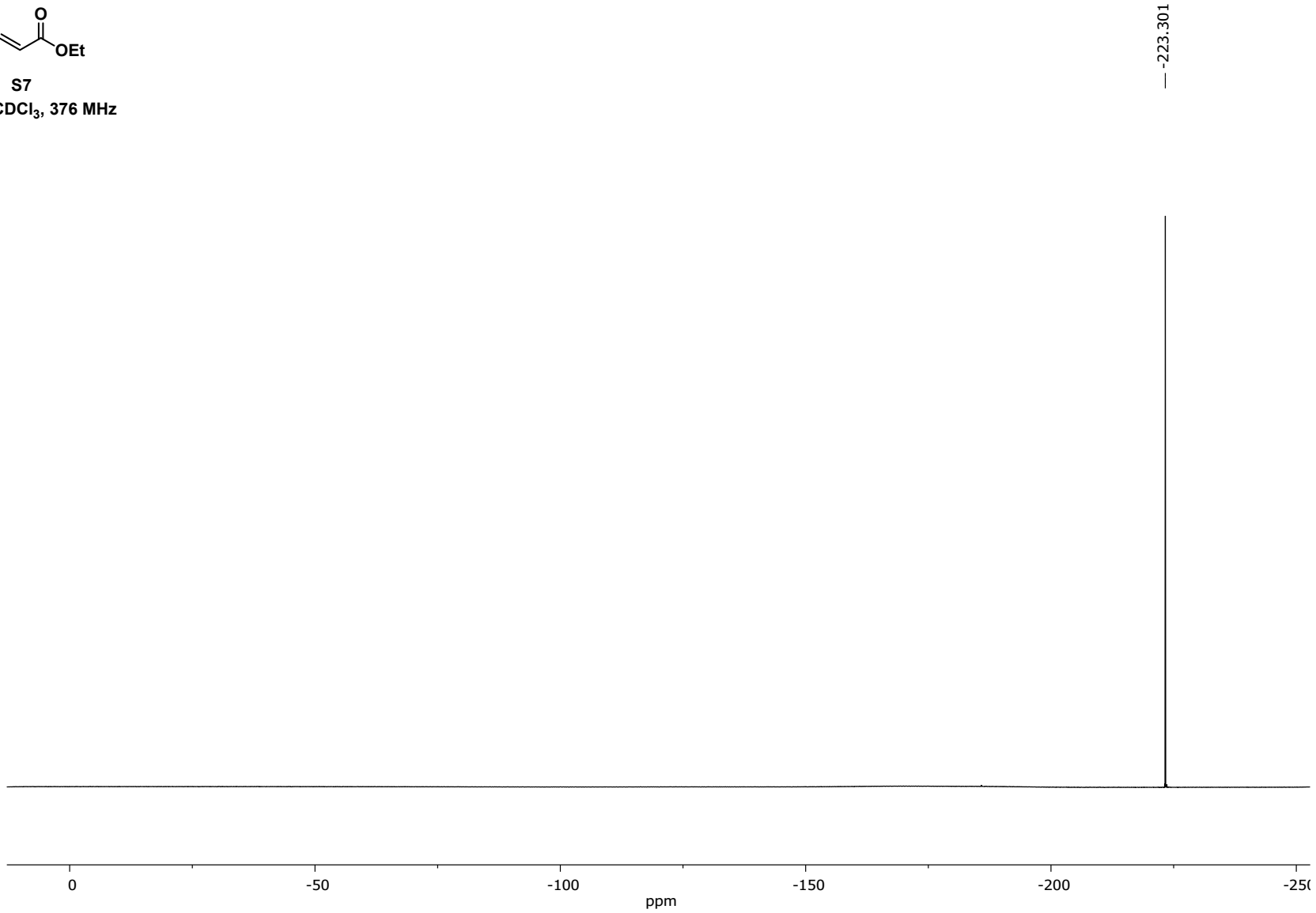


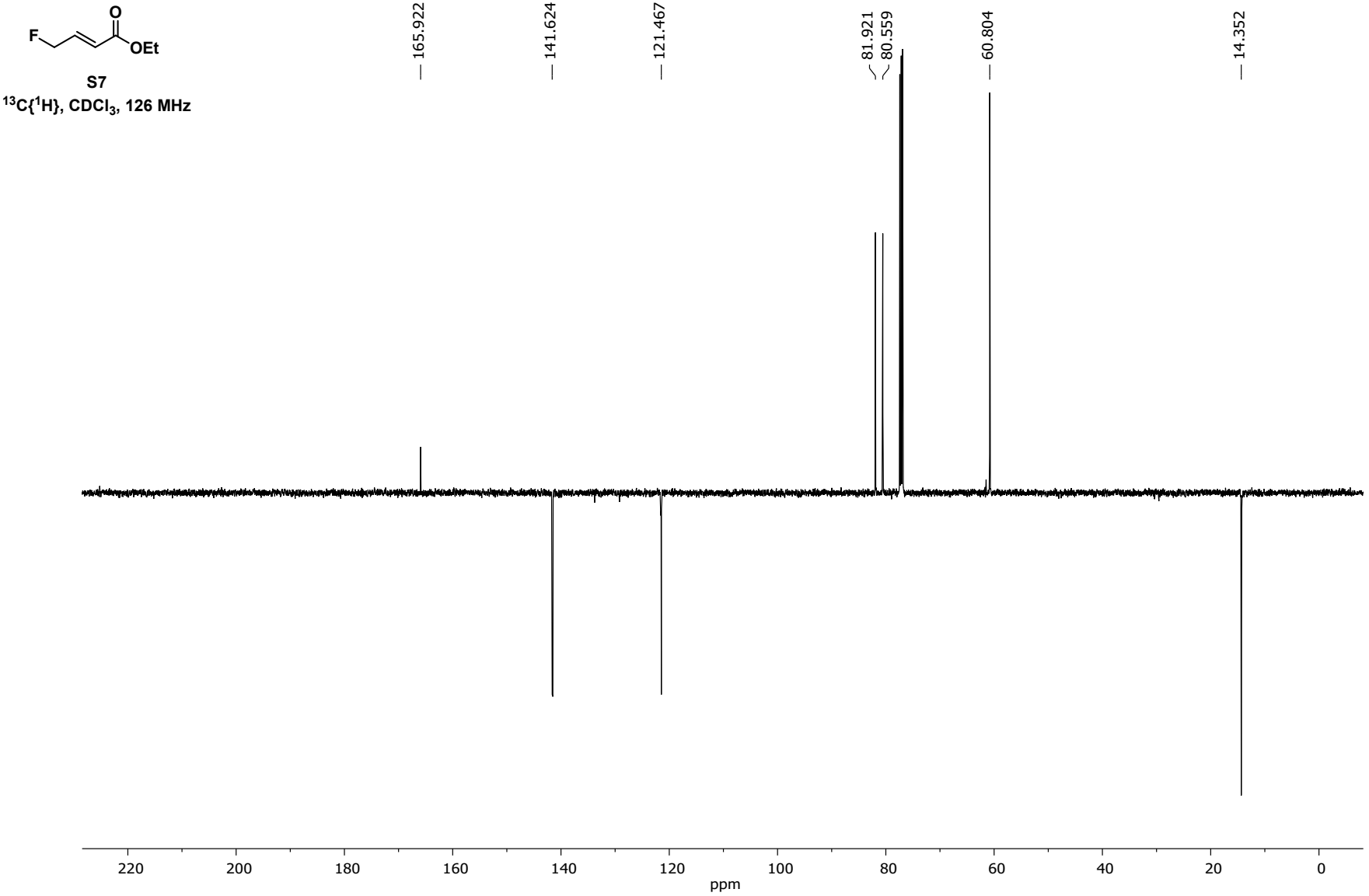

29
$^{13}C\{^{1}H\}$, $CDCl_3$, 126 MHz
159.895
147.352
147.318
147.258
147.223
147.166
147.130
145.368
145.333
145.275
145.241
145.181
145.148
141.690
141.652
141.564
141.525
139.689
139.646
139.562
139.522
135.721
135.433
135.146
134.857
129.183
129.150
129.119
129.072
129.040
129.007
128.959
128.928
128.896
126.072
126.023
125.973
125.924
124.824
122.671
120.519
118.365
104.286
104.105
103.924
7.004
6.997
6.989
6.973
6.965
6.958
6.951
6.943
6.927
6.919
6.912
6.135
6.131
6.127
6.123
6.103
6.099
6.095
6.091
5.106
5.101
5.098
5.094
5.013
5.009
5.006
5.001
4.239
4.225
4.211
4.196
1.313
1.299
1.284
S7
^{1}H, $CDCl_3$, 500 MHz
ppm
1.00
1.00
2.05
2.09
3.25
ppm

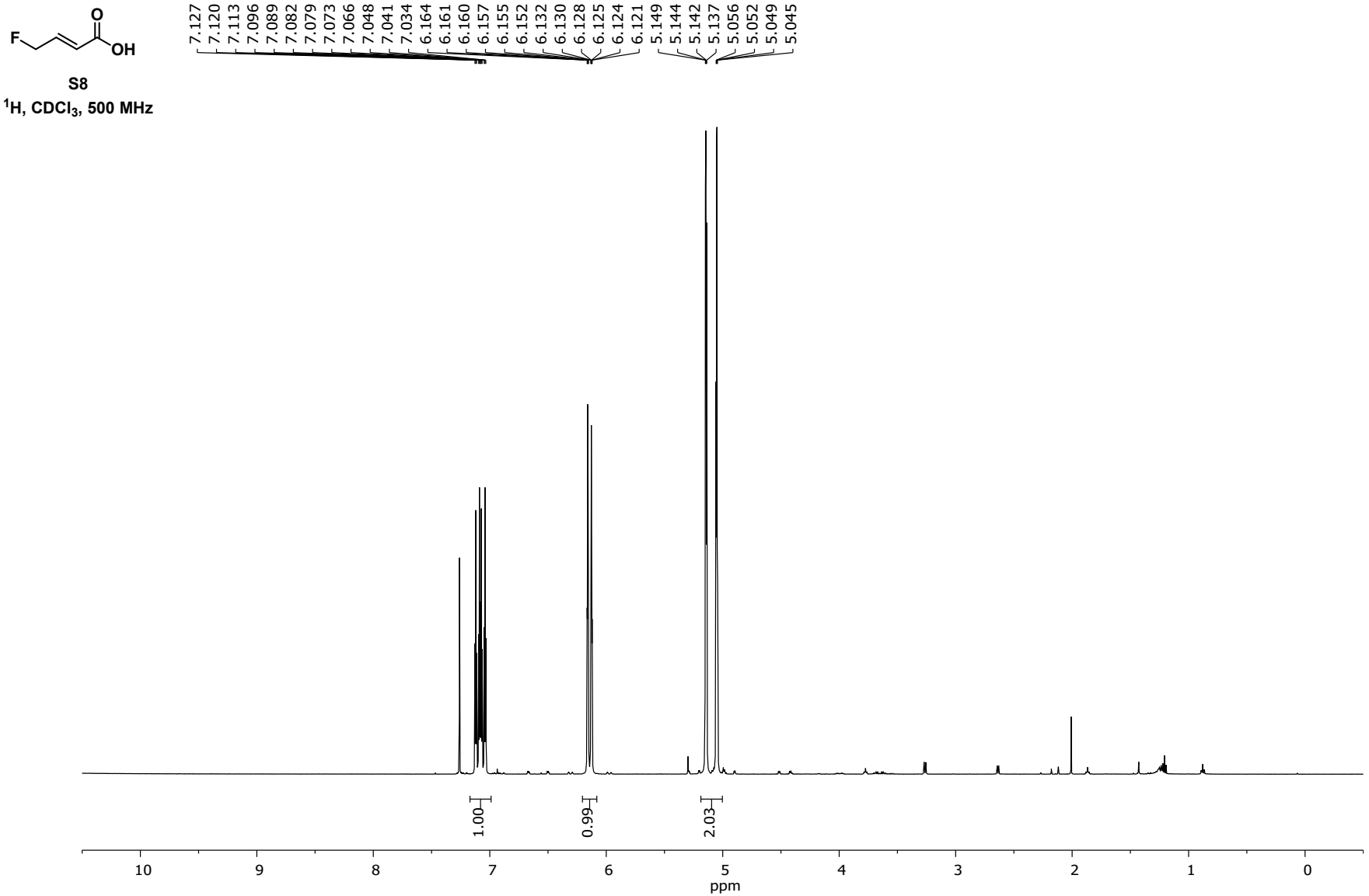


S7

$^{19}F\{^{1}H\}$, $CDCl_3$, 376 MHz

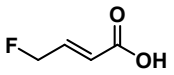



O
F
OEt
S7
13C{1H}, CDCl3, 126 MHz
165.922
141.624
121.467
81.921
80.559
60.804
14.352
220
200
180
160
140
120
100
80
60
40
20
0
ppm



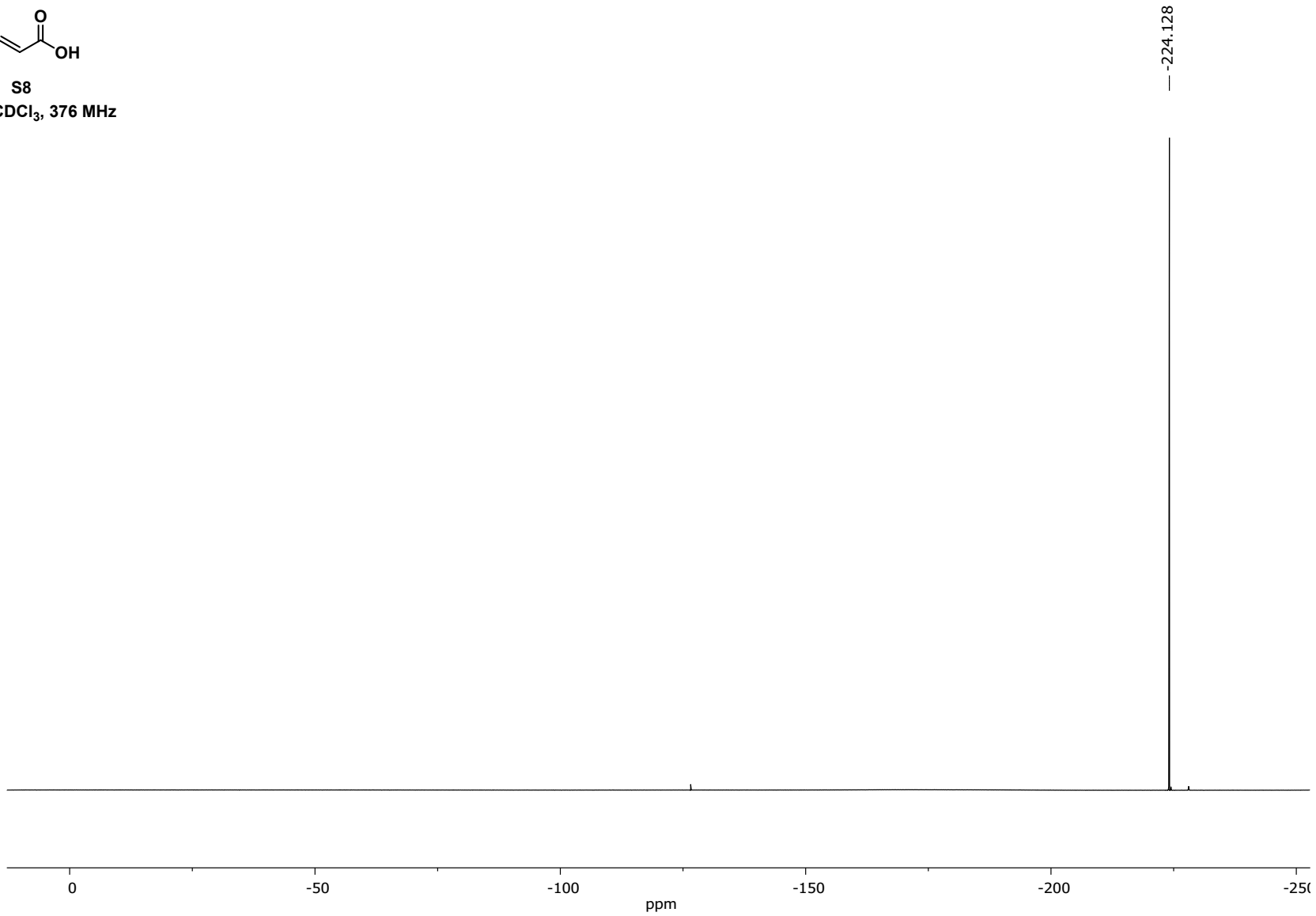
S8

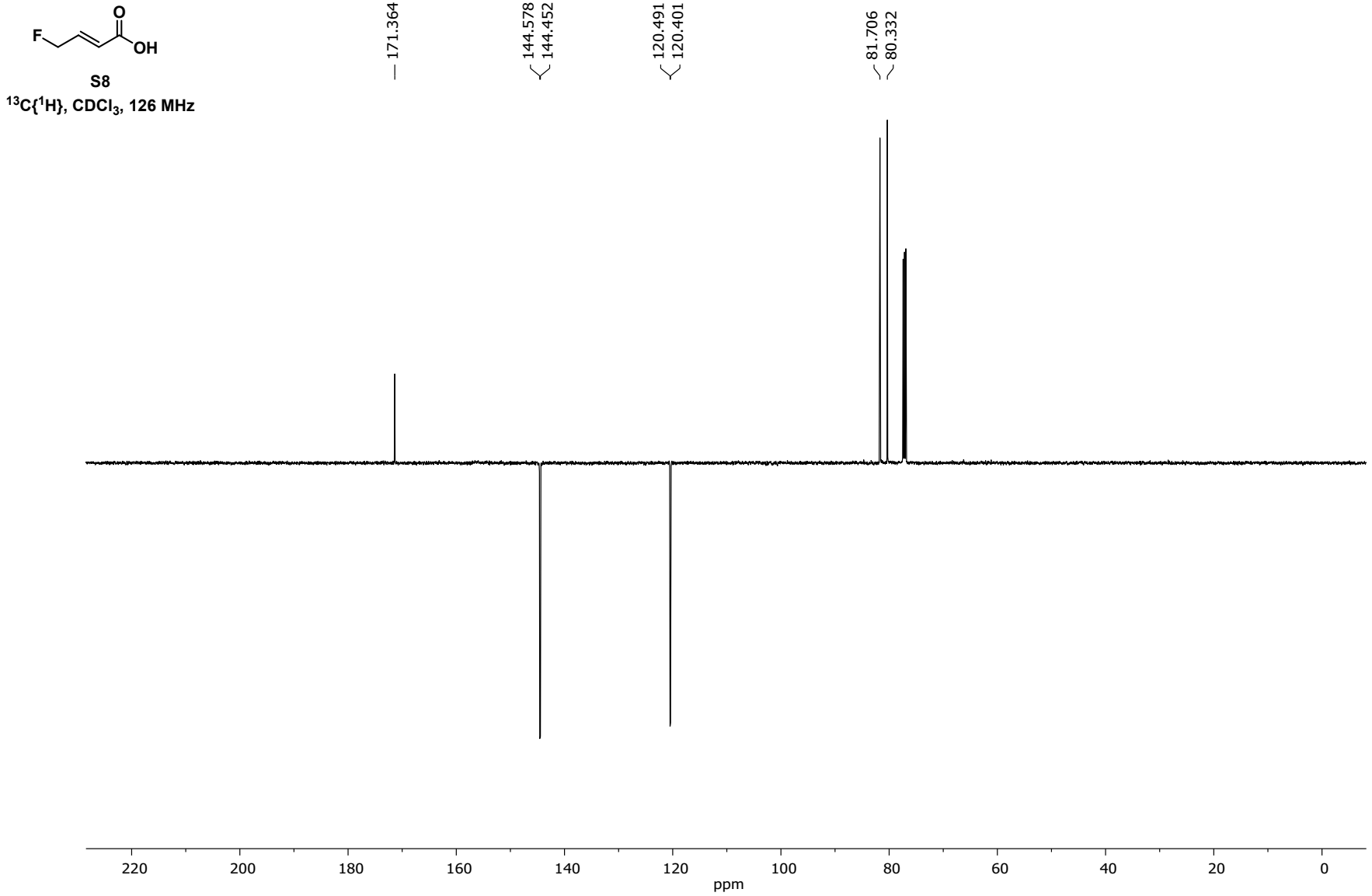
^{1}H, $CDCl_3$, 500 MHz

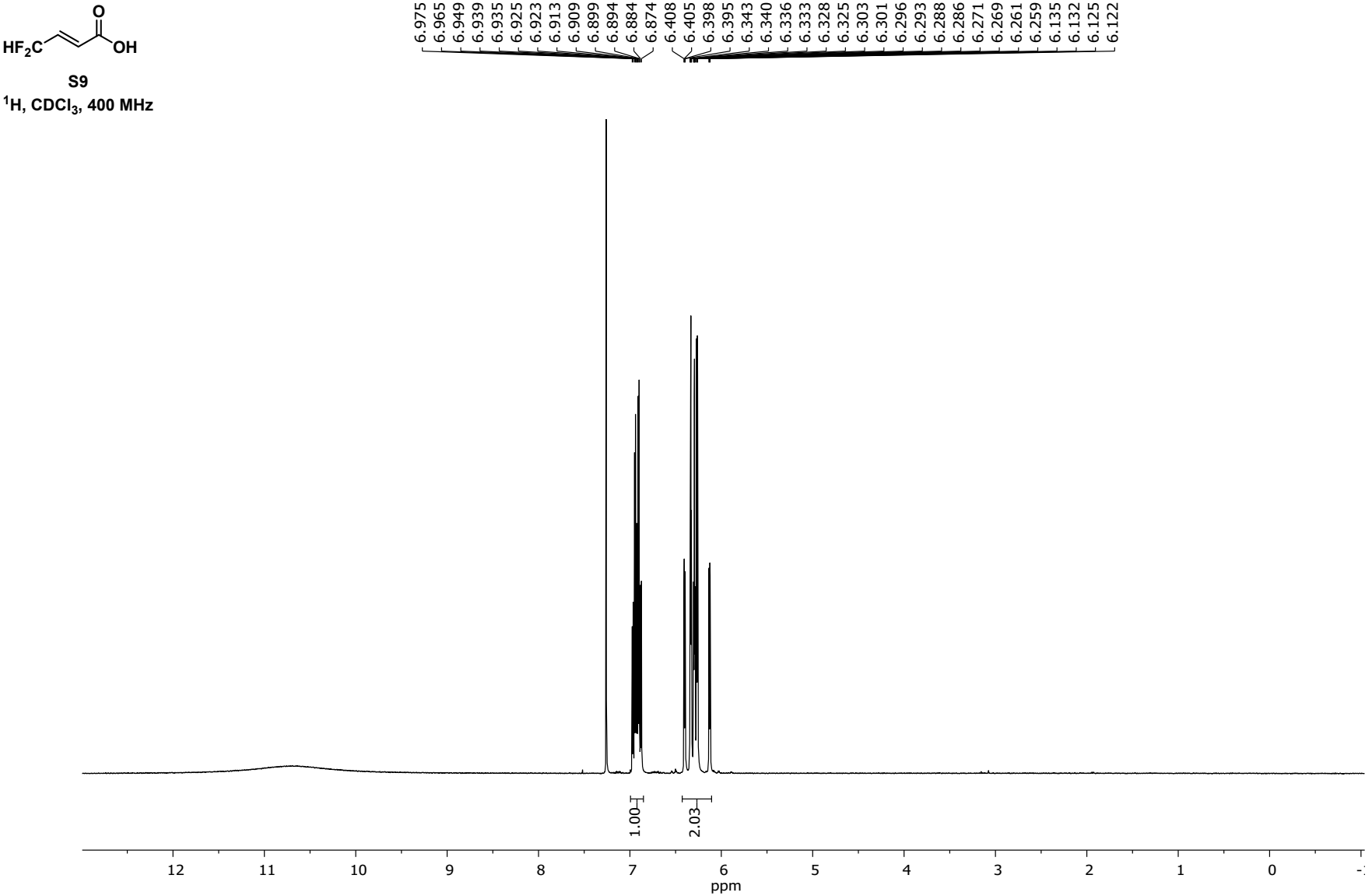


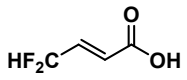
S8

$^{19}F\{^{1}H\}$, $CDCl_3$, 376 MHz



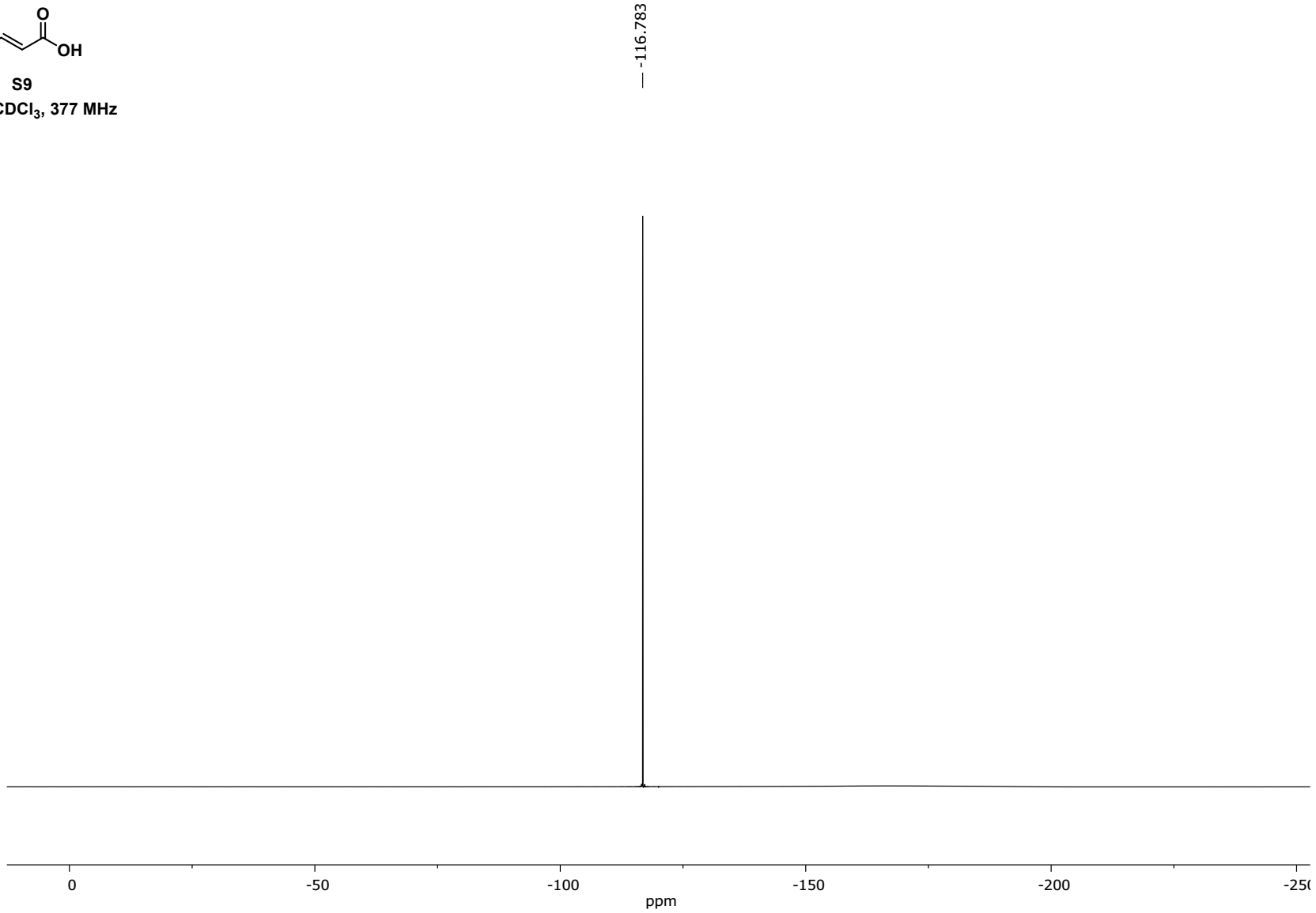

F
O
OH
S8
$^{13}C\{^{1}H\}$, $CDCl_3$, 126 MHz
171.364
144.578
144.452
120.491
120.401
81.706
80.332
220
200
180
160
140
120
100
80
60
40
20
0
ppm

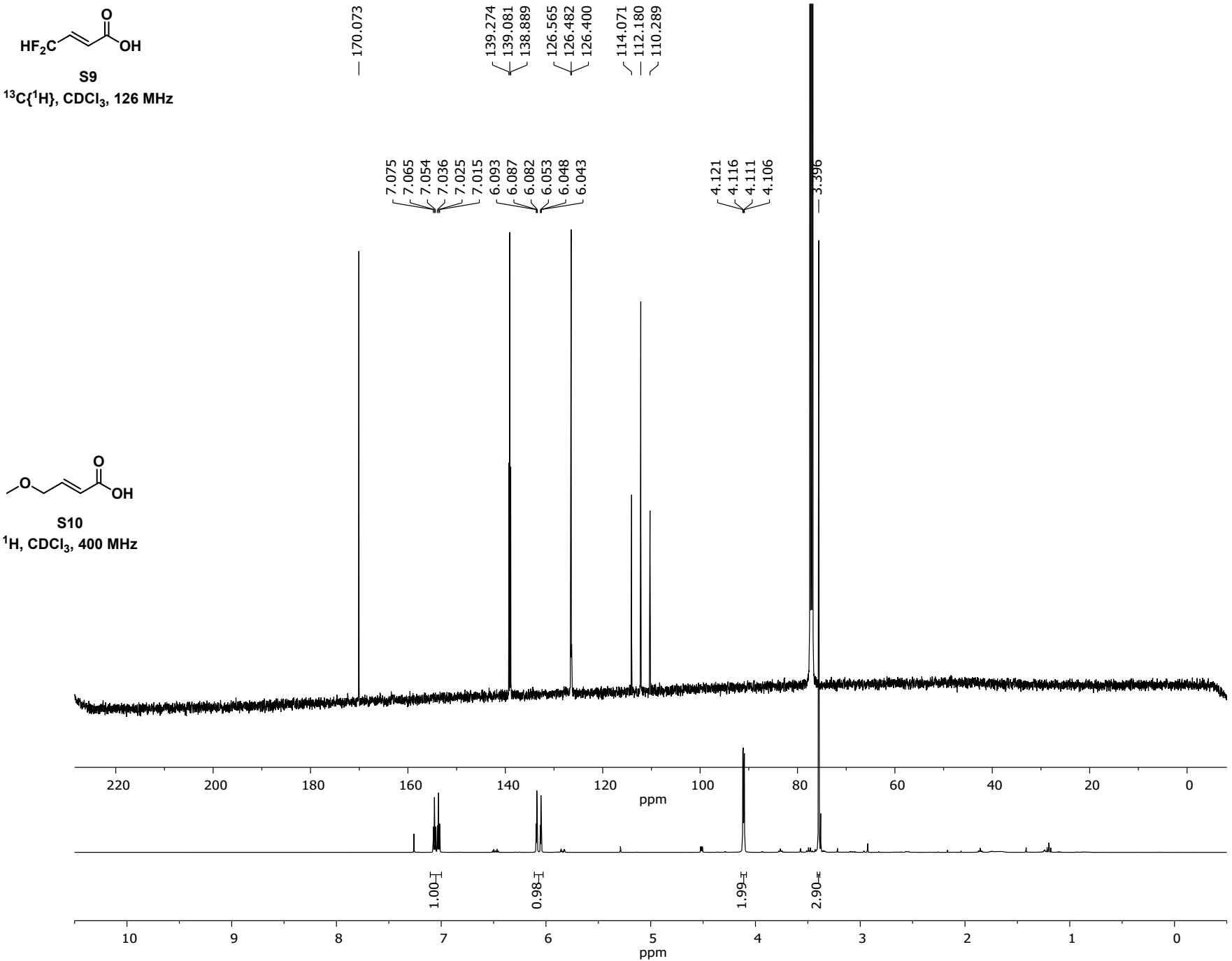

O
HF2C
OH
S9
1H, CDCl3, 400 MHz
6.975
6.965
6.949
6.939
6.935
6.925
6.923
6.913
6.909
6.899
6.894
6.884
6.874
6.408
6.405
6.398
6.395
6.343
6.340
6.336
6.333
6.328
6.325
6.303
6.301
6.296
6.293
6.288
6.286
6.271
6.269
6.261
6.259
6.135
6.132
6.125
6.122
1.00
2.03
12
11
10
9
8
7
6
5
4
3
2
1
0
ppm

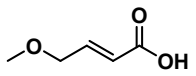


S9

$^{19}F\{^{1}H\}$, $CDCl_3$, 377 MHz

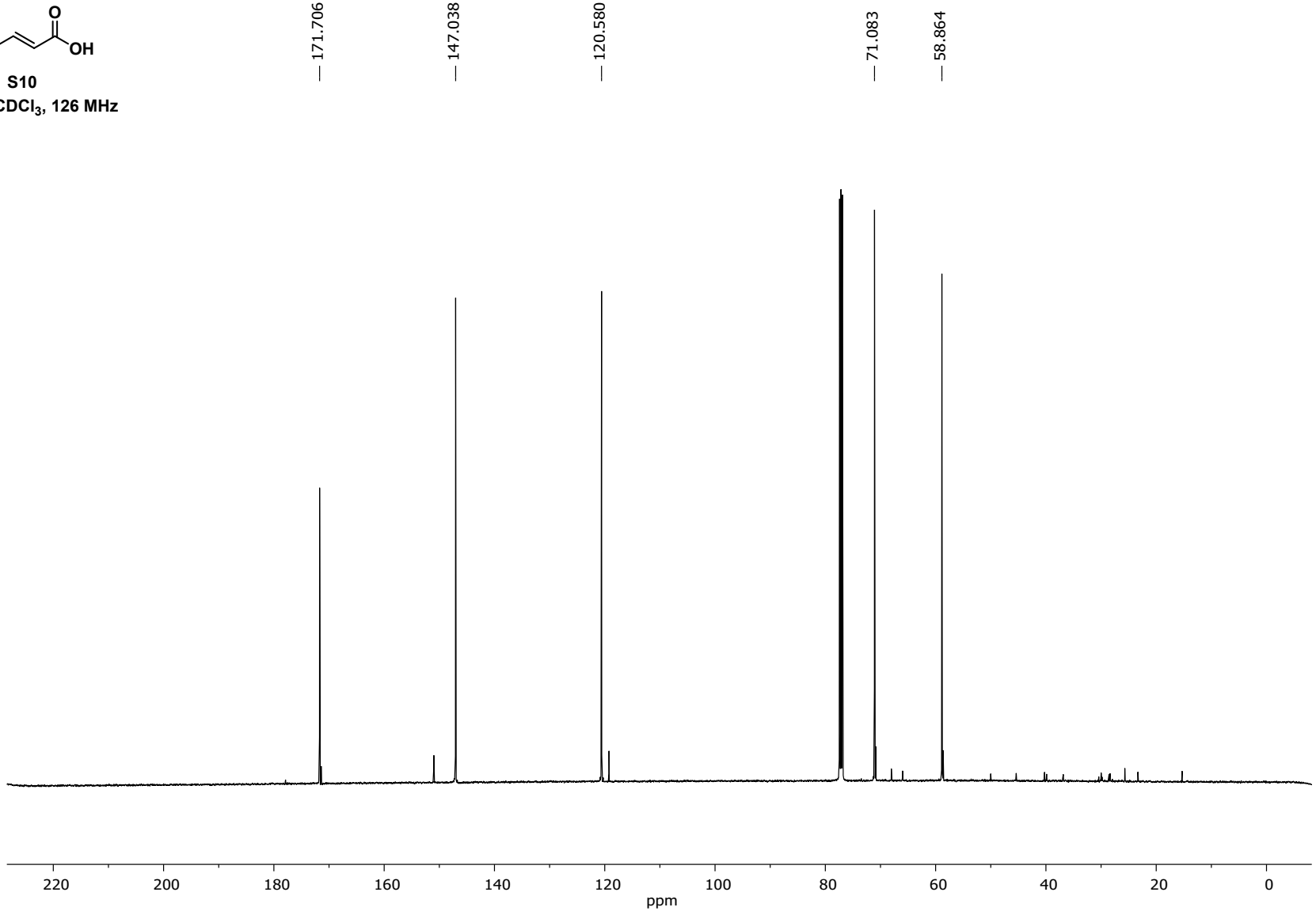


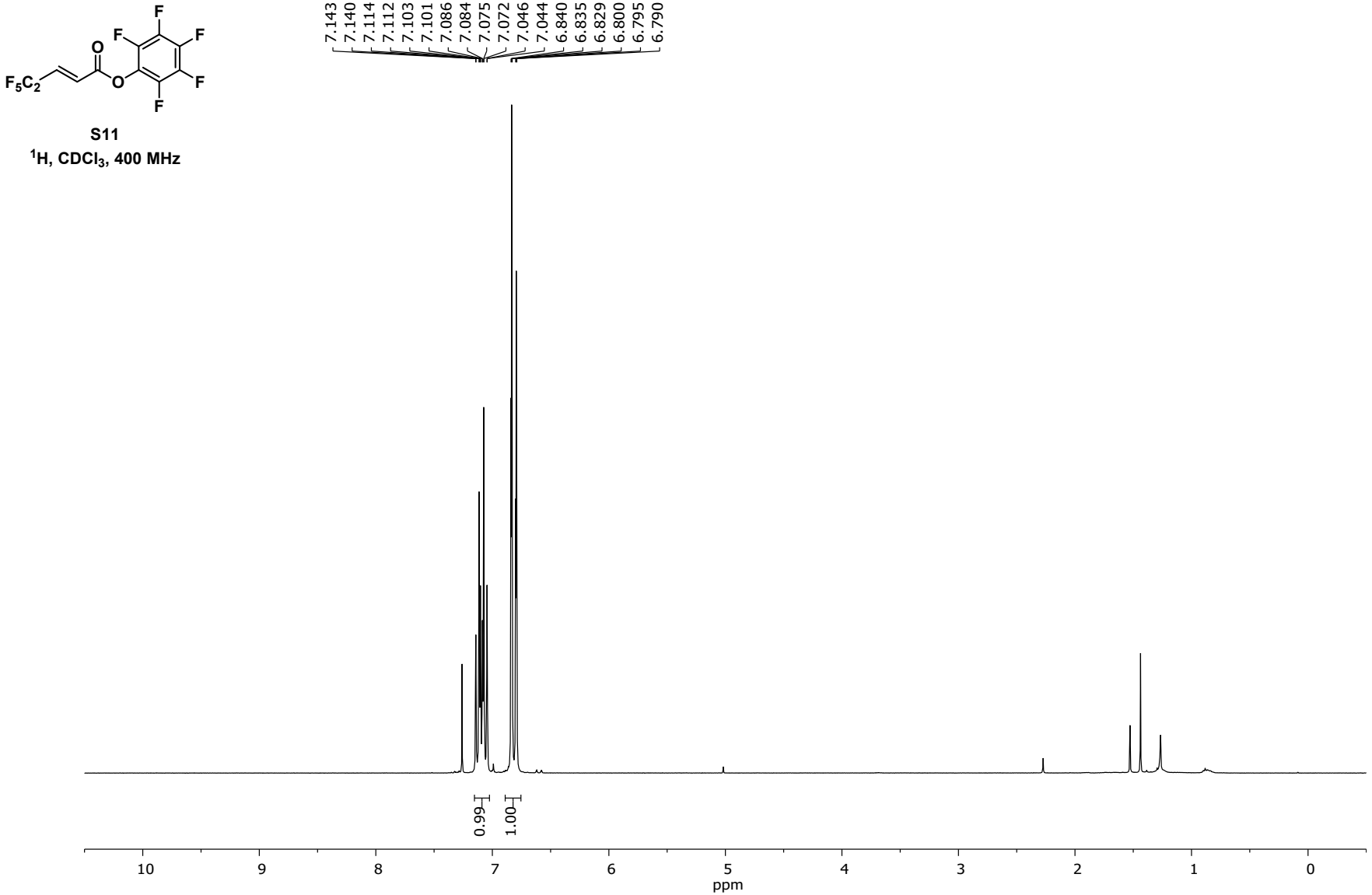

S9
13C{1H}, CDCl3, 126 MHz
170.073
139.274
139.081
138.889
126.565
126.482
126.400
114.071
112.180
110.289
7.075
7.065
7.054
7.036
7.025
7.015
6.093
6.087
6.082
6.053
6.048
6.043
4.121
4.116
4.111
4.106
3.396
S10
1H, CDCl3, 400 MHz
ppm
1.00
0.98
1.99
2.90
ppm

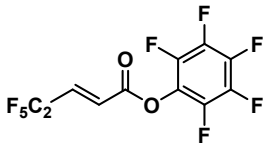


S10

$^{13}C\{^{1}H\}$, $CDCl_3$, 126 MHz

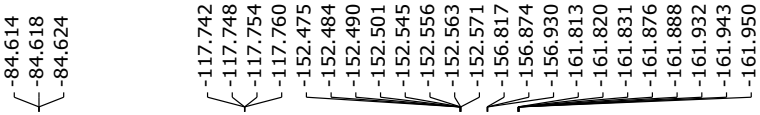


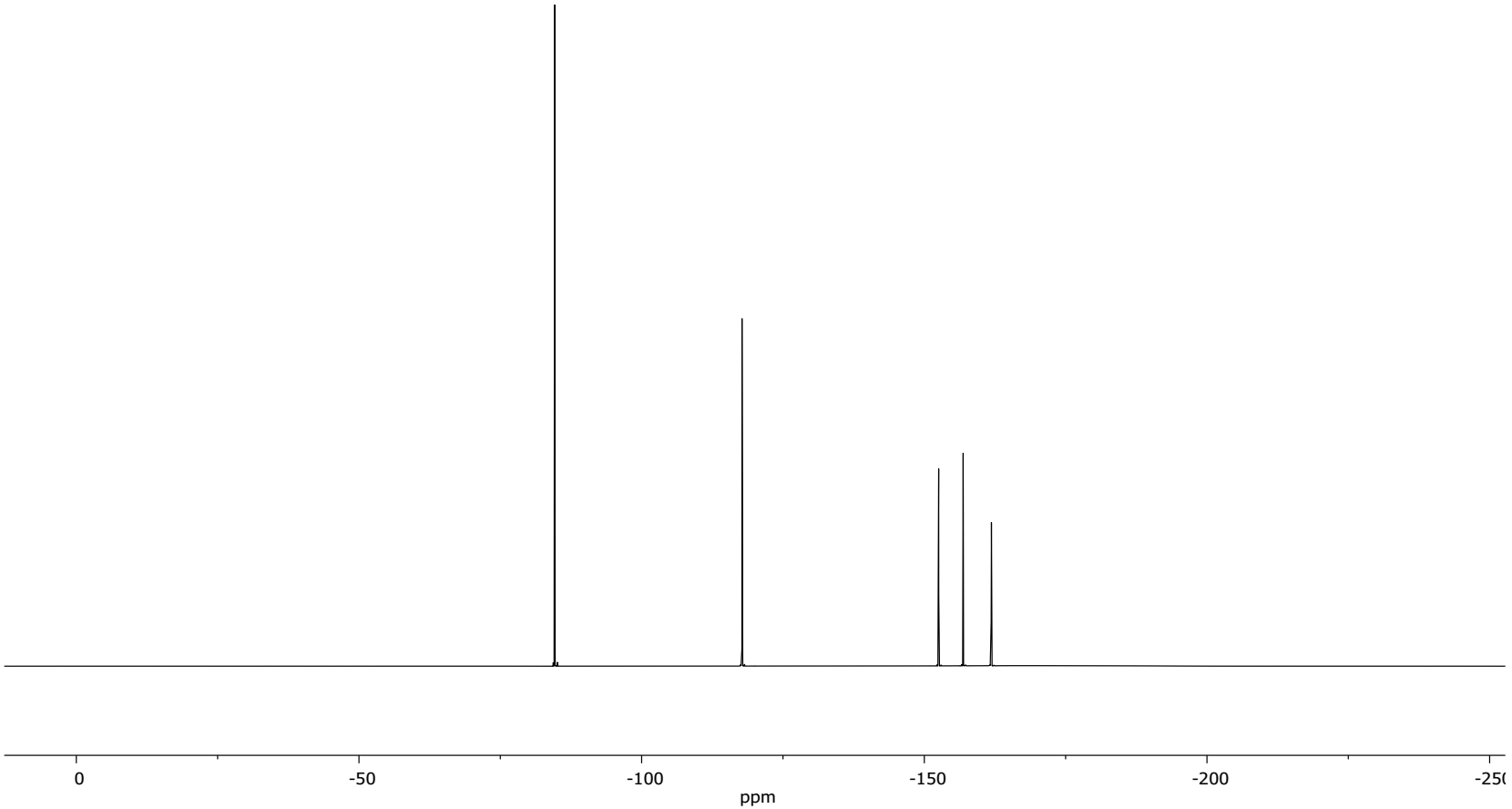

F
F
F
F
O
O
F
F5C2
S11
1H, CDCl3, 400 MHz
7.143
7.140
7.114
7.112
7.103
7.101
7.086
7.084
7.075
7.072
7.046
7.044
6.840
6.835
6.829
6.800
6.795
6.790
0.99
1.00
10
9
8
7
6
5
4
3
2
1
0
ppm

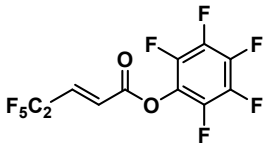


S11

$^{19}F\{^{1}H\}$, $CDCl_3$, 377 MHz

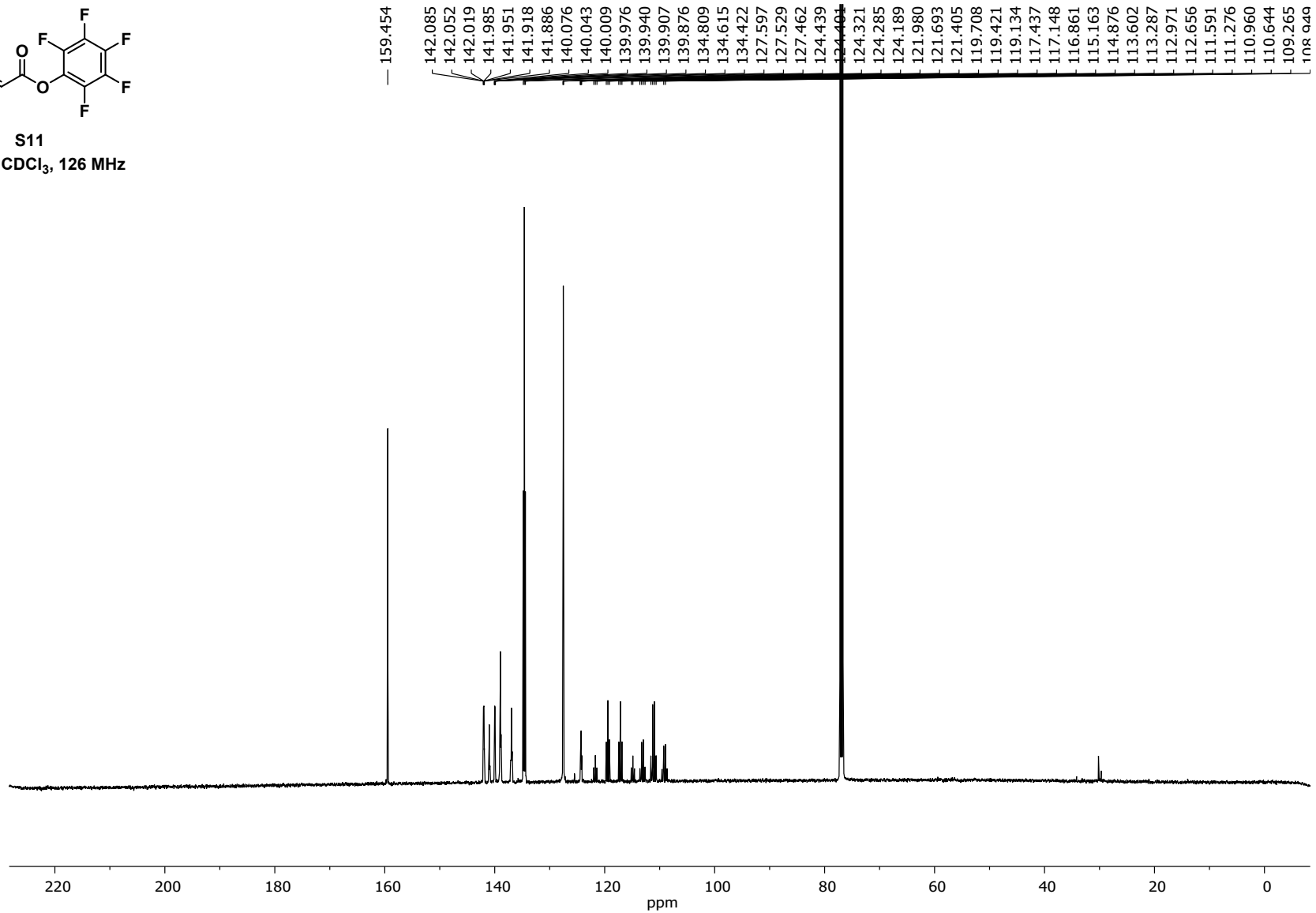


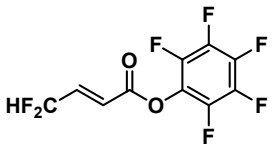




S11

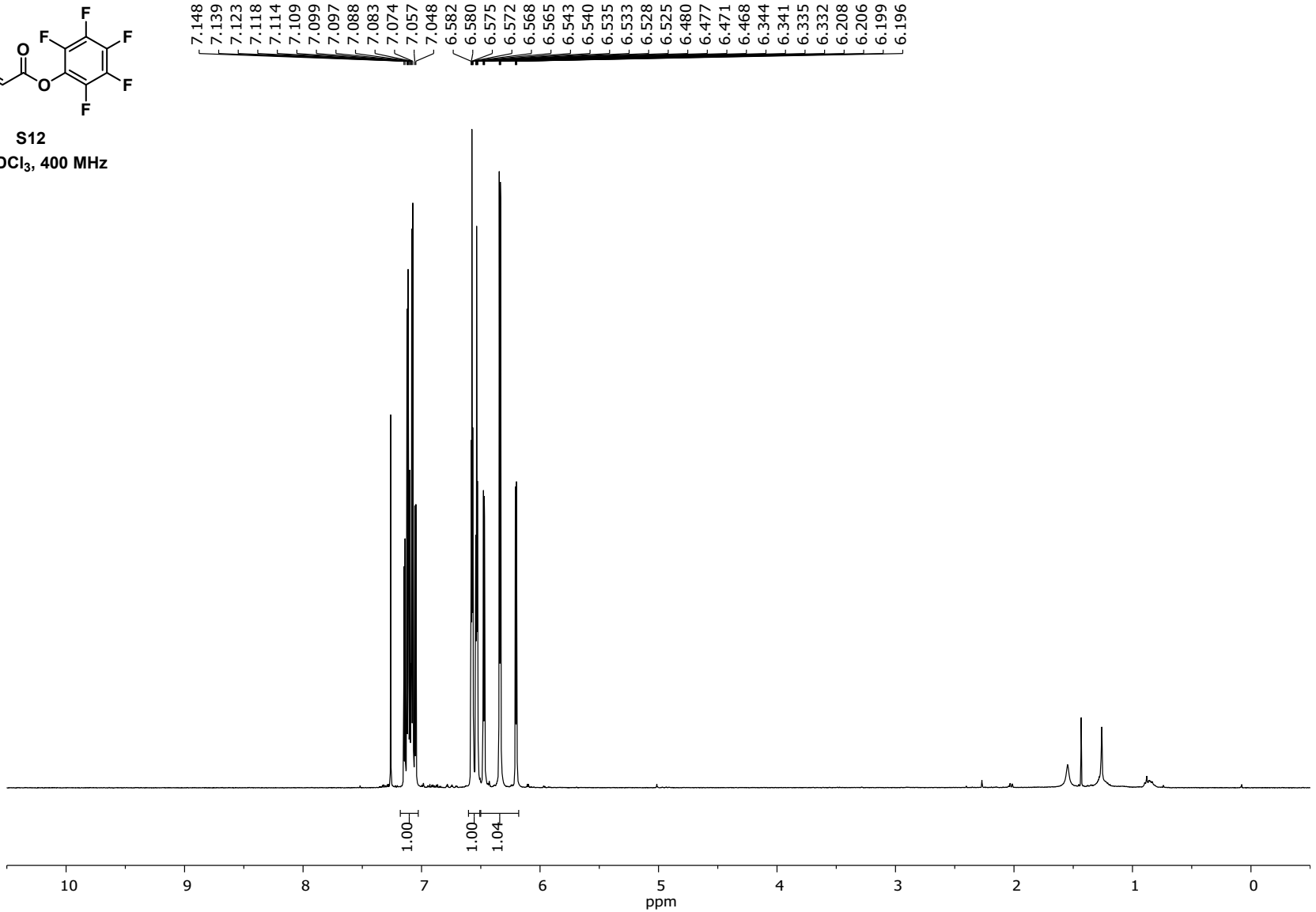
$^{13}C\{^{1}H\}$, $CDCl_3$, 126 MHz

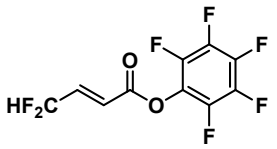




S12

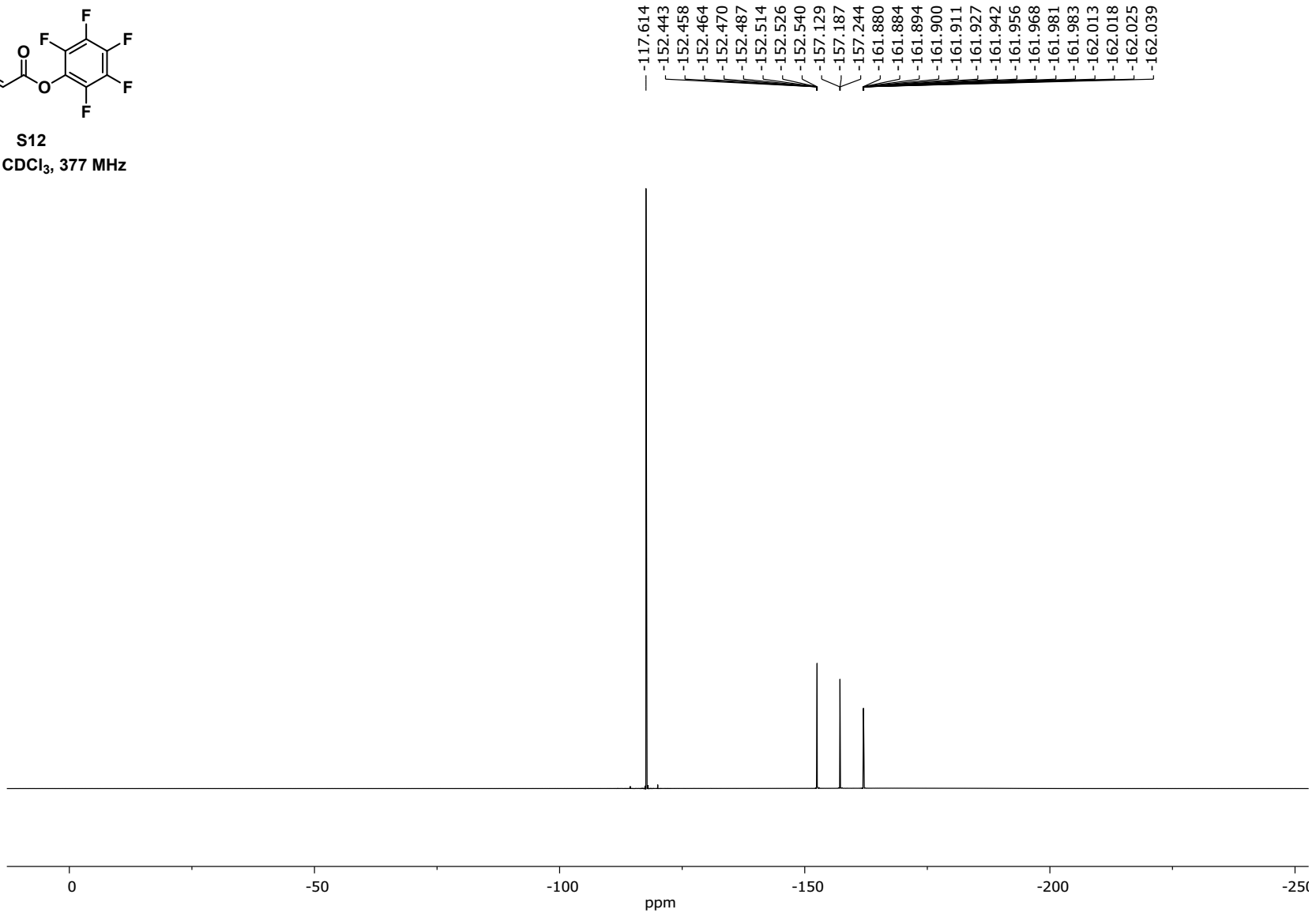
^{1}H, $CDCl_3$, 400 MHz

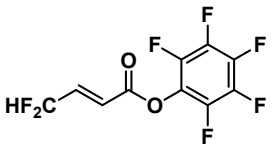




S12

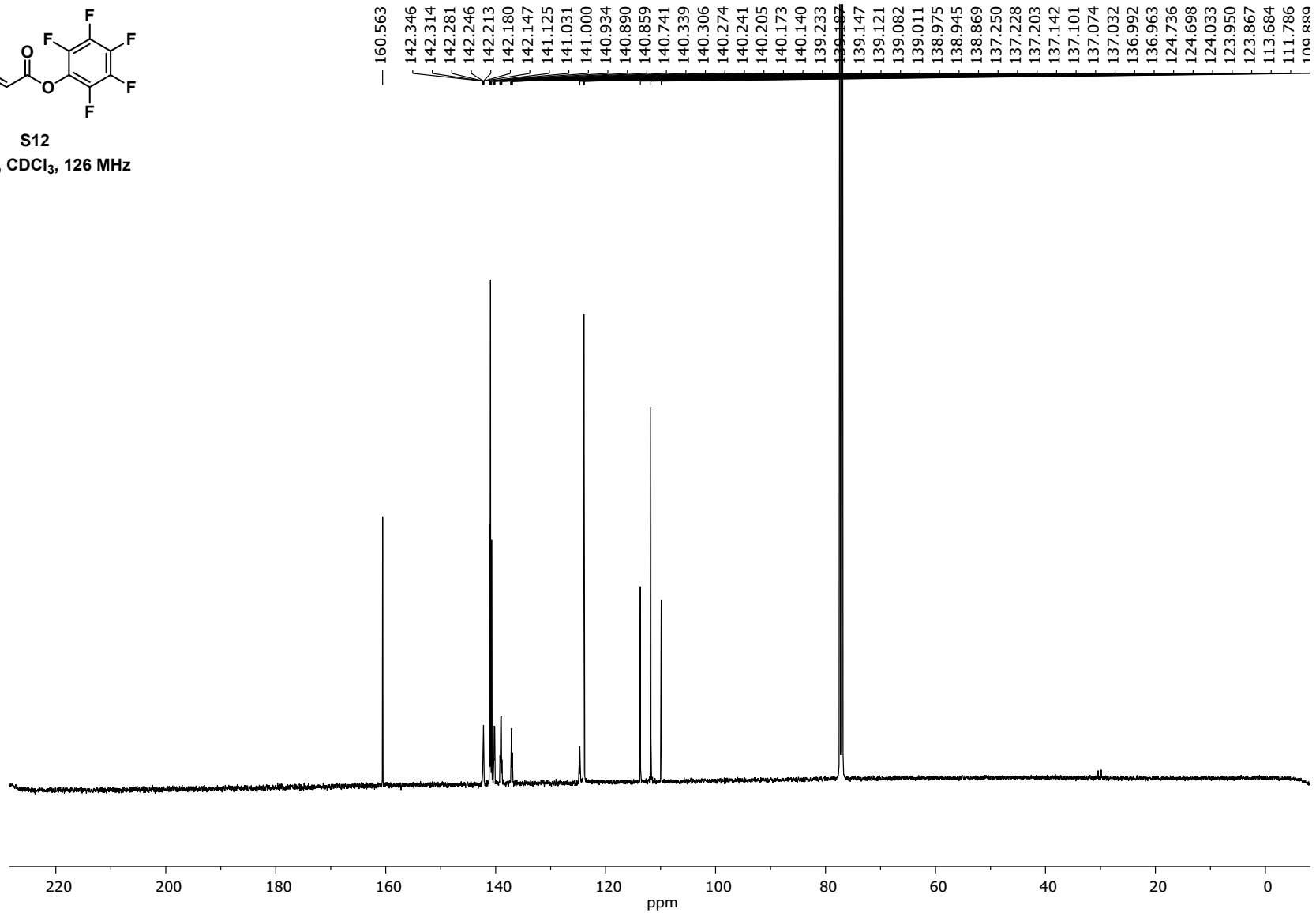
$^{19}F\{^{1}H\}$, $CDCl_3$, 377 MHz

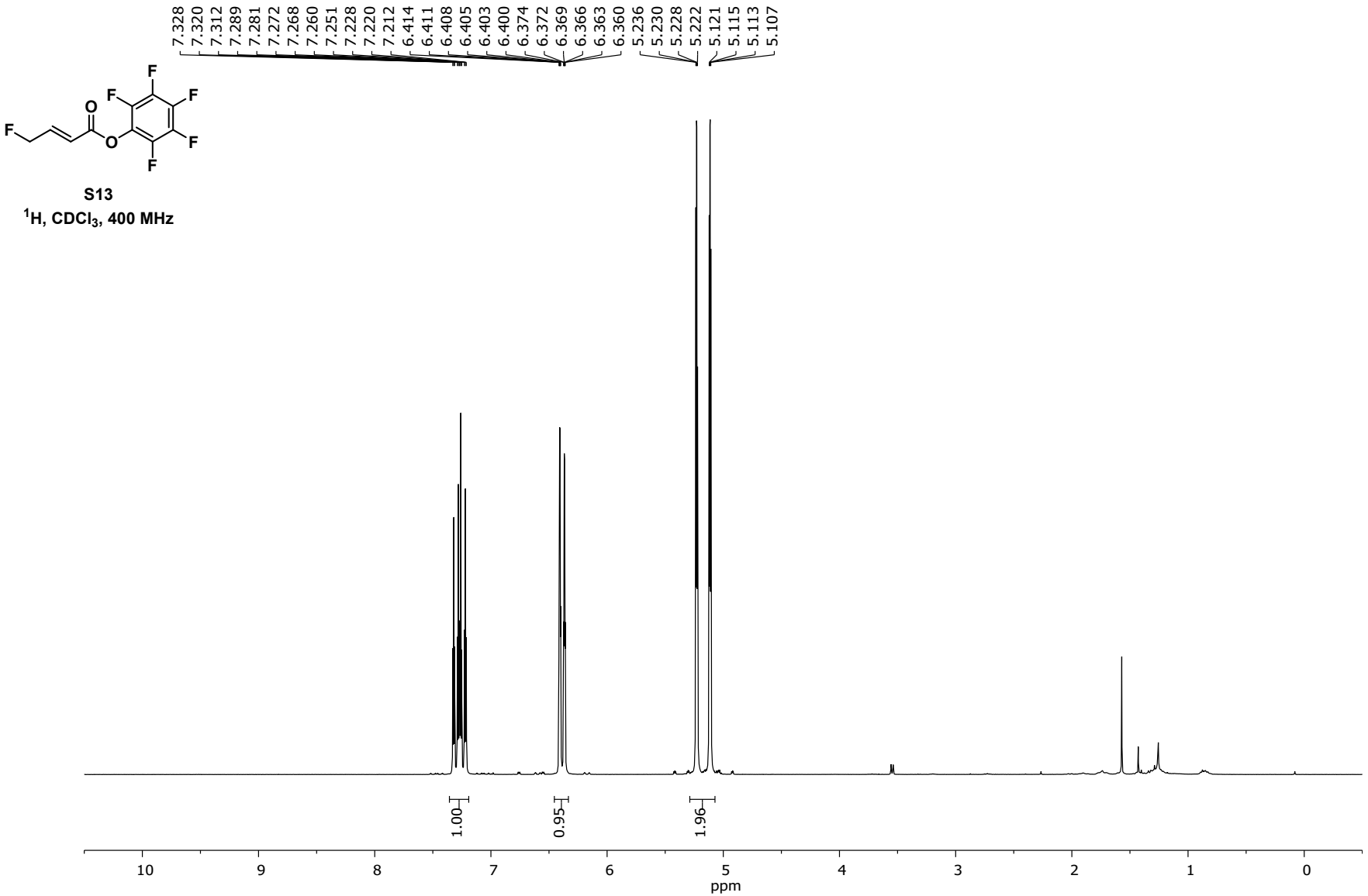




S12

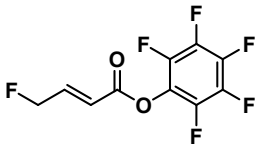
$^{13}C\{^{1}H\}$, $CDCl_3$, 126 MHz





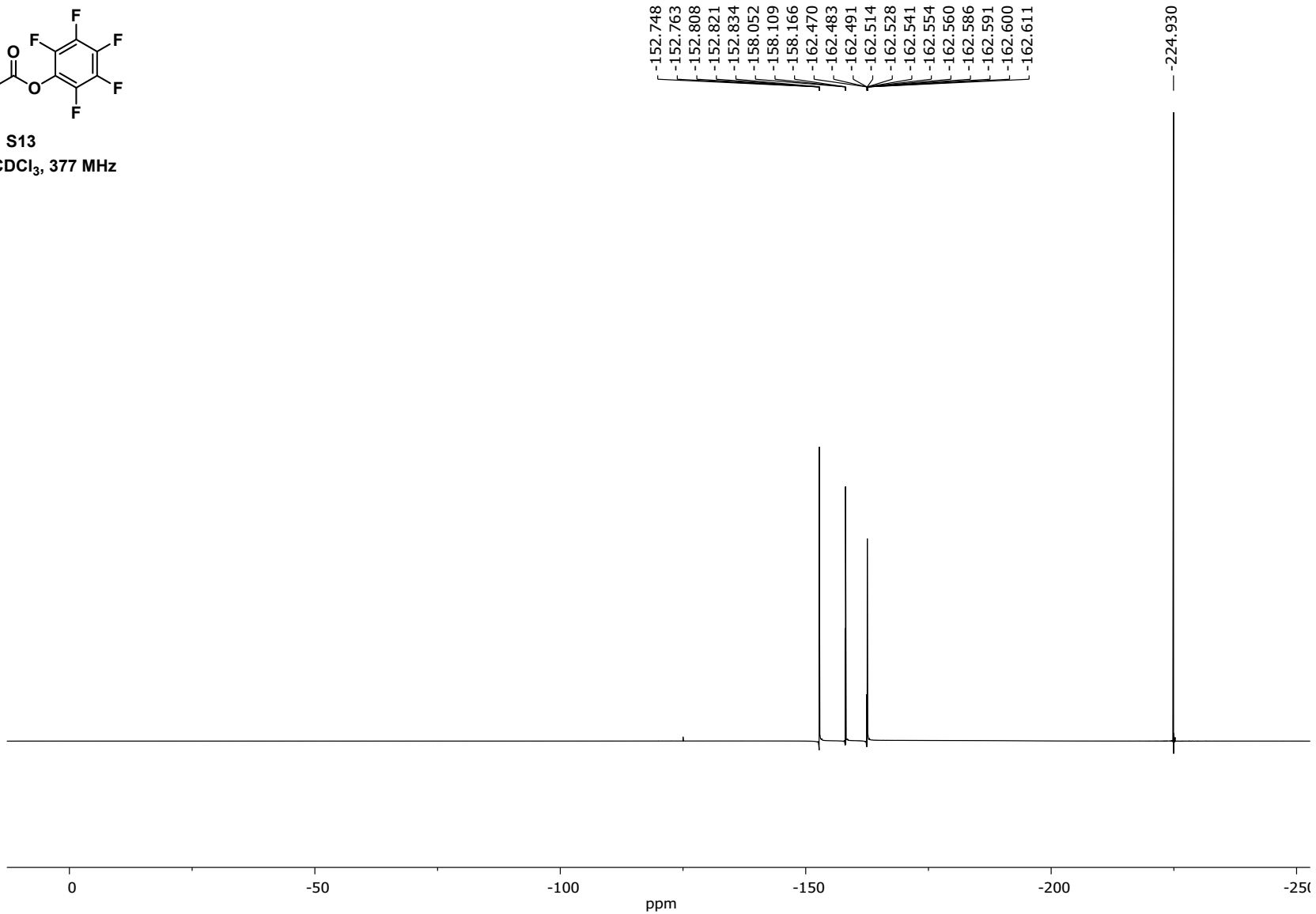
S13

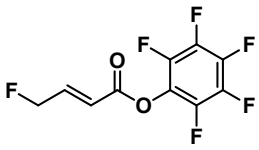
^{1}H, $CDCl_3$, 400 MHz



S13

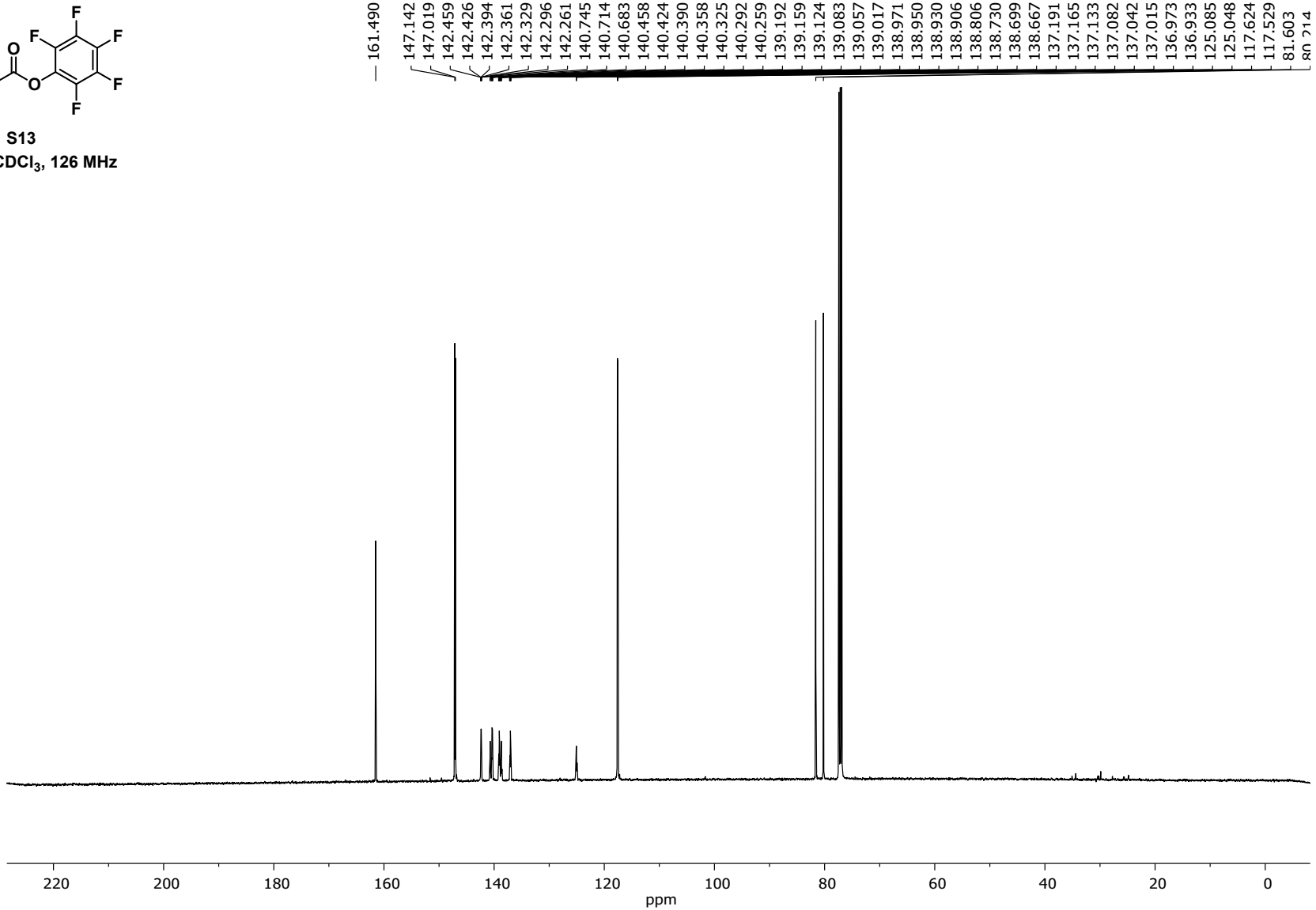
$^{19}F\{^{1}H\}$, $CDCl_3$, 377 MHz

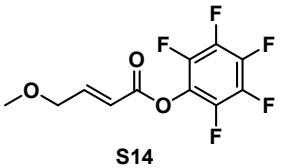




S13

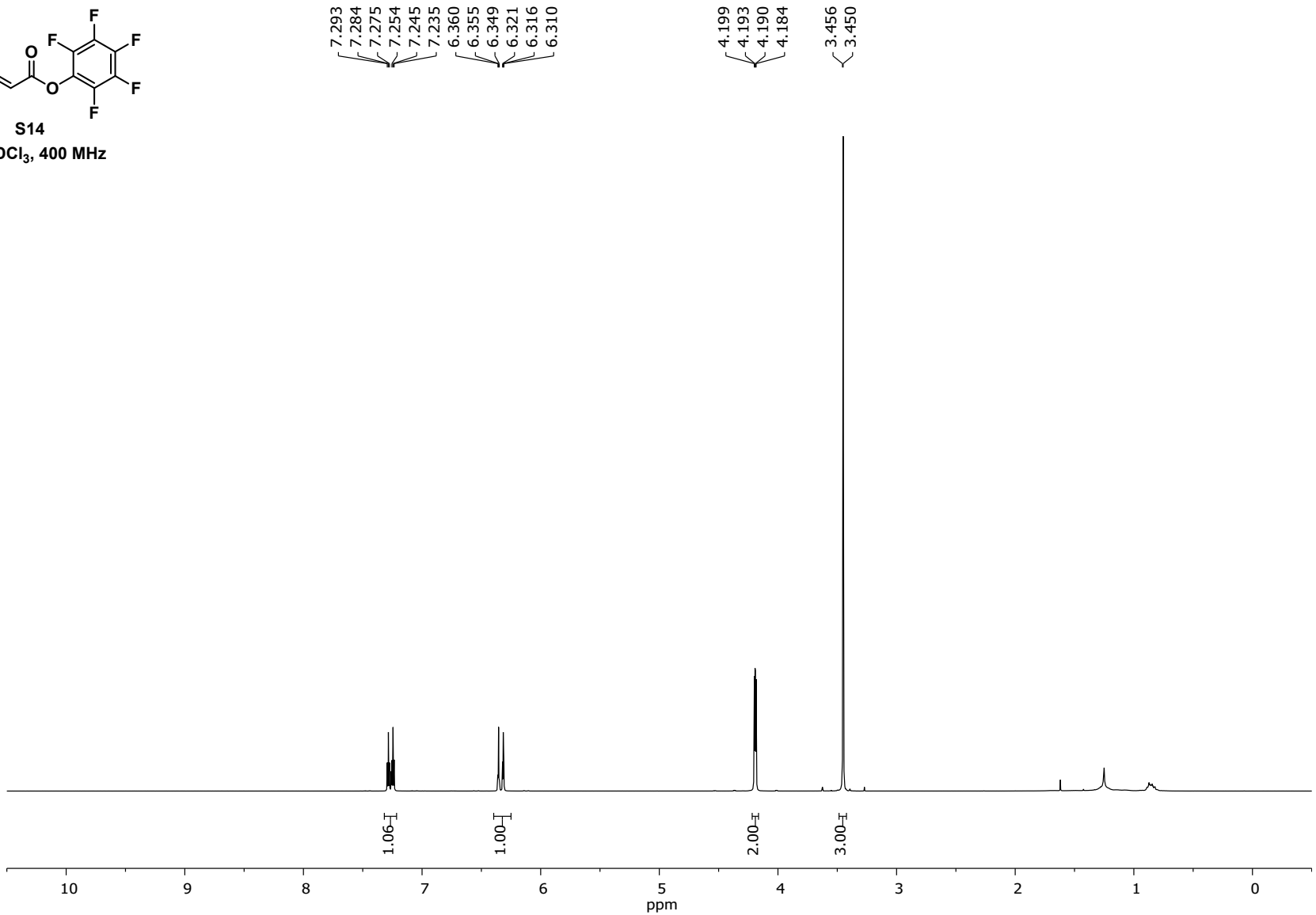
$^{13}C\{^{1}H\}$, $CDCl_3$, 126 MHz

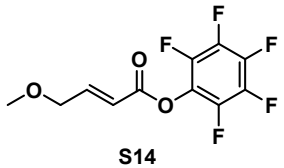




S14

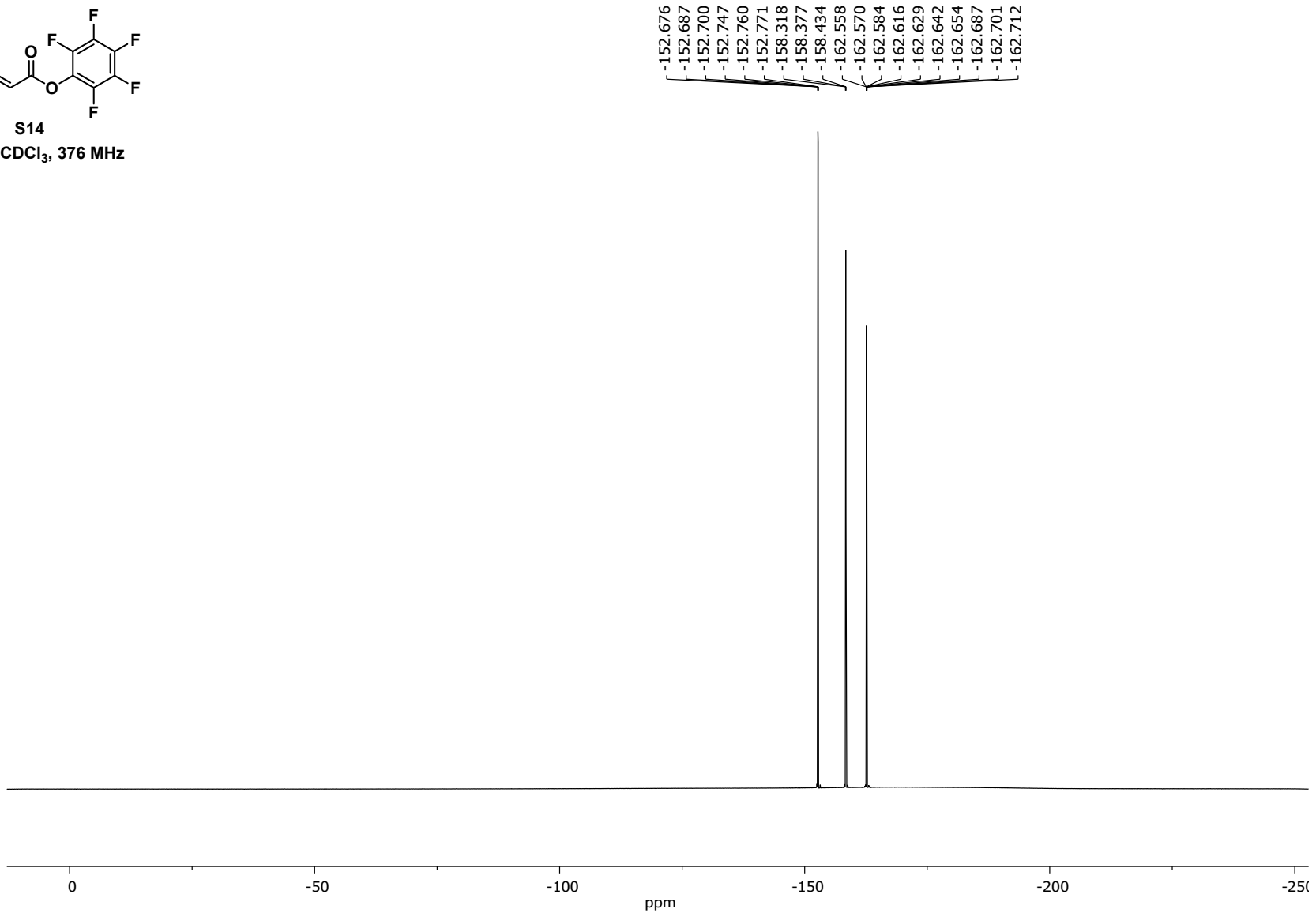
^{1}H, $CDCl_3$, 400 MHz

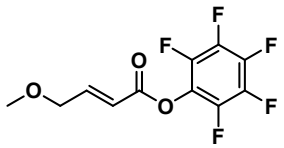




S14

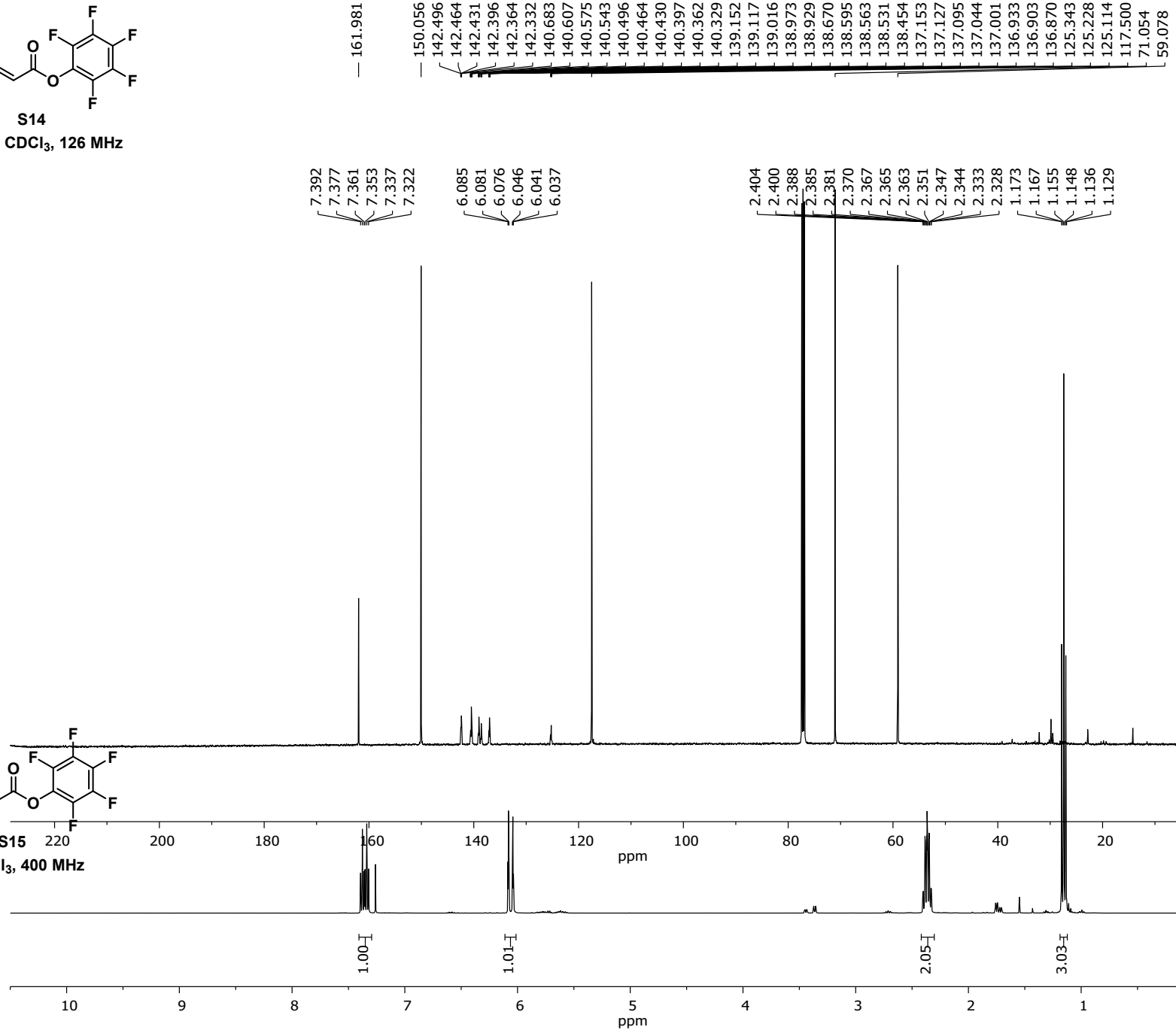
$^{19}F\{^{1}H\}$, $CDCl_3$, 376 MHz





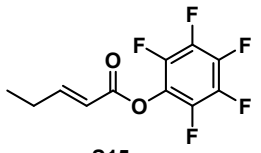
S14

$^{13}C\{^{1}H\}$, $CDCl_3$, 126 MHz



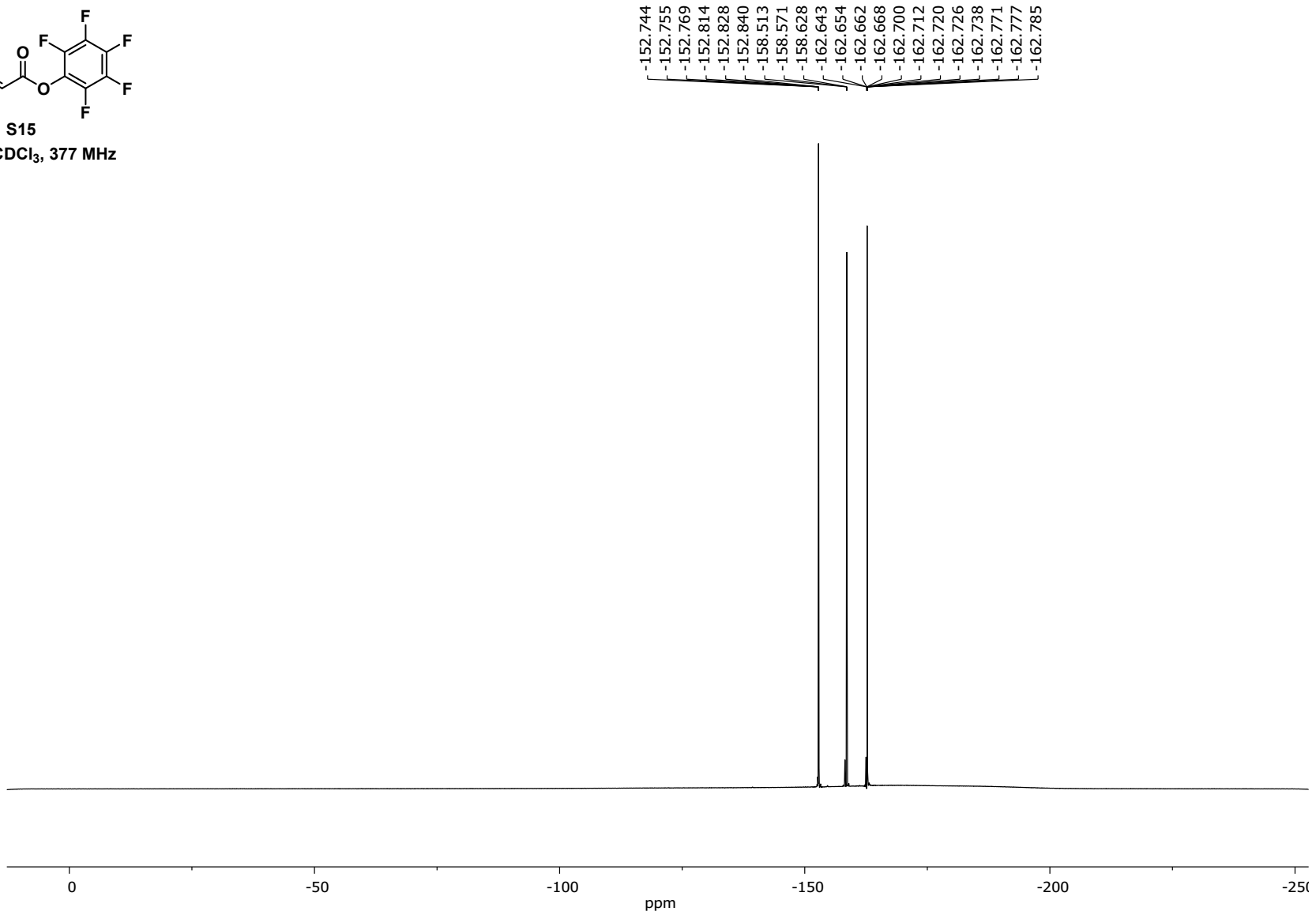
S15

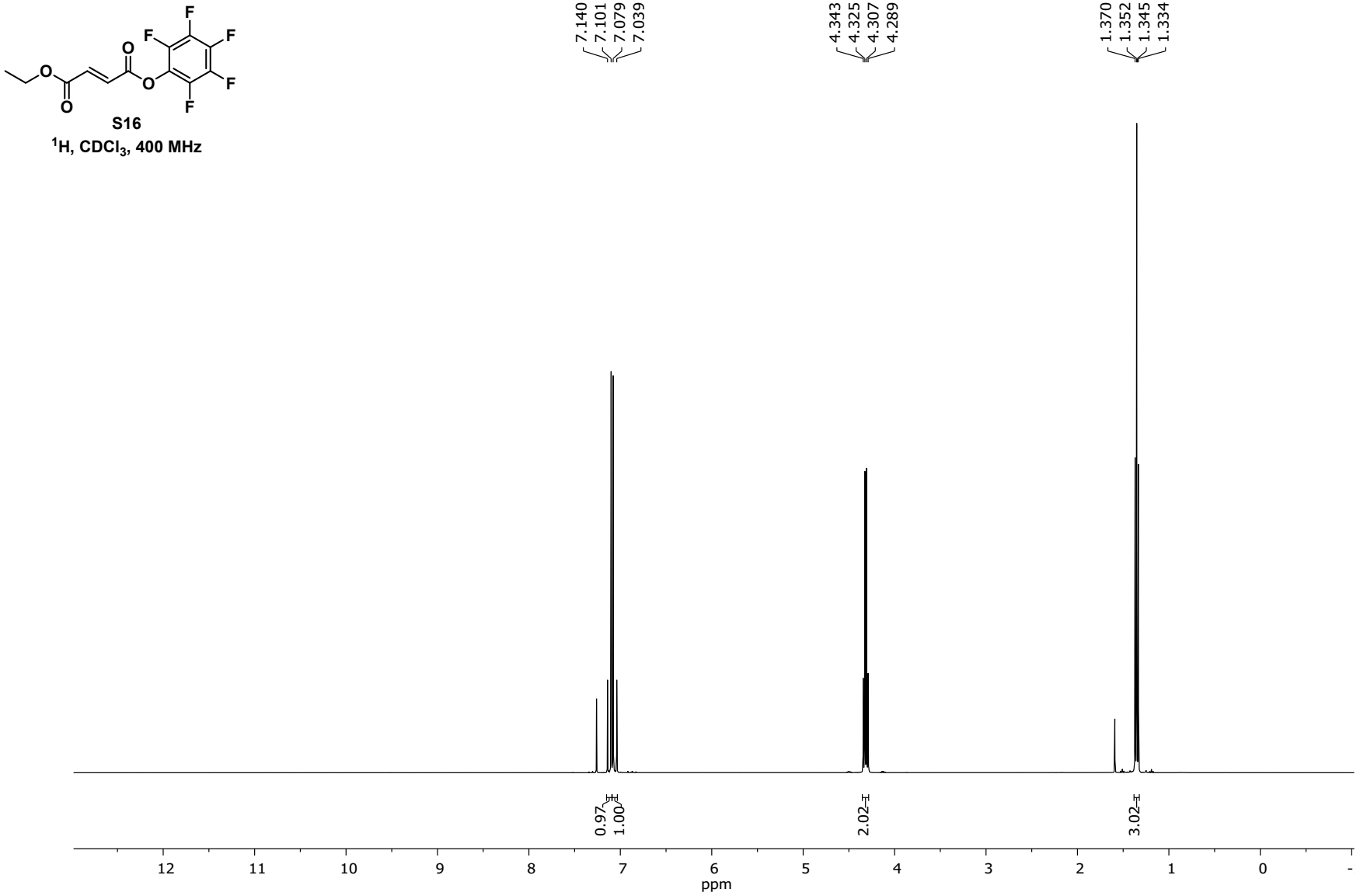
^{1}H, $CDCl_3$, 400 MHz

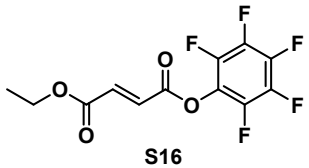


S15

$^{19}F\{^{1}H\}$, $CDCl_3$, 377 MHz



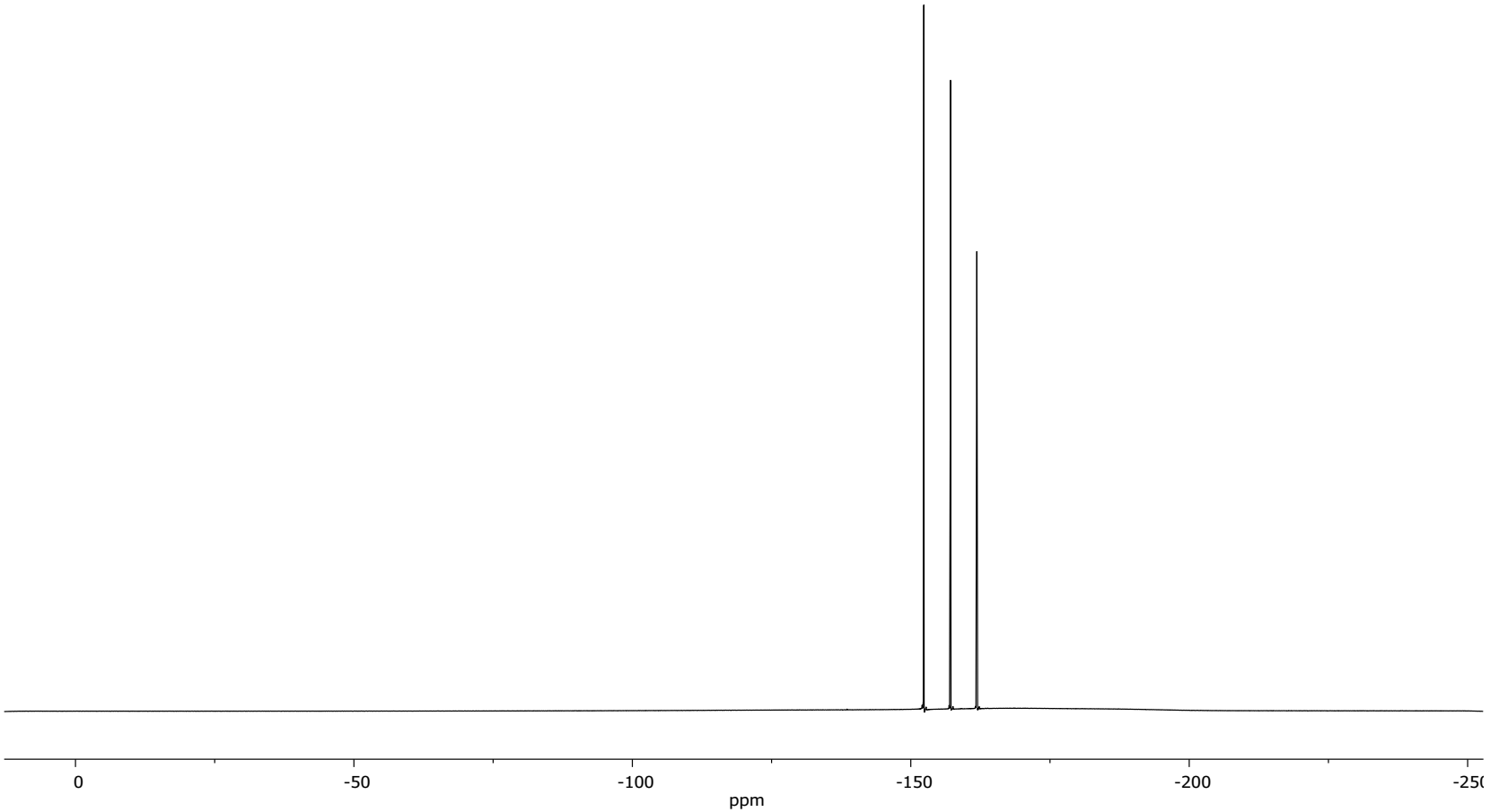

S16
1H, CDCl3, 400 MHz
7.140
7.101
7.079
7.039
4.343
4.325
4.307
4.289
1.370
1.352
1.345
1.334
0.97
1.00
2.02
3.02
12
11
10
9
8
7
6
5
4
3
2
1
0
-
ppm

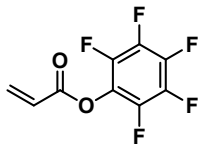


S16

$^{19}F\{^{1}H\}$, $CDCl_3$, 376 MHz

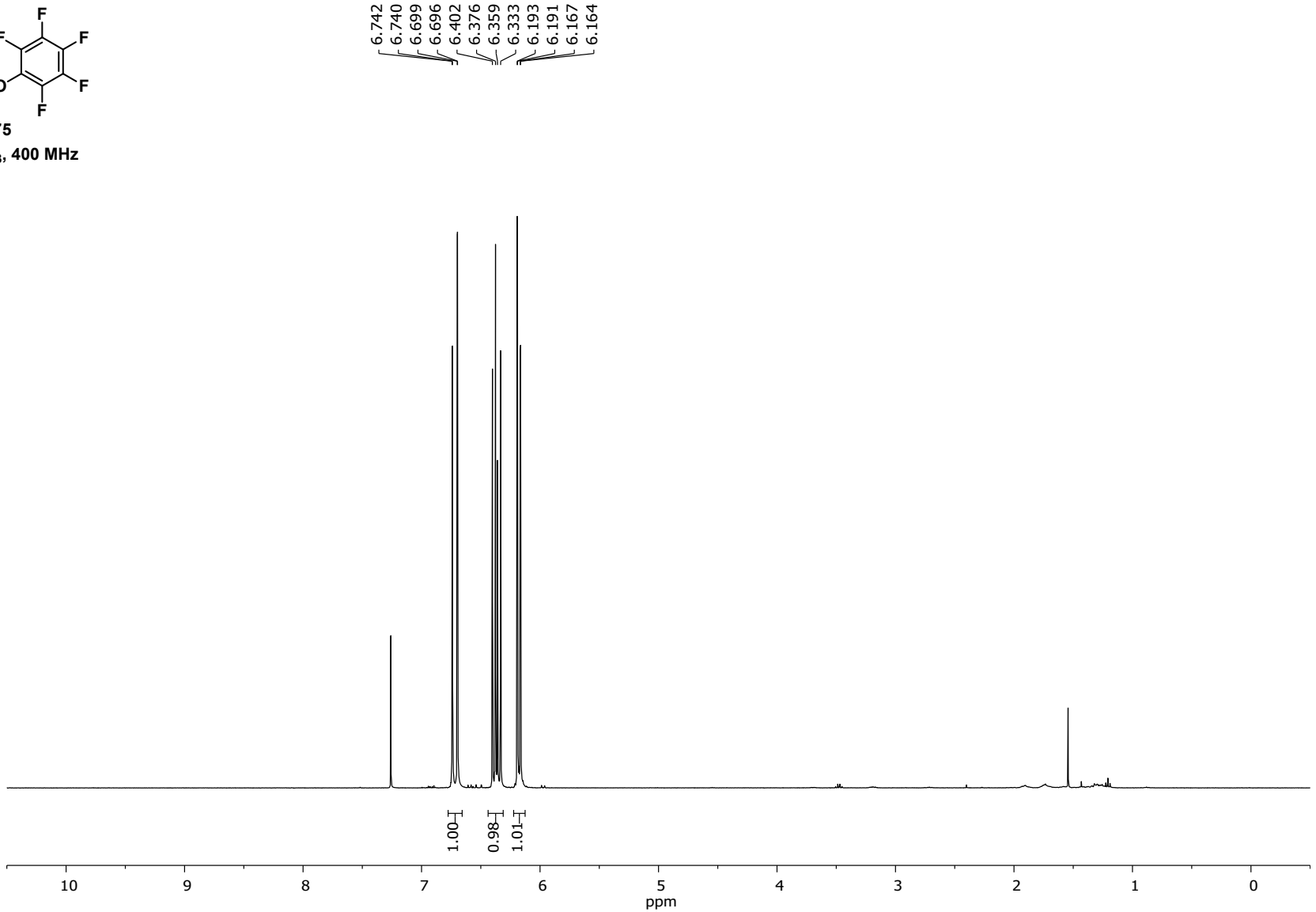
-152.271
-152.279
-152.285
-152.297
-152.323
-152.333
-152.342
-152.353
-152.358
-157.079
-157.137
-157.193
-161.796
-161.804
-161.810
-161.822
-161.853
-161.867
-161.873
-161.879
-161.893
-161.924
-161.936
-161.942
-161.950

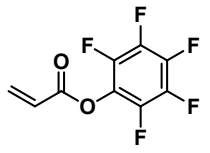




75

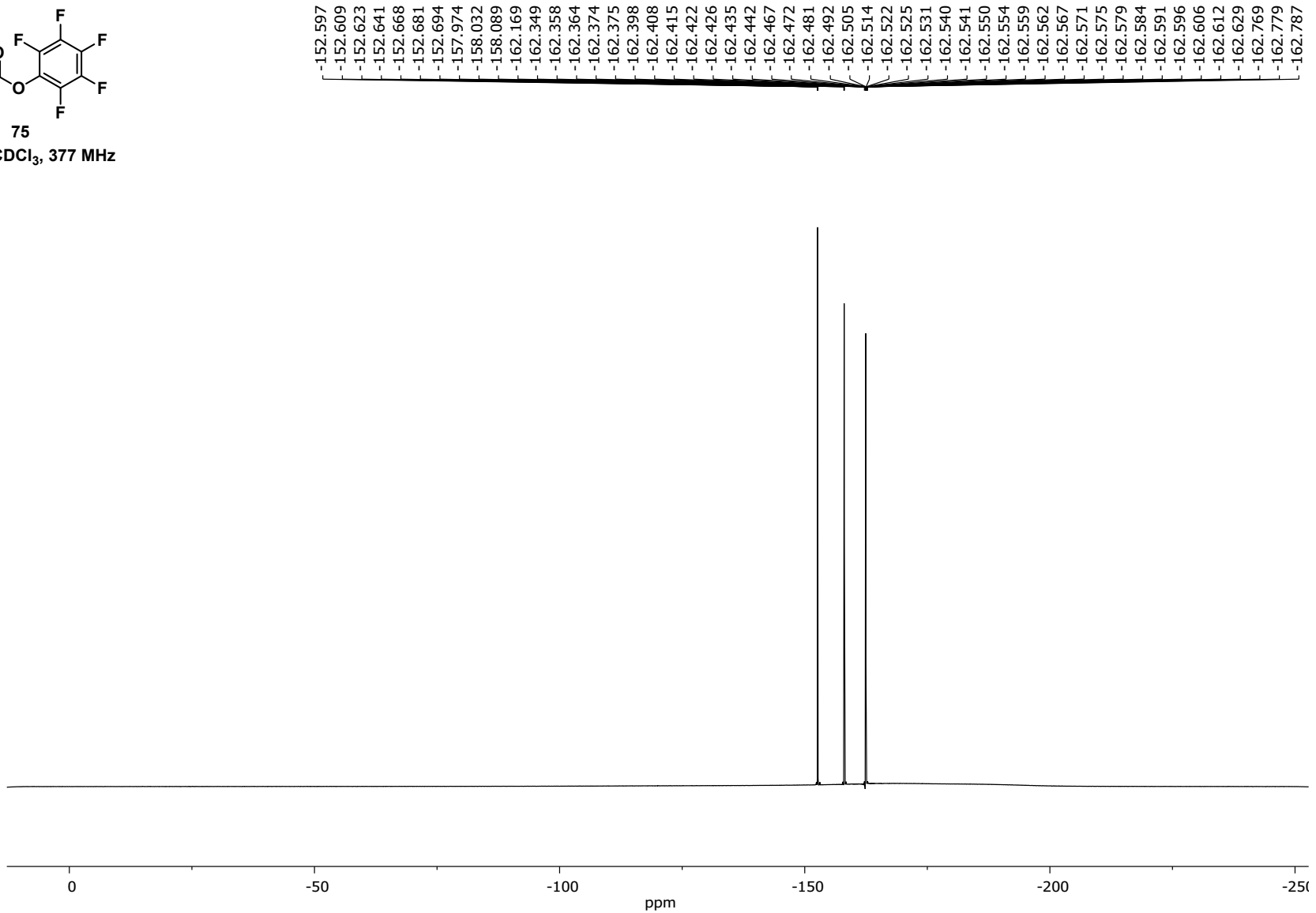
^{1}H, $CDCl_3$, 400 MHz

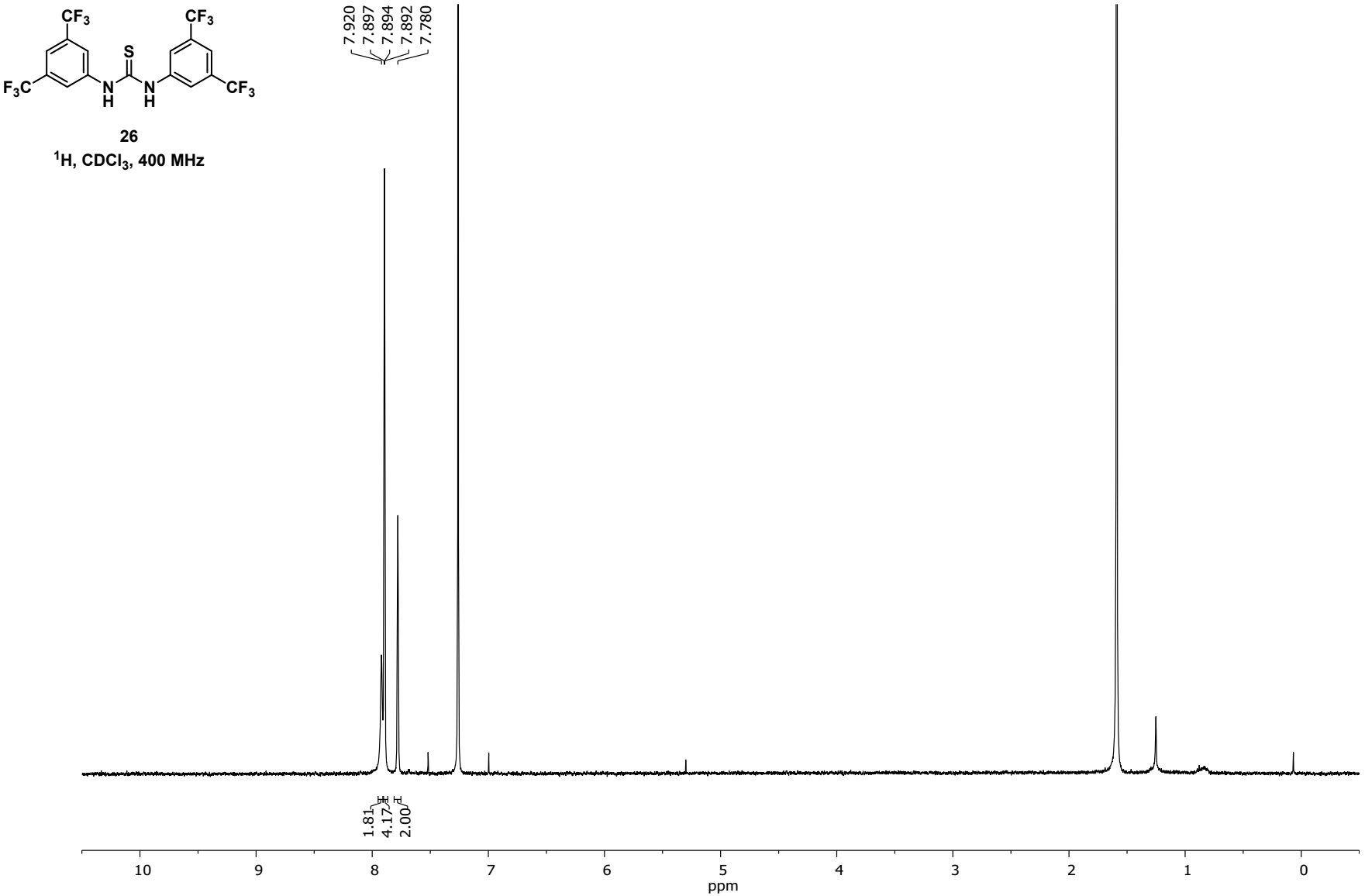


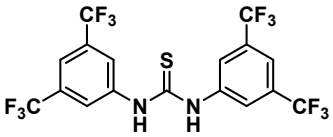


75

$^{19}F\{^{1}H\}$, $CDCl_3$, 377 MHz

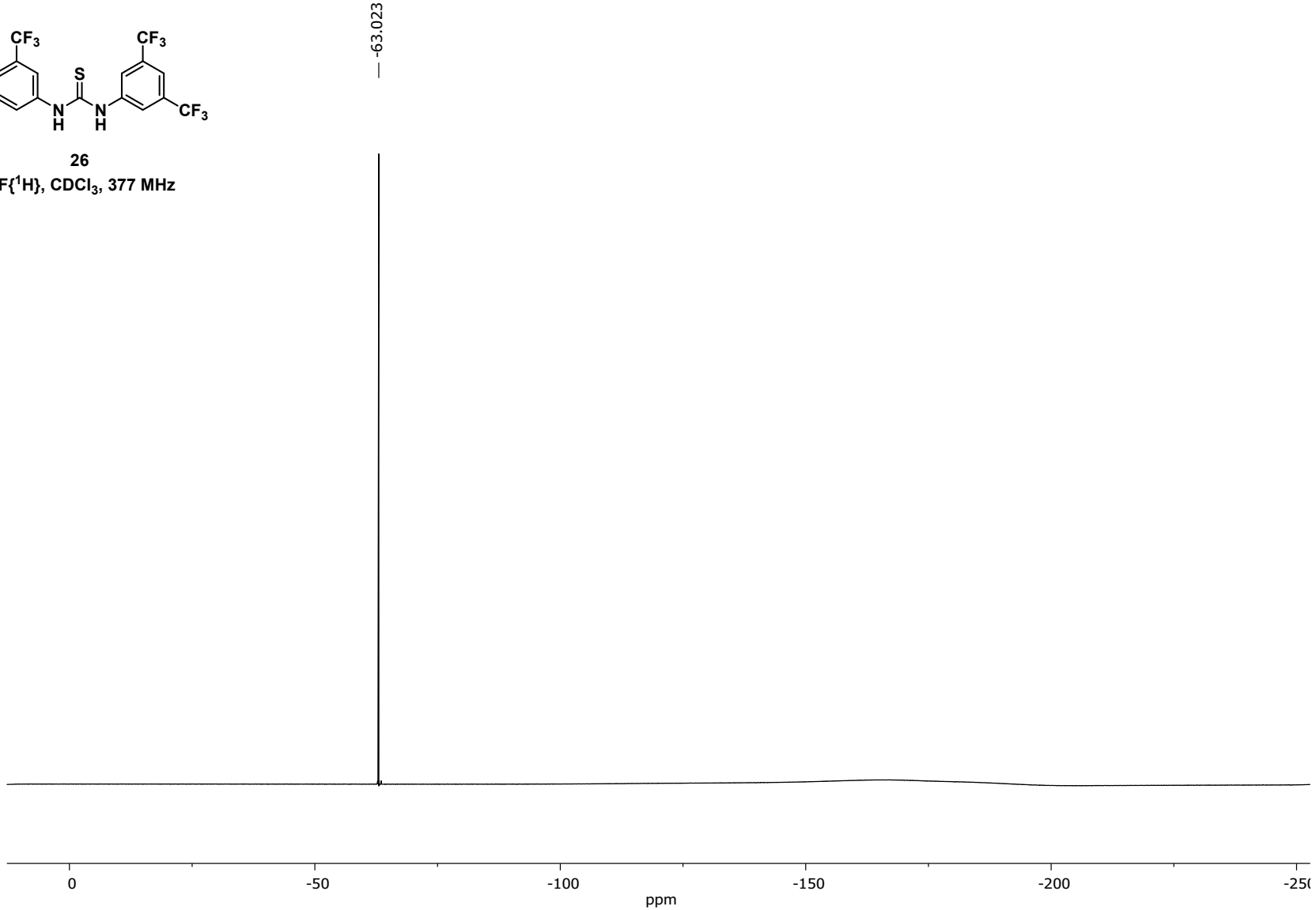


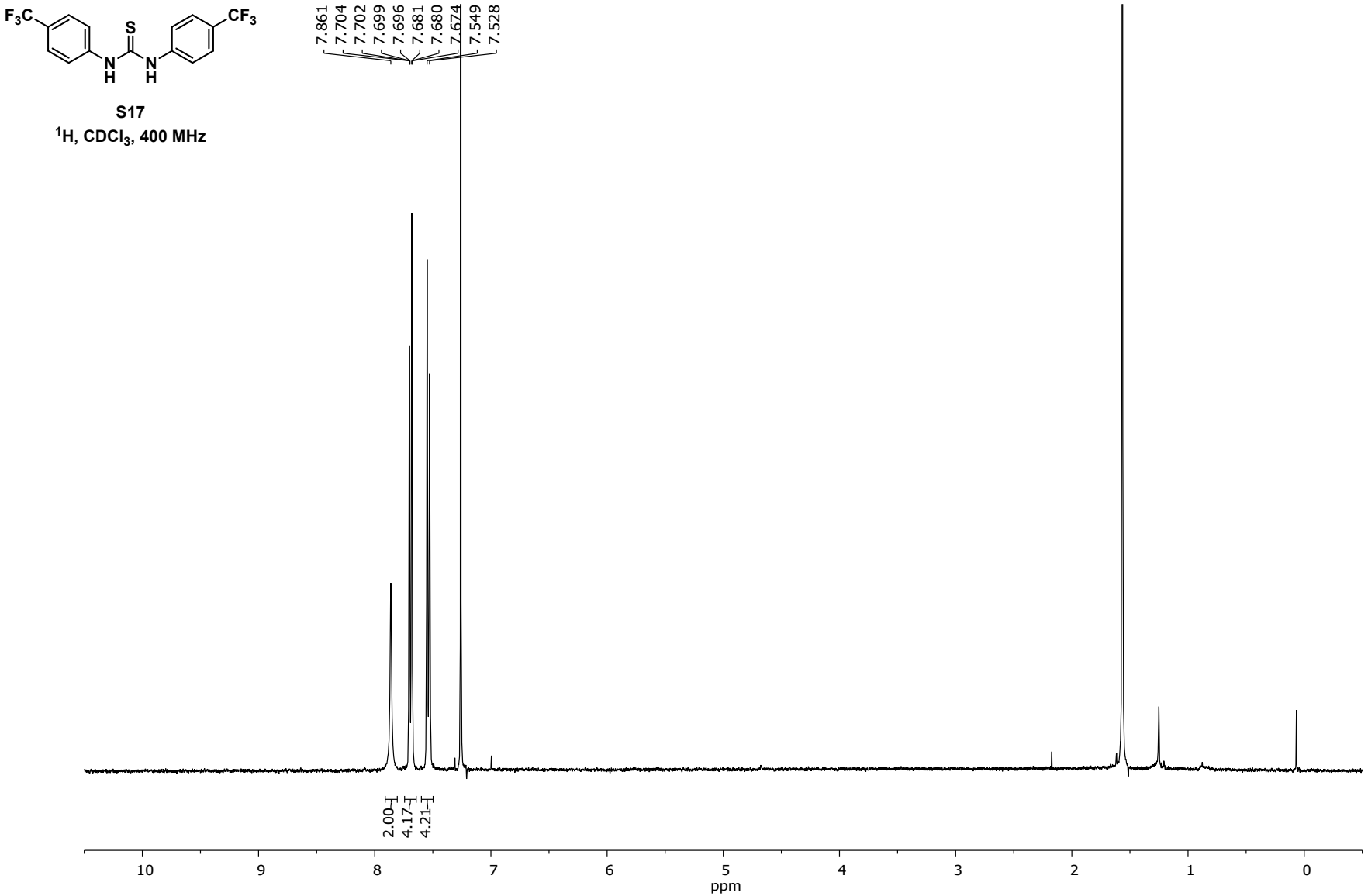

CF3
CF3
S
F3C
N
H
N
H
CF3
26
1H, CDCl3, 400 MHz
7.920
7.897
7.894
7.892
7.780
1.81
4.17
2.00
10
9
8
7
6
5
4
3
2
1
0
ppm

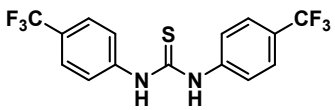


26

$^{19}F\{^{1}H\}$, $CDCl_3$, 377 MHz

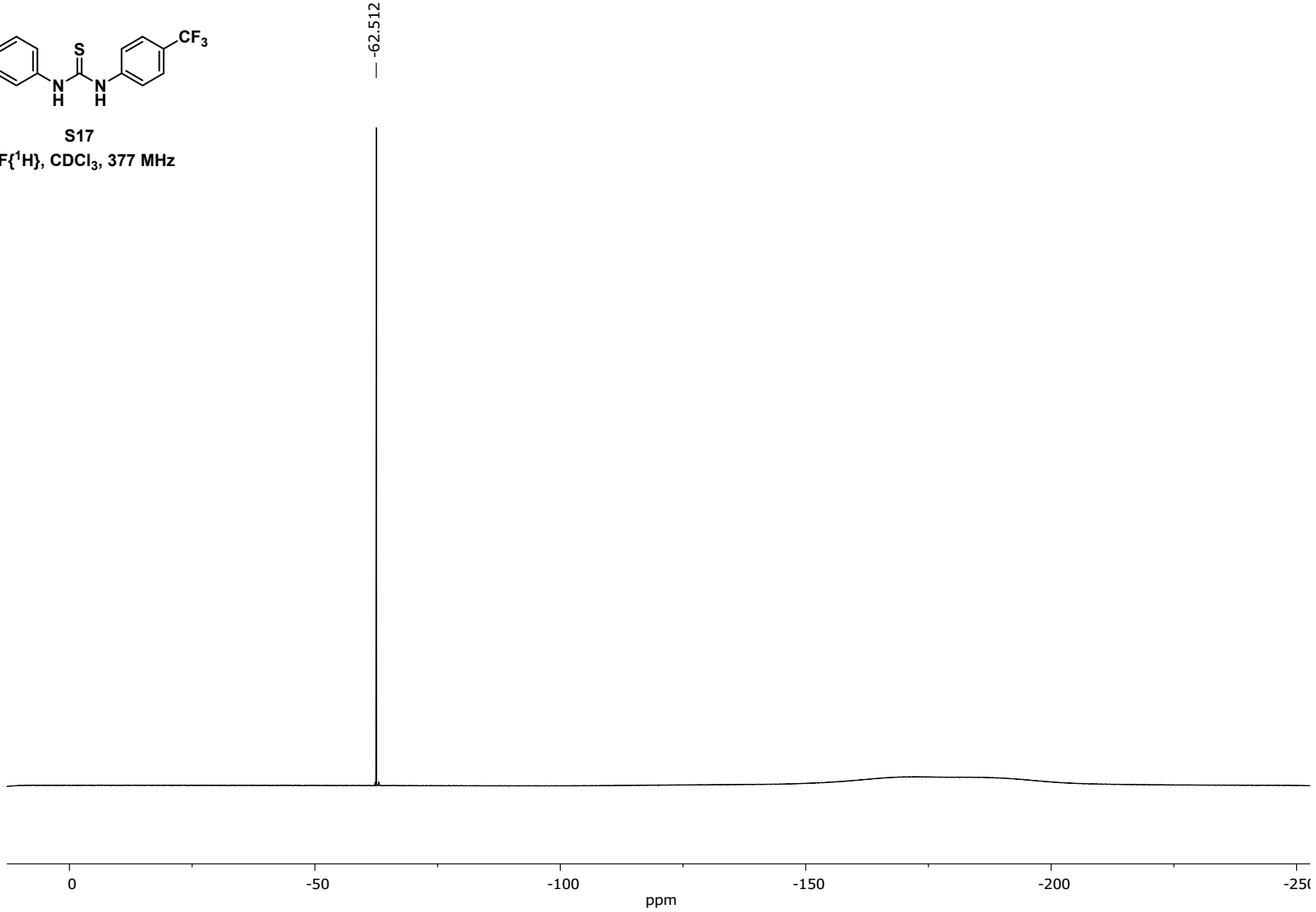


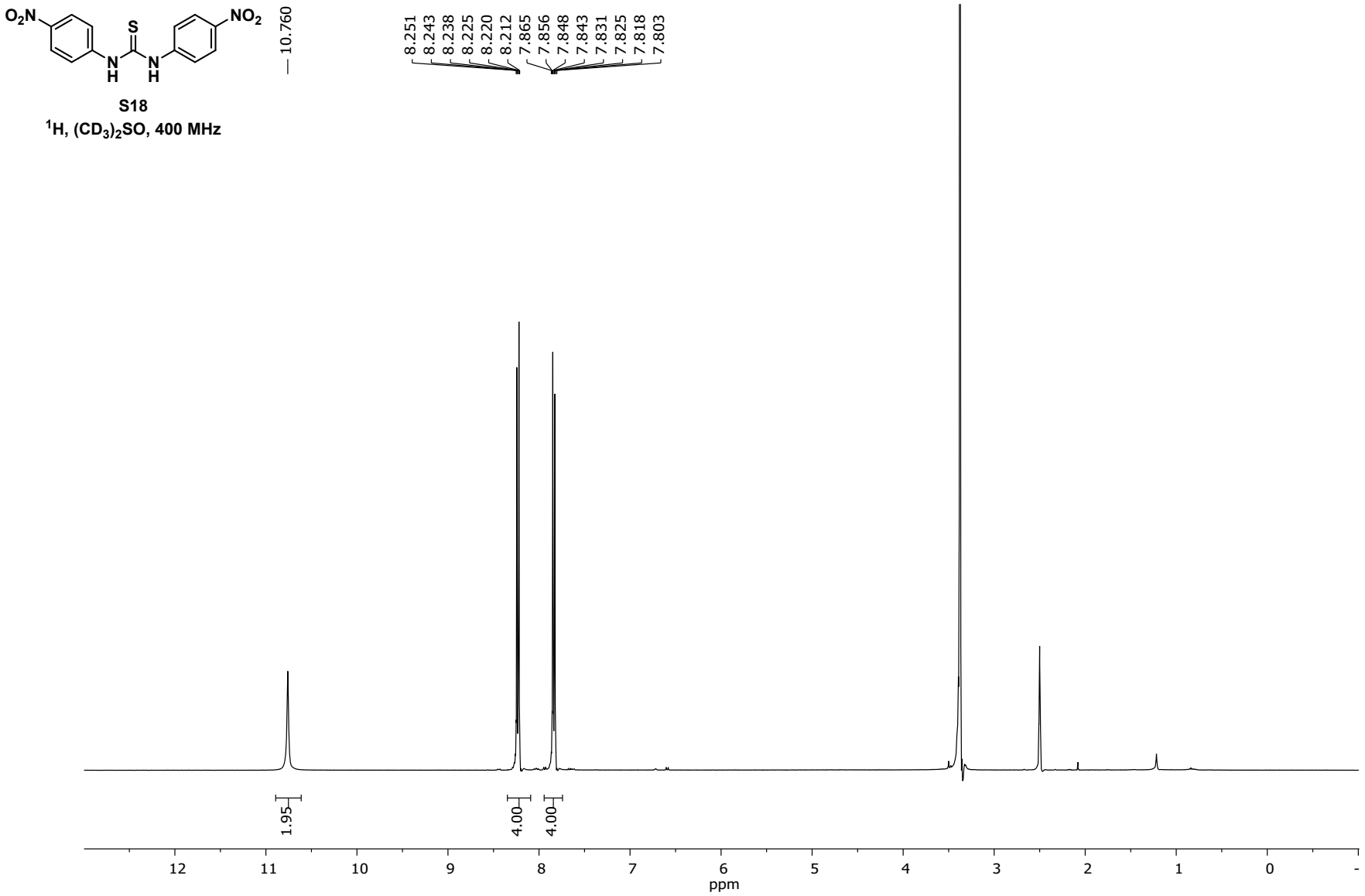

F3C
CF3
S
N
H
N
H
S17
1H, CDCl3, 400 MHz
7.861
7.704
7.702
7.699
7.696
7.681
7.680
7.624
7.549
7.528
2.00
4.17
4.21
10
9
8
7
6
5
4
3
2
1
0
ppm



S17

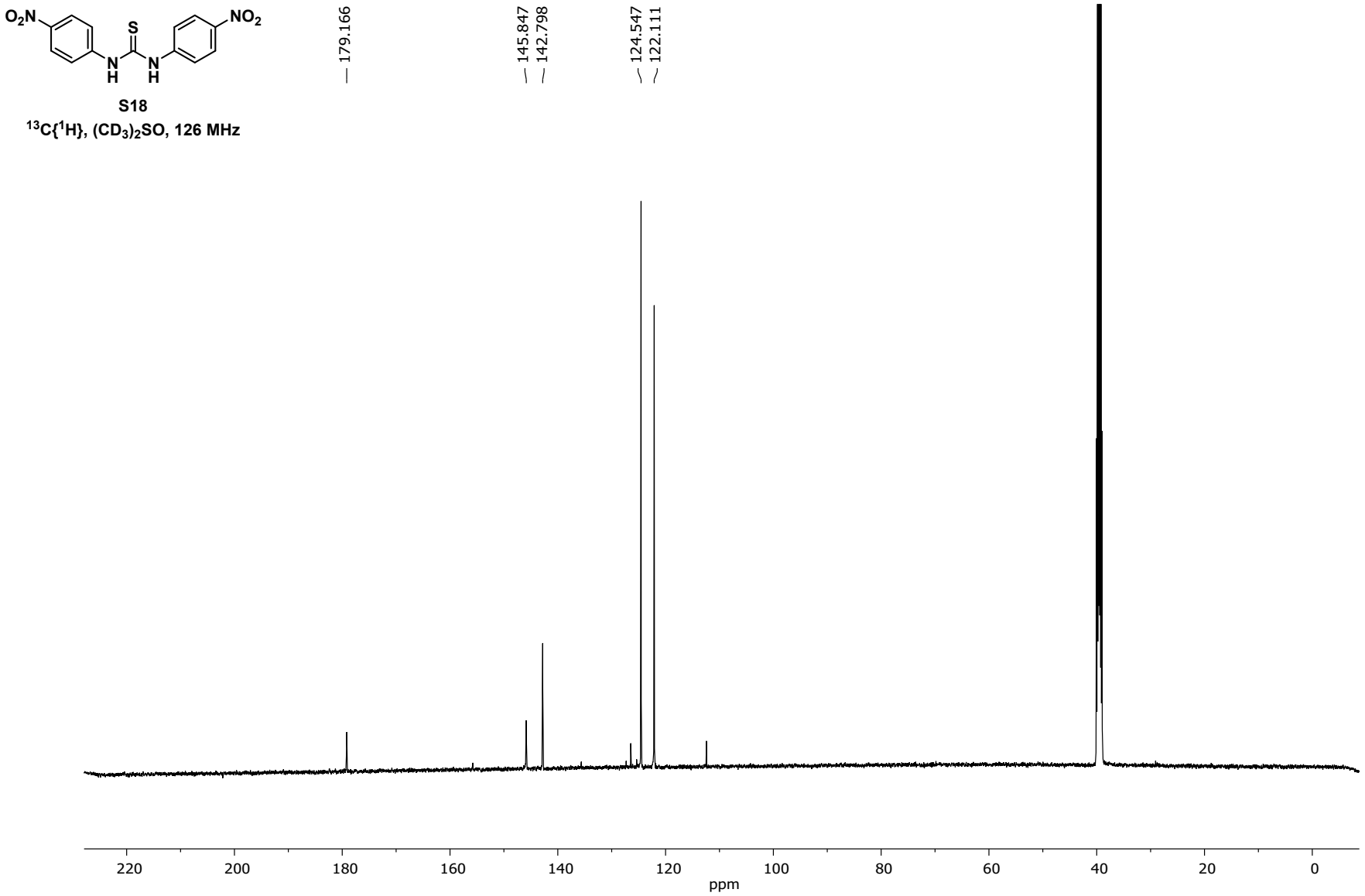
$^{19}F\{^{1}H\}$, $CDCl_3$, 377 MHz

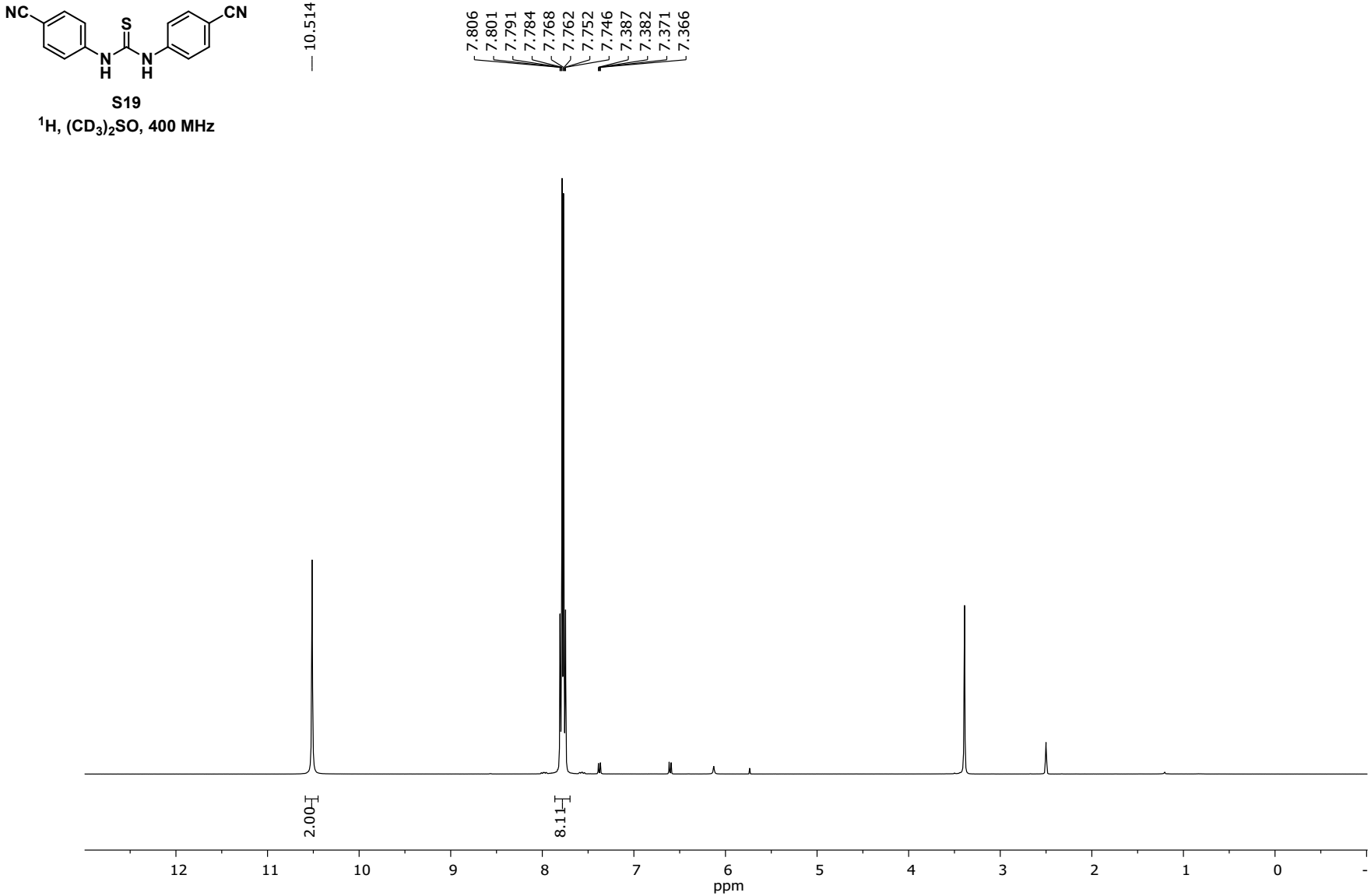


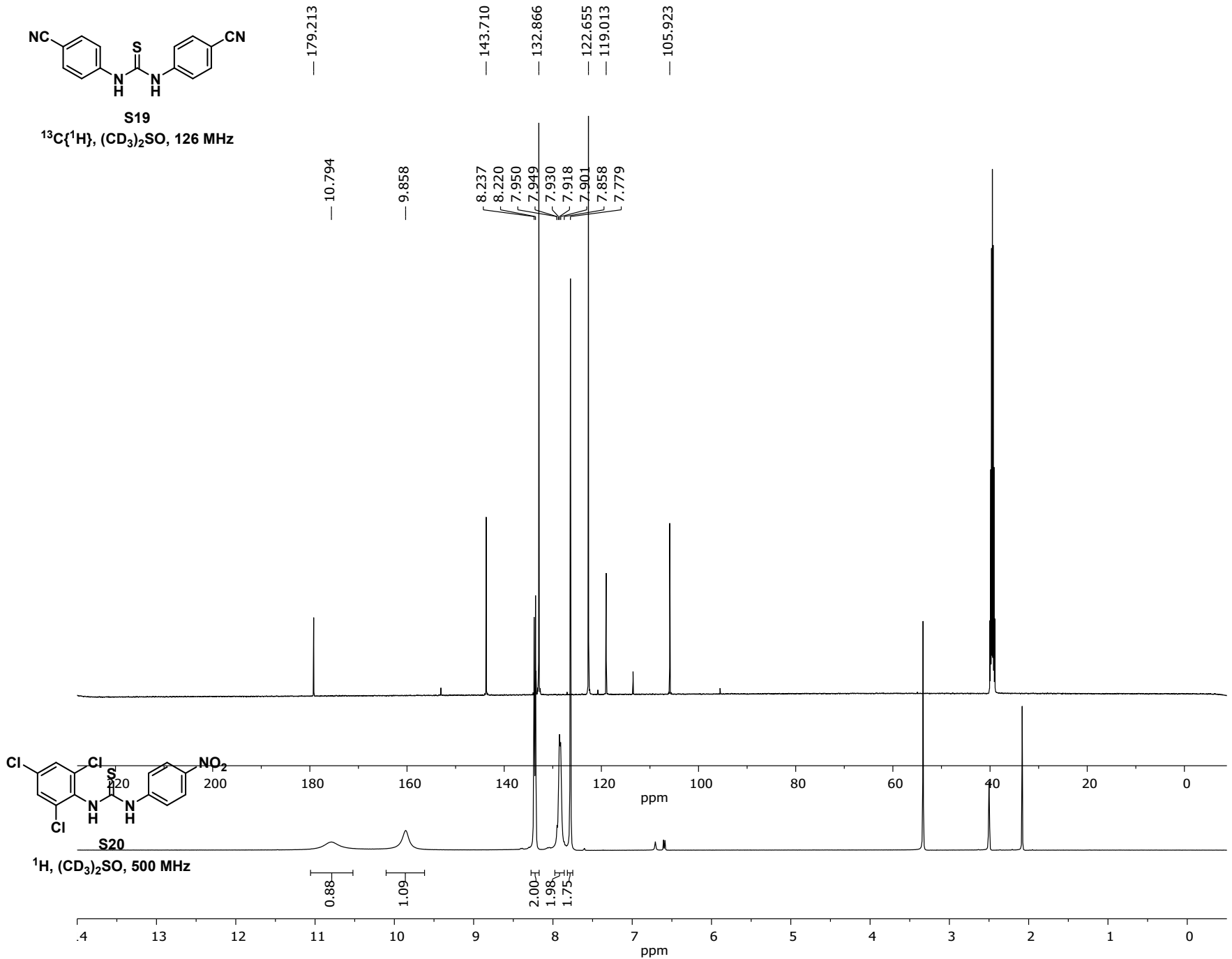


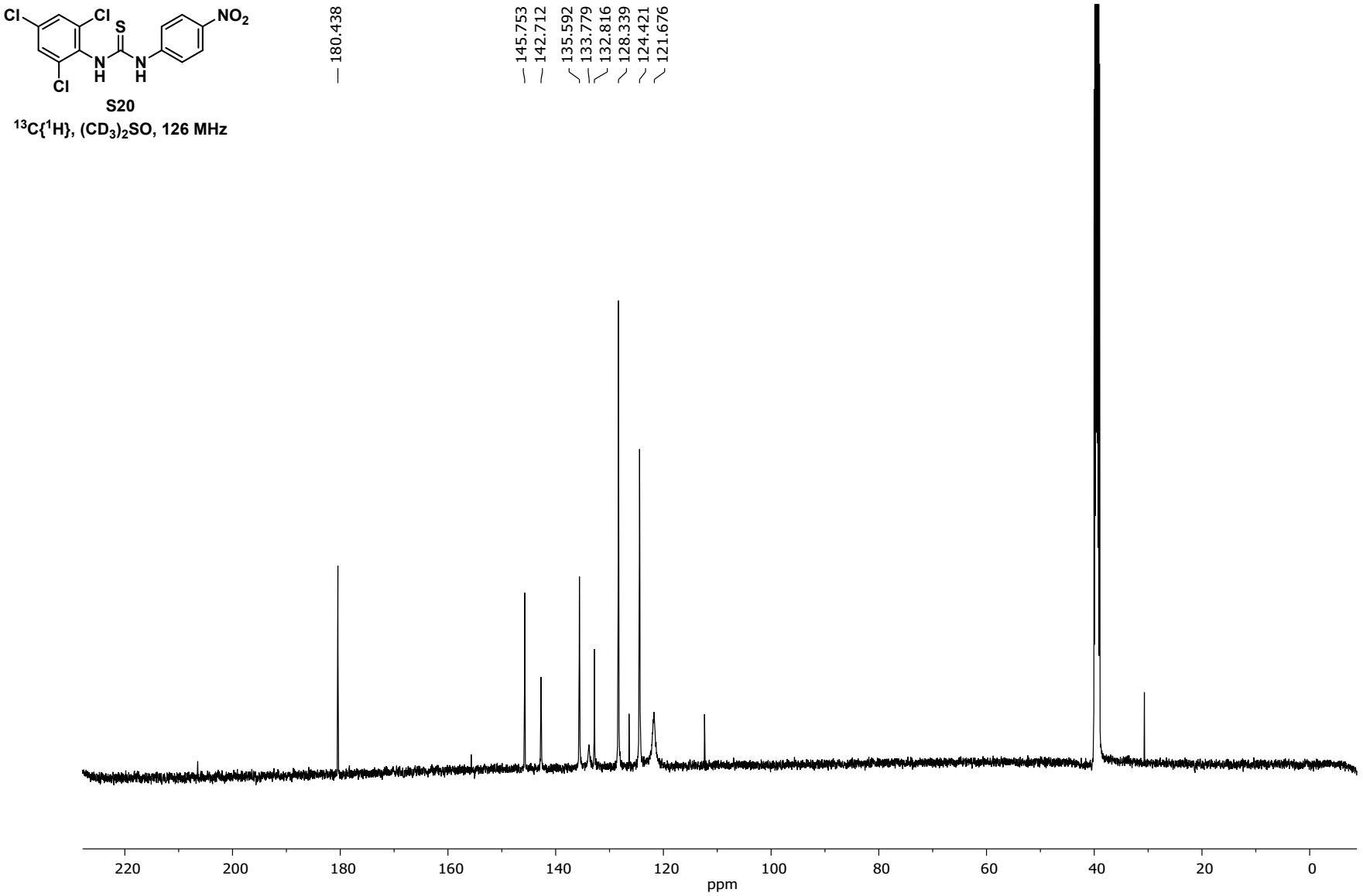
S18

^{1}H, $(CD_3)_2SO$, 400 MHz


O2N
NO2
S
N
H
N
H
S18
13C{1H}, (CD3)2SO, 126 MHz
179.166
145.847
142.798
124.547
122.111
220
200
180
160
140
120
100
80
60
40
20
0
ppm

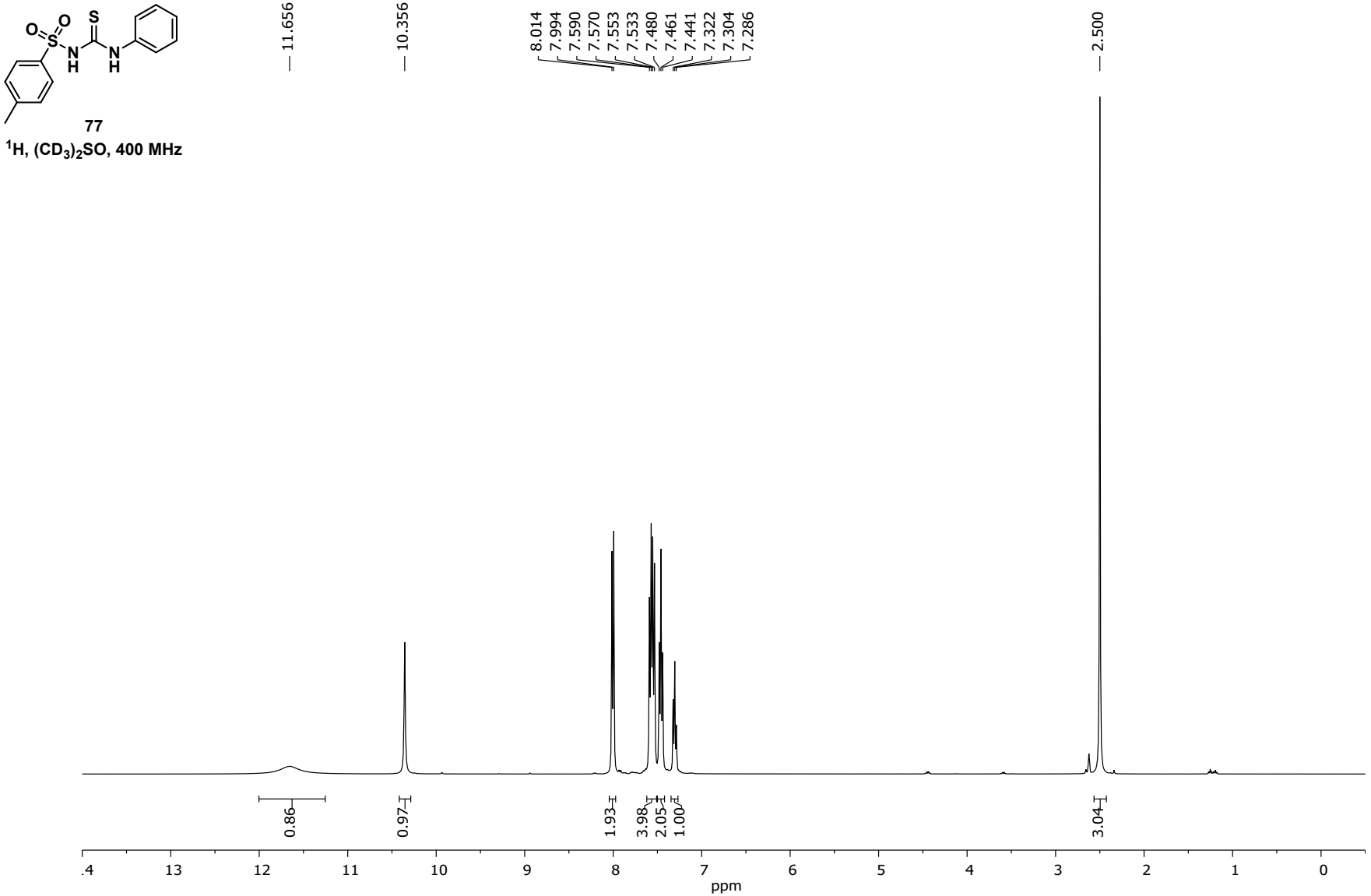

NC
S
CN
N
H
N
H
S19
^{1}H, $(CD_3)_2SO$, 400 MHz
10.514
7.806
7.801
7.791
7.784
7.768
7.762
7.752
7.746
7.387
7.382
7.371
7.366
2.00
8.11
12
11
10
9
8
7
6
5
4
3
2
1
0
-
ppm

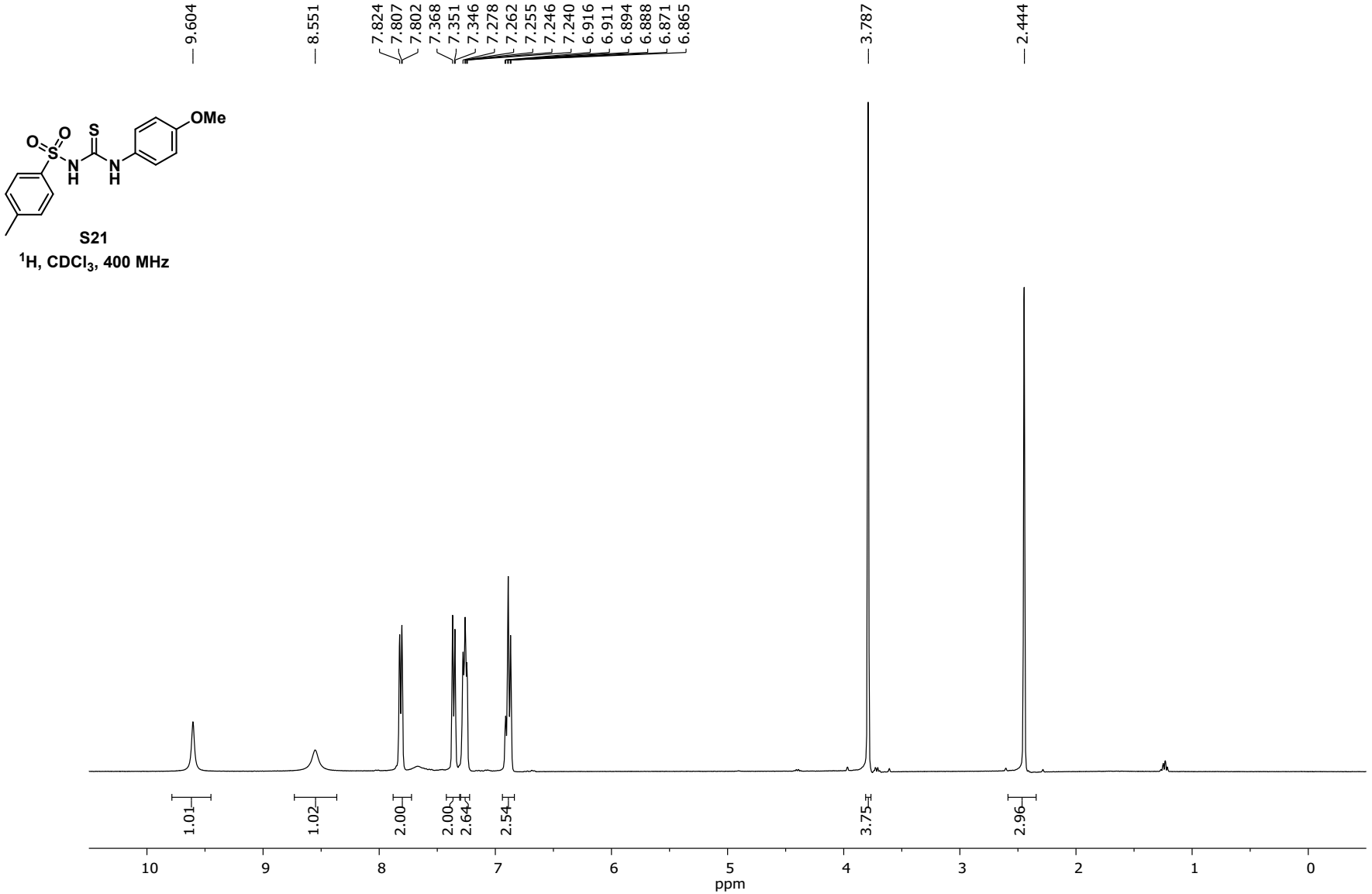

S19
$^{13}C\{^{1}H\}$, $(CD_3)_2SO$, 126 MHz
179.213
143.710
132.866
122.655
119.013
105.923
10.794
9.858
8.237
8.220
7.950
7.949
7.930
7.918
7.901
7.858
7.779
S20
^{1}H, $(CD_3)_2SO$, 500 MHz
0.88
1.09
2.00
1.98
1.75
ppm
ppm

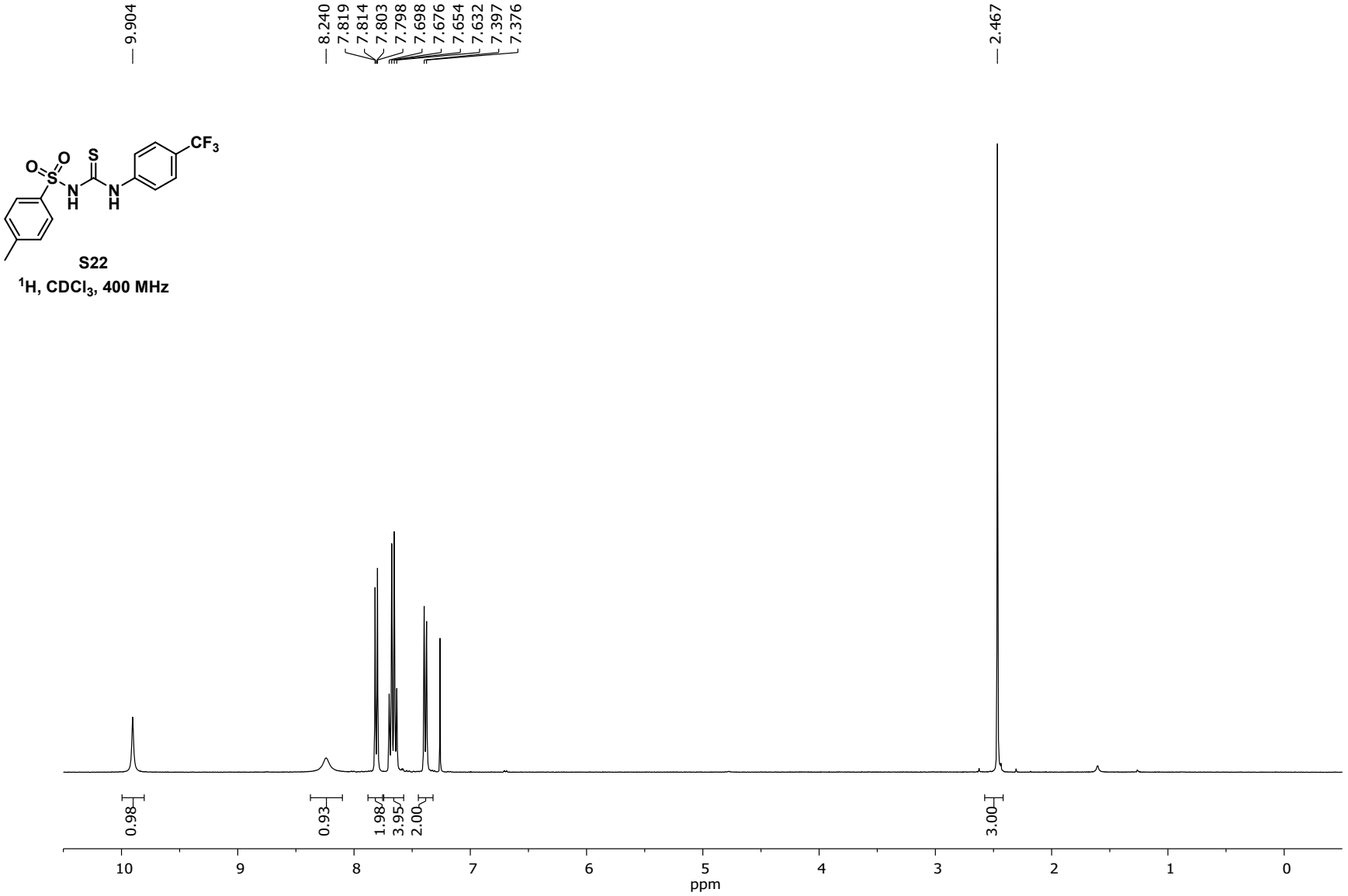


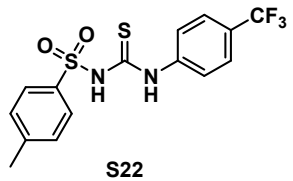
S20

$^{13}C\{^{1}H\}$, $(CD_3)_2SO$, 126 MHz


77
1H, (CD3)2SO, 400 MHz
11.656
10.356
8.014
7.994
7.590
7.570
7.553
7.533
7.480
7.461
7.441
7.322
7.304
7.286
2.500
0.86
0.97
1.93
3.98
2.05
1.00
3.04
ppm

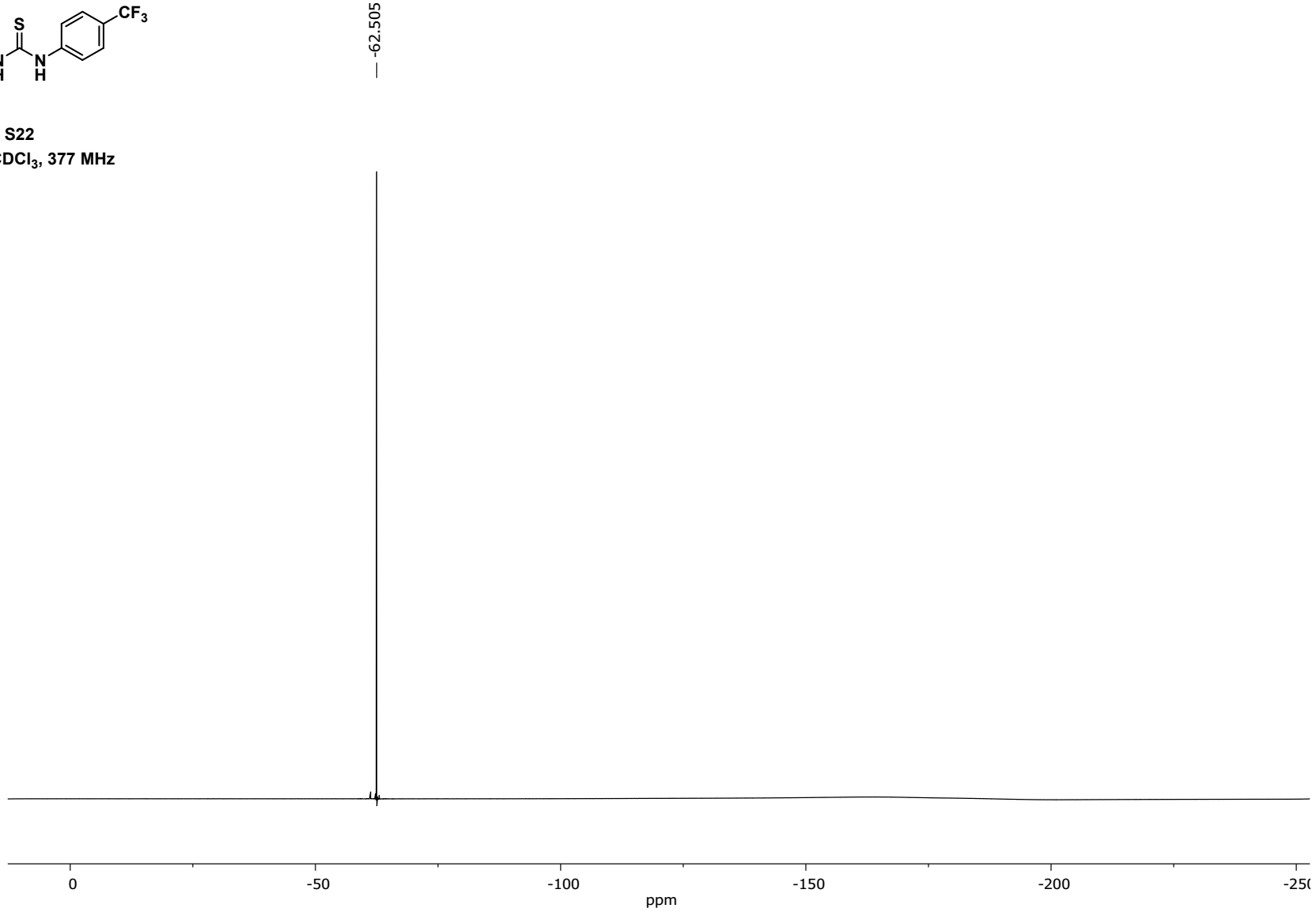

9.604
8.551
7.824
7.807
7.802
7.368
7.351
7.346
7.278
7.262
7.255
7.246
7.240
6.916
6.911
6.894
6.888
6.871
6.865
3.787
2.444
OMe
S
O
O
N
H
N
H
S21
1H, CDCl3, 400 MHz
1.01
1.02
2.00
2.00
2.64
2.54
3.75
2.96
10
9
8
7
6
5
4
3
2
1
0
ppm

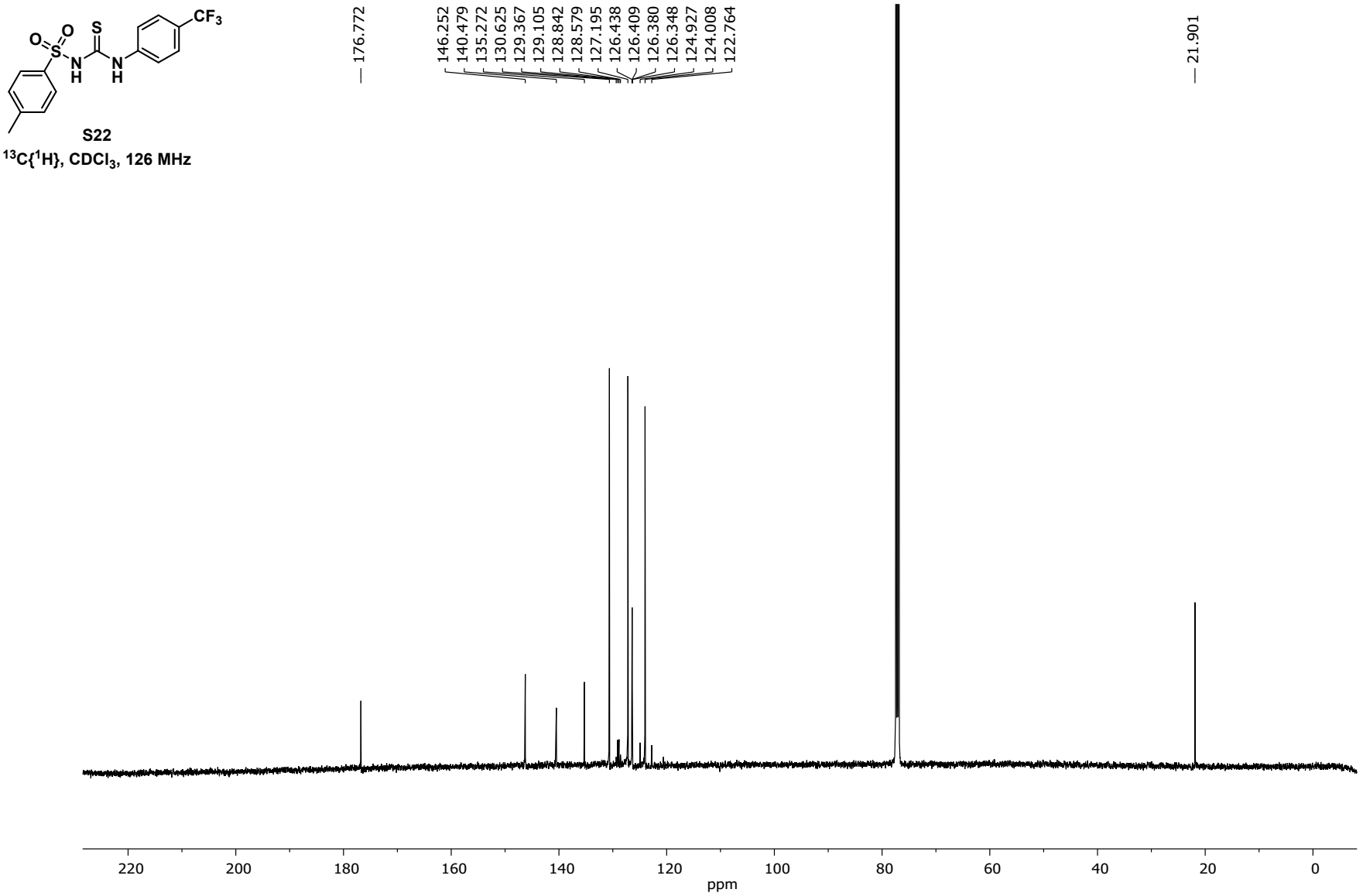

9.904
8.240
7.819
7.814
7.803
7.798
7.698
7.676
7.654
7.632
7.397
7.376
2.467
CF3
O
O
S
N
H
S
N
H
S22
1H, CDCl3, 400 MHz
0.98
0.93
1.98
3.95
2.00
3.00
10
9
8
7
6
5
4
3
2
1
0
ppm

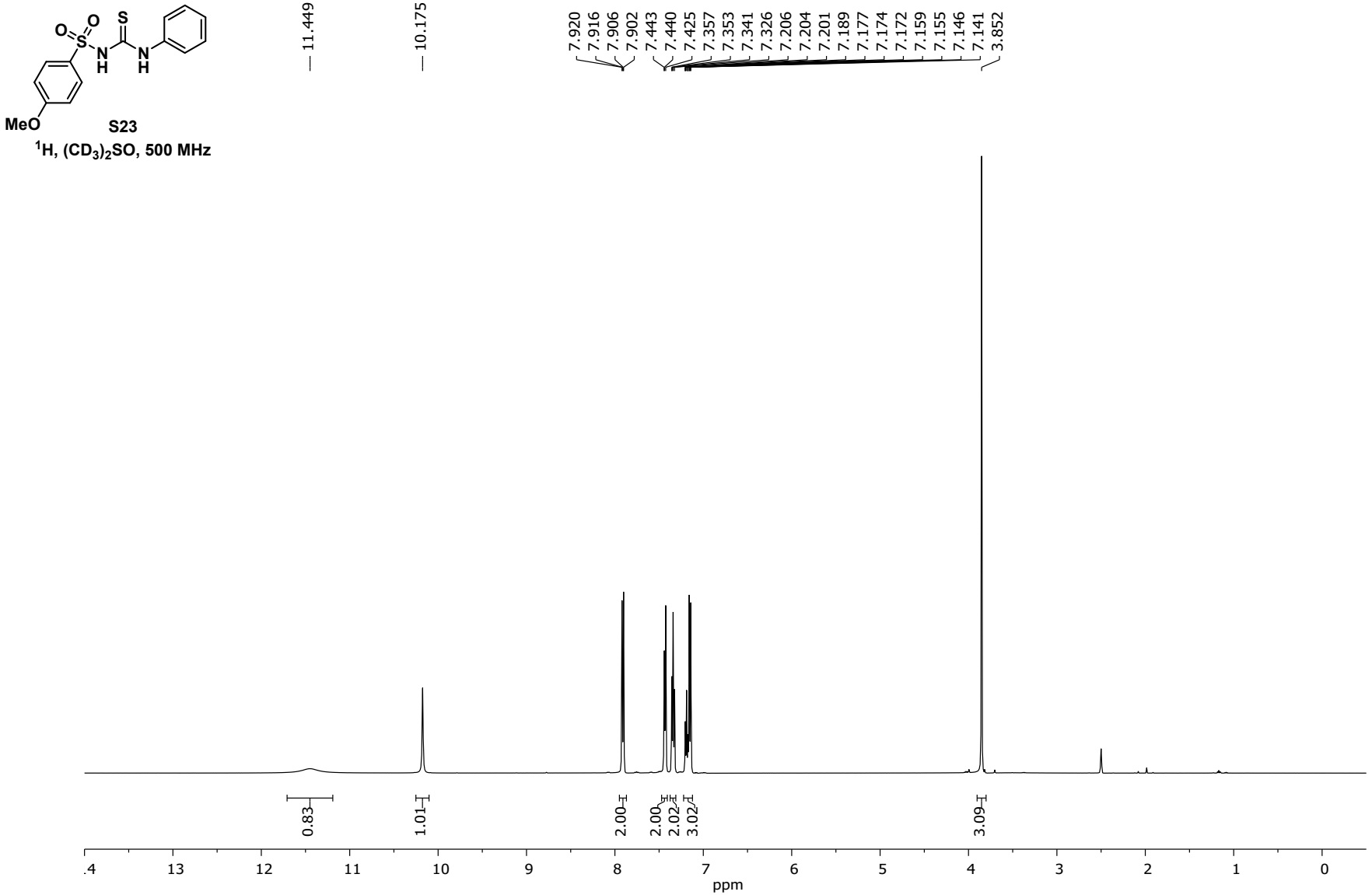


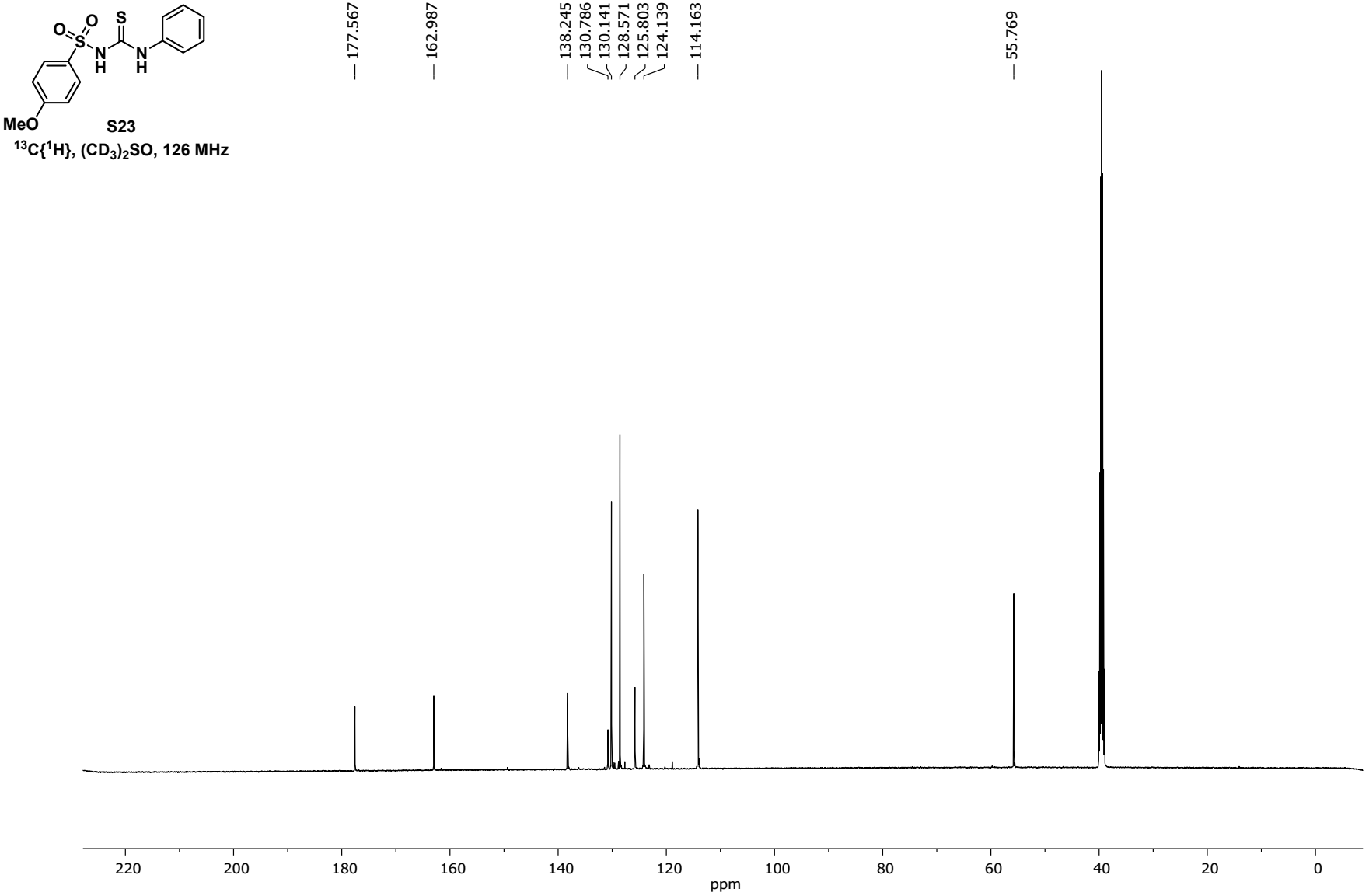
S22

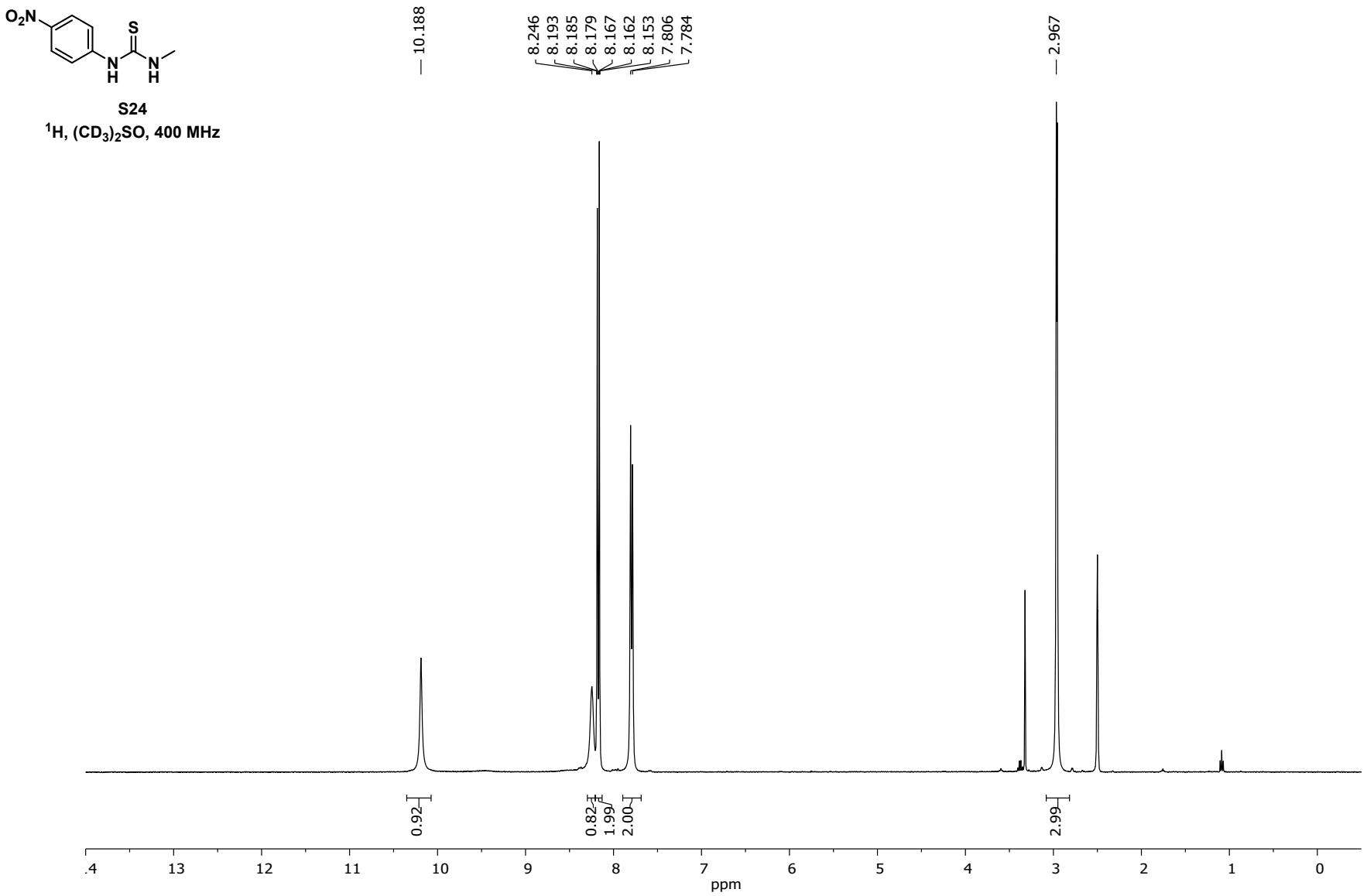
$^{19}F\{^{1}H\}$, $CDCl_3$, 377 MHz

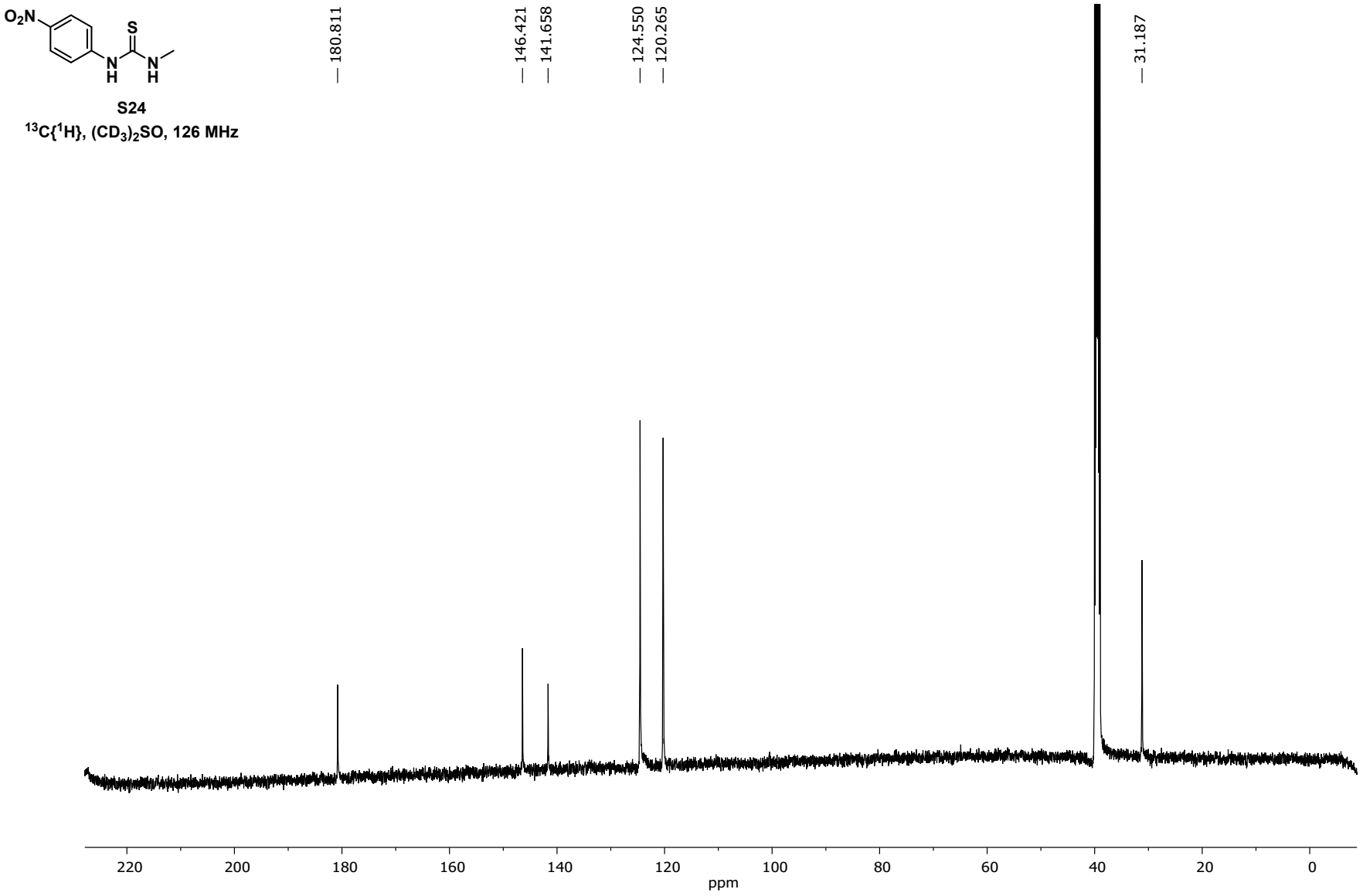



S22
$^{13}C\{^{1}H\}$, $CDCl_3$, 126 MHz
176.772
146.252
140.479
135.272
130.625
129.367
129.105
128.842
128.579
127.195
126.438
126.409
126.380
126.348
124.927
124.008
122.764
21.901
220
200
180
160
140
120
100
80
60
40
20
0
ppm


MeO
S23
^{1}H, $(CD_3)_2SO$, 500 MHz
11.449
10.175
7.920
7.916
7.906
7.902
7.443
7.440
7.425
7.357
7.353
7.341
7.326
7.206
7.204
7.201
7.189
7.177
7.174
7.172
7.159
7.155
7.146
7.141
3.852
0.83
1.01
2.00
2.00
2.02
3.02
3.09
ppm

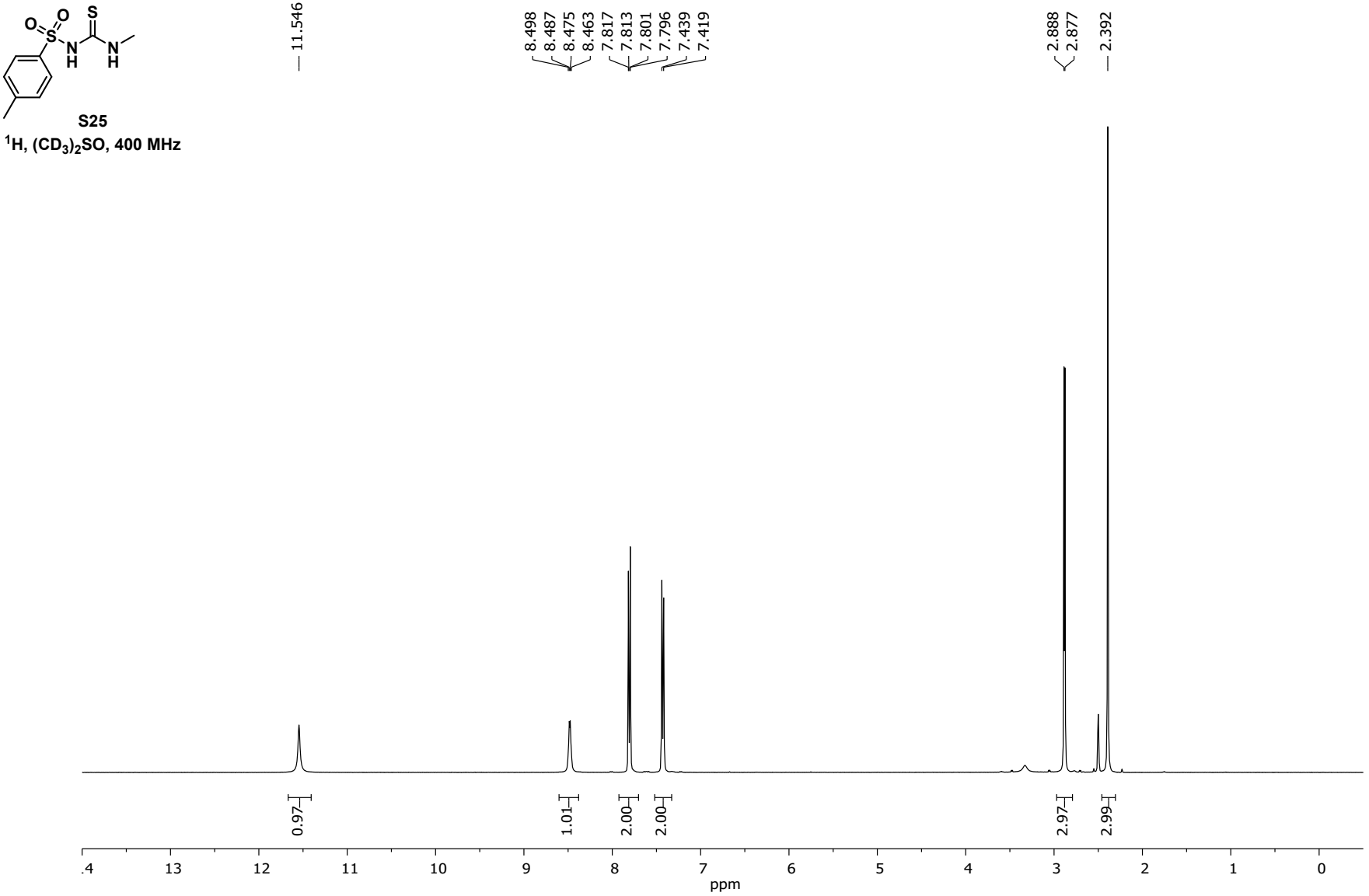

MeO
S23
$^{13}C\{^{1}H\}$, $(CD_3)_2SO$, 126 MHz
177.567
162.987
138.245
130.786
130.141
128.571
125.803
124.139
114.163
55.769
220
200
180
160
140
120
100
80
60
40
20
0
ppm


O2N
S
N
H
N
H
S24
1H, (CD3)2SO, 400 MHz
10.188
8.246
8.193
8.185
8.179
8.167
8.162
8.153
7.806
7.784
2.967
0.92
0.82
1.99
2.00
2.99
ppm



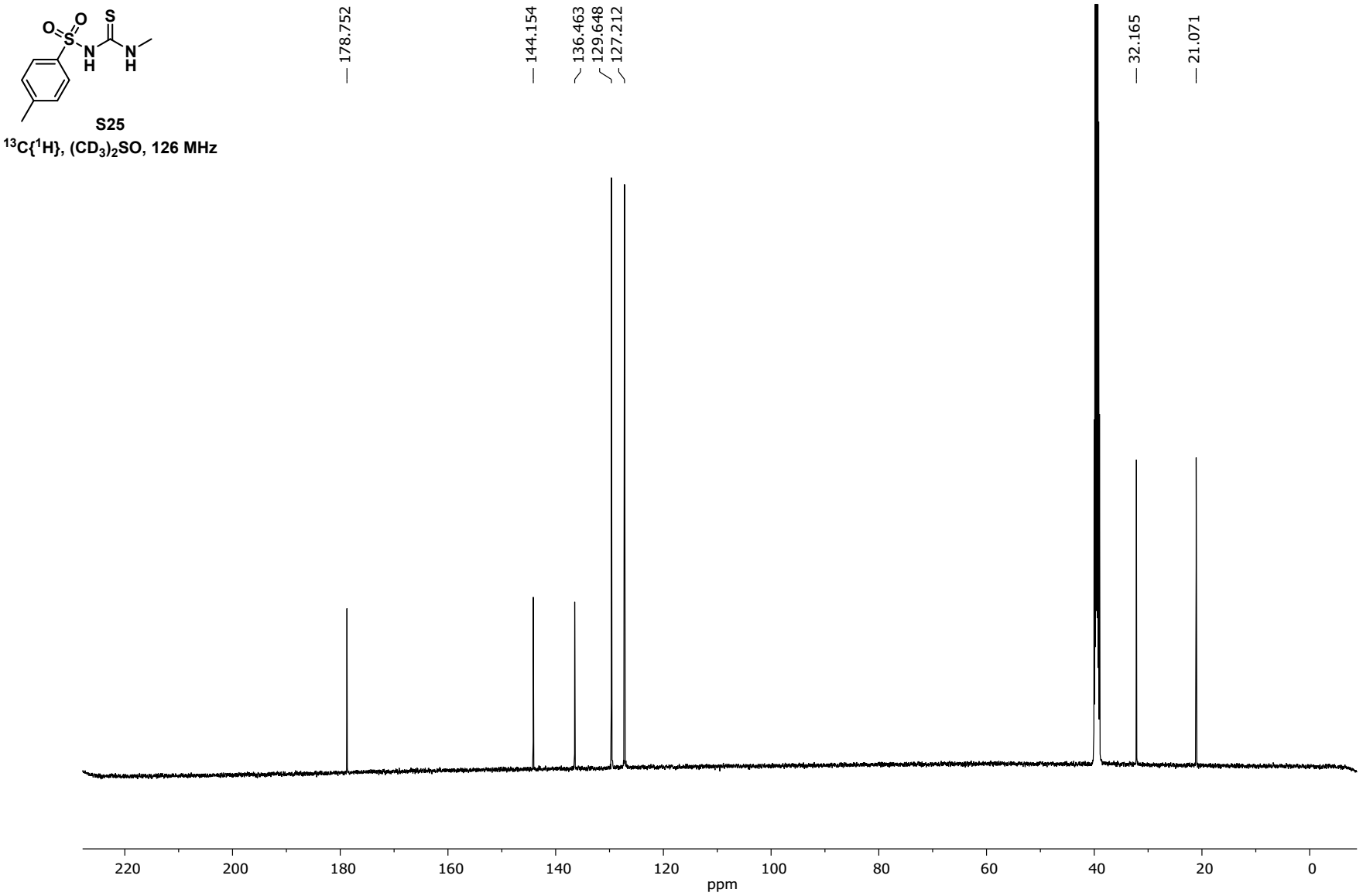
S24

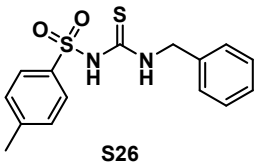
$^{13}C\{^{1}H\}$, $(CD_3)_2SO$, 126 MHz



S25

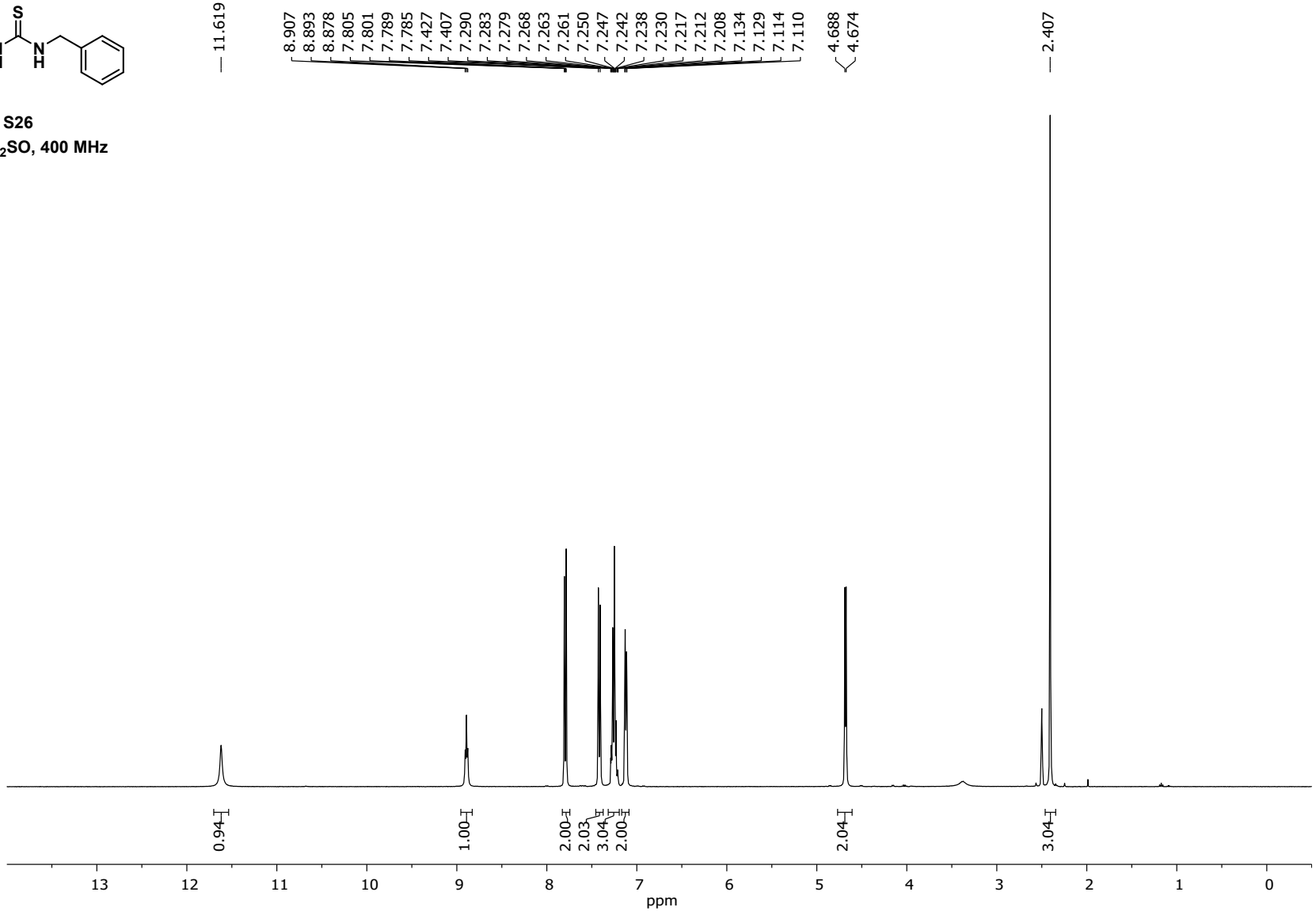
^{1}H, $(CD_3)_2SO$, 400 MHz

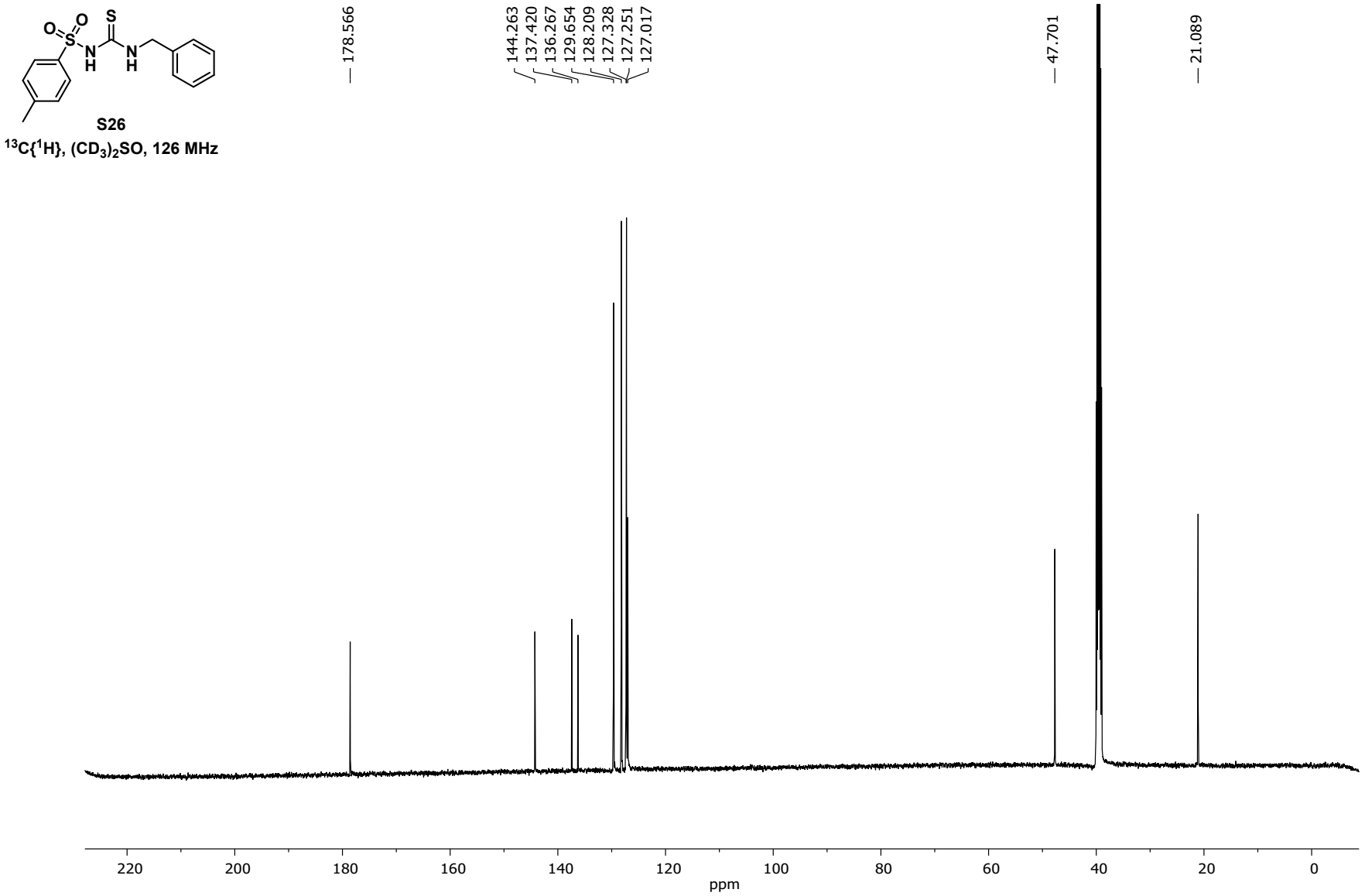

S25
$^{13}C\{^{1}H\}$, $(CD_3)_2SO$, 126 MHz
178.752
144.154
136.463
129.648
127.212
32.165
21.071
220
200
180
160
140
120
100
80
60
40
20
0
ppm

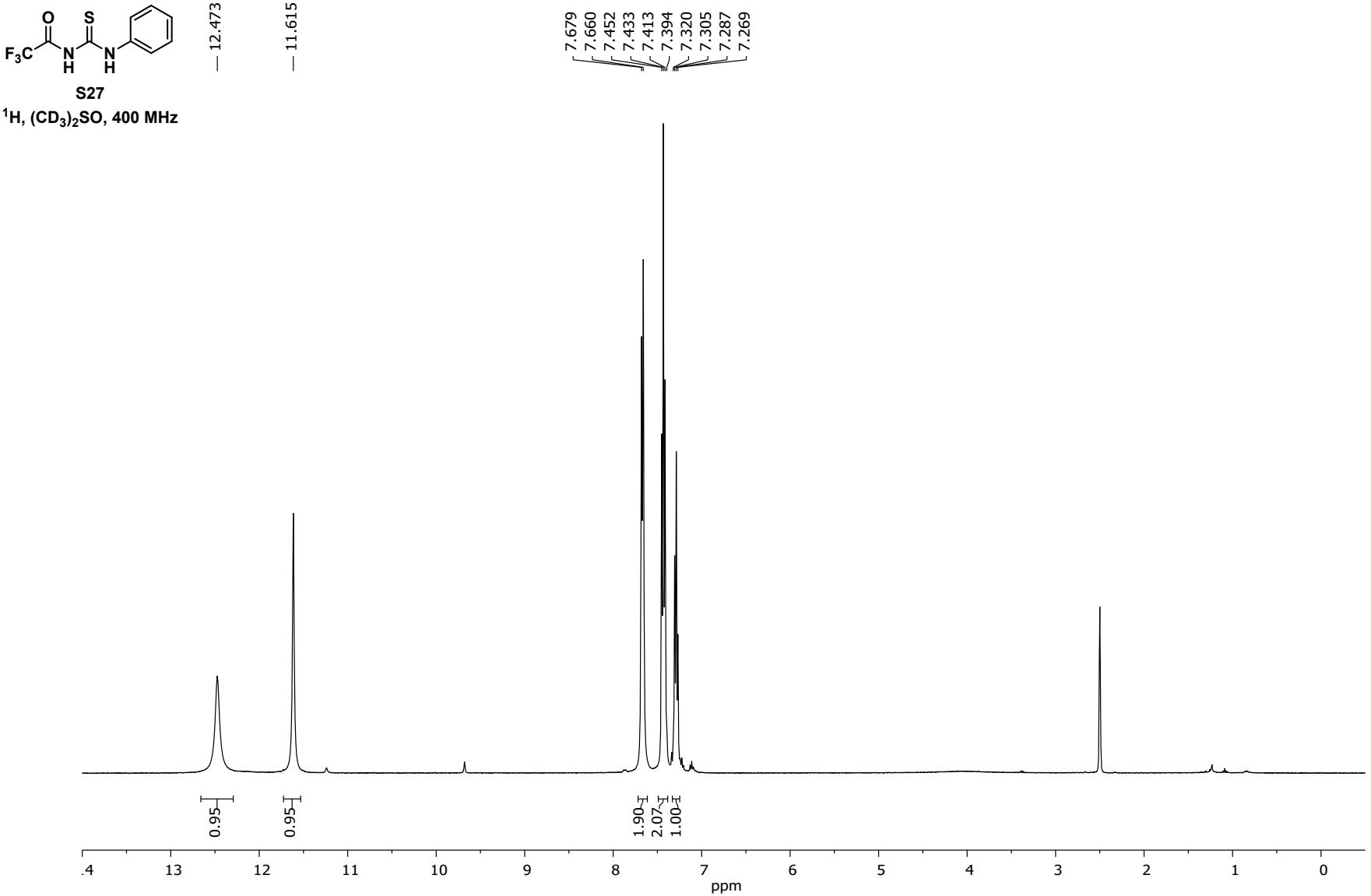


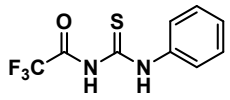
S26

^{1}H, $(CD_3)_2SO$, 400 MHz



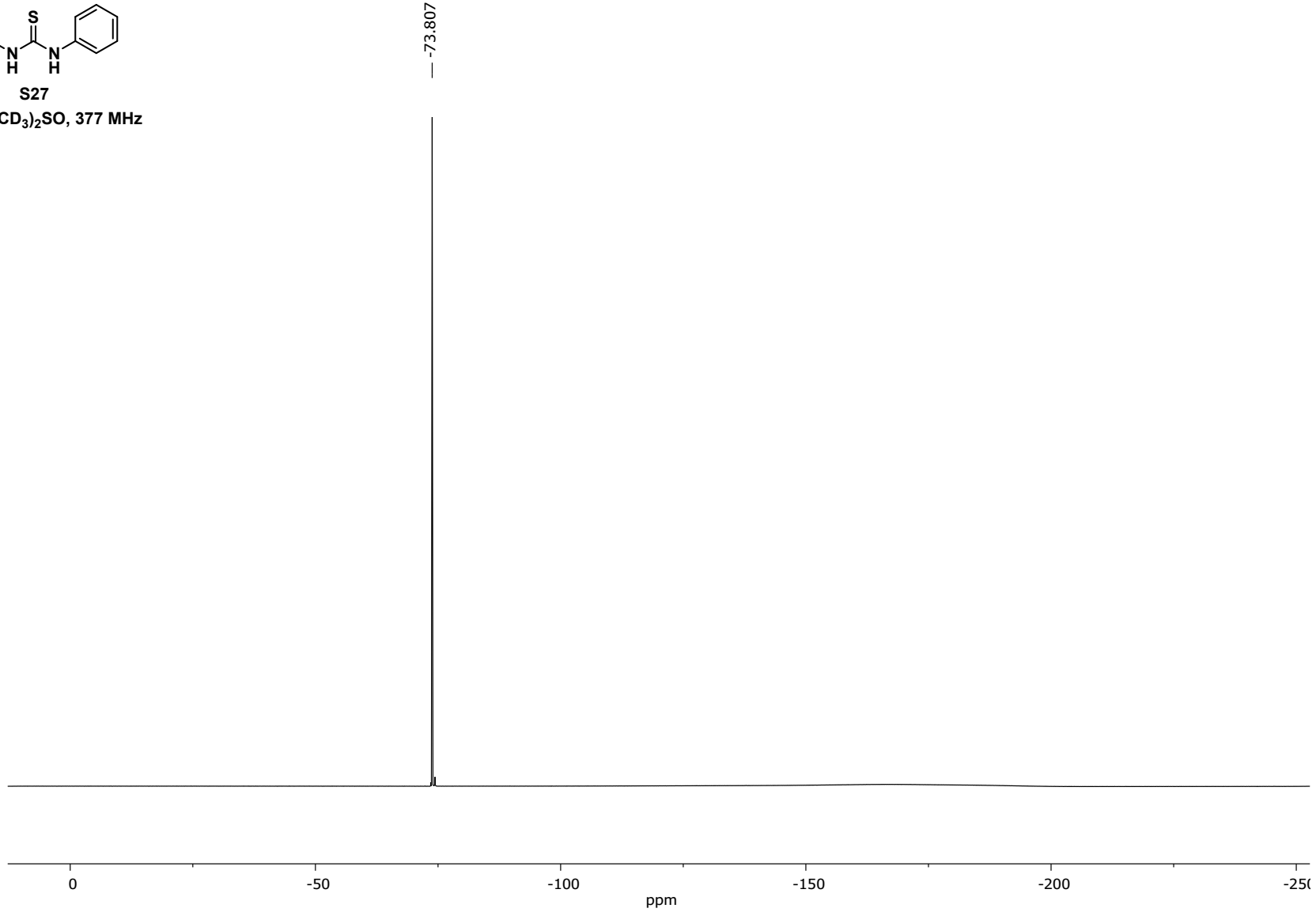

S26
$^{13}C\{^{1}H\}$, $(CD_3)_2SO$, 126 MHz
178.566
144.263
137.420
136.267
129.654
128.209
127.328
127.251
127.017
47.701
21.089
220
200
180
160
140
120
100
80
60
40
20
0
ppm

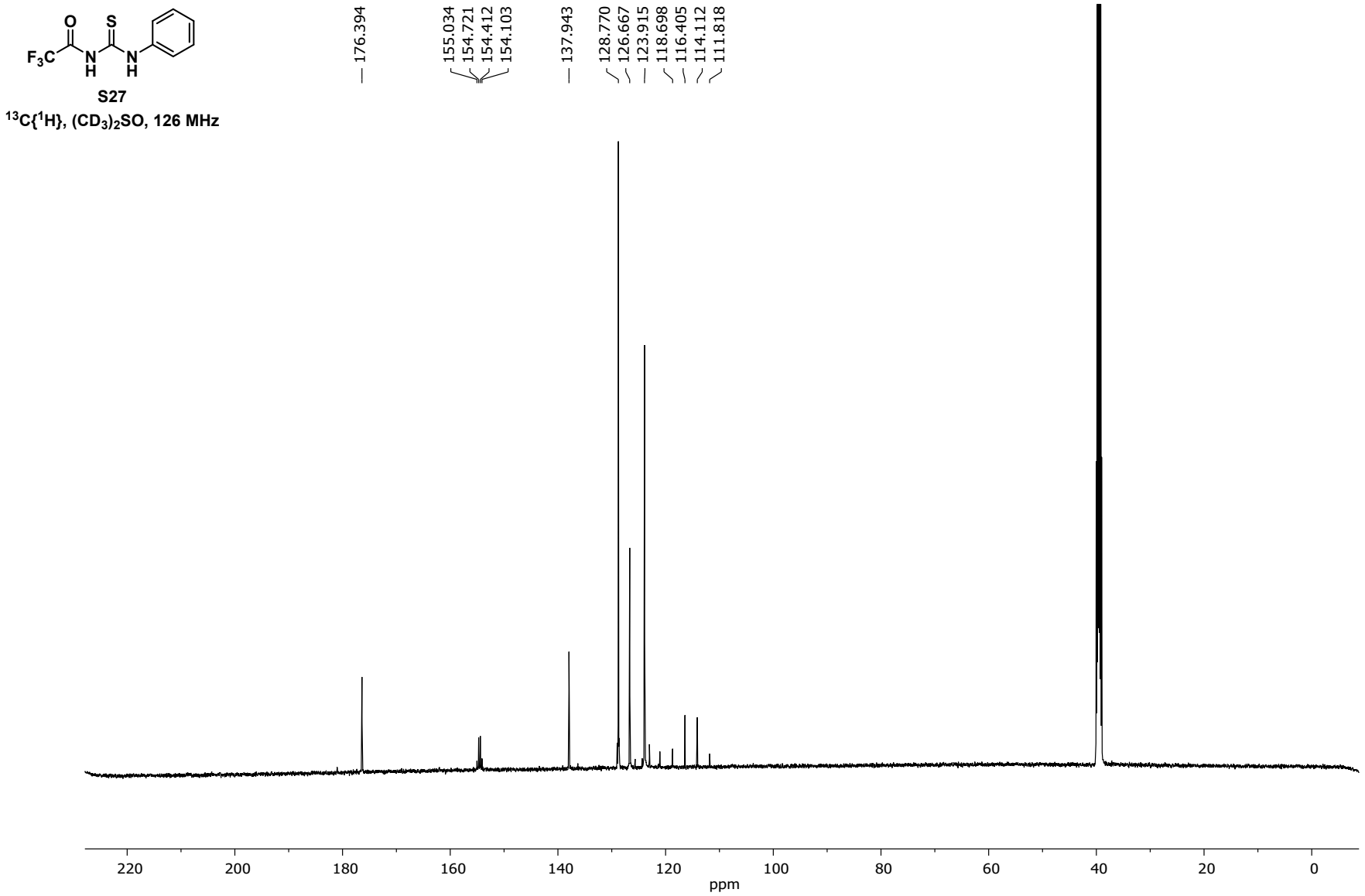

S27
^{1}H, $(CD_3)_2SO$, 400 MHz
12.473
11.615
7.679
7.660
7.452
7.433
7.413
7.394
7.320
7.305
7.287
7.269
0.95
0.95
1.90
2.07
1.00
ppm

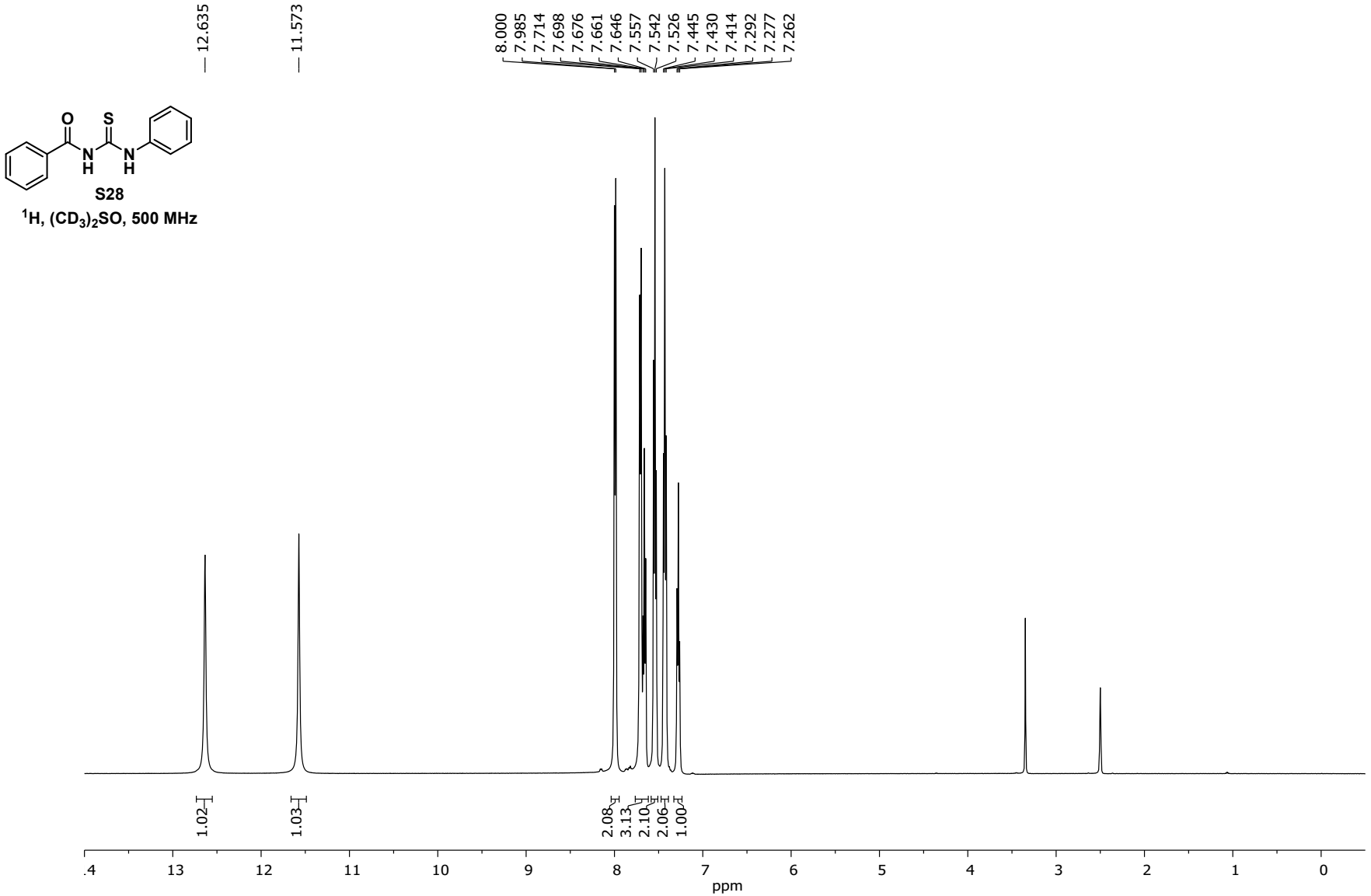


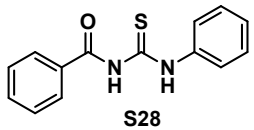
S27

$^{19}F\{^{1}H\}$, $(CD_3)_2SO$, 377 MHz



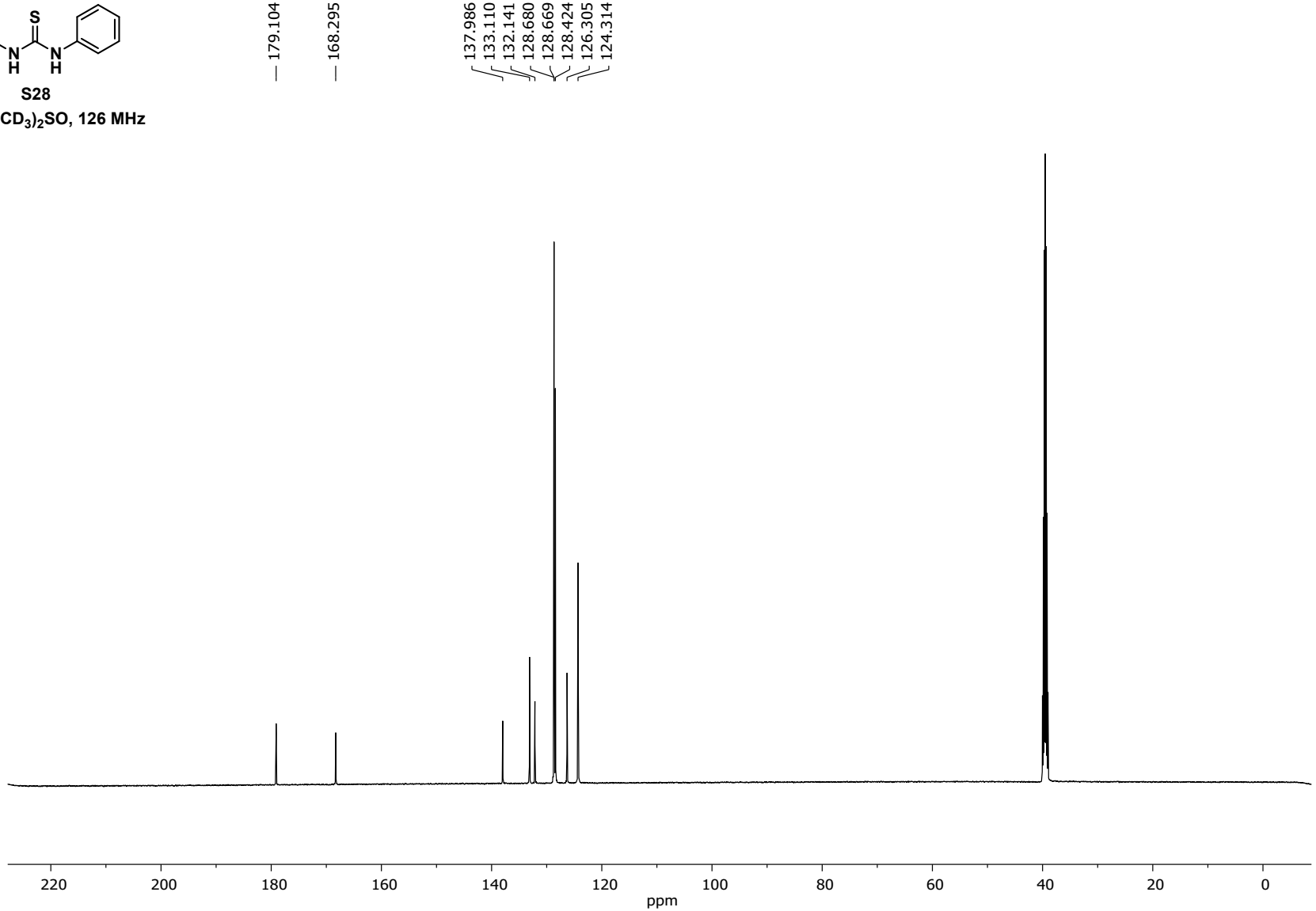

S27
$^{13}C\{^{1}H\}$, $(CD_3)_2SO$, 126 MHz
176.394
155.034
154.721
154.412
154.103
137.943
128.770
126.667
123.915
118.698
116.405
114.112
111.818
220
200
180
160
140
120
100
80
60
40
20
0
ppm

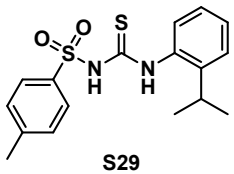

12.635
11.573
8.000
7.985
7.714
7.698
7.676
7.661
7.646
7.557
7.542
7.526
7.445
7.430
7.414
7.292
7.277
7.262
O
S
N
H
N
H
S28
1H, (CD3)2SO, 500 MHz
1.02
1.03
2.08
3.13
2.10
2.06
1.00
ppm



S28

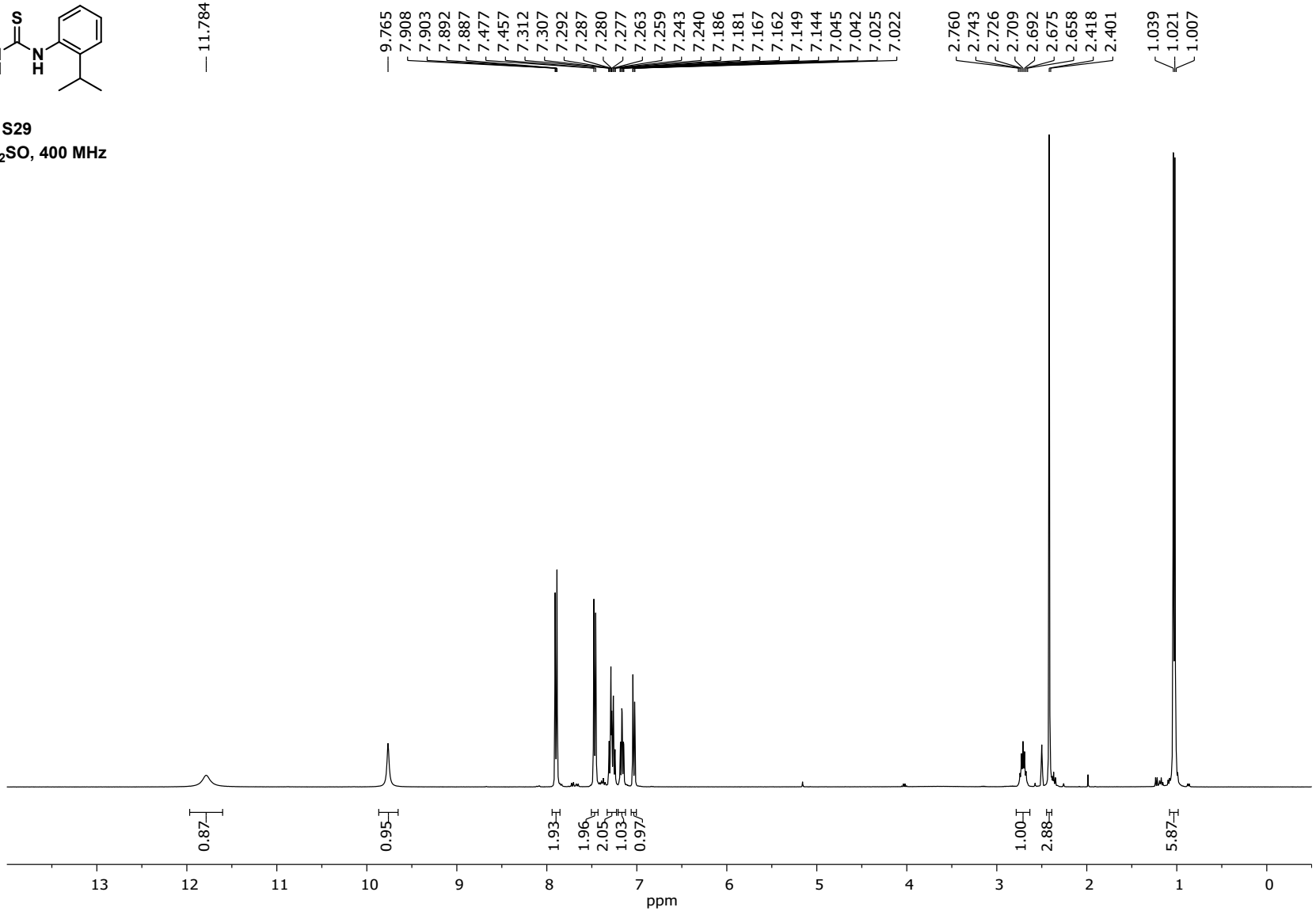
$^{13}C\{^{1}H\}$, $(CD_3)_2SO$, 126 MHz

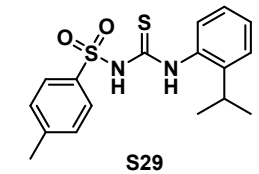




S29

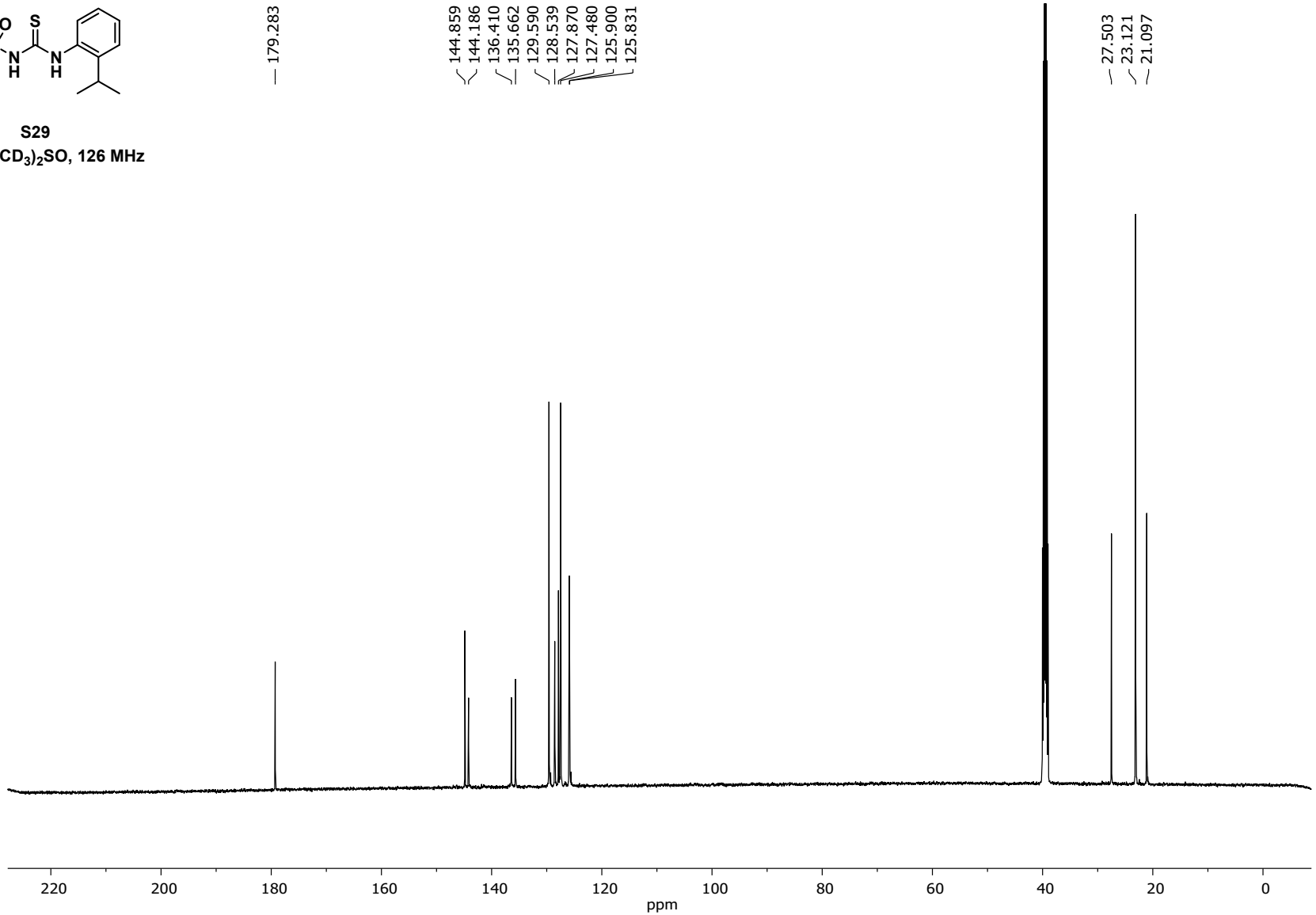
^{1}H, $(CD_3)_2SO$, 400 MHz

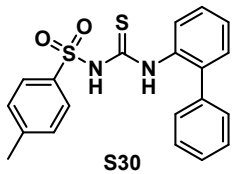




S29

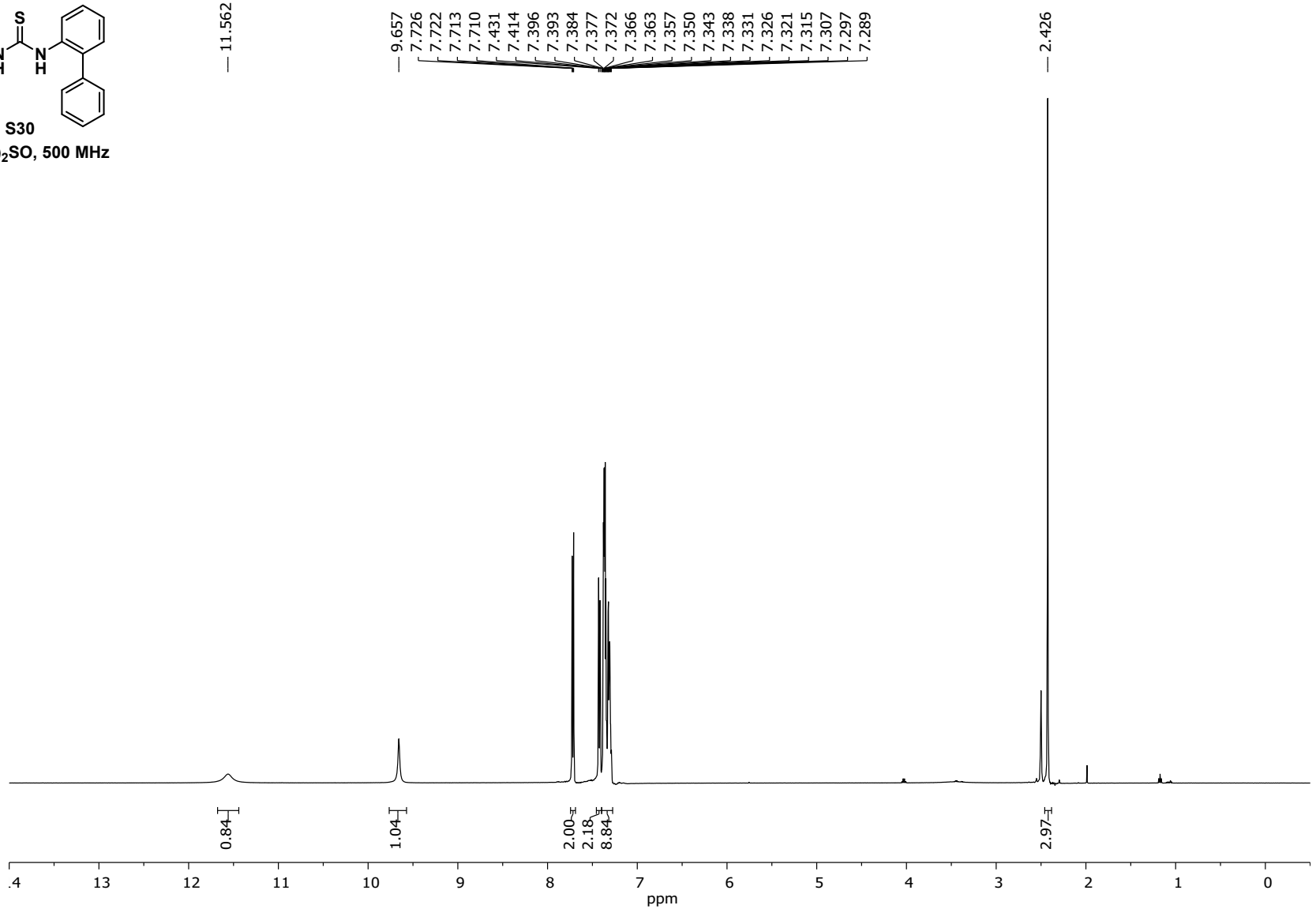
$^{13}C\{^{1}H\}$, $(CD_3)_2SO$, 126 MHz

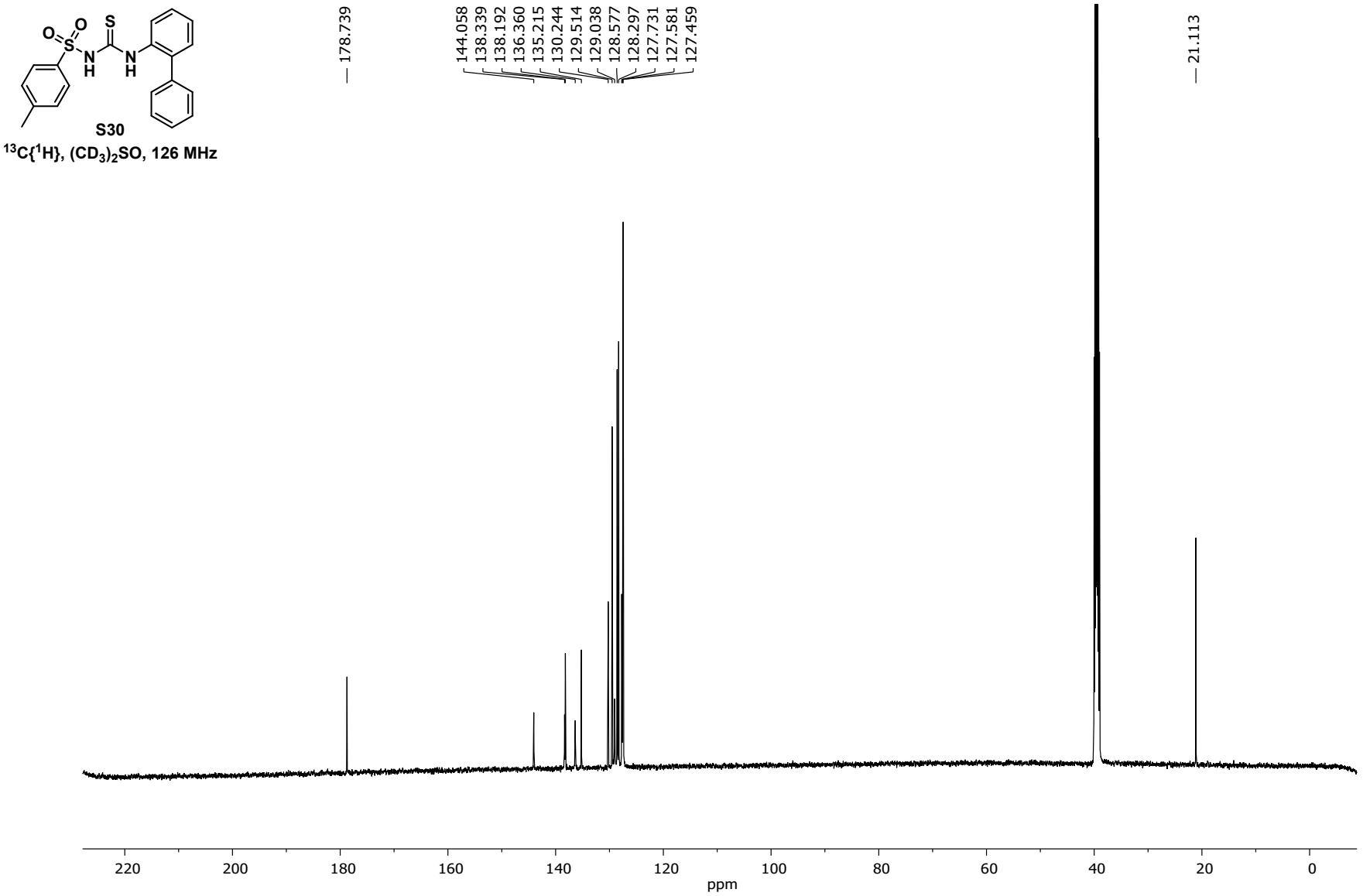


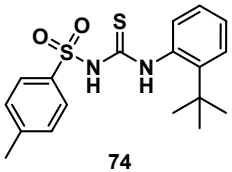


S30

^{1}H, $(CD_3)_2SO$, 500 MHz

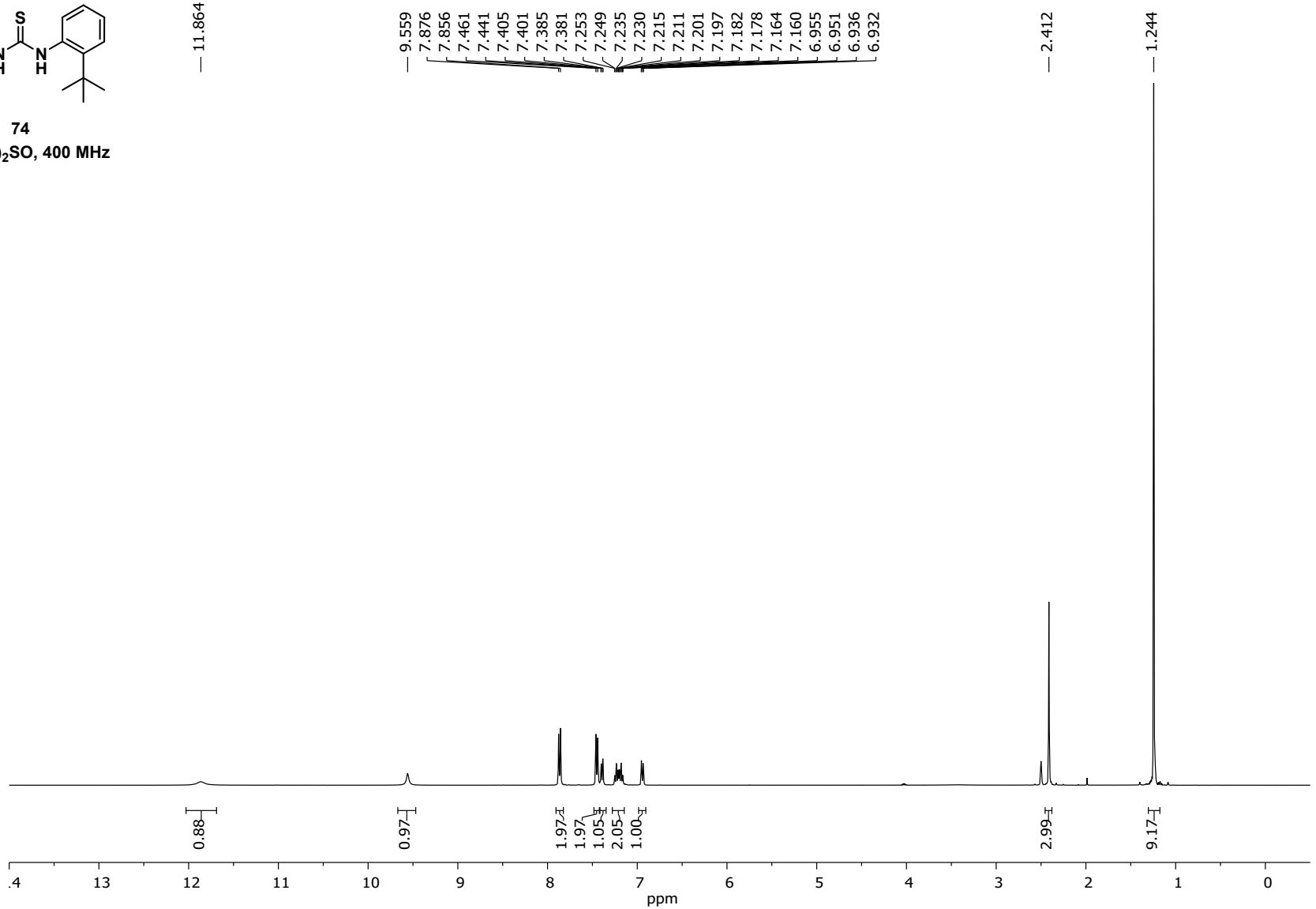


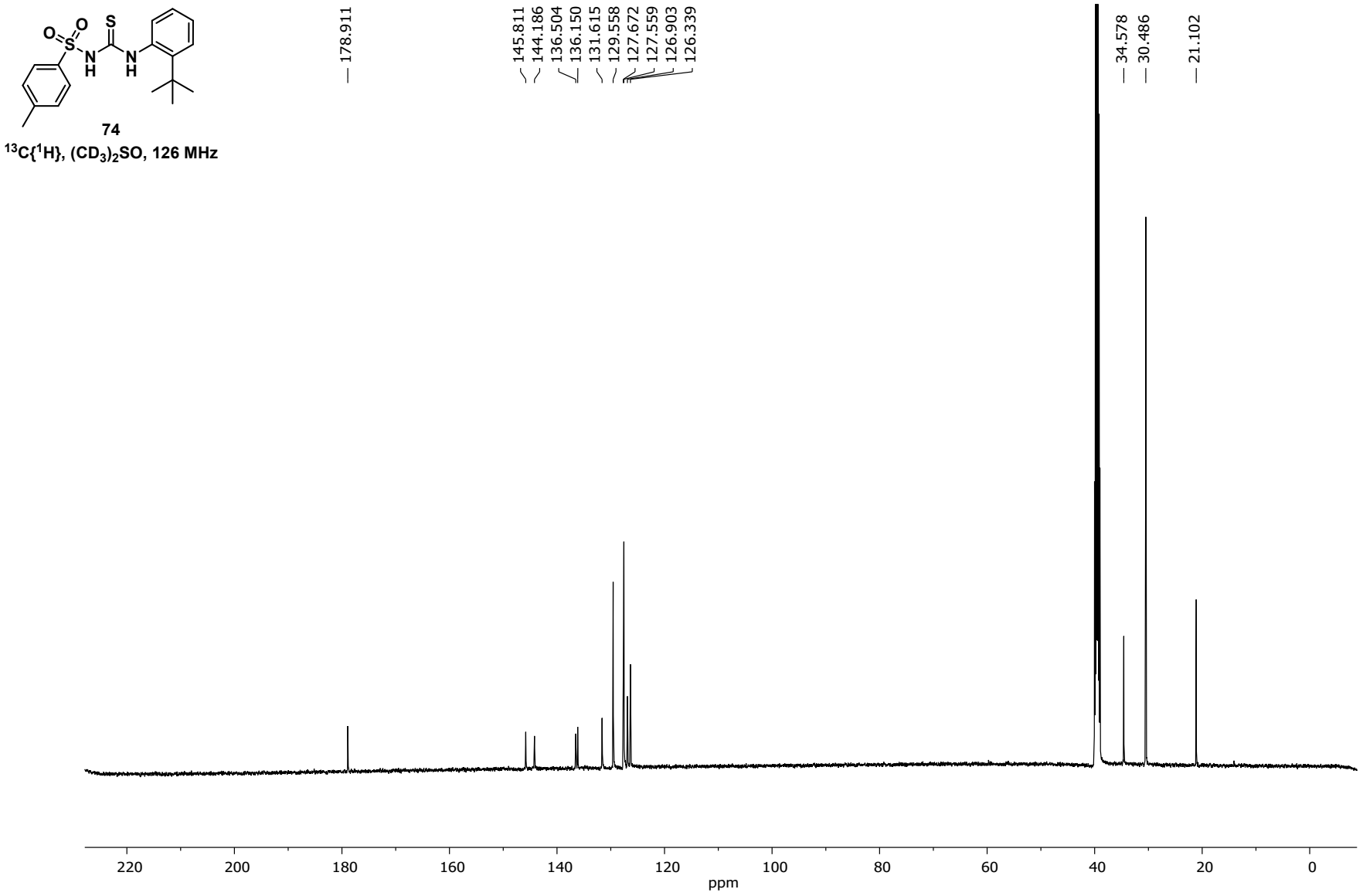

S30
$^{13}C\{^{1}H\}$, $(CD_3)_2SO$, 126 MHz
178.739
144.058
138.339
138.192
136.360
135.215
130.244
129.514
129.038
128.577
128.297
127.731
127.581
127.459
21.113
220
200
180
160
140
120
100
80
60
40
20
0
ppm

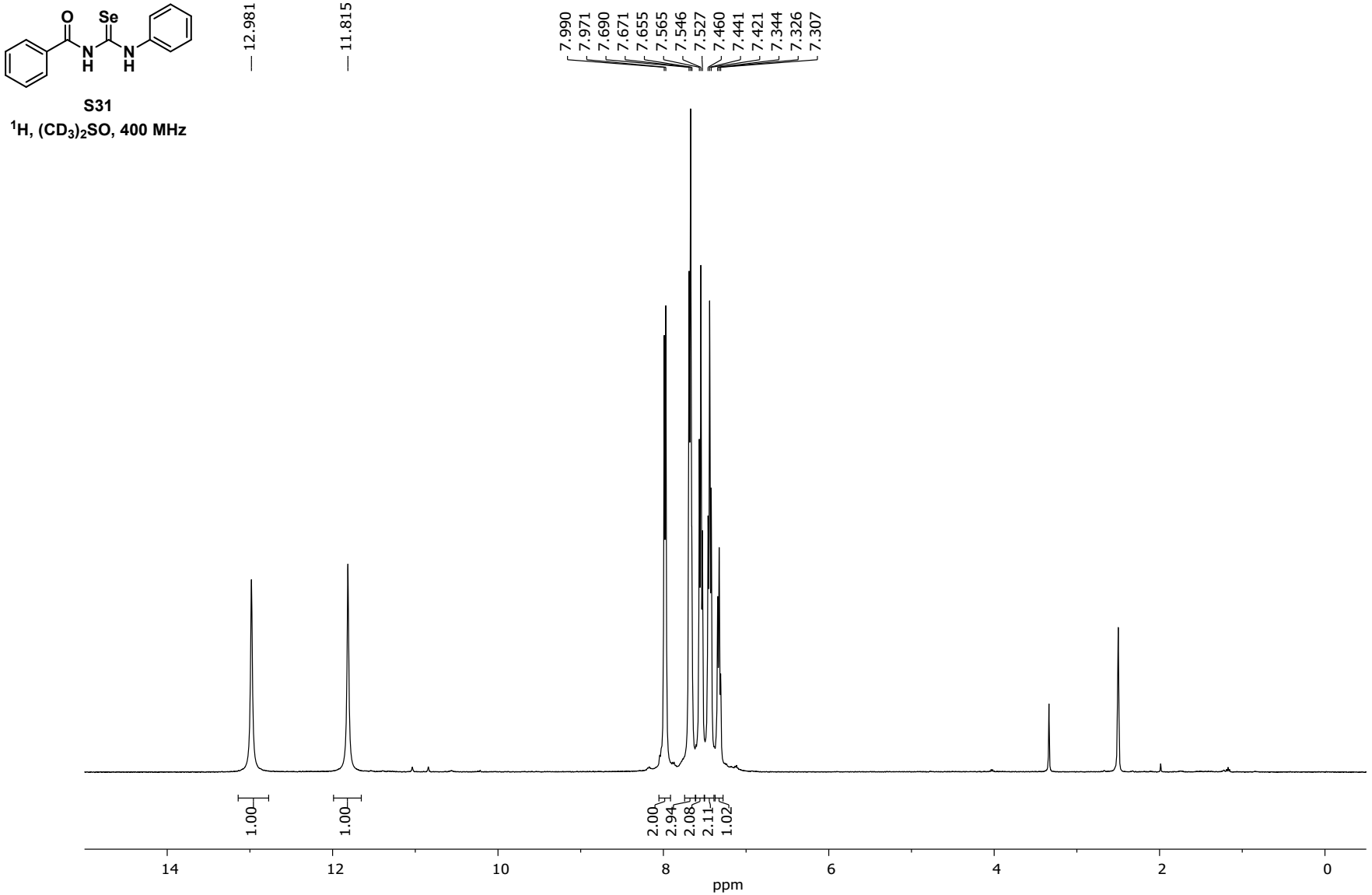


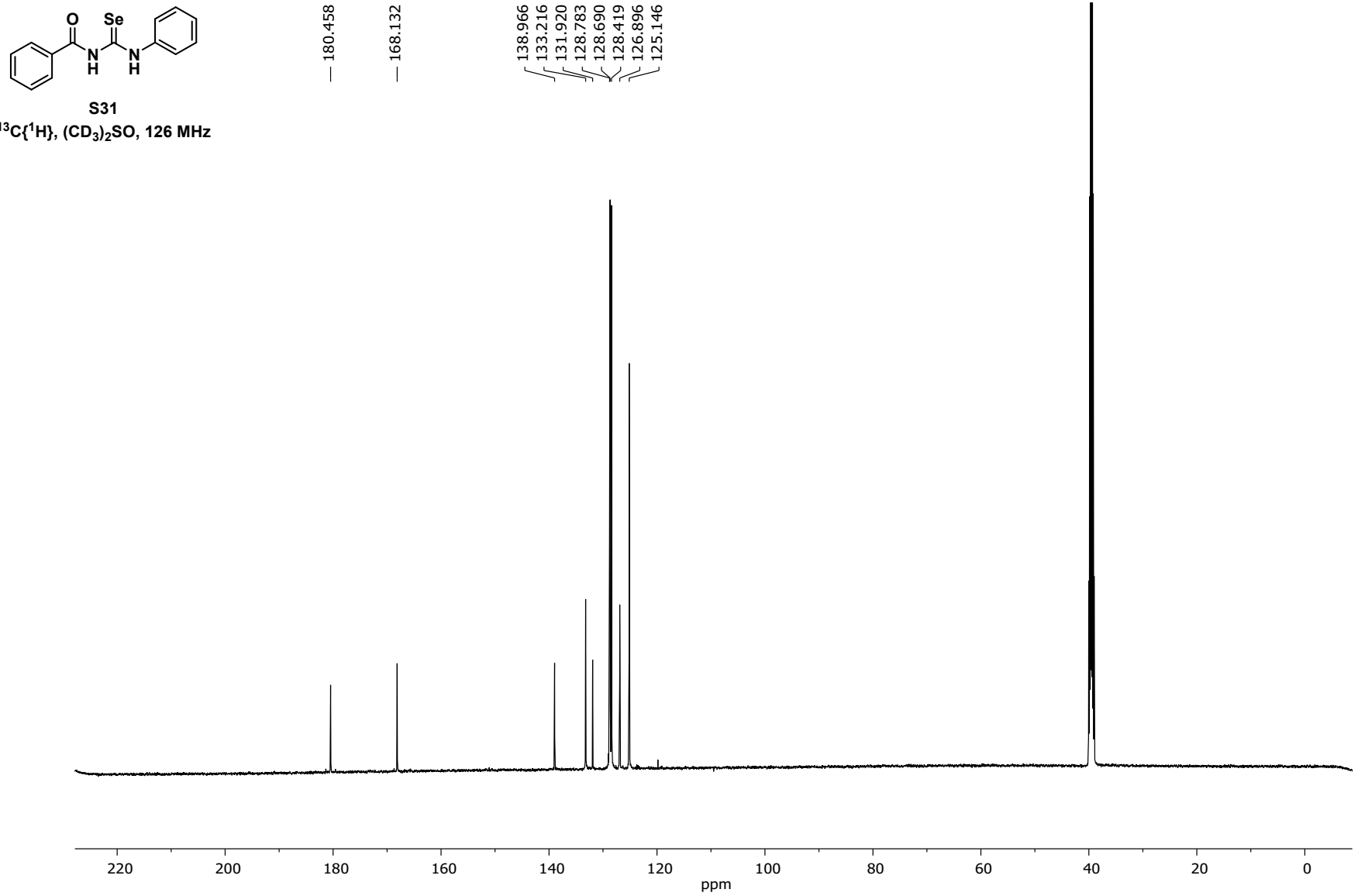
74

^{1}H, $(CD_3)_2SO$, 400 MHz



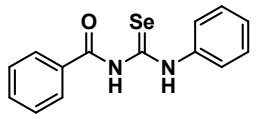

74
$^{13}C\{^{1}H\}$, $(CD_3)_2SO$, 126 MHz
178.911
145.811
144.186
136.504
136.150
131.615
129.558
127.672
127.559
126.903
126.339
34.578
30.486
21.102
220
200
180
160
140
120
100
80
60
40
20
0
ppm


S31
^{1}H, $(CD_3)_2SO$, 400 MHz
12.981
11.815
7.990
7.971
7.690
7.671
7.655
7.565
7.546
7.527
7.460
7.441
7.421
7.344
7.326
7.307
1.00
1.00
2.00
2.94
2.08
2.11
1.02
14
12
10
8
6
4
2
0
ppm



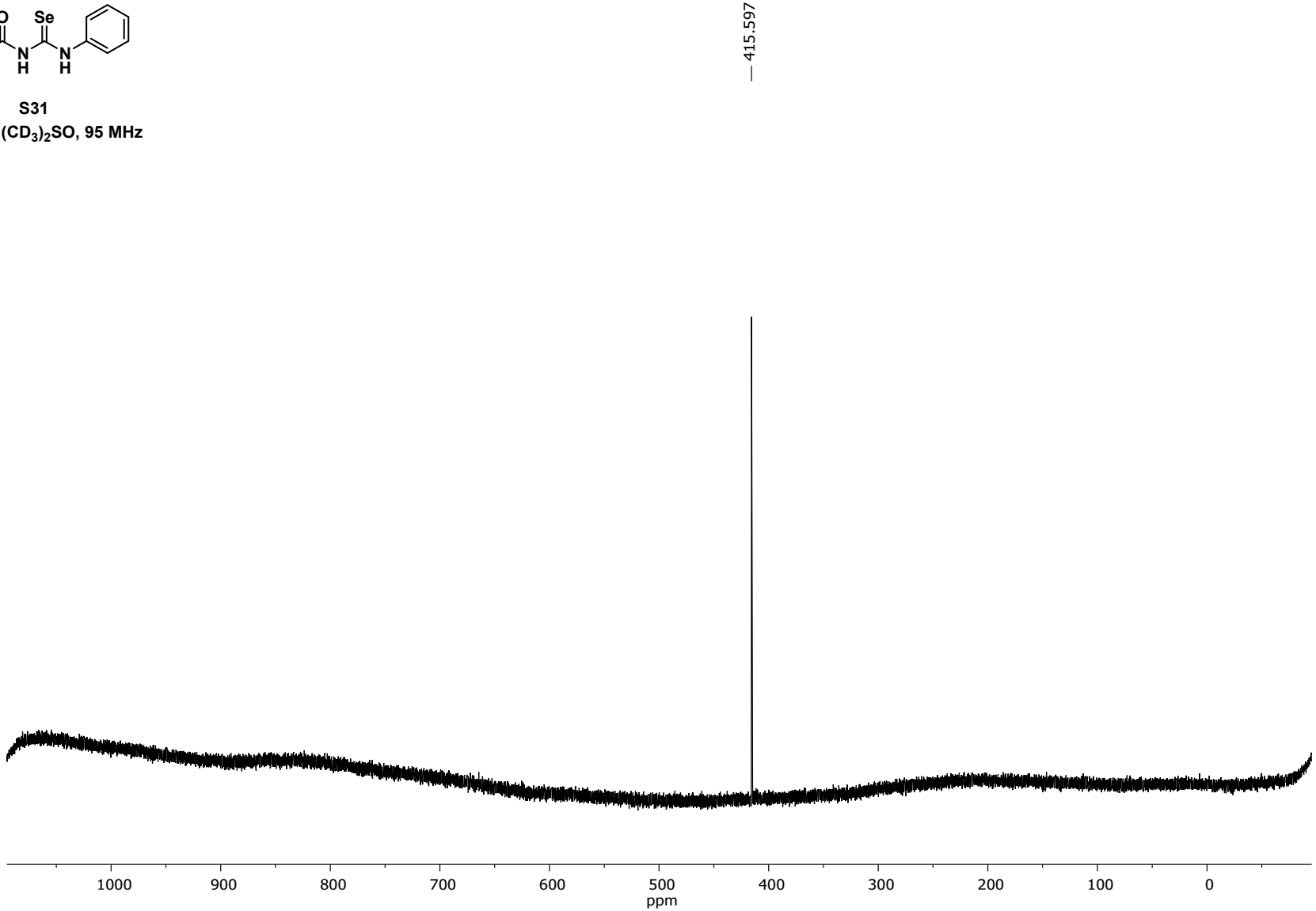
S31

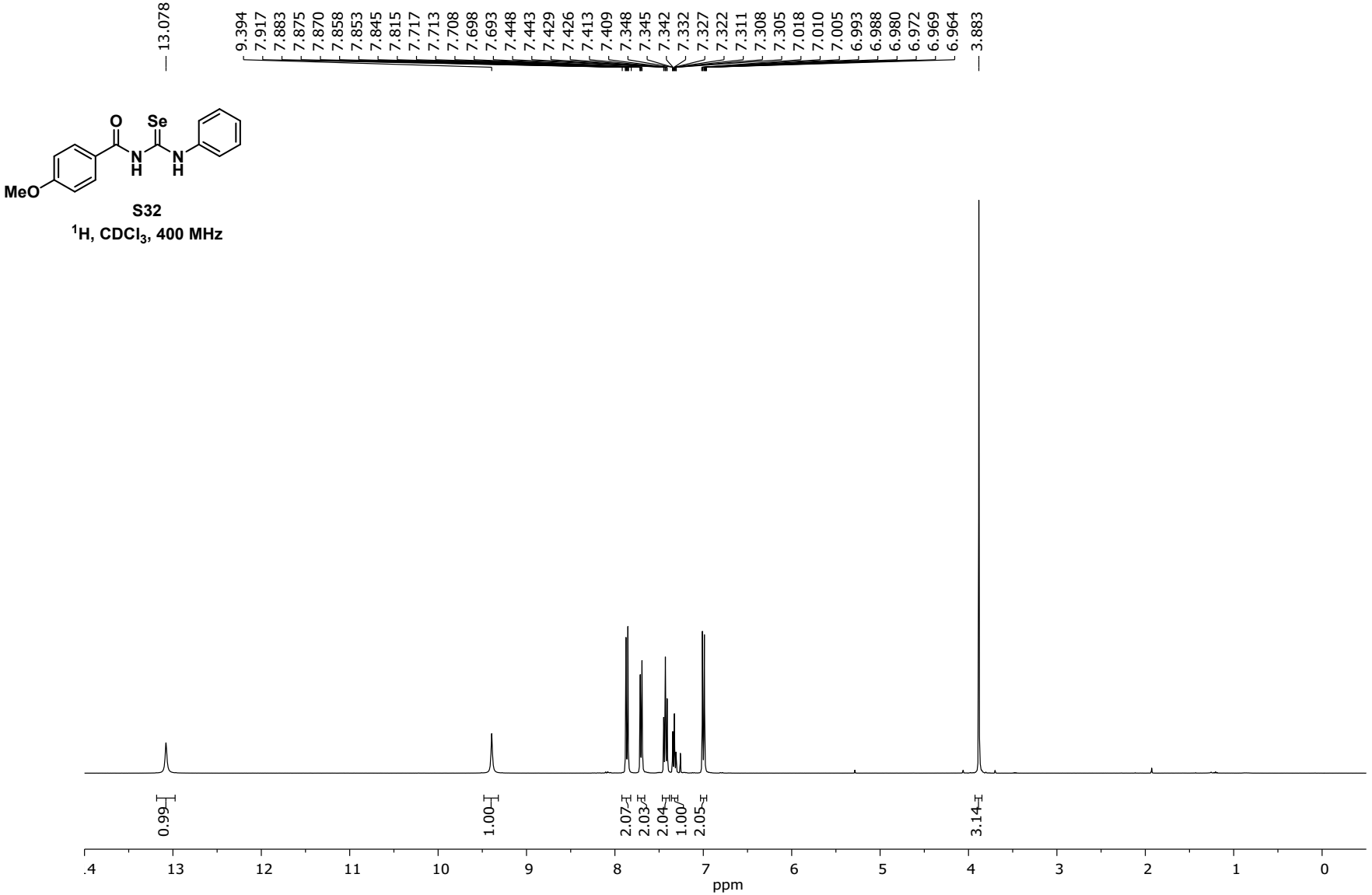
$^{13}C\{^{1}H\}$, $(CD_3)_2SO$, 126 MHz



S31

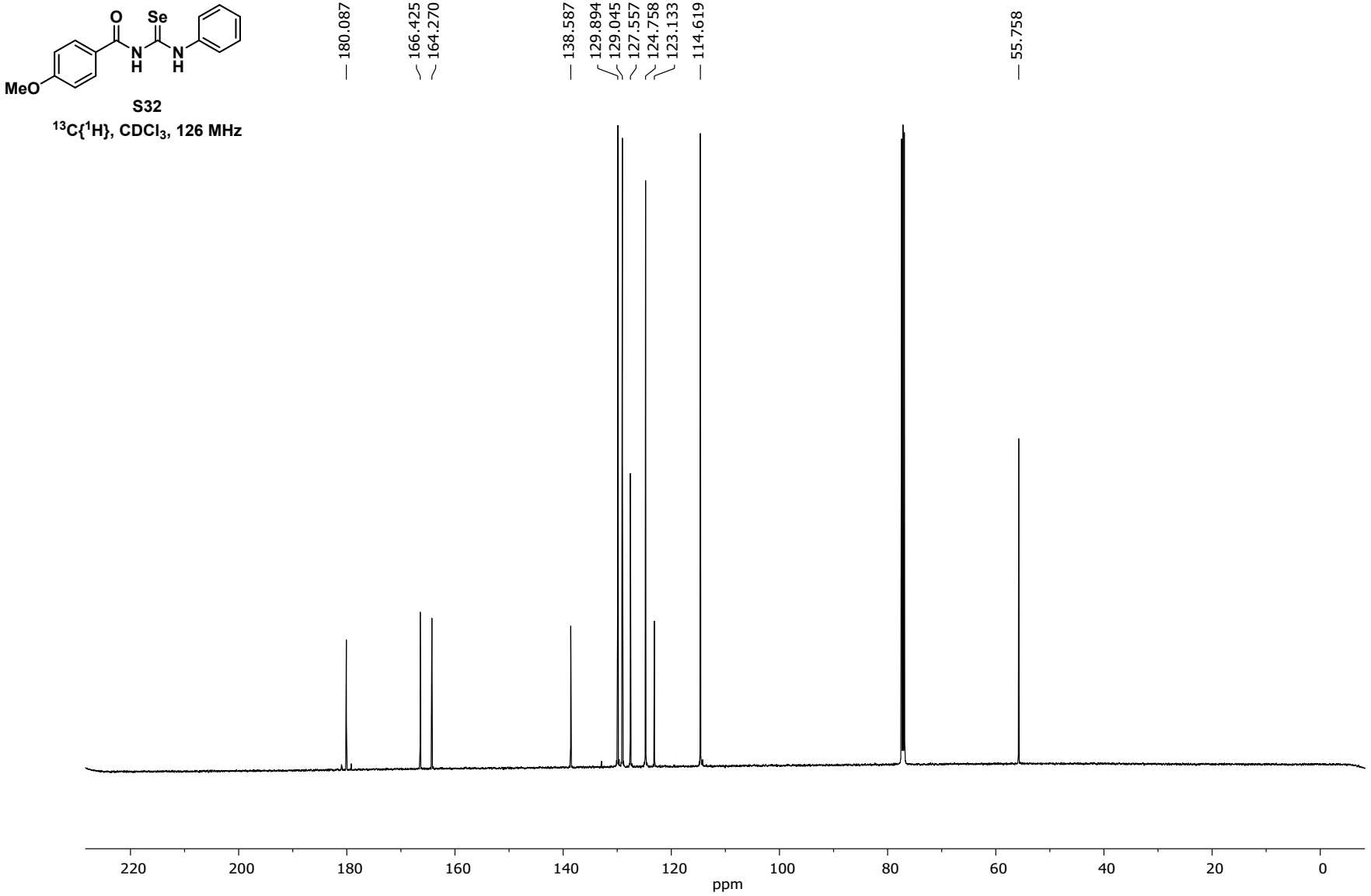
$^{77}Se\{^{1}H\}$, $(CD_3)_2SO$, 95 MHz





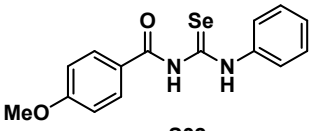
S32

^{1}H, $CDCl_3$, 400 MHz



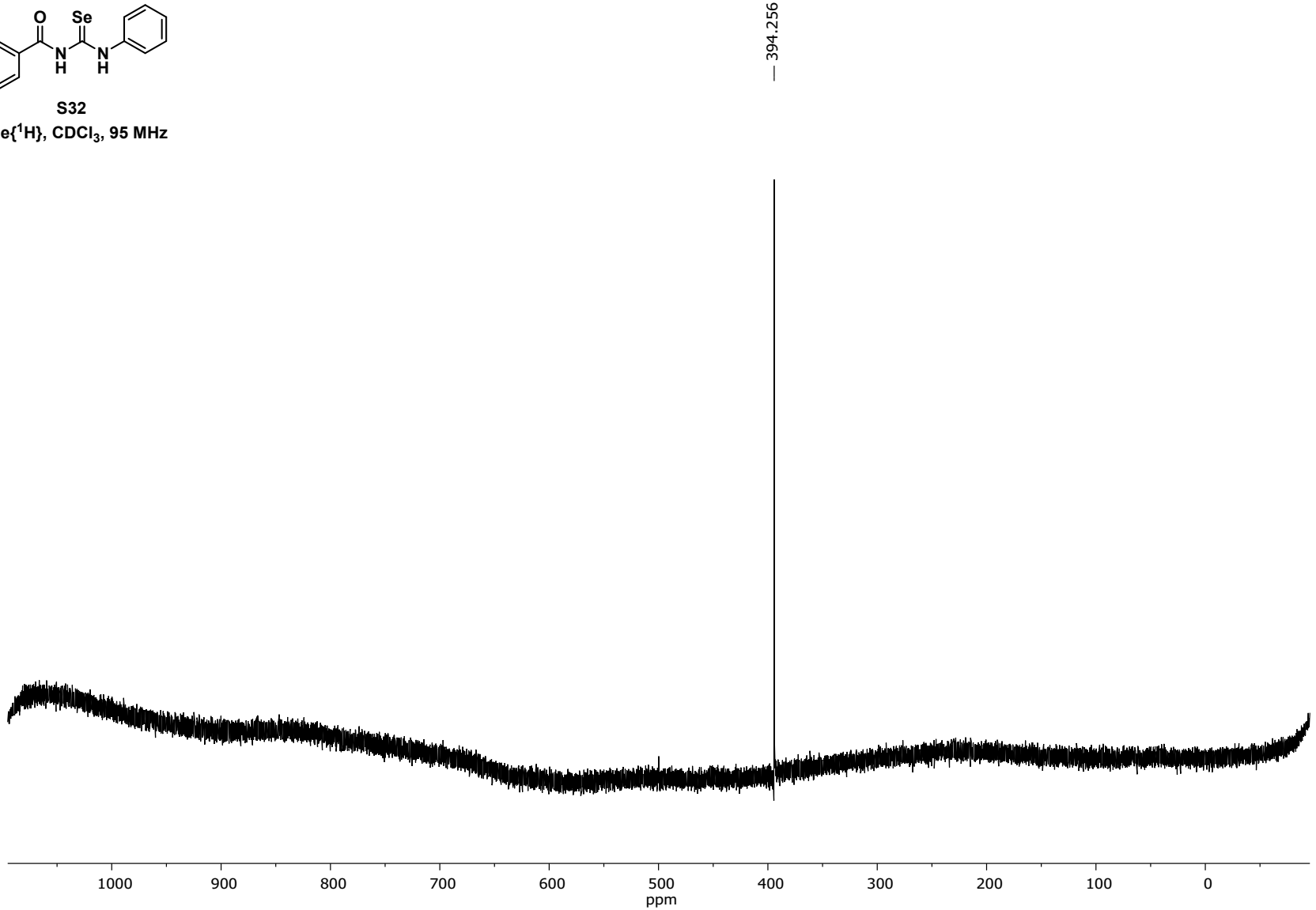
S32

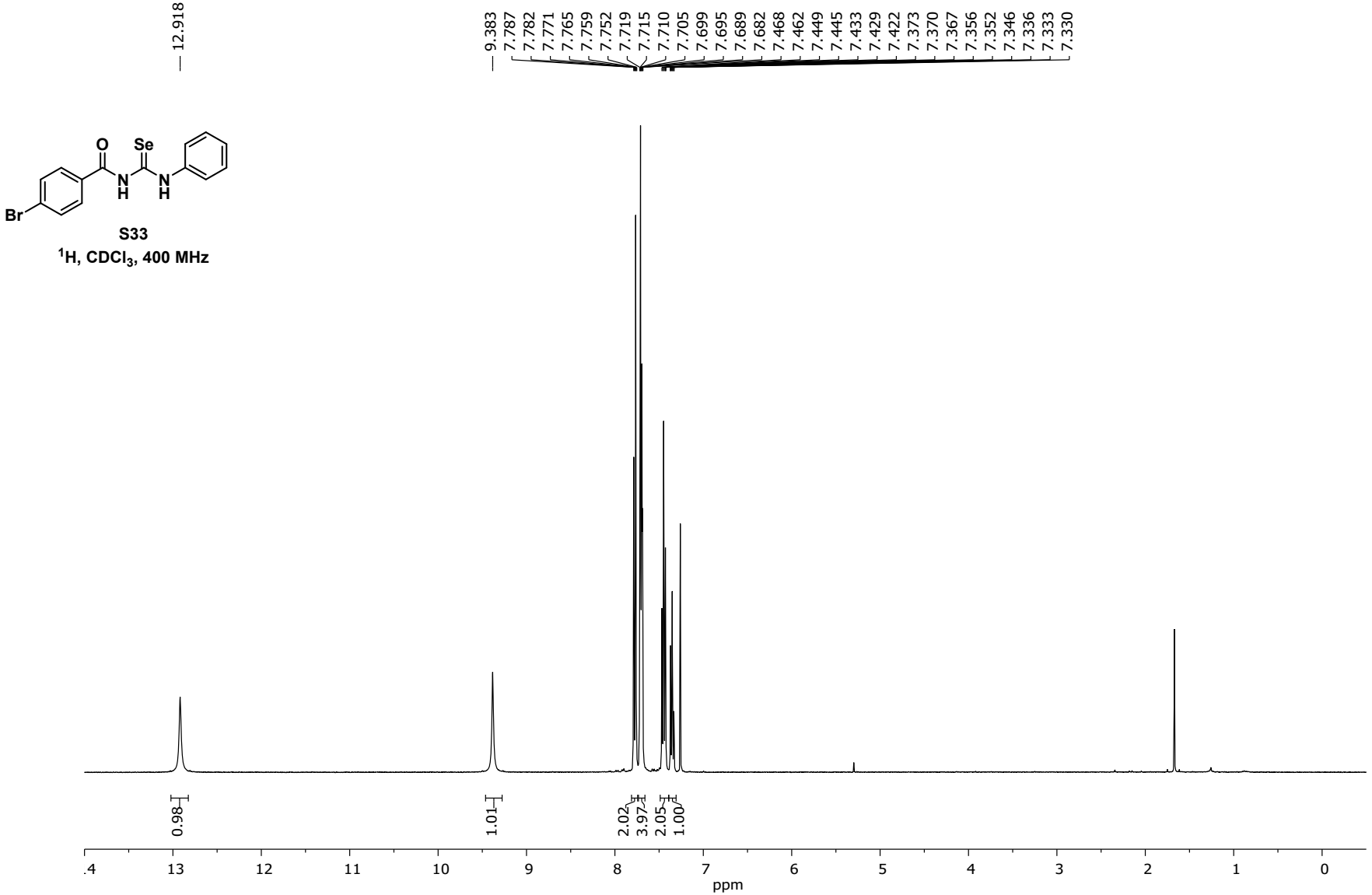
$^{13}C\{^{1}H\}$, $CDCl_3$, 126 MHz



S32

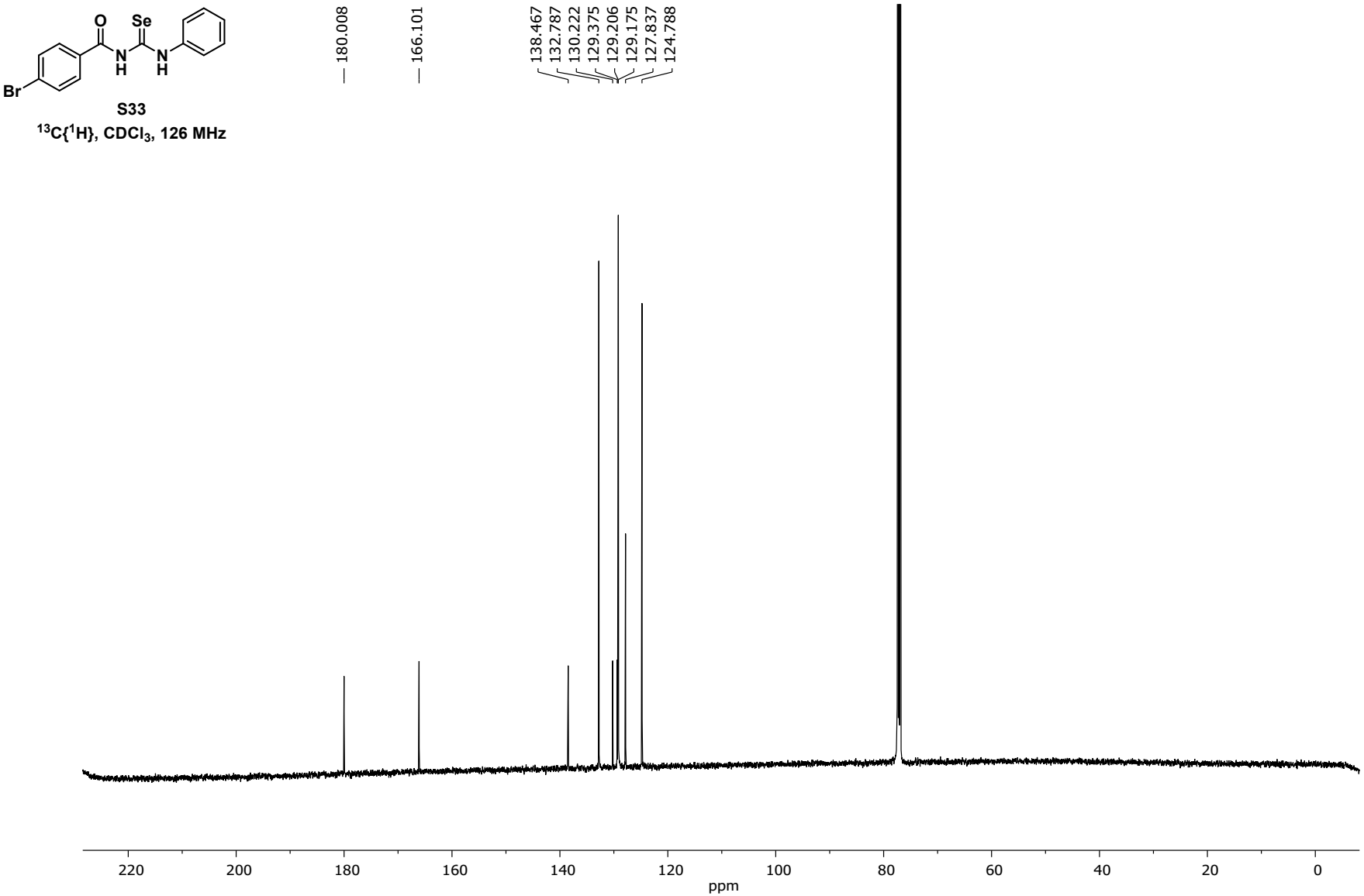
$^{77}Se\{^{1}H\}$, $CDCl_3$, 95 MHz





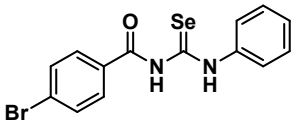
S33

^{1}H, $CDCl_3$, 400 MHz



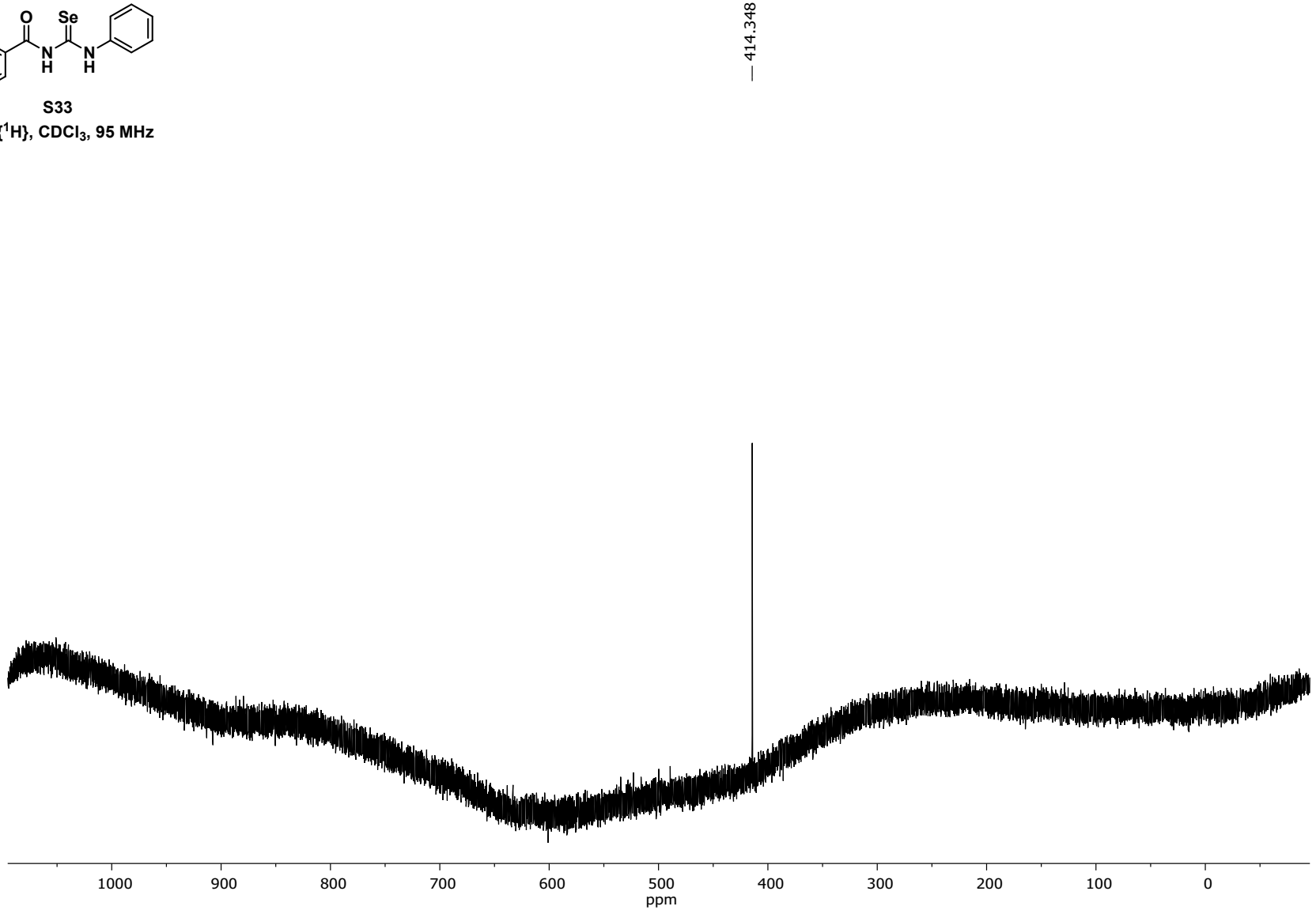
S33

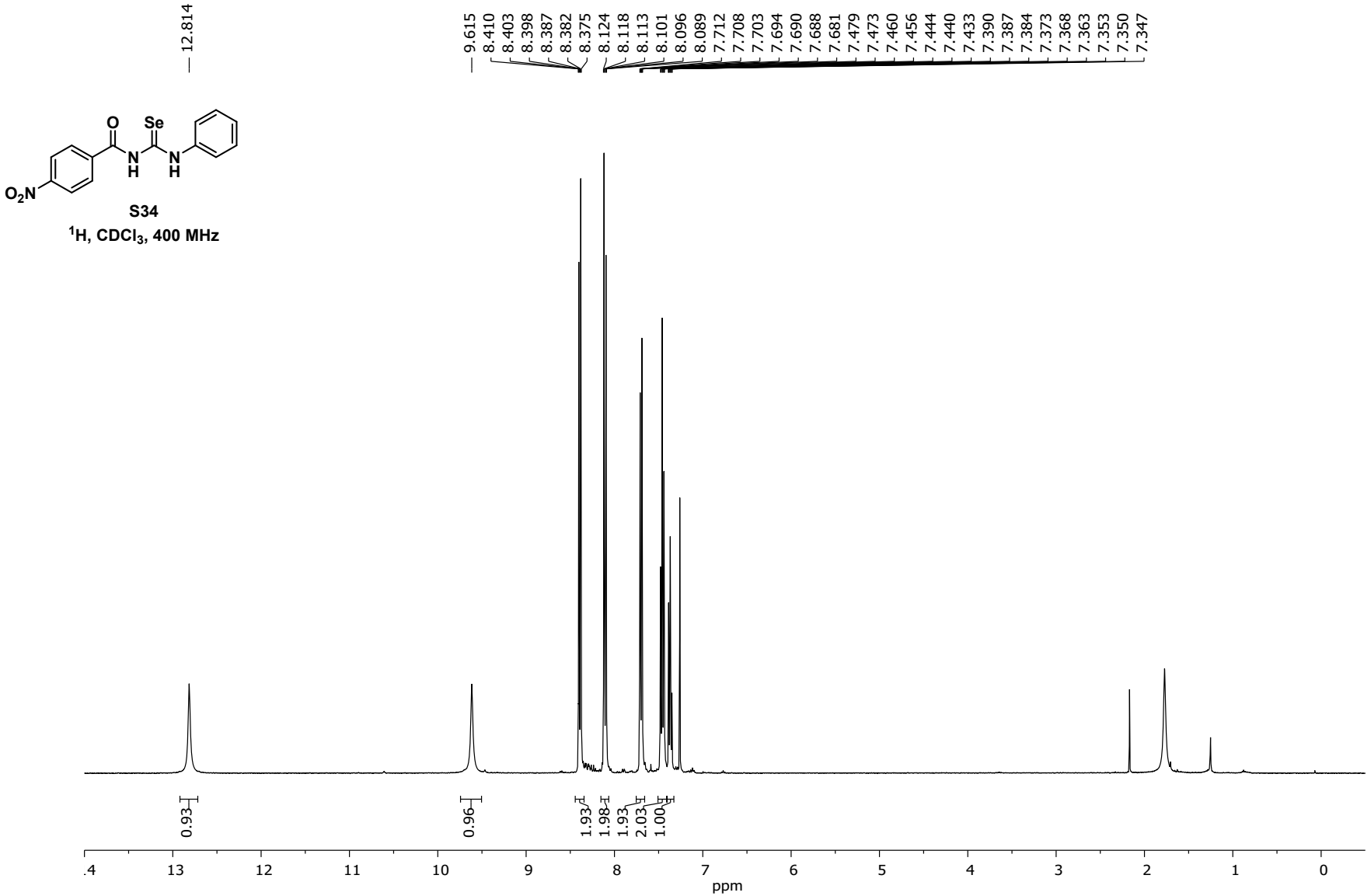
$^{13}C\{^{1}H\}$, $CDCl_3$, 126 MHz

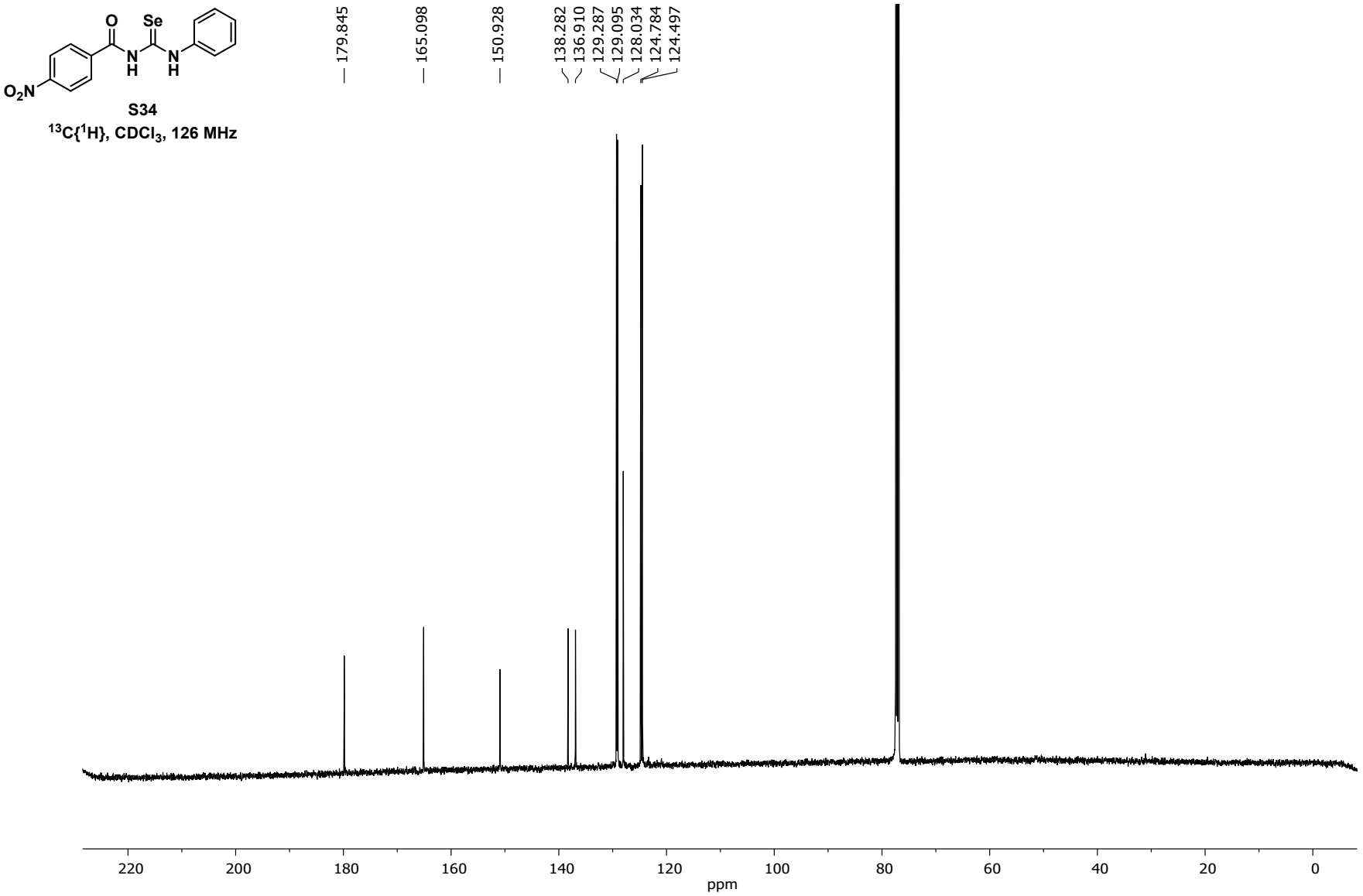


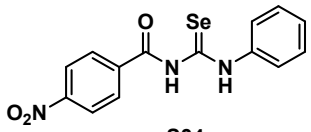
S33

$^{77}Se\{^{1}H\}$, $CDCl_3$, 95 MHz



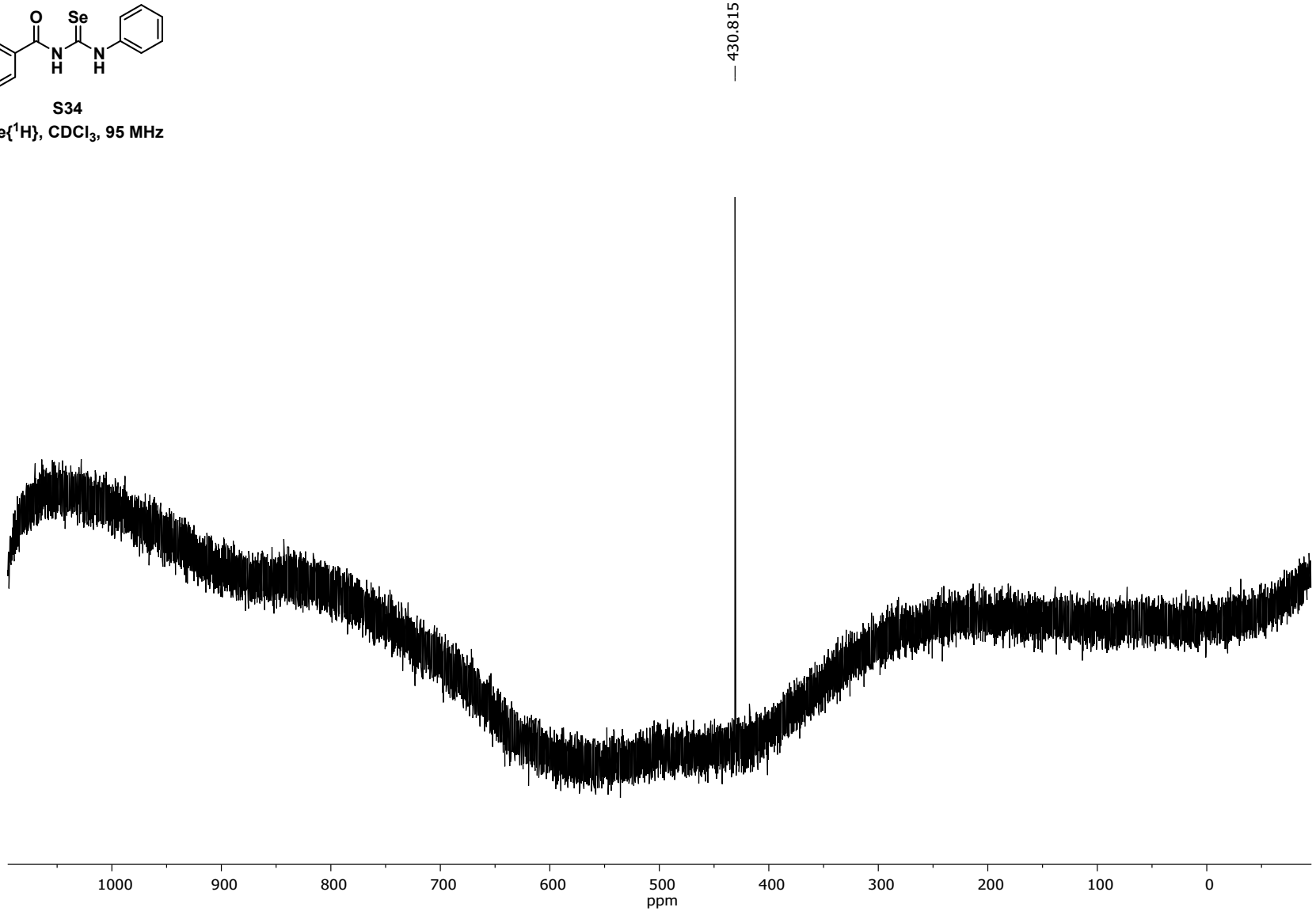

12.814
9.615
8.410
8.403
8.398
8.387
8.382
8.375
8.124
8.118
8.113
8.101
8.096
8.089
7.712
7.708
7.703
7.694
7.690
7.688
7.681
7.479
7.473
7.460
7.456
7.444
7.440
7.433
7.390
7.387
7.384
7.373
7.368
7.363
7.353
7.350
7.347
O
Se
N
H
N
H
O2N
S34
1H, CDCl3, 400 MHz
0.93
0.96
1.93
1.98
1.93
2.03
1.00
ppm

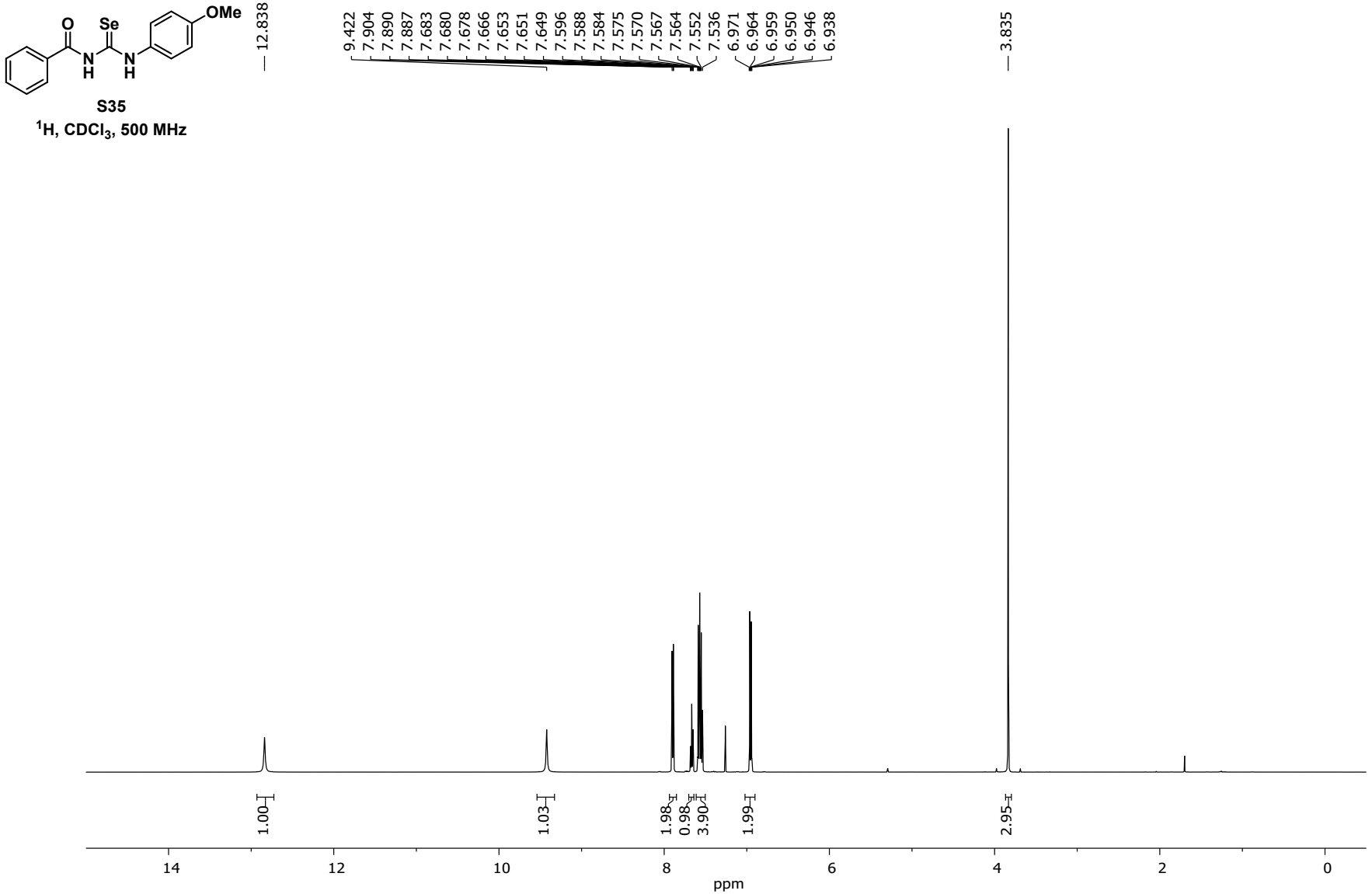

O
Se
N
H
N
H
O2N
S34
13C{1H}, CDCl3, 126 MHz
179.845
165.098
150.928
138.282
136.910
129.287
129.095
128.034
124.784
124.497
220
200
180
160
140
120
100
80
60
40
20
0
ppm



S34

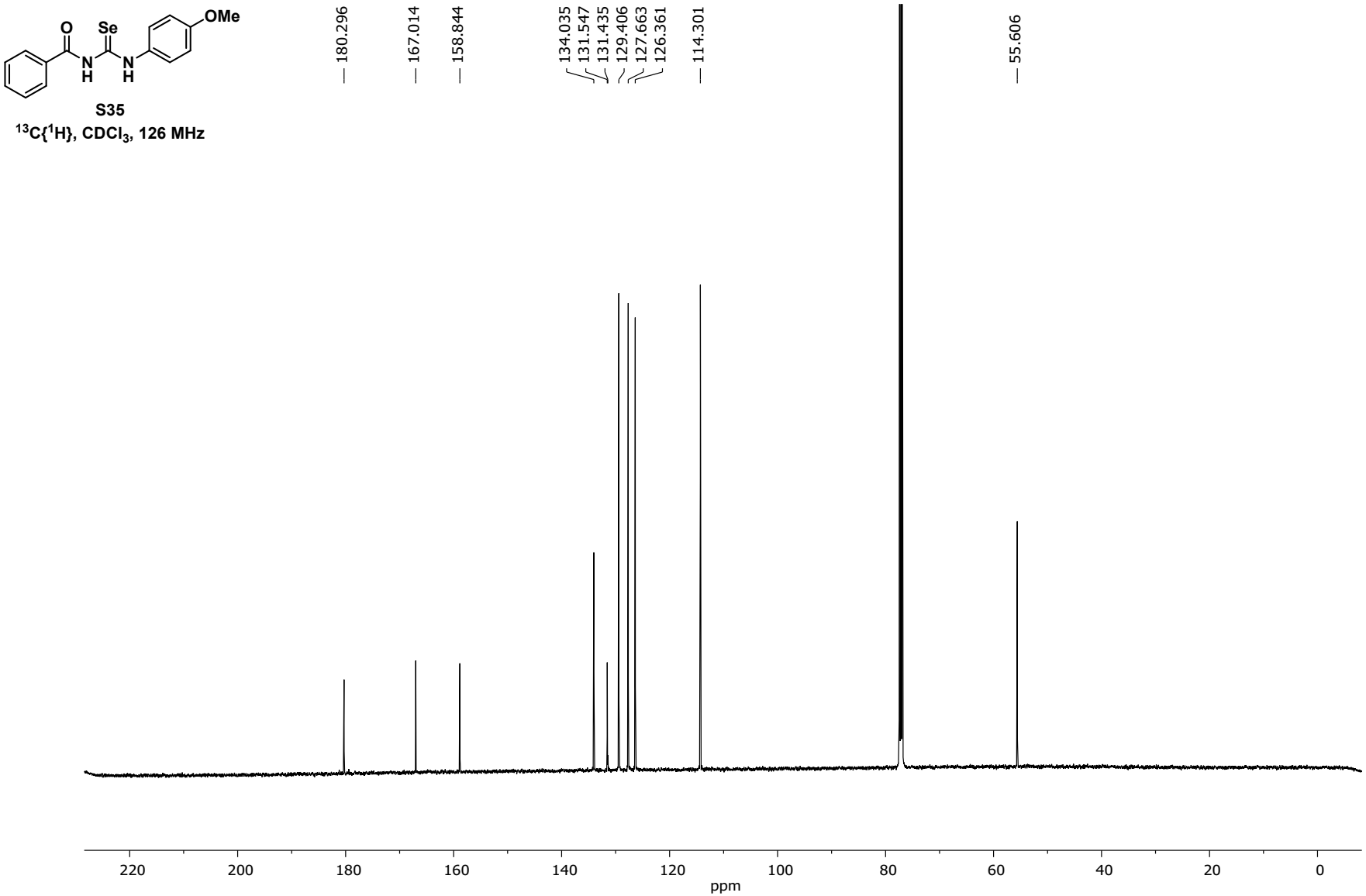
$^{77}Se\{^{1}H\}$, $CDCl_3$, 95 MHz





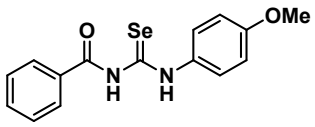
S35

^{1}H, $CDCl_3$, 500 MHz



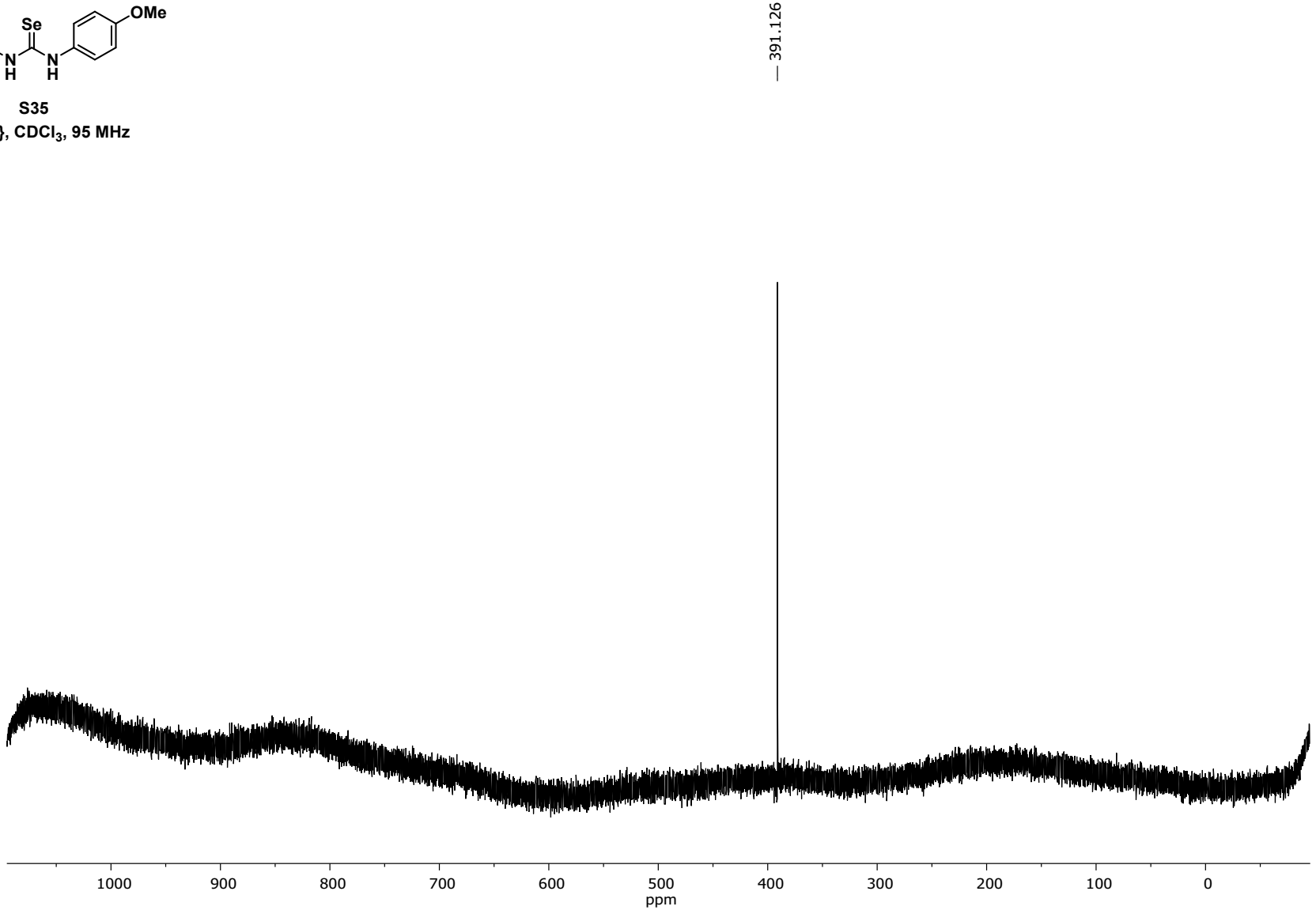
S35

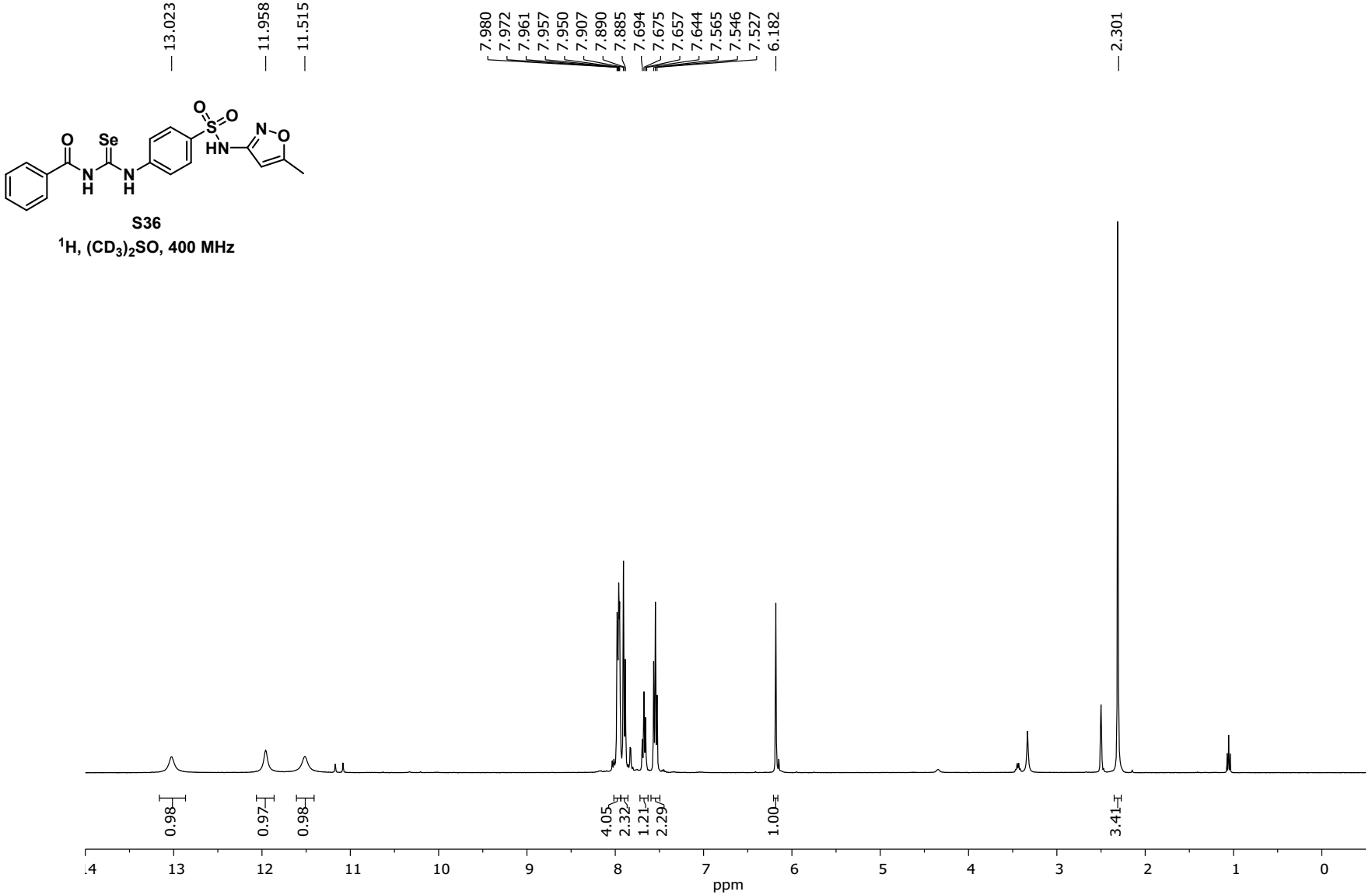
$^{13}C\{^{1}H\}$, $CDCl_3$, 126 MHz



S35

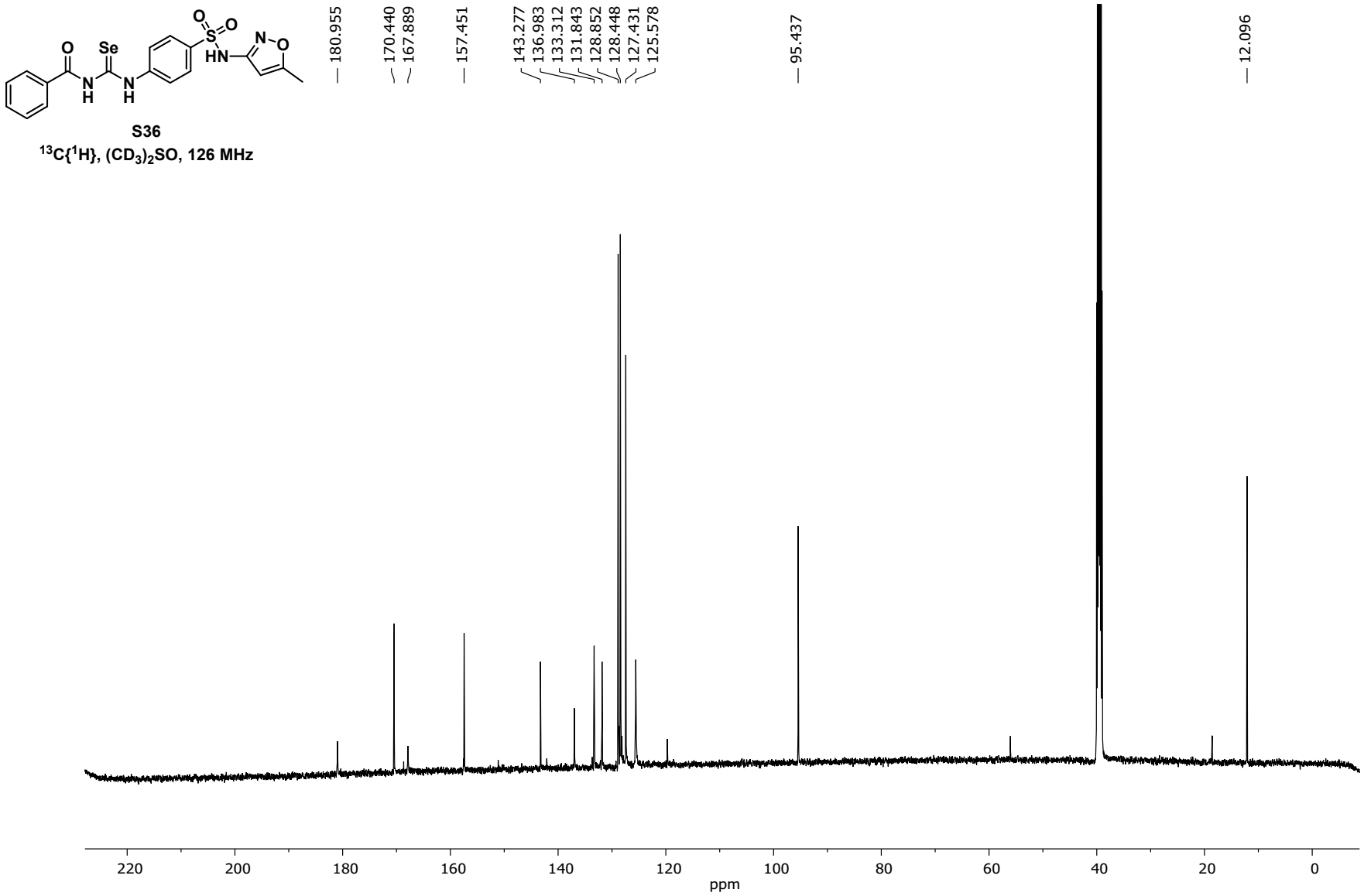
$^{77}Se\{^{1}H\}$, $CDCl_3$, 95 MHz





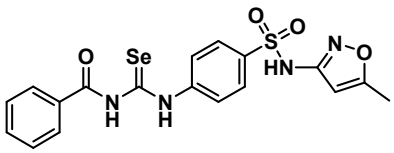
S36

^{1}H, $(CD_3)_2SO$, 400 MHz



S36

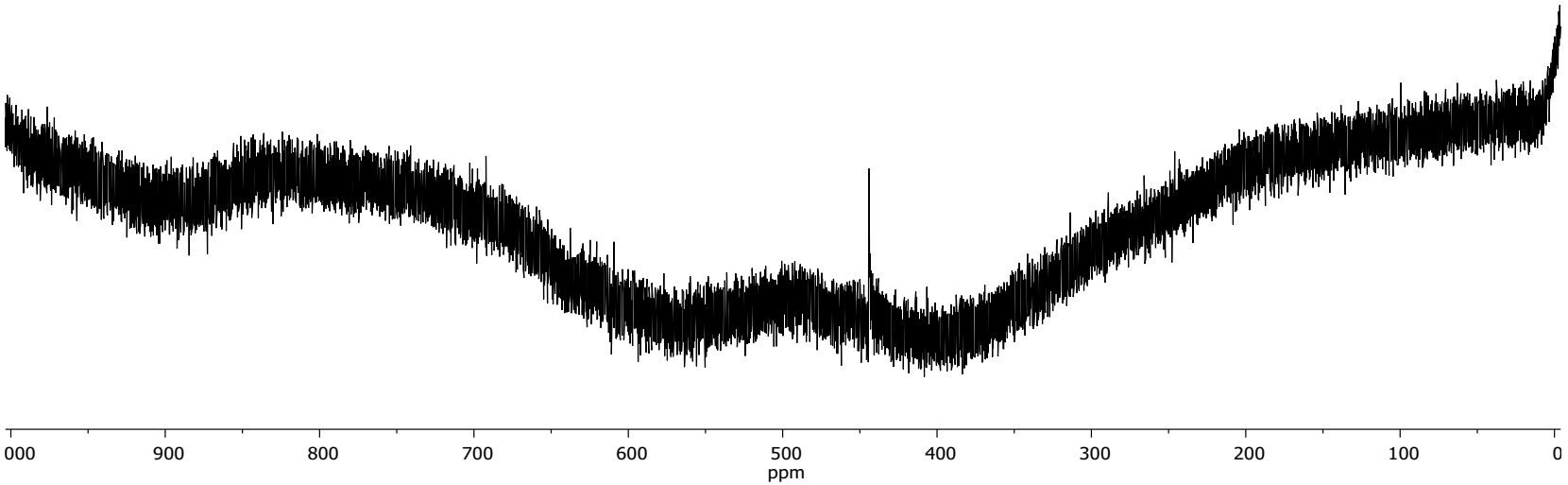
$^{13}C\{^{1}H\}$, $(CD_3)_2SO$, 126 MHz

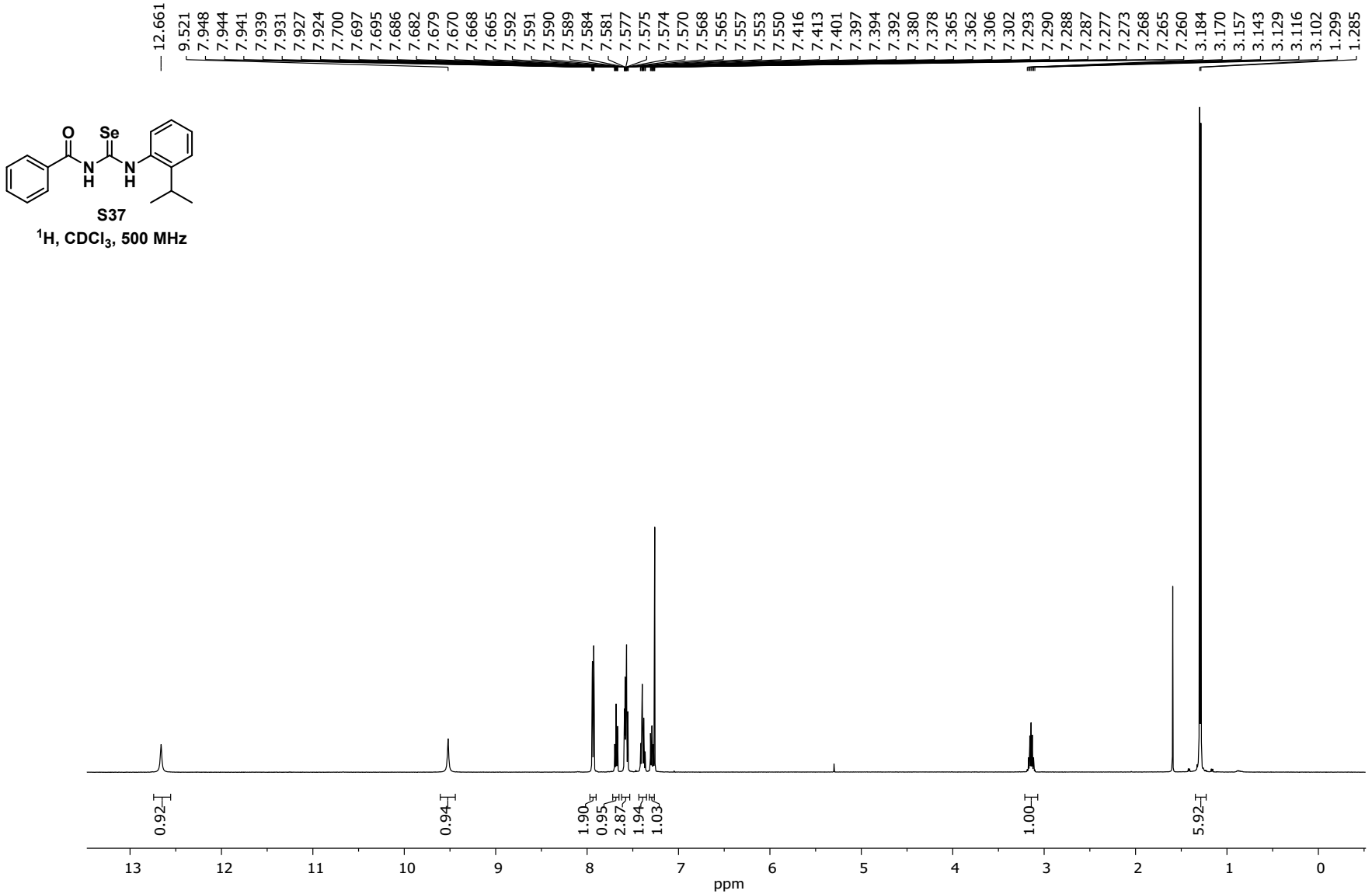


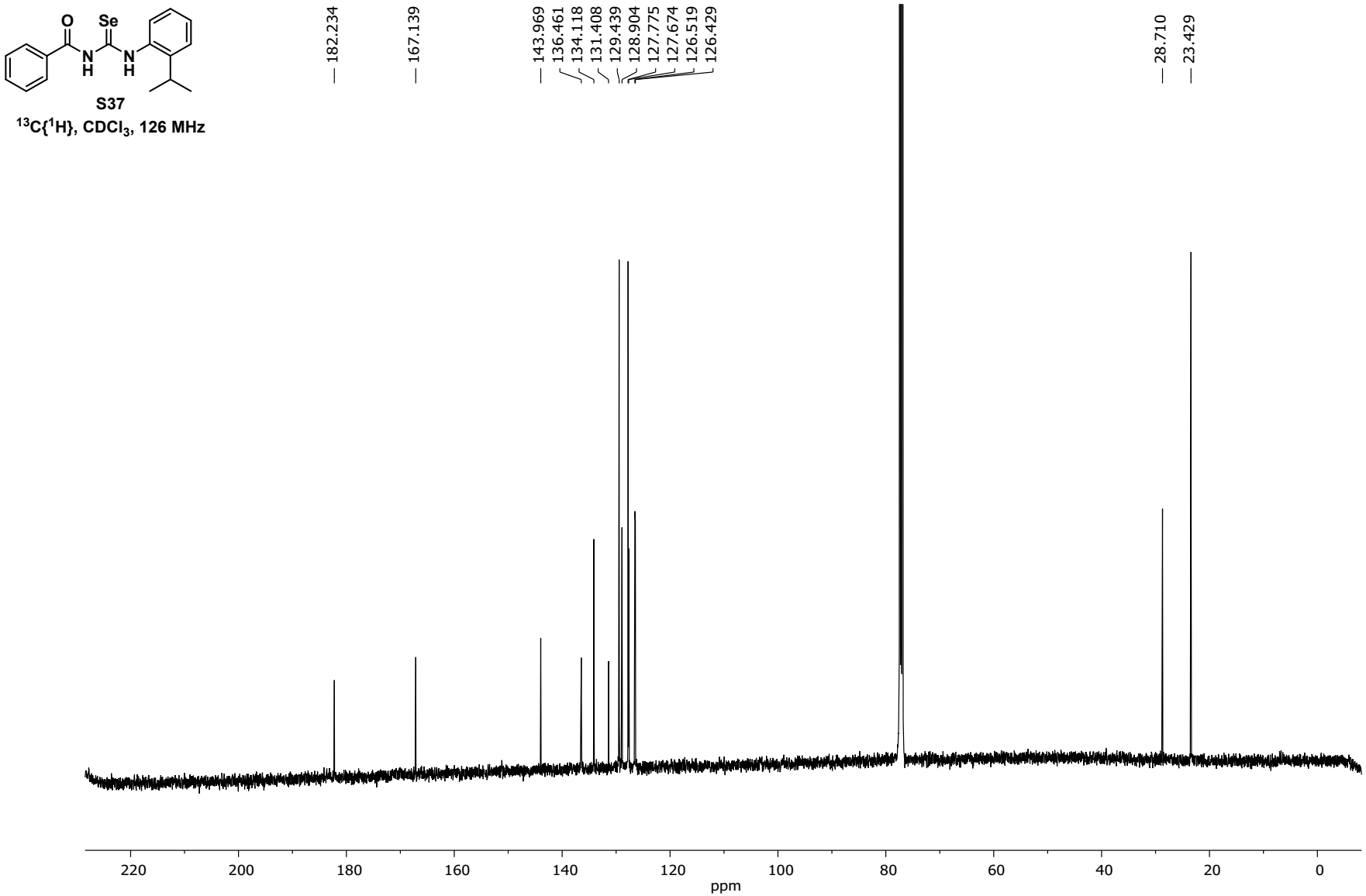
S36

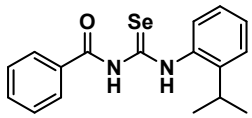
$^{77}Se\{^{1}H\}$, $(CD_3)_2SO$, 95 MHz

444.131



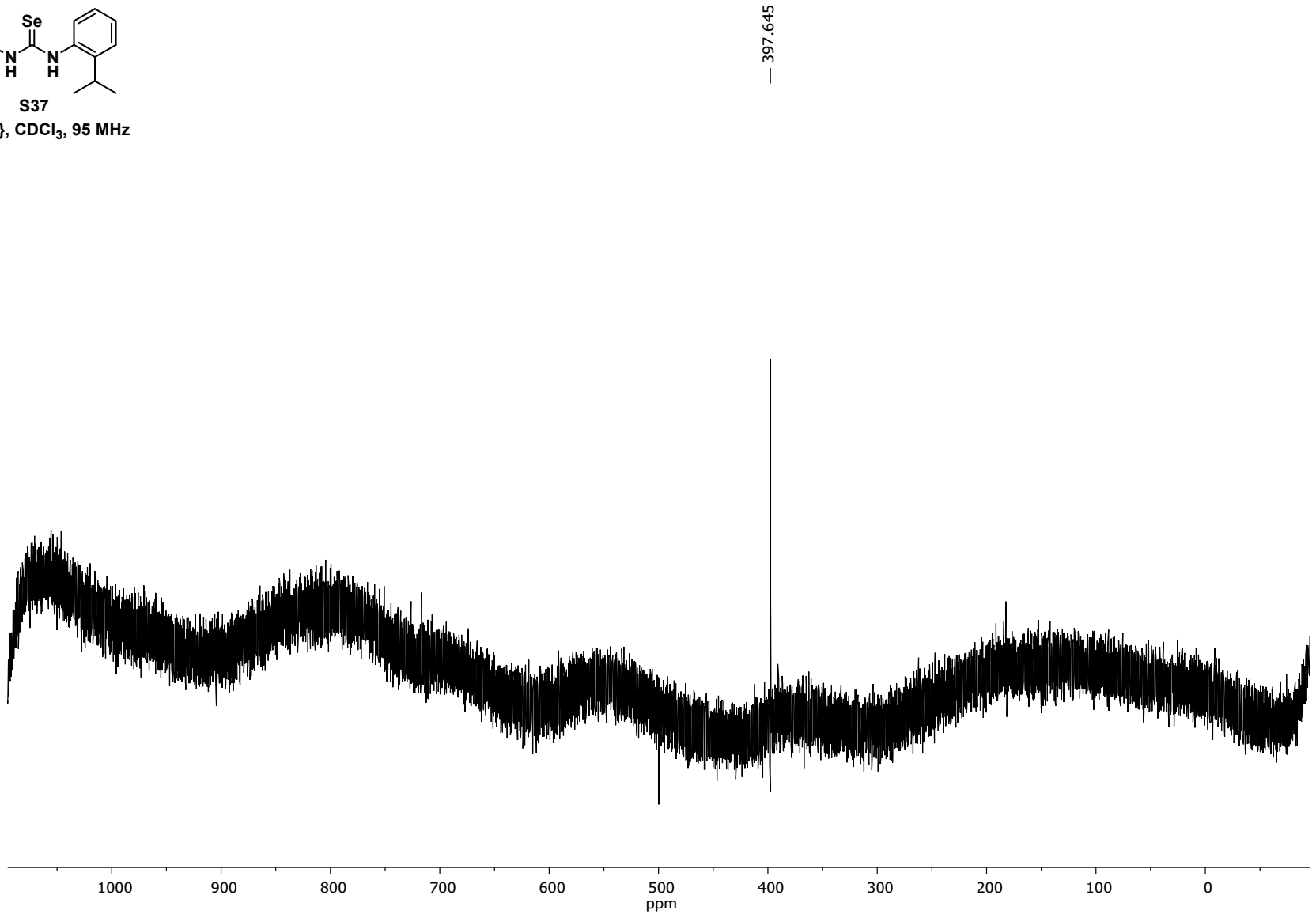

12.661
9.521
7.948
7.944
7.941
7.939
7.931
7.927
7.924
7.700
7.697
7.695
7.686
7.682
7.679
7.670
7.668
7.665
7.592
7.591
7.590
7.589
7.584
7.581
7.577
7.575
7.574
7.570
7.568
7.565
7.557
7.553
7.550
7.416
7.413
7.401
7.397
7.394
7.392
7.380
7.378
7.365
7.362
7.306
7.302
7.293
7.290
7.288
7.287
7.277
7.273
7.268
7.265
7.260
3.184
3.170
3.157
3.143
3.129
3.116
3.102
1.299
1.285
O
Se
N
H
N
H
S37
1H, CDCl3, 500 MHz
0.92
0.94
1.90
0.95
2.87
1.94
1.03
1.00
5.92
13
12
11
10
9
8
7
6
5
4
3
2
1
0
ppm

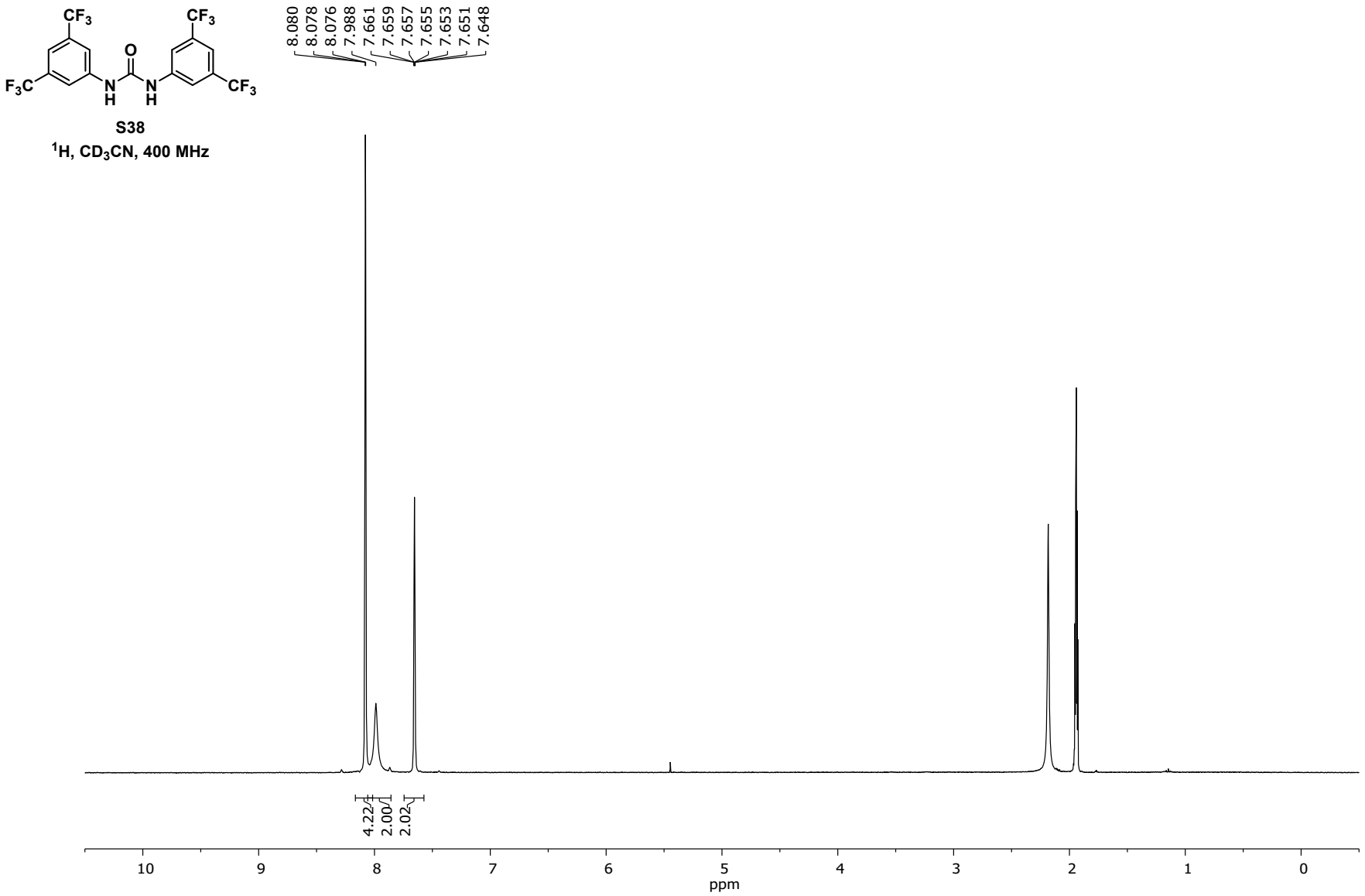

O
Se
N
H
N
H
S37
$^{13}C\{^{1}H\}$, $CDCl_3$, 126 MHz
182.234
167.139
143.969
136.461
134.118
131.408
129.439
128.904
127.775
127.674
126.519
126.429
28.710
23.429
220
200
180
160
140
120
100
80
60
40
20
0
ppm

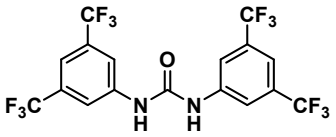


S37

$^{77}Se\{^{1}H\}$, $CDCl_3$, 95 MHz

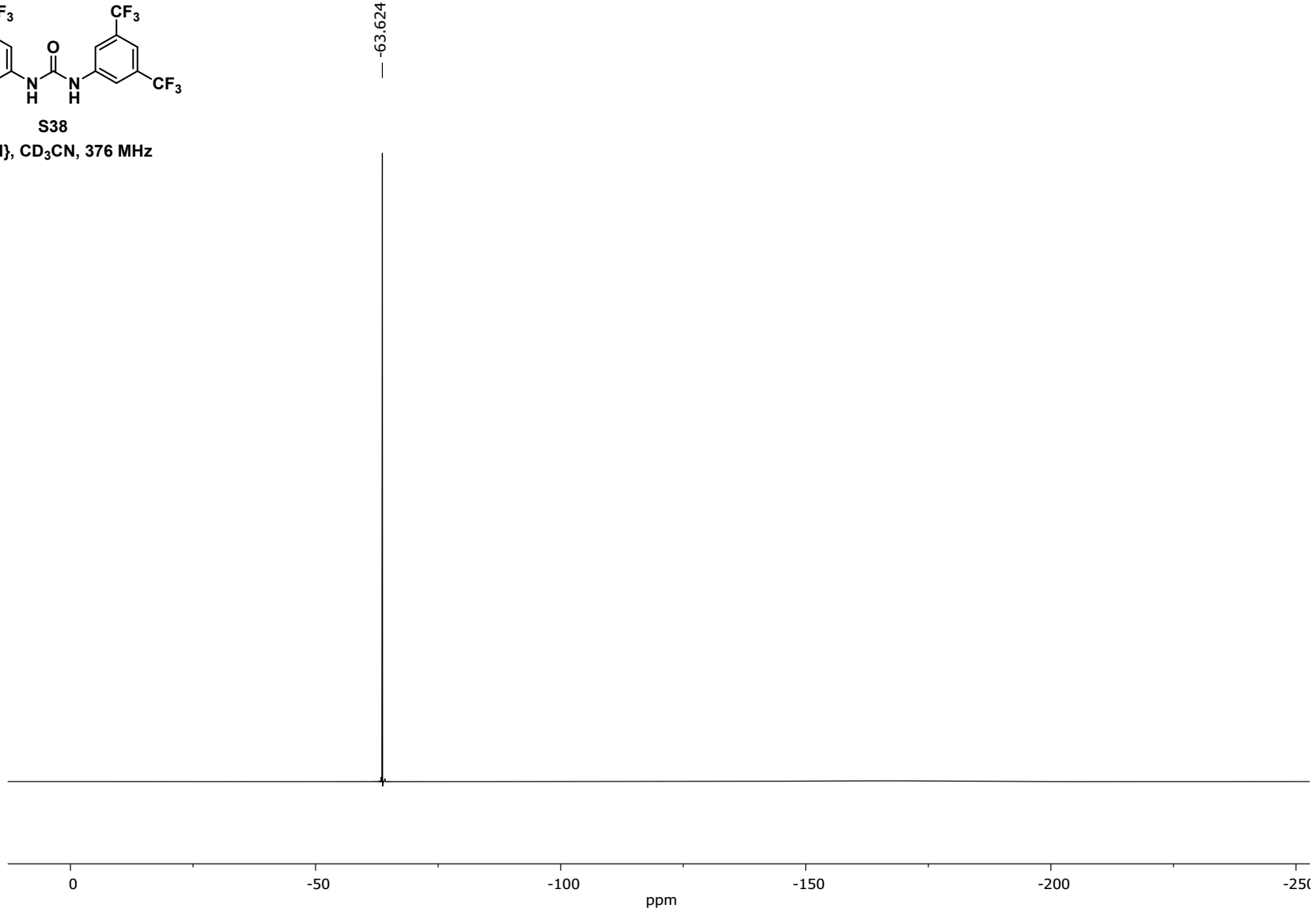


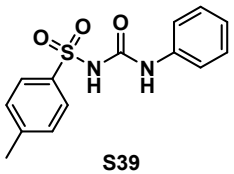

CF3
CF3
F3C
CF3
O
N
H
N
H
8.080
8.078
8.076
7.988
7.661
7.659
7.657
7.655
7.653
7.651
7.648
S38
1H, CD3CN, 400 MHz
4.22
2.00
2.02
10
9
8
7
6
5
4
3
2
1
0
ppm



S38

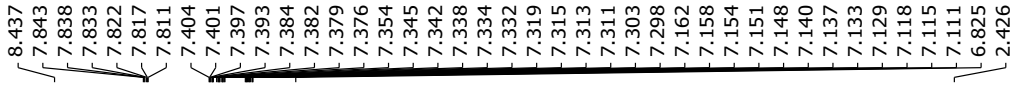
$^{19}F\{^{1}H\}$, CD_3CN, 376 MHz

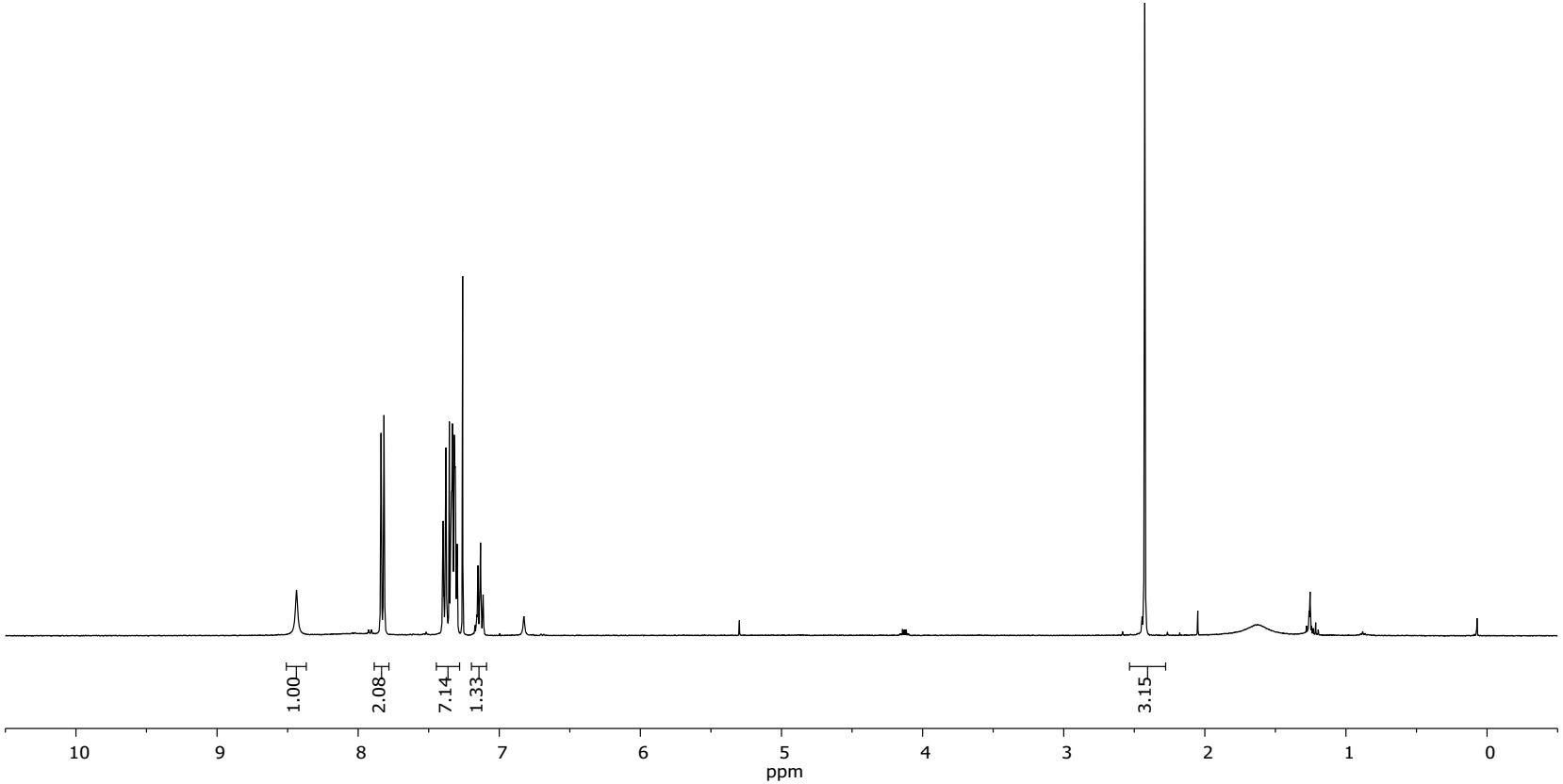


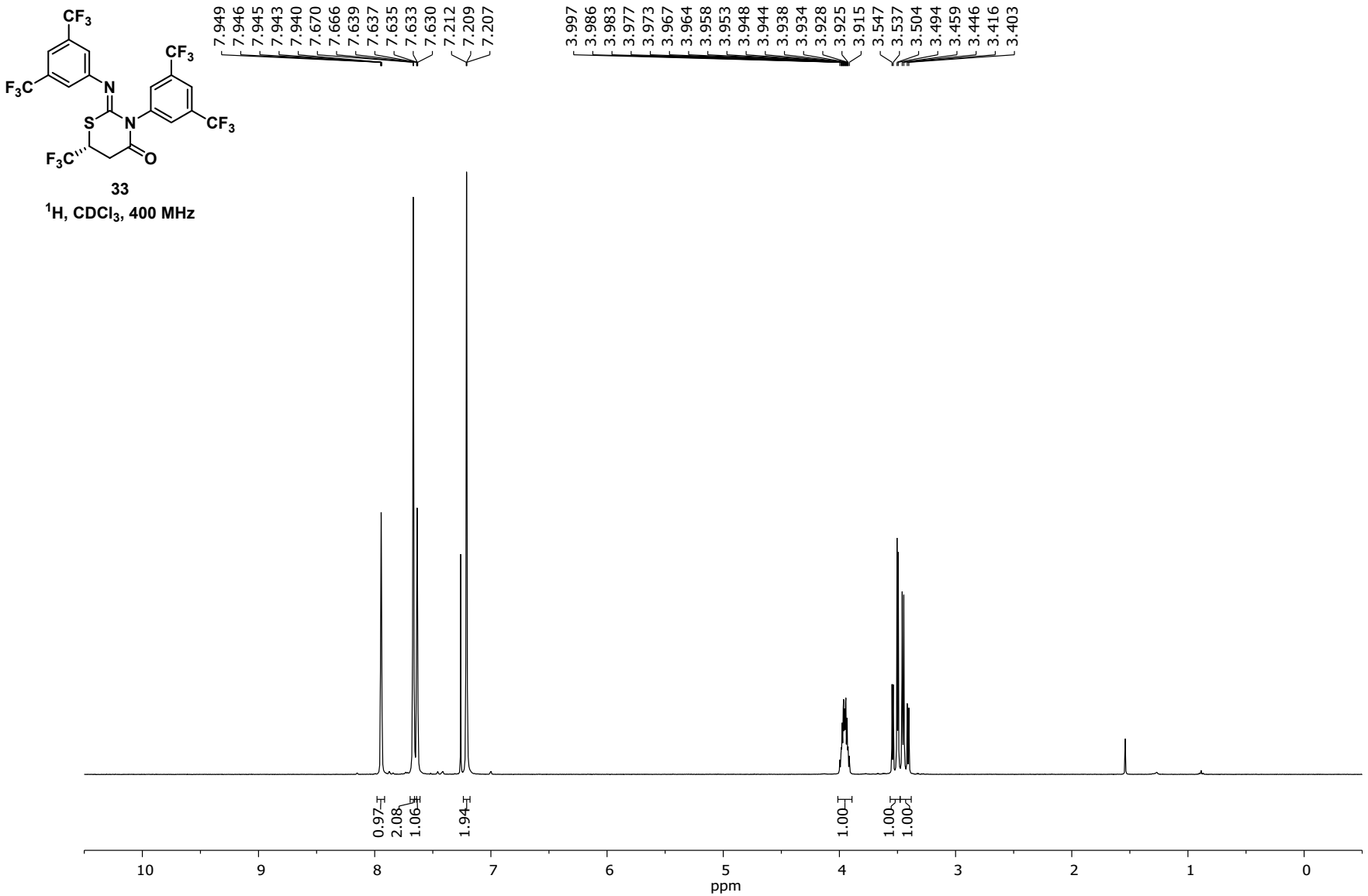


S39

^{1}H, $CDCl_3$, 400 MHz

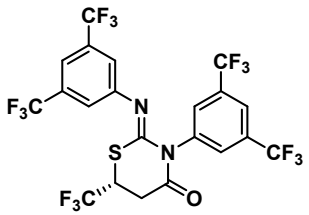






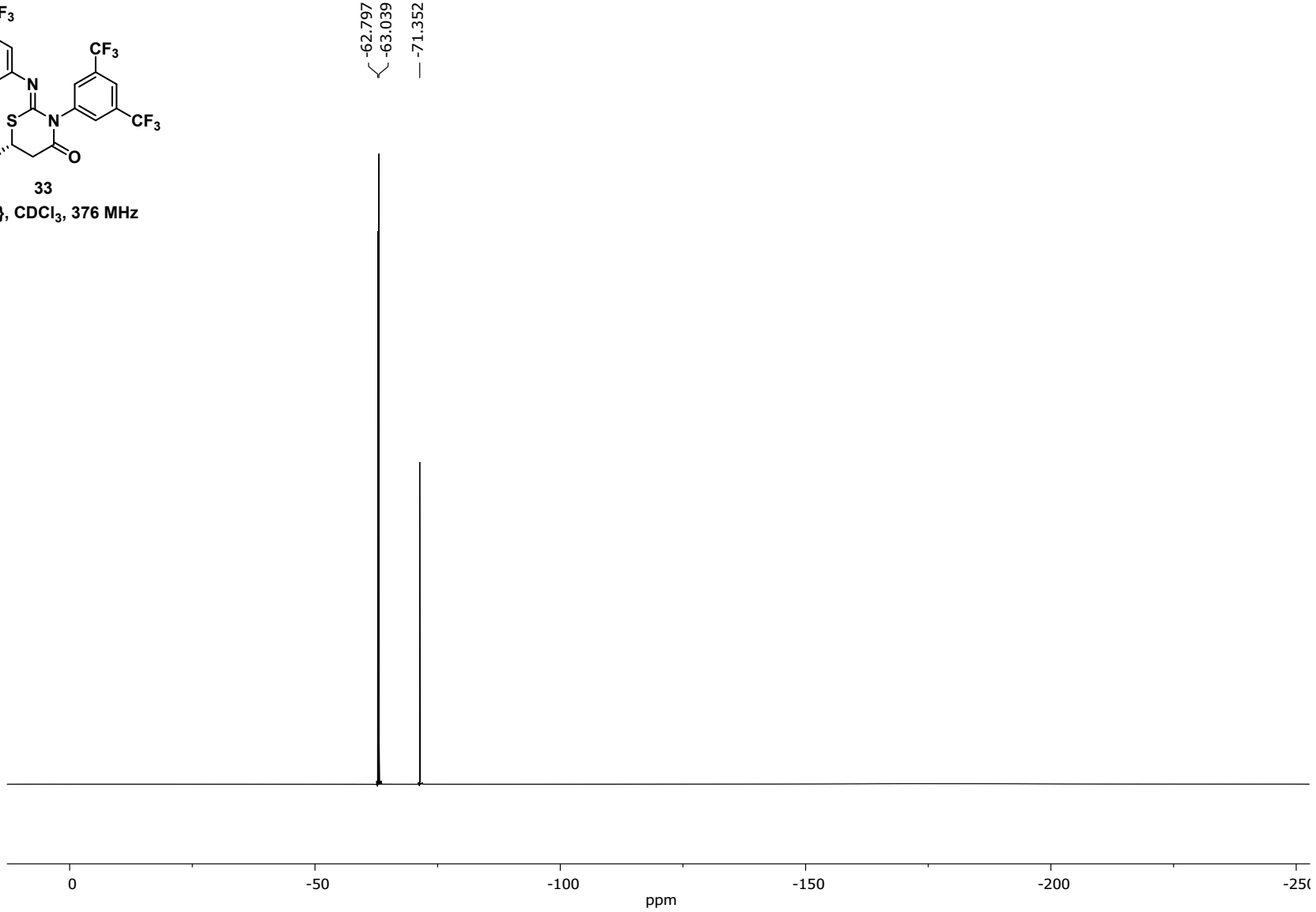
33

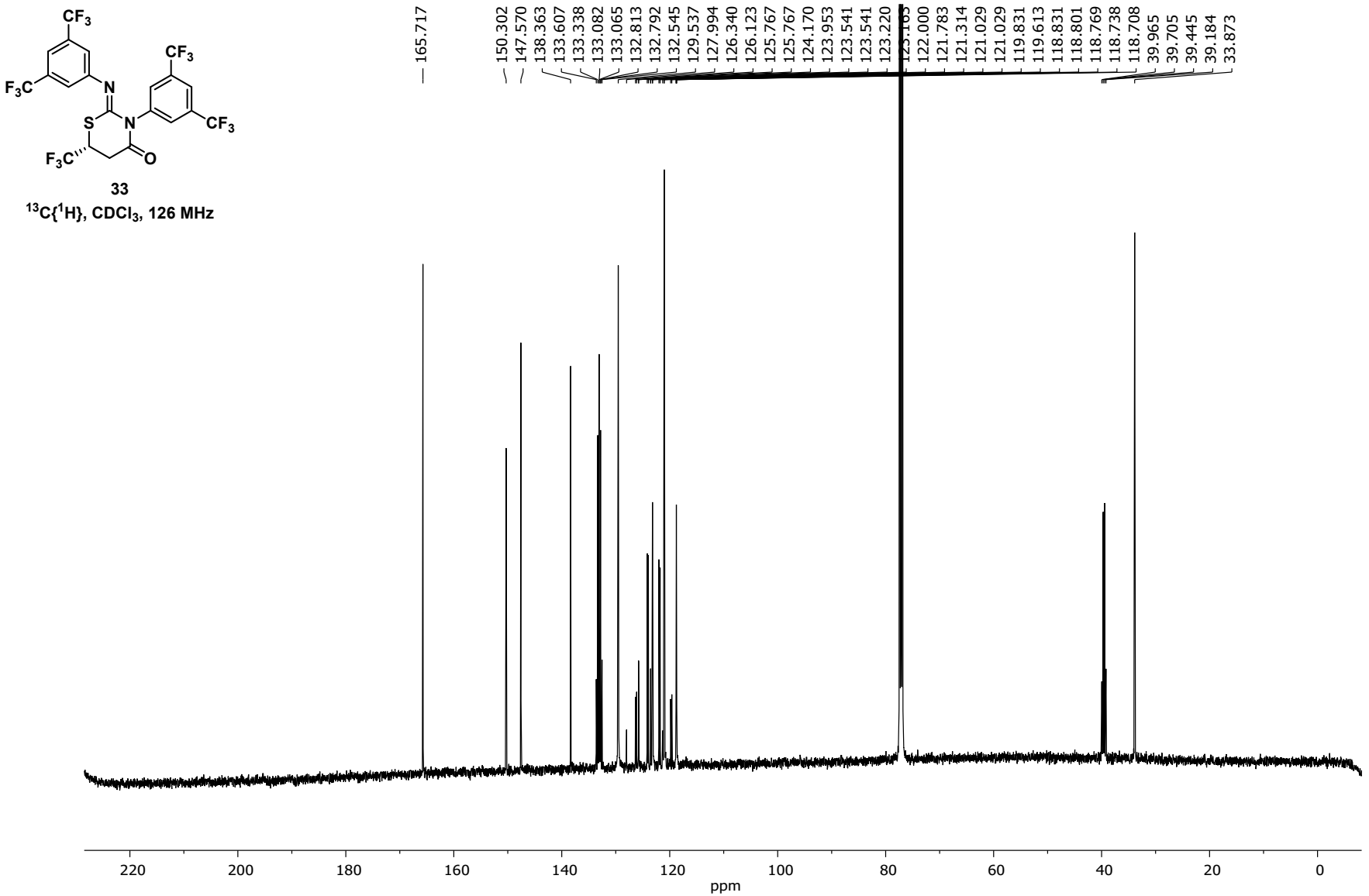
^{1}H, $CDCl_3$, 400 MHz



33

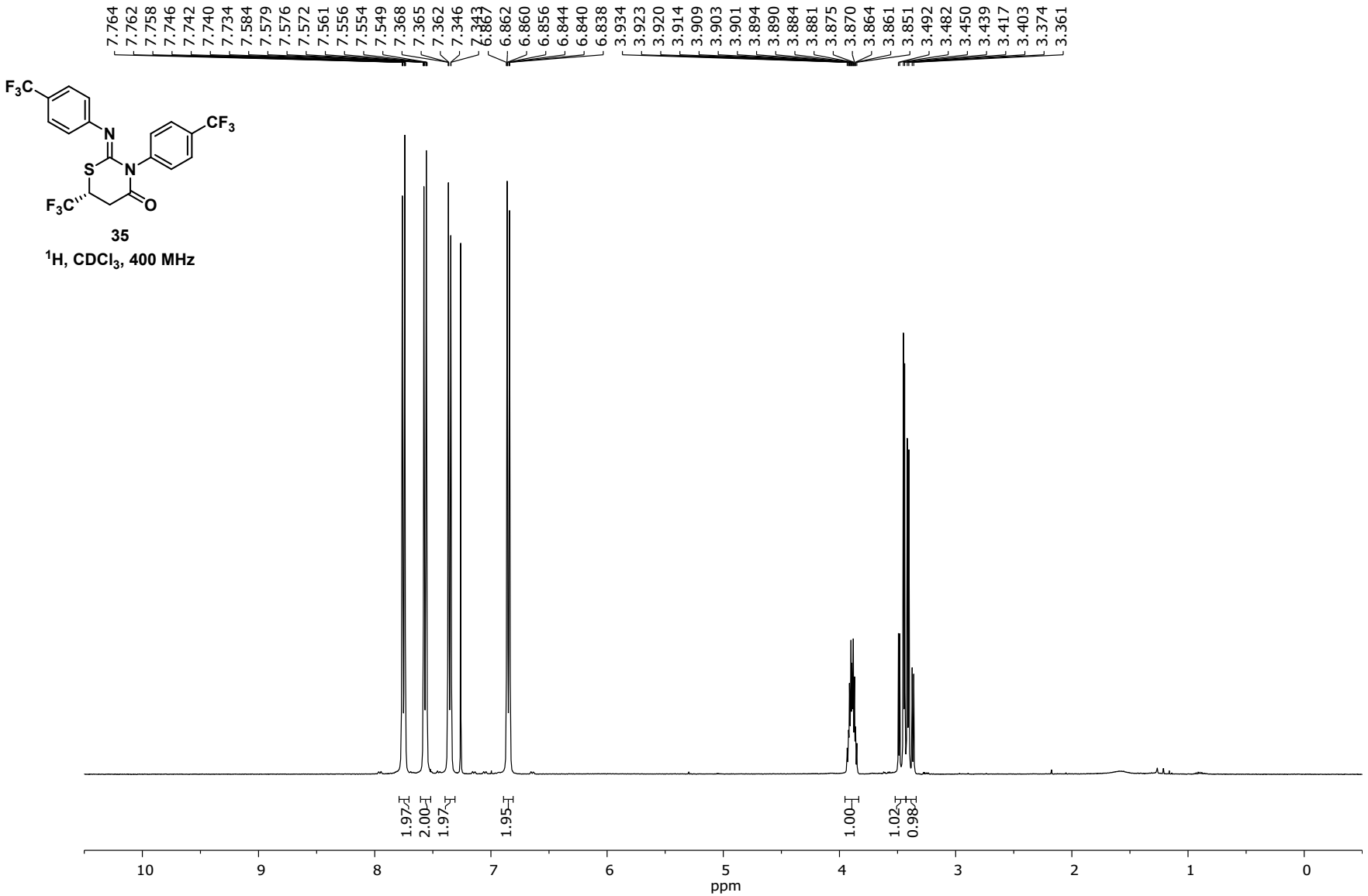
$^{19}F\{^{1}H\}$, $CDCl_3$, 376 MHz

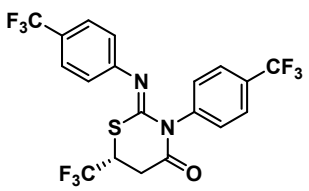




33

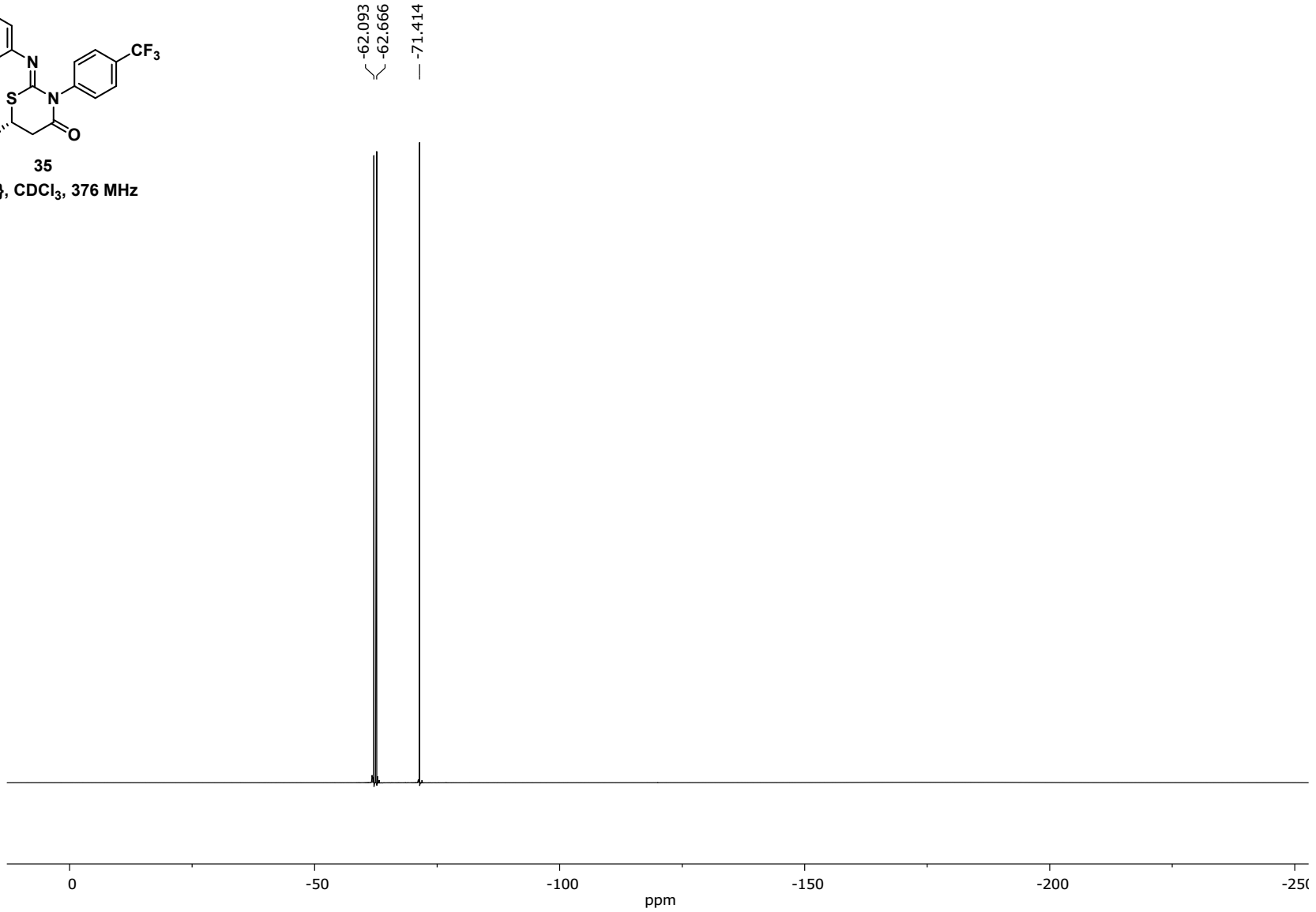
$^{13}C\{^{1}H\}$, $CDCl_3$, 126 MHz

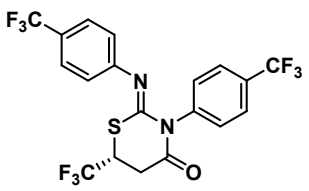

7.764
7.762
7.758
7.746
7.742
7.740
7.734
7.584
7.579
7.576
7.572
7.561
7.556
7.554
7.549
7.368
7.365
7.362
7.346
7.343
6.867
6.862
6.860
6.856
6.844
6.840
6.838
3.934
3.923
3.920
3.914
3.909
3.903
3.901
3.894
3.890
3.884
3.881
3.875
3.870
3.864
3.861
3.851
3.492
3.482
3.450
3.439
3.417
3.403
3.374
3.361
F3C
CF3
N
S
N
O
F3C
35
1H, CDCl3, 400 MHz
1.97
2.00
1.97
1.95
1.00
1.02
0.98
10
9
8
7
6
5
4
3
2
1
0
ppm



35

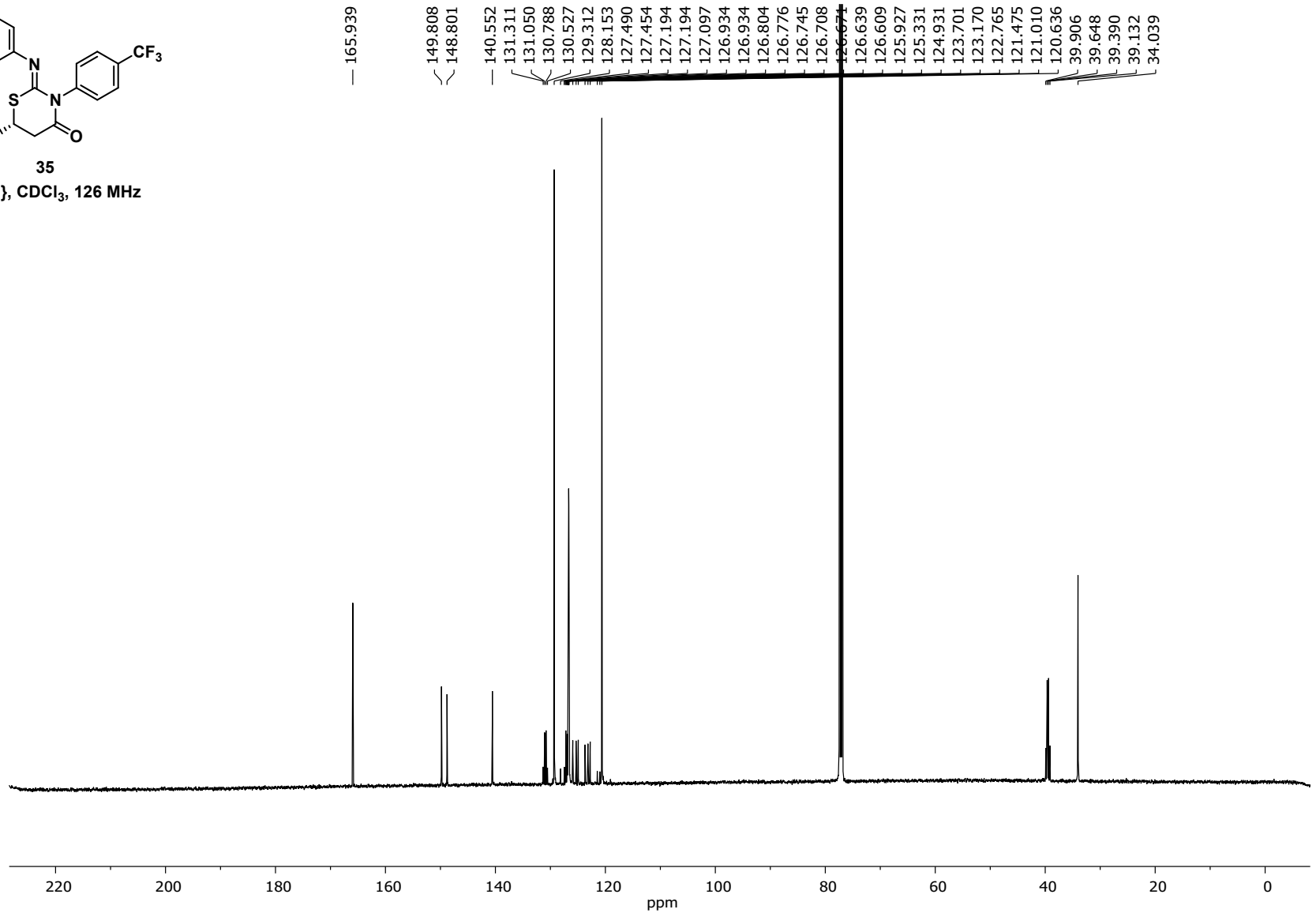
$^{19}F\{^{1}H\}$, $CDCl_3$, 376 MHz

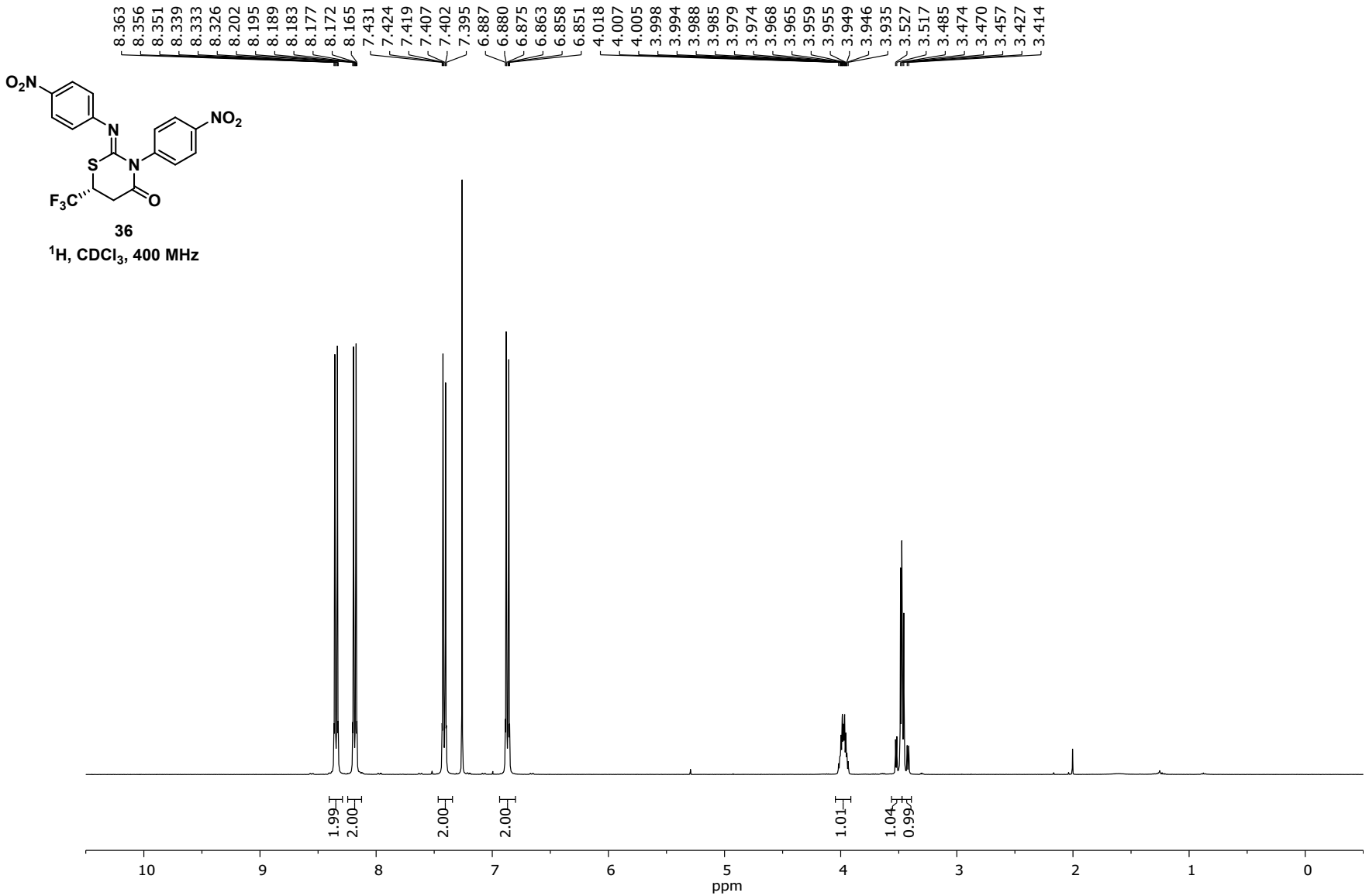


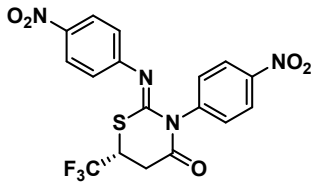


35

$^{13}C\{^{1}H\}$, $CDCl_3$, 126 MHz

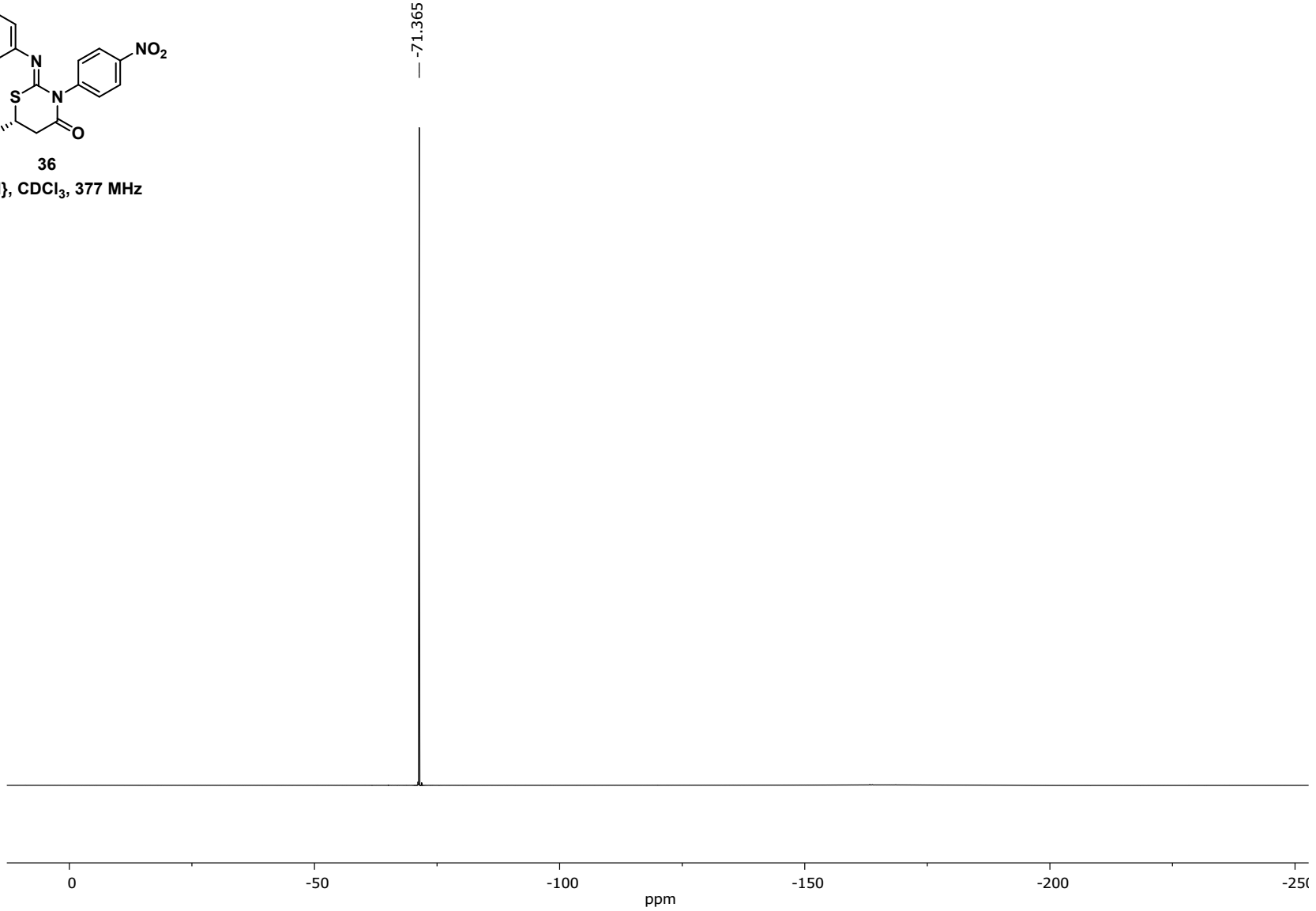


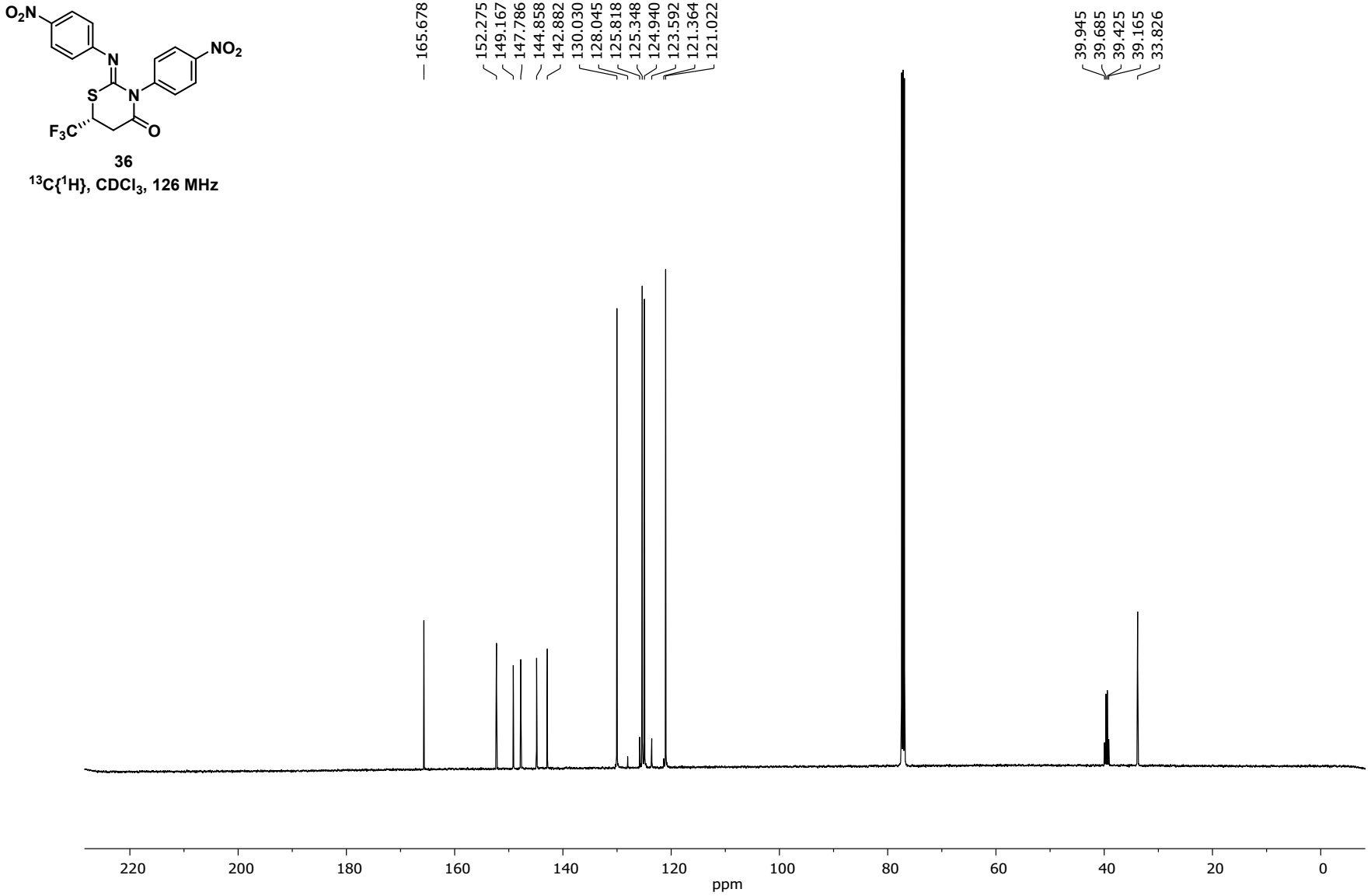

8.363
8.356
8.351
8.339
8.333
8.326
8.202
8.195
8.189
8.183
8.177
8.172
8.165
7.431
7.424
7.419
7.407
7.402
7.395
6.887
6.880
6.875
6.863
6.858
6.851
4.018
4.007
4.005
3.998
3.994
3.988
3.985
3.979
3.974
3.968
3.965
3.959
3.955
3.949
3.946
3.935
3.527
3.517
3.485
3.474
3.470
3.457
3.427
3.414
O2N
NO2
N
S
N
O
F3C
36
1H, CDCl3, 400 MHz
1.99
2.00
2.00
2.00
1.01
1.04
0.99
10
9
8
7
6
5
4
3
2
1
0
ppm

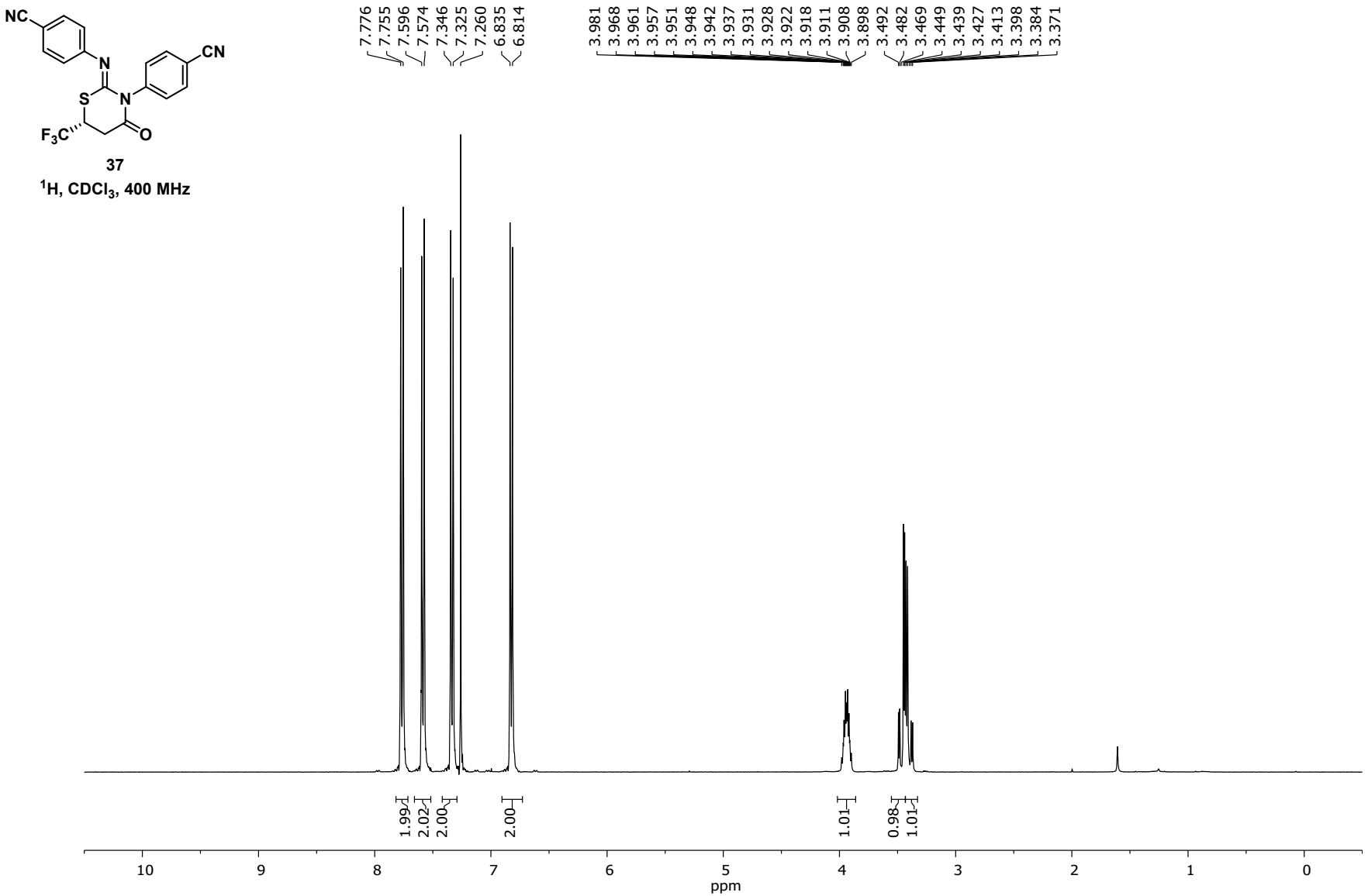


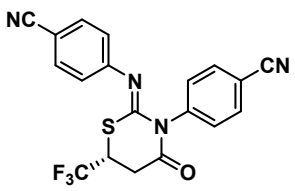
36

$^{19}F\{^{1}H\}$, $CDCl_3$, 377 MHz



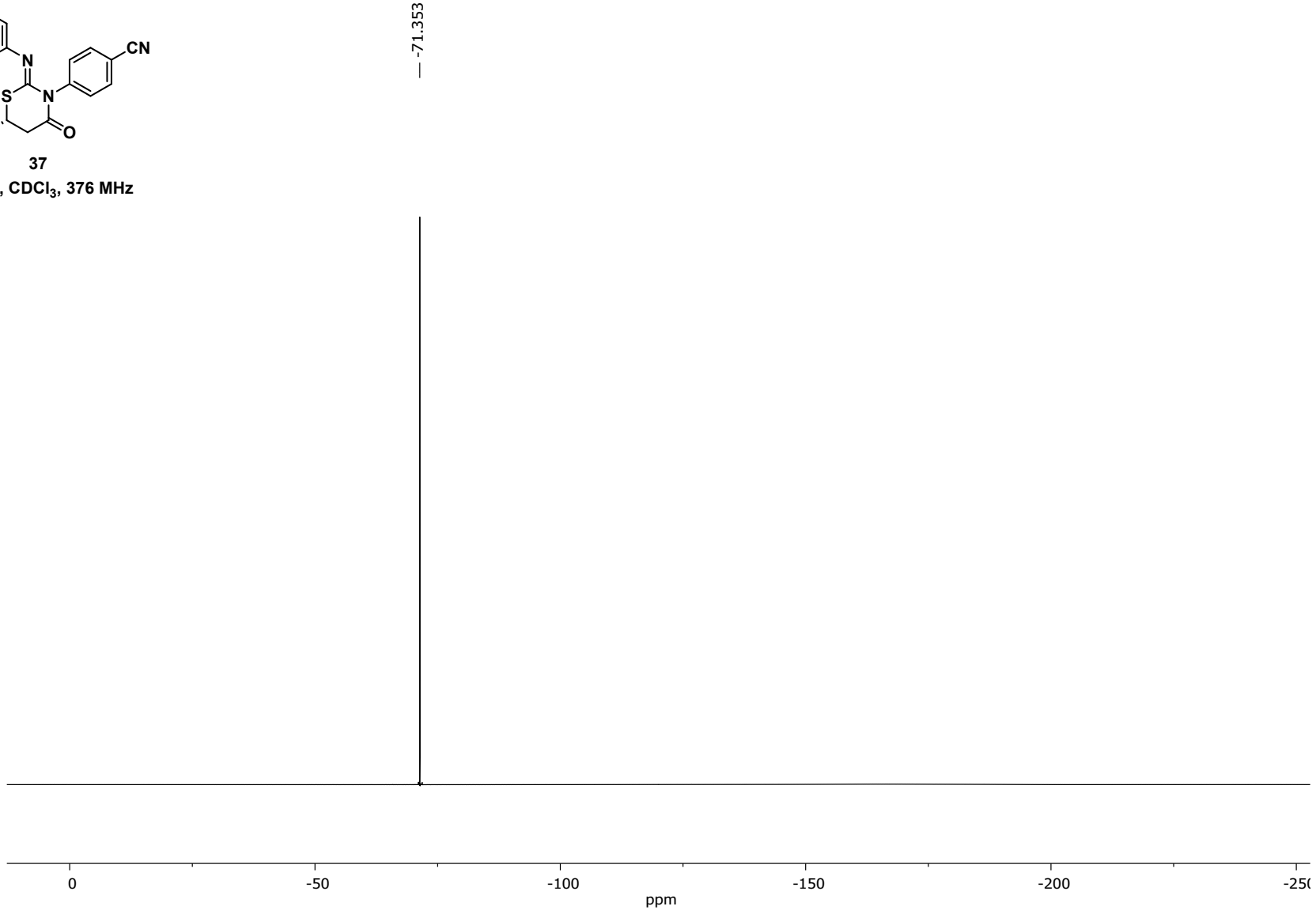

O2N
NO2
N
S
N
O
F3C
36
13C{1H}, CDCl3, 126 MHz
165.678
152.275
149.167
147.786
144.858
142.882
130.030
128.045
125.818
125.348
124.940
123.592
121.364
121.022
39.945
39.685
39.425
39.165
33.826
220
200
180
160
140
120
100
80
60
40
20
0
ppm

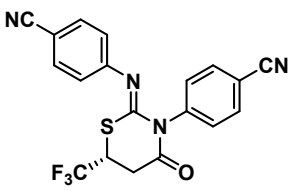

NC
CN
N
S
N
O
F3C
37
1H, CDCl3, 400 MHz
7.776
7.755
7.596
7.574
7.346
7.325
7.260
6.835
6.814
3.981
3.968
3.961
3.957
3.951
3.948
3.942
3.937
3.931
3.928
3.922
3.918
3.911
3.908
3.898
3.492
3.482
3.469
3.449
3.439
3.427
3.413
3.398
3.384
3.371
1.99
2.02
2.00
2.00
1.01
0.98
1.01
10
9
8
7
6
5
4
3
2
1
0
ppm



37

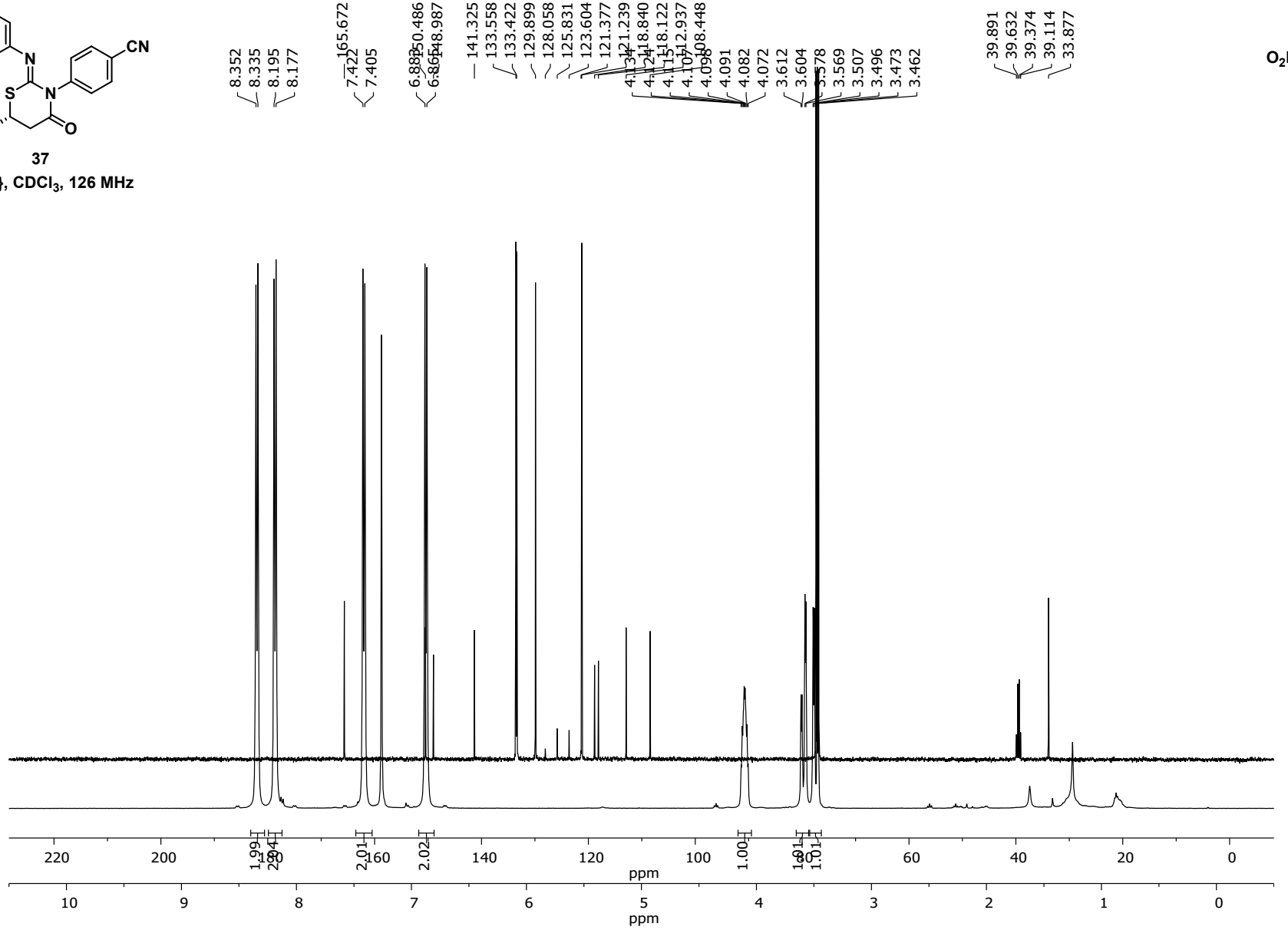
$^{19}F\{^{1}H\}$, $CDCl_3$, 376 MHz

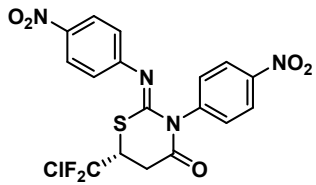




37

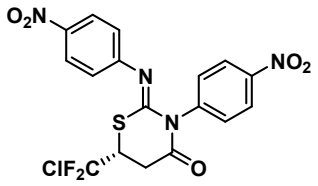
$^{13}C\{^{1}H\}$, $CDCl_3$, 126 MHz





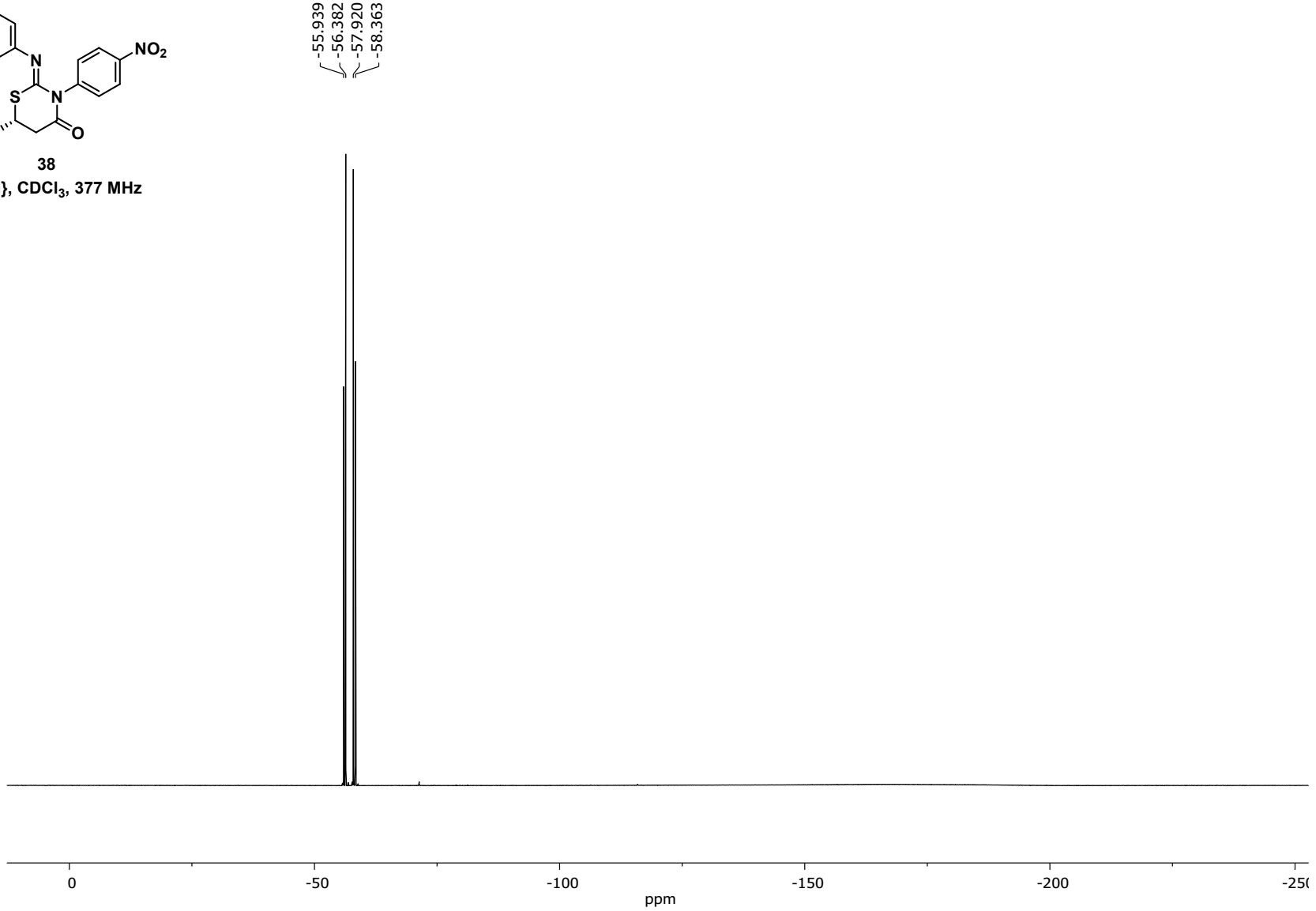
38

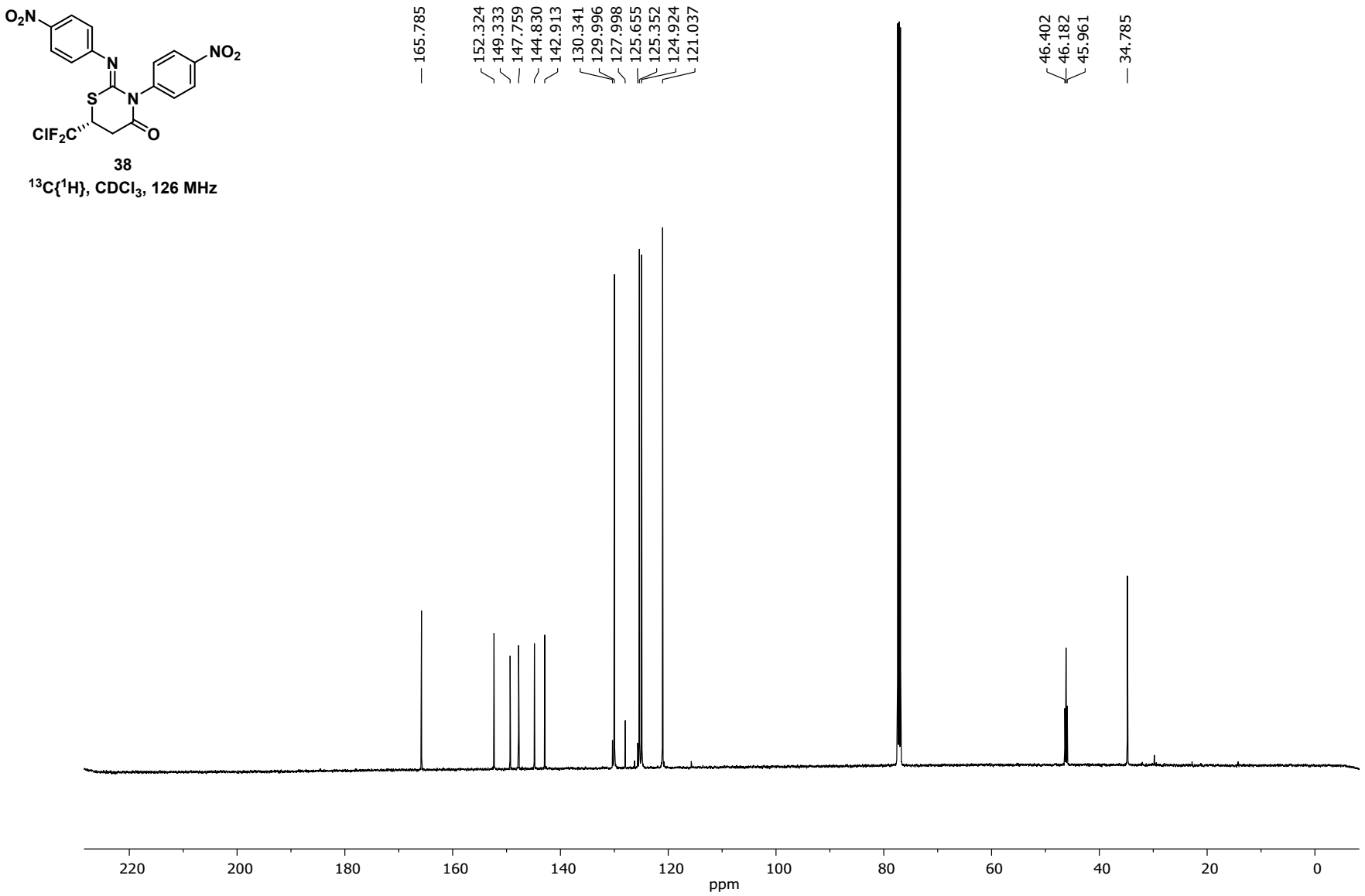
^{1}H, $CDCl_3$, 500 MHz

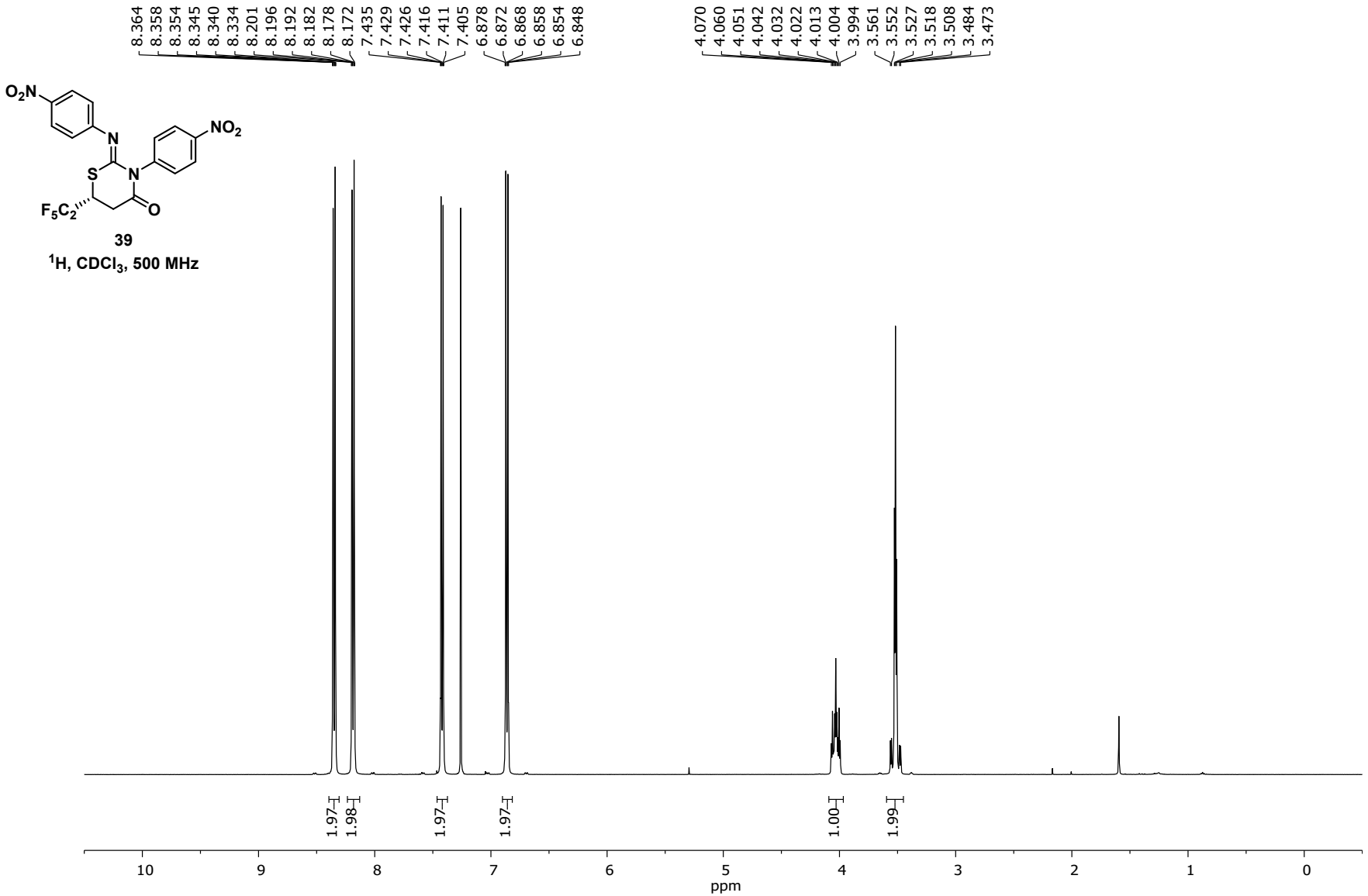


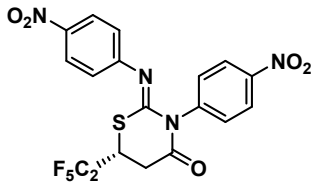
38

$^{19}F\{^{1}H\}$, $CDCl_3$, 377 MHz



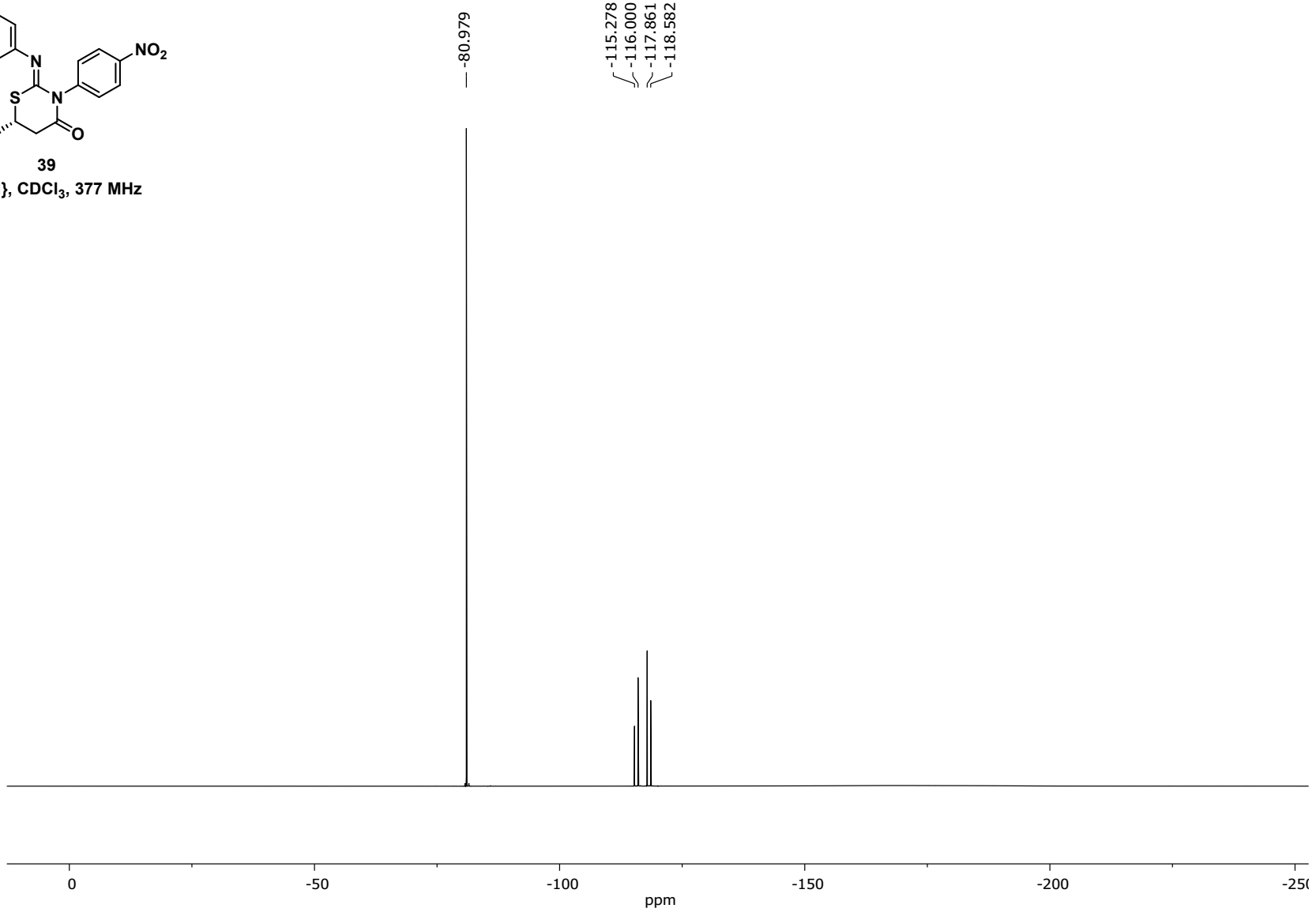

O2N
NO2
N
S
N
O
ClF2C
38
13C{1H}, CDCl3, 126 MHz
165.785
152.324
149.333
147.759
144.830
142.913
130.341
129.996
127.998
125.655
125.352
124.924
121.037
46.402
46.182
45.961
34.785
220
200
180
160
140
120
100
80
60
40
20
0
ppm

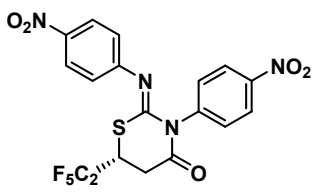

8.364
8.358
8.354
8.345
8.340
8.334
8.201
8.196
8.192
8.182
8.178
8.172
7.435
7.429
7.426
7.416
7.411
7.405
6.878
6.872
6.868
6.858
6.854
6.848
4.070
4.060
4.051
4.042
4.032
4.022
4.013
4.004
3.994
3.561
3.552
3.527
3.518
3.508
3.484
3.473
O2N
NO2
N
S
N
O
F5C2
39
1H, CDCl3, 500 MHz
1.97
1.98
1.97
1.97
1.00
1.99
10
9
8
7
6
5
4
3
2
1
0
ppm



39

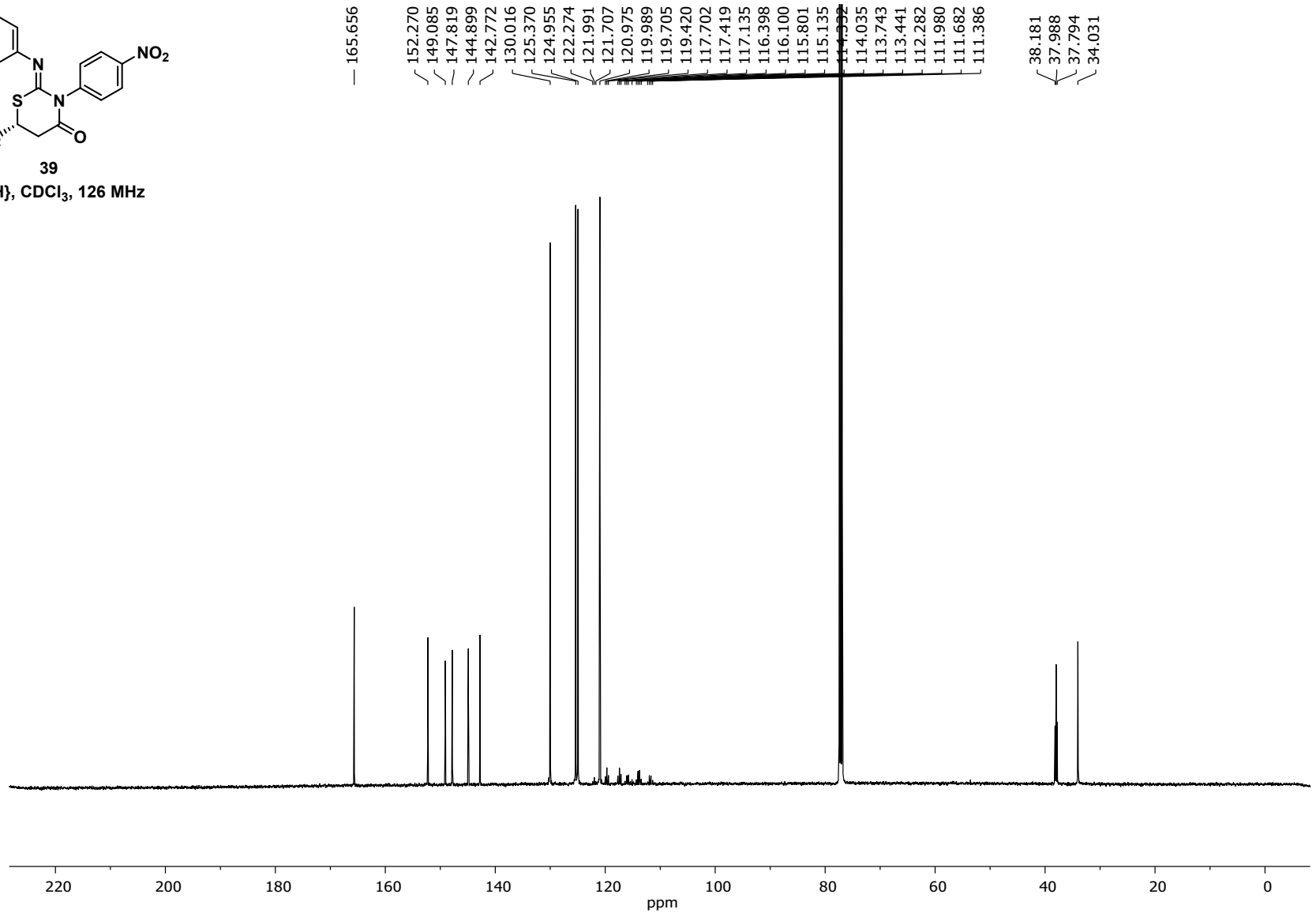
$^{19}F\{^{1}H\}$, $CDCl_3$, 377 MHz

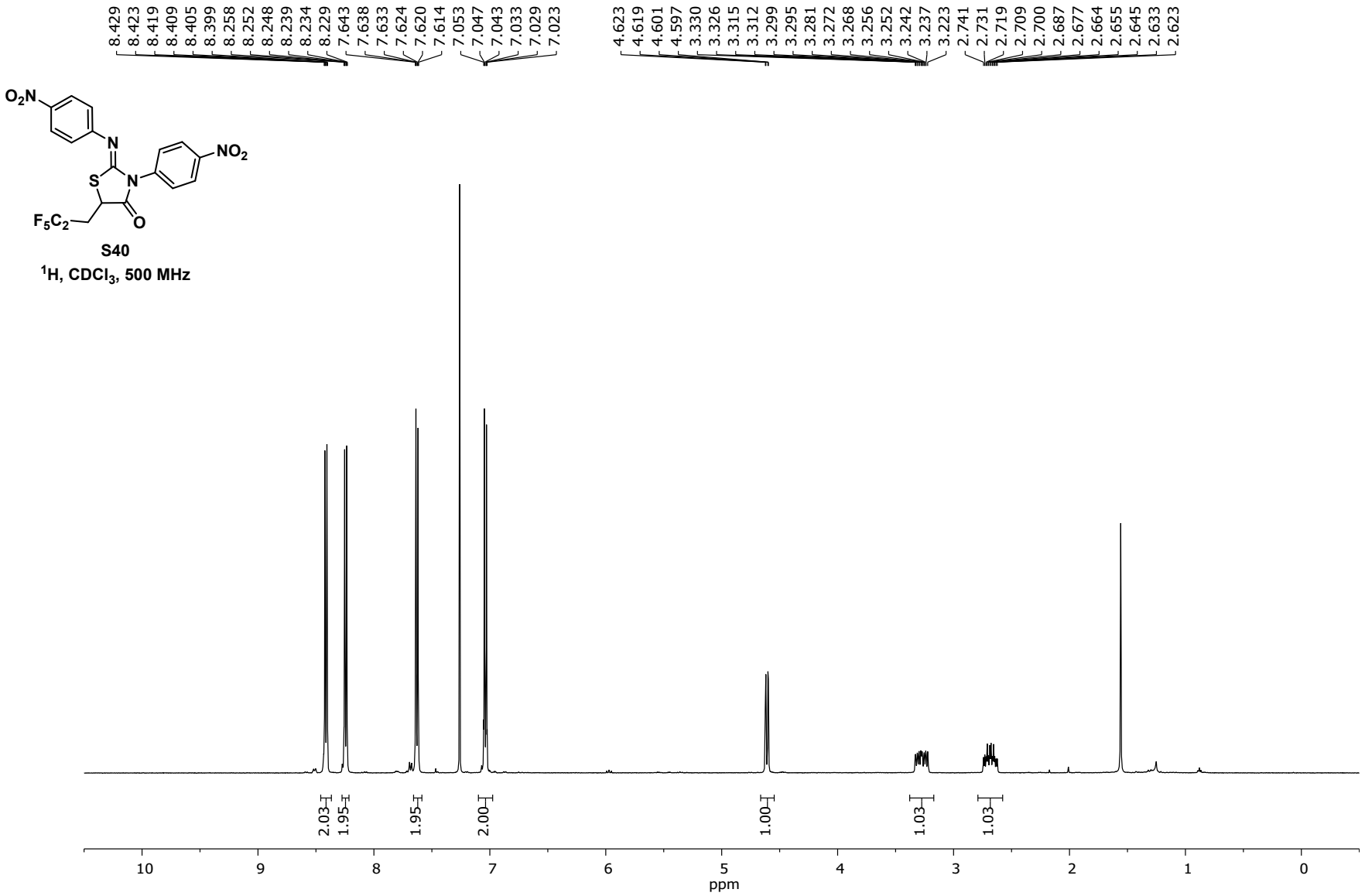


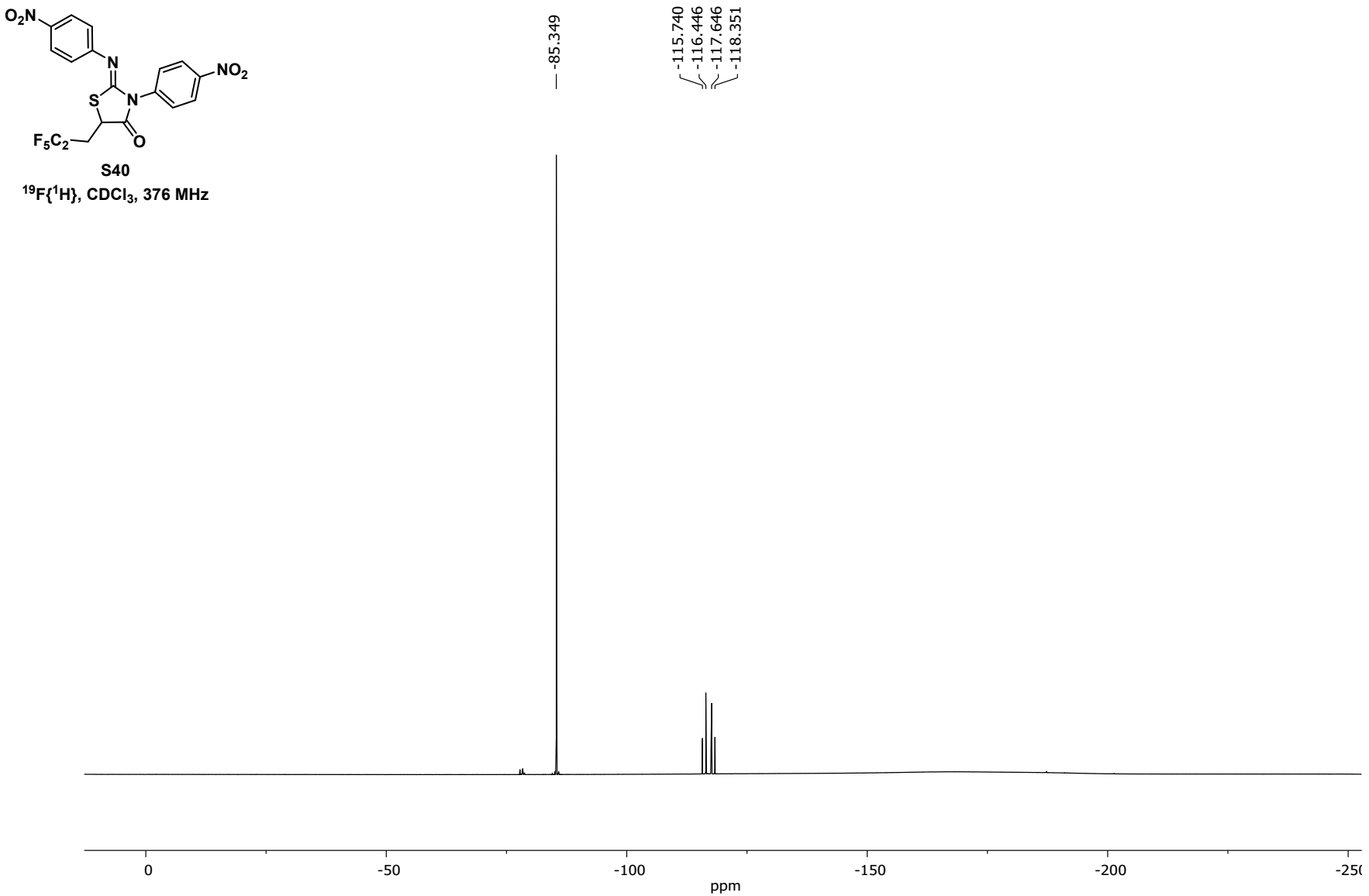


39

$^{13}C\{^{1}H\}$, $CDCl_3$, 126 MHz

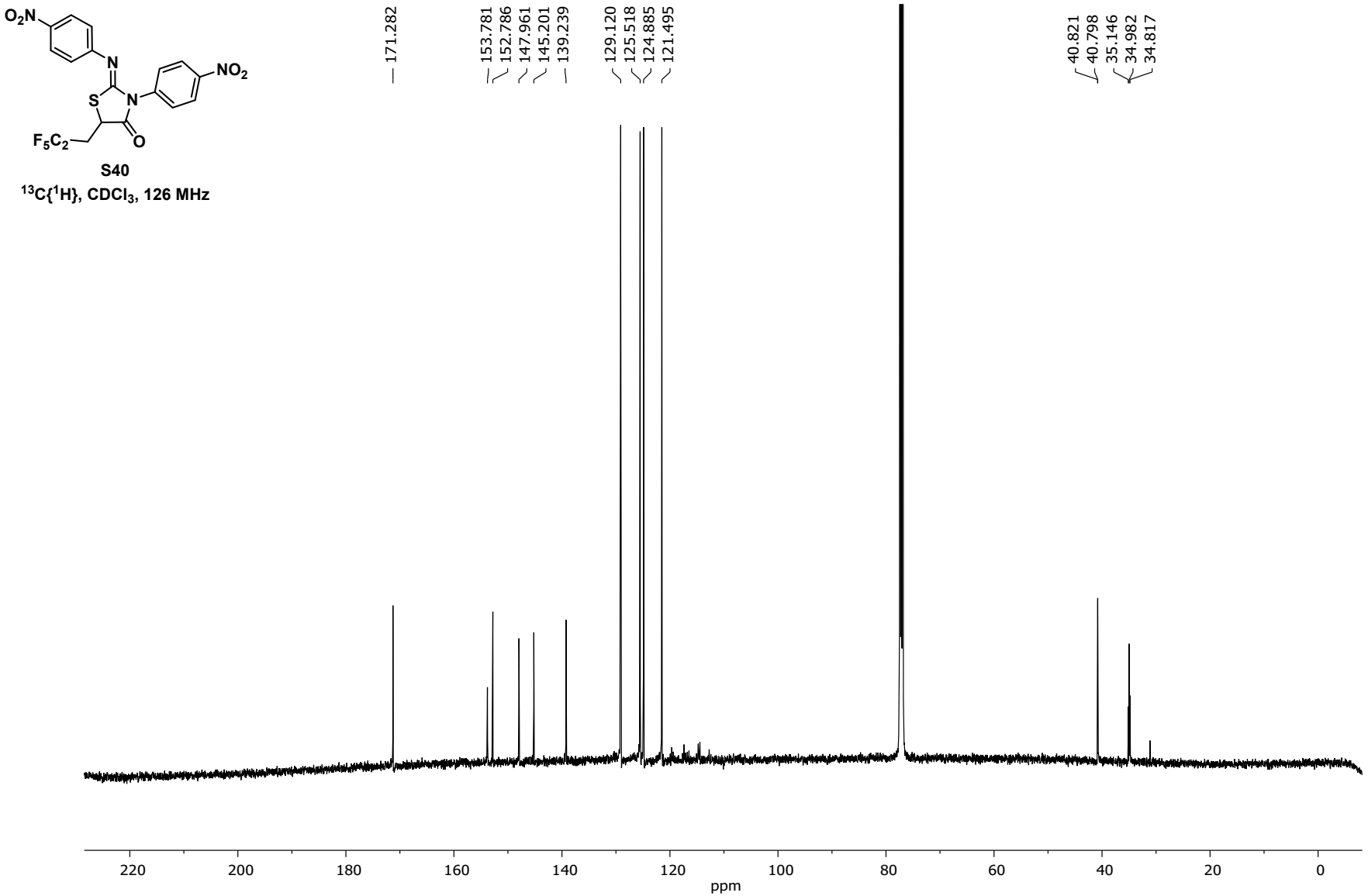



8.429
8.423
8.419
8.409
8.405
8.399
8.258
8.252
8.248
8.239
8.234
8.229
7.643
7.638
7.633
7.624
7.620
7.614
7.053
7.047
7.043
7.033
7.029
7.023
4.623
4.619
4.601
4.597
3.330
3.326
3.315
3.312
3.299
3.295
3.281
3.272
3.268
3.256
3.252
3.242
3.237
3.223
2.741
2.731
2.719
2.709
2.700
2.687
2.677
2.664
2.655
2.645
2.633
2.623
O2N
NO2
N
S
N
O
F5C2
S40
1H, CDCl3, 500 MHz
2.03
1.95
1.95
2.00
1.00
1.03
1.03
10
9
8
7
6
5
4
3
2
1
0
ppm



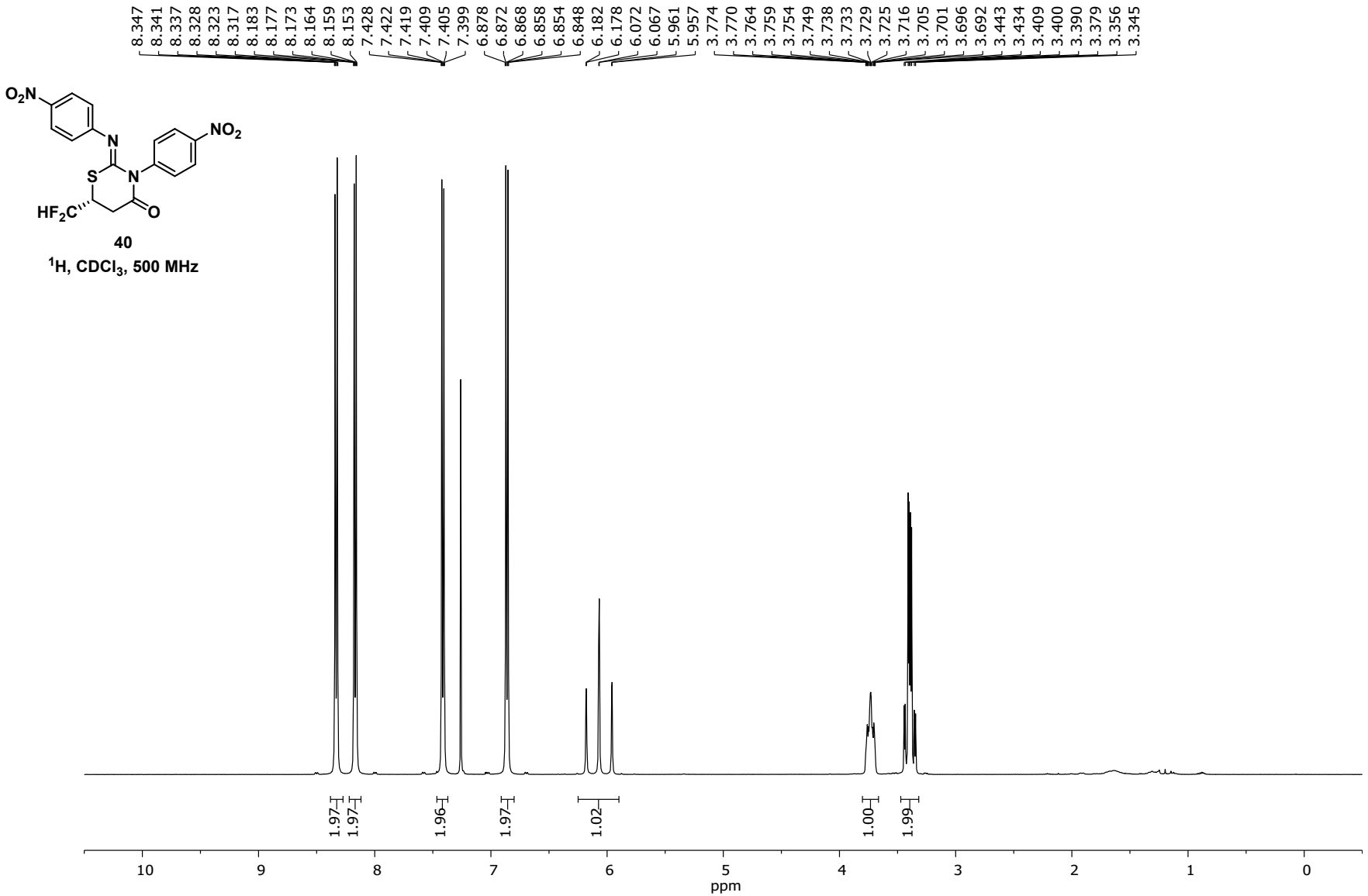
S40

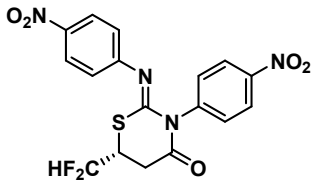
$^{19}F\{^{1}H\}$, $CDCl_3$, 376 MHz



S40

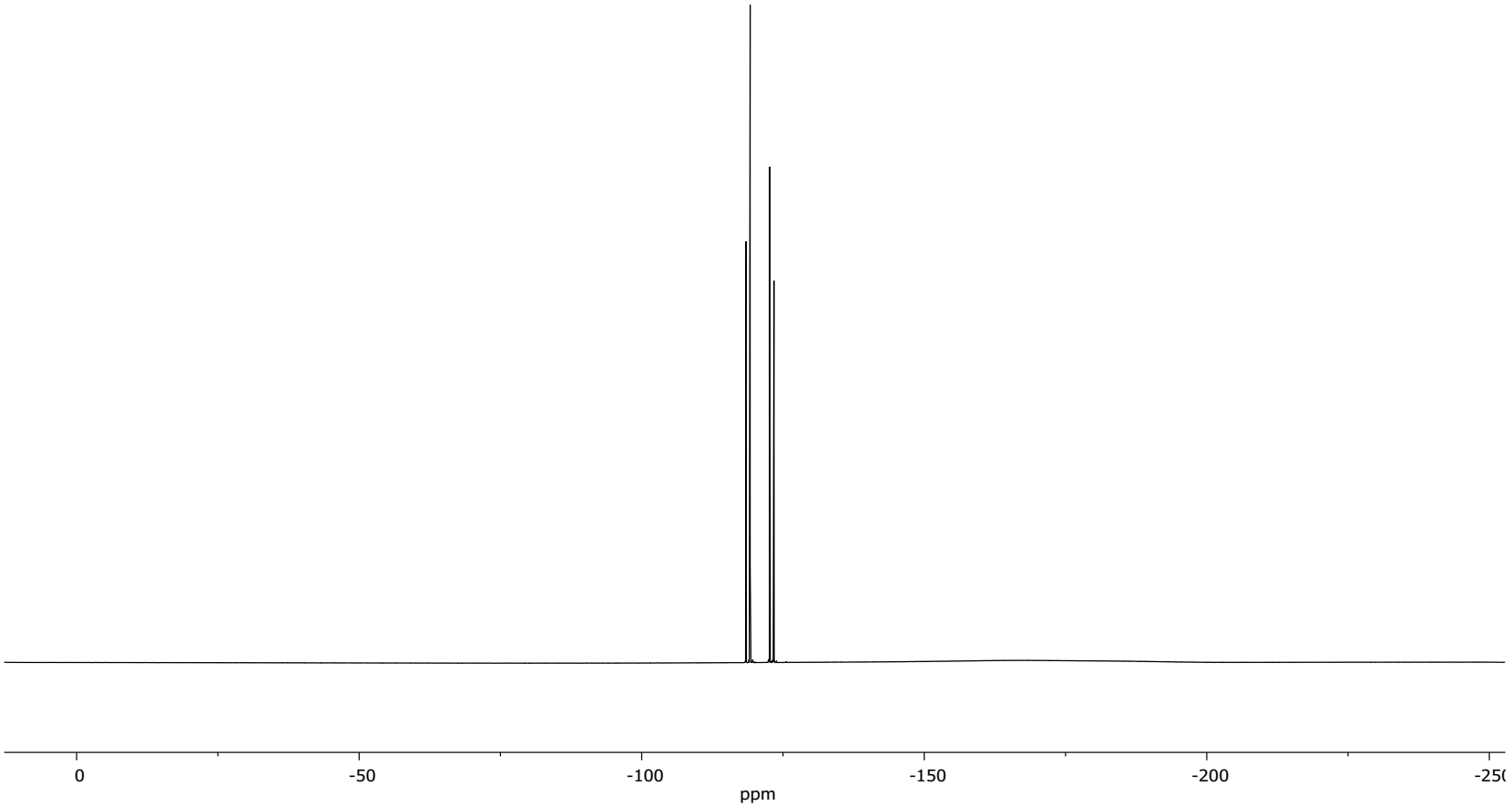
$^{13}C\{^{1}H\}$, $CDCl_3$, 126 MHz

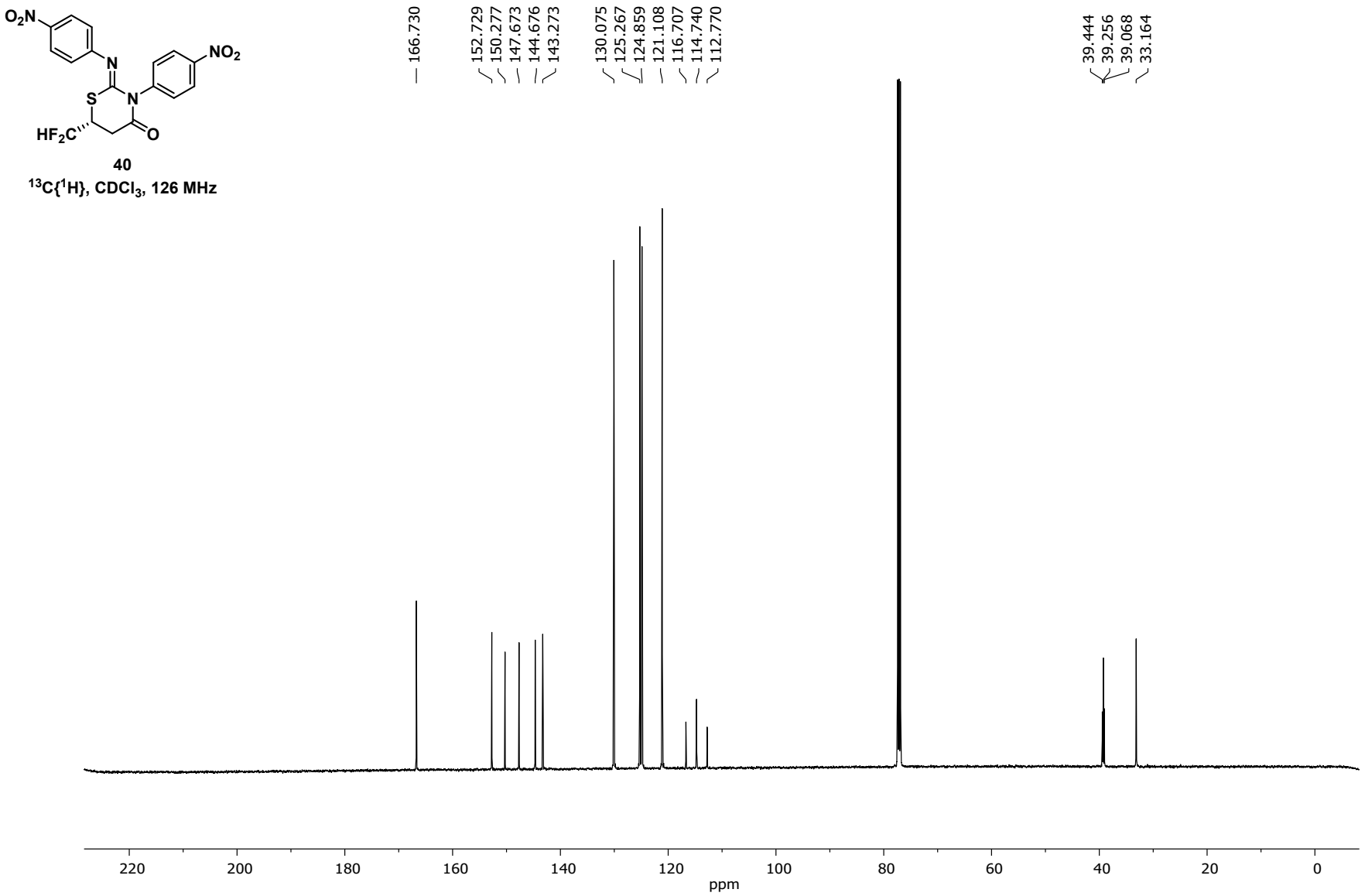

8.347
8.341
8.337
8.328
8.323
8.317
8.183
8.177
8.173
8.164
8.159
8.153
7.428
7.422
7.419
7.409
7.405
7.399
6.878
6.872
6.868
6.858
6.854
6.848
6.182
6.178
6.072
6.067
5.961
5.957
3.774
3.770
3.764
3.759
3.754
3.749
3.738
3.733
3.729
3.725
3.716
3.705
3.701
3.696
3.692
3.443
3.434
3.409
3.400
3.390
3.379
3.356
3.345
O2N
NO2
N
S
N
O
HF2C
40
1H, CDCl3, 500 MHz
1.97
1.97
1.96
1.97
1.02
1.00
1.99
10
9
8
7
6
5
4
3
2
1
0
ppm



40

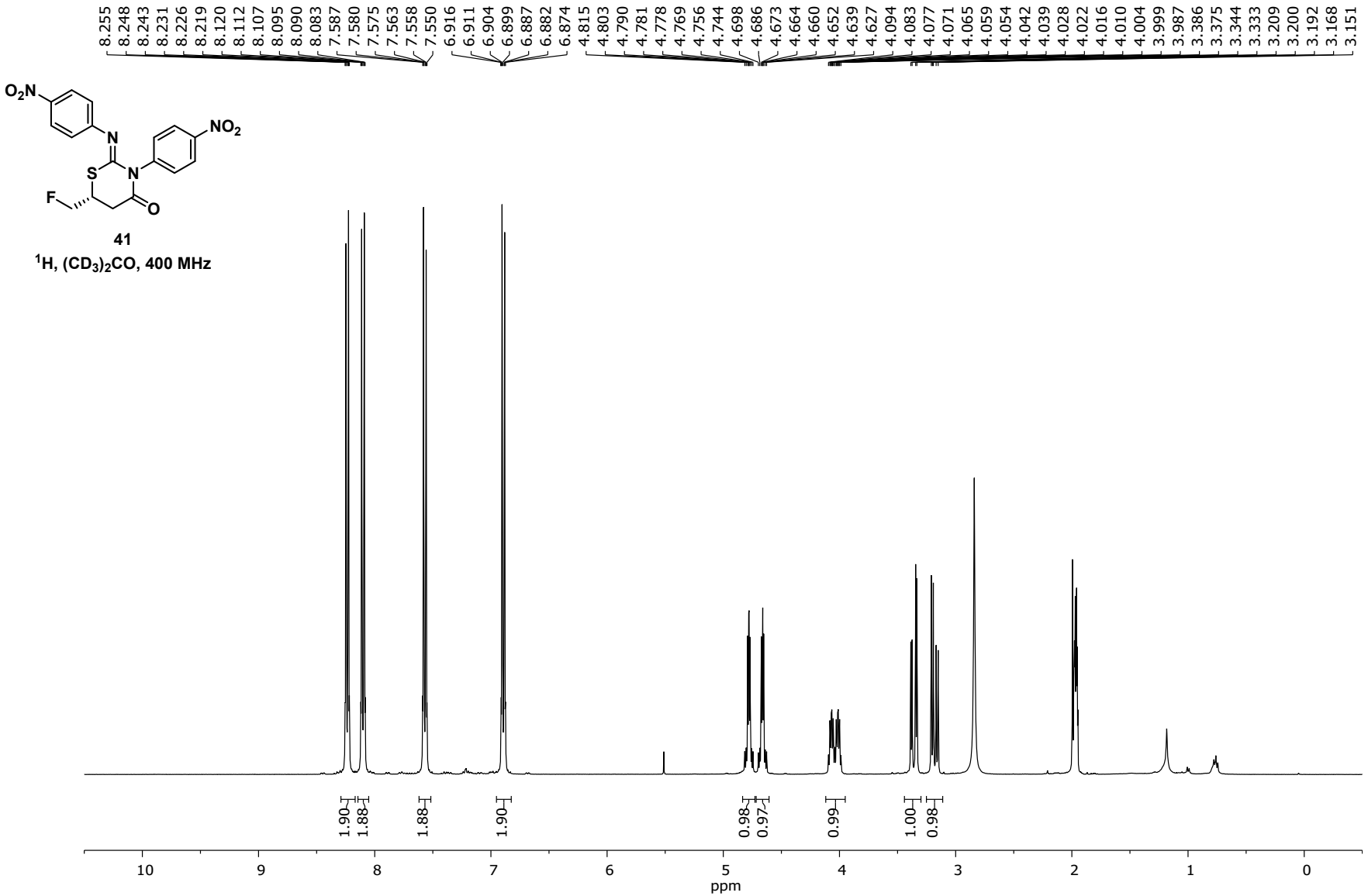
$^{19}F\{^{1}H\}$, $CDCl_3$, 376 MHz

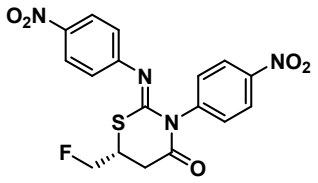




40

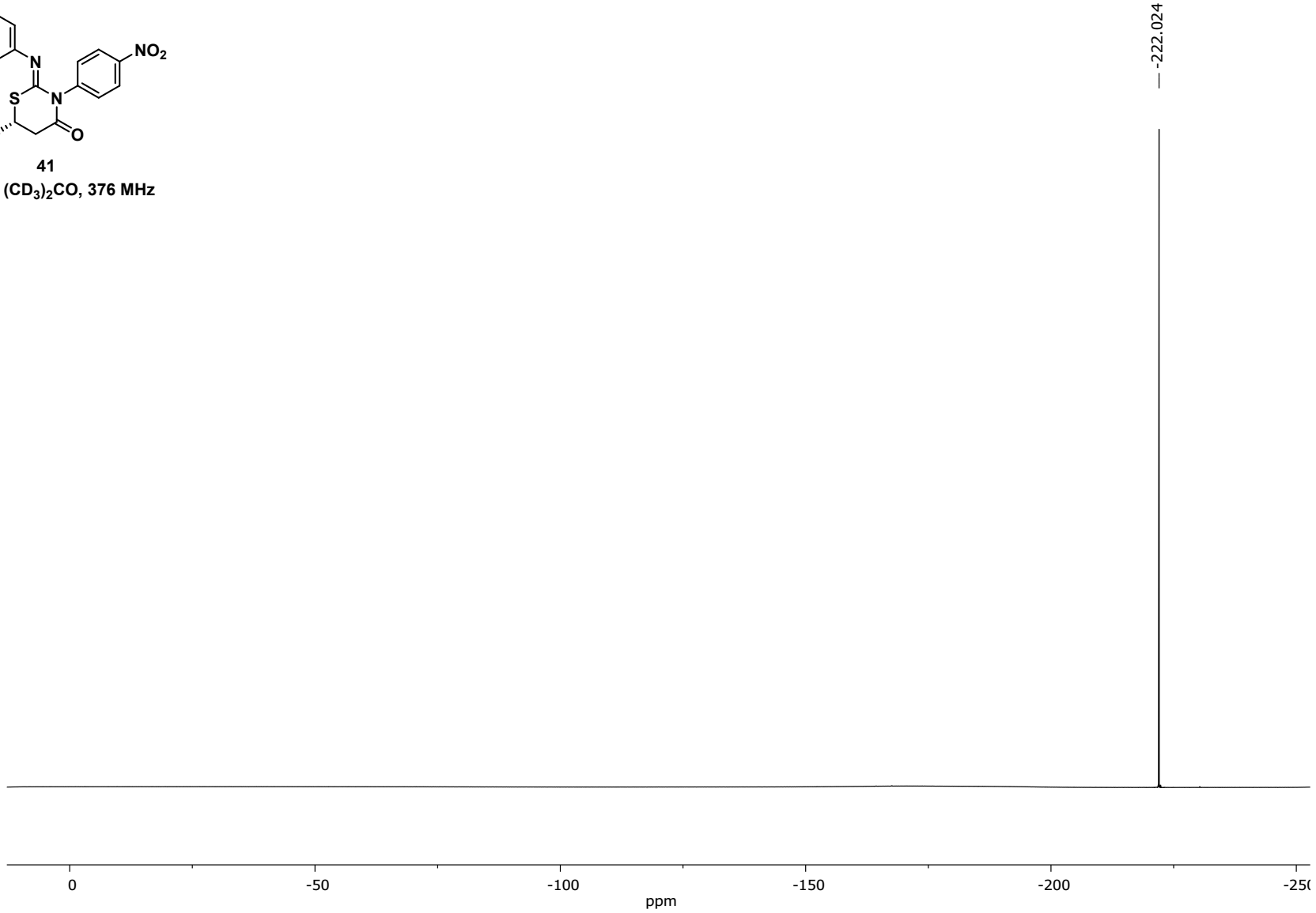
$^{13}C\{^{1}H\}$, $CDCl_3$, 126 MHz

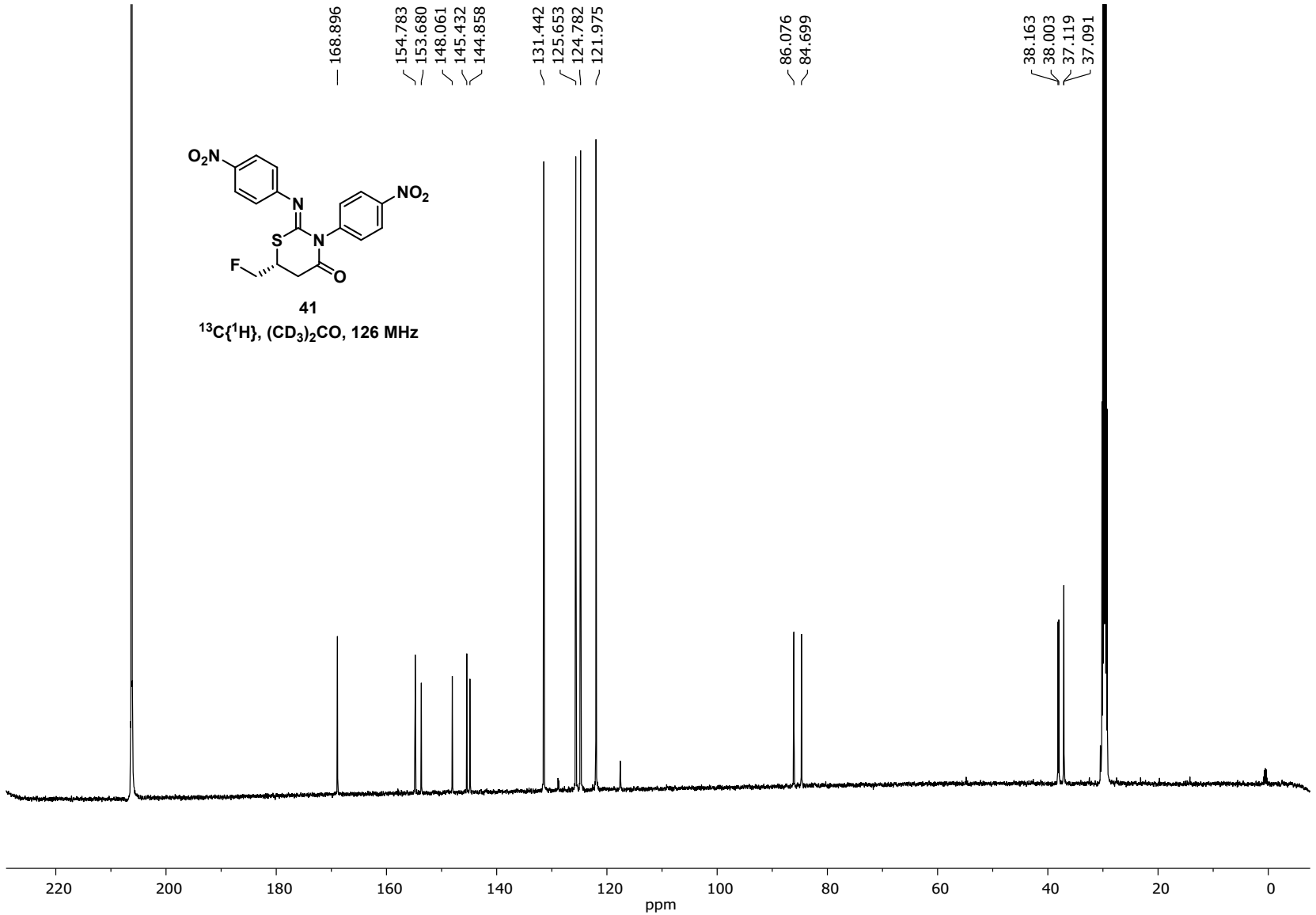

8.255
8.248
8.243
8.231
8.226
8.219
8.120
8.112
8.107
8.095
8.090
8.083
7.587
7.580
7.575
7.563
7.558
7.550
6.916
6.911
6.904
6.899
6.887
6.882
6.874
4.815
4.803
4.790
4.781
4.778
4.769
4.756
4.744
4.698
4.686
4.673
4.664
4.660
4.652
4.639
4.627
4.094
4.083
4.077
4.071
4.065
4.059
4.054
4.042
4.039
4.028
4.022
4.016
4.010
4.004
3.999
3.987
3.386
3.375
3.344
3.333
3.209
3.200
3.192
3.168
3.151
O2N
NO2
N
S
N
F
O
41
1H, (CD3)2CO, 400 MHz
1.90
1.88
1.88
1.90
0.98
0.97
0.99
1.00
0.98
10
9
8
7
6
5
4
3
2
1
0
ppm

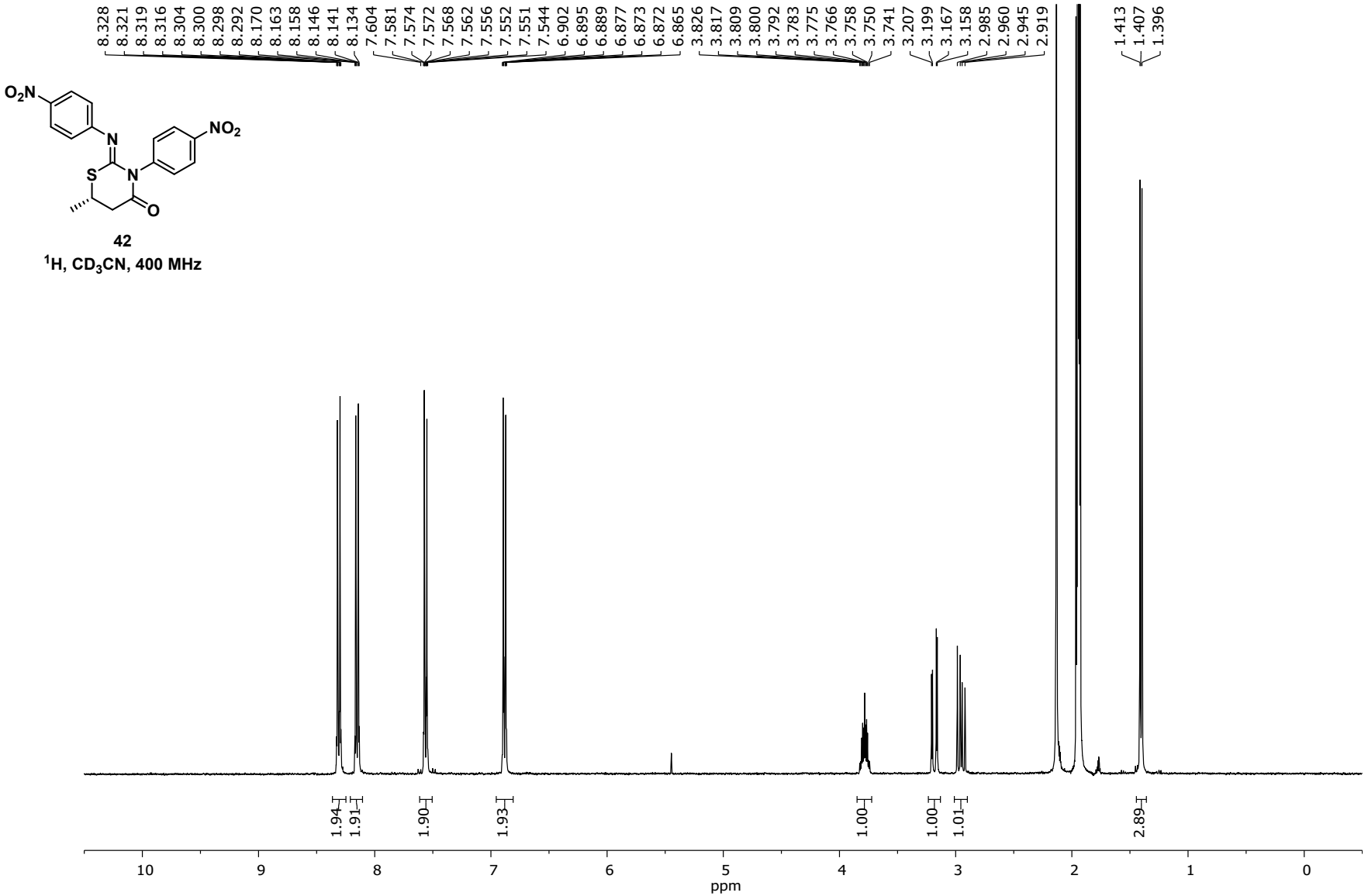


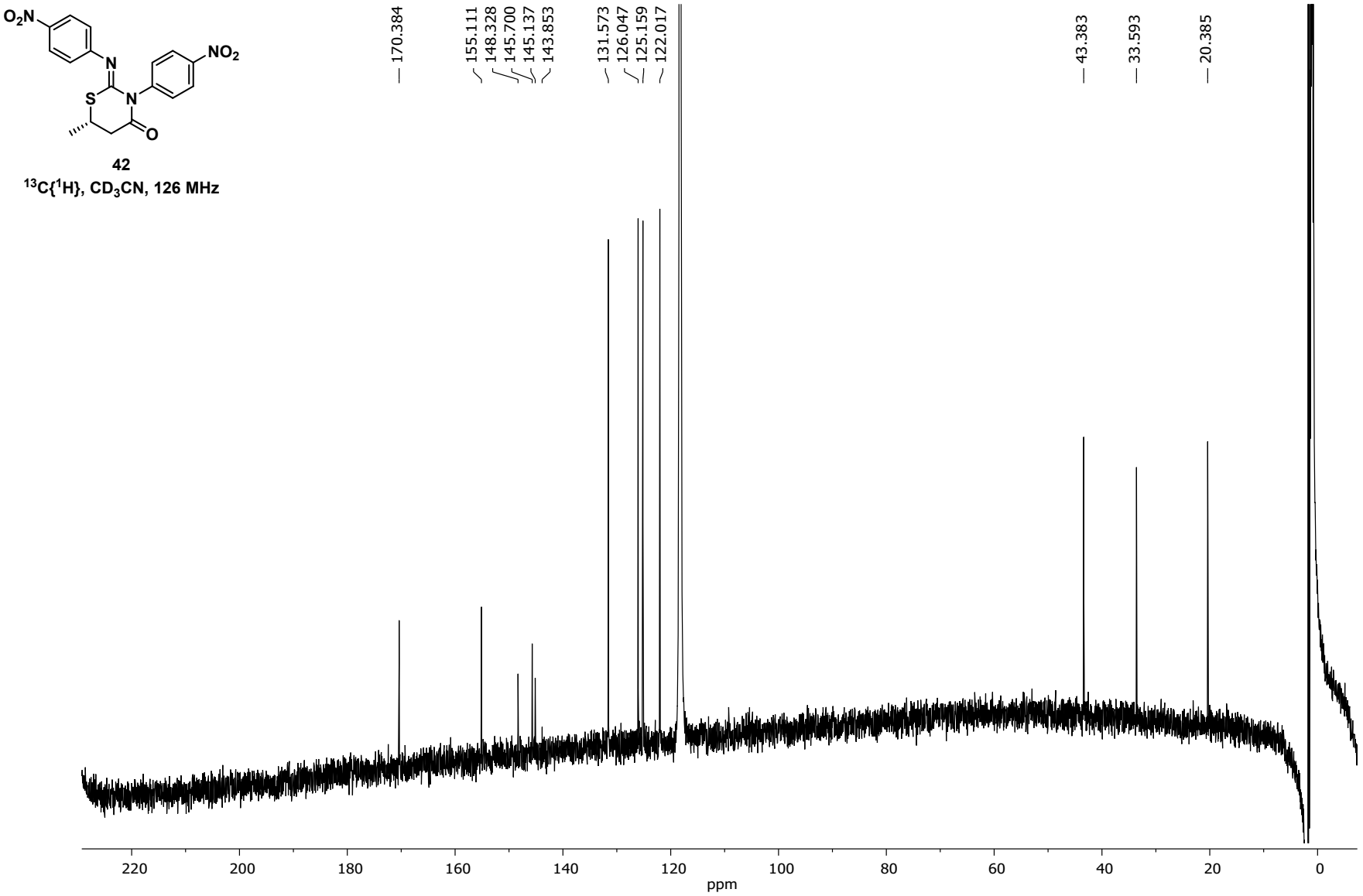
41

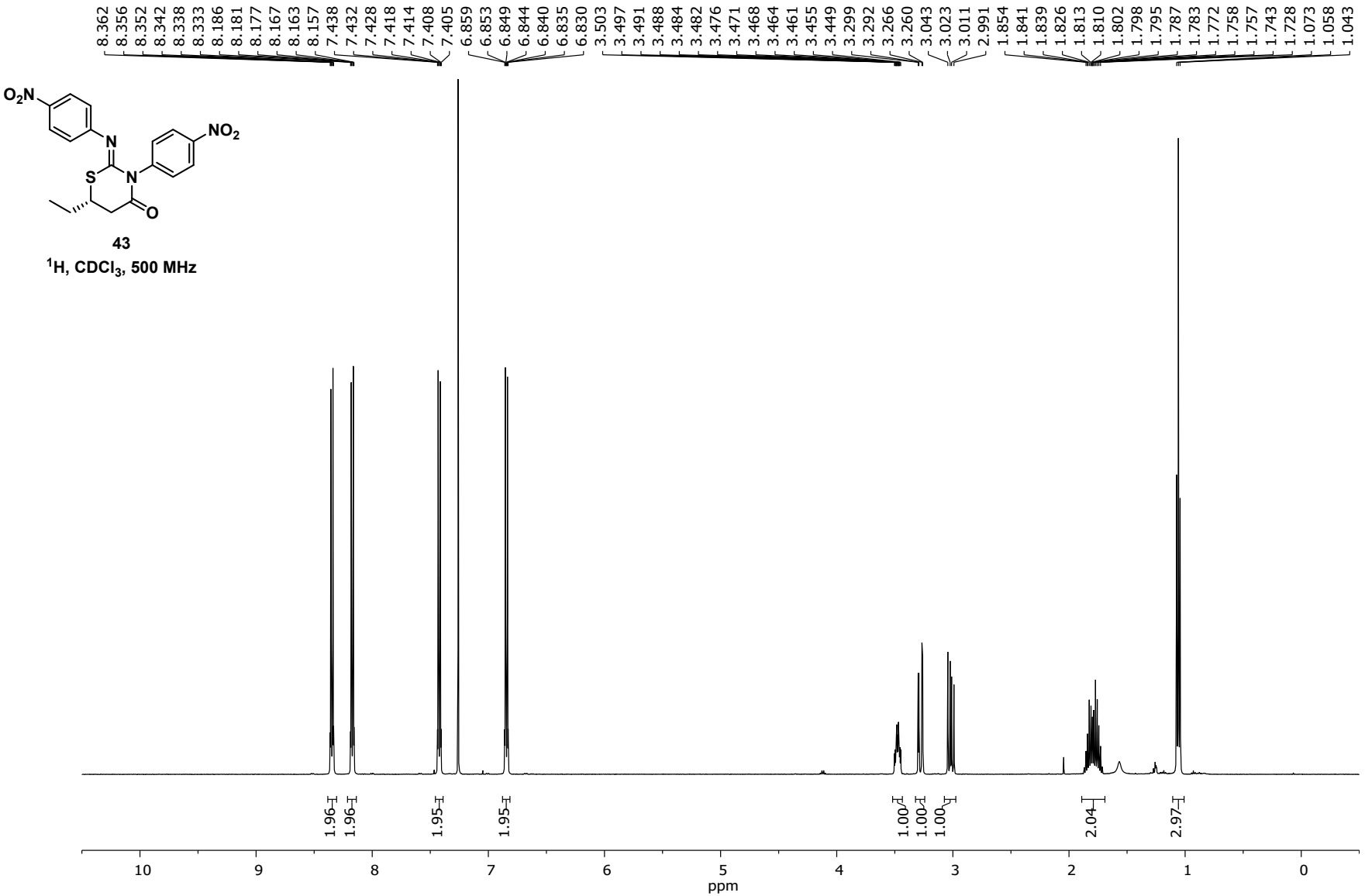
$^{19}F\{^{1}H\}$, $(CD_3)_2CO$, 376 MHz

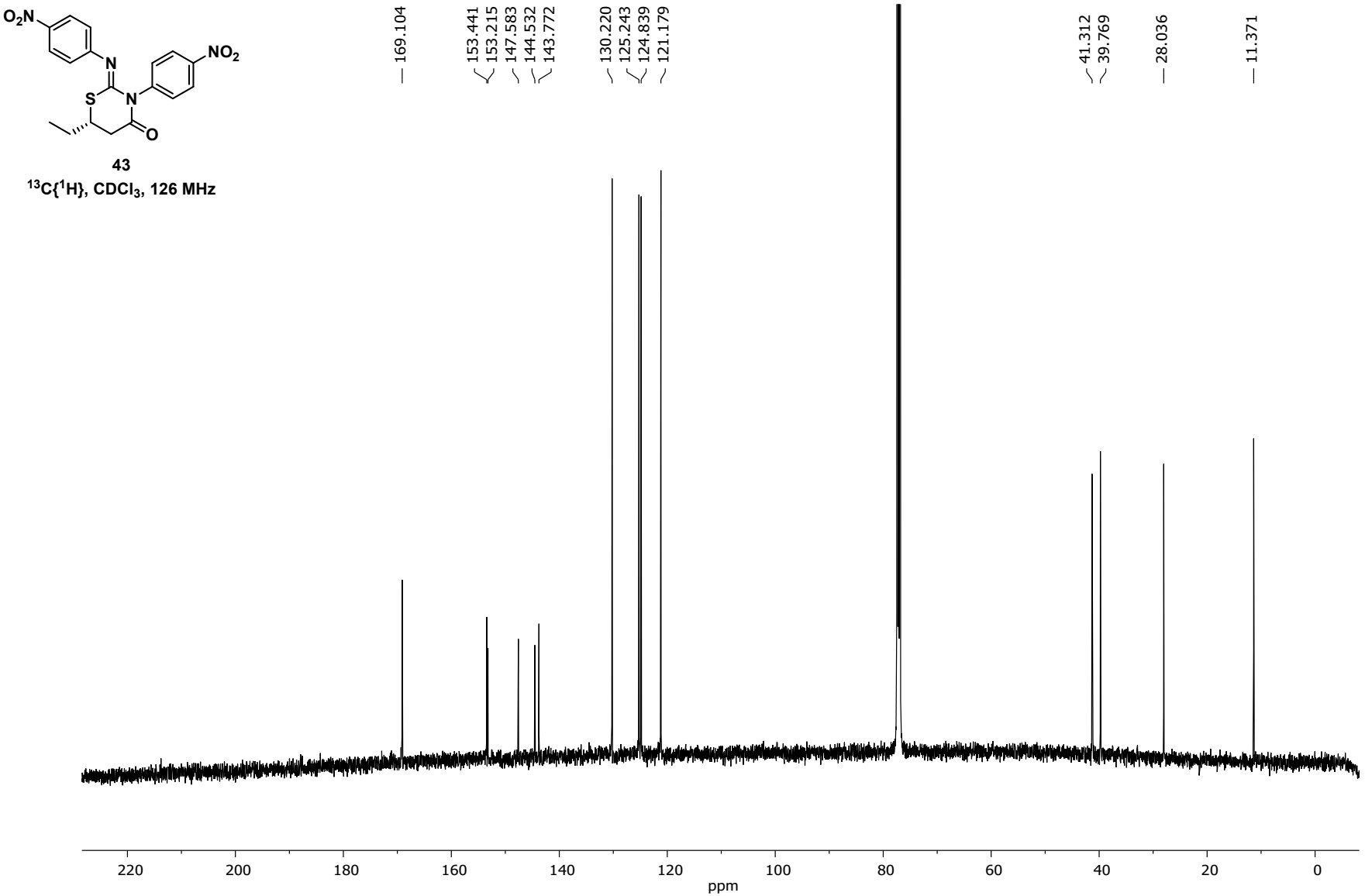


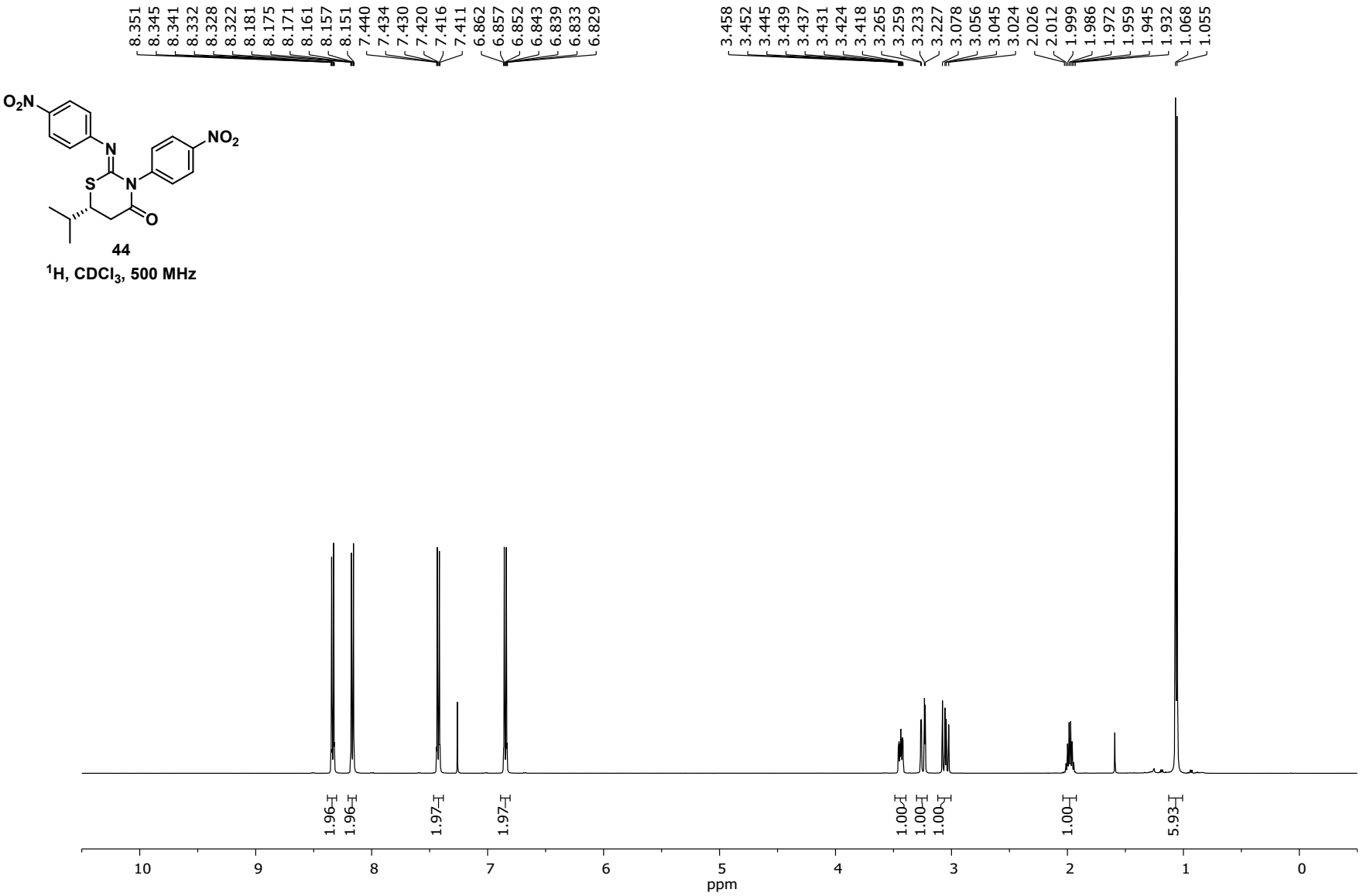

168.896
154.783
153.680
148.061
145.432
144.858
131.442
125.653
124.782
121.975
86.076
84.699
38.163
38.003
37.119
37.091
O2N
NO2
N
S
N
F
O
41
13C{1H}, (CD3)2CO, 126 MHz
220
200
180
160
140
120
100
80
60
40
20
0
ppm

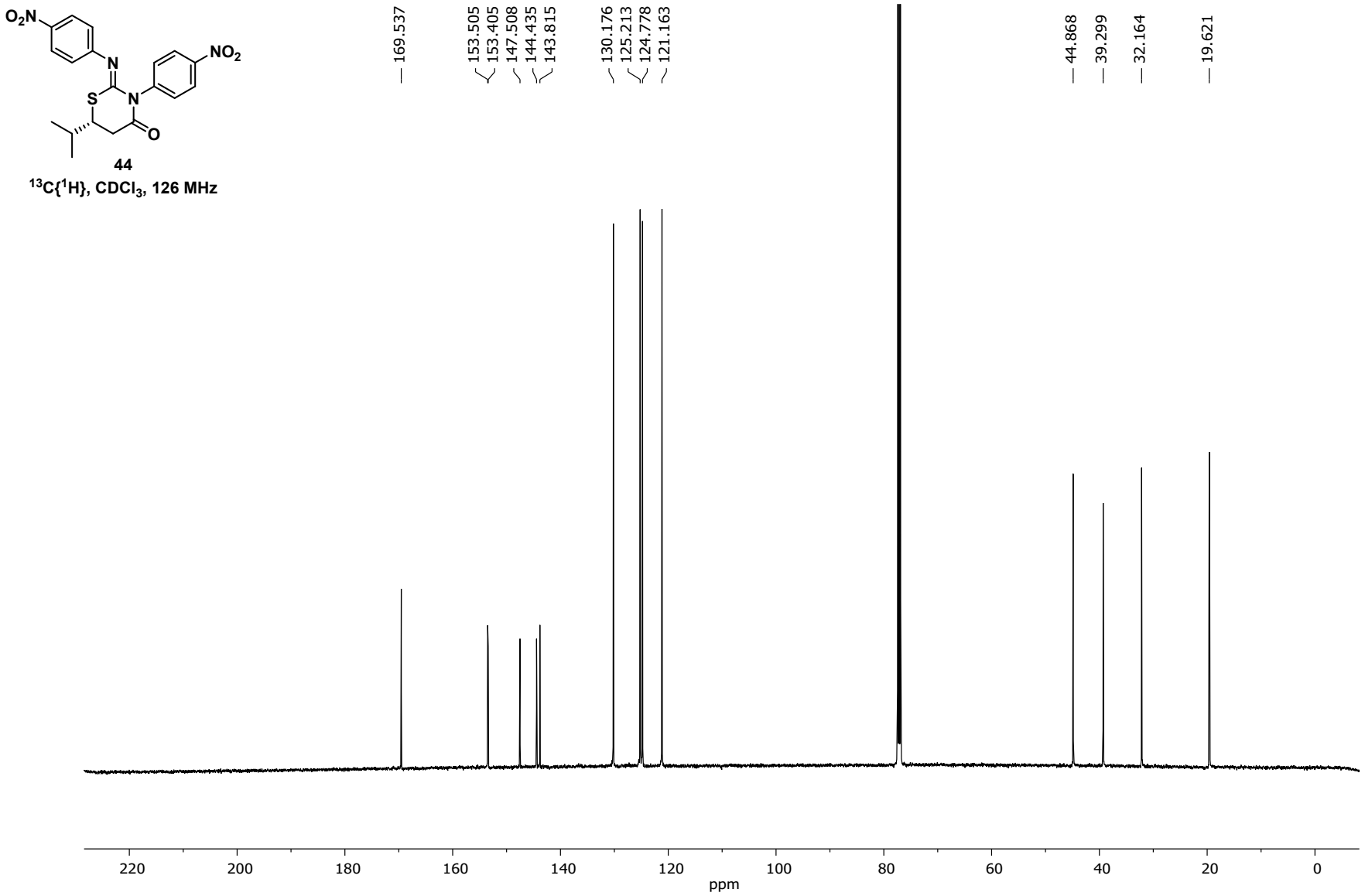

8.328
8.321
8.319
8.316
8.304
8.300
8.298
8.292
8.170
8.163
8.158
8.146
8.141
8.134
7.604
7.581
7.574
7.572
7.568
7.562
7.556
7.552
7.551
7.544
6.902
6.895
6.889
6.877
6.873
6.872
6.865
3.826
3.817
3.809
3.800
3.792
3.783
3.775
3.766
3.758
3.750
3.741
3.207
3.199
3.167
3.158
2.985
2.960
2.945
2.919
1.413
1.407
1.396
O2N
NO2
N
S
N
O
42
1H, CD3CN, 400 MHz
1.94
1.91
1.90
1.93
1.00
1.00
1.01
2.89
10
9
8
7
6
5
4
3
2
1
0
ppm

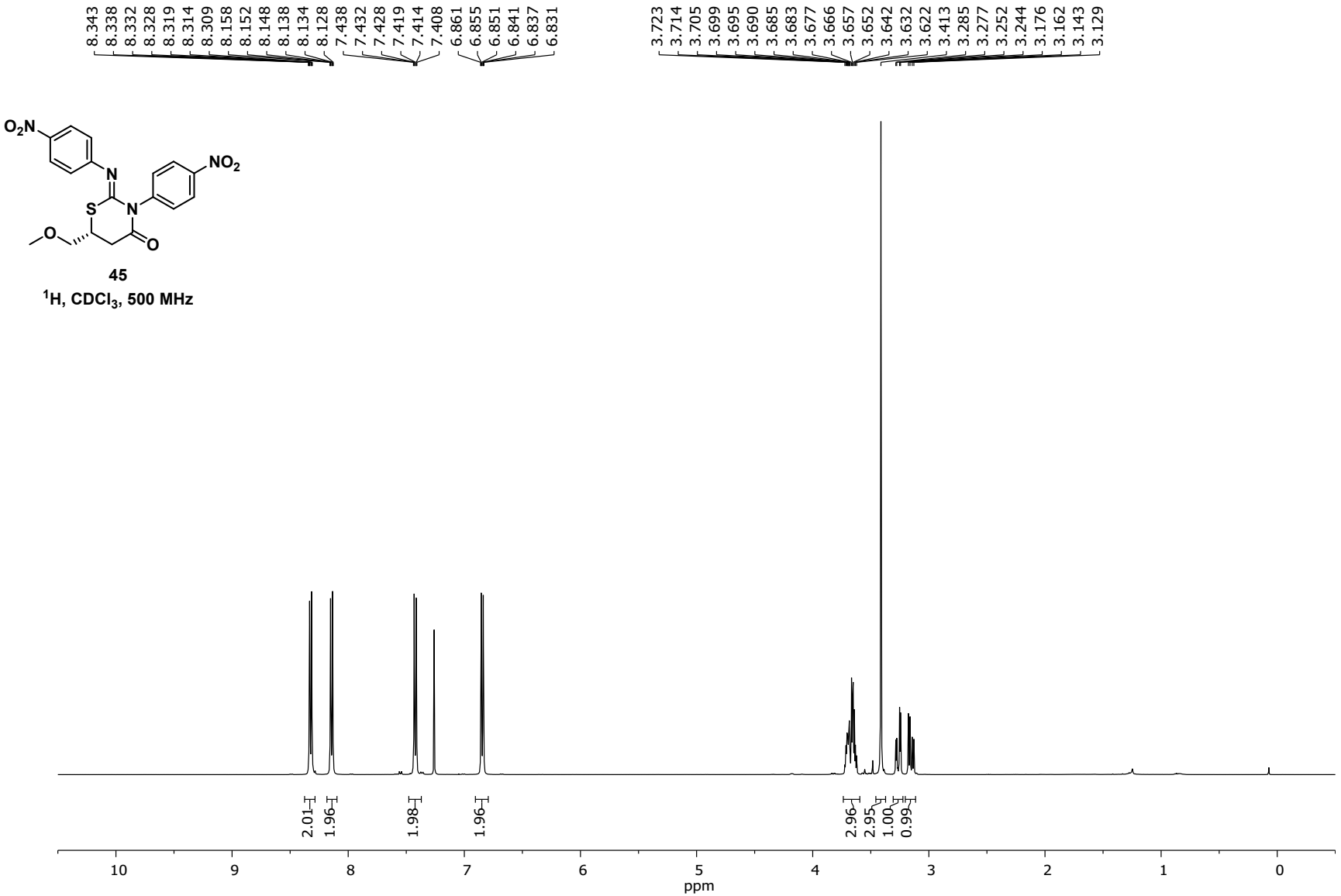

O2N
NO2
N
S
N
O
42
13C{1H}, CD3CN, 126 MHz
170.384
155.111
148.328
145.700
145.137
143.853
131.573
126.047
125.159
122.017
43.383
33.593
20.385
220
200
180
160
140
120
100
80
60
40
20
0
ppm

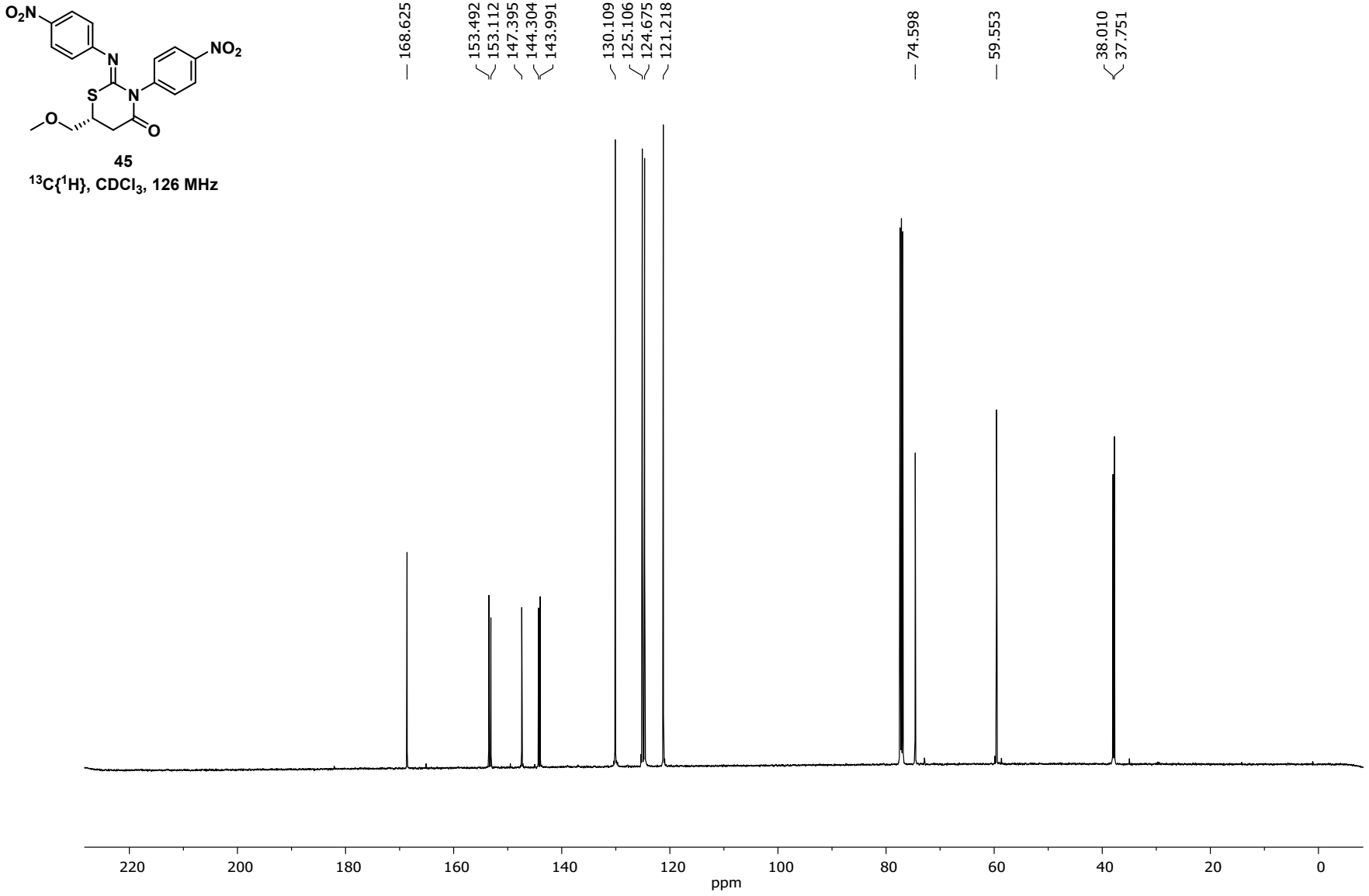

8.362
8.356
8.352
8.342
8.338
8.333
8.186
8.181
8.177
8.167
8.163
8.157
7.438
7.432
7.428
7.418
7.414
7.408
7.405
6.859
6.853
6.849
6.844
6.840
6.835
6.830
3.503
3.497
3.491
3.488
3.484
3.482
3.476
3.471
3.468
3.464
3.461
3.455
3.449
3.299
3.292
3.266
3.260
3.043
3.023
3.011
2.991
1.854
1.841
1.839
1.826
1.813
1.810
1.802
1.798
1.795
1.787
1.783
1.772
1.758
1.757
1.743
1.728
1.073
1.058
1.043
O2N
NO2
N
S
N
O
43
1H, CDCl3, 500 MHz
1.96
1.96
1.95
1.95
1.00
1.00
1.00
2.04
2.97
10
9
8
7
6
5
4
3
2
1
0
ppm

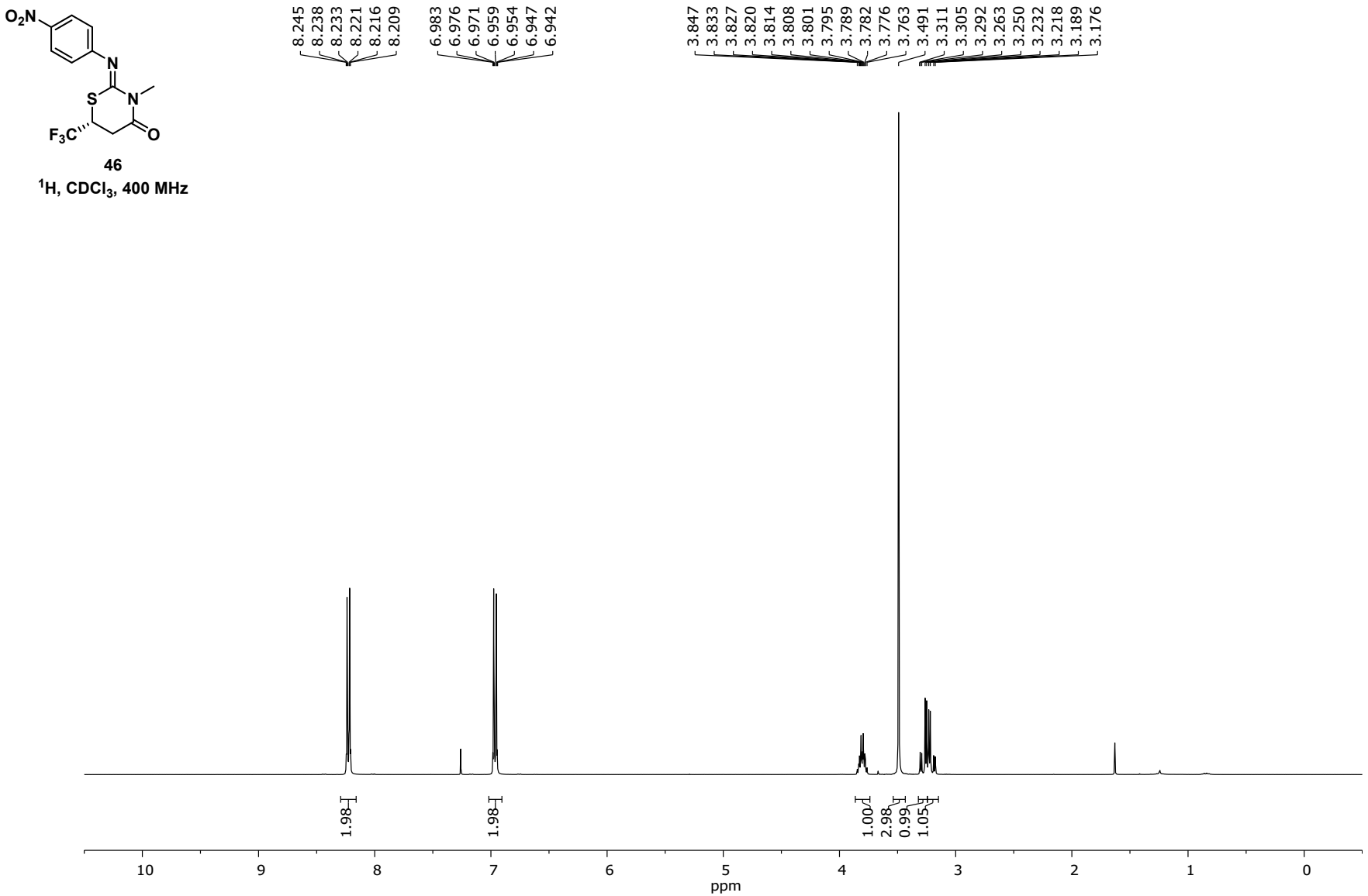

O2N
NO2
N
S
N
O
43
13C{1H}, CDCl3, 126 MHz
169.104
153.441
153.215
147.583
144.532
143.772
130.220
125.243
124.839
121.179
41.312
39.769
28.036
11.371
220
200
180
160
140
120
100
80
60
40
20
0
ppm


8.351
8.345
8.341
8.332
8.328
8.322
8.181
8.175
8.171
8.161
8.157
8.151
7.440
7.434
7.430
7.420
7.416
7.411
6.862
6.857
6.852
6.843
6.839
6.833
6.829
3.458
3.452
3.445
3.439
3.437
3.431
3.424
3.418
3.265
3.259
3.233
3.227
3.078
3.056
3.045
3.024
2.026
2.012
1.999
1.986
1.972
1.959
1.945
1.932
1.068
1.055
O2N
NO2
N
S
N
O
44
1H, CDCl3, 500 MHz
1.96
1.96
1.97
1.97
1.00
1.00
1.00
1.00
5.93
10
9
8
7
6
5
4
3
2
1
0
ppm


O2N
NO2
N
S
N
O
44
13C{1H}, CDCl3, 126 MHz
169.537
153.505
153.405
147.508
144.435
143.815
130.176
125.213
124.778
121.163
44.868
39.299
32.164
19.621
220
200
180
160
140
120
100
80
60
40
20
0
ppm

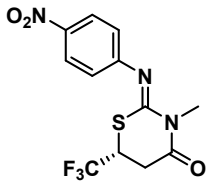

8.343
8.338
8.332
8.328
8.319
8.314
8.309
8.158
8.152
8.148
8.138
8.134
8.128
7.438
7.432
7.428
7.419
7.414
7.408
6.861
6.855
6.851
6.841
6.837
6.831
3.723
3.714
3.705
3.699
3.695
3.690
3.685
3.683
3.677
3.666
3.657
3.652
3.642
3.632
3.622
3.413
3.285
3.277
3.252
3.244
3.176
3.162
3.143
3.129
O2N
NO2
N
S
N
O
O
45
1H, CDCl3, 500 MHz
2.01
1.96
1.98
1.96
2.96
2.95
1.00
0.99
10
9
8
7
6
5
4
3
2
1
0
ppm


O2N
NO2
N
S
N
O
O
45
13C{1H}, CDCl3, 126 MHz
168.625
153.492
153.112
147.395
144.304
143.991
130.109
125.106
124.675
121.218
74.598
59.553
38.010
37.751
220
200
180
160
140
120
100
80
60
40
20
0
ppm



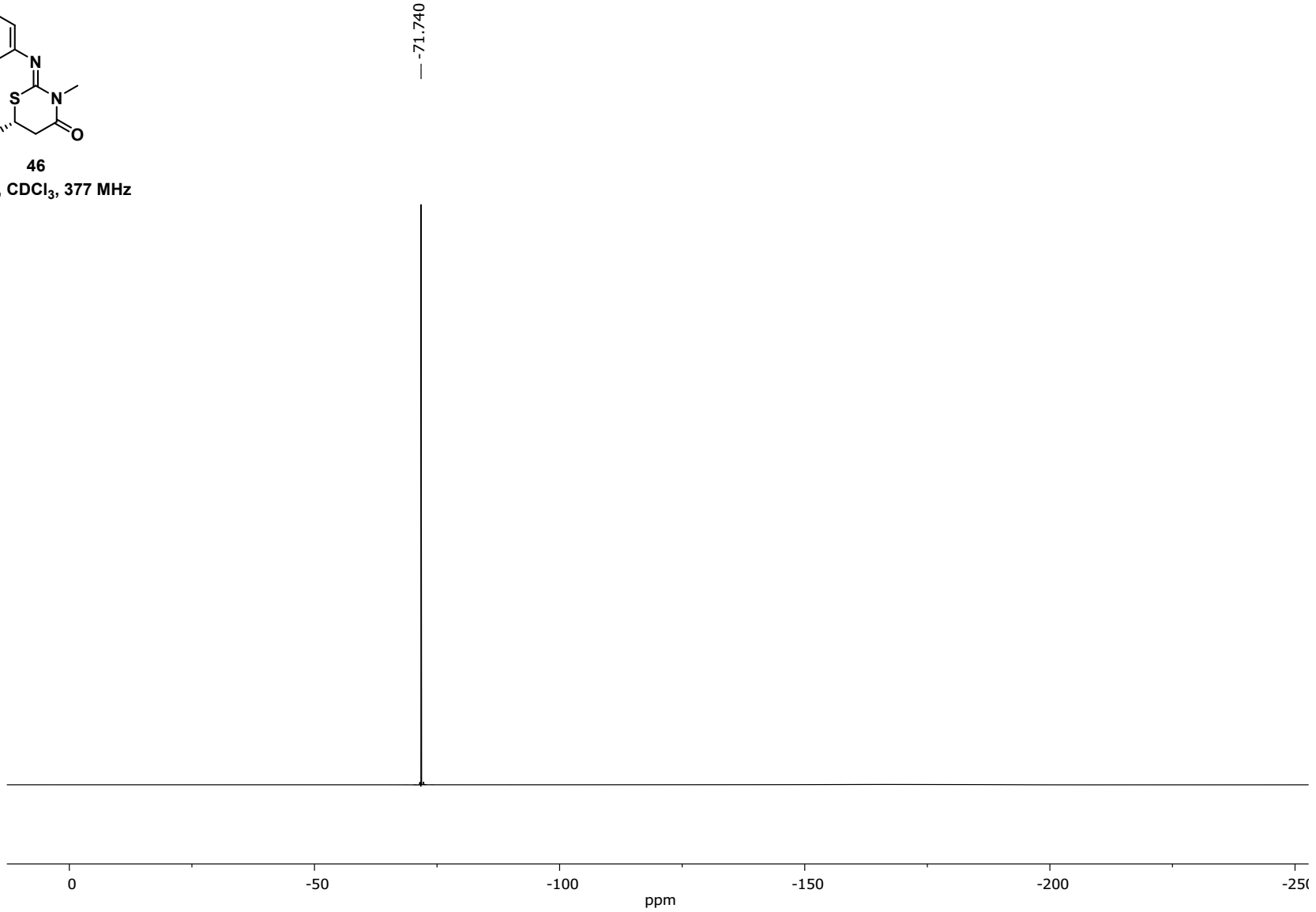
46

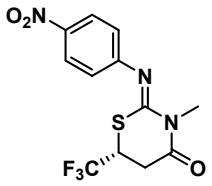
^{1}H, $CDCl_3$, 400 MHz



46

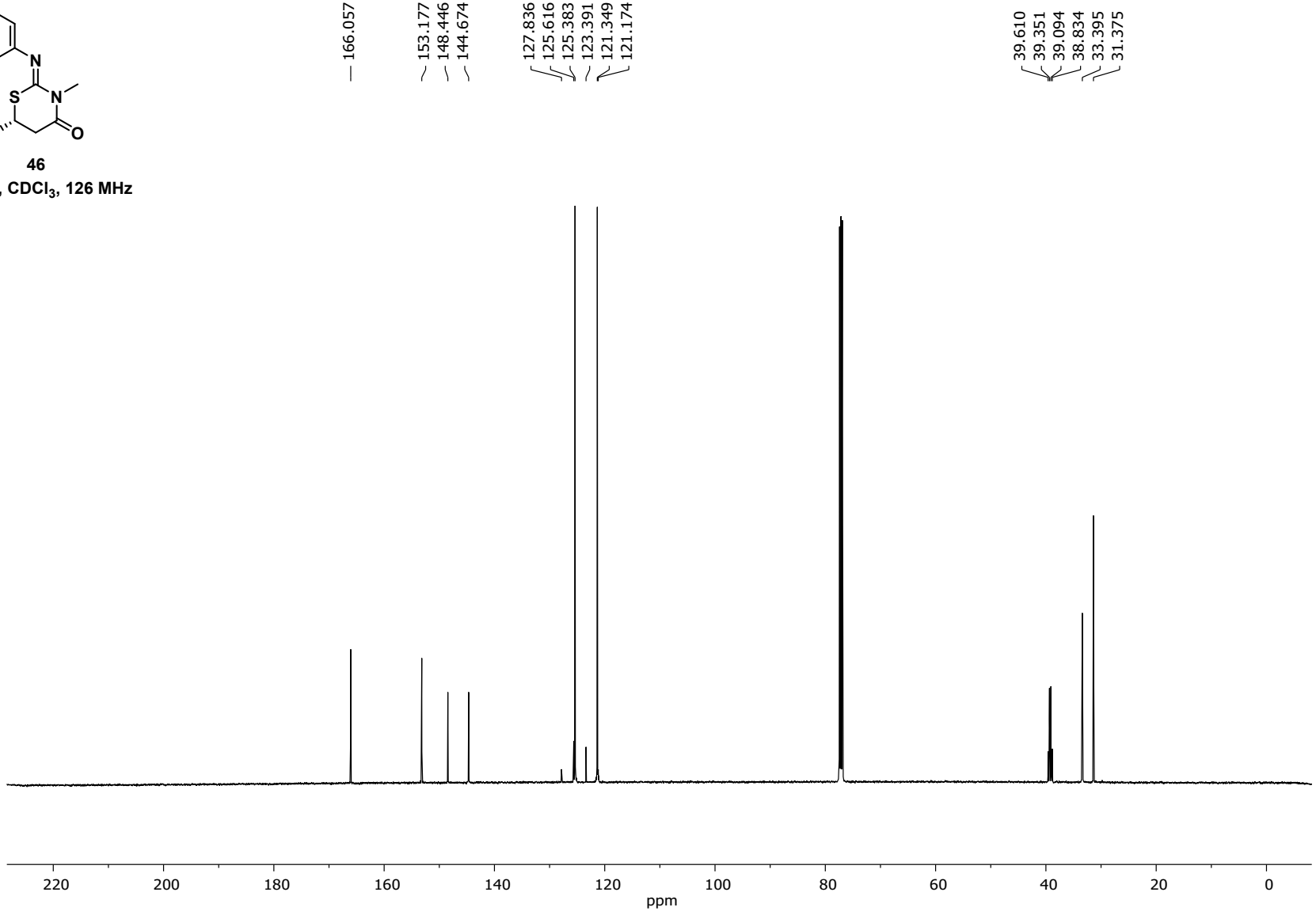
$^{19}F\{^{1}H\}$, $CDCl_3$, 377 MHz

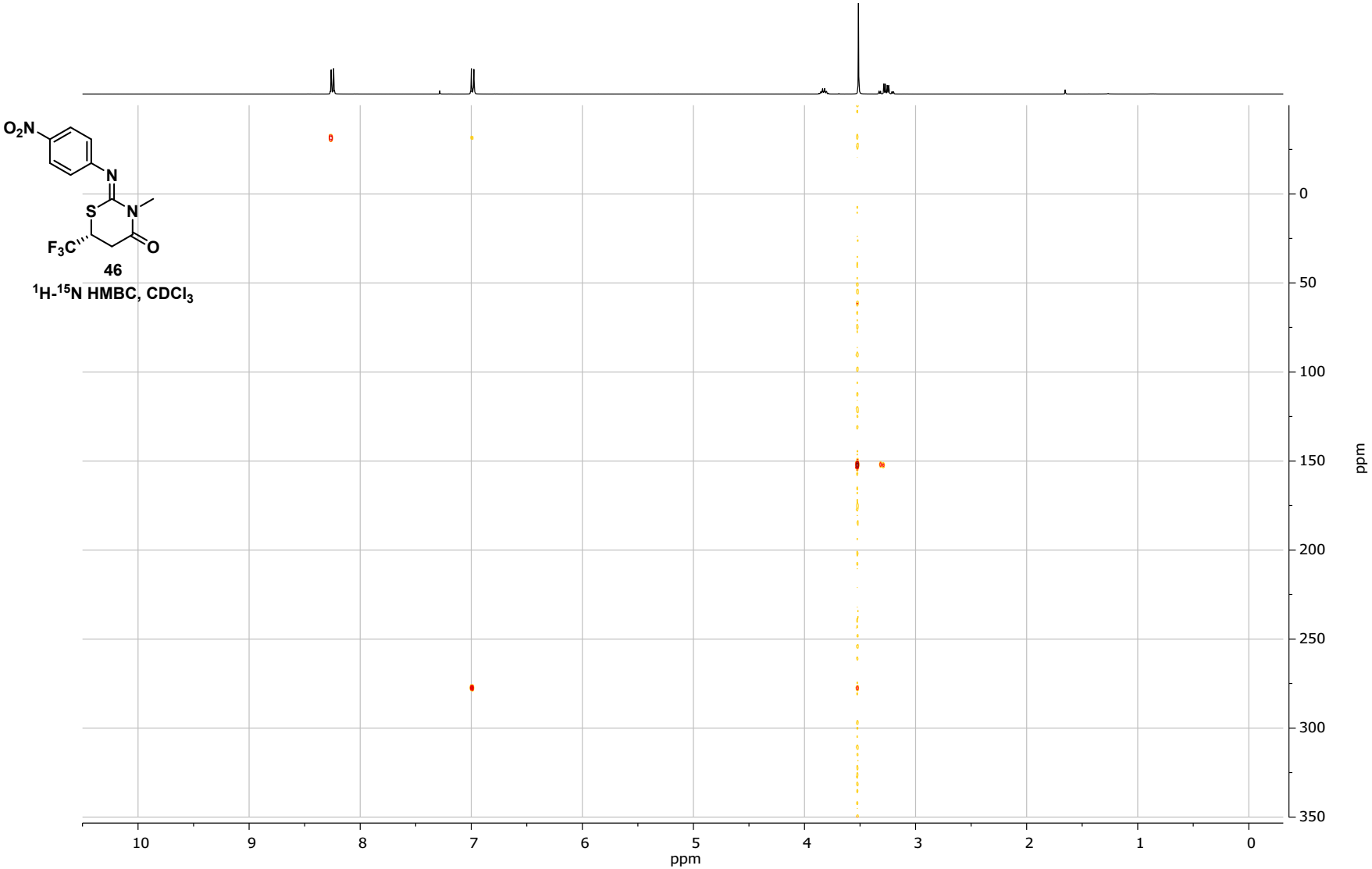


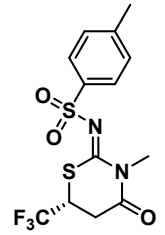


46

$^{13}C\{^{1}H\}$, $CDCl_3$, 126 MHz

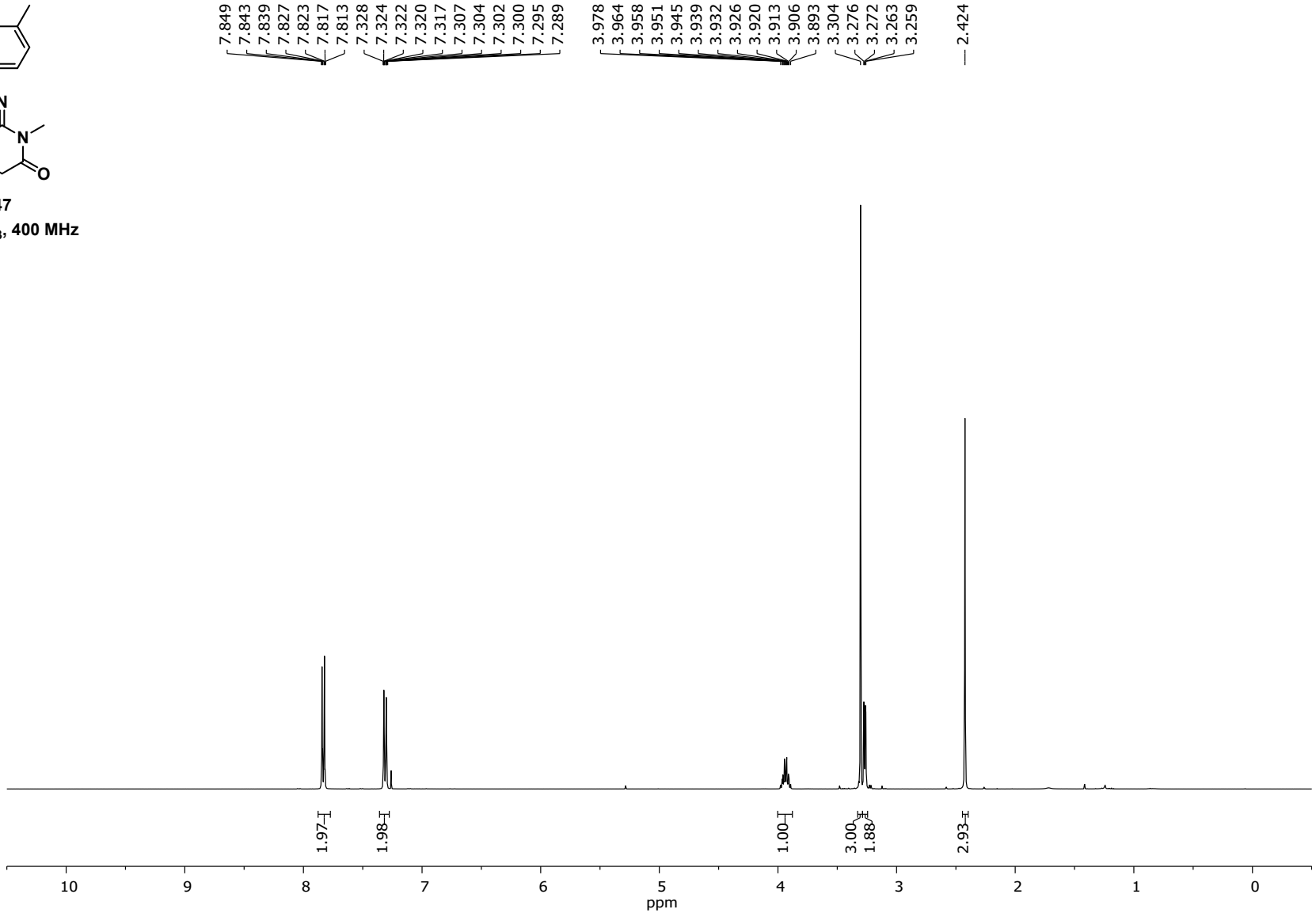


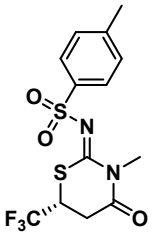

O2N
N
S
N
F3C
O
46
1H-15N HMBC, CDCl3
0
50
100
150
200
250
300
350
ppm
10
9
8
7
6
5
4
3
2
1
0
ppm



47

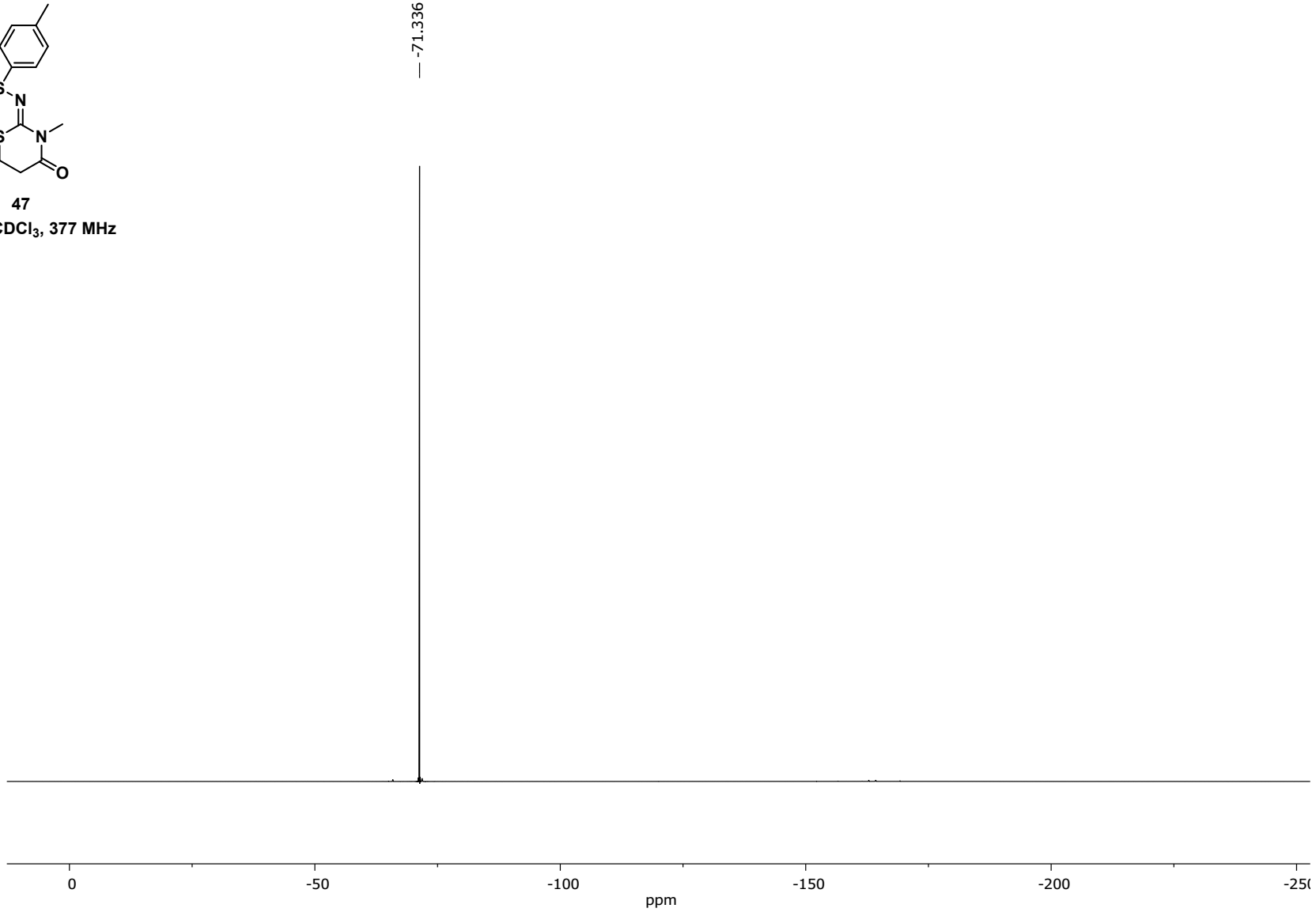
^{1}H, $CDCl_3$, 400 MHz

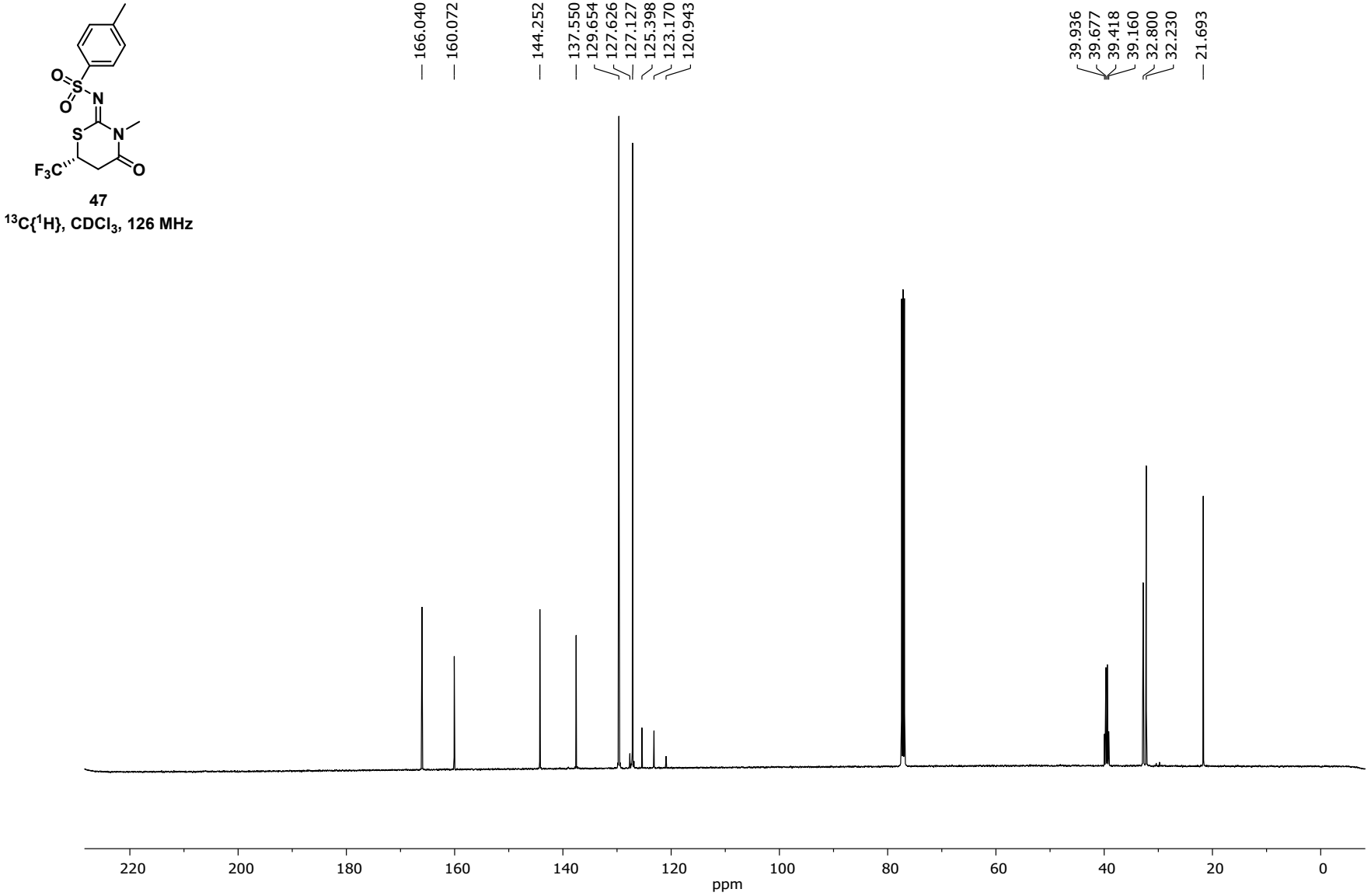




47

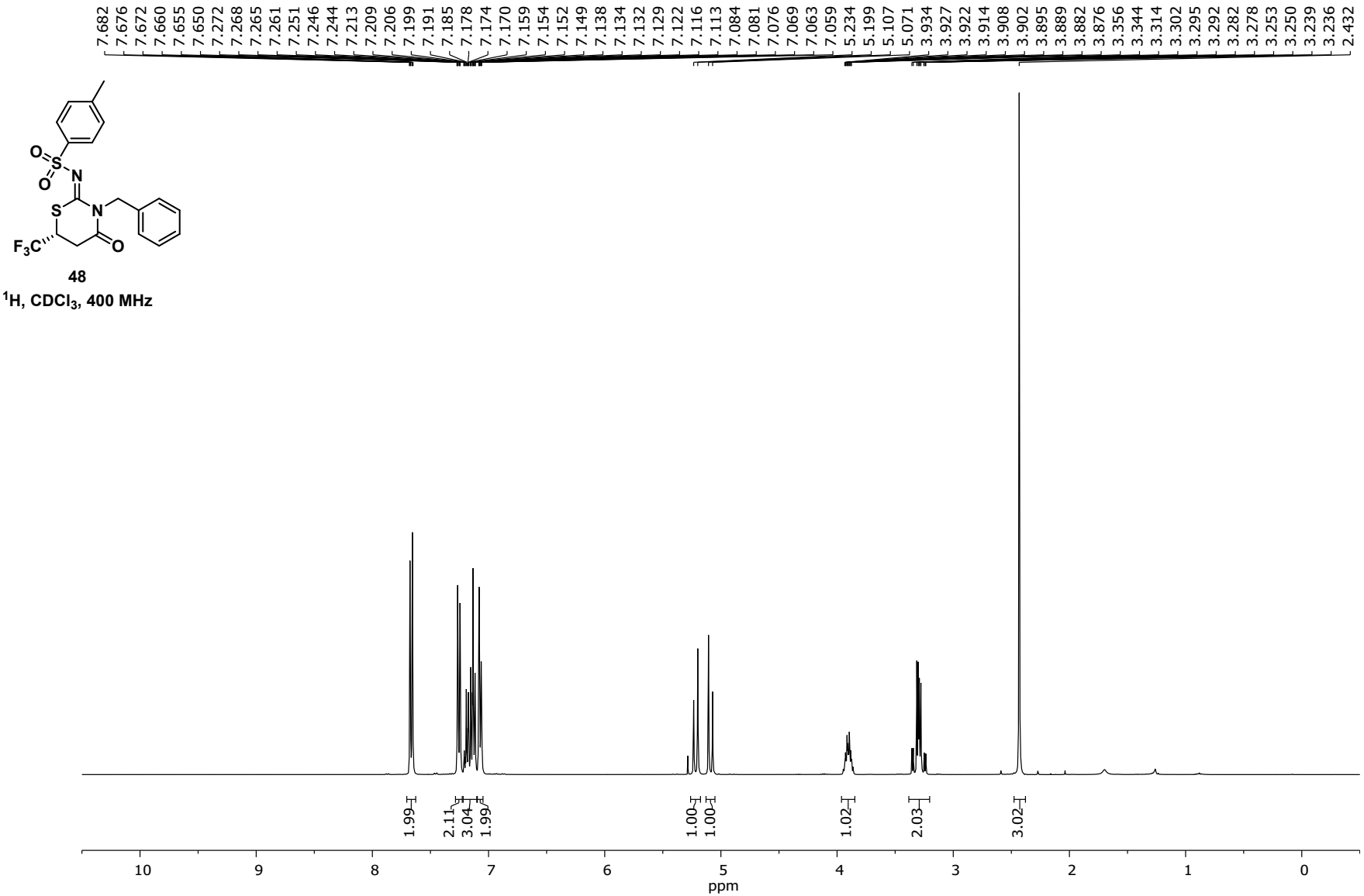
$^{19}F\{^{1}H\}$, $CDCl_3$, 377 MHz





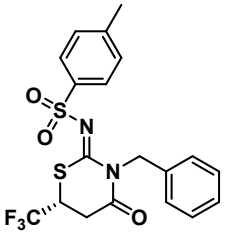
47

$^{13}C\{^{1}H\}$, $CDCl_3$, 126 MHz



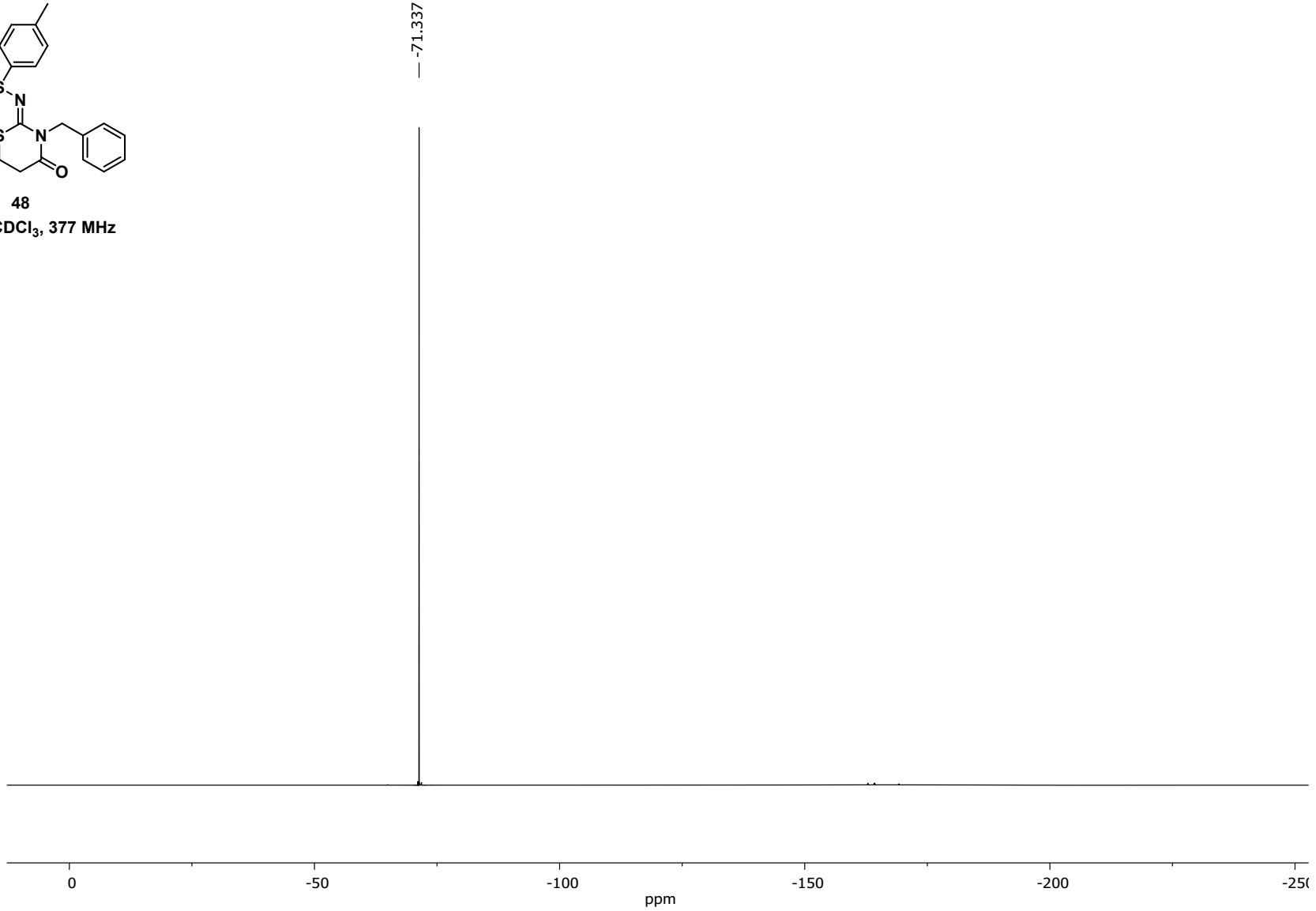
48

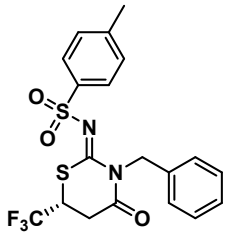
^{1}H, $CDCl_3$, 400 MHz



48

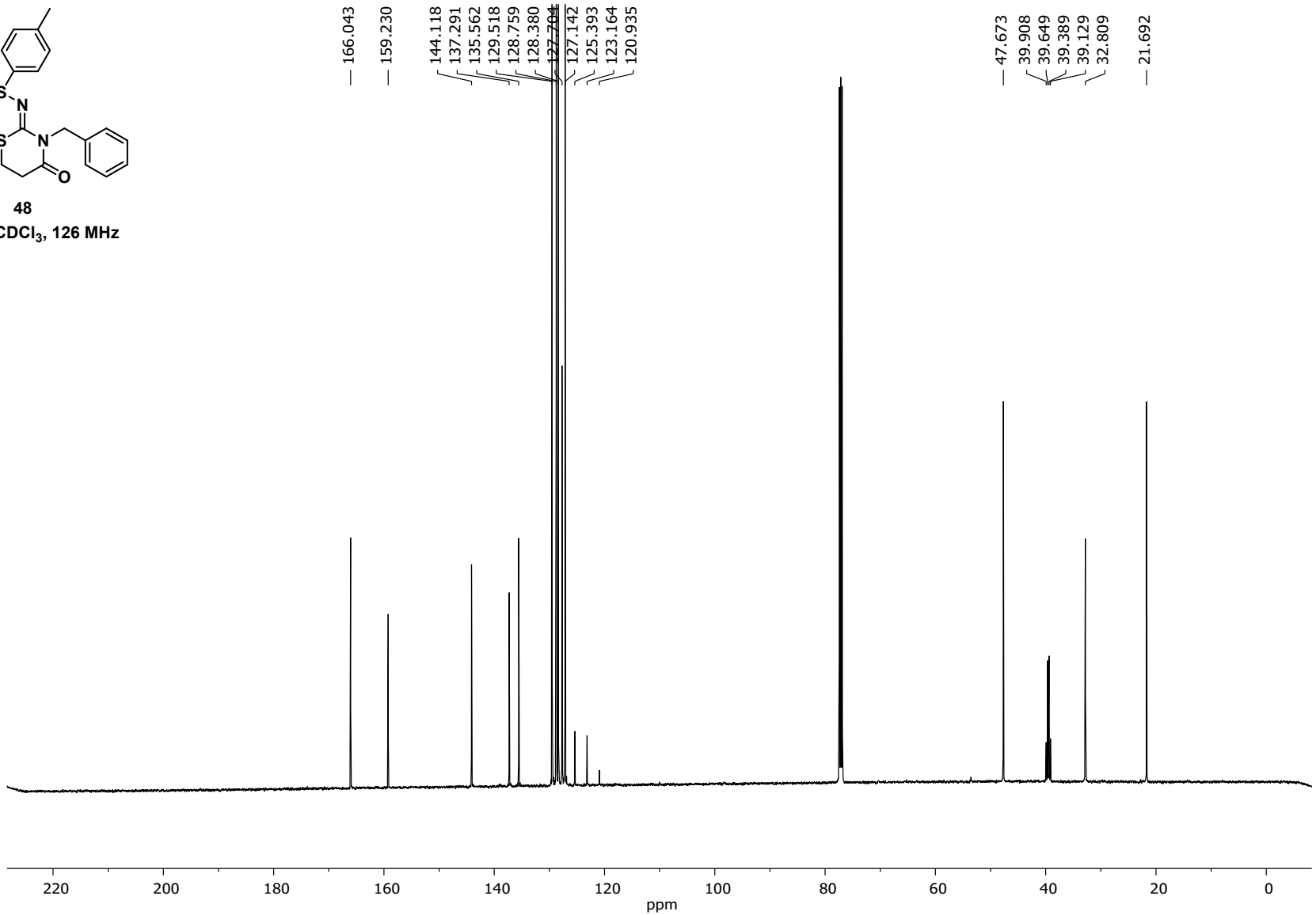
$^{19}F\{^{1}H\}$, $CDCl_3$, 377 MHz

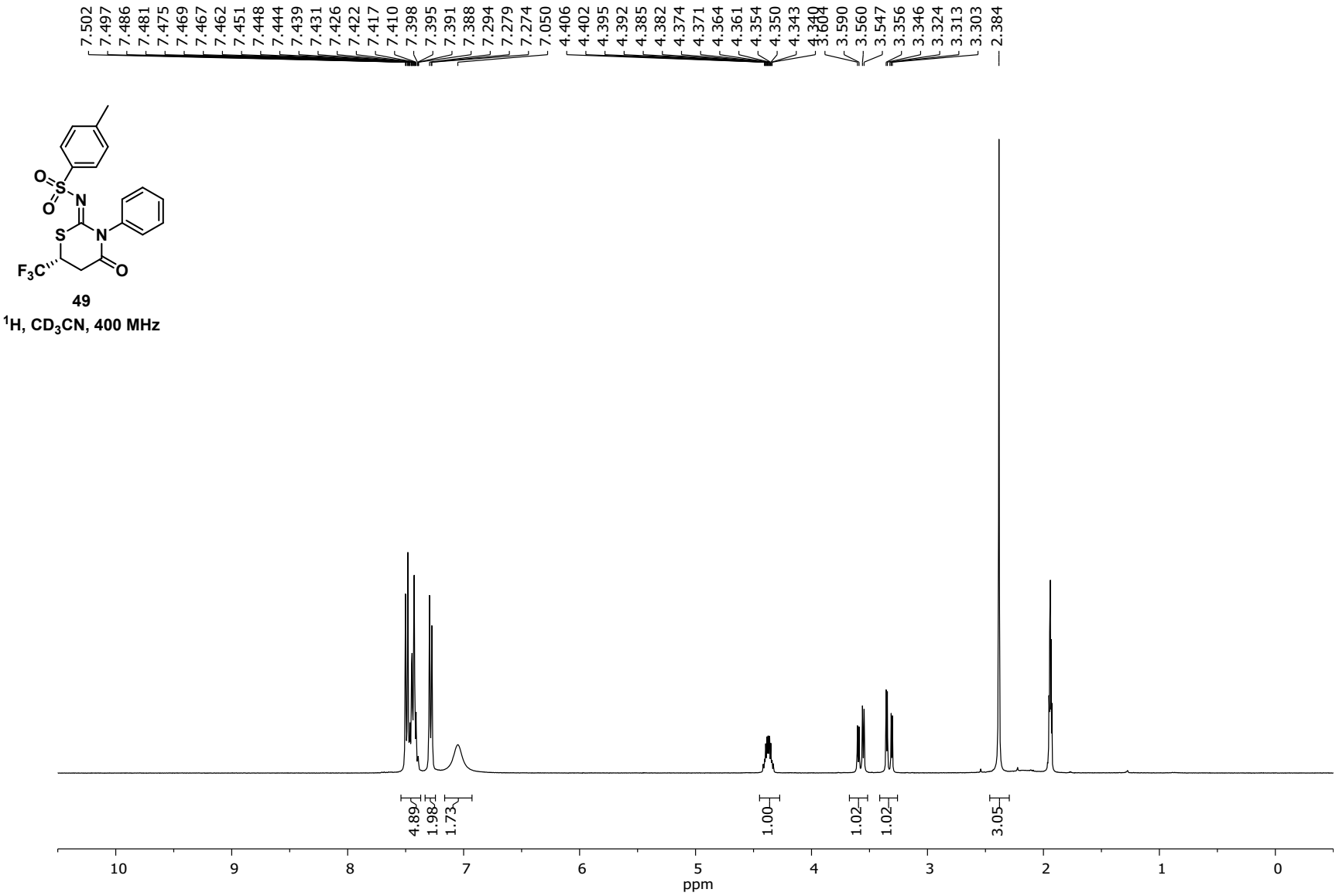


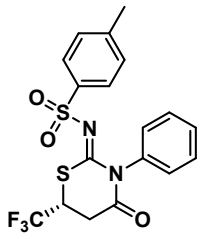


48

$^{13}C\{^{1}H\}$, $CDCl_3$, 126 MHz

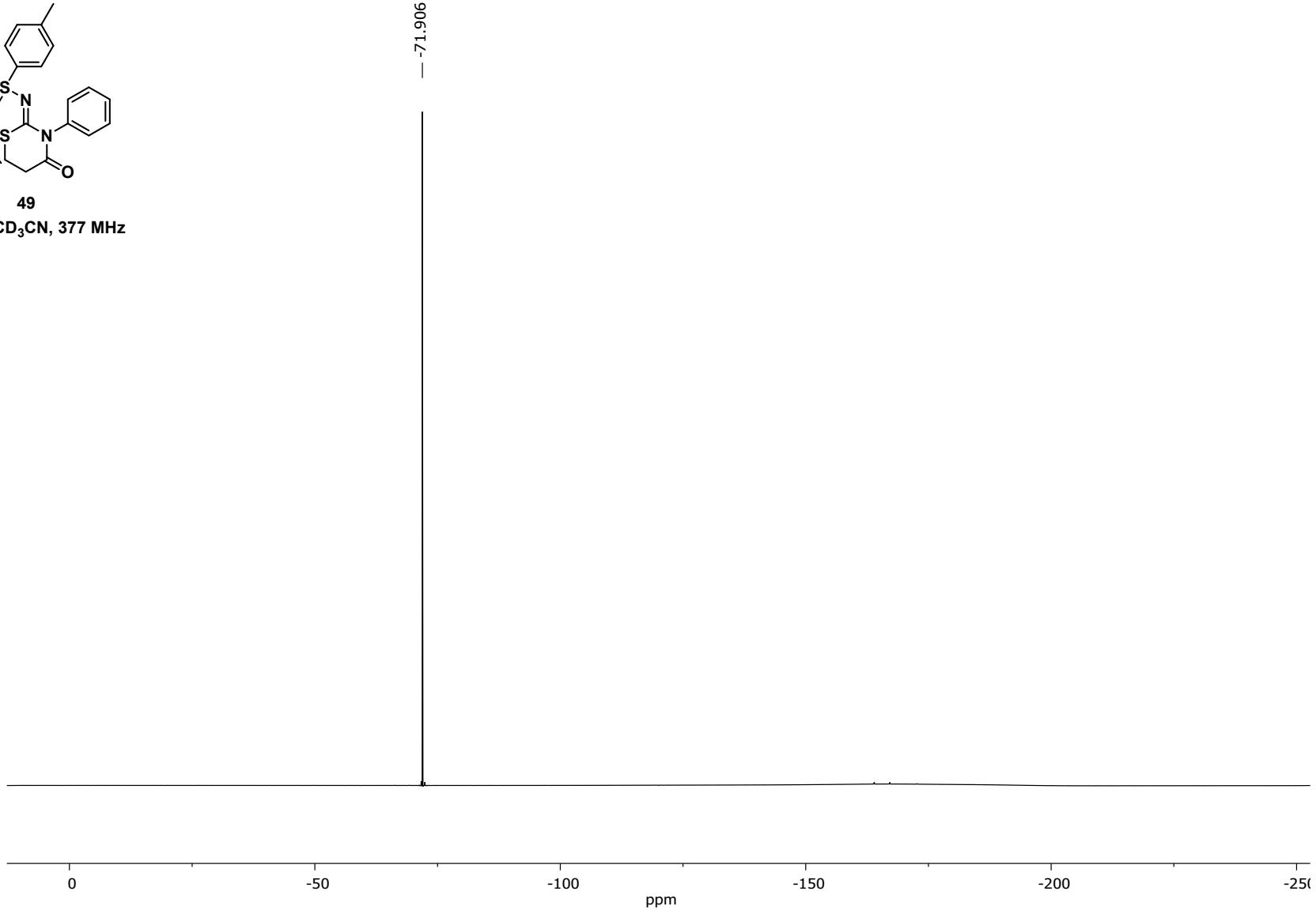


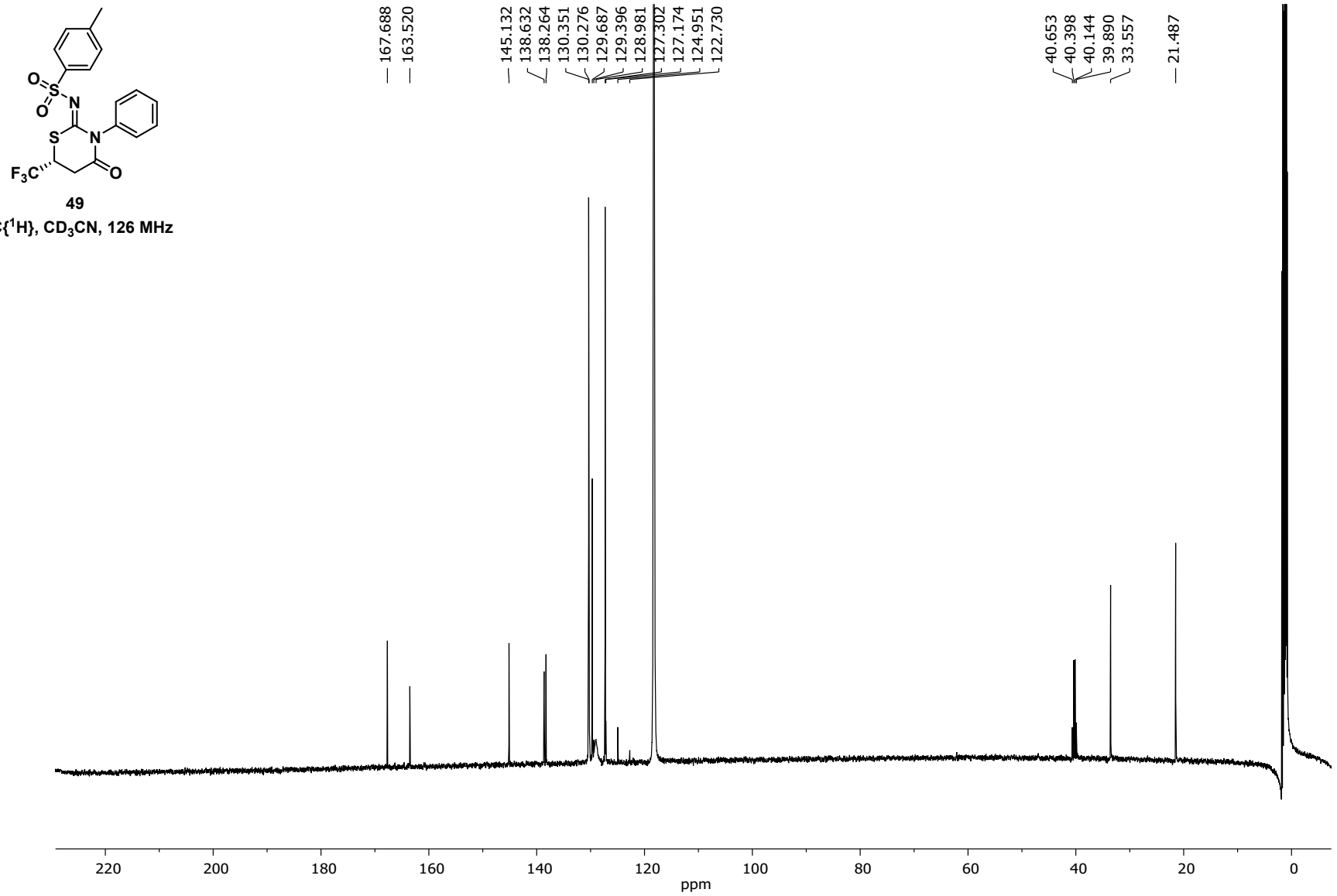

7.502
7.497
7.486
7.481
7.475
7.469
7.467
7.462
7.451
7.448
7.444
7.439
7.431
7.426
7.422
7.417
7.410
7.398
7.395
7.391
7.388
7.294
7.279
7.274
7.050
4.406
4.402
4.395
4.392
4.385
4.382
4.374
4.371
4.364
4.361
4.354
4.350
4.343
4.340
3.604
3.590
3.560
3.547
3.356
3.346
3.324
3.313
3.303
2.384
O
S
N
O
S
N
O
F3C
O
49
1H, CD3CN, 400 MHz
4.89
1.98
1.73
1.00
1.02
1.02
3.05
10
9
8
7
6
5
4
3
2
1
0
ppm



49

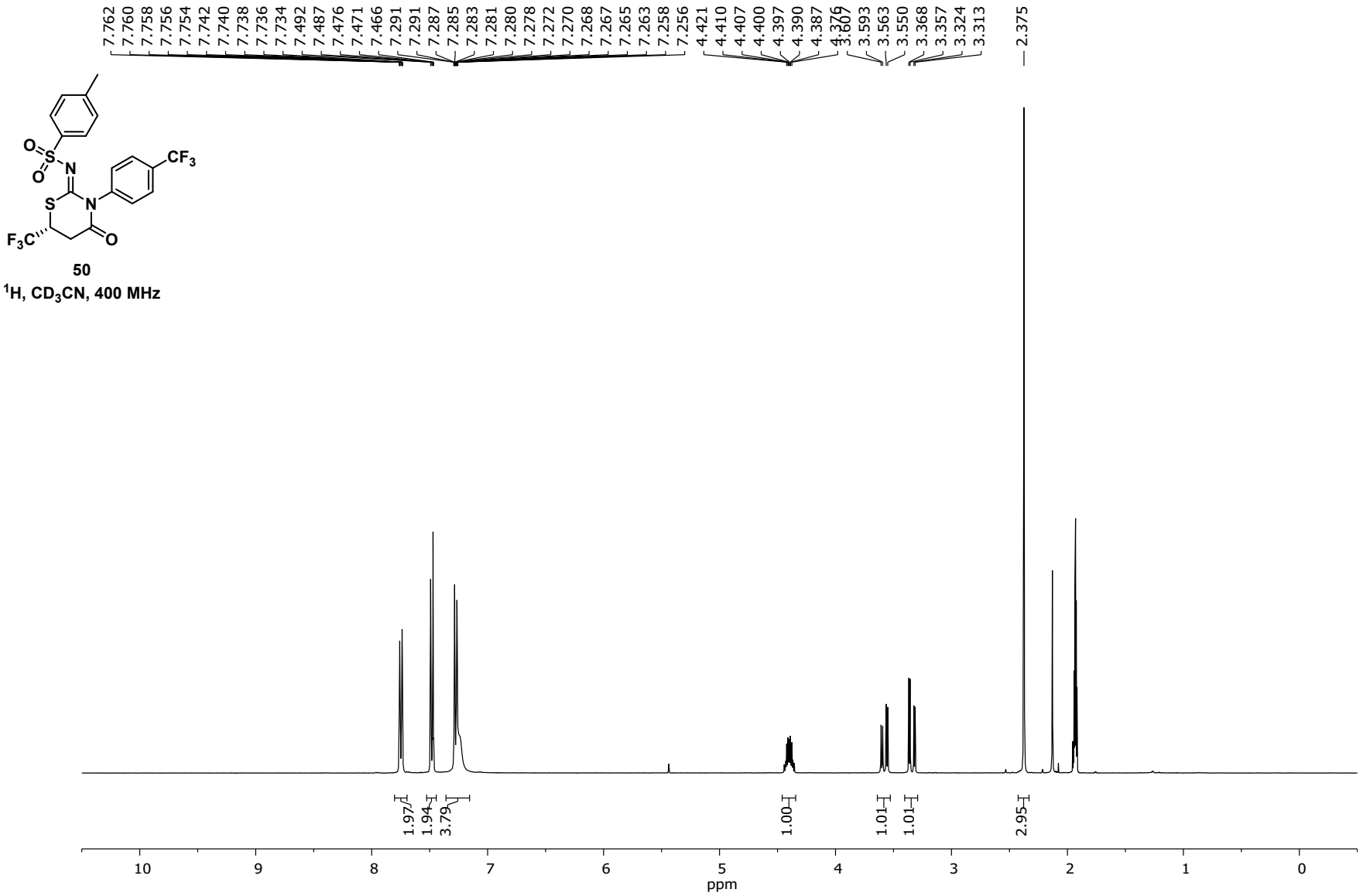
$^{19}F\{^{1}H\}$, CD_3CN, 377 MHz

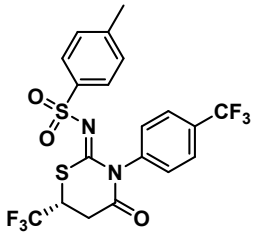




49

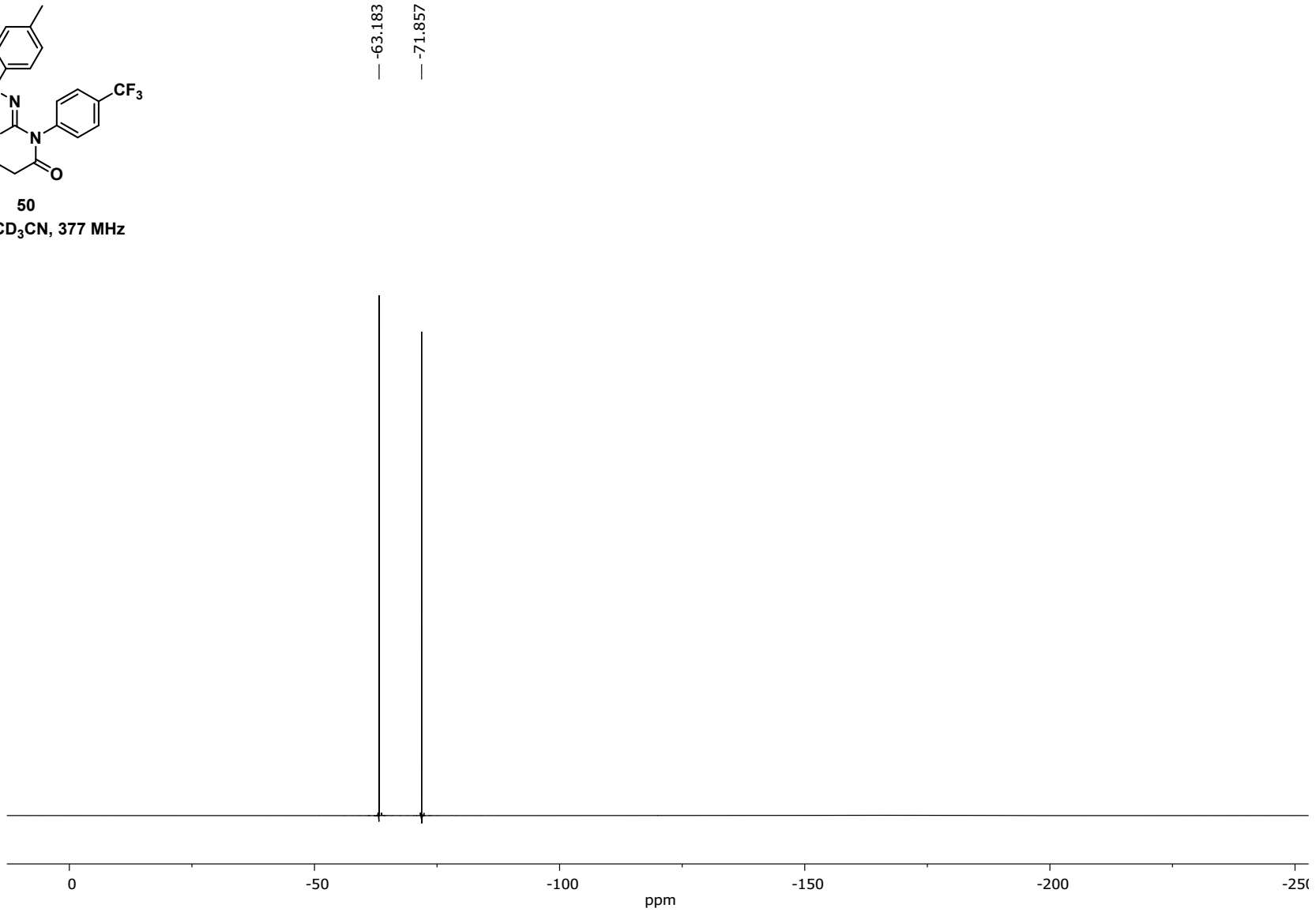
$^{13}C\{^{1}H\}$, CD_3CN, 126 MHz

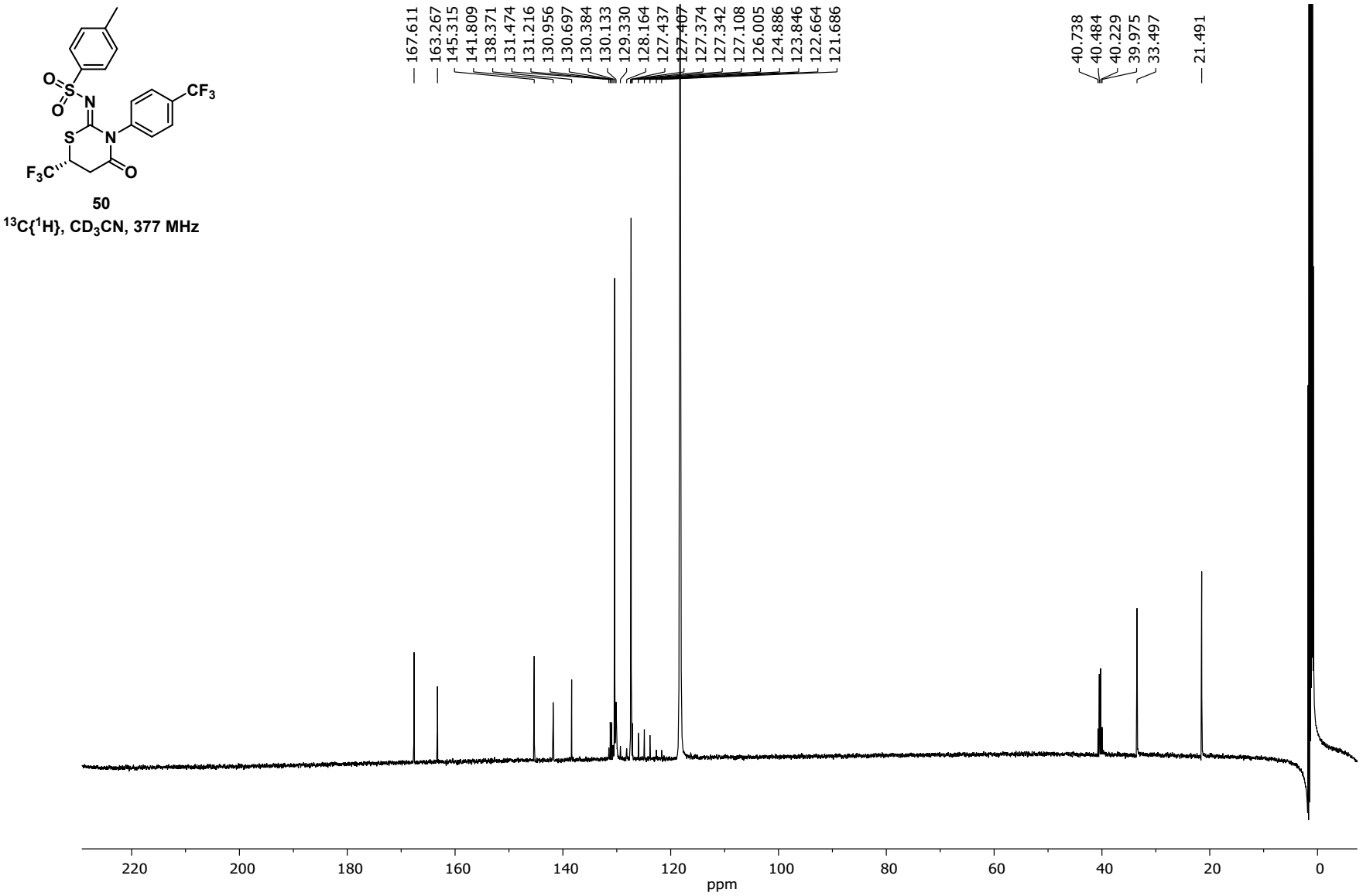

7.762
7.760
7.758
7.756
7.754
7.742
7.740
7.738
7.736
7.734
7.492
7.487
7.476
7.471
7.466
7.291
7.291
7.287
7.285
7.283
7.281
7.280
7.278
7.272
7.270
7.268
7.267
7.265
7.263
7.258
7.256
4.421
4.410
4.407
4.400
4.397
4.390
4.387
4.376
3.607
3.593
3.563
3.550
3.368
3.357
3.324
3.313
2.375
O
S
O
N
S
N
O
CF3
F3C
50
1H, CD3CN, 400 MHz
1.97
1.94
3.79
1.00
1.01
1.01
2.95
10
9
8
7
6
5
4
3
2
1
0
ppm

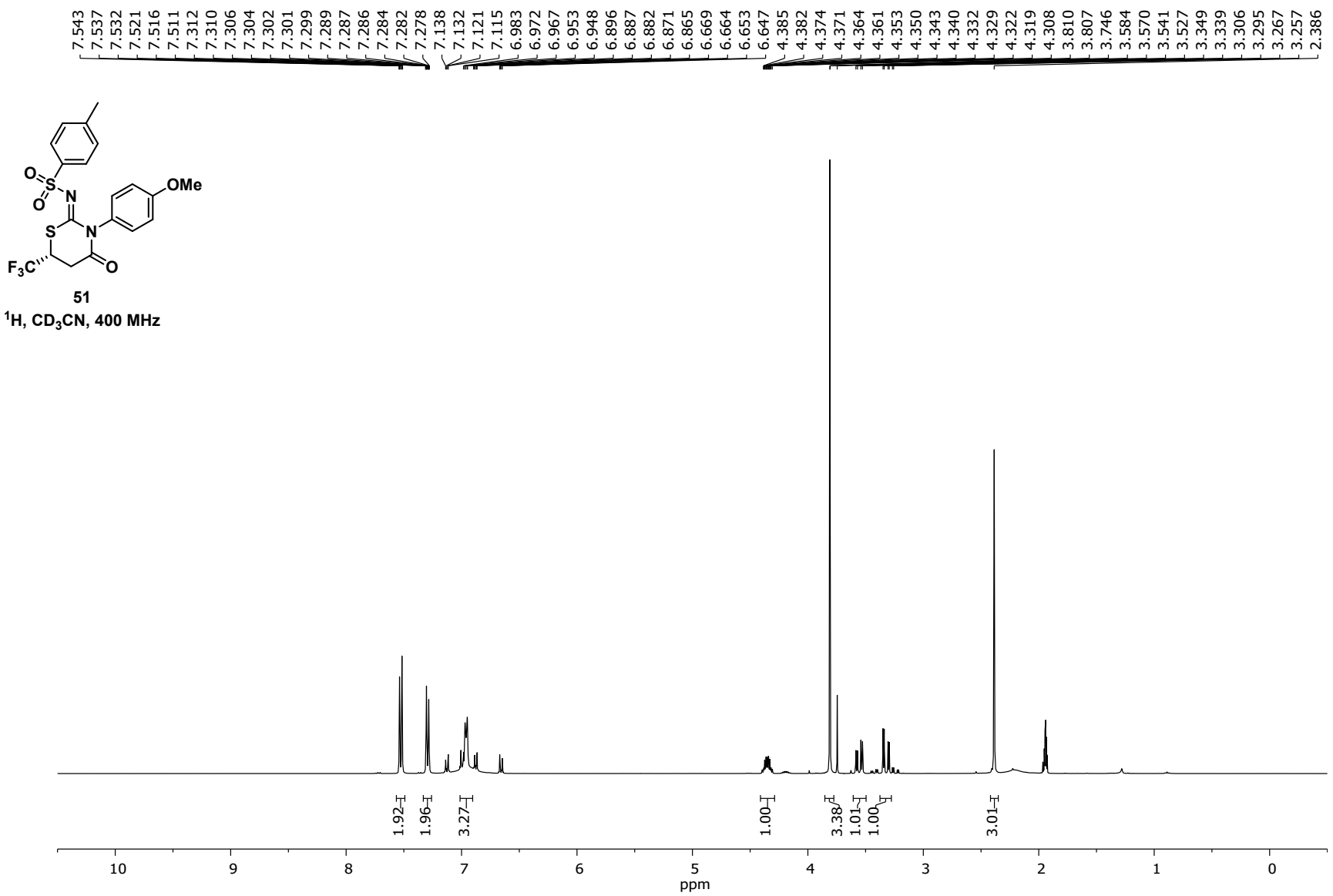


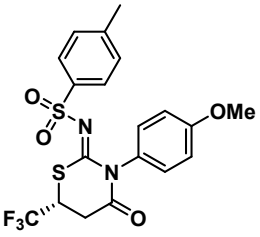
50

$^{19}F\{^{1}H\}$, CD_3CN, 377 MHz



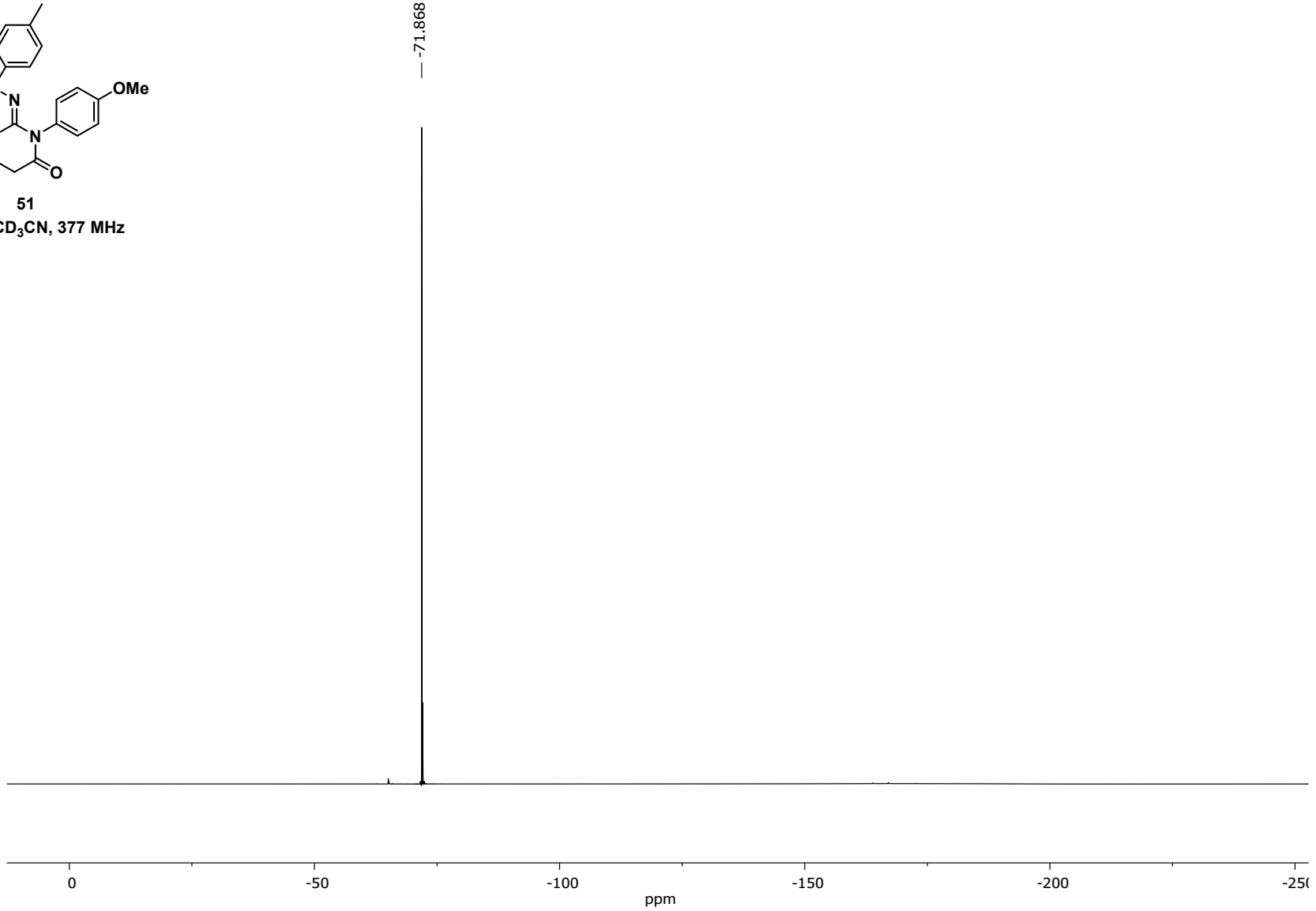

50
13C{1H}, CD3CN, 377 MHz
167.611
163.267
145.315
141.809
138.371
131.474
131.216
130.956
130.697
130.384
130.133
129.330
128.164
127.437
127.407
127.374
127.342
127.108
126.005
124.886
123.846
122.664
121.686
40.738
40.484
40.229
39.975
33.497
21.491
220
200
180
160
140
120
100
80
60
40
20
0
ppm

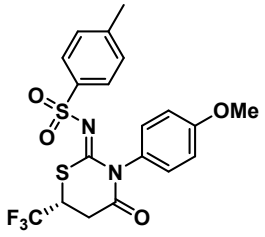

7.543
7.537
7.532
7.521
7.516
7.511
7.312
7.310
7.306
7.304
7.302
7.301
7.299
7.289
7.287
7.286
7.284
7.282
7.278
7.138
7.132
7.121
7.115
6.983
6.972
6.967
6.953
6.948
6.896
6.887
6.882
6.871
6.865
6.669
6.664
6.653
6.647
4.385
4.382
4.374
4.371
4.364
4.361
4.353
4.350
4.343
4.340
4.332
4.329
4.322
4.319
4.308
3.810
3.807
3.746
3.584
3.570
3.541
3.527
3.349
3.339
3.306
3.295
3.267
3.257
2.386
OMe
51
1H, CD3CN, 400 MHz
1.92
1.96
3.27
1.00
3.38
1.01
1.00
3.01
10
9
8
7
6
5
4
3
2
1
0
ppm



51

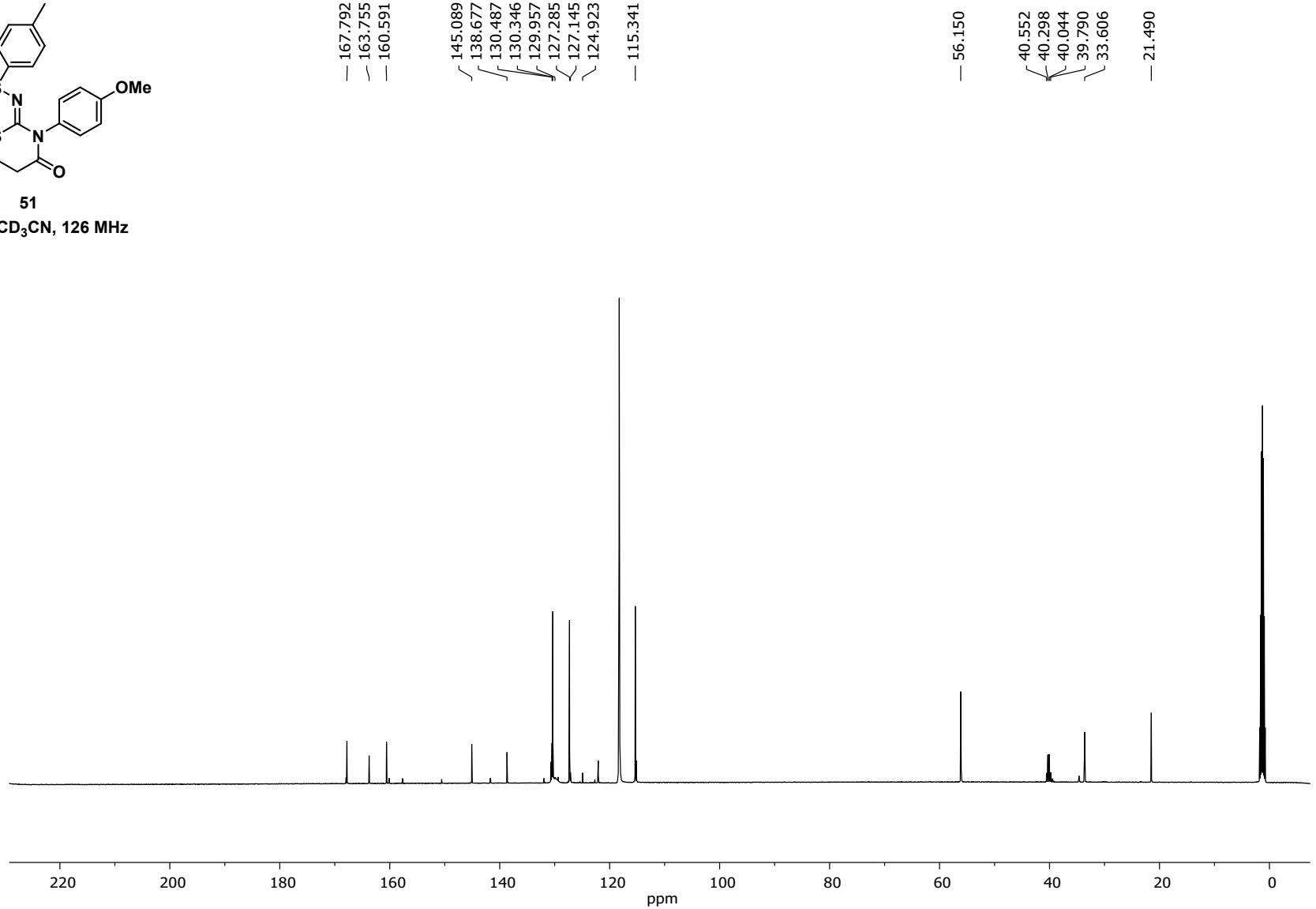
$^{19}F\{^{1}H\}$, CD_3CN, 377 MHz

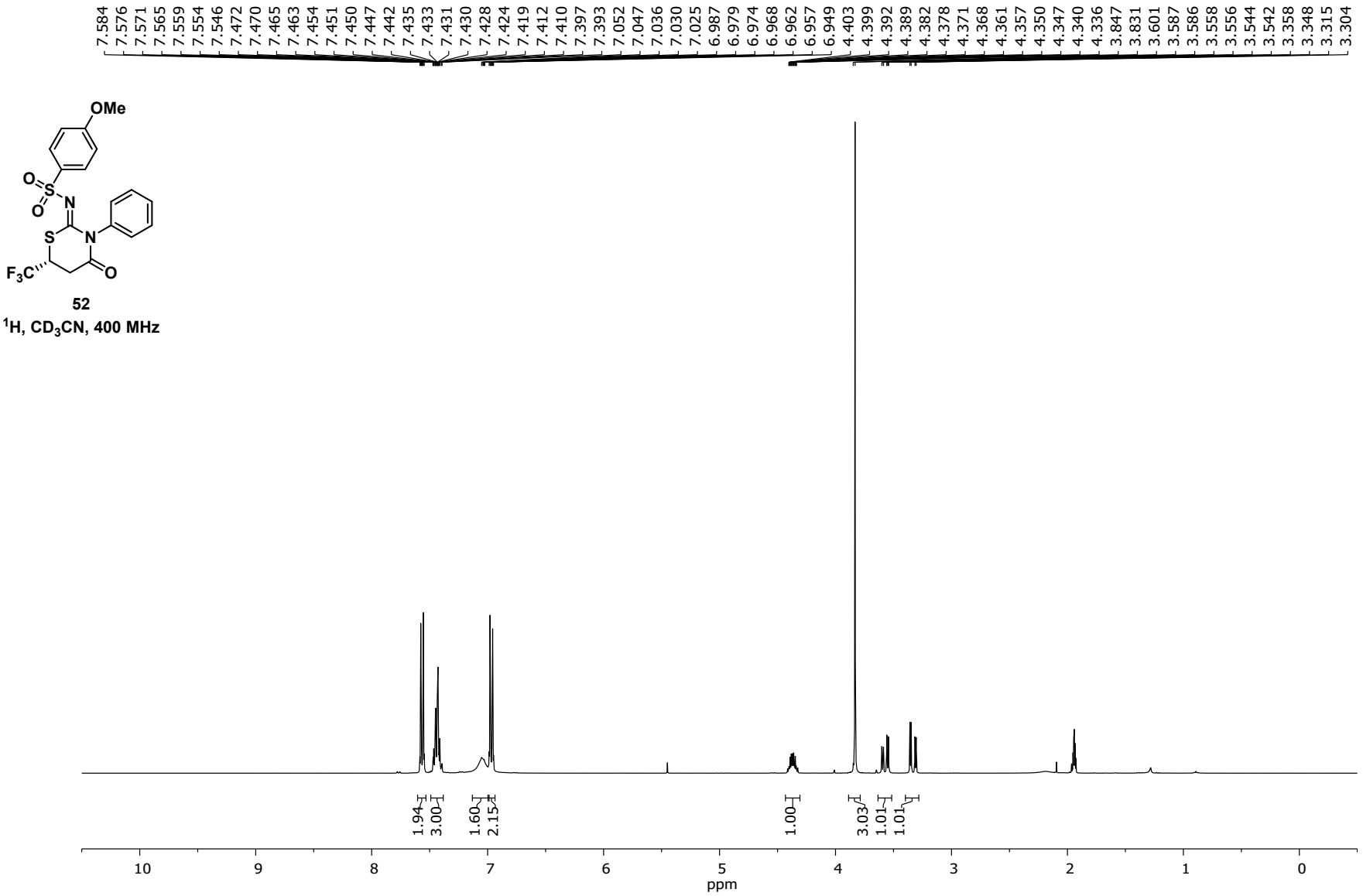




51

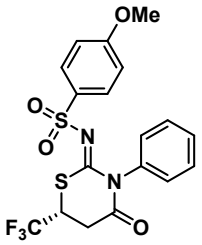
$^{13}C\{^{1}H\}$, CD_3CN, 126 MHz





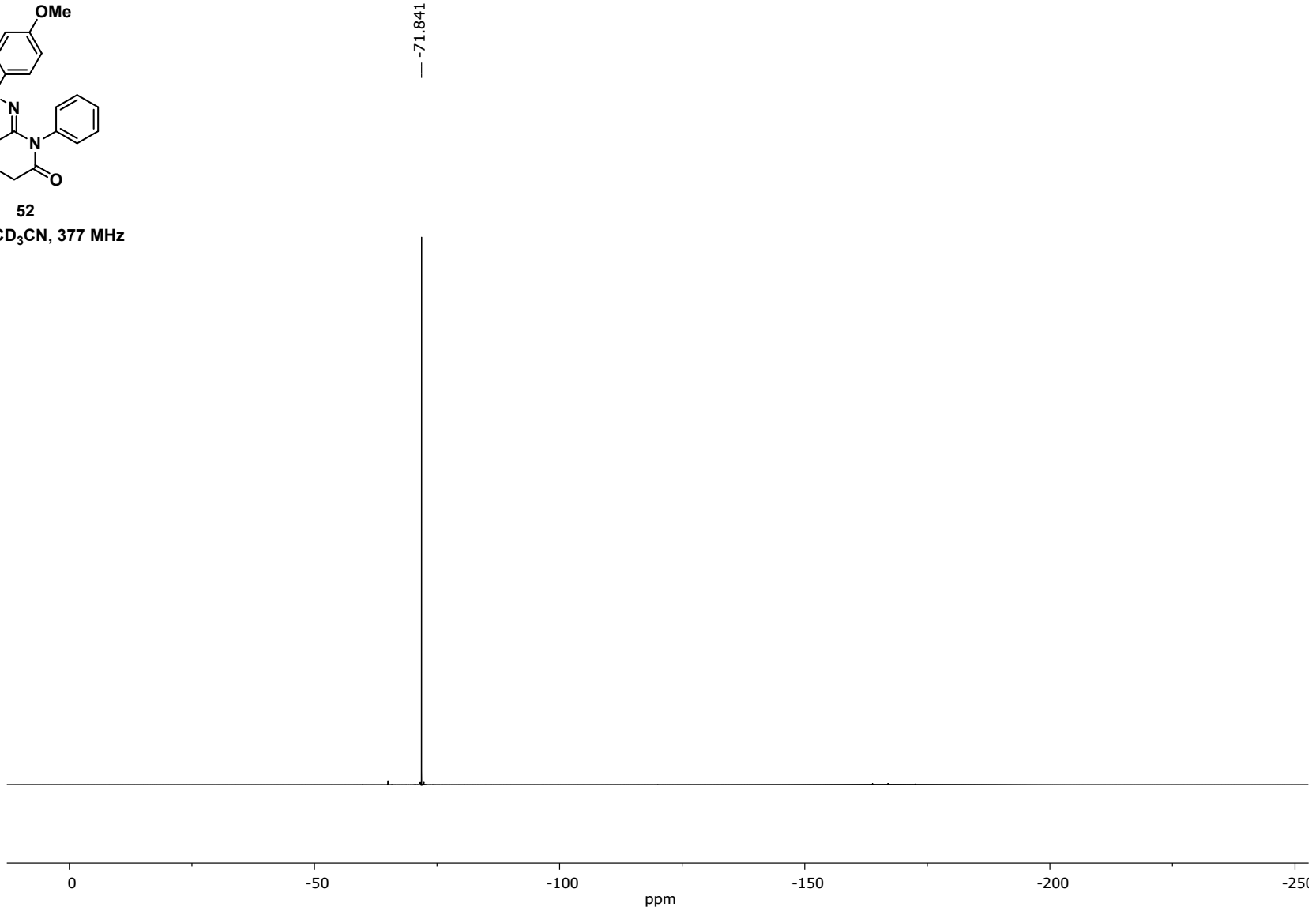
52

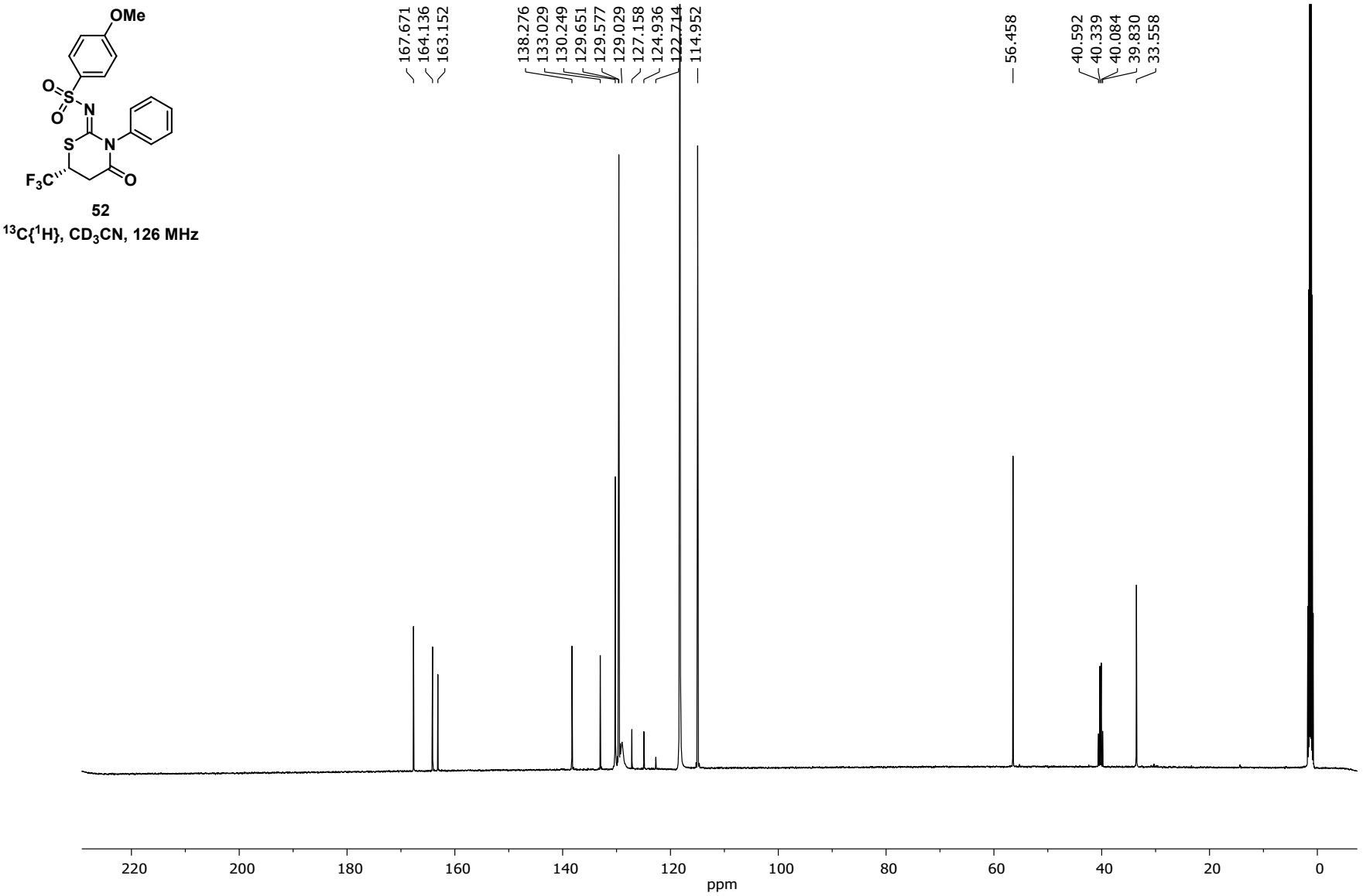
^{1}H, CD_3CN, 400 MHz

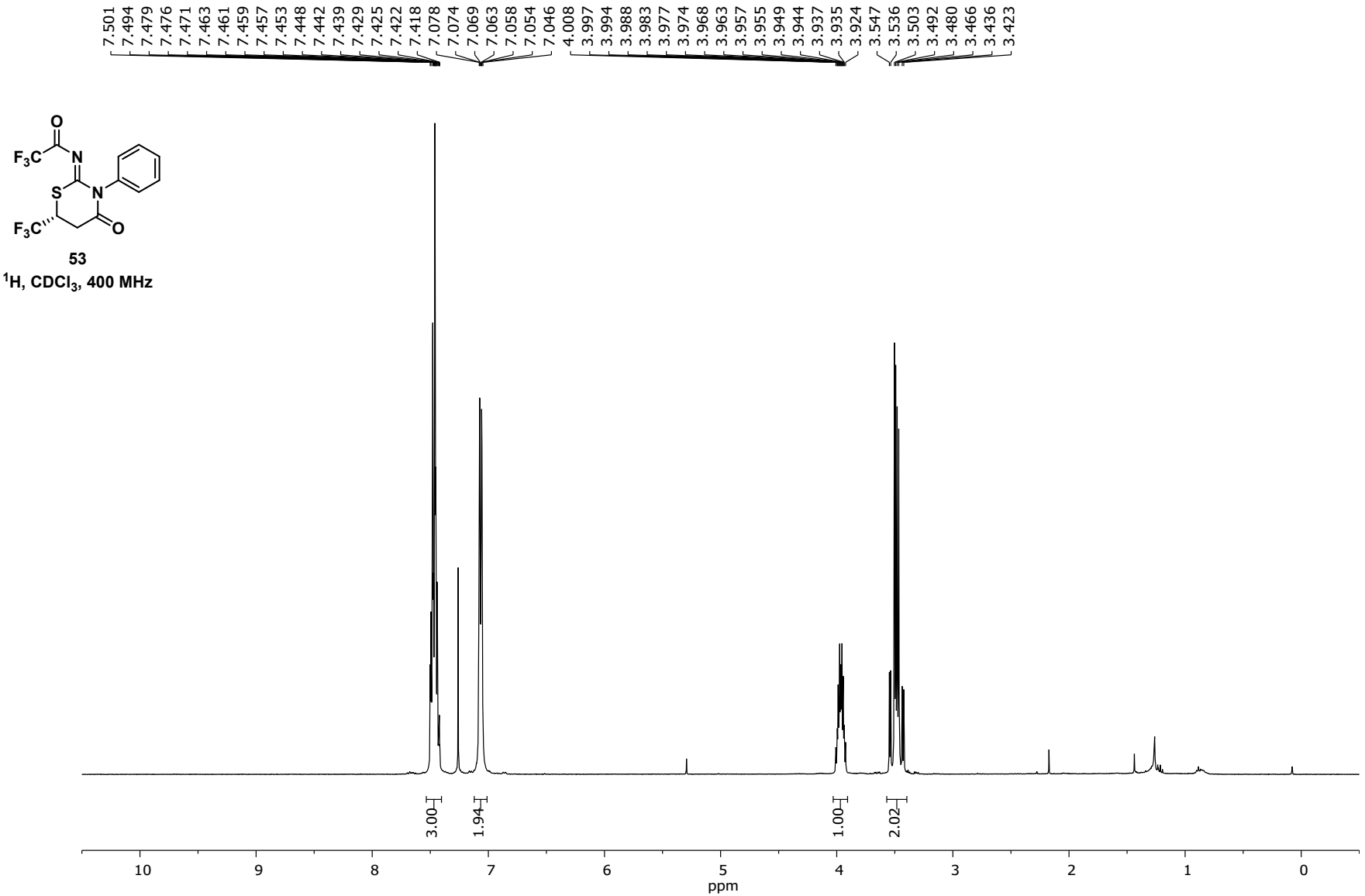


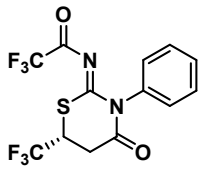
52

$^{19}F\{^{1}H\}$, CD_3CN, 377 MHz



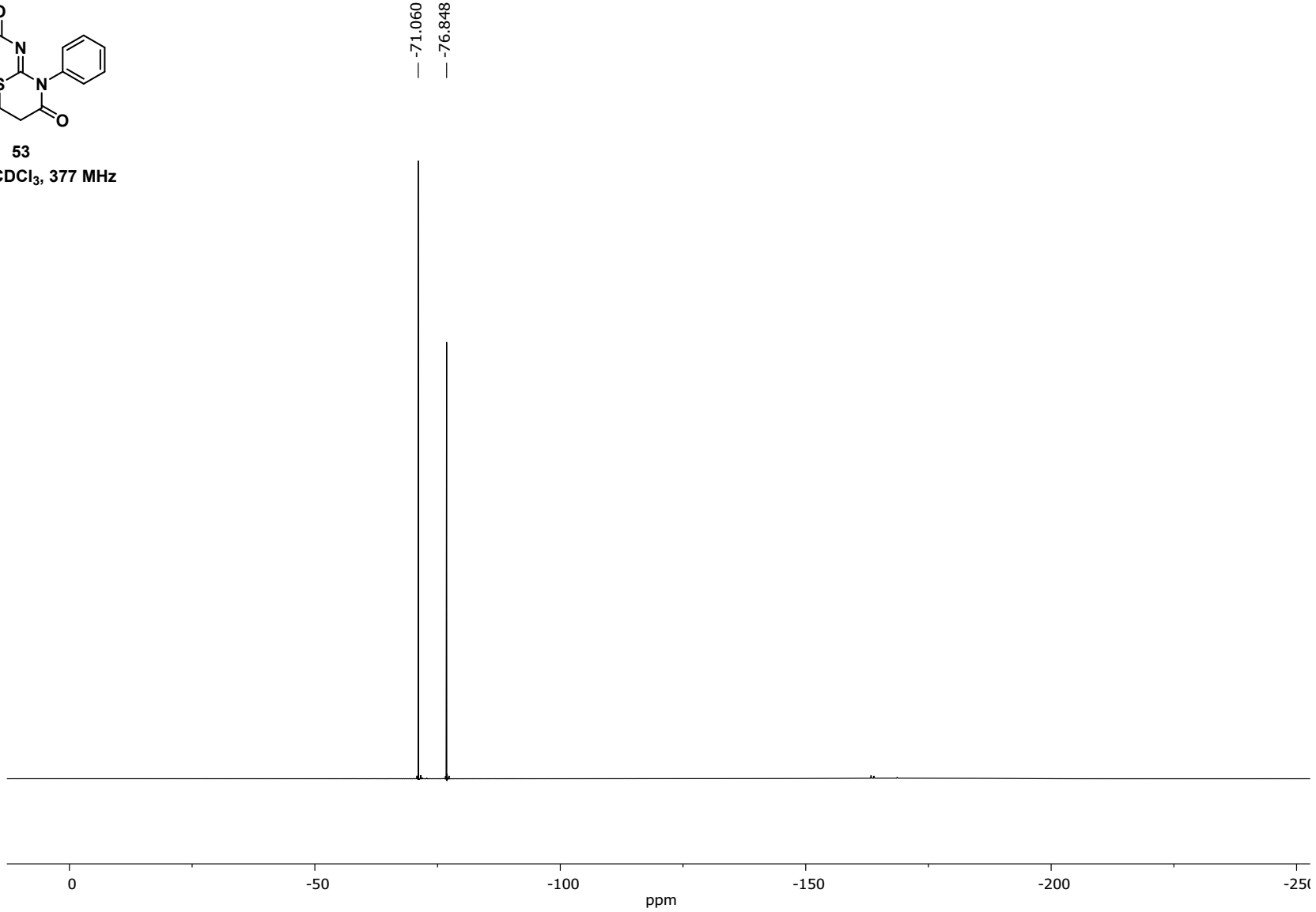

OMe
O
S
O
N
S
N
O
F3C
52
13C{1H}, CD3CN, 126 MHz
167.671
164.136
163.152
138.276
133.029
130.249
129.651
129.577
129.029
127.158
124.936
122.714
114.952
56.458
40.592
40.339
40.084
39.830
33.558
220
200
180
160
140
120
100
80
60
40
20
0
ppm

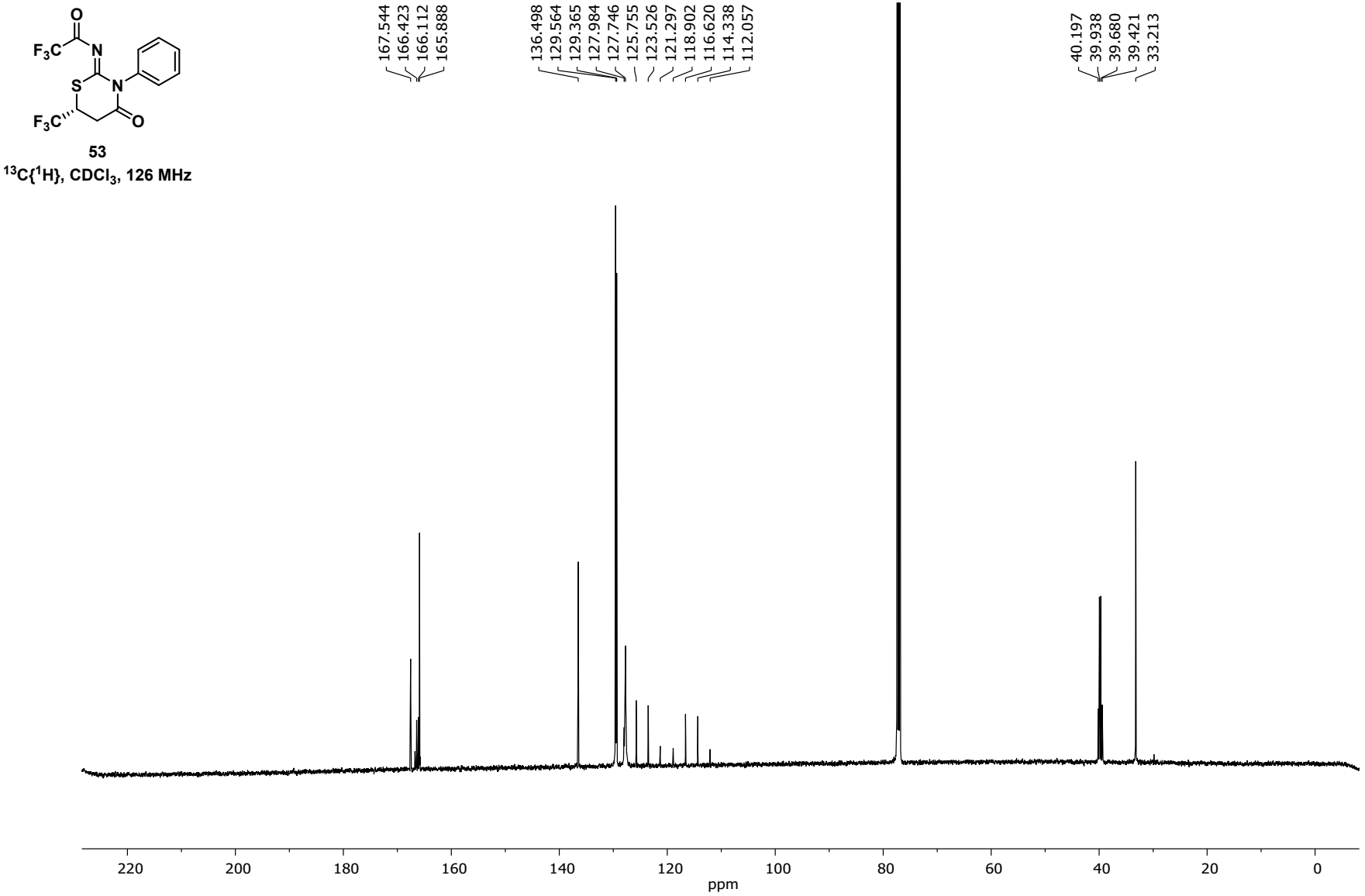

7.501
7.494
7.479
7.476
7.471
7.463
7.461
7.459
7.457
7.453
7.448
7.442
7.439
7.429
7.425
7.422
7.418
7.078
7.074
7.069
7.063
7.058
7.054
7.046
4.008
3.997
3.994
3.988
3.983
3.977
3.974
3.968
3.963
3.957
3.955
3.949
3.944
3.937
3.935
3.924
3.547
3.536
3.503
3.492
3.480
3.466
3.436
3.423
O
F3C
N
S
N
F3C
O
53
1H, CDCl3, 400 MHz
3.00
1.94
1.00
2.02
10
9
8
7
6
5
4
3
2
1
0
ppm



53

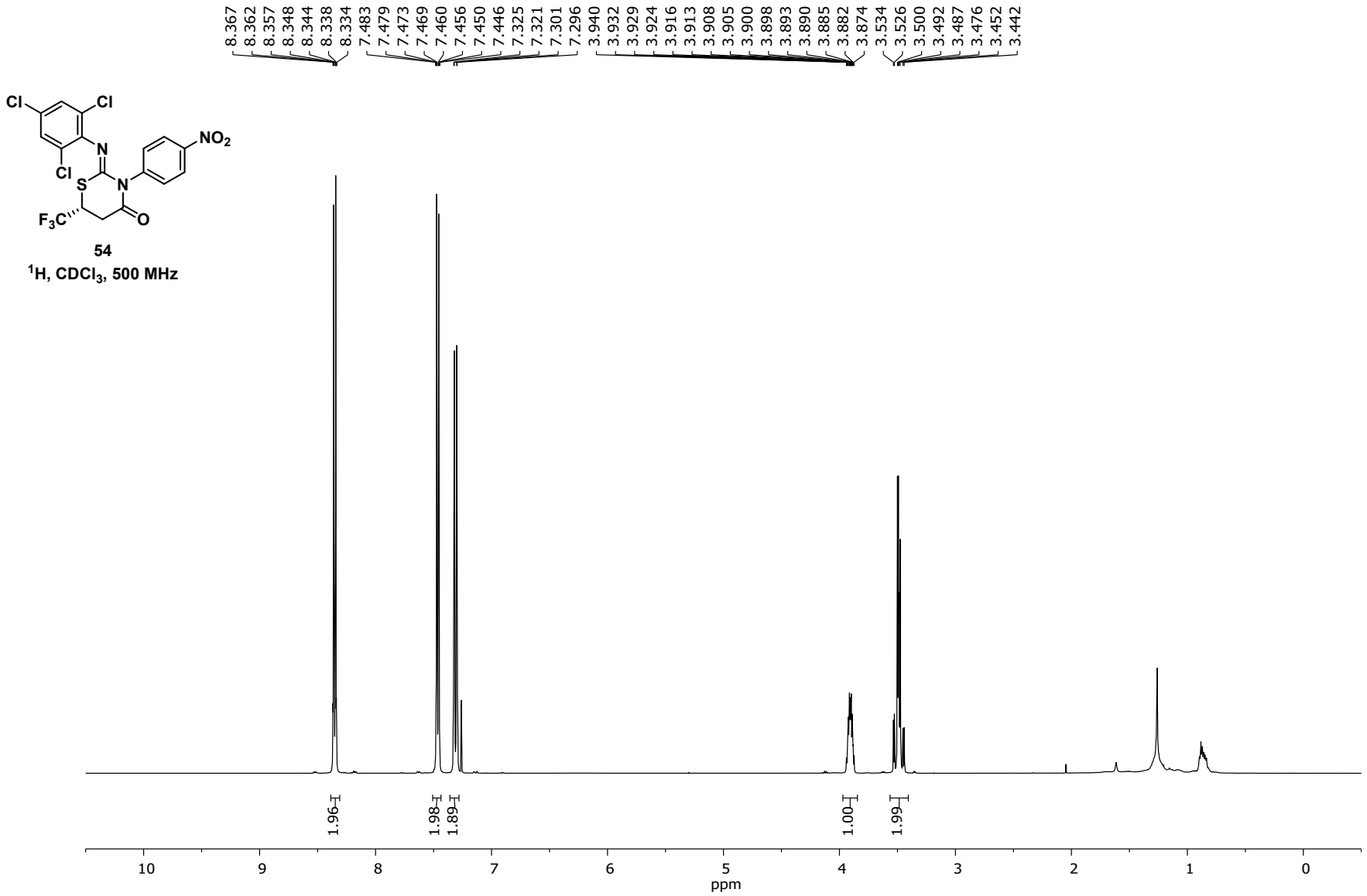
$^{19}F\{^{1}H\}$, $CDCl_3$, 377 MHz

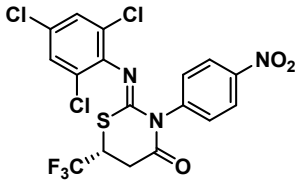




53

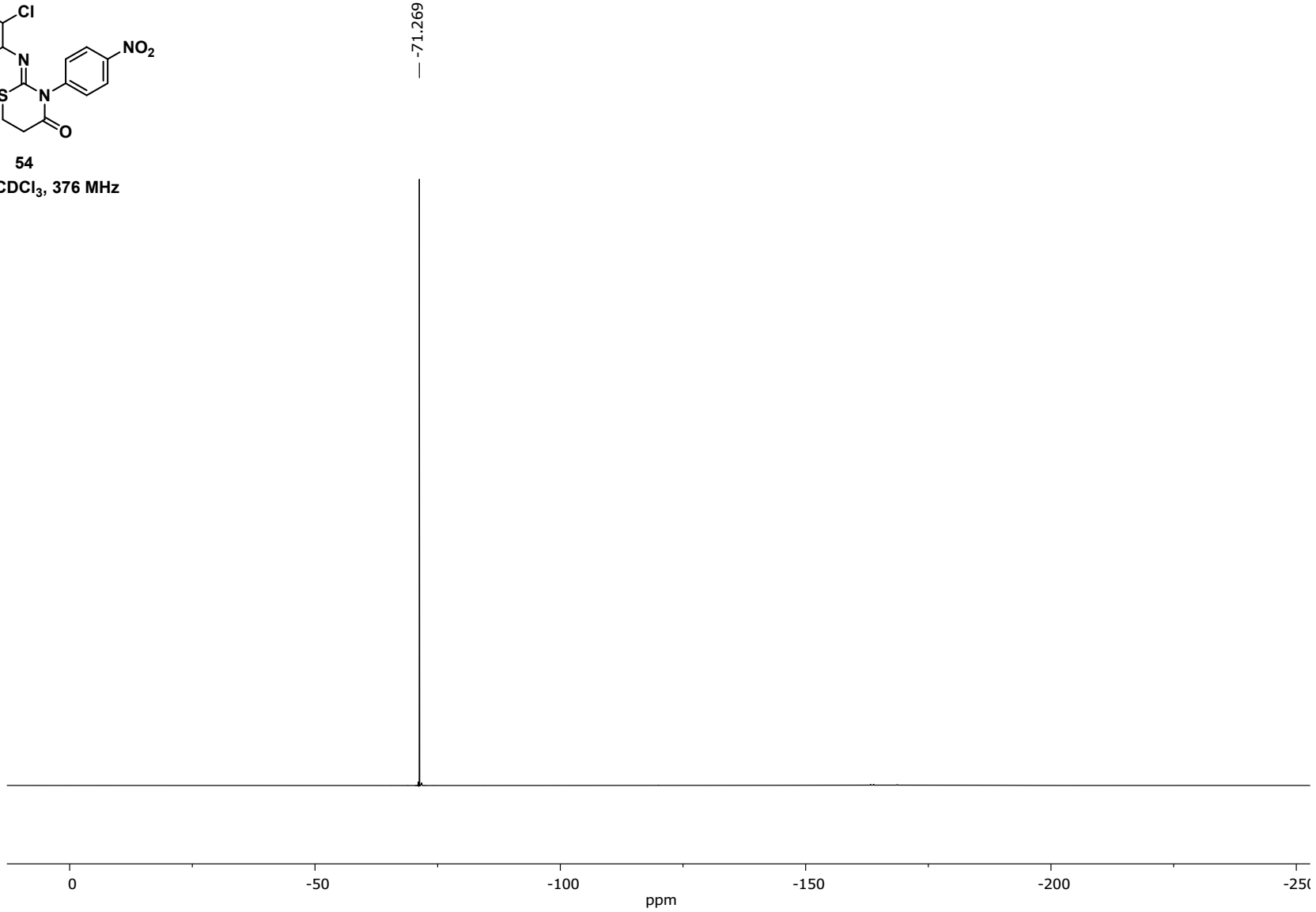
$^{13}C\{^{1}H\}$, $CDCl_3$, 126 MHz

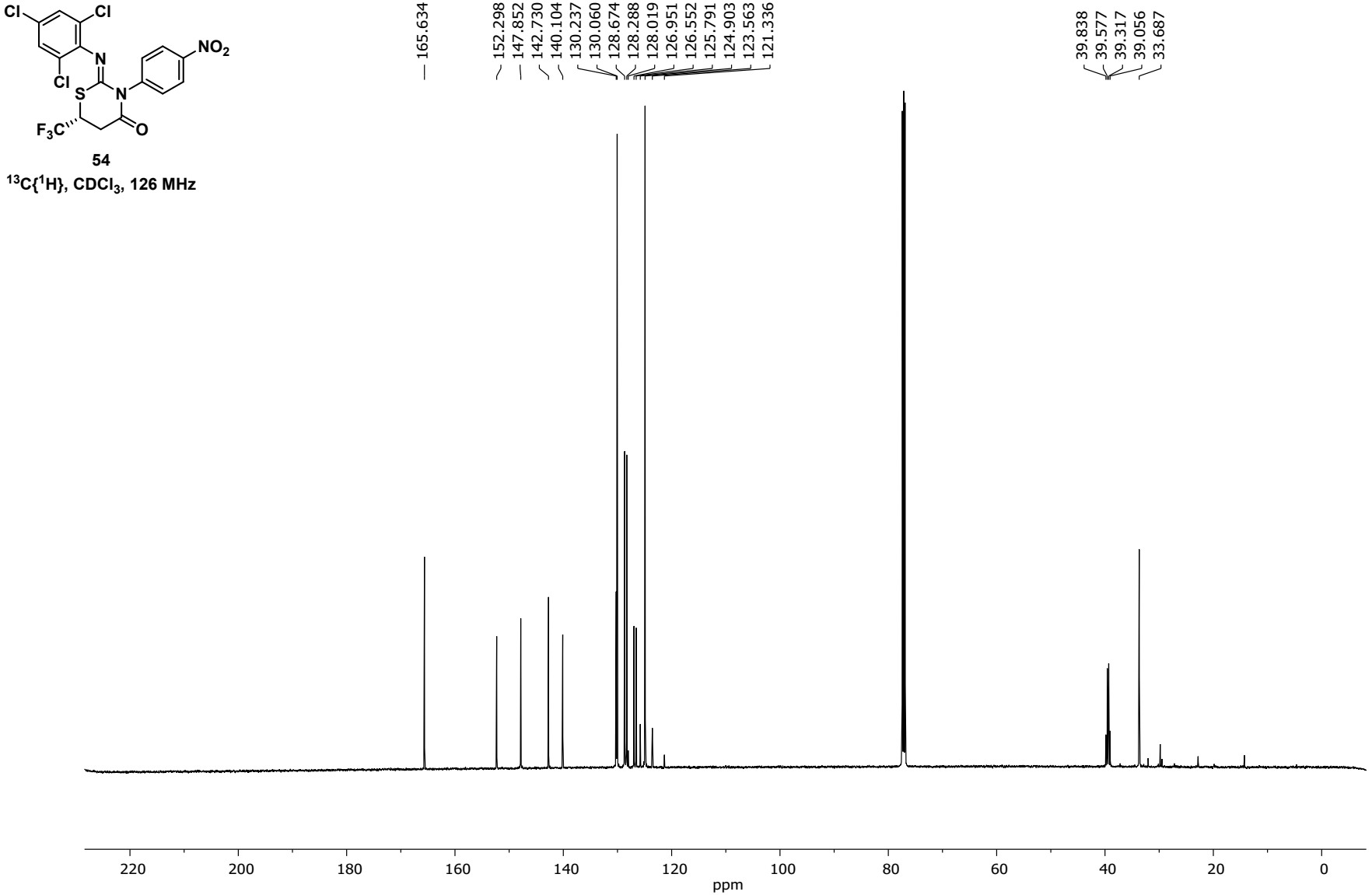

8.367
8.362
8.357
8.348
8.344
8.338
8.334
7.483
7.479
7.473
7.469
7.460
7.456
7.450
7.446
7.325
7.321
7.301
7.296
3.940
3.932
3.929
3.924
3.916
3.913
3.908
3.905
3.900
3.898
3.893
3.890
3.885
3.882
3.874
3.534
3.526
3.500
3.492
3.487
3.476
3.452
3.442
Cl
Cl
Cl
N
S
N
NO2
F3C
O
54
1H, CDCl3, 500 MHz
1.96
1.98
1.89
1.00
1.99
10
9
8
7
6
5
4
3
2
1
0
ppm

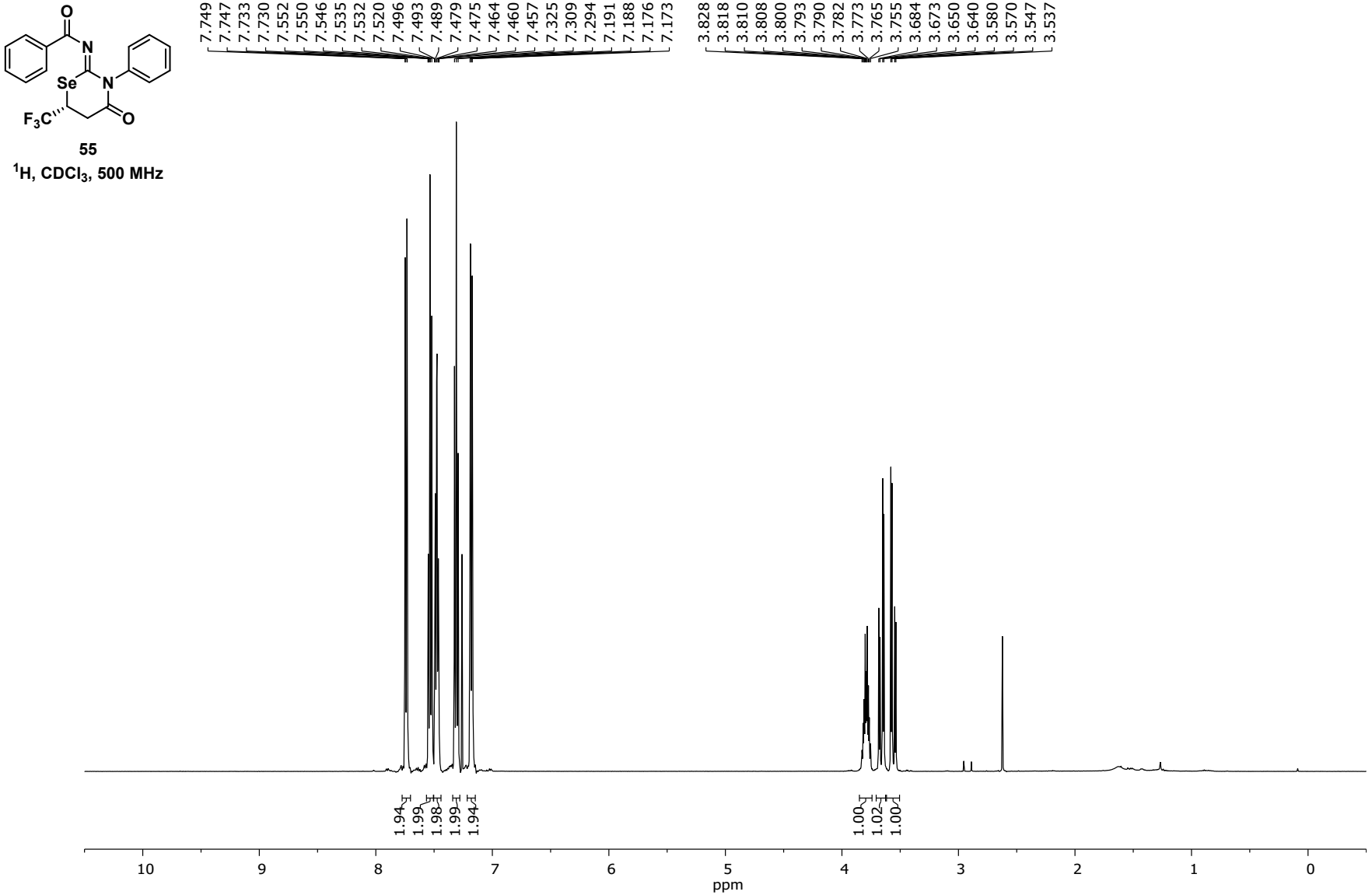


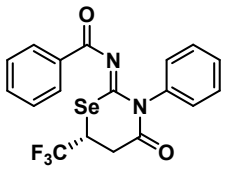
54

$^{19}F\{^{1}H\}$, $CDCl_3$, 376 MHz



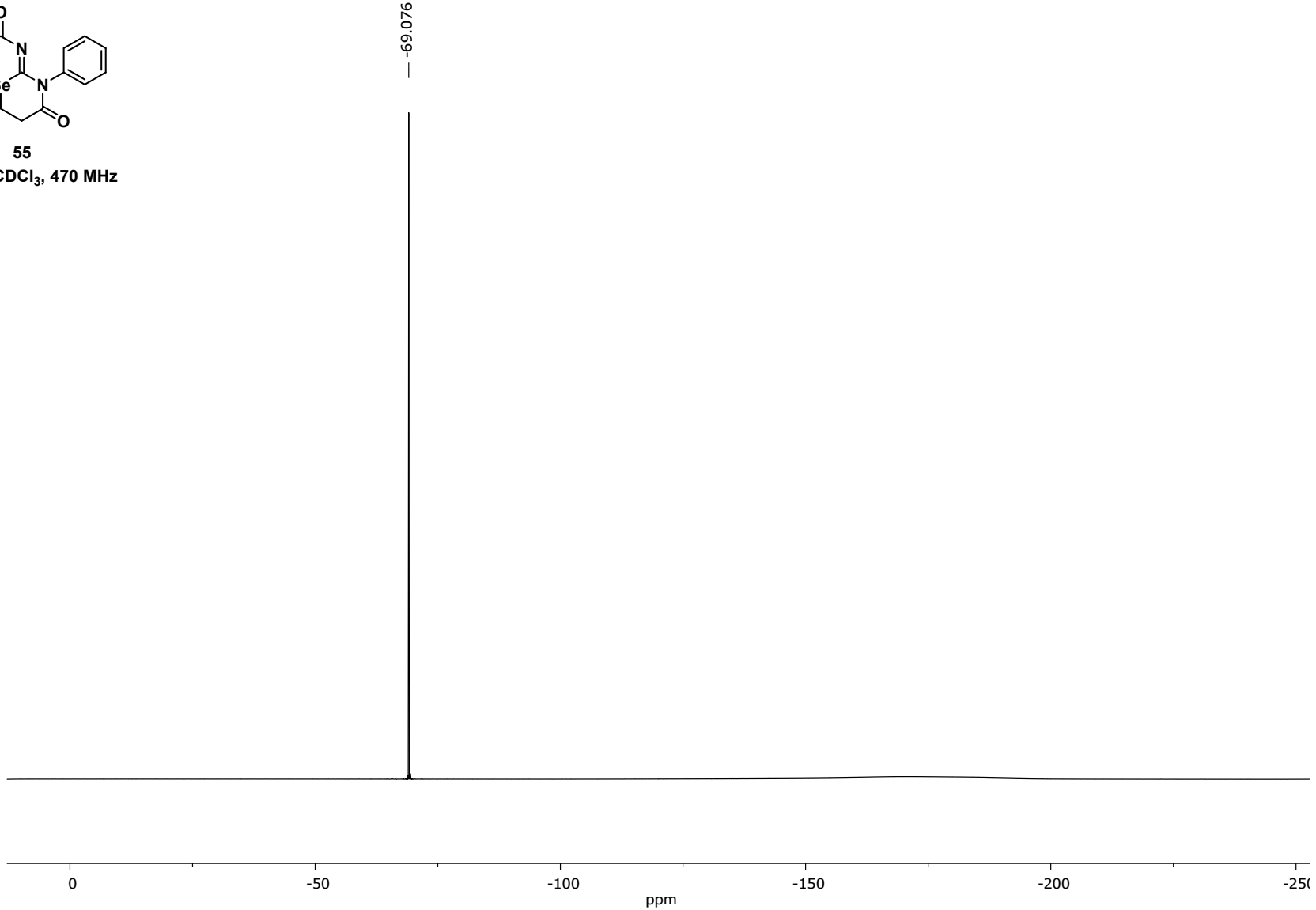

Cl
Cl
Cl
N
S
N
O
F_3C
NO_2
54
$^{13}C\{^1H\}$, $CDCl_3$, 126 MHz
165.634
152.298
147.852
142.730
140.104
130.237
130.060
128.674
128.288
128.019
126.951
126.552
125.791
124.903
123.563
121.336
39.838
39.577
39.317
39.056
33.687
220
200
180
160
140
120
100
80
60
40
20
0
ppm

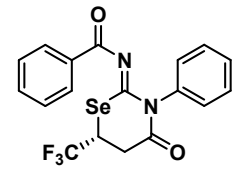

55
1H, CDCl3, 500 MHz
7.749
7.747
7.733
7.730
7.552
7.550
7.546
7.535
7.532
7.520
7.496
7.493
7.489
7.479
7.475
7.464
7.460
7.457
7.325
7.309
7.294
7.191
7.188
7.176
7.173
3.828
3.818
3.810
3.808
3.800
3.793
3.790
3.782
3.773
3.765
3.755
3.684
3.673
3.650
3.640
3.580
3.570
3.547
3.537
1.94
1.99
1.98
1.99
1.94
1.00
1.02
1.00
10
9
8
7
6
5
4
3
2
1
0
ppm



55

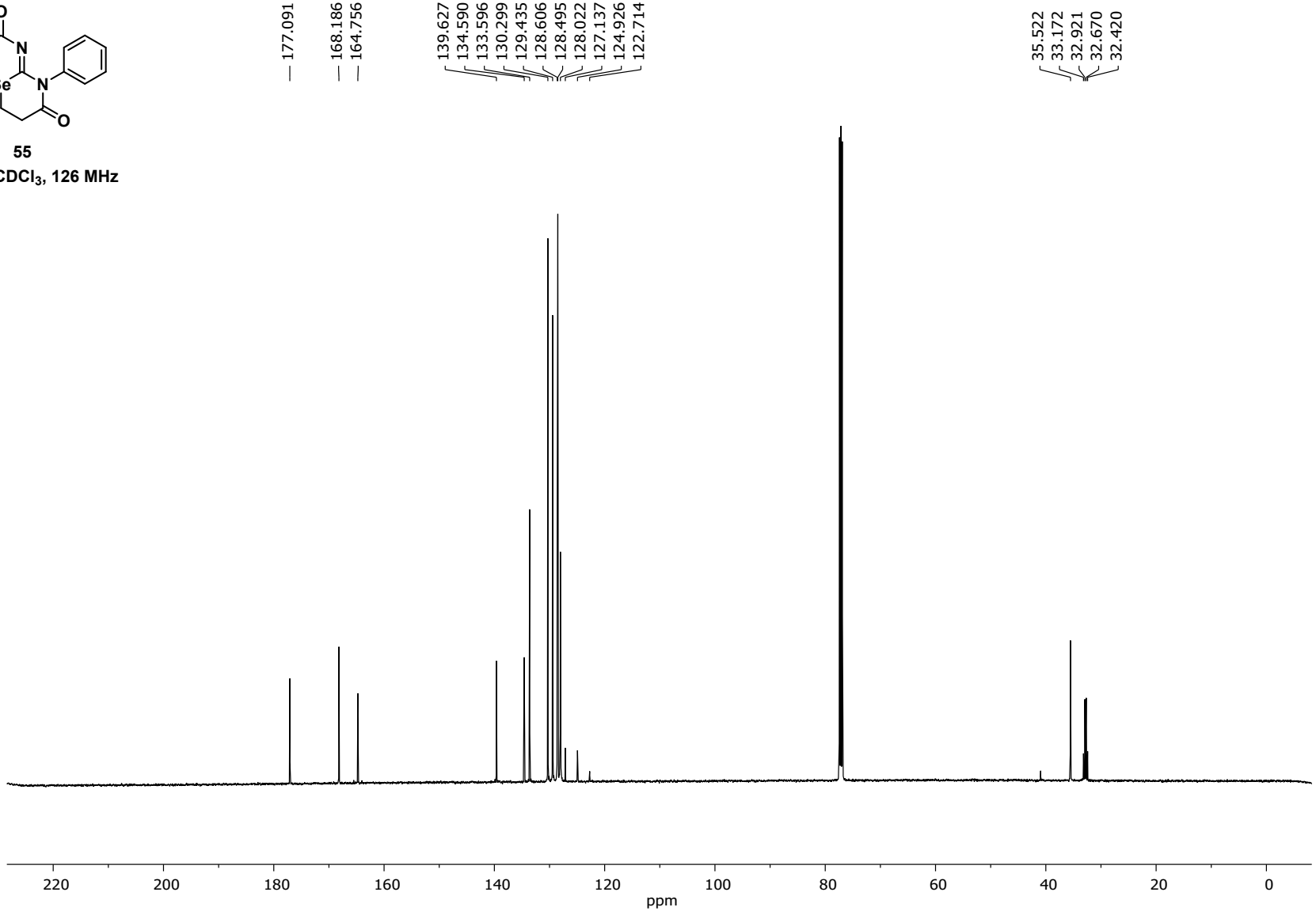
$^{19}F\{^{1}H\}$, $CDCl_3$, 470 MHz

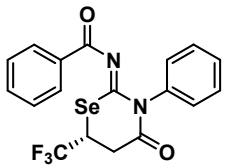




55

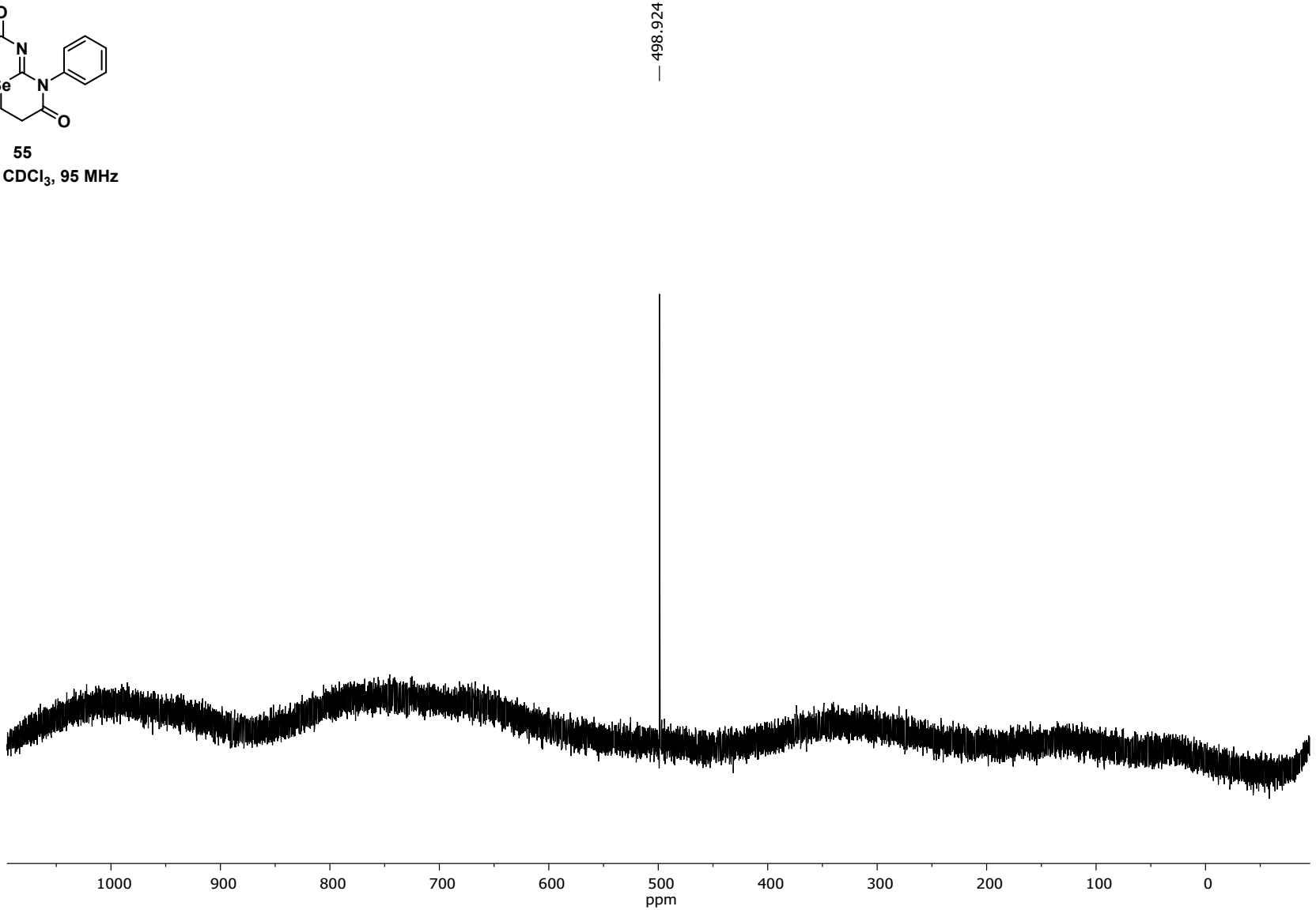
$^{13}C\{^{1}H\}$, $CDCl_3$, 126 MHz

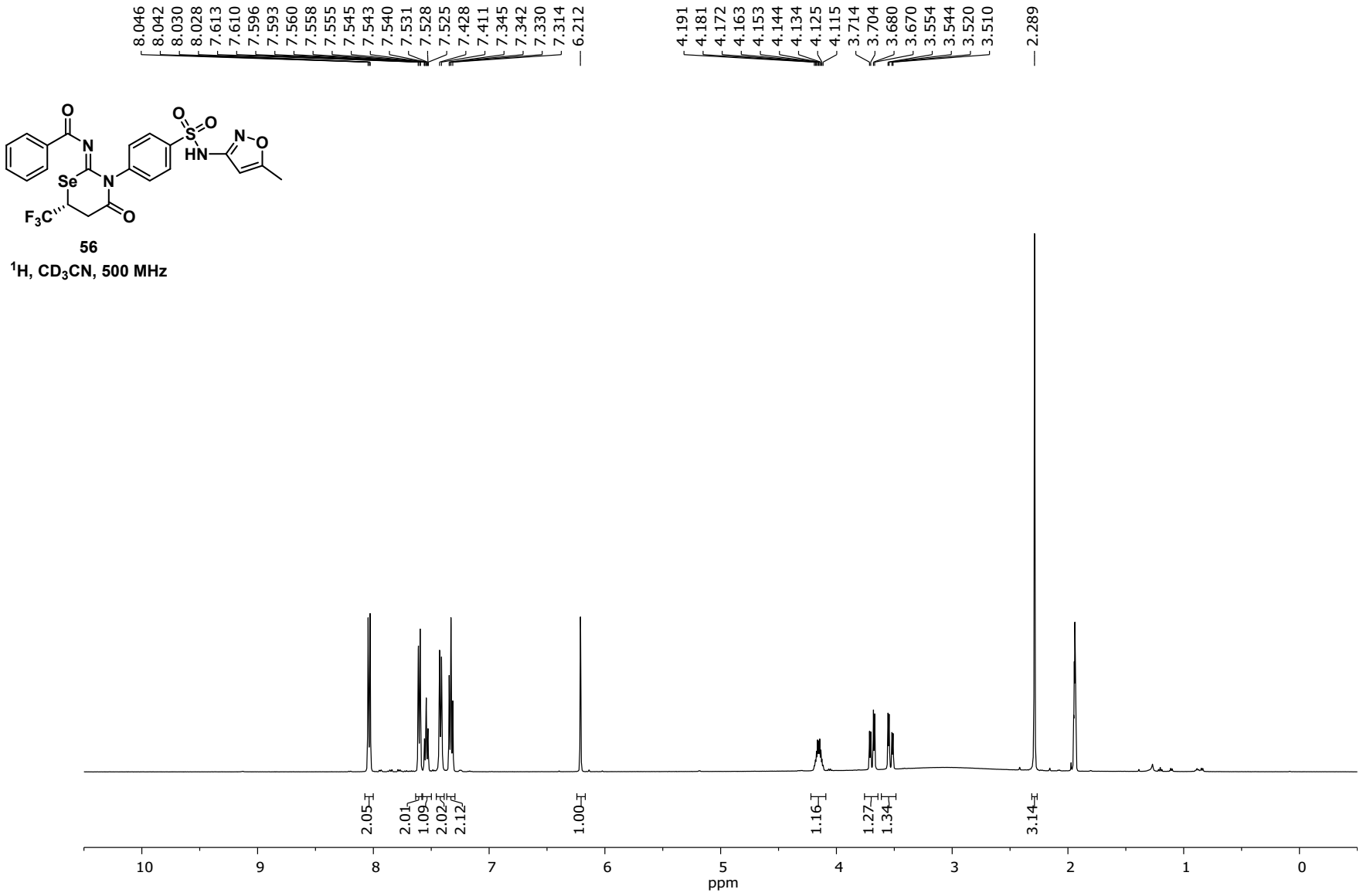


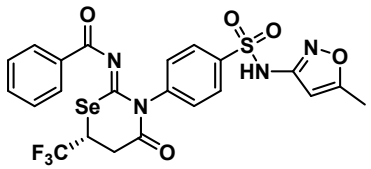


55

$^{77}Se\{^{1}H\}$, $CDCl_3$, 95 MHz

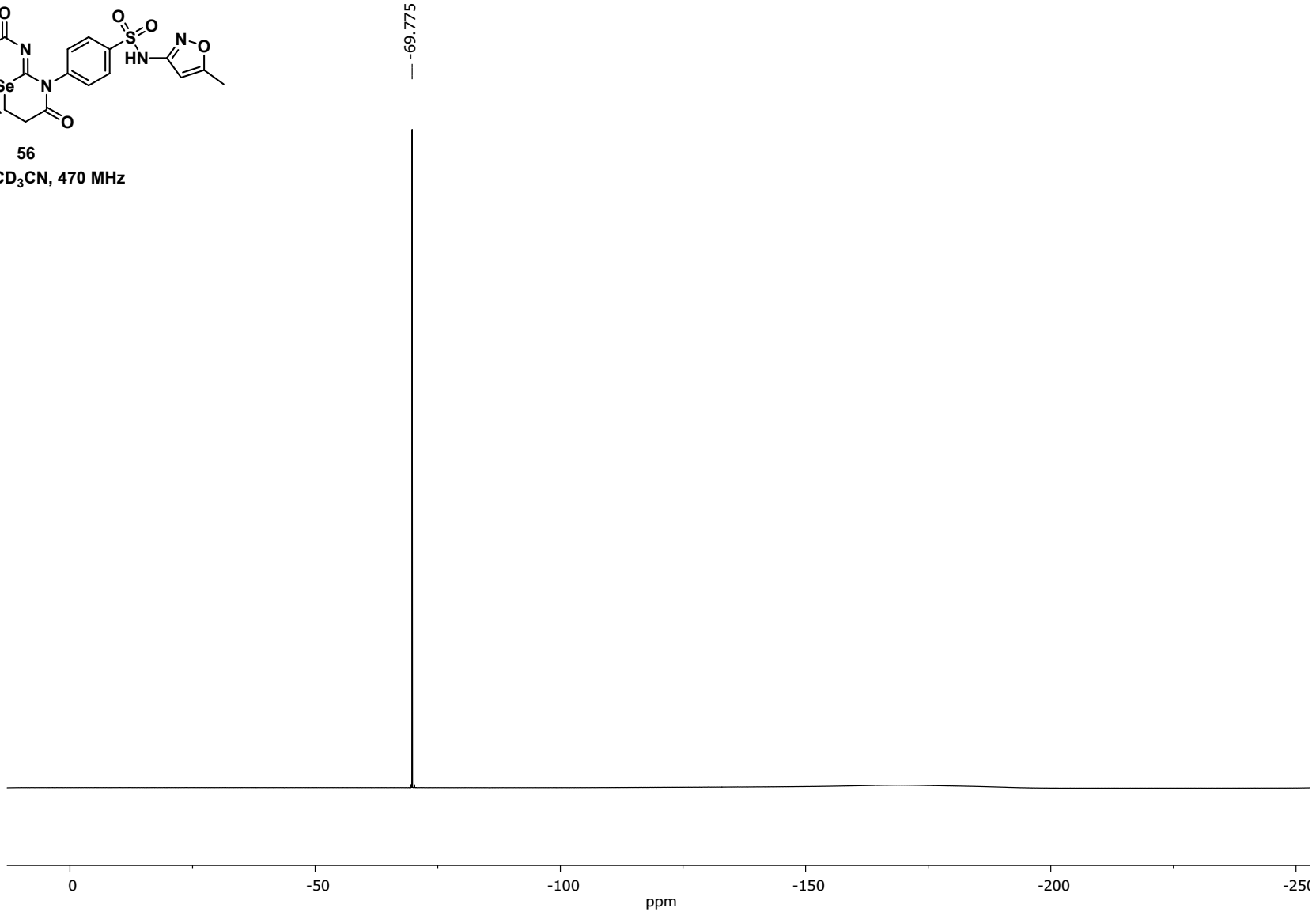


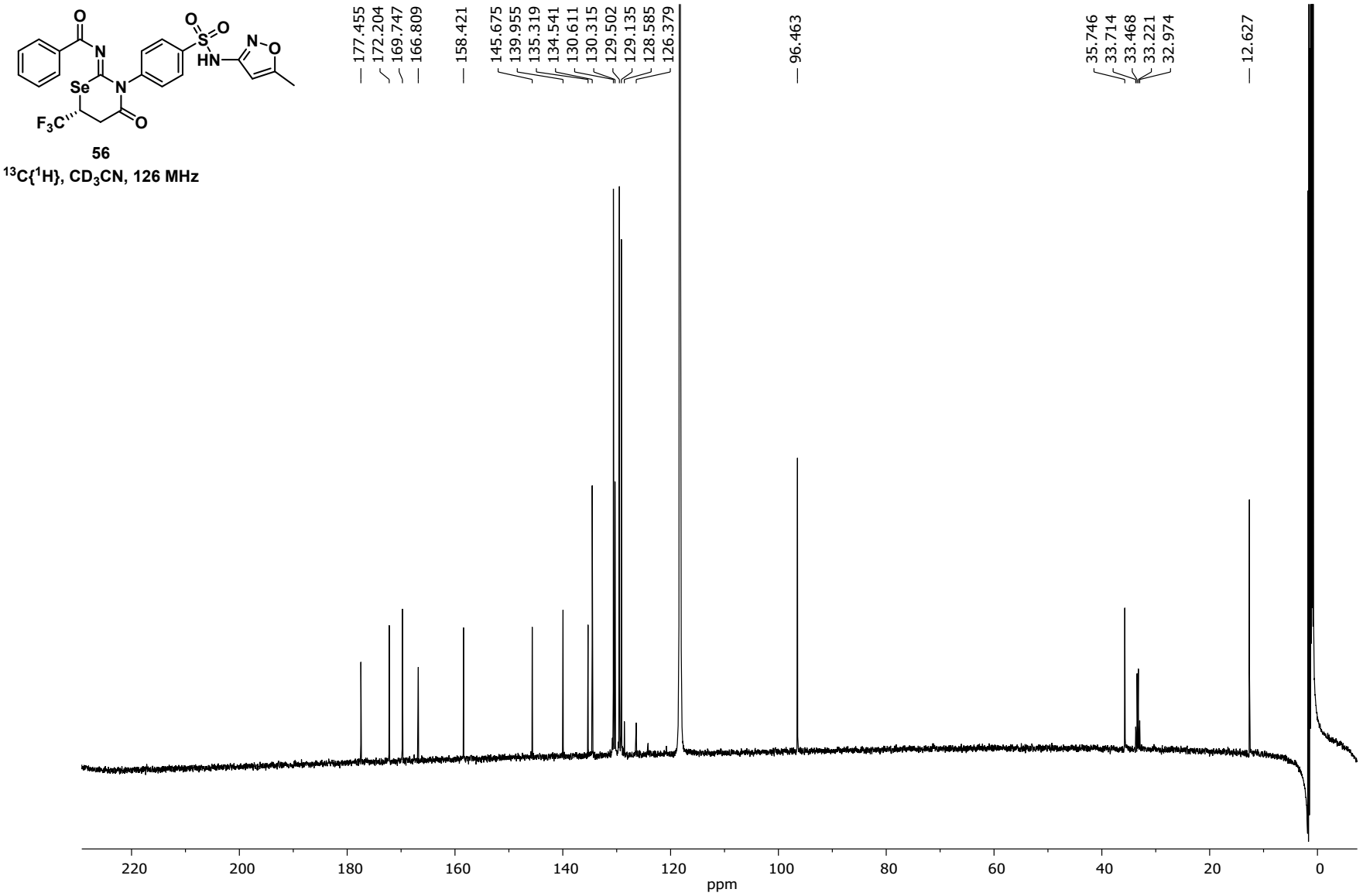

8.046
8.042
8.030
8.028
7.613
7.610
7.596
7.593
7.560
7.558
7.555
7.545
7.543
7.540
7.531
7.528
7.525
7.428
7.411
7.345
7.342
7.330
7.314
6.212
4.191
4.181
4.172
4.163
4.153
4.144
4.134
4.125
4.115
3.714
3.704
3.680
3.670
3.554
3.544
3.520
3.510
2.289
O
N
Se
N
O
F3C
O
S
O
HN
N
O
56
1H, CD3CN, 500 MHz
2.05
2.01
1.09
2.02
2.12
1.00
1.16
1.27
1.34
3.14
10
9
8
7
6
5
4
3
2
1
0
ppm

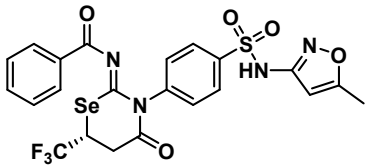


56

$^{19}F\{^{1}H\}$, CD_3CN, 470 MHz

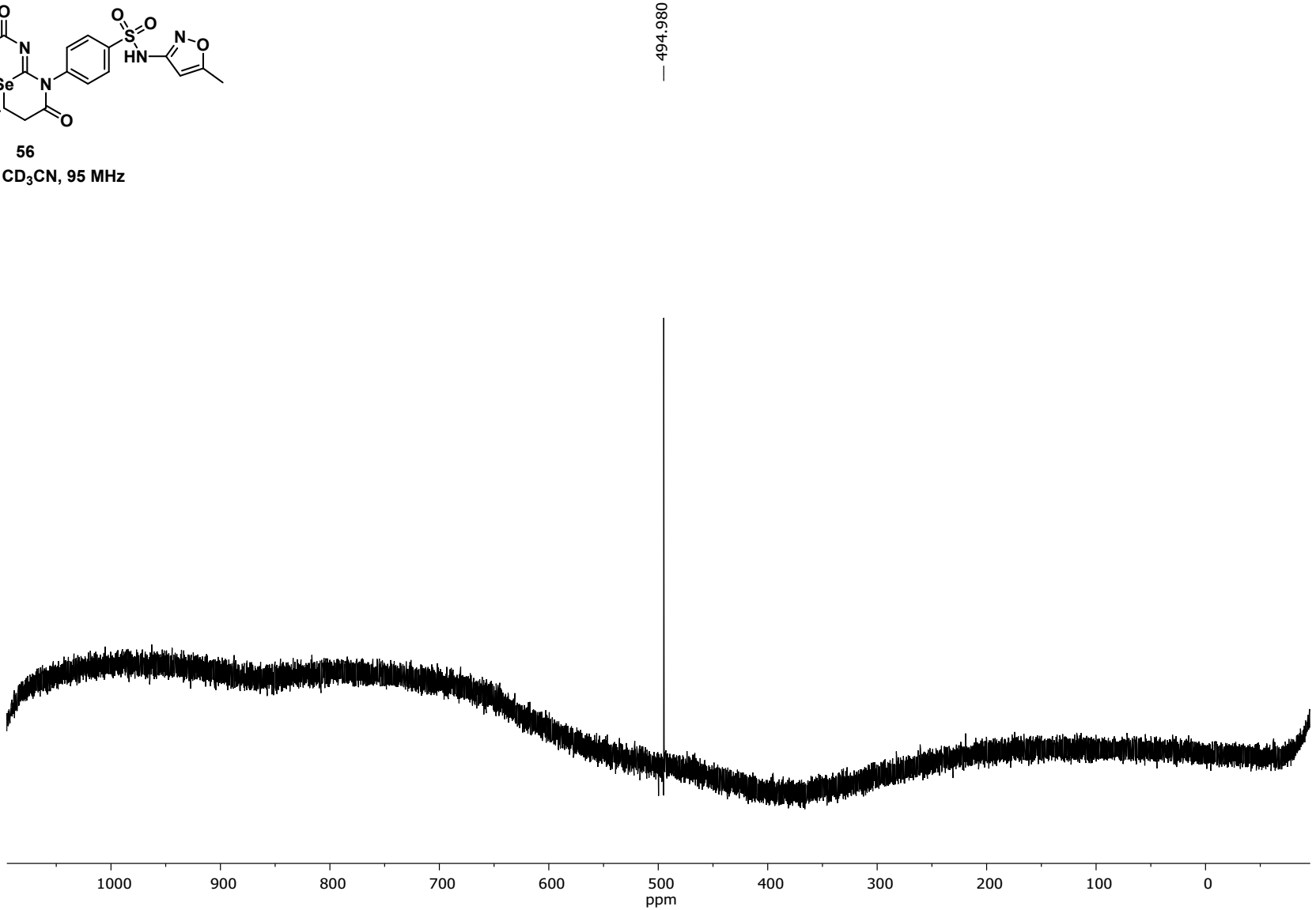


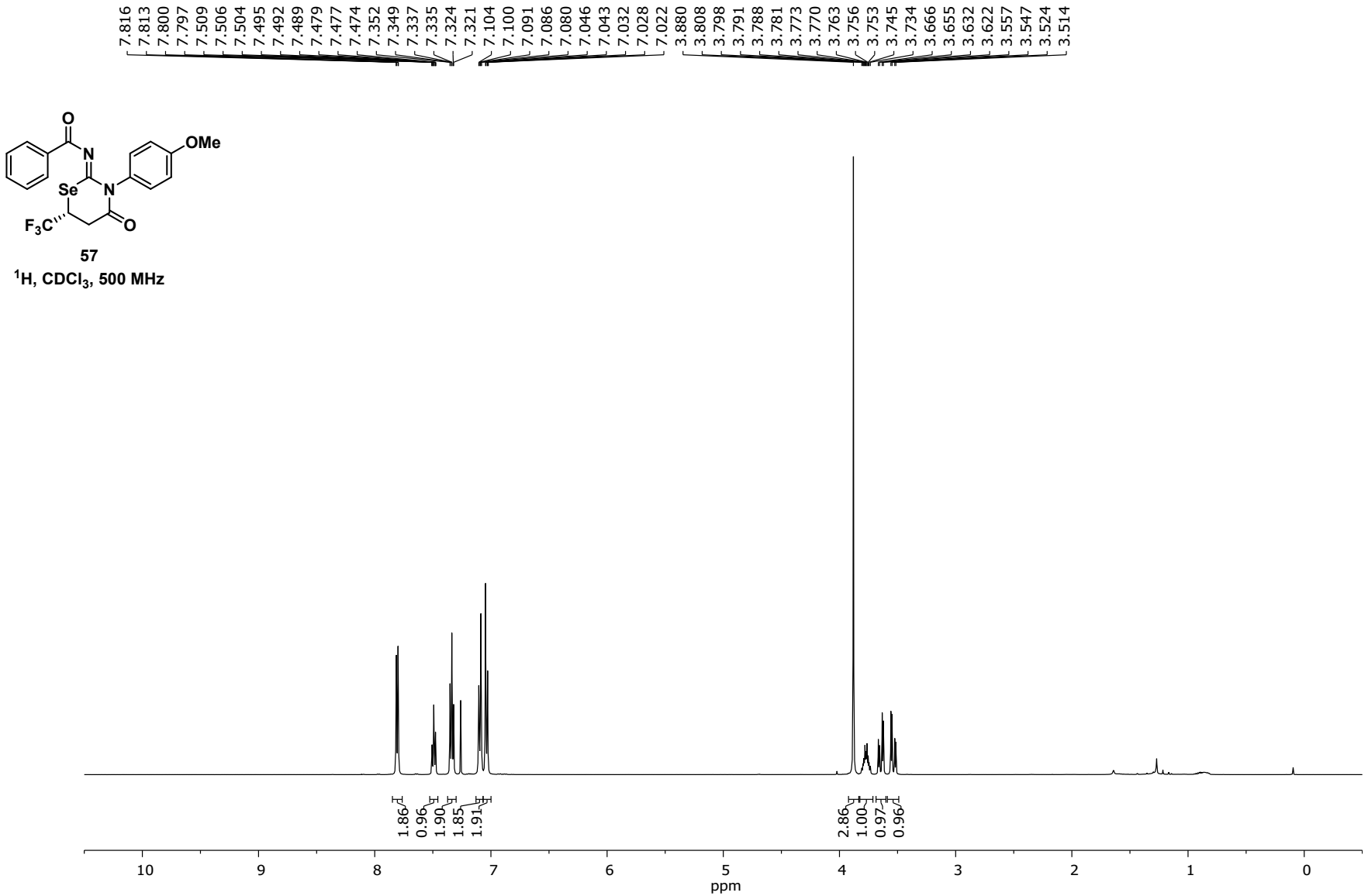

56
13C{1H}, CD3CN, 126 MHz
177.455
172.204
169.747
166.809
158.421
145.675
139.955
135.319
134.541
130.611
130.315
129.502
129.135
128.585
126.379
96.463
35.746
33.714
33.468
33.221
32.974
12.627
220
200
180
160
140
120
100
80
60
40
20
0
ppm

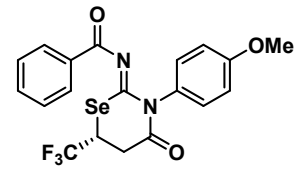


56

$^{77}Se\{^{1}H\}$, CD_3CN, 95 MHz

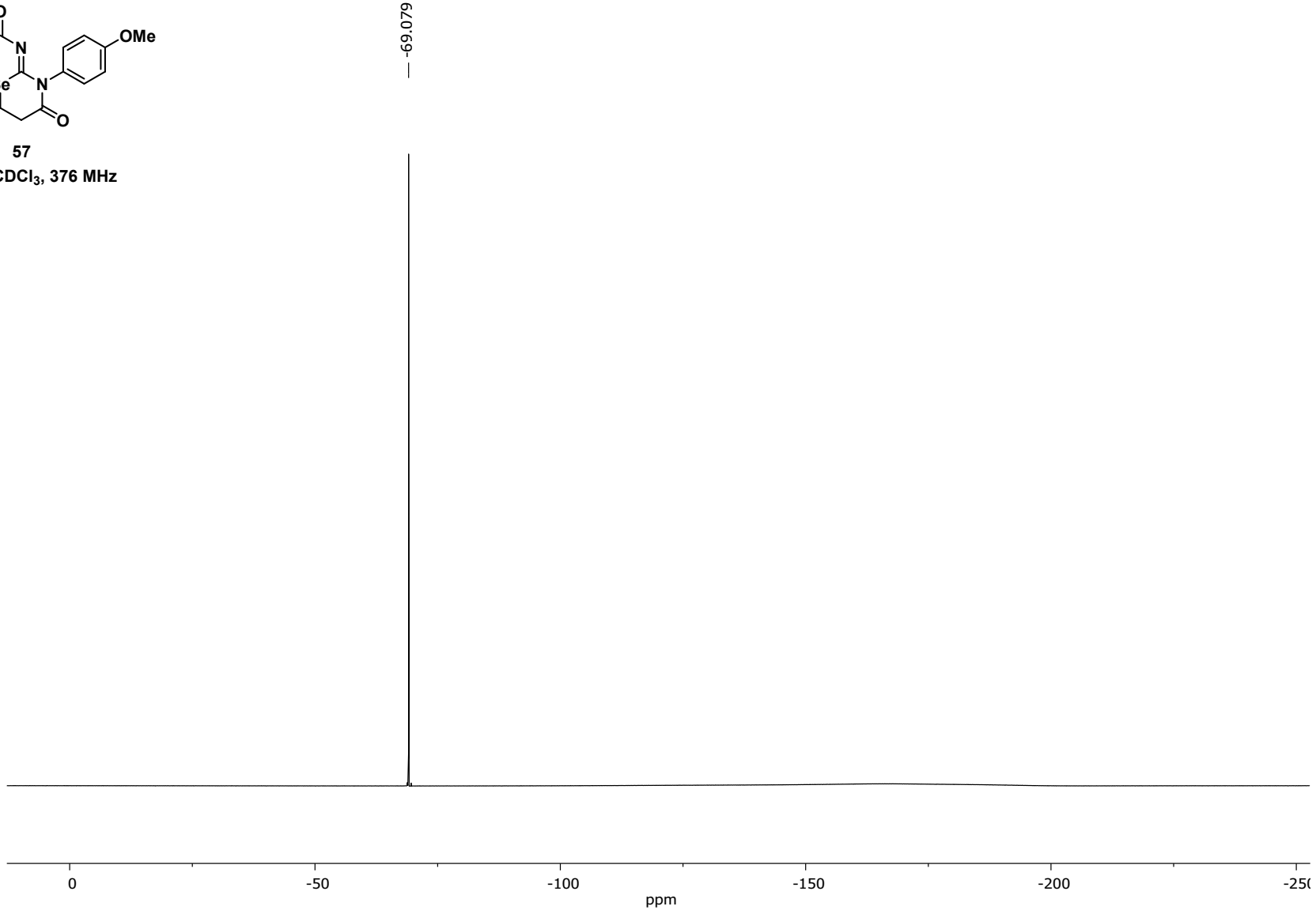


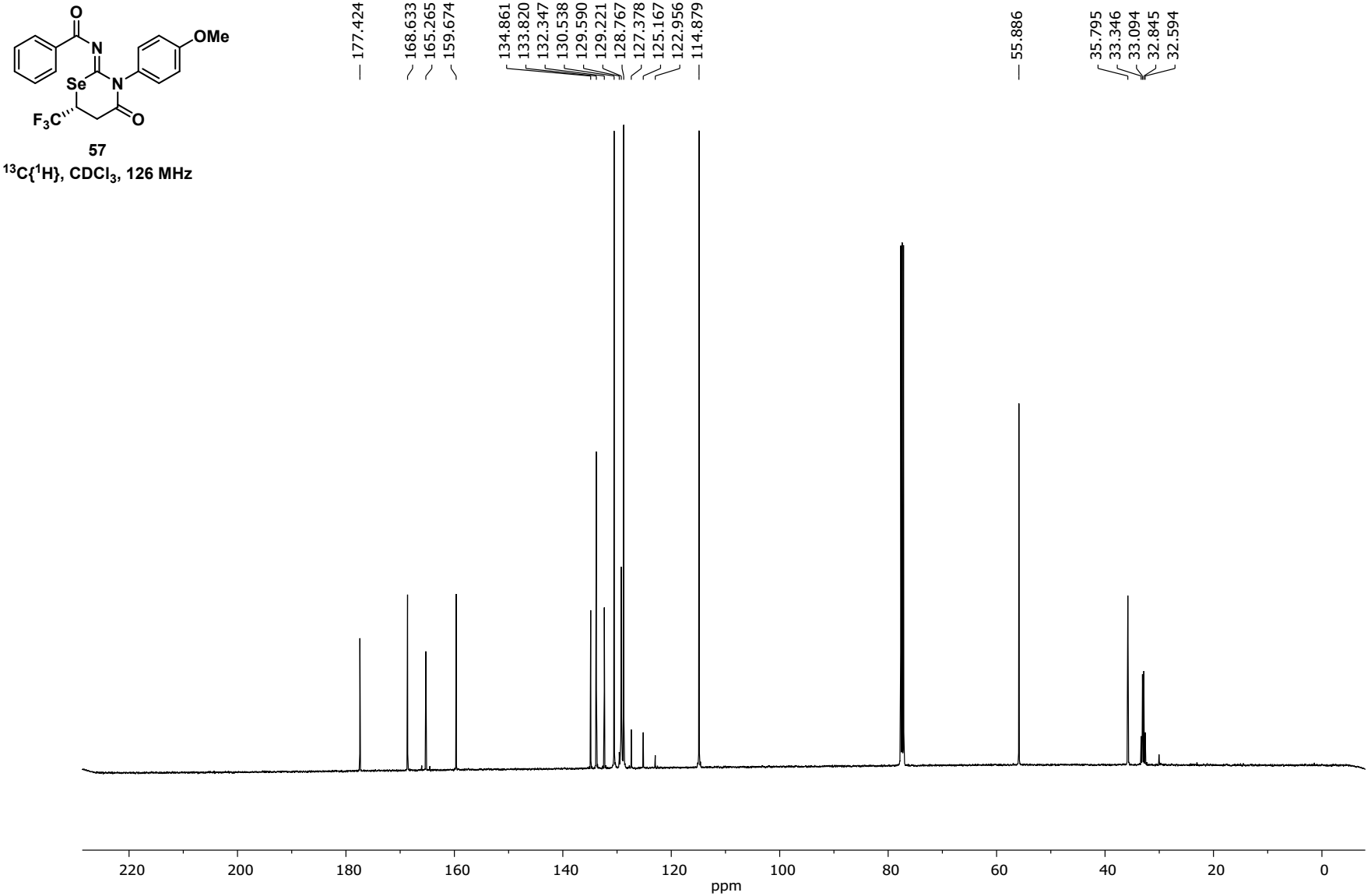

7.816
7.813
7.800
7.797
7.509
7.506
7.504
7.495
7.492
7.489
7.479
7.477
7.474
7.352
7.349
7.337
7.335
7.324
7.321
7.104
7.100
7.091
7.086
7.080
7.046
7.043
7.032
7.028
7.022
3.880
3.808
3.798
3.791
3.788
3.781
3.773
3.770
3.763
3.756
3.753
3.745
3.734
3.666
3.655
3.632
3.622
3.557
3.547
3.524
3.514
O
N
OMe
Se
N
F3C
O
57
1H, CDCl3, 500 MHz
1.86
0.96
1.90
1.85
1.91
2.86
1.00
0.97
0.96
10
9
8
7
6
5
4
3
2
1
0
ppm



57

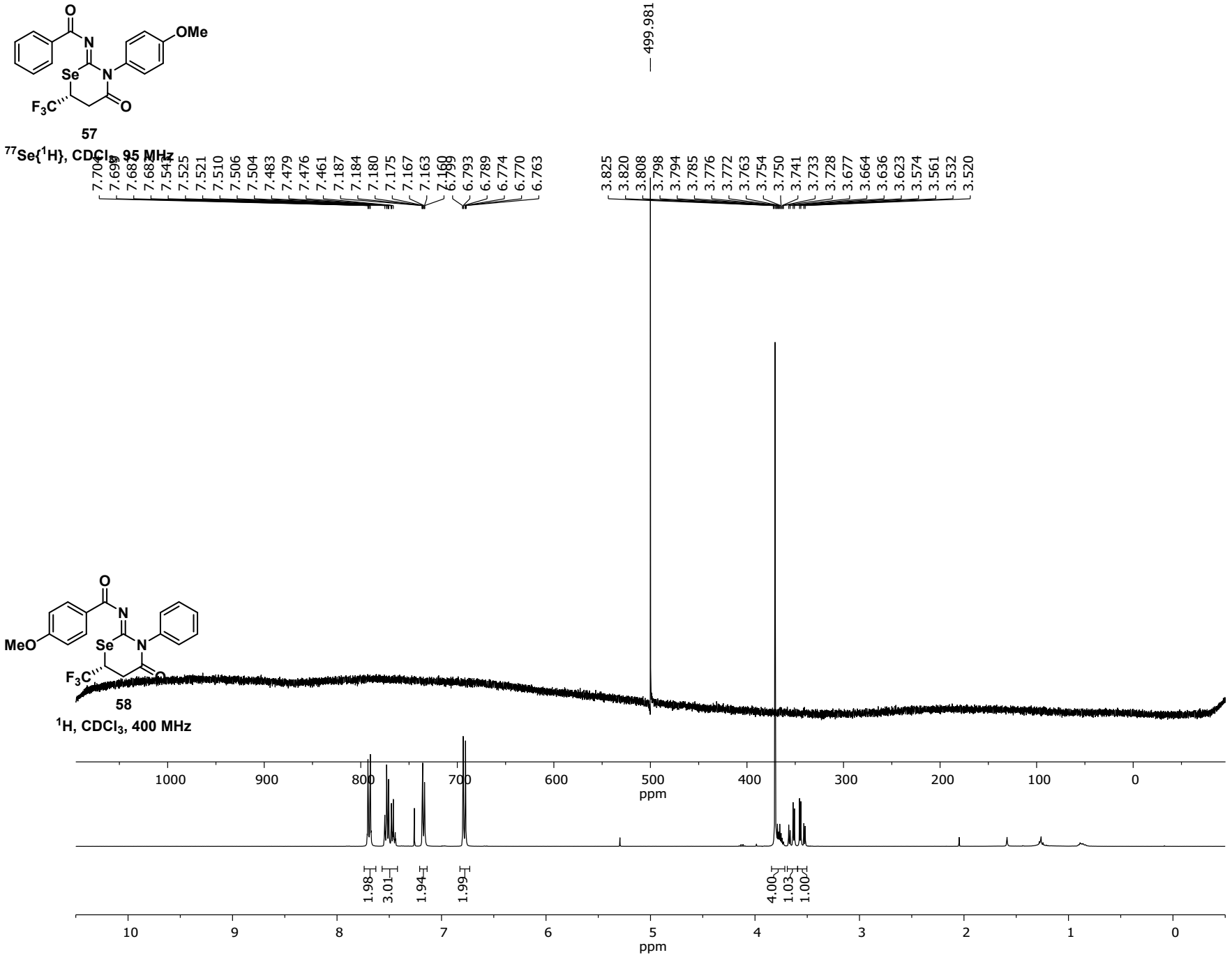
$^{19}F\{^{1}H\}$, $CDCl_3$, 376 MHz





57

$^{13}C\{^{1}H\}$, $CDCl_3$, 126 MHz

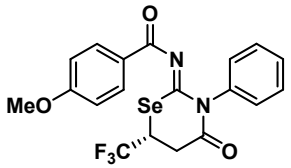


57

$^{77}Se\{^{1}H\}$, $CDCl_3$, 95 MHz

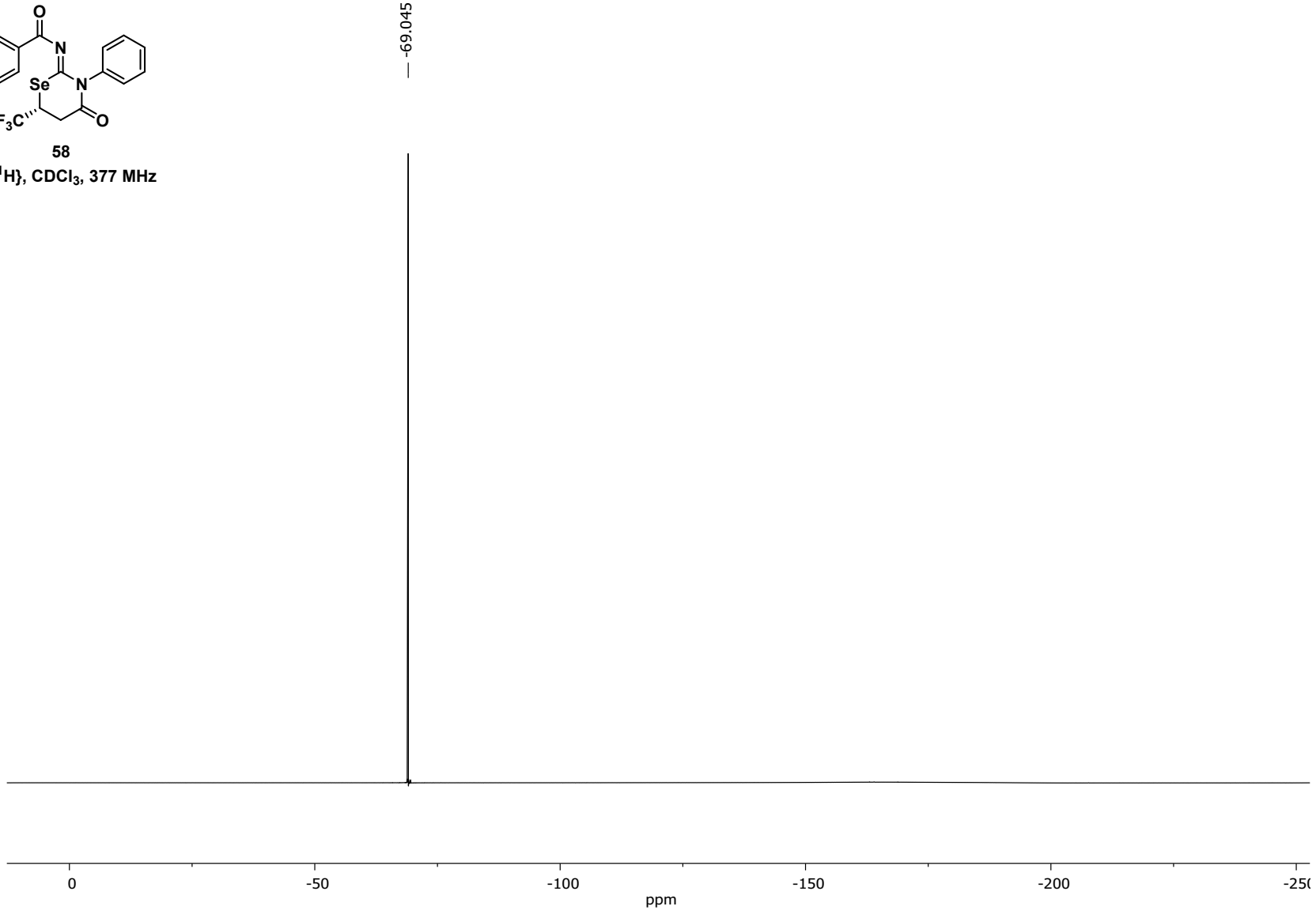
58

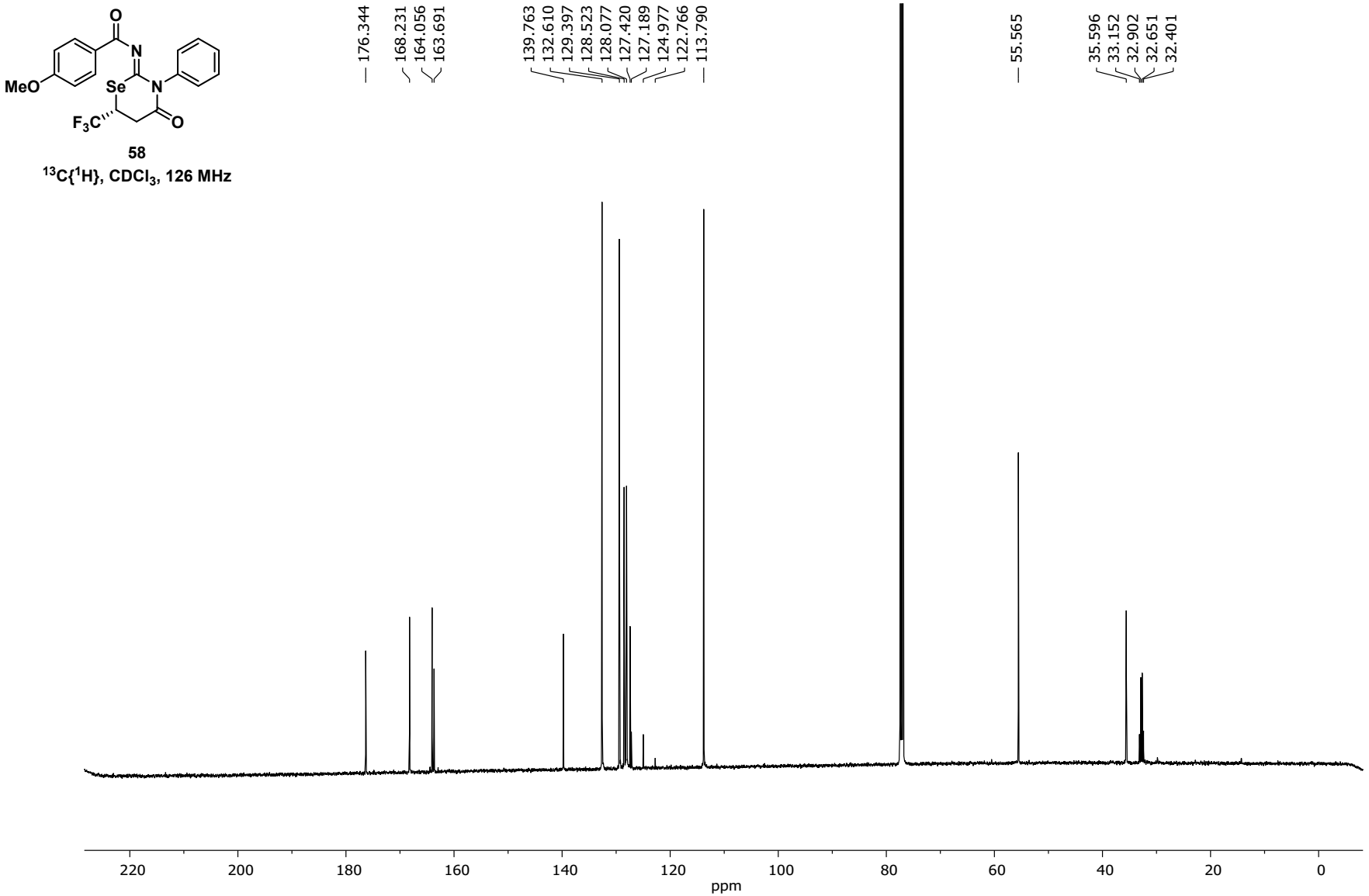
^{1}H, $CDCl_3$, 400 MHz

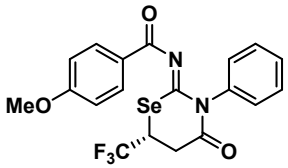


58

$^{19}F\{^{1}H\}$, $CDCl_3$, 377 MHz

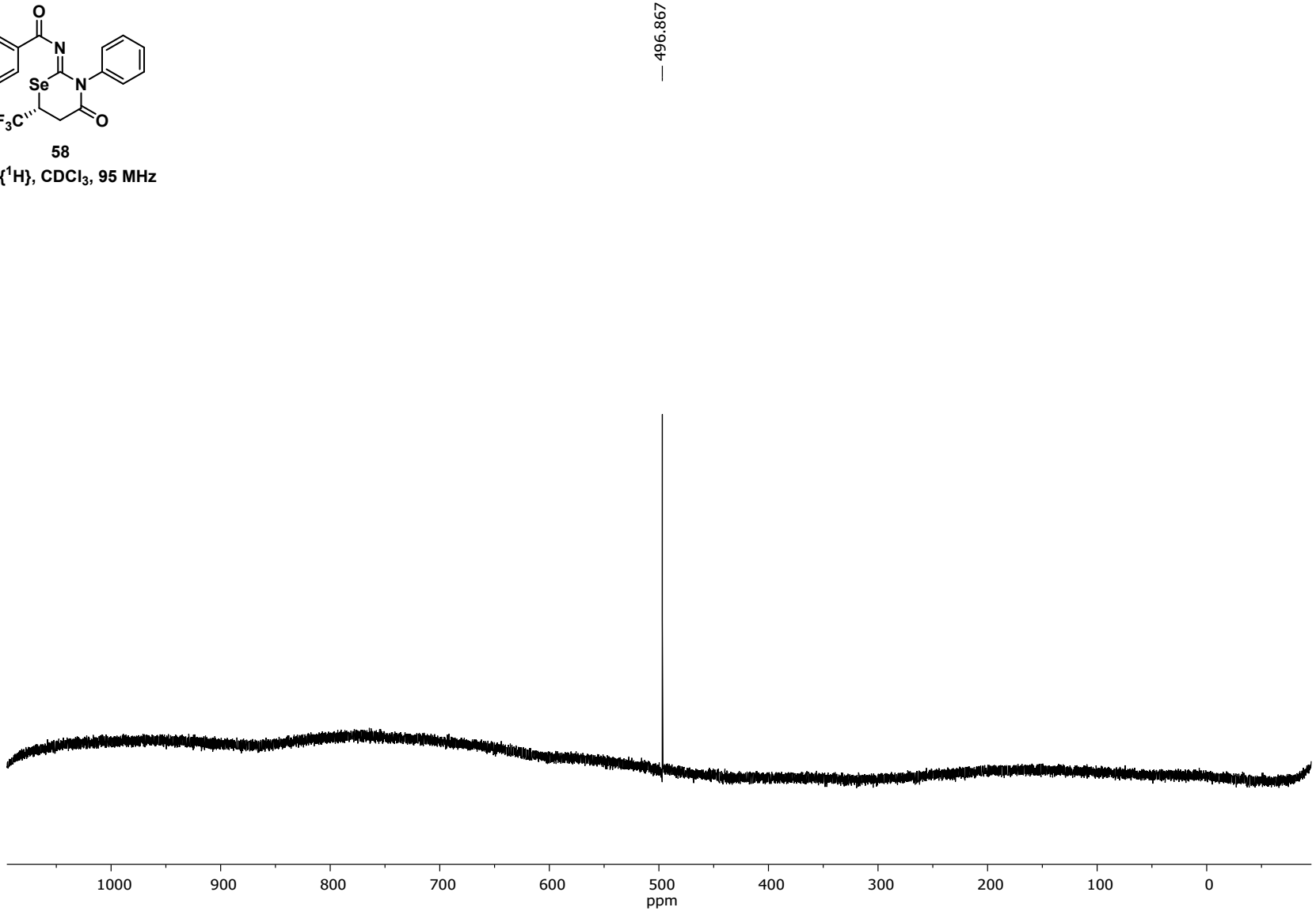


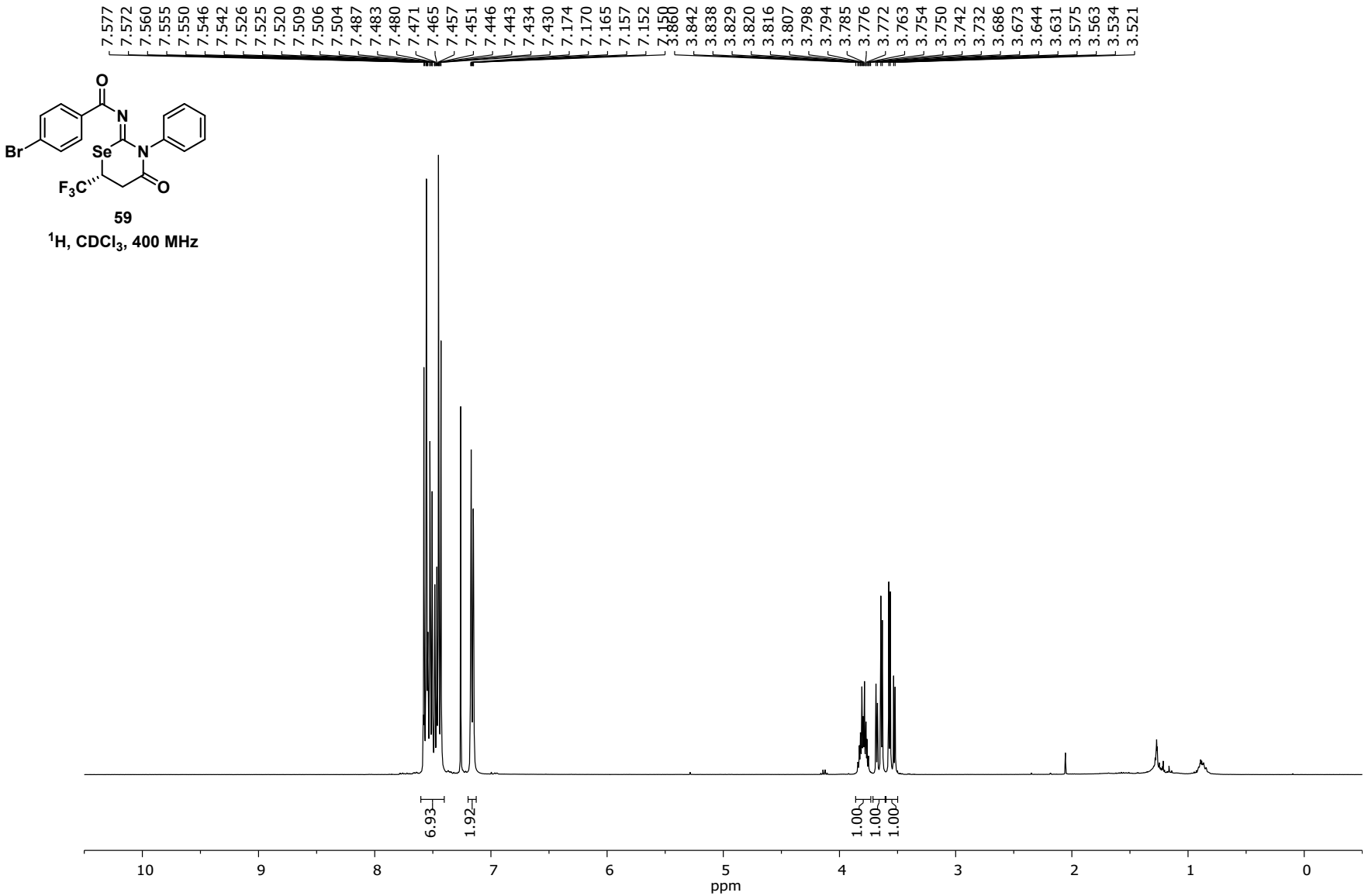

O
N
MeO
Se
N
F3C
O
58
13C{1H}, CDCl3, 126 MHz
176.344
168.231
164.056
163.691
139.763
132.610
129.397
128.523
128.077
127.420
127.189
124.977
122.766
113.790
55.565
35.596
33.152
32.902
32.651
32.401
220
200
180
160
140
120
100
80
60
40
20
0
ppm

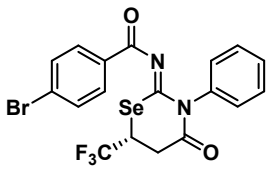


58

$^{77}Se\{^{1}H\}$, $CDCl_3$, 95 MHz

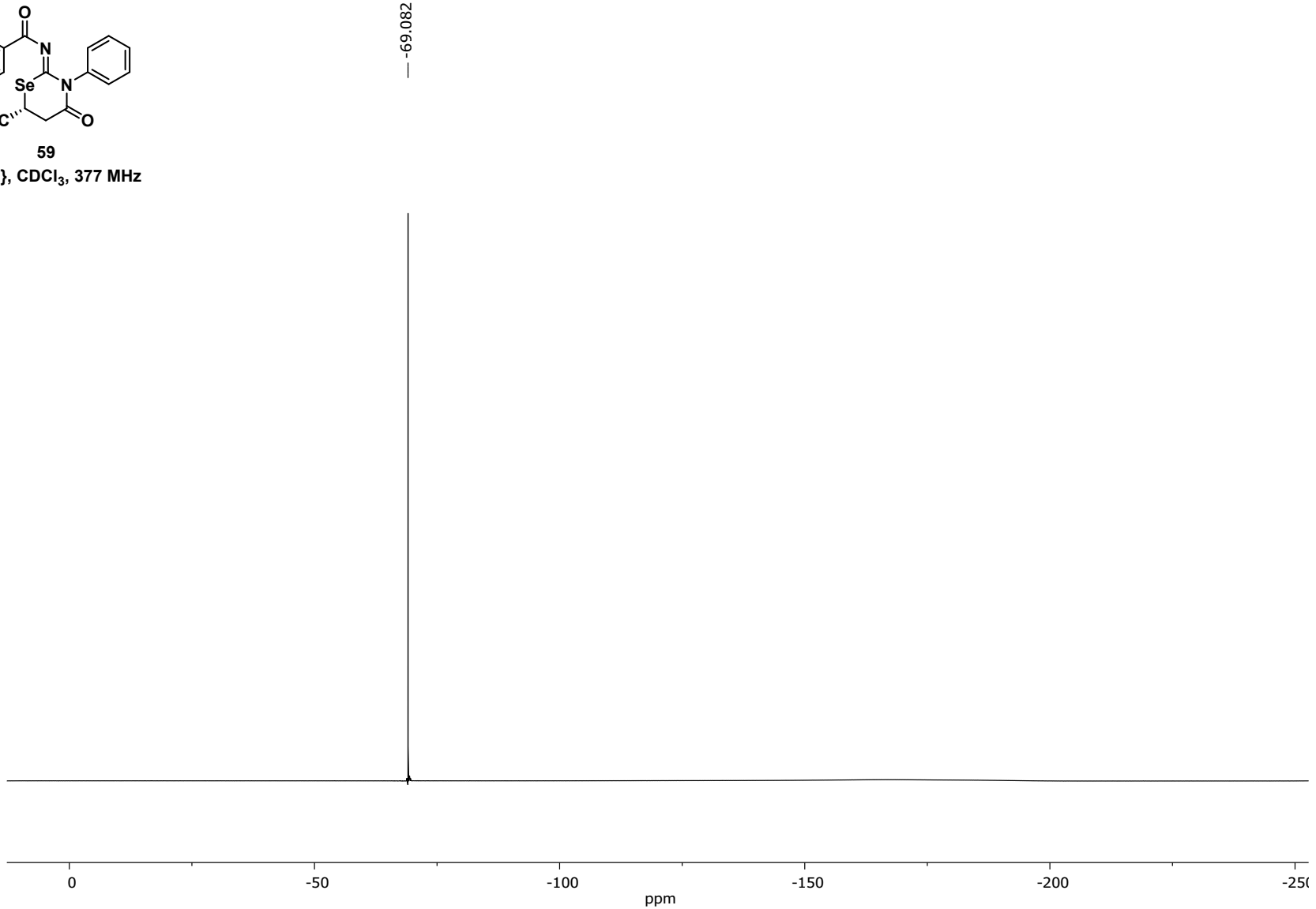


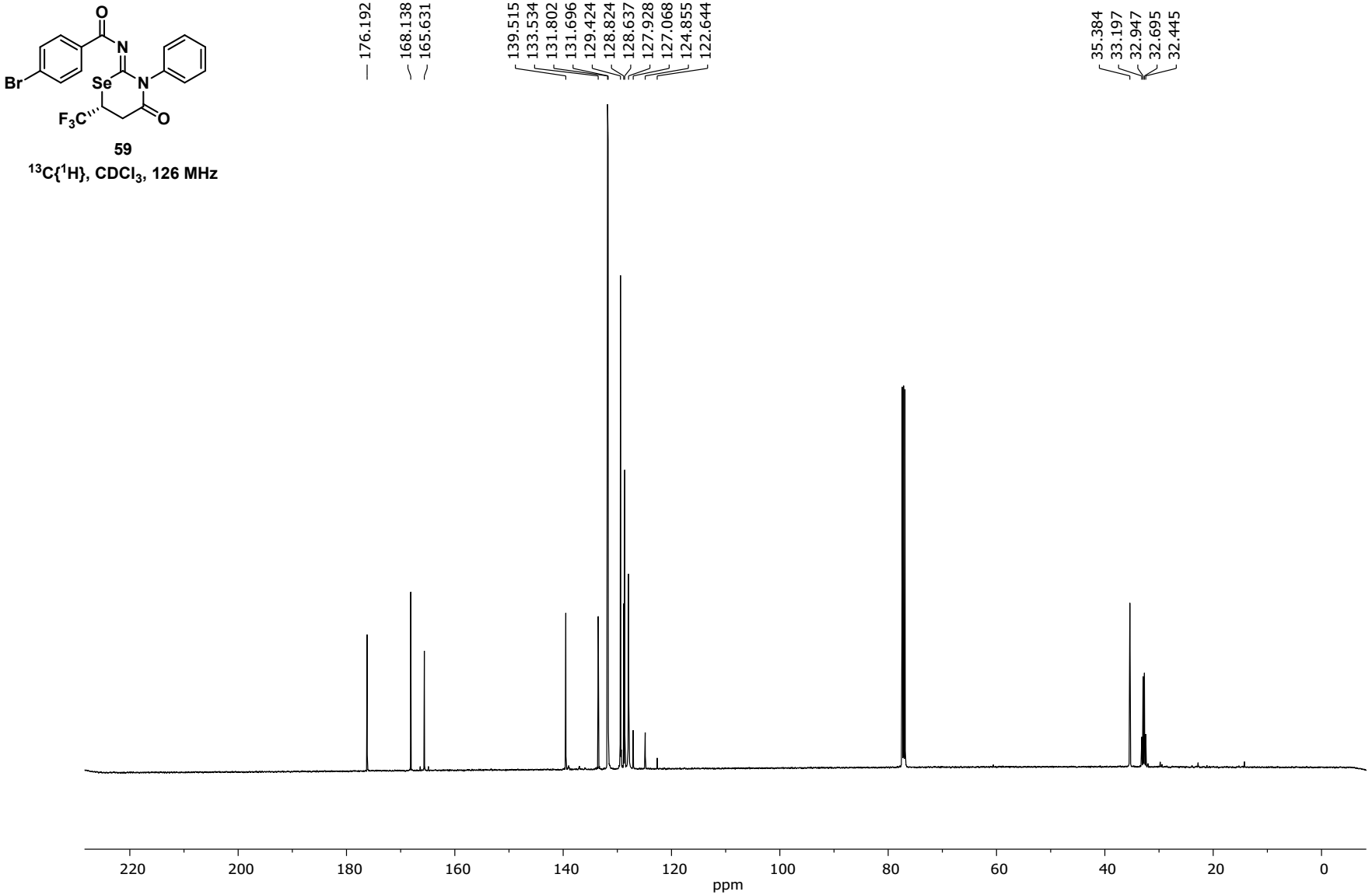

7.577
7.572
7.560
7.555
7.550
7.546
7.542
7.526
7.525
7.520
7.509
7.506
7.504
7.487
7.483
7.480
7.471
7.465
7.457
7.451
7.446
7.443
7.434
7.430
7.174
7.170
7.165
7.157
7.152
7.150
3.860
3.842
3.838
3.829
3.820
3.816
3.807
3.798
3.794
3.785
3.776
3.772
3.763
3.754
3.750
3.742
3.732
3.686
3.673
3.644
3.631
3.575
3.563
3.534
3.521
O
N
Br
Se
N
F3C
O
59
1H, CDCl3, 400 MHz
6.93
1.92
1.00
1.00
1.00
10
9
8
7
6
5
4
3
2
1
0
ppm

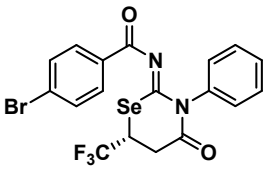


59

$^{19}F\{^{1}H\}$, $CDCl_3$, 377 MHz

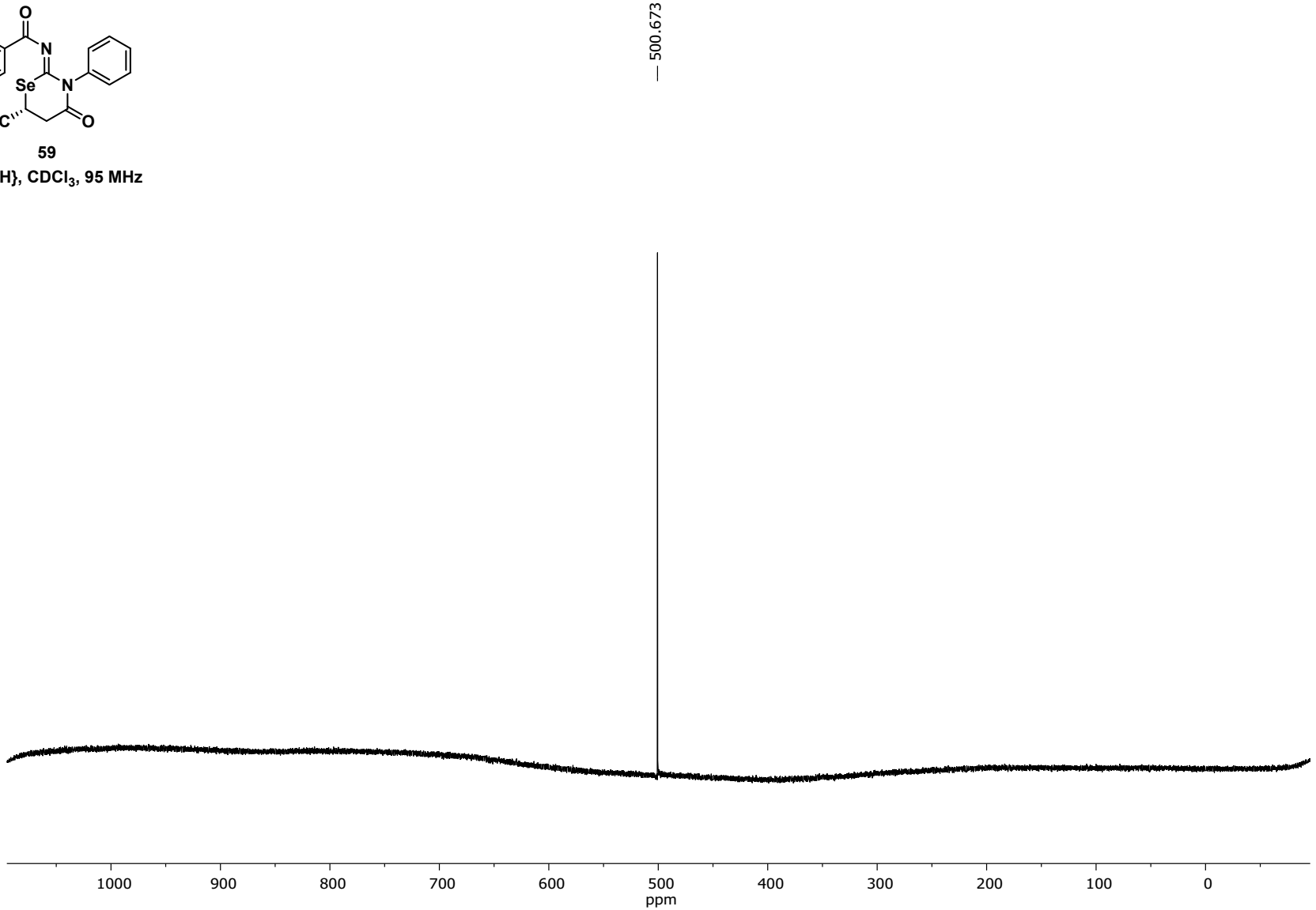


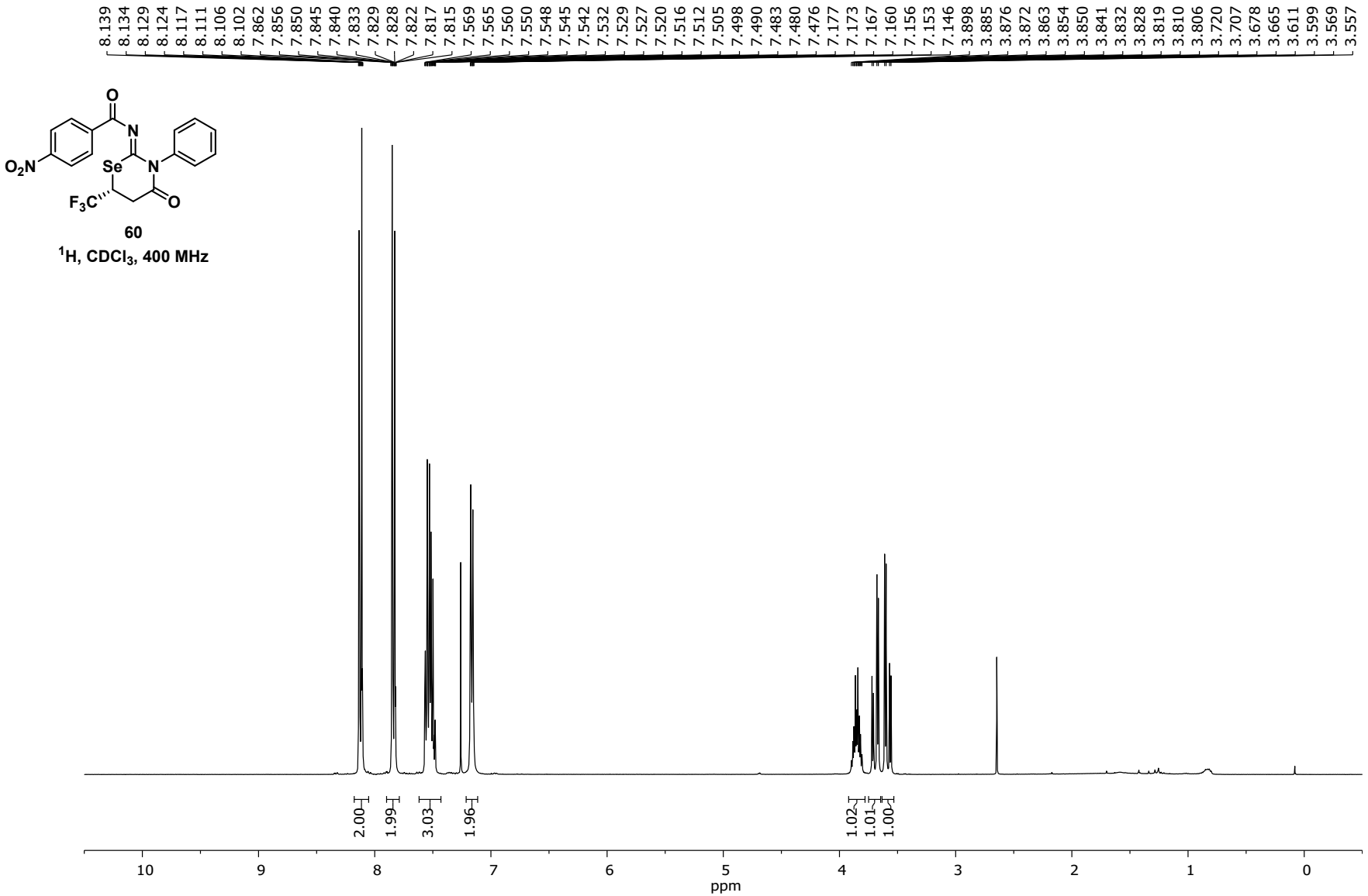

O
N
Br
Se
N
F3C
O
59
13C{1H}, CDCl3, 126 MHz
176.192
168.138
165.631
139.515
133.534
131.802
131.696
129.424
128.824
128.637
127.928
127.068
124.855
122.644
35.384
33.197
32.947
32.695
32.445
220
200
180
160
140
120
100
80
60
40
20
0
ppm

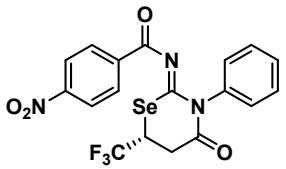


59

$^{77}Se\{^{1}H\}$, $CDCl_3$, 95 MHz

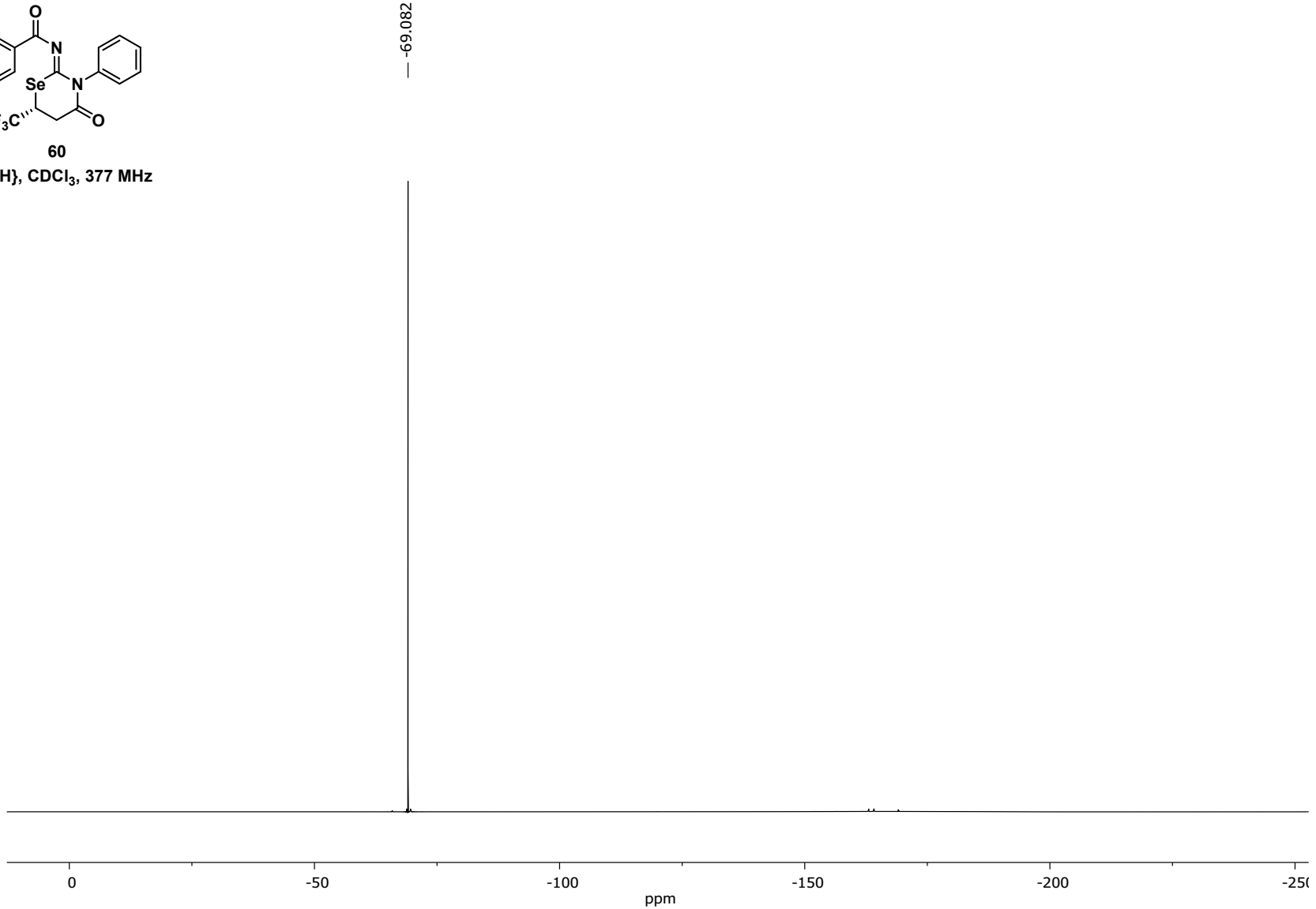


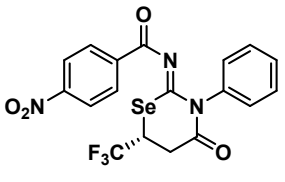

8.139
8.134
8.129
8.124
8.117
8.111
8.106
8.102
7.862
7.856
7.850
7.845
7.840
7.833
7.829
7.828
7.822
7.817
7.815
7.569
7.565
7.560
7.550
7.548
7.545
7.542
7.532
7.529
7.527
7.520
7.516
7.512
7.505
7.498
7.490
7.483
7.480
7.476
7.177
7.173
7.167
7.160
7.156
7.153
7.146
3.898
3.885
3.876
3.872
3.863
3.854
3.850
3.841
3.832
3.828
3.819
3.810
3.806
3.720
3.707
3.678
3.665
3.611
3.599
3.569
3.557
O
N
O2N
Se
N
F3C
O
60
1H, CDCl3, 400 MHz
2.00
1.99
3.03
1.96
1.02
1.01
1.00
10
9
8
7
6
5
4
3
2
1
0
ppm



60

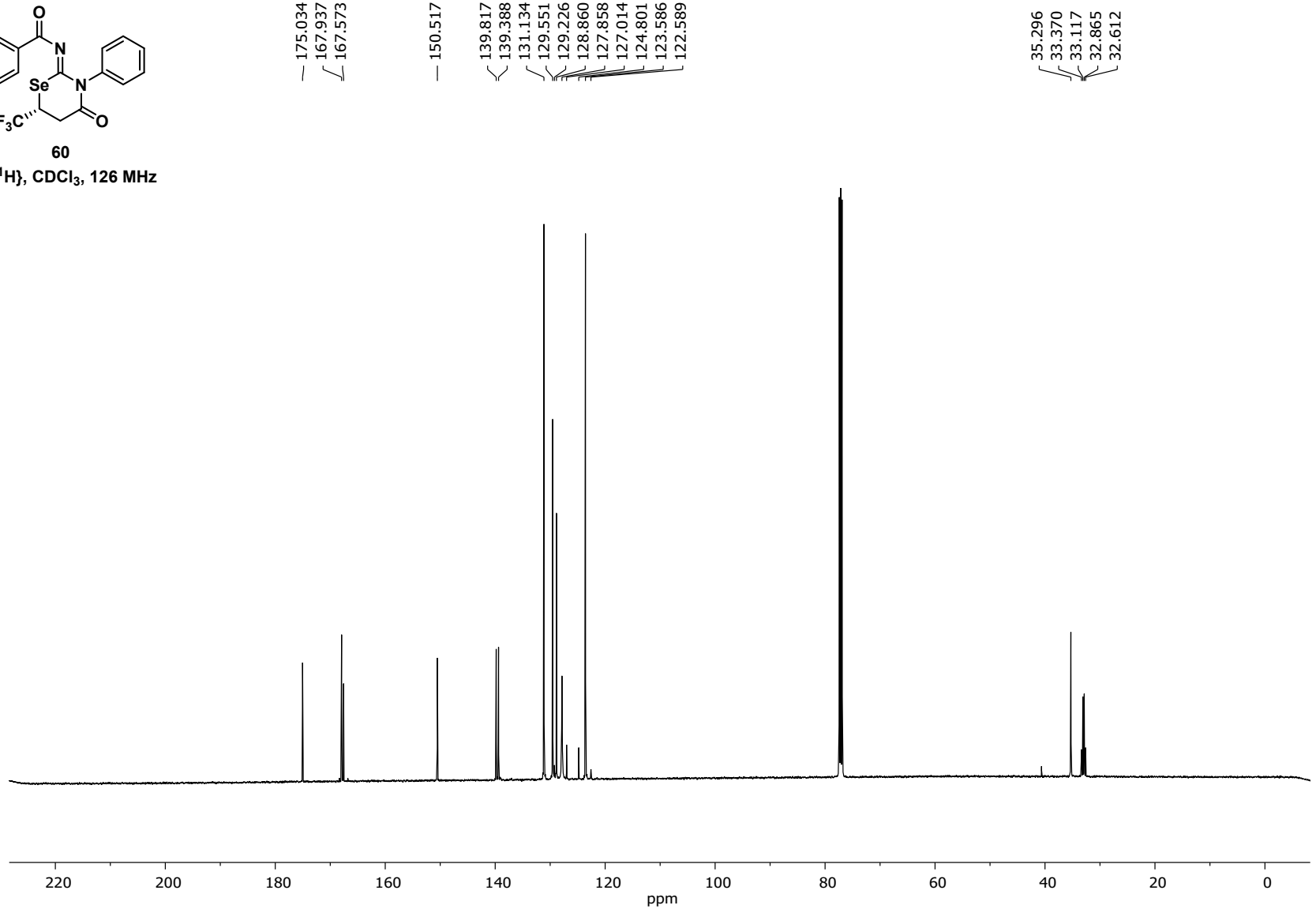
$^{19}F\{^{1}H\}$, $CDCl_3$, 377 MHz

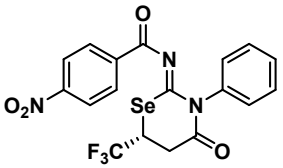




60

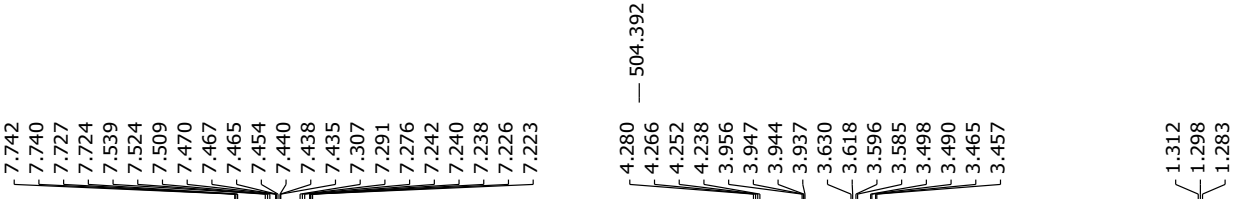
$^{13}C\{^{1}H\}$, $CDCl_3$, 126 MHz

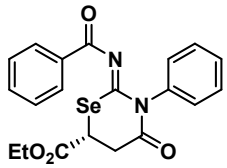




60

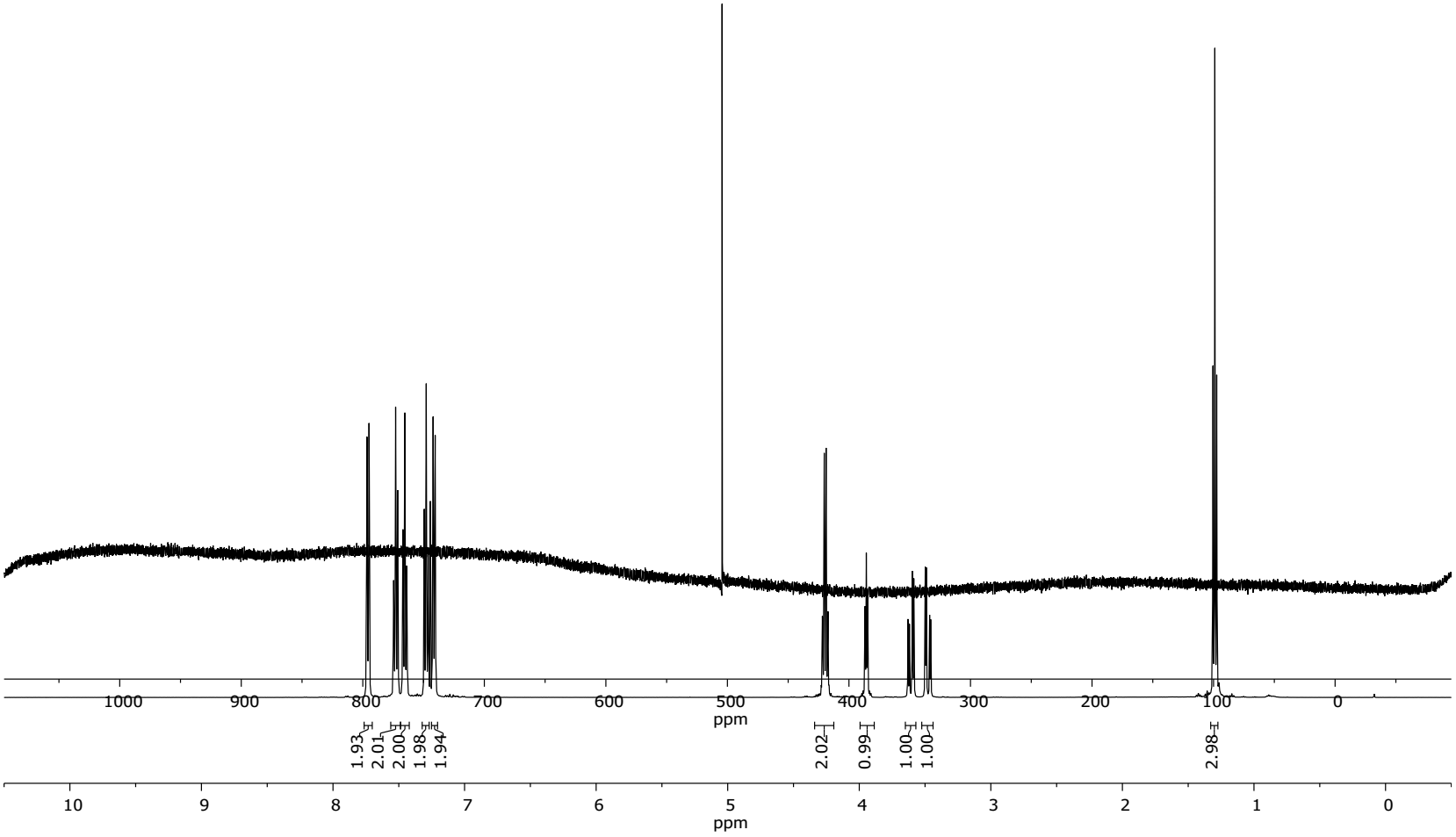
$^{77}Se\{^{1}H\}$, $CDCl_3$, 95 MHz

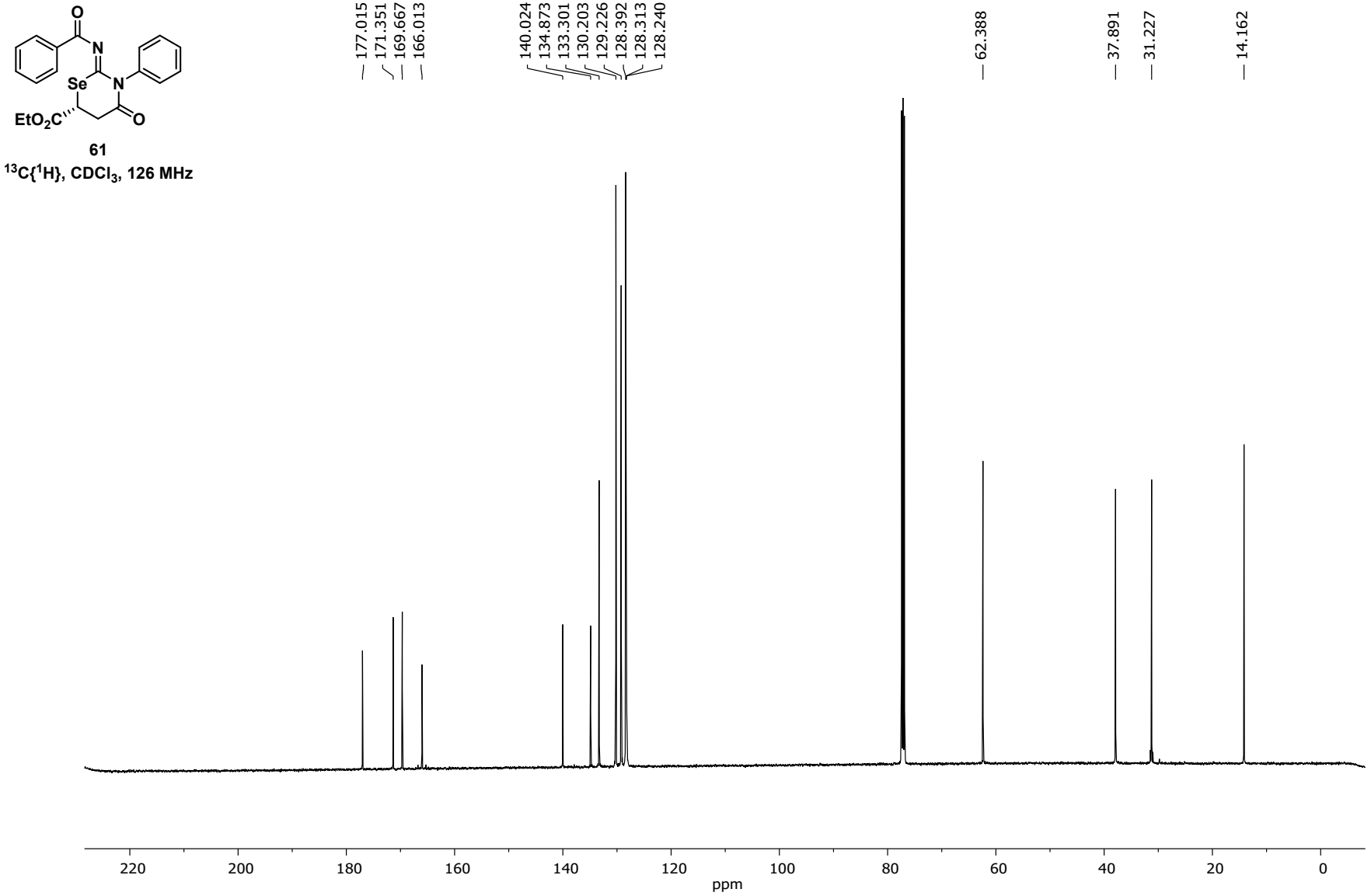


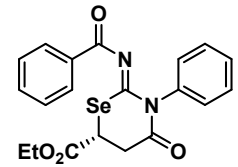


61

^{1}H, $CDCl_3$, 500 MHz

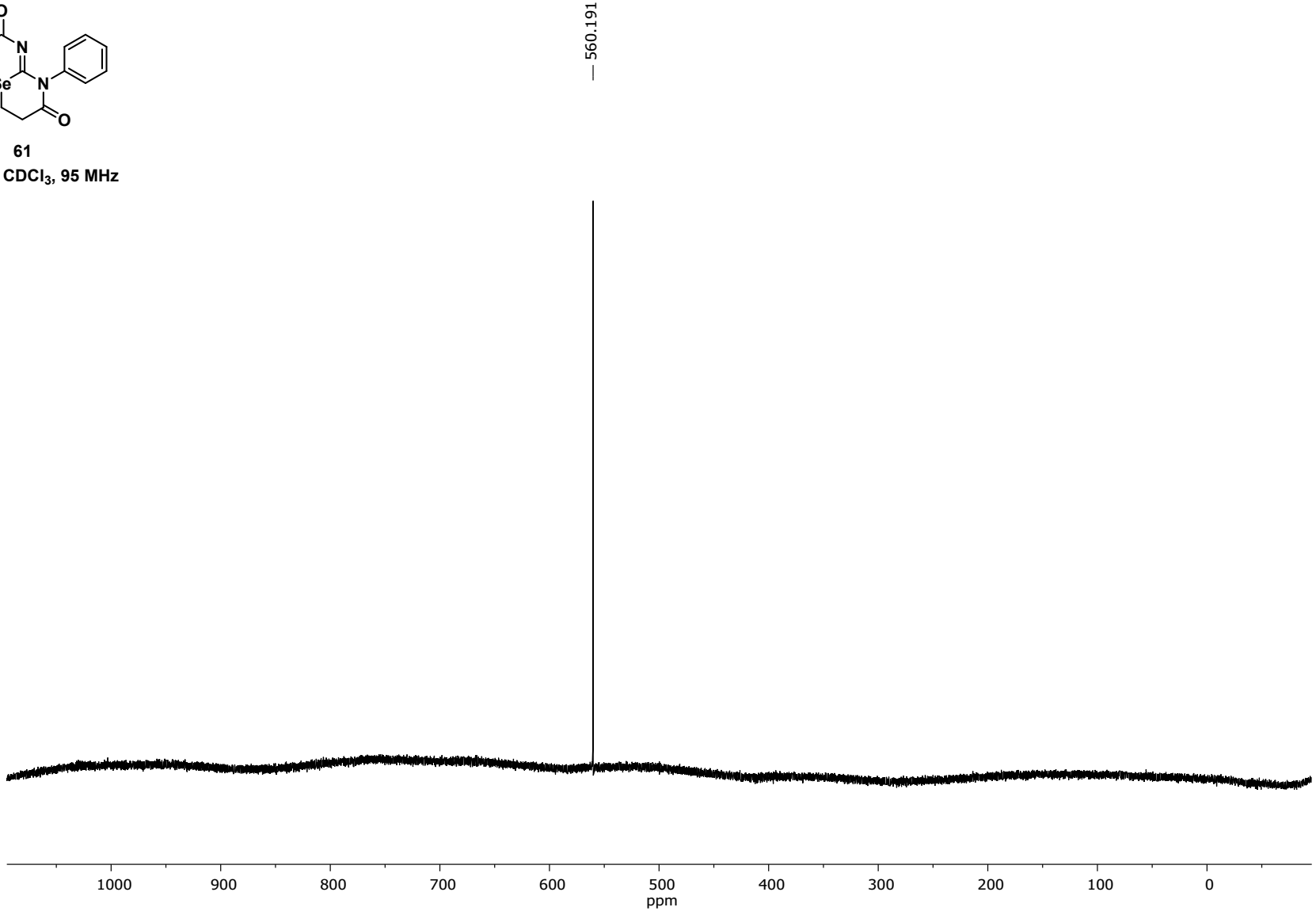


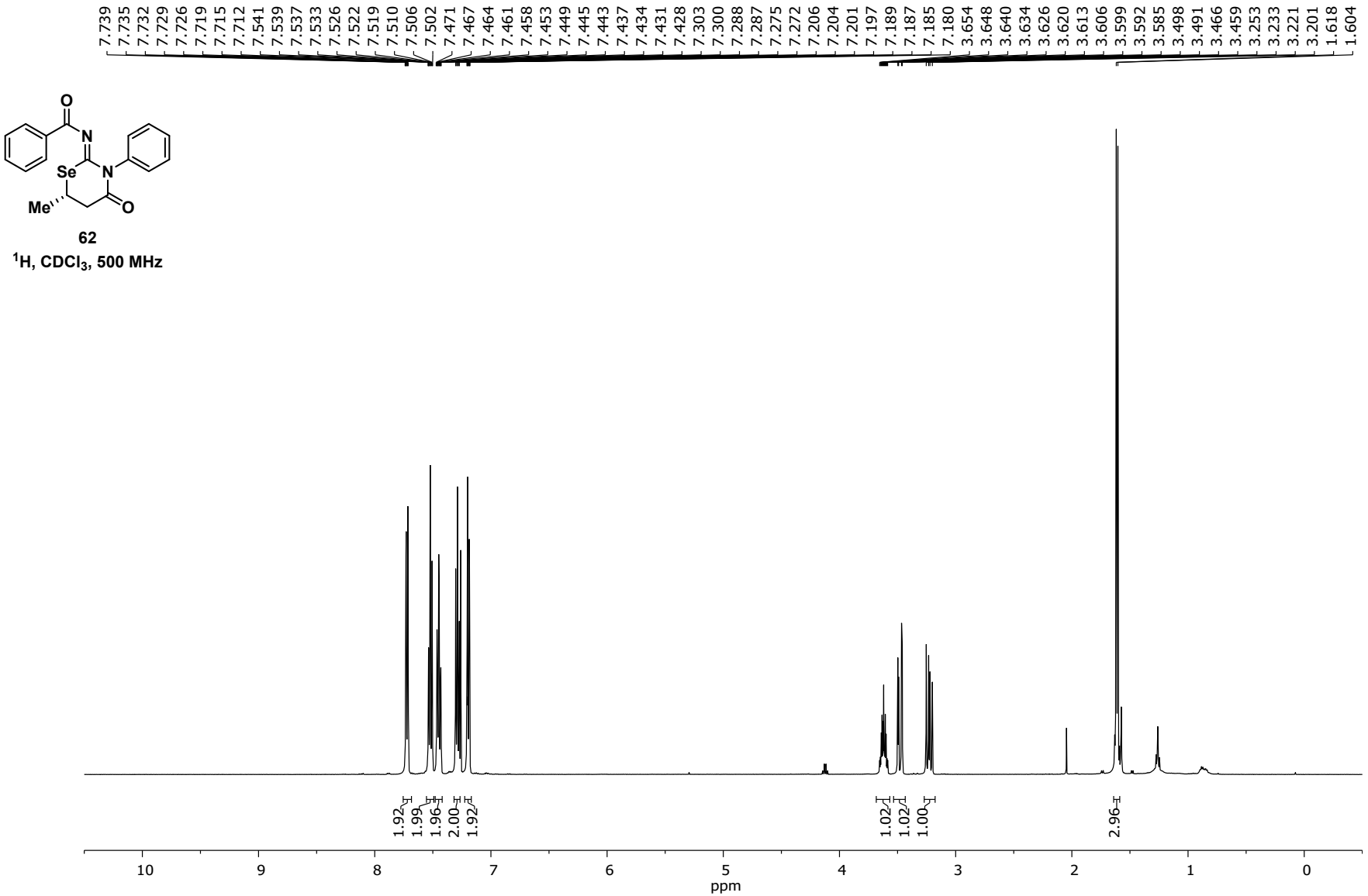

O
N
Se
N
O
EtO2C
61
13C{1H}, CDCl3, 126 MHz
177.015
171.351
169.667
166.013
140.024
134.873
133.301
130.203
129.226
128.392
128.313
128.240
62.388
37.891
31.227
14.162
220
200
180
160
140
120
100
80
60
40
20
0
ppm

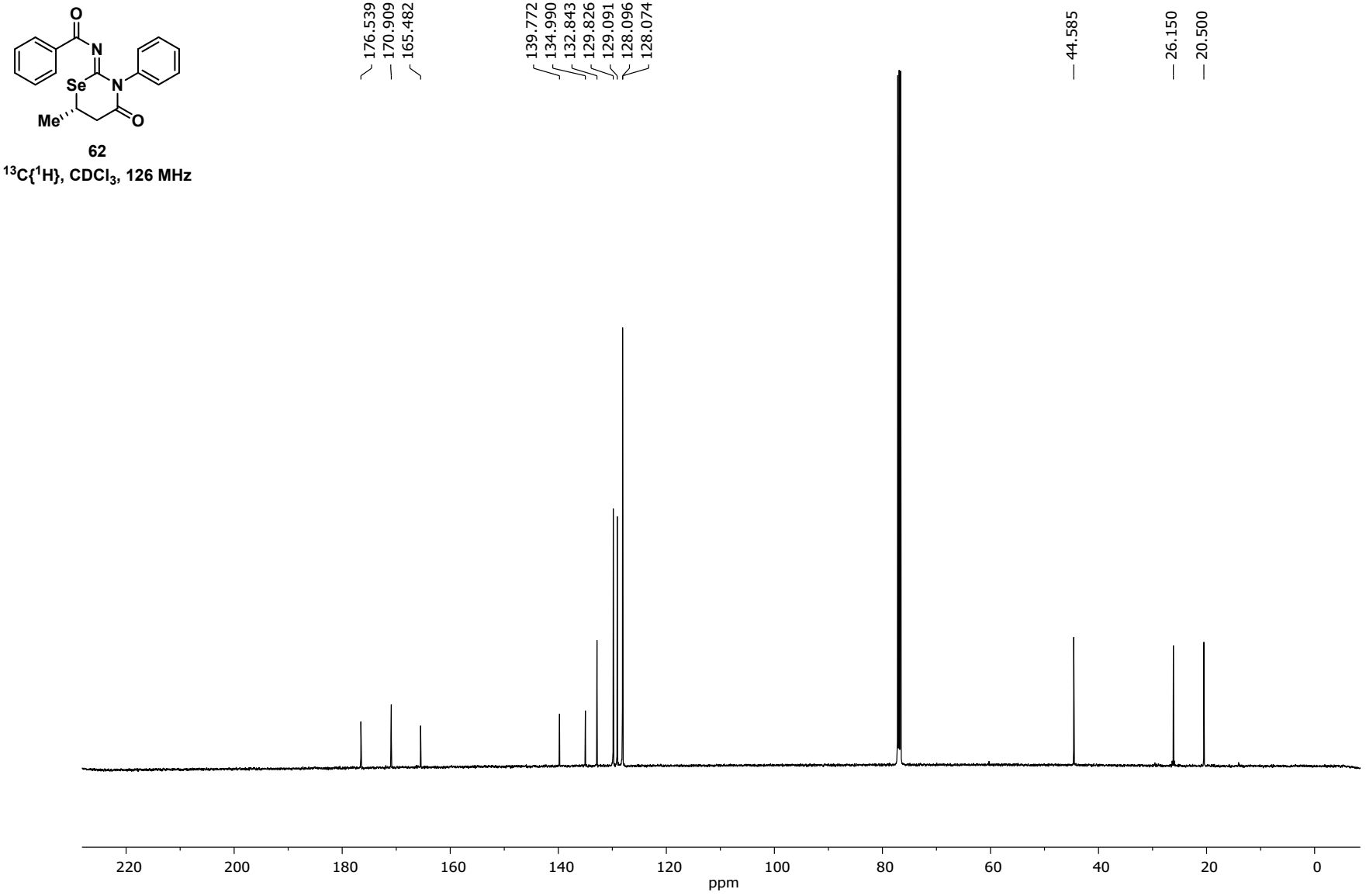


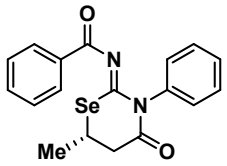
61

$^{77}Se\{^{1}H\}$, $CDCl_3$, 95 MHz



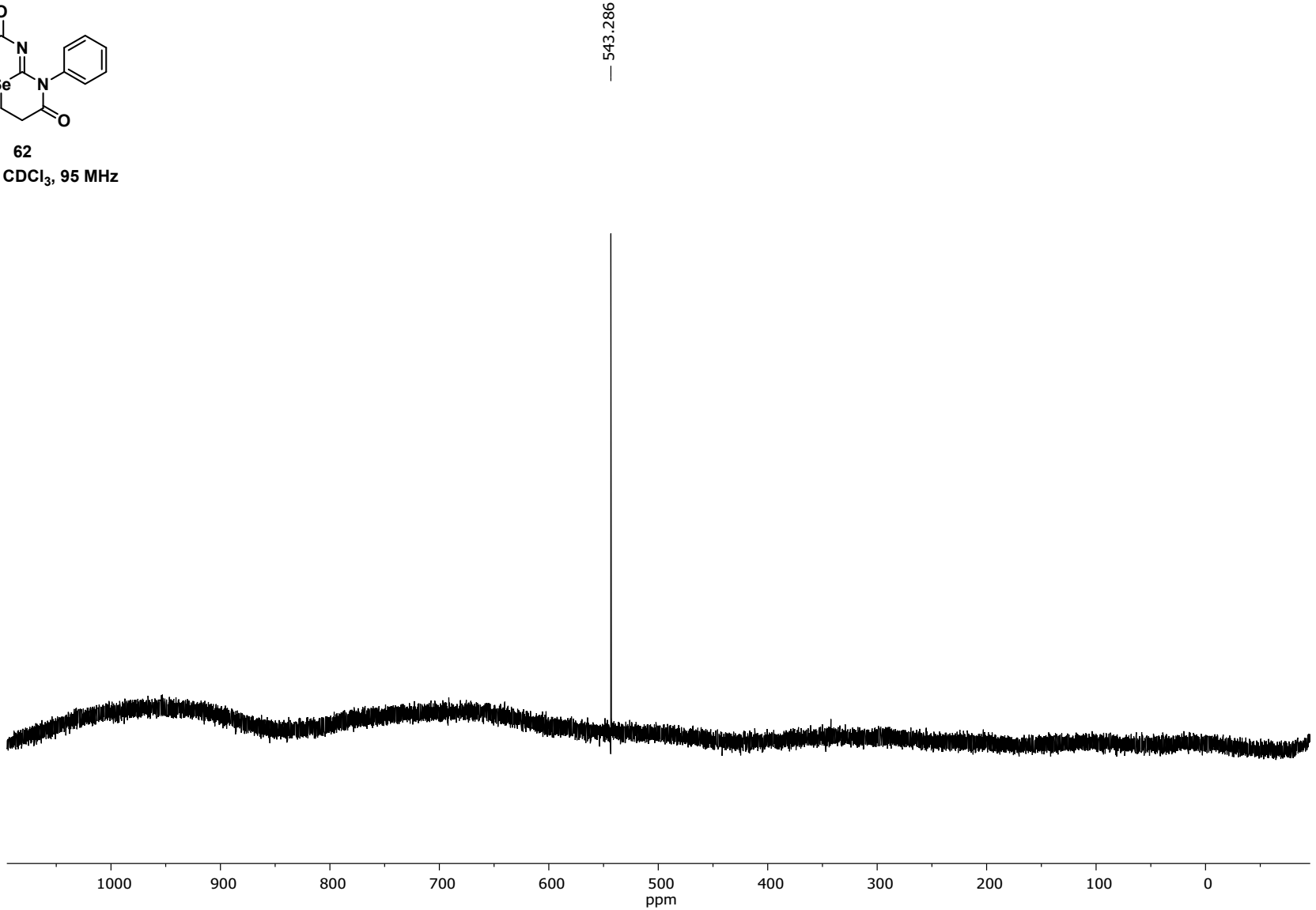

7.739
7.735
7.732
7.729
7.726
7.719
7.715
7.712
7.541
7.539
7.537
7.533
7.526
7.522
7.519
7.510
7.506
7.502
7.471
7.467
7.464
7.461
7.458
7.453
7.449
7.445
7.443
7.437
7.434
7.431
7.428
7.303
7.300
7.288
7.287
7.275
7.272
7.206
7.204
7.201
7.197
7.189
7.187
7.185
7.180
3.654
3.648
3.640
3.634
3.626
3.620
3.613
3.606
3.599
3.592
3.585
3.498
3.491
3.466
3.459
3.253
3.233
3.221
3.201
1.618
1.604
O
N
Se
N
Me
O
62
1H, CDCl3, 500 MHz
1.92
1.99
1.96
2.00
1.92
1.02
1.02
1.00
2.96
10
9
8
7
6
5
4
3
2
1
0
ppm

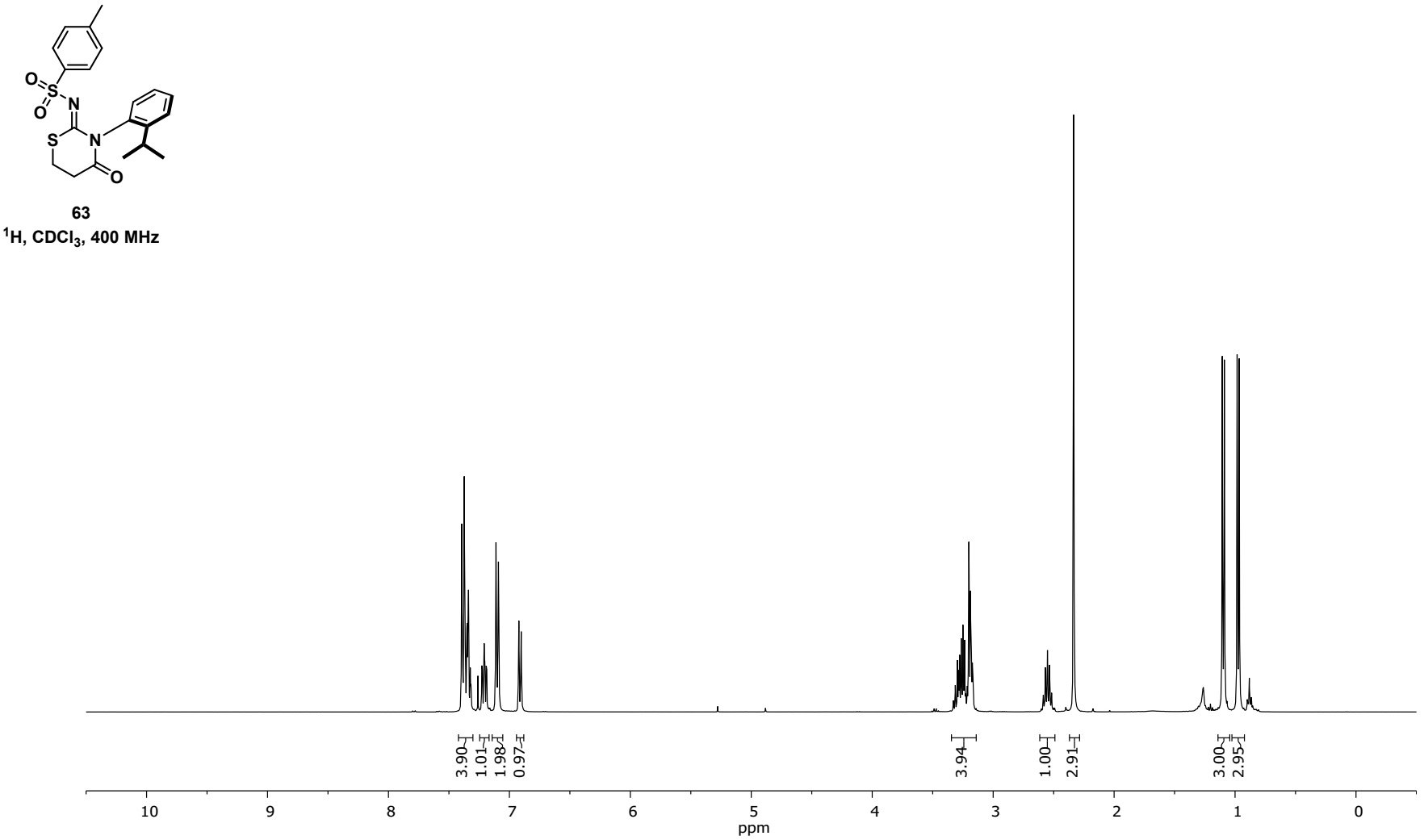

O
N
Se
N
Me
O
62
$^{13}C\{^{1}H\}$, $CDCl_3$, 126 MHz
176.539
170.909
165.482
139.772
134.990
132.843
129.826
129.091
128.096
128.074
44.585
26.150
20.500
220
200
180
160
140
120
100
80
60
40
20
0
ppm



62

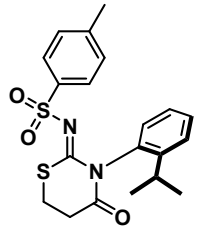
$^{77}Se\{^{1}H\}$, $CDCl_3$, 95 MHz





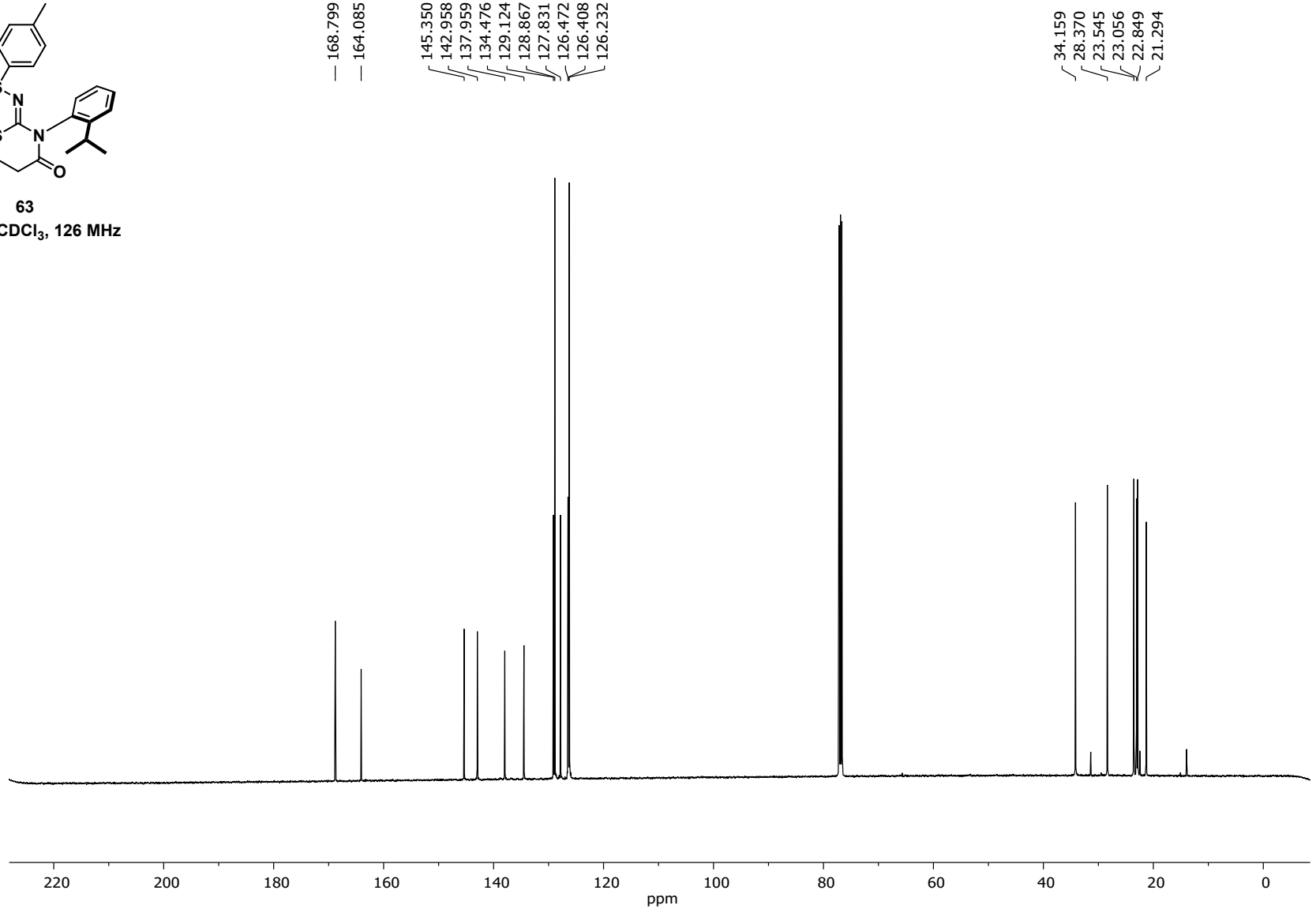
63

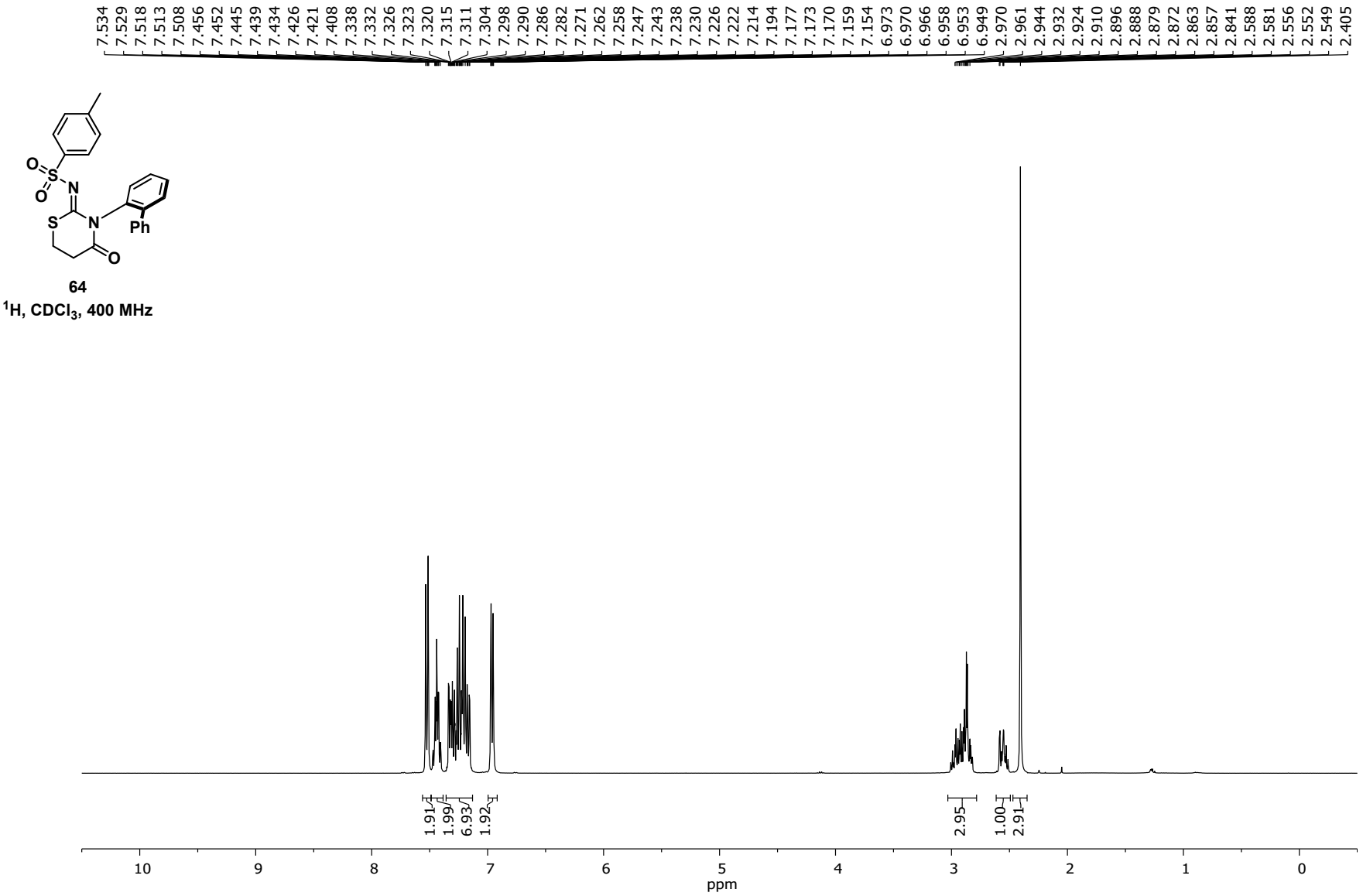
^{1}H, $CDCl_3$, 400 MHz



63

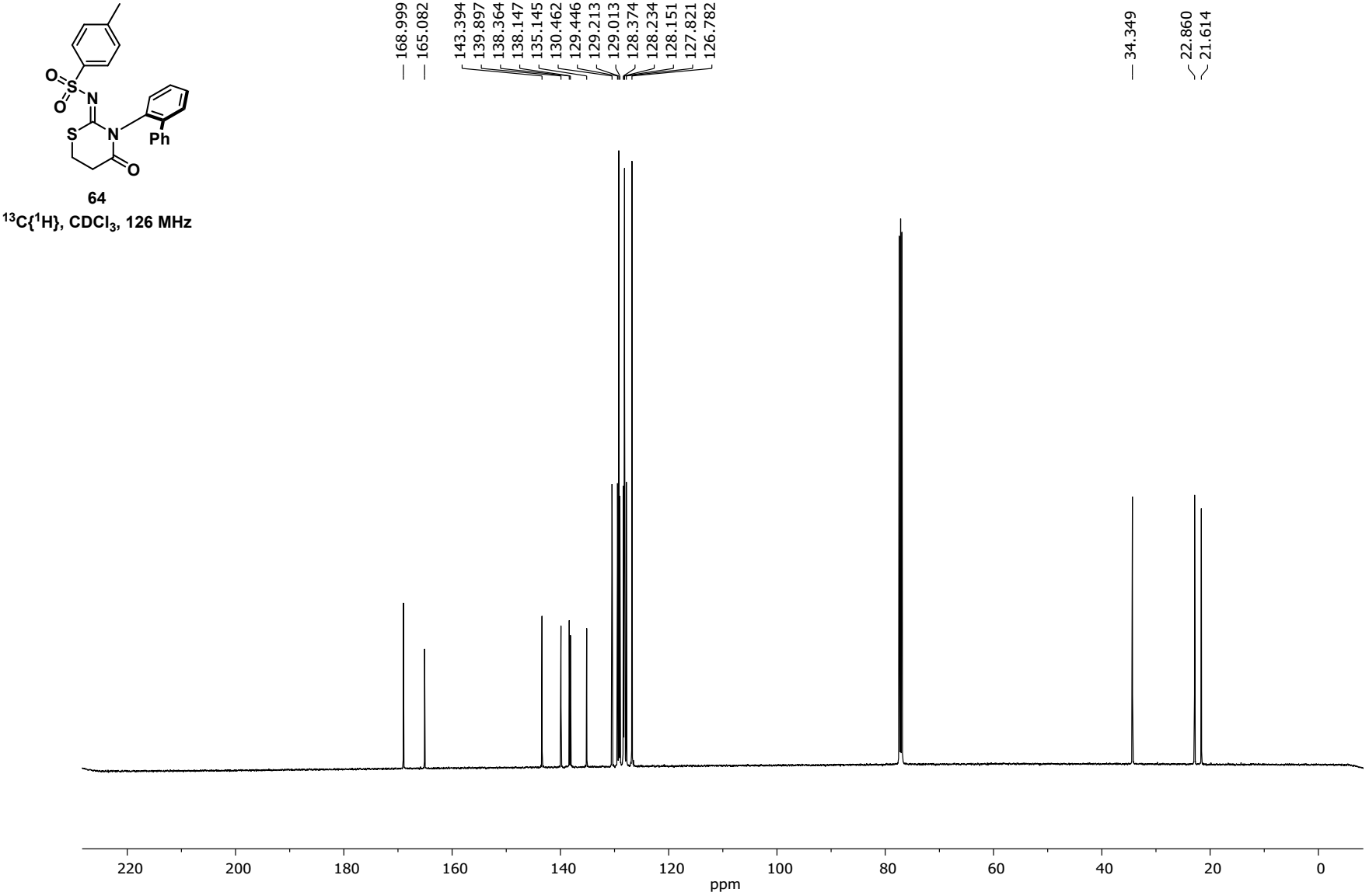
$^{13}C\{^{1}H\}$, $CDCl_3$, 126 MHz

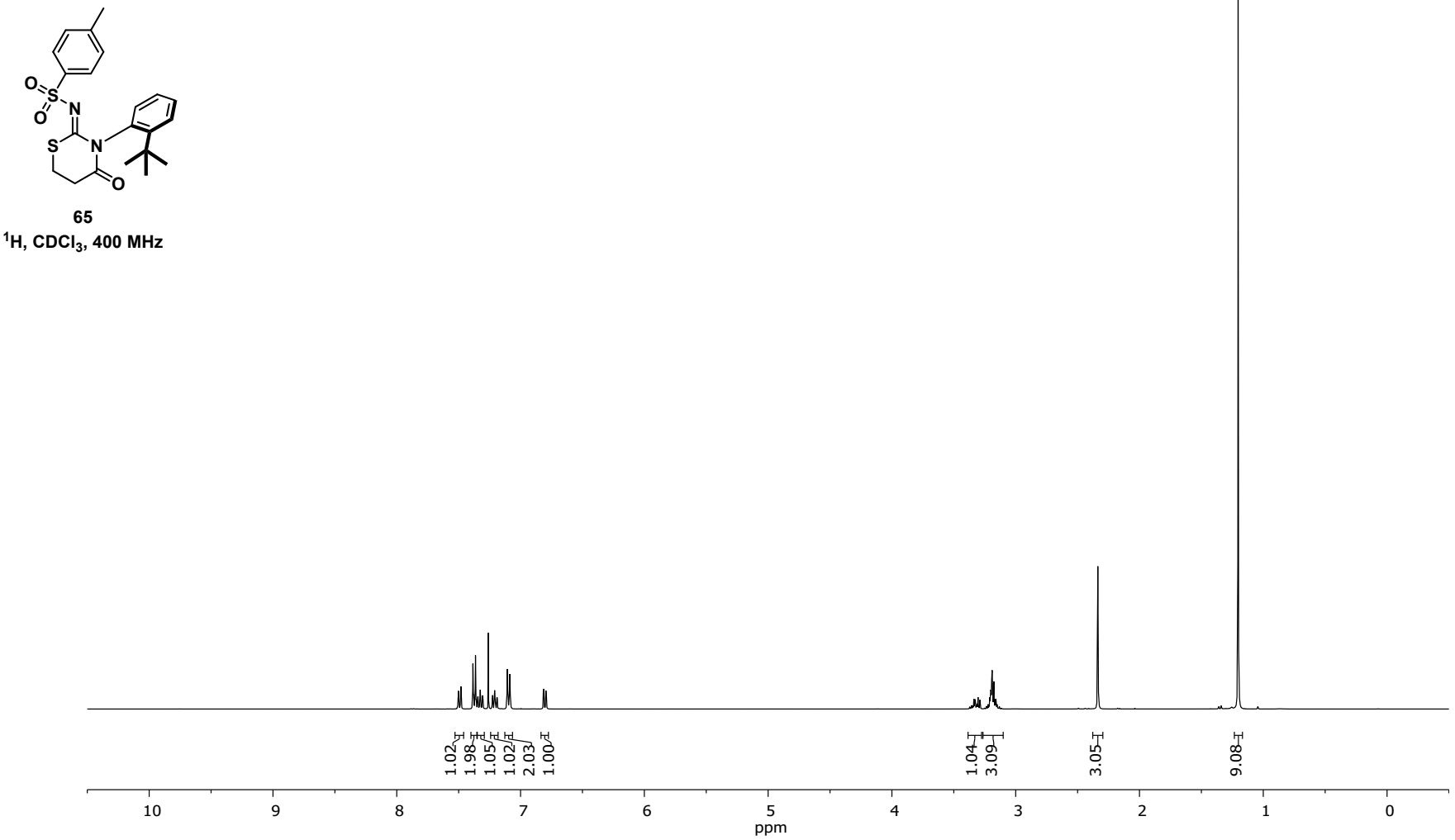




64

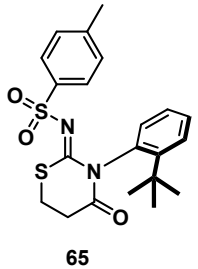
^{1}H, $CDCl_3$, 400 MHz


64
$^{13}C\{^{1}H\}$, $CDCl_3$, 126 MHz
168.999
165.082
143.394
139.897
138.364
138.147
135.145
130.462
129.446
129.213
129.013
128.374
128.234
128.151
127.821
126.782
34.349
22.860
21.614
220
200
180
160
140
120
100
80
60
40
20
0
ppm



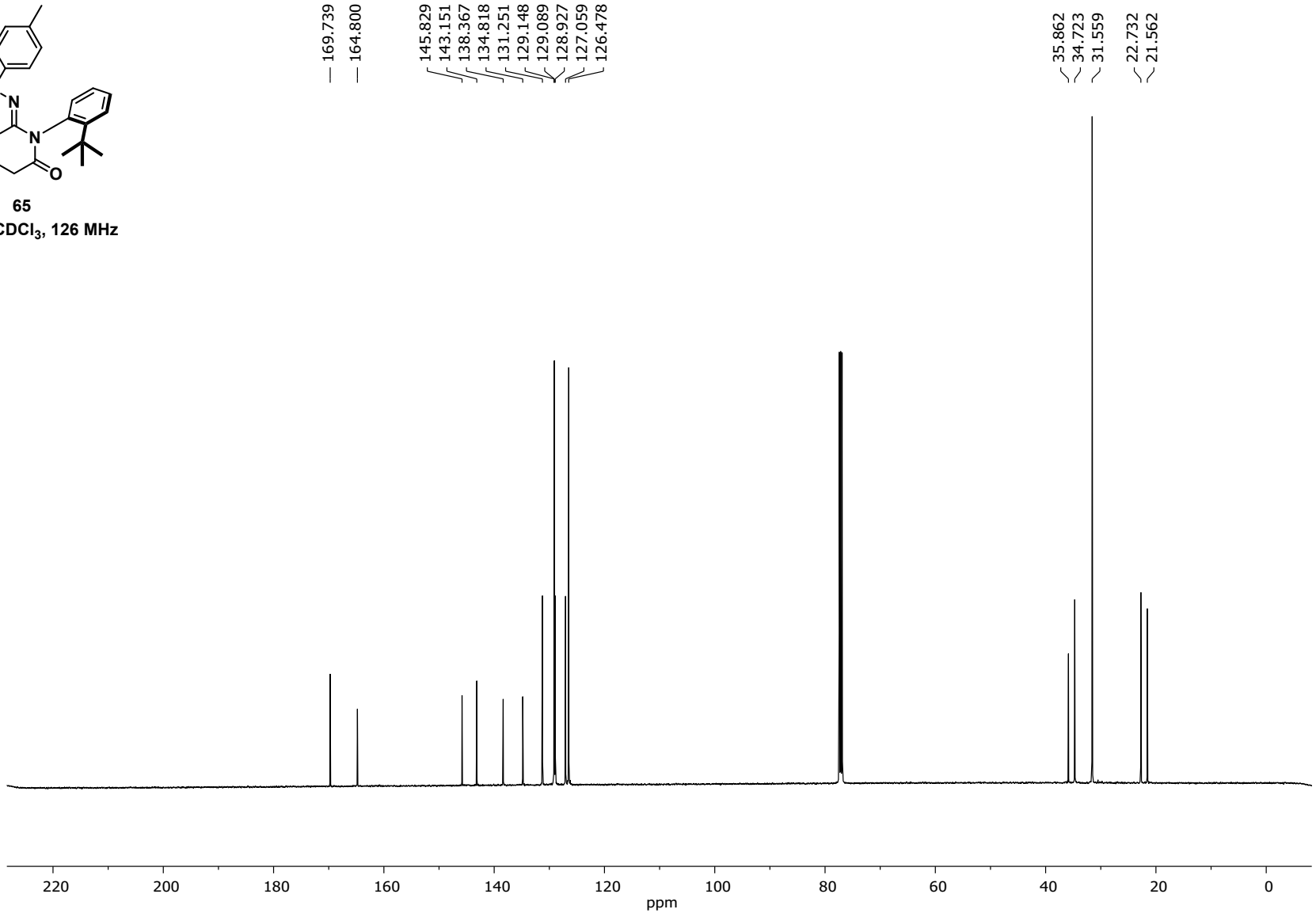
65

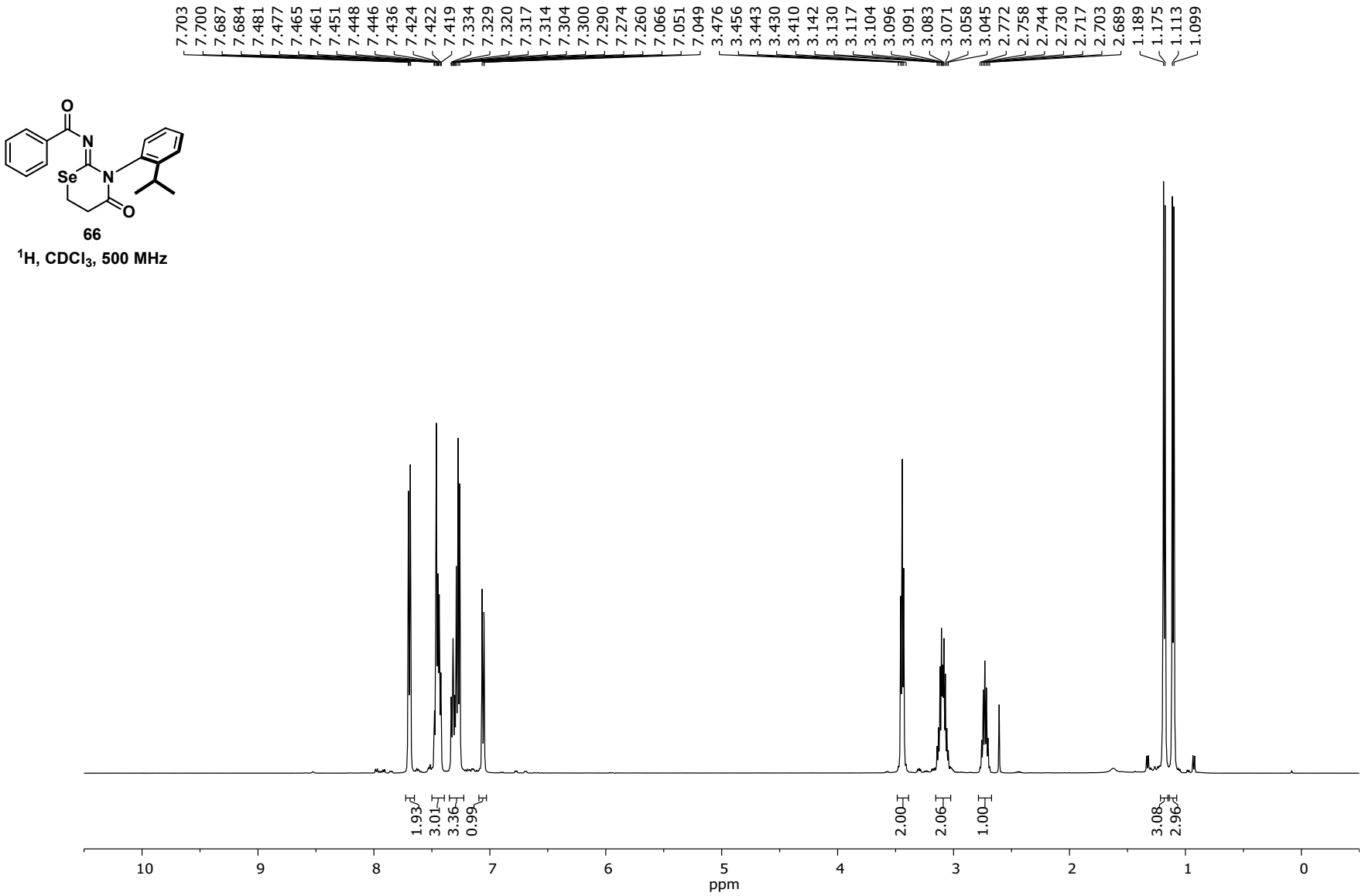
^{1}H, $CDCl_3$, 400 MHz

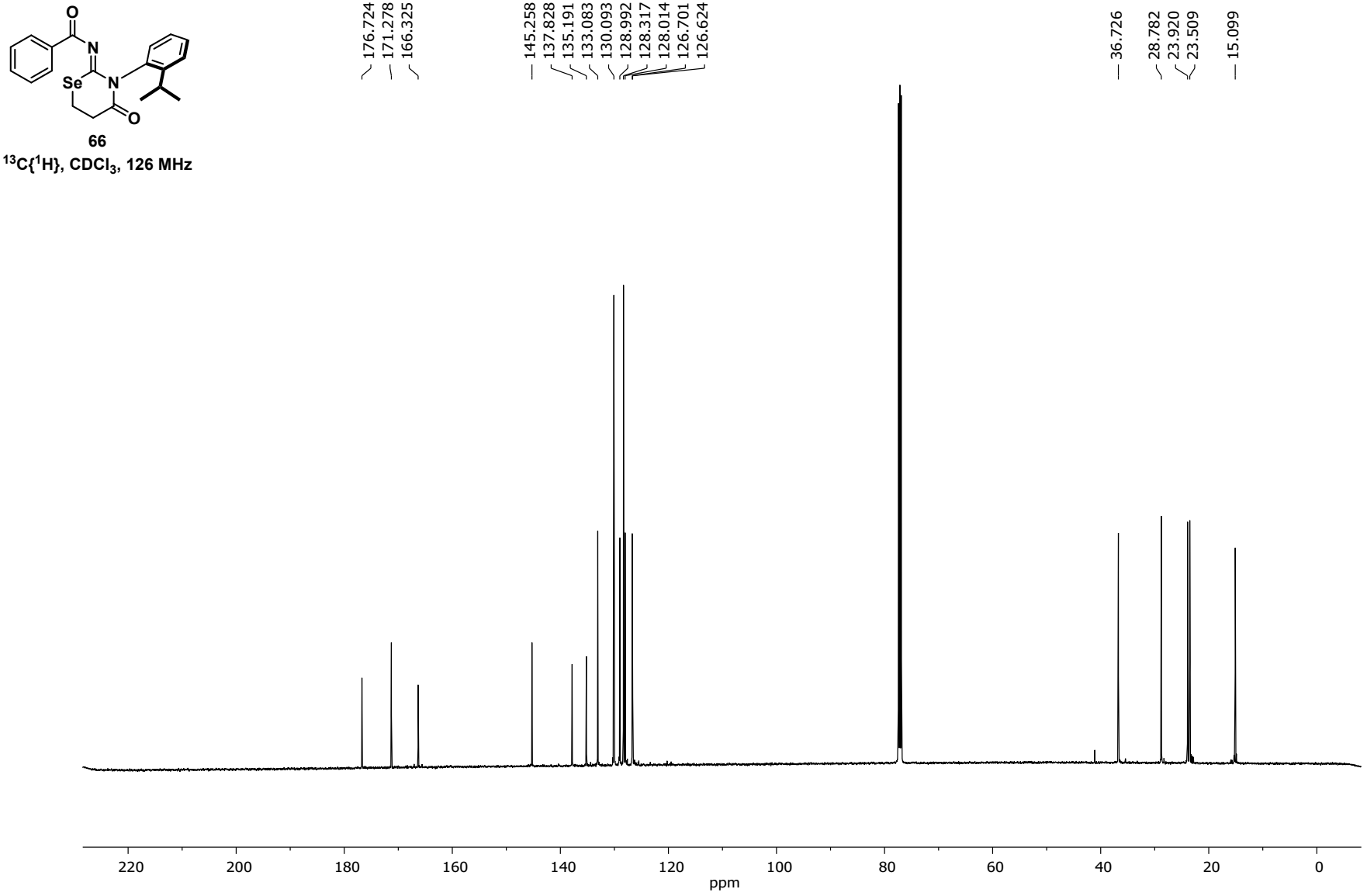


65

$^{13}C\{^{1}H\}$, $CDCl_3$, 126 MHz

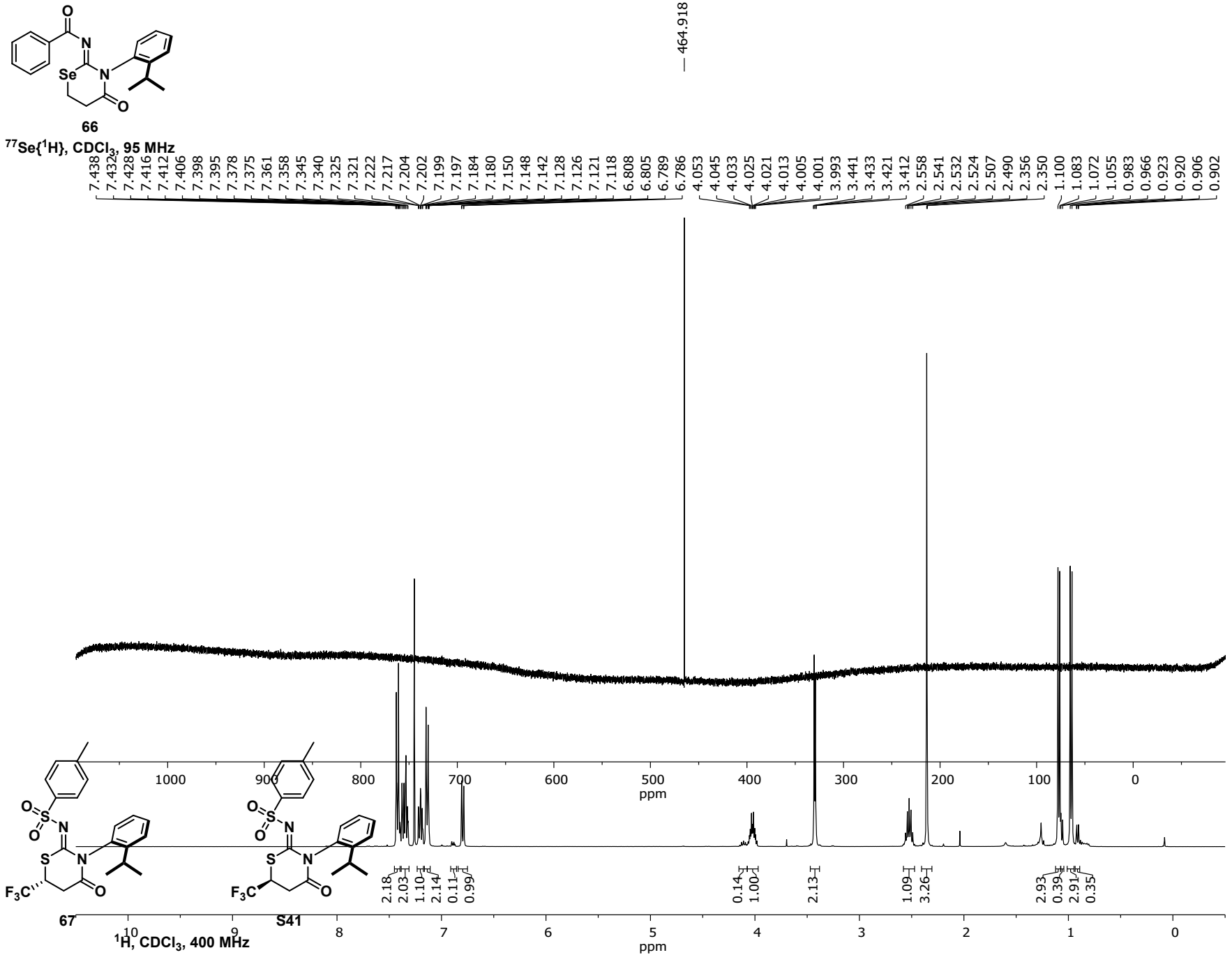


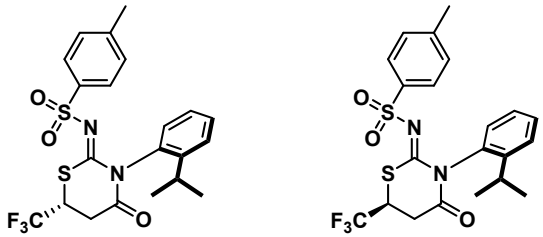

7.703
7.700
7.687
7.684
7.481
7.477
7.465
7.461
7.451
7.448
7.446
7.436
7.424
7.422
7.419
7.334
7.329
7.320
7.317
7.314
7.304
7.300
7.290
7.274
7.260
7.066
7.051
7.049
3.476
3.456
3.443
3.430
3.410
3.142
3.130
3.117
3.104
3.096
3.091
3.083
3.071
3.058
3.045
2.772
2.758
2.744
2.730
2.717
2.703
2.689
1.189
1.175
1.113
1.099
O
N
Se
N
O
66
1H, CDCl3, 500 MHz
1.93
3.01
3.36
0.99
2.00
2.06
1.00
3.08
2.96
10
9
8
7
6
5
4
3
2
1
0
ppm



66

$^{13}C\{^{1}H\}$, $CDCl_3$, 126 MHz

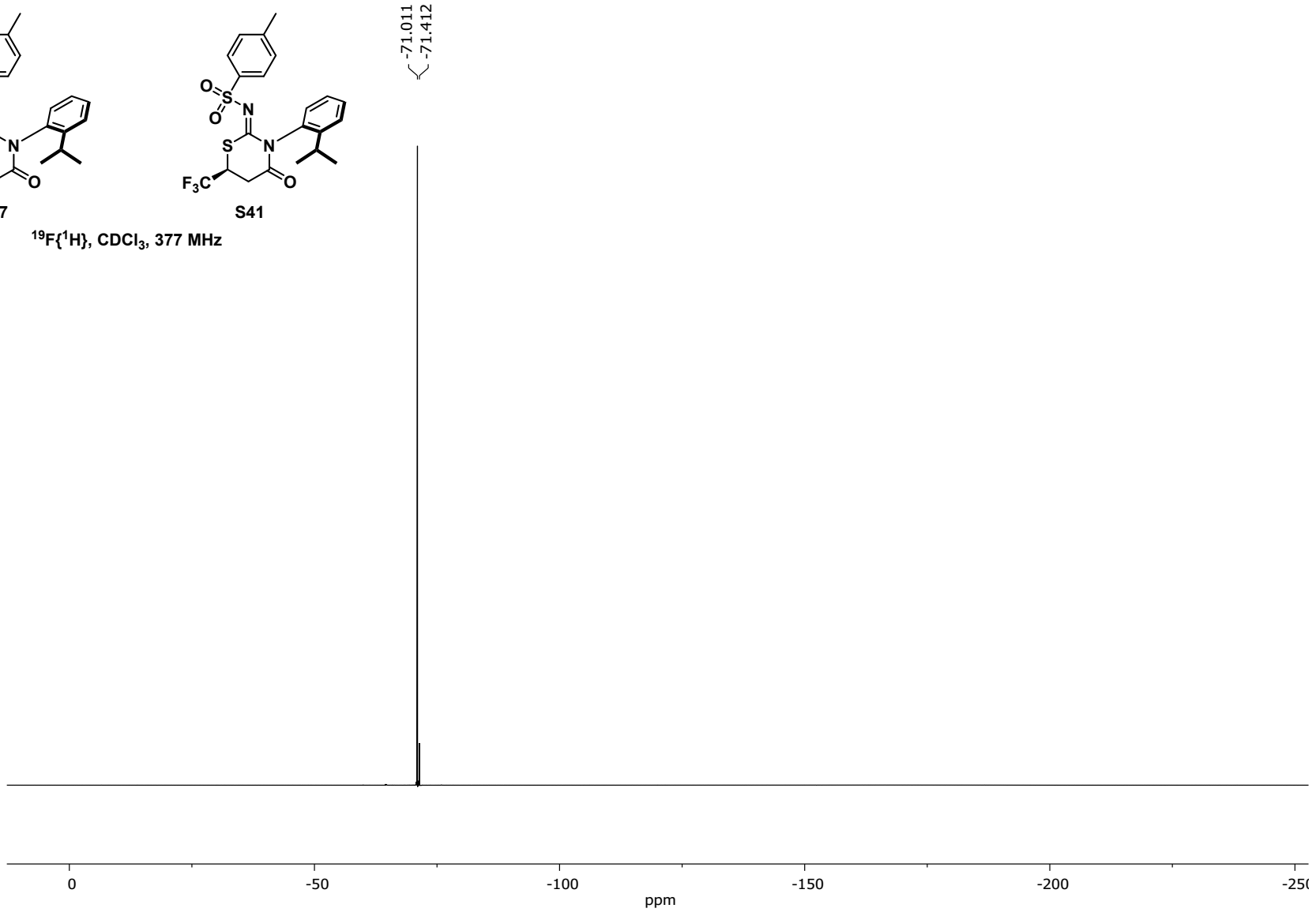

66
77Se{1H}, CDCl3, 95 MHz
464.918
7.438
7.432
7.428
7.416
7.412
7.406
7.398
7.395
7.378
7.375
7.361
7.358
7.345
7.340
7.325
7.321
7.222
7.217
7.204
7.202
7.199
7.197
7.184
7.180
7.150
7.148
7.142
7.128
7.126
7.121
7.118
6.808
6.805
6.789
6.786
4.053
4.045
4.033
4.025
4.021
4.013
4.005
4.001
3.993
3.441
3.433
3.421
3.412
2.558
2.541
2.532
2.524
2.507
2.490
2.356
2.350
1.100
1.083
1.072
1.055
0.983
0.966
0.923
0.920
0.906
0.902
1000
900
800
700
600
500
400
300
200
100
0
ppm
2.18
2.03
1.10
2.14
0.11
0.99
0.14
1.00
2.13
1.09
3.26
2.93
0.39
2.91
0.35
67
S41
10
9
8
7
6
5
4
3
2
1
0
ppm
1H, CDCl3, 400 MHz

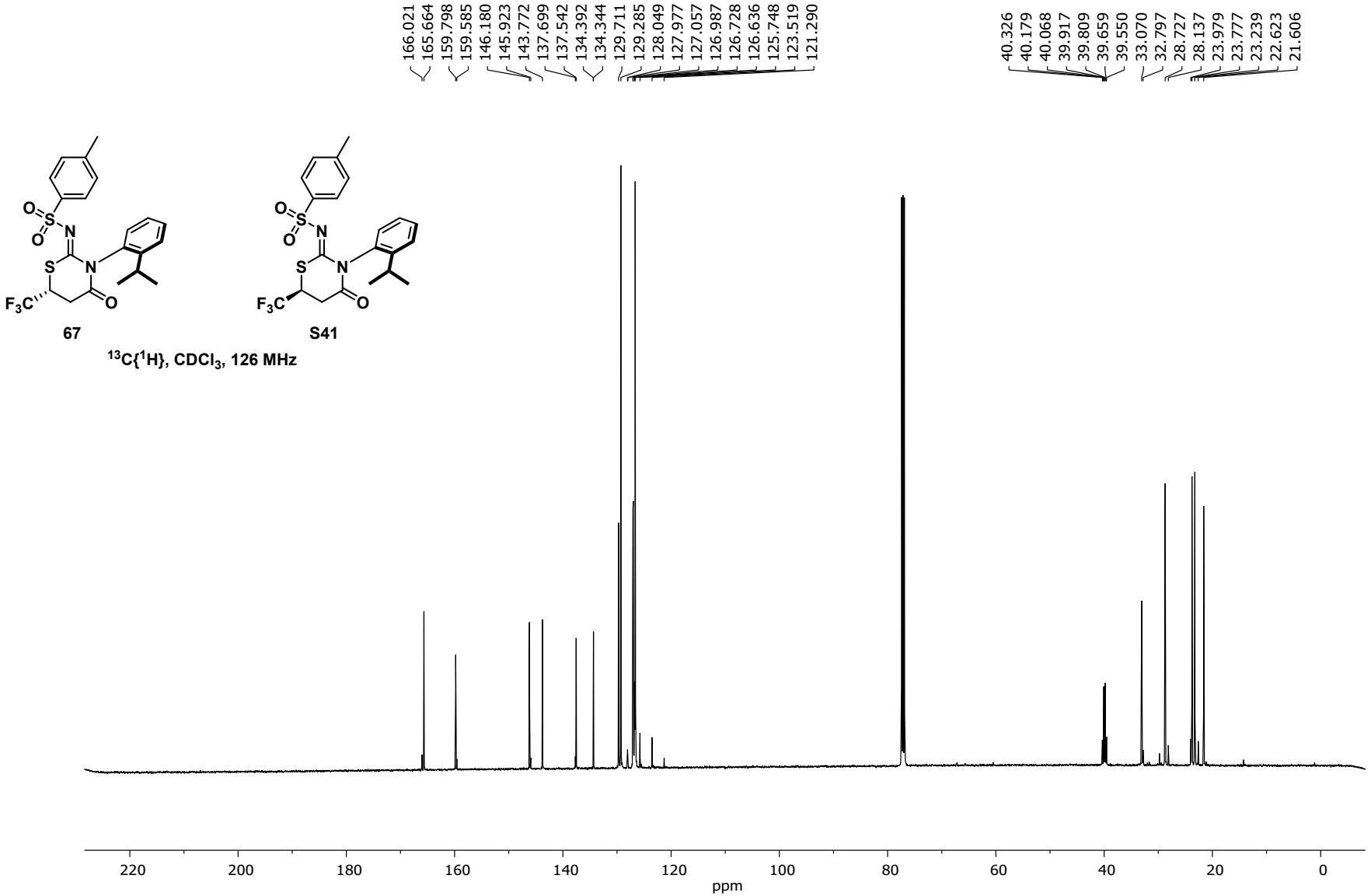


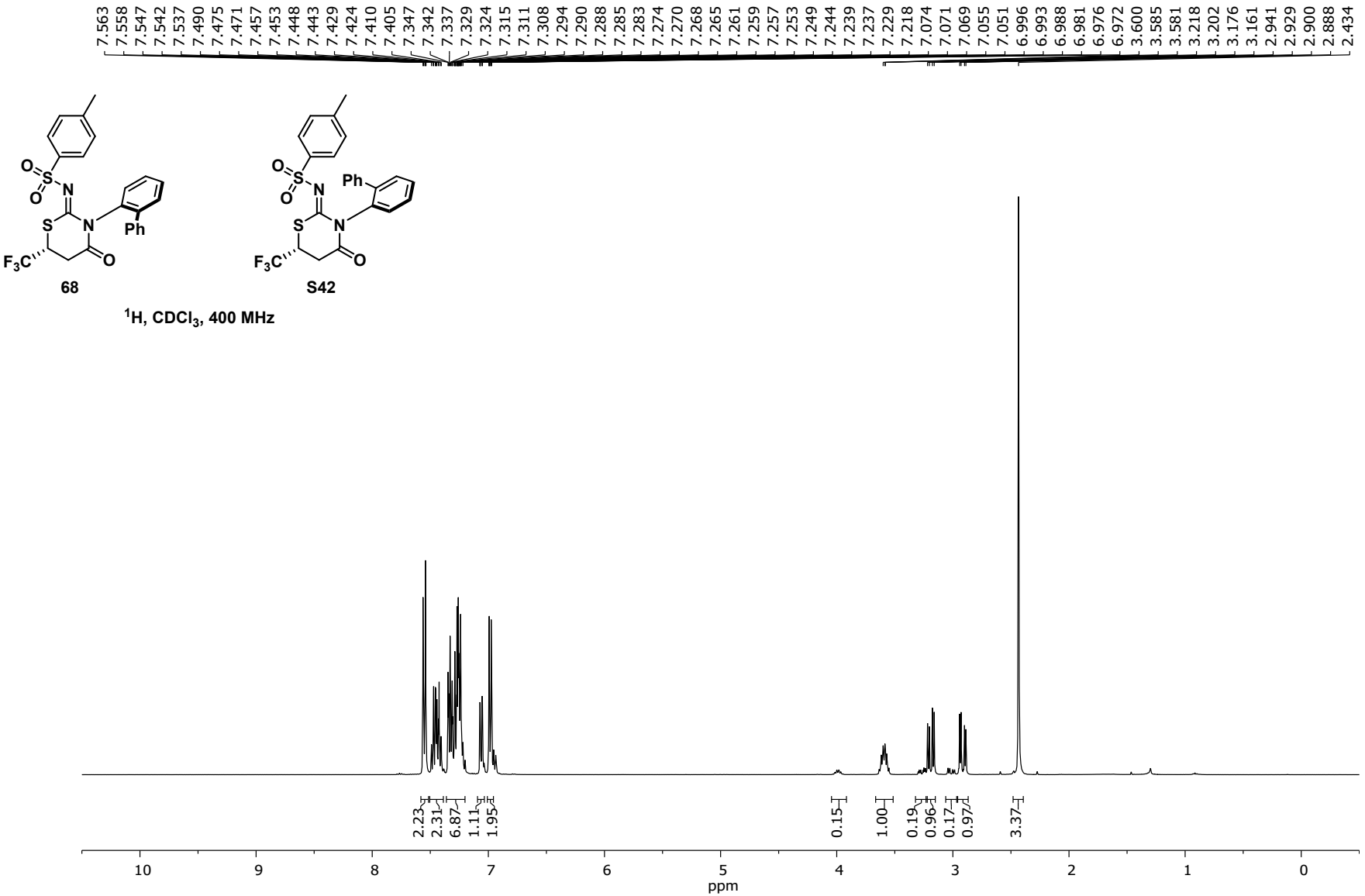
67

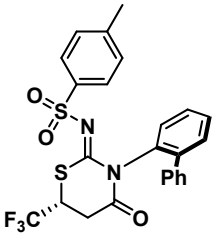
S41

$^{19}F\{^{1}H\}$, $CDCl_3$, 377 MHz

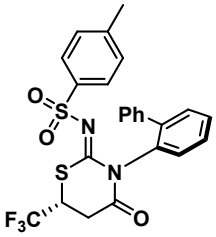



166.021
165.664
159.798
159.585
146.180
145.923
143.772
137.699
137.542
134.392
134.344
129.711
129.285
128.049
127.977
127.057
126.987
126.728
126.636
125.748
123.519
121.290
40.326
40.179
40.068
39.917
39.809
39.659
39.550
33.070
32.797
28.727
28.137
23.979
23.777
23.239
22.623
21.606
67
S41
$^{13}C\{^{1}H\}$, $CDCl_3$, 126 MHz
220
200
180
160
140
120
100
80
60
40
20
0
ppm


7.563
7.558
7.547
7.542
7.537
7.490
7.475
7.471
7.457
7.453
7.448
7.443
7.429
7.424
7.410
7.405
7.347
7.342
7.337
7.329
7.324
7.315
7.311
7.308
7.294
7.290
7.288
7.285
7.283
7.274
7.270
7.268
7.265
7.261
7.259
7.257
7.253
7.249
7.244
7.239
7.237
7.229
7.218
7.074
7.071
7.069
7.055
7.051
6.996
6.993
6.988
6.981
6.976
6.972
3.600
3.585
3.581
3.218
3.202
3.176
3.161
2.941
2.929
2.900
2.888
2.434
68
S42
1H, CDCl3, 400 MHz
2.23
2.31
6.87
1.11
1.95
0.15
1.00
0.19
0.96
0.17
0.97
3.37
10
9
8
7
6
5
4
3
2
1
0
ppm



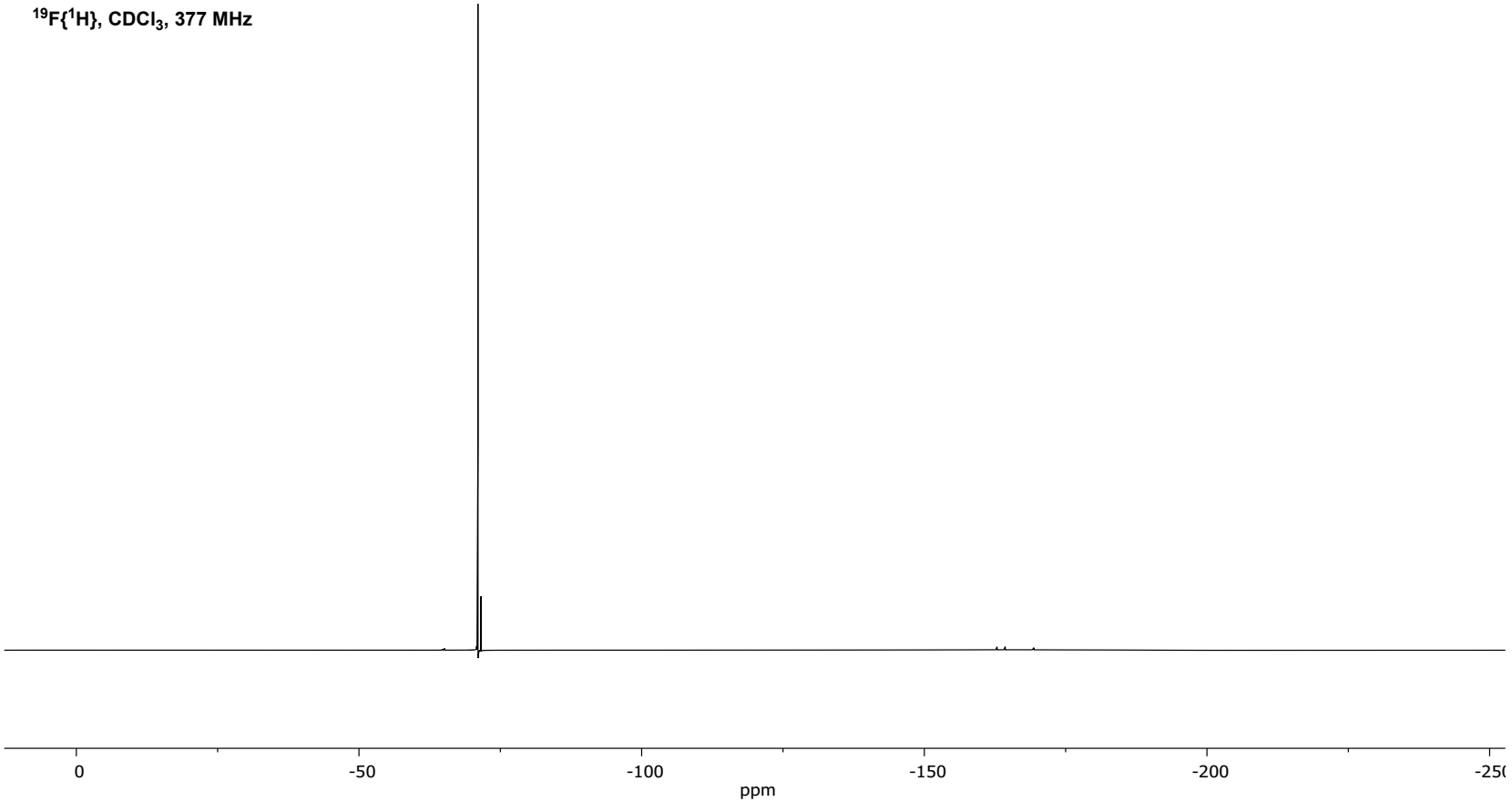
68

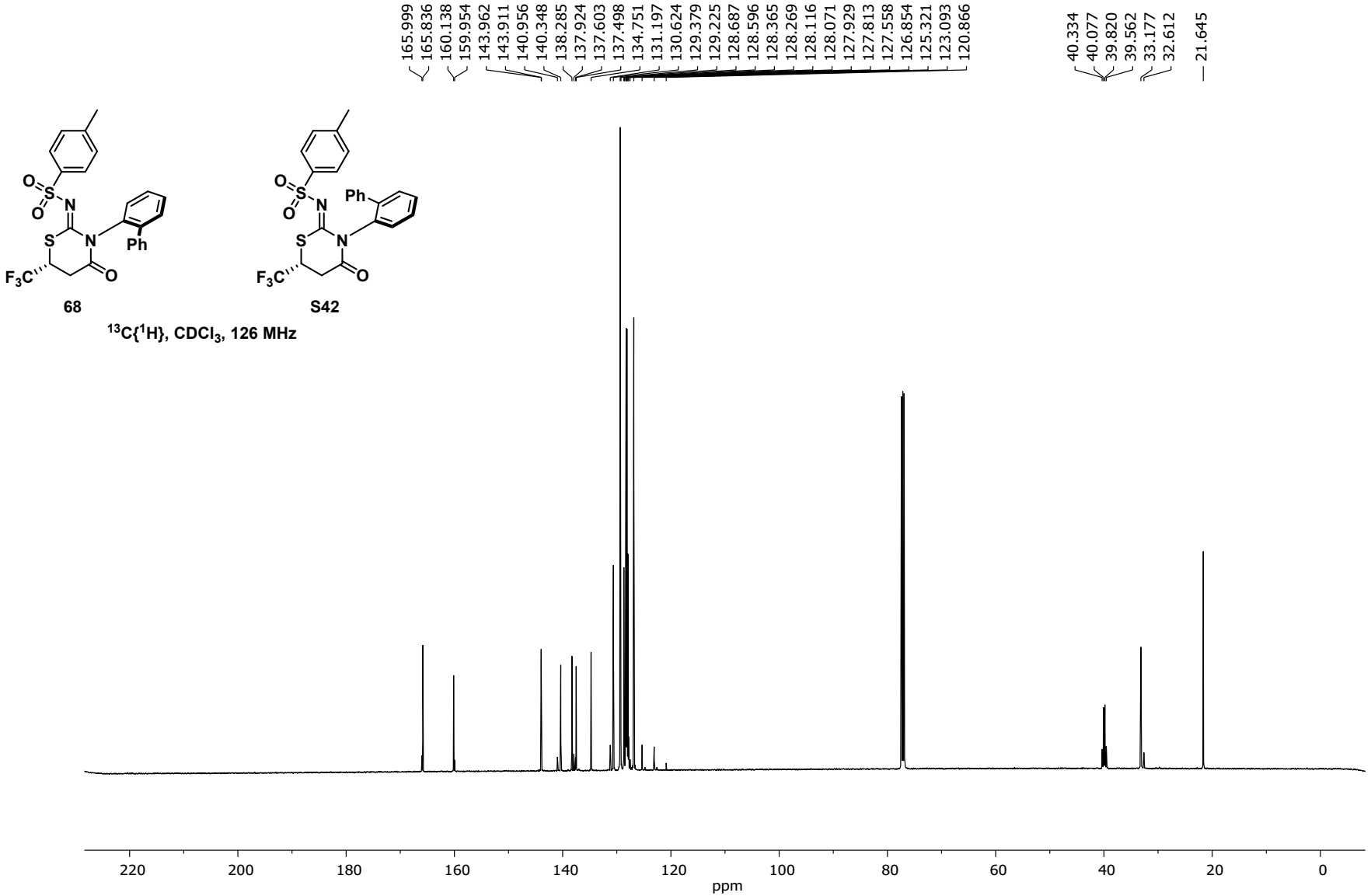


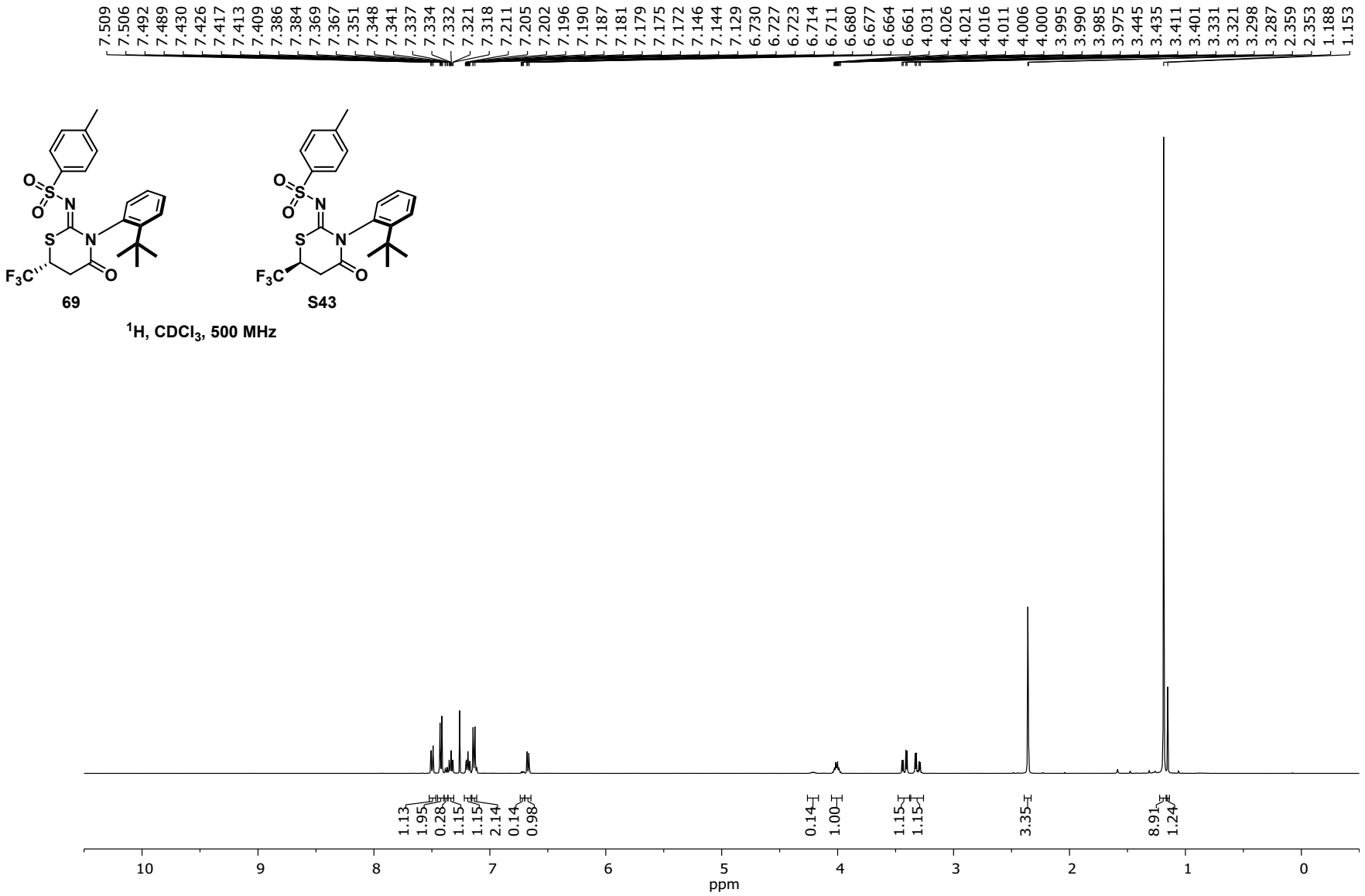
S42

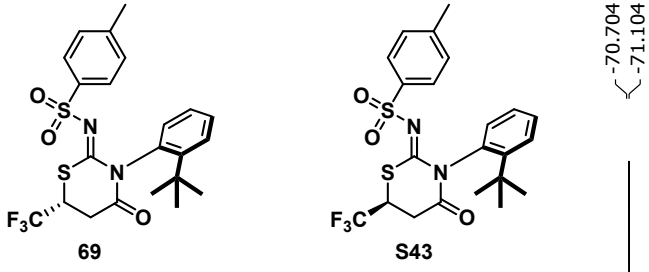
-71.043
-71.590

$^{19}F\{^{1}H\}$, $CDCl_3$, 377 MHz




165.999
165.836
160.138
159.954
143.962
143.911
140.956
140.348
138.285
137.924
137.603
137.498
134.751
131.197
130.624
129.379
129.225
128.687
128.596
128.365
128.269
128.116
128.071
127.929
127.813
127.558
126.854
125.321
123.093
120.866
40.334
40.077
39.820
39.562
33.177
32.612
21.645
Ph
Ph
68
S42
$^{13}C\{^{1}H\}$, $CDCl_3$, 126 MHz
220
200
180
160
140
120
100
80
60
40
20
0
ppm

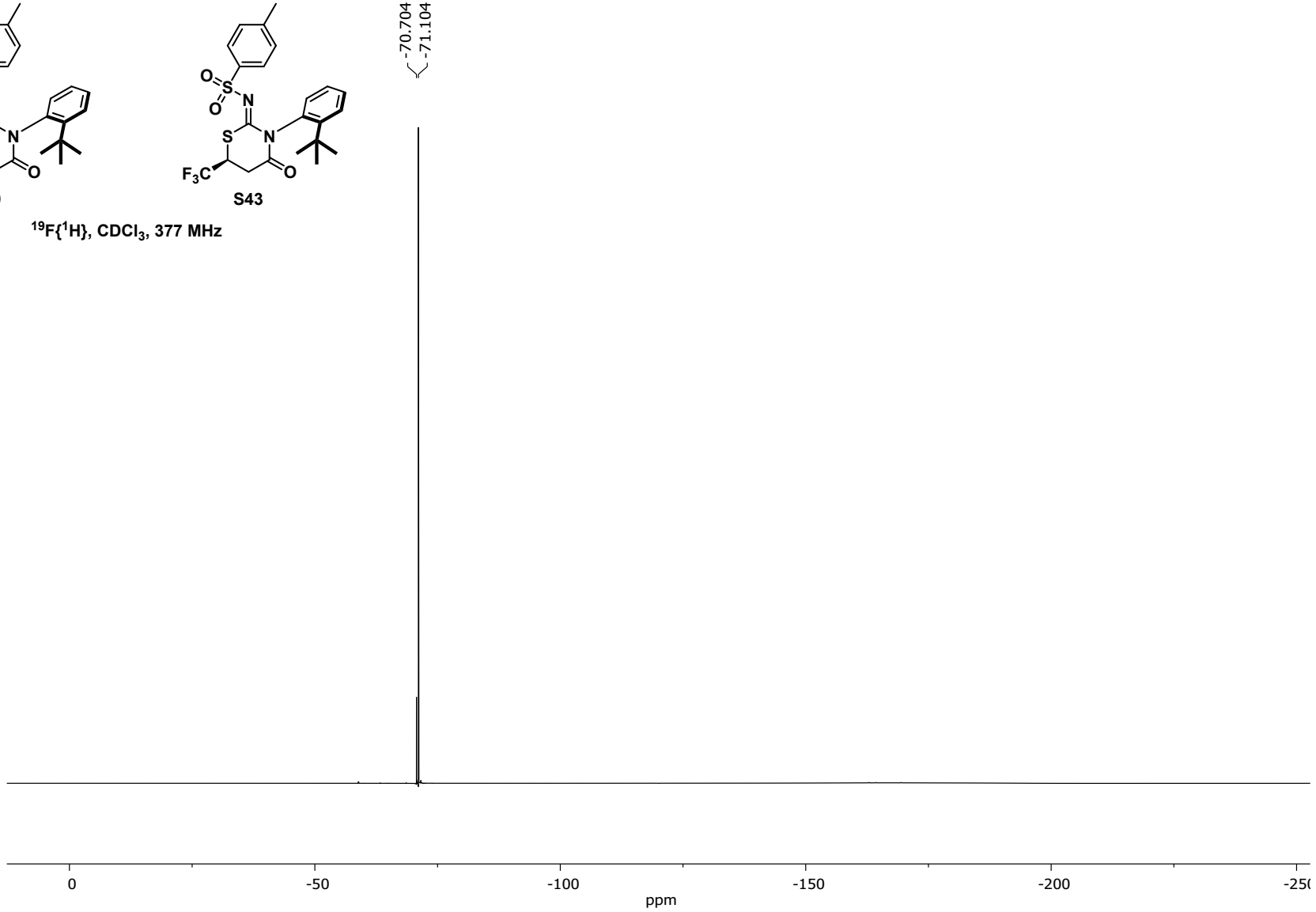

7.509
7.506
7.492
7.489
7.430
7.426
7.417
7.413
7.409
7.386
7.384
7.369
7.367
7.351
7.348
7.341
7.337
7.334
7.332
7.321
7.318
7.211
7.205
7.202
7.196
7.190
7.187
7.181
7.179
7.175
7.172
7.146
7.144
7.129
6.730
6.727
6.723
6.714
6.711
6.680
6.677
6.664
6.661
4.031
4.026
4.021
4.016
4.011
4.006
4.000
3.995
3.990
3.985
3.975
3.445
3.435
3.411
3.401
3.331
3.321
3.298
3.287
2.359
2.353
1.188
1.153
69
S43
1H, CDCl3, 500 MHz
1.13
1.95
0.28
1.15
1.15
2.14
0.14
0.98
0.14
1.00
1.15
1.15
3.35
8.91
1.24
10
9
8
7
6
5
4
3
2
1
0
ppm

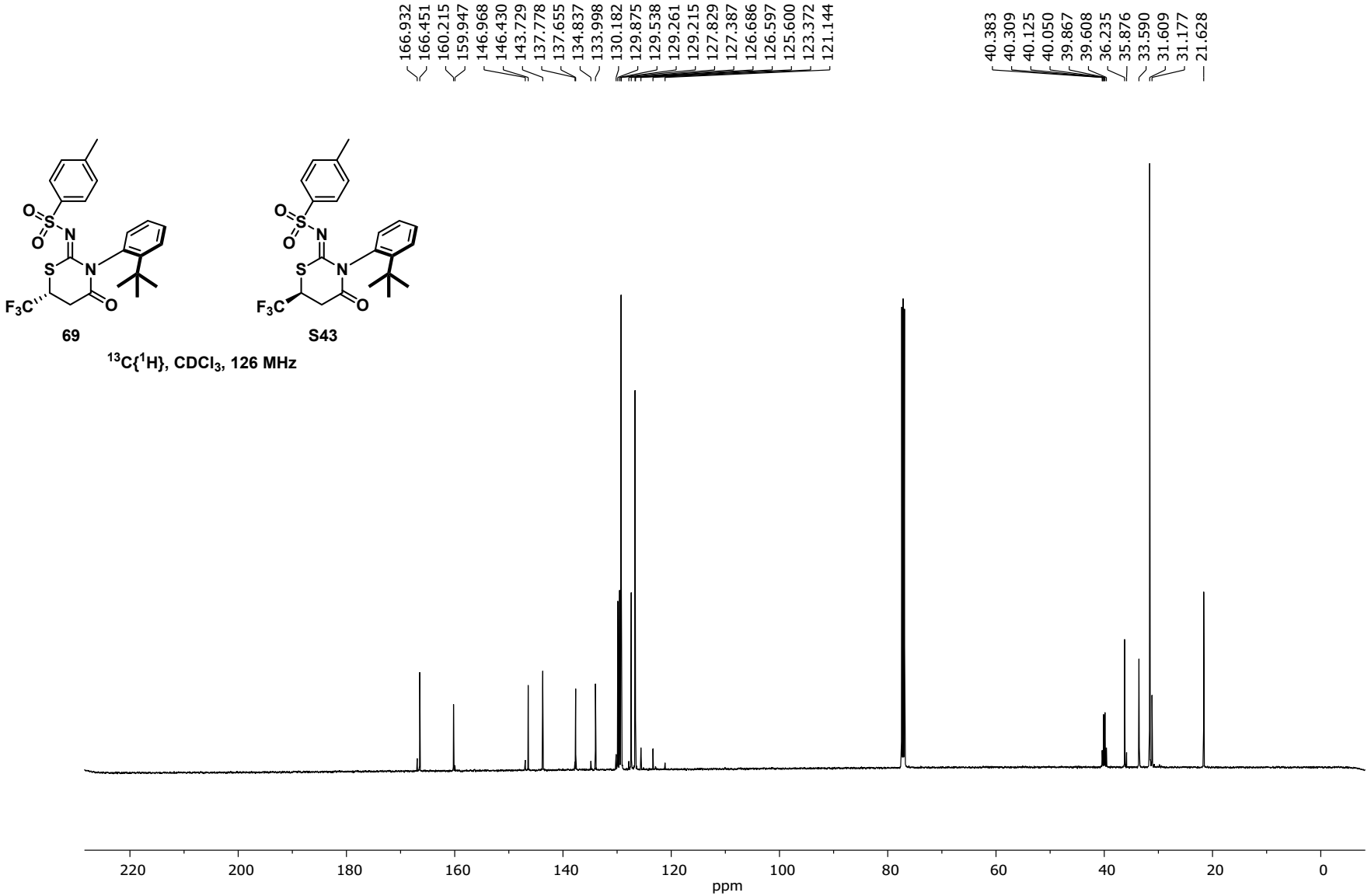


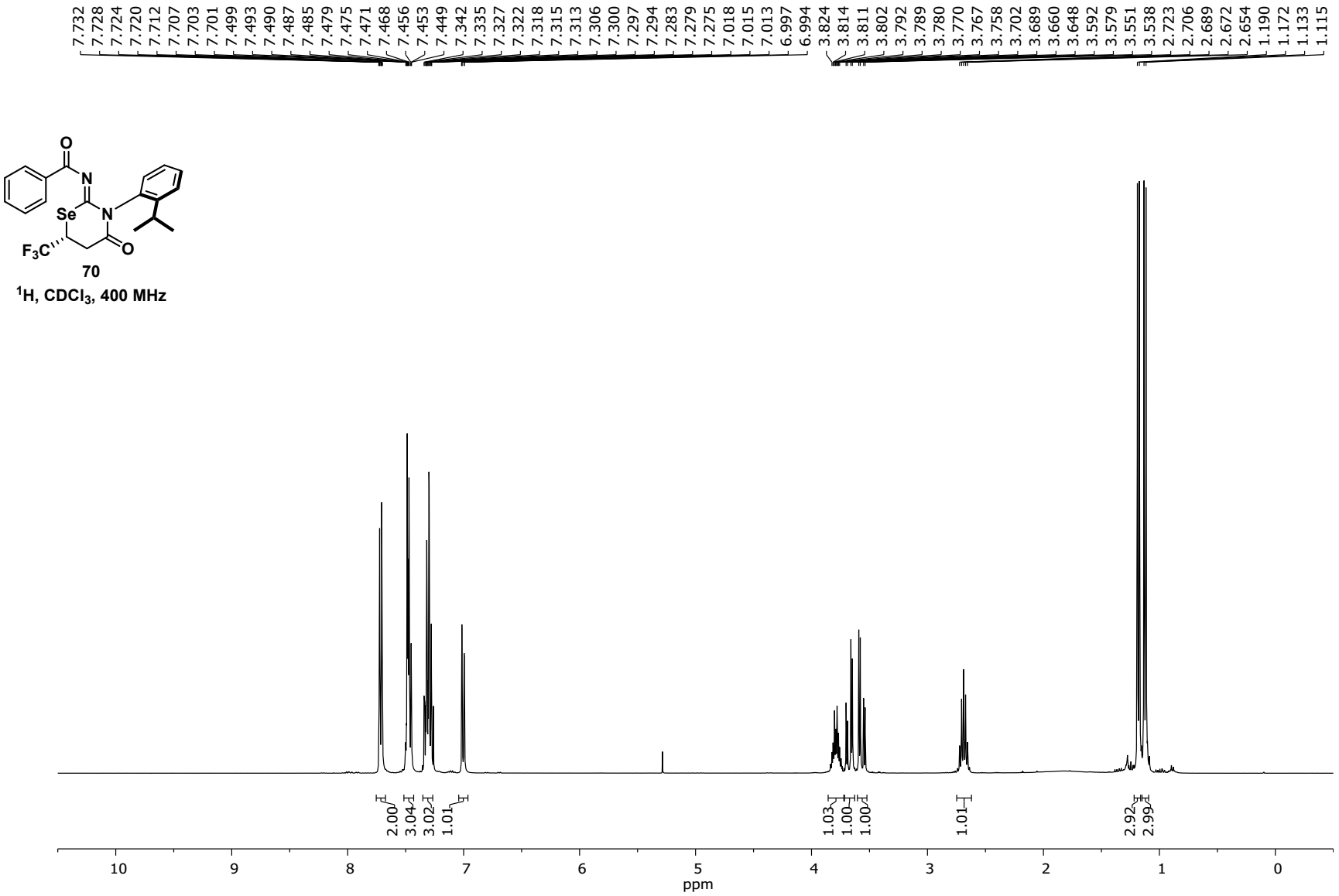
69

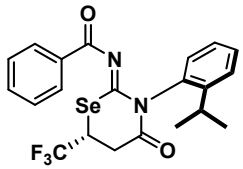
S43

$^{19}F\{^{1}H\}$, $CDCl_3$, 377 MHz



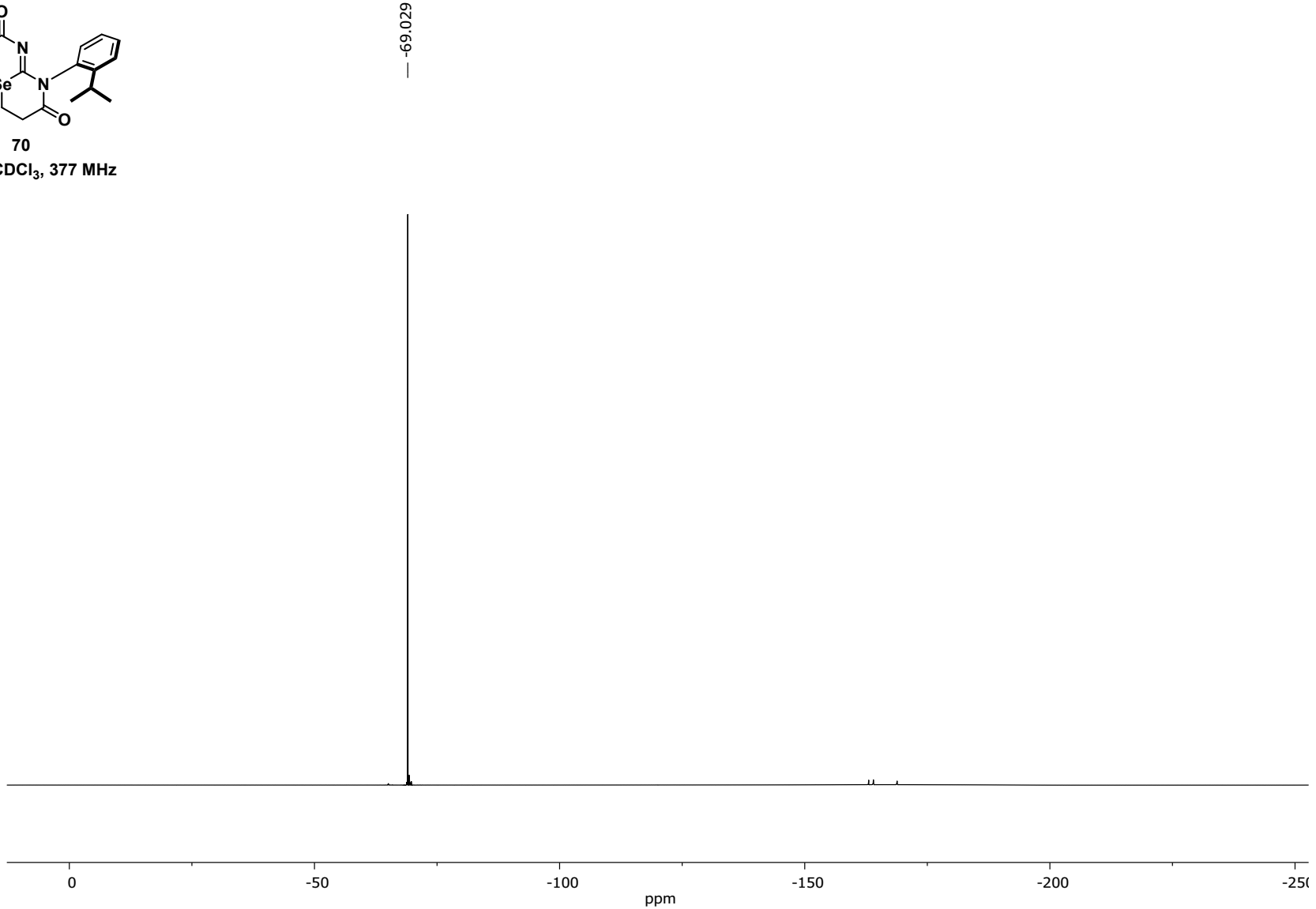

166.932
166.451
160.215
159.947
146.968
146.430
143.729
137.778
137.655
134.837
133.998
130.182
129.875
129.538
129.261
129.215
127.829
127.387
126.686
126.597
125.600
123.372
121.144
40.383
40.309
40.125
40.050
39.867
39.608
36.235
35.876
33.590
31.609
31.177
21.628
69
S43
13C{1H}, CDCl3, 126 MHz
220
200
180
160
140
120
100
80
60
40
20
0
ppm

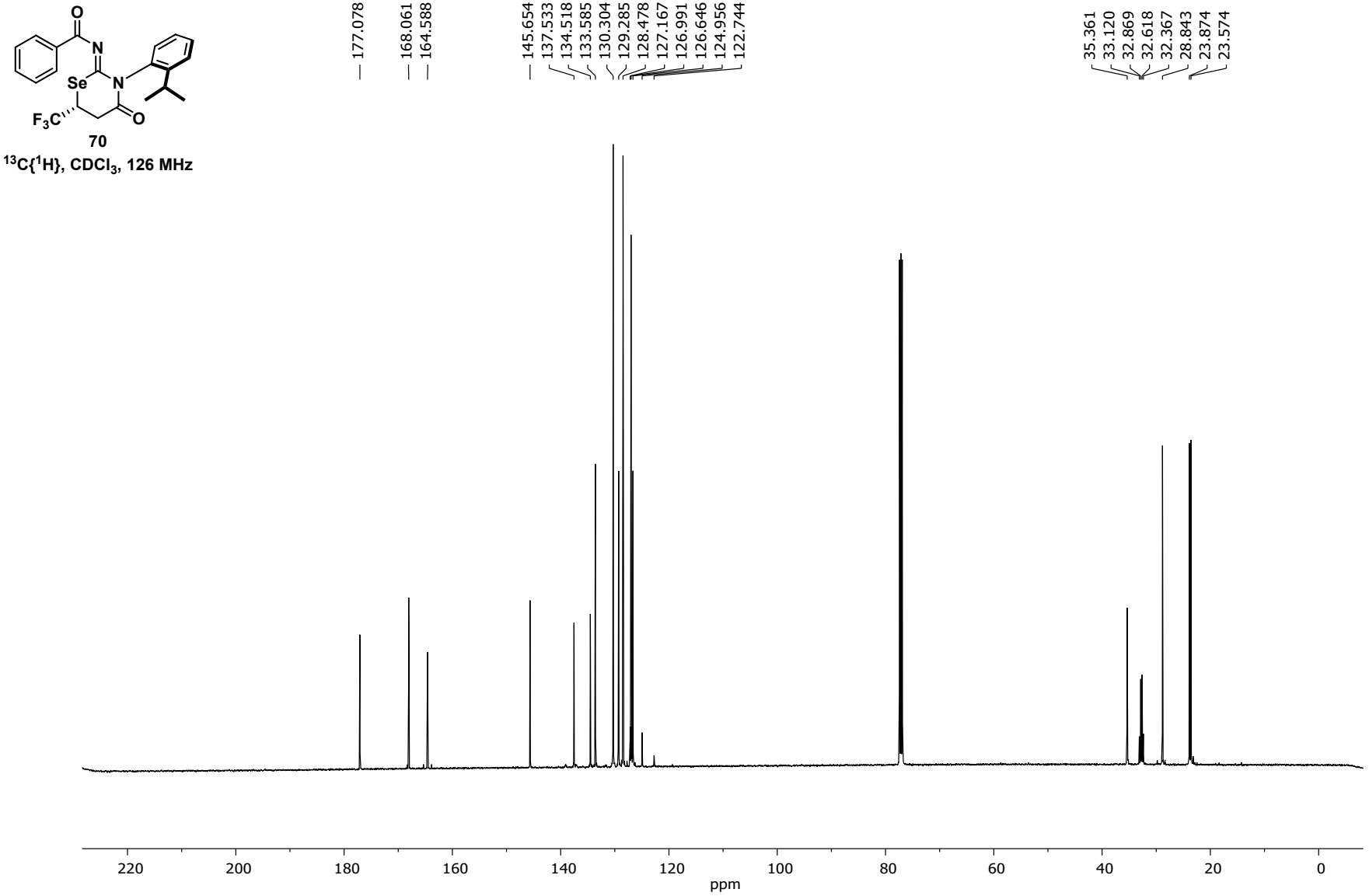

7.732
7.728
7.724
7.720
7.712
7.707
7.703
7.701
7.499
7.493
7.490
7.487
7.485
7.479
7.475
7.471
7.468
7.456
7.453
7.449
7.342
7.335
7.327
7.322
7.318
7.315
7.313
7.306
7.300
7.297
7.294
7.283
7.279
7.275
7.018
7.015
7.013
6.997
6.994
3.824
3.814
3.811
3.802
3.792
3.789
3.780
3.770
3.767
3.758
3.702
3.689
3.660
3.648
3.592
3.579
3.551
3.538
2.723
2.706
2.689
2.672
2.654
1.190
1.172
1.133
1.115
O
N
Se
N
O
F3C
70
1H, CDCl3, 400 MHz
2.00
3.04
3.02
1.01
1.03
1.00
1.00
1.01
2.92
2.99
10
9
8
7
6
5
4
3
2
1
0
ppm



70

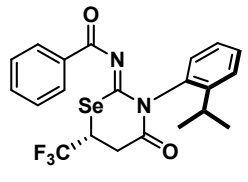
$^{19}F\{^{1}H\}$, $CDCl_3$, 377 MHz





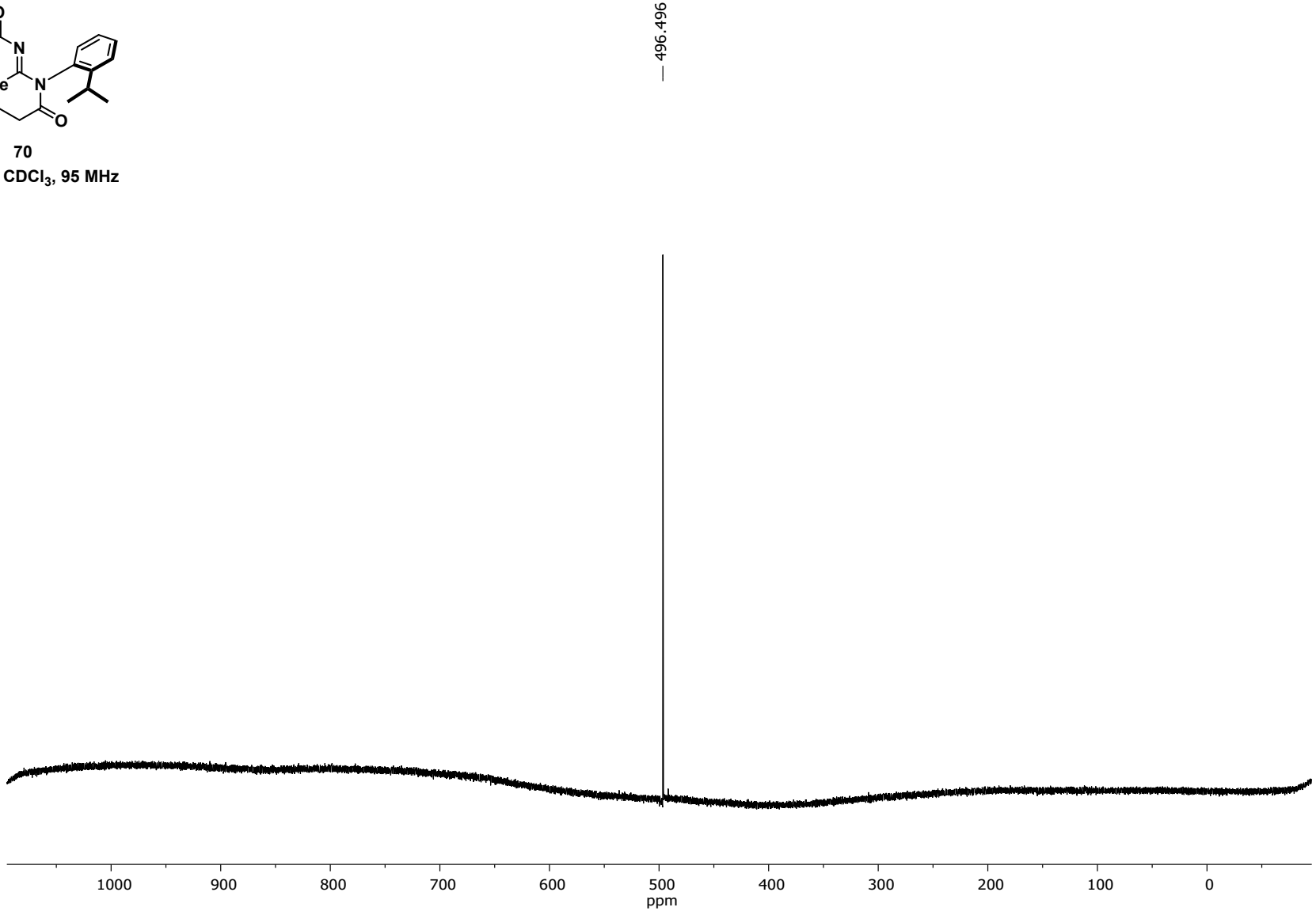
70

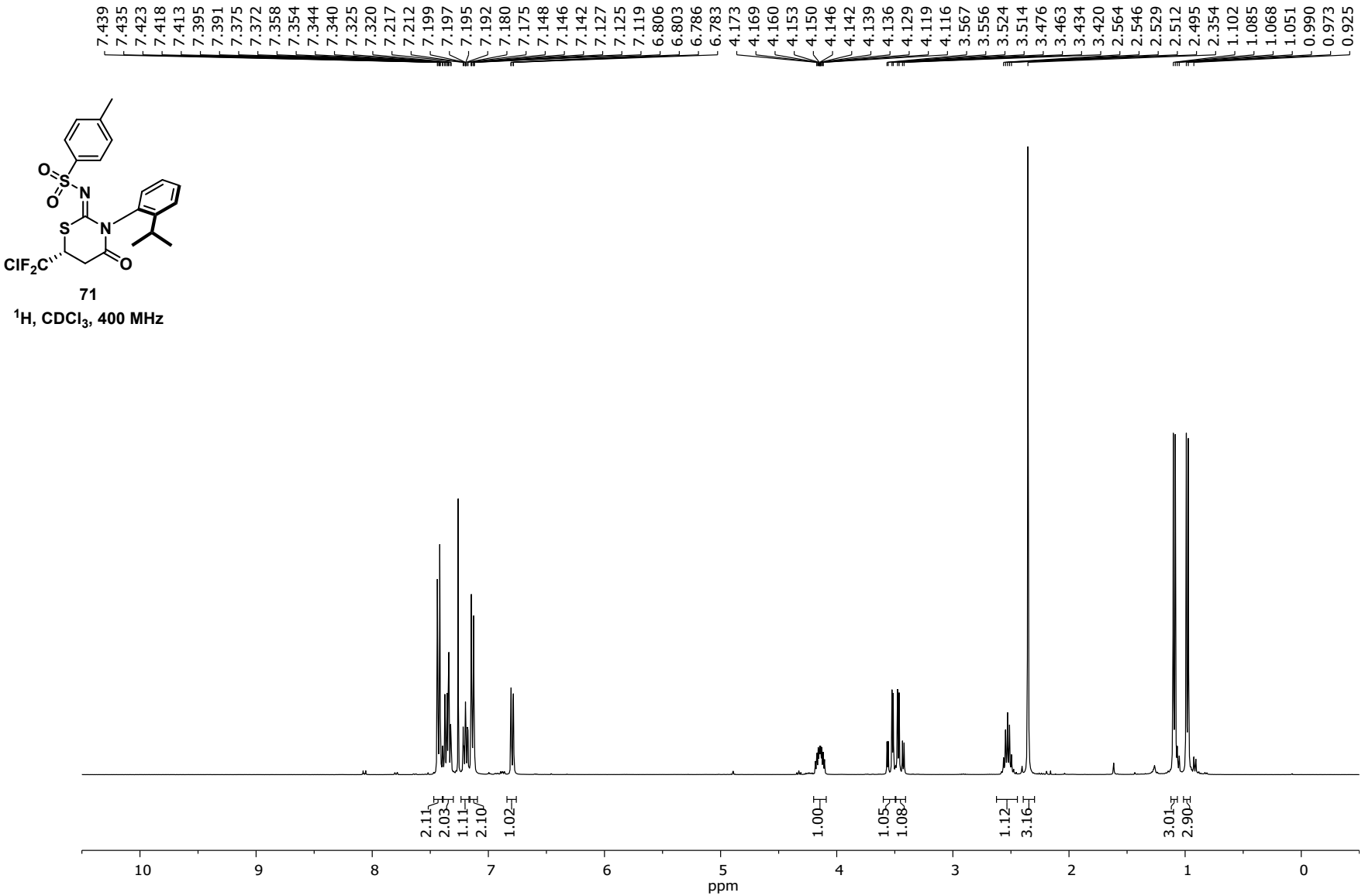
$^{13}C\{^{1}H\}$, $CDCl_3$, 126 MHz

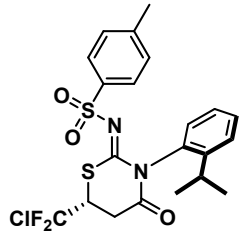


70

$^{77}Se\{^{1}H\}$, $CDCl_3$, 95 MHz

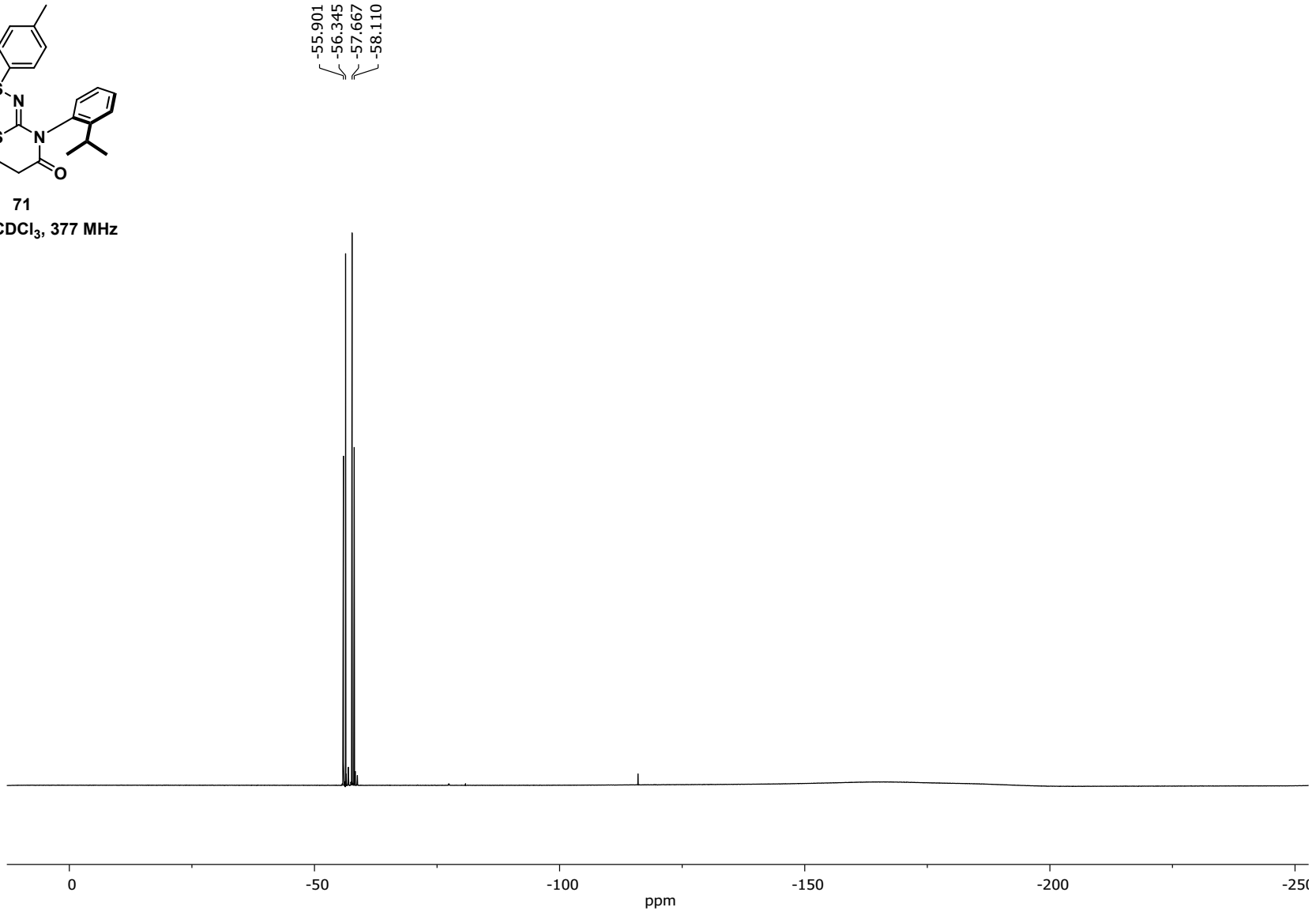


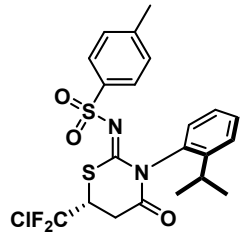

7.439
7.435
7.423
7.418
7.413
7.395
7.391
7.375
7.372
7.358
7.354
7.344
7.340
7.325
7.320
7.217
7.212
7.199
7.197
7.195
7.192
7.180
7.175
7.148
7.146
7.142
7.127
7.125
7.119
6.806
6.803
6.786
6.783
4.173
4.169
4.160
4.153
4.150
4.146
4.142
4.139
4.136
4.129
4.119
4.116
3.567
3.556
3.524
3.514
3.476
3.463
3.434
3.420
2.564
2.546
2.529
2.512
2.495
2.354
1.102
1.085
1.068
1.051
0.990
0.973
0.925
O
S
O
N
S
N
O
ClF2C
71
1H, CDCl3, 400 MHz
2.11
2.03
1.11
2.10
1.02
1.00
1.05
1.08
1.12
3.16
3.01
2.90
10
9
8
7
6
5
4
3
2
1
0
ppm



71

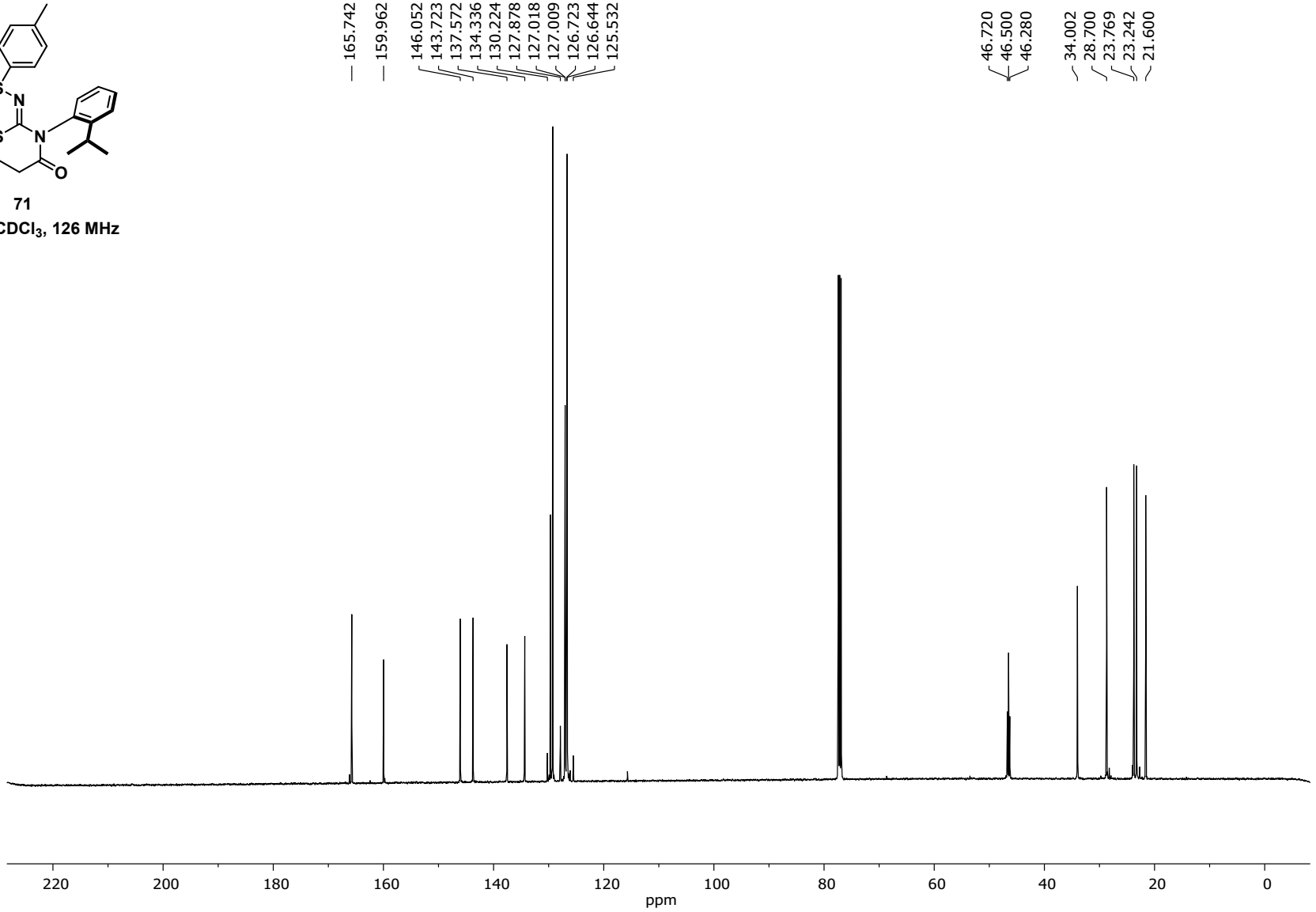
$^{19}F\{^{1}H\}$, $CDCl_3$, 377 MHz

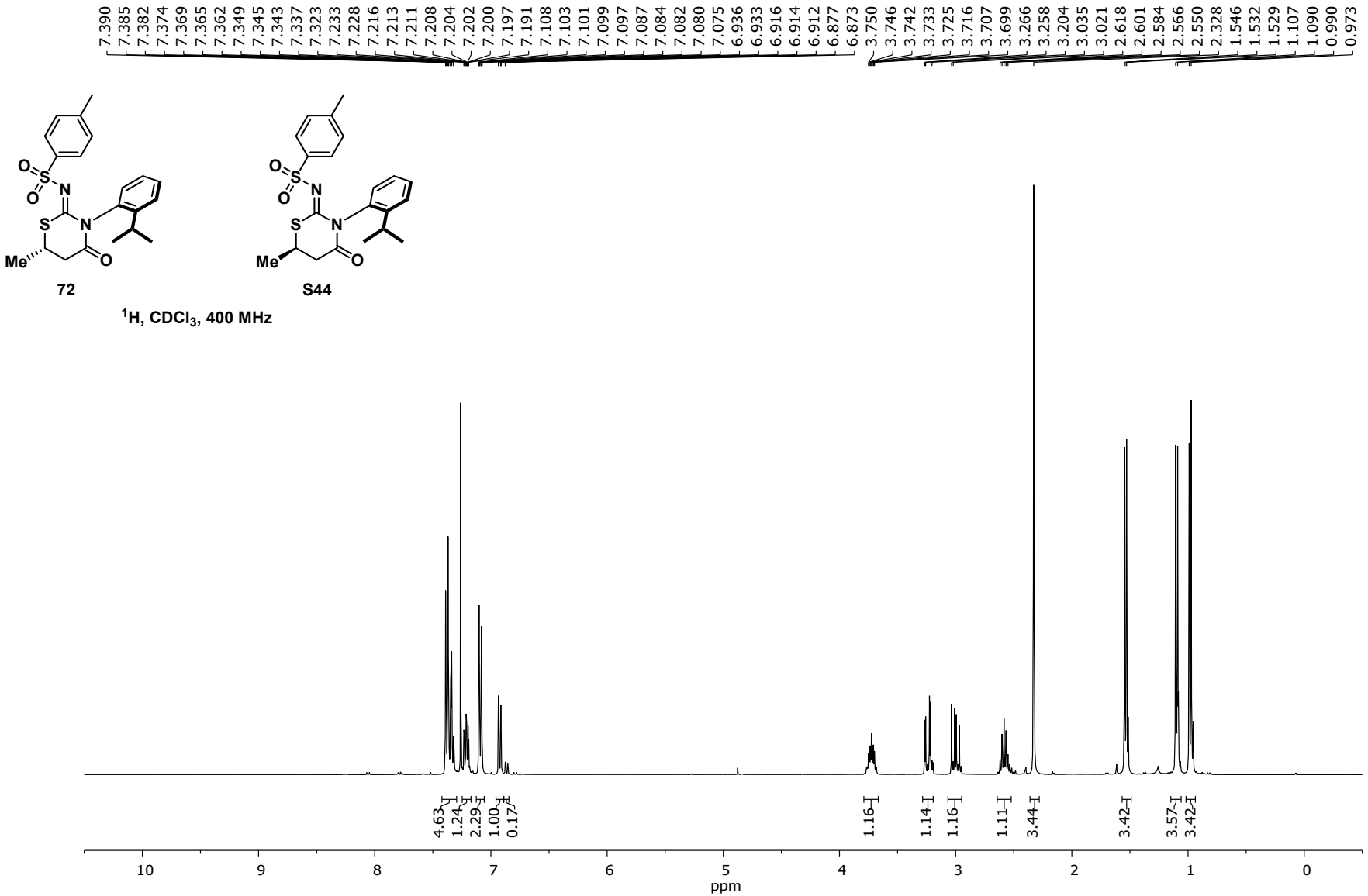


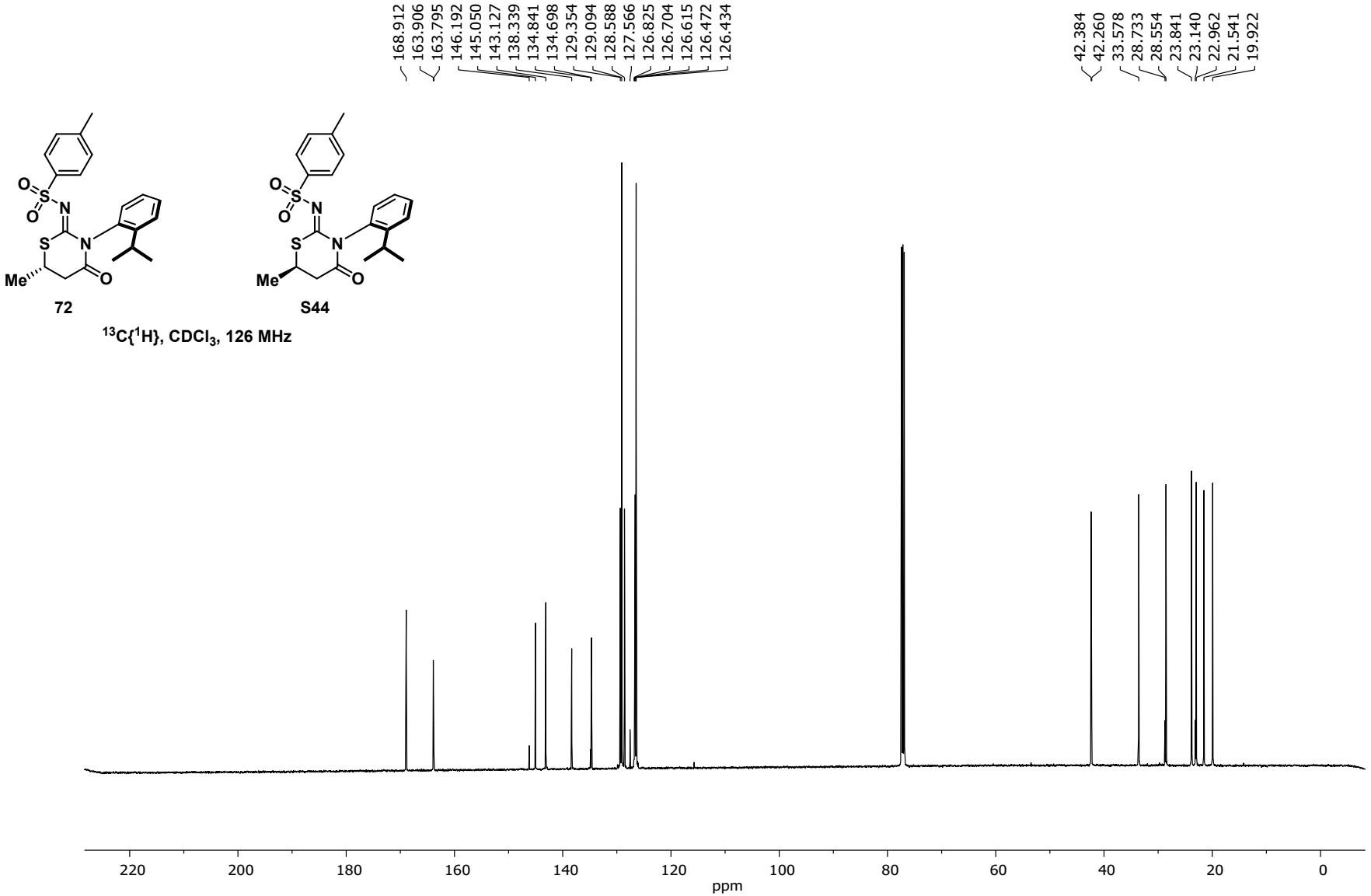


71

$^{13}C\{^{1}H\}$, $CDCl_3$, 126 MHz

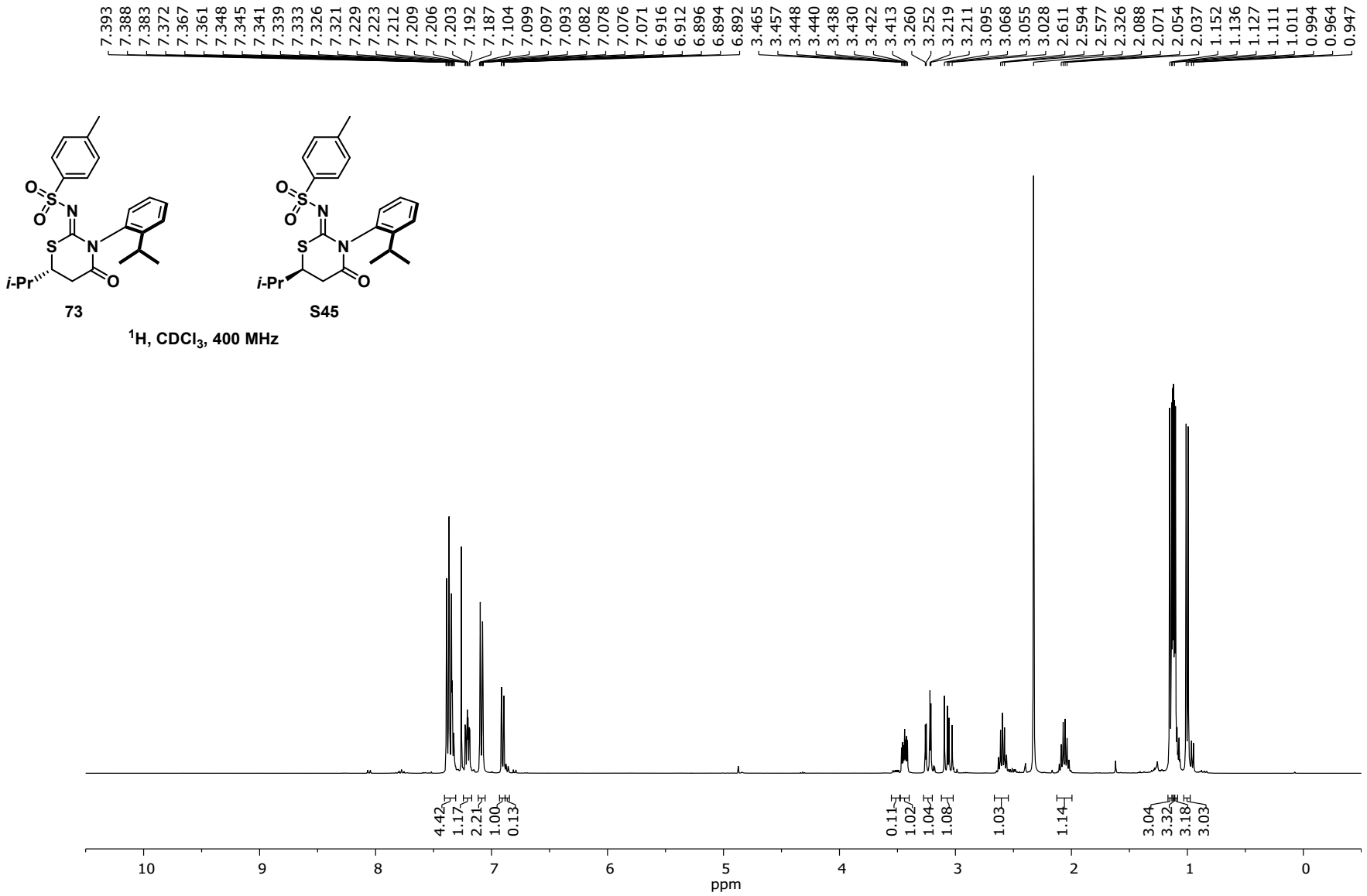


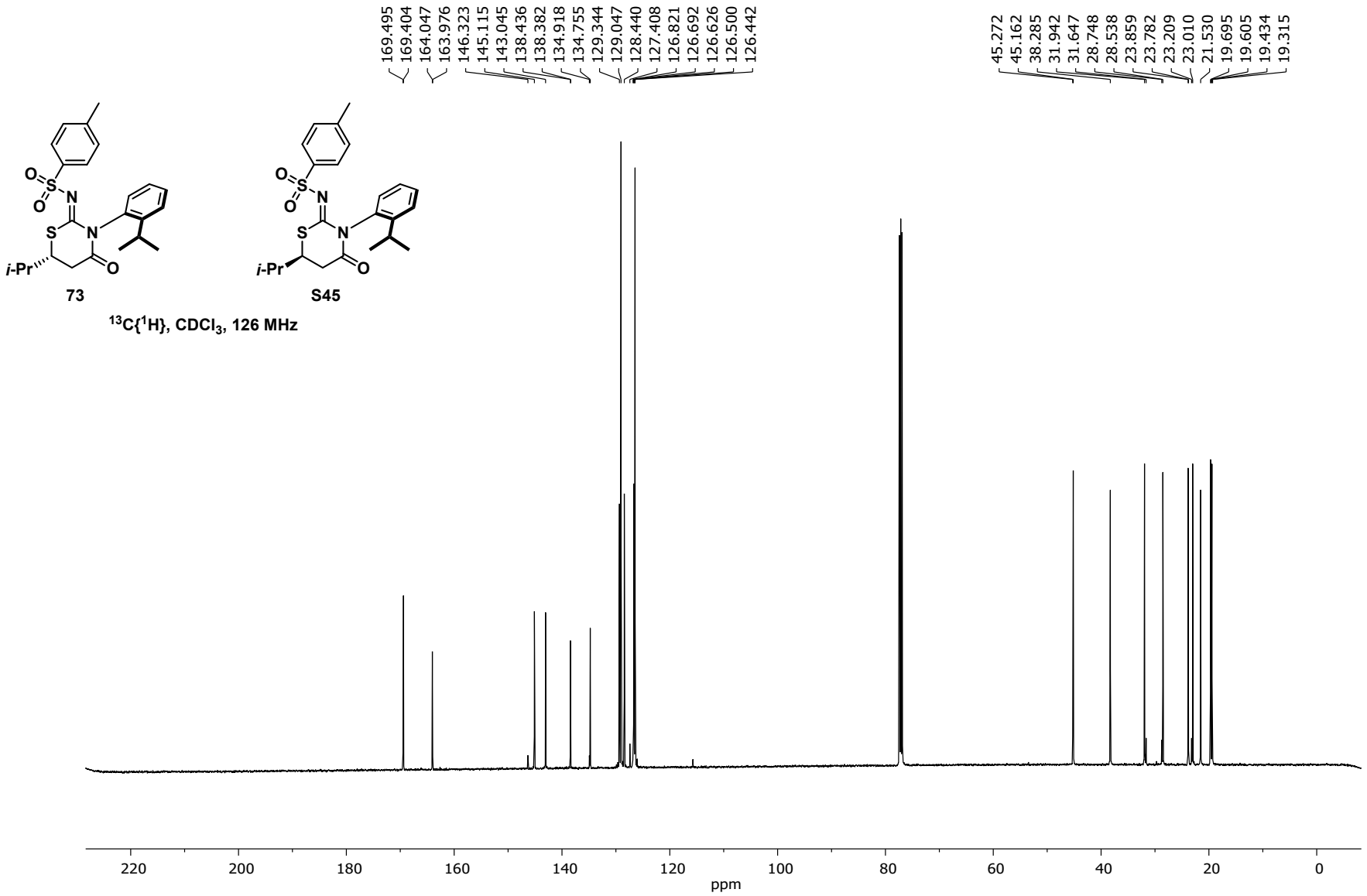

7.390
7.385
7.382
7.374
7.369
7.365
7.362
7.349
7.345
7.343
7.337
7.323
7.233
7.228
7.216
7.213
7.211
7.208
7.204
7.202
7.200
7.197
7.191
7.108
7.103
7.101
7.099
7.097
7.087
7.084
7.082
7.080
7.075
6.936
6.933
6.916
6.914
6.912
6.877
6.873
3.750
3.746
3.742
3.733
3.725
3.716
3.707
3.699
3.266
3.258
3.204
3.035
3.021
2.618
2.601
2.584
2.566
2.550
2.328
1.546
1.532
1.529
1.107
1.090
0.990
0.973
Me
72
S44
1H, CDCl3, 400 MHz
4.63
1.24
2.29
1.00
0.17
1.16
1.14
1.16
1.11
3.44
3.42
3.57
3.42
10
9
8
7
6
5
4
3
2
1
0
ppm



72 **S44**

$^{13}C\{^{1}H\}$, $CDCl_3$, 126 MHz


7.393
7.388
7.383
7.372
7.367
7.361
7.348
7.345
7.341
7.339
7.333
7.326
7.321
7.229
7.223
7.212
7.209
7.206
7.203
7.192
7.187
7.104
7.099
7.097
7.093
7.082
7.078
7.076
7.071
6.916
6.912
6.896
6.894
6.892
3.465
3.457
3.448
3.440
3.438
3.430
3.422
3.413
3.260
3.252
3.219
3.211
3.095
3.068
3.055
3.028
2.611
2.594
2.577
2.326
2.088
2.071
2.054
2.037
1.152
1.136
1.127
1.111
1.011
0.994
0.964
0.947
i-Pr
i-Pr
73
S45
1H, CDCl3, 400 MHz
4.42
1.17
2.21
1.00
0.13
0.11
1.02
1.04
1.08
1.03
1.14
3.04
3.32
3.18
3.03
10
9
8
7
6
5
4
3
2
1
0
ppm

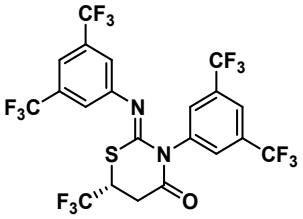


73 **S45**

$^{13}C\{^{1}H\}$, $CDCl_3$, 126 MHz

Appendix II: HPLC Traces of Novel Compounds

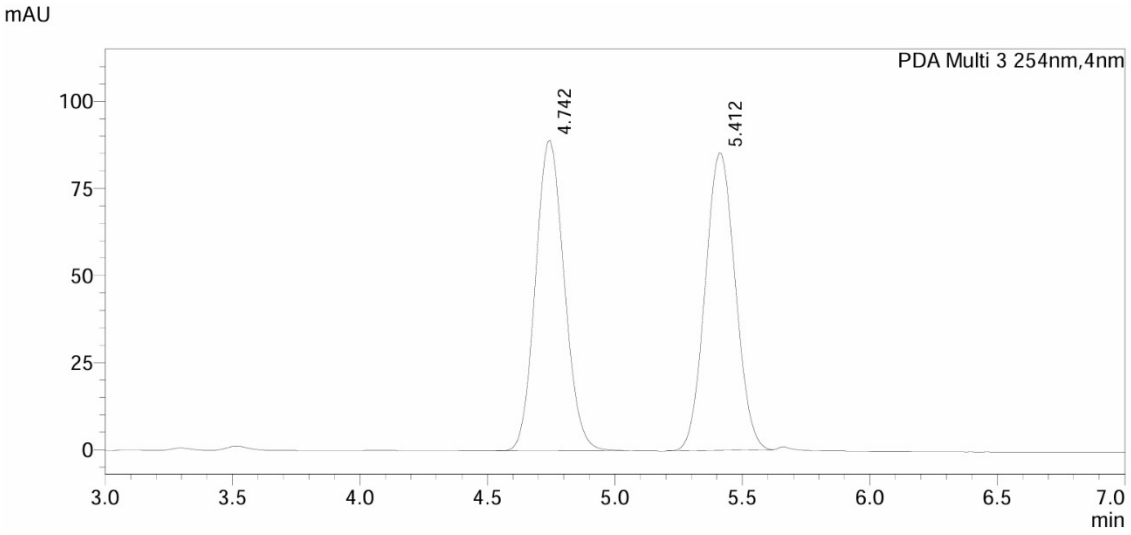
HPLC data for **33**: Chiralcel OD-H (90:10 *n*-hexane : IPA, flow rate 1.0 mLmin^{-1}, 254 nm, 30 °C) t_R (*S*) 4.7 min, t_R (*R*) 5.3 min, 95:5 er.



33

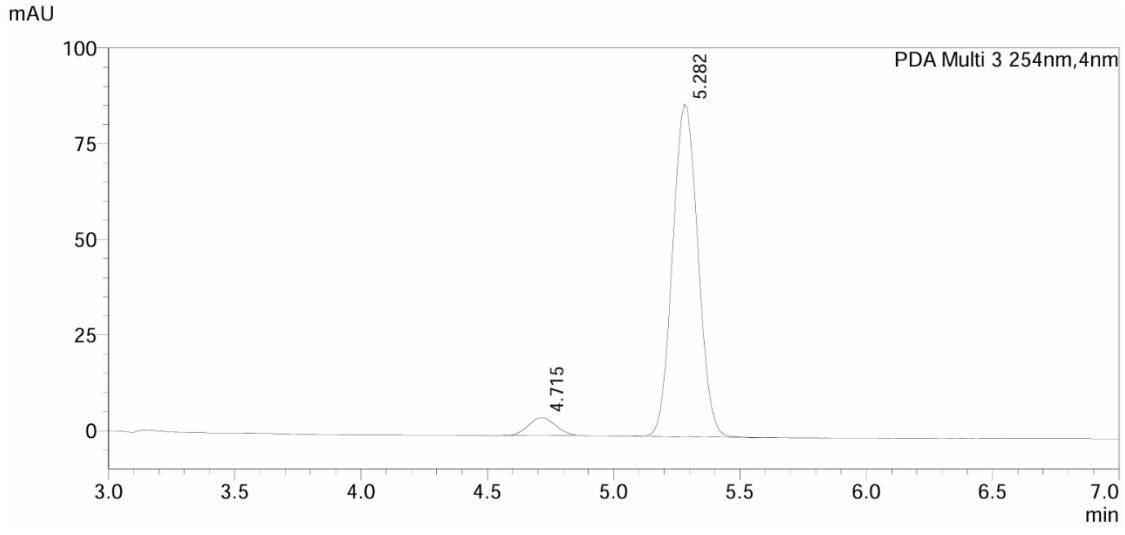
PDA Ch3 254nm

Peak#	Ret. Time	Area%
1	4.742	49.945
2	5.412	50.055
Total		100.000

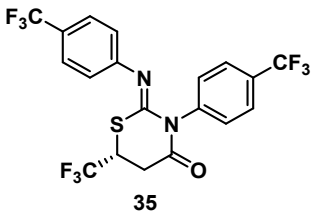


PDA Ch3 254nm

Peak#	Ret. Time	Area%
1	4.715	5.291
2	5.282	94.709
Total		100.000



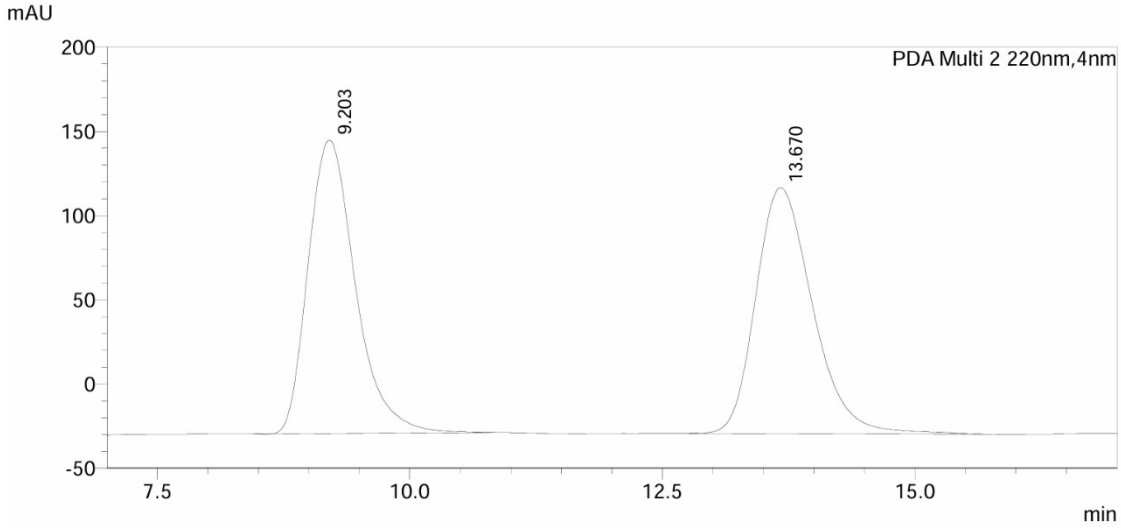
HPLC data for **35**: Chiralpak AD-H (97:3 *n*-hexane : IPA, flow rate 2.0 mLmin^{-1}, 220 nm, 40 °C) t_R (*R*) 9.1 min, t_R (*S*) 14.5 min, 95:5 er.



35

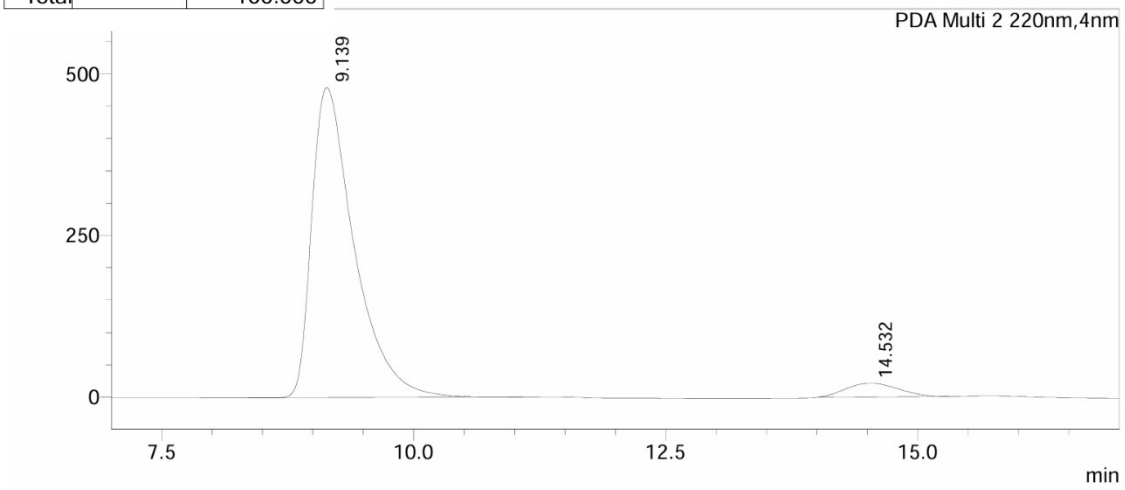
PDA Ch2 220nm

Peak#	Ret. Time	Area%
1	9.203	49.766
2	13.670	50.234
Total		100.000

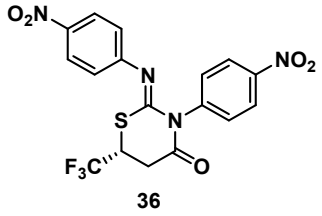


PDA Ch2 220nm

Peak#	Ret. Time	Area%
1	9.139	94.825
2	14.532	5.175
Total		100.000



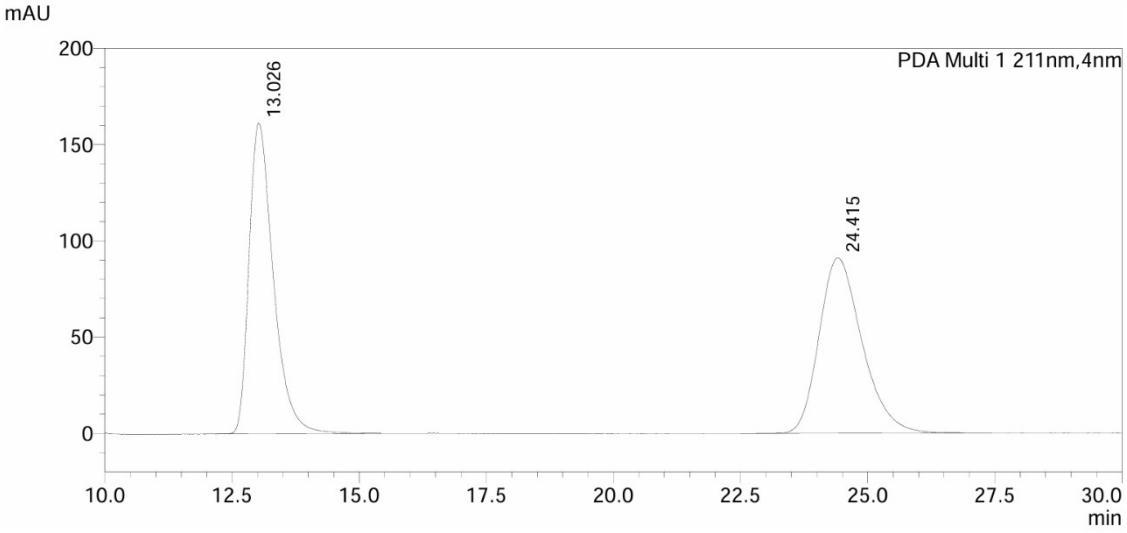
HPLC data for **36**: Chiralpak AD-H (70:30 *n*-hexane : IPA, flow rate 1.0 mLmin^{-1}, 211 nm, 30 °C) t_R (*R*) 13.1 min, t_R (*S*) 24.7 min, 98:2 er.



36

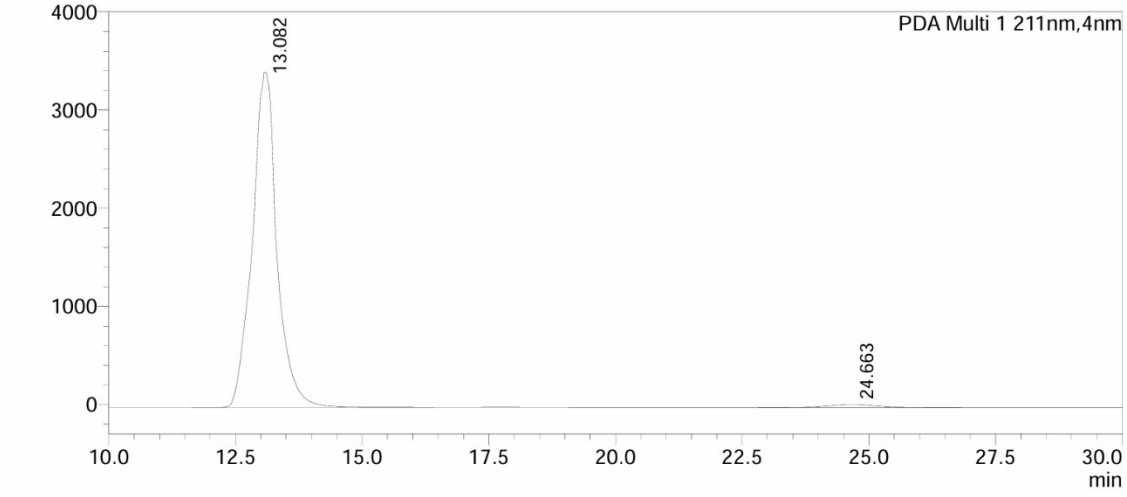
PDA Ch1 211nm

Peak#	Ret. Time	Area%
1	13.026	50.057
2	24.415	49.943
Total		100.000

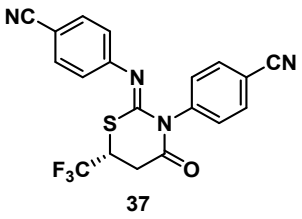


PDA Ch1 211nm

Peak#	Ret. Time	Area%
1	13.082	98.212
2	24.663	1.788
Total		100.000



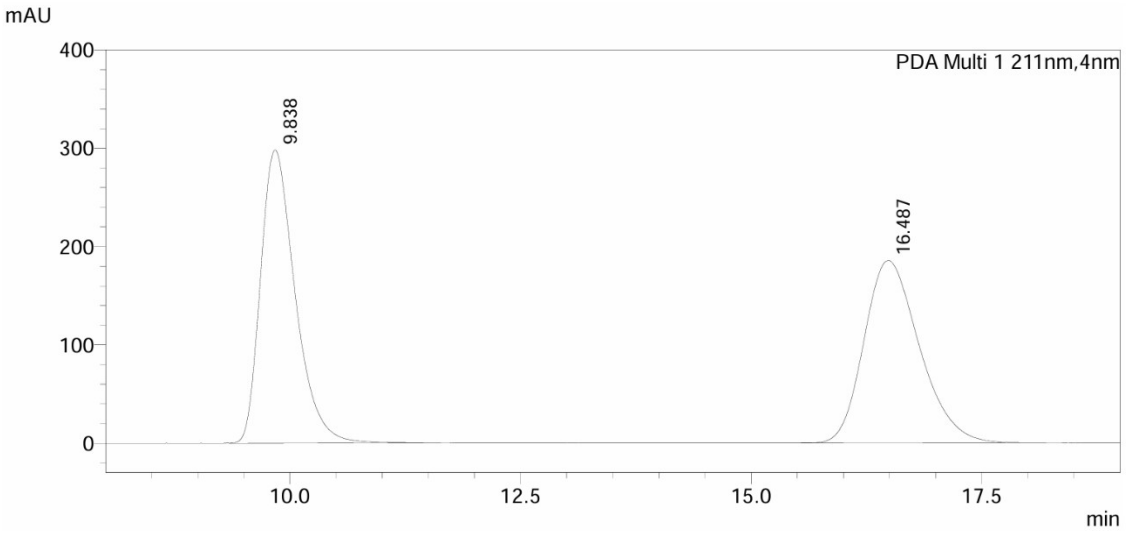
HPLC data for **37**: Chiralpak AD-H (70:30 *n*-hexane : IPA, flow rate 1.0 mLmin^{-1}, 211 nm, 30 °C) t_R (*R*) 9.8 min, t_R (*S*) 16.5 min, 97:3 er.



37

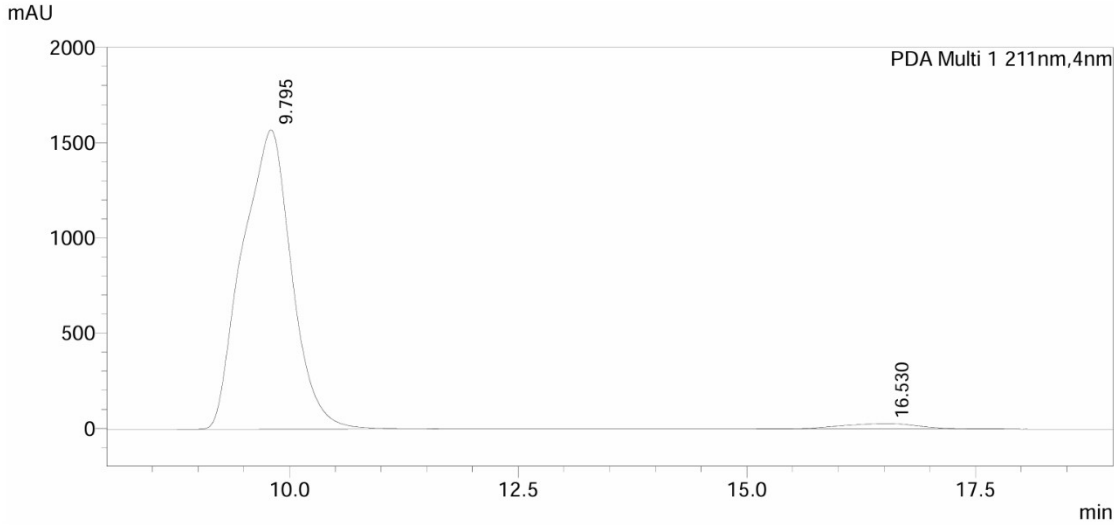
PDA Ch1 211nm

Peak#	Ret. Time	Area%
1	9.838	50.053
2	16.487	49.947
Total		100.000

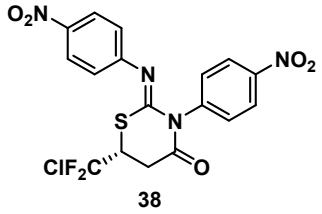


PDA Ch1 211nm

Peak#	Ret. Time	Area%
1	9.795	97.135
2	16.530	2.865
Total		100.000



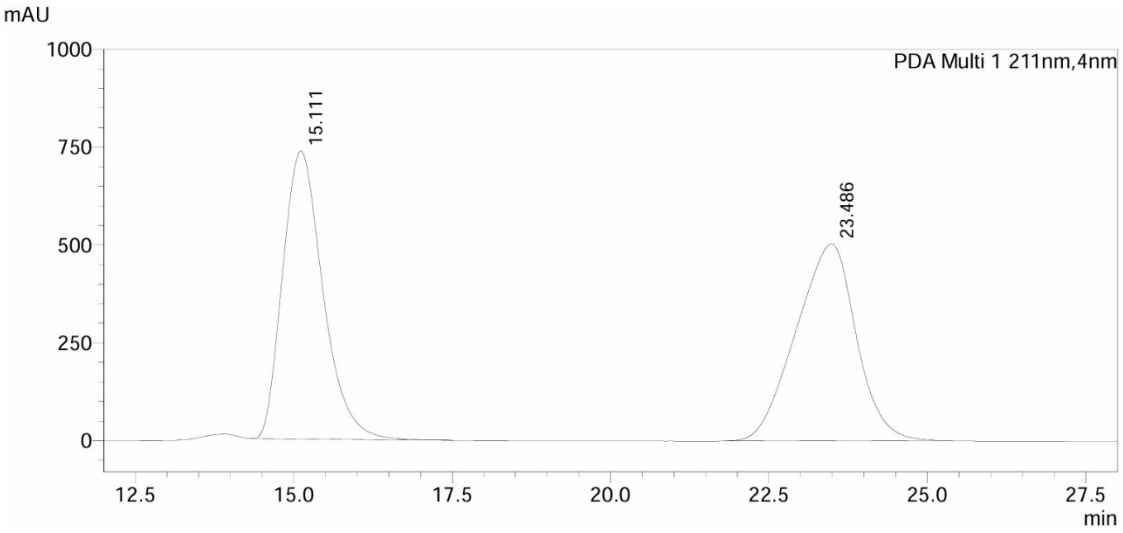
HPLC data for **38**: Chiralpak AD-H (70:30 *n*-hexane : IPA, flow rate 1.0 mLmin^{-1}, 211 nm, 30 °C) t_R (*R*) 15.3 min, t_R (*S*) 23.5 min, 98:2 er.



38

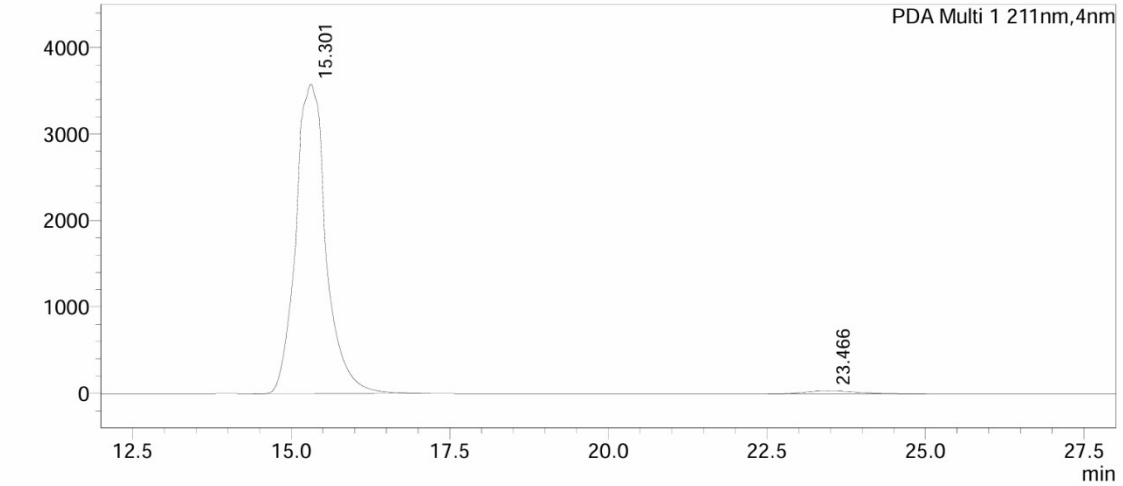
PDA Ch1 211nm

Peak#	Ret. Time	Area%
1	15.111	49.562
2	23.486	50.438
Total		100.000

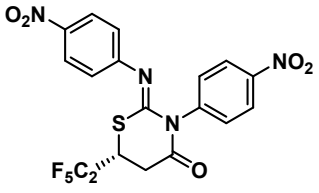


PDA Ch1 211nm

Peak#	Ret. Time	Area%
1	15.301	98.470
2	23.466	1.530
Total		100.000



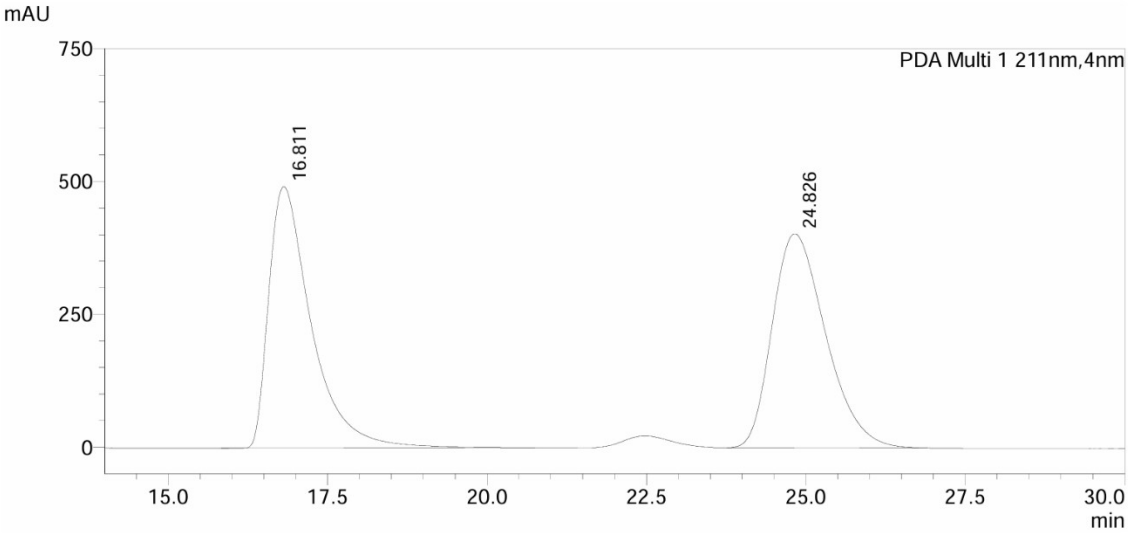
HPLC data for **39**: Chiralpak AD-H (80:20 *n*-hexane : IPA, flow rate 1.0 mLmin^{-1}, 211 nm, 30 °C) t_R (*R*) 16.9 min, t_R (*S*) 25.2 min, 98:2 er.



39

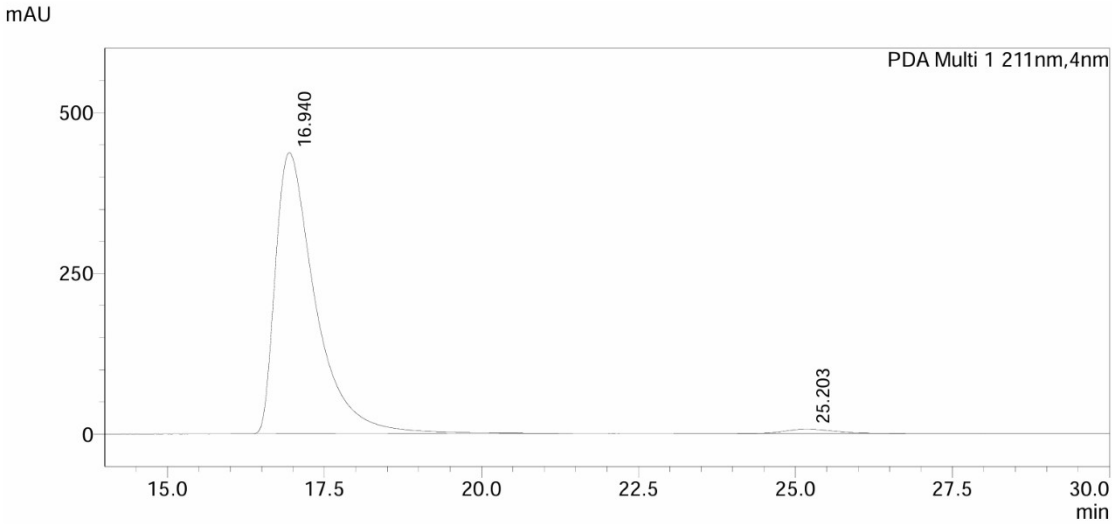
PDA Ch1 211nm

Peak#	Ret. Time	Area%
1	16.811	49.357
2	24.826	50.643
Total		100.000

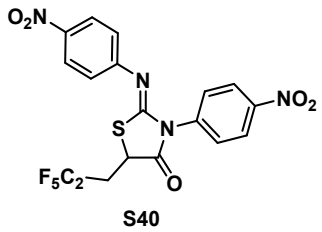


PDA Ch1 211nm

Peak#	Ret. Time	Area%
1	16.940	98.174
2	25.203	1.826
Total		100.000



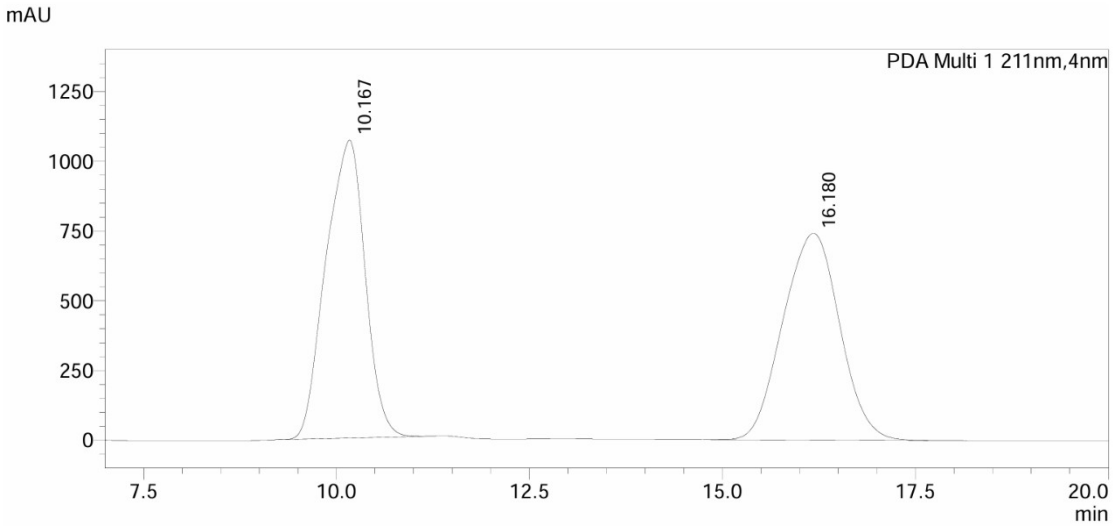
HPLC data for **S40**: Chiralpak AD-H (70:30 *n*-hexane : IPA, flow rate 1.0 mLmin^{-1}, 211 nm, 30 °C) t_R 10.2 min, t_R 16.2 min, 50:50 er.



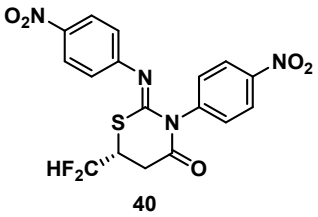
S40

PDA Ch1 211nm

Peak#	Ret. Time	Area%
1	10.167	49.986
2	16.180	50.014
Total		100.000



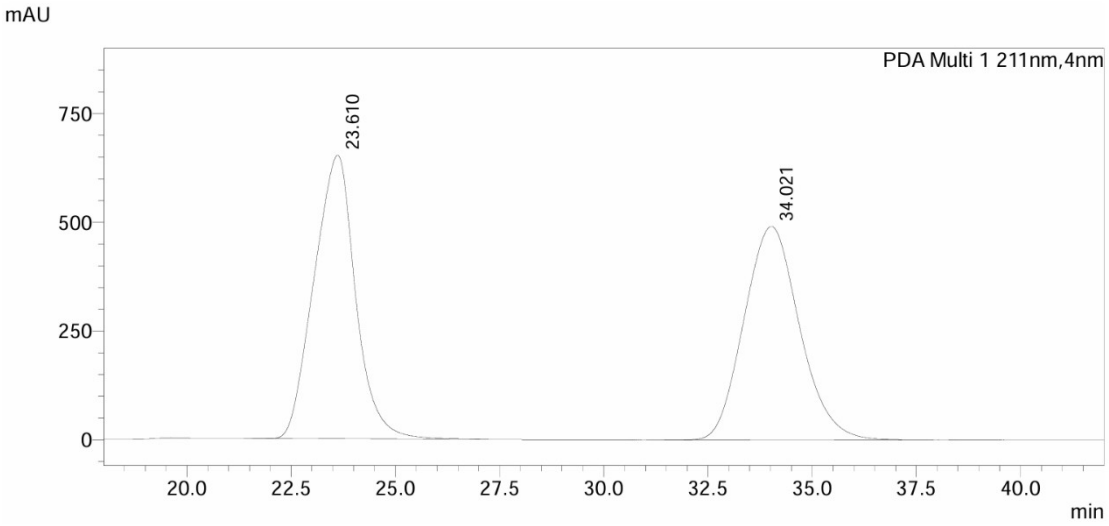
HPLC data for **40**: Chiralpak AD-H (70:30 *n*-hexane : IPA, flow rate 1.0 mLmin^{-1}, 211 nm, 30 °C) t_R (*R*) 24.4 min, t_R (*S*) 34.1 min, 80:20 er.



40

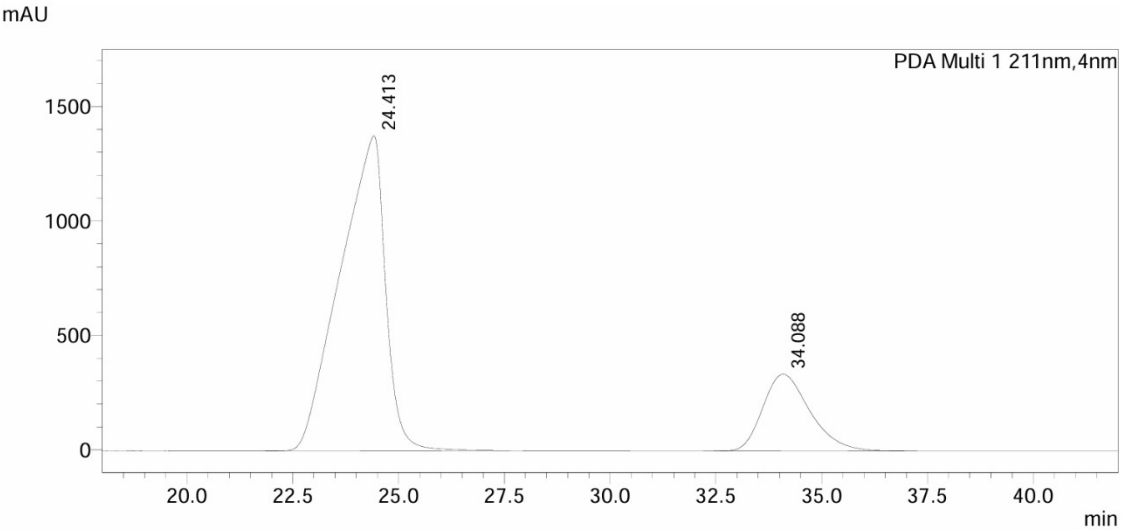
PDA Ch1 211nm

Peak#	Ret. Time	Area%
1	23.610	49.916
2	34.021	50.084
Total		100.000

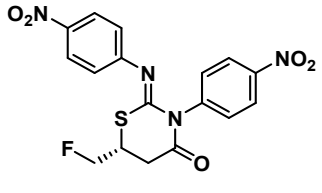


PDA Ch1 211nm

Peak#	Ret. Time	Area%
1	24.413	79.786
2	34.088	20.214
Total		100.000



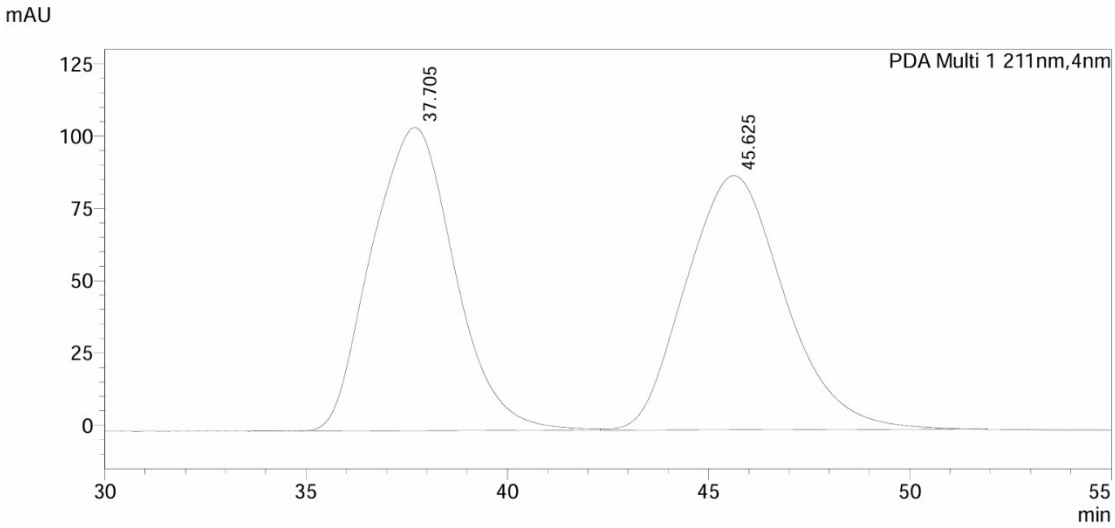
HPLC data for **41**: Chiralcel OJ-H (50:50 *n*-hexane : IPA, flow rate 0.7 mLmin^{-1}, 211 nm, 40 °C) t_R (*S*) 37.1 min, t_R (*R*) 44.5 min, 83:17 er.



41

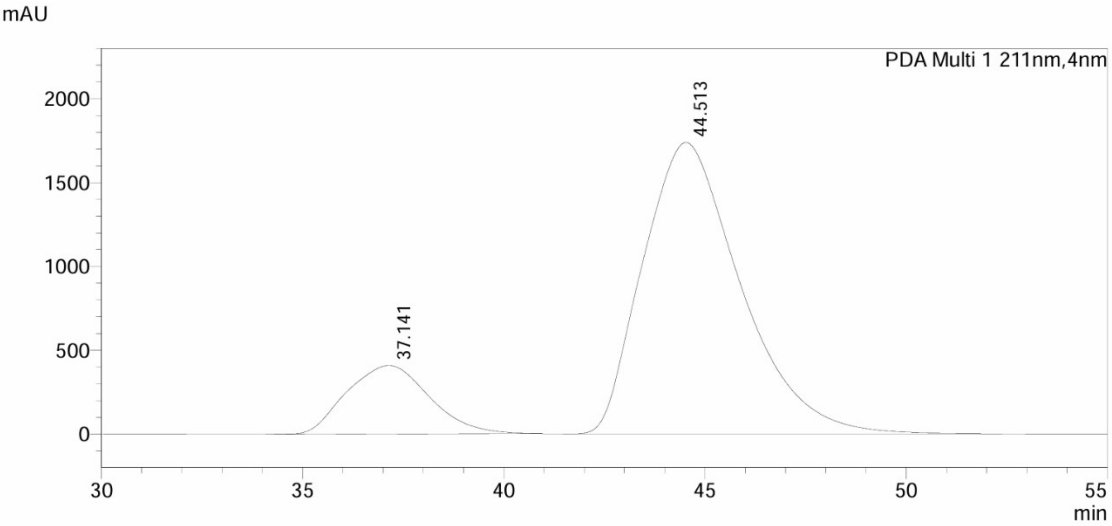
PDA Ch1 211nm

Peak#	Ret. Time	Area%
1	37.705	50.087
2	45.625	49.913
Total		100.000

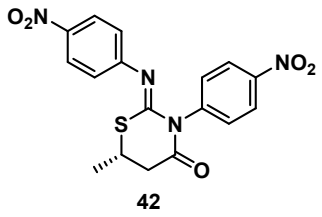


PDA Ch1 211nm

Peak#	Ret. Time	Area%
1	37.141	16.636
2	44.513	83.364
Total		100.000



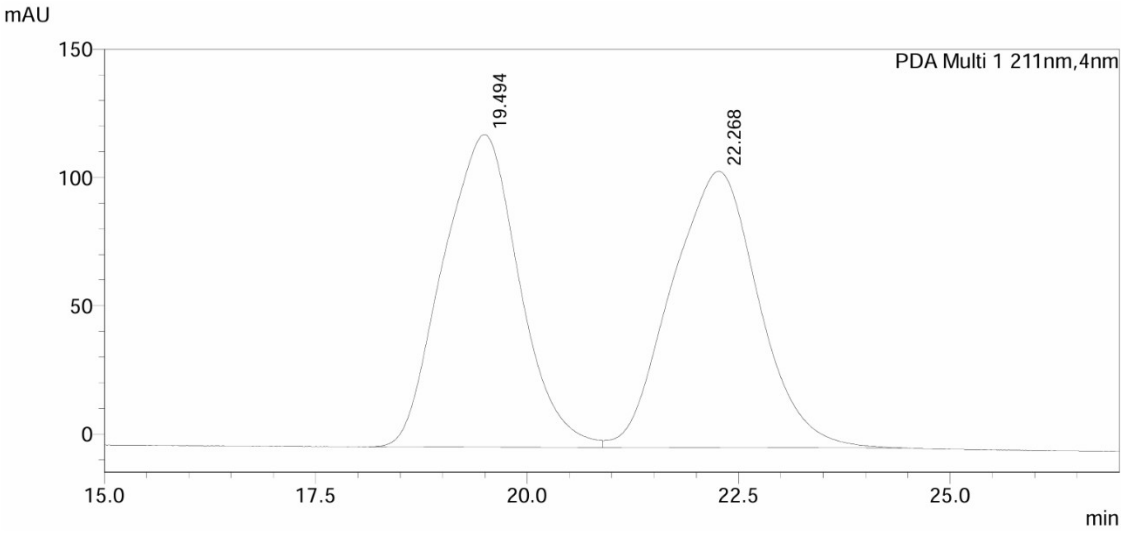
HPLC data for **42**: Chiralpak IB (80:20 *n*-hexane : IPA, flow rate 1.5 mLmin^{-1}, 211 nm, 30 °C) t_R (*R*) 19.3 min, t_R (*S*) 21.7 min, 86:14 er.



42

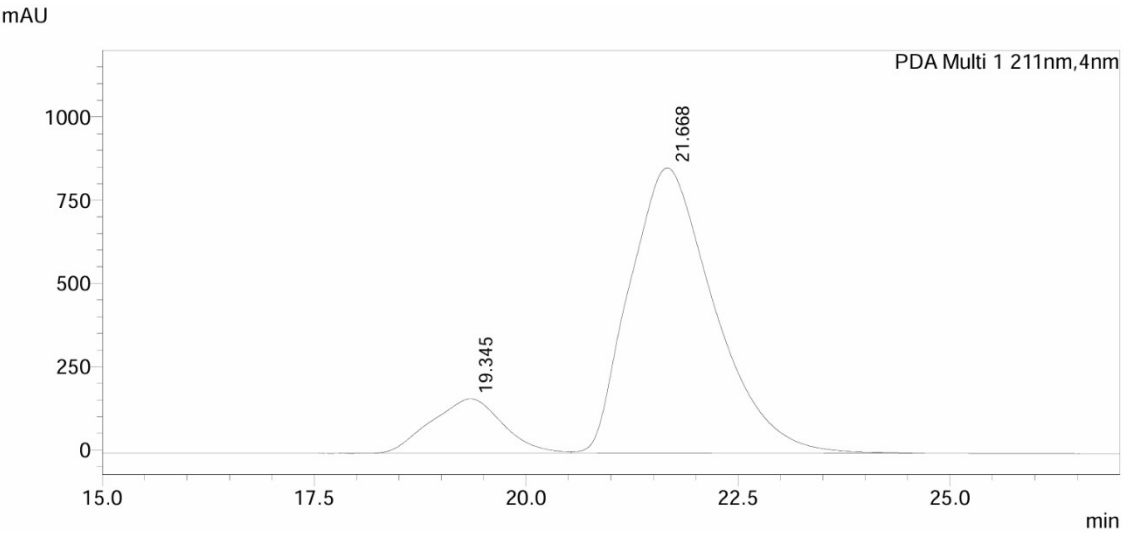
PDA Ch1 211nm

Peak#	Ret. Time	Area%
1	19.494	49.700
2	22.268	50.300
Total		100.000

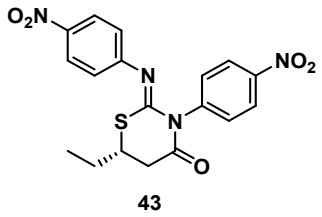


PDA Ch1 211nm

Peak#	Ret. Time	Area%
1	19.345	13.947
2	21.668	86.053
Total		100.000



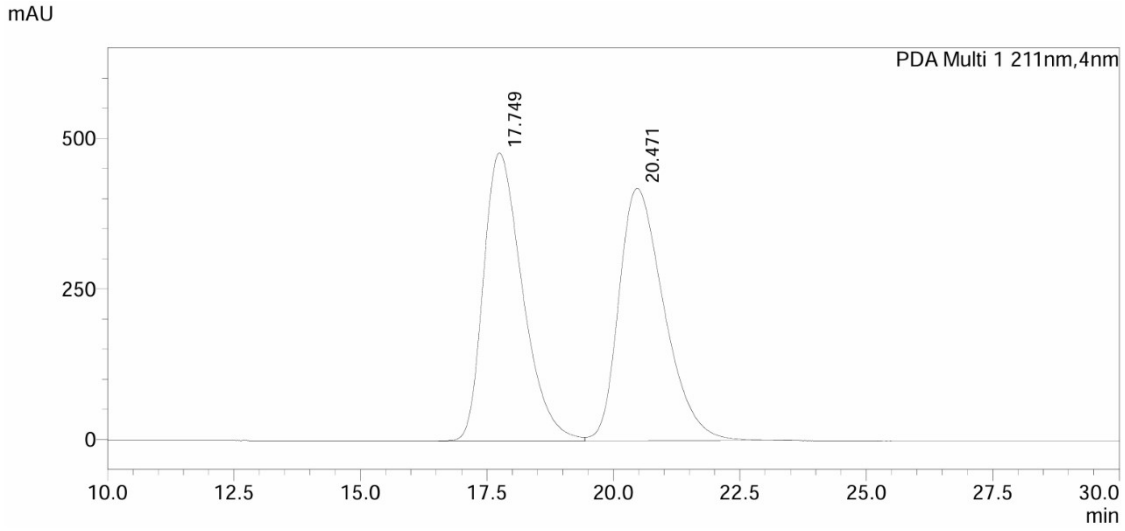
HPLC data for **43**: Chiralcel OD-H (70:30 *n*-hexane : IPA, flow rate 1.0 mLmin^{-1}, 211 nm, 30 °C) t_R (*R*) 18.1 min, t_R (*S*) 20.7 min, 89:11 er.



43

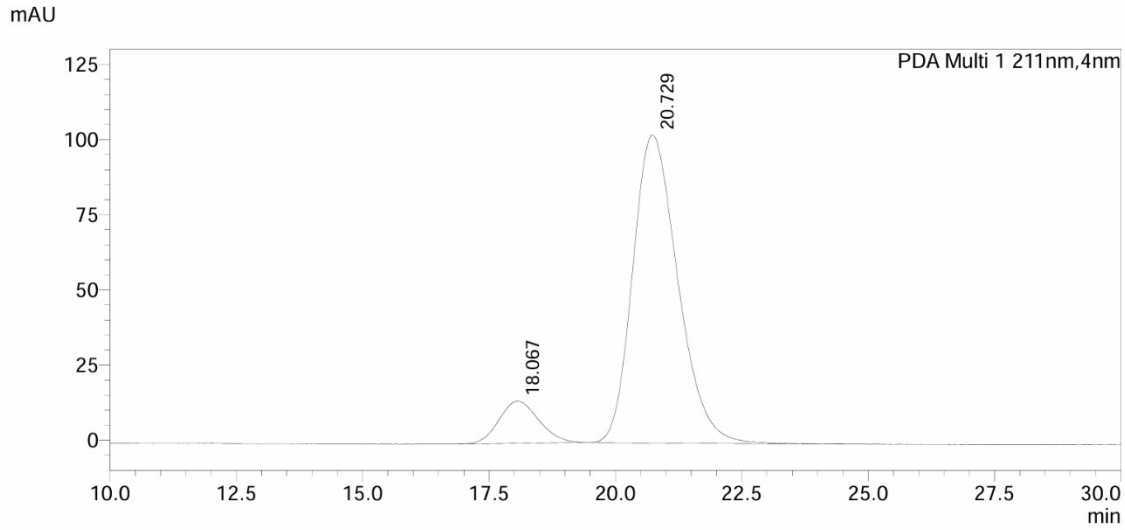
PDA Ch1 211nm

Peak#	Ret. Time	Area%
1	17.749	49.629
2	20.471	50.371
Total		100.000

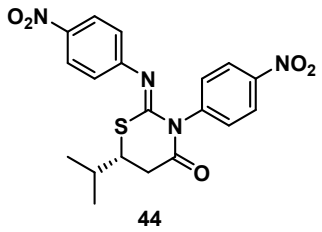


PDA Ch1 211nm

Peak#	Ret. Time	Area%
1	18.067	10.709
2	20.729	89.291
Total		100.000



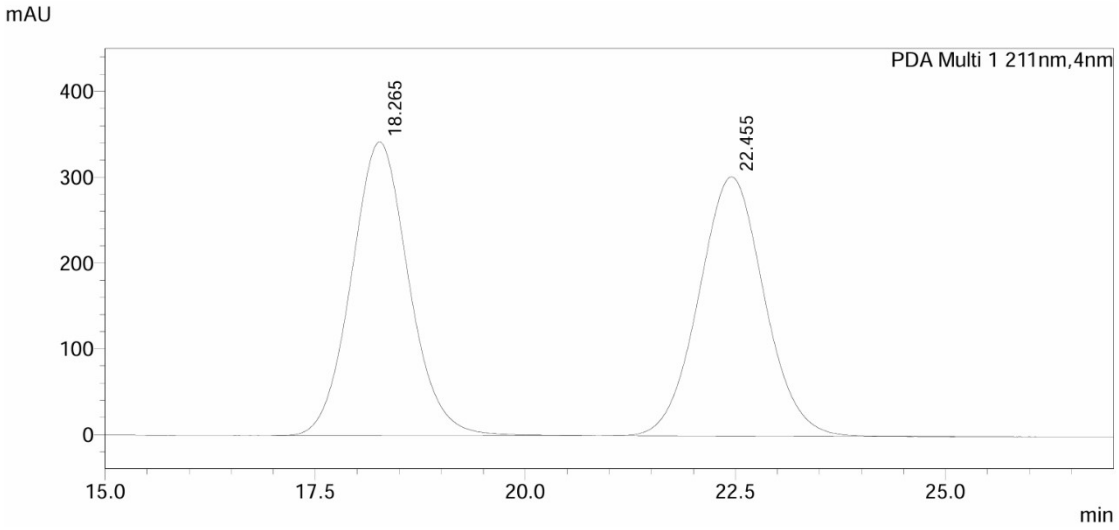
HPLC data for **44**: Chiralpak AD-H (60:40 *n*-hexane : IPA, flow rate 1.0 mLmin^{-1}, 211 nm, 30 °C) t_R (*R*) 18.3 min, t_R (*S*) 22.5 min, 94:6 er.



44

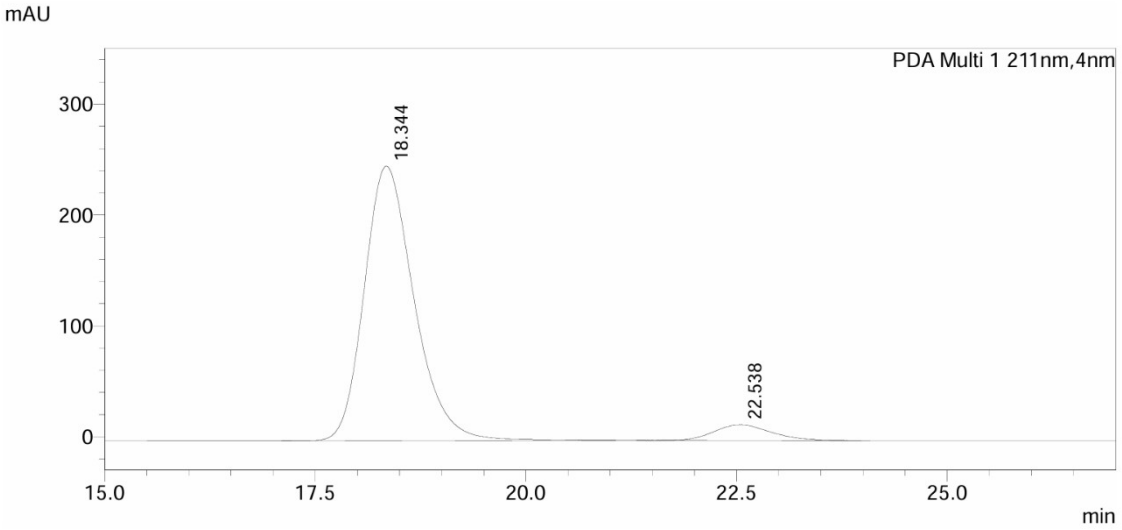
PDA Ch1 211nm

Peak#	Ret. Time	Area%
1	18.265	49.906
2	22.455	50.094
Total		100.000

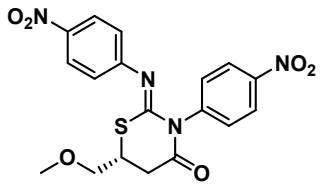


PDA Ch1 211nm

Peak#	Ret. Time	Area%
1	18.344	93.909
2	22.538	6.091
Total		100.000



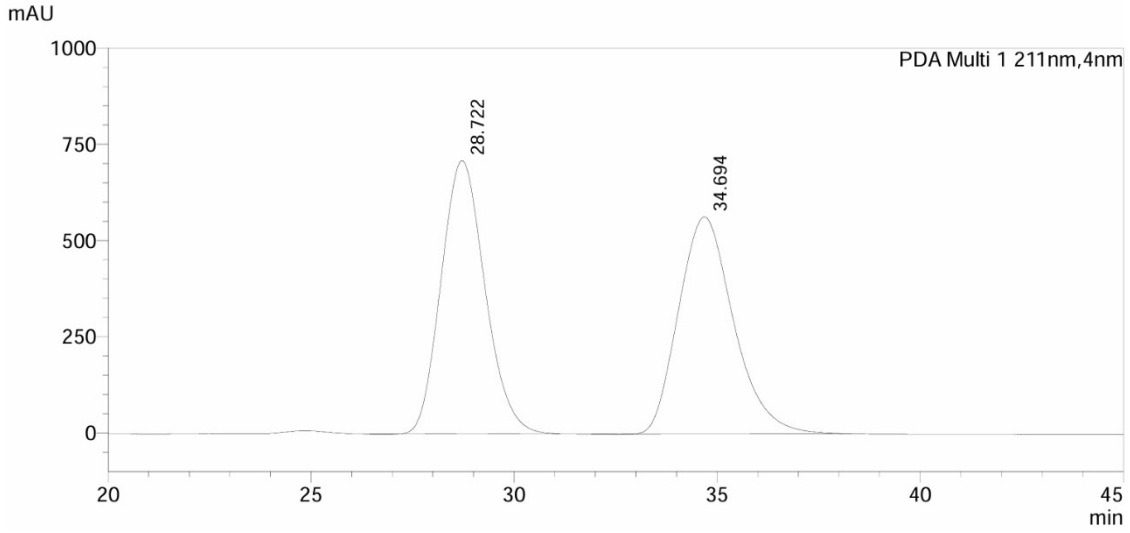
HPLC data for **45**: Chiralpak AD-H (70:30 *n*-hexane : IPA, flow rate 1.0 mLmin^{-1}, 211 nm, 30 °C) t_R (*S*) 28.8 min, t_R (*R*) 35.2 min, 86:14 er.



45

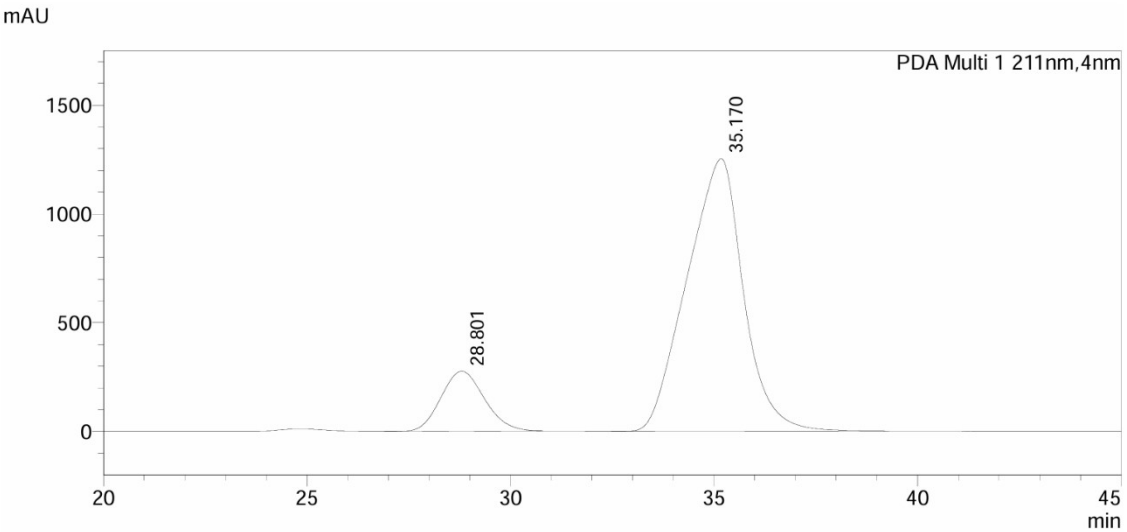
PDA Ch1 211nm

Peak#	Ret. Time	Area%
1	28.722	50.043
2	34.694	49.957
Total		100.000

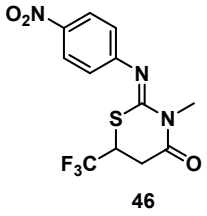


PDA Ch1 211nm

Peak#	Ret. Time	Area%
1	28.801	14.461
2	35.170	85.539
Total		100.000



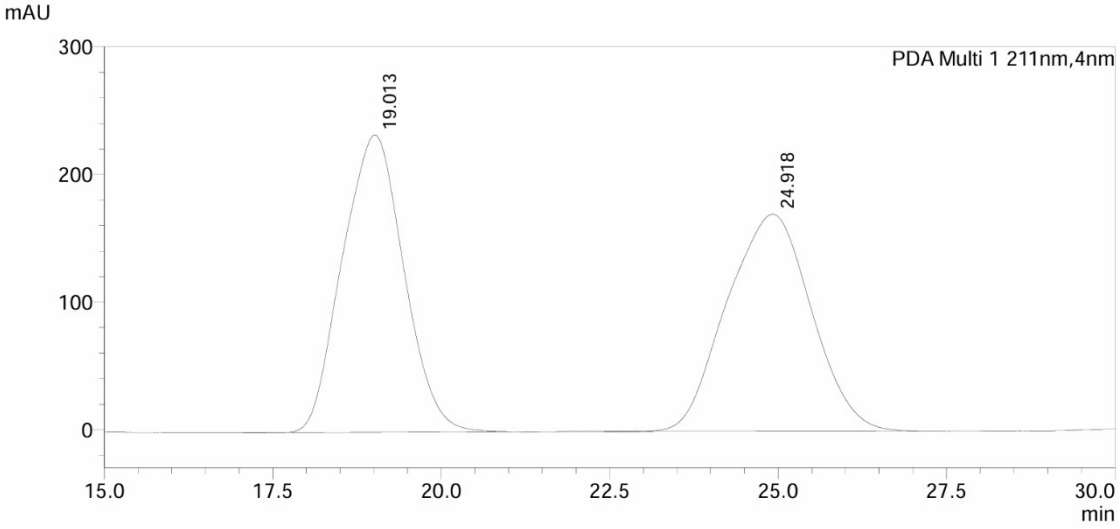
HPLC data for **46**: Chiralcel OD-H (90:10 *n*-hexane : IPA, flow rate 1.0 mLmin^{-1}, 211 nm, 30 °C) t_R 19.0 min, t_R 24.9 min, 50:50 er.



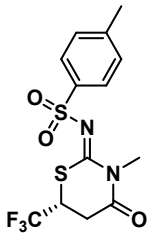
46

PDA Ch1 211nm

Peak#	Ret. Time	Area%
1	19.013	49.831
2	24.918	50.169
Total		100.000



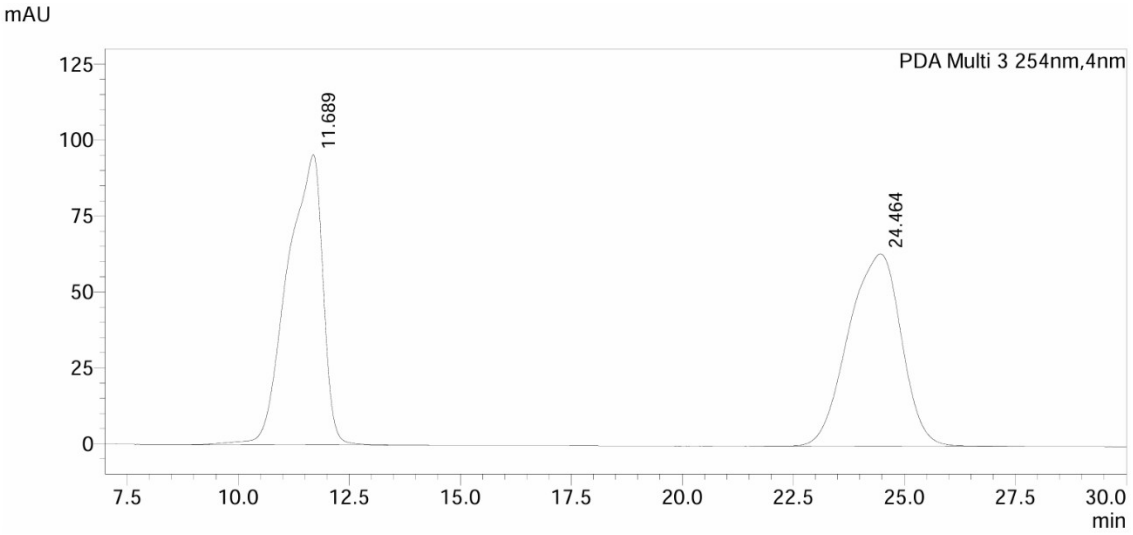
HPLC data for **47**: Chiralpak IB (80:20 *n*-hexane : IPA, flow rate 1.5 mLmin^{-1}, 254 nm, 30 °C) t_R (*S*) 11.6 min, t_R (*R*) 23.6 min, 67:33 er.



47

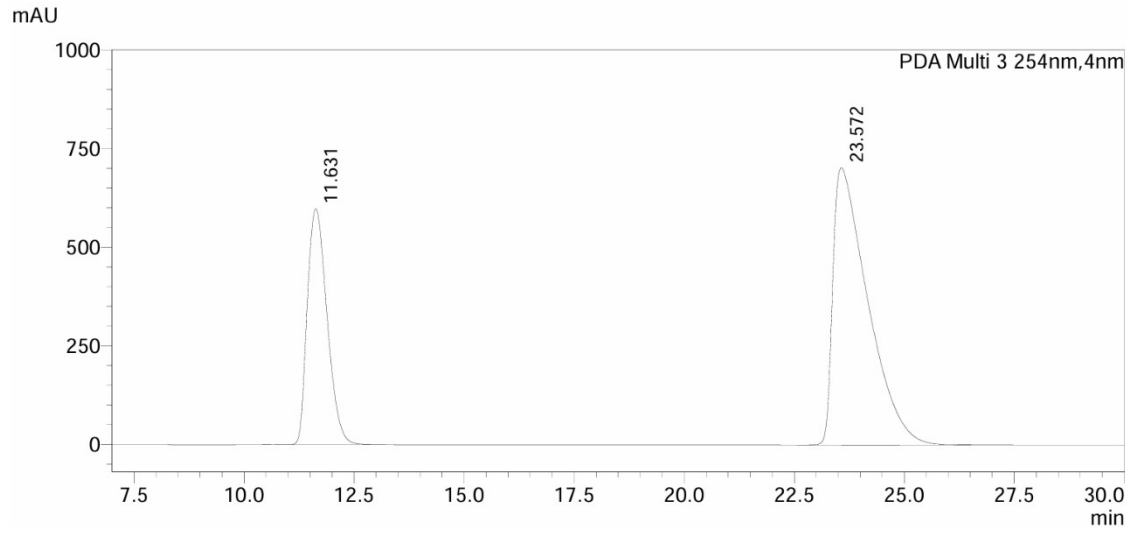
PDA Ch3 254nm

Peak#	Ret. Time	Area%
1	11.689	50.270
2	24.464	49.730
Total		100.000

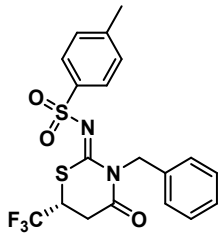


PDA Ch3 254nm

Peak#	Ret. Time	Area%
1	11.631	32.581
2	23.572	67.419
Total		100.000



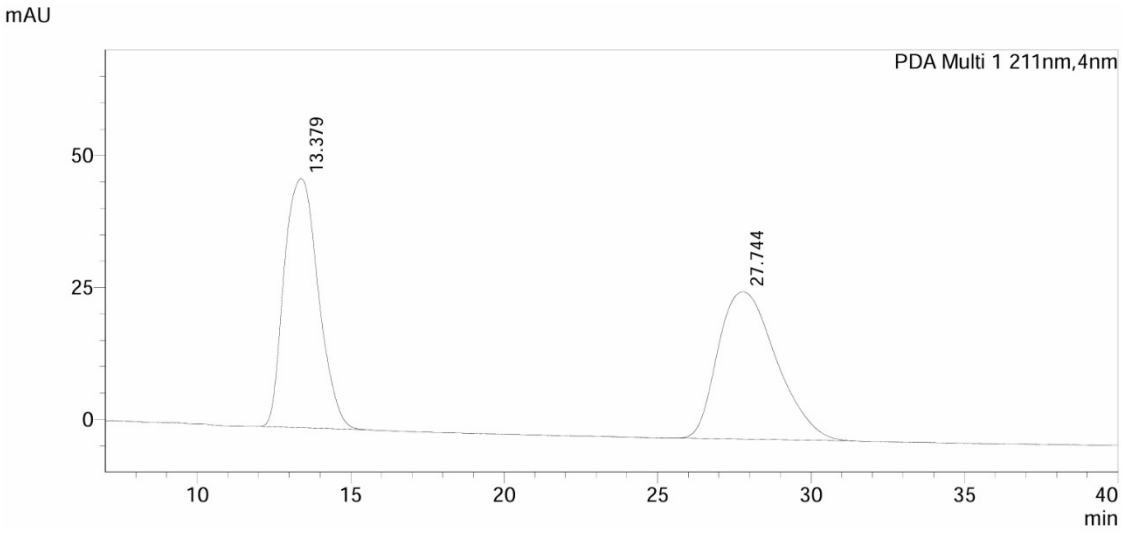
HPLC data for **48**: Chiralcel OD-H (70:30 *n*-hexane : IPA, flow rate 1.0 mLmin^{-1}, 211 nm, 30 °C) t_R (*S*) 13.4 min, t_R (*R*) 27.4 min, 78:22 er.



48

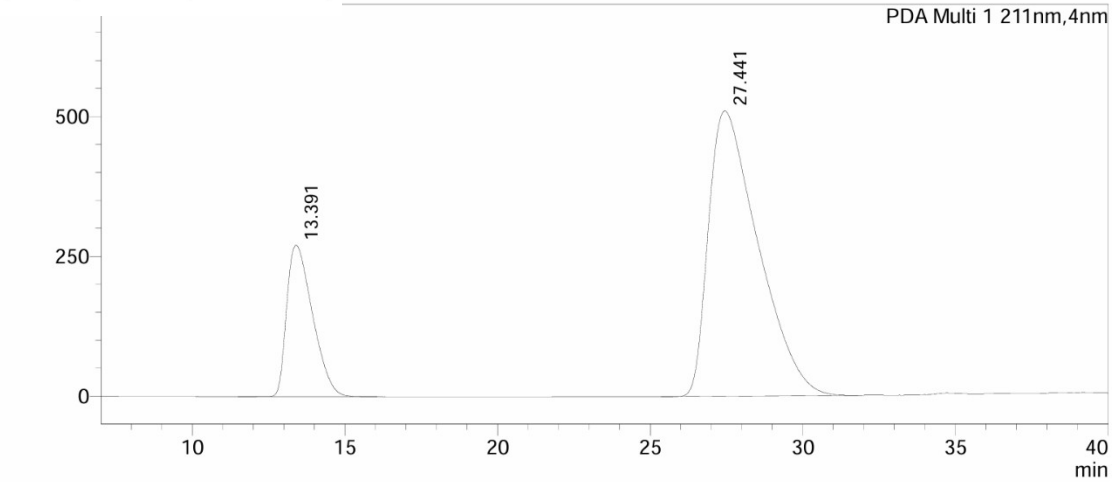
PDA Ch1 211nm

Peak#	Ret. Time	Area%
1	13.379	49.732
2	27.744	50.268
Total		100.000

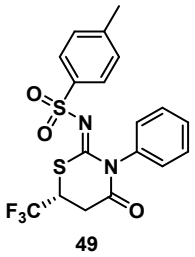


PDA Ch1 211nm

Peak#	Ret. Time	Area%
1	13.391	21.651
2	27.441	78.349
Total		100.000



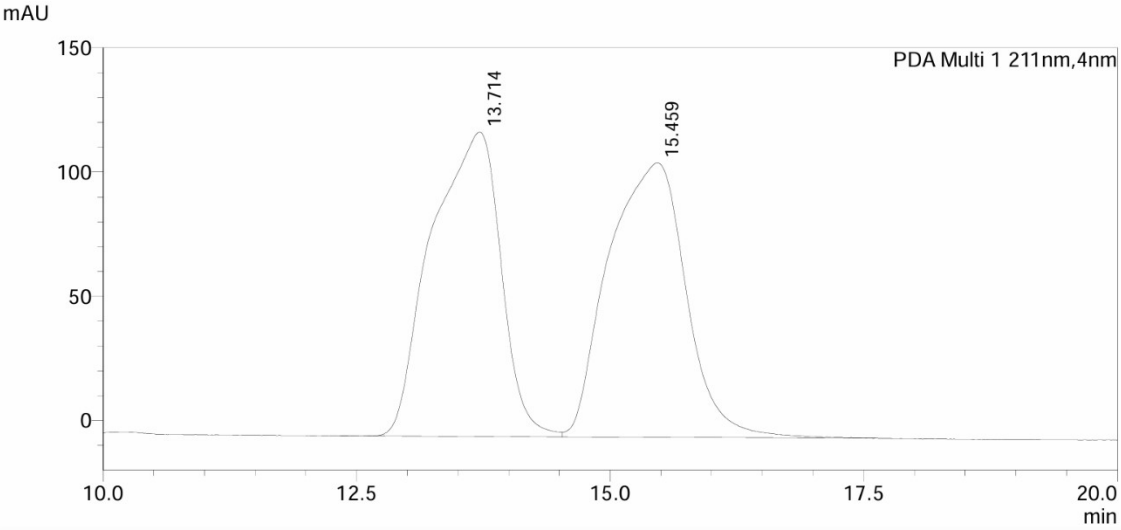
HPLC data for **49**: Chiralpak IA (80:20 *n*-hexane : IPA, flow rate 1.0 mLmin^{-1}, 211 nm, 30 °C) t_R (*S*) 13.7 min, t_R (*R*) 15.5 min, 91:9 er.



49

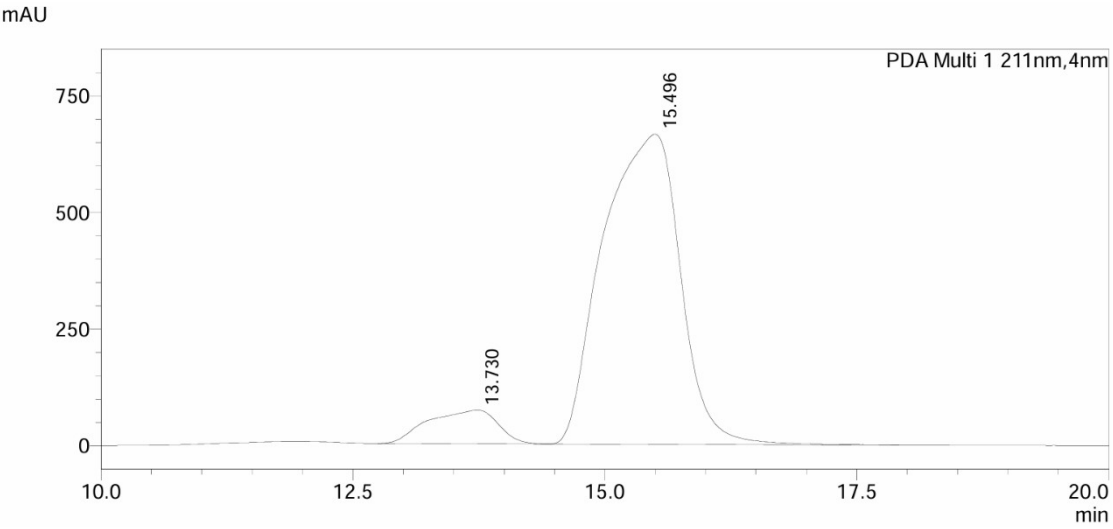
PDA Ch1 211nm

Peak#	Ret. Time	Area%
1	13.714	49.804
2	15.459	50.196
Total		100.000

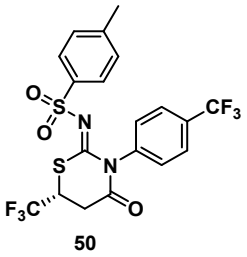


PDA Ch1 211nm

Peak#	Ret. Time	Area%
1	13.730	8.933
2	15.496	91.067
Total		100.000



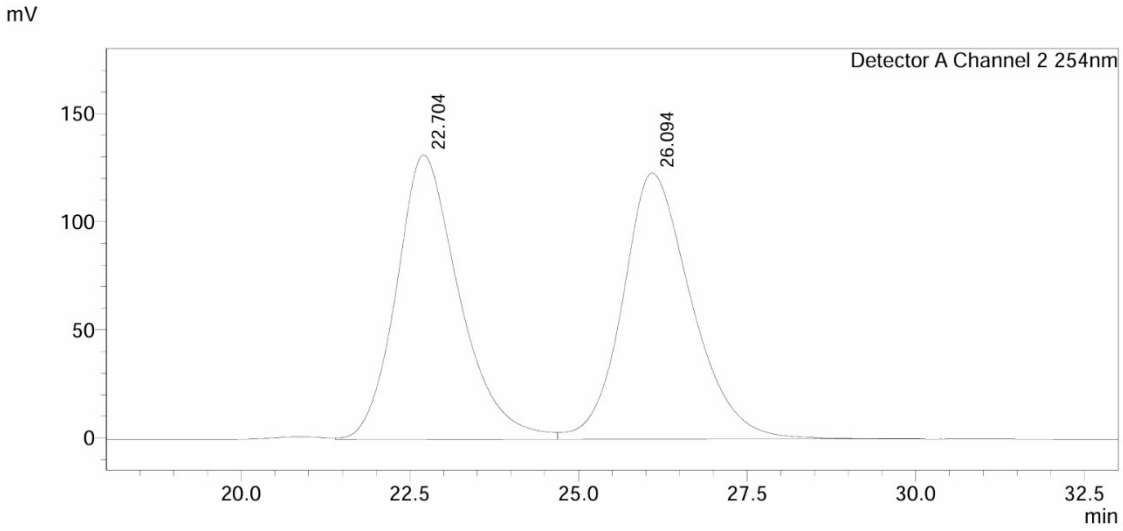
HPLC data for **50**: Chiralpak ID (93:7 *n*-hexane : IPA, flow rate 1.0 mLmin^{-1}, 254 nm, 40 °C) t_R (*S*) 22.9 min, t_R (*R*) 25.8 min, 88:12 er.



50

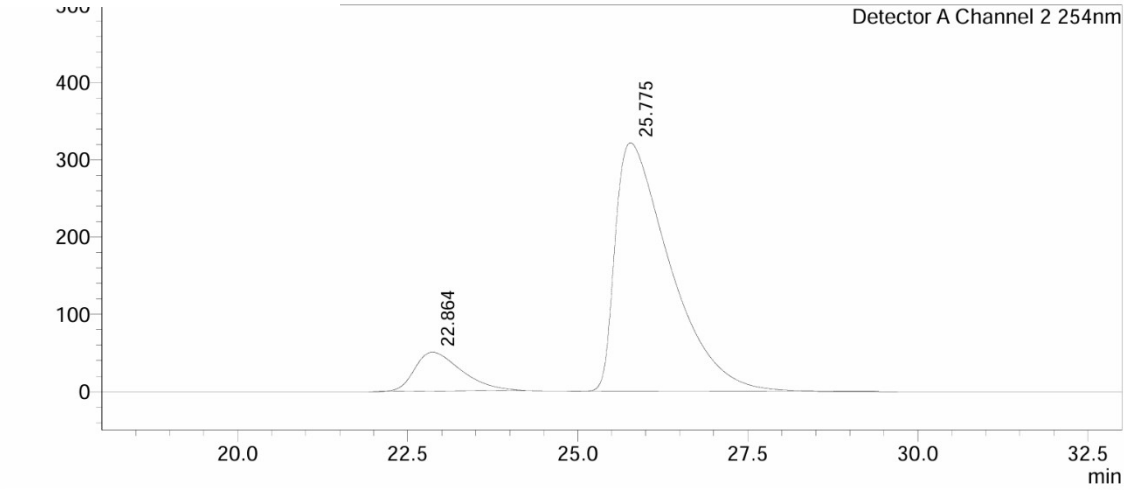
Detector A Channel 2 254nm

Peak#	Ret. Time	Area%
1	22.704	49.410
2	26.094	50.590
Total		100.000

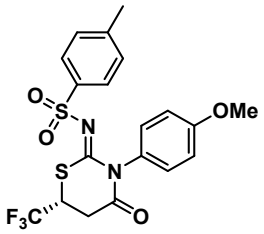


Detector A Channel 2 254nm

Peak#	Ret. Time	Area%
1	22.864	11.772
2	25.775	88.228
Total		100.000



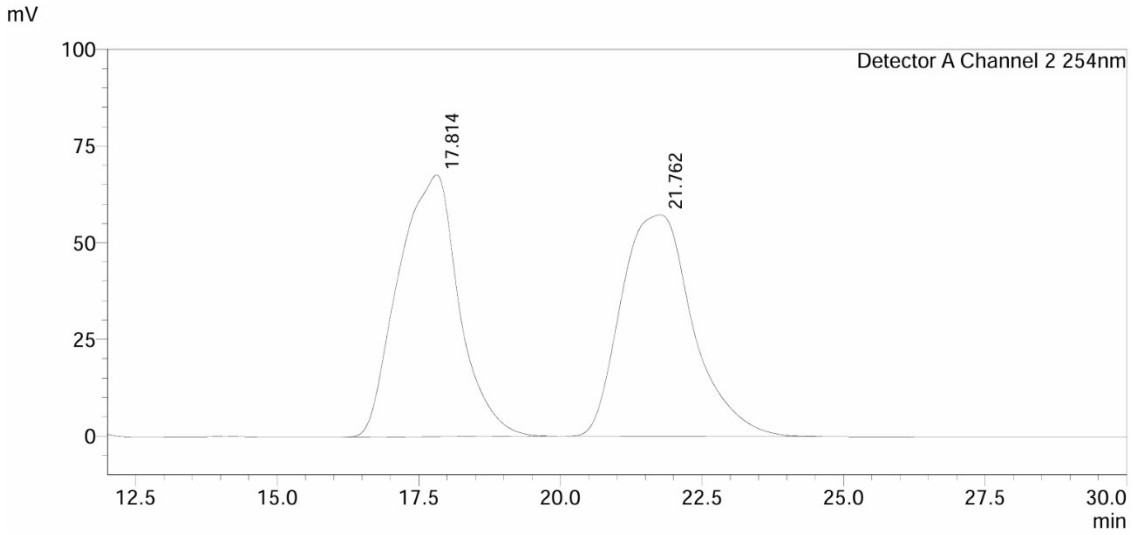
HPLC data for **51**: Chiralpak AD-H (80:20 *n*-hexane : IPA, flow rate 1.0 mLmin^{-1}, 254 nm, 30 °C) t_R (*S*) 18.0 min, t_R (*R*) 22.1 min, 90:10 er.



51

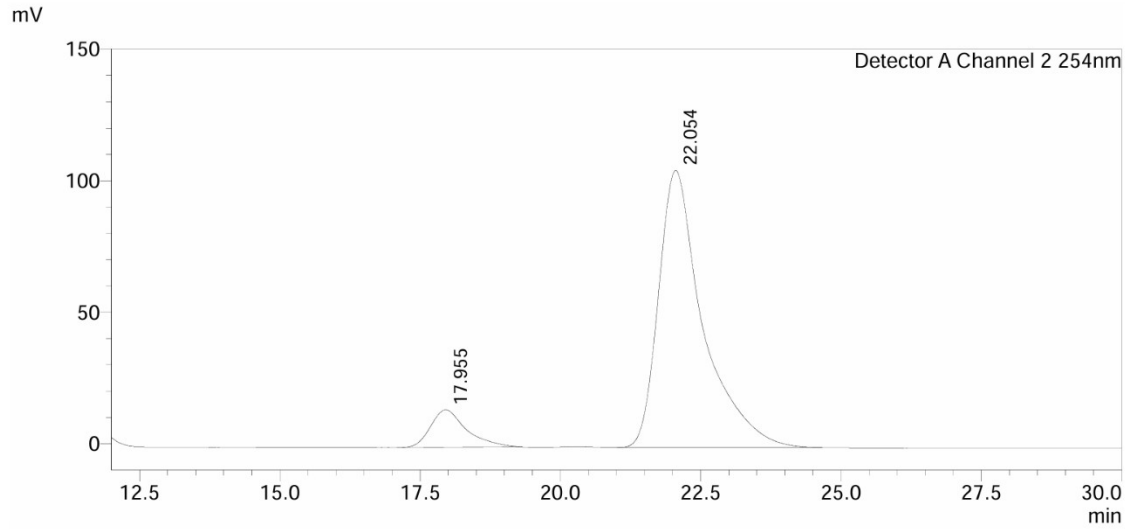
Detector A Channel 2 254nm

Peak#	Ret. Time	Area%
1	17.814	49.944
2	21.762	50.056
Total		100.000

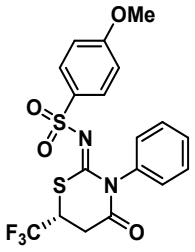


Detector A Channel 2 254nm

Peak#	Ret. Time	Area%
1	17.955	9.836
2	22.054	90.164
Total		100.000



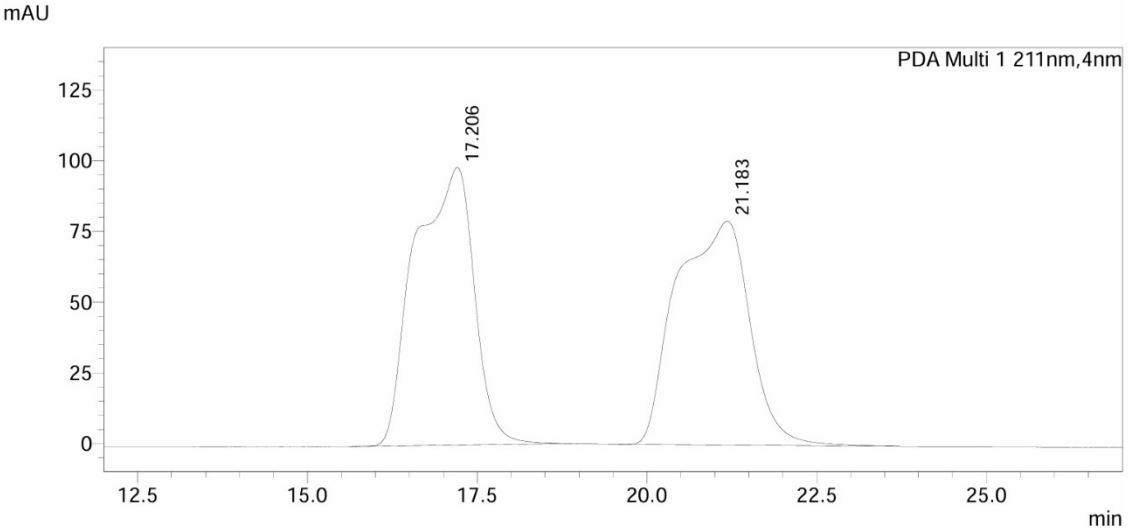
HPLC data for **52**: Chiralpak IA (80:20 *n*-hexane : IPA, flow rate 1.0 mLmin^{-1}, 211 nm, 30 °C) t_R (*S*) 17.2 min, t_R (*R*) 21.2 min, 91:9 er.



52

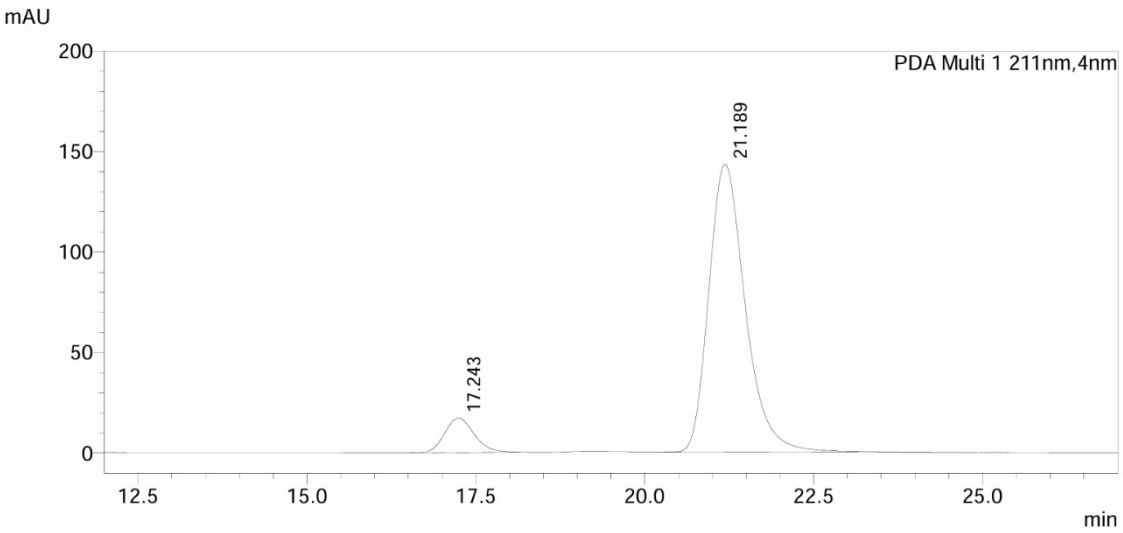
PDA Ch1 211nm

Peak#	Ret. Time	Area%
1	17.206	50.067
2	21.183	49.933
Total		100.000

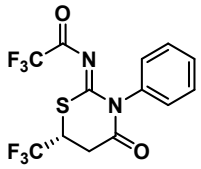


PDA Ch1 211nm

Peak#	Ret. Time	Area%
1	17.243	8.867
2	21.189	91.133
Total		100.000



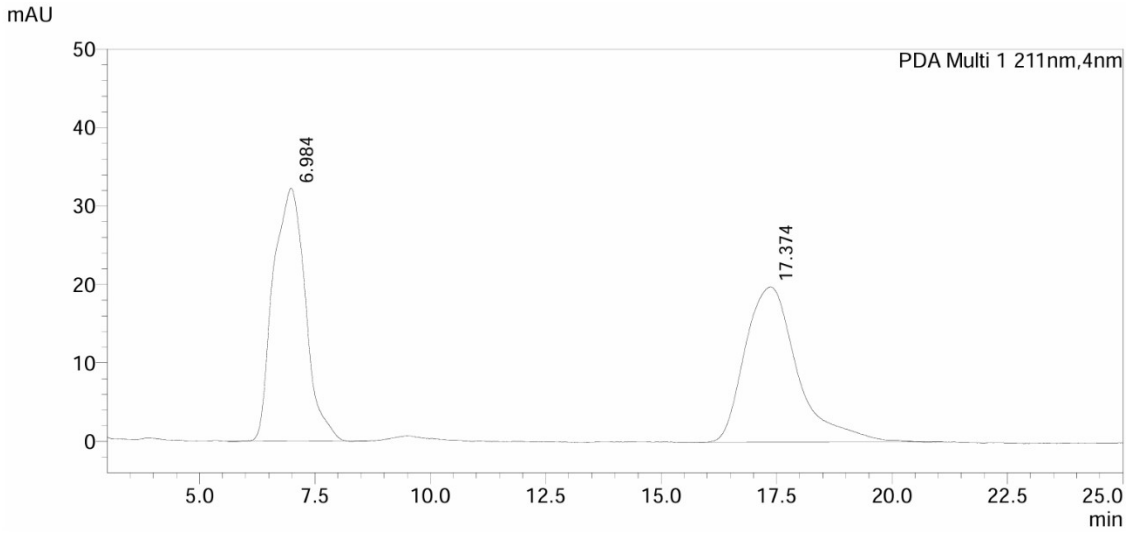
HPLC data for **53**: Chiralcel OD-H (90:10 *n*-hexane : IPA, flow rate 2.0 mLmin^{-1}, 211 nm, 40 °C) t_R (*S*) 7.0 min, t_R (*R*) 16.5 min, 96:4 er.



53

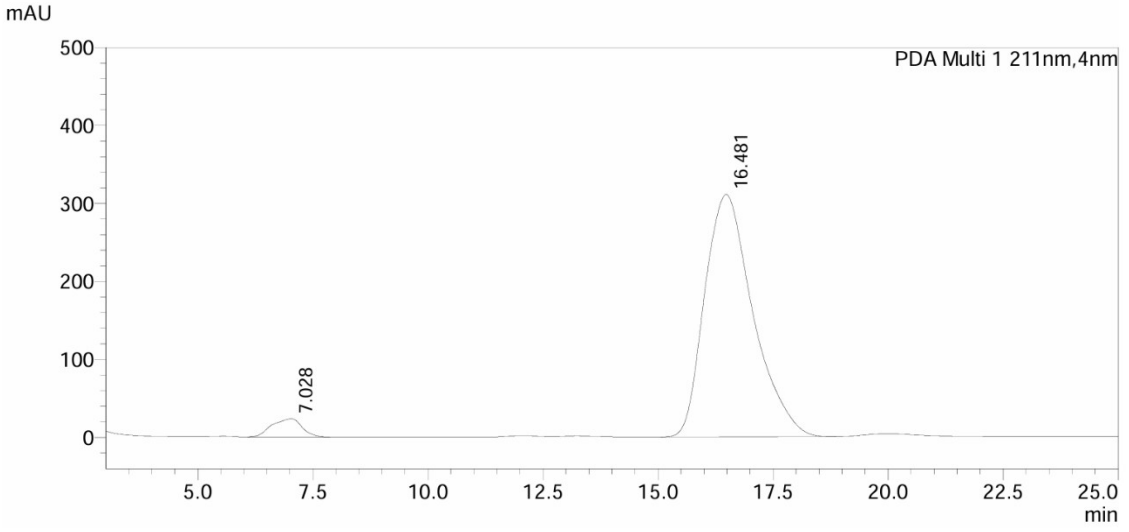
PDA Ch1 211nm

Peak#	Ret. Time	Area%
1	6.984	49.989
2	17.374	50.011
Total		100.000

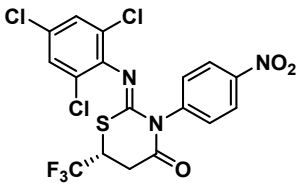


PDA Ch1 211nm

Peak#	Ret. Time	Area%
1	7.028	4.445
2	16.481	95.555
Total		100.000



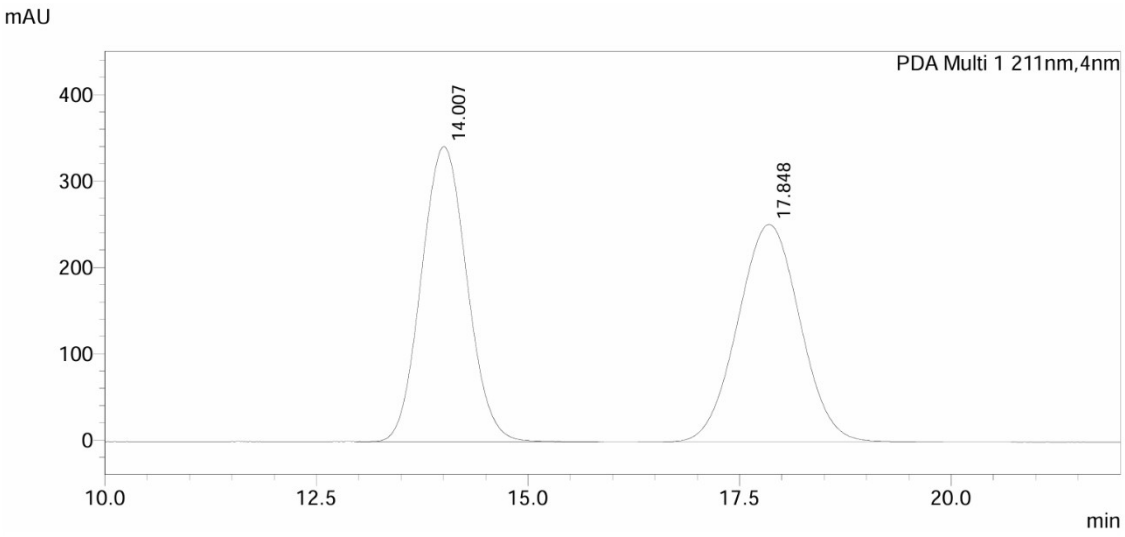
HPLC data for **54**: Chiralpak AD-H (90:10 *n*-hexane : IPA, flow rate 1.0 mLmin^{-1}, 211 nm, 30 °C) t_R (*R*) 14.0 min, t_R (*S*) 17.9 min, 98:2 er.



54

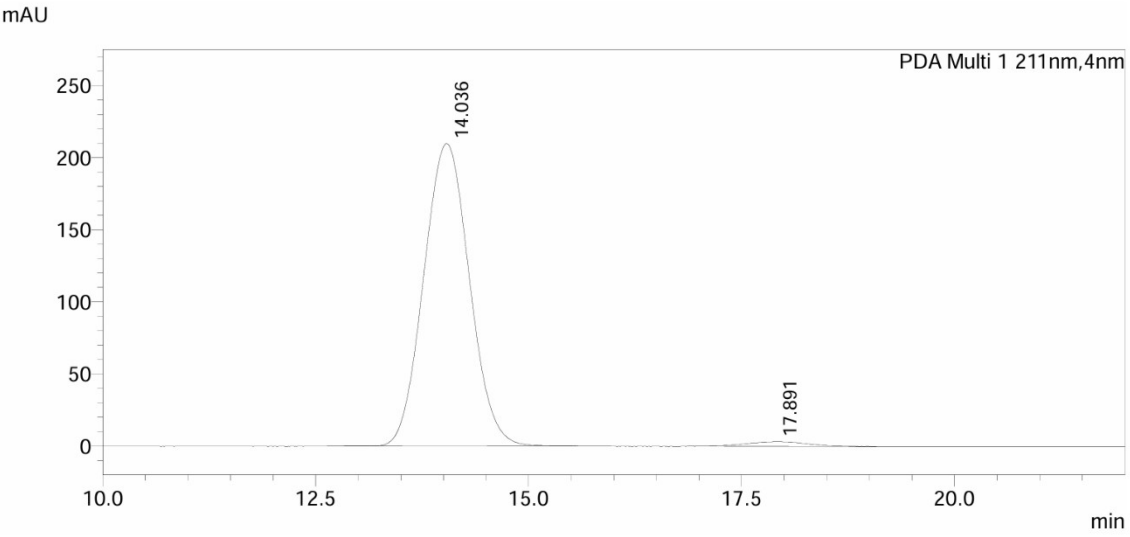
PDA Ch1 211nm

Peak#	Ret. Time	Area%
1	14.007	49.856
2	17.848	50.144
Total		100.000

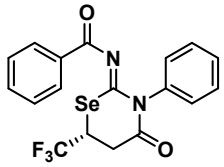


PDA Ch1 211nm

Peak#	Ret. Time	Area%
1	14.036	97.958
2	17.891	2.042
Total		100.000



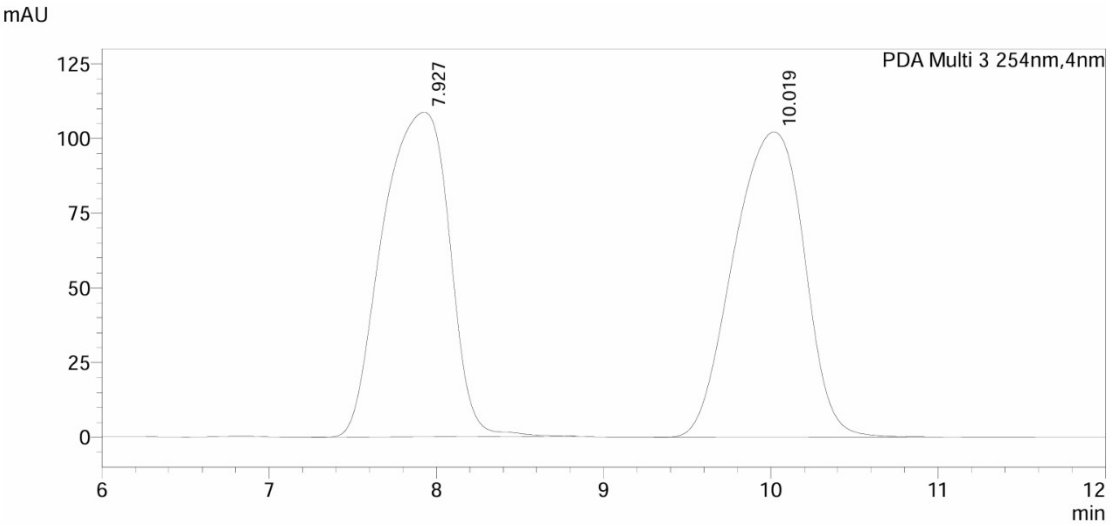
HPLC data for **55**: Chiralpak IA (80:20 *n*-hexane : IPA, flow rate 1.0 mLmin^{-1}, 254 nm, 30 °C) t_R (*S*) 8.0 min, t_R (*R*) 10.2 min, 99:1 er.



55

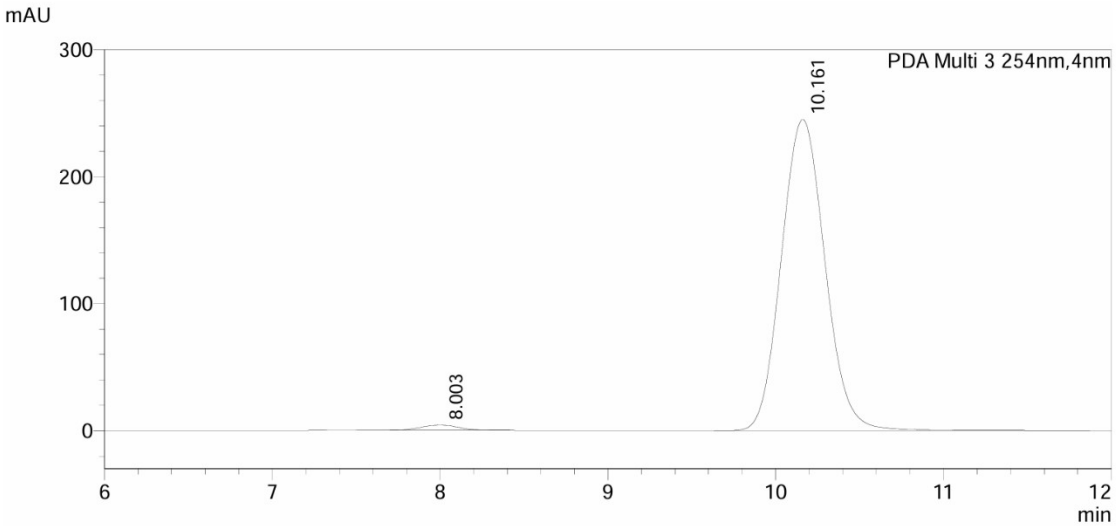
PDA Ch3 254nm

Peak#	Ret. Time	Area%
1	7.927	50.086
2	10.019	49.914
Total		100.000

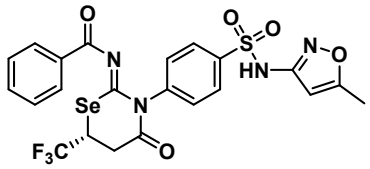


PDA Ch3 254nm

Peak#	Ret. Time	Area%
1	8.003	1.444
2	10.161	98.556
Total		100.000



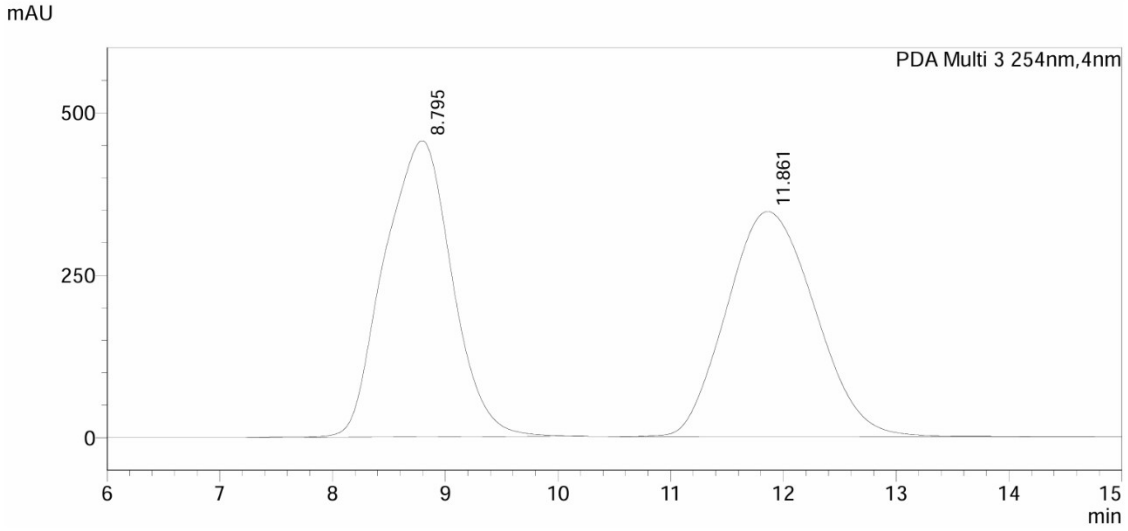
HPLC data for **56**: Chiralpak AD-H (60:40 *n*-hexane : IPA, flow rate 1.0 mLmin^{-1}, 254 nm, 30 °C) t_R (*S*) 8.8 min, t_R (*R*) 12.0 min, 98:2 er.



56

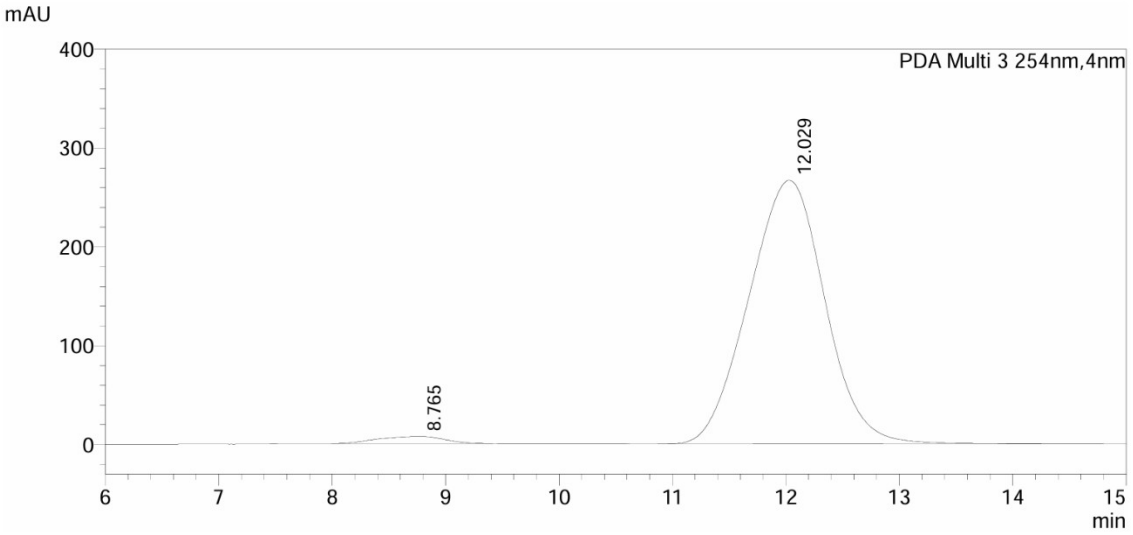
PDA Ch3 254nm

Peak#	Ret. Time	Area%
1	8.795	50.040
2	11.861	49.960
Total		100.000

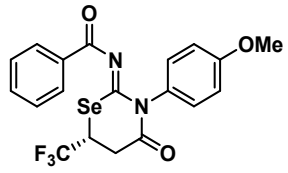


PDA Ch3 254nm

Peak#	Ret. Time	Area%
1	8.765	2.294
2	12.029	97.706
Total		100.000



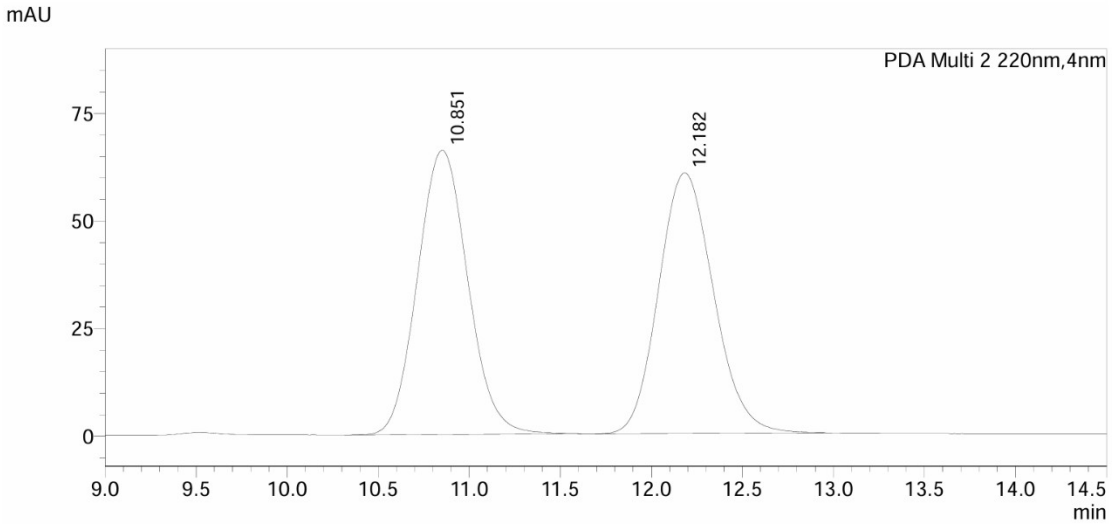
HPLC data for **57**: Chiralpak IA (80:20 *n*-hexane : IPA, flow rate 1.0 mLmin^{-1}, 220 nm, 30 °C) t_R (*S*) 10.8 min, t_R (*R*) 12.1 min, 98:2 er.



57

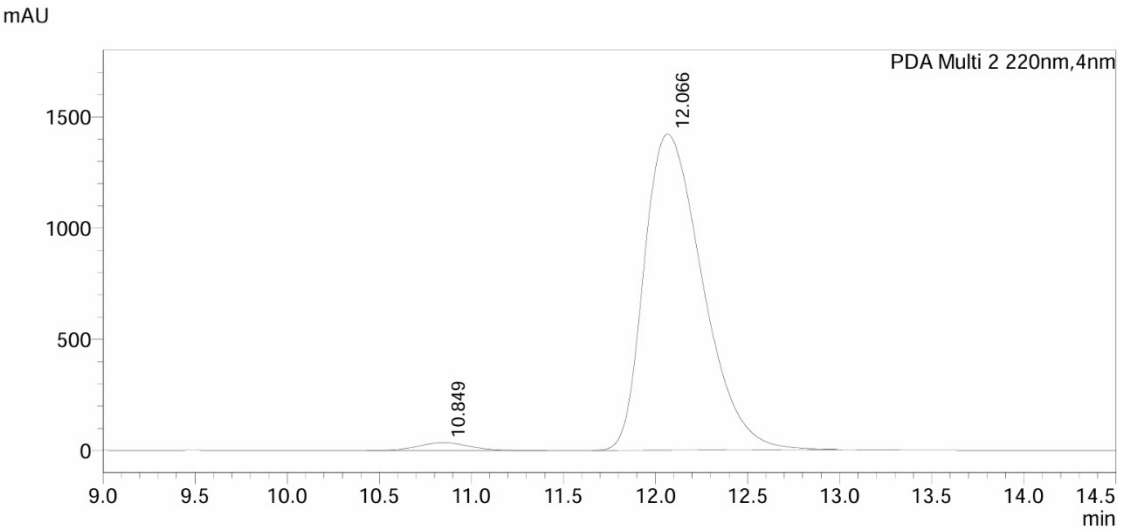
PDA Ch2 220nm

Peak#	Ret. Time	Area%
1	10.851	49.946
2	12.182	50.054
Total		100.000

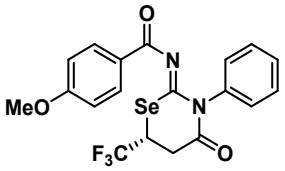


PDA Ch2 220nm

Peak#	Ret. Time	Area%
1	10.849	2.067
2	12.066	97.933
Total		100.000



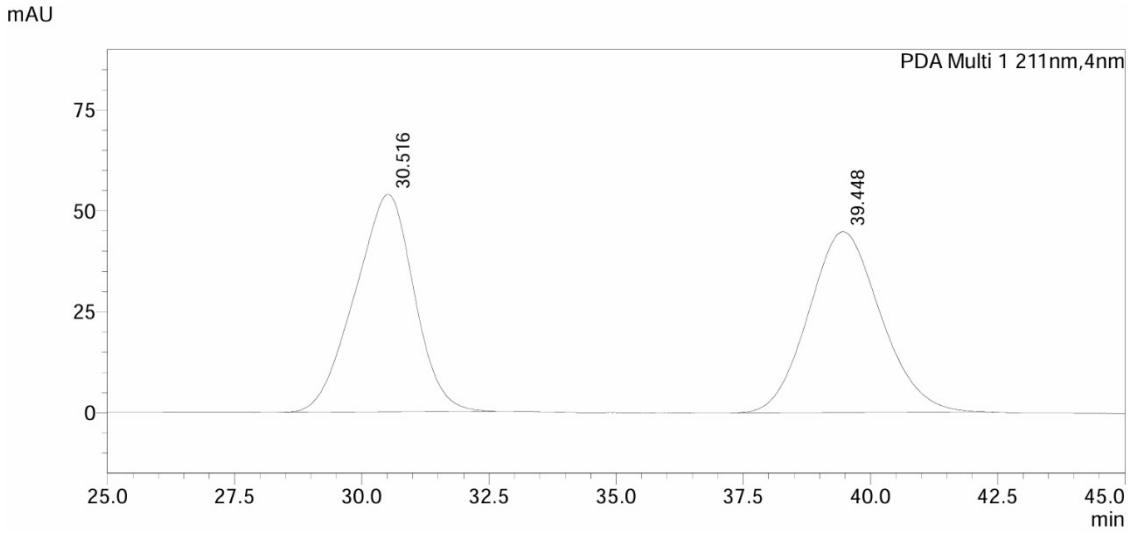
HPLC data for **58**: Chiralpak IB (90:10 *n*-hexane : IPA, flow rate 1.0 mLmin^{-1}, 211 nm, 30 °C) t_R (*S*) 30.6 min, t_R (*R*) 37.3 min, 99:1 er.



58

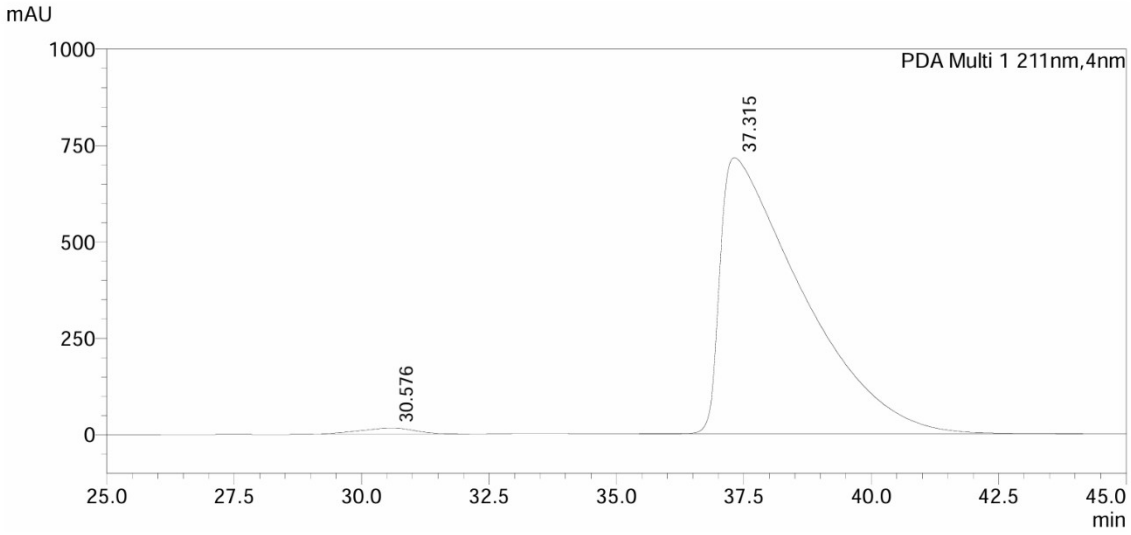
PDA Ch1 211nm

Peak#	Ret. Time	Area%
1	30.516	49.630
2	39.448	50.370
Total		100.000

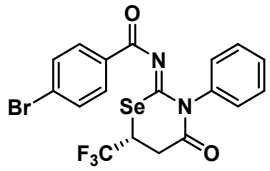


PDA Ch1 211nm

Peak#	Ret. Time	Area%
1	30.576	1.387
2	37.315	98.613
Total		100.000



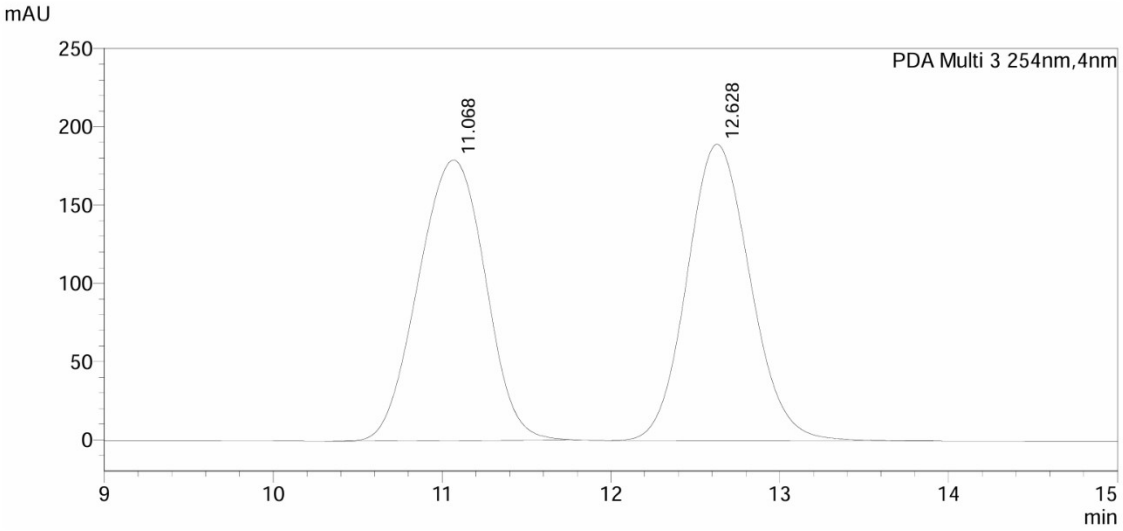
HPLC data for **59**: Chiralpak IA (80:20 *n*-hexane : IPA, flow rate 1.0 mLmin^{-1}, 254 nm, 30 °C) t_R (*S*) 11.1 min, t_R (*R*) 12.5 min, 98:2 er.



59

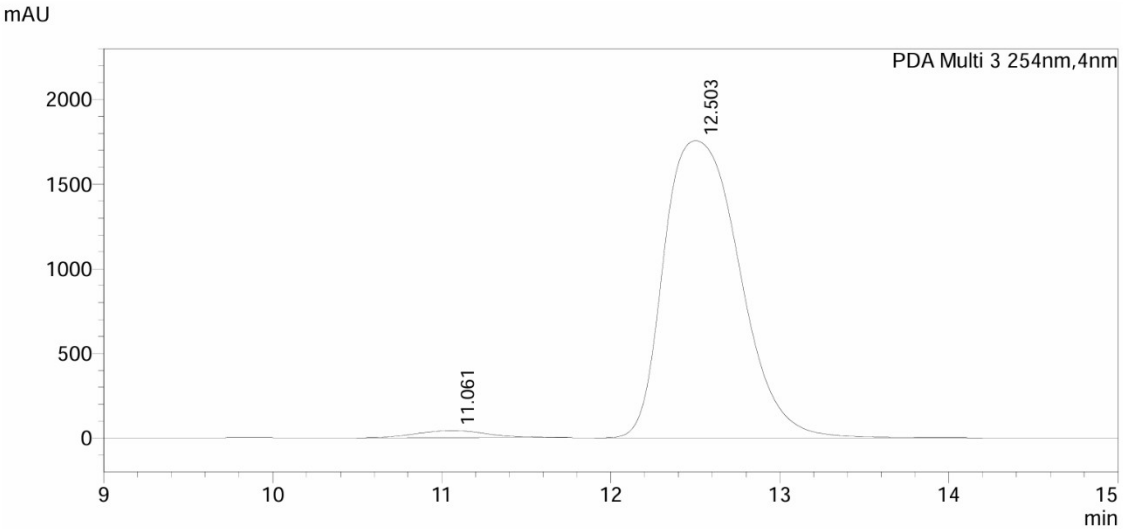
PDA Ch3 254nm

Peak#	Ret. Time	Area%
1	11.068	50.067
2	12.628	49.933
Total		100.000

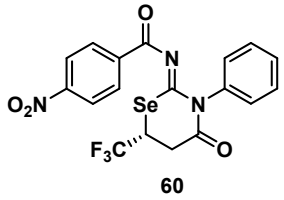


PDA Ch3 254nm

Peak#	Ret. Time	Area%
1	11.061	2.230
2	12.503	97.770
Total		100.000



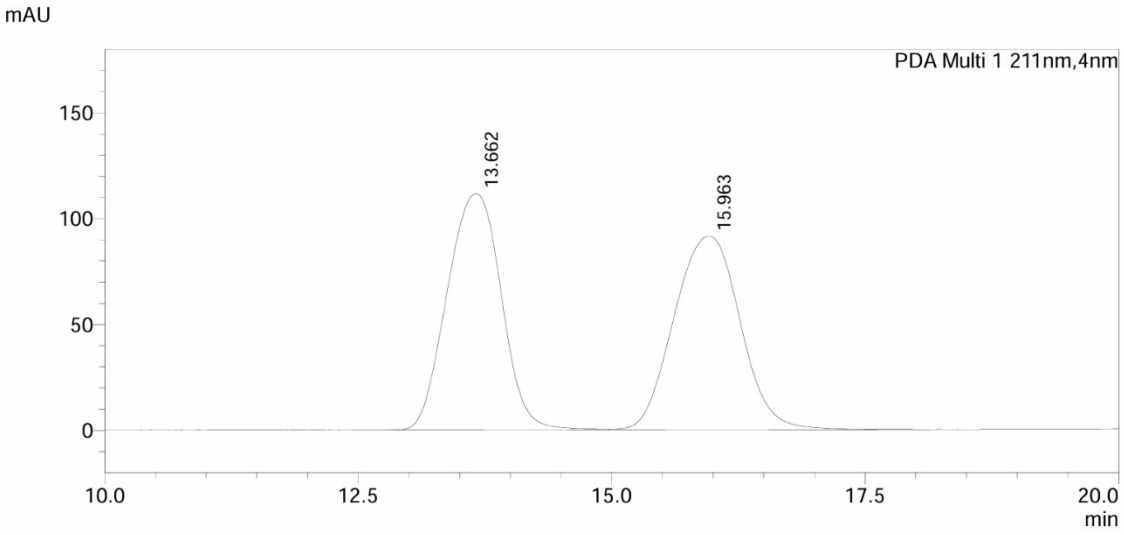
HPLC data for **60**: Chiralpak IA (80:20 *n*-hexane : IPA, flow rate 1.0 mLmin^{-1}, 211 nm, 30 °C) t_R (*S*) 13.8 min, t_R (*R*) 15.8 min, 97:3 er.



60

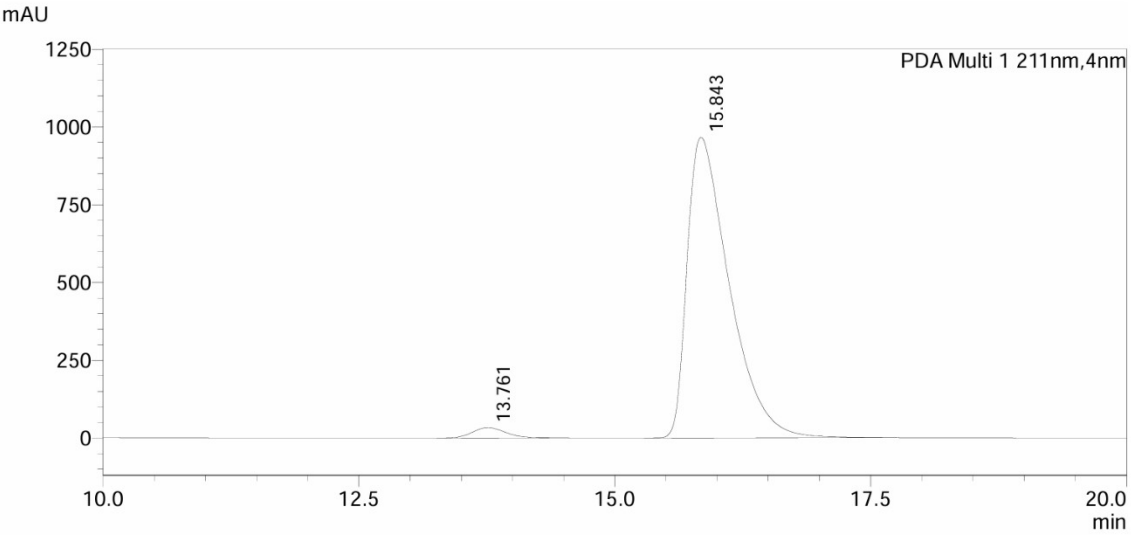
PDA Ch1 211nm

Peak#	Ret. Time	Area%
1	13.662	50.008
2	15.963	49.992
Total		100.000

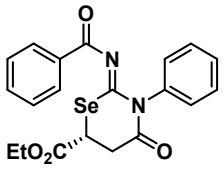


PDA Ch1 211nm

Peak#	Ret. Time	Area%
1	13.761	2.623
2	15.843	97.377
Total		100.000



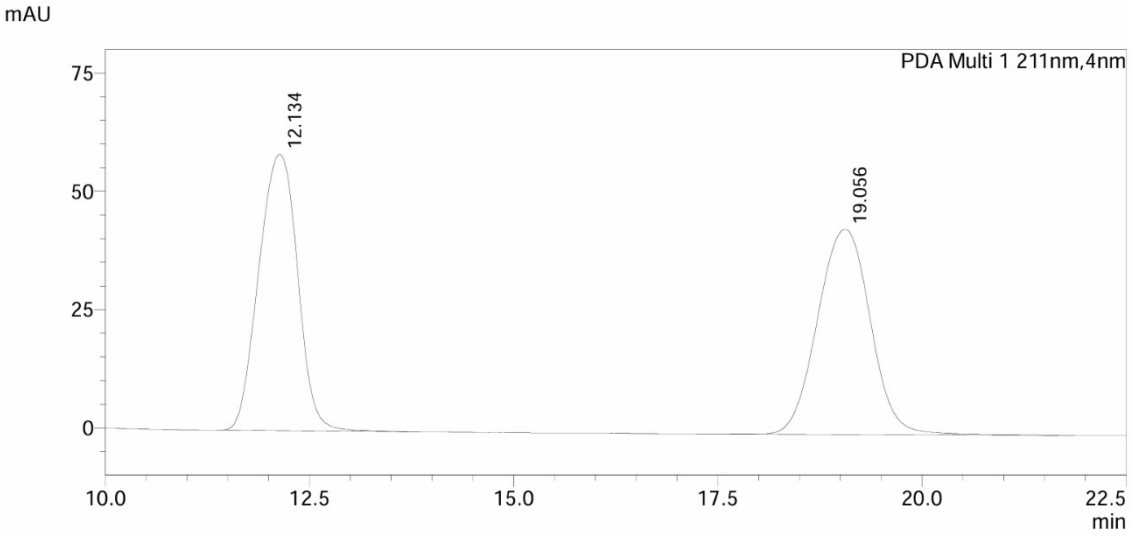
HPLC data for **61**: Chiralpak IA (80:20 *n*-hexane : IPA, flow rate 1.0 mLmin^{-1}, 211 nm, 30 °C) t_R (*S*) 12.1 min, t_R (*R*) 18.8 min, 93:7 er.



61

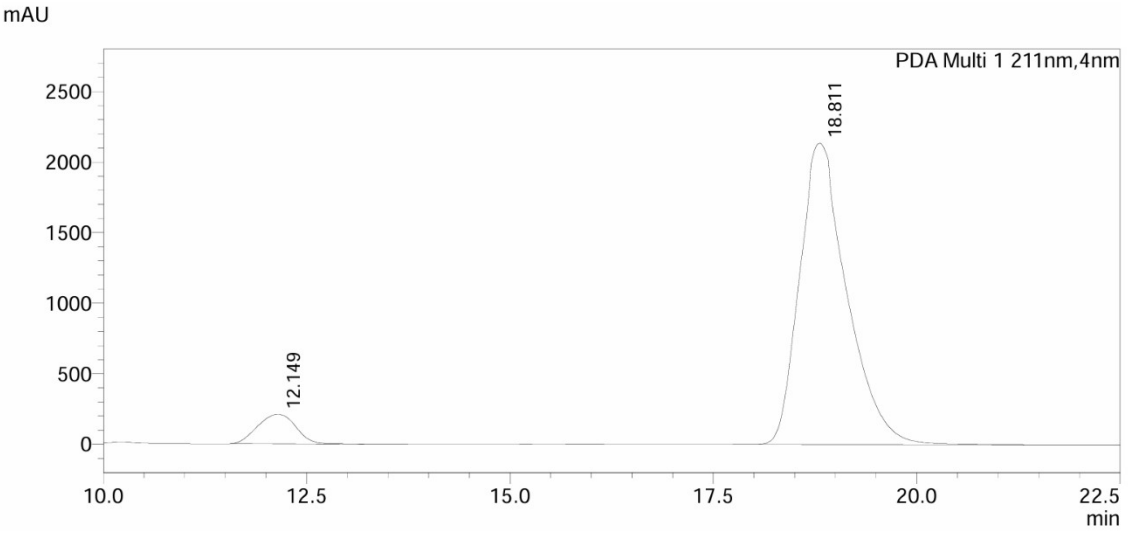
PDA Ch1 211nm

Peak#	Ret. Time	Area%
1	12.134	49.736
2	19.056	50.264
Total		100.000

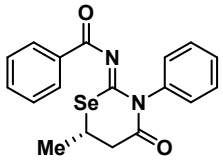


PDA Ch1 211nm

Peak#	Ret. Time	Area%
1	12.149	7.392
2	18.811	92.608
Total		100.000



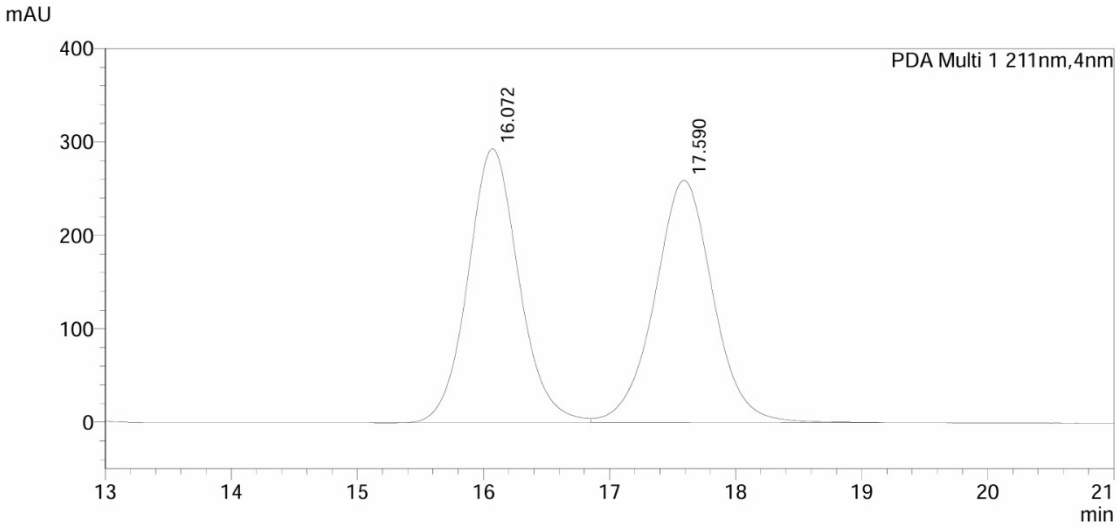
HPLC data for **62**: Chiralpak IA (90:10 *n*-hexane : IPA, flow rate 1.0 mLmin^{-1}, 211 nm, 30 °C) t_R (*R*) 16.0 min, t_R (*S*) 17.5 min, 87:13 er.



62

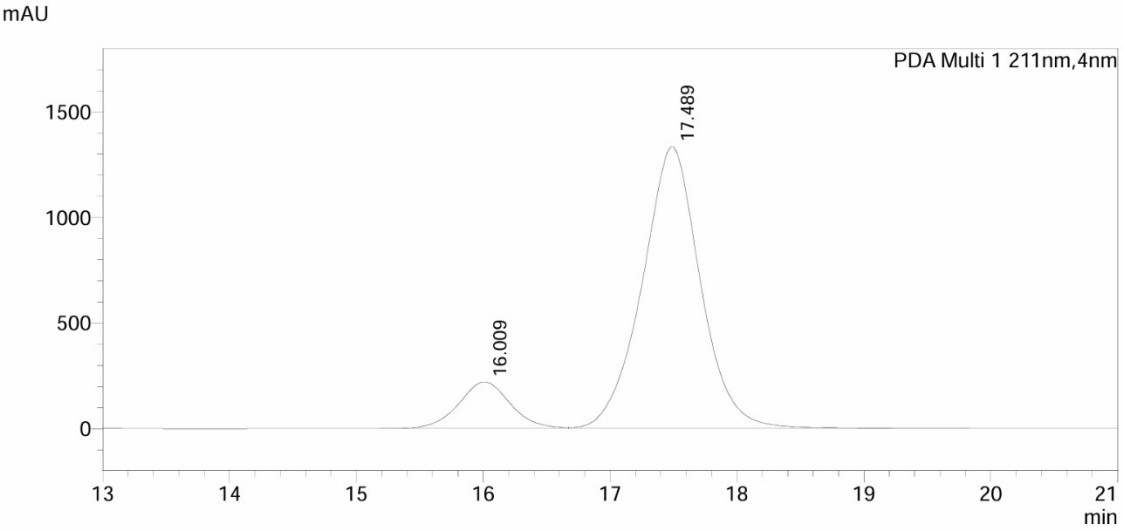
PDA Ch1 211nm

Peak#	Ret. Time	Area%
1	16.072	49.702
2	17.590	50.298
Total		100.000

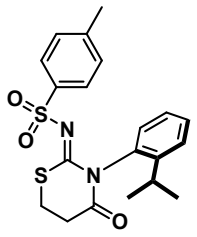


PDA Ch1 211nm

Peak#	Ret. Time	Area%
1	16.009	12.834
2	17.489	87.166
Total		100.000



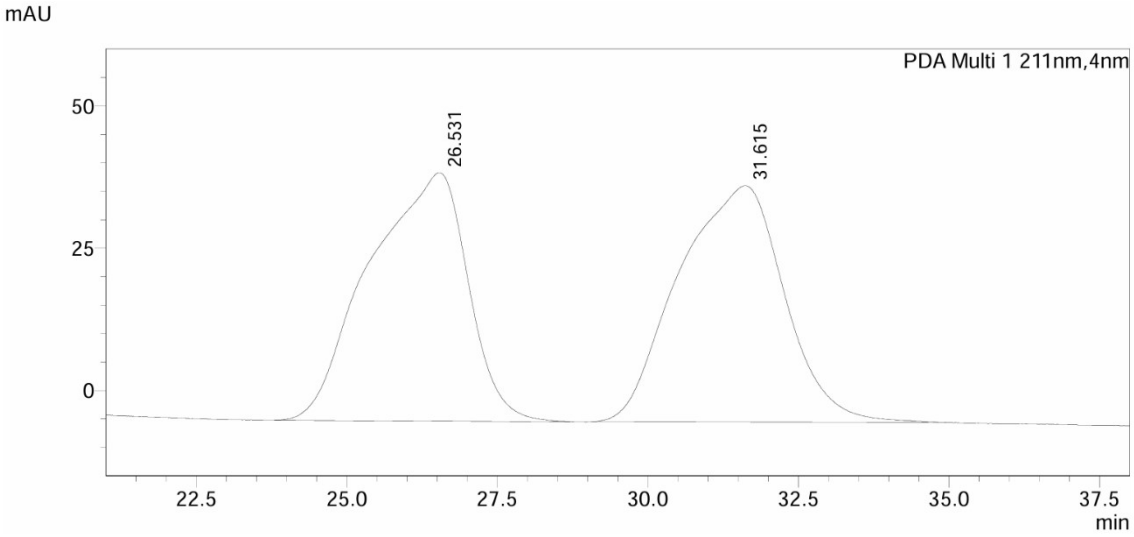
HPLC data for **63**: Chiralpak IB (80:20 *n*-hexane : IPA, flow rate 1.0 mLmin^{-1}, 211 nm, 30 °C) t_R (R_a) 26.0 min, t_R (S_a) 31.5 min, 87:13 er.



63

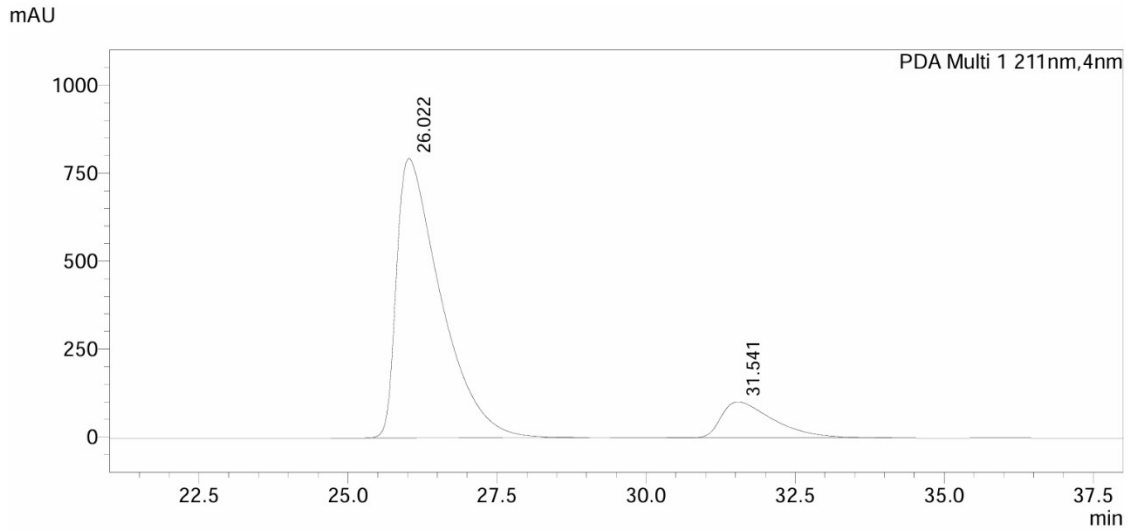
PDA Ch1 211nm

Peak#	Ret. Time	Area%
1	26.531	49.460
2	31.615	50.540
Total		100.000

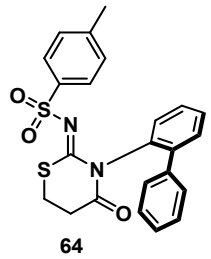


PDA Ch1 211nm

Peak#	Ret. Time	Area%
1	26.022	86.808
2	31.541	13.192
Total		100.000



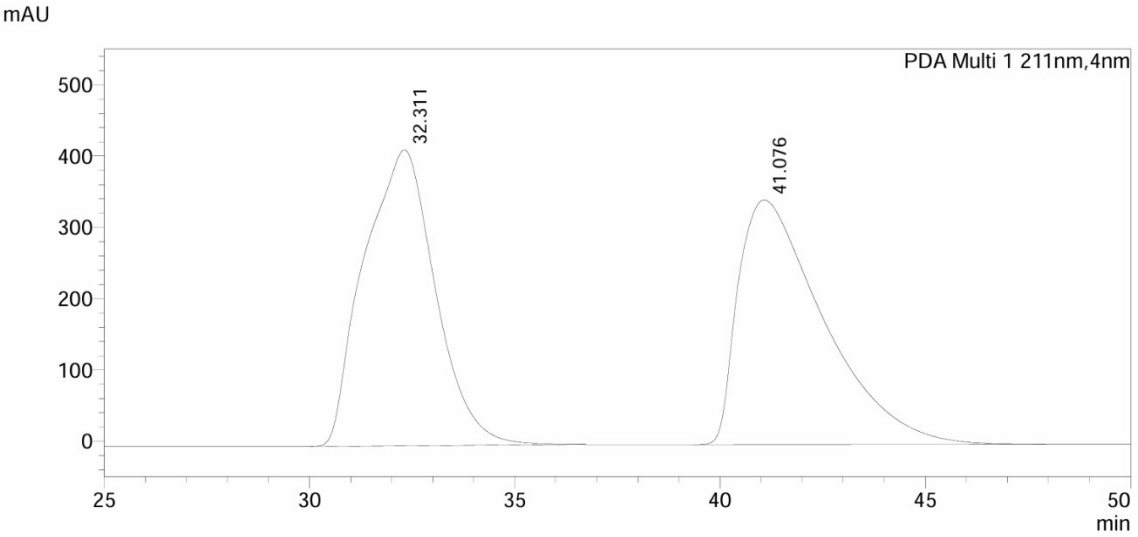
HPLC data for **64**: Chiralpak IB (80:20 *n*-hexane : IPA, flow rate 1.0 mLmin^{-1}, 211 nm, 30 °C) t_R (R_a) 31.9 min, t_R (S_a) 41.2 min, 73:27 er.



64

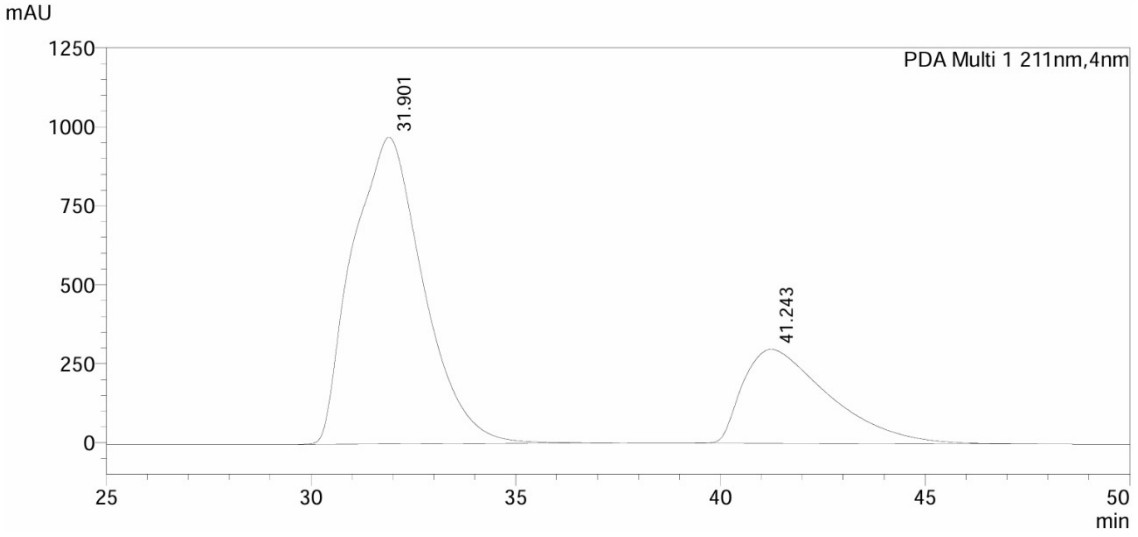
PDA Ch1 211nm

Peak#	Ret. Time	Area%
1	32.311	50.154
2	41.076	49.846
Total		100.000

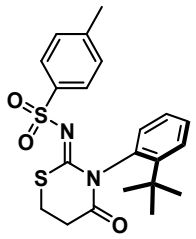


PDA Ch1 211nm

Peak#	Ret. Time	Area%
1	31.901	72.800
2	41.243	27.200
Total		100.000



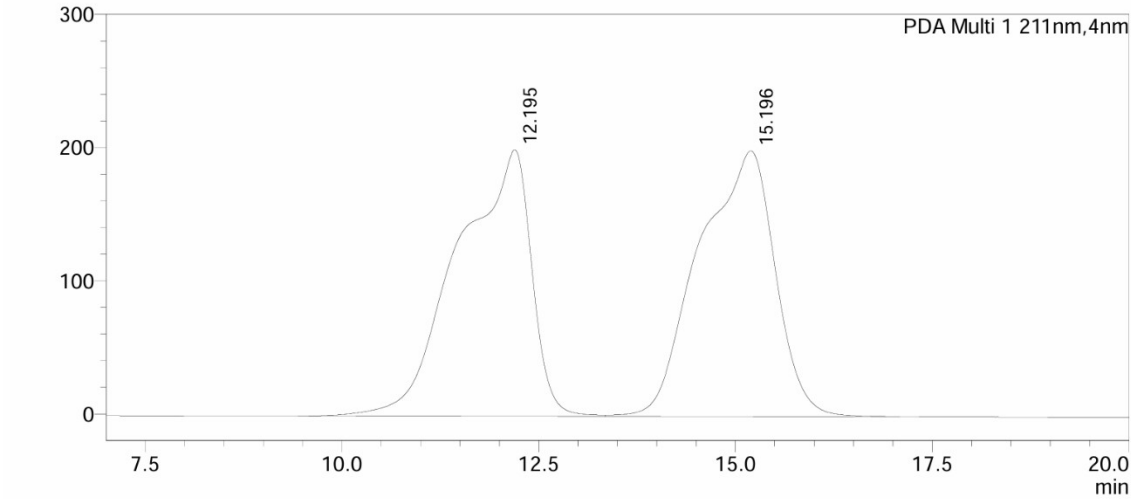
HPLC data for **65**: Chiralpak IB (60:40 *n*-hexane : IPA, flow rate 1.0 mLmin^{-1}, 211 nm, 30 °C) t_R (R_a) 12.1 min, t_R (S_a) 15.2 min, 80:20 er.



65

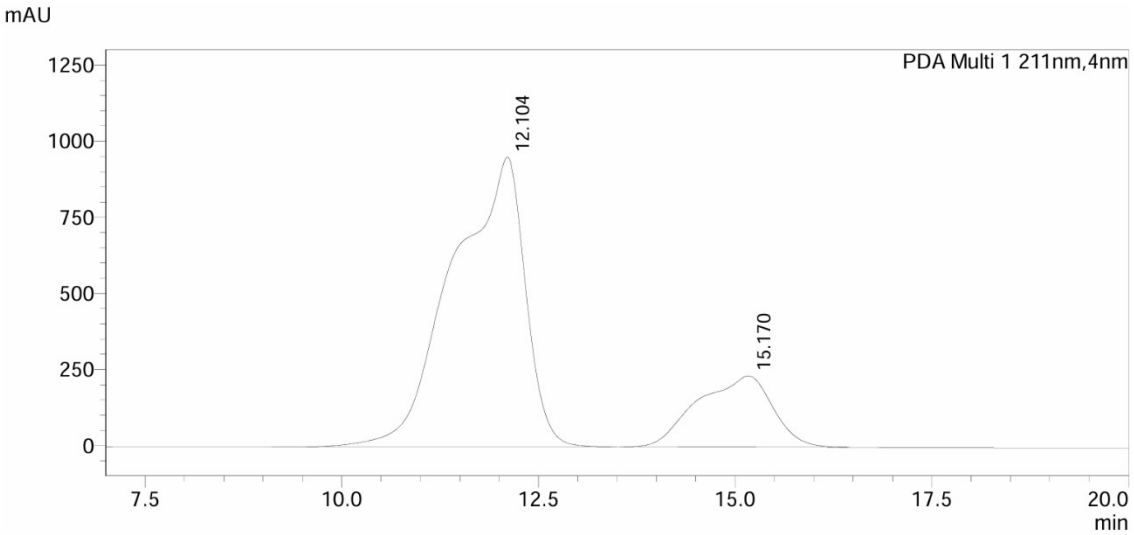
PDA Ch1 211nm

Peak#	Ret. Time	Area%
1	12.195	49.485
2	15.196	50.515
Total		100.000

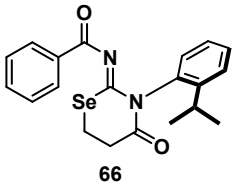


PDA Ch1 211nm

Peak#	Ret. Time	Area%
1	12.104	79.785
2	15.170	20.215
Total		100.000



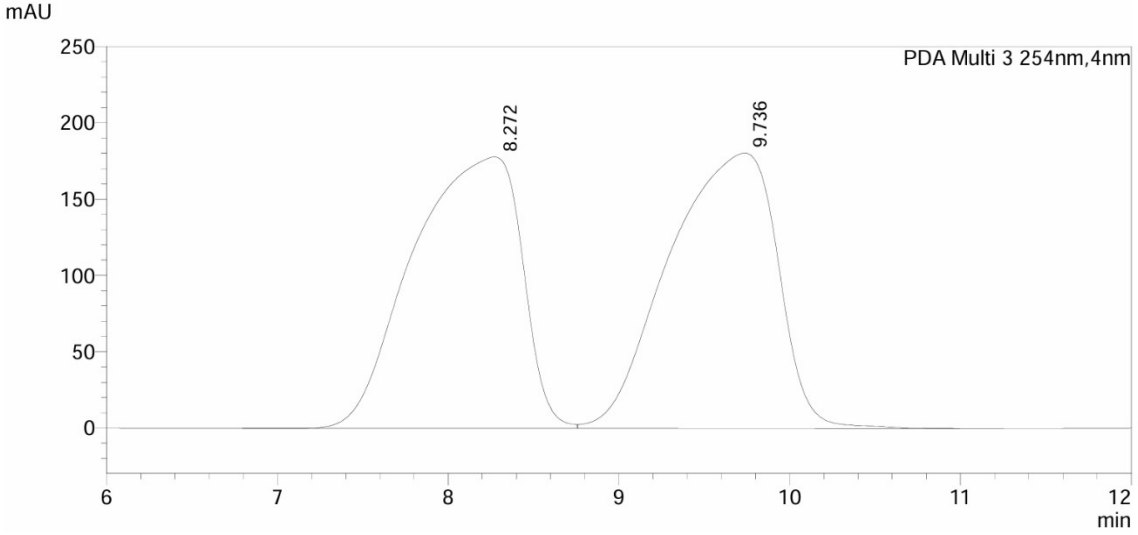
HPLC data for **66**: Chiralpak IB (80:20 *n*-hexane : IPA, flow rate 1.0 mLmin^{-1}, 254 nm, 30 °C) t_R (R_a) 8.3 min, t_R (S_a) 9.7 min, 77:23 er.



66

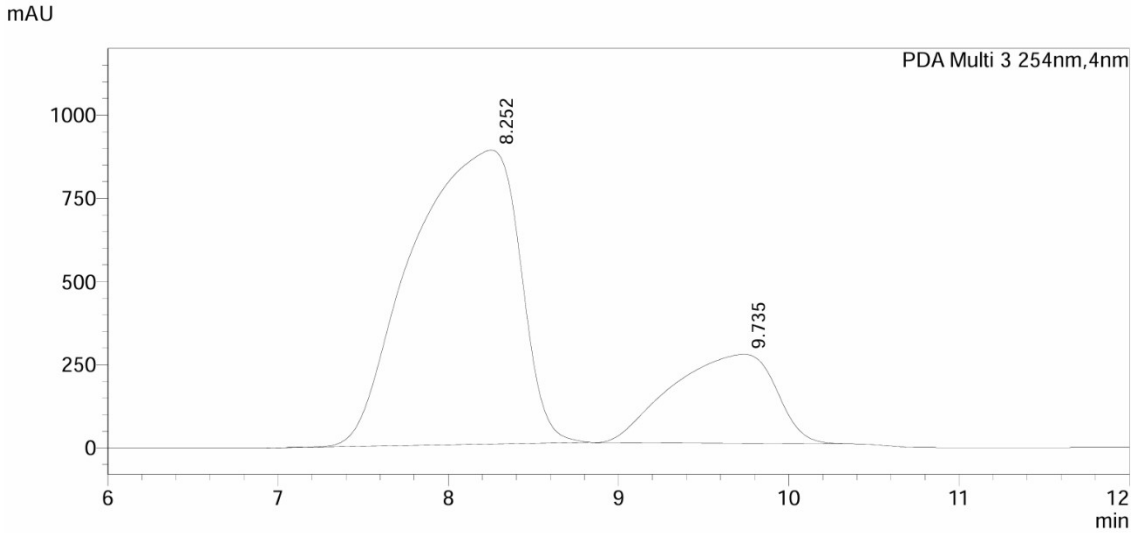
PDA Ch3 254nm

Peak#	Ret. Time	Area%
1	8.272	49.690
2	9.736	50.310
Total		100.000



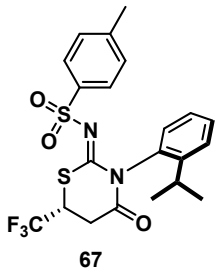
PDA Ch3 254nm

Peak#	Ret. Time	Area%
1	8.252	77.475
2	9.735	22.525
Total		100.000

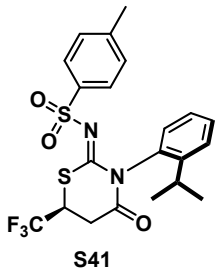


HPLC data for (*R*,R_a,*Z*)-**67**: Chiralpak AD-H (80:20 *n*-hexane : IPA, flow rate 1.0 mLmin^{-1}, 254 nm, 30 °C) t_R (*R*,R_a) 7.8 min, t_R (*S*,S_a) 17.5 min, 98:2 er.

HPLC data for (*S*,R_a,*Z*)-**S41**: er not determined.



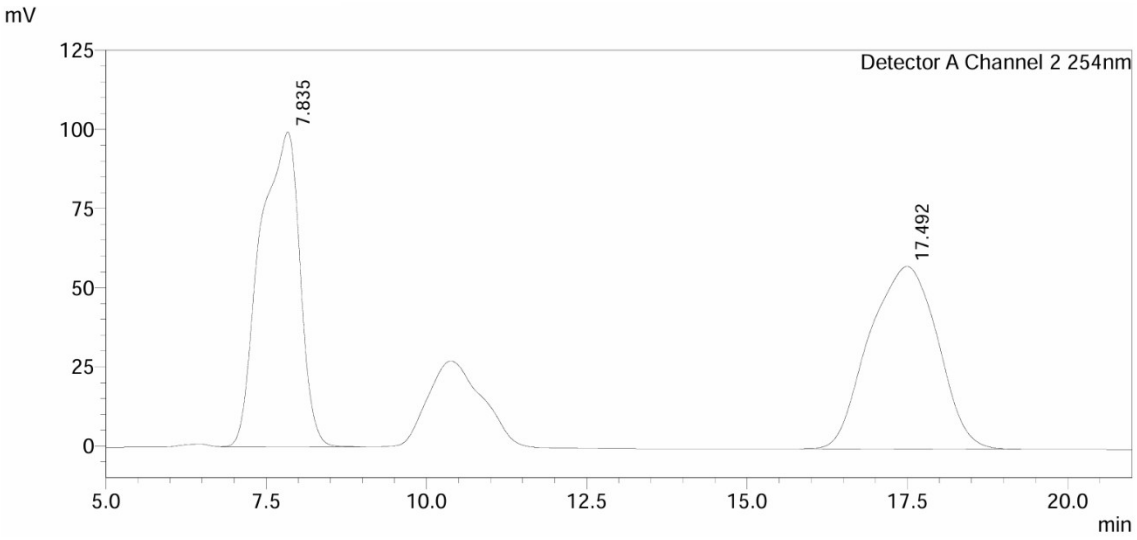
67



S41

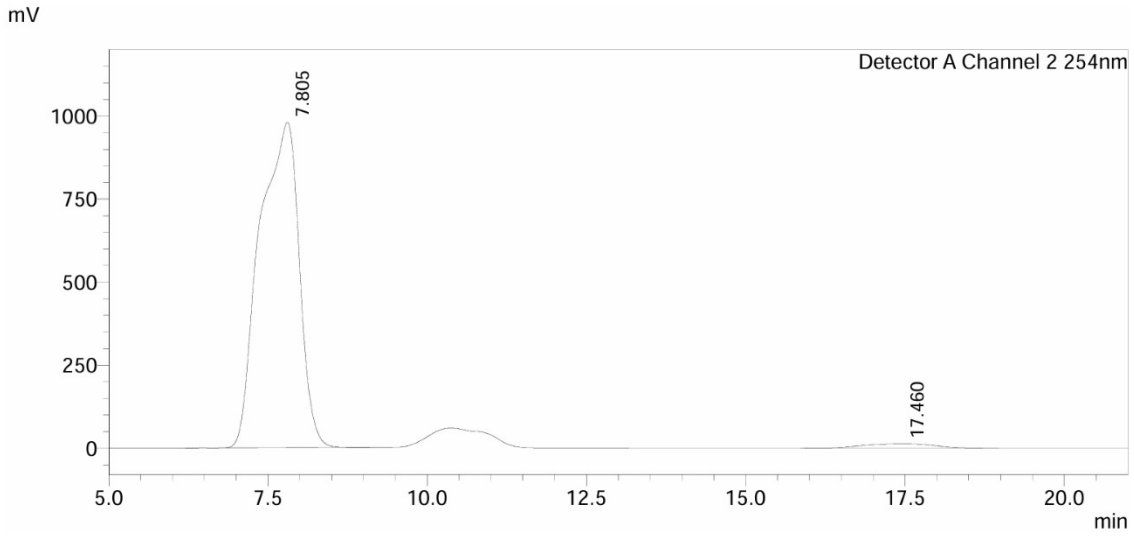
Detector A Channel 2 254nm

Peak#	Ret. Time	Area%
1	7.835	49.958
2	17.492	50.042
Total		100.000



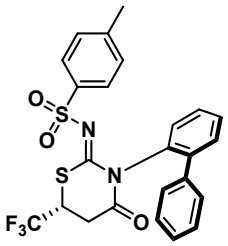
Detector A Channel 2 254nm

Peak#	Ret. Time	Area%
1	7.805	97.681
2	17.460	2.319
Total		100.000

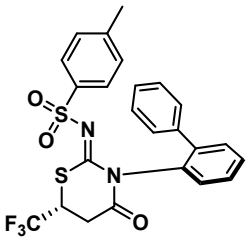


HPLC data for (*R*,R_a,*Z*)-**68**: Chiralcel OD-H (70:30 *n*-hexane : IPA, flow rate 1.0 mLmin^{-1}, 211 nm, 30 °C) t_R (*S*,S_a) 7.8 min, t_R (*R*,R_a) 18.5 min, 95:5 er.

HPLC data for (*R*,S_a,*Z*)-**S42**: Chiralcel OD-H (70:30 *n*-hexane : IPA, flow rate 1.0 mLmin^{-1}, 211 nm, 30 °C) t_R (*S*,R_a) 14.0 min, t_R (*R*,S_a) 33.2 min, 63:37 er.



68



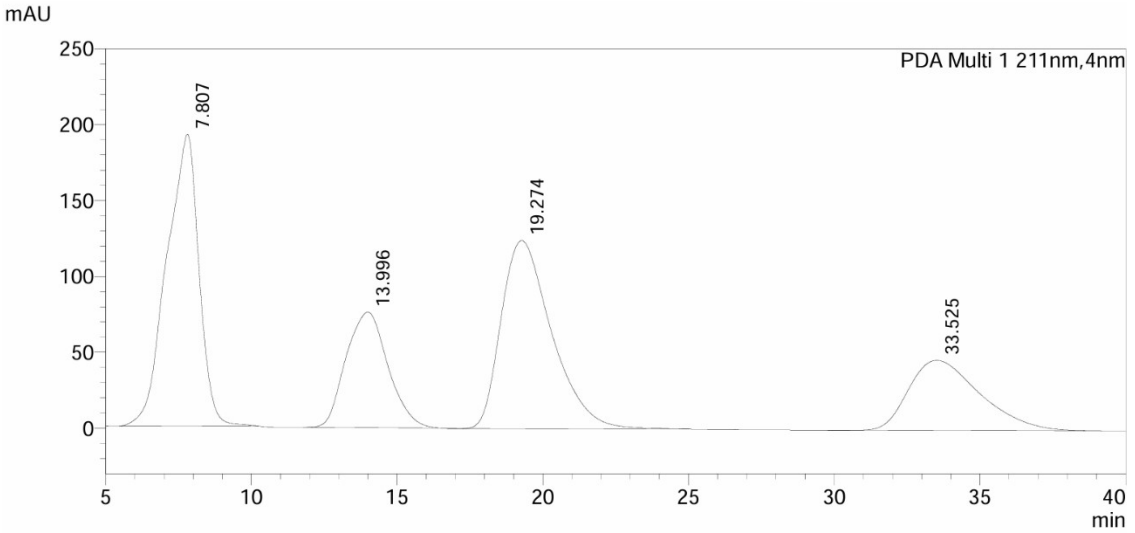
S42

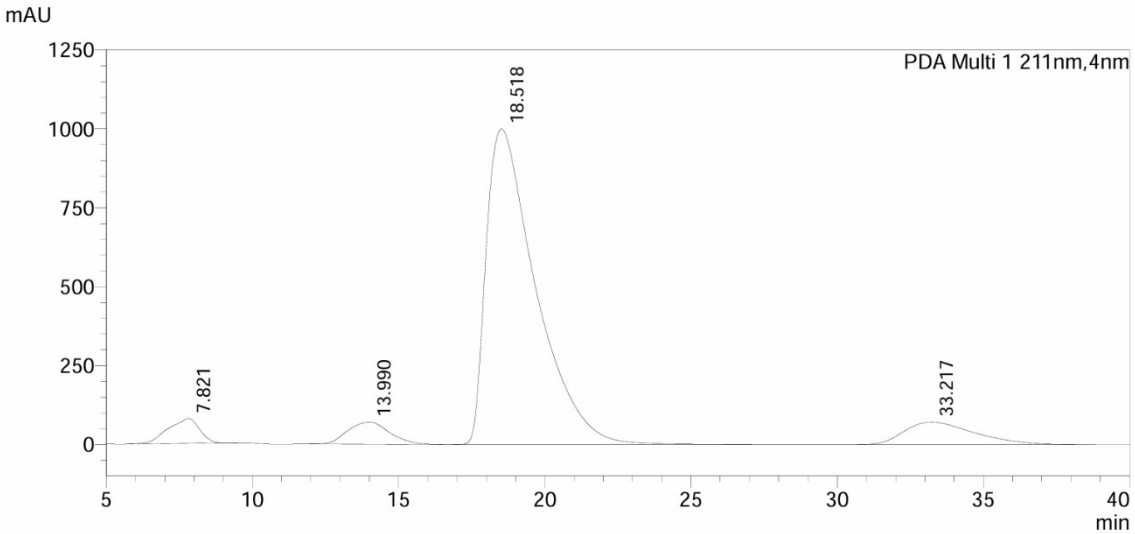
PDA Ch1 211nm

Peak#	Ret. Time	Area%
1	7.807	32.812
2	13.996	16.845
3	19.274	33.073
4	33.525	17.270
Total		100.000

PDA Ch1 211nm

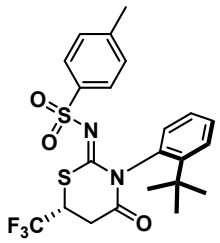
Peak#	Ret. Time	Area%
1	7.821	4.124
2	13.990	4.882
3	18.518	82.680
4	33.217	8.314
Total		100.000



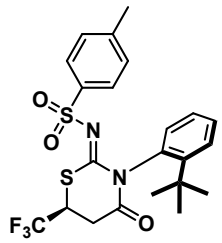


HPLC data for (*R*,R_a,*Z*)-**69**: Chiralpak IB (90:10 *n*-hexane : IPA, flow rate 1.0 mLmin^{-1}, 211 nm, 30 °C) t_R (*R*,R_a) 15.8 min, t_R (*S*,S_a) 20.3 min, 97:3 er.

HPLC data for (*S*,R_a,*Z*)-**S43**: Chiralpak IB (90:10 *n*-hexane : IPA, flow rate 1.0 mLmin^{-1}, 211 nm, 30 °C) t_R (*S*,R_a) 26.1 min, t_R (*R*,S_a) 40.6 min, 53:47 er.



69



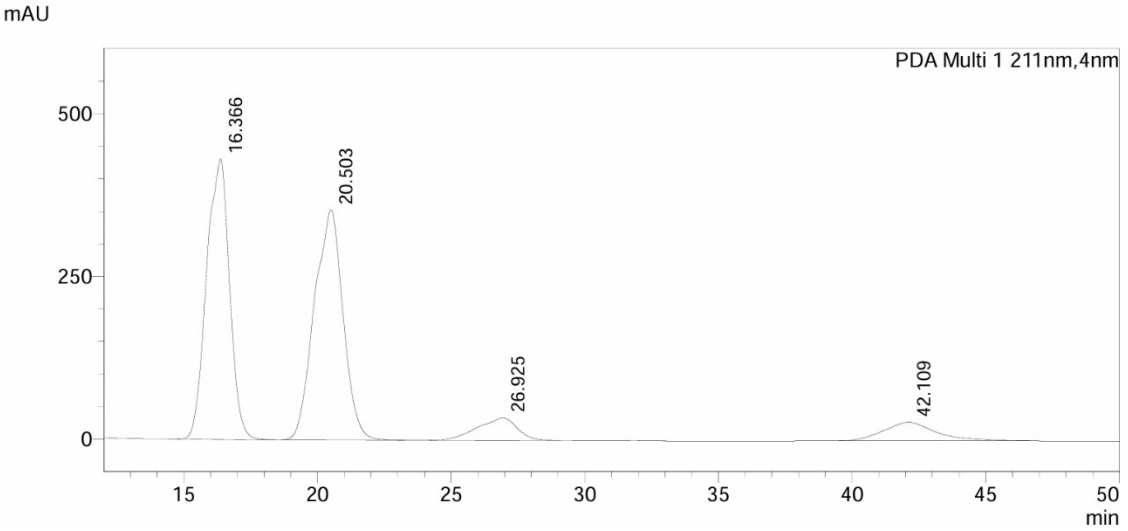
S43

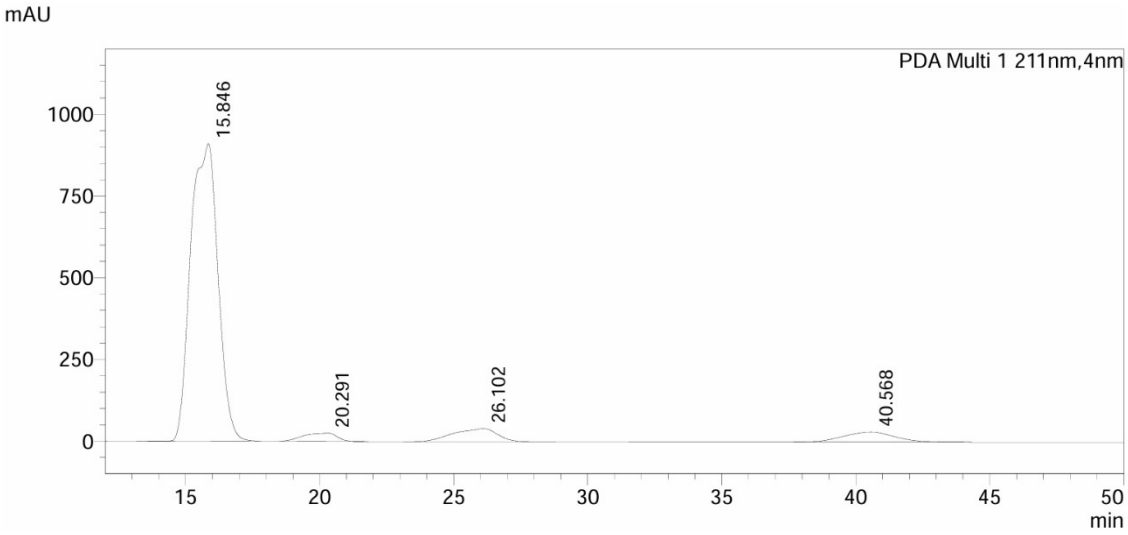
PDA Ch1 211nm

Peak#	Ret. Time	Area%
1	16.366	43.158
2	20.503	44.296
3	26.925	6.000
4	42.109	6.547
Total		100.000

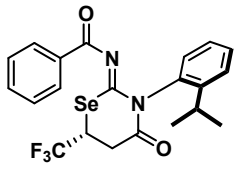
PDA Ch1 211nm

Peak#	Ret. Time	Area%
1	15.846	85.482
2	20.291	2.952
3	26.102	6.160
4	40.568	5.406
Total		100.000





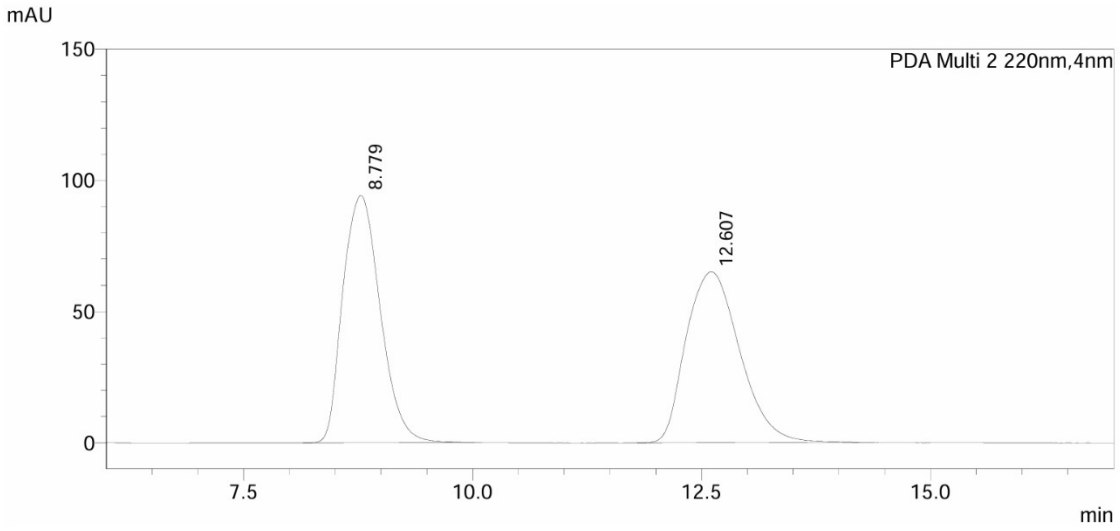
HPLC data for **70**: Chiralpak IB (98:2 *n*-hexane : IPA, flow rate 2.0 mLmin^{-1}, 220 nm, 30 °C) t_R (*S*,S_a) 8.6 min, t_R (*R*,R_a) 12.4 min, 98:2 er.



70

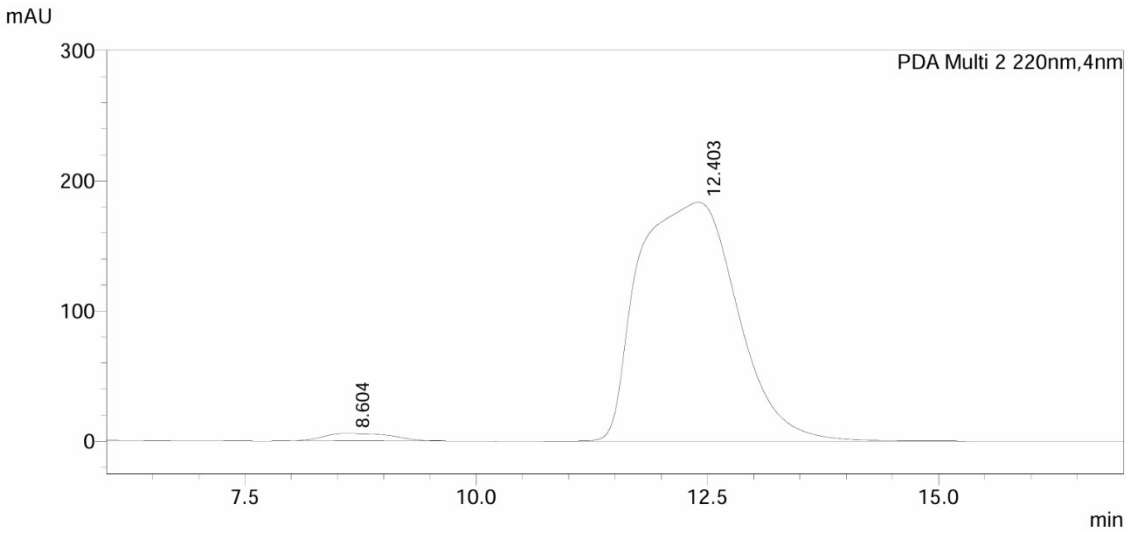
PDA Ch2 220nm

Peak#	Ret. Time	Area%
1	8.779	50.240
2	12.607	49.760
Total		100.000

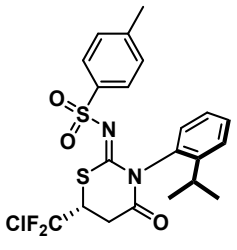


PDA Ch2 220nm

Peak#	Ret. Time	Area%
1	8.604	1.984
2	12.403	98.016
Total		100.000



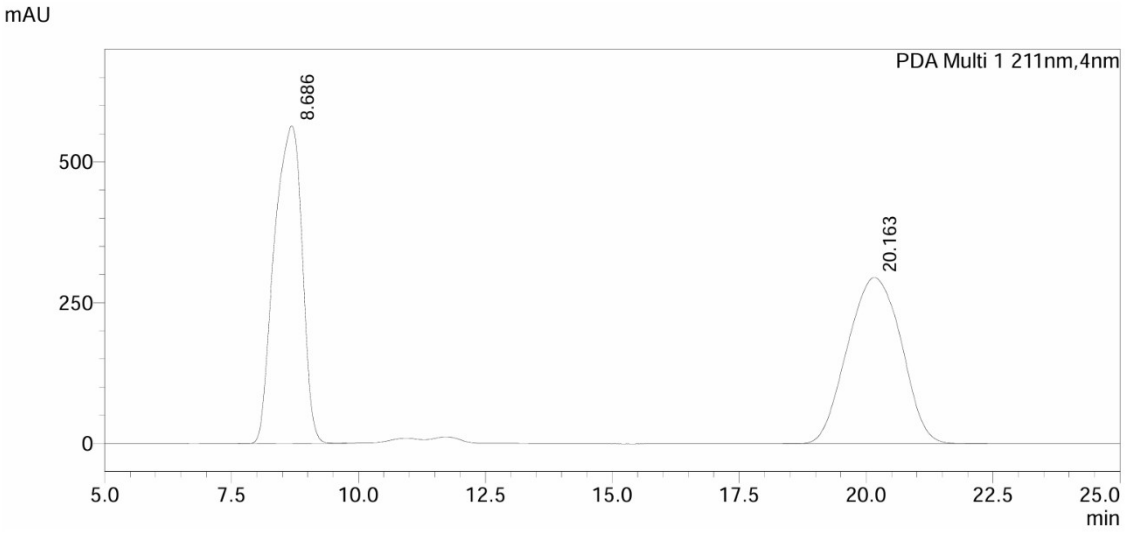
HPLC data for **71**: Chiralpak AD-H (80:20 *n*-hexane : IPA, flow rate 1.0 mLmin^{-1}, 211 nm, 30 °C) t_R (R,R_a) 8.7 min, t_R (S,S_a) 20.3 min, 98:2 er.



71

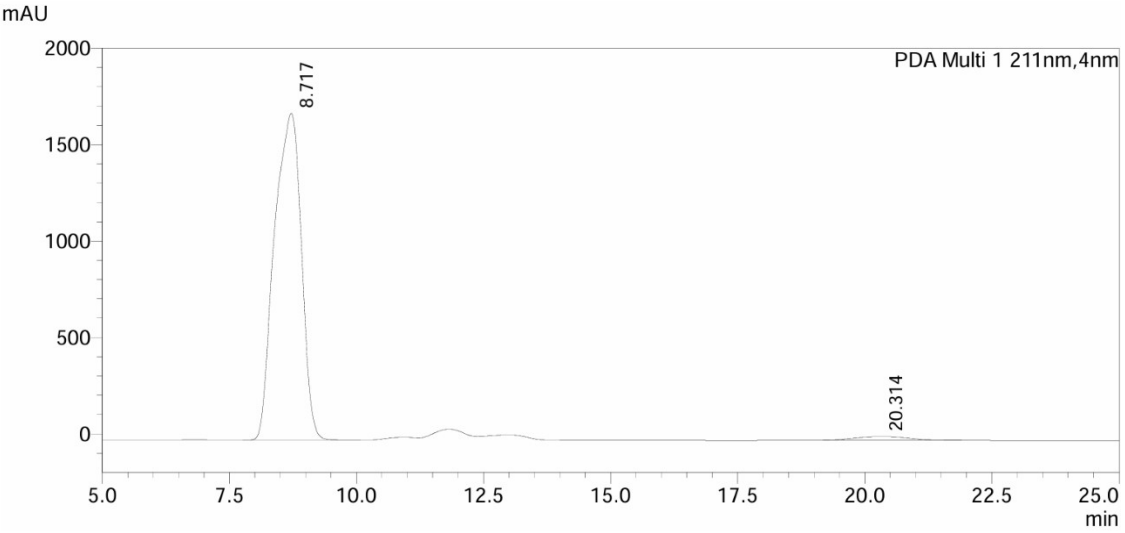
PDA Ch1 211nm

Peak#	Ret. Time	Area%
1	8.686	49.704
2	20.163	50.296
Total		100.000



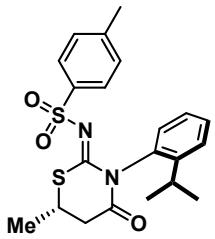
PDA Ch1 211nm

Peak#	Ret. Time	Area%
1	8.717	97.783
2	20.314	2.217
Total		100.000

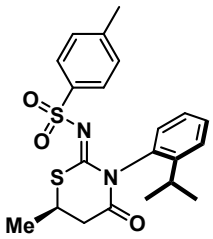


HPLC data for (*S*,R_a,*Z*)-**72**: Chiralpak IA (95:5 *n*-hexane : IPA, flow rate 1.0 mLmin^{-1}, 211 nm, 40 °C) t_R (*S*,R_a) 47.0 min, t_R (*R*,S_a) 58.5 min, 92:8 er.

HPLC data for (*R*,R_a,*Z*)-**S44**: Chiralpak IA (95:5 *n*-hexane : IPA, flow rate 1.0 mLmin^{-1}, 211 nm, 40 °C) t_R (*S*,S_a) 53.4 min, t_R (*R*,R_a) 76.0 min, 88:12 er.



72



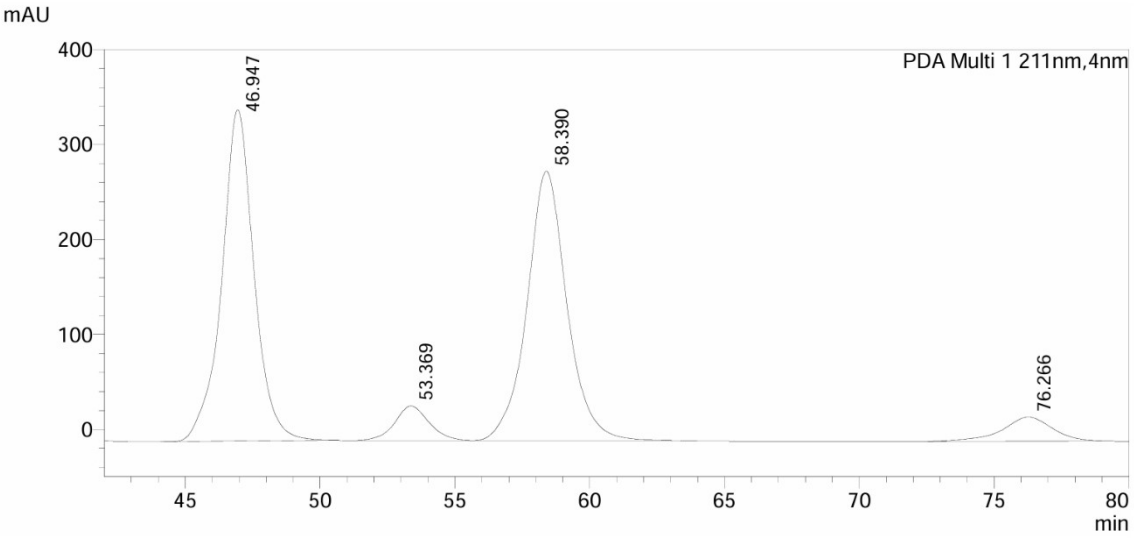
S44

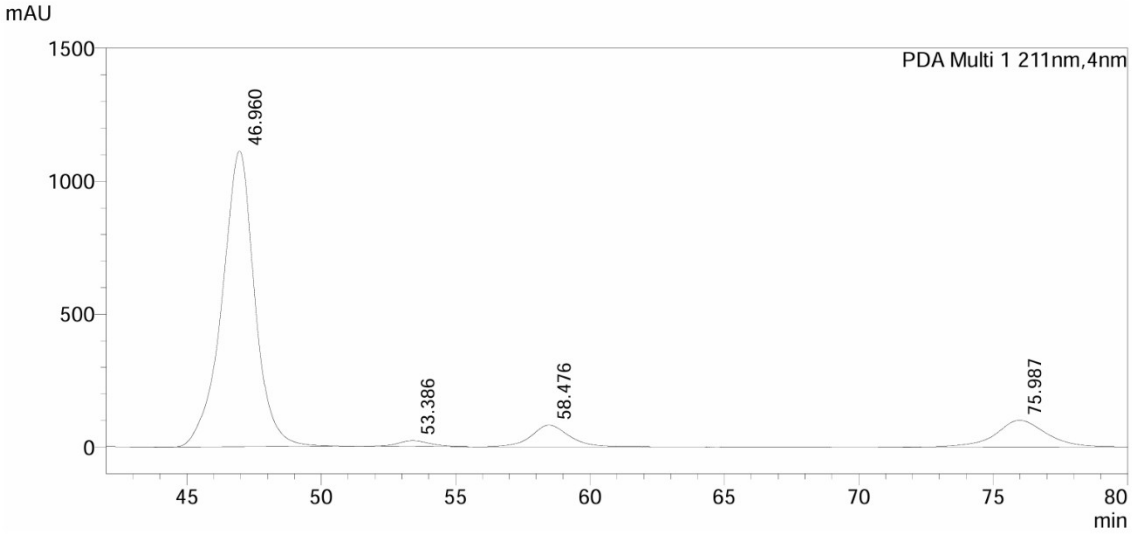
PDA Ch1 211nm

Peak#	Ret. Time	Area%
1	46.947	44.970
2	53.369	4.919
3	58.390	45.037
4	76.266	5.074
Total		100.000

PDA Ch1 211nm

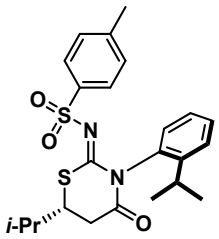
Peak#	Ret. Time	Area%
1	46.960	80.579
2	53.386	1.544
3	58.476	6.725
4	75.987	11.152
Total		100.000



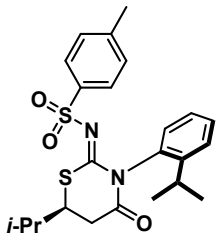


HPLC data for (*R*,R_a,*Z*)-**73**: Chiralpak AD-H (90:10 *n*-hexane : IPA, flow rate 1.0 mLmin^{-1}, 211 nm, 30 °C) t_R (*R*,R_a) 33.1 min, t_R (*S*,S_a) 47.1 min, 95:5 er.

HPLC data for (*S*,R_a,*Z*)-**S45**: Chiralpak AD-H (90:10 *n*-hexane : IPA, flow rate 1.0 mLmin^{-1}, 211 nm, 30 °C) t_R (*R*,S_a) 29.1 min, t_R (*S*,R_a) 54.7 min, 68:32 er.



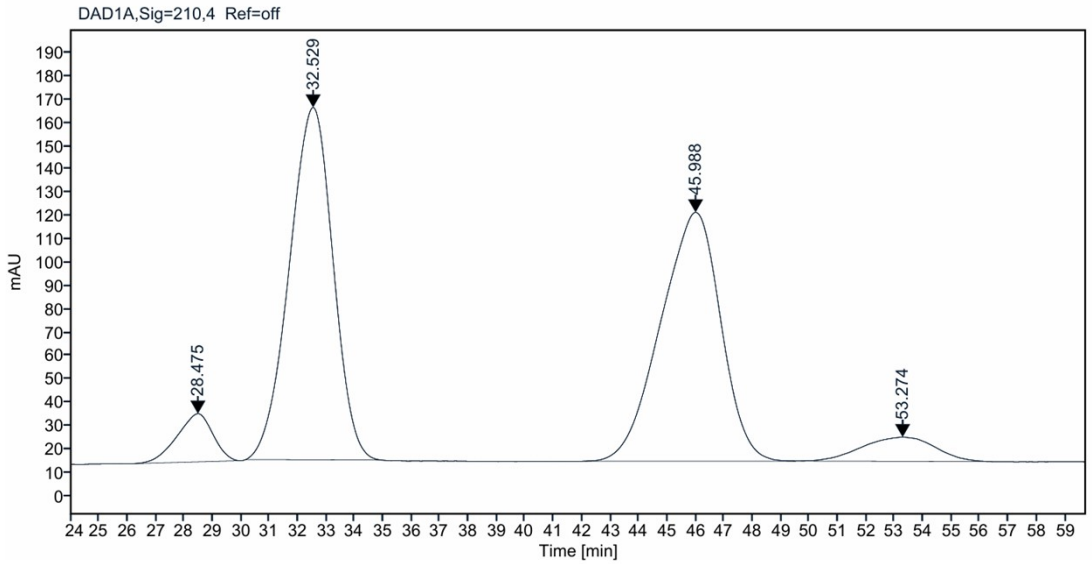
73



S45

RT [min]	Area%
28.475	5.0985
32.529	45.5746
45.988	44.1252
53.274	5.2018

RT [min]	Area%
29.136	2.4043
33.122	88.3377
47.125	4.2359
54.735	5.0221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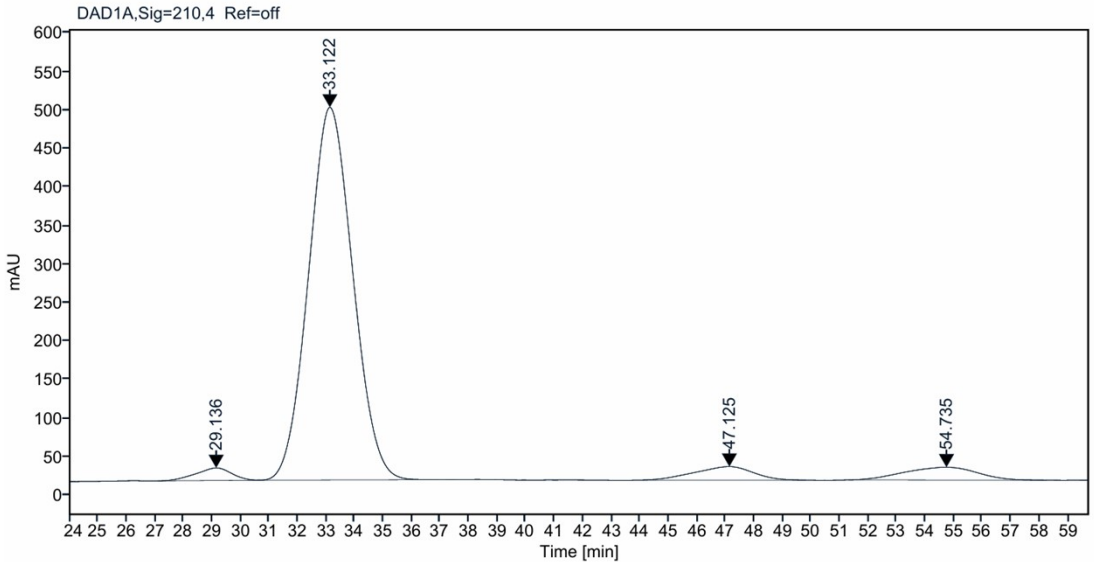
mAU
Time [min]
28.475
32.529
45.988
53.274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mAU
Time [min]
29.136
33.122
47.125
54.735

Appendix III: Computational Data

CF3_Michael_Acceptor/acyl_ammonium_ion_pair

Frequencies, energies and thermodynamic properties:

Lowest Vibrational Mode (1/cm) = 8.8127

2nd Lowest Vibrational Mode (1/cm) = 20.5513

E(RM062X) (a.u.) = -2572.63321020

Thermal correction to Enthalpy (a.u.) = 0.507813

Thermal correction to Gibbs Free Energy (a.u.) = 0.398690

Total Entropy (cal/Kmol) = 229.669

Esp(RM062X) (a.u.) = -2575.26059912

Optimised cartesian coordinates (Angstrom):

C	5.962400	-3.142995	-0.188524
C	5.388744	-4.049277	-1.092356
C	4.096110	-3.860571	-1.569888
C	3.392806	-2.742224	-1.122734
C	3.963289	-1.846183	-0.217057
C	5.261481	-2.030207	0.263490
H	6.979334	-3.310076	0.168376
H	5.962764	-4.913746	-1.427625
H	3.645507	-4.562373	-2.272984
H	5.714622	-1.326511	0.961372
C	1.913953	-0.854228	-0.534198
C	1.211367	1.259066	0.505206
C	2.120253	0.793209	1.652986
C	3.411125	0.219753	1.099938
H	3.989257	-0.269249	1.894416
S	1.759799	-2.265389	-1.546220
N	3.086642	-0.805374	0.104698
N	0.991963	0.116644	-0.417213
C	2.358843	1.868883	2.736006
C	3.559917	2.780976	2.471646
C	2.502589	1.201977	4.104443
H	1.451048	2.493803	2.762723
H	3.548835	3.228928	1.467834
H	3.568703	3.601559	3.203760
H	4.506821	2.230449	2.590911
H	1.601207	0.630068	4.367680
H	3.361110	0.511054	4.115272
H	2.671858	1.955065	4.887870
H	1.558019	-0.032292	2.119000
H	0.234841	1.436911	0.967372
C	1.679656	2.491262	-0.236501
C	1.175578	3.740093	0.144737
C	2.638088	2.425160	-1.253824
C	1.645626	4.906593	-0.456250
H	0.409818	3.795583	0.922840
C	3.107156	3.592190	-1.857340
H	3.024801	1.459285	-1.589722
C	2.617898	4.835052	-1.454613
H	1.246171	5.874167	-0.148073
H	3.855541	3.528662	-2.649052
H	2.985308	5.746967	-1.928114
C	-1.230644	1.078518	-0.999254
H	-0.960322	2.034821	-0.556506
C	-2.442316	0.886618	-1.521937
H	-2.735176	-0.059411	-1.983915
C	-3.474022	1.968012	-1.542540
F	-3.745758	2.344191	-2.799543
F	-4.629141	1.557074	-1.011354
F	-3.094011	3.060763	-0.880328

O -0.511192 -1.078013 -1.637743
C -0.278098 -0.058576 -1.032452
H 4.042490 0.984559 0.623134
O -1.046708 -0.310951 1.307385
C -2.178744 -0.848970 1.127617
C -2.346788 -2.219534 0.768356
C -3.399464 -0.111451 1.140164
C -3.588248 -2.805722 0.580875
C -4.646382 -0.688507 0.949732
C -4.751361 -2.039822 0.637173
F -3.336476 1.201078 1.405954
F -5.747892 0.058015 1.012326
F -3.678997 -4.106381 0.298834
F -1.257508 -2.993159 0.694765
F -5.947021 -2.605332 0.441127

CF3_Michael_Acceptor/C6F5OH

Frequencies, energies and thermodynamic properties:

Lowest Vibrational Mode (1/cm) = 111.0785
2nd Lowest Vibrational Mode (1/cm) = 141.1056
E(RM062X) (a.u.) = -802.732617403
Thermal correction to Enthalpy (a.u.) = 0.075937
Thermal correction to Gibbs Free Energy (a.u.) = 0.029109
Total Entropy (cal/Kmol) = 98.557
Esp(RM062X) (a.u.) = -803.686675322

Optimised cartesian coordinates (Angstrom):

C -0.234767 1.367630 -0.000143
C 1.071480 0.891834 0.000088
C 1.323220 -0.477089 -0.000141
C 0.255627 -1.367778 0.000104
C -1.046230 -0.882459 -0.000210
C -1.319165 0.486396 0.000091
O -2.565435 0.976289 -0.000016
F -2.074173 -1.730692 -0.000105
F 0.478209 -2.671996 0.000128
F 2.569392 -0.926193 -0.000068
F 2.082269 1.746196 0.000114
F -0.452829 2.675256 -0.000055
H -3.203310 0.245342 0.001266

CF3_Michael_Acceptor/CF3_ester

Frequencies, energies and thermodynamic properties:

Lowest Vibrational Mode (1/cm) = 20.0492
2nd Lowest Vibrational Mode (1/cm) = 25.5086
E(RM062X) (a.u.) = -1329.93763879
Thermal correction to Enthalpy (a.u.) = 0.132925
Thermal correction to Gibbs Free Energy (a.u.) = 0.066287
Total Entropy (cal/Kmol) = 140.252
Esp(RM062X) (a.u.) = -1331.50964551

Optimised cartesian coordinates (Angstrom):

C 2.439705 0.186295 -0.263914
H 2.562740 0.705547 -1.215776
C 3.469956 -0.210374 0.477319
H 3.334844 -0.731916 1.429016
O 0.150185 0.387174 -0.689292
C -1.172072 0.201388 -0.400663
C -1.986131 1.309892 -0.185503
C -1.721570 -1.077231 -0.336362
C -3.344355 1.143753 0.068010
C -3.074427 -1.248651 -0.069779
C -3.885756 -0.135611 0.134077
C 4.889532 0.027009 0.064287
F 4.985702 0.680750 -1.091690

F	5.537457	0.742225	0.986429
F	5.545170	-1.127737	-0.070479
O	0.750357	-0.617365	1.234228
C	1.060856	-0.080946	0.214767
F	-1.474006	2.526606	-0.230879
F	-0.950310	-2.131539	-0.536294
F	-5.172609	-0.295806	0.383838
F	-4.117529	2.199029	0.260061
F	-3.593468	-2.463001	-0.010561

CF3_Michael_Acceptor/cycl-R_rot

Frequencies, energies and thermodynamic properties:

Lowest Vibrational Mode (1/cm) = 14.6628

2nd Lowest Vibrational Mode (1/cm) = 16.1673

E(RM062X) (a.u.) = -3187.94058066

Thermal correction to Enthalpy (a.u.) = 0.681301

Thermal correction to Gibbs Free Energy (a.u.) = 0.555298

Total Entropy (cal/Kmol) = 265.196

Esp(RM062X) (a.u.) = -3190.93033339

Optimised cartesian coordinates (Angstrom):

C	-0.105535	0.585637	3.243174
C	1.363968	0.275974	3.442998
H	1.474872	-0.571169	4.135195
H	-0.633735	-0.337186	2.962171
H	-0.556069	0.957630	4.172777
N	0.431016	1.738794	1.076942
C	0.031255	2.709212	0.092562
C	-0.620550	2.279951	-1.062796
C	0.292345	4.057738	0.323682
C	-1.027639	3.215825	-2.005601
H	-0.798272	1.213112	-1.207471
C	-0.111907	5.003586	-0.612550
H	0.807520	4.359416	1.236588
C	-0.764478	4.559994	-1.757774
H	-1.543021	2.918181	-2.917209
H	0.072126	6.066240	-0.464384
N	-1.195337	5.556662	-2.751794
O	-0.946709	6.704341	-2.535034
O	-1.770907	5.164372	-3.721750
C	-0.430948	1.601530	2.174307
O	-1.414902	2.291587	2.254357
C	2.134277	1.426064	4.072709
F	1.607231	1.744249	5.255898
F	2.102219	2.528407	3.315103
F	3.411453	1.114798	4.270683
S	2.137250	-0.275625	1.900648
C	1.522894	0.940157	0.747865
N	2.065105	1.071601	-0.389320
C	3.205866	0.389976	-0.801305
C	4.476094	0.741911	-0.310109
C	3.086452	-0.613776	-1.775131
C	5.608915	0.092638	-0.779328
H	4.562009	1.531294	0.437887
C	4.215516	-1.271500	-2.243238
H	2.094538	-0.870899	-2.150791
C	5.460850	-0.907068	-1.738337
H	6.601017	0.350957	-0.412067
H	4.139619	-2.059176	-2.992052
N	6.657180	-1.596581	-2.234157
O	6.506663	-2.464716	-3.063790
O	7.729973	-1.260983	-1.786106
N	-1.463506	-0.725766	0.595754
C	-2.693595	-0.606912	0.283636

C -0.912388 -2.076641 0.678589
S -3.504749 0.978763 0.165058
N -3.589729 -1.610369 -0.020025
C -2.006222 -3.114717 1.035617
H -0.190716 -2.080366 1.511846
C -0.129445 -2.448626 -0.567746
C -4.993087 0.208651 -0.372569
C -4.851828 -1.189726 -0.411844
C -3.176303 -3.002500 0.063070
C -1.504076 -4.566120 1.202699
H -2.385009 -2.786135 2.018697
C 1.049916 -3.194979 -0.448036
C -0.606841 -2.147494 -1.849520
C -6.191321 0.816742 -0.725948
C -5.914466 -1.994357 -0.822610
H -4.027819 -3.597477 0.425018
H -2.906094 -3.369333 -0.940744
C -1.533561 -5.401514 -0.080788
C -2.299884 -5.278433 2.297624
H -0.456336 -4.501920 1.541399
C 1.702048 -3.686503 -1.578266
H 1.450883 -3.407466 0.546120
C 0.049436 -2.630619 -2.983465
H -1.509556 -1.542506 -1.967751
C -7.259079 0.009608 -1.128974
H -6.294259 1.902479 -0.690451
C -7.117143 -1.378387 -1.176972
H -5.806587 -3.078194 -0.871758
H -1.049118 -4.900576 -0.930954
H -1.015403 -6.357800 0.084756
H -2.569576 -5.639426 -0.370185
H -2.198359 -4.767275 3.266385
H -3.371717 -5.311839 2.043552
H -1.955489 -6.315917 2.422127
C 1.196472 -3.415248 -2.850626
H 2.613386 -4.277095 -1.465498
H -0.340825 -2.396353 -3.975608
H -8.205962 0.472049 -1.410146
H -7.955500 -1.997660 -1.499643
H 1.703212 -3.800521 -3.737474

CF3_Michael_Acceptor/cycl-R

Frequencies, energies and thermodynamic properties:

Lowest Vibrational Mode (1/cm) = 10.7067

2nd Lowest Vibrational Mode (1/cm) = 15.0479

E(RM062X) (a.u.) = -3187.94659271

Thermal correction to Enthalpy (a.u.) = 0.681766

Thermal correction to Gibbs Free Energy (a.u.) = 0.554742

Total Entropy (cal/Kmol) = 267.344

Esp(RM062X) (a.u.) = -3190.91181533

Optimised cartesian coordinates (Angstrom):

C 1.590975 -2.599093 -1.140928
C 2.184908 0.110322 -0.399450
C -0.118050 -0.836384 -0.954335
C 0.341272 -2.198945 -0.396155
H 0.518927 -2.187984 0.687664
H -0.455017 -2.923310 -0.621591
N 0.824075 0.234466 -0.334257
C 0.307325 1.545028 -0.148593
C -0.471013 2.140828 -1.148206
C 0.522491 2.212106 1.066082
C -1.082938 3.369450 -0.916623
H -0.597363 1.616114 -2.095350

C	-0.070427	3.444075	1.301676
H	1.149563	1.750119	1.829167
C	-0.881291	3.992447	0.309935
H	-1.706515	3.843422	-1.673350
H	0.075836	3.973423	2.242099
N	-1.554064	5.271564	0.577252
O	-1.483307	5.720339	1.699218
O	-2.148044	5.799367	-0.333837
O	-0.224977	-0.766009	-2.215572
S	2.970430	-1.453378	-0.803598
N	2.952355	1.114338	-0.200851
C	4.335811	1.063933	-0.174023
C	5.028606	0.471878	0.901371
C	5.071329	1.678347	-1.205775
C	6.415140	0.481676	0.939356
H	4.462787	0.007295	1.710035
C	6.457760	1.688849	-1.176974
H	4.529728	2.144993	-2.029056
C	7.112074	1.088697	-0.103098
H	6.961322	0.026376	1.764259
H	7.036691	2.155016	-1.972987
N	8.576389	1.100624	-0.066421
O	9.162109	1.631990	-0.983199
O	9.124146	0.578255	0.878731
H	1.385187	-2.594554	-2.220057
C	2.043477	-3.995335	-0.769055
F	3.196327	-4.313521	-1.363774
F	1.134897	-4.895771	-1.149020
F	2.223263	-4.142796	0.544798
N	-1.480835	-0.534385	-0.245717
C	-2.552706	-0.314622	-0.981067
C	-1.582055	-0.510366	1.223238
S	-2.623333	-0.440983	-2.735837
N	-3.746506	0.015132	-0.447796
C	-2.598021	0.580825	1.620197
H	-0.597283	-0.189035	1.588722
C	-1.863445	-1.878604	1.817631
C	-4.353940	-0.105894	-2.676960
C	-4.792879	0.113296	-1.370564
C	-3.939936	0.277776	0.977662
C	-2.702863	0.854244	3.136203
H	-2.215673	1.503629	1.152001
C	-1.183314	-2.255486	2.980848
C	-2.803636	-2.756926	1.267958
C	-5.243056	-0.039568	-3.747340
C	-6.131146	0.388453	-1.090753
H	-4.611842	1.142258	1.068265
H	-4.432843	-0.593940	1.434978
C	-3.694729	-0.042308	3.883594
C	-3.063873	2.321949	3.375206
H	-1.696142	0.681014	3.554137
C	-1.456738	-3.472488	3.602762
H	-0.430582	-1.584479	3.402421
C	-3.076770	-3.976850	1.888008
H	-3.328360	-2.505962	0.342917
C	-6.581755	0.239792	-3.477470
H	-4.899197	-0.205290	-4.769699
C	-7.018264	0.448794	-2.163914
H	-6.476604	0.545305	-0.068984
H	-3.547179	-1.112735	3.684436
H	-3.590380	0.114836	4.967132
H	-4.732306	0.215523	3.618093
H	-2.329694	3.004395	2.921695

H -4.050817 2.555902 2.944375
H -3.113242 2.540288 4.452030
C -2.410089 -4.334603 3.059884
H -0.918512 -3.751212 4.510257
H -3.812161 -4.652885 1.448678
H -7.295764 0.292906 -4.300260
H -8.070774 0.661218 -1.971790
H -2.624454 -5.289535 3.542516

CF3_Michael_Acceptor/cycl-S_rot

Frequencies, energies and thermodynamic properties:

Lowest Vibrational Mode (1/cm) = 6.5622
2nd Lowest Vibrational Mode (1/cm) = 9.5325
E(RM062X) (a.u.) = -3187.94262625
Thermal correction to Enthalpy (a.u.) = 0.681392
Thermal correction to Gibbs Free Energy (a.u.) = 0.553543
Total Entropy (cal/Kmol) = 269.081
Esp(RM062X) (a.u.) = -3190.90451915

Optimised cartesian coordinates (Angstrom):

C 1.586170 -2.595895 -1.414898
C 2.111908 -0.205305 -0.057811
C -0.227384 -0.860514 -1.029544
C 0.177710 -2.335673 -0.915665
H 0.136000 -2.724411 0.108098
H -0.549477 -2.885657 -1.529440
N 0.773469 0.018434 -0.221779
C 0.350116 1.372147 -0.044475
C 0.062349 2.178341 -1.150715
C 0.209995 1.880097 1.253679
C -0.402187 3.477674 -0.960135
H 0.194321 1.766181 -2.148583
C -0.239393 3.177996 1.455365
H 0.463257 1.246846 2.105904
C -0.546818 3.950971 0.337913
H -0.640718 4.121801 -1.805159
H -0.356038 3.593209 2.455233
N -1.031659 5.326072 0.542923
O -1.143684 5.719582 1.681128
O -1.292646 5.984416 -0.436704
O -0.434041 -0.449512 -2.207497
S 2.799787 -1.847478 -0.297577
N 2.886359 0.719702 0.372776
C 4.265459 0.638888 0.446732
C 4.905767 0.802287 1.689761
C 5.053933 0.482428 -0.713248
C 6.290021 0.791207 1.781466
H 4.293258 0.939931 2.581379
C 6.437227 0.475389 -0.630371
H 4.559237 0.369113 -1.679057
C 7.038770 0.626463 0.618468
H 6.794863 0.910901 2.739026
H 7.055395 0.356311 -1.519057
N 8.499922 0.617358 0.709043
O 9.130946 0.466499 -0.313479
O 9.001756 0.760097 1.802065
H 1.786422 -3.675285 -1.357060
C 1.898063 -2.218420 -2.859934
F 0.921999 -2.592771 -3.683406
F 3.009062 -2.859775 -3.255923
F 2.132771 -0.921680 -3.044696
N -1.543450 -0.700991 -0.152168
C -2.606192 -0.135755 -0.687008
C -1.573028 -1.149752 1.247489

S -2.740787 0.387744 -2.363829
N -3.740974 0.094623 0.007980
C -2.475659 -0.201039 2.061942
H -0.543942 -1.027972 1.618363
C -1.960650 -2.611522 1.391449
C -4.411236 0.867458 -2.066564
C -4.789202 0.636673 -0.743051
C -3.861303 -0.163291 1.441838
C -2.499158 -0.482543 3.581611
H -2.039269 0.799782 1.921674
C -1.303076 -3.397385 2.344964
C -2.986816 -3.184224 0.632697
C -5.309857 1.415257 -2.979200
C -6.076929 0.932836 -0.295574
H -4.450729 0.653412 1.880317
H -4.411080 -1.105122 1.590756
C -3.596604 -1.448711 4.035895
C -2.618068 0.834910 4.349456
H -1.523991 -0.930570 3.835413
C -1.684058 -4.720656 2.560668
H -0.481062 -2.966422 2.922193
C -3.367874 -4.509795 0.846304
H -3.496242 -2.604620 -0.140986
C -6.596892 1.719476 -2.539064
H -5.011942 1.598548 -4.012924
C -6.973692 1.477924 -1.212888
H -6.379881 0.741576 0.733807
H -3.607543 -2.387310 3.464038
H -3.449939 -1.703230 5.095737
H -4.591072 -0.983093 3.948487
H -1.772899 1.504956 4.132196
H -3.546493 1.362964 4.078687
H -2.640529 0.655358 5.434296
C -2.723513 -5.278731 1.815228
H -1.163186 -5.319872 3.309444
H -4.170786 -4.943629 0.247925
H -7.316796 2.147516 -3.237719
H -7.986785 1.717328 -0.887032
H -3.022582 -6.315076 1.980579

CF3_Michael_Acceptor/cycl-S

Frequencies, energies and thermodynamic properties:

Lowest Vibrational Mode (1/cm) = 13.2539

2nd Lowest Vibrational Mode (1/cm) = 14.6724

E(RM062X) (a.u.) = -3187.93779164

Thermal correction to Enthalpy (a.u.) = 0.681519

Thermal correction to Gibbs Free Energy (a.u.) = 0.554348

Total Entropy (cal/Kmol) = 267.653

Esp(RM062X) (a.u.) = -3190.90224164

Optimised cartesian coordinates (Angstrom):

C 0.228732 -1.974809 -1.873457
C -1.150749 -1.966066 -2.488517
H -1.226517 -1.226439 -3.299900
H 0.224307 -2.655576 -1.012529
H 0.969372 -2.335159 -2.600179
N -0.443525 0.376042 -1.067615
C -0.108585 1.767258 -1.009578
C -0.147958 2.475009 0.198384
C 0.248273 2.431751 -2.192084
C 0.199005 3.821165 0.237404
H -0.468104 1.976308 1.109216
C 0.599621 3.776347 -2.164125
H 0.251658 1.879542 -3.127287

C	0.576359	4.446042	-0.945458
H	0.177153	4.381117	1.171004
H	0.880108	4.305884	-3.073166
N	0.948610	5.869145	-0.909047
O	1.257164	6.399111	-1.951503
O	0.927098	6.431130	0.161940
C	0.715017	-0.534683	-1.562722
O	1.391345	-0.005007	-2.484131
C	-1.504806	-3.309905	-3.092688
F	-2.745469	-3.326583	-3.579672
F	-1.416792	-4.297494	-2.197123
F	-0.675484	-3.605054	-4.093124
S	-2.364635	-1.571671	-1.190487
C	-1.709291	0.022319	-0.684511
N	-2.458706	0.792728	0.006549
C	-3.807517	0.593779	0.244996
C	-4.759409	0.685423	-0.791444
C	-4.251803	0.374401	1.562771
C	-6.112056	0.545924	-0.521483
H	-4.420648	0.875096	-1.810622
C	-5.603281	0.227988	1.839905
H	-3.514066	0.329018	2.364385
C	-6.516628	0.313911	0.792052
H	-6.856052	0.616279	-1.313801
H	-5.956998	0.053217	2.854953
N	-7.944771	0.163606	1.080264
O	-8.273083	-0.040594	2.227829
O	-8.721861	0.250176	0.155899
N	1.607657	-0.704441	-0.242278
C	2.911343	-0.578156	-0.335037
C	1.021184	-1.245081	0.989378
S	3.757367	0.217830	-1.658711
N	3.759341	-1.017669	0.620306
C	1.932208	-2.370821	1.516828
H	0.066371	-1.705947	0.702363
C	0.700501	-0.174146	2.012064
C	5.282846	-0.014558	-0.804718
C	5.101301	-0.694361	0.401970
C	3.325579	-1.814387	1.768574
C	1.356675	-3.142282	2.726057
H	2.008925	-3.083272	0.678220
C	-0.540972	-0.215410	2.655401
C	1.614162	0.827195	2.364110
C	6.554478	0.380400	-1.213206
C	6.177087	-0.986592	1.239540
H	4.048102	-2.632246	1.898900
H	3.357983	-1.180738	2.667891
C	1.707671	-2.549735	4.093404
C	1.794733	-4.606407	2.668821
H	0.259204	-3.116300	2.616116
C	-0.862332	0.717144	3.642137
H	-1.266694	-0.982612	2.371965
C	1.294660	1.759574	3.350401
H	2.577829	0.909040	1.857261
C	7.635937	0.091569	-0.381744
H	6.698605	0.906914	-2.158178
C	7.446914	-0.582958	0.829846
H	6.031383	-1.510045	2.184549
H	1.478447	-1.477456	4.169443
H	1.138622	-3.070636	4.877222
H	2.776296	-2.689155	4.321649
H	1.452045	-5.093687	1.744280
H	2.892857	-4.688237	2.709565

H	1.387477	-5.168850	3.521715
C	0.056710	1.706662	3.993099
H	-1.834825	0.674036	4.135989
H	2.013213	2.538863	3.609934
H	8.639215	0.398105	-0.680228
H	8.305008	-0.798296	1.467932
H	-0.193480	2.439399	4.762035

CF3_Michael_Acceptor/HyperBTM

Frequencies, energies and thermodynamic properties:

Lowest Vibrational Mode (1/cm) = 26.7604

2nd Lowest Vibrational Mode (1/cm) = 57.9421

E(RM062X) (a.u.) = -1242.68108630

Thermal correction to Enthalpy (a.u.) = 0.371678

Thermal correction to Gibbs Free Energy (a.u.) = 0.305623

Total Entropy (cal/Kmol) = 139.024

Esp(RM062X) (a.u.) = -1243.74354485

Optimised cartesian coordinates (Angstrom):

C	-4.262530	0.973031	1.705921
C	-5.081884	0.026598	1.089062
C	-4.570448	-0.806552	0.088982
C	-3.238265	-0.667538	-0.277562
C	-2.412615	0.292849	0.336285
C	-2.921403	1.115944	1.340791
H	-4.669698	1.613207	2.490089
H	-6.126268	-0.070457	1.387912
H	-5.203340	-1.552803	-0.394046
H	-2.284078	1.850300	1.833836
C	-0.852054	-0.663172	-1.127167
C	1.406622	-0.103443	-1.317985
C	0.986323	1.302948	-0.824072
C	-0.065141	1.190869	0.277299
H	-0.509874	2.177247	0.477622
S	-2.342062	-1.583659	-1.484368
N	-1.120558	0.291010	-0.162611
N	0.251017	-0.908789	-1.701688
C	2.161531	2.231026	-0.444693
C	2.601261	2.139383	1.019395
C	1.826137	3.682431	-0.791325
H	3.015788	1.927239	-1.073553
H	2.788244	1.106938	1.347021
H	3.529866	2.711096	1.165556
H	1.842194	2.577462	1.687042
H	1.618759	3.801777	-1.864957
H	0.937651	4.022659	-0.235092
H	2.658630	4.352142	-0.528432
H	0.480326	1.757972	-1.692374
H	2.009511	0.051835	-2.226024
C	2.288128	-0.851872	-0.332650
C	3.679294	-0.826890	-0.482869
C	1.743460	-1.531774	0.763657
C	4.511225	-1.434125	0.457769
H	4.115252	-0.320870	-1.347869
C	2.572640	-2.139839	1.706383
H	0.659540	-1.591953	0.887188
C	3.959687	-2.086725	1.560541
H	5.594333	-1.401918	0.325517
H	2.131945	-2.662349	2.557484
H	4.607870	-2.563537	2.297932
H	0.371335	0.818121	1.218567

CF3_Michael_Acceptor/MA-product

Frequencies, energies and thermodynamic properties:

Lowest Vibrational Mode (1/cm) = 12.9010

2nd Lowest Vibrational Mode (1/cm) = 27.8348

E(RM062X) (a.u.) = -2748.01566672

Thermal correction to Enthalpy (a.u.) = 0.386975

Thermal correction to Gibbs Free Energy (a.u.) = 0.280216

Total Entropy (cal/Kmol) = 224.692

Esp(RM062X) (a.u.) = -2750.86693905

Optimised cartesian coordinates (Angstrom):

C	-0.917917	2.162890	-0.488778
H	-1.255076	1.216472	-0.935729
C	-1.770869	2.606724	0.692805
C	-2.960309	3.409949	0.184622
F	-2.547775	4.524841	-0.418976
F	-3.685298	2.723221	-0.699600
F	-3.768196	3.766660	1.180599
O	1.090522	2.340488	0.854832
C	0.545822	2.038522	-0.163601
H	-1.193708	3.288387	1.333634
S	-2.490650	1.278203	1.769744
C	-1.501665	-0.184245	1.339833
N	-1.982077	-1.241572	0.830636
N	-0.195394	-0.053209	1.721700
H	0.008692	0.772434	2.277579
C	-3.279725	-1.408839	0.354670
C	-4.025073	-2.493438	0.847713
C	-3.833630	-0.584472	-0.640207
C	-5.309223	-2.736315	0.382324
H	-3.578171	-3.137606	1.605368
C	-5.113317	-0.827789	-1.119736
H	-3.259310	0.248129	-1.043035
C	-5.834266	-1.897573	-0.597330
H	-5.901693	-3.566772	0.763220
H	-5.555016	-0.197252	-1.889969
N	-7.188604	-2.154786	-1.101555
O	-7.615847	-1.427749	-1.969151
O	-7.803303	-3.079870	-0.621831
C	0.906170	-0.872455	1.472366
C	0.854248	-2.074146	0.748841
C	2.140506	-0.410961	1.977838
C	2.026546	-2.791455	0.525652
H	-0.090872	-2.441076	0.360292
C	3.305215	-1.118246	1.747305
H	2.173587	0.521093	2.544105
C	3.230049	-2.303239	1.015846
H	2.010109	-3.718970	-0.045695
H	4.265237	-0.763012	2.120384
N	4.468977	-3.022042	0.713710
O	5.509450	-2.413277	0.838387
O	4.385259	-4.169369	0.344662
O	1.196724	1.519310	-1.238499
C	2.501497	1.127695	-1.121169
C	3.525915	1.971331	-0.694340
C	2.811011	-0.171415	-1.523192
C	4.827554	1.486432	-0.591852
C	4.114653	-0.645614	-1.444734
C	5.129952	0.184958	-0.981643
F	4.381310	-1.894282	-1.792761
F	1.853398	-0.971636	-1.956941
F	6.370211	-0.253670	-0.908305
F	5.793306	2.286474	-0.172168
F	3.286512	3.234580	-0.395435
H	-0.986231	2.916460	-1.291823

CF3_Michael_Acceptor/MA-R_pt_rot

Frequencies, energies and thermodynamic properties:

Lowest Vibrational Mode (1/cm) = 14.3681

2nd Lowest Vibrational Mode (1/cm) = 18.4051

E(RM062X) (a.u.) = -3187.94090470

Thermal correction to Enthalpy (a.u.) = 0.681771

Thermal correction to Gibbs Free Energy (a.u.) = 0.556928

Total Entropy (cal/Kmol) = 262.754

Esp(RM062X) (a.u.) = -3190.90298177

Optimised cartesian coordinates (Angstrom):

C	5.447228	-1.308211	-2.506161
C	5.679378	-2.213699	-1.457984
C	5.118730	-2.012853	-0.202107
C	4.304012	-0.892748	-0.027309
C	4.073513	0.004150	-1.071009
H	6.296141	-3.096062	-1.633089
H	5.284279	-2.721669	0.610479
C	2.673401	0.865456	0.529086
C	1.263271	2.865604	0.231911
C	2.446023	3.317487	-0.646001
C	2.893961	2.174703	-1.541264
H	3.822716	2.434710	-2.066148
S	3.393503	-0.450370	1.398131
N	3.184725	1.015333	-0.695269
N	1.675900	1.653510	0.996914
C	2.175938	4.621603	-1.432947
C	1.579397	4.408227	-2.827012
C	3.466184	5.435113	-1.540705
H	1.457505	5.209345	-0.838542
H	0.687521	3.766066	-2.822287
H	1.291174	5.378877	-3.255822
H	2.321233	3.961188	-3.507535
H	3.856270	5.705674	-0.548756
H	4.246408	4.864662	-2.069783
H	3.293038	6.363072	-2.104650
H	3.271963	3.520694	0.055385
H	1.113129	3.657636	0.977625
C	-0.019533	2.666262	-0.543037
C	-0.951241	3.707571	-0.602887
C	-0.253157	1.495647	-1.266549
C	-2.082724	3.593832	-1.409142
H	-0.784341	4.617362	-0.020175
C	-1.386866	1.376236	-2.068984
H	0.447543	0.662088	-1.193043
C	-2.296155	2.431949	-2.152535
H	-2.801238	4.413797	-1.455439
H	-1.564889	0.453504	-2.625543
H	-3.182766	2.339568	-2.782412
C	-0.207411	2.035126	2.616766
H	-0.550774	2.737585	1.855269
C	-1.439892	1.213084	3.019570
C	-1.244702	0.192812	4.136959
F	-2.429058	-0.081427	4.700507
F	-0.710789	-0.968625	3.795140
F	-0.474579	0.722325	5.099207
O	1.571255	0.488592	2.947686
C	1.042397	1.289275	2.222981
H	2.134852	1.897355	-2.286738
C	4.648216	-0.184638	-2.330108
H	4.455178	0.505803	-3.151284
H	5.893504	-1.494130	-3.483772
H	-2.088572	1.953622	3.513809
S	-2.574821	0.690999	1.697141

C -1.711349 -0.601830 0.731543
N -0.454671 -0.751219 1.043739
N -2.404182 -1.347835 -0.098851
C 0.314288 -1.741234 0.468316
C 1.048739 -2.593953 1.325132
C 0.483083 -1.902616 -0.927659
C 1.965351 -3.504057 0.826729
H 0.899548 -2.485871 2.399946
C 1.420486 -2.791203 -1.437056
H -0.126967 -1.311901 -1.610050
C 2.166129 -3.570601 -0.553492
H 2.546084 -4.144533 1.489933
H 1.584166 -2.886246 -2.509989
N 3.212544 -4.437923 -1.080795
O 3.350605 -4.504901 -2.283308
O 3.909644 -5.037280 -0.288269
C -3.692162 -1.212467 -0.508416
C -4.393240 -2.403325 -0.851743
C -4.383309 0.016932 -0.698425
C -5.694654 -2.380892 -1.311356
H -3.864833 -3.349740 -0.730189
C -5.688004 0.046619 -1.162960
H -3.874410 0.959735 -0.504988
C -6.341590 -1.149362 -1.461107
H -6.223375 -3.301033 -1.557349
H -6.208128 0.993086 -1.306995
N -7.710409 -1.113650 -1.945431
O -8.248836 -0.031706 -2.066305
O -8.253465 -2.167506 -2.207410
H 0.095575 2.626129 3.496572

CF3_Michael_Acceptor/MA-R_pt

Frequencies, energies and thermodynamic properties:

Lowest Vibrational Mode (1/cm) = 13.6087

2nd Lowest Vibrational Mode (1/cm) = 15.7017

E(RM062X) (a.u.) = -3187.95670984

Thermal correction to Enthalpy (a.u.) = 0.681533

Thermal correction to Gibbs Free Energy (a.u.) = 0.555523

Total Entropy (cal/Kmol) = 265.210

Esp(RM062X) (a.u.) = -3190.91949549

Optimised cartesian coordinates (Angstrom):

C 5.807566 -1.715154 1.593487
C 6.530882 -1.262845 0.480135
C 5.987246 -0.328248 -0.393896
C 4.701855 0.142104 -0.125707
C 3.978900 -0.319252 0.975998
H 7.528933 -1.658004 0.289059
H 6.540519 0.016596 -1.268417
C 2.398585 1.014147 -0.019449
C 0.189848 1.520864 0.932981
C 0.332919 0.172244 1.652752
C 1.758949 -0.053838 2.111723
H 1.900535 -1.099930 2.413260
S 3.742979 1.231142 -1.100493
N 2.686120 0.217026 1.009034
N 1.185694 1.602456 -0.163518
C -0.702815 -0.045202 2.778037
C -0.268208 0.457955 4.156461
C -1.076249 -1.526271 2.846912
H -1.605411 0.516317 2.481895
H 0.072399 1.503231 4.144615
H -1.112895 0.388610 4.857113
H 0.543819 -0.163617 4.565633

H	-1.471724	-1.880152	1.883098
H	-0.196102	-2.140012	3.100654
H	-1.839604	-1.702339	3.619075
H	0.126176	-0.577854	0.877274
H	-0.791823	1.482902	0.450387
C	0.245685	2.744991	1.820615
C	-0.957019	3.323098	2.241611
C	1.456992	3.276785	2.277102
C	-0.951970	4.395467	3.132632
H	-1.904813	2.924532	1.869544
C	1.461809	4.350785	3.166813
H	2.411746	2.862620	1.941945
C	0.258097	4.906393	3.602477
H	-1.896230	4.836095	3.456403
H	2.411392	4.756491	3.519355
H	0.264314	5.746144	4.299281
C	-0.522119	2.794975	-1.607006
H	-0.306741	3.685544	-2.213654
C	-1.464196	1.878473	-2.411117
C	-2.368521	2.729432	-3.289006
F	-3.143941	3.541382	-2.560553
F	-1.649328	3.505861	-4.105452
F	-3.166507	1.991504	-4.054096
O	1.674034	2.228395	-2.287182
C	0.850516	2.185729	-1.408768
H	2.041989	0.597108	2.953324
C	4.524912	-1.249947	1.861553
H	3.968091	-1.614348	2.724012
H	6.252227	-2.456051	2.258552
H	-0.886744	1.229607	-3.083690
S	-2.539592	0.802272	-1.404463
C	-1.498712	-0.717598	-1.246840
N	-2.056470	-1.782555	-0.755373
C	-3.340011	-1.899514	-0.281055
C	-4.133117	-2.976375	-0.741962
C	-3.885230	-1.050494	0.711186
C	-5.416739	-3.179746	-0.265868
H	-3.707699	-3.643507	-1.492303
C	-5.168519	-1.249394	1.197278
H	-3.279184	-0.236545	1.110551
C	-5.924255	-2.309544	0.700257
H	-6.031894	-4.001297	-0.630505
H	-5.589482	-0.597065	1.961124
N	-7.276880	-2.519205	1.208985
O	-7.694987	-1.751833	2.049179
O	-7.913789	-3.449924	0.765404
N	-0.273940	-0.554370	-1.700365
C	0.743239	-1.453919	-1.516856
C	0.795983	-2.480485	-0.531534
C	1.900575	-1.267033	-2.317670
C	1.965672	-3.191107	-0.302750
H	-0.086301	-2.693260	0.067423
C	3.058827	-1.993830	-2.113747
H	1.864895	-0.492654	-3.085749
C	3.093450	-2.936178	-1.083364
H	2.015024	-3.946763	0.481111
H	3.948649	-1.822719	-2.719347
N	4.338724	-3.633075	-0.796905
O	5.277508	-3.459266	-1.545931
O	4.380473	-4.351750	0.180579
H	-0.997901	3.135257	-0.680718

CF3_Michael_Acceptor/MA-R

Frequencies, energies and thermodynamic properties:

Lowest Vibrational Mode (1/cm) = 5.8319

2nd Lowest Vibrational Mode (1/cm) = 11.7034

E(RM062X) (a.u.) = -3187.94993819

Thermal correction to Enthalpy (a.u.) = 0.682306

Thermal correction to Gibbs Free Energy (a.u.) = 0.550292

Total Entropy (cal/Kmol) = 277.849

Esp(RM062X) (a.u.) = -3190.91703647

Optimised cartesian coordinates (Angstrom):

C	6.934837	2.976985	-1.928809
C	6.037967	4.052720	-1.898872
C	4.697315	3.853743	-1.579073
C	4.276106	2.556326	-1.293124
C	5.170476	1.485879	-1.332456
H	6.392293	5.059195	-2.124405
H	3.995971	4.689125	-1.549610
C	3.241158	0.379646	-0.710107
C	3.112684	-2.006822	-0.219214
C	4.271262	-2.127674	-1.224693
C	5.263751	-0.999247	-1.019218
H	5.986829	-0.974273	-1.844912
S	2.659788	2.027756	-0.845834
N	4.545288	0.274631	-1.017595
N	2.506663	-0.664393	-0.328212
C	4.941613	-3.520776	-1.242737
C	6.103708	-3.679790	-0.258212
C	5.413716	-3.853642	-2.658709
H	4.160517	-4.249732	-0.970609
H	5.844186	-3.380914	0.767074
H	6.421136	-4.732333	-0.229992
H	6.975191	-3.086758	-0.578169
H	6.152062	-3.115116	-3.010485
H	5.894659	-4.842306	-2.685018
H	4.575804	-3.862431	-3.370848
H	3.807739	-1.972820	-2.212831
H	2.343181	-2.709173	-0.560631
C	3.474552	-2.343198	1.213590
C	4.092207	-1.413255	2.056584
C	3.237610	-3.638130	1.686649
C	4.493746	-1.783493	3.340360
H	4.261215	-0.386057	1.722948
C	3.640659	-4.009729	2.968030
H	2.731783	-4.361835	1.042299
C	4.276644	-3.083976	3.795935
H	4.974627	-1.049348	3.988949
H	3.450807	-5.023792	3.323739
H	4.590609	-3.371701	4.800667
C	0.394919	-1.538519	0.538488
H	0.779978	-2.544895	0.668083
C	-1.017786	-1.250947	0.879591
C	-1.591282	-2.266094	1.847003
F	-0.874397	-2.306237	2.973521
F	-2.847800	-1.982003	2.194200
F	-1.589954	-3.502546	1.337137
O	0.668656	0.691287	-0.140454
C	1.108007	-0.479159	0.042636
H	5.817121	-1.093602	-0.072735
C	6.516700	1.679377	-1.645977
H	7.221141	0.848184	-1.664333
H	7.982357	3.154974	-2.175133
H	-1.122483	-0.269853	1.365307
S	-2.149686	-1.196149	-0.618692
C	-2.907747	0.433942	-0.403621

N	-1.989005	1.412857	-0.163328
H	-0.992984	1.118586	-0.213031
C	-2.183996	2.742228	0.185204
C	-1.020986	3.451004	0.561489
C	-3.425635	3.404535	0.183400
C	-1.088767	4.783743	0.921268
H	-0.067361	2.919394	0.572674
C	-3.492597	4.743470	0.551514
H	-4.325628	2.873317	-0.110042
C	-2.331824	5.418010	0.913186
H	-0.196724	5.335254	1.214210
H	-4.445677	5.270574	0.553288
N	-2.413625	6.828644	1.293037
O	-3.504414	7.354382	1.295864
O	-1.384328	7.396930	1.584483
N	-4.162660	0.645295	-0.480896
C	-5.112614	-0.332473	-0.730827
C	-6.125111	-0.554741	0.220576
C	-5.131453	-1.056806	-1.937302
C	-7.118412	-1.493466	-0.012464
H	-6.109660	0.018523	1.147884
C	-6.127244	-1.992293	-2.182204
H	-4.364247	-0.867316	-2.689686
C	-7.106127	-2.199480	-1.213969
H	-7.901026	-1.683170	0.720567
H	-6.152659	-2.559826	-3.111305
N	-8.159636	-3.186354	-1.468503
O	-9.005361	-3.344169	-0.616861
O	-8.128372	-3.791013	-2.516811

CF3_Michael_Acceptor/MA-S_pt_rot

Frequencies, energies and thermodynamic properties:

Lowest Vibrational Mode (1/cm) = 11.7212

2nd Lowest Vibrational Mode (1/cm) = 18.0102

E(RM062X) (a.u.) = -3187.95694997

Thermal correction to Enthalpy (a.u.) = 0.682217

Thermal correction to Gibbs Free Energy (a.u.) = 0.555784

Total Entropy (cal/Kmol) = 266.101

Esp(RM062X) (a.u.) = -3190.92099530

Optimised cartesian coordinates (Angstrom):

C	-3.769213	-4.339921	0.754915
C	-2.864528	-4.756088	1.744323
C	-1.966144	-3.861582	2.314739
C	-1.984257	-2.543191	1.858903
C	-2.869196	-2.136892	0.859989
H	-2.865209	-5.796505	2.070303
H	-1.261439	-4.180066	3.083996
C	-1.718199	-0.183264	1.206340
C	-2.207296	1.938804	0.073136
C	-2.693532	1.050204	-1.077409
C	-3.455486	-0.147441	-0.546771
H	-3.600197	-0.889922	-1.342841
S	-0.956159	-1.223274	2.369328
N	-2.678913	-0.794131	0.514662
N	-1.386031	1.112681	0.993691
C	-3.459377	1.816876	-2.176848
C	-4.965079	1.941916	-1.933100
C	-3.195351	1.166577	-3.535552
H	-3.030771	2.833056	-2.202106
H	-5.466461	0.967917	-2.047793
H	-5.206327	2.336782	-0.935686
H	-5.403722	2.621850	-2.677623
H	-2.125200	1.188850	-3.789092

H	-3.527057	0.115302	-3.541041
H	-3.744199	1.691218	-4.331024
H	-1.762716	0.668383	-1.525357
H	-1.535538	2.661826	-0.393186
C	-3.266429	2.722507	0.817204
C	-3.452930	4.067358	0.478889
C	-4.091965	2.138985	1.785405
C	-4.470854	4.811454	1.074237
H	-2.796098	4.532445	-0.261367
C	-5.107555	2.884715	2.382677
H	-3.950424	1.098911	2.090507
C	-5.304186	4.218734	2.022630
H	-4.608835	5.858582	0.800181
H	-5.747064	2.421013	3.135417
H	-6.100658	4.799065	2.491162
C	0.342411	2.898607	1.027137
H	1.108874	3.260097	1.721896
C	0.974308	2.545302	-0.334595
C	1.106320	3.782386	-1.196874
F	1.873785	4.716396	-0.632937
F	1.607930	3.512246	-2.396192
F	-0.103910	4.338795	-1.394048
O	0.285949	1.043458	2.531625
C	-0.229680	1.641104	1.624661
H	-4.438195	0.124692	-0.132841
C	-3.786296	-3.027914	0.297391
H	-4.483385	-2.715601	-0.479584
H	-4.460270	-5.062863	0.319974
H	0.356085	1.830036	-0.904554
S	2.569067	1.708263	-0.149790
C	2.116756	-0.059432	-0.479267
N	3.053438	-0.926404	-0.246706
N	0.881329	-0.263494	-0.886272
C	4.385838	-0.666200	-0.062748
C	5.152561	0.091556	-0.982034
C	5.055148	-1.244182	1.041956
C	6.512021	0.281346	-0.793311
H	4.663157	0.518977	-1.857997
C	6.412403	-1.056780	1.238858
H	4.472615	-1.841030	1.744763
C	7.129706	-0.290774	0.318695
H	7.103337	0.861506	-1.500567
H	6.925583	-1.493166	2.094771
N	8.561103	-0.092012	0.519234
O	9.077735	-0.604801	1.488983
O	9.163618	0.576750	-0.293063
C	0.356215	-1.523284	-1.051711
C	-0.671454	-1.690504	-2.019120
C	0.710275	-2.662465	-0.281302
C	-1.345297	-2.888843	-2.172910
H	-0.912813	-0.845931	-2.666112
C	0.041176	-3.867171	-0.432915
H	1.510926	-2.580103	0.449273
C	-0.991876	-3.971615	-1.363822
H	-2.136310	-3.002642	-2.913928
H	0.300409	-4.731423	0.178131
N	-1.740769	-5.212091	-1.465953
O	-2.723544	-5.228043	-2.179725
O	-1.361432	-6.168865	-0.823480
H	-0.428320	3.676829	0.932259

CF3_Michael_Acceptor/MA-S_pt

Frequencies, energies and thermodynamic properties:

Lowest Vibrational Mode (1/cm) = 15.7742

2nd Lowest Vibrational Mode (1/cm) = 17.2012

E(RM062X) (a.u.) = -3187.94879907

Thermal correction to Enthalpy (a.u.) = 0.681318

Thermal correction to Gibbs Free Energy (a.u.) = 0.555805

Total Entropy (cal/Kmol) = 264.163

Esp(RM062X) (a.u.) = -3190.91377171

Optimised cartesian coordinates (Angstrom):

C	5.658991	1.568418	2.061192
C	5.895732	2.201915	0.829958
C	5.272775	1.761821	-0.331554
C	4.389580	0.685781	-0.225641
C	4.156229	0.058040	0.998478
H	6.568409	3.059252	0.783660
H	5.442950	2.259791	-1.287565
C	2.669501	-1.069602	-0.334035
C	1.109070	-2.800269	0.472115
C	2.275582	-3.135067	1.421060
C	2.864996	-1.856416	1.990511
H	3.793386	-2.069714	2.536986
S	3.406507	-0.011943	-1.491241
N	3.207776	-0.962484	0.882065
N	1.617165	-1.887794	-0.589410
C	1.914787	-4.161190	2.520802
C	1.390706	-3.541240	3.819497
C	3.130126	-5.039150	2.821421
H	1.125602	-4.808900	2.104955
H	0.566383	-2.832190	3.659790
H	1.024118	-4.336781	4.484200
H	2.196308	-3.015850	4.356518
H	3.454779	-5.596883	1.930999
H	3.977736	-4.426040	3.167702
H	2.898299	-5.764862	3.614276
H	3.048876	-3.593515	0.782573
H	0.841947	-3.735951	-0.036282
C	-0.109572	-2.245267	1.174528
C	-1.133861	-3.117671	1.556377
C	-0.193977	-0.895065	1.522284
C	-2.204175	-2.654951	2.319744
H	-1.086245	-4.169418	1.262239
C	-1.265925	-0.429234	2.282553
H	0.574283	-0.192151	1.191378
C	-2.263568	-1.312484	2.697025
H	-2.994949	-3.344256	2.620132
H	-1.325015	0.628332	2.548647
H	-3.100357	-0.947631	3.295179
C	-0.326921	-2.510269	-2.072297
H	-0.747603	-2.961367	-1.171005
C	-1.346597	-1.535299	-2.688607
C	-2.170555	-2.242352	-3.748047
F	-1.380796	-2.773865	-4.688375
F	-2.890459	-3.246892	-3.233137
F	-3.013791	-1.419990	-4.364123
O	1.568346	-1.262964	-2.769147
C	1.004792	-1.825606	-1.867059
H	2.170307	-1.334845	2.664895
C	4.792966	0.486584	2.165944
H	4.600463	0.009384	3.126785
H	6.157291	1.937767	2.958202
H	-0.827650	-0.704752	-3.186250
S	-2.496446	-0.819326	-1.468480
C	-1.607367	0.708104	-0.976326
N	-0.391875	0.781221	-1.461243

N	-2.221175	1.628537	-0.277459
C	0.472361	1.798046	-1.140582
C	1.291191	2.328767	-2.167584
C	0.674338	2.281453	0.177237
C	2.304616	3.229810	-1.893817
H	1.125643	1.977375	-3.186938
C	1.703102	3.165855	0.464805
H	0.018008	1.935297	0.974469
C	2.520713	3.621793	-0.570189
H	2.944289	3.619896	-2.684931
H	1.886035	3.504478	1.484139
N	3.650450	4.483308	-0.256909
O	3.794861	4.848052	0.890656
O	4.409102	4.781282	-1.157822
C	-3.483879	1.650256	0.231727
C	-4.079447	2.932760	0.393294
C	-4.238197	0.530940	0.677971
C	-5.343138	3.094071	0.925187
H	-3.499675	3.798794	0.071913
C	-5.506046	0.685854	1.217528
H	-3.813787	-0.469646	0.634355
C	-6.055173	1.961818	1.333449
H	-5.790938	4.081222	1.032165
H	-6.075165	-0.177767	1.560161
N	-7.385369	2.119230	1.900149
O	-7.983246	1.121062	2.246061
O	-7.834429	3.242177	2.001201
H	-0.107708	-3.318759	-2.788754

CF3_Michael_Acceptor/MA-S

Frequencies, energies and thermodynamic properties:

Lowest Vibrational Mode (1/cm) = 11.3528

2nd Lowest Vibrational Mode (1/cm) = 20.5196

E(RM062X) (a.u.) = -3187.95028278

Thermal correction to Enthalpy (a.u.) = 0.682002

Thermal correction to Gibbs Free Energy (a.u.) = 0.555777

Total Entropy (cal/Kmol) = 265.663

Esp(RM062X) (a.u.) = -3190.91353033

Optimised cartesian coordinates (Angstrom):

C	-4.936250	-3.683418	-1.715028
C	-3.845238	-4.559349	-1.654702
C	-2.546498	-4.073436	-1.523544
C	-2.370008	-2.694429	-1.428306
C	-3.460669	-1.824333	-1.493549
H	-4.012047	-5.635784	-1.706920
H	-1.693539	-4.752370	-1.473594
C	-1.752096	-0.320819	-1.129802
C	-2.072958	2.069689	-0.815546
C	-3.193372	1.888575	-1.857653
C	-3.991880	0.630629	-1.555636
H	-4.641338	0.376297	-2.404923
S	-0.858378	-1.819241	-1.228618
N	-3.066005	-0.487890	-1.364338
N	-1.223990	0.858959	-0.816892
C	-4.078755	3.141860	-2.047637
C	-5.293723	3.218064	-1.119172
C	-4.534440	3.239348	-3.504303
H	-3.435097	4.012689	-1.838267
H	-5.034329	3.098009	-0.057933
H	-5.783530	4.195811	-1.235461
H	-6.038879	2.449749	-1.380135
H	-3.677760	3.304833	-4.190666
H	-5.131141	2.357273	-3.787515

H	-5.162975	4.128834	-3.656564
H	-2.666772	1.714803	-2.810357
H	-1.424254	2.876201	-1.179409
C	-2.571484	2.448867	0.564201
C	-2.478595	3.782635	0.976181
C	-3.197821	1.522983	1.406342
C	-3.017407	4.189187	2.196481
H	-1.978608	4.509924	0.331154
C	-3.733361	1.926074	2.629639
H	-3.268814	0.472764	1.115482
C	-3.650011	3.261873	3.024695
H	-2.938244	5.233516	2.502922
H	-4.218274	1.192560	3.276679
H	-4.071186	3.577526	3.980579
C	0.685692	2.099602	0.055065
H	0.030918	2.846649	0.496165
C	2.143686	2.288179	0.108973
C	2.493677	3.764059	0.123089
F	2.107919	4.351240	-1.011955
F	1.895325	4.415856	1.125857
F	3.806680	3.981343	0.248088
O	0.899603	-0.014363	-0.958433
C	0.226913	0.958879	-0.573323
H	-4.622236	0.736498	-0.660809
C	-4.762045	-2.303436	-1.639857
H	-5.615135	-1.625671	-1.678827
H	-5.944984	-4.086074	-1.815109
H	2.635036	1.848929	-0.769956
S	3.122296	1.559011	1.582785
C	2.470814	-0.123704	1.649419
N	3.158154	-1.159060	1.370209
N	1.203321	-0.189411	2.157934
H	0.792686	0.716010	2.366549
C	4.319548	-1.120114	0.615642
C	4.282185	-0.643509	-0.710024
C	5.519981	-1.630162	1.137907
C	5.428998	-0.655517	-1.489358
H	3.324985	-0.295571	-1.107007
C	6.672795	-1.636559	0.365228
H	5.534085	-2.011407	2.159350
C	6.611390	-1.147377	-0.937919
H	5.419817	-0.292825	-2.516206
H	7.615013	-2.016209	0.757690
N	7.825146	-1.159725	-1.758209
O	8.841402	-1.592706	-1.262112
O	7.748984	-0.736010	-2.890002
C	0.295941	-1.238243	2.078627
C	0.642016	-2.578832	1.833796
C	-1.059349	-0.893548	2.250430
C	-0.359873	-3.535407	1.706836
H	1.684958	-2.860816	1.727873
C	-2.056596	-1.842080	2.114033
H	-1.313571	0.144295	2.474483
C	-1.692919	-3.157434	1.826513
H	-0.110001	-4.575223	1.498610
H	-3.109106	-1.578451	2.218168
N	-2.745984	-4.148989	1.603236
O	-3.894411	-3.765522	1.612577
O	-2.413316	-5.297024	1.409142

CF3_Michael_Acceptor/pNO2_thiourea

Frequencies, energies and thermodynamic properties:

Lowest Vibrational Mode (1/cm) = 18.6815

2nd Lowest Vibrational Mode (1/cm) = 21.7203

E(RM062X) (a.u.) = -1418.04990065

Thermal correction to Enthalpy (a.u.) = 0.251465

Thermal correction to Gibbs Free Energy (a.u.) = 0.181252

Total Entropy (cal/Kmol) = 147.775

Esp(RM062X) (a.u.) = -1419.34300615

Optimised cartesian coordinates (Angstrom):

C	-0.010122	1.964661	0.081432
S	-0.923571	3.348093	-0.105177
N	1.353766	2.059251	0.123383
H	1.684195	3.016258	0.223140
N	-0.500866	0.708768	0.270880
H	0.140222	0.042540	0.699144
C	-1.817630	0.241178	0.178794
C	-2.757629	0.760615	-0.724929
C	-2.164941	-0.844466	0.999652
C	-4.030956	0.210625	-0.786694
H	-2.492443	1.585810	-1.380248
C	-3.433891	-1.399768	0.937124
H	-1.428459	-1.246755	1.697331
C	-4.353857	-0.856707	0.045689
H	-4.771858	0.598601	-1.484094
H	-3.715341	-2.237635	1.572957
C	2.349450	1.077612	0.045142
C	3.582038	1.360050	0.659970
C	2.187958	-0.124495	-0.666159
C	4.629343	0.455633	0.587476
H	3.706231	2.300119	1.199910
C	3.231832	-1.038536	-0.730380
H	1.261120	-0.339243	-1.196526
C	4.434327	-0.739726	-0.099629
H	5.586923	0.662590	1.063028
H	3.123355	-1.971243	-1.281951
N	5.535029	-1.708228	-0.170714
O	5.333037	-2.748914	-0.753086
O	6.581297	-1.410962	0.358233
N	-5.701693	-1.433283	-0.024638
O	-5.948306	-2.378536	0.689216
O	-6.490527	-0.932354	-0.792758

CF3_Michael_Acceptor/product

Frequencies, energies and thermodynamic properties:

Lowest Vibrational Mode (1/cm) = 19.1238

2nd Lowest Vibrational Mode (1/cm) = 22.6778

E(RM062X) (a.u.) = -1945.26747655

Thermal correction to Enthalpy (a.u.) = 0.307288

Thermal correction to Gibbs Free Energy (a.u.) = 0.220747

Total Entropy (cal/Kmol) = 182.142

Esp(RM062X) (a.u.) = -1947.17713409

Optimised cartesian coordinates (Angstrom):

C	0.198428	3.406049	-0.599559
C	0.078420	0.622002	-0.641485
C	-1.932075	2.076681	-1.057062
C	-1.073336	3.267513	-1.414322
H	-0.804175	3.182847	-2.478106
H	-1.708753	4.155132	-1.299960
N	-1.292894	0.877215	-0.709850
C	-2.159753	-0.227233	-0.383884
C	-2.488182	-0.452750	0.951322
C	-2.656782	-1.037356	-1.402710
C	-3.330073	-1.509419	1.280485
H	-2.084649	0.201107	1.725613
C	-3.500397	-2.095675	-1.085103

H	-2.380965	-0.836602	-2.438578
C	-3.817493	-2.308855	0.252375
H	-3.608614	-1.714148	2.312750
H	-3.907679	-2.749571	-1.854366
N	-4.710612	-3.431994	0.594680
O	-5.116450	-4.122134	-0.310283
O	-4.984132	-3.596707	1.759952
O	-3.133976	2.129106	-1.090590
S	1.261860	1.950377	-0.777346
N	0.472533	-0.573612	-0.499774
C	1.807153	-0.932470	-0.316536
C	2.498783	-1.581335	-1.352021
C	2.443272	-0.710294	0.917641
C	3.812721	-1.989474	-1.166277
H	1.990207	-1.761397	-2.299545
C	3.754327	-1.121234	1.110937
H	1.895795	-0.217474	1.722100
C	4.420037	-1.753082	0.063651
H	4.366917	-2.489583	-1.959133
H	4.263097	-0.958330	2.059918
N	5.807331	-2.188962	0.265267
O	6.314690	-1.976934	1.342908
O	6.367227	-2.735663	-0.657431
H	0.797963	4.243408	-0.984051
C	-0.070275	3.717824	0.864223
F	-0.776095	4.842281	0.978173
F	1.056552	3.873572	1.550032
F	-0.772784	2.745631	1.459810

CF3_Michael_Acceptor/TS-acyl

Frequencies, energies and thermodynamic properties:

Lowest Vibrational Mode (1/cm) = -121.9738

2nd Lowest Vibrational Mode (1/cm) = 10.1528

E(RM062X) (a.u.) = -2572.61729427

Thermal correction to Enthalpy (a.u.) = 0.505164

Thermal correction to Gibbs Free Energy (a.u.) = 0.396543

Total Entropy (cal/Kmol) = 228.612

Esp(RM062X) (a.u.) = -2575.24147968

Optimised cartesian coordinates (Angstrom):

C	6.671002	-1.747644	0.267353
C	6.324437	-2.999860	-0.246781
C	4.983837	-3.345754	-0.428728
C	4.007431	-2.416839	-0.086080
C	4.355512	-1.164910	0.438062
C	5.693530	-0.814013	0.615240
H	7.722674	-1.489020	0.398820
H	7.104436	-3.714268	-0.512543
H	4.707149	-4.320805	-0.833020
H	5.970014	0.164510	1.008306
C	2.035838	-0.945700	0.405474
C	0.831255	1.026580	0.959631
C	1.988461	1.314763	1.941465
C	3.319295	0.958535	1.289643
H	4.123398	0.965454	2.039387
S	2.261298	-2.599300	-0.218009
N	3.240783	-0.383063	0.722211
N	0.897138	-0.361531	0.512450
C	1.976932	2.735196	2.549439
C	2.761892	3.777749	1.748513
C	2.491010	2.695628	3.989270
H	0.921575	3.054321	2.580039
H	2.486652	3.797089	0.684510
H	2.576318	4.780310	2.161463

H	3.845804	3.593317	1.818154
H	1.870135	2.042528	4.619898
H	3.525824	2.318115	4.025464
H	2.488721	3.701854	4.434023
H	1.835133	0.602251	2.768710
H	-0.110457	1.124587	1.519091
C	0.765908	1.989858	-0.215705
C	-0.077103	3.104828	-0.145326
C	1.539661	1.801750	-1.367394
C	-0.128070	4.026521	-1.191226
H	-0.705075	3.248143	0.736876
C	1.490053	2.722326	-2.414305
H	2.179517	0.921170	-1.465131
C	0.659378	3.840076	-2.327445
H	-0.792405	4.889711	-1.120939
H	2.094396	2.557135	-3.307978
H	0.615913	4.556521	-3.149563
C	-1.065066	-0.438798	-1.136102
H	-1.376071	0.586532	-0.922510
C	-0.893625	-0.864402	-2.382700
H	-0.562563	-1.881448	-2.608310
C	-1.079847	0.044390	-3.551608
F	0.072450	0.219924	-4.213024
F	-1.952666	-0.456407	-4.433895
F	-1.520272	1.255024	-3.204115
O	-0.469124	-2.509642	-0.096755
C	-0.745108	-1.341388	0.023931
H	3.586142	1.671441	0.493229
O	-1.407306	-0.906091	1.232194
C	-2.750906	-0.805923	1.134082
C	-3.581394	-1.929947	1.182865
C	-3.349139	0.449692	0.998270
C	-4.965089	-1.795877	1.119299
C	-4.729632	0.593740	0.936349
C	-5.539632	-0.536173	0.985638
F	-2.580770	1.530575	0.933094
F	-5.273951	1.794013	0.815077
F	-5.739641	-2.867674	1.179639
F	-3.060253	-3.135911	1.320359
F	-6.854558	-0.411662	0.919231

CF3_Michael_Acceptor/TS-cycl-R_rot

Frequencies, energies and thermodynamic properties:

Lowest Vibrational Mode (1/cm) = -107.2018

2nd Lowest Vibrational Mode (1/cm) = 12.1212

E(RM062X) (a.u.) = -3187.93331614

Thermal correction to Enthalpy (a.u.) = 0.680738

Thermal correction to Gibbs Free Energy (a.u.) = 0.555516

Total Entropy (cal/Kmol) = 263.552

Esp(RM062X) (a.u.) = -3190.89449964

Optimised cartesian coordinates (Angstrom):

C	-0.167217	-1.461371	2.611883
C	1.337506	-1.394643	2.821634
H	1.618699	-2.308799	3.367011
H	-0.386767	-2.432652	2.153195
H	-0.653785	-1.464511	3.598063
N	0.619360	0.469257	0.727786
C	0.205944	1.696456	0.197015
C	0.190209	1.946068	-1.189862
C	-0.232927	2.707592	1.073700
C	-0.292181	3.146557	-1.689952
H	0.571078	1.187161	-1.870362
C	-0.722495	3.911596	0.581693

H	-0.169019	2.537882	2.145361
C	-0.755134	4.109598	-0.795166
H	-0.314704	3.343242	-2.761048
H	-1.062904	4.699689	1.251747
N	-1.272974	5.376645	-1.319826
O	-1.684389	6.194325	-0.526974
O	-1.266287	5.539376	-2.519970
C	-0.874298	-0.321788	1.873031
O	-1.345259	0.607552	2.501502
C	1.808319	-0.280027	3.747109
F	1.116731	-0.316822	4.892443
F	1.683870	0.948330	3.253386
F	3.096866	-0.444347	4.061121
S	2.314908	-1.510662	1.301099
C	1.812455	-0.006385	0.411036
N	2.617969	0.448864	-0.497460
C	3.966895	0.225759	-0.578363
C	4.836495	0.358673	0.533565
C	4.540027	-0.057180	-1.840127
C	6.203525	0.191565	0.392962
H	4.416944	0.606644	1.509527
C	5.906023	-0.229461	-1.987255
H	3.876163	-0.134667	-2.701988
C	6.727431	-0.107694	-0.865983
H	6.873997	0.296604	1.244992
H	6.346754	-0.454478	-2.957530
N	8.167016	-0.284929	-1.014807
O	8.599759	-0.539739	-2.118804
O	8.861487	-0.170632	-0.027315
N	-1.690484	-0.808382	0.729171
C	-2.981882	-0.489120	0.678159
C	-1.169294	-1.800778	-0.227853
S	-3.713426	0.878029	1.484916
N	-3.863320	-1.191843	-0.048903
C	-2.180461	-2.961735	-0.300837
H	-0.242413	-2.188380	0.210291
C	-0.803326	-1.214762	-1.578517
C	-5.258770	0.474571	0.751000
C	-5.158786	-0.663959	-0.051830
C	-3.529897	-2.429976	-0.761278
C	-1.693559	-4.176395	-1.125324
H	-2.296047	-3.300611	0.742294
C	0.417177	-1.595180	-2.147280
C	-1.661815	-0.388387	-2.315182
C	-6.474086	1.139341	0.903049
C	-6.264011	-1.166477	-0.738955
H	-4.326743	-3.155304	-0.547613
H	-3.541694	-2.211778	-1.839215
C	-2.021019	-4.118458	-2.619715
C	-2.245244	-5.470535	-0.524951
H	-0.595462	-4.197601	-1.020270
C	0.767160	-1.179615	-3.431636
H	1.106809	-2.218077	-1.571338
C	-1.316086	0.023231	-3.602043
H	-2.605394	-0.035025	-1.895623
C	-7.580743	0.643138	0.218930
H	-6.552276	2.025181	1.534808
C	-7.474518	-0.494709	-0.591786
H	-6.185178	-2.051952	-1.369620
H	-1.715008	-3.174464	-3.092051
H	-1.501610	-4.936325	-3.139872
H	-3.099630	-4.257531	-2.794895
H	-1.922741	-5.600849	0.518441

H -3.347072 -5.471579 -0.543166
H -1.902123 -6.343240 -1.099371
C -0.103799 -0.374498 -4.166442
H 1.723479 -1.486605 -3.858410
H -1.995191 0.669023 -4.161358
H -8.541369 1.150223 0.315625
H -8.354646 -0.864183 -1.119446
H 0.165794 -0.049766 -5.172767

CF3_Michael_Acceptor/TS-cycl-R

Frequencies, energies and thermodynamic properties:

Lowest Vibrational Mode (1/cm) = -158.3451
2nd Lowest Vibrational Mode (1/cm) = 9.8201
E(RM062X) (a.u.) = -3187.93917543
Thermal correction to Enthalpy (a.u.) = 0.680413
Thermal correction to Gibbs Free Energy (a.u.) = 0.554712
Total Entropy (cal/Kmol) = 264.560
Esp(RM062X) (a.u.) = -3190.90456649

Optimised cartesian coordinates (Angstrom):

C 1.707617 -2.526199 -1.147645
C 2.243743 0.203164 -0.329952
C -0.305280 -1.093178 -1.077964
C 0.399807 -2.270189 -0.428837
H 0.567778 -2.147790 0.645961
H -0.268186 -3.135431 -0.578371
N 0.915592 0.307736 -0.432702
C 0.316150 1.546344 -0.199038
C -0.578447 2.058402 -1.156724
C 0.505867 2.259349 1.003014
C -1.311005 3.212935 -0.908054
H -0.687182 1.527262 -2.102828
C -0.205410 3.422236 1.253741
H 1.215405 1.885395 1.739941
C -1.121507 3.873014 0.302959
H -2.015771 3.606514 -1.639771
H -0.070812 3.977620 2.181056
N -1.907800 5.074722 0.591911
O -1.792095 5.576428 1.688413
O -2.639455 5.496686 -0.275280
O -0.378831 -1.011402 -2.297945
S 3.045543 -1.390616 -0.646440
N 3.033617 1.167575 0.008338
C 4.408889 1.155420 -0.040094
C 5.148499 1.361139 1.144693
C 5.115051 1.029048 -1.258935
C 6.532948 1.420881 1.123215
H 4.606018 1.472578 2.084211
C 6.498963 1.090254 -1.289692
H 4.554435 0.890235 -2.184202
C 7.194571 1.282238 -0.096056
H 7.107041 1.572829 2.036197
H 7.047156 0.995304 -2.226097
N 8.654157 1.347378 -0.124948
O 9.208557 1.219699 -1.194862
O 9.236843 1.525155 0.922744
H 1.552300 -2.458637 -2.233548
C 2.191646 -3.936003 -0.865573
F 3.390022 -4.166002 -1.404226
F 1.345616 -4.832825 -1.378769
F 2.287641 -4.187773 0.441475
N -1.518877 -0.683244 -0.331148
C -2.615350 -0.335434 -1.007776
C -1.532777 -0.695779 1.148290

S	-2.778415	-0.367773	-2.752269
N	-3.746827	0.051158	-0.400766
C	-2.487106	0.408290	1.645938
H	-0.517676	-0.406971	1.454594
C	-1.829305	-2.075352	1.704230
C	-4.461742	0.110701	-2.600958
C	-4.820835	0.293336	-1.265377
C	-3.866603	0.207479	1.048826
C	-2.526033	0.579713	3.181089
H	-2.086523	1.344565	1.225218
C	-1.114475	-2.518918	2.821958
C	-2.822736	-2.896933	1.161737
C	-5.383894	0.310438	-3.626852
C	-6.117166	0.667465	-0.908751
H	-4.493709	1.088894	1.236043
H	-4.376600	-0.679015	1.455965
C	-3.530914	-0.323958	3.902970
C	-2.818240	2.039621	3.533393
H	-1.514297	0.338041	3.547928
C	-1.408229	-3.747691	3.409758
H	-0.318650	-1.892950	3.233450
C	-3.116414	-4.128811	1.748426
H	-3.374356	-2.591067	0.268982
C	-6.677425	0.688959	-3.278080
H	-5.099004	0.171627	-4.670844
C	-7.037296	0.862405	-1.935026
H	-6.405710	0.798038	0.134002
H	-3.444081	-1.383495	3.626278
H	-3.378798	-0.248058	4.989512
H	-4.563847	-0.000241	3.698416
H	-2.075566	2.723363	3.098161
H	-3.810906	2.339910	3.160516
H	-2.818687	2.182824	4.623768
C	-2.415908	-4.553201	2.877369
H	-0.843745	-4.080300	4.282371
H	-3.894081	-4.761012	1.316783
H	-7.418833	0.849269	-4.061590
H	-8.057721	1.154413	-1.684069
H	-2.646087	-5.517014	3.334306

CF3_Michael_Acceptor/TS-cycl-S_rot

Frequencies, energies and thermodynamic properties:

Lowest Vibrational Mode (1/cm) = -156.7463

2nd Lowest Vibrational Mode (1/cm) = 8.1342

E(RM062X) (a.u.) = -3187.93750850

Thermal correction to Enthalpy (a.u.) = 0.680296

Thermal correction to Gibbs Free Energy (a.u.) = 0.553889

Total Entropy (cal/Kmol) = 266.046

Esp(RM062X) (a.u.) = -3190.89948963

Optimised cartesian coordinates (Angstrom):

C	1.652237	-2.328958	-1.753183
C	2.128018	-0.164125	-0.016573
C	-0.452022	-0.928146	-1.318490
C	0.188999	-2.305513	-1.335471
H	0.133958	-2.825313	-0.375108
H	-0.408222	-2.881925	-2.059465
N	0.849102	0.074099	-0.296316
C	0.363312	1.370375	-0.050457
C	0.029146	2.207057	-1.126289
C	0.157863	1.824479	1.265126
C	-0.546932	3.453459	-0.896838
H	0.223884	1.861852	-2.140000
C	-0.408601	3.067102	1.506705

H	0.455389	1.185523	2.098078
C	-0.765898	3.857778	0.414761
H	-0.819891	4.111019	-1.721053
H	-0.578080	3.429170	2.519822
N	-1.380331	5.168970	0.661637
O	-1.571779	5.495642	1.811270
O	-1.666228	5.850054	-0.296446
O	-0.638142	-0.336664	-2.375873
S	2.777340	-1.800964	-0.433491
N	2.911099	0.657555	0.608965
C	4.281700	0.603845	0.647852
C	4.942778	0.777888	1.884952
C	5.073283	0.476817	-0.520384
C	6.325476	0.800432	1.963702
H	4.335961	0.895477	2.783502
C	6.455786	0.501256	-0.449848
H	4.578502	0.369424	-1.486590
C	7.070776	0.657838	0.793311
H	6.836142	0.927576	2.917357
H	7.067185	0.407640	-1.346412
N	8.527530	0.683871	0.868937
O	9.154722	0.550536	-0.160054
O	9.039569	0.836350	1.957469
H	1.925520	-3.382037	-1.914138
C	2.003162	-1.648064	-3.070601
F	1.129679	-1.969811	-4.025313
F	3.207373	-2.063345	-3.487807
F	2.069516	-0.320054	-2.999795
N	-1.573120	-0.816667	-0.334137
C	-2.649107	-0.097204	-0.650466
C	-1.483796	-1.473033	0.985350
S	-2.932266	0.675269	-2.198684
N	-3.675929	0.077662	0.197594
C	-2.239414	-0.623238	2.023855
H	-0.418832	-1.439210	1.255581
C	-1.936161	-2.920768	0.944312
C	-4.520973	1.186607	-1.648920
C	-4.761465	0.780580	-0.336051
C	-3.673153	-0.416145	1.574718
C	-2.130555	-1.146064	3.474247
H	-1.754013	0.363022	1.993523
C	-1.228530	-3.870705	1.690046
C	-3.066529	-3.324774	0.226392
C	-5.475773	1.910318	-2.361302
C	-5.966839	1.071211	0.303869
H	-4.163185	0.342345	2.199187
H	-4.266585	-1.341866	1.618435
C	-3.240926	-2.116248	3.886449
C	-2.087295	0.035705	4.443944
H	-1.167046	-1.676794	3.548866
C	-1.661340	-5.194126	1.746079
H	-0.326401	-3.567745	2.228016
C	-3.499378	-4.650687	0.280344
H	-3.620904	-2.611821	-0.389184
C	-6.679374	2.207885	-1.727421
H	-5.284474	2.231167	-3.386377
C	-6.920167	1.790741	-0.411746
H	-6.160986	0.744454	1.325338
H	-3.366172	-2.951057	3.182439
H	-3.011416	-2.542294	4.873977
H	-4.206795	-1.594061	3.974683
H	-1.228299	0.692387	4.240707
H	-3.004180	0.641529	4.362869

H -2.010134 -0.314474 5.483594
C -2.803528 -5.585793 1.046056
H -1.101145 -5.923776 2.333156
H -4.383805 -4.953004 -0.282885
H -7.443494 2.771070 -2.264415
H -7.871462 2.031118 0.064524
H -3.143573 -6.621818 1.087126

CF3_Michael_Acceptor/TS-cycl-S

Frequencies, energies and thermodynamic properties:

Lowest Vibrational Mode (1/cm) = -147.8870

2nd Lowest Vibrational Mode (1/cm) = 11.6807

E(RM062X) (a.u.) = -3187.93294578

Thermal correction to Enthalpy (a.u.) = 0.680546

Thermal correction to Gibbs Free Energy (a.u.) = 0.555204

Total Entropy (cal/Kmol) = 263.805

Esp(RM062X) (a.u.) = -3190.89656748

Optimised cartesian coordinates (Angstrom):

C 0.106479 -2.100773 -2.001132
C -1.338517 -1.890280 -2.404411
H -1.424812 -1.064198 -3.125643
H 0.156583 -2.838408 -1.190319
H 0.668925 -2.505225 -2.854976
N -0.539842 0.417566 -1.117527
C -0.029909 1.724556 -1.046786
C -0.005876 2.460745 0.153375
C 0.506133 2.305439 -2.211269
C 0.571333 3.722068 0.199692
H -0.455099 2.038203 1.049212
C 1.089170 3.566381 -2.174534
H 0.449359 1.755917 -3.147446
C 1.121281 4.252657 -0.964930
H 0.599525 4.295166 1.125420
H 1.504519 4.023778 -3.071183
N 1.737083 5.583502 -0.917849
O 2.199614 6.031396 -1.943040
O 1.753850 6.163144 0.144985
C 0.855306 -0.797423 -1.680733
O 1.469265 -0.239165 -2.580519
C -1.896586 -3.122644 -3.089812
F -3.161813 -2.954318 -3.468592
F -1.857903 -4.194316 -2.290895
F -1.189580 -3.418118 -4.182165
S -2.382533 -1.509452 -0.960894
C -1.761887 0.163995 -0.639602
N -2.501192 0.975160 0.038872
C -3.849122 0.846244 0.278629
C -4.794479 0.644981 -0.754825
C -4.326202 1.012938 1.597420
C -6.150692 0.589261 -0.477648
H -4.446779 0.543060 -1.783022
C -5.680601 0.953050 1.883738
H -3.600599 1.195336 2.390613
C -6.580648 0.737347 0.841025
H -6.881892 0.437755 -1.270539
H -6.050219 1.074580 2.901018
N -8.010124 0.677186 1.135169
O -8.360262 0.812744 2.287617
O -8.774111 0.493380 0.212548
N 1.596928 -0.894350 -0.379741
C 2.910784 -0.692710 -0.376687
C 0.959436 -1.424472 0.837507
S 3.794686 0.205794 -1.590425

N	3.702651	-1.139635	0.611551
C	1.854066	-2.552510	1.387974
H	0.012416	-1.874244	0.518013
C	0.619053	-0.357775	1.860067
C	5.271891	-0.007082	-0.660366
C	5.041439	-0.749709	0.499740
C	3.232120	-1.992730	1.707372
C	1.232866	-3.339456	2.565478
H	1.968479	-3.256296	0.546862
C	-0.633799	-0.416413	2.480216
C	1.531324	0.622660	2.271604
C	6.548739	0.457110	-0.970476
C	6.073099	-1.037658	1.393674
H	3.960372	-2.806301	1.829158
H	3.229189	-1.390551	2.627918
C	1.530721	-2.766924	3.953874
C	1.671186	-4.803374	2.504333
H	0.140762	-3.309486	2.413132
C	-0.960797	0.466769	3.509382
H	-1.362835	-1.162062	2.150928
C	1.204164	1.508456	3.297378
H	2.504614	0.726726	1.788829
C	7.583146	0.172594	-0.082362
H	6.730070	1.031669	-1.879949
C	7.345689	-0.564434	1.085052
H	5.890652	-1.610120	2.303088
H	1.304265	-1.694403	4.035657
H	0.926190	-3.294952	4.705565
H	2.587951	-2.916840	4.224915
H	1.364448	-5.276791	1.560195
H	2.766670	-4.888095	2.587719
H	1.229338	-5.376656	3.332311
C	-0.040213	1.429585	3.923722
H	-1.938918	0.401648	3.988990
H	1.924434	2.269288	3.602877
H	8.589675	0.531915	-0.299490
H	8.170249	-0.773422	1.767666
H	-0.294270	2.121507	4.728360

CF3_Michael_Acceptor/TS-MA-R

Frequencies, energies and thermodynamic properties:

Lowest Vibrational Mode (1/cm) = -184.9680

2nd Lowest Vibrational Mode (1/cm) = 4.5828

E(RM062X) (a.u.) = -3187.94763983

Thermal correction to Enthalpy (a.u.) = 0.680837

Thermal correction to Gibbs Free Energy (a.u.) = 0.554671

Total Entropy (cal/Kmol) = 265.539

Esp(RM062X) (a.u.) = -3190.90852411

Optimised cartesian coordinates (Angstrom):

C	-6.259958	1.915444	-0.150895
C	-6.694052	0.747207	0.489989
C	-5.781696	-0.132062	1.064980
C	-4.425367	0.175181	0.962355
C	-3.995925	1.327500	0.301765
H	-7.760193	0.524287	0.543591
H	-6.113839	-1.040997	1.568994
C	-1.966709	0.412469	0.899772
C	0.209002	1.406217	0.400107
C	-0.515613	2.041055	-0.797441
C	-1.897744	2.514267	-0.391653
H	-2.482579	2.794087	-1.277621
S	-3.070497	-0.756480	1.574161
N	-2.599442	1.417523	0.276649

N	-0.630780	0.338110	0.978540
C	0.315167	3.131977	-1.511390
C	0.108548	4.545724	-0.961797
H	-0.897355	4.921055	-1.208127
H	0.240130	4.605902	0.127793
H	0.833194	5.230749	-1.425252
H	-0.658629	1.212220	-1.512052
H	1.081225	0.901532	-0.026003
C	0.683971	2.377974	1.459038
C	2.006643	2.831314	1.415814
C	-0.176793	2.875070	2.443409
C	2.454274	3.793715	2.319269
H	2.690086	2.423882	0.665386
C	0.271184	3.836604	3.349268
H	-1.205487	2.512325	2.516432
C	1.584266	4.303791	3.283586
H	3.487850	4.140666	2.274429
H	-0.408771	4.219284	4.112202
H	1.933485	5.055694	3.993160
C	1.403948	-0.856679	1.672245
H	2.040631	-0.076448	1.266219
C	1.990754	-2.037930	2.132823
C	3.416755	-1.937475	2.605087
F	4.198728	-1.282290	1.744380
F	3.469957	-1.267056	3.764736
F	3.976600	-3.128184	2.831970
O	-0.777320	-1.666884	2.057337
C	-0.014651	-0.811661	1.619472
H	-1.861312	3.376375	0.291565
C	-4.907781	2.226003	-0.253125
H	-4.579527	3.136407	-0.753888
H	-6.994104	2.594722	-0.585819
H	1.383007	-2.691506	2.762137
S	2.307693	-3.596230	0.518241
C	1.209625	-2.789346	-0.602726
N	-0.078098	-3.286796	-0.517411
H	-0.159465	-4.073435	0.119142
C	-1.286154	-2.778861	-0.960085
C	-1.438251	-1.591835	-1.706007
C	-2.443195	-3.503698	-0.593065
C	-2.710110	-1.121894	-2.013109
H	-0.556919	-1.049027	-2.031300
C	-3.706722	-3.047140	-0.916528
H	-2.330823	-4.430550	-0.027400
C	-3.829699	-1.842569	-1.610223
H	-2.838213	-0.193544	-2.570594
H	-4.597794	-3.598850	-0.619957
N	-5.162083	-1.311993	-1.892294
O	-5.240297	-0.225726	-2.422683
O	-6.118954	-1.985178	-1.577568
N	1.438368	-1.779225	-1.365739
C	2.646658	-1.148208	-1.610850
C	2.554349	0.191891	-2.052471
C	3.929732	-1.733629	-1.539260
C	3.678887	0.945979	-2.344084
H	1.560269	0.623403	-2.180155
C	5.063242	-0.990030	-1.841013
H	4.037458	-2.774650	-1.248041
C	4.929288	0.342426	-2.222386
H	3.600119	1.981081	-2.675214
H	6.054753	-1.437248	-1.783496
N	6.128911	1.123463	-2.529444
O	5.982159	2.280302	-2.858002

O 7.203561 0.573766 -2.438562
H 1.375875 2.863099 -1.368574
C 0.027465 3.107229 -3.012564
H -1.039425 3.298199 -3.211459
H 0.606548 3.884003 -3.532976
H 0.285765 2.134485 -3.457445

CF3_Michael_Acceptor/TS-MA-S

Frequencies, energies and thermodynamic properties:

Lowest Vibrational Mode (1/cm) = -133.2872
2nd Lowest Vibrational Mode (1/cm) = 19.7386
E(RM062X) (a.u.) = -3187.94750675
Thermal correction to Enthalpy (a.u.) = 0.680593
Thermal correction to Gibbs Free Energy (a.u.) = 0.557801
Total Entropy (cal/Kmol) = 258.438
Esp(RM062X) (a.u.) = -3190.90928200

Optimised cartesian coordinates (Angstrom):

C 6.602875 0.840039 -0.451944
C 6.748102 -0.468436 0.029498
C 5.696515 -1.114920 0.671372
C 4.490800 -0.426113 0.800889
C 4.354067 0.880704 0.329827
H 7.694900 -0.991964 -0.106558
H 5.803413 -2.135871 1.041456
C 2.222061 0.498806 1.105459
C 0.388565 2.120461 0.975261
C 1.524990 3.141148 1.187851
C 2.708756 2.777673 0.308486
H 3.584389 3.388668 0.565647
S 3.000891 -1.002060 1.524151
N 3.066715 1.379811 0.556614
N 0.914245 0.764109 1.270226
C 1.091347 4.616840 1.021692
C 1.262249 5.173617 -0.394759
C 1.854092 5.492835 2.016306
H 0.021904 4.666059 1.283123
H 0.801406 6.170138 -0.456463
H 2.328601 5.293264 -0.643754
H 0.798574 4.543126 -1.166510
H 1.563536 6.547805 1.907017
H 1.655695 5.189339 3.054467
H 2.940375 5.426324 1.843143
H 1.843874 3.006500 2.234469
H -0.369733 2.317740 1.743886
C -0.256736 2.232169 -0.388371
C -1.392789 3.036930 -0.533202
C 0.313134 1.646371 -1.523342
C -1.922978 3.290353 -1.797715
H -1.858218 3.476020 0.352693
C -0.227035 1.885417 -2.787974
H 1.185626 0.995926 -1.426720
C -1.337901 2.718435 -2.928843
H -2.801648 3.929809 -1.898740
H 0.223575 1.418863 -3.665802
H -1.756483 2.908921 -3.918396
C -1.356685 -0.050597 1.781327
H -1.801748 0.684825 1.111894
C -2.141588 -0.914120 2.521826
C -3.576111 -0.530052 2.756669
F -3.631701 0.533985 3.578478
F -4.209354 -0.177453 1.638019
F -4.286496 -1.491123 3.345930
O 0.608850 -1.219648 2.351265

C	0.060544	-0.253458	1.845478
H	2.493561	2.908837	-0.761947
C	5.407840	1.537206	-0.306123
H	5.295731	2.550668	-0.691020
H	7.439715	1.321972	-0.958758
H	-1.683118	-1.453268	3.351376
S	-2.590511	-3.047323	1.494740
C	-1.562590	-2.661532	0.131031
N	-1.825583	-1.838590	-0.823519
N	-0.311247	-3.256281	0.188421
H	-0.211964	-3.901275	0.965739
C	-3.074879	-1.293128	-1.054507
C	-4.261331	-2.056901	-1.083936
C	-3.149317	0.077610	-1.365476
C	-5.478166	-1.459688	-1.373191
H	-4.216863	-3.124038	-0.872726
C	-4.362145	0.687605	-1.643396
H	-2.224523	0.652422	-1.370407
C	-5.517827	-0.090832	-1.638377
H	-6.399323	-2.040379	-1.394588
H	-4.422936	1.751825	-1.867985
N	-6.802790	0.541432	-1.930226
O	-6.811969	1.730891	-2.164183
O	-7.794769	-0.154242	-1.923745
C	0.857061	-2.970481	-0.487754
C	1.032085	-1.866796	-1.349762
C	1.958602	-3.822266	-0.241583
C	2.286249	-1.595490	-1.881543
H	0.186014	-1.224799	-1.576093
C	3.200758	-3.564668	-0.791422
H	1.821998	-4.687409	0.410079
C	3.359139	-2.434601	-1.594655
H	2.442238	-0.726586	-2.521901
H	4.050919	-4.215927	-0.591978
N	4.684532	-2.098291	-2.104319
O	5.578197	-2.899787	-1.936305
O	4.827289	-1.028746	-2.655743

CF3_Michael_Acceptor/TS-turn-R_rot

Frequencies, energies and thermodynamic properties:

Lowest Vibrational Mode (1/cm) = -158.3844

2nd Lowest Vibrational Mode (1/cm) = 11.5905

E(RM062X) (a.u.) = -3187.93994850

Thermal correction to Enthalpy (a.u.) = 0.680072

Thermal correction to Gibbs Free Energy (a.u.) = 0.554449

Total Entropy (cal/Kmol) = 264.396

Esp(RM062X) (a.u.) = -3190.90144270

Optimised cartesian coordinates (Angstrom):

C	-0.417053	-0.778291	2.647146
C	0.993656	-0.779774	3.201651
H	1.103253	-1.611794	3.913025
H	-0.598578	-1.783791	2.249605
H	-1.143636	-0.597317	3.450089
N	0.456555	0.680928	0.725989
C	0.297818	1.887907	-0.033388
C	0.321577	1.862293	-1.431349
C	0.148908	3.105356	0.643239
C	0.161502	3.037931	-2.156971
H	0.488145	0.923514	-1.953442
C	-0.012757	4.286352	-0.071798
H	0.157107	3.113124	1.729870
C	-0.011625	4.228953	-1.461551
H	0.174270	3.034454	-3.245746

H	-0.131898	5.242270	0.435394
N	-0.184688	5.476298	-2.223730
O	-0.323813	6.503673	-1.601146
O	-0.179414	5.405105	-3.431180
C	-0.702533	0.344138	1.626626
O	-1.346101	1.319338	2.043783
C	1.388922	0.462692	3.985442
F	0.474454	0.738580	4.915964
F	1.528712	1.550906	3.225223
F	2.552890	0.275853	4.611302
S	2.171886	-1.144554	1.878023
C	1.676362	0.056958	0.635416
N	2.487679	0.308901	-0.316550
C	3.807041	-0.108382	-0.373462
C	4.769552	0.384383	0.531296
C	4.214177	-0.978399	-1.401768
C	6.098522	0.005543	0.420521
H	4.456817	1.072336	1.318164
C	5.541485	-1.366482	-1.514914
H	3.468907	-1.337622	-2.112257
C	6.466441	-0.869835	-0.599965
H	6.851775	0.379973	1.112323
H	5.868045	-2.043253	-2.303061
N	7.869439	-1.274446	-0.718403
O	8.165823	-2.036636	-1.611400
O	8.658103	-0.826766	0.083580
N	-1.733936	-0.546425	0.485600
C	-3.018808	-0.368411	0.527619
C	-1.182929	-1.676876	-0.257236
S	-3.822823	1.001578	1.314134
N	-3.920366	-1.206105	-0.050251
C	-2.145832	-2.877826	-0.155104
H	-0.251410	-1.963579	0.255150
C	-0.802535	-1.303589	-1.675897
C	-5.381768	0.399790	0.756108
C	-5.249815	-0.792033	0.036330
C	-3.521735	-2.470676	-0.664444
C	-1.618980	-4.179177	-0.800361
H	-2.243296	-3.065111	0.927908
C	0.430092	-1.729875	-2.181840
C	-1.658260	-0.566575	-2.504007
C	-6.633374	0.970792	0.966377
C	-6.364539	-1.434920	-0.500613
H	-4.268497	-3.228560	-0.388961
H	-3.535611	-2.358290	-1.759538
C	-1.967853	-4.348338	-2.281438
C	-2.112074	-5.393509	-0.011897
H	-0.519747	-4.147112	-0.712657
C	0.799245	-1.436338	-3.495046
H	1.111925	-2.288568	-1.534526
C	-1.291763	-0.274518	-3.817380
H	-2.611230	-0.189988	-2.125696
C	-7.752979	0.331090	0.433198
H	-6.734254	1.898861	1.531383
C	-7.616790	-0.856785	-0.291840
H	-6.262936	-2.358869	-1.070003
H	-1.696682	-3.473870	-2.889507
H	-1.433440	-5.218913	-2.689105
H	-3.044918	-4.537727	-2.414295
H	-1.775718	-5.358430	1.034684
H	-3.213141	-5.440072	-0.013804
H	-1.739423	-6.326934	-0.458655
C	-0.062570	-0.708747	-4.316732

H 1.765272 -1.771505 -3.877290
H -1.964897 0.306387 -4.450249
H -8.741959 0.765952 0.582718
H -8.501680 -1.342616 -0.705276
H 0.225996 -0.474087 -5.342653

CF3_Michael_Acceptor/TS-turn-R

Frequencies, energies and thermodynamic properties:

Lowest Vibrational Mode (1/cm) = -113.4847
2nd Lowest Vibrational Mode (1/cm) = 10.1204
E(RM062X) (a.u.) = -3187.94123551
Thermal correction to Enthalpy (a.u.) = 0.680211
Thermal correction to Gibbs Free Energy (a.u.) = 0.552895
Total Entropy (cal/Kmol) = 267.959
Esp(RM062X) (a.u.) = -3190.90569267

Optimised cartesian coordinates (Angstrom):

C 1.698931 -2.592390 -1.436692
C 2.194302 0.157439 -0.702815
C 0.008278 -0.815068 -1.387137
C 0.386218 -2.167403 -0.811602
H 0.476025 -2.137625 0.281811
H -0.401879 -2.877146 -1.096434
N 0.822239 0.278471 -0.783732
C 0.232232 1.561411 -0.600508
C -0.680029 2.065085 -1.536663
C 0.507482 2.290354 0.567844
C -1.340786 3.265170 -1.291682
H -0.878989 1.500722 -2.445770
C -0.136393 3.494197 0.812150
H 1.219898 1.902517 1.293850
C -1.063544 3.956171 -0.118284
H -2.062829 3.663946 -2.002769
H 0.061597 4.065112 1.718137
N -1.781345 5.207102 0.160147
O -1.630361 5.711714 1.250399
O -2.488503 5.659176 -0.709841
O -0.357909 -0.703008 -2.545539
S 3.028801 -1.393048 -1.073776
N 2.930651 1.155271 -0.418183
C 4.310606 1.114245 -0.278389
C 4.906916 0.560406 0.870644
C 5.125633 1.696411 -1.266154
C 6.285477 0.578476 1.025177
H 4.274015 0.119530 1.642042
C 6.505164 1.713830 -1.120205
H 4.655091 2.133674 -2.147210
C 7.065919 1.154076 0.025395
H 6.761036 0.153854 1.908065
H 7.148311 2.155907 -1.879781
N 8.522945 1.175857 0.187415
O 9.183051 1.678845 -0.693585
O 8.987720 0.689702 1.193875
H 1.595382 -2.688440 -2.526911
C 2.140612 -3.948014 -0.917507
F 3.340815 -4.285392 -1.393065
F 1.277099 -4.891120 -1.293762
F 2.215426 -3.981261 0.412858
N -1.580266 -0.568596 -0.244131
C -2.739018 -0.447745 -0.793775
C -1.456110 -0.397185 1.201336
S -3.060012 -0.694555 -2.527219
N -3.890704 -0.126895 -0.133524
C -2.474750 0.662770 1.677370

H -0.452396 0.014491 1.383272
C -1.527119 -1.722532 1.939986
C -4.778797 -0.431112 -2.253498
C -5.045578 -0.138565 -0.910627
C -3.880541 0.233454 1.280468
C -2.360798 1.066784 3.161809
H -2.231929 1.558280 1.078626
C -0.635838 -1.968696 2.990846
C -2.476050 -2.699405 1.616914
C -5.803628 -0.479739 -3.192566
C -6.349427 0.097815 -0.476683
H -4.586507 1.063816 1.424224
H -4.232263 -0.623109 1.877377
C -3.147850 0.177453 4.128869
C -2.792445 2.523630 3.343741
H -1.290097 0.996078 3.421841
C -0.707945 -3.152531 3.724177
H 0.123427 -1.221862 3.237027
C -2.550246 -3.884267 2.349839
H -3.164830 -2.545357 0.782779
C -7.109880 -0.238784 -2.763018
H -5.590748 -0.703371 -4.239054
C -7.375911 0.044673 -1.420480
H -6.562588 0.312938 0.570507
H -2.944046 -0.893815 3.993457
H -2.892494 0.439413 5.166259
H -4.231696 0.336307 4.012458
H -2.199526 3.209504 2.720181
H -3.851838 2.653155 3.069161
H -2.682889 2.835994 4.392812
C -1.670779 -4.111795 3.408793
H -0.005769 -3.328674 4.540936
H -3.296548 -4.636168 2.087525
H -7.927600 -0.275653 -3.483748
H -8.402489 0.226263 -1.099190
H -1.727989 -5.040307 3.979281

CF3_Michael_Acceptor/TS-turn-S_rot

Frequencies, energies and thermodynamic properties:

Lowest Vibrational Mode (1/cm) = -166.8112
2nd Lowest Vibrational Mode (1/cm) = 7.5736
E(RM062X) (a.u.) = -3187.94087403
Thermal correction to Enthalpy (a.u.) = 0.680112
Thermal correction to Gibbs Free Energy (a.u.) = 0.553433
Total Entropy (cal/Kmol) = 266.618
Esp(RM062X) (a.u.) = -3190.90329525

Optimised cartesian coordinates (Angstrom):

C 1.623409 -1.897201 -2.404160
C 2.001606 0.067820 -0.447135
C -0.265490 -0.449607 -1.575146
C 0.217651 -1.873448 -1.830060
H 0.235812 -2.493972 -0.928520
H -0.500182 -2.302762 -2.541166
N 0.690294 0.350450 -0.737521
C 0.188957 1.619521 -0.311203
C -0.167026 2.583877 -1.258333
C 0.030585 1.877800 1.055733
C -0.712543 3.795491 -0.841228
H -0.021967 2.369417 -2.314205
C -0.507720 3.083894 1.483142
H 0.341018 1.125630 1.781399
C -0.876836 4.019532 0.519657
H -1.002426 4.561402 -1.558672

H	-0.644970	3.304174	2.540725
N	-1.455380	5.299140	0.963038
O	-1.578576	5.478810	2.152627
O	-1.776192	6.097501	0.114026
O	-0.816434	0.151326	-2.503910
S	2.810241	-1.378469	-1.137420
N	2.677121	0.817359	0.335906
C	4.039298	0.695647	0.563422
C	4.501763	0.280995	1.825903
C	4.975070	1.052413	-0.428271
C	5.861829	0.207888	2.091226
H	3.773708	0.018627	2.594179
C	6.335540	0.985837	-0.169205
H	4.615625	1.386417	-1.402588
C	6.761007	0.561308	1.088203
H	6.232489	-0.116528	3.062520
H	7.068619	1.259273	-0.926728
N	8.198138	0.488544	1.364870
O	8.962219	0.794269	0.477098
O	8.545348	0.125476	2.466513
H	1.900919	-2.933569	-2.644827
C	1.829623	-1.112368	-3.692703
F	0.879868	-1.398900	-4.581462
F	3.003183	-1.434667	-4.247300
F	1.841049	0.208157	-3.512799
N	-1.537867	-0.740219	-0.295145
C	-2.728485	-0.254866	-0.466439
C	-1.189550	-1.397546	0.963728
S	-3.283192	0.588266	-1.929084
N	-3.724336	-0.327639	0.459572
C	-2.017090	-0.794227	2.119724
H	-0.132129	-1.149175	1.153735
C	-1.300263	-2.910627	0.883212
C	-4.889829	0.747655	-1.227226
C	-4.950456	0.201352	0.058165
C	-3.498325	-0.888230	1.787874
C	-1.668896	-1.348218	3.519385
H	-1.767452	0.278365	2.119357
C	-0.319987	-3.704207	1.490246
C	-2.381773	-3.534346	0.251565
C	-6.011188	1.331906	-1.808680
C	-6.138110	0.216852	0.789015
H	-4.084918	-0.300591	2.507506
H	-3.864489	-1.926232	1.813828
C	-2.501958	-2.558497	3.949571
C	-1.790030	-0.237385	4.563784
H	-0.611169	-1.658956	3.483397
C	-0.434222	-5.093788	1.497073
H	0.544580	-3.225960	1.958082
C	-2.496665	-4.924992	0.256493
H	-3.142762	-2.937425	-0.257095
C	-7.200960	1.355415	-1.080149
H	-5.959229	1.759451	-2.811377
C	-7.260478	0.802312	0.202715
H	-6.192622	-0.219178	1.786416
H	-2.501803	-3.366154	3.203996
H	-2.103012	-2.968938	4.888834
H	-3.547461	-2.268291	4.139819
H	-1.113965	0.601465	4.339516
H	-2.818362	0.157068	4.597792
H	-1.544177	-0.613805	5.567654
C	-1.528082	-5.707751	0.885652
H	0.337184	-5.699279	1.976096

H -3.346259 -5.398975 -0.238125
H -8.091055 1.807751 -1.519078
H -8.198972 0.824149 0.758370
H -1.619178 -6.795200 0.888110

CF3_Michael_Acceptor/TS-turn-S

Frequencies, energies and thermodynamic properties:

Lowest Vibrational Mode (1/cm) = -180.4842
2nd Lowest Vibrational Mode (1/cm) = 9.2011
E(RM062X) (a.u.) = -3187.93662572
Thermal correction to Enthalpy (a.u.) = 0.680137
Thermal correction to Gibbs Free Energy (a.u.) = 0.553740
Total Entropy (cal/Kmol) = 266.025
Esp(RM062X) (a.u.) = -3190.90111371

Optimised cartesian coordinates (Angstrom):

C 0.330726 -1.784923 -2.028965
C -1.064152 -1.884935 -2.607621
H -1.223727 -1.163438 -3.423080
H 0.404250 -2.467007 -1.173204
H 1.079239 -2.078643 -2.777269
N -0.454176 0.481155 -1.147783
C -0.199441 1.888932 -1.038252
C -0.208383 2.527111 0.206274
C 0.046756 2.627828 -2.202167
C 0.055967 3.889595 0.296883
H -0.442851 1.961437 1.104190
C 0.313450 3.989572 -2.123772
H 0.032728 2.125137 -3.165860
C 0.320181 4.594486 -0.871441
H 0.055726 4.400730 1.258318
H 0.508976 4.580329 -3.017043
N 0.605670 6.035938 -0.781479
O 0.837219 6.630201 -1.808869
O 0.594293 6.545790 0.315073
C 0.687304 -0.321964 -1.706687
O 1.402822 0.275940 -2.518440
C -1.327312 -3.258533 -3.192795
F -2.577446 -3.376613 -3.639396
F -1.131547 -4.228407 -2.296215
F -0.508719 -3.490878 -4.217826
S -2.271121 -1.576448 -1.280000
C -1.693101 0.036822 -0.746881
N -2.461569 0.751440 -0.022455
C -3.795465 0.478543 0.237472
C -4.766620 0.539701 -0.782433
C -4.204356 0.215257 1.557651
C -6.105597 0.324718 -0.493955
H -4.455477 0.766286 -1.802895
C -5.541765 -0.007556 1.852873
H -3.453033 0.198185 2.347142
C -6.474961 0.047888 0.820998
H -6.865294 0.370634 -1.273004
H -5.869031 -0.217984 2.870015
N -7.888946 -0.182823 1.128575
O -8.186576 -0.424623 2.276936
O -8.684172 -0.120598 0.218021
N 1.661511 -0.581241 -0.205216
C 2.953740 -0.503486 -0.279491
C 1.045723 -1.184729 0.973688
S 3.843659 0.298486 -1.587747
N 3.803060 -1.003641 0.658386
C 1.934383 -2.336796 1.487638
H 0.095887 -1.632163 0.641738

C	0.698839	-0.156527	2.031736
C	5.359711	-0.026246	-0.751791
C	5.152839	-0.731287	0.438438
C	3.330163	-1.805541	1.784484
C	1.327071	-3.140076	2.659955
H	2.022987	-3.024227	0.629281
C	-0.547597	-0.224610	2.662896
C	1.601022	0.842639	2.417471
C	6.643206	0.328162	-1.156517
C	6.222921	-1.086516	1.258723
H	4.033524	-2.638599	1.924650
H	3.346658	-1.187680	2.695624
C	1.669971	-2.602098	4.051792
C	1.737075	-4.609885	2.557803
H	0.231773	-3.089661	2.537644
C	-0.884916	0.680694	3.669836
H	-1.263964	-0.990690	2.353422
C	1.265613	1.748166	3.423383
H	2.568466	0.939822	1.920116
C	7.718387	-0.027022	-0.340917
H	6.803553	0.874241	-2.087606
C	7.507424	-0.724770	0.852212
H	6.062149	-1.625550	2.192398
H	1.458809	-1.528925	4.161566
H	1.081570	-3.138892	4.810337
H	2.732959	-2.768171	4.288448
H	1.399459	-5.056775	1.611182
H	2.832630	-4.715552	2.611759
H	1.305605	-5.194451	3.383631
C	0.022048	1.669483	4.052885
H	-1.861200	0.617679	4.154374
H	1.975609	2.525994	3.709653
H	8.731358	0.246724	-0.638390
H	8.358465	-0.991526	1.480371
H	-0.241671	2.381150	4.836965

CF3_Michael_Acceptor_TS-MA-conf/TS-MA-R-iii

Frequencies, energies and thermodynamic properties:

Lowest Vibrational Mode (1/cm) = -50.7313

2nd Lowest Vibrational Mode (1/cm) = 10.3495

E(RM062X) (a.u.) = -3187.92983433

Thermal correction to Enthalpy (a.u.) = 0.681389

Thermal correction to Gibbs Free Energy (a.u.) = 0.549992

Total Entropy (cal/Kmol) = 276.550

Esp(RM062X) (a.u.) = -3190.89913858

Optimised cartesian coordinates (Angstrom):

C	7.257155	2.834692	-1.877399
C	6.371814	3.919596	-1.969072
C	5.013956	3.756677	-1.721569
C	4.563991	2.479975	-1.382794
C	5.444298	1.400423	-1.301472
H	6.753220	4.905954	-2.235087
H	4.322231	4.597473	-1.787406
C	3.472483	0.358948	-0.745675
C	3.272805	-2.019288	-0.127926
C	4.497132	-2.191191	-1.041429
C	5.484054	-1.062948	-0.820425
H	6.272070	-1.088695	-1.583636
S	2.926016	1.992470	-1.003247
N	4.782284	0.217106	-0.953858
N	2.685955	-0.669880	-0.347602
C	5.154352	-3.587266	-0.939708
C	6.238528	-3.698658	0.135771

C	5.726904	-3.988673	-2.299550
H	4.349393	-4.298512	-0.691752
H	5.904569	-3.351327	1.123713
H	6.548888	-4.748601	0.237122
H	7.133271	-3.121612	-0.146980
H	6.491961	-3.268399	-2.631383
H	6.204314	-4.977443	-2.241620
H	4.943075	-4.031928	-3.069487
H	4.108370	-2.083639	-2.067212
H	2.533626	-2.738373	-0.497714
C	3.517114	-2.272835	1.344362
C	4.064882	-1.292887	2.179267
C	3.230428	-3.537207	1.869613
C	4.351570	-1.586008	3.512515
H	4.267825	-0.286944	1.801868
C	3.518498	-3.830422	3.201197
H	2.778390	-4.297660	1.227684
C	4.086290	-2.856613	4.023497
H	4.779121	-0.815231	4.155668
H	3.291305	-4.820381	3.599824
H	4.309097	-3.083326	5.067332
C	0.514254	-1.519833	0.487621
H	0.872144	-2.545404	0.533251
C	-0.747692	-1.220719	0.848331
C	-1.636865	-2.259324	1.472460
F	-1.263764	-2.475018	2.744388
F	-2.910946	-1.885511	1.507054
F	-1.561425	-3.434126	0.848038
O	0.864895	0.681768	-0.278286
C	1.316452	-0.427050	-0.057028
H	5.952626	-1.098528	0.174404
C	6.811076	1.561731	-1.542838
H	7.507282	0.727019	-1.468948
H	8.319170	2.990237	-2.070558
H	-1.097918	-0.190847	0.919019
S	-2.318412	-1.011839	-1.513746
C	-3.042837	0.404608	-0.816010
N	-2.132693	1.439862	-0.591799
H	-1.177259	1.185802	-0.833343
C	-2.287821	2.694688	-0.040544
C	-1.099193	3.427151	0.197177
C	-3.526046	3.289687	0.283316
C	-1.137418	4.698943	0.734367
H	-0.140524	2.963676	-0.041945
C	-3.561983	4.567705	0.824245
H	-4.445260	2.740549	0.108211
C	-2.376138	5.261827	1.047125
H	-0.222734	5.259989	0.919834
H	-4.513654	5.035032	1.074396
N	-2.425758	6.603041	1.618464
O	-3.511896	7.072008	1.881135
O	-1.376042	7.181924	1.802082
N	-4.264374	0.573989	-0.419962
C	-5.273999	-0.334502	-0.636142
C	-6.110377	-0.676324	0.449197
C	-5.570547	-0.878134	-1.907332
C	-7.184870	-1.536040	0.286223
H	-5.884610	-0.251726	1.428250
C	-6.650949	-1.726987	-2.082649
H	-4.936286	-0.618823	-2.754133
C	-7.446169	-2.052682	-0.982508
H	-7.824588	-1.809535	1.124158
H	-6.888008	-2.143517	-3.060803

N -8.581018 -2.951572 -1.164998
O -9.262950 -3.214270 -0.197217
O -8.787646 -3.392388 -2.275608

CF3_Michael_Acceptor_TS-MA-conf/TS-MA-R-ii

Frequencies, energies and thermodynamic properties:

Lowest Vibrational Mode (1/cm) = -104.5920

2nd Lowest Vibrational Mode (1/cm) = 10.1083

E(RM062X) (a.u.) = -3187.94059886

Thermal correction to Enthalpy (a.u.) = 0.680773

Thermal correction to Gibbs Free Energy (a.u.) = 0.553113

Total Entropy (cal/Kmol) = 268.684

Esp(RM062X) (a.u.) = -3190.90402630

Optimised cartesian coordinates (Angstrom):

C 5.058498 -3.918405 -1.580405
C 3.936663 -4.594483 -2.081697
C 2.694216 -3.972695 -2.138131
C 2.598001 -2.667590 -1.654844
C 3.711507 -2.006371 -1.133791
H 4.038781 -5.620613 -2.436343
H 1.818852 -4.491460 -2.531703
C 2.086376 -0.410087 -0.802627
C 2.431912 1.731338 0.366084
C 3.639147 1.013134 0.993622
C 4.350834 0.164311 -0.040609
H 5.119521 -0.455707 0.436697
S 1.168369 -1.657417 -1.595544
N 3.375630 -0.733679 -0.658648
N 1.573050 0.749977 -0.342351
C 4.595971 1.953941 1.760223
C 5.711521 2.555818 0.901464
C 5.200376 1.212471 2.953005
H 3.982034 2.780291 2.154388
H 6.441495 1.784896 0.607403
H 5.338211 3.040781 -0.011527
H 6.256798 3.312727 1.483637
H 4.422415 0.869177 3.650654
H 5.770825 0.331180 2.618099
H 5.891403 1.864556 3.506469
H 3.207863 0.314340 1.728318
H 1.844604 2.095815 1.217282
C 2.768401 2.905074 -0.530719
C 2.784917 4.193655 0.013593
C 3.109602 2.727931 -1.875758
C 3.171961 5.284253 -0.762900
H 2.492679 4.343362 1.055993
C 3.495782 3.819538 -2.653694
H 3.070060 1.735932 -2.333174
C 3.535768 5.097841 -2.097099
H 3.181606 6.284402 -0.326703
H 3.760828 3.669584 -3.701512
H 3.836082 5.951251 -2.707208
C -0.364364 2.238915 0.010916
C -1.690619 2.507625 -0.179570
C -2.156186 3.916829 0.070589
F -3.478210 4.052915 0.083299
F -1.683815 4.410551 1.218323
F -1.701962 4.718361 -0.906608
O -0.466529 0.221251 -1.205382
C 0.176654 1.027131 -0.559140
H 4.823413 0.768643 -0.829695
C 4.967138 -2.615607 -1.104289
H 5.844477 -2.098276 -0.716708

H	6.024031	-4.424852	-1.556662
H	-2.277393	1.939955	-0.903097
S	-3.225325	1.555298	1.631508
C	-2.667669	-0.083999	1.375698
N	-3.300109	-1.053069	0.807538
N	-1.366371	-0.297241	1.817184
C	-4.607858	-0.981226	0.378067
C	-5.673024	-0.601292	1.223990
C	-4.906047	-1.389584	-0.938744
C	-6.981882	-0.623468	0.769345
H	-5.455189	-0.292942	2.246213
C	-6.211071	-1.401841	-1.406516
H	-4.081914	-1.689835	-1.587071
C	-7.237020	-1.019349	-0.543849
H	-7.809225	-0.336836	1.417139
H	-6.445467	-1.705539	-2.425801
N	-8.616230	-1.038638	-1.026166
O	-8.814643	-1.384828	-2.170688
O	-9.493155	-0.708027	-0.257772
C	-0.525669	-1.382423	1.671697
C	-0.904954	-2.634677	1.143190
C	0.816000	-1.199050	2.082006
C	0.040468	-3.640199	0.991198
H	-1.934278	-2.797909	0.842516
C	1.758886	-2.198641	1.924086
H	1.105070	-0.239223	2.519432
C	1.362918	-3.412615	1.360125
H	-0.242288	-4.603078	0.567096
H	2.797047	-2.050505	2.222801
N	2.365025	-4.447992	1.120717
O	3.520978	-4.188848	1.378974
O	1.991269	-5.510060	0.674267
H	0.237886	2.927575	0.596829
H	-0.956290	0.521133	2.255513

CF3_Michael_Acceptor_TS-MA-conf/TS-MA-R-i

Frequencies, energies and thermodynamic properties:

Lowest Vibrational Mode (1/cm) =	-184.9680
2nd Lowest Vibrational Mode (1/cm) =	4.5828
E(RM062X) (a.u.) =	-3187.94763983
Thermal correction to Enthalpy (a.u.) =	0.680837
Thermal correction to Gibbs Free Energy (a.u.) =	0.554671
Total Entropy (cal/Kmol) =	265.539
Esp(RM062X) (a.u.) =	-3190.90852411

Optimised cartesian coordinates (Angstrom):

C	-6.259958	1.915444	-0.150895
C	-6.694052	0.747207	0.489989
C	-5.781696	-0.132062	1.064980
C	-4.425367	0.175181	0.962355
C	-3.995925	1.327500	0.301765
H	-7.760193	0.524287	0.543591
H	-6.113839	-1.040997	1.568994
C	-1.966709	0.412469	0.899772
C	0.209002	1.406217	0.400107
C	-0.515613	2.041055	-0.797441
C	-1.897744	2.514267	-0.391653
H	-2.482579	2.794087	-1.277621
S	-3.070497	-0.756480	1.574161
N	-2.599442	1.417523	0.276649
N	-0.630780	0.338110	0.978540
C	0.315167	3.131977	-1.511390
C	0.108548	4.545724	-0.961797
H	-0.897355	4.921055	-1.208127

H	0.240130	4.605902	0.127793
H	0.833194	5.230749	-1.425252
H	-0.658629	1.212220	-1.512052
H	1.081225	0.901532	-0.026003
C	0.683971	2.377974	1.459038
C	2.006643	2.831314	1.415814
C	-0.176793	2.875070	2.443409
C	2.454274	3.793715	2.319269
H	2.690086	2.423882	0.665386
C	0.271184	3.836604	3.349268
H	-1.205487	2.512325	2.516432
C	1.584266	4.303791	3.283586
H	3.487850	4.140666	2.274429
H	-0.408771	4.219284	4.112202
H	1.933485	5.055694	3.993160
C	1.403948	-0.856679	1.672245
H	2.040631	-0.076448	1.266219
C	1.990754	-2.037930	2.132823
C	3.416755	-1.937475	2.605087
F	4.198728	-1.282290	1.744380
F	3.469957	-1.267056	3.764736
F	3.976600	-3.128184	2.831970
O	-0.777320	-1.666884	2.057337
C	-0.014651	-0.811661	1.619472
H	-1.861312	3.376375	0.291565
C	-4.907781	2.226003	-0.253125
H	-4.579527	3.136407	-0.753888
H	-6.994104	2.594722	-0.585819
H	1.383007	-2.691506	2.762137
S	2.307693	-3.596230	0.518241
C	1.209625	-2.789346	-0.602726
N	-0.078098	-3.286796	-0.517411
H	-0.159465	-4.073435	0.119142
C	-1.286154	-2.778861	-0.960085
C	-1.438251	-1.591835	-1.706007
C	-2.443195	-3.503698	-0.593065
C	-2.710110	-1.121894	-2.013109
H	-0.556919	-1.049027	-2.031300
C	-3.706722	-3.047140	-0.916528
H	-2.330823	-4.430550	-0.027400
C	-3.829699	-1.842569	-1.610223
H	-2.838213	-0.193544	-2.570594
H	-4.597794	-3.598850	-0.619957
N	-5.162083	-1.311993	-1.892294
O	-5.240297	-0.225726	-2.422683
O	-6.118954	-1.985178	-1.577568
N	1.438368	-1.779225	-1.365739
C	2.646658	-1.148208	-1.610850
C	2.554349	0.191891	-2.052471
C	3.929732	-1.733629	-1.539260
C	3.678887	0.945979	-2.344084
H	1.560269	0.623403	-2.180155
C	5.063242	-0.990030	-1.841013
H	4.037458	-2.774650	-1.248041
C	4.929288	0.342426	-2.222386
H	3.600119	1.981081	-2.675214
H	6.054753	-1.437248	-1.783496
N	6.128911	1.123463	-2.529444
O	5.982159	2.280302	-2.858002
O	7.203561	0.573766	-2.438562
H	1.375875	2.863099	-1.368574
C	0.027465	3.107229	-3.012564
H	-1.039425	3.298199	-3.211459

H 0.606548 3.884003 -3.532976

H 0.285765 2.134485 -3.457445

CF3_Michael_Acceptor_TS-MA-conf/TS-MA-R-iv

Frequencies, energies and thermodynamic properties:

Lowest Vibrational Mode (1/cm) = -87.8545

2nd Lowest Vibrational Mode (1/cm) = 12.3779

E(RM062X) (a.u.) = -3187.94336914

Thermal correction to Enthalpy (a.u.) = 0.681649

Thermal correction to Gibbs Free Energy (a.u.) = 0.556540

Total Entropy (cal/Kmol) = 263.314

Esp(RM062X) (a.u.) = -3190.90668472

Optimised cartesian coordinates (Angstrom):

C -7.219874 0.787081 -0.494897

C -7.262103 0.482659 -1.863967

C -6.142308 -0.014792 -2.520885

C -4.979745 -0.202347 -1.772294

C -4.939231 0.107494 -0.412786

H -8.185847 0.637885 -2.422391

H -6.170246 -0.252667 -3.585076

C -2.784157 -0.634270 -0.721416

C -1.132481 -0.898623 1.078128

C -1.893959 0.257082 1.747160

C -3.389131 0.106815 1.551684

H -3.906173 1.035734 1.828856

S -3.428450 -0.791988 -2.334798

N -3.677900 -0.144028 0.138800

N -1.532650 -0.978978 -0.349865

C -1.518949 0.490065 3.228245

C -2.333792 -0.332626 4.230591

C -1.642339 1.978900 3.557315

H -0.458234 0.207678 3.333160

H -3.371456 0.032550 4.289688

H -2.360412 -1.405045 3.991044

H -1.896558 -0.224708 5.233726

H -1.422634 2.161395 4.619297

H -0.945071 2.581128 2.958139

H -2.664128 2.345189 3.362901

H -1.580894 1.150884 1.186046

H -0.080516 -0.590555 1.077267

C -1.254393 -2.242018 1.764326

C -0.247771 -2.645168 2.647964

C -2.374389 -3.060956 1.584296

C -0.371529 -3.834427 3.364780

H 0.639462 -2.019755 2.776604

C -2.497540 -4.251514 2.300201

H -3.162909 -2.781388 0.881018

C -1.500346 -4.636771 3.196723

H 0.419918 -4.138003 4.051811

H -3.375707 -4.882263 2.153259

H -1.597708 -5.569142 3.755184

C 0.678809 -1.924080 -0.905164

H 0.944649 -2.005284 0.146304

C 1.566342 -2.299465 -1.868278

C 2.730628 -3.170417 -1.488176

F 3.651289 -3.270388 -2.440656

F 3.334933 -2.765161 -0.366957

F 2.292804 -4.418259 -1.252249

O -0.937564 -1.327507 -2.515913

C -0.601033 -1.412250 -1.345995

H -3.811023 -0.722802 2.139063

C -6.061628 0.605666 0.251649

H -6.036436 0.844677 1.314195

H	-8.111961	1.176200	-0.002913
H	1.255179	-2.372094	-2.910331
S	3.132549	-0.356504	-2.662180
C	2.423623	0.900216	-1.684176
N	1.071269	1.106549	-1.945512
H	0.721927	0.532541	-2.708228
C	0.137574	1.920101	-1.336674
C	-1.181792	1.847922	-1.845392
C	0.395594	2.782271	-0.248020
C	-2.228478	2.497669	-1.219383
H	-1.372496	1.231478	-2.725850
C	-0.650265	3.473200	0.350638
H	1.409825	2.889859	0.121674
C	-1.953391	3.290381	-0.103929
H	-3.254614	2.392792	-1.577360
H	-0.463376	4.128448	1.200934
N	-3.059595	3.850937	0.659097
O	-2.815504	4.703171	1.483104
O	-4.171598	3.408522	0.445047
N	2.999241	1.652070	-0.805864
C	4.297598	1.489734	-0.366762
C	5.121779	2.631565	-0.286171
C	4.809509	0.255611	0.090397
C	6.413669	2.550180	0.210550
H	4.721507	3.586158	-0.629898
C	6.094443	0.167604	0.601718
H	4.182282	-0.632345	0.036175
C	6.885893	1.315383	0.651764
H	7.056759	3.427459	0.264474
H	6.494088	-0.780107	0.960135
N	8.242459	1.222071	1.187252
O	8.627987	0.140958	1.576185
O	8.913827	2.230686	1.216771

CF3_Michael_Acceptor_TS-MA-conf/TS-MA-R-ix

Frequencies, energies and thermodynamic properties:

Lowest Vibrational Mode (1/cm) =	-184.9621
2nd Lowest Vibrational Mode (1/cm) =	10.8039
E(RM062X) (a.u.) =	-3187.93523408
Thermal correction to Enthalpy (a.u.) =	0.680928
Thermal correction to Gibbs Free Energy (a.u.) =	0.554318
Total Entropy (cal/Kmol) =	266.473
Esp(RM062X) (a.u.) =	-3190.89624583

Optimised cartesian coordinates (Angstrom):

C	-3.499284	-4.852767	1.323671
C	-2.177897	-5.267480	1.547710
C	-1.128303	-4.357862	1.499372
C	-1.432328	-3.024853	1.218217
C	-2.746426	-2.616775	0.990254
H	-1.970299	-6.316911	1.759787
H	-0.097424	-4.672329	1.669599
C	-1.635868	-0.623399	0.679506
C	-2.718793	1.513369	0.164802
C	-3.840802	0.650014	-0.437295
C	-4.089419	-0.583731	0.407102
H	-4.722884	-1.294033	-0.139106
S	-0.312116	-1.685202	1.080046
N	-2.817470	-1.252693	0.683550
N	-1.512508	0.683056	0.378702
C	-5.135068	1.436345	-0.746414
C	-6.132913	1.502490	0.412739
C	-5.811258	0.847355	-1.985253
H	-4.826081	2.466395	-0.990422

H	-6.948102	2.194893	0.157118
H	-6.590026	0.517195	0.596109
H	-5.679862	1.850966	1.351654
H	-6.072249	-0.211074	-1.824150
H	-6.740227	1.388588	-2.216425
H	-5.154818	0.902768	-2.865917
H	-3.442322	0.300272	-1.401344
H	-2.464371	2.236997	-0.615012
C	-3.085495	2.275666	1.420897
C	-3.100795	1.662819	2.679180
C	-3.470911	3.615347	1.310304
C	-3.523615	2.372929	3.802431
H	-2.779010	0.625061	2.799261
C	-3.896338	4.324924	2.432529
H	-3.438828	4.105231	0.334073
C	-3.929399	3.702450	3.680415
H	-3.532399	1.885236	4.778518
H	-4.195851	5.369494	2.332623
H	-4.259158	4.256497	4.560814
C	-0.029484	2.563689	-0.260341
H	-0.855446	3.180315	-0.602525
C	1.276588	2.917081	-0.564245
C	1.573847	4.354799	-0.895405
F	1.299932	5.140351	0.155618
F	2.855773	4.561688	-1.197527
F	0.837298	4.804925	-1.914326
O	0.743300	0.529333	0.610104
C	-0.188417	1.251420	0.281702
H	-4.568223	-0.344415	1.369062
C	-3.805223	-3.526240	1.043646
H	-4.834554	-3.217008	0.866630
H	-4.306595	-5.584992	1.363839
H	2.088973	2.416046	-0.032302
S	1.936436	1.972054	-2.616242
C	2.767040	0.602909	-1.882477
N	3.950025	0.990365	-1.275685
H	4.242514	1.935633	-1.507610
C	4.809173	0.290581	-0.441814
C	4.491087	-0.930109	0.187475
C	6.065870	0.883145	-0.189546
C	5.410837	-1.532574	1.034496
H	3.525384	-1.393114	0.011891
C	6.982640	0.281883	0.653841
H	6.313985	1.829841	-0.673760
C	6.644968	-0.928854	1.257021
H	5.173399	-2.472295	1.531241
H	7.953786	0.735662	0.845792
N	7.607309	-1.575189	2.147606
O	8.664778	-1.016791	2.341104
O	7.297505	-2.634752	2.646259
N	2.459432	-0.651949	-1.860635
C	1.245598	-1.252348	-2.096384
C	0.003750	-0.607869	-2.317271
C	1.235242	-2.668514	-1.996672
C	-1.176571	-1.332587	-2.342379
H	-0.032070	0.471190	-2.440772
C	0.058401	-3.396916	-2.003743
H	2.192372	-3.173155	-1.856696
C	-1.150324	-2.710859	-2.143403
H	-2.131346	-0.832942	-2.496013
H	0.058276	-4.478316	-1.870184
N	-2.412508	-3.427070	-2.011162
O	-3.441604	-2.777032	-2.038534

O -2.378142 -4.626822 -1.858327

CF3_Michael_Acceptor_TS-MA-conf/TS-MA-R-viii

Frequencies, energies and thermodynamic properties:

Lowest Vibrational Mode (1/cm) = -166.6097

2nd Lowest Vibrational Mode (1/cm) = 9.2326

E(RM062X) (a.u.) = -3187.93706911

Thermal correction to Enthalpy (a.u.) = 0.680759

Thermal correction to Gibbs Free Energy (a.u.) = 0.553743

Total Entropy (cal/Kmol) = 267.328

Esp(RM062X) (a.u.) = -3190.89903908

Optimised cartesian coordinates (Angstrom):

C 6.017677 -3.958980 -1.264156
C 5.200573 -4.509882 -2.261195
C 3.980928 -3.925899 -2.589495
C 3.602972 -2.774985 -1.901149
C 4.414793 -2.234254 -0.903233
H 5.522769 -5.409095 -2.787500
H 3.339536 -4.354434 -3.360653
C 2.653923 -0.752600 -0.844370
C 2.612649 1.292544 0.497203
C 3.463931 0.482199 1.487861
C 4.494154 -0.351750 0.751057
H 4.943339 -1.085740 1.432951
S 2.109899 -1.872110 -2.066905
N 3.835089 -1.102207 -0.320182
N 2.004850 0.364650 -0.483458
C 4.081366 1.326408 2.624712
C 5.461720 1.907995 2.307520
C 4.146521 0.493331 3.905592
H 3.389336 2.165875 2.804261
H 6.225791 1.115107 2.275676
H 5.490886 2.451081 1.351995
H 5.757245 2.610021 3.100783
H 4.592397 1.074880 4.725751
H 3.145489 0.166330 4.222941
H 4.763923 -0.407051 3.757913
H 2.760983 -0.225550 1.952042
H 1.774557 1.699733 1.076455
C 3.339159 2.435827 -0.180480
C 3.221949 3.723912 0.353534
C 4.168273 2.230914 -1.288447
C 3.945853 4.784221 -0.189218
H 2.556421 3.895557 1.203411
C 4.891798 3.292036 -1.833102
H 4.256171 1.241332 -1.743738
C 4.788343 4.568603 -1.280289
H 3.845996 5.783606 0.237437
H 5.536197 3.119454 -2.696649
H 5.354234 5.397716 -1.708164
C 0.131106 1.921571 -0.782642
H 0.750725 2.748225 -0.441926
C -1.238050 2.079654 -0.886830
C -1.781317 3.446320 -1.212251
F -3.113255 3.507198 -1.193111
F -1.314625 4.391286 -0.392826
F -1.409590 3.796192 -2.453542
O 0.129537 -0.298870 -1.598572
C 0.674399 0.617877 -1.005594
H 5.293883 0.258339 0.304338
C 5.638198 -2.815263 -0.568994
H 6.276961 -2.390828 0.205108
H 6.969354 -4.434820 -1.024715

H -1.820770 1.264789 -1.326266
S -2.229029 1.954380 1.256998
C -3.307676 0.594592 0.950819
N -4.612821 0.992327 0.720380
H -4.730313 2.000825 0.721751
C -5.756071 0.263308 0.442574
C -6.912768 1.010805 0.123757
C -5.840588 -1.143524 0.471509
C -8.112382 0.385817 -0.159363
H -6.849098 2.100233 0.098415
C -7.046398 -1.770711 0.185505
H -4.962515 -1.731302 0.716694
C -8.166739 -1.007882 -0.126767
H -9.003227 0.961091 -0.407003
H -7.123153 -2.856976 0.206807
N -9.430090 -1.679527 -0.424768
O -9.449959 -2.890432 -0.401235
O -10.392614 -0.989232 -0.679577
N -3.004729 -0.655457 0.870648
C -1.756645 -1.198034 1.089558
C -1.352288 -2.238536 0.227506
C -0.896915 -0.833719 2.152539
C -0.111981 -2.838715 0.356208
H -2.030732 -2.540008 -0.570871
C 0.345017 -1.432990 2.293117
H -1.214686 -0.074679 2.864107
C 0.738571 -2.410995 1.375482
H 0.211645 -3.621136 -0.328143
H 1.007963 -1.160283 3.113989
N 2.072942 -2.989988 1.470299
O 2.828239 -2.564345 2.324587
O 2.378667 -3.856443 0.679214

CF3_Michael_Acceptor_TS-MA-conf/TS-MA-R-vii

Frequencies, energies and thermodynamic properties:

Lowest Vibrational Mode (1/cm) = -157.2619

2nd Lowest Vibrational Mode (1/cm) = 5.8305

E(RM062X) (a.u.) = -3187.93673395

Thermal correction to Enthalpy (a.u.) = 0.680632

Thermal correction to Gibbs Free Energy (a.u.) = 0.551772

Total Entropy (cal/Kmol) = 271.210

Esp(RM062X) (a.u.) = -3190.89848612

Optimised cartesian coordinates (Angstrom):

C 6.402645 -3.770134 -1.023730
C 5.583199 -4.440652 -1.943348
C 4.320973 -3.951921 -2.263300
C 3.900515 -2.776299 -1.642936
C 4.713118 -2.117079 -0.720127
H 5.938895 -5.357170 -2.415312
H 3.678612 -4.468671 -2.977737
C 2.878800 -0.731098 -0.707771
C 2.699999 1.323825 0.604992
C 3.591164 0.563418 1.601635
C 4.692611 -0.173086 0.862156
H 5.206079 -0.868191 1.539614
S 2.363060 -1.957662 -1.837026
N 4.096047 -0.970949 -0.210260
N 2.161772 0.353916 -0.375839
C 4.124301 1.436279 2.759499
C 5.470402 2.109073 2.477609
C 4.215958 0.599990 4.036448
H 3.375200 2.227146 2.929244
H 6.283826 1.366690 2.452474

H	5.483707	2.664385	1.528890
H	5.704329	2.818920	3.284288
H	3.232331	0.204484	4.329285
H	4.897219	-0.254769	3.896539
H	4.603604	1.203169	4.870348
H	2.936087	-0.209326	2.035019
H	1.831644	1.681993	1.172841
C	3.364373	2.507653	-0.067869
C	3.179876	3.785595	0.471769
C	4.196280	2.352873	-1.181770
C	3.840020	4.886144	-0.071893
H	2.510595	3.918482	1.325536
C	4.856131	3.454439	-1.727297
H	4.333133	1.371491	-1.642605
C	4.685731	4.721398	-1.169363
H	3.687438	5.876983	0.359085
H	5.502606	3.320955	-2.596183
H	5.201135	5.582199	-1.598454
C	0.231551	1.819154	-0.767976
H	0.812038	2.682089	-0.447944
C	-1.126512	1.930935	-0.974804
C	-1.682697	3.260695	-1.412941
F	-1.303113	4.264224	-0.619178
F	-1.228148	3.552393	-2.642470
F	-3.012454	3.280527	-1.496530
O	0.336658	-0.428343	-1.497133
C	0.830978	0.526961	-0.923442
H	5.437032	0.507572	0.422653
C	5.982362	-2.600978	-0.398645
H	6.625514	-2.080913	0.310619
H	7.390210	-4.170497	-0.791467
H	-1.661728	1.071055	-1.388701
S	-2.317262	1.930895	1.112599
C	-3.423019	0.599128	0.788825
N	-4.732838	1.025257	0.647941
H	-4.830450	2.034770	0.693989
C	-5.908534	0.327565	0.435680
C	-7.077671	1.107146	0.277561
C	-6.014807	-1.077356	0.380465
C	-8.308586	0.515670	0.067004
H	-6.999676	2.195068	0.323191
C	-7.252719	-1.670590	0.169278
H	-5.126989	-1.688781	0.500995
C	-8.384088	-0.876475	0.013415
H	-9.208700	1.115919	-0.056548
H	-7.345523	-2.754974	0.125475
N	-9.680869	-1.511955	-0.209533
O	-9.722402	-2.721958	-0.249741
O	-10.648273	-0.794644	-0.342724
N	-3.151831	-0.652438	0.633818
C	-1.920317	-1.250005	0.804238
C	-0.977244	-0.897209	1.798005
C	-1.627554	-2.348297	-0.032994
C	0.233870	-1.565140	1.891289
H	-1.203391	-0.092823	2.493508
C	-0.427026	-3.030228	0.062001
H	-2.367494	-2.636963	-0.780321
C	0.503992	-2.615663	1.012796
H	0.960274	-1.297265	2.658726
H	-0.193108	-3.861377	-0.602286
N	1.800776	-3.274444	1.068902
O	1.941890	-4.322462	0.480584
O	2.692924	-2.726063	1.692478

CF3_Michael_Acceptor_TS-MA-conf/TS-MA-R-vi

Frequencies, energies and thermodynamic properties:

Lowest Vibrational Mode (1/cm) = -95.3079

2nd Lowest Vibrational Mode (1/cm) = 6.2238

E(RM062X) (a.u.) = -3187.92682929

Thermal correction to Enthalpy (a.u.) = 0.680852

Thermal correction to Gibbs Free Energy (a.u.) = 0.547975

Total Entropy (cal/Kmol) = 279.664

Esp(RM062X) (a.u.) = -3190.89573391

Optimised cartesian coordinates (Angstrom):

C	-8.632458	1.931228	0.368980
C	-8.175919	3.145884	-0.163178
C	-6.833732	3.327561	-0.478918
C	-5.959732	2.265264	-0.247913
C	-6.415052	1.061480	0.291319
H	-8.881883	3.959034	-0.335300
H	-6.474122	4.269060	-0.896030
C	-4.183385	0.570051	0.023210
C	-3.171786	-1.608181	0.522827
C	-4.268649	-1.689387	1.597678
C	-5.584751	-1.185921	1.038066
H	-6.325232	-1.077123	1.840868
S	-4.233594	2.215458	-0.554320
N	-5.375638	0.137614	0.446582
N	-3.088566	-0.213444	0.025192
C	-4.393764	-3.080966	2.258909
C	-5.361452	-4.034334	1.552429
C	-4.800154	-2.921019	3.724267
H	-3.387901	-3.531721	2.236681
H	-6.404677	-3.707409	1.687445
H	-5.168102	-4.125950	0.474402
H	-5.276989	-5.037983	1.993715
H	-4.901762	-3.903121	4.208344
H	-4.056544	-2.337783	4.286489
H	-5.771179	-2.406613	3.807139
H	-3.955644	-0.978977	2.380143
H	-2.225773	-1.799244	1.043010
C	-3.317681	-2.597893	-0.614287
C	-2.626603	-3.812382	-0.547065
C	-4.163801	-2.353195	-1.701077
C	-2.802377	-4.781679	-1.532849
H	-1.945161	-3.999517	0.286917
C	-4.339184	-3.322851	-2.688664
H	-4.690140	-1.399534	-1.793733
C	-3.665315	-4.541116	-2.602703
H	-2.258153	-5.725268	-1.468841
H	-5.001932	-3.121388	-3.531768
H	-3.801981	-5.297548	-3.377201
C	-0.744185	-0.604420	-0.631272
H	-0.840626	-1.669090	-0.434195
C	0.470378	-0.079888	-0.975073
C	1.536448	-0.997228	-1.504220
F	2.716044	-0.393991	-1.654414
F	1.722844	-2.077819	-0.739551
F	1.186510	-1.447255	-2.718419
O	-1.805965	1.500993	-0.743802
C	-1.845285	0.314779	-0.474998
H	-5.995634	-1.853168	0.265761
C	-7.762786	0.871813	0.604313
H	-8.127122	-0.071335	1.010151
H	-9.690935	1.810191	0.602362
H	0.543424	0.955690	-1.311276

S	1.654351	0.556469	1.146727
C	3.396957	0.433008	0.956335
N	3.858369	-0.872747	1.026474
H	3.117454	-1.542583	1.204376
C	5.098423	-1.418374	0.762421
C	5.178207	-2.830676	0.769726
C	6.264545	-0.672821	0.491299
C	6.370486	-3.481000	0.516767
H	4.275656	-3.410163	0.973335
C	7.461803	-1.327859	0.234987
H	6.219412	0.411366	0.487687
C	7.508465	-2.718509	0.249731
H	6.431591	-4.568203	0.520484
H	8.367793	-0.761027	0.024152
N	8.773570	-3.396431	-0.018688
O	9.748020	-2.714144	-0.248544
O	8.783973	-4.608293	0.002572
N	4.238601	1.394812	0.791948
C	3.867650	2.697446	0.536767
C	4.402774	3.732887	1.329101
C	3.036953	3.038847	-0.553441
C	4.101882	5.060683	1.065521
H	5.055813	3.468381	2.161557
C	2.740708	4.363024	-0.831490
H	2.644538	2.240317	-1.183467
C	3.271470	5.361068	-0.012869
H	4.502482	5.865275	1.680601
H	2.104740	4.635579	-1.672601
N	2.953954	6.758373	-0.298014
O	2.227502	6.997135	-1.238459
O	3.431625	7.609487	0.420665

CF3_Michael_Acceptor_TS-MA-conf/TS-MA-R-v

Frequencies, energies and thermodynamic properties:

Lowest Vibrational Mode (1/cm) = -193.4111

2nd Lowest Vibrational Mode (1/cm) = 12.8907

E(RM062X) (a.u.) = -3187.94497830

Thermal correction to Enthalpy (a.u.) = 0.680676

Thermal correction to Gibbs Free Energy (a.u.) = 0.556152

Total Entropy (cal/Kmol) = 262.083

Esp(RM062X) (a.u.) = -3190.90463753

Optimised cartesian coordinates (Angstrom):

C	-5.146113	-3.581970	-0.789316
C	-6.002275	-2.478170	-0.899672
C	-5.491165	-1.194895	-1.069269
C	-4.105887	-1.042760	-1.119530
C	-3.255062	-2.142223	-0.988935
H	-7.081895	-2.623889	-0.851040
H	-6.153123	-0.330956	-1.153033
C	-1.710133	-0.441319	-1.169893
C	0.723611	-0.716389	-0.977854
C	0.350391	-1.991318	-0.203251
C	-0.804873	-2.705806	-0.876685
H	-1.158088	-3.537683	-0.254357
S	-3.204379	0.450036	-1.310234
N	-1.910320	-1.759424	-1.023885
N	-0.487194	0.105498	-1.194815
C	1.542475	-2.920169	0.104437
C	1.896064	-3.907082	-1.012122
C	1.277867	-3.697350	1.396122
H	2.409481	-2.258539	0.280067
H	2.820715	-4.442274	-0.749460
H	1.105561	-4.665807	-1.125828

H	2.052308	-3.427885	-1.987796
H	0.485687	-4.448361	1.244833
H	2.183968	-4.228502	1.724239
H	0.960884	-3.032800	2.212412
H	-0.022905	-1.620516	0.765180
H	1.352951	-0.139620	-0.287540
C	1.487219	-0.929745	-2.267892
C	0.837526	-1.218709	-3.471804
C	2.885692	-0.885952	-2.241426
C	1.576421	-1.495103	-4.622671
H	-0.254271	-1.224253	-3.521516
C	3.624682	-1.162293	-3.390008
H	3.396744	-0.638889	-1.306632
C	2.970573	-1.475407	-4.582529
H	1.058670	-1.722305	-5.556074
H	4.714882	-1.128620	-3.355353
H	3.547168	-1.691355	-5.483509
C	0.928452	2.121510	-1.282566
H	1.839499	1.534926	-1.212847
C	0.965173	3.500578	-1.018091
C	2.269364	4.211018	-1.260478
F	2.571626	4.210839	-2.562975
F	2.250796	5.483527	-0.869949
F	3.300464	3.617551	-0.631307
O	-1.416901	2.180500	-1.391736
C	-0.366189	1.549845	-1.316138
H	-0.533082	-3.097986	-1.869001
C	-3.762591	-3.433238	-0.832444
H	-3.106046	-4.299001	-0.750584
H	-5.567666	-4.580148	-0.664550
H	0.109309	4.090361	-1.354594
S	0.608526	3.944343	1.126704
C	0.869690	2.266967	1.623048
N	0.027722	1.326350	1.869918
C	-1.358257	1.320422	1.879577
C	-2.232426	2.404886	1.643474
C	-1.934323	0.053913	2.146637
C	-3.608901	2.217340	1.654669
H	-1.830746	3.392774	1.438268
C	-3.305323	-0.143811	2.156314
H	-1.261151	-0.778329	2.358171
C	-4.129428	0.950166	1.900457
H	-4.284662	3.048209	1.456065
H	-3.740724	-1.122888	2.352883
N	-5.578499	0.747951	1.845486
O	-6.007766	-0.354614	2.105234
O	-6.272481	1.691028	1.534703
N	2.213658	1.945219	1.613615
C	2.835226	0.726281	1.856822
C	2.332976	-0.243563	2.745728
C	4.060371	0.490923	1.198746
C	3.046929	-1.413975	2.967315
H	1.401123	-0.062359	3.273843
C	4.763939	-0.684384	1.405479
H	4.445985	1.244544	0.509114
C	4.240584	-1.630356	2.285380
H	2.684200	-2.163554	3.668863
H	5.701986	-0.878773	0.887245
N	4.956712	-2.890720	2.485823
O	4.443462	-3.728766	3.195315
O	6.021970	-3.031619	1.929089
H	2.816430	2.673617	1.243475

CF3_Michael_Acceptor_TS-MA-conf/TS-MA-R-xiii

Frequencies, energies and thermodynamic properties:

Lowest Vibrational Mode (1/cm) = -134.8135

2nd Lowest Vibrational Mode (1/cm) = 13.8271

E(RM062X) (a.u.) = -3187.93706226

Thermal correction to Enthalpy (a.u.) = 0.681021

Thermal correction to Gibbs Free Energy (a.u.) = 0.555827

Total Entropy (cal/Kmol) = 263.494

Esp(RM062X) (a.u.) = -3190.89848931

Optimised cartesian coordinates (Angstrom):

C	-7.356309	1.833453	-1.309335
C	-6.842210	2.730698	-2.256411
C	-5.488537	2.733397	-2.575524
C	-4.663031	1.819386	-1.922637
C	-5.176486	0.930517	-0.978233
H	-7.511153	3.437042	-2.749299
H	-5.082681	3.430625	-3.309769
C	-2.946979	0.353699	-0.913927
C	-1.992349	-1.422027	0.490383
C	-3.232664	-1.195327	1.369154
C	-4.464343	-0.949870	0.523336
H	-5.295536	-0.614115	1.155923
S	-2.935704	1.610583	-2.123898
N	-4.174571	0.119470	-0.433500
N	-1.860092	-0.317597	-0.489473
C	-3.443300	-2.283803	2.444727
C	-4.306188	-3.462945	1.989153
C	-4.037929	-1.651409	3.703811
H	-2.444214	-2.671238	2.704571
H	-5.354892	-3.154062	1.853906
H	-3.956513	-3.910773	1.048136
H	-4.295936	-4.248356	2.758787
H	-3.370390	-0.881844	4.119309
H	-5.007267	-1.175227	3.485921
H	-4.205922	-2.412323	4.479840
H	-3.041117	-0.252161	1.897621
H	-1.137956	-1.332706	1.171597
C	-1.929885	-2.767908	-0.201803
C	-1.197619	-3.804454	0.385802
C	-2.629614	-3.013698	-1.388187
C	-1.193676	-5.077592	-0.181632
H	-0.626516	-3.611064	1.297448
C	-2.624322	-4.287074	-1.957584
H	-3.180473	-2.211633	-1.886627
C	-1.913745	-5.323193	-1.351182
H	-0.619742	-5.878542	0.287183
H	-3.174285	-4.468168	-2.882513
H	-1.909584	-6.318653	-1.798143
C	0.575259	-0.730332	-0.607419
H	0.562113	-1.339789	0.292345
C	1.758463	-0.520311	-1.279078
C	2.877443	-1.495822	-1.018617
F	3.100413	-1.668421	0.289622
F	2.544809	-2.701693	-1.509143
F	4.031488	-1.166507	-1.587548
O	-0.562101	0.775029	-2.010090
C	-0.580827	-0.038088	-1.101820
H	-4.781118	-1.841833	-0.039038
C	-6.534861	0.920189	-0.657359
H	-6.943821	0.225413	0.075114
H	-8.421511	1.849345	-1.075856
H	1.729281	-0.124203	-2.295253
S	2.950994	1.519634	-0.691869

C	3.117111	1.190357	1.013492
N	1.992634	1.169339	1.838254
H	2.213511	0.749360	2.739036
C	0.693431	1.609319	1.714185
C	-0.206222	1.173401	2.718373
C	0.210178	2.476492	0.709934
C	-1.545084	1.508149	2.675683
H	0.169116	0.545655	3.529029
C	-1.134663	2.810759	0.665944
H	0.884248	2.856647	-0.050685
C	-2.010796	2.298386	1.622380
H	-2.235786	1.153156	3.440210
H	-1.513796	3.460560	-0.122165
N	-3.440367	2.524577	1.481190
O	-3.819204	3.279283	0.611260
O	-4.192312	1.918136	2.221949
N	4.197595	0.836507	1.626105
C	5.434289	0.743668	1.020271
C	6.038782	1.824105	0.343490
C	6.155131	-0.461019	1.149923
C	7.313093	1.703420	-0.188403
H	5.494159	2.763197	0.248294
C	7.424809	-0.595851	0.609554
H	5.687428	-1.291780	1.679173
C	7.990322	0.491698	-0.053618
H	7.789155	2.534005	-0.707747
H	7.982467	-1.527207	0.696650
N	9.333095	0.360641	-0.617497
O	9.907081	-0.697833	-0.480908
O	9.804739	1.317137	-1.192663

CF3_Michael_Acceptor_TS-MA-conf/TS-MA-R-xii

Frequencies, energies and thermodynamic properties:

Lowest Vibrational Mode (1/cm) = -100.8931

2nd Lowest Vibrational Mode (1/cm) = 9.5552

E(RM062X) (a.u.) = -3187.92481392

Thermal correction to Enthalpy (a.u.) = 0.680856

Thermal correction to Gibbs Free Energy (a.u.) = 0.549230

Total Entropy (cal/Kmol) = 277.031

Esp(RM062X) (a.u.) = -3190.89242434

Optimised cartesian coordinates (Angstrom):

C	7.657144	0.033729	-2.523798
C	7.370915	1.395322	-2.701969
C	6.140132	1.921570	-2.325308
C	5.202351	1.051585	-1.768880
C	5.486589	-0.304131	-1.600676
H	8.123696	2.052717	-3.138290
H	5.914118	2.980587	-2.457015
C	3.353897	-0.225809	-0.741764
C	2.169390	-2.146942	0.230844
C	3.026206	-2.964671	-0.750745
C	4.446023	-2.433759	-0.775531
H	5.016841	-2.898476	-1.589790
S	3.590093	1.440490	-1.200593
N	4.409442	-0.992043	-1.031356
N	2.252582	-0.710786	-0.134158
C	2.963910	-4.490986	-0.512789
C	4.014011	-5.023350	0.466032
C	3.078516	-5.227656	-1.847711
H	1.966113	-4.706086	-0.096809
H	3.807520	-6.080375	0.687738
H	5.022657	-4.975346	0.025823
H	4.030860	-4.478526	1.420350

H	4.034445	-4.994200	-2.343587
H	3.041237	-6.315787	-1.693738
H	2.263135	-4.951041	-2.531544
H	2.589787	-2.767834	-1.743582
H	1.132662	-2.446941	0.039757
C	2.483009	-2.363094	1.697106
C	3.529578	-1.688375	2.334665
C	1.734821	-3.299649	2.418911
C	3.842709	-1.971352	3.664434
H	4.108901	-0.927577	1.804556
C	2.048583	-3.583561	3.746643
H	0.898444	-3.811063	1.935435
C	3.108534	-2.924343	4.370277
H	4.661303	-1.439336	4.151721
H	1.458063	-4.316908	4.298150
H	3.353354	-3.142864	5.410954
C	0.075452	-0.328494	0.970191
H	-0.001924	-1.371220	1.266409
C	-0.937704	0.541008	1.243984
C	-1.984070	0.159818	2.252382
F	-1.473089	0.255106	3.489922
F	-3.053135	0.954831	2.226818
F	-2.406086	-1.098763	2.109586
O	1.266011	1.336980	-0.198227
C	1.181456	0.187693	0.194561
H	4.977061	-2.606604	0.172635
C	6.723629	-0.836140	-1.971185
H	6.958368	-1.890305	-1.827323
H	8.632130	-0.354189	-2.821037
H	-0.803012	1.613150	1.095066
S	-2.512251	0.468844	-0.769975
C	-3.860325	1.548387	-0.563825
N	-5.112125	1.253474	-0.734127
C	-5.604501	-0.018936	-0.908381
C	-6.536716	-0.247029	-1.943196
C	-5.294911	-1.088447	-0.035576
C	-7.123429	-1.490350	-2.121132
H	-6.786629	0.582556	-2.605651
C	-5.885893	-2.330070	-0.198554
H	-4.589336	-0.921018	0.777374
C	-6.789772	-2.522148	-1.245292
H	-7.836368	-1.671361	-2.924340
H	-5.658266	-3.155258	0.474946
N	-7.406759	-3.833109	-1.421567
O	-7.091312	-4.719608	-0.656804
O	-8.203858	-3.972122	-2.324546
N	-3.672096	2.871034	-0.169972
C	-2.577652	3.701320	-0.040299
C	-1.289160	3.444842	-0.555268
C	-2.797131	4.921798	0.642984
C	-0.262940	4.358124	-0.360783
H	-1.089671	2.523092	-1.093651
C	-1.778979	5.838609	0.824579
H	-3.792336	5.134945	1.038066
C	-0.510044	5.543732	0.325111
H	0.734808	4.149727	-0.743687
H	-1.952973	6.773862	1.354660
N	0.575318	6.498908	0.521203
O	1.670755	6.213965	0.087545
O	0.326398	7.530180	1.107657
H	-4.559900	3.304789	0.073138

CF3_Michael_Acceptor_TS-MA-conf/TS-MA-R-xi

Frequencies, energies and thermodynamic properties:

Lowest Vibrational Mode (1/cm) = -127.6379

2nd Lowest Vibrational Mode (1/cm) = 11.7363

E(RM062X) (a.u.) = -3187.93273106

Thermal correction to Enthalpy (a.u.) = 0.680933

Thermal correction to Gibbs Free Energy (a.u.) = 0.554393

Total Entropy (cal/Kmol) = 266.324

Esp(RM062X) (a.u.) = -3190.89730460

Optimised cartesian coordinates (Angstrom):

C	3.680690	6.299501	-0.401985
C	2.416160	6.876891	-0.219468
C	1.298441	6.083919	0.018899
C	1.475251	4.701229	0.064383
C	2.733497	4.128657	-0.126804
H	2.305888	7.961029	-0.260429
H	0.313196	6.528137	0.167645
C	1.470728	2.232913	0.223438
C	2.344426	-0.069282	0.196372
C	3.412303	0.530014	-0.738227
C	3.859781	1.882863	-0.218278
H	4.519471	2.372522	-0.944776
S	0.251768	3.477975	0.360078
N	2.682732	2.733088	-0.043165
N	1.248550	0.917388	0.382506
C	4.605874	-0.405484	-1.035657
C	5.741255	-0.343076	-0.008313
C	5.174475	-0.106941	-2.423797
H	4.205952	-1.432823	-1.053650
H	6.284228	0.612288	-0.086428
H	5.401348	-0.458817	1.029387
H	6.465091	-1.144635	-0.215372
H	4.410829	-0.193350	-3.209485
H	5.586927	0.914346	-2.466072
H	5.988183	-0.806141	-2.662810
H	2.890592	0.705762	-1.694672
H	1.895242	-0.907886	-0.351405
C	2.874163	-0.597509	1.513201
C	3.229389	-1.949510	1.591763
C	3.062976	0.224245	2.627413
C	3.795812	-2.464618	2.755308
H	3.068724	-2.601107	0.727283
C	3.629046	-0.291995	3.794136
H	2.762032	1.274660	2.598678
C	4.002769	-1.633923	3.858056
H	4.071237	-3.519343	2.803077
H	3.772646	0.358255	4.658618
H	4.443326	-2.036505	4.771581
C	-0.229317	-0.892265	1.146723
H	0.580841	-1.608743	1.066527
C	-1.472089	-1.315240	1.585619
C	-1.491535	-2.583691	2.398118
F	-0.775948	-3.560446	1.829093
F	-0.950395	-2.361442	3.603398
F	-2.716659	-3.060459	2.615552
O	-0.958758	1.322802	0.806489
C	-0.076715	0.477141	0.783237
H	4.387615	1.806120	0.744385
C	3.860610	4.920823	-0.357084
H	4.850504	4.484778	-0.487990
H	4.544768	6.940737	-0.580021
H	-2.197154	-0.567510	1.911841
S	-2.995612	-2.084328	-0.054043
C	-2.611587	-0.891491	-1.275126

N	-3.390112	0.059115	-1.668769
C	-4.675057	0.262387	-1.208821
C	-5.003832	1.526486	-0.678868
C	-5.689218	-0.711894	-1.318030
C	-6.292775	1.808441	-0.252977
H	-4.216040	2.276735	-0.601699
C	-6.984103	-0.434621	-0.907138
H	-5.446760	-1.687973	-1.738532
C	-7.269937	0.822083	-0.374868
H	-6.551551	2.778711	0.168443
H	-7.774735	-1.178983	-0.991249
N	-8.634360	1.115840	0.063059
O	-9.469047	0.245613	-0.053472
O	-8.860622	2.215031	0.519971
N	-1.364910	-0.861698	-1.895053
C	-0.267436	-1.693146	-1.959444
C	-0.109240	-2.917444	-1.275256
C	0.790660	-1.242639	-2.785414
C	1.089429	-3.609144	-1.351177
H	-0.912274	-3.300394	-0.653696
C	1.977936	-1.944983	-2.880525
H	0.663197	-0.315077	-3.347860
C	2.131439	-3.112303	-2.133322
H	1.224504	-4.535725	-0.793907
H	2.790341	-1.595542	-3.515713
N	3.409947	-3.810750	-2.154730
O	4.295863	-3.355197	-2.848288
O	3.529235	-4.803271	-1.469444
H	-1.301555	-0.049839	-2.506137

CF3_Michael_Acceptor_TS-MA-conf/TS-MA-R-xiv

Frequencies, energies and thermodynamic properties:

Lowest Vibrational Mode (1/cm) = -193.8158

2nd Lowest Vibrational Mode (1/cm) = 17.5306

E(RM062X) (a.u.) = -3187.93578565

Thermal correction to Enthalpy (a.u.) = 0.681103

Thermal correction to Gibbs Free Energy (a.u.) = 0.556572

Total Entropy (cal/Kmol) = 262.098

Esp(RM062X) (a.u.) = -3190.89704171

Optimised cartesian coordinates (Angstrom):

C	-6.679174	-1.564870	0.685009
C	-7.012027	-0.478262	-0.135007
C	-6.031048	0.196731	-0.855360
C	-4.712109	-0.238874	-0.732461
C	-4.380791	-1.309336	0.100423
H	-8.050813	-0.154977	-0.209887
H	-6.283401	1.045654	-1.493480
C	-2.288684	-0.711106	-0.659458
C	-0.188738	-1.769214	0.029548
C	-0.976787	-2.146288	1.294190
C	-2.381989	-2.587068	0.932638
H	-2.990743	-2.708247	1.837369
S	-3.291085	0.444436	-1.499977
N	-3.001590	-1.545236	0.113289
N	-0.953611	-0.775325	-0.751550
C	-0.239308	-3.144824	2.212972
C	-0.527594	-4.616482	1.906011
C	-0.564157	-2.839408	3.675374
H	0.839584	-2.968958	2.067269
H	-1.562643	-4.881036	2.174750
H	-0.371961	-4.872067	0.848242
H	0.136139	-5.255627	2.506229
H	-0.247717	-1.822508	3.951685

H	-1.646756	-2.924028	3.864235
H	-0.053883	-3.547378	4.344414
H	-1.079627	-1.201392	1.852858
H	0.704488	-1.243407	0.391330
C	0.244246	-2.934167	-0.835486
C	1.529278	-3.460860	-0.671447
C	-0.623393	-3.529812	-1.757493
C	1.932425	-4.584757	-1.390626
H	2.218430	-2.981937	0.028081
C	-0.220778	-4.653620	-2.479041
H	-1.621942	-3.118152	-1.925619
C	1.054400	-5.187909	-2.291667
H	2.937972	-4.985445	-1.252760
H	-0.906130	-5.110480	-3.194841
H	1.368165	-6.066264	-2.858105
C	1.161820	0.220969	-1.543457
H	1.764559	-0.558656	-1.086147
C	1.753171	1.448827	-1.897466
C	3.194515	1.433727	-2.334275
F	3.983422	0.740923	-1.511464
F	3.292274	0.858136	-3.541345
F	3.713713	2.656726	-2.454596
O	-0.961121	1.073650	-2.082554
C	-0.253124	0.233408	-1.532663
H	-2.393976	-3.534894	0.373465
C	-5.362285	-1.997218	0.816187
H	-5.114072	-2.844738	1.454445
H	-7.464605	-2.084140	1.235533
H	1.156196	2.096697	-2.544220
S	1.785499	2.866767	-0.221933
C	1.353832	1.677218	1.002520
N	0.041877	1.522683	1.422695
H	0.002704	0.801146	2.141106
C	-1.198253	2.074531	1.135144
C	-2.282752	1.515256	1.854476
C	-1.463832	3.101338	0.209354
C	-3.582352	1.943041	1.652956
H	-2.084055	0.734615	2.592210
C	-2.768184	3.532161	0.006772
H	-0.655022	3.548929	-0.358727
C	-3.813070	2.950305	0.718147
H	-4.414157	1.502929	2.202054
H	-2.980909	4.315167	-0.719879
N	-5.187274	3.368178	0.451668
O	-5.375572	4.170110	-0.436611
O	-6.068730	2.884072	1.128050
N	2.150007	0.804923	1.522051
C	3.524922	0.764420	1.384760
C	4.357731	1.898170	1.485131
C	4.122840	-0.500497	1.216734
C	5.733635	1.773783	1.368325
H	3.915830	2.878349	1.655129
C	5.495722	-0.633538	1.085086
H	3.478795	-1.380169	1.178123
C	6.285751	0.511774	1.156015
H	6.385304	2.643470	1.439952
H	5.960726	-1.606532	0.934056
N	7.737467	0.383827	1.020765
O	8.195487	-0.723384	0.842538
O	8.405801	1.391067	1.094167

CF3_Michael_Acceptor_TS-MA-conf/TS-MA-R-xix

Frequencies, energies and thermodynamic properties:

Lowest Vibrational Mode (1/cm) = -126.3993

2nd Lowest Vibrational Mode (1/cm) = 16.1802

E(RM062X) (a.u.) = -3187.93115188

Thermal correction to Enthalpy (a.u.) = 0.680938

Thermal correction to Gibbs Free Energy (a.u.) = 0.556200

Total Entropy (cal/Kmol) = 262.533

Esp(RM062X) (a.u.) = -3190.89369923

Optimised cartesian coordinates (Angstrom):

C	2.551322	5.282020	1.137323
C	1.177194	5.500274	1.321785
C	0.277451	4.441857	1.296546
C	0.786422	3.160890	1.074842
C	2.151761	2.947954	0.884343
H	0.809619	6.513658	1.486874
H	-0.792288	4.602492	1.439662
C	1.362578	0.801117	0.638487
C	2.758891	-1.165418	0.145806
C	3.731089	-0.134012	-0.452035
C	3.794885	1.115081	0.402522
H	4.336505	1.906642	-0.129999
S	-0.112684	1.663823	0.971717
N	2.433520	1.600165	0.635550
N	1.443480	-0.525602	0.395352
C	5.126214	-0.710987	-0.780284
C	6.132844	-0.626953	0.370044
C	5.689423	-0.015551	-2.020299
H	4.977840	-1.774746	-1.029307
H	7.043777	-1.182621	0.104088
H	6.432056	0.416888	0.555403
H	5.747738	-1.045730	1.310693
H	5.784943	1.069200	-1.852409
H	6.688290	-0.405233	-2.264641
H	5.039918	-0.165493	-2.895147
H	3.275584	0.172673	-1.404492
H	2.594168	-1.898633	-0.651659
C	3.258027	-1.887449	1.379690
C	3.173252	-1.312713	2.652597
C	3.871213	-3.136219	1.233702
C	3.723610	-1.963854	3.756445
H	2.670149	-0.353075	2.798176
C	4.423203	-3.786102	2.336376
H	3.918279	-3.601371	0.245758
C	4.356674	-3.197147	3.599368
H	3.652678	-1.506628	4.744651
H	4.900567	-4.759082	2.209303
H	4.786255	-3.705387	4.464175
C	0.304255	-2.697032	0.013519
H	1.237565	-3.217552	-0.185723
C	-0.893843	-3.304372	-0.226997
C	-0.920484	-4.783009	-0.499663
F	-0.546833	-5.461877	0.597383
F	-2.126161	-5.229474	-0.831140
F	-0.070656	-5.132667	-1.469462
O	-0.811187	-0.711195	0.574154
C	0.237448	-1.296391	0.360371
H	4.272595	0.940586	1.378672
C	3.060603	4.008310	0.917587
H	4.128436	3.850910	0.771267
H	3.237320	6.129545	1.160892
H	-1.837350	-2.871618	0.113869
S	-1.744868	-2.552147	-2.522845
C	-2.780911	-1.367002	-1.804787
N	-3.770571	-1.728468	-1.047191

C	-4.527761	-0.855682	-0.289802
C	-3.952439	0.104229	0.578043
C	-5.934446	-0.975768	-0.319526
C	-4.751852	0.916788	1.366800
H	-2.865740	0.170987	0.637870
C	-6.739477	-0.160264	0.459830
H	-6.375767	-1.727589	-0.974724
C	-6.138184	0.781821	1.294145
H	-4.315509	1.650112	2.043911
H	-7.825047	-0.244104	0.432724
N	-6.981259	1.644089	2.119036
O	-8.182043	1.495238	2.055674
O	-6.436821	2.466619	2.823603
N	-2.614511	0.000313	-2.098423
C	-1.490326	0.782168	-2.256680
C	-0.189003	0.294164	-2.503981
C	-1.666870	2.183081	-2.128620
C	0.888287	1.164200	-2.523882
H	-0.037761	-0.768641	-2.670592
C	-0.589435	3.049732	-2.137442
H	-2.673437	2.576528	-1.970700
C	0.694795	2.525130	-2.296918
H	1.890727	0.789529	-2.723685
H	-0.727297	4.120315	-1.986992
N	1.854891	3.392222	-2.162841
O	2.952978	2.866383	-2.112694
O	1.674782	4.585280	-2.078249
H	-3.440110	0.551827	-1.876724

CF3_Michael_Acceptor_TS-MA-conf/TS-MA-R-x

Frequencies, energies and thermodynamic properties:

Lowest Vibrational Mode (1/cm) = -193.2876

2nd Lowest Vibrational Mode (1/cm) = 9.6698

E(RM062X) (a.u.) = -3187.93221907

Thermal correction to Enthalpy (a.u.) = 0.680603

Thermal correction to Gibbs Free Energy (a.u.) = 0.552822

Total Entropy (cal/Kmol) = 268.936

Esp(RM062X) (a.u.) = -3190.89592756

Optimised cartesian coordinates (Angstrom):

C	-0.183871	7.032676	-1.058549
C	-1.540101	7.044240	-0.705485
C	-2.164643	5.893206	-0.233545
C	-1.400476	4.732480	-0.123198
C	-0.052504	4.722213	-0.485428
H	-2.114537	7.966687	-0.797072
H	-3.219183	5.899048	0.045926
C	-0.300588	2.540946	0.212305
C	1.525168	0.938336	0.358677
C	2.078305	1.680232	-0.868137
C	1.914433	3.176981	-0.681153
H	2.116586	3.710884	-1.619199
S	-1.925553	3.150498	0.434183
N	0.525871	3.461098	-0.305929
N	0.107737	1.313737	0.546451
C	3.514947	1.260935	-1.252120
C	4.619887	2.051856	-0.546549
C	3.700925	1.357124	-2.766921
H	3.610692	0.195757	-0.972411
H	4.663783	3.085453	-0.925522
H	4.494830	2.092962	0.544307
H	5.595561	1.589042	-0.754605
H	2.967091	0.737813	-3.302604
H	3.586319	2.397937	-3.111242

H	4.707787	1.020631	-3.055676
H	1.419299	1.373059	-1.698319
H	1.514750	-0.120637	0.084405
C	2.322400	1.102419	1.636174
C	3.270681	0.129261	1.971207
C	2.168501	2.217036	2.467132
C	4.073951	0.281624	3.100088
H	3.380179	-0.753900	1.336144
C	2.971750	2.369936	3.597506
H	1.414079	2.976496	2.247280
C	3.930433	1.406896	3.912492
H	4.810225	-0.484473	3.348465
H	2.842857	3.244271	4.237580
H	4.556583	1.527076	4.798068
C	-0.329914	-0.888173	1.512726
H	0.734013	-1.009249	1.695562
C	-1.172911	-2.006279	1.628673
C	-0.786295	-3.019203	2.676121
F	0.518290	-3.317276	2.633601
F	-1.034007	-2.535066	3.897872
F	-1.457567	-4.167782	2.575704
O	-2.038080	0.674336	0.997724
C	-0.860273	0.335958	1.041432
H	2.577718	3.575031	0.101960
C	0.580435	5.874226	-0.954504
H	1.636652	5.873839	-1.222648
H	0.286618	7.947870	-1.419896
H	-2.251788	-1.819815	1.617702
S	-1.065438	-3.363645	-0.136288
C	-0.867702	-1.981753	-1.207093
N	-1.958100	-1.167504	-1.435712
H	-1.682847	-0.276957	-1.844973
C	-3.320146	-1.295860	-1.189260
C	-4.056767	-0.097725	-1.091120
C	-4.000918	-2.524814	-1.104621
C	-5.426654	-0.117147	-0.896763
H	-3.526466	0.853255	-1.144654
C	-5.373610	-2.547539	-0.896348
H	-3.461026	-3.460304	-1.216031
C	-6.071214	-1.348217	-0.791856
H	-5.997270	0.806384	-0.813146
H	-5.909701	-3.493443	-0.833869
N	-7.519096	-1.379216	-0.582336
O	-8.052659	-2.459716	-0.464403
O	-8.107920	-0.321602	-0.539068
N	0.228132	-1.556670	-1.737630
C	1.497710	-2.103136	-1.632082
C	2.078472	-2.611061	-0.449340
C	2.297454	-2.033577	-2.793214
C	3.403136	-3.029702	-0.436057
H	1.490351	-2.673406	0.462911
C	3.617122	-2.457100	-2.791780
H	1.848475	-1.629764	-3.701433
C	4.156618	-2.947454	-1.604314
H	3.857918	-3.414996	0.475868
H	4.231754	-2.404739	-3.689347
N	5.555866	-3.380910	-1.583086
O	6.190187	-3.296007	-2.611012
O	6.004575	-3.798653	-0.539154

CF3_Michael_Acceptor_TS-MA-conf/TS-MA-R-xviii

Frequencies, energies and thermodynamic properties:

Lowest Vibrational Mode (1/cm) = -148.6875

2nd Lowest Vibrational Mode (1/cm) = 6.2819

E(RM062X) (a.u.) = -3187.93009767

Thermal correction to Enthalpy (a.u.) = 0.680889

Thermal correction to Gibbs Free Energy (a.u.) = 0.552791

Total Entropy (cal/Kmol) = 269.604

Esp(RM062X) (a.u.) = -3190.89200629

Optimised cartesian coordinates (Angstrom):

C	-6.954814	-4.161836	-0.695958
C	-6.112165	-5.239794	-1.002791
C	-4.729668	-5.085778	-1.007449
C	-4.211177	-3.827081	-0.703939
C	-5.052827	-2.754306	-0.408053
H	-6.544252	-6.213202	-1.237495
H	-4.069769	-5.922725	-1.239867
C	-3.000211	-1.732985	-0.188210
C	-2.663860	0.619024	0.439652
C	-4.059580	0.823872	-0.180395
C	-4.977958	-0.321544	0.198349
H	-5.913515	-0.266156	-0.371718
S	-2.522269	-3.360270	-0.608418
N	-4.329154	-1.588681	-0.136518
N	-2.151745	-0.726049	0.078832
C	-4.694984	2.201670	0.121121
C	-5.457401	2.281874	1.448093
C	-5.629606	2.604721	-1.021768
H	-3.866524	2.929959	0.146740
H	-6.393611	1.703384	1.397248
H	-4.880910	1.923047	2.311201
H	-5.736387	3.327429	1.644259
H	-6.068623	3.593540	-0.823584
H	-5.096386	2.656605	-1.979661
H	-6.460395	1.886886	-1.118551
H	-3.900636	0.770381	-1.271020
H	-2.002549	1.337691	-0.061847
C	-2.583196	0.852462	1.933606
C	-2.161629	2.101173	2.402140
C	-2.964841	-0.129675	2.852501
C	-2.154885	2.377554	3.767763
H	-1.834882	2.861703	1.687417
C	-2.957482	0.146047	4.220082
H	-3.268127	-1.122842	2.510260
C	-2.560565	1.401819	4.679612
H	-1.824910	3.355497	4.121934
H	-3.258873	-0.626586	4.929236
H	-2.553531	1.615593	5.749653
C	0.140736	0.032242	0.593068
H	-0.170221	1.068490	0.694628
C	1.452091	-0.327964	0.843241
C	2.253142	0.589142	1.732094
F	3.565749	0.364483	1.716936
F	2.063783	1.878057	1.436390
F	1.857687	0.424403	3.003907
O	-0.375135	-2.136358	-0.154368
C	-0.732234	-1.007176	0.144972
H	-5.220905	-0.325748	1.272018
C	-6.440899	-2.905354	-0.392749
H	-7.102416	-2.075435	-0.146663
H	-8.035536	-4.308255	-0.691351
H	1.677096	-1.384229	1.004065
S	2.843335	-0.502072	-1.070882
C	3.570355	1.089869	-1.172180
N	4.926016	1.237309	-0.926945
H	5.176451	2.215174	-0.794437

C	5.934594	0.330547	-0.640183
C	6.989305	0.786805	0.177095
C	5.996114	-0.975068	-1.164804
C	8.060035	-0.034362	0.487408
H	6.947885	1.801138	0.577558
C	7.062239	-1.804264	-0.848293
H	5.215639	-1.332460	-1.830472
C	8.079084	-1.330497	-0.022832
H	8.870828	0.313132	1.125792
H	7.119944	-2.814045	-1.252160
N	9.200780	-2.209259	0.306391
O	9.187631	-3.336857	-0.135407
O	10.084874	-1.763265	1.004200
N	2.957312	2.214929	-1.358079
C	1.619242	2.353053	-1.641139
C	0.914788	3.382589	-0.976704
C	0.934014	1.589697	-2.615684
C	-0.423465	3.623385	-1.238564
H	1.453531	3.984385	-0.244371
C	-0.405460	1.819133	-2.880757
H	1.468836	0.813939	-3.159942
C	-1.073563	2.829161	-2.184814
H	-0.966229	4.419902	-0.730411
H	-0.937057	1.237563	-3.633045
N	-2.475750	3.085288	-2.479039
O	-3.059202	2.309180	-3.210952
O	-2.995394	4.063243	-1.984146

CF3_Michael_Acceptor_TS-MA-conf/TS-MA-R-xvii

Frequencies, energies and thermodynamic properties:

Lowest Vibrational Mode (1/cm) = -127.1767

2nd Lowest Vibrational Mode (1/cm) = 7.8233

E(RM062X) (a.u.) = -3187.92885559

Thermal correction to Enthalpy (a.u.) = 0.680578

Thermal correction to Gibbs Free Energy (a.u.) = 0.552275

Total Entropy (cal/Kmol) = 270.035

Esp(RM062X) (a.u.) = -3190.89178255

Optimised cartesian coordinates (Angstrom):

C	7.334890	1.487493	-1.941947
C	6.856328	2.769959	-1.634140
C	5.577137	2.950553	-1.119115
C	4.789651	1.815311	-0.924964
C	5.266428	0.539682	-1.231978
H	7.495614	3.638095	-1.798503
H	5.186468	3.938429	-0.870005
C	3.170607	0.016157	-0.440437
C	2.206123	-2.250427	-0.367741
C	3.213957	-2.534923	-1.495864
C	4.545601	-1.873135	-1.193843
H	5.223785	-1.960261	-2.051477
S	3.165301	1.751441	-0.272039
N	4.314746	-0.448211	-0.952305
N	2.138031	-0.789936	-0.120968
C	3.353904	-4.035066	-1.841459
C	4.422258	-4.773717	-1.030320
C	3.629685	-4.198688	-3.336444
H	2.378351	-4.501774	-1.628556
H	5.433439	-4.445945	-1.319808
H	4.314053	-4.633720	0.054419
H	4.360518	-5.852160	-1.236314
H	2.814287	-3.780042	-3.943975
H	4.563752	-3.688866	-3.622233
H	3.738459	-5.261602	-3.596487

H	2.801416	-2.029558	-2.384361
H	1.227795	-2.536515	-0.771222
C	2.441270	-3.018245	0.917567
C	1.760660	-4.224850	1.115515
C	3.354764	-2.585265	1.884780
C	2.014726	-5.005313	2.241627
H	1.025122	-4.555924	0.377991
C	3.608004	-3.365493	3.013462
H	3.875042	-1.630505	1.772005
C	2.945760	-4.580245	3.190082
H	1.478292	-5.945068	2.382431
H	4.323633	-3.017975	3.760321
H	3.144857	-5.188494	4.073907
C	-0.154904	-1.058155	0.785939
H	-0.175323	-2.123249	0.571113
C	-1.270173	-0.424138	1.264145
C	-2.353360	-1.247152	1.902450
F	-2.763517	-2.259483	1.136927
F	-1.900031	-1.789732	3.043811
F	-3.425969	-0.525494	2.236647
O	0.995519	0.987828	0.718322
C	0.971542	-0.208376	0.492071
H	5.037454	-2.304588	-0.309002
C	6.552219	0.354588	-1.745338
H	6.935395	-0.638129	-1.980213
H	8.343274	1.371471	-2.341067
H	-1.194101	0.599164	1.636211
S	-2.698323	0.441241	-0.614352
C	-3.574210	1.667751	0.265527
N	-4.854330	1.829145	0.337012
C	-5.798132	0.981972	-0.207523
C	-6.858224	1.564761	-0.934303
C	-5.810449	-0.416653	-0.007819
C	-7.878999	0.791677	-1.464890
H	-6.855535	2.646731	-1.071535
C	-6.834671	-1.195811	-0.522951
H	-5.009725	-0.880971	0.563086
C	-7.854704	-0.585669	-1.252825
H	-8.692763	1.239135	-2.033765
H	-6.853744	-2.273583	-0.367018
N	-8.928905	-1.409882	-1.802039
O	-8.882835	-2.606153	-1.612795
O	-9.812592	-0.856452	-2.420096
N	-2.840991	2.553240	1.058310
C	-1.577646	3.090776	0.871353
C	-0.941396	3.158899	-0.383786
C	-0.929091	3.639419	1.997232
C	0.318265	3.723136	-0.497133
H	-1.439980	2.763846	-1.265258
C	0.327819	4.206975	1.887790
H	-1.425741	3.595346	2.968091
C	0.946671	4.233335	0.638073
H	0.817743	3.780154	-1.463499
H	0.838716	4.615604	2.758540
N	2.288887	4.783750	0.525152
O	2.784791	5.302688	1.498618
O	2.860768	4.681213	-0.547107
H	-3.397679	2.983941	1.793539

CF3_Michael_Acceptor_TS-MA-conf/TS-MA-R-xvi

Frequencies, energies and thermodynamic properties:

Lowest Vibrational Mode (1/cm) = -149.4170

2nd Lowest Vibrational Mode (1/cm) = 13.0627

E(RM062X) (a.u.) = -3187.93072656

Thermal correction to Enthalpy (a.u.) = 0.680763

Thermal correction to Gibbs Free Energy (a.u.) = 0.553534

Total Entropy (cal/Kmol) = 267.774

Esp(RM062X) (a.u.) = -3190.89294073

Optimised cartesian coordinates (Angstrom):

C	7.579373	-1.241955	1.373229
C	7.123592	-2.544656	1.120759
C	5.799762	-2.782491	0.765708
C	4.945190	-1.683574	0.677287
C	5.398542	-0.388700	0.933206
H	7.816815	-3.383010	1.198467
H	5.424182	-3.785860	0.557644
C	3.205263	0.043436	0.391135
C	2.164612	2.267782	0.388931
C	3.240720	2.592412	1.440752
C	4.572682	1.983444	1.041908
H	5.298198	2.073126	1.861055
S	3.252984	-1.690689	0.222980
N	4.377947	0.556755	0.779150
N	2.116740	0.803890	0.173030
C	3.345020	4.097648	1.777316
C	4.325814	4.877135	0.896768
C	3.714852	4.274840	3.250151
H	2.339337	4.524705	1.630892
H	5.366935	4.597363	1.123532
H	4.155828	4.723769	-0.178255
H	4.228356	5.953323	1.100768
H	2.959689	3.826162	3.911680
H	4.685008	3.801221	3.470231
H	3.800626	5.341550	3.503244
H	2.912995	2.071512	2.355474
H	1.208510	2.538703	0.852139
C	2.300803	3.012053	-0.923854
C	1.584227	4.198887	-1.110345
C	3.162606	2.569751	-1.933147
C	1.751940	4.951618	-2.271186
H	0.889361	4.536110	-0.337067
C	3.329669	3.322045	-3.096066
H	3.707635	1.628182	-1.826075
C	2.631305	4.517820	-3.263949
H	1.188138	5.876375	-2.404143
H	4.005143	2.967750	-3.876394
H	2.761730	5.104175	-4.174941
C	-0.236486	0.991887	-0.575502
H	-0.276067	2.056297	-0.359114
C	-1.367396	0.318455	-0.973716
C	-2.520290	1.120405	-1.513664
F	-2.869021	2.127223	-0.707644
F	-2.185841	1.669667	-2.690610
F	-3.611089	0.385958	-1.739778
O	0.955435	-1.029307	-0.510739
C	0.919471	0.175606	-0.332107
H	4.997729	2.452975	0.142016
C	6.728365	-0.145090	1.281816
H	7.092395	0.865533	1.465513
H	8.624080	-1.080870	1.642083
H	-1.275234	-0.688283	-1.388917
S	-2.527003	-0.644665	0.933266
C	-3.366576	-1.886325	0.039840
N	-4.750986	-1.871637	-0.070493
H	-5.084075	-2.724747	-0.514923
C	-5.756545	-0.994817	0.292195

C -7.071810 -1.513660 0.236957
C -5.583091 0.354975 0.664755
C -8.169465 -0.733943 0.549905
H -7.216400 -2.555581 -0.055496
C -6.684399 1.136585 0.983958
H -4.589954 0.790085 0.697234
C -7.964043 0.591992 0.928926
H -9.178786 -1.140607 0.509116
H -6.554938 2.180242 1.267365
N -9.114284 1.425925 1.264824
O -8.908186 2.571074 1.603158
O -10.217250 0.929480 1.188086
N -2.819809 -2.868270 -0.607382
C -1.503889 -3.263553 -0.526278
C -0.808696 -3.428381 0.693082
C -0.847172 -3.618184 -1.726047
C 0.493791 -3.897864 0.707316
H -1.308595 -3.180875 1.628399
C 0.457068 -4.079612 -1.722172
H -1.393713 -3.511127 -2.664049
C 1.117838 -4.214496 -0.500599
H 1.035715 -4.021552 1.644281
H 0.970203 -4.335190 -2.648286
N 2.501813 -4.658855 -0.493041
O 3.010367 -4.992110 -1.539879
O 3.101036 -4.652253 0.569705

CF3_Michael_Acceptor_TS-MA-conf/TS-MA-R-xv

Frequencies, energies and thermodynamic properties:

Lowest Vibrational Mode (1/cm) = -182.1758

2nd Lowest Vibrational Mode (1/cm) = 11.7370

E(RM062X) (a.u.) = -3187.93347488

Thermal correction to Enthalpy (a.u.) = 0.680278

Thermal correction to Gibbs Free Energy (a.u.) = 0.553472

Total Entropy (cal/Kmol) = 266.887

Esp(RM062X) (a.u.) = -3190.89406859

Optimised cartesian coordinates (Angstrom):

C -6.751729 -1.334829 0.742888
C -7.056106 -0.263364 -0.107057
C -6.058667 0.361655 -0.850120
C -4.752565 -0.108412 -0.720162
C -4.449368 -1.163047 0.143170
H -8.085243 0.088255 -0.187401
H -6.288643 1.200156 -1.510352
C -2.343592 -0.655022 -0.646007
C -0.287512 -1.792423 0.026422
C -1.054192 -2.087747 1.324395
C -2.490623 -2.465513 1.020057
H -3.079976 -2.502606 1.945195
S -3.314267 0.508991 -1.513057
N -3.078215 -1.439475 0.159090
N -1.016304 -0.774467 -0.755402
C -0.344672 -3.095169 2.254914
C -0.701997 -4.560759 1.994705
C -0.628246 -2.738038 3.714521
H 0.738602 -2.972688 2.084220
H -1.740839 -4.772369 2.293985
H -0.583048 -4.850837 0.941133
H -0.052732 -5.212246 2.597593
H -0.273816 -1.725025 3.956842
H -1.709295 -2.778925 3.924822
H -0.131258 -3.445998 4.393668
H -1.077892 -1.118649 1.848353

H	0.641859	-1.310066	0.348942
C	0.058381	-2.998628	-0.820563
C	1.327270	-3.574676	-0.701880
C	-0.876966	-3.583007	-1.681764
C	1.647402	-4.735925	-1.403717
H	2.071480	-3.106553	-0.052464
C	-0.557305	-4.743547	-2.386144
H	-1.864109	-3.132883	-1.815188
C	0.702107	-5.326874	-2.242423
H	2.640921	-5.175497	-1.301406
H	-1.294877	-5.191107	-3.054359
H	0.951199	-6.234177	-2.795244
C	1.125102	0.123134	-1.575870
H	1.694904	-0.663703	-1.091788
C	1.787742	1.311882	-1.971313
C	3.231805	1.161449	-2.379052
F	3.929751	0.394100	-1.535780
F	3.301910	0.575431	-3.581878
F	3.876199	2.324437	-2.484168
O	-0.960891	1.064851	-2.106928
C	-0.280987	0.201328	-1.554094
H	-2.569800	-3.440534	0.515643
C	-5.446906	-1.801001	0.882212
H	-5.219350	-2.636280	1.544225
H	-7.549456	-1.814790	1.311112
H	1.249729	1.932897	-2.693575
S	1.808788	2.802789	-0.438218
C	1.321857	1.731524	0.878155
N	0.144909	1.516324	1.361676
C	-1.087982	2.086277	1.084967
C	-2.157944	1.548855	1.843153
C	-1.387551	3.113291	0.161749
C	-3.463744	1.983076	1.685759
H	-1.924456	0.780504	2.581435
C	-2.693329	3.559313	0.000787
H	-0.598523	3.555017	-0.438559
C	-3.714506	2.987413	0.753439
H	-4.281986	1.558708	2.266668
H	-2.928134	4.340226	-0.721312
N	-5.096056	3.419959	0.533849
O	-5.307108	4.219385	-0.351393
O	-5.957191	2.949485	1.244043
N	2.284187	0.879940	1.390184
C	3.671766	0.836353	1.304186
C	4.490395	1.958576	1.082005
C	4.273209	-0.421409	1.505689
C	5.867475	1.808798	1.006485
H	4.052449	2.945732	0.967581
C	5.647824	-0.573443	1.441391
H	3.638849	-1.288725	1.699311
C	6.431101	0.547485	1.177322
H	6.511366	2.669186	0.830002
H	6.116303	-1.546147	1.582794
N	7.884563	0.397071	1.094104
O	8.350395	-0.706513	1.272513
O	8.543689	1.383229	0.852344
H	1.868283	0.150523	1.966577

CF3_Michael_Acceptor_TS-MA-conf/TS-MA-R-xxiii

Frequencies, energies and thermodynamic properties:

Lowest Vibrational Mode (1/cm) = -106.1505

2nd Lowest Vibrational Mode (1/cm) = 9.1193

E(RM062X) (a.u.) = -3187.91489894

Thermal correction to Enthalpy (a.u.) = 0.680869

Thermal correction to Gibbs Free Energy (a.u.) = 0.549440

Total Entropy (cal/Kmol) = 276.615

Esp(RM062X) (a.u.) = -3190.88530730

Optimised cartesian coordinates (Angstrom):

C	-6.669691	3.760229	-1.102498
C	-5.721976	4.483462	-1.841916
C	-4.430699	3.998185	-2.016036
C	-4.111719	2.773157	-1.430412
C	-5.051346	2.062386	-0.682816
H	-6.000216	5.438464	-2.288821
H	-3.688694	4.555278	-2.589358
C	-3.247964	0.642940	-0.524729
C	-3.270341	-1.515771	0.648410
C	-4.331669	-0.839787	1.531964
C	-5.289800	-0.033545	0.677637
H	-5.941678	0.582493	1.310088
S	-2.580361	1.925723	-1.498708
N	-4.516754	0.872691	-0.175176
N	-2.591095	-0.481169	-0.171032
C	-5.057542	-1.814063	2.488019
C	-6.319988	-2.452277	1.902318
C	-5.394664	-1.097137	3.795717
H	-4.342847	-2.620111	2.721374
H	-6.690976	-3.228935	2.586618
H	-7.123406	-1.706757	1.791245
H	-6.150704	-2.922326	0.923204
H	-6.048833	-0.230217	3.609132
H	-5.924087	-1.772332	4.483434
H	-4.487667	-0.735908	4.301609
H	-3.771412	-0.122545	2.153803
H	-2.511548	-1.900279	1.339378
C	-3.775521	-2.656327	-0.210230
C	-4.401685	-2.432950	-1.441125
C	-3.652673	-3.966133	0.266037
C	-4.927103	-3.502037	-2.167161
H	-4.480794	-1.422958	-1.852334
C	-4.178616	-5.034058	-0.458645
H	-3.139996	-4.148884	1.214016
C	-4.823788	-4.802742	-1.674032
H	-5.414739	-3.316663	-3.125581
H	-4.077323	-6.050964	-0.076227
H	-5.233684	-5.637860	-2.244335
C	-0.602937	-1.937599	-0.311953
H	-1.130819	-2.755612	0.171165
C	0.726509	-2.054913	-0.583241
C	1.365321	-3.415250	-0.563297
F	0.990076	-4.095476	-1.662665
F	2.690631	-3.373670	-0.582207
F	0.981399	-4.147582	0.482707
O	-0.698390	0.248219	-1.197628
C	-1.237557	-0.670838	-0.606251
H	-5.917852	-0.668063	0.034479
C	-6.351990	2.541973	-0.512259
H	-7.096675	1.984713	0.055339
H	-7.678349	4.158276	-0.986008
H	1.244500	-1.308694	-1.187227
S	1.922292	-1.175869	1.519130
C	3.504332	-0.567421	1.146012
N	4.510626	-1.358696	0.940599
C	5.733493	-0.950969	0.457420
C	5.878298	-0.114694	-0.677585
C	6.905384	-1.463005	1.060634

C	7.132317	0.201890	-1.174208
H	4.987222	0.269114	-1.176130
C	8.162514	-1.141937	0.576399
H	6.794727	-2.122633	1.921980
C	8.264048	-0.308850	-0.538124
H	7.246833	0.837129	-2.051578
H	9.065610	-1.530048	1.045512
N	9.585874	0.031008	-1.056291
O	10.554683	-0.430053	-0.492240
O	9.648649	0.758989	-2.023669
N	3.718884	0.817592	1.181881
C	2.837428	1.874432	1.052292
C	1.623075	1.778420	0.343290
C	3.207990	3.121151	1.598207
C	0.795897	2.880747	0.219506
H	1.327426	0.841340	-0.117370
C	2.386346	4.229843	1.467726
H	4.153067	3.205700	2.137985
C	1.177763	4.095525	0.786782
H	-0.140569	2.804252	-0.330354
H	2.666918	5.191365	1.895308
N	0.296119	5.250998	0.651750
O	-0.758027	5.097371	0.072007
O	0.660906	6.304870	1.125797
H	4.679889	1.092209	1.375021

CF3_Michael_Acceptor_TS-MA-conf/TS-MA-R-xxii

Frequencies, energies and thermodynamic properties:

Lowest Vibrational Mode (1/cm) = -135.3890

2nd Lowest Vibrational Mode (1/cm) = 13.6187

E(RM062X) (a.u.) = -3187.92987472

Thermal correction to Enthalpy (a.u.) = 0.680795

Thermal correction to Gibbs Free Energy (a.u.) = 0.554807

Total Entropy (cal/Kmol) = 265.163

Esp(RM062X) (a.u.) = -3190.89123648

Optimised cartesian coordinates (Angstrom):

C	6.612791	4.759427	-0.606570
C	5.666309	5.786808	-0.730305
C	4.303760	5.510192	-0.688478
C	3.911106	4.181580	-0.526068
C	4.855295	3.160678	-0.413382
H	6.000995	6.817040	-0.856565
H	3.563407	6.306489	-0.777835
C	2.911157	1.938320	-0.223628
C	2.802131	-0.509185	0.054080
C	4.185144	-0.484844	-0.629942
C	5.009242	0.674427	-0.103907
H	5.934471	0.778118	-0.683792
S	2.275657	3.555768	-0.412424
N	4.247132	1.910973	-0.258641
N	2.168285	0.832077	-0.039079
C	4.967166	-1.818865	-0.555431
C	5.828337	-1.985739	0.701013
C	5.842928	-1.976817	-1.799007
H	4.227754	-2.634017	-0.574182
H	6.698339	-1.310223	0.676636
H	5.279883	-1.802655	1.635295
H	6.218929	-3.013036	0.739730
H	6.413111	-2.916077	-1.746631
H	5.231421	-2.000756	-2.710241
H	6.570014	-1.152419	-1.879960
H	3.980825	-0.285032	-1.694629
H	2.173729	-1.173411	-0.554671

C	2.816291	-1.033076	1.474223
C	2.591203	-2.398032	1.683057
C	3.098997	-0.210384	2.567569
C	2.677077	-2.939752	2.963582
H	2.350145	-3.041362	0.831501
C	3.183035	-0.752288	3.850831
H	3.250404	0.863204	2.427903
C	2.979298	-2.117545	4.050416
H	2.501226	-4.006093	3.114198
H	3.404278	-0.102176	4.698904
H	3.043551	-2.539062	5.054867
C	-0.024492	-0.142064	0.582618
H	0.369129	-1.155597	0.600725
C	-1.323454	0.118632	0.985088
C	-1.946854	-0.858300	1.949441
F	-3.275029	-0.778695	2.046536
F	-1.647437	-2.128794	1.668315
F	-1.469052	-0.615491	3.179748
O	0.277206	2.104589	-0.033345
C	0.737440	0.986917	0.145676
H	5.270462	0.554521	0.958396
C	6.224655	3.433591	-0.445109
H	6.966884	2.642720	-0.339276
H	7.676019	5.000868	-0.634020
H	-1.584710	1.153841	1.212723
S	-2.982915	0.327959	-0.731150
C	-3.849892	-1.192892	-0.816130
N	-3.128208	-2.381440	-0.858960
H	-3.670862	-3.191265	-0.567092
C	-1.819184	-2.622446	-1.225852
C	-1.182737	-3.758559	-0.685445
C	-1.114134	-1.809469	-2.136584
C	0.143646	-4.030583	-0.969278
H	-1.737196	-4.402067	-0.000757
C	0.213775	-2.073887	-2.420386
H	-1.607393	-0.961627	-2.603089
C	0.838406	-3.164715	-1.814284
H	0.649006	-4.889448	-0.529318
H	0.770339	-1.444409	-3.113632
N	2.252670	-3.392561	-2.061359
O	2.841359	-2.597903	-2.767010
O	2.784940	-4.346352	-1.532063
N	-5.129999	-1.344432	-0.811818
C	-6.047695	-0.339803	-0.573958
C	-7.124385	-0.194563	-1.471771
C	-6.007053	0.481864	0.573568
C	-8.117574	0.747816	-1.252059
H	-7.159845	-0.842394	-2.348365
C	-7.003369	1.416087	0.808503
H	-5.183565	0.368196	1.276975
C	-8.045257	1.543472	-0.110590
H	-8.946970	0.870535	-1.947087
H	-6.984166	2.049421	1.694370
N	-9.093668	2.532724	0.134020
O	-9.016273	3.208089	1.137078
O	-9.987477	2.627570	-0.678841

CF3_Michael_Acceptor_TS-MA-conf/TS-MA-R-xxi

Frequencies, energies and thermodynamic properties:

Lowest Vibrational Mode (1/cm) =	-127.8148
2nd Lowest Vibrational Mode (1/cm) =	11.9306
E(RM062X) (a.u.) =	-3187.92890664
Thermal correction to Enthalpy (a.u.) =	0.680916

Thermal correction to Gibbs Free Energy (a.u.) = 0.554696

Total Entropy (cal/Kmol) = 265.653

Esp(RM062X) (a.u.) = -3190.89295423

Optimised cartesian coordinates (Angstrom):

C	7.188267	-2.228404	0.076349
C	7.083906	-2.591961	-1.274046
C	5.984598	-2.206699	-2.033766
C	4.992135	-1.454008	-1.408217
C	5.095454	-1.098221	-0.063274
H	7.874651	-3.183708	-1.736488
H	5.898314	-2.485023	-3.084906
C	3.066120	-0.142705	-0.586311
C	1.653003	1.129980	0.979068
C	2.424639	0.368152	2.069421
C	3.887047	0.209596	1.707223
H	4.372191	-0.488705	2.400197
S	3.520335	-0.830469	-2.122617
N	3.985177	-0.359966	0.361815
N	1.921861	0.528642	-0.350669
C	2.210224	0.931759	3.491778
C	3.194558	2.033006	3.893813
C	2.253670	-0.209526	4.508777
H	1.193634	1.358440	3.511237
H	4.208285	1.624565	4.032015
H	3.250179	2.848698	3.159130
H	2.887452	2.468788	4.855666
H	1.470106	-0.955306	4.308763
H	3.225633	-0.727300	4.481299
H	2.108355	0.173744	5.529216
H	2.004262	-0.646808	2.062638
H	0.596265	0.934087	1.195448
C	1.869324	2.629624	0.945582
C	0.957128	3.460263	1.604756
C	2.976812	3.202241	0.310455
C	1.167042	4.836884	1.662501
H	0.073780	3.023114	2.077141
C	3.186369	4.580082	0.365879
H	3.686214	2.577395	-0.239461
C	2.286847	5.399025	1.048661
H	0.448493	5.473838	2.180882
H	4.054513	5.015400	-0.131656
H	2.451166	6.477002	1.089814
C	-0.244950	1.406712	-1.160316
C	-1.022896	1.765596	-2.226497
C	-2.207975	2.651293	-1.944955
F	-3.040642	2.792752	-2.967210
F	-2.917558	2.220190	-0.893468
F	-1.780661	3.886353	-1.629157
O	1.374958	0.438714	-2.562030
C	1.019896	0.778241	-1.449363
H	4.437915	1.162699	1.718497
C	6.200021	-1.476402	0.702142
H	6.292423	-1.195429	1.750797
H	8.061324	-2.539448	0.651171
H	-0.583117	1.872257	-3.217992
S	-2.277714	-0.148786	-3.302267
C	-3.241333	-0.484601	-1.901673
N	-2.621893	-0.913967	-0.719498
N	-4.507963	-0.225202	-1.885457
C	-1.407637	-1.505351	-0.445295
C	-0.542011	-2.071677	-1.406803
C	-1.045170	-1.588311	0.921754
C	0.672058	-2.614830	-1.016615

H	-0.815485	-2.054030	-2.456874
C	0.159746	-2.140317	1.311299
H	-1.731008	-1.199962	1.678268
C	1.032292	-2.618885	0.331102
H	1.350464	-3.035667	-1.757909
H	0.435120	-2.195959	2.364081
N	2.360047	-3.071020	0.715873
O	2.684597	-2.973162	1.884635
O	3.094439	-3.495441	-0.151195
C	-5.351127	-0.547770	-0.843341
C	-5.498962	-1.869807	-0.360817
C	-6.155790	0.467575	-0.280133
C	-6.408513	-2.161881	0.643826
H	-4.899132	-2.668308	-0.800410
C	-7.060089	0.184289	0.730786
H	-6.044559	1.483711	-0.660289
C	-7.176419	-1.130233	1.182793
H	-6.533124	-3.178672	1.013990
H	-7.677716	0.964942	1.172930
N	-8.129493	-1.435488	2.248036
O	-8.794597	-0.526104	2.693879
O	-8.204100	-2.582088	2.633034
H	-0.626369	1.517764	-0.148462
H	-3.188663	-0.760402	0.111393

CF3_Michael_Acceptor_TS-MA-conf/TS-MA-R-xxiv

Frequencies, energies and thermodynamic properties:

Lowest Vibrational Mode (1/cm) = -124.2677

2nd Lowest Vibrational Mode (1/cm) = 14.8989

E(RM062X) (a.u.) = -3187.93316292

Thermal correction to Enthalpy (a.u.) = 0.680557

Thermal correction to Gibbs Free Energy (a.u.) = 0.555180

Total Entropy (cal/Kmol) = 263.879

Esp(RM062X) (a.u.) = -3190.89754500

Optimised cartesian coordinates (Angstrom):

C	-0.967582	5.951171	-1.001928
C	-0.286409	5.694273	-2.199836
C	-0.176298	4.398724	-2.693292
C	-0.746793	3.366074	-1.949098
C	-1.407639	3.623166	-0.746634
H	0.162774	6.519257	-2.753732
H	0.353228	4.191900	-3.624391
C	-1.553568	1.323016	-0.815736
C	-2.583539	-0.077973	0.921728
C	-2.335222	1.136887	1.834292
C	-2.626695	2.429249	1.098790
H	-2.310918	3.291262	1.699410
S	-0.723373	1.651747	-2.313749
N	-1.857358	2.443048	-0.144910
N	-1.872369	0.097986	-0.367065
C	-3.044666	1.049947	3.203911
C	-4.457475	1.639296	3.222394
C	-2.184610	1.725015	4.273144
H	-3.114384	-0.020263	3.457620
H	-4.427123	2.735394	3.116685
H	-5.102434	1.236628	2.428667
H	-4.936914	1.419952	4.187533
H	-1.200580	1.241345	4.362257
H	-2.021316	2.788165	4.033185
H	-2.677067	1.678353	5.255323
H	-1.253345	1.130415	2.027664
H	-2.091004	-0.922879	1.418766
C	-4.044565	-0.420422	0.706127

C	-4.644159	-1.378638	1.530958
C	-4.823777	0.232951	-0.254178
C	-6.006469	-1.652294	1.425507
H	-4.034822	-1.915728	2.262437
C	-6.187444	-0.041731	-0.362143
H	-4.372141	0.960079	-0.933459
C	-6.783464	-0.977820	0.482810
H	-6.461127	-2.400805	2.076523
H	-6.784842	0.475791	-1.114587
H	-7.849947	-1.192415	0.396757
C	-1.851884	-2.344831	-0.645110
C	-1.333873	-3.469011	-1.263515
C	-2.096299	-4.753115	-1.075716
F	-1.430292	-5.833401	-1.489538
F	-2.441670	-4.960774	0.197176
F	-3.233697	-4.717350	-1.784883
O	-0.837639	-0.852914	-2.166524
C	-1.468590	-1.065208	-1.140227
H	-3.693570	2.544683	0.853706
C	-1.540813	4.924546	-0.259637
H	-2.064954	5.134778	0.672065
H	-1.045486	6.975996	-0.636928
H	-0.898315	-3.364632	-2.259406
S	0.668379	-4.274748	-0.335850
C	1.530910	-2.781620	-0.118357
N	2.861545	-2.860450	-0.523686
N	0.984756	-1.718761	0.380946
C	3.970373	-2.209607	-0.003148
C	3.962720	-1.566094	1.249567
C	5.158623	-2.230319	-0.758576
C	5.108670	-0.943296	1.719451
H	3.063642	-1.570449	1.863401
C	6.306123	-1.612218	-0.289884
H	5.165588	-2.734369	-1.726531
C	6.265255	-0.965605	0.943538
H	5.116077	-0.446498	2.688504
H	7.226859	-1.617872	-0.871303
N	7.469856	-0.301195	1.440206
O	8.471346	-0.362493	0.761976
O	7.402461	0.274703	2.503437
C	1.430579	-0.430368	0.169929
C	2.056448	0.007359	-1.021270
C	1.146453	0.533450	1.162143
C	2.349228	1.346540	-1.218297
H	2.280775	-0.711657	-1.808547
C	1.407344	1.880263	0.961440
H	0.692745	0.187765	2.092518
C	1.999470	2.275455	-0.238002
H	2.807308	1.689850	-2.145327
H	1.155917	2.626400	1.715364
N	2.203187	3.698061	-0.498808
O	1.752331	4.492300	0.298097
O	2.806976	4.012201	-1.501845
H	-2.445666	-2.467709	0.254957
H	3.058588	-3.615489	-1.175123

CF3_Michael_Acceptor_TS-MA-conf/TS-MA-R-xx

Frequencies, energies and thermodynamic properties:

Lowest Vibrational Mode (1/cm) = -146.6720

2nd Lowest Vibrational Mode (1/cm) = 12.1869

E(RM062X) (a.u.) = -3187.93246125

Thermal correction to Enthalpy (a.u.) = 0.680836

Thermal correction to Gibbs Free Energy (a.u.) = 0.555957

Total Entropy (cal/Kmol) = 262.830

Esp(RM062X) (a.u.) = -3190.89586022

Optimised cartesian coordinates (Angstrom):

C	-5.182923	3.260798	-1.936029
C	-4.131548	4.151854	-2.192222
C	-2.807252	3.753084	-2.046020
C	-2.564301	2.451035	-1.609213
C	-3.613358	1.572666	-1.333502
H	-4.352260	5.169881	-2.514780
H	-1.983994	4.439314	-2.249282
C	-1.810303	0.241988	-0.793527
C	-1.966055	-1.985576	0.244998
C	-3.374300	-1.522311	0.656384
C	-4.033487	-0.752213	-0.471015
H	-4.974192	-0.302817	-0.130310
S	-1.008080	1.687982	-1.350153
N	-3.142483	0.337002	-0.872143
N	-1.188205	-0.842016	-0.292715
C	-4.263885	-2.655113	1.217127
C	-5.089265	-3.392402	0.159662
C	-5.184351	-2.096510	2.302768
H	-3.588024	-3.383393	1.694316
H	-5.590840	-4.256061	0.619835
H	-5.876603	-2.740016	-0.250398
H	-4.481955	-3.764726	-0.677338
H	-5.839700	-1.309229	1.896532
H	-5.830096	-2.887962	2.709956
H	-4.608700	-1.664285	3.134296
H	-3.216424	-0.801702	1.473535
H	-1.473347	-2.273717	1.181148
C	-1.931395	-3.161581	-0.709620
C	-2.097202	-2.992826	-2.088489
C	-1.784214	-4.453241	-0.193047
C	-2.150497	-4.102296	-2.932314
H	-2.180730	-1.991586	-2.519157
C	-1.839731	-5.562161	-1.035543
H	-1.623861	-4.590146	0.879453
C	-2.030697	-5.388916	-2.406876
H	-2.281629	-3.959031	-4.006124
H	-1.724881	-6.564750	-0.620408
H	-2.071045	-6.256040	-3.068151
C	0.900065	-1.987651	0.352102
H	0.339290	-2.779884	0.838230
C	2.278435	-2.022902	0.401701
C	2.922106	-3.363075	0.634363
F	2.810078	-4.115848	-0.471607
F	4.222945	-3.291514	0.908536
F	2.337448	-4.045150	1.622213
O	0.830850	0.052487	-0.836451
C	0.256439	-0.877486	-0.282471
H	-4.242151	-1.381340	-1.349203
C	-4.943164	1.960015	-1.506770
H	-5.769009	1.276412	-1.312184
H	-6.213183	3.593284	-2.068222
H	2.860808	-1.350799	-0.234375
S	3.142280	-1.005839	2.438695
C	2.167411	0.365804	2.009282
N	0.958749	0.455561	2.476409
C	0.052352	1.460618	2.197736
C	0.348152	2.821511	1.939427
C	-1.310566	1.080754	2.236356
C	-0.663511	3.721140	1.628130
H	1.377312	3.176907	1.978584

C	-2.324939	1.966775	1.921126
H	-1.529888	0.046807	2.508616
C	-1.983362	3.278457	1.587672
H	-0.436551	4.762381	1.401725
H	-3.372326	1.662593	1.920837
N	-3.036409	4.198384	1.161109
O	-4.175590	3.786230	1.144290
O	-2.714854	5.320609	0.837484
N	2.622363	1.229435	1.017990
C	3.847855	1.273948	0.365947
C	5.077693	1.114504	1.032537
C	3.844365	1.559175	-1.013406
C	6.268282	1.219838	0.330385
H	5.092466	0.915400	2.101184
C	5.033346	1.671444	-1.717576
H	2.889110	1.670674	-1.528941
C	6.234450	1.492988	-1.036216
H	7.226126	1.104391	0.835439
H	5.039158	1.882508	-2.785785
N	7.493591	1.602636	-1.773085
O	8.525126	1.425395	-1.163906
O	7.438611	1.865667	-2.954305
H	1.865421	1.632294	0.469054

CF3_Michael_Acceptor_TS-MA-conf/TS-MA-R-xxvii

Frequencies, energies and thermodynamic properties:

Lowest Vibrational Mode (1/cm) = -57.6559

2nd Lowest Vibrational Mode (1/cm) = 16.9159

E(RM062X) (a.u.) = -3187.92165898

Thermal correction to Enthalpy (a.u.) = 0.681381

Thermal correction to Gibbs Free Energy (a.u.) = 0.554798

Total Entropy (cal/Kmol) = 266.416

Esp(RM062X) (a.u.) = -3190.89108182

Optimised cartesian coordinates (Angstrom):

C	-0.977195	6.464947	-1.031389
C	-0.648447	6.290565	-2.384377
C	-0.568486	5.020058	-2.942247
C	-0.822262	3.928776	-2.110770
C	-1.139513	4.103517	-0.763387
H	-0.454648	7.163171	-3.008990
H	-0.317826	4.878428	-3.994281
C	-1.225078	1.810519	-0.905043
C	-1.890802	0.325414	0.942799
C	-1.321119	1.437543	1.837296
C	-1.709602	2.800300	1.302132
H	-1.160948	3.590542	1.829380
S	-0.814549	2.233144	-2.545381
N	-1.348629	2.879643	-0.116818
N	-1.442928	0.550251	-0.459838
C	-1.659764	1.263921	3.336031
C	-2.990070	1.892684	3.761502
C	-0.526306	1.825855	4.195611
H	-1.715889	0.178280	3.521602
H	-2.925485	2.992447	3.752316
H	-3.835356	1.593475	3.126173
H	-3.223570	1.591814	4.792909
H	0.425228	1.301662	4.024797
H	-0.367238	2.895811	3.984863
H	-0.773447	1.733553	5.263207
H	-0.227042	1.352393	1.735428
H	-1.398141	-0.594853	1.277259
C	-3.391729	0.133978	1.010154
C	-3.909341	-0.863244	1.843471

C	-4.272894	0.954110	0.297001
C	-5.286490	-1.018994	1.988329
H	-3.225123	-1.523021	2.383233
C	-5.651456	0.797268	0.440986
H	-3.897561	1.722267	-0.384376
C	-6.160567	-0.183862	1.291727
H	-5.677614	-1.800413	2.641696
H	-6.329902	1.442714	-0.119072
H	-7.239266	-0.306577	1.401333
C	-1.799180	-1.850911	-0.901111
C	-2.005218	-2.834957	-1.802479
C	-2.728499	-4.078195	-1.361355
F	-2.655299	-5.071605	-2.239557
F	-2.311014	-4.525871	-0.179324
F	-4.036784	-3.794700	-1.220945
O	-1.043162	-0.310538	-2.528331
C	-1.389783	-0.536551	-1.384486
H	-2.788515	2.998484	1.391924
C	-1.228489	5.379098	-0.200984
H	-1.488865	5.524511	0.846680
H	-1.039072	7.472685	-0.619193
H	-1.957212	-2.657913	-2.877232
S	0.279716	-4.363088	-2.248141
C	1.184362	-3.278991	-1.258496
N	1.441797	-2.039568	-1.860890
N	1.567540	-3.578620	-0.052191
C	2.519890	-1.185874	-1.714133
C	3.745147	-1.579782	-1.140248
C	2.380357	0.132740	-2.191865
C	4.778823	-0.665794	-1.007671
H	3.889094	-2.607626	-0.811260
C	3.410940	1.048096	-2.063332
H	1.438453	0.425051	-2.658727
C	4.598902	0.641274	-1.457661
H	5.729543	-0.959646	-0.564819
H	3.303416	2.071785	-2.419467
N	5.686446	1.605200	-1.305698
O	5.506339	2.732231	-1.713349
O	6.710249	1.229065	-0.779483
C	1.982671	-2.717678	0.927189
C	1.479467	-1.403340	1.117044
C	2.946870	-3.187946	1.852791
C	1.947897	-0.600321	2.141919
H	0.734872	-1.013888	0.422650
C	3.417654	-2.391398	2.881658
H	3.321391	-4.204201	1.724108
C	2.914753	-1.096263	3.017315
H	1.589099	0.420480	2.268702
H	4.168368	-2.756562	3.581468
N	3.405992	-0.243353	4.089335
O	4.255218	-0.687834	4.830319
O	2.940950	0.875021	4.190167
H	-1.960900	-2.053009	0.154719
H	0.828416	-1.840938	-2.647650

CF3_Michael_Acceptor_TS-MA-conf/TS-MA-R-xxvi

Frequencies, energies and thermodynamic properties:

Lowest Vibrational Mode (1/cm) = -80.0818

2nd Lowest Vibrational Mode (1/cm) = 13.6227

E(RM062X) (a.u.) = -3187.93068206

Thermal correction to Enthalpy (a.u.) = 0.680787

Thermal correction to Gibbs Free Energy (a.u.) = 0.554840

Total Entropy (cal/Kmol) = 265.080

Esp(RM062X) (a.u.) = -3190.89540926

Optimised cartesian coordinates (Angstrom):

C	-1.993114	5.787293	-1.727463
C	-1.184397	5.559564	-2.850324
C	-0.732611	4.280762	-3.156909
C	-1.105361	3.238550	-2.308654
C	-1.904016	3.469299	-1.188363
H	-0.905360	6.395356	-3.492852
H	-0.104892	4.096573	-4.029872
C	-1.535369	1.206344	-0.970961
C	-2.465046	-0.210923	0.811882
C	-2.627284	1.102350	1.592669
C	-3.038293	2.241525	0.684851
H	-2.955882	3.194278	1.222337
S	-0.686711	1.543479	-2.456143
N	-2.126854	2.293498	-0.461303
N	-1.599619	-0.002465	-0.377971
C	-3.524554	0.973305	2.844215
C	-5.013528	1.218903	2.588365
C	-3.017747	1.915871	3.936866
H	-3.407583	-0.060006	3.211453
H	-5.203988	2.278639	2.355924
H	-5.415319	0.609387	1.766649
H	-5.587327	0.978461	3.495183
H	-1.983668	1.677653	4.225876
H	-3.036810	2.962730	3.594883
H	-3.649301	1.844627	4.834327
H	-1.620207	1.354468	1.949288
H	-1.907230	-0.870052	1.486651
C	-3.755303	-0.898117	0.413243
C	-4.245736	-1.938667	1.208044
C	-4.488580	-0.490843	-0.706733
C	-5.466292	-2.542159	0.909812
H	-3.664273	-2.279378	2.068426
C	-5.709231	-1.095226	-1.006589
H	-4.113658	0.298590	-1.363819
C	-6.203834	-2.116732	-0.195353
H	-5.837959	-3.353417	1.537838
H	-6.273142	-0.769427	-1.882069
H	-7.157582	-2.590774	-0.432749
C	-1.049228	-2.410847	-0.347709
C	-0.714487	-3.539036	-1.040704
C	-1.131014	-4.852921	-0.440118
F	-0.640641	-5.911181	-1.078583
F	-0.790386	-4.952956	0.848840
F	-2.469266	-4.969045	-0.486000
O	-0.471959	-0.962364	-2.114107
C	-0.988661	-1.136987	-1.027523
H	-4.064015	2.135211	0.299249
C	-2.366533	4.749633	-0.880932
H	-2.994245	4.939806	-0.011457
H	-2.336034	6.799120	-1.508510
H	-0.615035	-3.517886	-2.125949
S	1.763866	-4.244955	-1.083948
C	2.529306	-2.787356	-0.571687
N	3.601614	-2.325395	-1.130865
N	1.902326	-2.152222	0.513345
C	4.480386	-1.441399	-0.549726
C	4.838486	-1.483017	0.819905
C	5.119689	-0.489023	-1.376241
C	5.767897	-0.597450	1.338888
H	4.377654	-2.224697	1.472773
C	6.041730	0.407022	-0.862172

H	4.863804	-0.473480	-2.436639
C	6.354723	0.347388	0.495870
H	6.047565	-0.627535	2.391218
H	6.525461	1.148210	-1.496954
N	7.325580	1.287103	1.045949
O	7.823704	2.097597	0.294332
O	7.585438	1.212211	2.227958
C	1.684878	-0.804476	0.698710
C	1.962891	0.163122	-0.289062
C	1.103330	-0.391052	1.918928
C	1.616195	1.488243	-0.081472
H	2.391897	-0.132990	-1.243593
C	0.744958	0.928967	2.119425
H	0.929381	-1.131332	2.702135
C	0.976142	1.856330	1.100046
H	1.797407	2.235592	-0.853018
H	0.286999	1.249933	3.054517
N	0.442159	3.205440	1.220662
O	-0.318838	3.434815	2.142272
O	0.747584	4.021571	0.379333
H	-1.344804	-2.496496	0.695499
H	1.320080	-2.770688	1.071243

CF3_Michael_Acceptor_TS-MA-conf/TS-MA-R-xxv

Frequencies, energies and thermodynamic properties:

Lowest Vibrational Mode (1/cm) = -94.6578

2nd Lowest Vibrational Mode (1/cm) = 4.3796

E(RM062X) (a.u.) = -3187.91930276

Thermal correction to Enthalpy (a.u.) = 0.680468

Thermal correction to Gibbs Free Energy (a.u.) = 0.547318

Total Entropy (cal/Kmol) = 280.238

Esp(RM062X) (a.u.) = -3190.88995171

Optimised cartesian coordinates (Angstrom):

C	7.166796	4.718867	0.899953
C	6.095270	5.458703	1.421657
C	4.808958	4.931006	1.448533
C	4.620895	3.645613	0.939924
C	5.687289	2.915353	0.414140
H	6.271388	6.460736	1.814252
H	3.972757	5.501478	1.855050
C	3.979110	1.401003	0.132182
C	4.258368	-0.859061	-0.790220
C	5.416042	-0.216898	-1.573925
C	6.203636	0.711764	-0.670491
H	6.929445	1.293845	-1.252342
S	3.122802	2.739199	0.851930
N	5.278202	1.658671	-0.044606
N	3.425798	0.215283	-0.192204
C	6.314564	-1.236135	-2.311536
C	7.490487	-1.760748	-1.482881
C	6.830318	-0.620423	-3.612970
H	5.671231	-2.091186	-2.576577
H	7.982831	-2.582944	-2.022027
H	8.246787	-0.974285	-1.331563
H	7.189218	-2.140478	-0.496577
H	6.003190	-0.347829	-4.284291
H	7.418342	0.289354	-3.409778
H	7.483724	-1.327332	-4.144441
H	4.931839	0.410547	-2.340214
H	3.626256	-1.351624	-1.538514
C	4.676557	-1.881096	0.246859
C	4.688223	-3.235028	-0.106029
C	5.096652	-1.506219	1.527359

C	5.145289	-4.196622	0.792954
H	4.335396	-3.536909	-1.095579
C	5.553484	-2.468962	2.427940
H	5.065130	-0.459953	1.842101
C	5.586371	-3.813935	2.060294
H	5.149980	-5.249115	0.505231
H	5.879488	-2.165042	3.423946
H	5.942301	-4.565478	2.766797
C	1.502680	-1.336437	-0.131506
C	0.164883	-1.512312	0.016448
C	-0.369867	-2.917004	0.077815
F	-1.698246	-2.986745	0.058115
F	0.097238	-3.689245	-0.906500
F	0.018281	-3.494467	1.228454
O	1.373381	0.946340	0.458142
C	2.028364	0.000252	0.071973
H	6.740606	0.170956	0.123305
C	6.981632	3.438893	0.389232
H	7.819772	2.868066	-0.009199
H	8.167623	5.152123	0.894776
H	-0.489279	-0.733309	0.414322
S	-1.211758	-0.910384	-2.185604
C	-2.648608	-0.495115	-1.327117
N	-2.642991	-0.122894	-0.080424
N	-3.822413	-0.609094	-2.078526
C	-3.695525	-0.247581	0.789489
C	-4.587946	-1.348847	0.775962
C	-3.858161	0.727276	1.801780
C	-5.609361	-1.448069	1.704877
H	-4.465304	-2.126622	0.021538
C	-4.882604	0.638746	2.728169
H	-3.157247	1.562929	1.829161
C	-5.755630	-0.448545	2.668629
H	-6.297796	-2.292228	1.696017
H	-5.016580	1.396851	3.498720
N	-6.835422	-0.549598	3.642000
O	-6.942432	0.330827	4.469463
O	-7.574913	-1.508874	3.578092
C	-4.998809	0.114515	-1.983650
C	-5.095557	1.334625	-1.284878
C	-6.135007	-0.383010	-2.653183
C	-6.301146	2.016786	-1.235723
H	-4.218846	1.755087	-0.795828
C	-7.338854	0.299503	-2.611061
H	-6.059033	-1.323571	-3.201240
C	-7.412200	1.491357	-1.892103
H	-6.385537	2.961095	-0.699783
H	-8.221913	-0.084310	-3.119794
N	-8.681449	2.213328	-1.836316
O	-9.628400	1.743057	-2.428015
O	-8.721103	3.245225	-1.203049
H	2.137194	-2.168252	-0.426272
H	-3.729021	-1.195294	-2.902944

CF3_Michael_Acceptor_TS-MA-conf/TS-MA-S-iii

Frequencies, energies and thermodynamic properties:

Lowest Vibrational Mode (1/cm) = -140.1437

2nd Lowest Vibrational Mode (1/cm) = 15.4918

E(RM062X) (a.u.) = -3187.94160125

Thermal correction to Enthalpy (a.u.) = 0.680667

Thermal correction to Gibbs Free Energy (a.u.) = 0.556302

Total Entropy (cal/Kmol) = 261.750

Esp(RM062X) (a.u.) = -3190.90181159

Optimised cartesian coordinates (Angstrom):

C	5.930896	2.657108	-0.954982
C	6.437236	1.361950	-1.132636
C	5.740951	0.251190	-0.665410
C	4.523782	0.469464	-0.019704
C	4.021655	1.761202	0.153599
H	7.387262	1.218843	-1.648559
H	6.130756	-0.759097	-0.806972
C	2.316143	0.528069	1.079422
C	0.209260	1.474044	1.892523
C	1.094406	2.670171	2.295649
C	2.088783	2.982181	1.190436
H	2.848510	3.690376	1.547487
S	3.442470	-0.732256	0.661283
N	2.785046	1.752208	0.807655
N	1.088020	0.323531	1.583092
C	0.295992	3.915187	2.748354
C	-0.050068	4.894158	1.622859
C	1.058544	4.645582	3.854511
H	-0.648159	3.544111	3.180000
H	-0.736600	5.664172	2.003667
H	0.852071	5.413420	1.262213
H	-0.534157	4.410365	0.762583
H	0.507231	5.538997	4.181837
H	1.213876	3.999405	4.730628
H	2.046555	4.976317	3.495804
H	1.674368	2.316925	3.164046
H	-0.355176	1.187737	2.788692
C	-0.763151	1.785484	0.775584
C	-2.073388	2.152850	1.098077
C	-0.350025	1.835254	-0.560225
C	-2.939571	2.623202	0.110223
H	-2.411774	2.088989	2.135493
C	-1.212559	2.309451	-1.546948
H	0.657199	1.516426	-0.840069
C	-2.502412	2.723592	-1.210450
H	-3.956570	2.918680	0.374998
H	-0.876458	2.356002	-2.584731
H	-3.173466	3.101137	-1.984293
C	-0.717905	-1.238072	2.196102
H	-1.480047	-0.472621	2.058877
C	-1.055219	-2.534027	2.522019
C	-2.375425	-2.793427	3.190739
F	-2.374732	-2.270756	4.426804
F	-3.405426	-2.225854	2.545559
F	-2.649959	-4.086843	3.328465
O	1.496971	-1.908091	1.766511
C	0.657321	-1.026582	1.849650
H	1.607225	3.407666	0.297882
C	4.717365	2.878586	-0.310477
H	4.322455	3.886826	-0.185615
H	6.493924	3.510931	-1.333849
H	-0.262329	-3.215532	2.832571
S	-1.357726	-3.901050	0.562518
C	-1.645308	-2.502096	-0.448774
N	-0.838843	-1.797450	-1.172592
N	-2.954874	-2.057904	-0.352361
C	0.488930	-2.000666	-1.487188
C	1.308450	-3.102663	-1.143331
C	1.066403	-0.971349	-2.274547
C	2.637413	-3.145030	-1.541115
H	0.899415	-3.914167	-0.548465
C	2.388695	-1.008221	-2.680565

H 0.424885 -0.137077 -2.560787
C 3.166575 -2.099256 -2.294528
H 3.276681 -3.979444 -1.254290
H 2.827073 -0.206914 -3.274490
N 4.588830 -2.096127 -2.614273
O 4.993716 -1.287319 -3.420183
O 5.304180 -2.887047 -2.032250
C -3.621729 -1.054862 -1.032429
C -3.223756 -0.547169 -2.285425
C -4.808671 -0.569271 -0.440569
C -3.989226 0.423861 -2.913388
H -2.319374 -0.919532 -2.756455
C -5.574436 0.396410 -1.068692
H -5.114136 -0.963088 0.531001
C -5.147852 0.892320 -2.300060
H -3.689959 0.826848 -3.880467
H -6.485505 0.780634 -0.612015
N -5.913354 1.956358 -2.940853
O -7.001536 2.229558 -2.484081
O -5.416557 2.519400 -3.893964
H -3.497197 -2.531435 0.362233

CF3_Michael_Acceptor_TS-MA-conf/TS-MA-S-ii

Frequencies, energies and thermodynamic properties:

Lowest Vibrational Mode (1/cm) = -120.4338

2nd Lowest Vibrational Mode (1/cm) = 11.9005

E(RM062X) (a.u.) = -3187.93569739

Thermal correction to Enthalpy (a.u.) = 0.681112

Thermal correction to Gibbs Free Energy (a.u.) = 0.553134

Total Entropy (cal/Kmol) = 269.353

Esp(RM062X) (a.u.) = -3190.89979260

Optimised cartesian coordinates (Angstrom):

C -7.017676 3.237141 -0.727025
C -6.083932 4.283081 -0.771775
C -4.735574 4.050131 -0.522079
C -4.346818 2.743271 -0.225616
C -5.279892 1.706988 -0.164397
H -6.417528 5.294296 -1.007470
H -3.993745 4.849389 -0.550749
C -3.355843 0.554439 0.341738
C -3.236792 -1.869940 0.718371
C -4.680336 -1.699765 1.224405
C -5.444595 -0.751687 0.319742
H -6.413954 -0.493624 0.765175
S -2.728998 2.166281 0.124699
N -4.680167 0.487999 0.172273
N -2.605052 -0.533434 0.603860
C -5.422563 -3.037315 1.449208
C -6.179057 -3.557076 0.223450
C -6.381197 -2.905631 2.633313
H -4.655413 -3.781153 1.719683
H -6.548597 -4.573361 0.423067
H -7.058087 -2.929302 0.007320
H -5.557438 -3.599087 -0.681894
H -6.921417 -3.848502 2.801823
H -5.845013 -2.648478 3.558323
H -7.131220 -2.120592 2.444548
H -4.585537 -1.205638 2.205144
H -2.696429 -2.391011 1.517854
C -3.101057 -2.665939 -0.563791
C -2.831191 -4.036733 -0.483320
C -3.288548 -2.079921 -1.819878
C -2.783564 -4.817155 -1.636771

H	-2.657136	-4.494221	0.494208
C	-3.239796	-2.861006	-2.974887
H	-3.467297	-1.005753	-1.913908
C	-2.995681	-4.231248	-2.885371
H	-2.572725	-5.885082	-1.560847
H	-3.387618	-2.393278	-3.949575
H	-2.956214	-4.839983	-3.790114
C	-0.379899	-1.582946	0.834677
H	-0.800093	-2.576416	0.698384
C	0.970968	-1.415224	0.919144
C	1.821399	-2.606538	1.264550
F	1.627071	-2.938742	2.553130
F	1.512199	-3.685689	0.545258
F	3.127785	-2.383868	1.132487
O	-0.727456	0.744855	0.749875
C	-1.179717	-0.382747	0.740369
H	-5.618350	-1.176497	-0.680299
C	-6.632958	1.935697	-0.422519
H	-7.362720	1.127191	-0.392244
H	-8.068330	3.444618	-0.933657
H	1.395444	-0.440781	1.172081
S	1.983383	-1.063024	-1.396354
C	3.360559	-0.150190	-0.823182
N	3.364274	1.006950	-0.244736
N	4.561481	-0.833419	-0.948000
H	4.443969	-1.776741	-1.303491
C	2.296077	1.870767	-0.173516
C	1.449251	2.165509	-1.266631
C	2.100041	2.574311	1.036481
C	0.435638	3.099535	-1.143135
H	1.600630	1.646846	-2.211801
C	1.086256	3.505817	1.170362
H	2.767271	2.359050	1.872322
C	0.259461	3.759039	0.075080
H	-0.222601	3.327576	-1.980724
H	0.924643	4.037325	2.107308
N	-0.829405	4.708719	0.217067
O	-0.914008	5.349045	1.240365
O	-1.628713	4.804207	-0.701167
C	5.856039	-0.481824	-0.621875
C	6.256132	0.789032	-0.157457
C	6.839368	-1.485417	-0.788215
C	7.592930	1.034660	0.126015
H	5.514675	1.569181	-0.021922
C	8.169116	-1.239891	-0.505349
H	6.533038	-2.470646	-1.144827
C	8.536068	0.026278	-0.047359
H	7.911226	2.013519	0.482392
H	8.924409	-2.014078	-0.632072
N	9.938673	0.297035	0.254254
O	10.738695	-0.597892	0.086372
O	10.232004	1.401765	0.656430

CF3_Michael_Acceptor_TS-MA-conf/TS-MA-S-i

Frequencies, energies and thermodynamic properties:

Lowest Vibrational Mode (1/cm) = -133.2872

2nd Lowest Vibrational Mode (1/cm) = 19.7386

E(RM062X) (a.u.) = -3187.94750675

Thermal correction to Enthalpy (a.u.) = 0.680593

Thermal correction to Gibbs Free Energy (a.u.) = 0.557801

Total Entropy (cal/Kmol) = 258.438

Esp(RM062X) (a.u.) = -3190.90928200

Optimised cartesian coordinates (Angstrom):

C	6.602875	0.840039	-0.451944
C	6.748102	-0.468436	0.029498
C	5.696515	-1.114920	0.671372
C	4.490800	-0.426113	0.800889
C	4.354067	0.880704	0.329827
H	7.694900	-0.991964	-0.106558
H	5.803413	-2.135871	1.041456
C	2.222061	0.498806	1.105459
C	0.388565	2.120461	0.975261
C	1.524990	3.141148	1.187851
C	2.708756	2.777673	0.308486
H	3.584389	3.388668	0.565647
S	3.000891	-1.002060	1.524151
N	3.066715	1.379811	0.556614
N	0.914245	0.764109	1.270226
C	1.091347	4.616840	1.021692
C	1.262249	5.173617	-0.394759
C	1.854092	5.492835	2.016306
H	0.021904	4.666059	1.283123
H	0.801406	6.170138	-0.456463
H	2.328601	5.293264	-0.643754
H	0.798574	4.543126	-1.166510
H	1.563536	6.547805	1.907017
H	1.655695	5.189339	3.054467
H	2.940375	5.426324	1.843143
H	1.843874	3.006500	2.234469
H	-0.369733	2.317740	1.743886
C	-0.256736	2.232169	-0.388371
C	-1.392789	3.036930	-0.533202
C	0.313134	1.646371	-1.523342
C	-1.922978	3.290353	-1.797715
H	-1.858218	3.476020	0.352693
C	-0.227035	1.885417	-2.787974
H	1.185626	0.995926	-1.426720
C	-1.337901	2.718435	-2.928843
H	-2.801648	3.929809	-1.898740
H	0.223575	1.418863	-3.665802
H	-1.756483	2.908921	-3.918396
C	-1.356685	-0.050597	1.781327
H	-1.801748	0.684825	1.111894
C	-2.141588	-0.914120	2.521826
C	-3.576111	-0.530052	2.756669
F	-3.631701	0.533985	3.578478
F	-4.209354	-0.177453	1.638019
F	-4.286496	-1.491123	3.345930
O	0.608850	-1.219648	2.351265
C	0.060544	-0.253458	1.845478
H	2.493561	2.908837	-0.761947
C	5.407840	1.537206	-0.306123
H	5.295731	2.550668	-0.691020
H	7.439715	1.321972	-0.958758
H	-1.683118	-1.453268	3.351376
S	-2.590511	-3.047323	1.494740
C	-1.562590	-2.661532	0.131031
N	-1.825583	-1.838590	-0.823519
N	-0.311247	-3.256281	0.188421
H	-0.211964	-3.901275	0.965739
C	-3.074879	-1.293128	-1.054507
C	-4.261331	-2.056901	-1.083936
C	-3.149317	0.077610	-1.365476
C	-5.478166	-1.459688	-1.373191
H	-4.216863	-3.124038	-0.872726
C	-4.362145	0.687605	-1.643396

H	-2.224523	0.652422	-1.370407
C	-5.517827	-0.090832	-1.638377
H	-6.399323	-2.040379	-1.394588
H	-4.422936	1.751825	-1.867985
N	-6.802790	0.541432	-1.930226
O	-6.811969	1.730891	-2.164183
O	-7.794769	-0.154242	-1.923745
C	0.857061	-2.970481	-0.487754
C	1.032085	-1.866796	-1.349762
C	1.958602	-3.822266	-0.241583
C	2.286249	-1.595490	-1.881543
H	0.186014	-1.224799	-1.576093
C	3.200758	-3.564668	-0.791422
H	1.821998	-4.687409	0.410079
C	3.359139	-2.434601	-1.594655
H	2.442238	-0.726586	-2.521901
H	4.050919	-4.215927	-0.591978
N	4.684532	-2.098291	-2.104319
O	5.578197	-2.899787	-1.936305
O	4.827289	-1.028746	-2.655743

CF3_Michael_Acceptor_TS-MA-conf/TS-MA-S-iv

Frequencies, energies and thermodynamic properties:

Lowest Vibrational Mode (1/cm) = -114.6001

2nd Lowest Vibrational Mode (1/cm) = 8.0403

E(RM062X) (a.u.) = -3187.92742926

Thermal correction to Enthalpy (a.u.) = 0.681189

Thermal correction to Gibbs Free Energy (a.u.) = 0.551827

Total Entropy (cal/Kmol) = 272.267

Esp(RM062X) (a.u.) = -3190.89499663

Optimised cartesian coordinates (Angstrom):

C	7.898594	-3.743939	-0.764131
C	7.338657	-4.827986	-0.073134
C	6.128901	-4.695925	0.600386
C	5.498140	-3.452355	0.572366
C	6.062162	-2.372429	-0.108039
H	7.854476	-5.788743	-0.066357
H	5.684372	-5.537524	1.133275
C	4.138929	-1.390421	0.692561
C	3.473493	0.931890	0.266640
C	4.982372	1.182058	0.120280
C	5.638372	0.044203	-0.636326
H	6.730627	0.134873	-0.589166
S	3.960289	-3.018984	1.296442
N	5.269224	-1.224095	-0.004496
N	3.248901	-0.400795	0.878549
C	5.324185	2.569744	-0.469102
C	5.399002	2.606724	-1.997772
C	6.636348	3.078915	0.128257
H	4.521952	3.254728	-0.148510
H	5.501851	3.647924	-2.336089
H	6.282062	2.058106	-2.362299
H	4.508008	2.183733	-2.482675
H	6.893472	4.065005	-0.284830
H	6.571204	3.172916	1.221975
H	7.466223	2.392836	-0.106512
H	5.378949	1.154328	1.148624
H	3.129692	1.669420	0.999978
C	2.650199	1.077574	-0.998161
C	1.977340	2.279514	-1.240787
C	2.556579	0.042780	-1.935685
C	1.244298	2.455767	-2.412825
H	2.020673	3.081825	-0.499713

C 1.818759 0.216990 -3.106343
H 3.044140 -0.919417 -1.758150
C 1.164655 1.424613 -3.349494
H 0.725385 3.399129 -2.589963
H 1.748468 -0.599002 -3.827348
H 0.584219 1.558296 -4.263850
C 1.042401 0.377064 1.642505
H 1.269595 1.393824 1.339564
C -0.257738 0.059907 1.960005
C -1.162601 1.151974 2.456005
F -0.834122 1.461466 3.722756
F -1.059629 2.277576 1.750672
F -2.444636 0.790385 2.480769
O 1.799726 -1.845127 1.884427
C 1.983702 -0.697338 1.516404
H 5.331511 0.008333 -1.692615
C 7.271202 -2.502943 -0.795126
H 7.710780 -1.670769 -1.344049
H 8.844133 -3.872958 -1.292130
H -0.495495 -0.929688 2.353423
S -1.276895 -0.328320 -0.174369
C -3.042551 -0.432778 -0.198823
N -3.888698 0.533089 -0.115455
N -3.502715 -1.737515 -0.282828
C -3.552436 1.872016 -0.116620
C -2.703160 2.456166 -1.080459
C -4.149852 2.705635 0.851240
C -2.438360 3.816454 -1.055768
H -2.250437 1.826172 -1.845063
C -3.880250 4.063879 0.891794
H -4.816722 2.251805 1.585032
C -3.020864 4.604575 -0.063571
H -1.786000 4.278484 -1.795423
H -4.324832 4.708782 1.648414
N -2.729145 6.035756 -0.029631
O -3.267129 6.706949 0.824047
O -1.962178 6.481365 -0.856147
C -4.781473 -2.252470 -0.383945
C -5.958122 -1.477836 -0.450752
C -4.889777 -3.662094 -0.430130
C -7.193609 -2.102414 -0.561027
H -5.891699 -0.395687 -0.412979
C -6.119613 -4.282060 -0.539913
H -3.981119 -4.264893 -0.377782
C -7.267253 -3.490958 -0.604728
H -8.107879 -1.512771 -0.614506
H -6.202748 -5.367227 -0.575653
N -8.572481 -4.136273 -0.721640
O -8.605015 -5.346928 -0.766191
O -9.555000 -3.429115 -0.768321
H -2.756293 -2.425117 -0.274281

CF3_Michael_Acceptor_TS-MA-conf/TS-MA-S-ix

Frequencies, energies and thermodynamic properties:

Lowest Vibrational Mode (1/cm) = -117.2044

2nd Lowest Vibrational Mode (1/cm) = 10.6628

E(RM062X) (a.u.) = -3187.92969015

Thermal correction to Enthalpy (a.u.) = 0.681013

Thermal correction to Gibbs Free Energy (a.u.) = 0.554315

Total Entropy (cal/Kmol) = 266.660

Esp(RM062X) (a.u.) = -3190.89371566

Optimised cartesian coordinates (Angstrom):

C 3.244744 5.058515 -0.817826

C	1.919962	5.456379	-0.590296
C	0.882580	4.529195	-0.603866
C	1.206791	3.192732	-0.835325
C	2.526574	2.801715	-1.066031
H	1.698036	6.505622	-0.393018
H	-0.149862	4.832689	-0.422218
C	1.481528	0.752763	-1.091344
C	2.658971	-1.383975	-1.286181
C	3.621732	-0.591143	-2.186761
C	3.903285	0.768921	-1.574398
H	4.424696	1.416341	-2.292140
S	0.122443	1.815326	-0.839377
N	2.633042	1.418139	-1.242987
N	1.423106	-0.590050	-1.091944
C	4.910107	-1.365674	-2.550231
C	6.072043	-1.162693	-1.573862
C	5.352625	-0.998977	-3.967050
H	4.644875	-2.436002	-2.547611
H	5.792426	-1.346302	-0.526818
H	6.889591	-1.852901	-1.827696
H	6.475855	-0.140488	-1.648149
H	4.578080	-1.246593	-4.707358
H	5.564558	0.079591	-4.043530
H	6.271072	-1.538879	-4.239519
H	3.064957	-0.418210	-3.122339
H	2.358147	-2.271715	-1.856176
C	3.256646	-1.824884	0.034670
C	3.748732	-3.127647	0.162631
C	3.379331	-0.942228	1.112777
C	4.372055	-3.536299	1.340734
H	3.639045	-3.829688	-0.668029
C	3.999211	-1.350726	2.293629
H	2.991793	0.077152	1.042272
C	4.502001	-2.647083	2.407870
H	4.750358	-4.556099	1.427763
H	4.089263	-0.651876	3.127304
H	4.986118	-2.966812	3.331999
C	0.181598	-2.650132	-0.567496
H	1.101903	-3.216111	-0.448322
C	-1.030191	-3.205938	-0.199533
C	-1.115722	-4.700711	-0.057685
F	-0.906316	-5.290455	-1.246380
F	-0.190853	-5.185522	0.775373
F	-2.305150	-5.115598	0.366945
O	-0.826704	-0.533867	-0.744842
C	0.169635	-1.244842	-0.809689
H	4.511420	0.701078	-0.660397
C	3.569314	3.728176	-1.062921
H	4.602551	3.421018	-1.223778
H	4.041004	5.803467	-0.794227
H	-1.970321	-2.734713	-0.499673
S	-1.547505	-2.574911	2.060157
C	-2.707225	-1.395554	1.526478
N	-3.708695	-1.760426	0.791472
N	-2.605404	-0.065698	1.945439
H	-3.469944	0.450789	1.800772
C	-4.541388	-0.866269	0.141392
C	-5.938487	-1.023545	0.254397
C	-4.039102	0.156418	-0.697946
C	-6.807862	-0.181072	-0.421678
H	-6.322003	-1.823625	0.888472
C	-4.903540	0.996964	-1.382155
H	-2.958267	0.252146	-0.815876

C	-6.279290	0.823359	-1.231044
H	-7.887666	-0.291862	-0.332322
H	-4.526762	1.782241	-2.036311
N	-7.191552	1.715100	-1.945578
O	-6.709900	2.588574	-2.633714
O	-8.382281	1.537026	-1.811493
C	-1.528832	0.776538	2.161380
C	-1.824115	2.160164	2.162644
C	-0.190013	0.375899	2.354400
C	-0.829587	3.112500	2.295671
H	-2.859785	2.479470	2.027740
C	0.807684	1.331849	2.481702
H	0.062352	-0.680238	2.393122
C	0.490634	2.686205	2.428159
H	-1.061841	4.176722	2.273655
H	1.842898	1.029062	2.632186
O	2.695933	3.284814	2.264748
N	1.561940	3.674318	2.450596
O	1.263662	4.833348	2.638302

CF3_Michael_Acceptor_TS-MA-conf/TS-MA-S-viii

Frequencies, energies and thermodynamic properties:

Lowest Vibrational Mode (1/cm) = -117.2204

2nd Lowest Vibrational Mode (1/cm) = 10.6675

E(RM062X) (a.u.) = -3187.92969022

Thermal correction to Enthalpy (a.u.) = 0.681014

Thermal correction to Gibbs Free Energy (a.u.) = 0.554320

Total Entropy (cal/Kmol) = 266.649

Esp(RM062X) (a.u.) = -3190.89371057

Optimised cartesian coordinates (Angstrom):

C	-3.506258	4.917444	0.818063
C	-2.188389	5.391318	0.739745
C	-1.108840	4.518348	0.816290
C	-1.381795	3.158040	0.964528
C	-2.694079	2.691839	1.053585
H	-2.005618	6.458023	0.606781
H	-0.081917	4.880716	0.746749
C	-1.546113	0.701608	1.142599
C	-2.610313	-1.511651	1.303603
C	-3.698240	-0.744253	2.072966
C	-3.996167	0.571752	1.378917
H	-4.644517	1.198131	2.005691
S	-0.232333	1.838391	1.020020
N	-2.740250	1.299611	1.182929
N	-1.413255	-0.642598	1.165027
C	-4.972208	-1.577653	2.345059
C	-6.039411	-1.479032	1.251236
C	-5.573236	-1.177519	3.692701
H	-4.651326	-2.629700	2.419638
H	-5.646468	-1.678218	0.244443
H	-6.837896	-2.208620	1.449378
H	-6.505704	-0.481154	1.246050
H	-4.864606	-1.347523	4.516229
H	-5.850565	-0.111187	3.695530
H	-6.483741	-1.758404	3.899335
H	-3.247003	-0.500749	3.048919
H	-2.305990	-2.343537	1.951272
C	-3.050190	-2.062356	-0.037602
C	-3.515498	-3.378546	-0.124837
C	-3.031817	-1.266951	-1.185843
C	-3.980073	-3.881596	-1.338635
H	-3.509210	-4.014344	0.764479
C	-3.493275	-1.769726	-2.402503

H -2.642804 -0.247630 -1.136542
C -3.974150 -3.076589 -2.479016
H -4.339191 -4.910304 -1.396818
H -3.470593 -1.139542 -3.293472
H -4.331803 -3.472749 -3.430665
C -0.049551 -2.651688 0.728864
H -0.936974 -3.276698 0.677948
C 1.148215 -3.138016 0.311574
C 1.297759 -4.613007 0.067729
F 1.271230 -5.278444 1.235497
F 0.303123 -5.107235 -0.673078
F 2.444903 -4.926849 -0.522480
O 0.837592 -0.473958 0.892638
C -0.121626 -1.222159 0.947754
H -4.478699 0.432274 0.400250
C -3.780669 3.564522 0.980207
H -4.806851 3.201101 1.024664
H -4.335289 5.621976 0.742774
H 2.083006 -2.586861 0.437032
S 1.444710 -2.335400 -2.148657
C 2.612024 -1.192431 -1.601424
N 3.676437 -1.587727 -0.962095
N 2.473888 0.172268 -1.884847
H 3.334610 0.690432 -1.726154
C 4.528809 -0.745511 -0.281347
C 5.923777 -0.915658 -0.433423
C 4.069222 0.232904 0.636276
C 6.823206 -0.133914 0.272976
H 6.277930 -1.680451 -1.125550
C 4.964299 1.013407 1.350465
H 2.994785 0.340947 0.792479
C 6.333603 0.828101 1.156883
H 7.898449 -0.257678 0.150712
H 4.616694 1.760600 2.062886
N 7.276487 1.656466 1.902231
O 6.827564 2.502545 2.645747
O 8.461203 1.459150 1.739153
C 1.391055 1.009263 -2.057342
C 1.681068 2.395059 -2.014408
C 0.048809 0.610908 -2.242330
C 0.685780 3.347908 -2.118354
H 2.717384 2.712067 -1.878917
C -0.950935 1.570217 -2.340638
H -0.196589 -0.446506 -2.303233
C -0.634501 2.923832 -2.265512
H 0.916892 4.411429 -2.071713
H -1.991231 1.277762 -2.483835
O -2.846549 3.522207 -2.208048
N -1.702522 3.914973 -2.299257
O -1.392775 5.081443 -2.409282

CF3_Michael_Acceptor_TS-MA-conf/TS-MA-S-vii

Frequencies, energies and thermodynamic properties:

Lowest Vibrational Mode (1/cm) = -99.1496

2nd Lowest Vibrational Mode (1/cm) = 7.3018

E(RM062X) (a.u.) = -3187.92478746

Thermal correction to Enthalpy (a.u.) = 0.680730

Thermal correction to Gibbs Free Energy (a.u.) = 0.548046

Total Entropy (cal/Kmol) = 279.257

Esp(RM062X) (a.u.) = -3190.89247641

Optimised cartesian coordinates (Angstrom):

C -7.376249 -0.360297 -2.878083
C -6.951026 0.859931 -3.423978

C	-5.763955	1.453496	-3.009014
C	-5.014258	0.797214	-2.032669
C	-5.444657	-0.411857	-1.484488
H	-7.556273	1.349619	-4.187578
H	-5.426802	2.399705	-3.434324
C	-3.467171	-0.129427	-0.345197
C	-2.544063	-1.744656	1.260572
C	-4.021753	-2.074264	1.532529
C	-4.792530	-2.126887	0.227181
H	-5.870952	-2.187893	0.421306
S	-3.489739	1.307182	-1.332834
N	-4.549405	-0.891928	-0.522327
N	-2.467696	-0.477845	0.490148
C	-4.229915	-3.338445	2.398260
C	-4.350129	-4.640164	1.600827
C	-5.461177	-3.158033	3.286861
H	-3.349408	-3.418753	3.056626
H	-4.343499	-5.496251	2.290845
H	-5.302399	-4.675841	1.048194
H	-3.531153	-4.783140	0.881756
H	-5.629292	-4.052853	3.903399
H	-5.349008	-2.295215	3.959358
H	-6.364766	-2.999365	2.676280
H	-4.409515	-1.215224	2.104169
H	-2.094522	-1.527605	2.237223
C	-1.757497	-2.853678	0.592288
C	-1.029179	-3.742157	1.391234
C	-1.781427	-3.044035	-0.792963
C	-0.361294	-4.822923	0.819028
H	-0.985584	-3.582655	2.471722
C	-1.111686	-4.125331	-1.366220
H	-2.314959	-2.346010	-1.443157
C	-0.407308	-5.020492	-0.561510
H	0.204126	-5.508164	1.452511
H	-1.135777	-4.263728	-2.448225
H	0.118763	-5.863494	-1.012231
C	-0.195696	-0.107398	1.379416
H	-0.114062	-1.144591	1.696889
C	0.851126	0.746842	1.536618
C	1.964804	0.388884	2.479215
F	1.551987	0.555141	3.747068
F	2.348656	-0.884115	2.368299
F	3.043178	1.156924	2.333634
O	-1.351716	1.451798	0.039072
C	-1.322011	0.376762	0.607844
H	-4.497785	-2.979671	-0.402677
C	-6.632666	-1.015398	-1.902715
H	-6.964845	-1.968140	-1.491413
H	-8.307370	-0.809335	-3.225597
H	0.739745	1.811269	1.326481
S	2.296147	0.532234	-0.603694
C	3.660615	1.605221	-0.543792
N	3.509937	2.952774	-0.219472
N	4.898993	1.289867	-0.773902
C	2.435369	3.804488	-0.072195
C	1.107440	3.524708	-0.459656
C	2.716432	5.072207	0.493207
C	0.105705	4.462113	-0.253459
H	0.856832	2.565644	-0.903152
C	1.721522	6.011823	0.685918
H	3.742238	5.303496	0.786654
C	0.413964	5.694266	0.316228
H	-0.921089	4.234456	-0.535847

H	1.943022	6.983012	1.126136
N	-0.646860	6.672365	0.528998
O	-0.346369	7.740909	1.016452
O	-1.775644	6.368110	0.208237
C	5.372548	0.005724	-0.906626
C	5.101000	-1.017088	0.032584
C	6.249996	-0.282168	-1.974397
C	5.675291	-2.270261	-0.097957
H	4.437815	-0.804848	0.870204
C	6.818551	-1.537902	-2.120099
H	6.471222	0.511536	-2.688974
C	6.523559	-2.522256	-1.178149
H	5.475987	-3.059146	0.626061
H	7.488208	-1.764756	-2.948533
N	7.121766	-3.845710	-1.320155
O	7.861425	-4.040239	-2.261184
O	6.849436	-4.687155	-0.490553
H	4.416347	3.390285	-0.069741

CF3_Michael_Acceptor_TS-MA-conf/TS-MA-S-vi

Frequencies, energies and thermodynamic properties:

Lowest Vibrational Mode (1/cm) = -138.9866

2nd Lowest Vibrational Mode (1/cm) = 11.7384

E(RM062X) (a.u.) = -3187.93203755

Thermal correction to Enthalpy (a.u.) = 0.680944

Thermal correction to Gibbs Free Energy (a.u.) = 0.553373

Total Entropy (cal/Kmol) = 268.497

Esp(RM062X) (a.u.) = -3190.89576817

Optimised cartesian coordinates (Angstrom):

C	-2.352822	-6.163568	-1.918722
C	-3.492823	-5.423582	-2.263092
C	-3.651383	-4.111648	-1.827194
C	-2.641842	-3.557939	-1.040690
C	-1.513643	-4.301355	-0.691149
H	-4.266020	-5.879854	-2.882176
H	-4.536980	-3.532216	-2.092293
C	-1.021971	-2.306504	0.345307
C	1.068881	-1.836691	1.532167
C	1.013959	-3.338322	1.874803
C	0.601355	-4.132739	0.649788
H	0.393391	-5.176696	0.918936
S	-2.585006	-1.945057	-0.348491
N	-0.633921	-3.563957	0.108292
N	-0.255133	-1.427188	1.007373
C	2.301498	-3.888429	2.530550
C	3.331202	-4.438674	1.539624
C	1.938440	-4.966609	3.552444
H	2.763258	-3.050836	3.077522
H	4.268321	-4.664401	2.068899
H	2.977902	-5.379878	1.089340
H	3.566607	-3.737156	0.726959
H	2.844103	-5.378990	4.020450
H	1.294546	-4.565954	4.348802
H	1.403909	-5.800281	3.068703
H	0.201158	-3.434133	2.613400
H	1.191304	-1.305763	2.484277
C	2.204279	-1.455255	0.604740
C	3.427231	-1.062259	1.162782
C	2.095413	-1.572783	-0.784018
C	4.539236	-0.847887	0.351173
H	3.508468	-0.934461	2.245228
C	3.208251	-1.350793	-1.597791
H	1.140363	-1.831012	-1.248936

C	4.435254	-1.005899	-1.031894
H	5.487768	-0.541172	0.796175
H	3.112547	-1.446252	-2.680777
H	5.303859	-0.833694	-1.670933
C	0.175387	0.899569	1.675794
H	1.235255	0.682291	1.784545
C	-0.308862	2.180475	1.881834
C	0.464024	3.078631	2.808644
F	0.294462	2.671460	4.075324
F	1.779948	3.050685	2.571835
F	0.073482	4.350994	2.766130
O	-1.936613	0.107400	0.980225
C	-0.753410	-0.083718	1.213779
H	1.369563	-4.117403	-0.137804
C	-1.346982	-5.616276	-1.128555
H	-0.460238	-6.193712	-0.868232
H	-2.248262	-7.188514	-2.276526
H	-1.391112	2.315585	1.949176
S	-0.148518	3.622857	-0.013848
C	-0.339491	2.288426	-1.125062
N	-1.599363	1.803507	-1.451968
N	0.606408	1.648383	-1.733637
C	-2.897080	2.046166	-1.051831
C	-3.325276	3.034032	-0.140495
C	-3.875167	1.206250	-1.636433
C	-4.669884	3.151698	0.181286
H	-2.605449	3.711875	0.306798
C	-5.214002	1.322179	-1.317025
H	-3.556349	0.449734	-2.356164
C	-5.603170	2.297801	-0.399377
H	-5.002071	3.912278	0.886722
H	-5.959844	0.669907	-1.768860
N	-7.013038	2.428162	-0.049407
O	-7.800667	1.668270	-0.571416
O	-7.326164	3.287609	0.745442
C	1.961852	1.916804	-1.675687
C	2.686396	2.173771	-0.493684
C	2.672586	1.840490	-2.893887
C	4.063490	2.334957	-0.528734
H	2.164713	2.233633	0.455743
C	4.046801	2.010327	-2.940757
H	2.110091	1.630937	-3.804599
C	4.729062	2.247963	-1.748685
H	4.628751	2.509976	0.385681
H	4.596135	1.944219	-3.878810
N	6.187551	2.338560	-1.768430
O	6.750018	2.233197	-2.836947
O	6.762777	2.502332	-0.714263
H	-1.513405	1.034493	-2.113033

CF3_Michael_Acceptor_TS-MA-conf/TS-MA-S-v

Frequencies, energies and thermodynamic properties:

Lowest Vibrational Mode (1/cm) = -167.7310

2nd Lowest Vibrational Mode (1/cm) = 13.2661

E(RM062X) (a.u.) = -3187.93151947

Thermal correction to Enthalpy (a.u.) = 0.680602

Thermal correction to Gibbs Free Energy (a.u.) = 0.553802

Total Entropy (cal/Kmol) = 266.872

Esp(RM062X) (a.u.) = -3190.89262992

Optimised cartesian coordinates (Angstrom):

C	7.678746	0.441137	0.754706
C	7.469220	1.762423	0.333614
C	6.268693	2.143265	-0.256622

C	5.287706	1.165807	-0.422844
C	5.494752	-0.146436	0.004189
H	8.254732	2.505156	0.477443
H	6.081450	3.174114	-0.558850
C	3.336469	-0.308734	-0.781054
C	1.950510	-2.325470	-0.650359
C	3.293791	-3.072626	-0.689712
C	4.322276	-2.358371	0.165569
H	5.319930	-2.786092	0.004379
S	3.681543	1.371636	-1.095019
N	4.372856	-0.949931	-0.227401
N	2.161452	-0.910190	-1.034000
C	3.178971	-4.577081	-0.354310
C	3.303322	-4.903844	1.136411
C	4.221850	-5.365694	-1.147288
H	2.182166	-4.901830	-0.695827
H	3.059590	-5.963070	1.303355
H	4.336011	-4.749646	1.487379
H	2.633759	-4.302503	1.767233
H	4.159361	-6.438118	-0.912193
H	4.079667	-5.244361	-2.230981
H	5.240839	-5.028617	-0.897346
H	3.634108	-2.993402	-1.735308
H	1.343792	-2.774846	-1.444397
C	1.186238	-2.409395	0.656522
C	0.181014	-3.371527	0.801142
C	1.473494	-1.558123	1.729268
C	-0.507962	-3.500582	2.005544
H	-0.067426	-4.020798	-0.042401
C	0.783061	-1.685974	2.934703
H	2.229728	-0.774223	1.634894
C	-0.205171	-2.659776	3.077352
H	-1.292372	-4.252812	2.103669
H	1.014080	-1.013972	3.763028
H	-0.748720	-2.754471	4.018745
C	-0.219827	-0.764499	-1.656559
H	-0.333190	-1.844233	-1.635033
C	-1.344443	0.038398	-1.663362
C	-2.598535	-0.486547	-2.308639
F	-2.417183	-0.584717	-3.634643
F	-2.934553	-1.704900	-1.878025
F	-3.652584	0.313200	-2.134835
O	1.226858	1.093012	-1.590323
C	1.033427	-0.104500	-1.454843
H	4.084608	-2.410234	1.239094
C	6.696180	-0.531695	0.602639
H	6.859639	-1.552340	0.947663
H	8.626681	0.168809	1.220454
H	-1.212225	1.118432	-1.780159
S	-2.198286	0.209364	0.521441
C	-2.889216	1.809716	0.372647
N	-4.262782	2.001290	0.335381
N	-2.218975	2.909660	0.230656
C	-5.381617	1.189439	0.378541
C	-5.396196	-0.219984	0.315558
C	-6.619091	1.869511	0.476573
C	-6.600972	-0.907196	0.361485
H	-4.467481	-0.773144	0.224467
C	-7.819204	1.185603	0.518845
H	-6.618383	2.960275	0.522324
C	-7.799400	-0.207409	0.464131
H	-6.615112	-1.995079	0.310516
H	-8.766883	1.716315	0.596444

N	-9.059302	-0.943220	0.510468
O	-10.086488	-0.305402	0.593827
O	-9.014073	-2.153219	0.463935
C	-0.857199	3.051068	0.385778
C	-0.173497	3.876150	-0.532300
C	-0.126483	2.496224	1.462678
C	1.185647	4.112859	-0.414514
H	-0.742664	4.318765	-1.350755
C	1.228650	2.745691	1.600756
H	-0.639305	1.873613	2.193904
C	1.873479	3.547014	0.657388
H	1.717651	4.728583	-1.138289
H	1.795209	2.326430	2.431640
N	3.308949	3.756271	0.770884
O	3.882942	3.311001	1.740630
O	3.874406	4.344567	-0.132199
H	-4.479118	2.995162	0.289030

CF3_Michael_Acceptor_TS-MA-conf/TS-MA-S-xiii

Frequencies, energies and thermodynamic properties:

Lowest Vibrational Mode (1/cm) = -64.6455

2nd Lowest Vibrational Mode (1/cm) = 9.4812

E(RM062X) (a.u.) = -3187.91769616

Thermal correction to Enthalpy (a.u.) = 0.681201

Thermal correction to Gibbs Free Energy (a.u.) = 0.550663

Total Entropy (cal/Kmol) = 274.741

Esp(RM062X) (a.u.) = -3190.88959644

Optimised cartesian coordinates (Angstrom):

C	4.759820	5.680671	0.148532
C	3.446811	6.125832	-0.067123
C	2.427774	5.227913	-0.363846
C	2.755930	3.874280	-0.443004
C	4.064076	3.434875	-0.236007
H	3.219672	7.190165	0.002303
H	1.403932	5.566915	-0.526941
C	3.016614	1.426667	-0.630591
C	4.129318	-0.769959	-0.562441
C	5.371149	0.033815	-0.983294
C	5.439176	1.334565	-0.207382
H	6.232433	1.979441	-0.605639
S	1.679995	2.534425	-0.783723
N	4.169071	2.045990	-0.365840
N	2.923926	0.082485	-0.734944
C	6.690552	-0.768992	-0.915778
C	7.407581	-0.690733	0.434679
C	7.630568	-0.309671	-2.030970
H	6.432029	-1.822850	-1.108392
H	8.248523	-1.399050	0.447329
H	7.826892	0.314594	0.598365
H	6.753581	-0.931878	1.284454
H	8.580905	-0.861190	-1.988869
H	7.185736	-0.469962	-3.023807
H	7.862414	0.762916	-1.930484
H	5.198401	0.296570	-2.039885
H	4.037184	-1.577977	-1.298791
C	4.184016	-1.370045	0.828222
C	4.654218	-2.679308	0.982494
C	3.808935	-0.641735	1.961536
C	4.781522	-3.239779	2.251414
H	4.920824	-3.264603	0.098629
C	3.933851	-1.204297	3.232305
H	3.401823	0.368323	1.867856
C	4.427187	-2.499857	3.380401

H 5.148944 -4.261624 2.358426
H 3.634433 -0.628165 4.109083
H 4.520003 -2.939150 4.374879
C 1.537928 -1.963856 -0.836711
H 2.402345 -2.595230 -0.647713
C 0.296317 -2.492300 -0.823456
C 0.115467 -3.982287 -0.867061
F 0.420200 -4.442970 -2.091510
F 0.905592 -4.624336 -0.010751
F -1.143901 -4.360867 -0.632598
O 0.688671 0.220361 -1.118799
C 1.636666 -0.510720 -0.925414
H 5.617636 1.175320 0.866830
C 5.089914 4.332569 0.069240
H 6.110445 3.994396 0.247102
H 5.540393 6.404064 0.386595
H -0.583023 -1.890503 -1.058008
S -0.623669 -2.285161 1.763737
C -2.033465 -1.384392 1.371133
N -2.780125 -1.913875 0.303303
N -2.387554 -0.298991 1.996162
C -3.501777 -1.253453 -0.671874
C -3.378768 0.130872 -0.912571
C -4.362592 -2.016248 -1.489034
C -4.115035 0.731456 -1.921245
H -2.688156 0.727329 -0.319235
C -5.093981 -1.418666 -2.500706
H -4.452072 -3.089254 -1.309924
C -4.969805 -0.044584 -2.702189
H -4.024088 1.799043 -2.116713
H -5.765267 -2.001510 -3.129596
N -5.741692 0.592462 -3.765180
O -6.455484 -0.109387 -4.448346
O -5.627568 1.789854 -3.912001
C -3.660473 0.202981 2.045823
C -4.822980 -0.608180 2.109785
C -3.831631 1.607531 2.109699
C -6.083177 -0.043648 2.198326
H -4.719137 -1.693434 2.087985
C -5.089235 2.178915 2.189290
H -2.938914 2.234281 2.085157
C -6.209578 1.346789 2.227577
H -6.976272 -0.665536 2.246022
H -5.219300 3.259785 2.224096
N -7.536371 1.940428 2.312222
O -7.620193 3.150416 2.346514
O -8.494731 1.197154 2.343985
H -2.624262 -2.904696 0.142960

CF3_Michael_Acceptor_TS-MA-conf/TS-MA-S-xii

Frequencies, energies and thermodynamic properties:

Lowest Vibrational Mode (1/cm) = -43.1607

2nd Lowest Vibrational Mode (1/cm) = 9.9637

E(RM062X) (a.u.) = -3187.91958643

Thermal correction to Enthalpy (a.u.) = 0.680543

Thermal correction to Gibbs Free Energy (a.u.) = 0.549410

Total Entropy (cal/Kmol) = 275.993

Esp(RM062X) (a.u.) = -3190.89060599

Optimised cartesian coordinates (Angstrom):

C 3.353560 5.813001 1.271547
C 1.958510 5.957374 1.305436
C 1.122054 4.893711 0.985721
C 1.715601 3.682415 0.629644

C	3.103614	3.544711	0.586871
H	1.521694	6.915572	1.588666
H	0.036835	5.000676	1.013515
C	2.464843	1.421509	-0.016724
C	4.020713	-0.427720	-0.478527
C	4.961256	0.699043	-0.938752
C	4.888095	1.866935	0.027047
H	5.424239	2.735421	-0.377315
S	0.912142	2.188795	0.186417
N	3.484897	2.255356	0.198963
N	2.649303	0.122526	-0.333119
C	6.411029	0.231260	-1.203550
C	7.333248	0.300488	0.016733
C	7.010446	1.038064	-2.355688
H	6.348946	-0.820709	-1.527262
H	8.293006	-0.180965	-0.220101
H	7.552353	1.345926	0.285942
H	6.916912	-0.201210	0.901736
H	8.046386	0.725144	-2.550618
H	6.433525	0.906234	-3.282455
H	7.026738	2.113112	-2.114583
H	4.545982	1.046584	-1.898968
H	3.969672	-1.140761	-1.310204
C	4.464505	-1.159833	0.770786
C	5.181608	-2.353615	0.635505
C	4.223257	-0.649337	2.050577
C	5.679220	-3.010718	1.759235
H	5.350585	-2.770915	-0.360575
C	4.720186	-1.307697	3.175574
H	3.640711	0.265649	2.185860
C	5.455074	-2.484503	3.031875
H	6.237097	-3.940918	1.640677
H	4.527095	-0.900447	4.169285
H	5.841079	-2.999132	3.913234
C	1.730158	-2.137966	-0.746174
H	2.683648	-2.607856	-0.509619
C	0.668530	-2.871608	-1.144256
C	0.865653	-4.322622	-1.483929
F	1.672509	-4.439074	-2.554957
F	1.452779	-5.006389	-0.499334
F	-0.267605	-4.939729	-1.796371
O	0.408662	-0.197964	-0.512058
C	1.505108	-0.713670	-0.533097
H	5.305617	1.624446	1.015667
C	3.947648	4.608311	0.913046
H	5.031442	4.499478	0.895450
H	3.988229	6.660562	1.532791
H	-0.278685	-2.417096	-1.450275
S	-1.048634	-3.457479	0.927697
C	-2.155891	-2.240943	0.432330
N	-2.311560	-1.868006	-0.808302
N	-2.893067	-1.671634	1.482055
C	-2.785821	-0.647552	-1.212479
C	-2.546357	0.562072	-0.509673
C	-3.493781	-0.570360	-2.435734
C	-3.012290	1.771023	-0.992532
H	-1.974180	0.531704	0.416758
C	-3.970358	0.635538	-2.921076
H	-3.664039	-1.494868	-2.989626
C	-3.728189	1.800823	-2.192368
H	-2.828153	2.700968	-0.455523
H	-4.526012	0.689366	-3.856379
N	-4.219029	3.074374	-2.697090

O -4.838657 3.076995 -3.740166
O -3.983784 4.074922 -2.051123
C -4.194586 -1.206733 1.484257
C -5.108159 -1.460814 0.440205
C -4.630219 -0.473778 2.608083
C -6.402985 -0.972050 0.510519
H -4.805580 -2.059290 -0.416739
C -5.924556 0.010697 2.683051
H -3.928601 -0.284515 3.422378
C -6.798686 -0.235104 1.625118
H -7.115440 -1.166405 -0.289995
H -6.262860 0.582788 3.545756
N -8.163032 0.280472 1.693004
O -8.487526 0.900698 2.682474
O -8.901294 0.061319 0.757698
H -2.477509 -1.814368 2.397843

CF3_Michael_Acceptor_TS-MA-conf/TS-MA-S-xi

Frequencies, energies and thermodynamic properties:

Lowest Vibrational Mode (1/cm) = -110.5018

2nd Lowest Vibrational Mode (1/cm) = 10.3080

E(RM062X) (a.u.) = -3187.92199084

Thermal correction to Enthalpy (a.u.) = 0.680431

Thermal correction to Gibbs Free Energy (a.u.) = 0.551262

Total Entropy (cal/Kmol) = 271.858

Esp(RM062X) (a.u.) = -3190.88812167

Optimised cartesian coordinates (Angstrom):

C -6.587421 3.856023 -0.553634
C -5.533404 4.777521 -0.642183
C -4.214795 4.376740 -0.455844
C -3.979338 3.029285 -0.179860
C -5.030474 2.116024 -0.077513
H -5.748628 5.823886 -0.861631
H -3.381851 5.078363 -0.517949
C -3.243301 0.730218 0.333998
C -3.408452 -1.697698 0.685538
C -4.788566 -1.352047 1.272348
C -5.475505 -0.308099 0.411735
H -6.377951 0.066488 0.911388
S -2.432379 2.254971 0.102333
N -4.571106 0.828681 0.226044
N -2.620795 -0.447582 0.547718
C -5.681265 -2.586373 1.539113
C -6.572715 -2.988880 0.361067
C -6.539522 -2.345186 2.781451
H -5.002888 -3.427077 1.758129
H -7.060988 -3.949436 0.580320
H -7.371629 -2.247479 0.201268
H -6.017456 -3.103041 -0.580614
H -7.185147 -3.212498 2.981687
H -5.918582 -2.168384 3.671655
H -7.192545 -1.468639 2.641732
H -4.577155 -0.880562 2.246142
H -2.894472 -2.294133 1.449491
C -3.446936 -2.485794 -0.607410
C -3.353850 -3.881023 -0.550931
C -3.624765 -1.863227 -1.847189
C -3.469045 -4.644931 -1.710691
H -3.189400 -4.371477 0.412011
C -3.739224 -2.627976 -3.008378
H -3.668202 -0.773895 -1.924355
C -3.669192 -4.019311 -2.941778
H -3.394084 -5.731998 -1.653678

H -3.877147 -2.131728 -3.970288
H -3.755438 -4.615382 -3.851654
C -0.535424 -1.767780 0.663940
H -1.078793 -2.690806 0.473835
C 0.815845 -1.778117 0.791920
C 1.508513 -3.084026 1.068570
F 1.204742 -3.493479 2.315260
F 1.120816 -4.058885 0.248027
F 2.834206 -2.998421 1.020785
O -0.600729 0.588854 0.692367
C -1.188338 -0.471768 0.643900
H -5.755573 -0.697984 -0.578325
C -6.355428 2.514572 -0.269166
H -7.181491 1.806710 -0.206109
H -7.612392 4.194682 -0.709590
H 1.360576 -0.875903 1.076195
S 2.034983 -1.470581 -1.554157
C 3.489862 -0.807665 -0.894656
N 3.405331 0.335807 -0.082854
N 4.632412 -1.408165 -1.016909
C 2.490832 1.372044 -0.066901
C 1.687517 1.717451 -1.172759
C 2.409376 2.151401 1.106812
C 0.804260 2.779088 -1.085701
H 1.756860 1.140462 -2.090844
C 1.534687 3.218940 1.194038
H 3.038910 1.892279 1.960287
C 0.727876 3.516707 0.096204
H 0.176826 3.050135 -1.933978
H 1.459301 3.812664 2.104012
N -0.232073 4.602064 0.197680
O -0.206859 5.310340 1.177807
O -1.037078 4.737972 -0.709617
C 5.840872 -0.857074 -0.657115
C 6.759712 -1.654502 0.064005
C 6.248678 0.442525 -1.048505
C 8.015937 -1.178483 0.399985
H 6.450719 -2.660108 0.351765
C 7.507877 0.921519 -0.725012
H 5.565705 1.064896 -1.628473
C 8.378280 0.109107 0.002162
H 8.720721 -1.789424 0.962582
H 7.828012 1.916534 -1.031495
N 9.702015 0.617069 0.349297
O 9.991112 1.741114 -0.001019
O 10.445865 -0.109540 0.972337
H 4.156667 0.429421 0.597850

CF3_Michael_Acceptor_TS-MA-conf/TS-MA-S-xiv

Frequencies, energies and thermodynamic properties:

Lowest Vibrational Mode (1/cm) = -82.8939

2nd Lowest Vibrational Mode (1/cm) = 13.2831

E(RM062X) (a.u.) = -3187.92204605

Thermal correction to Enthalpy (a.u.) = 0.680551

Thermal correction to Gibbs Free Energy (a.u.) = 0.552231

Total Entropy (cal/Kmol) = 270.073

Esp(RM062X) (a.u.) = -3190.89068423

Optimised cartesian coordinates (Angstrom):

C 0.065352 5.942300 -1.378623
C -1.164813 5.486291 -1.874155
C -1.399587 4.128875 -2.068039
C -0.373664 3.239742 -1.748739
C 0.851526 3.696858 -1.260496

H	-1.952118	6.203536	-2.108033
H	-2.356864	3.770872	-2.449987
C	1.228491	1.428585	-1.235033
C	3.240489	0.381990	-0.314708
C	3.945799	1.639364	-0.853358
C	3.113248	2.872251	-0.554952
H	3.495508	3.741721	-1.106255
S	-0.380466	1.493320	-1.904481
N	1.736904	2.643167	-1.005484
N	1.887642	0.297837	-0.924200
C	5.413694	1.776984	-0.386430
C	5.596393	2.526900	0.935923
C	6.244365	2.446622	-1.482015
H	5.797257	0.751663	-0.253815
H	6.646360	2.456507	1.254864
H	5.364640	3.597358	0.817553
H	4.972587	2.128149	1.748269
H	7.292423	2.549308	-1.165496
H	6.224623	1.864501	-2.414757
H	5.862486	3.456503	-1.702044
H	3.959662	1.512505	-1.948284
H	3.795216	-0.476625	-0.710831
C	3.201059	0.277689	1.195321
C	4.126212	-0.553223	1.835917
C	2.316322	1.035951	1.970716
C	4.184317	-0.608604	3.227621
H	4.807450	-1.162762	1.236232
C	2.368637	0.976043	3.362814
H	1.567175	1.677234	1.498368
C	3.308033	0.159996	3.993746
H	4.911077	-1.261013	3.714157
H	1.668374	1.566689	3.955928
H	3.347792	0.113980	5.083188
C	1.979363	-2.150728	-0.755374
H	2.643156	-2.078531	0.104622
C	1.732412	-3.360636	-1.335580
C	2.718409	-4.467088	-1.082281
F	3.844904	-4.229470	-1.780453
F	3.079116	-4.553142	0.197564
F	2.290958	-5.666586	-1.470746
O	0.335477	-0.981861	-1.997838
C	1.312061	-0.981974	-1.272131
H	3.092509	3.118010	0.516835
C	1.091947	5.057732	-1.065065
H	2.043312	5.415884	-0.672831
H	0.222693	7.011363	-1.231017
H	1.197172	-3.421960	-2.283791
S	-0.177614	-4.685291	-0.317912
C	-1.127438	-3.312587	0.138170
N	-2.459951	-3.363036	-0.295818
N	-0.633047	-2.335990	0.827929
C	-3.313948	-2.323945	-0.624352
C	-2.835851	-1.050246	-0.987676
C	-4.702159	-2.562134	-0.621385
C	-3.724148	-0.032511	-1.291367
H	-1.762123	-0.881288	-1.056513
C	-5.593247	-1.548712	-0.936272
H	-5.072504	-3.552223	-0.350615
C	-5.094118	-0.286729	-1.254030
H	-3.369965	0.958999	-1.570797
H	-6.668600	-1.720564	-0.924953
N	-6.026083	0.792178	-1.572552
O	-7.211419	0.544323	-1.551410

O	-5.565167	1.880383	-1.842660
C	-1.347837	-1.382756	1.503492
C	-2.499297	-1.671713	2.276448
C	-0.878999	-0.050875	1.485640
C	-3.164440	-0.667791	2.959653
H	-2.868357	-2.696907	2.325097
C	-1.541174	0.961041	2.157483
H	0.029281	0.154907	0.921080
C	-2.687610	0.642909	2.886845
H	-4.053544	-0.884229	3.550684
H	-1.186401	1.991293	2.129148
N	-3.392139	1.699859	3.601461
O	-2.945225	2.826085	3.538973
O	-4.389338	1.402616	4.223443
H	-2.782487	-4.296259	-0.534782

CF3_Michael_Acceptor_TS-MA-conf/TS-MA-S-x

Frequencies, energies and thermodynamic properties:

Lowest Vibrational Mode (1/cm) = -89.8842

2nd Lowest Vibrational Mode (1/cm) = 13.0595

E(RM062X) (a.u.) = -3187.92330888

Thermal correction to Enthalpy (a.u.) = 0.680228

Thermal correction to Gibbs Free Energy (a.u.) = 0.552868

Total Entropy (cal/Kmol) = 268.053

Esp(RM062X) (a.u.) = -3190.89001089

Optimised cartesian coordinates (Angstrom):

C	8.013971	-1.688748	-1.985323
C	7.530727	-2.710757	-2.815716
C	6.209207	-3.136324	-2.731235
C	5.382153	-2.512270	-1.797362
C	5.868796	-1.501798	-0.967169
H	8.198454	-3.177627	-3.540559
H	5.828736	-3.929601	-3.376156
C	3.681501	-1.585740	-0.263985
C	2.704383	-0.052747	1.375926
C	4.111421	-0.080101	2.002666
C	5.164937	-0.003685	0.913955
H	6.160805	-0.218922	1.323154
S	3.692825	-2.848239	-1.467201
N	4.881445	-1.020397	-0.101595
N	2.593399	-1.178597	0.417608
C	4.323224	0.975627	3.112844
C	4.876196	2.314656	2.617490
C	5.234246	0.406052	4.200830
H	3.335182	1.160804	3.565041
H	4.299456	2.735894	1.781633
H	4.858787	3.046103	3.438341
H	5.924636	2.212624	2.295362
H	4.799985	-0.495058	4.657808
H	6.219063	0.136907	3.786129
H	5.399122	1.146982	4.996494
H	4.197081	-1.074497	2.470494
H	2.003702	-0.278056	2.187723
C	2.333523	1.276740	0.755577
C	1.612060	2.197832	1.523002
C	2.787432	1.653143	-0.513994
C	1.395221	3.492981	1.054040
H	1.229611	1.898927	2.502476
C	2.573408	2.949222	-0.981267
H	3.313256	0.940677	-1.154476
C	1.891713	3.875903	-0.192032
H	0.830779	4.204931	1.659531
H	2.934981	3.234229	-1.970782

H	1.719184	4.887916	-0.564746
C	0.190632	-1.401688	0.963327
H	0.113185	-0.361387	1.278241
C	-0.837581	-2.277204	1.125662
C	-1.954218	-1.928652	2.068050
F	-1.488802	-1.832403	3.325356
F	-2.525609	-0.749824	1.793536
F	-2.916938	-2.849559	2.097901
O	1.379235	-2.918965	-0.397112
C	1.360674	-1.904784	0.268862
H	5.191040	0.980553	0.424029
C	7.193526	-1.069118	-1.048873
H	7.570803	-0.270012	-0.411286
H	9.052900	-1.369218	-2.074625
H	-0.687622	-3.341968	0.950306
S	-2.376112	-2.416310	-0.959658
C	-2.481249	-0.701895	-1.109964
N	-1.418759	0.028885	-1.282376
N	-3.732496	-0.072481	-1.120534
H	-3.717548	0.852350	-1.544669
C	-1.424964	1.401466	-1.167497
C	-0.828149	2.185076	-2.180924
C	-1.950998	2.065467	-0.030244
C	-0.764402	3.564659	-2.074967
H	-0.413716	1.675185	-3.051479
C	-1.884523	3.443518	0.084641
H	-2.402127	1.472333	0.766101
C	-1.290352	4.180922	-0.939892
H	-0.297182	4.169893	-2.850961
H	-2.271513	3.955270	0.965044
N	-1.138904	5.620727	-0.778553
O	-1.624825	6.140930	0.203058
O	-0.521725	6.229516	-1.628844
C	-5.008751	-0.506681	-0.812435
C	-6.080402	0.215045	-1.383884
C	-5.302783	-1.565777	0.071328
C	-7.396089	-0.109206	-1.104203
H	-5.859953	1.039997	-2.064061
C	-6.621028	-1.896305	0.347728
H	-4.497817	-2.122387	0.539533
C	-7.655446	-1.172876	-0.241789
H	-8.220189	0.444829	-1.551027
H	-6.854808	-2.710229	1.032629
O	-9.239669	-2.463524	0.801054
N	-9.039668	-1.527690	0.057697
O	-9.918862	-0.867132	-0.452081

CF3_Michael_Acceptor_TS-MA-conf/TS-MA-S-xvi

Frequencies, energies and thermodynamic properties:

Lowest Vibrational Mode (1/cm) = -115.9437

2nd Lowest Vibrational Mode (1/cm) = 5.6041

E(RM062X) (a.u.) = -3187.91917952

Thermal correction to Enthalpy (a.u.) = 0.680569

Thermal correction to Gibbs Free Energy (a.u.) = 0.551373

Total Entropy (cal/Kmol) = 271.916

Esp(RM062X) (a.u.) = -3190.88588653

Optimised cartesian coordinates (Angstrom):

C	8.237596	-1.972564	-2.025653
C	7.691356	-3.088342	-2.676241
C	6.367546	-3.460746	-2.466344
C	5.603661	-2.688726	-1.591366
C	6.152712	-1.583774	-0.939207
H	8.310436	-3.671969	-3.358414

H	5.937527	-4.326592	-2.971887
C	4.001982	-1.508330	-0.126414
C	3.138770	0.252328	1.342120
C	4.581115	0.290253	1.879829
C	5.567460	0.194439	0.730811
H	6.585541	0.031397	1.108133
S	3.925586	-2.928070	-1.138113
N	5.220190	-0.957239	-0.105386
N	2.961249	-0.983414	0.542618
C	4.868101	1.486647	2.816770
C	5.388240	2.739280	2.106529
C	5.850279	1.063490	3.909760
H	3.912894	1.741733	3.304430
H	5.425781	3.576828	2.818015
H	6.413039	2.583499	1.733875
H	4.758557	3.047739	1.259850
H	6.072360	1.906578	4.579951
H	5.445959	0.241130	4.517664
H	6.803335	0.725962	3.471453
H	4.687824	-0.629709	2.477831
H	2.488779	0.138572	2.217531
C	2.726149	1.495069	0.582343
C	2.041170	2.505469	1.265702
C	3.095243	1.702754	-0.751643
C	1.783707	3.728865	0.648098
H	1.720134	2.335867	2.296761
C	2.837990	2.926129	-1.370045
H	3.593609	0.914115	-1.321297
C	2.203682	3.948873	-0.664137
H	1.251678	4.513216	1.189303
H	3.134720	3.082270	-2.408518
H	2.004055	4.906228	-1.147893
C	0.571839	-1.002427	1.133306
H	0.577872	0.065107	1.345637
C	-0.569229	-1.743592	1.310002
C	-1.614030	-1.196320	2.242694
F	-1.197764	-1.349665	3.511969
F	-1.821424	0.111779	2.068504
F	-2.792343	-1.808721	2.162566
O	1.645216	-2.758693	-0.013807
C	1.689570	-1.663811	0.517970
H	5.567974	1.095340	0.099414
C	7.479773	-1.203791	-1.148537
H	7.908208	-0.334766	-0.649880
H	9.276781	-1.697745	-2.210102
H	-0.517846	-2.832595	1.284223
S	-1.865124	-2.064819	-0.792644
C	-3.444614	-1.385487	-0.519990
N	-3.562161	-0.015099	-0.268289
N	-4.488601	-2.142037	-0.432417
C	-2.751926	1.048993	-0.616421
C	-1.863912	1.029262	-1.711502
C	-2.884372	2.238487	0.131759
C	-1.143453	2.165171	-2.045591
H	-1.751628	0.124065	-2.301461
C	-2.161677	3.372287	-0.195574
H	-3.567317	2.255182	0.983228
C	-1.298387	3.325532	-1.289271
H	-0.469971	2.164178	-2.901682
H	-2.262023	4.290914	0.380800
N	-0.556652	4.520814	-1.661422
O	-0.558003	5.458440	-0.891120
O	0.035671	4.518979	-2.719080

C -5.781186 -1.662460 -0.364685
C -6.308532 -0.742171 -1.301512
C -6.642090 -2.174513 0.630801
C -7.635646 -0.347492 -1.239636
H -5.663080 -0.353838 -2.090660
C -7.967119 -1.776087 0.705858
H -6.236676 -2.893980 1.343067
C -8.450210 -0.864360 -0.232259
H -8.049659 0.353966 -1.962846
H -8.632087 -2.163199 1.476781
N -9.847512 -0.442193 -0.161243
O -10.539769 -0.911494 0.715607
O -10.242470 0.357521 -0.981577
H -4.370490 0.242314 0.294326

CF3_Michael_Acceptor_TS-MA-conf/TS-MA-S-xv

Frequencies, energies and thermodynamic properties:

Lowest Vibrational Mode (1/cm) = -82.0437
2nd Lowest Vibrational Mode (1/cm) = 5.3567
E(RM062X) (a.u.) = -3187.92592216
Thermal correction to Enthalpy (a.u.) = 0.680024
Thermal correction to Gibbs Free Energy (a.u.) = 0.551067
Total Entropy (cal/Kmol) = 271.413
Esp(RM062X) (a.u.) = -3190.89293419

Optimised cartesian coordinates (Angstrom):

C -5.849265 -3.300040 -2.718221
C -5.240471 -3.076770 -3.961376
C -4.273463 -2.088335 -4.117840
C -3.925137 -1.335164 -2.997759
C -4.539241 -1.554341 -1.762816
H -5.525835 -3.686271 -4.819492
H -3.797159 -1.910642 -5.082995
C -3.083201 0.130707 -1.197844
C -2.695958 0.885688 1.089018
C -4.212001 0.650887 1.254767
C -4.616068 -0.645903 0.575128
H -5.708680 -0.704305 0.476079
S -2.774194 -0.014218 -2.907706
N -4.055404 -0.684824 -0.779059
N -2.396945 0.925838 -0.362897
C -4.708523 0.739212 2.716947
C -4.681116 -0.584435 3.486270
C -6.120495 1.325782 2.748081
H -4.038661 1.447806 3.231771
H -4.907398 -0.396685 4.545862
H -5.450891 -1.276081 3.108523
H -3.708404 -1.094253 3.437410
H -6.490673 1.392645 3.781383
H -6.147764 2.333845 2.309433
H -6.820676 0.689081 2.183495
H -4.687697 1.473968 0.696876
H -2.493607 1.897444 1.459381
C -1.846193 -0.095109 1.868512
C -1.345635 0.303823 3.113073
C -1.672774 -1.424196 1.462142
C -0.743905 -0.620921 3.966529
H -1.450098 1.345897 3.425572
C -1.087432 -2.351950 2.323101
H -2.007678 -1.757367 0.476677
C -0.635910 -1.957821 3.583828
H -0.366969 -0.296346 4.937913
H -0.971970 -3.388828 1.999892
H -0.176247 -2.687199 4.252789

C -0.650601 2.618971 0.003751
H -0.331547 2.104853 0.912269
C -0.110141 3.811178 -0.376629
C 0.717110 4.564094 0.624825
F -0.046170 4.974917 1.654115
F 1.681960 3.804961 1.160842
F 1.286839 5.656326 0.124344
O -1.686644 2.242708 -2.086890
C -1.558442 1.972688 -0.914352
H -4.267593 -1.534304 1.120960
C -5.510652 -2.543026 -1.601106
H -5.982607 -2.720471 -0.634695
H -6.602403 -4.082864 -2.620833
H -0.575777 4.406828 -1.160246
S 1.779040 3.520368 -2.053756
C 2.187778 1.984014 -1.392983
N 1.346916 0.995155 -1.357295
N 3.480462 1.916040 -0.846473
C 1.478614 -0.089783 -0.519320
C 1.865012 0.032839 0.837236
C 1.171412 -1.375434 -1.016605
C 2.018279 -1.087882 1.633429
H 2.067225 1.024387 1.245001
C 1.320794 -2.502514 -0.224533
H 0.840367 -1.462292 -2.052758
C 1.759622 -2.347206 1.089426
H 2.323597 -1.003098 2.675593
H 1.100786 -3.498271 -0.607556
N 1.855874 -3.517323 1.949588
O 1.483696 -4.585220 1.507743
O 2.288627 -3.368012 3.072810
C 4.364611 0.856391 -0.818007
C 4.207910 -0.293987 -1.618319
C 5.488490 0.950874 0.029322
C 5.125467 -1.329507 -1.541577
H 3.373328 -0.364839 -2.313676
C 6.410631 -0.078604 0.101988
H 5.617722 1.846104 0.640173
C 6.212894 -1.218093 -0.676990
H 5.012170 -2.221992 -2.155454
H 7.274554 -0.015546 0.761953
N 7.174805 -2.313219 -0.595428
O 8.126825 -2.179593 0.142504
O 6.972815 -3.299435 -1.269982
H 3.864879 2.822551 -0.596712

Me_Michael_Acceptor/acyl_ammonium_ion_pair

Frequencies, energies and thermodynamic properties:

Lowest Vibrational Mode (1/cm) = 17.2774

2nd Lowest Vibrational Mode (1/cm) = 23.2636

E(RM062X) (a.u.) = -2275.21374105

Thermal correction to Enthalpy (a.u.) = 0.527841

Thermal correction to Gibbs Free Energy (a.u.) = 0.423224

Total Entropy (cal/Kmol) = 220.185

Esp(RM062X) (a.u.) = -2277.48416201

Optimised cartesian coordinates (Angstrom):

C -5.157437 3.666703 0.426376
C -4.540885 4.584538 -0.436178
C -3.331258 4.282575 -1.053210
C -2.755431 3.040167 -0.788730
C -3.368146 2.131269 0.075701
C -4.582849 2.429161 0.696333
H -6.107075 3.924398 0.896789

H	-5.014833	5.547862	-0.627808
H	-2.847085	4.993498	-1.724061
H	-5.069472	1.719376	1.364466
C	-1.507142	0.923472	-0.530577
C	-1.014569	-1.355786	0.233865
C	-1.749850	-0.897641	1.501758
C	-2.996768	-0.117985	1.130652
H	-3.439290	0.353123	2.018096
S	-1.241019	2.408176	-1.407565
N	-2.621452	0.956909	0.208371
N	-0.722650	-0.163045	-0.599398
C	-2.030675	-2.037419	2.505291
C	-3.371052	-2.747860	2.299583
C	-1.934734	-1.501541	3.934100
H	-1.225472	-2.778499	2.372787
H	-3.521819	-3.089284	1.265323
H	-3.427760	-3.629536	2.954597
H	-4.212283	-2.089265	2.569032
H	-0.935334	-1.090983	4.138147
H	-2.673470	-0.701156	4.102833
H	-2.134652	-2.299281	4.664496
H	-1.040122	-0.199992	1.974183
H	-0.035057	-1.698214	0.583941
C	-1.707292	-2.439108	-0.562334
C	-1.347070	-3.773547	-0.341035
C	-2.729740	-2.152884	-1.473554
C	-2.018903	-4.806218	-0.993147
H	-0.532651	-4.001120	0.351480
C	-3.401134	-3.185814	-2.128575
H	-3.007348	-1.117568	-1.686992
C	-3.052529	-4.514261	-1.884129
H	-1.729743	-5.842412	-0.809857
H	-4.197810	-2.950135	-2.836156
H	-3.577929	-5.321199	-2.397583
C	1.305892	-1.315291	-1.450180
H	0.887383	-2.280305	-1.167936
C	2.563821	-1.219732	-1.906192
H	2.940104	-0.224208	-2.166893
C	3.496143	-2.370165	-2.060266
O	0.835653	0.978866	-1.795881
C	0.517592	-0.080465	-1.305244
H	-3.760456	-0.746559	0.648032
O	1.313422	-0.054906	1.239489
C	2.500680	0.285086	0.984724
C	2.895231	1.629447	0.700504
C	3.570581	-0.651342	0.838335
C	4.198915	1.998605	0.410078
C	4.874091	-0.290772	0.537254
C	5.203728	1.039433	0.296002
F	3.296368	-1.953918	1.009625
F	5.813318	-1.234383	0.411403
F	4.498385	3.282223	0.197572
F	1.963501	2.589045	0.776061
F	6.461086	1.395176	0.004057
H	3.021129	-3.321866	-1.788554
H	4.382918	-2.223420	-1.423409
H	3.861378	-2.431854	-3.097272

Me_Michael_Acceptor/C6F5OH

Frequencies, energies and thermodynamic properties:

Lowest Vibrational Mode (1/cm) = 111.0785

2nd Lowest Vibrational Mode (1/cm) = 141.1056

E(RM062X) (a.u.) = -802.732617403

Thermal correction to Enthalpy (a.u.) = 0.075937

Thermal correction to Gibbs Free Energy (a.u.) = 0.029109

Total Entropy (cal/Kmol) = 98.557

Esp(RM062X) (a.u.) = -803.686675322

Optimised cartesian coordinates (Angstrom):

C	-0.234767	1.367630	-0.000143
C	1.071480	0.891834	0.000088
C	1.323220	-0.477089	-0.000141
C	0.255627	-1.367778	0.000104
C	-1.046230	-0.882459	-0.000210
C	-1.319165	0.486396	0.000091
O	-2.565435	0.976289	-0.000016
F	-2.074173	-1.730692	-0.000105
F	0.478209	-2.671996	0.000128
F	2.569392	-0.926193	-0.000068
F	2.082269	1.746196	0.000114
F	-0.452829	2.675256	-0.000055
H	-3.203310	0.245342	0.001266

Me_Michael_Acceptor/cycl-R_rot

Frequencies, energies and thermodynamic properties:

Lowest Vibrational Mode (1/cm) = 14.6168

2nd Lowest Vibrational Mode (1/cm) = 18.9956

E(RM062X) (a.u.) = -2890.51631942

Thermal correction to Enthalpy (a.u.) = 0.701812

Thermal correction to Gibbs Free Energy (a.u.) = 0.581546

Total Entropy (cal/Kmol) = 253.121

Esp(RM062X) (a.u.) = -2893.12138078

Optimised cartesian coordinates (Angstrom):

C	0.307192	-1.149736	-2.851552
C	-1.069551	-1.018909	-3.474428
H	-1.251361	-1.891297	-4.118839
H	0.373470	-2.127154	-2.356401
H	1.080851	-1.114365	-3.631567
N	-0.520046	0.582444	-1.129076
C	-0.274693	1.826265	-0.464566
C	-0.400805	1.941307	0.926232
C	0.076170	2.954445	-1.221584
C	-0.145951	3.151524	1.561355
H	-0.718545	1.084021	1.513192
C	0.336312	4.168896	-0.596917
H	0.150320	2.864703	-2.301276
C	0.228395	4.243943	0.787452
H	-0.236462	3.250206	2.641987
H	0.610400	5.052246	-1.171368
N	0.503510	5.525672	1.454091
O	0.832287	6.462878	0.763535
O	0.387748	5.573093	2.657463
C	0.683813	0.038736	-1.932409
O	1.358005	0.944980	-2.489699
C	-1.301791	0.257305	-4.270520
S	-2.291397	-1.245114	-2.134638
C	-1.776125	0.042891	-1.007496
N	-2.595230	0.443329	-0.106938
C	-3.933343	0.105098	-0.043504
C	-4.856123	0.558353	-1.010255
C	-4.409181	-0.638993	1.053787
C	-6.205647	0.266554	-0.891240
H	-4.494683	1.150067	-1.852194
C	-5.757629	-0.940219	1.177155
H	-3.696126	-0.969173	1.809887
C	-6.640189	-0.484342	0.200640
H	-6.925710	0.613673	-1.630978

H -6.133568 -1.519086 2.019512
N -8.064250 -0.795953 0.328337
O -8.419457 -1.447168 1.285964
O -8.814070 -0.387767 -0.530737
N 1.575492 -0.658058 -0.752165
C 2.867314 -0.453125 -0.727213
C 0.991766 -1.696109 0.101783
S 3.697009 0.859156 -1.565231
N 3.723174 -1.218640 -0.010280
C 1.955292 -2.898699 0.151447
H 0.073693 -2.030730 -0.401508
C 0.579444 -1.177015 1.464436
C 5.216463 0.350037 -0.827926
C 5.049222 -0.778635 -0.021276
C 3.308339 -2.441385 0.677399
C 1.397173 -4.132593 0.896576
H 2.094958 -3.187545 -0.904072
C -0.673080 -1.542450 1.968608
C 1.421171 -0.380146 2.250577
C 6.471817 0.931685 -0.985020
C 6.124689 -1.346263 0.661068
H 4.072578 -3.208014 0.486429
H 3.283028 -2.245910 1.760118
C 1.680728 -4.158936 2.400959
C 1.919388 -5.416348 0.249661
H 0.302799 -4.108754 0.758427
C -1.075184 -1.132809 3.240388
H -1.344139 -2.145709 1.350986
C 1.021273 0.029011 3.522236
H 2.389695 -0.047625 1.870859
C 7.553016 0.368693 -0.307334
H 6.603502 1.809664 -1.619684
C 7.378454 -0.755968 0.506372
H 5.991892 -2.220266 1.298748
H 1.390189 -3.228897 2.909617
H 1.122375 -4.984136 2.866663
H 2.749413 -4.338571 2.598589
H 1.625354 -5.482974 -0.808076
H 3.019297 -5.460575 0.299914
H 1.526875 -6.302864 0.769059
C -0.226694 -0.347313 4.021563
H -2.056121 -1.423371 3.621246
H 1.684126 0.655431 4.121696
H 8.543303 0.813541 -0.412399
H 8.234607 -1.181287 1.031726
H -0.540292 -0.022572 5.015090
H -2.299301 0.249977 -4.730841
H -0.548234 0.334338 -5.068692
H -1.211305 1.150152 -3.636671

Me_Michael_Acceptor/cycl-R

Frequencies, energies and thermodynamic properties:

Lowest Vibrational Mode (1/cm) = 9.9210

2nd Lowest Vibrational Mode (1/cm) = 15.8179

E(RM062X) (a.u.) = -2890.52310822

Thermal correction to Enthalpy (a.u.) = 0.701846

Thermal correction to Gibbs Free Energy (a.u.) = 0.580234

Total Entropy (cal/Kmol) = 255.953

Esp(RM062X) (a.u.) = -2893.13007809

Optimised cartesian coordinates (Angstrom):

C 1.512266 -2.842279 -1.678695
C 2.298332 -0.283019 -0.609000
C -0.086601 -0.995988 -1.217775

C	0.290826	-2.449764	-0.882997
H	0.459590	-2.616017	0.190968
H	-0.560712	-3.069185	-1.205546
N	0.946702	-0.066050	-0.523238
C	0.521380	1.244940	-0.182665
C	-0.272592	1.983622	-1.069162
C	0.834464	1.771636	1.080363
C	-0.799937	3.211283	-0.678793
H	-0.478808	1.566960	-2.054738
C	0.326914	3.000739	1.473569
H	1.470343	1.200707	1.757246
C	-0.500851	3.692345	0.590900
H	-1.433519	3.792868	-1.347102
H	0.550885	3.419275	2.453732
N	-1.084750	4.968065	1.025356
O	-0.937151	5.289079	2.183448
O	-1.688523	5.622453	0.207250
O	-0.269841	-0.738643	-2.445216
S	2.953771	-1.872569	-1.096827
N	3.125564	0.658704	-0.333963
C	4.498218	0.519501	-0.277758
C	5.124161	-0.253953	0.722876
C	5.304046	1.228648	-1.191048
C	6.506506	-0.327778	0.800573
H	4.507932	-0.793287	1.443652
C	6.686882	1.156613	-1.122866
H	4.816852	1.835290	-1.954960
C	7.272054	0.377212	-0.126397
H	6.998655	-0.922127	1.569110
H	7.316949	1.695159	-1.829376
N	8.731244	0.300527	-0.047679
O	9.377387	0.928686	-0.856865
O	9.217608	-0.387723	0.822497
H	1.341339	-2.567333	-2.727752
C	1.872366	-4.314167	-1.558780
N	-1.400003	-0.706218	-0.379039
C	-2.497438	-0.353054	-1.012210
C	-1.411407	-0.831901	1.086873
S	-2.678215	-0.280287	-2.763987
N	-3.639611	-0.023983	-0.371557
C	-2.334822	0.263859	1.659420
H	-0.388774	-0.606137	1.416814
C	-1.739696	-2.236681	1.559451
C	-4.382371	0.127303	-2.557383
C	-4.730761	0.226636	-1.209378
C	-3.729647	0.097872	1.082310
C	-2.329312	0.384412	3.198470
H	-1.929033	1.208647	1.259892
C	-1.019363	-2.766488	2.636128
C	-2.759953	-3.002335	0.985047
C	-5.327500	0.352495	-3.555392
C	-6.032482	0.539016	-0.817742
H	-4.343451	0.981160	1.305738
H	-4.241970	-0.790494	1.483099
C	-3.328290	-0.528061	3.916693
C	-2.585010	1.837004	3.606616
H	-1.311644	0.112995	3.528425
C	-1.330106	-4.023965	3.150656
H	-0.204900	-2.184286	3.075093
C	-3.070695	-4.262747	1.497592
H	-3.318914	-2.628502	0.123687
C	-6.630501	0.668325	-3.173148
H	-5.053640	0.280185	-4.609408

C	-6.976270	0.758370	-1.819865
H	-6.308733	0.604577	0.234650
H	-3.261952	-1.578299	3.600686
H	-3.148720	-0.492021	5.001217
H	-4.361428	-0.184779	3.748507
H	-1.840965	2.523049	3.175213
H	-3.580820	2.165906	3.267894
H	-2.555788	1.945528	4.700750
C	-2.362212	-4.773724	2.585101
H	-0.760397	-4.422260	3.991949
H	-3.869144	-4.849332	1.040049
H	-7.387284	0.844249	-3.938574
H	-8.001712	1.002781	-1.539560
H	-2.606615	-5.759715	2.983736
H	2.018782	-4.600820	-0.506948
H	1.055344	-4.921253	-1.975720
H	2.789913	-4.551496	-2.116983

Me_Michael_Acceptor/cycl-S_rot

Frequencies, energies and thermodynamic properties:

Lowest Vibrational Mode (1/cm) = 10.9628

2nd Lowest Vibrational Mode (1/cm) = 14.6435

E(RM062X) (a.u.) = -2890.52022205

Thermal correction to Enthalpy (a.u.) = 0.701973

Thermal correction to Gibbs Free Energy (a.u.) = 0.580378

Total Entropy (cal/Kmol) = 255.919

Esp(RM062X) (a.u.) = -2893.12557609

Optimised cartesian coordinates (Angstrom):

C	1.534535	-3.005647	-1.488856
C	2.302094	-0.371386	-0.565671
C	-0.083181	-1.064129	-1.189929
C	0.258456	-2.516341	-0.825959
H	0.343995	-2.650537	0.260764
H	-0.586069	-3.125037	-1.184223
N	0.950898	-0.135242	-0.508426
C	0.540813	1.193633	-0.216465
C	-0.242087	1.915231	-1.126466
C	0.860710	1.756992	1.029279
C	-0.749640	3.163427	-0.776276
H	-0.456473	1.470323	-2.097382
C	0.373442	3.006105	1.381776
H	1.487248	1.199341	1.725700
C	-0.442716	3.681998	0.476380
H	-1.374169	3.732190	-1.463887
H	0.604114	3.452527	2.347926
N	-1.004489	4.981316	0.867623
O	-0.849549	5.339319	2.013875
O	-1.598561	5.617376	0.028228
O	-0.285132	-0.807370	-2.413090
S	2.954266	-1.997780	-0.911077
N	3.134615	0.579106	-0.346288
C	4.505802	0.434281	-0.265421
C	5.115586	-0.231022	0.818916
C	5.324969	1.031329	-1.244296
C	6.496565	-0.307142	0.917029
H	4.487782	-0.683455	1.587922
C	6.706512	0.954552	-1.156549
H	4.849934	1.555019	-2.074331
C	7.276075	0.285036	-0.074941
H	6.976922	-0.817605	1.750544
H	7.347032	1.406780	-1.912437
N	8.733997	0.205896	0.025751
O	9.392471	0.715150	-0.853908

O	9.206756	-0.365152	0.983756
H	1.767365	-3.996360	-1.072385
C	1.506285	-3.103964	-3.008224
N	-1.405590	-0.745533	-0.332895
C	-2.503362	-0.398202	-0.965942
C	-1.406759	-0.820081	1.136431
S	-2.702738	-0.379275	-2.718753
N	-3.636828	-0.033687	-0.326852
C	-2.309125	0.307626	1.680782
H	-0.377928	-0.598961	1.450256
C	-1.752657	-2.201757	1.662051
C	-4.400531	0.050554	-2.509115
C	-4.733320	0.201003	-1.161863
C	-3.711298	0.141279	1.122103
C	-2.288106	0.479359	3.215007
H	-1.894197	1.232909	1.246411
C	-1.027654	-2.704289	2.748588
C	-2.792828	-2.970552	1.128615
C	-5.353110	0.252669	-3.504880
C	-6.026959	0.543860	-0.768722
H	-4.310401	1.040828	1.319198
H	-4.232536	-0.724234	1.559579
C	-3.292106	-0.394850	3.972845
C	-2.522189	1.947802	3.576705
H	-1.270918	0.206162	3.545280
C	-1.353063	-3.936224	3.313482
H	-0.197933	-2.120545	3.155628
C	-3.118233	-4.205483	1.691613
H	-3.356942	-2.619247	0.261193
C	-6.648301	0.597686	-3.121035
H	-5.091070	0.140668	-4.558416
C	-6.978574	0.739672	-1.768471
H	-6.291745	0.650405	0.283291
H	-3.240676	-1.456545	3.694842
H	-3.103634	-0.321744	5.053990
H	-4.322411	-0.045456	3.799977
H	-1.774514	2.609783	3.115346
H	-3.517328	2.277219	3.236659
H	-2.480870	2.092460	4.666260
C	-2.405034	-4.688117	2.788991
H	-0.779490	-4.312886	4.162083
H	-3.932330	-4.794604	1.265991
H	-7.410865	0.755944	-3.884599
H	-7.997871	1.006904	-1.486543
H	-2.661338	-5.654050	3.227271
H	1.345214	-2.120975	-3.463746
H	0.679453	-3.764010	-3.314172
H	2.446034	-3.537348	-3.379081

Me_Michael_Acceptor/cycl-S

Frequencies, energies and thermodynamic properties:

Lowest Vibrational Mode (1/cm) = 7.9531

2nd Lowest Vibrational Mode (1/cm) = 18.1811

E(RM062X) (a.u.) = -2890.51608262

Thermal correction to Enthalpy (a.u.) = 0.701853

Thermal correction to Gibbs Free Energy (a.u.) = 0.579743

Total Entropy (cal/Kmol) = 257.002

Esp(RM062X) (a.u.) = -2893.12243592

Optimised cartesian coordinates (Angstrom):

C	-0.273153	-1.363709	2.731307
C	1.089343	-1.235253	3.373373
H	1.191577	-0.251845	3.856404
H	-0.299686	-2.298019	2.152776

H	-1.050920	-1.421191	3.506350
N	0.523311	0.538139	1.186017
C	0.251615	1.831328	0.637275
C	0.363056	2.075375	-0.737886
C	-0.116160	2.876856	1.497533
C	0.075810	3.332842	-1.257434
H	0.694521	1.282588	-1.402736
C	-0.409166	4.136908	0.988867
H	-0.173387	2.685957	2.565009
C	-0.316153	4.340567	-0.383786
H	0.154247	3.532039	-2.325126
H	-0.697129	4.957706	1.643676
N	-0.627920	5.671041	-0.927645
O	-0.970186	6.533007	-0.150997
O	-0.527311	5.831072	-2.122622
C	-0.676770	-0.103326	1.927395
O	-1.361385	0.735256	2.571739
C	1.386617	-2.341917	4.372867
S	2.331366	-1.321679	2.037614
C	1.785135	0.030893	1.005961
N	2.587680	0.510780	0.129316
C	3.931242	0.203482	0.031482
C	4.851493	0.583877	1.031716
C	4.414252	-0.430313	-1.130204
C	6.204890	0.325321	0.883312
H	4.485359	1.092330	1.924355
C	5.766595	-0.698415	-1.283433
H	3.703902	-0.701048	-1.912036
C	6.646144	-0.318640	-0.272227
H	6.922724	0.616632	1.648886
H	6.148149	-1.193248	-2.175363
N	8.073997	-0.597058	-0.430662
O	8.433675	-1.163281	-1.439326
O	8.822238	-0.248485	0.455595
N	-1.555834	-0.694035	0.693732
C	-2.850227	-0.496550	0.685594
C	-0.964985	-1.645980	-0.251864
S	-3.690852	0.729137	1.634907
N	-3.698406	-1.201033	-0.098691
C	-1.918342	-2.847477	-0.408917
H	-0.042810	-2.016404	0.217612
C	-0.565282	-1.002311	-1.564047
C	-5.204617	0.279502	0.848329
C	-5.027457	-0.772288	-0.054211
C	-3.274243	-2.354117	-0.892319
C	-1.353221	-4.004031	-1.264915
H	-2.054501	-3.232417	0.615869
C	0.686853	-1.308117	-2.107195
C	-1.420504	-0.147425	-2.270587
C	-6.464197	0.838018	1.050040
C	-6.096352	-1.283977	-0.789241
H	-4.033219	-3.139638	-0.771515
H	-3.248516	-2.061694	-1.953021
C	-1.639782	-3.895137	-2.765126
C	-1.867611	-5.344762	-0.738148
H	-0.258671	-3.986060	-1.126881
C	1.075522	-0.781538	-3.339452
H	1.368493	-1.957800	-1.551399
C	-1.034447	0.378016	-3.502967
H	-2.389183	0.140411	-1.856963
C	-7.538756	0.331562	0.319349
H	-6.603964	1.655654	1.759160
C	-7.354024	-0.715970	-0.589638

H	-5.955633	-2.097076	-1.501579
H	-1.356317	-2.921089	-3.188207
H	-1.077167	-4.671238	-3.304364
H	-2.707720	-4.063556	-2.976366
H	-1.574285	-5.505750	0.309548
H	-2.967289	-5.390578	-0.794155
H	-1.469291	-6.177757	-1.335783
C	0.213719	0.061589	-4.041829
H	2.056704	-1.026178	-3.750633
H	-1.708347	1.048308	-4.039338
H	-8.532011	0.760453	0.457626
H	-8.205234	-1.097164	-1.155364
H	0.517043	0.477406	-5.004094
H	0.662619	-2.288163	5.198565
H	1.297695	-3.332080	3.901117
H	2.396975	-2.243514	4.794194

Me_Michael_Acceptor/HyperBTM

Frequencies, energies and thermodynamic properties:

Lowest Vibrational Mode (1/cm) = 26.7604

2nd Lowest Vibrational Mode (1/cm) = 57.9421

E(RM062X) (a.u.) = -1242.68108630

Thermal correction to Enthalpy (a.u.) = 0.371678

Thermal correction to Gibbs Free Energy (a.u.) = 0.305623

Total Entropy (cal/Kmol) = 139.024

Esp(RM062X) (a.u.) = -1243.74354485

Optimised cartesian coordinates (Angstrom):

C	-4.262530	0.973031	1.705921
C	-5.081884	0.026598	1.089062
C	-4.570448	-0.806552	0.088982
C	-3.238265	-0.667538	-0.277562
C	-2.412615	0.292849	0.336285
C	-2.921403	1.115944	1.340791
H	-4.669698	1.613207	2.490089
H	-6.126268	-0.070457	1.387912
H	-5.203340	-1.552803	-0.394046
H	-2.284078	1.850300	1.833836
C	-0.852054	-0.663172	-1.127167
C	1.406622	-0.103443	-1.317985
C	0.986323	1.302948	-0.824072
C	-0.065141	1.190869	0.277299
H	-0.509874	2.177247	0.477622
S	-2.342062	-1.583659	-1.484368
N	-1.120558	0.291010	-0.162611
N	0.251017	-0.908789	-1.701688
C	2.161531	2.231026	-0.444693
C	2.601261	2.139383	1.019395
C	1.826137	3.682431	-0.791325
H	3.015788	1.927239	-1.073553
H	2.788244	1.106938	1.347021
H	3.529866	2.711096	1.165556
H	1.842194	2.577462	1.687042
H	1.618759	3.801777	-1.864957
H	0.937651	4.022659	-0.235092
H	2.658630	4.352142	-0.528432
H	0.480326	1.757972	-1.692374
H	2.009511	0.051835	-2.226024
C	2.288128	-0.851872	-0.332650
C	3.679294	-0.826890	-0.482869
C	1.743460	-1.531774	0.763657
C	4.511225	-1.434125	0.457769
H	4.115252	-0.320870	-1.347869
C	2.572640	-2.139839	1.706383

H 0.659540 -1.591953 0.887188
C 3.959687 -2.086725 1.560541
H 5.594333 -1.401918 0.325517
H 2.131945 -2.662349 2.557484
H 4.607870 -2.563537 2.297932
H 0.371335 0.818121 1.218567

Me_Michael_Acceptor/MA-R_pt_rot

Frequencies, energies and thermodynamic properties:

Lowest Vibrational Mode (1/cm) = 12.3327
2nd Lowest Vibrational Mode (1/cm) = 17.2725
E(RM062X) (a.u.) = -2890.52043429
Thermal correction to Enthalpy (a.u.) = 0.701818
Thermal correction to Gibbs Free Energy (a.u.) = 0.581463
Total Entropy (cal/Kmol) = 253.307
Esp(RM062X) (a.u.) = -2893.12629120

Optimised cartesian coordinates (Angstrom):

C 5.062028 -1.448523 -2.428759
C 5.366933 -2.298905 -1.353776
C 4.907980 -2.022167 -0.071151
C 4.122628 -0.881646 0.106210
C 3.825346 -0.036311 -0.963292
H 5.956120 -3.200222 -1.527651
H 5.129476 -2.689406 0.763168
C 2.581150 0.946406 0.694956
C 1.167941 2.938778 0.389149
C 2.282283 3.330655 -0.600526
C 2.661734 2.135888 -1.459252
H 3.559344 2.357172 -2.052403
S 3.341607 -0.340215 1.574896
N 2.992546 1.016665 -0.574166
N 1.640747 1.779570 1.196278
C 1.959873 4.590147 -1.438754
C 1.246750 4.306562 -2.763841
C 3.245025 5.376917 -1.700262
H 1.299414 5.221955 -0.822274
H 0.349455 3.682878 -2.647525
H 0.937649 5.255732 -3.225041
H 1.923338 3.806421 -3.474601
H 3.719484 5.697617 -0.761408
H 3.972251 4.764787 -2.257765
H 3.035197 6.273551 -2.301218
H 3.159072 3.568263 0.024019
H 1.070616 3.776508 1.091913
C -0.166148 2.690256 -0.274681
C -1.111644 3.718977 -0.315512
C -0.435341 1.485033 -0.926054
C -2.293782 3.559329 -1.036995
H -0.916523 4.655954 0.212593
C -1.617619 1.321116 -1.645106
H 0.275207 0.658790 -0.859039
C -2.542020 2.364704 -1.713959
H -3.023753 4.369860 -1.070015
H -1.822801 0.372908 -2.146811
H -3.467294 2.236691 -2.278719
C -0.109127 2.242644 2.956852
H -0.488225 2.952457 2.218042
C -1.279751 1.347967 3.416493
C -0.930263 0.246674 4.407469
O 1.751089 0.784640 3.232403
C 1.133953 1.520776 2.506702
H 1.856132 1.830008 -2.141826
C 4.294469 -0.303326 -2.251599

H 4.048707 0.347326 -3.090694
H 5.426270 -1.694329 -3.426917
H -1.951710 2.051583 3.932137
S -2.421789 0.836955 2.077132
C -1.657504 -0.558427 1.207742
N -0.392997 -0.768744 1.492654
N -2.388474 -1.335254 0.433460
C 0.316342 -1.774201 0.876416
C 1.119625 -2.622780 1.677697
C 0.373475 -1.956770 -0.528225
C 1.985611 -3.545190 1.118231
H 1.063916 -2.510672 2.761537
C 1.256840 -2.860781 -1.100885
H -0.283229 -1.367075 -1.166529
C 2.067798 -3.637221 -0.273271
H 2.614339 -4.181490 1.740312
H 1.330762 -2.969490 -2.182561
N 3.060609 -4.516522 -0.870268
O 3.091756 -4.612899 -2.078957
O 3.828990 -5.096524 -0.129602
C -3.684418 -1.223605 0.048290
C -4.346134 -2.436300 -0.306131
C -4.433669 -0.021731 -0.106247
C -5.653444 -2.462474 -0.746250
H -3.776051 -3.361297 -0.210244
C -5.744371 -0.040746 -0.554297
H -3.969157 0.939569 0.100319
C -6.353633 -1.256630 -0.866473
H -6.146164 -3.399920 -1.001479
H -6.305560 0.885697 -0.672700
N -7.727797 -1.269269 -1.332491
O -8.311015 -0.208207 -1.433030
O -8.232749 -2.340705 -1.601490
H 0.218434 2.817478 3.838941
H -0.359782 0.670552 5.247897
H -0.327600 -0.535664 3.935213
H -1.854933 -0.198164 4.800559

Me_Michael_Acceptor/MA-R_pt

Frequencies, energies and thermodynamic properties:

Lowest Vibrational Mode (1/cm) = 10.4402
2nd Lowest Vibrational Mode (1/cm) = 19.1989
E(RM062X) (a.u.) = -2890.53315300
Thermal correction to Enthalpy (a.u.) = 0.702243
Thermal correction to Gibbs Free Energy (a.u.) = 0.581687
Total Entropy (cal/Kmol) = 253.731
Esp(RM062X) (a.u.) = -2893.13820633

Optimised cartesian coordinates (Angstrom):

C -5.415150 -1.251116 -2.256225
C -6.257495 -1.156030 -1.139106
C -5.840646 -0.506763 0.017911
C -4.560026 0.044992 0.028984
C -3.719098 -0.062500 -1.080373
H -7.249612 -1.607092 -1.171887
H -6.487736 -0.441135 0.893597
C -2.301754 0.964101 0.405969
C -0.061696 1.801534 -0.148479
C -0.058903 0.716584 -1.235208
C -1.427608 0.569330 -1.868726
H -1.476902 -0.359063 -2.452939
S -3.746490 0.825831 1.366426
N -2.456914 0.488011 -0.829372
N -1.143944 1.523801 0.825649

C	1.070688	0.881224	-2.276671
C	0.712824	1.749891	-3.485131
C	1.544421	-0.497285	-2.738844
H	1.910132	1.364660	-1.748317
H	0.299846	2.729439	-3.204543
H	1.613581	1.927183	-4.090536
H	-0.018105	1.241470	-4.133905
H	1.883557	-1.105863	-1.887612
H	0.729993	-1.041787	-3.244756
H	2.377372	-0.406504	-3.451580
H	0.144208	-0.215145	-0.690843
H	0.879732	1.662497	0.394587
C	-0.128668	3.226920	-0.652013
C	1.062097	3.950837	-0.778640
C	-1.333567	3.818342	-1.048034
C	1.055227	5.234242	-1.323394
H	2.002147	3.499147	-0.450230
C	-1.340744	5.103184	-1.590760
H	-2.281730	3.286079	-0.933890
C	-0.146360	5.809994	-1.736774
H	1.990758	5.787510	-1.420354
H	-2.285123	5.554959	-1.898574
H	-0.154438	6.814800	-2.162257
C	0.349496	2.353244	2.700594
H	0.010852	3.026886	3.500740
C	1.334154	1.353845	3.343578
C	2.176525	2.068390	4.398256
O	-1.841125	1.492100	2.981901
C	-0.945271	1.742657	2.214915
H	-1.683727	1.415694	-2.524959
C	-4.136513	-0.703811	-2.247695
H	-3.485457	-0.790275	-3.116974
H	-5.761810	-1.774320	-3.147941
H	0.770504	0.529679	3.797785
S	2.515879	0.591881	2.169216
C	1.598795	-0.829401	1.469213
N	2.251043	-1.690558	0.737939
C	3.554308	-1.608773	0.322992
C	4.368808	-2.761320	0.442517
C	4.112468	-0.470556	-0.310744
C	5.674677	-2.774135	-0.014618
H	3.937015	-3.646145	0.911555
C	5.417549	-0.476342	-0.776623
H	3.497299	0.419000	-0.448485
C	6.190383	-1.626602	-0.620208
H	6.301815	-3.658776	0.088116
H	5.844474	0.397635	-1.266985
N	7.563654	-1.634301	-1.110251
O	7.990928	-0.624110	-1.627955
O	8.211469	-2.650427	-0.975991
N	0.333515	-0.875207	1.843388
C	-0.598580	-1.727033	1.317060
C	-0.506964	-2.436673	0.083765
C	-1.828760	-1.823478	2.022398
C	-1.608545	-3.089117	-0.449958
H	0.434261	-2.441716	-0.459958
C	-2.919919	-2.498656	1.509017
H	-1.904603	-1.300740	2.977277
C	-2.813105	-3.104025	0.254253
H	-1.545891	-3.590592	-1.415559
H	-3.866225	-2.538319	2.048265
N	-3.986539	-3.722472	-0.341310
O	-4.995743	-3.801015	0.328680

O	-3.903463	-4.128090	-1.483005
H	0.850401	2.974110	1.947752
H	1.520220	2.488733	5.173973
H	2.880114	1.372792	4.874401
H	2.752341	2.895072	3.954208

Me_Michael_Acceptor/MA-R

Frequencies, energies and thermodynamic properties:

Lowest Vibrational Mode (1/cm) = 8.8863

2nd Lowest Vibrational Mode (1/cm) = 12.1737

E(RM062X) (a.u.) = -2890.52259154

Thermal correction to Enthalpy (a.u.) = 0.702426

Thermal correction to Gibbs Free Energy (a.u.) = 0.576570

Total Entropy (cal/Kmol) = 264.886

Esp(RM062X) (a.u.) = -2893.13184347

Optimised cartesian coordinates (Angstrom):

C	6.577701	2.997548	-2.120738
C	5.637128	4.034692	-2.081844
C	4.325800	3.791619	-1.680447
C	3.978398	2.490242	-1.323161
C	4.915241	1.457122	-1.374527
H	5.933553	5.045420	-2.364692
H	3.589784	4.596438	-1.643659
C	3.070762	0.295438	-0.607290
C	3.071954	-2.073112	-0.034224
C	4.172948	-2.181164	-1.103936
C	5.129327	-1.009540	-0.989465
H	5.802759	-0.983442	-1.856100
S	2.412356	1.913523	-0.767721
N	4.360729	0.233736	-0.984660
N	2.405004	-0.760861	-0.147232
C	4.897147	-3.546816	-1.123641
C	6.124781	-3.628069	-0.211787
C	5.292866	-3.905843	-2.556542
H	4.165716	-4.296899	-0.780513
H	5.919913	-3.302792	0.817850
H	6.484826	-4.666383	-0.169752
H	6.949991	-3.014807	-0.607429
H	5.977043	-3.150149	-2.975125
H	5.811470	-4.875242	-2.585240
H	4.413246	-3.969073	-3.213488
H	3.646243	-2.073808	-2.066308
H	2.311697	-2.815835	-0.303659
C	3.535578	-2.348470	1.382369
C	4.155028	-1.365049	2.160619
C	3.393673	-3.639101	1.903885
C	4.650602	-1.676507	3.427121
H	4.252517	-0.341388	1.789913
C	3.890397	-3.951797	3.167994
H	2.889075	-4.405994	1.310736
C	4.526814	-2.971536	3.930452
H	5.132494	-0.900593	4.024312
H	3.774539	-4.963087	3.561473
H	4.914841	-3.213359	4.921308
C	0.387227	-1.674102	0.894832
H	0.854775	-2.640177	1.063559
C	-1.011118	-1.480421	1.358770
C	-1.439629	-2.521580	2.383310
O	0.523853	0.527359	0.076950
C	1.017582	-0.617965	0.298397
H	5.738503	-1.053777	-0.073858
C	6.233156	1.695099	-1.767629
H	6.973870	0.895801	-1.791669

H 7.601867 3.209698 -2.430149
H -1.151731 -0.468803 1.765303
S -2.261270 -1.558979 -0.073707
C -3.014726 0.074181 -0.063376
N -2.125248 1.089266 0.136627
H -1.115989 0.821391 0.110636
C -2.354481 2.439601 0.349226
C -1.212362 3.206430 0.678511
C -3.607579 3.077374 0.264078
C -1.311456 4.564775 0.911781
H -0.249540 2.697345 0.753104
C -3.705889 4.442618 0.505718
H -4.491064 2.503849 0.003095
C -2.565285 5.171801 0.823750
H -0.435523 5.158870 1.167756
H -4.668364 4.948543 0.441740
N -2.679852 6.608273 1.070098
O -3.779497 7.111607 1.002920
O -1.667279 7.221434 1.328923
N -4.268081 0.277362 -0.230678
C -5.212518 -0.705120 -0.461046
C -6.353668 -0.749943 0.364370
C -5.114002 -1.610732 -1.536412
C -7.351413 -1.686975 0.146834
H -6.433560 -0.036315 1.185036
C -6.112522 -2.546200 -1.767213
H -4.250411 -1.562686 -2.201421
C -7.216742 -2.575772 -0.918658
H -8.231202 -1.736697 0.786780
H -6.045569 -3.250123 -2.595531
N -8.270128 -3.564602 -1.156874
O -9.224258 -3.567538 -0.411125
O -8.131997 -4.328448 -2.086375
H -0.759040 -2.480915 3.247468
H -1.385985 -3.535307 1.958229
H -2.465999 -2.346299 2.731348

Me_Michael_Acceptor/MA-S_pt_rot

Frequencies, energies and thermodynamic properties:

Lowest Vibrational Mode (1/cm) = 6.8077

2nd Lowest Vibrational Mode (1/cm) = 14.0310

E(RM062X) (a.u.) = -2890.51922515

Thermal correction to Enthalpy (a.u.) = 0.702591

Thermal correction to Gibbs Free Energy (a.u.) = 0.579968

Total Entropy (cal/Kmol) = 258.082

Esp(RM062X) (a.u.) = -2893.13771810

Optimised cartesian coordinates (Angstrom):

C -3.377495 4.150335 -1.178237
C -2.415560 4.415104 -2.165073
C -1.549423 3.421388 -2.605833
C -1.657543 2.158974 -2.021874
C -2.600910 1.904249 -1.026811
H -2.344796 5.415682 -2.592327
H -0.801341 3.625430 -3.373214
C -1.541818 -0.131510 -1.121872
C -2.207963 -2.097245 0.178415
C -2.679531 -1.076964 1.222252
C -3.347130 0.105014 0.546067
H -3.467068 0.933458 1.257903
S -0.678984 0.744977 -2.346680
N -2.497450 0.595566 -0.540507
N -1.299365 -1.415904 -0.773192
C -3.534854 -1.688682 2.353917

C	-5.036721	-1.733427	2.061833
C	-3.272995	-0.943712	3.663640
H	-3.185061	-2.726418	2.489256
H	-5.476887	-0.723921	2.085130
H	-5.273032	-2.189751	1.089842
H	-5.545872	-2.322535	2.837950
H	-2.219074	-1.020584	3.969404
H	-3.527369	0.125182	3.573717
H	-3.888455	-1.357843	4.475121
H	-1.741103	-0.706420	1.664455
H	-1.598202	-2.812875	0.735258
C	-3.293825	-2.869707	-0.539473
C	-3.618389	-4.151359	-0.082325
C	-4.019051	-2.321845	-1.604430
C	-4.667741	-4.865216	-0.659033
H	-3.050780	-4.597418	0.739200
C	-5.067135	-3.036338	-2.182887
H	-3.775039	-1.333639	-2.003010
C	-5.397725	-4.305637	-1.706989
H	-4.911208	-5.863050	-0.290985
H	-5.626034	-2.599735	-3.011907
H	-6.218768	-4.862436	-2.161423
C	0.311389	-3.307717	-0.576377
H	1.063969	-3.777440	-1.221762
C	0.939779	-2.951529	0.789800
C	1.159735	-4.208259	1.623486
O	0.448044	-1.571313	-2.213333
C	-0.143967	-2.067759	-1.292153
H	-4.334228	-0.145364	0.126576
C	-3.486911	2.894138	-0.594303
H	-4.232105	2.704742	0.178488
H	-4.040326	4.949598	-0.844414
H	0.316185	-2.226397	1.334832
S	2.527361	-2.085031	0.560650
C	2.114213	-0.305363	0.713994
N	3.071059	0.526677	0.432355
N	0.880910	-0.019394	1.105043
C	4.391007	0.224008	0.238637
C	5.175009	-0.440139	1.214634
C	5.036960	0.663670	-0.941412
C	6.525867	-0.668979	1.013479
H	4.701599	-0.765902	2.141524
C	6.385595	0.435025	-1.152418
H	4.441423	1.185342	-1.691400
C	7.120226	-0.233176	-0.171489
H	7.129983	-1.177303	1.764007
H	6.879551	0.763993	-2.065839
N	8.541457	-0.475596	-0.386961
O	9.037947	-0.079756	-1.420294
O	9.158243	-1.062018	0.477092
C	0.413366	1.267133	1.149933
C	-0.618208	1.565189	2.086028
C	0.820695	2.326352	0.290696
C	-1.254798	2.792201	2.116088
H	-0.884454	0.796795	2.813314
C	0.191803	3.560484	0.321273
H	1.634809	2.151917	-0.407763
C	-0.855737	3.784066	1.215504
H	-2.048885	3.003091	2.832483
H	0.490549	4.358252	-0.358625
N	-1.572392	5.043414	1.178890
O	-2.583646	5.143916	1.845854
O	-1.144986	5.930929	0.469576

H -0.514245 -4.025366 -0.455590
H 1.603087 -3.954317 2.595110
H 1.830428 -4.913341 1.109561
H 0.203066 -4.724559 1.800916

Me_Michael_Acceptor/MA-S_pt

Frequencies, energies and thermodynamic properties:

Lowest Vibrational Mode (1/cm) = 14.3743

2nd Lowest Vibrational Mode (1/cm) = 19.5632

E(RM062X) (a.u.) = -2890.52375835

Thermal correction to Enthalpy (a.u.) = 0.701771

Thermal correction to Gibbs Free Energy (a.u.) = 0.581304

Total Entropy (cal/Kmol) = 253.542

Esp(RM062X) (a.u.) = -2893.13094811

Optimised cartesian coordinates (Angstrom):

C 5.270854 -1.163463 -2.469429
C 5.574754 -2.044310 -1.418401
C 5.059158 -1.840712 -0.143969
C 4.214193 -0.746139 0.047141
C 3.913424 0.126953 -0.998739
H 6.213429 -2.908558 -1.604811
H 5.279636 -2.530948 0.671801
C 2.576712 0.987232 0.655561
C 1.045678 2.893333 0.359660
C 2.152317 3.385532 -0.592573
C 2.633668 2.238433 -1.463729
H 3.526051 2.531648 -2.032465
S 3.360680 -0.303034 1.507289
N 3.018015 1.122506 -0.597445
N 1.583519 1.758881 1.159093
C 1.758007 4.633236 -1.417725
C 1.130504 4.318508 -2.778504
C 2.979010 5.534738 -1.603969
H 1.017824 5.189673 -0.820089
H 0.287771 3.615893 -2.713019
H 0.757790 5.246718 -3.235238
H 1.877852 3.894993 -3.467814
H 3.378188 5.876446 -0.637911
H 3.782976 4.999403 -2.134340
H 2.719700 6.421647 -2.200033
H 2.993002 3.672538 0.060077
H 0.863900 3.707761 1.072711
C -0.246510 2.548482 -0.344900
C -1.252136 3.515733 -0.439619
C -0.419000 1.316459 -0.979566
C -2.393678 3.271685 -1.201302
H -1.134359 4.470580 0.079259
C -1.562878 1.067457 -1.736580
H 0.337168 0.534754 -0.876040
C -2.543885 2.051845 -1.862891
H -3.169778 4.035133 -1.276882
H -1.691105 0.099433 -2.225620
H -3.437632 1.857227 -2.458234
C -0.201388 2.120622 2.911774
H -0.658872 2.774086 2.164172
C -1.246323 1.112656 3.432319
C -2.033143 1.712248 4.594630
O 1.690776 0.707778 3.166279
C 1.070094 1.452347 2.452676
H 1.864282 1.893086 -2.169306
C 4.442494 -0.063838 -2.277788
H 4.196068 0.607813 -3.100235
H 5.684568 -1.349361 -3.461251

H -0.740222 0.190282 3.742623
S -2.469501 0.644396 2.152662
C -1.677112 -0.724394 1.257388
N -0.432397 -0.943265 1.614871
N -2.367809 -1.470699 0.422508
C 0.351982 -1.893810 1.015191
C 1.202723 -2.675063 1.837607
C 0.448748 -2.079472 -0.388456
C 2.148029 -3.529974 1.300672
H 1.117483 -2.555244 2.918525
C 1.409509 -2.915466 -0.936520
H -0.237075 -1.541269 -1.040699
C 2.263095 -3.623696 -0.089146
H 2.812230 -4.112387 1.938593
H 1.513404 -3.023378 -2.015816
N 3.323053 -4.434415 -0.665161
O 3.370726 -4.546987 -1.872184
O 4.126069 -4.947101 0.089355
C -3.654852 -1.349049 0.004899
C -4.298443 -2.548636 -0.417407
C -4.405650 -0.145456 -0.117574
C -5.595008 -2.562961 -0.889708
H -3.725110 -3.473841 -0.346290
C -5.705682 -0.152067 -0.597049
H -3.951693 0.809038 0.137780
C -6.299057 -1.356752 -0.974679
H -6.075814 -3.491144 -1.196238
H -6.269510 0.775657 -0.690104
N -7.662595 -1.356606 -1.473725
O -8.248650 -0.295030 -1.544565
O -8.154562 -2.418374 -1.798172
H 0.121163 2.750690 3.757599
H -1.346355 1.962572 5.416546
H -2.552468 2.634887 4.291958
H -2.781986 1.001836 4.969097

Me_Michael_Acceptor/MA-S

Frequencies, energies and thermodynamic properties:

Lowest Vibrational Mode (1/cm) = 14.8782
2nd Lowest Vibrational Mode (1/cm) = 22.6976
E(RM062X) (a.u.) = -2890.52409555
Thermal correction to Enthalpy (a.u.) = 0.702364
Thermal correction to Gibbs Free Energy (a.u.) = 0.581886
Total Entropy (cal/Kmol) = 253.566
Esp(RM062X) (a.u.) = -2893.12972629

Optimised cartesian coordinates (Angstrom):

C -4.365833 3.834896 1.759681
C -3.188680 4.591451 1.709615
C -1.948884 3.972944 1.564291
C -1.918211 2.584783 1.447421
C -3.094561 1.834051 1.504073
H -3.240308 5.678530 1.779567
H -1.029550 4.559331 1.520053
C -1.553943 0.162274 1.112431
C -2.120790 -2.179324 0.795822
C -3.217043 -1.884024 1.838034
C -3.880875 -0.550591 1.534914
H -4.508226 -0.231937 2.379171
S -0.506795 1.558773 1.224604
N -2.843452 0.465807 1.354582
N -1.153344 -1.062188 0.789862
C -4.227767 -3.038882 2.026399
C -5.449239 -2.978697 1.105236

C	-4.681594	-3.099580	3.485699
H	-3.681898	-3.971475	1.806166
H	-5.184099	-2.880790	0.043113
H	-6.040666	-3.898925	1.218789
H	-6.105794	-2.136047	1.374471
H	-3.832114	-3.264597	4.164292
H	-5.175854	-2.160462	3.782281
H	-5.402355	-3.916625	3.635628
H	-2.676422	-1.764116	2.791317
H	-1.557210	-3.046802	1.160501
C	-2.660146	-2.510213	-0.580709
C	-2.722447	-3.848305	-0.984394
C	-3.177820	-1.523824	-1.427212
C	-3.305787	-4.196835	-2.202167
H	-2.309279	-4.624531	-0.334988
C	-3.756631	-1.868812	-2.648645
H	-3.125928	-0.471746	-1.139137
C	-3.827504	-3.207472	-3.036187
H	-3.348623	-5.245036	-2.502665
H	-4.154457	-1.087668	-3.299376
H	-4.282825	-3.477931	-3.990289
C	0.628822	-2.494376	-0.083176
H	-0.107439	-3.190927	-0.479353
C	2.061421	-2.841815	-0.154905
C	2.314034	-4.338940	-0.266507
O	1.046990	-0.394890	0.905517
C	0.285513	-1.309284	0.531746
H	-4.511791	-0.589367	0.635085
C	-4.337915	2.445423	1.661389
H	-5.257335	1.860475	1.691499
H	-5.326254	4.340105	1.869651
H	2.597020	-2.421690	0.706904
S	3.067556	-2.123883	-1.625684
C	2.603618	-0.386446	-1.676274
N	3.391045	0.580070	-1.399596
N	1.344487	-0.183829	-2.177186
H	0.842009	-1.043392	-2.380322
C	4.536362	0.422509	-0.639902
C	4.448920	-0.087555	0.672239
C	5.780596	0.849514	-1.135864
C	5.584859	-0.190253	1.460031
H	3.461682	-0.366662	1.049910
C	6.922397	0.740649	-0.354778
H	5.835758	1.258398	-2.145238
C	6.809626	0.219713	0.932815
H	5.536076	-0.579422	2.476120
H	7.895818	1.055295	-0.728306
N	8.011617	0.108989	1.760879
O	9.065311	0.470582	1.285155
O	7.891359	-0.339575	2.879621
C	0.549270	0.948877	-2.082001
C	1.030310	2.245846	-1.826959
C	-0.835952	0.747880	-2.248217
C	0.131871	3.297220	-1.681034
H	2.097276	2.418360	-1.726059
C	-1.731003	1.790742	-2.094238
H	-1.196027	-0.256318	-2.479184
C	-1.233938	3.059264	-1.794644
H	0.488212	4.303469	-1.463351
H	-2.805756	1.635992	-2.192875
N	-2.178043	4.150029	-1.553675
O	-3.360445	3.888972	-1.571090
O	-1.728704	5.254079	-1.338410

H 1.909099 -4.838690 0.625909
H 1.809772 -4.753859 -1.152048
H 3.386741 -4.571534 -0.334495

Me_Michael_Acceptor/Me_ester

Frequencies, energies and thermodynamic properties:

Lowest Vibrational Mode (1/cm) = 33.1391
2nd Lowest Vibrational Mode (1/cm) = 48.3949
E(RM062X) (a.u.) = -1032.52305687
Thermal correction to Enthalpy (a.u.) = 0.153117
Thermal correction to Gibbs Free Energy (a.u.) = 0.092635
Total Entropy (cal/Kmol) = 127.296
Esp(RM062X) (a.u.) = -1033.73601298

Optimised cartesian coordinates (Angstrom):

C 3.451144 0.252262 -0.305519
H 3.550568 0.741158 -1.276484
C 4.508333 -0.100783 0.437082
H 4.311778 -0.587517 1.399266
O 1.157257 0.426042 -0.727929
C -0.153968 0.219346 -0.424956
C -0.987937 1.310966 -0.197347
C -0.682790 -1.068107 -0.351227
C -2.340485 1.121444 0.070130
C -2.029442 -1.264306 -0.070885
C -2.858777 -0.166763 0.143136
C 5.929578 0.115958 0.055906
O 1.767910 -0.531330 1.215664
C 2.090639 -0.016150 0.185567
F -0.500241 2.538600 -0.247101
F 0.103196 -2.110724 -0.559152
F -4.140739 -0.349972 0.407075
F -3.130201 2.163788 0.271313
F -2.525724 -2.488774 -0.005615
H 6.023148 0.611255 -0.918925
H 6.436372 0.725175 0.820483
H 6.462415 -0.847228 0.023762

Me_Michael_Acceptor/pNO2_thiourea

Frequencies, energies and thermodynamic properties:

Lowest Vibrational Mode (1/cm) = 18.6815
2nd Lowest Vibrational Mode (1/cm) = 21.7203
E(RM062X) (a.u.) = -1418.04990065
Thermal correction to Enthalpy (a.u.) = 0.251465
Thermal correction to Gibbs Free Energy (a.u.) = 0.181252
Total Entropy (cal/Kmol) = 147.775
Esp(RM062X) (a.u.) = -1419.34300615

Optimised cartesian coordinates (Angstrom):

C -0.010122 1.964661 0.081432
S -0.923571 3.348093 -0.105177
N 1.353766 2.059251 0.123383
H 1.684195 3.016258 0.223140
N -0.500866 0.708768 0.270880
H 0.140222 0.042540 0.699144
C -1.817630 0.241178 0.178794
C -2.757629 0.760615 -0.724929
C -2.164941 -0.844466 0.999652
C -4.030956 0.210625 -0.786694
H -2.492443 1.585810 -1.380248
C -3.433891 -1.399768 0.937124
H -1.428459 -1.246755 1.697331
C -4.353857 -0.856707 0.045689
H -4.771858 0.598601 -1.484094
H -3.715341 -2.237635 1.572957

C	2.349450	1.077612	0.045142
C	3.582038	1.360050	0.659970
C	2.187958	-0.124495	-0.666159
C	4.629343	0.455633	0.587476
H	3.706231	2.300119	1.199910
C	3.231832	-1.038536	-0.730380
H	1.261120	-0.339243	-1.196526
C	4.434327	-0.739726	-0.099629
H	5.586923	0.662590	1.063028
H	3.123355	-1.971243	-1.281951
N	5.535029	-1.708228	-0.170714
O	5.333037	-2.748914	-0.753086
O	6.581297	-1.410962	0.358233
N	-5.701693	-1.433283	-0.024638
O	-5.948306	-2.378536	0.689216
O	-6.490527	-0.932354	-0.792758

Me_Michael_Acceptor/product

Frequencies, energies and thermodynamic properties:

Lowest Vibrational Mode (1/cm) = 17.2658

2nd Lowest Vibrational Mode (1/cm) = 22.7400

E(RM062X) (a.u.) = -1647.84535300

Thermal correction to Enthalpy (a.u.) = 0.327796

Thermal correction to Gibbs Free Energy (a.u.) = 0.246591

Total Entropy (cal/Kmol) = 170.911

Esp(RM062X) (a.u.) = -1649.39867118

Optimised cartesian coordinates (Angstrom):

C	0.173755	3.883215	0.248719
C	0.085389	1.140167	-0.238252
C	-1.897136	2.662081	-0.523514
C	-0.993586	3.852644	-0.723723
H	-0.628686	3.835811	-1.762868
H	-1.626452	4.741025	-0.598939
N	-1.287107	1.421115	-0.267592
C	-2.170658	0.291130	-0.142496
C	-2.471276	-0.200732	1.126487
C	-2.712219	-0.288754	-1.289117
C	-3.326179	-1.289800	1.258045
H	-2.034459	0.269932	2.008213
C	-3.570836	-1.375072	-1.170334
H	-2.458862	0.113037	-2.270785
C	-3.857994	-1.853829	0.103879
H	-3.581711	-1.697817	2.234512
H	-4.011176	-1.850539	-2.045103
N	-4.764881	-3.009181	0.236059
O	-5.229521	-3.477027	-0.776555
O	-4.990466	-3.421615	1.349294
O	-3.098192	2.736596	-0.584606
S	1.265038	2.457104	-0.096666
N	0.455406	-0.072846	-0.312706
C	1.787479	-0.466071	-0.209144
C	2.501155	-0.816639	-1.367459
C	2.406086	-0.574864	1.049095
C	3.815072	-1.254859	-1.275762
H	2.008234	-0.741235	-2.337169
C	3.717686	-1.016259	1.148083
H	1.842917	-0.313497	1.945892
C	4.404114	-1.347490	-0.017645
H	4.383675	-1.526303	-2.164099
H	4.212359	-1.106487	2.114018
N	5.792310	-1.811657	0.084369
O	6.280590	-1.895792	1.188419
O	6.374056	-2.083998	-0.941089

H 0.813674 4.742600 0.005577
C -0.248402 3.947330 1.708810
H 0.628689 3.989734 2.367787
H -0.850008 3.070110 1.993239
H -0.855338 4.849449 1.877713

Me_Michael_Acceptor/TS-acyl

Frequencies, energies and thermodynamic properties:

Lowest Vibrational Mode (1/cm) = -159.1750

2nd Lowest Vibrational Mode (1/cm) = 11.2941

E(RM062X) (a.u.) = -2275.19404571

Thermal correction to Enthalpy (a.u.) = 0.525426

Thermal correction to Gibbs Free Energy (a.u.) = 0.421019

Total Entropy (cal/Kmol) = 219.744

Esp(RM062X) (a.u.) = -2277.46016117

Optimised cartesian coordinates (Angstrom):

C -6.549765 -1.764538 -0.222148
C -6.203621 -3.037891 0.237824
C -4.864833 -3.380013 0.439112
C -3.888678 -2.426129 0.171478
C -4.236959 -1.153916 -0.299577
C -5.573026 -0.805763 -0.495620
H -7.600204 -1.509598 -0.369712
H -6.982908 -3.772259 0.444897
H -4.589291 -4.372246 0.800411
H -5.848373 0.188749 -0.847341
C -1.922000 -0.915738 -0.192626
C -0.730971 1.102054 -0.607976
C -1.858240 1.419013 -1.615633
C -3.204407 1.013553 -1.028497
H -3.981268 1.038681 -1.806196
S -2.144200 -2.601291 0.338116
N -3.122729 -0.349514 -0.515978
N -0.789318 -0.308370 -0.233431
C -1.849633 2.866368 -2.157168
C -2.673136 3.861442 -1.334458
C -2.321387 2.886596 -3.611998
H -0.798481 3.200165 -2.141639
H -2.431359 3.836183 -0.262536
H -2.488857 4.883936 -1.695955
H -3.751811 3.667233 -1.446379
H -1.675537 2.268628 -4.252818
H -3.350487 2.500820 -3.694752
H -2.317798 3.911860 -4.010887
H -1.664238 0.748751 -2.469139
H 0.227522 1.239023 -1.127468
C -0.724911 2.010806 0.610450
C 0.102248 3.139549 0.619493
C -1.544026 1.765985 1.719113
C 0.095874 4.019238 1.701971
H 0.762838 3.327119 -0.229932
C -1.550995 2.643654 2.803403
H -2.175825 0.874813 1.751576
C -0.734228 3.775397 2.796490
H 0.747570 4.894821 1.693112
H -2.194024 2.437962 3.661089
H -0.737909 4.459753 3.646662
C 1.122266 -0.507889 1.498387
H 1.386414 0.549155 1.399555
C 1.051282 -1.101271 2.691410
H 0.768955 -2.160175 2.710675
C 1.308393 -0.419694 3.995058
O 0.525076 -2.448506 0.228605

C	0.780318	-1.262600	0.246820
H	-3.513007	1.687158	-0.213143
O	1.514629	-0.716230	-0.907157
C	2.849126	-0.659624	-0.752881
C	3.662344	-1.793171	-0.861955
C	3.470869	0.564829	-0.486910
C	5.044766	-1.697520	-0.730130
C	4.850012	0.671372	-0.358514
C	5.639888	-0.468403	-0.468406
F	2.724956	1.656875	-0.361609
F	5.412917	1.845554	-0.113747
F	5.799395	-2.779911	-0.851007
F	3.129484	-2.973299	-1.127465
F	6.954755	-0.380101	-0.340830
H	1.575411	0.636799	3.852698
H	2.119158	-0.919967	4.547492
H	0.414425	-0.469857	4.637002

Me_Michael_Acceptor/TS-cycl-R_rot

Frequencies, energies and thermodynamic properties:

Lowest Vibrational Mode (1/cm) = -131.1259

2nd Lowest Vibrational Mode (1/cm) = 12.8276

E(RM062X) (a.u.) = -2890.50993623

Thermal correction to Enthalpy (a.u.) = 0.700989

Thermal correction to Gibbs Free Energy (a.u.) = 0.581795

Total Entropy (cal/Kmol) = 250.865

Esp(RM062X) (a.u.) = -2893.11486570

Optimised cartesian coordinates (Angstrom):

C	-0.176948	-1.345251	2.950155
C	1.277308	-1.129128	3.343037
H	1.573527	-1.996932	3.951270
H	-0.276909	-2.323497	2.463760
H	-0.783376	-1.381893	3.868238
N	0.664898	0.605208	1.146849
C	0.240409	1.786509	0.528409
C	0.345779	2.000252	-0.862028
C	-0.344081	2.795949	1.320864
C	-0.148343	3.158321	-1.444264
H	0.826696	1.247110	-1.481781
C	-0.845636	3.957008	0.746164
H	-0.390561	2.659202	2.398144
C	-0.748685	4.118727	-0.632505
H	-0.076064	3.322942	-2.518572
H	-1.295036	4.740329	1.354688
N	-1.276160	5.340281	-1.245645
O	-1.793212	6.162314	-0.521726
O	-1.171700	5.464498	-2.446025
C	-0.852248	-0.236307	2.138513
O	-1.436426	0.668067	2.713978
C	1.534378	0.138803	4.146299
S	2.377022	-1.300482	1.893405
C	1.885651	0.125098	0.901592
N	2.709594	0.565582	0.002264
C	4.053513	0.302920	-0.063457
C	4.933069	0.530678	1.023927
C	4.611505	-0.123991	-1.290480
C	6.295644	0.322024	0.895539
H	4.523553	0.886491	1.969890
C	5.972940	-0.340584	-1.425486
H	3.939551	-0.278849	-2.135396
C	6.804310	-0.118643	-0.327667
H	6.974285	0.500288	1.728729
H	6.401822	-0.677056	-2.368417

N	8.239099	-0.341797	-0.464051
O	8.658177	-0.722223	-1.536604
O	8.942890	-0.137754	0.502082
N	-1.559325	-0.777144	0.930115
C	-2.858045	-0.537799	0.789717
C	-0.919941	-1.758113	0.036382
S	-3.723074	0.789343	1.533498
N	-3.648295	-1.295292	0.011347
C	-1.861767	-2.972503	-0.084447
H	-0.006453	-2.085404	0.546503
C	-0.494092	-1.181502	-1.300261
C	-5.187852	0.293762	0.696134
C	-4.967936	-0.842303	-0.086320
C	-3.195415	-2.518227	-0.659055
C	-1.253664	-4.175808	-0.841991
H	-2.040232	-3.295416	0.954820
C	0.767713	-1.532533	-1.792657
C	-1.334254	-0.394217	-2.098353
C	-6.446575	0.888907	0.755171
C	-5.992320	-1.410455	-0.843962
H	-3.968526	-3.283267	-0.503749
H	-3.129193	-2.309557	-1.737079
C	-1.489893	-4.172410	-2.354511
C	-1.766980	-5.485122	-0.240845
H	-0.165190	-4.130087	-0.668711
C	1.174643	-1.129189	-3.064384
H	1.443417	-2.123036	-1.168141
C	-0.928834	0.009770	-3.370041
H	-2.310582	-0.065250	-1.737700
C	-7.473268	0.326850	0.000263
H	-6.620550	1.773324	1.369825
C	-7.246426	-0.807742	-0.789363
H	-5.819024	-2.292332	-1.460513
H	-1.204257	-3.224821	-2.832672
H	-0.898491	-4.974073	-2.820216
H	-2.547590	-4.371240	-2.589565
H	-1.504753	-5.569847	0.823912
H	-2.863395	-5.552753	-0.327619
H	-1.337688	-6.350011	-0.767327
C	0.323870	-0.360792	-3.859607
H	2.160523	-1.415743	-3.434604
H	-1.593769	0.626761	-3.976912
H	-8.465153	0.779550	0.023745
H	-8.064593	-1.229751	-1.374248
H	0.639707	-0.044122	-4.855020
H	0.895934	0.141519	5.042960
H	1.303543	1.037821	3.560295
H	2.583975	0.183007	4.468359

Me_Michael_Acceptor/TS-cycl-R

Frequencies, energies and thermodynamic properties:

Lowest Vibrational Mode (1/cm) = -161.0763

2nd Lowest Vibrational Mode (1/cm) = 7.7267

E(RM062X) (a.u.) = -2890.51587789

Thermal correction to Enthalpy (a.u.) = 0.701037

Thermal correction to Gibbs Free Energy (a.u.) = 0.580622

Total Entropy (cal/Kmol) = 253.435

Esp(RM062X) (a.u.) = -2893.12312690

Optimised cartesian coordinates (Angstrom):

C	1.658466	-2.813996	-1.546840
C	2.393819	-0.250062	-0.391208
C	-0.245518	-1.228057	-1.285921
C	0.351950	-2.545018	-0.827198

H	0.491275	-2.608177	0.258503
H	-0.384539	-3.313622	-1.120525
N	1.076044	-0.025869	-0.478956
C	0.573400	1.221118	-0.108108
C	-0.284090	1.905463	-0.989684
C	0.816403	1.775060	1.166959
C	-0.932919	3.070655	-0.598375
H	-0.434671	1.497729	-1.989493
C	0.189544	2.946003	1.560849
H	1.500151	1.268608	1.846762
C	-0.696550	3.568034	0.680227
H	-1.610722	3.595486	-1.270864
H	0.365520	3.376804	2.545722
N	-1.401190	4.773484	1.119648
O	-1.268064	5.117959	2.273850
O	-2.089329	5.356308	0.311817
O	-0.325501	-0.964492	-2.480587
S	3.038596	-1.882677	-0.789978
N	3.246885	0.629393	0.033959
C	4.614254	0.548507	-0.050324
C	5.391246	0.724586	1.117244
C	5.292171	0.390397	-1.283913
C	6.775718	0.722692	1.066825
H	4.874411	0.863088	2.067642
C	6.675511	0.391038	-1.343551
H	4.708293	0.276056	-2.197728
C	7.406273	0.552439	-0.165358
H	7.374981	0.851271	1.967200
H	7.199048	0.273091	-2.291476
N	8.864119	0.551170	-0.225311
O	9.390466	0.391507	-1.305796
O	9.477836	0.708365	0.808576
H	1.562034	-2.486668	-2.590633
C	2.050906	-4.284646	-1.495938
N	-1.431063	-0.825343	-0.471966
C	-2.502640	-0.328038	-1.087484
C	-1.439083	-1.007428	0.995313
S	-2.674335	-0.137443	-2.822744
N	-3.605124	0.057830	-0.426224
C	-2.309293	0.098775	1.626963
H	-0.403838	-0.830393	1.317876
C	-1.834409	-2.415979	1.395807
C	-4.326238	0.417794	-2.595342
C	-4.666714	0.463207	-1.243151
C	-3.704136	0.058210	1.032771
C	-2.325649	0.109598	3.171872
H	-1.847849	1.045464	1.302327
C	-1.154730	-3.035698	2.450294
C	-2.885469	-3.095479	0.771906
C	-5.240202	0.791538	-3.578911
C	-5.936840	0.867550	-0.829833
H	-4.270011	0.952308	1.325525
H	-4.270400	-0.831988	1.346534
C	-3.378979	-0.802126	3.810391
C	-2.526916	1.539821	3.678185
H	-1.327440	-0.228468	3.497929
C	-1.537962	-4.299542	2.895028
H	-0.316068	-2.520976	2.926224
C	-3.269022	-4.362105	1.215137
H	-3.412726	-2.647595	-0.074401
C	-6.507178	1.202561	-3.172967
H	-4.969633	0.759957	-4.635394
C	-6.849072	1.236836	-1.814841

H -6.213463 0.890504 0.223932
H -3.359816 -1.830502 3.424807
H -3.214595 -0.848641 4.896850
H -4.391527 -0.396974 3.654757
H -1.750218 2.222054 3.304324
H -3.503986 1.934456 3.355104
H -2.507634 1.567898 4.777455
C -2.601395 -4.963669 2.281588
H -1.000377 -4.770468 3.719683
H -4.091329 -4.881544 0.720386
H -7.241229 1.498700 -3.923137
H -7.848829 1.556685 -1.518496
H -2.901668 -5.954392 2.626707
H 2.108010 -4.640567 -0.456532
H 3.024614 -4.456492 -1.976933
H 1.297151 -4.882861 -2.028477

Me_Michael_Acceptor/TS-cycl-S_rot

Frequencies, energies and thermodynamic properties:

Lowest Vibrational Mode (1/cm) = -178.4552

2nd Lowest Vibrational Mode (1/cm) = 8.9078

E(RM062X) (a.u.) = -2890.51286395

Thermal correction to Enthalpy (a.u.) = 0.700937

Thermal correction to Gibbs Free Energy (a.u.) = 0.580229

Total Entropy (cal/Kmol) = 254.052

Esp(RM062X) (a.u.) = -2893.11865574

Optimised cartesian coordinates (Angstrom):

C -1.612026 1.791975 -2.821236
C -2.152635 -0.011340 -0.726095
C 0.489245 0.685808 -1.874690
C -0.227610 1.983810 -2.213886
H -0.319814 2.662250 -1.361522
H 0.434331 2.467284 -2.950692
N -0.877143 -0.319378 -1.002238
C -0.341845 -1.513038 -0.494625
C 0.264259 -2.422921 -1.378057
C -0.336564 -1.799298 0.885407
C 0.895042 -3.566552 -0.898616
H 0.238024 -2.215813 -2.445654
C 0.286479 -2.937503 1.374480
H -0.834713 -1.114530 1.570632
C 0.904645 -3.801769 0.471240
H 1.370739 -4.275241 -1.575089
H 0.302961 -3.162333 2.440105
N 1.572401 -5.003896 0.983111
O 1.573128 -5.184403 2.180291
O 2.090693 -5.749161 0.182705
O 0.952313 -0.005603 -2.779409
S -2.826635 1.465169 -1.495230
N -2.906325 -0.683456 0.087267
C -4.271675 -0.582009 0.191371
C -4.853663 -0.382152 1.463642
C -5.135644 -0.763472 -0.915989
C -6.228865 -0.341745 1.626941
H -4.192529 -0.258751 2.322261
C -6.511136 -0.729571 -0.760568
H -4.703373 -0.942160 -1.901082
C -7.046300 -0.513343 0.510234
H -6.678110 -0.179976 2.605890
H -7.178504 -0.873259 -1.609346
N -8.495669 -0.474545 0.675321
O -9.185944 -0.627417 -0.309537
O -8.938252 -0.290005 1.788953

H	-1.940600	2.777033	-3.184114
C	-1.709697	0.787542	-3.961365
N	1.406121	0.825905	-0.681373
C	2.575762	0.196078	-0.679242
C	1.000512	1.628389	0.488188
S	3.236600	-0.716353	-2.025283
N	3.417095	0.230642	0.369753
C	1.578413	0.987627	1.763989
H	-0.093203	1.533212	0.545146
C	1.354814	3.096651	0.337934
C	4.714538	-0.985076	-1.111684
C	4.644399	-0.405951	0.156002
C	3.086051	0.868948	1.643743
C	1.128383	1.663503	3.078784
H	1.181647	-0.037789	1.771378
C	0.441954	4.061694	0.779547
C	2.584872	3.512180	-0.181681
C	5.852010	-1.679335	-1.519575
C	5.712782	-0.487746	1.049710
H	3.481970	0.232534	2.446830
H	3.592692	1.844808	1.690895
C	2.042777	2.792412	3.562438
C	0.984747	0.607212	4.175516
H	0.128932	2.089104	2.889563
C	0.765097	5.416386	0.735594
H	-0.534341	3.743845	1.155101
C	2.908485	4.869243	-0.228021
H	3.303468	2.782209	-0.562903
C	6.920046	-1.770344	-0.630214
H	5.903666	-2.136013	-2.509099
C	6.849457	-1.178844	0.637395
H	5.667115	-0.024671	2.035145
H	2.246077	3.544881	2.787352
H	1.575174	3.306992	4.414528
H	3.007551	2.393613	3.914047
H	0.243167	-0.158366	3.902946
H	1.945822	0.099422	4.356638
H	0.667205	1.067394	5.122577
C	2.004027	5.823127	0.237744
H	0.044253	6.157404	1.085070
H	3.872131	5.180968	-0.634312
H	7.821598	-2.307355	-0.927351
H	7.698538	-1.257179	1.317542
H	2.258747	6.883557	0.200552
H	-0.971849	1.032318	-4.739930
H	-2.714262	0.817969	-4.405286
H	-1.501641	-0.232073	-3.612639

Me_Michael_Acceptor/TS-cycl-S

Frequencies, energies and thermodynamic properties:

Lowest Vibrational Mode (1/cm) = -139.0151

2nd Lowest Vibrational Mode (1/cm) = 10.9724

E(RM062X) (a.u.) = -2890.51047329

Thermal correction to Enthalpy (a.u.) = 0.700886

Thermal correction to Gibbs Free Energy (a.u.) = 0.580752

Total Entropy (cal/Kmol) = 252.843

Esp(RM062X) (a.u.) = -2893.11617929

Optimised cartesian coordinates (Angstrom):

C	-0.183796	-1.471817	2.879129
C	1.262504	-1.245735	3.277043
H	1.375928	-0.231916	3.687399
H	-0.273685	-2.434336	2.356535
H	-0.789735	-1.545120	3.795204

N	0.640069	0.600422	1.247837
C	0.198438	1.821039	0.721916
C	0.267739	2.126930	-0.652439
C	-0.372479	2.766344	1.596621
C	-0.252032	3.316452	-1.142489
H	0.743815	1.423674	-1.331786
C	-0.897856	3.958908	1.115328
H	-0.387394	2.552920	2.662401
C	-0.838996	4.212772	-0.251575
H	-0.208462	3.554735	-2.204458
H	-1.338218	4.695041	1.786186
N	-1.394547	5.467391	-0.766920
O	-1.901888	6.231429	0.023998
O	-1.321357	5.674241	-1.958016
C	-0.860832	-0.327129	2.115857
O	-1.482339	0.522742	2.737613
C	1.732214	-2.278722	4.292197
S	2.361167	-1.348672	1.820355
C	1.858303	0.144994	0.942043
N	2.662828	0.665834	0.069496
C	4.007804	0.425548	-0.045022
C	4.904737	0.516776	1.048186
C	4.548694	0.171792	-1.326853
C	6.266193	0.336806	0.871307
H	4.512450	0.743568	2.039632
C	5.908678	-0.014396	-1.511243
H	3.864572	0.130374	-2.175091
C	6.756933	0.064805	-0.406809
H	6.957705	0.410140	1.709750
H	6.323694	-0.216727	-2.497715
N	8.190400	-0.128106	-0.594101
O	8.594590	-0.348928	-1.715942
O	8.907810	-0.060203	0.381115
N	-1.542470	-0.809857	0.866252
C	-2.840599	-0.575208	0.715701
C	-0.878272	-1.733252	-0.068598
S	-3.734428	0.698106	1.518437
N	-3.608109	-1.292601	-0.121876
C	-1.805722	-2.947508	-0.273313
H	0.028637	-2.082127	0.439302
C	-0.436547	-1.077197	-1.362938
C	-5.175490	0.243213	0.618402
C	-4.928755	-0.843560	-0.223664
C	-3.132312	-2.473905	-0.848064
C	-1.172498	-4.102460	-1.083646
H	-2.000522	-3.326581	0.743906
C	0.835912	-1.387778	-1.854553
C	-1.271961	-0.252183	-2.127912
C	-6.440166	0.825003	0.682754
C	-5.930583	-1.372937	-1.037487
H	-3.900863	-3.252845	-0.748590
H	-3.047615	-2.207028	-1.911898
C	-1.379550	-4.016289	-2.598083
C	-1.685379	-5.447550	-0.566840
H	-0.087984	-4.058318	-0.886759
C	1.257310	-0.910101	-3.095601
H	1.507809	-2.007149	-1.254390
C	-0.850860	0.228609	-3.367179
H	-2.256386	0.048287	-1.764700
C	-7.444724	0.301494	-0.127706
H	-6.635519	1.670126	1.344459
C	-7.190510	-0.782935	-0.977131
H	-5.736230	-2.215554	-1.700976

H -1.094134 -3.040673 -3.016617
H -0.771498 -4.785309 -3.096279
H -2.430566 -4.210959 -2.864486
H -1.445409 -5.588784 0.497140
H -2.778890 -5.520798 -0.681730
H -1.235755 -6.277941 -1.130582
C 0.412128 -0.103782 -3.858211
H 2.250359 -1.169230 -3.466823
H -1.512335 0.873875 -3.947866
H -8.440603 0.745172 -0.100777
H -7.991544 -1.175053 -1.605005
H 0.739697 0.271299 -4.829237
H 2.779404 -2.108543 4.577397
H 1.642210 -3.298728 3.888412
H 1.111515 -2.214516 5.197632

Me_Michael_Acceptor/TS-MA-R

Frequencies, energies and thermodynamic properties:

Lowest Vibrational Mode (1/cm) = -195.9971
2nd Lowest Vibrational Mode (1/cm) = 5.0630
E(RM062X) (a.u.) = -2890.51804246
Thermal correction to Enthalpy (a.u.) = 0.700697
Thermal correction to Gibbs Free Energy (a.u.) = 0.577658
Total Entropy (cal/Kmol) = 258.957
Esp(RM062X) (a.u.) = -2893.12342069

Optimised cartesian coordinates (Angstrom):

C 4.582473 -3.920101 -1.676015
C 3.404609 -4.502772 -2.162725
C 2.210232 -3.789019 -2.179250
C 2.218014 -2.489335 -1.673487
C 3.388206 -1.921704 -1.167093
H 3.422563 -5.526953 -2.536779
H 1.291065 -4.235950 -2.561234
C 1.891262 -0.212762 -0.768149
C 2.426715 1.873307 0.398531
C 3.584035 1.062005 1.006576
C 4.212315 0.167114 -0.043008
H 4.931377 -0.519780 0.421299
S 0.863664 -1.378602 -1.562277
N 3.159560 -0.636766 -0.661704
N 1.477736 0.965605 -0.281144
C 4.620697 1.918978 1.766927
C 5.768782 2.441213 0.898716
C 5.182139 1.122132 2.945117
H 4.077782 2.787163 2.175763
H 6.434580 1.619378 0.590977
H 5.423058 2.959648 -0.006633
H 6.376912 3.150159 1.479209
H 4.389413 0.833782 3.650987
H 5.677484 0.202352 2.594113
H 5.929772 1.712676 3.494296
H 3.108890 0.393329 1.742591
H 1.889332 2.294640 1.255691
C 2.847165 3.009052 -0.511763
C 2.969453 4.297610 0.018428
C 3.169398 2.792102 -1.855718
C 3.438914 5.346673 -0.770137
H 2.695417 4.479323 1.060724
C 3.637397 3.841937 -2.646352
H 3.051246 1.801442 -2.302277
C 3.780864 5.118991 -2.103655
H 3.531471 6.346950 -0.343813
H 3.886293 3.660555 -3.693231

H 4.146352 5.939321 -2.723597
C -0.365432 2.547037 0.164028
C -1.701234 2.931679 -0.016364
C -2.086341 4.367863 0.206761
O -0.619429 0.562969 -1.084534
C 0.073504 1.342087 -0.437369
H 4.729504 0.739637 -0.827952
C 4.594805 -2.622014 -1.176225
H 5.515021 -2.177276 -0.799424
H 5.509258 -4.495034 -1.681702
H -2.241990 2.403888 -0.805281
S -3.168542 2.046796 1.578471
C -2.771470 0.342030 1.397907
N -3.500500 -0.578846 0.873382
N -1.504592 0.030542 1.866853
C -4.788094 -0.385540 0.418500
C -5.819911 0.112682 1.242738
C -5.105525 -0.782593 -0.896593
C -7.118070 0.215962 0.768037
H -5.586139 0.411311 2.264583
C -6.398651 -0.671213 -1.383981
H -4.306207 -1.172852 -1.527735
C -7.392586 -0.173493 -0.542873
H -7.921120 0.595504 1.398414
H -6.648230 -0.965859 -2.402334
N -8.759953 -0.060702 -1.047194
O -8.976366 -0.407748 -2.187977
O -9.608706 0.374198 -0.299562
C -0.740429 -1.108315 1.702737
C -1.216226 -2.331896 1.187616
C 0.619834 -1.013824 2.077238
C -0.341712 -3.394909 1.003555
H -2.262672 -2.428356 0.918333
C 1.491792 -2.070900 1.890508
H 0.984933 -0.074771 2.500836
C 1.002543 -3.253841 1.334335
H -0.697055 -4.336095 0.585618
H 2.545973 -1.989229 2.156776
N 1.928934 -4.350043 1.062300
O 3.103116 -4.173873 1.306674
O 1.477665 -5.377203 0.605600
H 0.288596 3.187343 0.750071
H -1.014557 0.833834 2.247982
H -1.671298 4.748099 1.150986
H -1.669176 4.973194 -0.614753
H -3.175134 4.504900 0.214339

Me_Michael_Acceptor/TS-MA-S

Frequencies, energies and thermodynamic properties:

Lowest Vibrational Mode (1/cm) = -224.1195

2nd Lowest Vibrational Mode (1/cm) = 10.0597

E(RM062X) (a.u.) = -2890.52036486

Thermal correction to Enthalpy (a.u.) = 0.700564

Thermal correction to Gibbs Free Energy (a.u.) = 0.580812

Total Entropy (cal/Kmol) = 252.040

Esp(RM062X) (a.u.) = -2893.12581797

Optimised cartesian coordinates (Angstrom):

C 6.274168 0.857810 -0.724597
C 6.461744 -0.428342 -0.202061
C 5.459724 -1.051640 0.537058
C 4.260695 -0.365455 0.723249
C 4.082511 0.920039 0.209003
H 7.400401 -0.953572 -0.381536

H	5.599775	-2.055660	0.941290
C	2.006415	0.561251	1.145596
C	0.163165	2.155638	1.066615
C	1.296387	3.198484	1.153751
C	2.426440	2.805146	0.218069
H	3.309606	3.433983	0.394924
S	2.827864	-0.919190	1.575567
N	2.810843	1.423084	0.502414
N	0.719809	0.822239	1.387526
C	0.834706	4.660336	0.950139
C	0.895663	5.150468	-0.499609
C	1.655757	5.589952	1.844843
H	-0.213277	4.713186	1.287274
H	0.413125	6.135671	-0.576810
H	1.939730	5.273789	-0.828778
H	0.392022	4.475131	-1.205585
H	1.349576	6.636746	1.703369
H	1.530752	5.338191	2.908045
H	2.728531	5.520534	1.602973
H	1.683738	3.116555	2.182614
H	-0.546395	2.379524	1.873148
C	-0.576966	2.195365	-0.253369
C	-1.731629	2.979566	-0.360160
C	-0.083522	1.553264	-1.393437
C	-2.355933	3.156741	-1.594415
H	-2.138437	3.462778	0.531780
C	-0.716774	1.716208	-2.626762
H	0.802857	0.918112	-1.324679
C	-1.846720	2.528430	-2.732353
H	-3.248438	3.780979	-1.665921
H	-0.323860	1.206330	-3.508301
H	-2.338159	2.659686	-3.697739
C	-1.492047	0.000126	2.074978
H	-1.968852	0.724290	1.415546
C	-2.289610	-0.857273	2.877590
C	-3.715843	-0.441227	3.137265
O	0.523753	-1.116178	2.593242
C	-0.099602	-0.190211	2.075061
H	2.143617	2.892171	-0.841227
C	5.085199	1.553779	-0.524382
H	4.939693	2.550796	-0.940210
H	7.070194	1.323312	-1.307019
H	-1.760608	-1.283268	3.734198
S	-2.604924	-2.898360	2.037460
C	-1.705793	-2.646915	0.544100
N	-2.084315	-1.941251	-0.458705
N	-0.450375	-3.224644	0.552524
H	-0.266456	-3.766784	1.390447
C	-3.359545	-1.421498	-0.592321
C	-4.519876	-2.221058	-0.519414
C	-3.498138	-0.055948	-0.901474
C	-5.773910	-1.666390	-0.723933
H	-4.422761	-3.283502	-0.299024
C	-4.748662	0.511726	-1.094459
H	-2.594991	0.547476	-0.978687
C	-5.875276	-0.302865	-0.999951
H	-6.675281	-2.275369	-0.670727
H	-4.859782	1.571306	-1.321894
N	-7.197949	0.286085	-1.206163
O	-7.261203	1.473134	-1.442155
O	-8.163361	-0.441647	-1.129873
C	0.657194	-2.974528	-0.234567
C	0.744350	-1.922923	-1.169311

C	1.785620	-3.798114	-0.024422
C	1.951422	-1.662519	-1.805497
H	-0.127717	-1.305970	-1.365649
C	2.979127	-3.554970	-0.678902
H	1.712152	-4.624130	0.685887
C	3.056823	-2.469526	-1.551898
H	2.044854	-0.827753	-2.500729
H	3.853789	-4.181471	-0.508557
N	4.336187	-2.146464	-2.176826
O	5.252075	-2.926650	-2.030184
O	4.420289	-1.110248	-2.798721
H	-4.286060	-1.221200	3.658187
H	-4.229886	-0.203200	2.194137
H	-3.715903	0.463955	3.766806

Me_Michael_Acceptor/TS-turn-R_rot

Frequencies, energies and thermodynamic properties:

Lowest Vibrational Mode (1/cm) = -183.4658

2nd Lowest Vibrational Mode (1/cm) = 10.5148

E(RM062X) (a.u.) = -2890.51652502

Thermal correction to Enthalpy (a.u.) = 0.700641

Thermal correction to Gibbs Free Energy (a.u.) = 0.580451

Total Entropy (cal/Kmol) = 252.961

Esp(RM062X) (a.u.) = -2893.12190628

Optimised cartesian coordinates (Angstrom):

C	0.347980	-0.991013	-2.896015
C	-1.029327	-0.939626	-3.534996
H	-1.162584	-1.833559	-4.161157
H	0.455486	-1.945940	-2.368482
H	1.128911	-0.937662	-3.667341
N	-0.539030	0.695705	-1.190781
C	-0.330311	1.928629	-0.489658
C	-0.388996	1.977304	0.907448
C	-0.075578	3.097723	-1.218155
C	-0.166043	3.174475	1.578589
H	-0.629999	1.079495	1.470320
C	0.149495	4.300431	-0.558290
H	-0.046511	3.054570	-2.303948
C	0.107105	4.314617	0.831625
H	-0.205119	3.226691	2.665504
H	0.350777	5.218257	-1.108149
N	0.348082	5.583887	1.536303
O	0.582572	6.564671	0.868631
O	0.299832	5.576405	2.744821
C	0.623452	0.233886	-2.010819
O	1.335044	1.128301	-2.477159
C	-1.309146	0.308789	-4.358841
S	-2.254275	-1.191767	-2.202672
C	-1.773504	0.094924	-1.061241
N	-2.586255	0.453053	-0.141080
C	-3.912784	0.066591	-0.062949
C	-4.858586	0.489049	-1.020514
C	-4.350472	-0.693651	1.037937
C	-6.195759	0.148347	-0.890419
H	-4.526697	1.094974	-1.864467
C	-5.686182	-1.044231	1.171900
H	-3.620342	-0.996291	1.788745
C	-6.592442	-0.619970	0.203285
H	-6.934406	0.470520	-1.623059
H	-6.033675	-1.636718	2.016981
N	-8.003485	-0.985097	0.341724
O	-8.325253	-1.653903	1.298727
O	-8.774861	-0.600894	-0.508960

N	1.609331	-0.588517	-0.678830
C	2.891862	-0.430785	-0.661808
C	1.013980	-1.658480	0.116462
S	3.752839	0.893941	-1.474593
N	3.761697	-1.240394	0.007608
C	1.957745	-2.879914	0.134806
H	0.093800	-1.966066	-0.405011
C	0.592564	-1.184113	1.493241
C	5.273419	0.321366	-0.795428
C	5.093839	-0.832762	-0.024311
C	3.320601	-2.463352	0.672881
C	1.381098	-4.127110	0.841325
H	2.094579	-3.139268	-0.929049
C	-0.665715	-1.550833	1.981944
C	1.434096	-0.409255	2.301530
C	6.537699	0.877695	-0.962486
C	6.173854	-1.447180	0.608557
H	4.064844	-3.246982	0.470320
H	3.294978	-2.291094	1.760150
C	1.657394	-4.198883	2.345664
C	1.890661	-5.399296	0.162260
H	0.287650	-4.086662	0.699475
C	-1.073584	-1.163828	3.259208
H	-1.336440	-2.137983	1.348415
C	1.028059	-0.021268	3.577821
H	2.407637	-0.078380	1.932899
C	7.622689	0.265002	-0.333324
H	6.675067	1.774842	-1.568433
C	7.439279	-0.882877	0.443094
H	6.035281	-2.340035	1.218329
H	1.375948	-3.279707	2.878616
H	1.087462	-5.029939	2.786533
H	2.723120	-4.396198	2.542478
H	1.603043	-5.432774	-0.898855
H	2.989594	-5.459080	0.218193
H	1.483671	-6.295154	0.653952
C	-0.226355	-0.398208	4.060980
H	-2.058805	-1.455999	3.628034
H	1.690997	0.588350	4.194360
H	8.620551	0.689983	-0.448256
H	8.296455	-1.348462	0.931516
H	-0.545224	-0.089957	5.058096
H	-0.549831	0.405477	-5.149581
H	-1.271734	1.217329	-3.740865
H	-2.299088	0.248382	-4.830945

TS-turn-R

Frequencies, energies and thermodynamic properties:

Lowest Vibrational Mode (1/cm) = -136.0175

2nd Lowest Vibrational Mode (1/cm) = 9.5511

E(RM062X) (a.u.) = -2890.51995560

Thermal correction to Enthalpy (a.u.) = 0.700836

Thermal correction to Gibbs Free Energy (a.u.) = 0.578777

Total Entropy (cal/Kmol) = 256.895

Esp(RM062X) (a.u.) = -2893.12619392

Optimised cartesian coordinates (Angstrom):

C	1.617310	-2.792974	-1.896581
C	2.319574	-0.215232	-0.790204
C	0.035236	-0.937508	-1.534120
C	0.339668	-2.385960	-1.192962
H	0.429394	-2.549533	-0.109753
H	-0.497833	-2.983963	-1.580952
N	0.955807	0.006177	-0.814101

C	0.471066	1.296902	-0.465834
C	-0.410735	1.984461	-1.310277
C	0.814055	1.850431	0.779471
C	-0.976780	3.188346	-0.900625
H	-0.660300	1.555199	-2.278669
C	0.266081	3.056123	1.189313
H	1.505229	1.321068	1.433625
C	-0.635968	3.700557	0.345544
H	-1.675004	3.726944	-1.539850
H	0.517773	3.490155	2.155908
N	-1.255699	4.952476	0.797055
O	-1.055123	5.300278	1.939680
O	-1.938528	5.563187	0.007961
O	-0.317979	-0.631840	-2.669146
S	3.011661	-1.806151	-1.229394
N	3.121432	0.720102	-0.451980
C	4.492930	0.579604	-0.328917
C	5.062405	-0.133283	0.745301
C	5.341488	1.221768	-1.250802
C	6.439732	-0.212658	0.888615
H	4.407797	-0.620917	1.469178
C	6.719607	1.142905	-1.116929
H	4.894744	1.781925	-2.072707
C	7.251171	0.425310	-0.047255
H	6.891885	-0.760668	1.714046
H	7.385521	1.630050	-1.827797
N	8.706035	0.342732	0.101012
O	9.392798	0.903059	-0.723768
O	9.145532	-0.282056	1.040631
H	1.531434	-2.551682	-2.965234
C	1.965451	-4.261295	-1.715237
N	-1.473826	-0.724207	-0.383918
C	-2.622818	-0.451251	-0.904331
C	-1.336712	-0.754323	1.070796
S	-2.966594	-0.446827	-2.650590
N	-3.744435	-0.140868	-0.192085
C	-2.271982	0.309036	1.689177
H	-0.304216	-0.448896	1.292579
C	-1.508015	-2.151978	1.638999
C	-4.662436	-0.107805	-2.319447
C	-4.902478	0.026350	-0.947297
C	-3.705202	0.036059	1.255931
C	-2.128568	0.509369	3.212200
H	-1.964208	1.254078	1.208376
C	-0.635758	-2.585707	2.644282
C	-2.528349	-3.010253	1.213412
C	-5.692675	0.036154	-3.243068
C	-6.184670	0.292605	-0.467825
H	-4.349624	0.889771	1.509493
H	-4.116851	-0.862098	1.743163
C	-2.983209	-0.433521	4.064496
C	-2.448132	1.959469	3.582396
H	-1.066731	0.324911	3.451897
C	-0.795725	-3.838089	3.235890
H	0.177535	-1.930121	2.966479
C	-2.689488	-4.264470	1.803614
H	-3.205582	-2.709456	0.410355
C	-6.976997	0.307782	-2.768416
H	-5.499513	-0.063349	-4.312441
C	-7.216551	0.432254	-1.396826
H	-6.379176	0.384514	0.600929
H	-2.863980	-1.491033	3.790680
H	-2.708944	-0.327846	5.124503

H	-4.051140	-0.177093	3.979273
H	-1.803901	2.673267	3.047503
H	-3.494010	2.202542	3.334725
H	-2.317400	2.125382	4.661986
C	-1.828546	-4.679316	2.820207
H	-0.108486	-4.160308	4.020155
H	-3.490808	-4.922670	1.463155
H	-7.798624	0.420845	-3.476699
H	-8.226602	0.640300	-1.040981
H	-1.955754	-5.661030	3.279576
H	2.922073	-4.510336	-2.197163
H	2.030775	-4.520016	-0.648309
H	1.180814	-4.877368	-2.178157

Me_Michael_Acceptor/TS-turn-S_rot

Frequencies, energies and thermodynamic properties:

Lowest Vibrational Mode (1/cm) = -141.4351

2nd Lowest Vibrational Mode (1/cm) = 9.5114

E(RM062X) (a.u.) = -2890.51856759

Thermal correction to Enthalpy (a.u.) = 0.700674

Thermal correction to Gibbs Free Energy (a.u.) = 0.579274

Total Entropy (cal/Kmol) = 255.508

Esp(RM062X) (a.u.) = -2893.12343797

Optimised cartesian coordinates (Angstrom):

C	1.587880	-2.948724	-1.713243
C	2.312075	-0.329523	-0.741546
C	-0.004596	-1.027609	-1.457505
C	0.283004	-2.475533	-1.091682
H	0.323537	-2.612393	-0.003333
H	-0.551689	-3.067575	-1.494390
N	0.952900	-0.085037	-0.772669
C	0.501845	1.230106	-0.470497
C	-0.359851	1.914940	-1.337219
C	0.857855	1.812983	0.758044
C	-0.894996	3.145104	-0.964695
H	-0.618712	1.462527	-2.292365
C	0.341481	3.043910	1.130612
H	1.535864	1.286483	1.428711
C	-0.543066	3.685536	0.265968
H	-1.578118	3.682156	-1.621317
H	0.603852	3.500902	2.083636
N	-1.130263	4.966224	0.678488
O	-0.928357	5.338862	1.813010
O	-1.789513	5.574518	-0.132274
O	-0.353704	-0.735794	-2.603627
S	2.972688	-1.968634	-1.016131
N	3.130169	0.620253	-0.490467
C	4.496636	0.474929	-0.335773
C	5.044386	-0.182685	0.784504
C	5.365357	1.062591	-1.275602
C	6.418436	-0.261863	0.955315
H	4.375278	-0.627038	1.522918
C	6.740300	0.982550	-1.114753
H	4.935850	1.581298	-2.133100
C	7.249672	0.320179	0.000536
H	6.852961	-0.766887	1.816863
H	7.421091	1.427059	-1.839367
N	8.700962	0.237613	0.177929
O	9.405459	0.748784	-0.663754
O	9.120543	-0.338181	1.157213
H	1.799181	-3.958837	-1.334149
C	1.623066	-2.965137	-3.234753
N	-1.468058	-0.754165	-0.337381

C	-2.614190	-0.472170	-0.866884
C	-1.332553	-0.754414	1.118857
S	-2.963653	-0.509476	-2.610108
N	-3.725018	-0.123382	-0.158808
C	-2.241485	0.347312	1.708573
H	-0.292774	-0.470464	1.333894
C	-1.543584	-2.131900	1.722802
C	-4.652825	-0.136108	-2.281287
C	-4.884629	0.041412	-0.913382
C	-3.680264	0.095089	1.283586
C	-2.093676	0.584789	3.226182
H	-1.913010	1.272054	1.202867
C	-0.689322	-2.559618	2.745925
C	-2.582567	-2.975406	1.313334
C	-5.685206	-0.001760	-3.204308
C	-6.159476	0.342581	-0.435193
H	-4.304300	0.970662	1.511926
H	-4.113030	-0.778606	1.796069
C	-2.971355	-0.313056	4.103571
C	-2.379398	2.051637	3.556088
H	-1.036837	0.381842	3.472544
C	-0.885618	-3.790359	3.370853
H	0.138902	-1.916819	3.055434
C	-2.779706	-4.208179	1.936741
H	-3.246229	-2.680903	0.496772
C	-6.962334	0.303905	-2.731762
H	-5.498980	-0.134816	-4.271266
C	-7.193342	0.471867	-1.363147
H	-6.346779	0.469004	0.631296
H	-2.879934	-1.380328	3.858734
H	-2.693062	-0.185841	5.160133
H	-4.032375	-0.031366	4.012271
H	-1.716161	2.734914	3.004960
H	-3.418230	2.312894	3.297302
H	-2.248585	2.243080	4.631403
C	-1.936895	-4.616146	2.971014
H	-0.211957	-4.108062	4.168606
H	-3.595102	-4.855076	1.608327
H	-7.785599	0.409791	-3.439244
H	-8.198166	0.706607	-1.009197
H	-2.092313	-5.581058	3.456549
H	0.812169	-3.607312	-3.611956
H	2.579522	-3.371893	-3.591271
H	1.482531	-1.959673	-3.650255

Me_Michael_Acceptor/TS-turn-S

Frequencies, energies and thermodynamic properties:

Lowest Vibrational Mode (1/cm) = -160.5560

2nd Lowest Vibrational Mode (1/cm) = 9.9181

E(RM062X) (a.u.) = -2890.51570127

Thermal correction to Enthalpy (a.u.) = 0.700510

Thermal correction to Gibbs Free Energy (a.u.) = 0.578922

Total Entropy (cal/Kmol) = 255.903

Esp(RM062X) (a.u.) = -2893.12208291

Optimised cartesian coordinates (Angstrom):

C	-0.320730	-1.265136	2.765807
C	1.043855	-1.208276	3.418149
H	1.185311	-0.245543	3.931903
H	-0.380504	-2.182520	2.164536
H	-1.106413	-1.306983	3.533710
N	0.529745	0.606548	1.235429
C	0.293647	1.900088	0.666829
C	0.377750	2.107973	-0.715092

C	-0.013559	2.973685	1.513965
C	0.125795	3.364871	-1.254108
H	0.660335	1.288158	-1.370039
C	-0.268857	4.234152	0.986421
H	-0.055303	2.807706	2.586901
C	-0.202109	4.404972	-0.392175
H	0.183432	3.538988	-2.327447
H	-0.510121	5.078427	1.630087
N	-0.474665	5.735929	-0.956975
O	-0.748662	6.629823	-0.189641
O	-0.411318	5.863402	-2.158219
C	-0.648671	0.022884	1.987155
O	-1.357424	0.861050	2.570145
C	1.289869	-2.355825	4.384856
S	2.289277	-1.308816	2.086306
C	1.777154	0.054415	1.052911
N	2.583469	0.509892	0.169445
C	3.917743	0.163458	0.058364
C	4.854981	0.509134	1.054735
C	4.372840	-0.473106	-1.112452
C	6.199296	0.212533	0.894141
H	4.510831	1.021274	1.953940
C	5.715775	-0.779409	-1.277686
H	3.650105	-0.714244	-1.892456
C	6.612873	-0.434365	-0.269658
H	6.930652	0.476828	1.656642
H	6.076207	-1.276813	-2.176945
N	8.031399	-0.752554	-0.441156
O	8.367064	-1.318986	-1.457742
O	8.795295	-0.434376	0.442990
N	-1.584653	-0.636954	0.642216
C	-2.873030	-0.477552	0.638542
C	-0.979574	-1.603092	-0.272235
S	-3.743058	0.742181	1.585233
N	-3.725136	-1.211186	-0.126152
C	-1.913471	-2.822861	-0.416242
H	-0.053376	-1.953362	0.208334
C	-0.577988	-0.977344	-1.593042
C	-5.253548	0.245101	0.826137
C	-5.060693	-0.813223	-0.067625
C	-3.276329	-2.358657	-0.912032
C	-1.325799	-3.984317	-1.249398
H	-2.050136	-3.193033	0.614116
C	0.675773	-1.282169	-2.133044
C	-1.433511	-0.126656	-2.304207
C	-6.522554	0.775751	1.038405
C	-6.128257	-1.355297	-0.782314
H	-4.019616	-3.159764	-0.792886
H	-3.247817	-2.073943	-1.975092
C	-1.616572	-3.909565	-2.750776
C	-1.809724	-5.325417	-0.695453
H	-0.231594	-3.940979	-1.114224
C	1.066456	-0.757029	-3.365301
H	1.357419	-1.929005	-1.573901
C	-1.045267	0.398076	-3.536296
H	-2.404309	0.157109	-1.892384
C	-7.595649	0.235843	0.328392
H	-6.671802	1.597724	1.740505
C	-7.397411	-0.815863	-0.571605
H	-5.977684	-2.171486	-1.489078
H	-1.351896	-2.938049	-3.191571
H	-1.040593	-4.684671	-3.277280
H	-2.681659	-4.100954	-2.956811

H -1.509648 -5.459538 0.354173
H -2.908294 -5.396683 -0.746152
H -1.395314 -6.161442 -1.277867
C 0.205427 0.084115 -4.070982
H 2.049057 -1.000697 -3.773780
H -1.719408 1.065402 -4.076114
H -8.596750 0.642647 0.476323
H -8.246175 -1.223778 -1.122233
H 0.510898 0.499704 -5.032679
H 0.566153 -2.294929 5.210229
H 1.160144 -3.326585 3.883308
H 2.302038 -2.313173 4.811182

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atropisomerism/CF3_S_Ts_iPr_B

Frequencies, energies and thermodynamic properties:

Lowest Vibrational Mode (1/cm) = 14.5004
2nd Lowest Vibrational Mode (1/cm) = 28.5553
E(RM062X) (a.u.) = -2202.77184649
Thermal correction to Enthalpy (a.u.) = 0.398532
Thermal correction to Gibbs Free Energy (a.u.) = 0.310903
Total Entropy (cal/Kmol) = 184.432
Esp(RM062X) (a.u.) = -2204.69678720

Optimised cartesian coordinates (Angstrom):

N 0.788958 -0.815802 -0.245034
C 0.104007 0.173525 0.201473
S 0.517234 1.856735 -0.185593
C -0.755331 2.798089 0.703630
C -1.166524 2.129635 1.998751
N -1.011003 -0.134419 0.966627
C -1.459587 -1.511750 0.938296
C -2.064008 -2.023864 -0.215915
C -2.494406 -3.357240 -0.170802
C -2.329165 -4.140601 0.968015
C -1.715793 -3.606166 2.102171
C -1.276386 -2.287305 2.082406
C -1.722838 0.739678 1.813699
O -2.703687 0.359276 2.393076
H -2.969691 -3.788742 -1.054871
H -1.577257 -4.214148 2.997201
H -0.791364 -1.844792 2.954034
H -1.939650 2.717723 2.508490
H -0.290362 2.067407 2.661854
H -0.285926 3.769234 0.917063
C -1.939900 3.091549 -0.204524
F -2.588800 1.972009 -0.549339
F -2.815140 3.882753 0.413786
F -1.562110 3.698126 -1.323799
H -2.677342 -5.174858 0.969702
C -2.244259 -1.207287 -1.482472
H -1.825108 -0.206473 -1.313799
C -3.728117 -1.016379 -1.806818
H -4.215789 -1.981305 -2.015619
H -4.258008 -0.540240 -0.968397
H -3.845737 -0.378519 -2.695695
C -1.484554 -1.836544 -2.653193
H -1.551927 -1.191967 -3.542338
H -0.421451 -1.977567 -2.408361
H -1.906459 -2.819138 -2.915836
S 2.061814 -0.719644 -1.315920
O 2.250382 -2.076093 -1.796056
O 1.852838 0.355219 -2.278755
C 3.429658 -0.296134 -0.266477
C 3.904624 -1.259811 0.624721

C	3.999138	0.970834	-0.365597
C	4.975037	-0.930137	1.450893
H	3.443915	-2.248498	0.663756
C	5.075728	1.283297	0.464859
H	3.609558	1.689841	-1.087887
C	5.557354	0.337929	1.370056
H	5.362098	-1.667176	2.155838
H	5.540565	2.267992	0.399678
H	6.399600	0.588194	2.017246

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atropisomerism/CF3_S_Ts_iPr_F

Frequencies, energies and thermodynamic properties:

Lowest Vibrational Mode (1/cm) = 25.1148

2nd Lowest Vibrational Mode (1/cm) = 26.1756

E(RM062X) (a.u.) = -2202.77047290

Thermal correction to Enthalpy (a.u.) = 0.398604

Thermal correction to Gibbs Free Energy (a.u.) = 0.311726

Total Entropy (cal/Kmol) = 182.849

Esp(RM062X) (a.u.) = -2204.69687963

Optimised cartesian coordinates (Angstrom):

N	0.616682	-0.527506	-0.889683
C	-0.122289	0.332815	-0.291855
S	0.296739	2.056504	-0.211080
C	-1.011897	2.715234	0.861711
C	-1.419641	1.722757	1.932224
N	-1.299225	-0.134849	0.277422
C	-1.847217	-1.372910	-0.241354
C	-1.395436	-2.615748	0.214101
C	-2.009974	-3.752864	-0.328370
C	-3.022341	-3.654120	-1.279367
C	-3.449765	-2.401288	-1.719867
C	-2.857348	-1.256931	-1.196182
C	-1.965786	0.427387	1.381015
O	-2.907809	-0.134328	1.872778
H	-1.682606	-4.740697	0.004077
H	-4.240021	-2.313996	-2.466731
H	-3.171271	-0.262255	-1.516882
H	-2.196502	2.146266	2.580885
H	-0.543396	1.493079	2.557540
H	-0.564636	3.604510	1.328799
C	-2.189194	3.218600	0.040584
F	-2.808798	2.226101	-0.606745
F	-3.090516	3.800787	0.830882
F	-1.805526	4.111417	-0.865571
H	-3.478159	-4.560637	-1.681260
C	-0.289989	-2.761972	1.241632
H	0.079323	-1.754722	1.486701
C	0.881921	-3.561028	0.664901
H	0.584395	-4.599705	0.452977
H	1.238531	-3.107285	-0.272086
H	1.714126	-3.595883	1.384787
C	-0.821054	-3.395698	2.530310
H	-0.024517	-3.454402	3.287323
H	-1.652943	-2.809140	2.946796
H	-1.184979	-4.418124	2.344536
S	2.044336	-0.189002	-1.683899
O	2.413255	-1.430890	-2.335410
O	1.911955	1.030450	-2.471929
C	3.194420	0.115464	-0.359639
C	3.574158	-0.951619	0.455857
C	3.708782	1.398249	-0.187668
C	4.478673	-0.713883	1.487212
H	3.171401	-1.950515	0.281038

C 4.621062 1.619149 0.844314
H 3.402308 2.202809 -0.857510
C 4.999136 0.568604 1.680083
H 4.786301 -1.534309 2.137094
H 5.038594 2.616096 0.991936
H 5.711678 0.747562 2.487014

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atropisomerism/CF3_S_Ts_iPr-TS_O_rot

Frequencies, energies and thermodynamic properties:

Lowest Vibrational Mode (1/cm) = -24.4501

2nd Lowest Vibrational Mode (1/cm) = 14.0916

E(RM062X) (a.u.) = -2202.72742026

Thermal correction to Enthalpy (a.u.) = 0.397352

Thermal correction to Gibbs Free Energy (a.u.) = 0.312409

Total Entropy (cal/Kmol) = 178.777

Esp(RM062X) (a.u.) = -2204.65205304

Optimised cartesian coordinates (Angstrom):

N 1.071035 -1.213602 -0.200145
C 0.414243 -0.123547 -0.206545
S 0.969833 1.394352 -0.952538
C -0.147572 2.542540 -0.090581
C -0.383045 2.112849 1.346313
N -0.872329 -0.130381 0.394543
C -1.850186 -1.042616 -0.167907
C -3.080329 -1.446396 0.415817
C -3.874711 -2.339329 -0.326220
C -3.545239 -2.802105 -1.592189
C -2.377253 -2.335920 -2.183707
C -1.557792 -1.466910 -1.480569
C -0.925434 0.708698 1.543152
O -1.318108 0.358414 2.618908
H -4.809830 -2.679966 0.115186
H -2.094062 -2.635712 -3.193573
H -0.664328 -1.112295 -1.989525
H -1.098364 2.786533 1.840860
H 0.561961 2.196483 1.903777
H 0.401760 3.494800 -0.084819
C -1.403932 2.831507 -0.901106
F -2.137130 1.752228 -1.168227
F -2.186133 3.690109 -0.242090
F -1.084014 3.389025 -2.068069
H -4.204834 -3.496728 -2.113918
C -3.661761 -0.908290 1.715899
H -2.864692 -0.899464 2.461714
C -4.797824 -1.743905 2.305035
H -5.714562 -1.697463 1.698429
H -4.512585 -2.799609 2.422577
H -5.048058 -1.350110 3.301060
C -4.145438 0.533400 1.503902
H -4.421781 0.996667 2.463326
H -3.391576 1.173136 1.021453
H -5.031130 0.539105 0.848852
S 2.547495 -1.412486 -0.996131
O 2.752590 -2.843696 -1.056363
O 2.542824 -0.623661 -2.223420
C 3.699007 -0.709246 0.152646
C 3.964169 -1.407213 1.332326
C 4.319642 0.499278 -0.156071
C 4.869054 -0.859340 2.236711
H 3.472978 -2.361066 1.532535
C 5.230047 1.029575 0.757683
H 4.099519 1.003773 -1.097754
C 5.498283 0.354902 1.948654

H	5.090577	-1.385269	3.166295
H	5.733503	1.971144	0.534394
H	6.210792	0.775750	2.660047

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atropisomerism/CF3_S_Ts_iPr-TS

Frequencies, energies and thermodynamic properties:

Lowest Vibrational Mode (1/cm) = -31.4408

2nd Lowest Vibrational Mode (1/cm) = 20.9720

E(RM062X) (a.u.) = -2202.73182653

Thermal correction to Enthalpy (a.u.) = 0.397246

Thermal correction to Gibbs Free Energy (a.u.) = 0.313818

Total Entropy (cal/Kmol) = 175.587

Esp(RM062X) (a.u.) = -2204.65424962

Optimised cartesian coordinates (Angstrom):

N	0.616048	-1.339076	0.617215
C	-0.014400	-0.370224	0.106810
S	0.410181	0.527505	-1.389612
C	0.564933	2.130978	-0.491592
C	0.643879	1.959171	1.029235
N	-1.068166	0.215370	0.862803
C	-2.462803	-0.098013	0.654281
C	-2.923594	-1.265607	-0.010560
C	-4.312640	-1.418860	-0.145836
C	-5.235468	-0.493520	0.324867
C	-4.766396	0.656621	0.947654
C	-3.400190	0.850516	1.100532
C	-0.610404	1.314872	1.613792
O	-1.165274	1.746102	2.587572
H	-4.686832	-2.310827	-0.646428
H	-5.455557	1.418298	1.315496
H	-3.063147	1.759894	1.585473
H	0.758309	2.937572	1.512589
H	1.536840	1.360428	1.271044
H	1.510471	2.561097	-0.851314
C	-0.523915	3.100400	-0.914252
F	-1.731548	2.724442	-0.485881
F	-0.284581	4.313453	-0.413991
F	-0.584778	3.213636	-2.238530
H	-6.304344	-0.669256	0.196184
C	-2.041230	-2.394354	-0.539707
H	-1.145199	-1.962308	-0.998110
C	-2.675692	-3.214283	-1.665344
H	-3.499853	-3.848066	-1.307628
H	-3.054368	-2.572863	-2.474485
H	-1.912739	-3.883379	-2.089155
C	-1.617773	-3.320531	0.607325
H	-0.831251	-4.017064	0.277231
H	-1.234415	-2.761197	1.470245
H	-2.486209	-3.910280	0.941064
S	1.927869	-2.093051	-0.181089
O	2.181056	-3.285881	0.598118
O	1.625189	-2.195072	-1.601634
C	3.221005	-0.918085	0.099140
C	3.699595	-0.772851	1.403032
C	3.712392	-0.168959	-0.968096
C	4.690743	0.175568	1.641425
H	3.304104	-1.391133	2.210978
C	4.712087	0.768996	-0.712166
H	3.318453	-0.325790	-1.972664
C	5.191950	0.943233	0.586824
H	5.078918	0.310230	2.651765
H	5.118719	1.362535	-1.532048
H	5.972069	1.681417	0.779835

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atropisomerism/H_Se_Bz_iPr_B

Frequencies, energies and thermodynamic properties:

Lowest Vibrational Mode (1/cm) = 16.2527

2nd Lowest Vibrational Mode (1/cm) = 29.5052

E(RM062X) (a.u.) = -3434.27237340

Thermal correction to Enthalpy (a.u.) = 0.386962

Thermal correction to Gibbs Free Energy (a.u.) = 0.308404

Total Entropy (cal/Kmol) = 165.339

Esp(RM062X) (a.u.) = -3435.71101244

Optimised cartesian coordinates (Angstrom):

N	-0.534700	-0.044986	0.805845
C	0.127546	0.919703	0.314362
C	0.854250	3.499358	-0.781044
C	1.504675	2.534115	-1.749830
N	1.466498	0.716651	-0.032915
C	2.136521	-0.400915	0.594535
C	2.081163	-1.681437	0.030417
C	2.778519	-2.702085	0.689974
C	3.491021	-2.460225	1.862561
C	3.522437	-1.177997	2.410482
C	2.841716	-0.146640	1.770329
C	2.169114	1.365477	-1.061987
O	3.266832	0.975701	-1.376283
H	2.760904	-3.712141	0.274268
H	4.075019	-0.980042	3.330043
H	2.851012	0.868092	2.172135
H	2.298086	3.031806	-2.322137
H	0.760401	2.146459	-2.464268
H	0.435916	4.368138	-1.303474
H	4.022256	-3.278332	2.352093
C	1.317725	-1.970588	-1.247540
H	0.736063	-1.069832	-1.498550
C	0.329410	-3.123769	-1.058835
H	0.856053	-4.075121	-0.886862
H	-0.334453	-2.939252	-0.201078
H	-0.292300	-3.248366	-1.958764
C	2.284462	-2.245883	-2.403335
H	1.731197	-2.406041	-3.341225
H	2.976753	-1.403529	-2.543801
H	2.880613	-3.150114	-2.203333
C	-2.890407	-0.612125	0.516124
C	-2.638342	-1.124186	-0.761565
C	-4.176876	-0.695640	1.061026
C	-3.669020	-1.718256	-1.488107
H	-1.633904	-1.058333	-1.183122
C	-5.202562	-1.295461	0.336311
H	-4.353807	-0.284801	2.056109
C	-4.948720	-1.806803	-0.938841
H	-3.472275	-2.116256	-2.484946
H	-6.204089	-1.365174	0.763810
H	-5.753631	-2.276650	-1.506991
H	1.556741	3.850553	-0.014566
Se	-0.666041	2.655092	0.091618
C	-1.822553	0.066584	1.320467
O	-2.056109	0.622399	2.369549

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atropisomerism/H_Se_Bz_iPr_F

Frequencies, energies and thermodynamic properties:

Lowest Vibrational Mode (1/cm) = 19.6295

2nd Lowest Vibrational Mode (1/cm) = 25.5982

E(RM062X) (a.u.) = -3434.27774264

Thermal correction to Enthalpy (a.u.) = 0.386817

Thermal correction to Gibbs Free Energy (a.u.) = 0.308216

Total Entropy (cal/Kmol) = 165.430

Esp(RM062X) (a.u.) = -3435.71439007

Optimised cartesian coordinates (Angstrom):

N	-0.551923	0.560023	-0.472564
C	0.691875	0.873116	-0.357999
C	3.170192	2.153009	0.367343
C	3.628679	1.309754	-0.801343
N	1.606476	-0.154321	-0.575094
C	1.052961	-1.490105	-0.664960
C	0.715366	-2.182805	0.503162
C	0.168716	-3.465466	0.352042
C	-0.027168	-4.032255	-0.904424
C	0.321611	-3.320478	-2.053955
C	0.860815	-2.044830	-1.929748
C	2.998883	-0.058225	-0.794831
O	3.637556	-1.062798	-0.980089
H	-0.110000	-4.030780	1.244666
H	0.171173	-3.755967	-3.042867
H	1.134801	-1.462442	-2.811081
H	4.712628	1.140487	-0.773329
H	3.382480	1.806087	-1.754200
H	3.688337	3.119814	0.388966
H	-0.453780	-5.033328	-0.987937
C	0.894323	-1.586712	1.887635
H	1.371737	-0.601858	1.775273
C	1.820578	-2.450294	2.747607
H	1.383594	-3.444734	2.926778
H	2.797072	-2.589690	2.260530
H	1.986943	-1.976300	3.726560
C	-0.461284	-1.373369	2.567545
H	-0.329477	-0.886529	3.545554
H	-1.117919	-0.740552	1.951588
H	-0.972360	-2.334499	2.734717
C	-2.937607	0.854689	-0.213945
C	-3.129291	-0.519972	-0.403513
C	-4.038460	1.686558	0.024891
C	-4.415748	-1.054329	-0.351200
H	-2.265389	-1.158956	-0.593084
C	-5.321359	1.149424	0.075692
H	-3.868913	2.754584	0.169363
C	-5.510308	-0.222098	-0.112265
H	-4.564625	-2.125133	-0.499402
H	-6.178055	1.799015	0.262479
H	-6.516627	-0.643301	-0.072702
H	3.333892	1.647614	1.328766
Se	1.286457	2.608135	0.181639
C	-1.572995	1.468417	-0.253967
O	-1.408255	2.667272	-0.110579

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atropisomerism/H_Se_Bz_iPr-TS

Frequencies, energies and thermodynamic properties:

Lowest Vibrational Mode (1/cm) = -32.7217

2nd Lowest Vibrational Mode (1/cm) = 7.1759

E(RM062X) (a.u.) = -3434.23733501

Thermal correction to Enthalpy (a.u.) = 0.386033

Thermal correction to Gibbs Free Energy (a.u.) = 0.309916

Total Entropy (cal/Kmol) = 160.200

Esp(RM062X) (a.u.) = -3435.67374676

Optimised cartesian coordinates (Angstrom):

N	0.821989	0.322419	-0.395054
C	-0.057741	-0.383827	0.170299
C	-0.528458	-2.858273	1.285818

C	-0.155436	-3.029298	-0.184138
N	-1.187976	-0.829479	-0.574703
C	-2.428325	-0.100854	-0.653507
C	-2.601930	1.249593	-0.243788
C	-3.885670	1.803567	-0.387108
C	-4.980161	1.102251	-0.873672
C	-4.806655	-0.232126	-1.222172
C	-3.554329	-0.818031	-1.105982
C	-1.017983	-2.142151	-1.068980
O	-1.557949	-2.549983	-2.064267
H	-4.029367	2.843285	-0.094176
H	-5.642340	-0.832699	-1.585092
H	-3.452986	-1.858859	-1.392275
H	-0.345077	-4.058554	-0.515418
H	0.914452	-2.818568	-0.341478
H	-0.007705	-3.593196	1.911265
H	-5.951696	1.589698	-0.965030
C	-1.521138	2.185083	0.298020
H	-0.791029	1.607603	0.870660
C	-2.043510	3.225509	1.293845
H	-2.632644	4.017510	0.809155
H	-2.660928	2.763899	2.078532
H	-1.185390	3.713142	1.779492
C	-0.796495	2.884360	-0.857551
H	0.039157	3.493542	-0.479191
H	-0.398856	2.164879	-1.585521
H	-1.496197	3.552852	-1.384464
C	3.238149	0.640303	-0.296968
C	3.375856	0.013563	-1.541526
C	4.371291	1.072236	0.403645
C	4.646414	-0.182746	-2.079017
H	2.487914	-0.308436	-2.087484
C	5.637323	0.874903	-0.137796
H	4.241079	1.558006	1.371848
C	5.774399	0.246956	-1.378652
H	4.756794	-0.668570	-3.049580
H	6.521712	1.209635	0.406414
H	6.768354	0.093468	-1.802863
H	-1.610204	-2.958774	1.442943
Se	0.066230	-1.104872	1.956743
C	1.902586	0.848106	0.326794
O	1.729937	1.451293	1.362508

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atropisomerism/H_Se_Ts_iPr_B

Frequencies, energies and thermodynamic properties:

Lowest Vibrational Mode (1/cm) = 20.2580

2nd Lowest Vibrational Mode (1/cm) = 28.6182

E(RM062X) (a.u.) = -3869.31272382

Thermal correction to Enthalpy (a.u.) = 0.388449

Thermal correction to Gibbs Free Energy (a.u.) = 0.307775

Total Entropy (cal/Kmol) = 169.793

Esp(RM062X) (a.u.) = -3870.99459938

Optimised cartesian coordinates (Angstrom):

N	0.118997	-0.305623	-0.912689
C	-0.111628	0.820472	-0.338715
C	0.087572	3.412339	0.913444
C	-0.590937	2.580370	1.979822
N	-1.373748	0.976564	0.232723
C	-2.446897	0.158862	-0.295544
C	-2.677351	-1.135715	0.182761
C	-3.760655	-1.835393	-0.364513
C	-4.572419	-1.273730	-1.347540
C	-4.316222	0.015415	-1.813791

C	-3.248381	0.732318	-1.282057
C	-1.672117	1.700615	1.406367
O	-2.758966	1.589784	1.913642
H	-3.970696	-2.847866	-0.011997
H	-4.944202	0.462344	-2.585752
H	-3.025352	1.745112	-1.622379
H	-1.083918	3.219612	2.723242
H	0.143653	1.947957	2.504143
H	0.824495	4.098698	1.348113
H	-5.407617	-1.847262	-1.753302
C	-1.807938	-1.776724	1.246362
H	-0.973737	-1.090648	1.456874
C	-1.208493	-3.090720	0.739108
H	-1.991556	-3.847702	0.577668
H	-0.680989	-2.933379	-0.213847
H	-0.499795	-3.499596	1.475637
C	-2.594430	-1.978622	2.544334
H	-1.946014	-2.400464	3.327190
H	-3.003603	-1.024491	2.906720
H	-3.433625	-2.674681	2.389439
S	1.541782	-0.695553	-1.682815
O	1.269297	-1.932379	-2.389693
O	2.064402	0.453665	-2.417676
C	2.651654	-1.049118	-0.336166
C	2.420701	-2.186676	0.438878
C	3.733710	-0.203610	-0.103818
C	3.288889	-2.465822	1.490771
H	1.578071	-2.843196	0.216709
C	4.600224	-0.500632	0.948658
H	3.893936	0.664714	-0.744155
C	4.374582	-1.623199	1.744644
H	3.123152	-3.349031	2.109328
H	5.455374	0.147907	1.143942
H	5.054274	-1.849411	2.567873
H	-0.633018	3.993426	0.323462
Se	1.121732	2.284385	-0.288892

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atropisomerism/H_Se_Ts_iPr_F

Frequencies, energies and thermodynamic properties:

Lowest Vibrational Mode (1/cm) =	18.0506
2nd Lowest Vibrational Mode (1/cm) =	32.4274
E(RM062X) (a.u.) =	-3869.31341149
Thermal correction to Enthalpy (a.u.) =	0.388678
Thermal correction to Gibbs Free Energy (a.u.) =	0.307761
Total Entropy (cal/Kmol) =	170.306
Esp(RM062X) (a.u.) =	-3870.99411460

Optimised cartesian coordinates (Angstrom):

N	0.286715	-0.624536	-0.235902
C	-0.104390	0.565326	0.056860
C	-0.369517	3.448036	0.354223
C	-0.727826	2.932093	1.729990
N	-1.245692	0.652186	0.848881
C	-2.059742	-0.541884	0.938389
C	-2.827985	-0.945004	-0.160919
C	-3.591817	-2.111602	-0.013640
C	-3.593835	-2.839022	1.172960
C	-2.817901	-2.415754	2.253476
C	-2.045584	-1.266541	2.130040
C	-1.647460	1.741776	1.655109
O	-2.682371	1.680489	2.266358
H	-4.196642	-2.457095	-0.855432
H	-2.809436	-2.981962	3.185894
H	-1.423760	-0.918436	2.956485

H -1.265898 3.696181 2.304638
H 0.180497 2.649702 2.285746
H 0.258166 4.345652 0.414451
H -4.200284 -3.742733 1.254055
C -2.832976 -0.193358 -1.480093
H -2.211229 0.706939 -1.365531
C -4.243314 0.274368 -1.848951
H -4.916953 -0.581307 -2.009381
H -4.674003 0.902985 -1.055530
H -4.219883 0.860848 -2.779633
C -2.221656 -1.048331 -2.594761
H -2.142890 -0.466804 -3.525592
H -1.217944 -1.405794 -2.322449
H -2.849999 -1.929504 -2.798922
S 1.540103 -1.001333 -1.257360
O 1.294562 -2.367419 -1.683577
O 1.731466 0.032715 -2.271909
C 2.938499 -0.988454 -0.163620
C 3.065479 -2.022995 0.764772
C 3.867411 0.045205 -0.256849
C 4.153783 -2.007641 1.632337
H 2.325249 -2.824254 0.800142
C 4.955008 0.043613 0.617107
H 3.742629 0.825991 -1.008427
C 5.094124 -0.976285 1.558107
H 4.272832 -2.806395 2.365731
H 5.697119 0.841007 0.557737
H 5.947017 -0.972229 2.238922
H -1.261852 3.680480 -0.241270
Se 0.716100 2.161087 -0.621439

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atropisomerism/H_Se_Ts_iPr-TS

Frequencies, energies and thermodynamic properties:

Lowest Vibrational Mode (1/cm) = -32.1300

2nd Lowest Vibrational Mode (1/cm) = 22.7746

E(RM062X) (a.u.) = -3869.27506226

Thermal correction to Enthalpy (a.u.) = 0.387447

Thermal correction to Gibbs Free Energy (a.u.) = 0.309747

Total Entropy (cal/Kmol) = 163.532

Esp(RM062X) (a.u.) = -3870.95334510

Optimised cartesian coordinates (Angstrom):

N 0.420884 0.640289 -0.809963
C -0.143930 -0.185044 -0.029953
C 0.093068 -2.573276 1.312460
C 0.358298 -2.819760 -0.170789
N -1.204408 -0.968198 -0.572507
C -2.592994 -0.598818 -0.459532
C -3.061731 0.698699 -0.115051
C -4.453445 0.878443 -0.044437
C -5.375272 -0.135358 -0.268606
C -4.900383 -1.408803 -0.558985
C -3.533235 -1.631637 -0.643140
C -0.772827 -2.244538 -1.006998
O -1.305852 -2.850565 -1.897616
H -4.829631 1.870124 0.204228
H -5.585862 -2.242671 -0.718399
H -3.196447 -2.636582 -0.874667
H 0.382926 -3.895144 -0.390188
H 1.329783 -2.393852 -0.471107
H 0.822645 -3.103312 1.936812
H -6.444920 0.068291 -0.203916
C -2.199261 1.934298 0.142753
H -1.281366 1.630134 0.653435

C	-2.834887	2.951296	1.095123
H	-3.674294	3.492541	0.635171
H	-3.192187	2.475888	2.020475
H	-2.077934	3.701210	1.367954
C	-1.830737	2.616803	-1.179890
H	-1.090498	3.414485	-1.013314
H	-1.407499	1.908496	-1.903562
H	-2.732315	3.066562	-1.625791
S	1.641679	1.688622	-0.262453
O	1.716257	2.726845	-1.270014
O	1.381474	2.044315	1.129599
C	3.083995	0.668204	-0.368154
C	3.528195	0.292178	-1.637677
C	3.735325	0.275895	0.799118
C	4.652659	-0.522651	-1.730748
H	3.002928	0.632438	-2.531920
C	4.867665	-0.530541	0.686226
H	3.362325	0.603575	1.769937
C	5.318314	-0.931163	-0.571664
H	5.016016	-0.833600	-2.711038
H	5.398566	-0.845112	1.585660
H	6.202525	-1.565609	-0.652098
H	-0.918862	-2.884514	1.602602
Se	0.357764	-0.675178	1.764711

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atropisomerism/H_S_Ts_biPh-B

Frequencies, energies and thermodynamic properties:

Lowest Vibrational Mode (1/cm) = 13.5691

2nd Lowest Vibrational Mode (1/cm) = 26.1489

E(RM062X) (a.u.) = -1979.08573915

Thermal correction to Enthalpy (a.u.) = 0.386982

Thermal correction to Gibbs Free Energy (a.u.) = 0.304869

Total Entropy (cal/Kmol) = 172.821

Esp(RM062X) (a.u.) = -1980.72922013

Optimised cartesian coordinates (Angstrom):

N	0.764693	-0.807187	-0.358412
C	0.258224	0.063893	0.444647
S	0.908375	1.683748	0.654345
C	-0.369892	2.431190	1.699492
C	-0.741244	1.496199	2.828956
N	-0.890173	-0.318307	1.126611
C	-1.642821	-1.424221	0.579809
C	-2.670680	-1.135759	-0.328430
C	-3.447831	-2.201107	-0.799457
C	-3.191176	-3.507877	-0.389110
C	-2.155803	-3.772427	0.508091
C	-1.381658	-2.724342	0.999216
C	-1.423479	0.262378	2.300884
O	-2.389187	-0.230155	2.821242
H	-4.256613	-1.994561	-1.503163
H	-1.953259	-4.794976	0.829559
H	-0.574667	-2.902533	1.711434
H	-1.449220	1.969389	3.520570
H	0.153429	1.200129	3.399547
H	0.079154	3.360091	2.073094
H	-3.803037	-4.325425	-0.773752
S	1.950061	-0.499866	-1.480709
O	2.112650	-1.745672	-2.205454
O	1.638245	0.720515	-2.218620
C	3.426486	-0.227468	-0.524815
C	3.945463	-1.293169	0.211862
C	4.044800	1.019168	-0.561157
C	5.109085	-1.089564	0.948470

H	3.445988	-2.263812	0.205044
C	5.215416	1.205637	0.174018
H	3.610549	1.823569	-1.156945
C	5.741577	0.156459	0.927667
H	5.529224	-1.907956	1.534818
H	5.717240	2.174069	0.155782
H	6.656472	0.308299	1.502830
H	-1.238119	2.687083	1.073469
C	-2.947518	0.269071	-0.745595
C	-2.007465	1.002051	-1.485005
C	-4.152212	0.882156	-0.378038
C	-2.265069	2.326140	-1.837703
H	-1.071768	0.533734	-1.797947
C	-4.408803	2.206672	-0.734044
H	-4.884430	0.317582	0.203443
C	-3.464500	2.932883	-1.460455
H	-1.522114	2.882512	-2.412418
H	-5.349559	2.674169	-0.437696
H	-3.664928	3.969695	-1.736415

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atropisomerism/H_S_Ts_biPh-F

Frequencies, energies and thermodynamic properties:

Lowest Vibrational Mode (1/cm) = 17.7158

2nd Lowest Vibrational Mode (1/cm) = 20.3934

E(RM062X) (a.u.) = -1979.08504145

Thermal correction to Enthalpy (a.u.) = 0.387013

Thermal correction to Gibbs Free Energy (a.u.) = 0.305436

Total Entropy (cal/Kmol) = 171.693

Esp(RM062X) (a.u.) = -1980.72976950

Optimised cartesian coordinates (Angstrom):

N	-0.085482	-0.555458	-1.051727
C	0.253533	-1.278723	-0.044133
S	-0.798028	-2.506088	0.658116
C	0.271158	-3.221619	1.934587
C	1.032216	-2.141846	2.667820
N	1.527169	-1.059005	0.479395
C	2.452924	-0.307630	-0.342434
C	2.411443	1.093906	-0.389445
C	3.318283	1.740631	-1.240442
C	4.240040	1.023680	-1.999825
C	4.268958	-0.368007	-1.930521
C	3.366911	-1.031806	-1.103135
C	1.993434	-1.424815	1.759631
O	3.111443	-1.127198	2.094008
H	3.300592	2.830990	-1.292763
H	4.986460	-0.938104	-2.522159
H	3.357987	-2.121420	-1.042920
H	1.628706	-2.563152	3.486213
H	0.337894	-1.397415	3.091428
H	-0.414380	-3.754520	2.605610
H	4.938927	1.556117	-2.646847
S	-1.506428	-0.700144	-1.905967
O	-1.365612	0.217199	-3.021190
O	-1.817099	-2.100598	-2.166791
C	-2.737188	-0.044039	-0.800056
C	-2.721543	1.324590	-0.532752
C	-3.689603	-0.895932	-0.246510
C	-3.675604	1.846860	0.336292
H	-1.973750	1.965045	-1.002375
C	-4.647076	-0.357346	0.613007
H	-3.677719	-1.958703	-0.492808
C	-4.635035	1.006420	0.907013
H	-3.675660	2.914382	0.562973

H -5.404645 -1.007034 1.053603
H -5.384214 1.421041 1.583642
H 0.944683 -3.955625 1.471263
C 1.429700 1.899151 0.386139
C 1.300077 1.766319 1.775700
C 0.634553 2.842492 -0.279806
C 0.383182 2.547480 2.479129
H 1.951169 1.077028 2.316085
C -0.272742 3.630955 0.426469
H 0.719516 2.941479 -1.364447
C -0.407040 3.480300 1.807169
H 0.298057 2.436268 3.561634
H -0.886216 4.359690 -0.107510
H -1.121243 4.093541 2.359713

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atropisomerism/H_S_Ts_biPh-TS

Frequencies, energies and thermodynamic properties:

Lowest Vibrational Mode (1/cm) = -22.5131
2nd Lowest Vibrational Mode (1/cm) = 31.5509
E(RM062X) (a.u.) = -1979.05058148
Thermal correction to Enthalpy (a.u.) = 0.385365
Thermal correction to Gibbs Free Energy (a.u.) = 0.308268
Total Entropy (cal/Kmol) = 162.265
Esp(RM062X) (a.u.) = -1980.68994854

Optimised cartesian coordinates (Angstrom):

N 0.354791 0.497795 -0.565687
C -0.069605 -0.332640 0.292833
S 0.493578 -0.532111 1.968592
C 0.648192 -2.357312 1.847963
C 0.933029 -2.779120 0.409687
N -0.974508 -1.353127 -0.153137
C -2.398273 -1.206262 -0.240110
C -3.064444 0.039545 -0.219069
C -4.465291 0.059323 -0.313337
C -5.222732 -1.100144 -0.405743
C -4.562881 -2.326365 -0.380288
C -3.178283 -2.378069 -0.292242
C -0.307832 -2.564100 -0.440029
O -0.723234 -3.380464 -1.219368
H -4.957949 1.033689 -0.302322
H -5.124420 -3.260917 -0.425115
H -2.698950 -3.351698 -0.277991
H 1.168444 -3.849167 0.352465
H 1.792946 -2.220129 0.001660
H 1.490364 -2.609510 2.505336
H -6.309450 -1.047091 -0.481563
S 1.643547 1.572716 -0.244714
O 1.672986 2.467054 -1.383894
O 1.585789 2.107765 1.106591
C 2.996746 0.429693 -0.369017
C 3.307030 -0.091286 -1.626545
C 3.687198 0.059718 0.783103
C 4.332619 -1.027990 -1.722089
H 2.752595 0.231455 -2.509562
C 4.717936 -0.873626 0.668348
H 3.418019 0.500795 1.743053
C 5.033001 -1.418008 -0.577048
H 4.590225 -1.451579 -2.693721
H 5.276761 -1.173778 1.555896
H 5.837552 -2.150755 -0.659546
H -0.259483 -2.839405 2.236257
C -2.400351 1.367560 -0.062134
C -2.124830 2.157463 -1.182382

C -2.071174 1.842313 1.212493
C -1.481422 3.384104 -1.033719
H -2.383233 1.787808 -2.176775
C -1.426875 3.070245 1.359187
H -2.299932 1.233362 2.090043
C -1.122468 3.837972 0.236192
H -1.242300 3.981692 -1.914856
H -1.149126 3.421586 2.354284
H -0.598104 4.788367 0.349235

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atropisomerism/H_S_Ts_iPr_alkene_B

Frequencies, energies and thermodynamic properties:

Lowest Vibrational Mode (1/cm) = 14.6793
2nd Lowest Vibrational Mode (1/cm) = 30.1239
E(RM062X) (a.u.) = -1864.86136113
Thermal correction to Enthalpy (a.u.) = 0.365591
Thermal correction to Gibbs Free Energy (a.u.) = 0.286735
Total Entropy (cal/Kmol) = 165.967
Esp(RM062X) (a.u.) = -1866.38702476

Optimised cartesian coordinates (Angstrom):

N -0.320206 -0.247210 0.522570
C 0.075162 0.908951 0.120685
S -0.796396 2.408259 0.515402
C 0.111111 3.602847 -0.355958
C 1.237324 3.393174 -1.042680
N 1.223508 0.951796 -0.640132
C 1.855175 -0.323501 -0.921273
C 2.651201 -0.946950 0.045068
C 3.230210 -2.174561 -0.305184
C 3.024263 -2.750116 -1.556022
C 2.221901 -2.106652 -2.499311
C 1.633422 -0.888824 -2.176173
C 1.881097 2.085191 -1.188395
O 2.930087 1.941337 -1.765873
H 3.854884 -2.691674 0.426790
H 2.053428 -2.551178 -3.481143
H 0.998728 -0.363277 -2.891824
H 3.490545 -3.707360 -1.795367
C 2.883454 -0.358425 1.424133
H 2.359489 0.607493 1.476495
C 4.371214 -0.086840 1.663740
H 4.950965 -1.022689 1.656253
H 4.784734 0.576659 0.890010
H 4.519260 0.391111 2.643663
C 2.301244 -1.267674 2.510622
H 2.419480 -0.802552 3.500963
H 1.231321 -1.456691 2.340181
H 2.824033 -2.236831 2.530489
S -1.661263 -0.545318 1.451152
O -1.452220 -1.865498 2.017313
O -1.944516 0.575245 2.343224
C -2.949572 -0.644632 0.233105
C -2.965164 -1.745182 -0.625706
C -3.901094 0.369531 0.160169
C -3.962947 -1.819023 -1.592880
H -2.208568 -2.526503 -0.533443
C -4.897795 0.277999 -0.812198
H -3.864790 1.205209 0.860547
C -4.925171 -0.809244 -1.685020
H -3.993725 -2.669710 -2.275104
H -5.656342 1.058768 -0.883835
H -5.706764 -0.874902 -2.443824
H 1.751634 4.218638 -1.534849

H -0.325888 4.601252 -0.265557

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atropisomerism/H_S_Ts_iPr_alkene_F

Frequencies, energies and thermodynamic properties:

Lowest Vibrational Mode (1/cm) = 12.5367

2nd Lowest Vibrational Mode (1/cm) = 24.2657

E(RM062X) (a.u.) = -1864.86113145

Thermal correction to Enthalpy (a.u.) = 0.365329

Thermal correction to Gibbs Free Energy (a.u.) = 0.285883

Total Entropy (cal/Kmol) = 167.208

Esp(RM062X) (a.u.) = -1866.38793284

Optimised cartesian coordinates (Angstrom):

N 0.302318 -0.757978 0.859083
C -0.670709 -1.332824 0.248372
S -0.561990 -2.981820 -0.425347
C -2.132545 -3.190701 -1.131853
C -3.128730 -2.301076 -1.146428
N -1.840615 -0.610296 0.117856
C -1.840462 0.721935 0.690581
C -1.426035 1.812185 -0.081193
C -1.462808 3.073889 0.528236
C -1.889936 3.236218 1.843617
C -2.296318 2.129391 2.590325
C -2.270013 0.866530 2.008246
C -3.039878 -0.967017 -0.551292
O -3.943139 -0.168597 -0.612816
H -1.149750 3.949044 -0.046052
H -2.631764 2.248240 3.621482
H -2.579306 -0.018616 2.566744
H -1.906325 4.232561 2.288713
C -0.964988 1.665572 -1.519206
H -0.964241 0.593746 -1.769364
C 0.464817 2.182178 -1.697763
H 0.521321 3.266048 -1.511598
H 1.154924 1.680335 -1.003415
H 0.813058 1.999540 -2.725755
C -1.938128 2.363784 -2.473246
H -1.629480 2.210630 -3.518308
H -2.958363 1.972440 -2.350506
H -1.961900 3.448139 -2.283163
S 1.821893 -1.358223 1.128023
O 2.101298 -1.169513 2.539230
O 1.989330 -2.685117 0.539608
C 2.788023 -0.202711 0.191004
C 3.197679 0.980131 0.802931
C 3.076057 -0.493474 -1.141154
C 3.914194 1.905115 0.045824
H 2.956139 1.165700 1.850506
C 3.794240 0.441405 -1.884544
H 2.746434 -1.436619 -1.580279
C 4.207931 1.636608 -1.292711
H 4.245511 2.838316 0.503461
H 4.033211 0.234902 -2.928786
H 4.768785 2.365506 -1.880147
H -4.079925 -2.533314 -1.625423
H -2.242931 -4.175000 -1.596152

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atropisomerism/H_S_Ts_iPr_alkene-TS

Frequencies, energies and thermodynamic properties:

Lowest Vibrational Mode (1/cm) = -36.1523

2nd Lowest Vibrational Mode (1/cm) = 16.8551

E(RM062X) (a.u.) = -1864.81305094

Thermal correction to Enthalpy (a.u.) = 0.364085

Thermal correction to Gibbs Free Energy (a.u.) = 0.287828

Total Entropy (cal/Kmol) = 160.498

Esp(RM062X) (a.u.) = -1866.33485304

Optimised cartesian coordinates (Angstrom):

N	0.451056	0.521159	-0.812184
C	-0.139958	-0.203474	0.032562
S	0.382529	-0.513850	1.737918
C	0.730553	-2.194699	1.353592
C	0.329799	-2.850303	0.251370
N	-1.190853	-1.045959	-0.399019
C	-2.585535	-0.731558	-0.215981
C	-3.069805	0.573541	0.067570
C	-4.455693	0.724109	0.227721
C	-5.356441	-0.329909	0.133875
C	-4.863618	-1.604720	-0.116252
C	-3.498286	-1.799219	-0.281606
C	-0.733609	-2.370700	-0.660348
O	-1.240198	-3.079005	-1.491941
H	-4.845262	1.719611	0.437823
H	-5.533731	-2.463348	-0.181612
H	-3.146420	-2.806002	-0.482214
H	-6.425048	-0.153497	0.263067
C	-2.207016	1.829301	0.162096
H	-1.275361	1.582669	0.685058
C	-2.816277	2.950144	1.006923
H	-3.680523	3.419906	0.515721
H	-3.130997	2.590089	1.997303
H	-2.059475	3.734582	1.153233
C	-1.865018	2.355245	-1.237291
H	-1.088524	3.134523	-1.183009
H	-1.503345	1.560900	-1.902853
H	-2.765860	2.796015	-1.692680
S	1.692230	1.616433	-0.360962
O	1.860754	2.454009	-1.528544
O	1.345620	2.211626	0.922369
C	3.088745	0.544894	-0.191285
C	3.590732	-0.066708	-1.341329
C	3.647573	0.347703	1.069330
C	4.681750	-0.921356	-1.210986
H	3.136691	0.122397	-2.315842
C	4.746808	-0.502371	1.178699
H	3.226579	0.852786	1.939416
C	5.255691	-1.136453	0.044428
H	5.089587	-1.415982	-2.093332
H	5.206900	-0.668082	2.153710
H	6.113514	-1.804447	0.137806
H	0.672089	-3.869455	0.069826
H	1.379851	-2.674247	2.092108

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atropisomerism/H_S_Ts_iPr_B

Frequencies, energies and thermodynamic properties:

Lowest Vibrational Mode (1/cm) = 16.6340

2nd Lowest Vibrational Mode (1/cm) = 25.9087

E(RM062X) (a.u.) = -1866.08181850

Thermal correction to Enthalpy (a.u.) = 0.389342

Thermal correction to Gibbs Free Energy (a.u.) = 0.309368

Total Entropy (cal/Kmol) = 168.319

Esp(RM062X) (a.u.) = -1867.60936744

Optimised cartesian coordinates (Angstrom):

N	0.192360	0.226040	0.912359
C	-0.064659	-0.942100	0.439005
S	1.085578	-2.275690	0.454098
C	0.123881	-3.566309	-0.381894

C -0.615645 -2.996976 -1.571902
N -1.339070 -1.133341 -0.090598
C -2.378974 -0.215129 0.326190
C -2.548741 1.023056 -0.303434
C -3.602832 1.828688 0.147225
C -4.444921 1.421834 1.179455
C -4.250125 0.185553 1.794974
C -3.211874 -0.634100 1.363060
C -1.672718 -2.012961 -1.143322
O -2.759237 -1.949248 -1.656345
H -3.764453 2.801290 -0.323421
H -4.902414 -0.140416 2.606291
H -3.036472 -1.608404 1.822693
H -1.132168 -3.785610 -2.133060
H 0.083540 -2.490907 -2.257319
H 0.866922 -4.313101 -0.689178
H -5.255782 2.075061 1.506443
C -1.644628 1.500592 -1.423061
H -0.862652 0.740934 -1.572297
C -0.951350 2.810661 -1.039123
H -1.682403 3.626496 -0.927635
H -0.410666 2.700279 -0.087066
H -0.237860 3.110936 -1.822011
C -2.423338 1.638511 -2.734092
H -1.750440 1.935716 -3.552610
H -2.905255 0.688729 -3.007842
H -3.207138 2.407025 -2.646696
S 1.618749 0.664536 1.646101
O 1.407343 2.030849 2.088214
O 2.036245 -0.345594 2.611033
C 2.800065 0.692768 0.311948
C 2.654681 1.653563 -0.689702
C 3.853378 -0.217789 0.315225
C 3.583680 1.683577 -1.726364
H 1.829440 2.366919 -0.654460
C 4.782466 -0.169555 -0.724238
H 3.938970 -0.946745 1.122383
C 4.644478 0.774063 -1.741994
H 3.485182 2.425160 -2.520442
H 5.616924 -0.872205 -0.736441
H 5.372519 0.805696 -2.554366
H -0.559812 -4.033016 0.340596

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atropisomerism/H_S_Ts_iPr_F

Frequencies, energies and thermodynamic properties:

Lowest Vibrational Mode (1/cm) = 14.3572

2nd Lowest Vibrational Mode (1/cm) = 31.0530

E(RM062X) (a.u.) = -1866.08203469

Thermal correction to Enthalpy (a.u.) = 0.389514

Thermal correction to Gibbs Free Energy (a.u.) = 0.309311

Total Entropy (cal/Kmol) = 168.800

Esp(RM062X) (a.u.) = -1867.60824851

Optimised cartesian coordinates (Angstrom):

N -0.320262 -0.551453 0.059812
C 0.030411 0.683970 0.152465
S -0.855654 1.870907 1.107077
C 0.151479 3.359337 0.864953
C 0.628602 3.466389 -0.565441
N 1.199897 1.044361 -0.511244
C 2.061694 -0.036560 -0.939765
C 2.793441 -0.764225 0.007437
C 3.617757 -1.791173 -0.474251
C 3.709820 -2.078612 -1.832942

C	2.964912	-1.341871	-2.755242
C	2.135659	-0.322144	-2.303064
C	1.578222	2.348517	-0.904959
O	2.613271	2.523428	-1.491677
H	4.198117	-2.381693	0.238580
H	3.025956	-1.563514	-3.821626
H	1.539089	0.265752	-3.002377
H	1.176172	4.402436	-0.729269
H	-0.224884	3.435386	-1.261579
H	-0.513935	4.191015	1.129516
H	4.362060	-2.884474	-2.173824
C	2.696635	-0.506448	1.500630
H	2.029770	0.353490	1.661307
C	4.059400	-0.137604	2.092826
H	4.774197	-0.968462	1.991170
H	4.487212	0.742975	1.591116
H	3.960642	0.089602	3.164873
C	2.087695	-1.714073	2.220839
H	1.915627	-1.481588	3.282440
H	1.128955	-2.009412	1.771408
H	2.766018	-2.580159	2.170092
S	-1.562297	-1.264207	0.904076
O	-1.367710	-2.691893	0.721341
O	-1.657475	-0.731149	2.258220
C	-3.006108	-0.773649	-0.008699
C	-3.201233	-1.311110	-1.282102
C	-3.906264	0.119992	0.565727
C	-4.327980	-0.924292	-2.002005
H	-2.482672	-2.021125	-1.695457
C	-5.034337	0.492927	-0.165547
H	-3.724782	0.505325	1.570133
C	-5.240603	-0.024587	-1.444129
H	-4.498961	-1.330917	-2.999752
H	-5.754434	1.188316	0.268019
H	-6.124145	0.271305	-2.012242
H	0.989862	3.346411	1.575584

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atropisomerism/H_S_Ts_iPr-TS

Frequencies, energies and thermodynamic properties:

Lowest Vibrational Mode (1/cm) = -34.9357

2nd Lowest Vibrational Mode (1/cm) = 19.6019

E(RM062X) (a.u.) = -1866.04239348

Thermal correction to Enthalpy (a.u.) = 0.388298

Thermal correction to Gibbs Free Energy (a.u.) = 0.311606

Total Entropy (cal/Kmol) = 161.412

Esp(RM062X) (a.u.) = -1867.56611539

Optimised cartesian coordinates (Angstrom):

N	0.444993	0.584961	-0.688493
C	-0.100479	-0.227709	0.120093
S	0.403058	-0.601791	1.782934
C	0.181482	-2.413094	1.576710
C	0.423129	-2.829357	0.128061
N	-1.162487	-1.036478	-0.382371
C	-2.555806	-0.682409	-0.261193
C	-3.039283	0.628241	0.000760
C	-4.431496	0.789155	0.097038
C	-5.338777	-0.254388	-0.030835
C	-4.847952	-1.536906	-0.244315
C	-3.479088	-1.741906	-0.347513
C	-0.721004	-2.332882	-0.741171
O	-1.250773	-3.000730	-1.587352
H	-4.820398	1.789239	0.284710
H	-5.521684	-2.391215	-0.326861

H -3.128601 -2.755183 -0.514910
H 0.439914 -3.922169 0.030089
H 1.391476 -2.444904 -0.232692
H 0.928499 -2.859910 2.245123
H -6.410137 -0.065211 0.048016
C -2.186844 1.888364 0.141133
H -1.265243 1.637711 0.674525
C -2.825700 2.985597 0.996608
H -3.675336 3.470493 0.494527
H -3.168853 2.599218 1.967625
H -2.074734 3.766221 1.187444
C -1.828362 2.446925 -1.241704
H -1.070953 3.241425 -1.156535
H -1.429345 1.671280 -1.907459
H -2.729716 2.873366 -1.710245
S 1.680057 1.641657 -0.193764
O 1.800422 2.598108 -1.275160
O 1.397060 2.105212 1.159909
C 3.101128 0.584883 -0.190367
C 3.582710 0.128767 -1.419275
C 3.696091 0.239843 1.021018
C 4.687212 -0.718471 -1.423958
H 3.101432 0.432675 -2.350640
C 4.809323 -0.599712 0.996616
H 3.292718 0.627546 1.956904
C 5.296657 -1.079841 -0.219315
H 5.079066 -1.091343 -2.371088
H 5.296854 -0.878215 1.931825
H 6.165553 -1.740007 -0.230714
H -0.819203 -2.709578 1.920164

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atropisomerism/H_S_Ts_tBu-B

Frequencies, energies and thermodynamic properties:

Lowest Vibrational Mode (1/cm) = 19.7510
2nd Lowest Vibrational Mode (1/cm) = 24.2685
E(RM062X) (a.u.) = -1905.33910729
Thermal correction to Enthalpy (a.u.) = 0.419017
Thermal correction to Gibbs Free Energy (a.u.) = 0.337456
Total Entropy (cal/Kmol) = 171.659
Esp(RM062X) (a.u.) = -1906.90908701

Optimised cartesian coordinates (Angstrom):

N -0.466582 -0.572225 0.232313
C -0.096274 0.643689 0.024989
S -0.907034 2.039088 0.737895
C 0.029664 3.420552 0.023039
C 0.420872 3.137677 -1.409501
N 1.041534 0.821123 -0.753628
C 1.852260 -0.354419 -1.000029
C 2.830701 -0.799406 -0.093127
C 3.503709 -1.978610 -0.465441
C 3.244221 -2.656933 -1.651856
C 2.281623 -2.175853 -2.536714
C 1.587482 -1.023798 -2.197229
C 1.375121 1.976107 -1.492610
O 2.376010 1.993552 -2.160147
H 4.263890 -2.389436 0.196323
H 2.068640 -2.693417 -3.472954
H 0.814843 -0.622417 -2.855858
H 0.933200 3.999615 -1.853680
H -0.470107 2.910144 -2.016561
H -0.651930 4.278217 0.088271
H 3.802217 -3.565720 -1.883692
C 3.171463 -0.144243 1.262902

C	4.643778	-0.409107	1.627686
H	4.847509	-1.468848	1.829467
H	5.322615	-0.067874	0.830952
H	4.889501	0.143057	2.546146
C	2.289085	-0.772279	2.355965
H	2.560083	-0.354574	3.338516
H	1.221383	-0.575596	2.186386
H	2.429567	-1.863061	2.393967
S	-1.702212	-1.038068	1.241647
O	-1.550298	-2.472636	1.392233
O	-1.748110	-0.197762	2.434467
C	-3.156182	-0.729826	0.266652
C	-3.395544	-1.550188	-0.837189
C	-4.020776	0.300563	0.626678
C	-4.529879	-1.314642	-1.608523
H	-2.704786	-2.359395	-1.080771
C	-5.157502	0.519803	-0.152264
H	-3.806354	0.909055	1.506404
C	-5.407142	-0.281920	-1.265828
H	-4.735423	-1.942981	-2.476295
H	-5.850368	1.318762	0.115344
H	-6.297230	-0.104704	-1.871849
H	0.907222	3.627444	0.651280
C	2.984646	1.384380	1.281119
H	3.410802	1.857339	0.383086
H	1.932027	1.676916	1.379647
H	3.507212	1.794355	2.157664

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atropisomerism/H_S_Ts_tBu-F

Frequencies, energies and thermodynamic properties:

Lowest Vibrational Mode (1/cm) = 15.3711

2nd Lowest Vibrational Mode (1/cm) = 33.2207

E(RM062X) (a.u.) = -1905.33867110

Thermal correction to Enthalpy (a.u.) = 0.418772

Thermal correction to Gibbs Free Energy (a.u.) = 0.338466

Total Entropy (cal/Kmol) = 169.018

Esp(RM062X) (a.u.) = -1906.91039091

Optimised cartesian coordinates (Angstrom):

N	-0.263877	0.021854	-1.009601
C	-0.017671	-1.071748	-0.375462
S	-1.193469	-2.370353	-0.195399
C	-0.240833	-3.587398	0.752163
C	0.559458	-2.911653	1.841813
N	1.248689	-1.188398	0.185808
C	2.290021	-0.331936	-0.349730
C	2.555596	0.966104	0.113979
C	3.603310	1.639671	-0.543324
C	4.346512	1.071967	-1.571370
C	4.065448	-0.224304	-1.998647
C	3.032773	-0.915177	-1.381565
C	1.621531	-2.013937	1.266617
O	2.741382	-1.957549	1.703856
H	3.842226	2.660109	-0.242526
H	4.637129	-0.689219	-2.802814
H	2.777154	-1.930326	-1.691007
H	1.075347	-3.647852	2.470330
H	-0.098788	-2.305658	2.486106
H	-0.994698	-4.267334	1.168954
H	5.145938	1.648041	-2.040347
C	1.804490	1.754778	1.205867
C	1.064193	2.910349	0.507565
H	1.768750	3.609764	0.033919
H	0.397027	2.519090	-0.275398

H 0.466738 3.475554 1.240595
C 2.825078 2.323007 2.209208
H 2.296440 2.893749 2.987642
H 3.381454 1.508963 2.699048
H 3.550353 3.000513 1.739609
S -1.694449 0.387926 -1.772186
O -1.450224 1.654945 -2.436974
O -2.182075 -0.746443 -2.547771
C -2.827708 0.679321 -0.427548
C -2.652647 1.817926 0.360695
C -3.872409 -0.215377 -0.209633
C -3.538067 2.047084 1.410587
H -1.839020 2.514328 0.151473
C -4.757778 0.031773 0.839808
H -3.987021 -1.084386 -0.858946
C -4.586920 1.154973 1.648756
H -3.415527 2.930188 2.039263
H -5.584377 -0.656236 1.022825
H -5.281076 1.342146 2.469755
H 0.400109 -4.157485 0.065504
C 0.783025 0.964514 2.036387
H -0.073691 0.618848 1.444861
H 1.247554 0.116191 2.559677
H 0.383918 1.638406 2.809501

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atropisomerism/H_S_Ts_tBu-TS

Frequencies, energies and thermodynamic properties:

Lowest Vibrational Mode (1/cm) = -44.1563
2nd Lowest Vibrational Mode (1/cm) = 18.9238
E(RM062X) (a.u.) = -1905.28604529
Thermal correction to Enthalpy (a.u.) = 0.417610
Thermal correction to Gibbs Free Energy (a.u.) = 0.339841
Total Entropy (cal/Kmol) = 163.678
Esp(RM062X) (a.u.) = -1906.85245391

Optimised cartesian coordinates (Angstrom):

N -0.415334 -0.626310 -0.282984
C -0.042855 0.298537 0.505446
S -0.830124 0.736656 2.038956
C -0.391898 2.502890 1.976065
C -0.562260 3.013130 0.558129
N 1.013449 1.155853 0.091607
C 2.395022 0.834708 -0.210056
C 3.061529 -0.427529 -0.280832
C 4.396126 -0.385478 -0.738458
C 5.110090 0.770055 -1.013881
C 4.496954 1.992705 -0.771325
C 3.173952 2.004015 -0.368816
C 0.448499 2.389317 -0.386206
O 0.771222 2.896539 -1.421931
H 4.920360 -1.328369 -0.867462
H 5.032761 2.935736 -0.888307
H 2.720931 2.972666 -0.176143
H -0.396810 4.098272 0.499013
H -1.581546 2.819034 0.185723
H -1.088823 2.992226 2.668520
H 6.140536 0.707861 -1.366056
C 2.549808 -1.830671 0.140197
C 3.717654 -2.796135 0.446026
H 4.287442 -3.087843 -0.445902
H 4.410750 -2.379215 1.192284
H 3.285880 -3.718402 0.861799
C 1.787823 -2.490959 -1.026786
H 1.350992 -3.447488 -0.699770

H	0.983557	-1.870297	-1.427144
H	2.498154	-2.702069	-1.841169
S	-1.702768	-1.669139	0.055119
O	-1.563431	-2.758859	-0.890410
O	-1.769222	-1.956725	1.483987
C	-3.091019	-0.670548	-0.410624
C	-3.295134	-0.417603	-1.768404
C	-3.935919	-0.170662	0.577832
C	-4.375383	0.377667	-2.139225
H	-2.621366	-0.838691	-2.516544
C	-5.018967	0.616982	0.187737
H	-3.746677	-0.403108	1.626195
C	-5.232815	0.892454	-1.162963
H	-4.553336	0.591267	-3.193970
H	-5.698330	1.014061	0.943185
H	-6.080788	1.511353	-1.461003
H	0.632827	2.649788	2.342919
C	1.751956	-1.756100	1.472179
H	2.296369	-2.280689	2.269663
H	1.618796	-0.730704	1.839021
H	0.760264	-2.220760	1.400218