SUPPORTING INFORMATION

Unexpected metal-free synthesis of trifluoroarenes via tandem coupling of dicyanoalkenes and conjugated fluorinated sulfinylimines

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Contents

General remarks.

Reactions were carried out under a nitrogen atmosphere unless otherwise indicated. Solvents were purified prior to use: THF and PhMe were distilled from sodium, and CH_2Cl_2 was distilled from calcium hydride. The reactions were monitored with by means of TLC on 0.25 mm precoated silica gel plates. Visualization was carried out with UV light and potassium permanganate stain. Flash column chromatography was performed with the indicated solvents on silica gel 60 (particle size 0.040−0.063 mm). ^{1}H and ^{13}C-NMR spectra were recorded on a 300 MHz spectrometer. Chemical shifts are given in ppm (δ), referenced to the residual proton resonances of the solvents. Coupling constants (J) are given in hertz (Hz). The letters m, s, d, t, and q stand for multiplet, singlet, doublet, triplet, and quartet, respectively. The designation br indicates that the signal is broad. The abbreviations DCM and THF indicate dichloromethane and tetrahydrofuran, respectively. A QTOF mass analyzer system has been used for the HRMS measurements. Dicyanoalkenes **1** were prepared following known methodologies.[1] Imines **2a**,[2] **2b**,[3] **2e**,[2] **2f**[2], **2k**[4] and **2i**[5] were previously described.

[1] a) D. Xue, Y.-C. Chen, X. Cui, Q.-W. Wang, J. Zhu, J.-G. Deng, *J. Org. Chem,* 2005, **70**, 3584; b) J. Lu, F. Liu, T.-P. Loh, *Adv. Synth. Catal.* 2008, **350**, 1781. c) M. D. Kilde, P. G. Arroyo, A. S. Gertsen, K. V. Mikkelsen, M. B. Nielsen, *RSC Adv.* 2018, **8**, 6356.

[2] Z.-J. Liu, J.-T. Liu, *Chem. Commun.* 2008, 5233.

[3] D. Enders, K. Gottfried, G. Raabe, *Adv. Synth. Catal.* 2010, **352**, 3147.

[4] P. Liu, Z.-G. Liu, F. Wu, *Adv. Synth. Catal.* 2015, **357**, 818.

[5] L. G. Borrego, R. Recio, M. Alcarranza, N. Khiar, I. Fernández, *Adv. Synth. Catal.* 2018, **360**, 1273.

Starting dicyanoalkenes **1** and sulfinyl imines **2**.

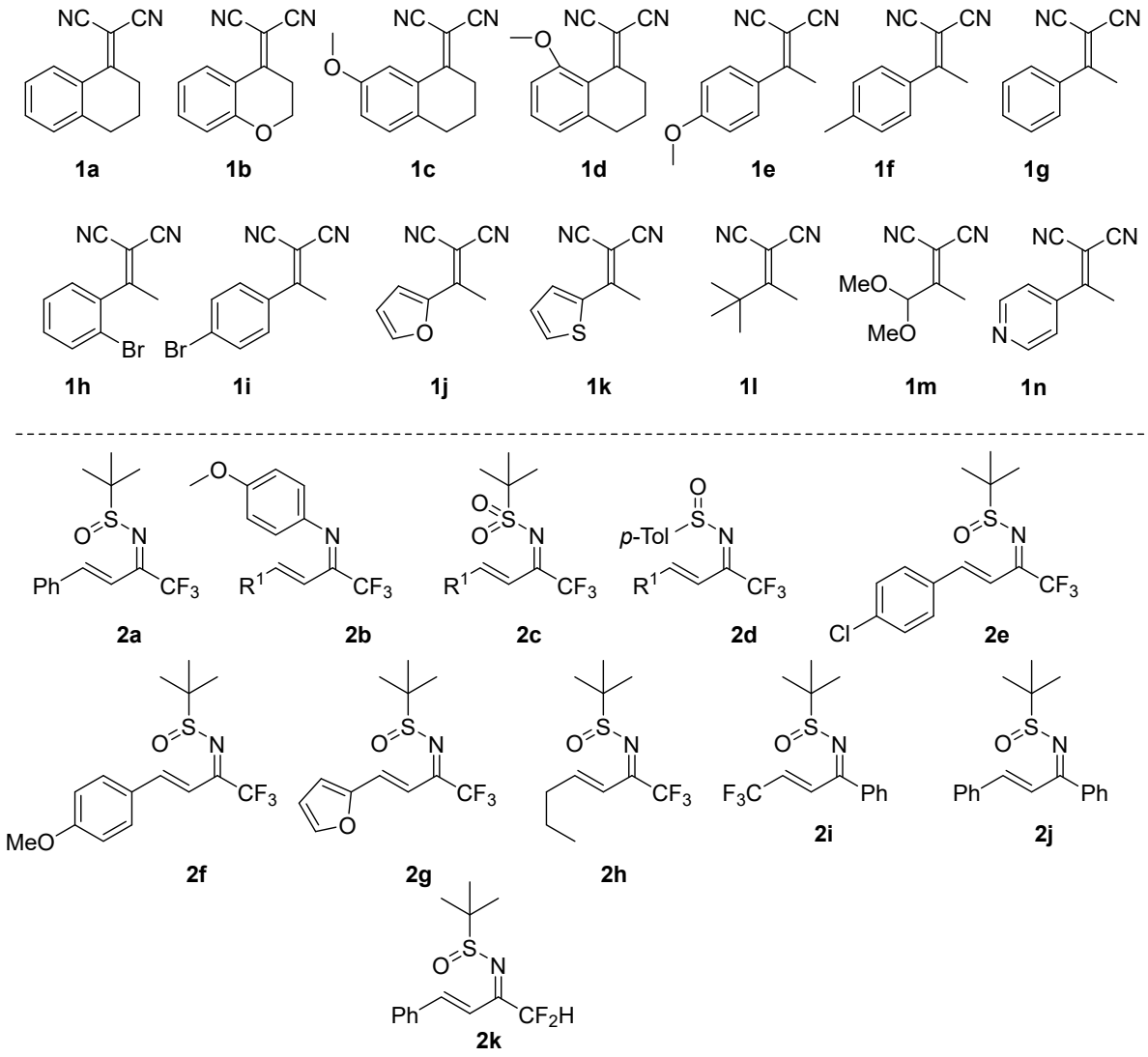
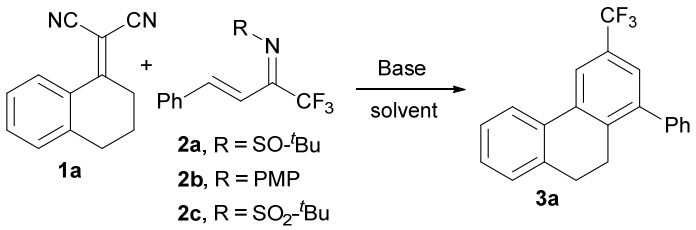


Table S1. Optimization of the reaction of dicyanoalkene **1a** with fluorinated imines **2a-c**[a]



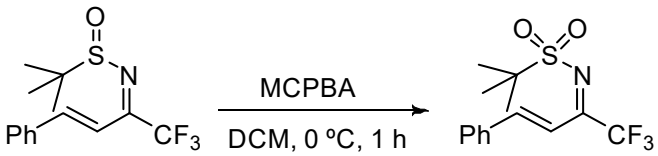
Entry	base	solvent	**2**	**3a** (yield %)[b]
1	*t*-BuOK	DCM	**2a**	-[c]
2	NaH	THF	**2a**	45
3	P_2-*t*Bu	DCM	**2a**	75
4	KHMDS	DCM	**2a**	0

5	Na_2CO_3	DCM	**2a**	0
6	DBU	DCM	**2a**	88
7	Et_3N	DCM	**2a**	0
8	DABCO	DCM	**2a**	0
9	TBAF	DCM	**2a**	0
10	DBU	DCE	**2a**	85
11	DBU	THF	**2a**	75
12	DBU	Acetone	**2a**	85
13	DBU	Toluene	**2a**	65
14	DBU	CH_3CN	**2a**	73
15	DBU	DCM	**2b**	-[c]
16	DBU	DCM	**2c**	-[c]

P_2-^{t}Bu = $(Me_2N)_3P$=N-$(Et_2N)_2P$=N-CMe_3. PMP= 4-MeO-C_6H_4.

[a] Reactions were carried out with **1a** (2 equiv.) and **2** (1 equiv.) in the corresponding solvent (0.1 M) and base (1.1 equiv.) at room temperature for 12 h. [b] Isolated yields of **3a**. [c] Complex mixture of products.

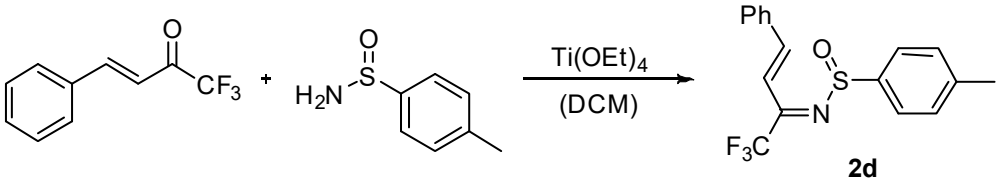
Preparation of conjugated sulfonyl imine **2c**.



2a **2c**

To a 100 mL round bottom flask fitted with a magnetic stirring bar, sulfinyl imine **2a** (303 mg, 1mmol) was dissolved in DCM (30 mL). m-CPBA (344 mg, 2 mmol) was then added and the mixture stirred for 10 min at room temperature. The mixture was quenched with $NaHCO_3$, extracted with DCM, dried over Na_2SO_4 and solvents removed under vacuum. Imine **2c** (303 mg) was obtained in 95% yield as an orange oil, after purification by column chromatography with Hex:EtOAc (4:1) as eluent. M. p. = 83-85 °C. ^{1}H NMR (300 MHz, $CDCl_3$) δ: 7.65 – 7.61 (m, 4H), 7.48 – 7.41 (m, 3H), 1.53 (s, 9H). ^{19}F NMR (282 MHz, $CDCl_3$) δ -66.2. ^{13}C NMR (75 MHz, $CDCl_3$) δ 148.8 (s), 134.0 (s), 132.4 (s), 129.4 (s), 129.4 (s), 119.4 (q, *J* = 283.2 Hz), 116.4 (s), 116.4 (s), 60.3 (s), 23.9 (s).

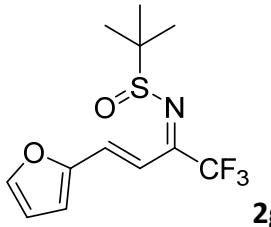
Preparation of conjugated imine **2d**.



2d

To a stirred solution of 1,1,1-trifluoro-4-phenyl-3-buten-2-one (5 mmol, 1,0 g) and $Ti(OEt)_4$ (20 mmol, 4,2 mL), p-tolyl sulfinamide (5 mmol, 775 mg) was added, and the neat reaction mixture was stirred at rt for 24h under N_2 atmosphere. The reaction mixture was diluted with 10 mL of DCM and quenched with 20 mL of a saturated NH_4Cl solution. The formed titanium salts were filtered over a Celite pad and the mixture extracted with more DCM, dried over sodium sulfate and evaporated under vacuum. Imine **2d** (1,35 g) was obtained in 80% as a yellow solid, after purification by column chromatography with Hex:EtOAc (4:1) as eluent. M. p. = 72-74 °C. ^{1}H NMR (300 MHz, $CDCl_3$) δ: 8.08 (dd, *J* = 16.9, 1.4 Hz, 1H), 7.74 – 7.69 (m, 2H), 7.59 (dd, *J* = 6.7, 2.9 Hz, 2H), 7.45 – 7.34 (m, 6H), 2.43 (s, 3H). ^{19}F NMR (282 MHz, $CDCl_3$) δ: -66.3. ^{13}C NMR (75 MHz, $CDCl_3$) δ 157.00 (q, *J* = 33.4 Hz), 144.74 (q, *J* = 2.6 Hz), 142.18, 141.31, 134.73, 131.29, 130.15, 129.19, 128.66, 125.49, 118.98 (q, *J* = 282.2 Hz), 114.98, 21.53.

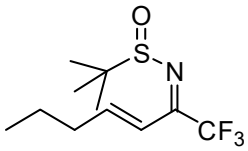
Preparation of conjugated imine **2g**.



2g

Starting from conjugated ketone 1(-2-furyl)-4,4-dimethyl-3-penten-2-one (890 mg, 5 mmol) and Ellman's reagent (5 mmol, 605 mg) and following the general procedure employed for the preparation of imine **2d**, imine **2g** (1.13 g, 77%) was obtained as an orange oil. ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.86 (dq, *J* = 16.6, 1.7 Hz, 1H), 7.52 (d, *J* = 1.7 Hz, 1H), 7.07 (dq, *J* = 16.6, 1.9 Hz, 1H), 6.70 (d, *J* = 3.5 Hz, 1H), 6.49 (dd, *J* = 3.5, 1.8 Hz, 1H), 1.33 (s, 9H). ^{19}F NMR (282 MHz, $CDCl_3$) δ -66.45. ^{13}C NMR (75 MHz, $CDCl_3$) δ 158.61 (q, *J* = 33.1 Hz), 151.25 (q, *J* = 1.3 Hz), 146.07, 129.83 (q, *J* = 3.0 Hz), 119.16 (q, *J* = 282.0 Hz), 116.69, 113.01, 112.90, 60.67, 23.09.

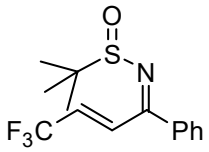
Preparation of conjugated imine **2h**.



2h

Starting from conjugated ketone 2,2-dimethyl-4-octen-3-one (770 mg, 5 mmol) and Ellman's reagent (5 mmol, 605 mg) and following the general procedure employed for the preparation of imine **2d**, imine **2h** (0.77 g, 57%) was obtained as a yellow oil. ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.24 (dh, *J* = 16.5, 1.6 Hz, 1H), 6.65 (dtq, *J* = 16.5, 6.9, 2.2 Hz, 1H), 2.25 (qd, *J* = 7.1, 1.5 Hz, 2H), 1.51 (h, *J* = 7.4 Hz, 2H), 1.30 (s, 9H), 0.93 (t, *J* = 7.4 Hz, 3H). ^{19}F NMR (282 MHz, $CDCl_3$) δ -66.69. ^{13}C NMR (75 MHz, $CDCl_3$) δ 159.21 (q, *J* = 32.8 Hz), 150.09 (q, *J* = 2.3 Hz), 119.03 (q, *J* = 282.0 Hz), 118.81, 60.22, 36.22, 23.00, 21.48, 13.74.

Preparation of conjugated imine **2i**.



2i

Starting from conjugated ketone 4,4,4-trifluoro-1-phenyl-2-buten-1-one (1 g, 5 mmol) and Ellman's reagent (5 mmol, 605 mg) and following the general procedure employed for the preparation of imine **2d**, imine **2i** (1.24 g, 82%) was obtained as a yellow oil. ^{1}H NMR (300 MHz, $CDCl_3$) δ: 8.02 (d, *J* = 16.3 Hz, 1H), 7.79 – 7.40 (m, 5H), 5.99 (dq, *J* = 16.3, 6.3 Hz, 1H), 1.33 (s, 9H). ^{19}F NMR (282 MHz, $CDCl_3$) δ -64.7. ^{13}C NMR (75 MHz, $CDCl_3$) δ 170.5, 137.2, 131.9, 128.8, 127.6 (q, *J* = 35.0 Hz), 122.5 (q, *J* = 270.5 Hz), 59.5, 23.0.

Preparation of polycyclic trifluoroarenes **3**.

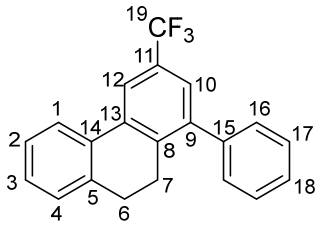
General procedure A for the cycloaromatization reaction

In a 50 mL round bottom flask fitted with a magnetic stirring bar, the corresponding dicyanoalkene **1** (0.6 mmol), DCM (6 mL) and DBU (0.6 mmol) were loaded. After stirring

the reaction mixture for 5 min at room temperature, a solution of the corresponding sulfinylimine **2** (0.3 mmol) in DCM (3 mL) was added. After stirring for 16 h at rt, the solvents were removed and the crude product purified by means of flash column chromatography.

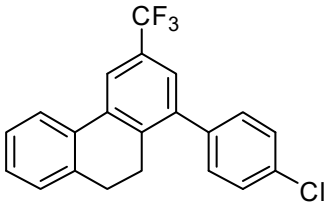
General procedure B for the cycloaromatization reaction

In a 50 mL round bottom flask fitted with a magnetic stirring bar, the corresponding sulfinylimine **2** (0.3 mmol), DCM (6 mL) and DBU (0.6 mmol) were loaded. After stirring the reaction mixture for 5 min at room temperature, a solution of the corresponding dicyanoalkene **1** (0.6 mmol) in DCM (3 mL) was slowly added with a syringe pump over 3 h (1 mL/h). After stirring for 3 additional hours at rt, the solvents were removed and the crude product purified by means of flash column chromatography.



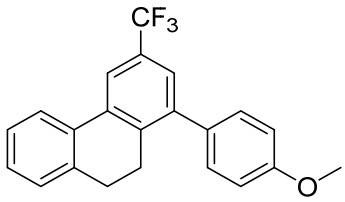
1-Phenyl-3-(trifluoromethyl)-9,10-dihydrophenanthrene (3a):

Starting from 2-(3,4-dihydronaphthalen-1(2H)-ylidene)malononitrile **1a** (116.5 mg), 2-methyl-N-((2Z,3E)-1,1,1-trifluoro-4-phenylbut-3-en-2-ylidene)propane-2-sulfinamide **2a** (91.0 mg) and DBU (90 µL), following the general procedure **A** mentioned above, the titled compound **3a** was obtained as a white solid (85.6 mg, 0.264 mmol, 88%) after purification by column chromatography with Hex:EtOAc (10:1) as eluent. M.p. = 89-91 °C. ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.0 (dcd, 1H, $^{4}J_{HH}$ 1.9, $^{4}J_{FH}$ 0.6, $^{5}J_{HH}$ 0.5, Hz, H12), 7.82 (ddt, 1H, $^{3}J_{HH}$ 7.5, $^{4}J_{HH}$ 1.4, $^{5}J_{HH}$ 0.5, Hz, H1), 7.5 (m, 1H, H10), 7.46 (m, 2H, H17), 7.43 (m, 1H, H18), 7.37 (m, 1H, H2), 7.36 (m, 2H, H16), 7.31 (td, 2H, $^{3}J_{HH}$ 7.2, $^{4}J_{HH}$ 1.4 Hz, H3), 7.26 (m, 1H, H4), 2.85 (m, 2H, H7), 2.77 (m, 2H, H6), ppm. ^{13}C{^{1}H} NMR (75.48 MHz, $CDCl_3$) δ 141.96 (C9), 140.3 (C15), 138.95 (c, $^{2}J_{FC}$ 1.4 Hz, C11), 137.53 (C5 + C8), 136.12 (C13), 133.91 (C14), 129.37 (C16), 128.5 (C17), 128.42 (C3), 128.13 (c, $^{1}J_{FC}$ 272.3 Hz, C19), 128.11 (C4), 127.74 (C18), 127.38 (C2), 124.44 (C1), 125.59 (c, $^{3}J_{FC}$ 3.8 Hz, C10), 120.02 (c, $^{3}J_{FC}$ 3.8 Hz, C12), 26.6 (C7), 28.75 (C6) ppm. ^{19}F{^{1}H} NMR (282.4 MHz, $CDCl_3$) δ -62.4 ppm. HRMS (ES): calculated for ($M - H_2 + H^+$) $C_{21}H_{14}F_3$: 323.1048; found 323.1058.



1-(4-Chlorophenyl)-3-(trifluoromethyl)-9,10-dihydrophenanthrene (3b):

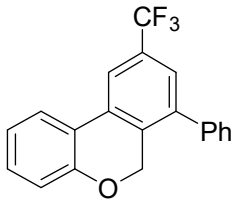
Starting from 2-(3,4-dihydronaphthalen-1(2H)-ylidene)malononitrile **1a** (116.5 mg), N-((2Z,3E)-4-(4-chlorophenyl)-1,1,1-trifluorobut-3-en-2-ylidene)-2-methylpropane-2-sulfinamide **2e** (101.3 mg) and DBU (90 µL), following the general procedure **A** mentioned above, the titled compound **3b** was obtained as a yellowish oil (91.5 mg, 0.255 mmol, 85%) after purification by column chromatography with Hex:EtOAc (10:1) as eluent. ^{1}H NMR (500 MHz, $CDCl_3$) δ: 7.91 (s, 1H), 7.71 (d, *J* = 7.6 Hz, 1H), 7.35 – 7.33 (m, 3H), 7.27 (td, *J* = 7.5, 1.0 Hz, 1H), 7.22 – 7.15 (m, 3H), 2.73 – 2.70 (m, 2H), 2.68 – 2.65 (m, 2H). ^{19}F NMR (282 MHz, $CDCl_3$) δ: -62.4 (s). ^{13}C NMR (126 MHz, $CDCl_3$) δ: 140.6, 138.8, 138.6, 137.3, 136.2, 133.8, 133.6, 130.6, 129.0 (q, *J* = 32.7 Hz), 128.6, 128.4, 128.0, 127.3, 125.3 (q, *J* = 3.7 Hz), 124.3, 124.3 (q, *J* = 273.4 Hz), 120.2 (q, *J* = 3.7 Hz), 28.6, 26.5. HRMS (ES): calculated for ($M - H_2 + H^+$) $C_{21}H_{13}ClF_3$: 357.0652; found 357.0655.



1-(4-Methoxyphenyl)-3-(trifluoromethyl)-9,10-dihydrophenanthrene (3c):

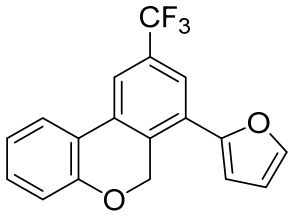
Starting from 2-(3,4-dihydronaphthalen-1(2H)-ylidene)malononitrile **1a** (116.5 mg), 2-methyl-N-((2Z,3E)-1,1,1-trifluoro-4-(4-methoxyphenyl)but-3-en-2-ylidene)propane-2-sulfinamide **2f** (100.0 mg) and DBU (90 µL), following the general procedure **A** mentioned above, the titled compound **3c** was obtained as a white solid (70.2 mg, 0.198 mmol, 66%) after purification by column chromatography with Hex:EtOAc (10:1) as eluent. M.p. = 89-91 °C. ^{1}H NMR (300 MHz, $CDCl_3$) δ: 7.89 (s, 1H), 7.73 (d, *J* = 7.4 Hz, 1H), 7.40 (s, 1H), 7.28 (ddd, *J* = 13.4, 6.7, 1.6 Hz, 1H), 7.22 – 7.18 (m, 3H), 6.92 (d, *J* = 8.8 Hz, 2H), 3.80 (s, 3H), 2.80 – 2.75 (m, 2H), 2.70 – 2.65 (m, 2H). ^{19}F NMR (282 MHz, $CDCl_3$) δ: -62.4 (s). ^{13}C NMR (75 MHz, $CDCl_3$) δ: 159.1, 141.5, 138.9, 137.4, 136.0, 133.9, 132.5, 130.4, 128.8 (q, *J* = 32.2 Hz), 128.2, 127.9, 127.2, 125.5 (q, *J* = 3.7 Hz), 124.4 (q, *J* = 272.2

Hz), 124.3, 119.6 (q, *J* = 3.7 Hz), 113.8, 55.4, 28.7, 26.5. HRMS (ES): calculated for (M – H_2 + H^+) $C_{22}H_{16}F_3O$: 353.1153; found 353.1162.



7-Phenyl-9-(trifluoromethyl)-6H-benzo[c]chromene (3d):

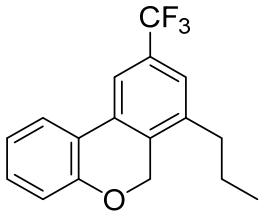
Starting from 2-(chroman-4-ylidene)malononitrile **1b** (117.7 mg), 2-methyl-N-((2Z,3E)-1,1,1-trifluoro-4-phenylbut-3-en-2-ylidene)propane-2-sulfinamide **2a** (91.0 mg) and DBU (90 µL), following the general procedure **A** mentioned above, the titled compound **3d** was obtained as a colourless solid (88.1 mg, 0.27 mmol, 90%) after purification by column chromatography with Hex:EtOAc (10:1) as eluent. M.p. = 73-75 °C. ^{1}H NMR (500 MHz, $CDCl_3$) δ: 7.86 (s, 1H), 7.74 (dd, *J* = 7.8, 1.4 Hz, 1H), 7.45 (br s, 1H), 7.45 – 7.42 (m, 3H), 7.25 – 7.21 (m, 3H), 7.05 (td, *J* = 7.7, 1.0 Hz, 1H), 6.94 – 6.92 (m, 1H), 5.02 (s, 2H). ^{19}F NMR (282 MHz, $CDCl_3$) δ: -62.6 (s). ^{13}C NMR (126 MHz, $CDCl_3$) δ: 154.9, 140.1, 138.3, 132.7, 131.7, 130.4, 130.4 (q, *J* = 32.4 Hz), 128.9, 128.7, 128.2, 125.6 (q, *J* = 3.7 Hz), 124.1 (q, J = 273.4 Hz), 123.8, 122.6, 122.3, 118.1 (q, *J* = 3.8 Hz), 117.4, 66.1. HRMS (ES): calculated for (M + H^+) $C_{20}H_{14}F_3O$: 327.0997; found 327.0995.



7-(Furan-2-yl)-9-(trifluoromethyl)-6H-benzo[c]chromene (3e):

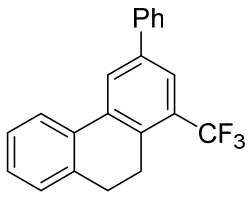
Starting from 2-(chroman-4-ylidene)malononitrile **1b** (117.7 mg), 2-methyl-N-((2Z,3E)-1,1,1-trifluoro-4-(furan-2-yl)but-3-en-2-ylidene)propane-2-sulfinamide **2g** (87.9 mg) and DBU (90 µL), following the general procedure **A** mentioned above, the titled compound **3e** was obtained as a white solid (75.8 mg, 0.24 mmol, 80%) after purification by column chromatography with Hex:EtOAc (10:1) as eluent. M.p. = 79-81 °C. ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.87 (d, *J* = 1.8 Hz, 1H), 7.82 (dd, *J* = 1.8, 0.8 Hz, 1H), 7.76 (dd, *J* = 7.7, 1.6 Hz, 1H), 7.59 (dd, *J* = 1.8, 0.8 Hz, 1H), 7.31 (ddd, *J* = 8.1, 7.4, 1.6 Hz, 1H), 7.11 (td, *J* =

7.5, 1.3 Hz, 1H), 7.03 (dd, *J* = 8.1, 1.2 Hz, 1H), 6.57 (dd, *J* = 3.4, 1.8 Hz, 1H), 6.53 (dd, *J* = 3.4, 0.8 Hz, 1H), 5.39 (s, 1H). ^{19}F NMR (282 MHz, $CDCl_3$) δ -62.84. ^{13}C NMR (75 MHz, $CDCl_3$) δ 154.85, 151.03, 143.48, 132.10, 132.06 (q, *J* = 1.2 Hz), 130.75 (q, *J* = 32.6 Hz), 130.61, 128.56, 124.09 (q, *J* = 272.3 Hz), 123.89, 123.36 (q, *J* = 3.9 Hz), 122.70, 122.15, 118.39 (q, *J* = 3.7 Hz), 117.53, 111.97, 110.29, 66.08. HRMS (ES): calculated for (M + H^+) $C_{18}H_{12}F_3O_2$: 317.0789; found 317.0798.



7-Propyl-9-(trifluoromethyl)-6H-benzo[c]chromene (3f):

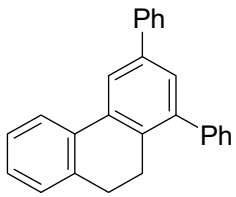
Starting from 2-(chroman-4-ylidene)malononitrile **1b** (117.7 mg), 2-methyl-N-((2Z,3E)-1,1,1-trifluorohept-3-en-2-ylidene)propane-2-sulfinamide **2h** (81.3 mg) and DBU (90 µL), following the general procedure **A** mentioned above, the titled compound **3f** was obtained as a white solid (38.7 mg, 0.13 mmol, 44%) after purification by column chromatography with Hex:EtOAc (10:1) as eluent. M.p. = 50-52 °C. ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.79 (s, 1H), 7.75 (dd, *J* = 7.8, 1.6 Hz, 1H), 7.37 (s, 1H), 7.28 (ddd, *J* = 8.1, 7.4, 1.6 Hz, 1H), 7.09 (td, *J* = 7.6, 1.2 Hz, 1H), 7.01 (dd, *J* = 8.1, 1.2 Hz, 1H), 5.18 (s, 2H), 2.70 – 2.60 (m, 2H), 1.70 – 1.53 (m, 2H), 1.00 (t, *J* = 7.3 Hz, 3H). ^{19}F NMR (282 MHz, $CDCl_3$) δ -62.66. ^{13}C NMR (75 MHz, $CDCl_3$) δ 154.73, 139.11, 133.30 (q, *J* = 1.4 Hz), 131.26, 130.40 (q, *J* = 32.1 Hz), 130.30, 125.29 (q, *J* = 3.8 Hz), 124.35 (q, *J* = 272.5 Hz), 123.82, 122.60, 122.34, 117.44, 116.99 (q, *J* = 3.9 Hz), 65.25, 34.65, 23.95, 13.97. HRMS (ES): calculated for (M + H^+) $C_{17}H_{16}F_3O$: 294.1187; found 294.1180.



3-Phenyl-1-(trifluoromethyl)-9,10-dihydrophenanthrene (3g):

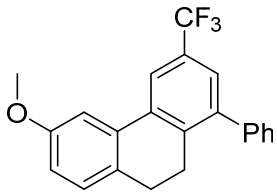
Starting from 2-(3,4-dihydronaphthalen-1(2H)-ylidene)malononitrile **1a** (116.5 mg), 2-methyl-*N*-((1E,2E)-4,4,4-trifluoro-1-phenylbut-2-en-1-ylidene)propane-2-sulfinamide **2i**

(93.4 mg) and DBU (90 µL), following the general procedure **A** mentioned above, the titled compound **3g** was obtained as a white solid (38.9 mg, 0.120 mmol, 40%) after purification by column chromatography with Hex:EtOAc (10:1) as eluent. M. p. = 111–112 °C. ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.14 (d, *J* = 1.3 Hz, 1H), 7.85 – 7.77 (m, *2*H), 7.71 – 7.61 (m, 2H), 7.56 – 7.45 (m, 2H), 7.46 – 7.27 (m, 4H), 3.24 – 3.03 (m, 2H), 2.97 – 2.87 (m, 2H). ^{19}F NMR (282 MHz, $CDCl_3$) δ -60.1. ^{13}C NMR (75 MHz, $CDCl_3$) δ 140.2, 139.9, 137.5, 137.0, 135.2 (q, *J* = 1.69 Hz), 133.7, 129.1, 128.7, 128.4, 128.1, 128.0, 127.4, 127.2, 126.3, 124.7 (q, *J* = 275.0 Hz), 124.4, 123.6 (q, *J* = 5.7 Hz), 28.4, 24.9 (q, *J* = 2.3 Hz). HRMS (ES): calculated for (M – H_2 + H^+) $C_{21}H_{14}F_3$: 323.1048; found 323.1056.



1,3-Diphenyl-9,10-dihydrophenanthrene (3h):

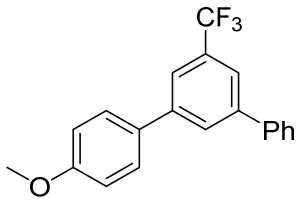
Starting from 2-(3,4-dihydronaphthalen-1(2H)-ylidene)malononitrile **1a** (116.5 mg), N-((1Z,2E)-1,3-diphenylallylidene)-2-methylpropane-2-sulfinamide **2j** (93.4 mg) and DBU (90 µL), following the general procedure **A** mentioned above, the titled compound **3h** was obtained as a yellowish oil (40.9 mg, 0.123 mmol, 41%) after purification by column chromatography with Hex:EtOAc (10:1) as eluent. ^{1}H NMR (300 MHz, $CDCl_3$) δ: 7.92 (d, *J* = 1.8 Hz, 1H), 7.78 (d, *J* = 7.6 Hz, 1H), 7.61 – 7.58 (m, 2H), 7.41 – 7.14 (m, 12H), 2.79 – 2.74 (m, 2H), 2.71 – 2.66 (m, 2H). ^{13}C NMR (75 MHz, $CDCl_3$) δ: 141.6, 141.4, 141.2, 139.4, 137.6, 135.6, 134.9, 134.2, 129.4, 128.8, 128.2, 128.0, 127.9, 127.6, 127.3, 127.2, 127.1, 127.0, 124.2, 122.1, 29.2, 26.3. HRMS (ES): calculated for (M – H_2 + H^+) $C_{21}H_{19}$: 331.1487; found 331.1489.



6-Methoxy-1-phenyl-3-(trifluoromethyl)-9,10-dihydrophenanthrene (3i):

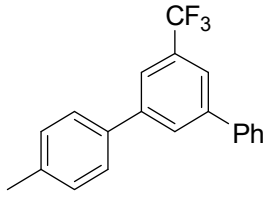
Starting from 2-(7-methoxy-3,4-dihydronaphthalen-1(2H)-ylidene)malononitrile **1c** (134.6 mg), 2-methyl-N-((2Z,3E)-1,1,1-trifluoro-4-phenylbut-3-en-2-ylidene)propane-2-

sulfinamide **2a** (91.0 mg) and DBU (90 µL), following the general procedure **A** mentioned above, the titled compound **3i** was obtained as a yellowish solid (97.8 mg, 0.276 mmol, 92%) after purification by column chromatography with Hex:EtOAc (10:1) as eluent. M.p. = 80-82 °C. ^{1}H NMR (500 MHz, $CDCl_3$) δ: 7.97 (br s, 1H), 7.51 (br s, 1H), 7.49 – 7.46 (m, 2H), 7.44 – 7.40 (m, 1H), 7.37 – 7.35 (m, 3H), 7.18 (d, *J* = 8.2 Hz, 1H), 6.87 (dd, *J* = 8.2, 2.6 Hz, 1H), 3.91 (s, 3H), 2.85 – 2.82 (m, 2H), 2.72 – 2.69 (m, 2H). ^{19}F NMR (282 MHz, $CDCl_3$) δ: -62.4 (s). ^{13}C NMR (126 MHz, $CDCl_3$) δ: 158.9, 141.9, 140.2, 136.0, 134.7, 129.7, 129.2, 128.8, 128.8 (q, *J* = 32.7 Hz), 128.4, 127.6, 125.6 (q, *J* = 3.7 Hz), 124.4 (q, *J* = 273.4 Hz), 119.9 (q, *J* = 3.7 Hz), 113.69, 110.01, 55.55, 27.75, 26.84. HRMS (ES): calculated for ($M - H_2 + H^+$) $C_{22}H_{16}F_3O$: 353.1153; found 353.1152.



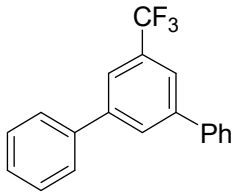
4-Methoxy-5'-(trifluoromethyl)-1,1':3',1''-terphenyl (3k):

Starting from 2-(1-(4-methoxyphenyl)ethylidene)malononitrile **1e** (118.9 mg), 2-methyl-N-((2Z,3E)-1,1,1-trifluoro-4-phenylbut-3-en-2-ylidene)propane-2-sulfinamide **2a** (91.0 mg) and DBU (90 µL), following the general procedure **B** mentioned above, the titled compound **3k** was obtained as a white solid (60.1 mg, 0.183 mmol, 61%) after purification by column chromatography with Hex:EtOAc (10:1) as eluent. M. p. = 84-86 °C. ^{1}H NMR (500 MHz, $CDCl_3$) δ: 7.92 (s, 1H), 7.77 (br s, 2H), 7.65 (d, *J* = 7.1 Hz, H), 7.60 (d, *J* = 8.8 Hz, 2H), 7.50 (t, *J* = 7.5 Hz, 2H), 7.42 (t, *J* = 7.4 Hz, 1H), 7.03 (d, *J* = 8.8 Hz, 2H), 3.88 (s, 3H). ^{19}F NMR (471 MHz, $CDCl_3$) δ: -62.5. ^{13}C NMR (126 MHz, $CDCl_3$) δ: 159.8, 142.6, 142.2, 139.9, 132.2, 131.6 (q, *J* = 32.0 Hz), 129.0, 128.8, 128.4, 128.1, 127.3, 124.3 (q, *J* = 273.4 Hz), 122.3 (q, *J* = 3.7 Hz), 122.1 (q, *J* = 3.8 Hz), 114.5, 55.4. HRMS (ES): calculated for ($M + H^+$) $C_{20}H_{16}F_3O$: 329.1153; found 329.1156.



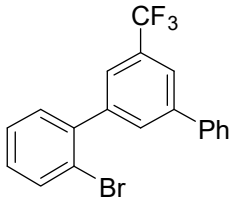
4-Methyl-5'-(trifluoromethyl)-1,1':3',1''-terphenyl (3l):

Starting from 2-(1-(p-tolyl)ethylidene)malononitrile **1f** (109.3 mg), 2-methyl-N-((2Z,3E)-1,1,1-trifluoro-4-phenylbut-3-en-2-ylidene)propane-2-sulfinamide **2a** (91.0 mg) and DBU (90 µL), following the general procedure **B** mentioned above, the titled compound **3l** was obtained as a white solid (75.9 mg, 0.243 mmol, 81%) after purification by column chromatography with Hex:EtOAc (10:1) as eluent. M. p. = 83-85 °C. ^{1}H NMR (500 MHz, $CDCl_3$) δ: 7.96 (s, 0H), 7.80 (d, *J* = 5.1 Hz, 1H), 7.66 (d, *J* = 7.2 Hz, 1H), 7.56 (d, *J* = 8.1 Hz, 1H), 7.50 (t, *J* = 7.6 Hz, 1H), 7.43 (t, *J* = 7.4 Hz, 0H), 7.31 (d, *J* = 8.0 Hz, 1H), 2.44 (s, 1H). ^{19}F NMR (471 MHz, $CDCl_3$) δ: -62.5. ^{13}C NMR (126 MHz, $CDCl_3$) δ: 142.6, 142.6, 139.9, 138.1, 136.9, 131.7 (q, *J* = 32.0 Hz), 129.8, 129.1, 129.0, 128.1, 127.3, 127.1, 124.3 (q, *J* = 272.6 Hz), 122.5 (dq, *J* = 7.6, 3.8 Hz), 21.2. HRMS (ES): calculated for (M + H^+) $C_{20}H_{16}F_3$: 313.1204; found 313.1210.



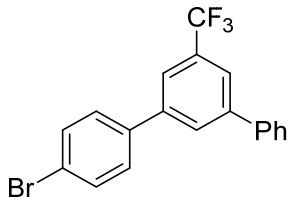
5'-(Trifluoromethyl)-1,1':3',1''-terphenyl (3m):

Starting from 2-(1-phenylethylidene)malononitrile **1g** (100.9 mg), 2-methyl-N-((2Z,3E)-1,1,1-trifluoro-4-phenylbut-3-en-2-ylidene)propane-2-sulfinamide **2a** (91.0 mg) and DBU (90 µL), following the general procedure **B** mentioned above, the titled compound **3m** was obtained as a colorless solid (69.8 mg, 0.234 mmol, 78%) after purification by column chromatography with Hex:EtOAc (10:1) as eluent. M. p. = 80-82 °C. ^{1}H NMR (500 MHz, $CDCl_3$) δ: 7.98 (s, 1H), 7.83 (s, 1H), 7.68 – 7.66 (m, 2H), 7.51 (t, *J* = 7.5 Hz, 2H), 7.43 (t, *J* = 7.4 Hz, 1H). ^{19}F NMR (471 MHz, $CDCl_3$) δ: -62.5 (s). ^{13}C NMR (126 MHz, $CDCl_3$) δ: 142.7, 139.8, 131.7 (q, *J* = 32.1 Hz), 129.3, 129.1, 128.2, 127.3, 124.2 (q, *J* = 272.7 Hz), 122.8 (q, *J* = 3.7 Hz). HRMS (ES): calculated for (M + H^+) $C_{19}H_{14}F_3$: 299.1048; found 299.2052.



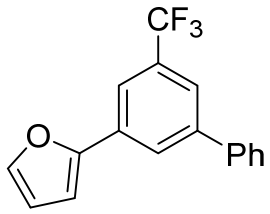
2-Bromo-5'-(trifluoromethyl)-1,1':3',1''-terphenyl (3n):

Starting from 2-(1-(2-bromophenyl)ethylidene)malononitrile **1h** (148.3 mg), 2-methyl-N-((2Z,3E)-1,1,1-trifluoro-4-phenylbut-3-en-2-ylidene)propane-2-sulfinamide **2a** (91.0 mg) and DBU (90 µL), following the general procedure **B** mentioned above, the titled compound **3n** was obtained as a colorless oil (80.3 mg, 0.213 mmol, 78%) after purification by column chromatography with Hex:EtOAc (10:1) as eluent. ^{1}H NMR (500 MHz, $CDCl_3$) δ: 7.85 (d, *J* = 9.2 Hz, 2H), 7.72 (d, *J* = 8.6 Hz, 1H), 7.66 – 7.64 (m, 3H), 7.49 (t, *J* = 7.6 Hz, 2H), 7.43 – 7.38 (m, 3H), 7.29 – 7.25 (m, 1H). ^{19}F NMR (471 MHz, $CDCl_3$) δ: -62.4 (s). ^{13}C NMR (126 MHz, $CDCl_3$) δ: 142.2, 141.8, 141.0, 139.5, 133.4, 131.6, 131.1 (q, *J* = 33.8 Hz), 131.2, 129.5, 129.0, 128.2, 127.7, 127.3, 125.0 (q, *J* = 3.8 Hz), 124.1 (q, *J* = 272.6 Hz), 123.1 (q, *J* = 3.8 Hz), 122.5. HRMS (ES): calculated for (M + H^+) $C_{19}H_{13}BrF_3$: 377.0153; found 377.0152.



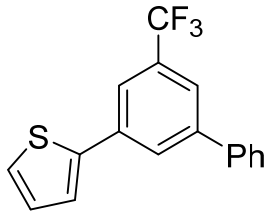
4-Bromo-5'-(trifluoromethyl)-1,1':3',1''-terphenyl (3o):

Starting from 2-(1-(4-bromophenyl)ethylidene)malononitrile **1i** (148.3 mg), 2-methyl-N-((2Z,3E)-1,1,1-trifluoro-4-phenylbut-3-en-2-ylidene)propane-2-sulfinamide **2a** (91.0 mg) and DBU (90 µL), following the general procedure **B** mentioned above, the titled compound **3o** was obtained as a colourless solid (55.5 mg, 0.147 mmol, 49%) after purification by column chromatography with Hex:EtOAc (10:1) as eluent. M. p. = 78-80 °C. ^{1}H NMR (500 MHz, $CDCl_3$) δ: 7.92 (s, 1H), 7.83 (s, 1H), 7.77 (s, 1H), 7.65 – 7.62 (m, 4H), 7.53 – 7.49 (m, 4H), 7.43 (t, *J* = 7.3 Hz, 1H). ^{19}F NMR (471 MHz, $CDCl_3$) δ: -62.5 (s). ^{13}C NMR (126 MHz, $CDCl_3$) δ: 142.9, 141.4, 139.6, 138.7, 132.2, 131.9 (q, *J* = 32.2 Hz), 129.1, 129.0, 128.9, 128.3, 127.3, 124.1 (q, *J* = 273.4 Hz), 123.1 (q, *J* = 3.7 Hz), 122.6, 122.5 (q, *J* = 3.7 Hz). HRMS (ES): calculated for (M + H^+) $C_{19}H_{13}BrF_3$: 377.0153; found 377.0158.



2-(5-(Trifluoromethyl)-[1,1'-biphenyl]-3-yl)furan (3p)

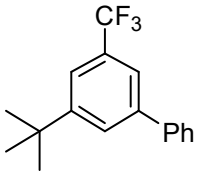
Starting from 3-(furan-2-yl)-2-isocyano-2-butenenitrile **1j** (95 mg), 2-methyl-N-((2Z,3E)-1,1,1-trifluoro-4-phenylbut-3-en-2-ylidene)propane-2-sulfinamide **2a** (91.0 mg) and DBU (90 µL), following the general procedure **A** mentioned above, the titled compound **3p** was obtained as a white solid (45 mg, 0.12 mmol, 52%) after purification by column chromatography with Hex:EtOAc (10:1) as eluent. M. p. = 57 – 59 ºC. ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.05 (t, *J* = 1.7 Hz, 1H), 7.89 (td, *J* = 1.7, 0.8 Hz, 1H), 7.71 (td, *J* = 1.7, 0.8 Hz, 1H), 7.68 – 7.61 (m, 2H), 7.56 – 7.46 (m, 3H), 7.46 – 7.39 (m, 1H), 6.80 (dd, *J* = 3.4, 0.8 Hz, 1H), 6.53 (dd, *J* = 3.4, 1.8 Hz, 1H). ^{19}F NMR (282 MHz, $CDCl_3$) δ -62.75. ^{13}C NMR (75 MHz, $CDCl_3$) δ 152.63, 143.03, 142.75, 139.74, 132.18, 131.87 (q, *J* = 32.3 Hz), 129.16, 128.36, 127.36, 125.59 (q, *J* = 1.0 Hz), 124.21 (q, *J* = 272.6 Hz) 122.69 (q, *J* = 3.8 Hz), 119.43 (q, *J* = 3.9 Hz), 112.09, 106.70. HRMS (ES): calculated for (M + H^+) $C_{17}H_{12}F_3O$: 289.0840; found 289.0850.



2-(5-(Trifluoromethyl)-[1,1'-biphenyl]-3-yl)thiophene (3q)

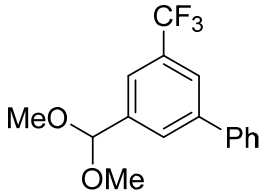
Starting from 2-isocyano-3-(thiophen-2-yl)but-2-enenitrileitrile **1k** (104 mg), 2-methyl-N-((2Z,3E)-1,1,1-trifluoro-4-phenylbut-3-en-2-ylidene)propane-2-sulfinamide **2a** (91.0 mg) and DBU (90 µL), following the general procedure **A** mentioned above, the titled compound **3q** was obtained as a white solid (52 mg, 0.12 mmol, 57%) after purification by column chromatography with Hex:EtOAc (10:1) as eluent. M. p. = 67 – 69 ºC. ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.97 (t, *J* = 1.8 Hz, 1H), 7.83 (td, *J* = 1.7, 0.8 Hz, 1H), 7.74 (td, *J* = 1.7, 0.8 Hz, 1H), 7.68 – 7.60 (m, 2H), 7.55 – 7.41 (m, 4H), 7.37 (dd, *J* = 5.1, 1.2 Hz, 1H), 7.14 (dd, *J* = 5.1, 3.6 Hz, 1H). ^{19}F NMR (282 MHz, $CDCl_3$) δ -62.65. ^{13}C NMR (75 MHz, $CDCl_3$) δ 143.01, 142.77, 139.66, 135.88, 132.00 (q, *J* = 32.3 Hz), 129.19, 128.43, 128.41, 127.98

(q, *J* = 1.4 Hz), 127.39, 126.12, 124.48, 124.17 (q, *J* = 272.6 Hz), 122.93 (q, *J* = 3.7 Hz), 121.48 (q, *J* = 3.8 Hz). HRMS (ES): calculated for (M + H^+) $C_{17}H_{12}F_3S$: 305.0612; found 305.0615.



3-(*tert*-Butyl)-5-(trifluoromethyl)-1,1'-biphenyl (3r):

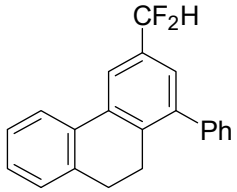
Starting from 2-isocyano-3,4,4-trimethyl-2-pentenenitrile **1l** (89 mg), 2-methyl-N-((2Z,3E)-1,1,1-trifluoro-4-phenylbut-3-en-2-ylidene)propane-2-sulfinamide **2a** (91.0 mg) and DBU (90 µL), following the general procedure **A** mentioned above, the titled compound **3r** was obtained as a colourless oil (33.4 mg, 0.12 mmol, 40%) after purification by column chromatography with Hex:EtOAc (10:1) as eluent. ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.77 (t, *J* = 1.8 Hz, 1H), 7.68 – 7.56 (m, 4H), 7.52 – 7.44 (m, 2H), 7.43 – 7.36 (m, 1H), 1.41 (s, 9H). ^{19}F NMR (282 MHz, $CDCl_3$) δ -62.30. ^{13}C NMR (75 MHz, $CDCl_3$) δ 152.77, 141.97, 140.61, 130.98 (q, *J* = 31.6 Hz), 129.07, 128.00, 127.90 (q, *J* = 1.4 Hz), 127.47, 124.58 (q, *J* = 272.5 Hz), 121.46 (q, *J* = 3.8 Hz), 121.04 (q, *J* = 3.8 Hz), 35.21, 31.41. HRMS (ES): calculated for (M + H^+) $C_{17}H_{18}F_3$: 279.1361; found 279.1357.



3-(Dimethoxymethyl)-5-(trifluoromethyl)-1,1'-biphenyl (3s):

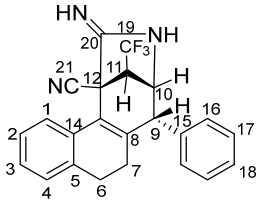
Starting from (Z)-2-isocyano-4,4-dimethoxy-3-methyl-2-butenenitrile **1m** (89 mg), 2-methyl-N-((2Z,3E)-1,1,1-trifluoro-4-phenylbut-3-en-2-ylidene)propane-2-sulfinamide **2a** (91.0 mg) and DBU (90 µL), following the general procedure **A** mentioned above, the titled compound **3s** was obtained as a colourless oil (26.8 mg, 0.09 mmol, 30%) after purification by column chromatography with Hex:EtOAc (10:1) as eluent. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.87 (t, *J* = 1.7 Hz, 1H), 7.80 (t, *J* = 1.8 Hz, 1H), 7.71 (t, *J* = 1.7 Hz, 1H), 7.64 – 7.60 (m, 2H), 7.50 – 7.44 (m, 2H), 7.43 – 7.38 (m, 1H), 5.50 (s, 1H), 3.37 (s, 6H). ^{19}F NMR (471 MHz, $CDCl_3$) δ -62.48. ^{13}C NMR (126 MHz, $CDCl_3$) δ 142.25, 139.97, 139.71, 131.38

(q, *J* = 32.4 Hz), 129.14, 128.94, 128.27, 127.39, 124.11 (q, *J* = 3.7 Hz), 124.28 (d, *J* = 272.5 Hz), 122.64 (q, *J* = 3.8 Hz), 102.29, 52.92. HRMS (ES): calculated for (M + H^+) $C_{16}H_{16}F_3O_2$: 297.1102; found 297.1108.



3-(Difluoromethyl)-1-phenyl-9,10-dihydrophenanthrene (3u):

Starting from 2-(3,4-dihydronaphthalen-1(2H)-ylidene)malononitrile **1a** (116.5 mg), N-((2Z,3E)-1,1-difluoro-4-phenylbut-3-en-2-ylidene)-2-methylpropane-2-sulfinamide **2k** (85.6 mg) and DBU (90 µL), following the general procedure **A** mentioned above, the titled compound **3u** was obtained as a yellowish oil (56.1 mg, 0.183 mmol, 61%) after purification by column chromatography with Hex:EtOAc (10:1) as eluent. ^{1}H NMR (300 MHz, $CDCl_3$) δ: 7.82 (s, 1H), 7.74 (d, *J* = 8.4 Hz, 1H), 7.41 – 7.15 (m, 9H), 6.65 (t, *J* = 56.6 Hz, 1H), 2.78 – 2.73 (m, 2H), 2.70 – 2.65 (m, 2H). ^{19}F NMR (282 MHz, $CDCl_3$) δ: -110.2 (dt, *J* = 56.7, 1.2 Hz). ^{13}C NMR (75 MHz, $CDCl_3$) δ: 141.7, 140.6, 137.7, 137.4, 135.8, 134.1, 132.6 (t, *J* = 22.4 Hz), 129.3, 128.3, 128.0, 127.9, 127.4, 127.2, 126.0 (t, *J* = 6.0 Hz), 124.3, 120.3 (t, *J* = 6.0 Hz), 114.9 (t, *J* = 238.8 Hz), 28.8, 26.5. HRMS (ES): calculated for (M – H_2 + H^+) $C_{21}H_{15}F_2$: 305.1142; found 305.1152.



(1S*,4S*,5S*,12R*)-2-imino-5-phenyl-12-(trifluoromethyl)-2,3,4,5-tetrahydro-1H-1,4-methanonaphtho[1,2-d]azepine-1-carbonitrile (4). In a 50 mL round bottom flask fitted with a magnetic stirring bar, sulfinylimine **2g** (106 mg, 0.3 mmol), DCM (6 mL) and DBU (90 µL, 0.6 mmol) were loaded. After stirring the reaction mixture for 5 min at room temperature, a solution of the corresponding dicyanoalkene **1a** (116.5 mg, 0.6 mmol) in DCM (3 mL) was slowly added with a syringe pump over 3 h (1 mL/h). After stirring over night, the solvents were removed and the crude product purified by means of flash

column chromatography to afford the title compound **8** (71 mg, 60%; together with 29 mg of **3a**) as a light yellow oil. ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.84 (bd, 1H, $^{3}J_{HH}$ 7.7 Hz, H1), 7.36 (m, 2H, H17), 7.33 (m, 1H, H2), 7.30 (m, 1H, H3), 7.26 (m, 2H, H4 + H18), 7.17 (m, 2H, H16), 4.38 (cd, 1H, $^{3}J_{FH}$ 7.3, $^{3}J_{HH}$ 4.1 Hz, H11), 3.98 (m, 1H, H9), 3.55 (dd, $^{3}J_{HH}$ 4.2 and 2.9 Hz, H10), 2.89 (m, 1H, H6^{a}), 2.81 (m, 1H, H6^{e}), 2.19 (m, 1H, H7^{e}), 2.16 (m, 1H, H7^{a}) ppm. ^{13}C{^{1}H} NMR (75.48 MHz, $CDCl_3$) δ 163.85 (C20), 147.66 (C8), 139.71 (C15), 136.68 (C5), 130.04 (C14), 129.53 (C13), 129.49 (C17), 129.08 (C4), 128.53 (C18), 128.04 (C3), 127.44 (C16), 127.21 (C2), 125.32 (c, $^{1}J_{FC}$ 280.5 Hz, C19), 121.93 (C1), 118.43 (c, $^{4}J_{FC}$ 25.4 Hz, C21), 75.63 (c, $^{2}J_{FC}$ 4.1 Hz, C11), 61.0 (C9), 59.84 (c, $^{3}J_{FC}$ 1.6 Hz, C10), 58.77 (C12), 28.25 (C6), 23.71 (C7) ppm. ^{19}F{^{1}H} NMR (282.4 MHz, $CDCl_3$) δ -76.0 ppm. HRMS (ESI) calcd. for $C_{23}H_{19}F_3N_3$: 394.1519; calcd: 394.1526. The superscripts a/e stand for axial/equatorial.

The structural assignment of compound **4** was based on the analysis of the 1D (^{1}H, ^{13}C, ^{19}F) and 2D (COSY, HSQC-edited, HMBC NOESY) set of NMR spectra. The identification of the dihydronaphthalene (**A**) and phenyl (**B**) fragments was straightforward. The three proton spin systems present in these fragments are easily recognizable in the COSY spectrum (Fig. S1, blue arrows). The correlations observed in the HMBC spectrum for the methylenic protons of **A** (δ 2.89, 2.81, H6 and δ 2.16, 2.19, H7 ppm, red arrows) confirmed the connectivity in this substructure and allowed to assign all the quaternary carbons. In addition, the correlation of H4 (δ 7.26 ppm) with C6 (δ 28.25 ppm) provided the reference for the sequence of assignment of the aromatic protons.

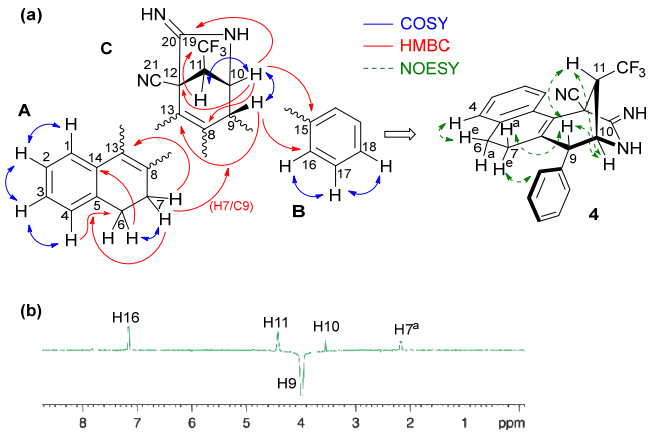


Figure S1. (a) Selected correlations observed in the 2D COSY, HMBC and NOESY NMR spectra of **8** including the numbering scheme used. **(b)** Row extracted from the 2D NOESY spectrum showing the NOEs of H9.

The same assignment strategy afforded the structure of the azabicyclo[3.2.1]octene system **C**. Thus, the short chain of three methine protons at δ 4.38 (H11), 3.98 (H9) and 3. 55 (H10) ppm is evidenced in the COSY spectrum by the correlations of H10 with H9 and H11 (blue arrows). On the other hand, the correlations detected in the HMBC spectrum (Fig. 2, red arrows) of H10 with C12, C20 and C21 fixed the position of these carbon atoms. Interestingly, the correlation H10-C21 involved a $^4J_{CH}$ probably favoured by the rigidity of the molecule and the zigzag arrangement of H10 and C21. The location of the CF_3 substituent was established by the cross-peaks of negative slope existing between H11 and the C19 quartet.[15] This assignment was further supported by the doublet observed in the ^{19}F NMR spectrum measured without ^1H decoupling at δ -76.0 ppm ($^3J_{FH}$ 7.3 Hz) The same assignment strategy afforded the structure of the azabicyclo[3.2.1]octene system **C**. Thus, the short chain of three methine protons at δ 4.38 (H11), 3.98 (H9) and 3. 55 (H10) ppm is evidenced in the COSY spectrum by the correlations of H10 with H9 and H11 (blue arrows). On the other hand, the correlations detected in the HMBC spectrum (Fig. S1, red arrows) of H10 with C12, C20 and C21 fixed the position of these carbon atoms. Interestingly, the correlation H10-C21 involved a $^4J_{CH}$ probably favoured by the rigidity of the molecule and the zigzag arrangement of H10 and C21. The location of the CF_3 substituent was established by the cross-peaks of negative slope existing between H11 and the C19 quartet.[15] This assignment was further supported by the doublet observed in the ^{19}F NMR spectrum measured without ^1H decoupling at δ -76.0 ppm ($^3J_{FH}$ 7.3 Hz).

The assembly of the three substructures was achieved through the correlations shown in the HMBC spectrum between H9-C13, H10-C8 and H7-C9 for fragments **A**-**C**, and H9-C16 and H10-C15 for the binding of the phenyl ring **B** to carbon C9 of the molecule. Finally, the NOESY spectrum showed correlations of H10 with H9 and H11 (Fig. S1, green arrows) indicating the *syn* arrangement of H9 and H11. Furthermore, the correlations between H4-H6^e and H9-H7^a allowed to unravel the assignment of axial and equatorial protons of the methylene groupsThe assembly of the three substructures was achieved through the correlations shown in the HMBC spectrum between H9-C13, H10-C8 and H7-C9 for fragments **A**-**C**, and H9-C16 and H10-C15 for the binding of the phenyl ring **B** to carbon C9 of the molecule. Finally, the NOESY spectrum showed correlations of H10

with H9 and H11 (Fig. S1, green arrows) indicating the *syn* arrangement of H9 and H11. Furthermore, the correlations between H4-H6^{e} and H9-H7^{a} allowed to unravel the assignment of axial and equatorial protons of the methylene groups.

X-RAY STRUCTURE OF COMPOUND 3d[6]

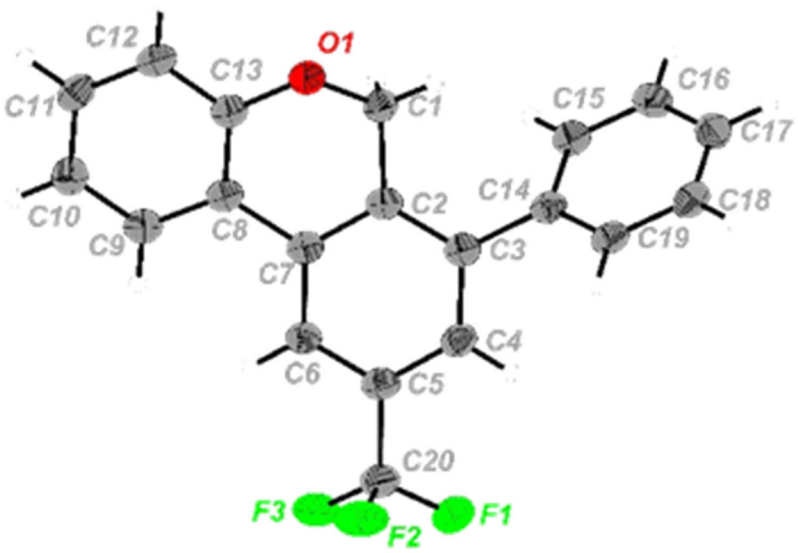


Figure S1. Ortep diagram for compound **3i**

[6] CCDC 1989940 contains the supplementary crystallographic data of compound **3d**. These data can be obtained free of charge at www.ccdc.cam.ac.uk/conts/retrieving.html [or from the Cambridge Crystallographic Data Centre, 12 Union Road, Cambridge CB2 1EZ, UK; fax: (internat.) +44(1223)336-033, e-mail: deposit@ccdc.cam.ac.uk].

X-RAY STRUCTURE OF COMPOUND 3i[7]

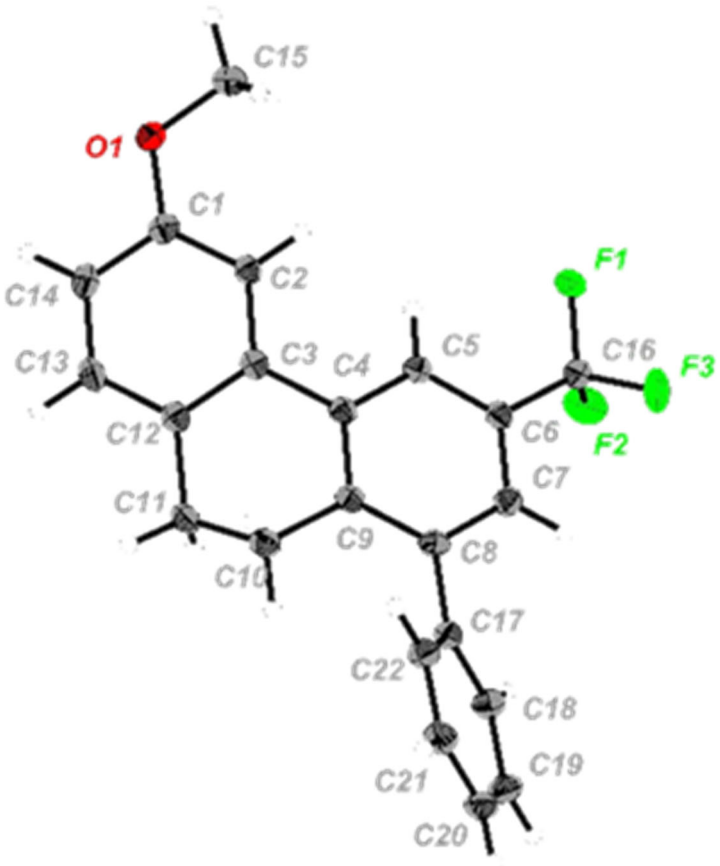


Figure S1. Ortep diagram for compound **3i**

[7] CCDC 1989936 contains the supplementary crystallographic data of compound **3i**. These data can be obtained free of charge at www.ccdc.cam.ac.uk/conts/retrieving.html [or from the Cambridge Crystallographic Data Centre, 12 Union Road, Cambridge CB2 1EZ, UK; fax: (internat.) +44(1223)336-033, e-mail: deposit@ccdc.cam.ac.uk].

COMPUTATIONAL SUPPORTING INFORMATION

- *Computational details*

All structures were optimized using density functional theory (DFT) as implemented in Gaussian[8] with B3LYP[9] as functional and 6-31G** as basis set. Final energies were obtained performing single-point calculations on the previously optimized structures using the M06-2X[10] functional and the basis set Def2TZVPP[11]. Solvation factors were introduced with the IEF-PCM[12] method, using tetrahydrofuran as solvent. The stationary points were characterized by frequency calculations in order to verify that they have the right number of imaginary frequencies. The intrinsic reaction coordinates (IRC)[13] were followed to verify the energy profiles connecting each TS to the correct associated local minima.

Cartesian coordinates of the optimized structures are shown below, as well as their single point energy and correction to Gibbs free energy (in Hartrees). Negative frequencies of transition states are also displayed.

[8] Gaussian 16, Revision B.01, M. J. Frisch, G. W. Trucks, 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. Nakai, T. Vreven, K. Throssell, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. J. Bearpark, J. J. Heyd, E. N. Brothers, K. N. Kudin, V. N. Staroverov, T. A. Keith, R. Kobayashi, J. Normand, K. Raghavachari, A. P. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, J. M. Millam, M. Klene, C. Adamo, R. Cammi, J. W. Ochterski, R. L. Martin, K. Morokuma, O. Farkas, J. B. Foresman, and D. J. Fox, Gaussian, Inc., Wallingford CT, 2016.

[9] (a) C. Lee, W. Yang, R. G. Parr, *Phys. Rev. B* 1988, **37**, 785-789; (b) A. D. Becke, *J. Chem. Phys*. 1993, **98**, 5648-5652; (c) W. Khon, A. D. Becke, G. R. Parr, *J. Phys. Chem*. 1996, **100**, 12974-12980

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

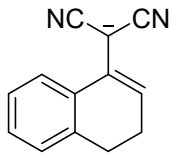
[11] (a) F. Furche and R. Ahlrichs, *J. Chem. Phys*. 2003, **119**, 12753; (b) F. Weigend and R. Ahlrichs, *Phys. Chem. Chem. Phys.* 2005, **7**, 3297

[12] (a) E. Cancès, B. Mennucci, J. Tomasi, *J. Chem. Phys.* 1997, **107**, 3032-3047; (b) J. Tomasi, B. Mennucci, E. Cancès, *J. Mol. Struct. (Theochem)* 1999, **464**, 211-226; (c) M. Cossi, V. Barone, B. Mennucci, J. Tomasi, J. *Chem. Phys. Lett.* 1998, **286**, 253-260

[13] C. Gonzalez, H. B. Schlegel, *J. Phys. Chem.* 1990, **94**, 5523.

Cartesian coordinates and energies

Molecule **I**:



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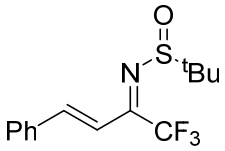
Molecule **2a**:



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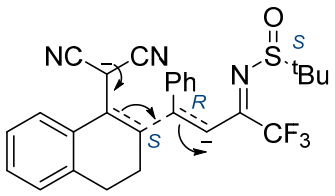

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C	1.56426	4.02834	-0.89996
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H	-0.63831	3.63558	-2.26320
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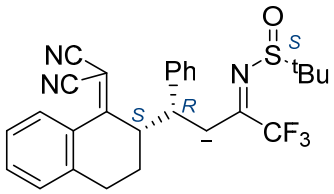
Molecule **II**:



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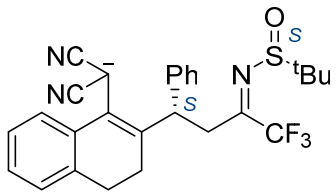
H	0.11362	-0.77539	0.97571
C	1.43872	-3.59293	-0.43645
O	-4.00740	0.63765	-1.71713
N	-1.71587	-0.04679	-0.45991
C	0.51967	-0.63567	-1.07246
H	1.89242	-5.62063	-0.99106
S	-3.04275	0.98027	-0.59010
C	-0.71077	-0.08050	-1.35715
C	-3.92430	0.30503	0.95164
H	2.14969	-3.17239	-1.14289
H	1.24709	-0.75529	-1.86482
C	-0.88021	0.45886	-2.77715
H	-2.12106	-0.00762	2.11240
H	-5.80141	0.98552	0.10072
F	0.27085	0.43109	-3.50115
C	-3.05220	0.55757	2.18096
C	-5.23088	1.10538	1.02526
H	-3.58672	0.25735	3.09294
H	-5.84150	0.75710	1.86783
F	-1.78994	-0.23742	-3.48689

H	-2.79485	1.61910	2.27741
H	-5.03585	2.17503	1.16990
H	3.61212	-0.55731	2.35979
H	2.99243	-1.37845	0.14977
C	2.56789	-0.85025	2.19450
H	1.43590	3.07281	-0.60000
C	1.22114	2.87851	0.44372
H	0.15839	4.72266	0.70795
C	0.48993	3.80187	1.17752
C	2.26485	-0.76160	0.68446
H	2.47154	-1.89035	2.52517
C	1.64684	1.66572	1.01995
C	2.44714	0.68549	0.26754
C	0.16969	3.53118	2.51084
C	4.27506	0.06912	-1.25283
N	4.93666	-0.71712	-1.80473
C	3.48482	1.05106	-0.57488
C	1.28717	1.37306	2.35700
H	-0.39785	4.25040	3.09494
C	0.56416	2.32600	3.08396
C	1.63517	0.05045	3.01851
C	3.89520	2.39825	-0.82370
H	2.07493	0.23944	4.00604
H	0.29941	2.10728	4.11615
N	4.28490	3.47569	-1.04065
H	0.69411	-0.48010	3.21327

Molecule **III**:



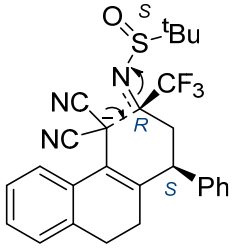
E = -1981.189151

G_{corr} = 0.396308

H	3.77366	0.71094	-3.01279
H	5.09376	-0.46749	-2.94989
C	4.83995	0.58768	-2.81434
H	-1.28355	-4.20318	2.82599
C	-0.75465	-3.73664	1.99889
H	5.40667	1.18267	-3.54056
C	-0.99400	-2.39902	1.69344
H	-1.71396	-1.82937	2.27538
C	0.16542	-4.47380	1.24841
H	0.35938	-5.51602	1.48814
C	-0.32390	-1.76320	0.63503
C	0.83626	-3.85773	0.19381

C	-0.66966	-0.30038	0.35039
F	1.06312	1.22421	2.23068
C	0.59207	-2.51565	-0.11252
O	4.81581	-1.56682	-0.69066
N	2.77421	0.03883	-0.69958
C	0.44253	0.51476	-0.38623
H	1.56069	-4.41507	-0.39385
S	4.45503	-0.20342	-0.16589
C	1.85741	0.39498	0.12107
C	5.19447	1.03560	-1.39580
H	1.13836	-2.05873	-0.93063
C	2.13927	0.75551	1.59469
H	3.60452	2.52672	-1.25447
H	7.05502	-0.09678	-1.30871
F	2.58146	-0.32902	2.26933
C	4.67734	2.43814	-1.06833
C	6.70665	0.92728	-1.14799
H	5.19003	3.16944	-1.70438
H	7.24022	1.58718	-1.84145
F	3.10264	1.70755	1.68141
H	4.86785	2.71017	-0.02562
H	6.97082	1.22681	-0.12762
H	-7.69553	1.00226	-0.23998
C	-6.77848	0.69012	-0.73326
H	-5.55365	1.26201	0.92760
H	-2.49261	-2.08327	-1.33546
C	-5.56119	0.83906	-0.06890
C	-6.82151	0.14942	-2.01764
H	-7.76830	0.03329	-2.53930
C	-4.35258	0.43435	-0.66260
C	-2.13725	-1.08380	-1.63200
C	-3.03155	0.56969	0.02912
C	-5.62893	-0.23930	-2.62847
C	-2.87094	1.56736	1.11964
C	-1.98954	-0.20214	-0.40690
C	-1.85515	2.53079	1.00437
C	-4.40547	-0.10519	-1.97021
N	-0.99330	3.31908	0.85549
C	-3.69295	1.60804	2.25997
N	-4.38113	1.62577	3.21342
H	-1.16212	-1.24885	-2.10704
H	-5.64237	-0.65156	-3.63582
C	-3.10680	-0.47352	-2.64202
H	-3.28592	-1.15661	-3.48104
H	-2.64972	0.43589	-3.06264
H	-0.83584	0.18243	1.31446
H	0.48279	0.25208	-1.44643
H	0.14859	1.56952	-0.30231

TS_2:



E = -1981.190085

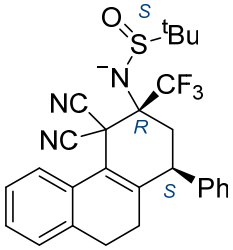
G_{corr} = 0.399824

Freq= -141.6457

H	4.59210	-1.31277	1.30923
H	5.55410	0.14019	0.98864
C	5.30392	-0.85828	0.61698
H	-1.79879	6.20718	0.78044
C	-1.71677	5.31346	0.16727
H	6.21849	-1.46546	0.58207
C	-1.40885	4.08918	0.76446
H	-1.24897	4.03749	1.83882
C	-1.91706	5.38864	-1.21082
H	-2.15660	6.33966	-1.67884
C	-1.29302	2.92238	0.00020
C	-1.80276	4.23174	-1.98564
C	-0.91678	1.59132	0.65127
F	1.25160	0.68412	2.96222
H	-0.98785	1.74238	1.73810
C	-1.49258	3.01246	-1.38568
O	3.82201	1.72188	-0.07786
N	2.38352	-0.43783	0.46989
C	0.54955	1.26744	0.30766
H	-1.95187	4.27950	-3.06102
S	3.22810	0.45256	-0.68802
C	1.08907	-0.10784	0.73117
C	4.68839	-0.75016	-0.77852
H	-1.39993	2.11700	-1.99487
H	0.68606	1.33706	-0.77580
C	0.84424	-0.39298	2.23706
H	3.47712	-2.53841	-0.58804
H	5.94308	0.90109	-1.42210
F	-0.46407	-0.58510	2.57949
C	4.18011	-2.09630	-1.29688
C	5.66926	-0.10132	-1.76303
H	5.02372	-2.78597	-1.43788
H	6.58014	-0.70786	-1.84450
F	1.50937	-1.45805	2.69531
H	3.66911	-1.98627	-2.26009

H	5.23020	-0.01500	-2.76404
H	-3.79630	1.24278	-0.46338
C	-3.38050	0.88946	0.49178
H	-1.53990	-2.99965	-1.68833
C	-2.51564	-2.81210	-1.25714
H	-3.38696	-4.51514	-2.23352
C	-3.56746	-3.67177	-1.57296
C	-1.92120	0.50293	0.31341
H	-3.45172	1.73693	1.18193
C	-2.70878	-1.70967	-0.40888
C	-1.61315	-0.75810	-0.06386
C	-4.83829	-3.44998	-1.04630
C	0.28869	-1.17459	-1.55597
N	0.60935	-1.08547	-2.67229
C	-0.15421	-1.22961	-0.17229
C	-4.00470	-1.48507	0.11062
H	-5.66042	-4.11844	-1.28785
C	-5.04776	-2.35323	-0.20814
C	-4.19990	-0.29169	1.01149
C	0.05015	-2.56888	0.36037
H	-5.26210	-0.03202	1.08546
H	-6.03669	-2.16422	0.20448
N	0.21793	-3.63372	0.79883
H	-3.85601	-0.53976	2.02697
H	1.20293	2.02958	0.74121

Molecule **IV**:

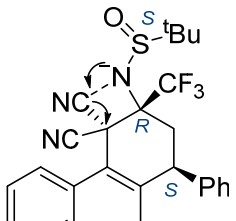


E = -1981.193780

G_{corr} = 0.399456

H	1.46861	-1.29053	-2.93165
H	2.97882	-2.21508	-2.94626
C	2.54264	-1.22667	-3.12086
H	-4.41953	-4.24126	-2.33146
C	-4.23864	-3.46736	-1.58989
H	2.70705	-0.94035	-4.16876
C	-2.99050	-2.84365	-1.52976
H	-2.20467	-3.13716	-2.22137
C	-5.24972	-3.09757	-0.70295
H	-6.22253	-3.57987	-0.74845
C	-2.72694	-1.84487	-0.58434
C	-5.00064	-2.10292	0.24598
C	-1.34776	-1.19961	-0.49659

F	2.55095	-0.92423	2.52259
H	-0.76370	-1.50288	-1.37555
C	-3.75189	-1.48573	0.30473
O	3.74085	-2.28218	-0.56294
N	1.42932	-1.00785	-0.33953
C	-0.59077	-1.72595	0.72469
H	-5.78012	-1.80868	0.94395
S	3.10451	-0.90313	-0.41075
C	0.75924	-0.99598	0.87987
C	3.19253	-0.21277	-2.18000
H	-3.56291	-0.71600	1.04882
H	-1.19902	-1.61935	1.62800
C	1.47650	-1.62809	2.10620
H	1.44421	1.04480	-1.98410
H	5.18238	-1.05940	-2.34934
F	0.66030	-1.75105	3.19137
C	2.50496	1.15017	-2.22240
C	4.69329	-0.08950	-2.47297
H	2.60322	1.59618	-3.22216
H	4.85402	0.26189	-3.50074
F	1.89189	-2.87493	1.81360
H	2.94588	1.84390	-1.49821
H	5.17234	0.62436	-1.79258
H	-3.29439	1.08195	-1.26408
C	-2.28064	0.89371	-1.64781
H	-0.38045	3.14238	2.17790
C	-0.72176	3.51105	1.21910
H	-0.77712	5.53885	1.92194
C	-0.95622	4.87861	1.07805
C	-1.41097	0.31258	-0.54658
H	-2.39315	0.15341	-2.44691
C	-0.93899	2.62050	0.15424
C	-0.72403	1.14801	0.26567
C	-1.41813	5.39158	-0.13173
C	-0.44849	0.66503	2.64120
N	-1.05855	0.71528	3.63184
C	0.24972	0.61246	1.34939
C	-1.42530	3.14935	-1.06480
H	-1.60085	6.45660	-0.24710
C	-1.65392	4.51836	-1.19468
C	-1.68204	2.18776	-2.19696
C	1.45012	1.45418	1.43221
H	-2.34292	2.64020	-2.94499
H	-2.02413	4.90219	-2.14301
N	2.39039	2.13321	1.49708
H	-0.73387	1.95351	-2.70261
H	-0.38227	-2.79076	0.58642



TS_3:

E = -1981.173520

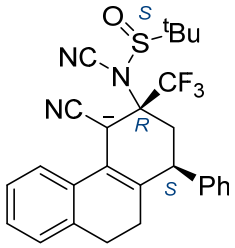
G_{corr} = 0.401924

Freq= -159.7186

H	3.24837	1.46759	-1.97116
H	3.02361	0.30900	-3.31157
C	3.69189	0.61802	-2.50211
H	-3.54354	-5.14986	-1.70705
C	-3.52654	-4.29850	-1.03136
H	4.65333	0.92099	-2.93860
C	-2.47962	-3.37694	-1.10463
H	-1.68517	-3.51267	-1.83435
C	-4.54816	-4.12613	-0.09714
H	-5.36548	-4.84020	-0.03998
C	-2.43135	-2.27054	-0.24746
C	-4.51278	-3.02623	0.76361
C	-1.25546	-1.29906	-0.30312
F	2.47102	0.04012	2.68207
H	-0.69617	-1.51491	-1.22501
C	-3.46398	-2.11067	0.68880
O	1.46613	-1.37753	-2.39040
N	1.67438	-0.17087	0.00357
C	-0.32538	-1.58061	0.88211
H	-5.30439	-2.88113	1.49434
S	2.25538	-1.33438	-1.08928
C	0.73693	-0.50292	1.08922
C	3.92331	-0.54974	-1.54195
H	-3.44167	-1.25483	1.35901
H	-0.91373	-1.63535	1.80415
C	1.56128	-0.88614	2.33938
H	4.15429	0.74556	0.18401
H	4.10324	-2.05543	-3.11197
F	0.78638	-1.11811	3.42956
C	4.63914	-0.12685	-0.25784
C	4.66758	-1.69815	-2.24522
H	5.67883	0.13259	-0.49772
H	5.64314	-1.34001	-2.59449
F	2.24316	-2.04072	2.10529
H	4.65906	-0.93563	0.48181
H	4.83991	-2.54468	-1.57051
H	-3.75929	0.48649	-0.80785
C	-2.81121	0.43304	-1.36567

H	-0.29085	3.56201	1.48328
C	-0.97801	3.69811	0.66266
H	-1.03012	5.81904	0.97614
C	-1.39199	4.99626	0.36582
C	-1.66845	0.15757	-0.40475
H	-2.92057	-0.40702	-2.05948
C	-1.42088	2.59462	-0.08707
C	-1.02694	1.18088	0.21345
C	-2.24822	5.23653	-0.70497
C	0.07052	1.53878	2.42643
N	-0.01844	1.99562	3.49433
C	0.19584	0.95472	1.10117
C	-2.24580	2.85934	-1.20798
H	-2.57894	6.24571	-0.93736
C	-2.65711	4.16118	-1.49311
C	-2.59249	1.72605	-2.13874
C	1.51168	1.38140	0.15268
H	-3.47234	1.97633	-2.74342
H	-3.29539	4.33084	-2.35807
N	2.07222	2.37364	-0.22742
H	-1.75479	1.58101	-2.83745
H	0.14848	-2.55958	0.75616

Molecule **V**:

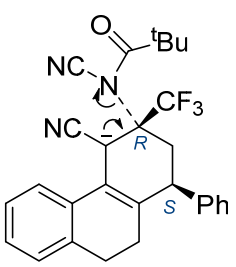


E = -1981.203327

G_{corr} = 0.400302

H	-1.93657	-1.51968	2.94779
H	-3.66892	-1.84349	2.76390
C	-2.93148	-1.07307	3.00611
H	4.38057	-4.50431	1.73718
C	4.24719	-3.61332	1.12870
H	-3.09756	-0.74334	4.03933
C	3.02952	-2.93065	1.15877
H	2.21684	-3.29763	1.78112
C	5.28833	-3.15499	0.32076
H	6.23871	-3.68201	0.29835
C	2.82586	-1.78085	0.38492
C	5.09784	-2.01143	-0.45887
C	1.47157	-1.07356	0.38733
F	-2.48496	-0.77323	-2.61494
H	0.92174	-1.47293	1.25517
C	3.87981	-1.33366	-0.42618

O	-4.23093	-1.55060	0.28540
N	-1.57611	-1.26041	0.08164
C	0.71764	-1.48813	-0.88662
H	5.90160	-1.64521	-1.09289
S	-3.18792	-0.46780	0.26211
C	-0.62076	-0.74570	-1.06577
C	-3.07629	0.12133	2.06434
H	3.73405	-0.44143	-1.02930
H	1.32664	-1.23264	-1.75877
C	-1.24311	-1.24468	-2.39009
H	-0.95938	0.64842	1.98991
H	-5.25915	0.10936	2.15619
F	-0.48022	-0.89826	-3.45089
C	-1.92599	1.12049	2.17643
C	-4.43330	0.81612	2.27251
H	-1.91732	1.54268	3.18940
H	-4.47247	1.23508	3.28478
F	-1.34092	-2.60009	-2.41161
H	-2.03743	1.94510	1.46598
H	-4.57580	1.63918	1.56357
H	3.56637	1.18589	0.96469
C	2.57993	1.02213	1.43299
H	0.29252	3.13591	-2.22547
C	0.77565	3.54135	-1.34674
H	0.90304	5.51109	-2.19448
C	1.12391	4.89245	-1.32846
C	1.56546	0.43472	0.47533
H	2.76193	0.31054	2.24947
C	1.03414	2.70542	-0.24750
C	0.71974	1.23955	-0.25567
C	1.74881	5.44361	-0.21178
C	-1.39104	1.58643	-1.54339
N	-2.21311	2.31129	-1.97085
C	-0.40569	0.72960	-1.02530
C	1.70267	3.26616	0.86650
H	2.01833	6.49674	-0.19044
C	2.04134	4.61980	0.87642
C	2.07274	2.34855	2.00427
C	-1.50011	-2.52544	0.50769
H	2.82380	2.82243	2.64856
H	2.55220	5.02778	1.74667
N	-1.38558	-3.61470	0.92367
H	1.18851	2.14819	2.62769
H	0.56412	-2.56873	-0.90002



TS_4:

E = -1981.198178

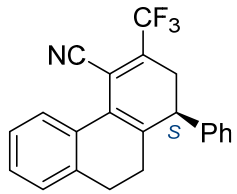
G_{corr} = 0.401924

Freq= -234.4029

H	2.14000	-1.55017	-2.94926
H	3.87902	-1.78007	-2.70895
C	3.11143	-1.05259	-2.98854
H	-3.97669	-4.83226	-1.64636
C	-3.94566	-3.90822	-1.07465
H	3.29200	-0.73344	-4.02299
C	-2.78705	-3.12942	-1.08209
H	-1.91502	-3.45523	-1.64385
C	-5.05838	-3.50453	-0.33545
H	-5.96293	-4.10721	-0.33174
C	-2.71639	-1.93514	-0.35264
C	-4.99846	-2.31982	0.40190
C	-1.42101	-1.12739	-0.32899
F	2.48658	-0.47774	2.66135
H	-0.81934	-1.49094	-1.17544
C	-3.83830	-1.54575	0.39399
O	4.34338	-1.43833	-0.21955
N	1.68140	-1.19537	-0.08177
C	-0.67011	-1.46367	0.96991
H	-5.85790	-1.99709	0.98437
S	3.24674	-0.40420	-0.24563
C	0.57276	-0.60145	1.18587
C	3.17033	0.15988	-2.06083
H	-3.79406	-0.62479	0.96929
H	-1.33002	-1.26820	1.82319
C	1.29052	-1.05928	2.46093
H	1.03010	0.57572	-2.04886
H	5.34981	0.25573	-2.08382
F	0.52533	-0.78613	3.54936
C	1.97428	1.09826	-2.21558
C	4.49508	0.91868	-2.24272
H	1.96774	1.51437	-3.23112
H	4.54986	1.32038	-3.26163
F	1.49921	-2.39777	2.47236
H	2.02444	1.93283	-1.50891
H	4.57361	1.76006	-1.54530
H	-3.64345	0.98723	-0.99538
C	-2.64548	0.86693	-1.44934
H	-0.53506	3.22311	2.16699

C	-1.02571	3.57348	1.26866
H	-1.26880	5.56093	2.04716
C	-1.44483	4.90258	1.20051
C	-1.61704	0.36978	-0.45513
H	-2.77334	0.11767	-2.24095
C	-1.22595	2.69019	0.19496
C	-0.83756	1.24625	0.25433
C	-2.08310	5.38156	0.05835
C	1.26284	1.75036	1.51252
N	2.04256	2.54825	1.87557
C	0.30667	0.81121	1.06650
C	-1.90682	3.17637	-0.94592
H	-2.40750	6.41744	-0.00160
C	-2.31672	4.50840	-1.00560
C	-2.20330	2.20065	-2.05663
C	1.56877	-2.44362	-0.52329
H	-2.96744	2.60682	-2.73043
H	-2.83529	4.86044	-1.89533
N	1.36664	-3.53192	-0.91842
H	-1.29687	2.03057	-2.65674
H	-0.41671	-2.52425	0.99272

Molecule **VI**:



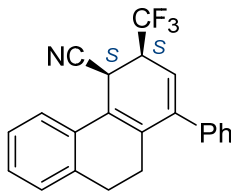
E = -1202.252502

G_{corr} = 0.272913

H	4.18422	-4.35037	2.18423
C	4.12104	-3.57210	1.42935
C	2.94188	-2.83748	1.28929
H	2.09483	-3.05119	1.93649
C	5.21242	-3.30693	0.60292
H	6.13091	-3.87609	0.71020
C	2.83241	-1.82988	0.32393
C	5.11655	-2.30378	-0.36398
C	1.52597	-1.06490	0.15179
F	-2.53361	-0.56677	-2.45635
H	0.84088	-1.40837	0.94496
C	3.93706	-1.57361	-0.50224
C	0.88313	-1.40506	-1.20559
H	5.96173	-2.08905	-1.01146
C	-0.36540	-0.59344	-1.43303
H	3.87606	-0.79423	-1.25754
H	1.59921	-1.19708	-2.01387
C	-1.47728	-1.32367	-2.13215

F	-1.00389	-1.87576	-3.27764
F	-1.92645	-2.34790	-1.36497
H	3.64710	1.19494	0.62012
C	2.72990	1.01393	1.20082
H	-0.01278	3.23749	-2.10490
C	0.53664	3.62309	-1.25375
H	0.42979	5.64807	-1.96463
C	0.79320	4.99164	-1.17999
C	1.65822	0.44519	0.29982
H	3.00161	0.27236	1.95883
C	0.98986	2.75136	-0.25225
C	0.78021	1.28222	-0.31447
C	1.51630	5.50966	-0.10727
C	-1.58545	1.50158	-1.10750
N	-2.52639	2.18437	-1.12533
C	-0.39820	0.69438	-1.01488
C	1.74610	3.27791	0.81855
H	1.71742	6.57493	-0.04429
C	1.99456	4.64804	0.88181
C	2.26113	2.31503	1.86099
H	3.07422	2.76838	2.43659
H	2.57347	5.04352	1.71268
H	1.45778	2.08042	2.57499
H	0.65933	-2.47322	-1.25414

Molecule **VII**:

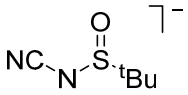


E = -1202.261483

G_{corr} = 0.273704

H	1.56317	-4.28861	4.07137
C	2.08214	-3.55912	3.45645
C	1.35607	-2.75183	2.58072
H	0.27585	-2.84631	2.52194
C	3.46803	-3.42585	3.54689
H	4.03377	-4.05350	4.22898
C	2.00363	-1.79755	1.78095
C	4.12385	-2.47965	2.75659
C	1.22955	-0.96952	0.81266
F	-2.46151	-1.66039	-0.34721
C	3.39858	-1.67024	1.88413
C	0.39472	-1.56945	-0.06039
H	5.20331	-2.37520	2.81497
C	-0.39117	-0.77415	-1.07046

H	3.91822	-0.95004	1.25906
H	0.27425	-2.64709	-0.05717
C	-1.81687	-0.49855	-0.58527
F	-1.86091	0.23044	0.54649
F	-2.52600	0.17388	-1.52351
H	3.03694	1.34204	1.88351
C	1.95310	1.21496	2.02259
H	0.94887	2.94437	-2.42193
C	1.07587	3.44755	-1.46880
H	1.22043	5.38316	-2.39225
C	1.24035	4.83169	-1.45722
C	1.36442	0.50521	0.81774
H	1.83019	0.60242	2.91935
C	1.10974	2.70762	-0.27468
C	0.95092	1.24441	-0.24324
C	1.43533	5.50066	-0.24976
C	1.38506	0.24809	-2.46011
N	2.20206	0.02793	-3.25524
C	0.34443	0.53609	-1.45526
C	1.31157	3.39176	0.94721
H	1.56342	6.57885	-0.23496
C	1.46898	4.77602	0.94406
C	1.29569	2.58365	2.22303
H	1.79072	3.13117	3.03138
H	1.61878	5.29404	1.88807
H	0.25166	2.43098	2.53551
H	-0.38187	1.19967	-1.93660
H	-0.52706	-1.36805	-1.97990

Leaving group: 

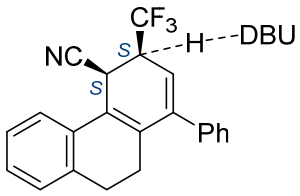
E = -778.957079

G_{corr} = 0.103223

N	0.33097	-0.98217	3.73946
C	-0.68918	-0.47350	3.42808
H	-1.87375	2.69843	3.33914
N	-1.84824	0.11857	3.20713
C	-2.27877	3.00500	2.37214
H	-1.43734	3.17369	1.68848
H	-3.97652	1.36745	3.78066
H	-2.80976	3.96009	2.49047
S	-2.23092	0.33002	1.58500
C	-4.37028	1.63065	2.79617
C	-3.22309	1.93184	1.83153
H	-5.03513	2.50085	2.89013
O	-3.29079	-0.64985	1.09379

H	-4.94748	0.77969	2.42142
C	-3.75882	2.29909	0.44325
H	-2.94040	2.50499	-0.25782
H	-4.38904	3.19695	0.49849
H	-4.35218	1.47433	0.03937

TS_5:



E = -1664.315305

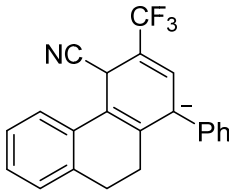
G_{corr} = 0.50129

Freq= -834.3117

H	-1.92333	5.44272	-1.22677
C	-0.92102	5.02469	-1.18187
C	-0.72874	3.74771	-0.65697
H	-1.58420	3.17745	-0.30630
C	0.16456	5.75984	-1.66081
H	0.01616	6.75278	-2.07506
C	0.55275	3.17128	-0.58068
C	1.44374	5.20430	-1.59833
C	0.76305	1.83174	0.02493
F	-0.24964	-1.24404	3.59375
C	1.63492	3.93187	-1.06236
C	0.13106	1.49165	1.19577
H	2.30032	5.76962	-1.95520
C	0.30633	0.20355	1.81875
H	2.64002	3.52845	-0.98694
H	-0.56222	2.19867	1.64495
C	-0.17976	0.06681	3.21492
F	0.56423	0.68155	4.17351
F	-1.44544	0.57909	3.35877
H	2.99312	1.38543	-2.14471
C	1.99074	0.93785	-2.07522
H	3.59921	-2.22358	1.24280
C	3.57379	-2.27657	0.15947
H	4.92409	-3.94747	0.10621
C	4.33809	-3.24929	-0.48470
C	1.59193	0.81177	-0.61390
H	1.31450	1.61705	-2.60014
C	2.81343	-1.34529	-0.57375
C	1.99192	-0.30845	0.06852
C	4.36123	-3.31642	-1.87689
C	2.79558	0.22254	2.34378

N	3.68758	0.69578	2.91877
C	1.68764	-0.40777	1.56545
C	2.84900	-1.41773	-1.98951
H	4.95844	-4.06943	-2.38261
C	3.61568	-2.39530	-2.61867
C	2.00813	-0.43012	-2.76276
H	2.37105	-0.33980	-3.79229
H	3.63250	-2.43523	-3.70570
H	0.97273	-0.80378	-2.82674
H	1.67479	-1.45819	1.87723
H	-0.70619	-0.76567	1.05405
H	-0.98149	-2.42386	-2.10754
H	-2.96778	0.97150	-1.11133
H	-4.47061	-0.84244	-2.58968
H	-5.35850	1.31079	-1.72929
C	-1.21374	-3.18663	-1.35648
C	-3.75521	0.87181	-0.35442
H	-0.75379	-4.12318	-1.68357
H	-3.16969	-3.46276	-2.24389
C	-5.14487	-0.83483	-1.72369
C	-5.09685	0.52377	-1.01285
H	-3.84879	1.85567	0.11764
H	0.40181	-2.48689	-0.08754
C	-2.72402	-3.36483	-1.24870
C	-0.65486	-2.74984	-0.00620
H	-6.15730	-0.99391	-2.11424
N	-1.36948	-1.57228	0.48076
C	-2.62929	-1.36588	0.19027
N	-3.35099	-2.20624	-0.58743
C	-3.29176	-0.12203	0.73405
H	-2.58215	0.35607	1.40653
C	-4.79460	-2.02338	-0.81632
H	-5.87985	0.54107	-0.24155
H	-5.14692	-2.95370	-1.26806
H	-2.96984	-4.27695	-0.68807
H	-0.74236	-3.55837	0.73160
H	-4.14605	-0.41828	1.35655
H	-5.31286	-1.93491	0.14560

Molecule **VIII**:

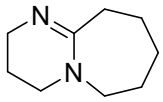


E = -1664.322412

G_{corr} = 0.504175

H	-2.38154	5.21263	-1.17363
C	-1.34522	4.88416	-1.18608
C	-1.00641	3.65208	-0.63043
H	-1.78612	3.03002	-0.19960
C	-0.36496	5.68871	-1.77024
H	-0.62780	6.64675	-2.20913
C	0.32347	3.18492	-0.62201
C	0.95865	5.24534	-1.77697
C	0.68841	1.89573	0.01018
F	-0.18768	-1.26073	3.51756
C	1.29731	4.01946	-1.20650
C	0.10419	1.52454	1.21598
H	1.73735	5.86515	-2.21353
C	0.43135	0.32862	1.88789
H	2.33785	3.71132	-1.18333
H	-0.66775	2.16160	1.64071
C	-0.09802	0.08164	3.24220
F	0.62770	0.59944	4.27128
F	-1.36552	0.58687	3.40027
H	2.95679	1.53058	-2.15220
C	1.96521	1.06064	-2.07536
H	3.75038	-2.00881	1.23634
C	3.69937	-2.07530	0.15474
H	5.09712	-3.70536	0.09055
C	4.47748	-3.03256	-0.49593
C	1.57653	0.93577	-0.60993
H	1.27046	1.71645	-2.60494
C	2.89230	-1.17330	-0.56934
C	2.04514	-0.16585	0.07923
C	4.47513	-3.11613	-1.88754
C	2.91478	0.42179	2.33405
N	3.79445	0.94058	2.88890
C	1.80582	-0.25265	1.58655
C	2.90361	-1.26401	-1.98664
H	5.08497	-3.85580	-2.39787
C	3.68688	-2.22397	-2.62154
C	2.01794	-0.31138	-2.75296
H	2.36097	-0.21726	-3.78921

H	3.68290	-2.27318	-3.70860
H	0.99308	-0.71775	-2.79906
H	1.83791	-1.29962	1.91228
H	-0.70921	-0.90323	0.93508
H	-0.92097	-2.35097	-2.24579
H	-3.10879	0.84544	-0.95198
H	-4.53024	-1.01531	-2.45558
H	-5.54736	1.00782	-1.43423
C	-1.04303	-3.15819	-1.51595
C	-3.84416	0.63601	-0.16606
H	-0.53010	-4.03961	-1.90913
H	-3.02062	-3.56866	-2.29790
C	-5.15964	-1.10866	-1.56142
C	-5.18555	0.20955	-0.77669
H	-3.99154	1.57935	0.36967
H	0.58229	-2.35147	-0.31327
C	-2.52443	-3.46866	-1.32791
C	-0.43229	-2.73302	-0.18592
H	-6.17369	-1.32959	-1.91515
N	-1.23555	-1.65605	0.39254
C	-2.52923	-1.53063	0.18881
N	-3.21060	-2.39061	-0.58688
C	-3.24318	-0.37261	0.83918
H	-2.53237	0.12573	1.49755
C	-4.67642	-2.31291	-0.74062
H	-5.92603	0.12020	0.03058
H	-4.97433	-3.24368	-1.22807
H	-2.66194	-4.41417	-0.78733
H	-0.39502	-3.57330	0.51852
H	-4.03335	-0.76958	1.48938
H	-5.14802	-2.31813	0.24860

DBU: 

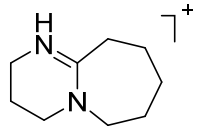
E = -462.061789

G_{corr} = 0.210705

C	-7.33977	1.85620	0.21819
C	-6.67965	0.49208	0.46100
C	-6.38391	3.05572	0.22130
H	-8.12026	2.01894	0.97189
H	-7.85647	1.82509	-0.75230
C	-5.23345	2.94182	-0.79325
H	-5.95185	3.19849	1.22030
H	-6.95786	3.96350	-0.00682
C	-5.62067	0.08941	-0.58763
H	-7.46635	-0.27191	0.46201

H	-6.22392	0.46280	1.45919
C	-4.24152	0.68280	-0.36717
H	-5.98920	0.33868	-1.59307
H	-5.46444	-0.99014	-0.56515
N	-4.13884	2.06581	-0.37816
H	-4.79517	3.93186	-0.95112
H	-5.62964	2.63012	-1.76968
C	-2.85550	2.70552	-0.08247
C	-1.96676	1.77227	0.73445
H	-3.04759	3.63202	0.47301
H	-2.34565	2.99237	-1.01637
C	-1.94500	0.39201	0.07219
H	-2.37277	1.67864	1.74870
H	-0.96044	2.19675	0.81987
N	-3.27956	-0.14906	-0.15475
H	-1.38652	-0.31870	0.69293
H	-1.40447	0.44860	-0.88606

DBUH$^+$:



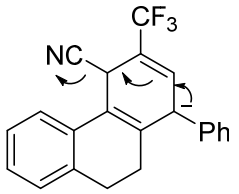
E = -462.530203

G_{corr} = 0.226186

C	-7.34171	1.84941	0.23221
C	-6.69663	0.47384	0.44282
C	-6.37259	3.03828	0.25988
H	-8.10797	1.99771	0.99976
H	-7.87132	1.84716	-0.72993
C	-5.25891	2.96308	-0.79192
H	-5.92030	3.15177	1.25304
H	-6.93760	3.95749	0.07104
C	-5.63545	0.09496	-0.61963
H	-7.47778	-0.29133	0.40221
H	-6.24962	0.40422	1.44203
C	-4.28935	0.73615	-0.39681
H	-5.99296	0.36415	-1.62115
H	-5.49197	-0.98907	-0.62937
N	-4.14098	2.05392	-0.42711
H	-4.80262	3.94379	-0.93473
H	-5.65798	2.65973	-1.76573
C	-2.83516	2.69101	-0.13070
C	-1.95100	1.78683	0.72277
H	-3.04301	3.62506	0.39631
H	-2.35007	2.94477	-1.08064
C	-1.88464	0.39115	0.11177
H	-2.35147	1.72556	1.73971
H	-0.94879	2.21681	0.78781

N	-3.25602	-0.06803	-0.14591
H	-1.41225	-0.32130	0.79124
H	-1.31862	0.39065	-0.82674
H	-3.44197	-1.06072	-0.12887

TS_6:



E = -1201.754664

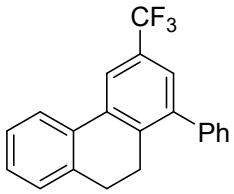
G_{corr} = 0.255612

Freq= -241.7360

H	-4.41666	-2.38895	-0.61713
C	-3.74849	-2.00169	0.14854
C	-2.43524	-1.67775	-0.18624
H	-2.09360	-1.80073	-1.20972
C	-4.21269	-1.81595	1.45266
H	-5.23870	-2.06128	1.71410
C	-1.53183	-1.16582	0.76906
C	-3.33669	-1.31177	2.41594
C	-0.12744	-0.88777	0.38445
F	3.87812	-2.96433	-1.01939
C	-2.01945	-0.99945	2.08185
C	0.55772	-1.87871	-0.34438
H	-3.67541	-1.17489	3.44044
C	1.87744	-1.73125	-0.72566
H	-1.34505	-0.64877	2.85611
H	0.05527	-2.81950	-0.54606
C	2.58352	-2.82988	-1.43592
F	1.99244	-4.04372	-1.24075
F	2.65175	-2.66345	-2.78126
H	0.17558	1.20837	2.65749
C	-0.04239	1.37705	1.59075
H	4.66047	0.84187	0.44434
C	4.09170	1.69772	0.79038
H	5.86849	2.83087	1.20785
C	4.78138	2.82679	1.22823
C	0.59371	0.28216	0.74963
H	-1.13007	1.34964	1.48951
C	2.68525	1.64240	0.80263
C	1.92961	0.45547	0.35743
C	4.08436	3.94351	1.68848
C	2.63349	0.51575	-2.43185
N	2.47480	1.09855	-3.43864

C	2.55223	-0.48315	-0.54427
C	1.98921	2.79032	1.25435
H	4.61665	4.82658	2.03249
C	2.68793	3.91349	1.69344
C	0.48398	2.75822	1.19461
H	0.05326	3.53633	1.83646
H	2.12700	4.78182	2.03485
H	0.16079	2.97412	0.16535
H	3.63006	-0.52267	-0.57576

Molecule **3a**:

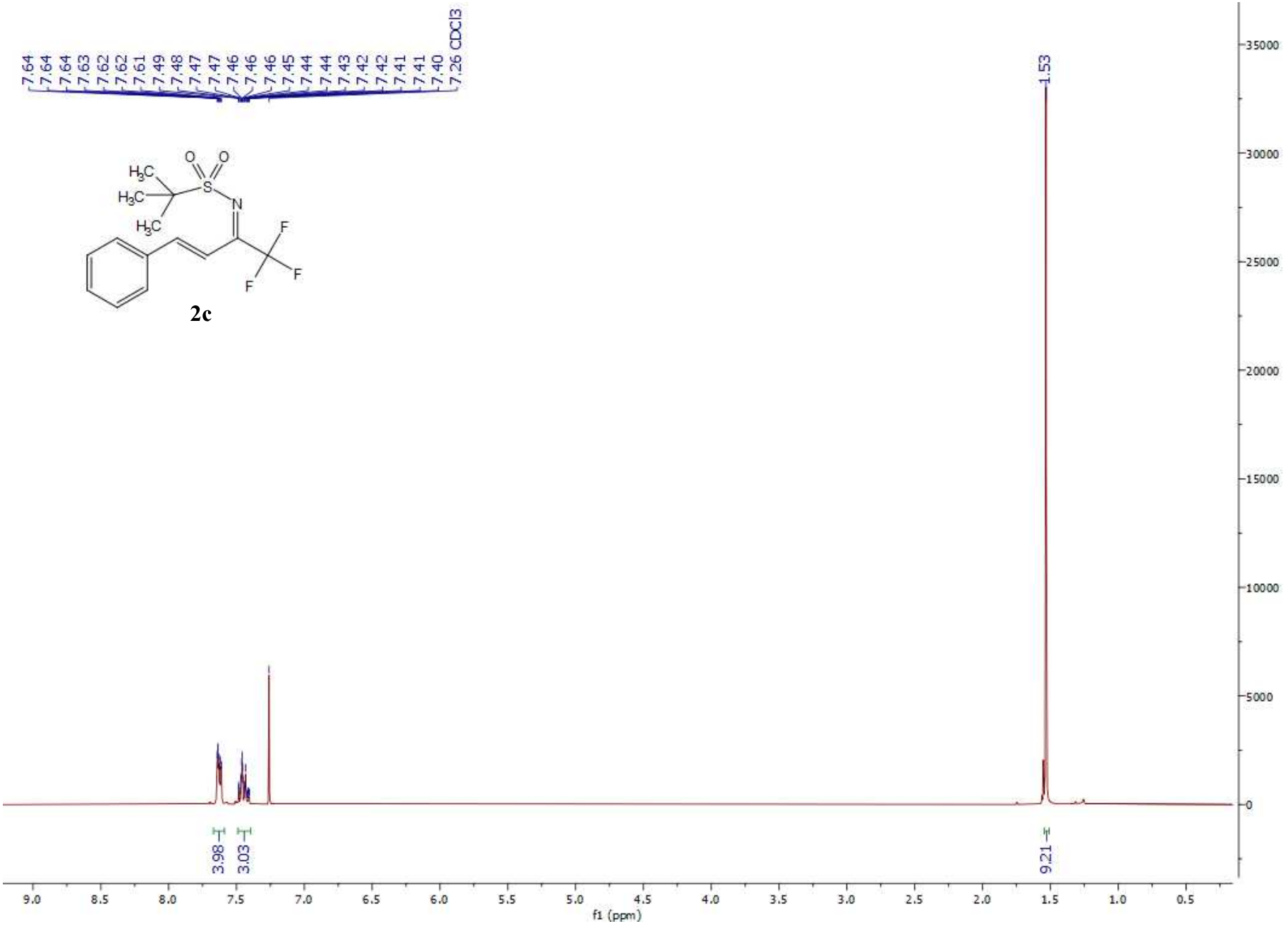


E = -1108.841160

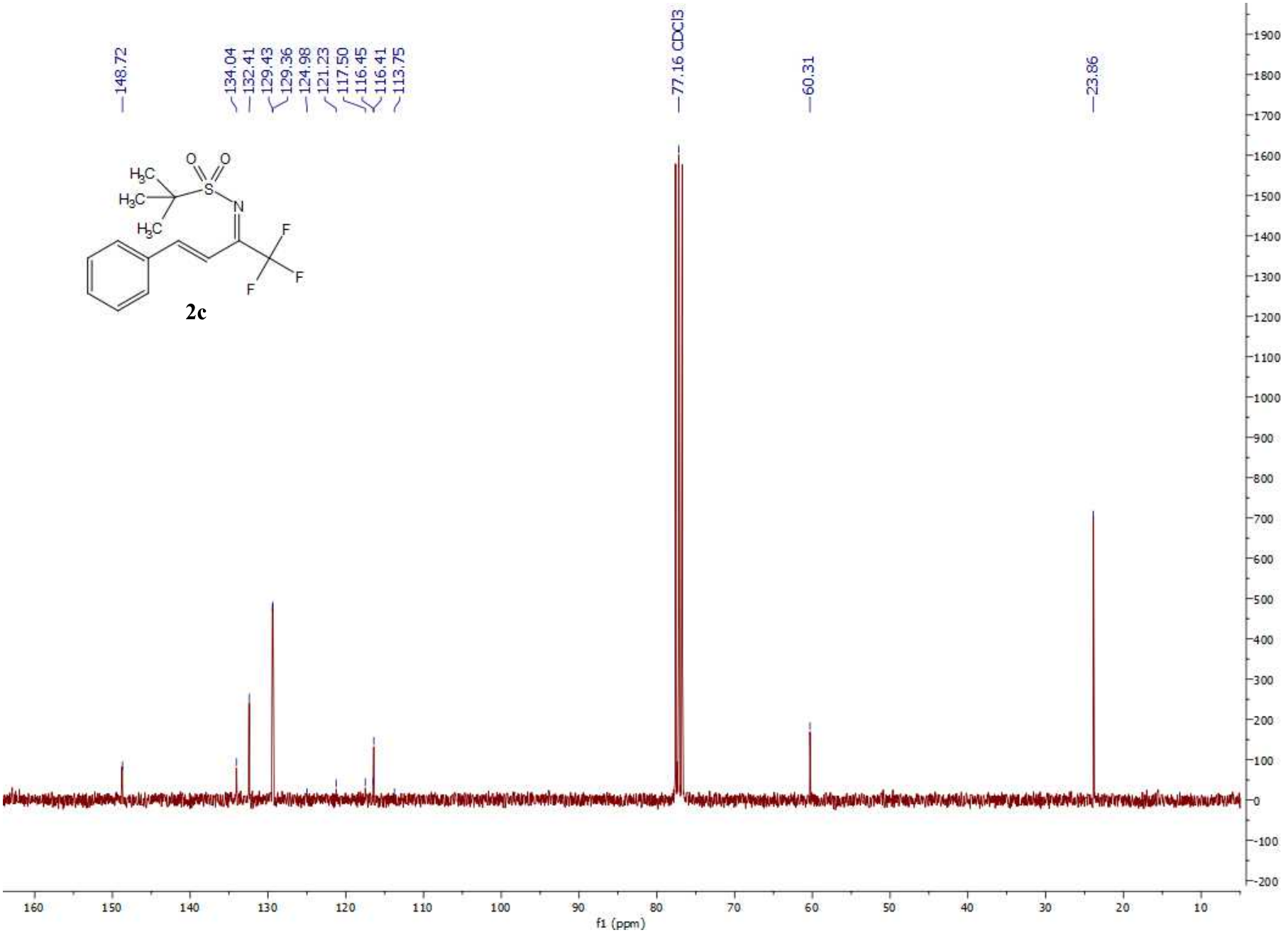
G_{corr} = 0.254685

H	5.31723	-2.64614	2.71826
C	4.23258	-2.66080	2.66260
C	3.57464	-1.79846	1.78628
H	4.15132	-1.12796	1.15629
C	3.50261	-3.54559	3.45797
H	4.01531	-4.21647	4.14088
C	2.17401	-1.80398	1.68773
C	2.11015	-3.56434	3.36791
C	1.45700	-0.91974	0.72220
F	-1.23549	-0.72560	-3.21335
C	1.45289	-2.70348	2.48932
C	0.58636	-1.52253	-0.19626
H	1.53313	-4.24794	3.98392
C	-0.10305	-0.75526	-1.13192
H	0.36841	-2.71539	2.42938
H	0.46511	-2.59997	-0.18771
C	-1.08933	-1.41256	-2.05740
F	-0.71795	-2.67242	-2.37915
F	-2.32044	-1.50073	-1.49808
H	3.48081	1.39812	1.28575
C	2.48314	1.21578	1.71141
H	0.63145	2.97645	-2.39480
C	0.92723	3.47631	-1.47793
H	0.93193	5.41899	-2.39845
C	1.10724	4.85754	-1.48563
C	1.62134	0.48167	0.70262
H	2.63151	0.60265	2.60276
C	1.15207	2.72465	-0.31373
C	0.94326	1.25501	-0.27037

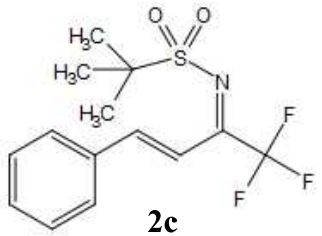
C	1.52377	5.51217	-0.32594
C	0.07611	0.62429	-1.17113
C	1.59238	3.38890	0.85076
H	1.66973	6.58831	-0.32610
C	1.76882	4.77361	0.83169
C	1.85409	2.56346	2.08745
H	2.50575	3.10740	2.77885
H	2.10638	5.27658	1.73454
H	0.90940	2.38120	2.62059
H	-0.47597	1.20877	-1.89719


7.64
7.64
7.64
7.63
7.62
7.62
7.61
7.49
7.48
7.47
7.47
7.46
7.46
7.46
7.45
7.44
7.44
7.43
7.42
7.42
7.41
7.41
7.40
7.26 CDCl3
1.53
3.98
3.03
9.21
f1 (ppm)

2c

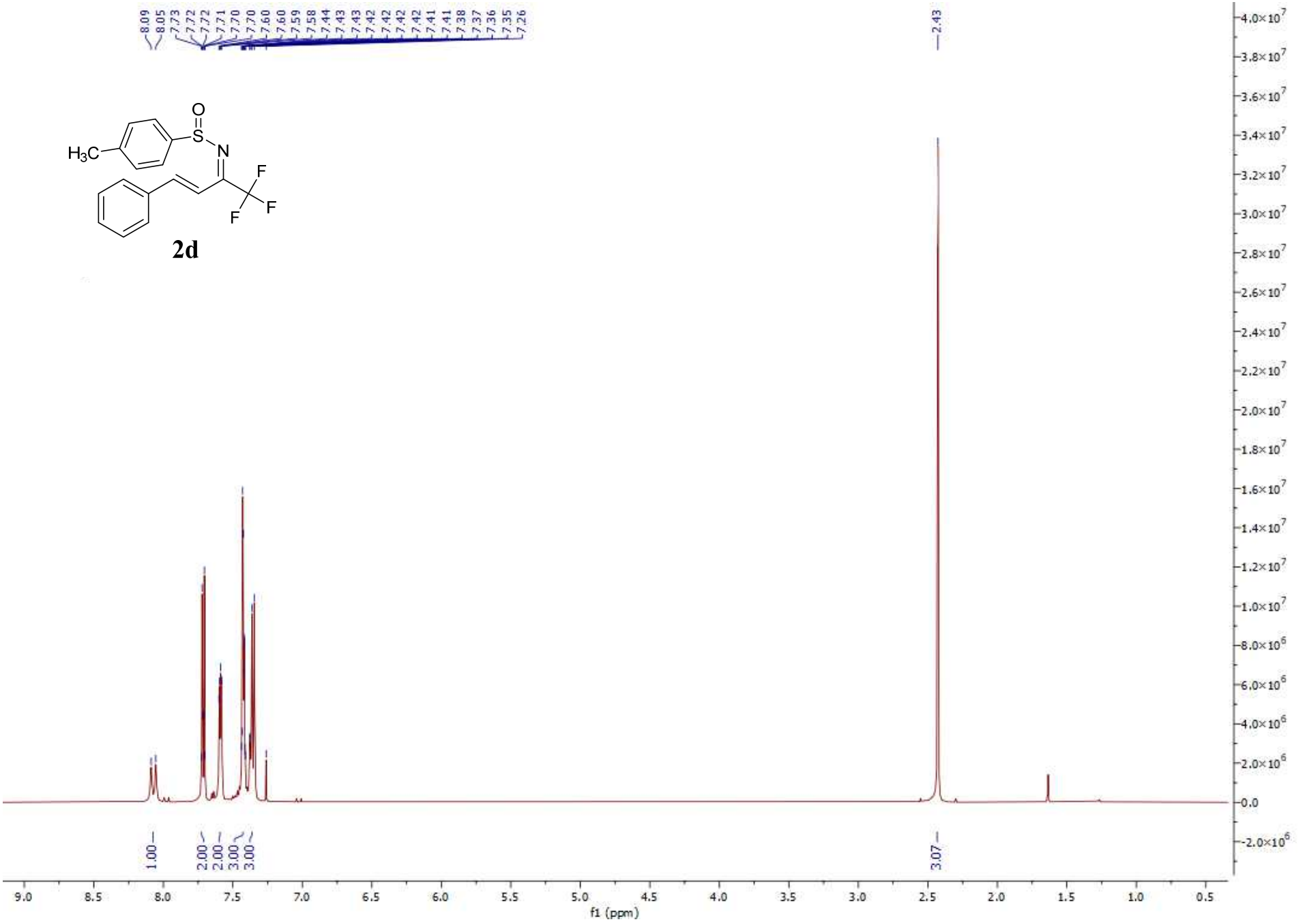

148.72
134.04
132.41
129.43
129.36
124.98
121.23
117.50
116.45
116.41
113.75
77.16 CDCl3
60.31
23.86
f1 (ppm)

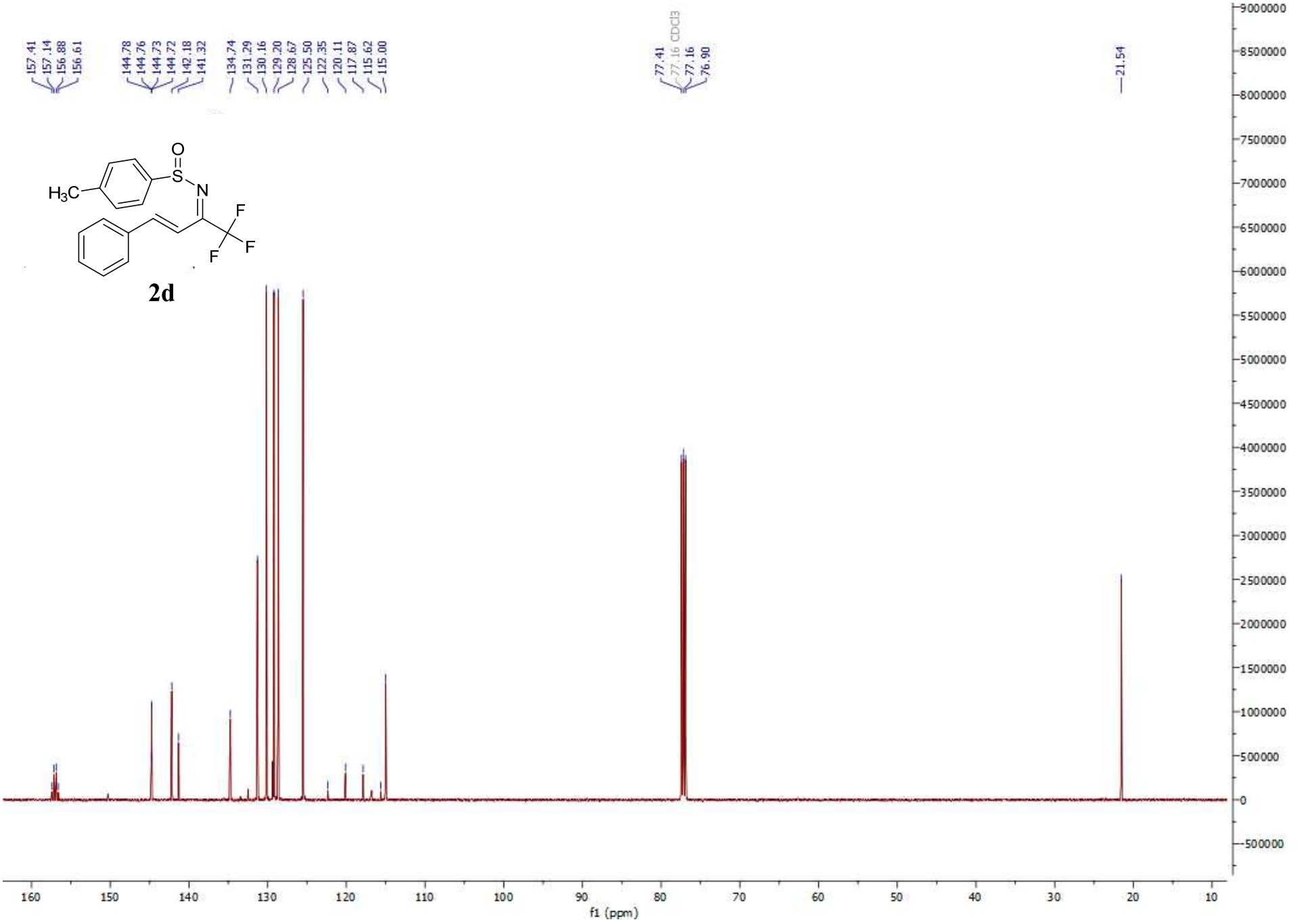
2c

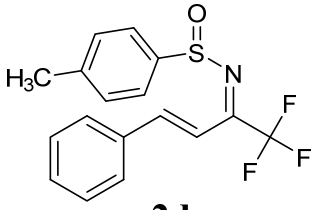

O
O
S
N
H3C
H3C
H3C
F
F
F

2c

-66.15
24000
23000
22000
21000
20000
19000
18000
17000
16000
15000
14000
13000
12000
11000
10000
9000
8000
7000
6000
5000
4000
3000
2000
1000
0
-1000
-2000
-3000
-50 -51 -52 -53 -54 -55 -56 -57 -58 -59 -60 -61 -62 -63 -64 -65 -66 -67 -68 -69 -70 -71 -72 -73 -74 -75 -76 -77 -78 -79 -80 -81 -82 -83
f1 (ppm)

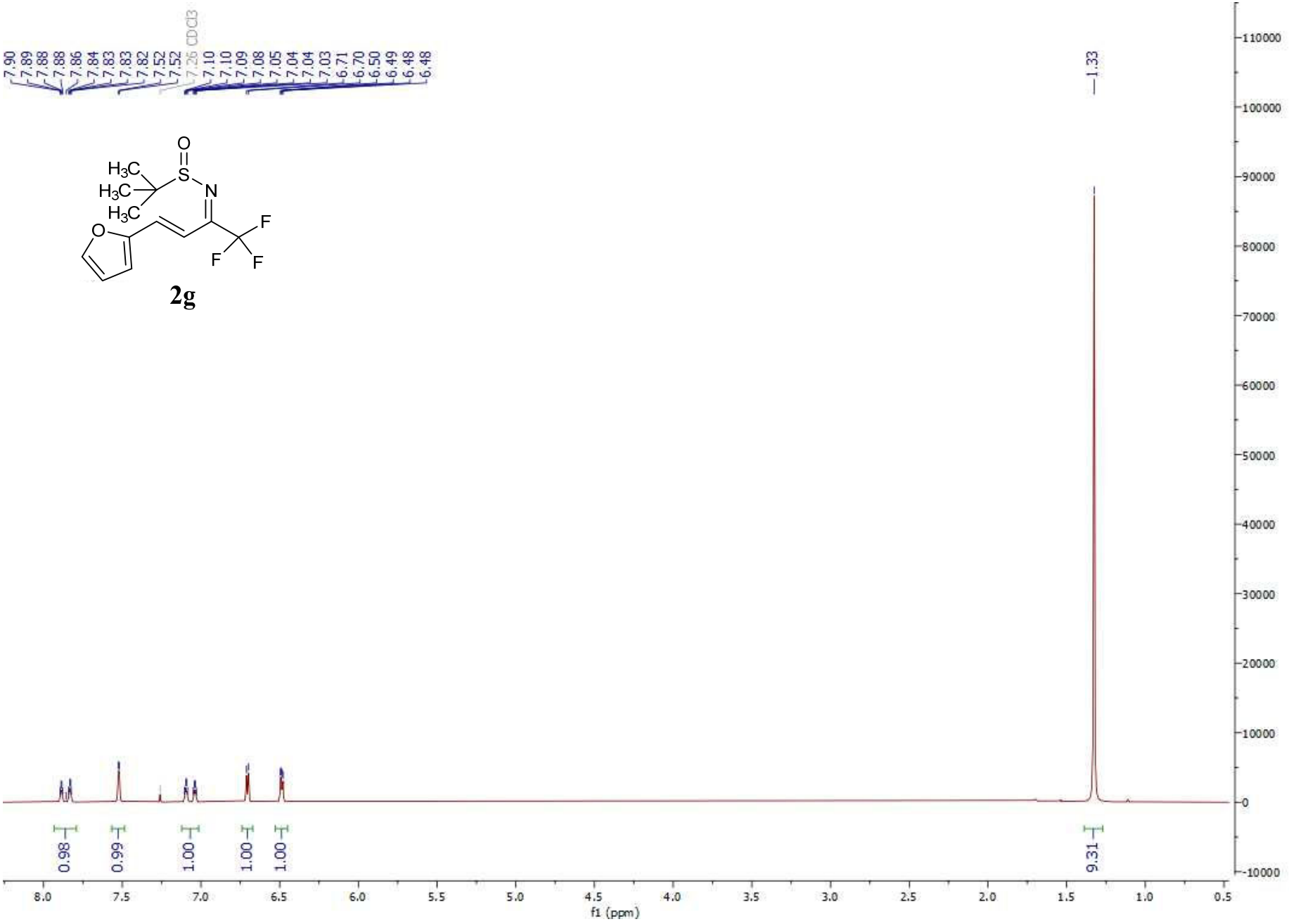

8.09
8.05
7.73
7.72
7.72
7.71
7.70
7.70
7.60
7.60
7.59
7.58
7.44
7.43
7.43
7.42
7.42
7.42
7.42
7.41
7.41
7.38
7.37
7.36
7.35
7.26
2.43
O
S
N
H3C
F
F
F
2d
1.00
2.00
2.00
3.00
3.00
3.07
f1 (ppm)

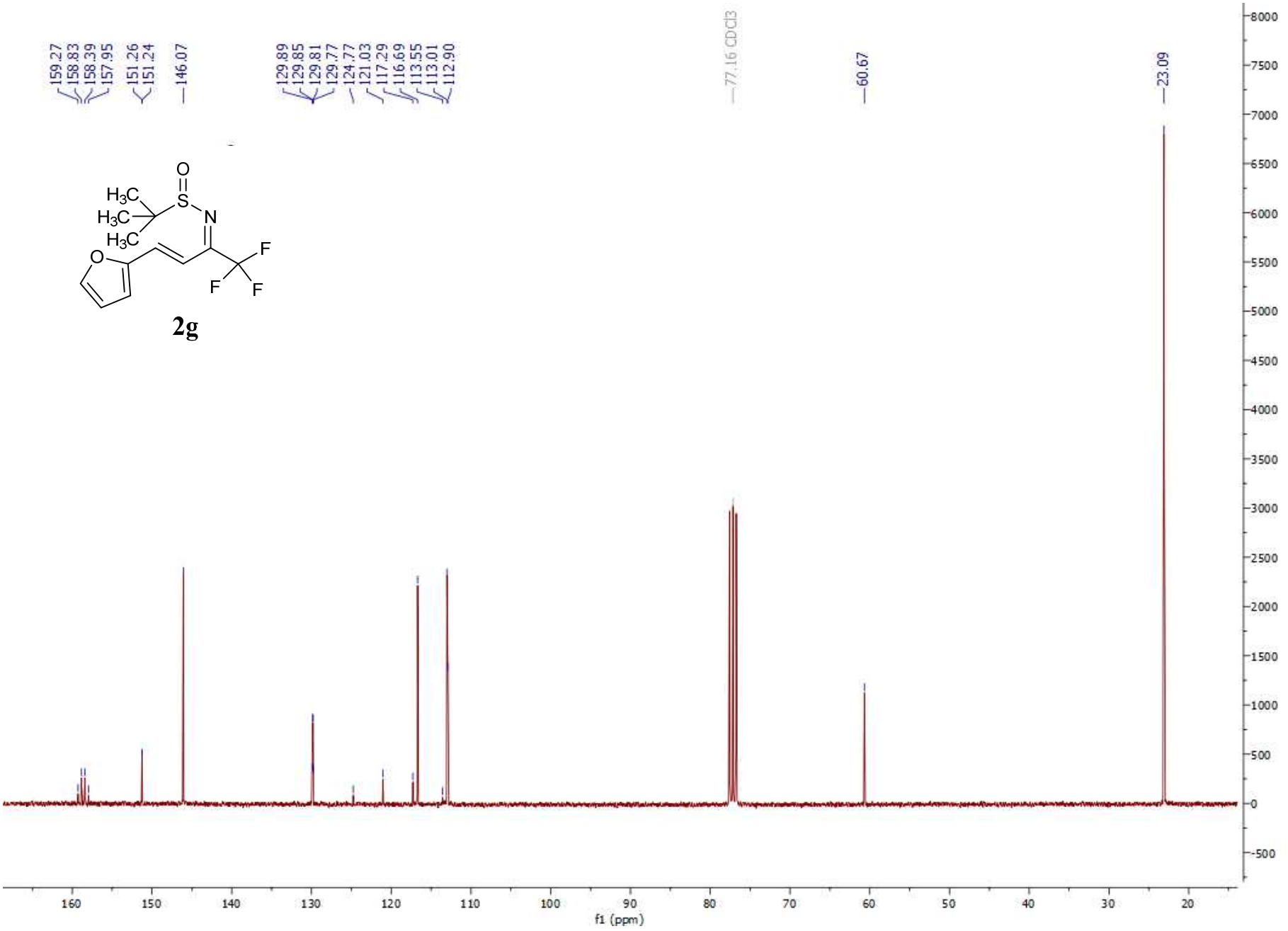

157.41
157.14
156.88
156.61
144.78
144.76
144.73
144.72
142.18
141.32
134.74
131.29
130.16
129.20
128.67
125.50
122.35
120.11
117.87
115.62
115.00
77.41
77.16 CDCl3
77.16
76.90
21.54
O
S
N
H3C
F
F
F
2d
f1 (ppm)


O
S
N
H3C
F
F
F

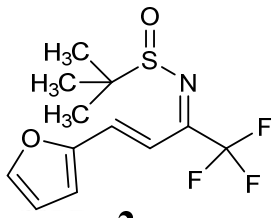
2d

-66.32
20000000
19000000
18000000
17000000
16000000
15000000
14000000
13000000
12000000
11000000
10000000
9000000
8000000
7000000
6000000
5000000
4000000
3000000
2000000
1000000
0
-1000000
-2000000
-53
-54
-55
-56
-57
-58
-59
-60
-61
-62
-63
-64
-65
-66
-67
-68
-69
-70
-71
-72
-73
-74
-75
-76
-77
f1 (ppm)


7.90
7.89
7.88
7.88
7.86
7.84
7.83
7.83
7.82
7.52
7.52
7.26 CDCl3
7.10
7.10
7.09
7.08
7.05
7.04
7.04
7.03
6.71
6.70
6.50
6.49
6.48
6.48
1.33
O
S
N
H3C
H3C
H3C
O
F
F
F
2g
0.98
0.99
1.00
1.00
1.00
9.31
f1 (ppm)

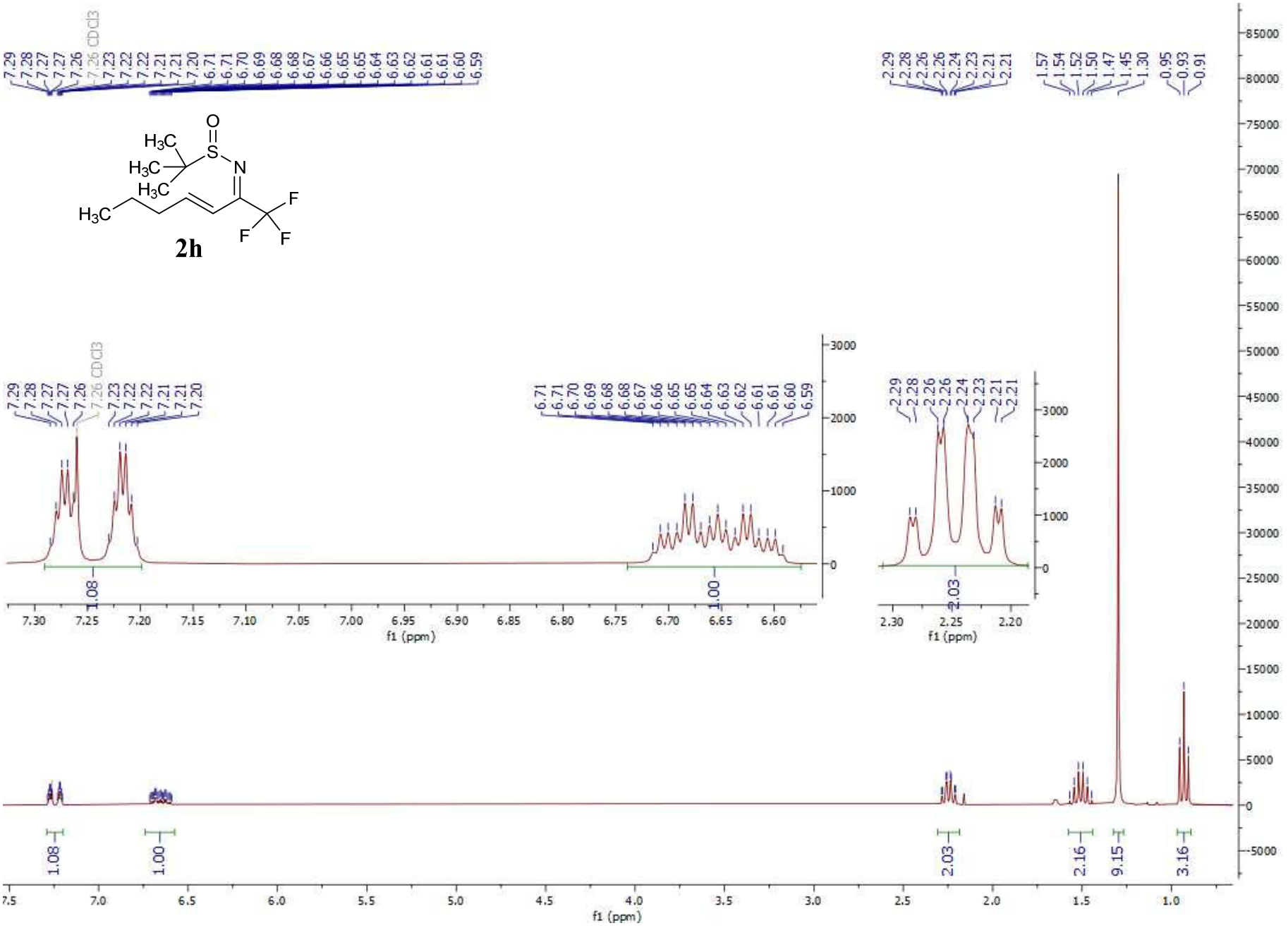

159.27
158.83
158.39
157.95
151.26
151.24
146.07
129.89
129.85
129.81
129.77
124.77
121.03
117.29
116.69
113.55
113.01
112.90
77.16 CDCl3
60.67
23.09
f1 (ppm)

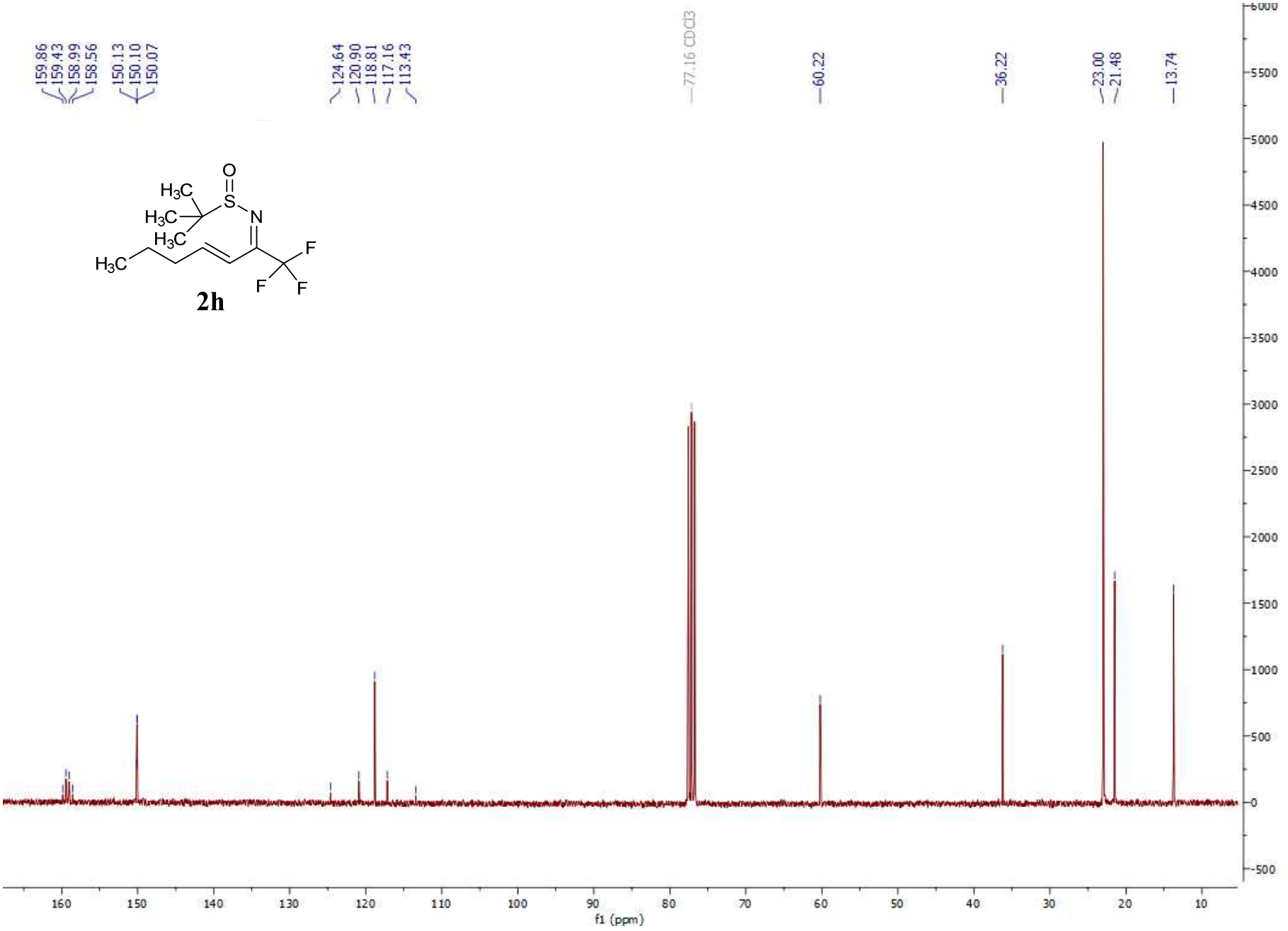
2g

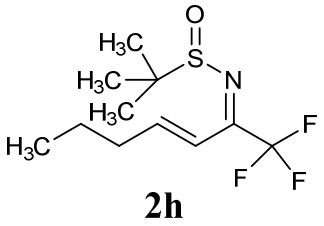

O
H3C
S
N
H3C
H3C
O
F
F
F

2g

-66.45
50000
45000
40000
35000
30000
25000
20000
15000
10000
5000
0
-5 -10 -15 -20 -25 -30 -35 -40 -45 -50 -55 -60 -65 -70 -75 -80 -85 -90 -95 -100 -105 -110 -115 -120 -125 -130 -135
f1 (ppm)

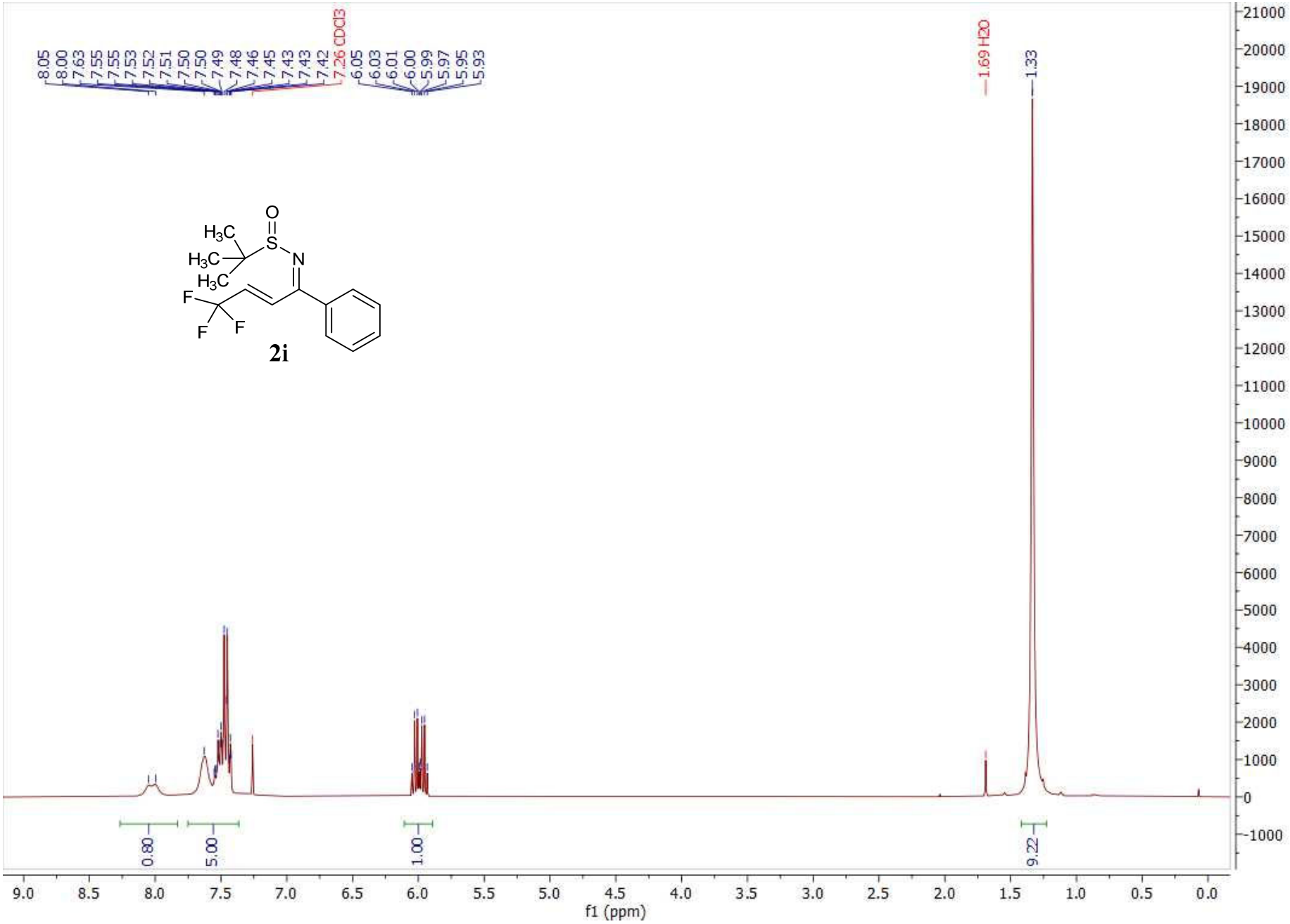

7.29 7.28 7.27 7.27 7.26 7.26 CDCl3 7.23 7.22 7.22 7.21 7.21 7.20 6.71 6.70 6.69 6.68 6.68 6.67 6.66 6.65 6.65 6.64 6.63 6.62 6.61 6.61 6.60 6.59
2.29 2.28 2.26 2.26 2.24 2.23 2.21 2.21
1.57 1.54 1.52 1.50 1.47 1.45 1.30
0.95 0.93 0.91
O
S
N
F
F
F
2h
1.08
1.00
2.03
2.16
9.15
3.16
f1 (ppm)

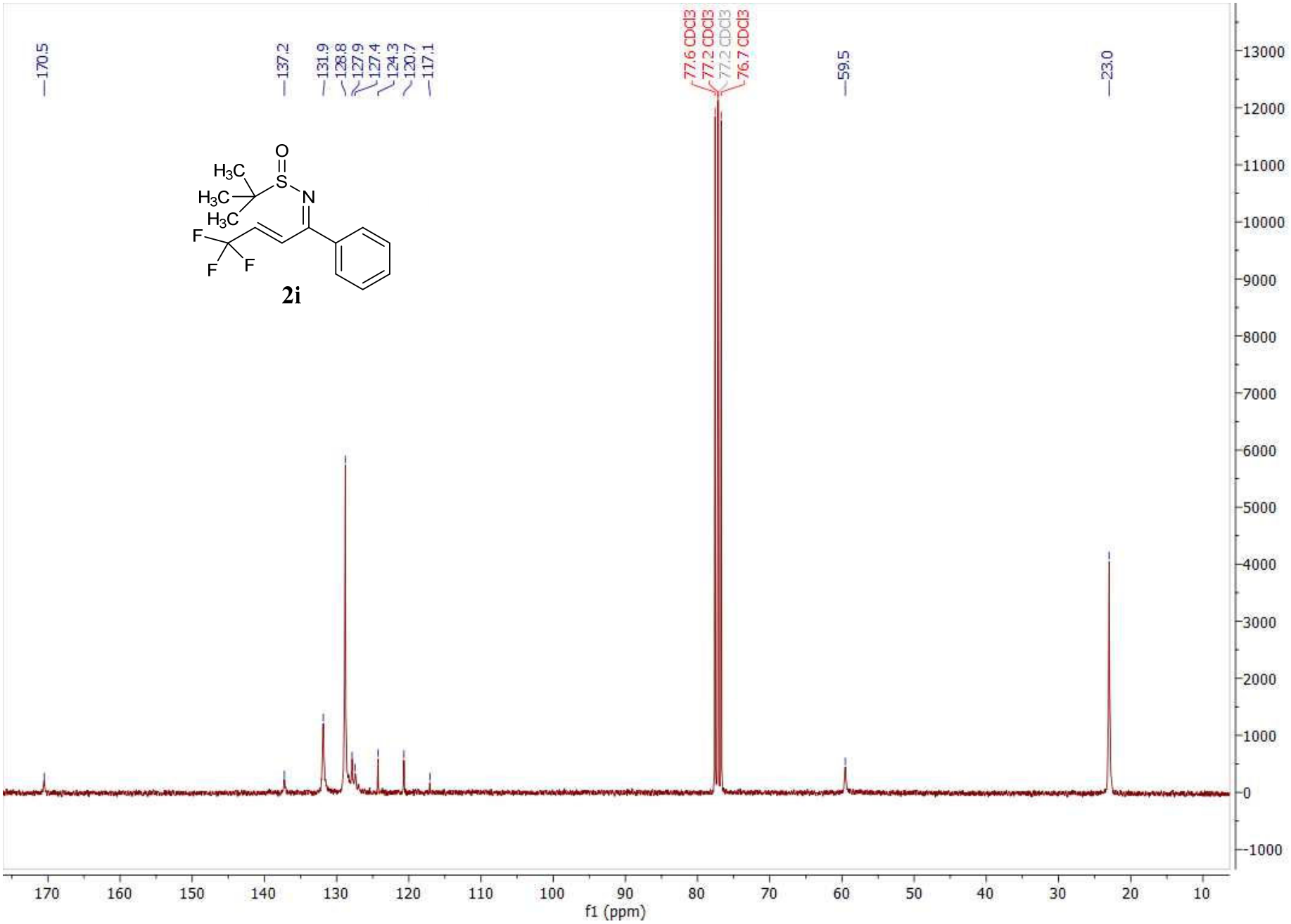

159.86
159.43
158.99
158.56
150.13
150.10
150.07
124.64
120.90
118.81
117.16
113.43
77.16 CDCl3
60.22
36.22
23.00
21.48
13.74
O
S
N
H3C
H3C
H3C
H3C
F
F
F
2h
f1 (ppm)

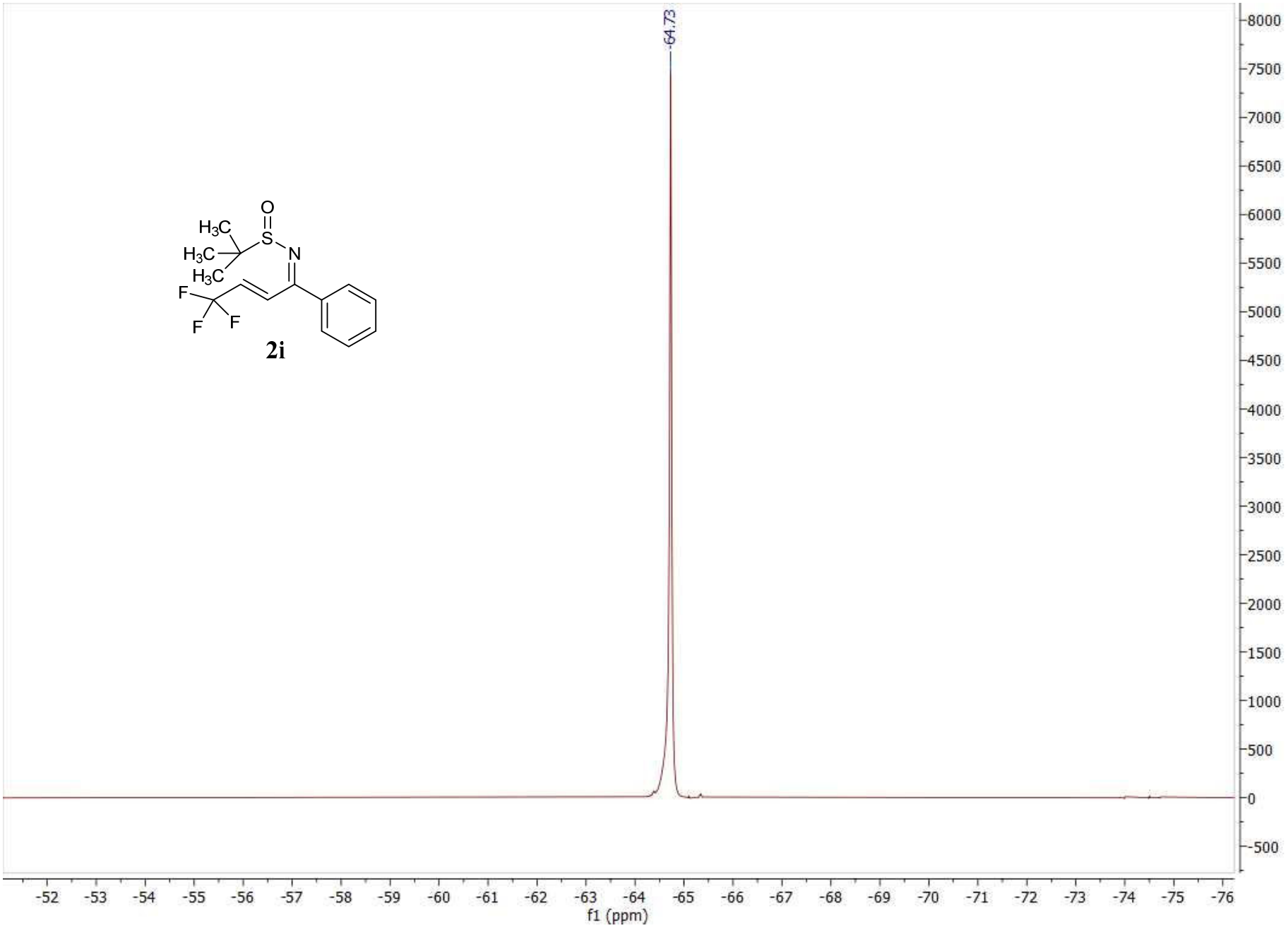

O
H3C
S
N
H3C
H3C
H3C
F
F
F

2h

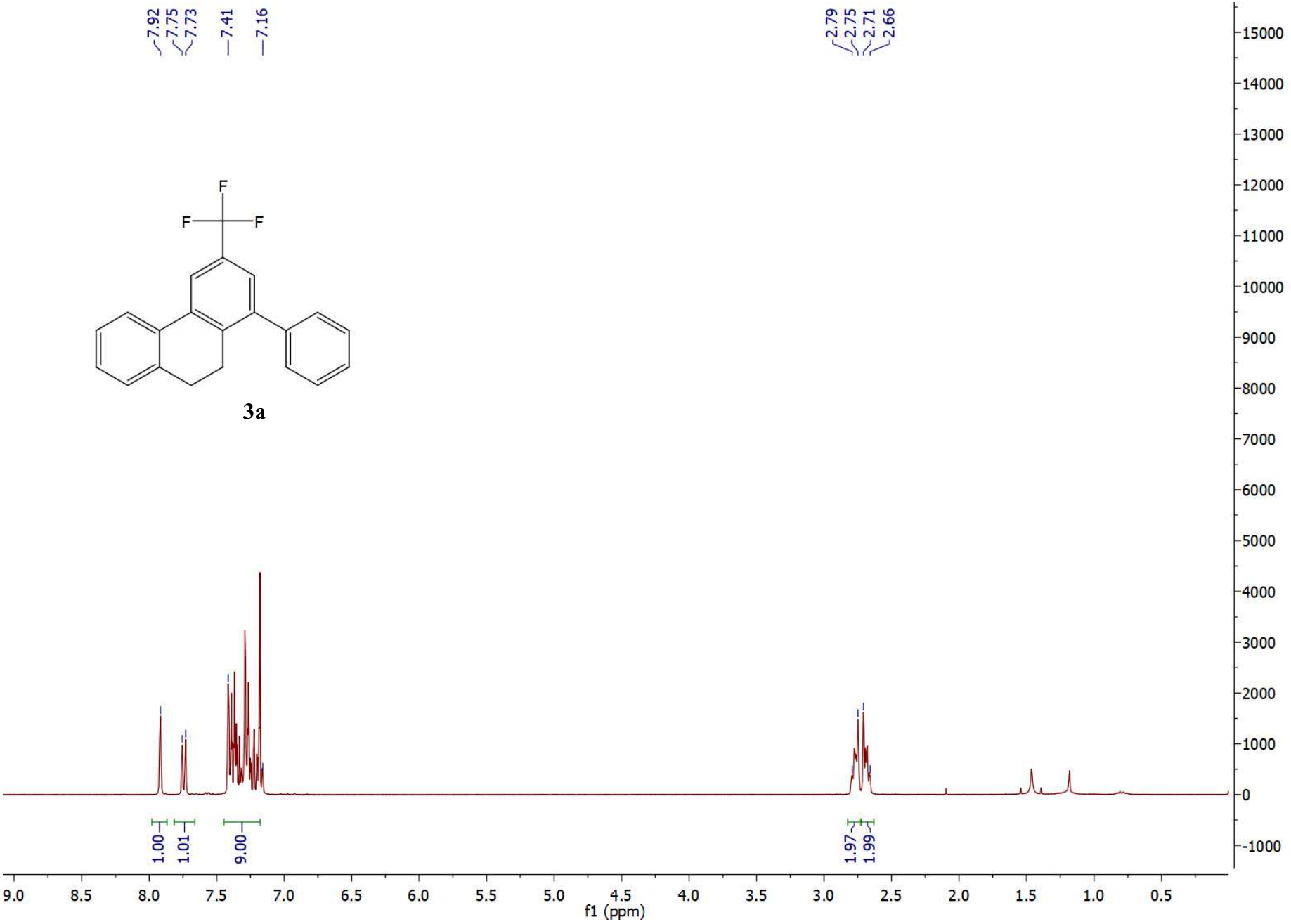
-66.69
8000
7500
7000
6500
6000
5500
5000
4500
4000
3500
3000
2500
2000
1500
1000
500
0
-500
-35
-40
-45
-50
-55
-60
-65
-70
-75
-80
-85
-90
-95
-100
-105
f1 (ppm)


8.05
8.00
7.63
7.55
7.55
7.53
7.52
7.51
7.50
7.50
7.49
7.48
7.46
7.45
7.43
7.43
7.42
7.26 CDCl3
6.05
6.03
6.01
6.00
5.99
5.97
5.95
5.93
1.69 H2O
1.33
O
S
N
H3C
H3C
H3C
F
F
F
2i
0.80
5.00
1.00
9.22
f1 (ppm)

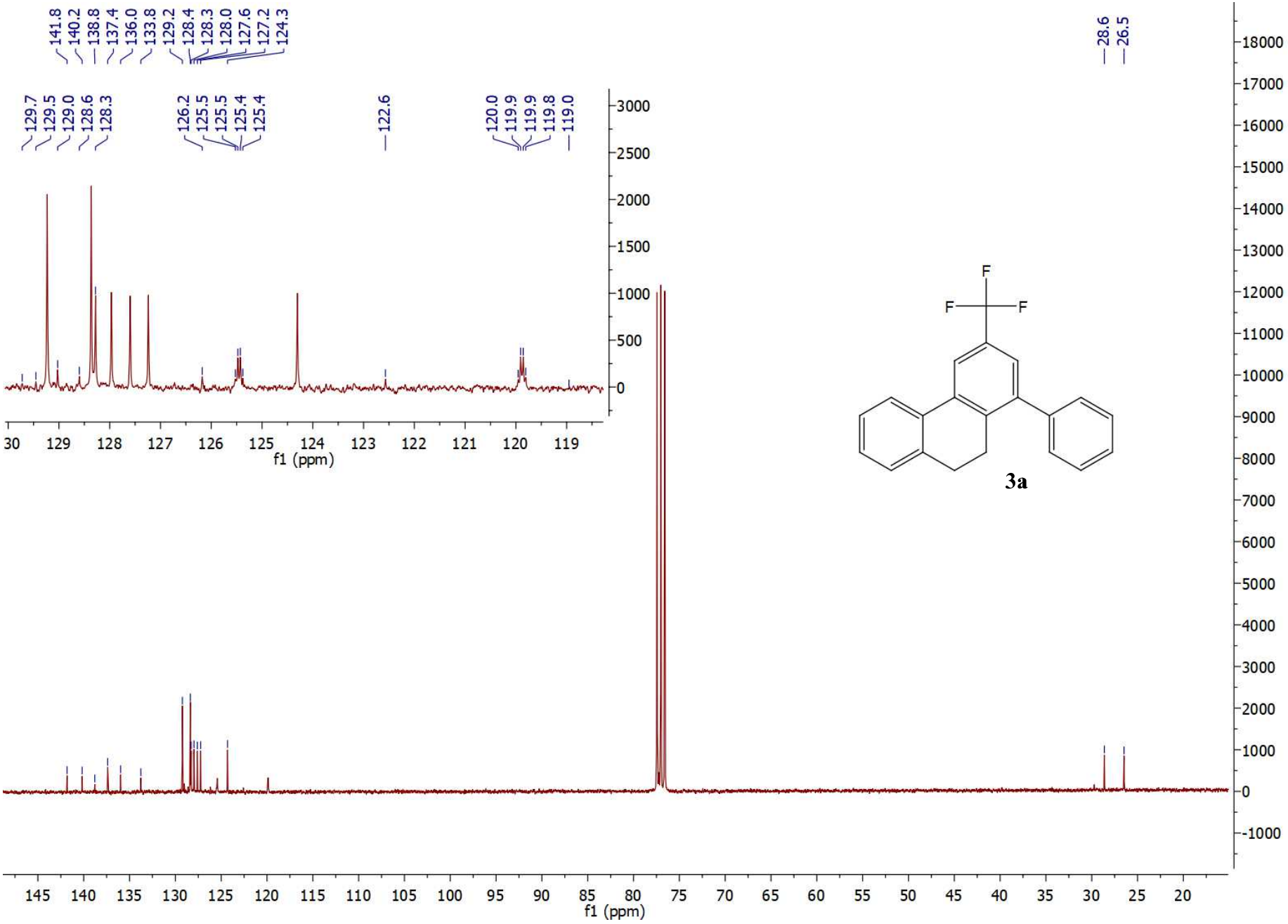

170.5
137.2
131.9
128.8
127.9
127.4
124.3
120.7
117.1
77.6 CDCl3
77.2 CDCl3
77.2 CDCl3
76.7 CDCl3
59.5
23.0
O
S
N
H3C
H3C
H3C
F
F
F
2i
f1 (ppm)

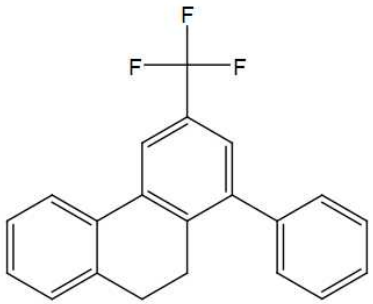

-64.73
8000
7500
7000
6500
6000
5500
5000
4500
4000
3500
3000
2500
2000
1500
1000
500
0
-500
-52 -53 -54 -55 -56 -57 -58 -59 -60 -61 -62 -63 -64 -65 -66 -67 -68 -69 -70 -71 -72 -73 -74 -75 -76
f1 (ppm)
O
S
N
H3C
H3C
H3C
F
F
F

2i


7.92
7.75
7.73
7.41
7.16
2.79
2.75
2.71
2.66
F
F
F
1.00
1.01
9.00
1.97
1.99
f1 (ppm)

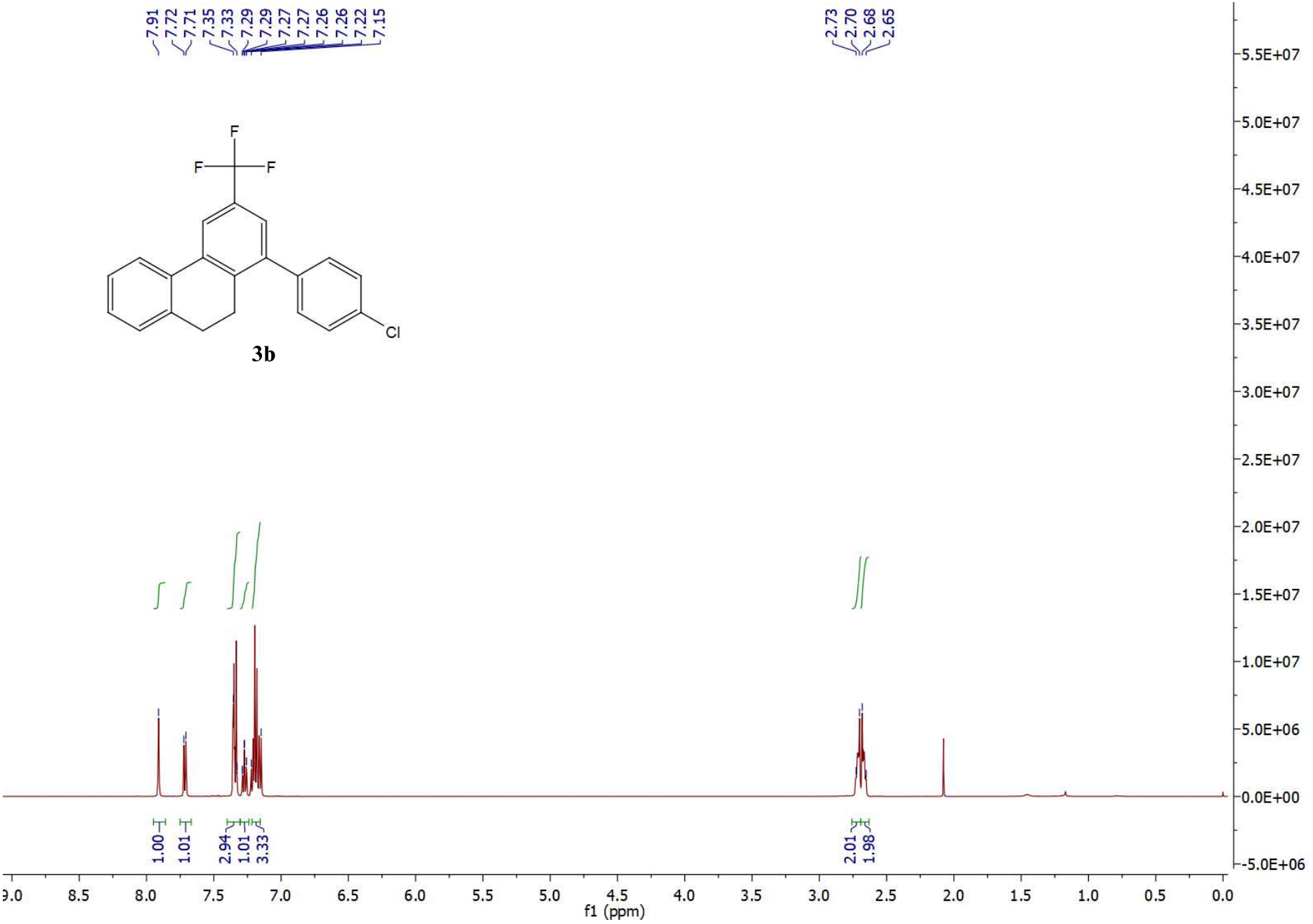
3a

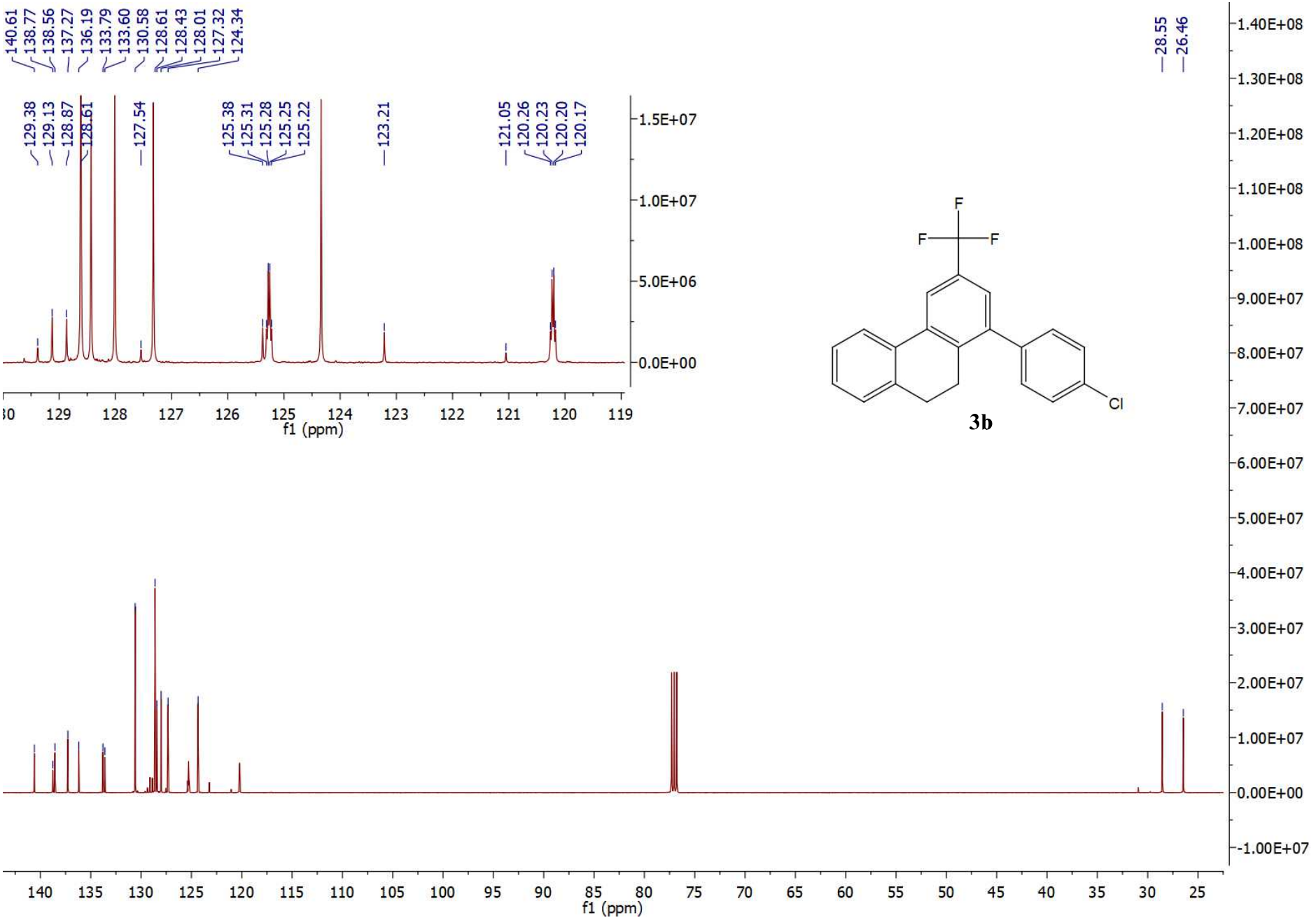

141.8
140.2
138.8
137.4
136.0
133.8
129.2
128.4
128.3
128.0
127.6
127.2
124.3
129.7
129.5
129.0
128.6
128.3
126.2
125.5
125.5
125.4
125.4
122.6
120.0
119.9
119.9
119.8
119.0
28.6
26.5
f1 (ppm)
F
F
F
3a

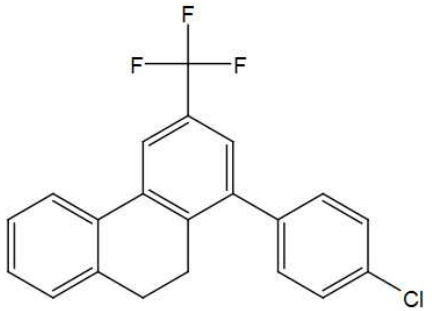

F
F
F

3a

-62.38
17000
16000
15000
14000
13000
12000
11000
10000
9000
8000
7000
6000
5000
4000
3000
2000
1000
0
-1000
-53
-54
-55
-56
-57
-58
-59
-60
-61
-62
-63
-64
-65
-66
-67
-68
-69
-70
-71
-72
f1 (ppm)

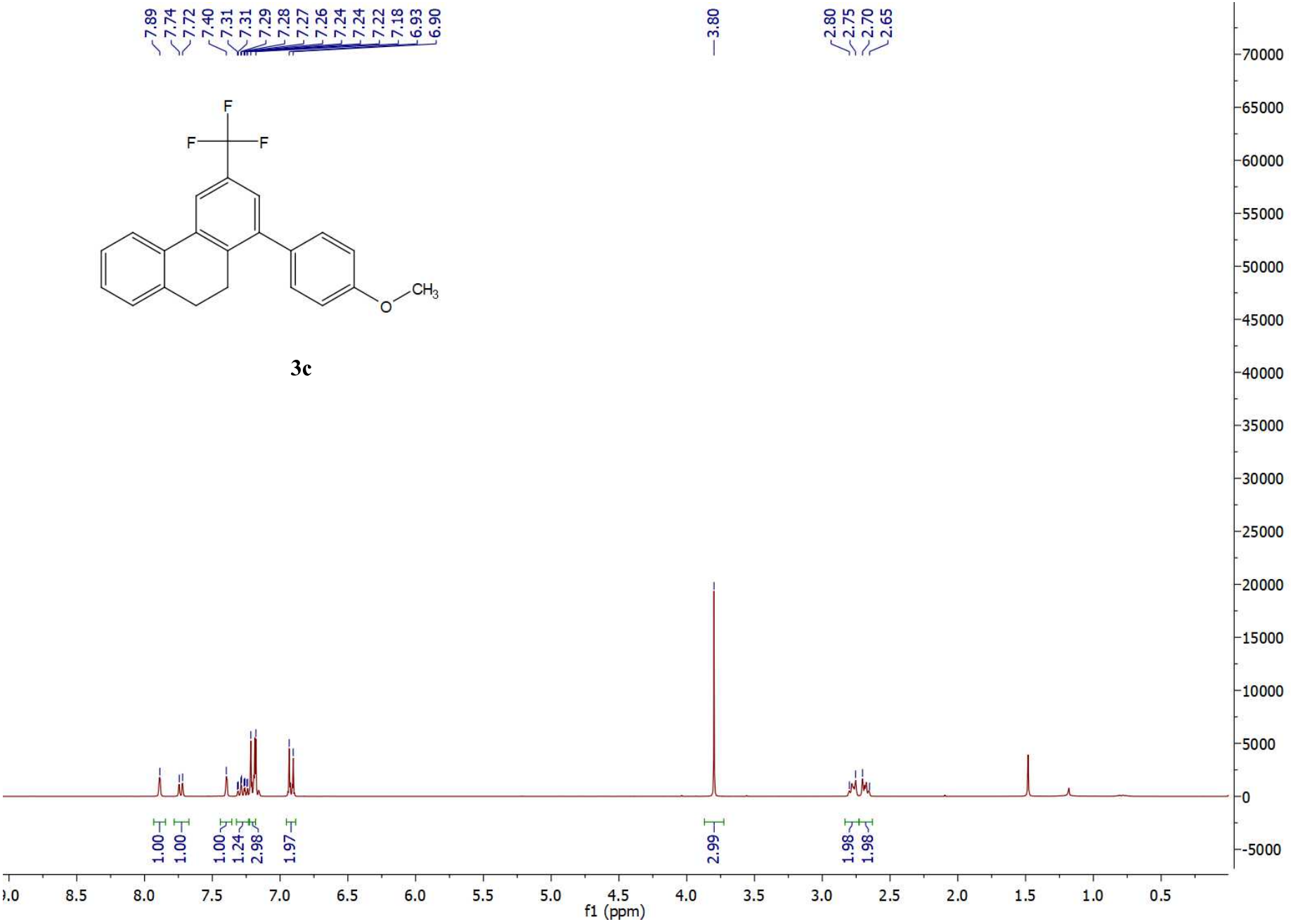

7.91
7.72
7.71
7.35
7.33
7.29
7.29
7.27
7.27
7.26
7.26
7.22
7.15
2.73
2.70
2.68
2.65
F
F
F
Cl
3b
5.5E+07
5.0E+07
4.5E+07
4.0E+07
3.5E+07
3.0E+07
2.5E+07
2.0E+07
1.5E+07
1.0E+07
5.0E+06
0.0E+00
-5.0E+06
1.00
1.01
2.94
1.01
3.33
2.01
1.98
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


140.61
138.77
138.56
137.27
136.19
133.79
133.60
130.58
128.61
128.43
128.01
127.32
124.34
129.38
129.13
128.87
128.61
127.54
125.38
125.31
125.28
125.25
125.22
123.21
121.05
120.26
120.23
120.20
120.17
28.55
26.46
F
F
F
Cl
3b
f1 (ppm)
f1 (ppm)


F
F
F
Cl

3b

-62.38
140000
130000
120000
110000
100000
90000
80000
70000
60000
50000
40000
30000
20000
10000
0
-10000
-53
-54
-55
-56
-57
-58
-59
-60
-61
-62
-63
-64
-65
-66
-67
-68
-69
-70
-71
-72
f1 (ppm)


7.89
7.74
7.72
7.40
7.31
7.31
7.29
7.28
7.27
7.26
7.24
7.24
7.22
7.18
6.93
6.90
3.80
2.80
2.75
2.70
2.65
F
F
F
CH3
O
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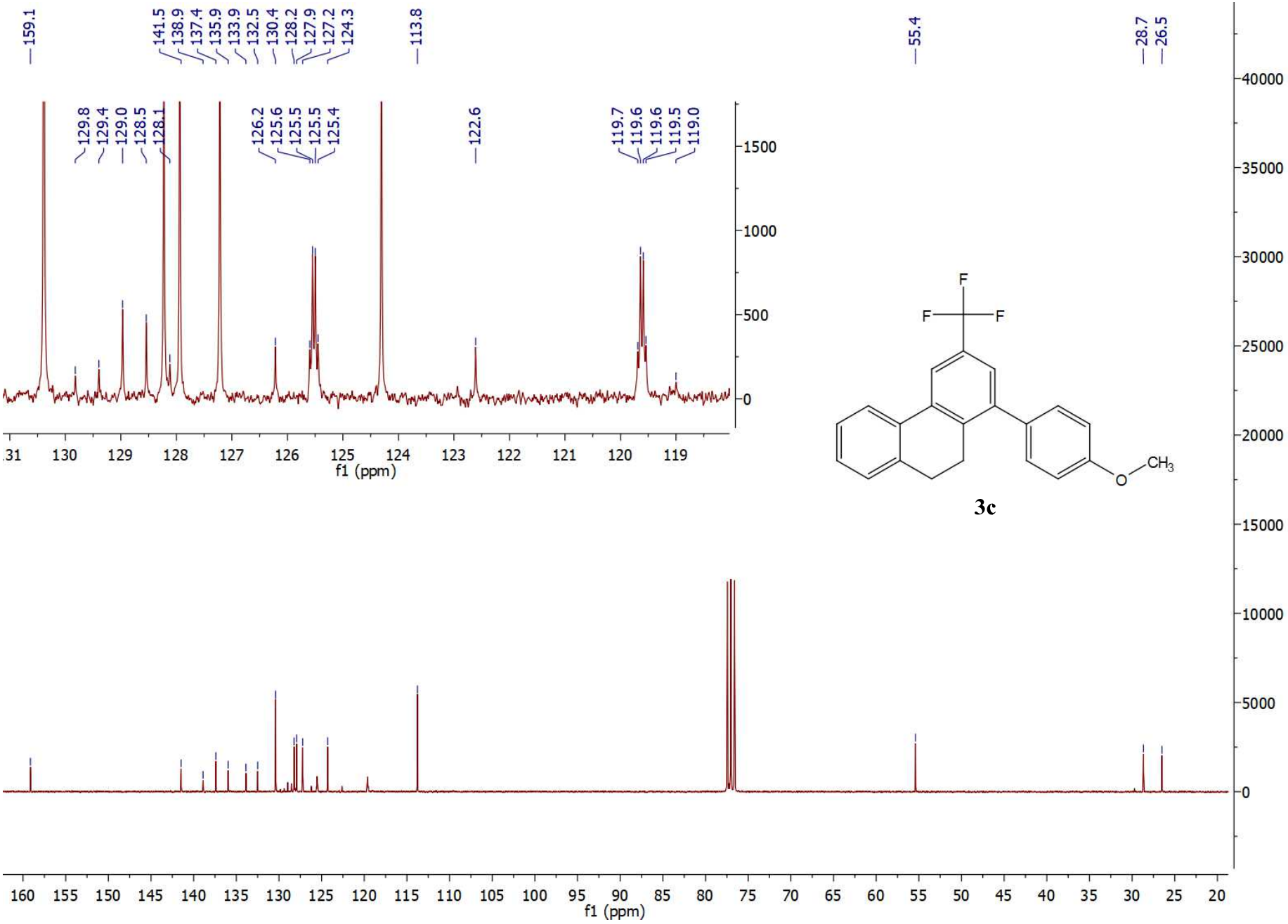
1.00
1.00
1.24
2.98
1.97
2.99
1.98
1.98
f1 (ppm)

3c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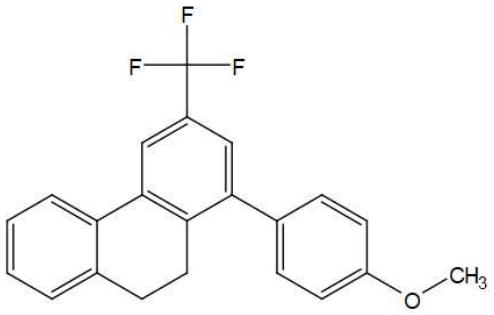
141.5
138.9
137.4
135.9
133.9
132.5
130.4
128.2
127.9
127.2
124.3
113.8
55.4
28.7
26.5
129.8
129.4
129.0
128.5
128.1
126.2
125.6
125.5
125.5
125.4
122.6
119.7
119.6
119.6
119.5
119.0
F
F
F
O
CH3
f1 (ppm)
f1 (ppm)

3c


F
F
F
O
CH3

3c

-62.37
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36000
34000
32000
30000
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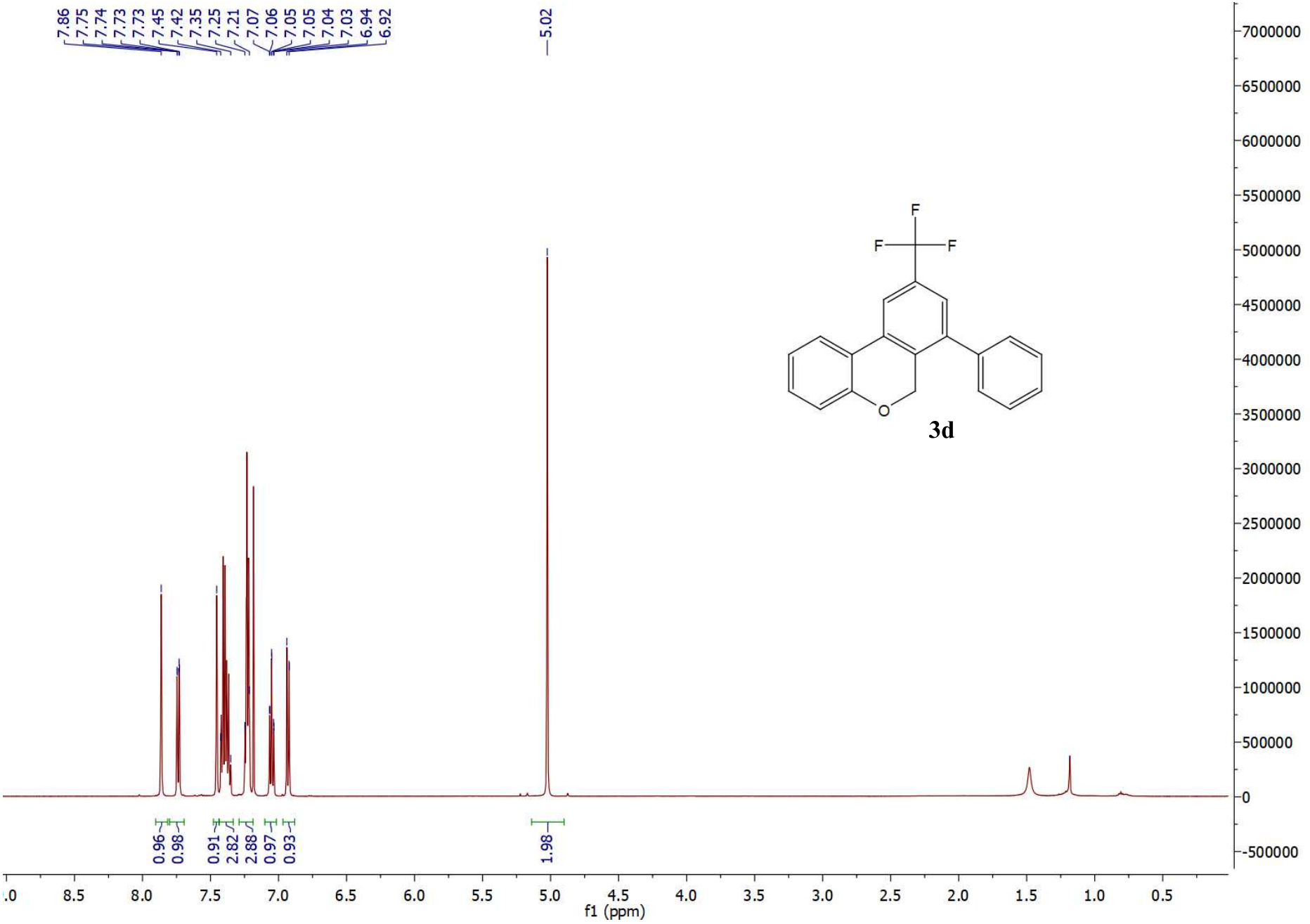
24000
22000
20000
18000
16000
14000
12000
10000
8000
6000
4000
2000
0
-2000
-52
-53
-54
-55
-56
-57
-58
-59
-60
-61
-62
-63
-64
-65
-66
-67
-68
-69
-70
-71
f1 (ppm)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7.74
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7.45
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7.35
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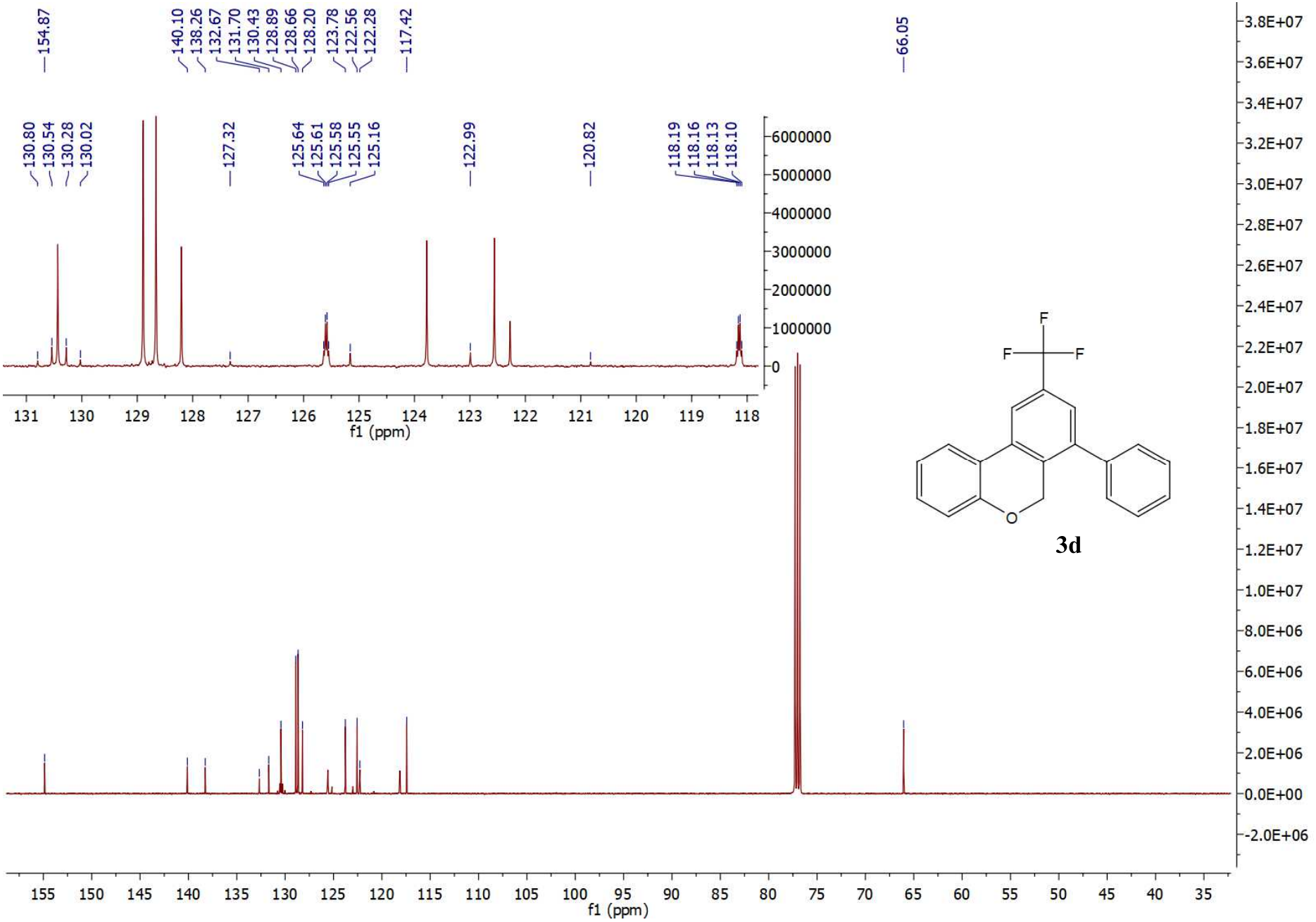
7.21
7.07
7.06
7.05
7.05
7.04
7.03
6.94
6.92
5.02
F
F
F
O
3d
0.96
0.98
0.91
2.82
2.88
0.97
0.93
1.98
f1 (ppm)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130.43
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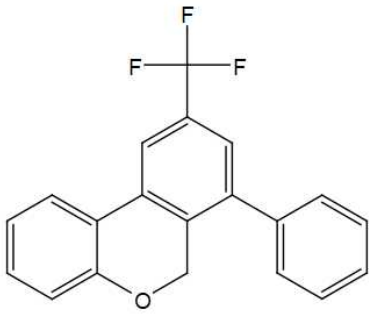
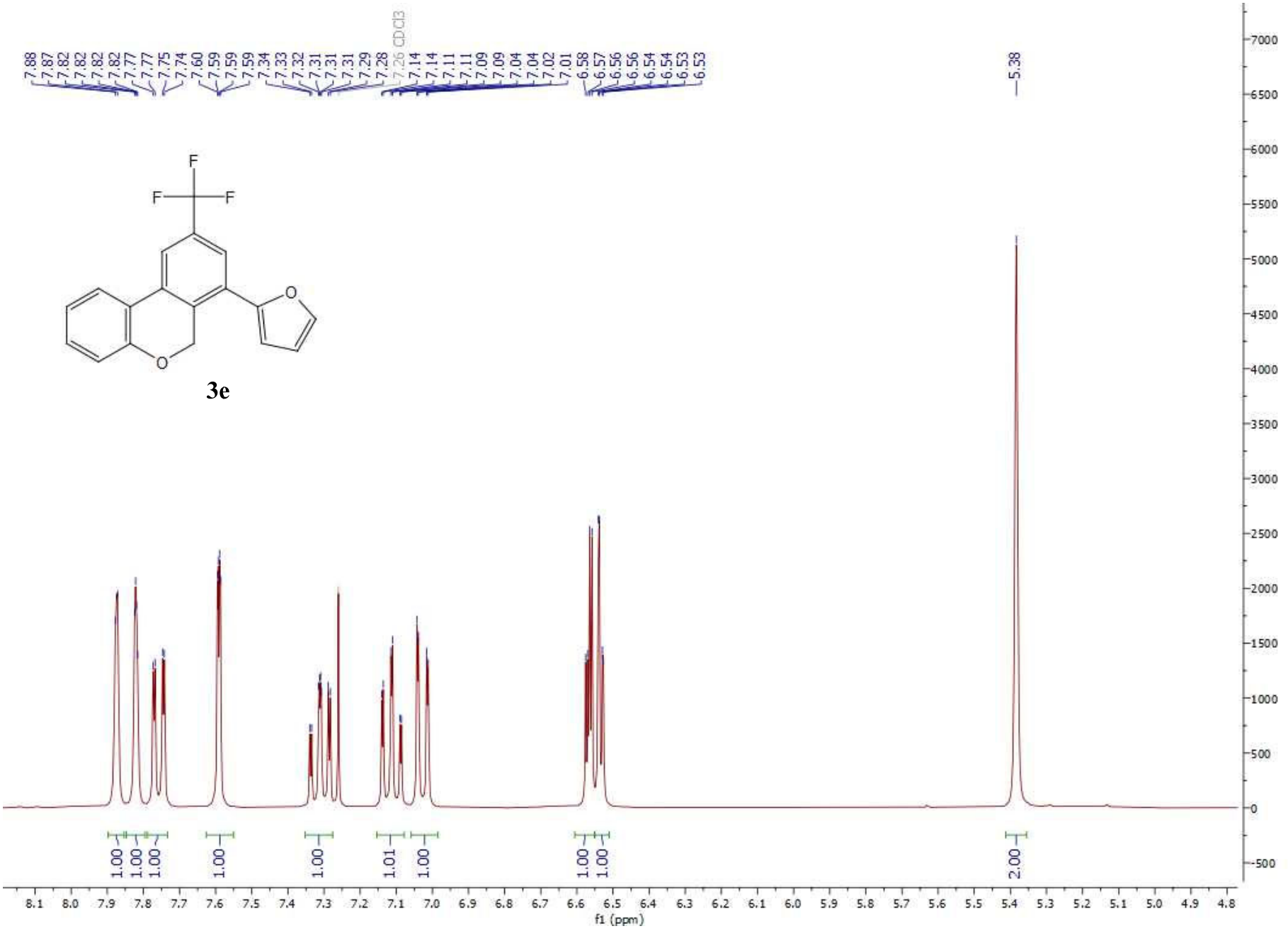
128.66
128.20
123.78
122.56
122.28
117.42
66.05
130.80
130.54
130.28
130.02
127.32
125.64
125.61
125.58
125.55
125.16
122.99
120.82
118.19
118.16
118.13
118.10
f1 (ppm)
F
F
F
O
3d


F
F
F
O

3d

-62.62
65000
60000
55000
50000
45000
40000
35000
30000
25000
20000
15000
10000
5000
0
-5000
-53
-54
-55
-56
-57
-58
-59
-60
-61
-62
-63
-64
-65
-66
-67
-68
-69
-70
-71
-72
f1 (ppm)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7.87
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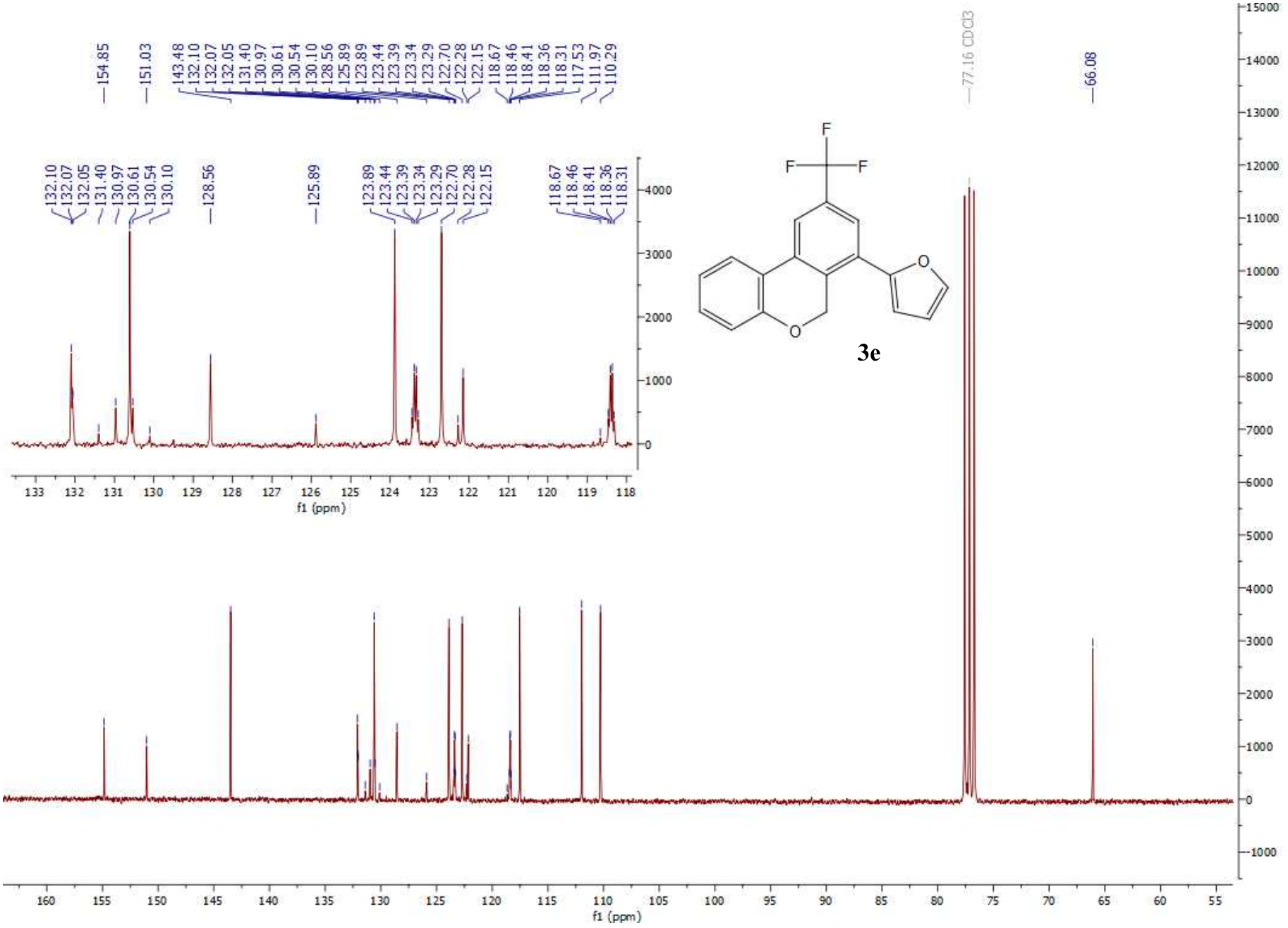
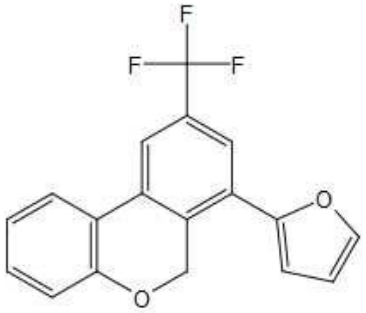
7.77
7.75
7.74
7.60
7.59
7.59
7.59
7.34
7.33
7.32
7.31
7.31
7.31
7.29
7.28
7.26 CDCl3
7.14
7.14
7.11
7.11
7.09
7.09
7.04
7.04
7.02
7.01
6.58
6.57
6.56
6.56
6.54
6.54
6.53
6.53
5.38
F
F
F
O
O
1.00
1.00
1.00
1.00
1.00
1.01
1.00
1.00
1.00
2.00
f1 (ppm)

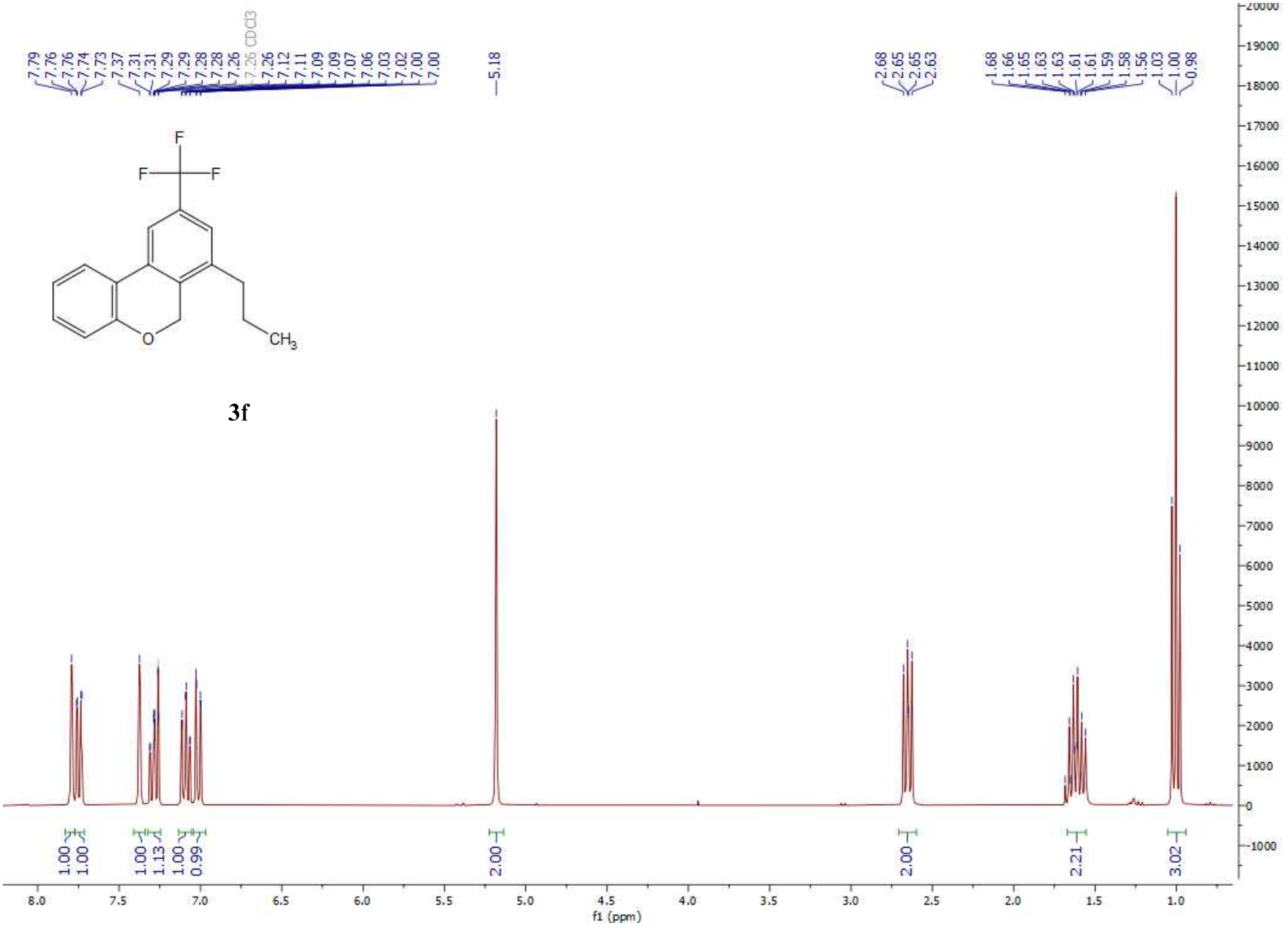
3e


154.85
151.03
143.48
132.10
132.07
132.05
131.40
130.97
130.61
130.54
130.10
128.56
125.89
123.89
123.44
123.39
123.34
123.29
122.70
122.28
122.15
118.67
118.46
118.41
118.36
118.31
117.53
111.97
110.29
77.16 CDCl3
66.08
F
F
F
O
O
3e
f1 (ppm)


F
F
F
O
O

3e

40000
35000
30000
25000
20000
15000
10000
5000
0
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
f1 (ppm)


7.79
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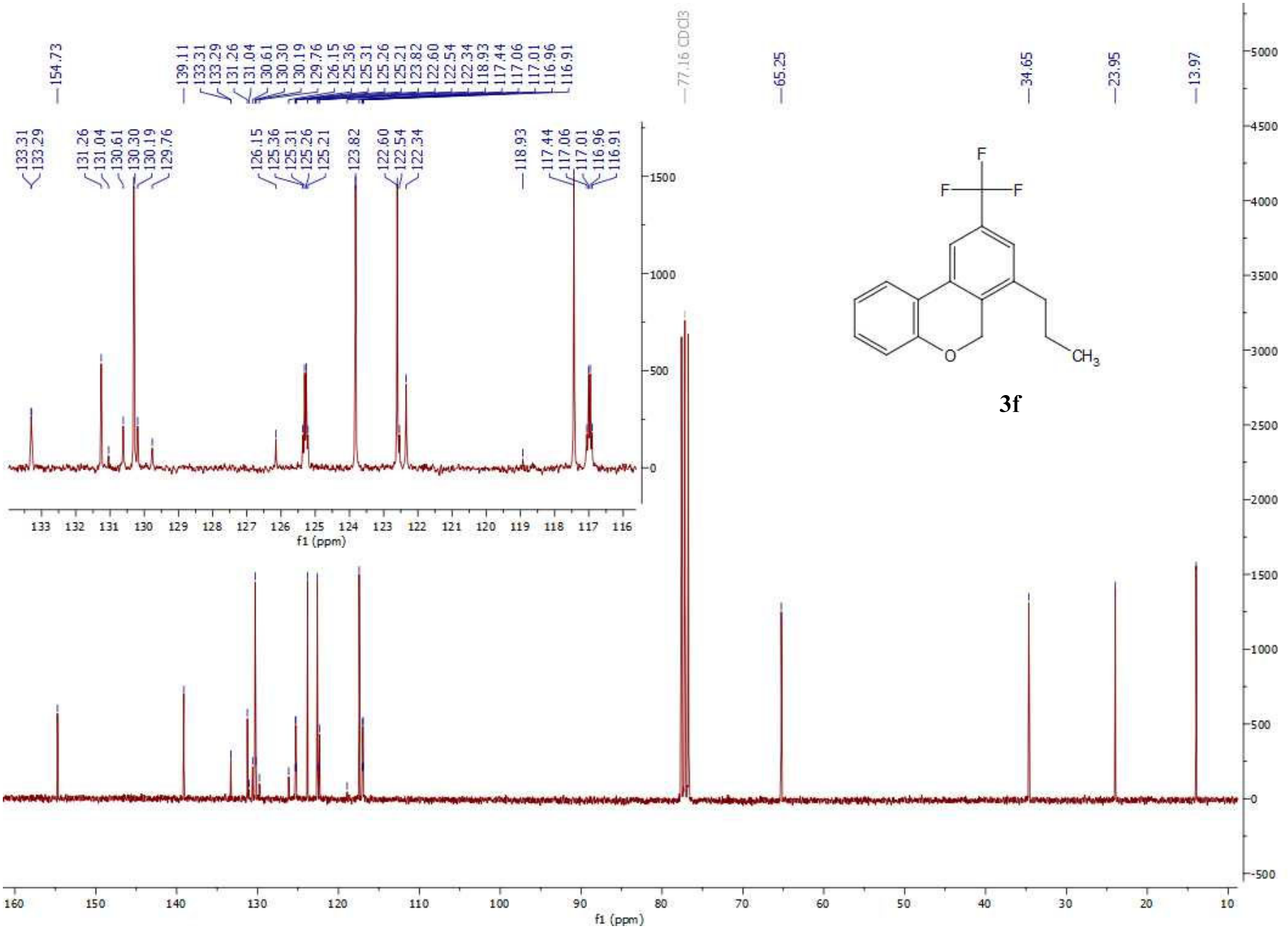
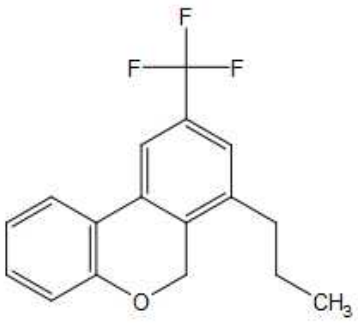
7.76
7.74
7.73
7.37
7.31
7.31
7.29
7.29
7.28
7.28
7.26
CDCl3
7.26
7.12
7.11
7.09
7.09
7.07
7.06
7.03
7.02
7.00
7.00
5.18
2.68
2.65
2.65
2.63
1.68
1.66
1.65
1.63
1.63
1.61
1.61
1.59
1.58
1.56
1.03
1.00
0.98
F
F
F
O
CH3
1.00
1.00
1.00
1.13
1.00
0.99
2.00
2.00
2.21
3.02
f1 (ppm)

3f

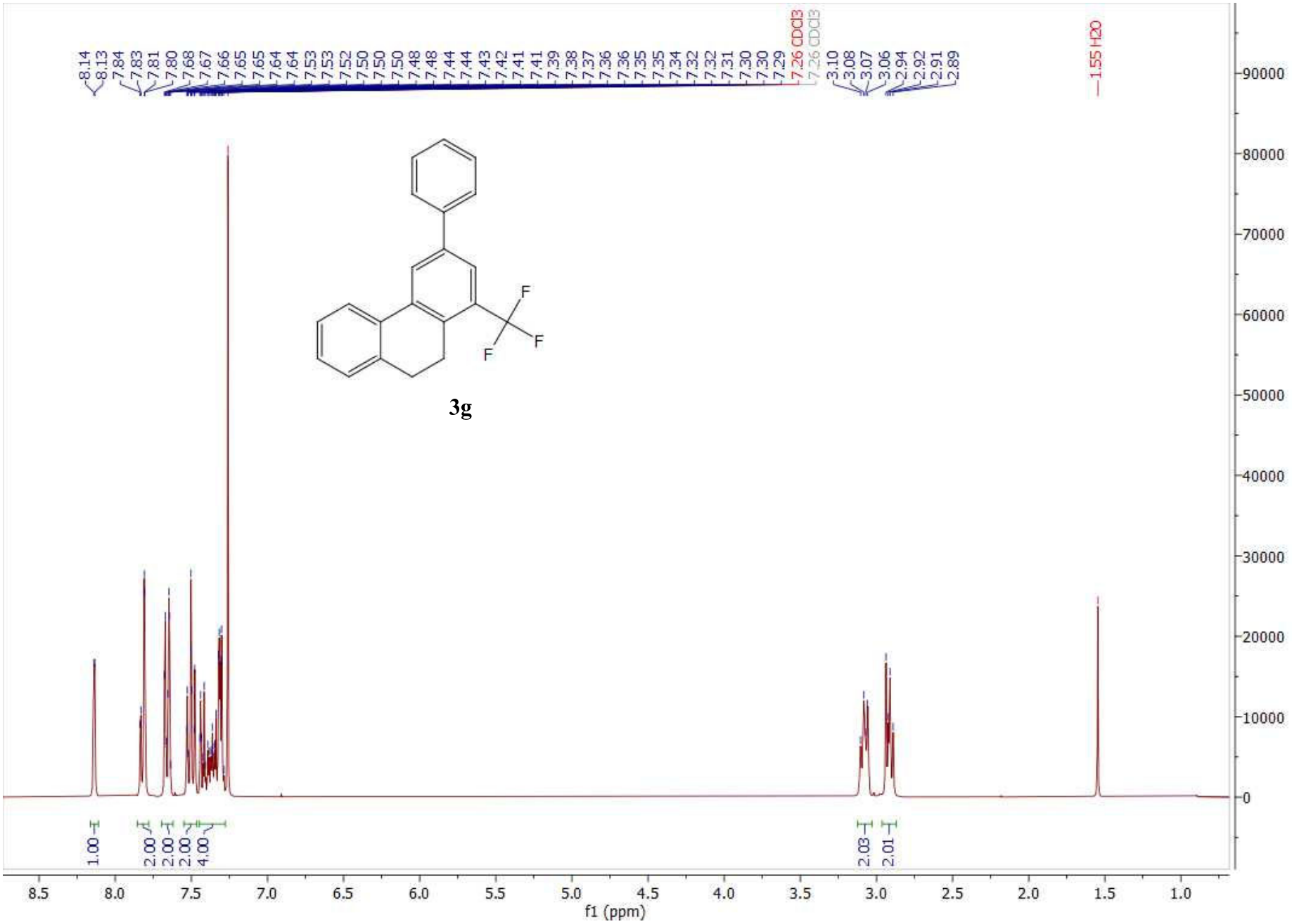

154.73
139.11
133.31
133.29
131.26
131.04
130.61
130.30
130.19
129.76
126.15
125.36
125.31
125.26
125.21
123.82
122.60
122.54
122.34
118.93
117.44
117.06
117.01
116.96
116.91
77.16 CDCl3
65.25
34.65
23.95
13.97
F
F
F
O
CH3
f1 (ppm)

3f


F
F
F
O
CH3

3f

-62.66
70000
65000
60000
55000
50000
45000
40000
35000
30000
25000
20000
15000
10000
5000
0
-5000
-20
-25
-30
-35
-40
-45
-50
-55
-60
-65
-70
-75
-80
-85
-90
-95
-100
-105
-110
f1 (ppm)


8.14
8.13
7.84
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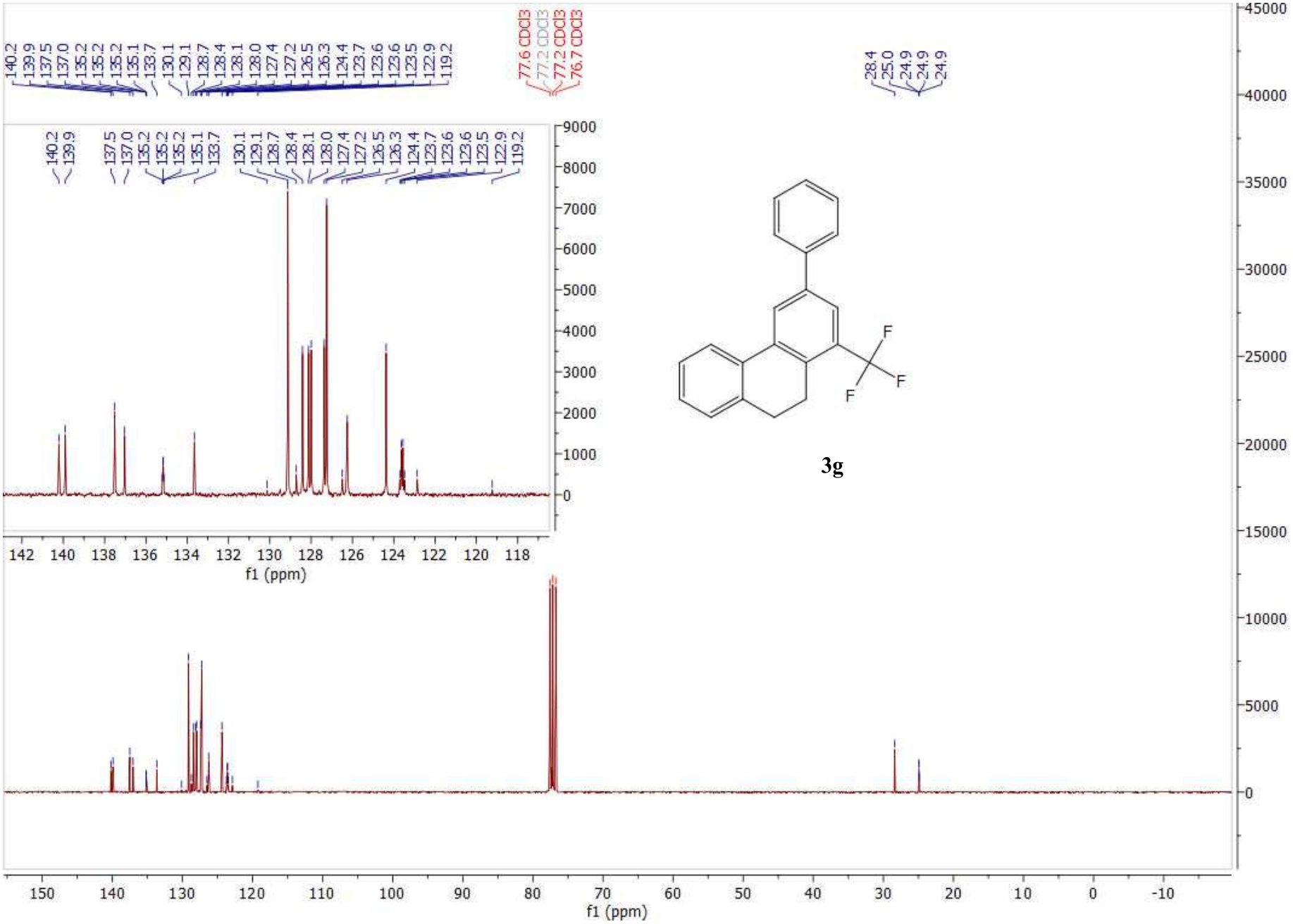
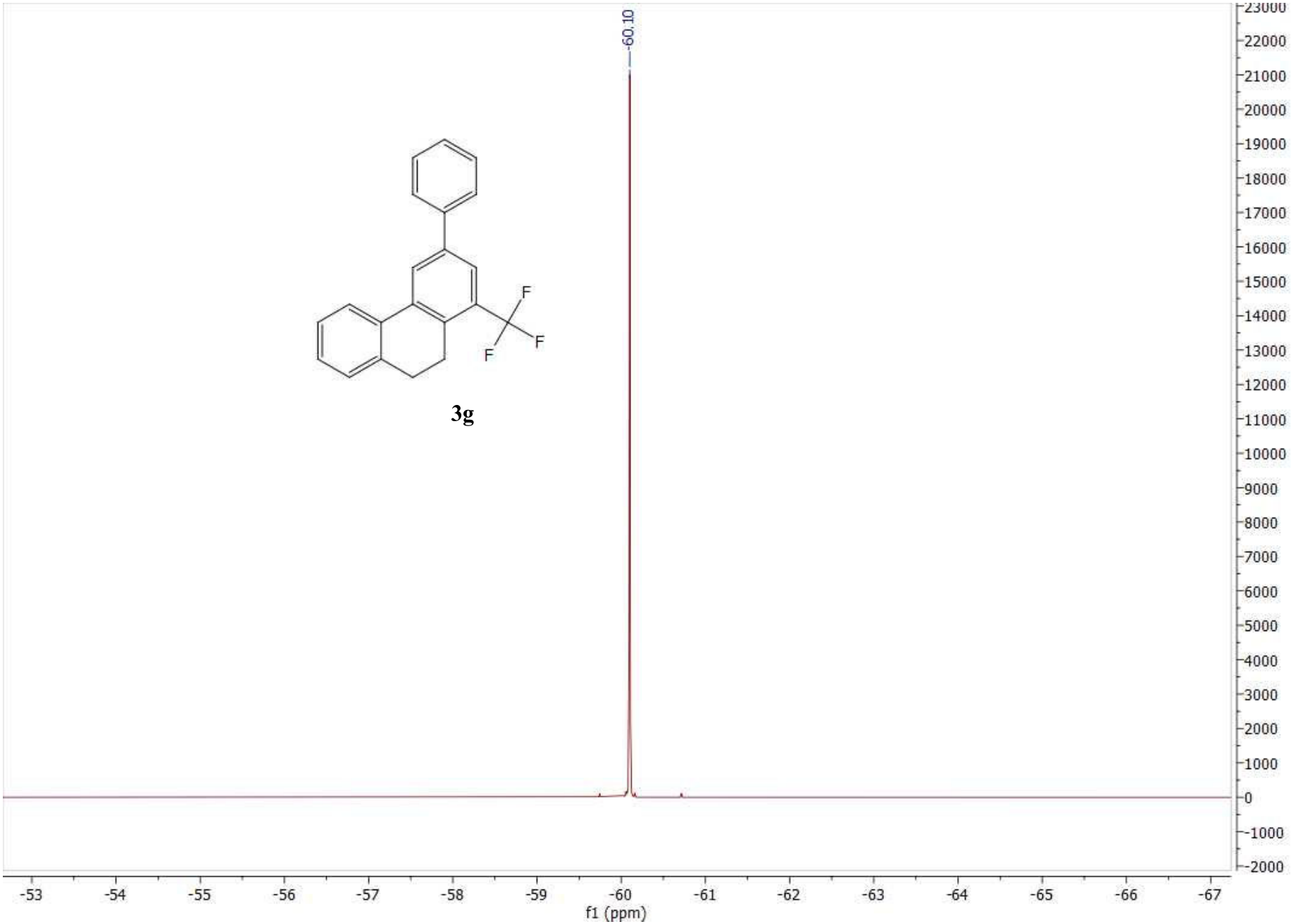
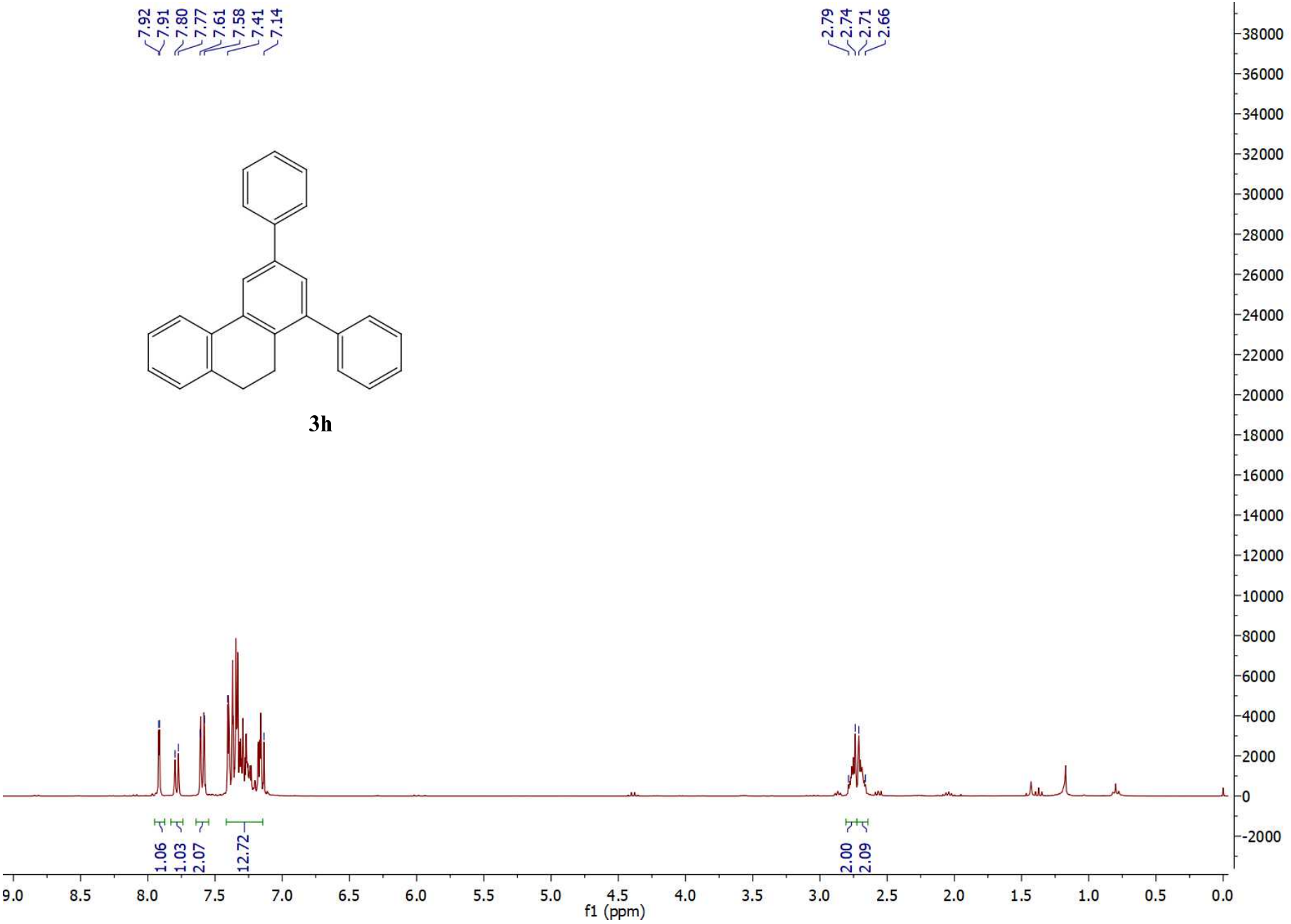
7.81
7.80
7.68
7.67
7.66
7.65
7.65
7.64
7.64
7.53
7.53
7.52
7.50
7.50
7.50
7.48
7.48
7.44
7.44
7.43
7.42
7.41
7.41
7.39
7.38
7.37
7.36
7.36
7.35
7.35
7.34
7.32
7.32
7.31
7.30
7.30
7.29
7.26 CDCl3
7.26 CDCl3
3.10
3.08
3.07
3.06
2.94
2.92
2.91
2.89
1.55 H2O
F
F
F
1.00
2.00
2.00
2.00
4.00
2.03
2.01
f1 (ppm)

3g

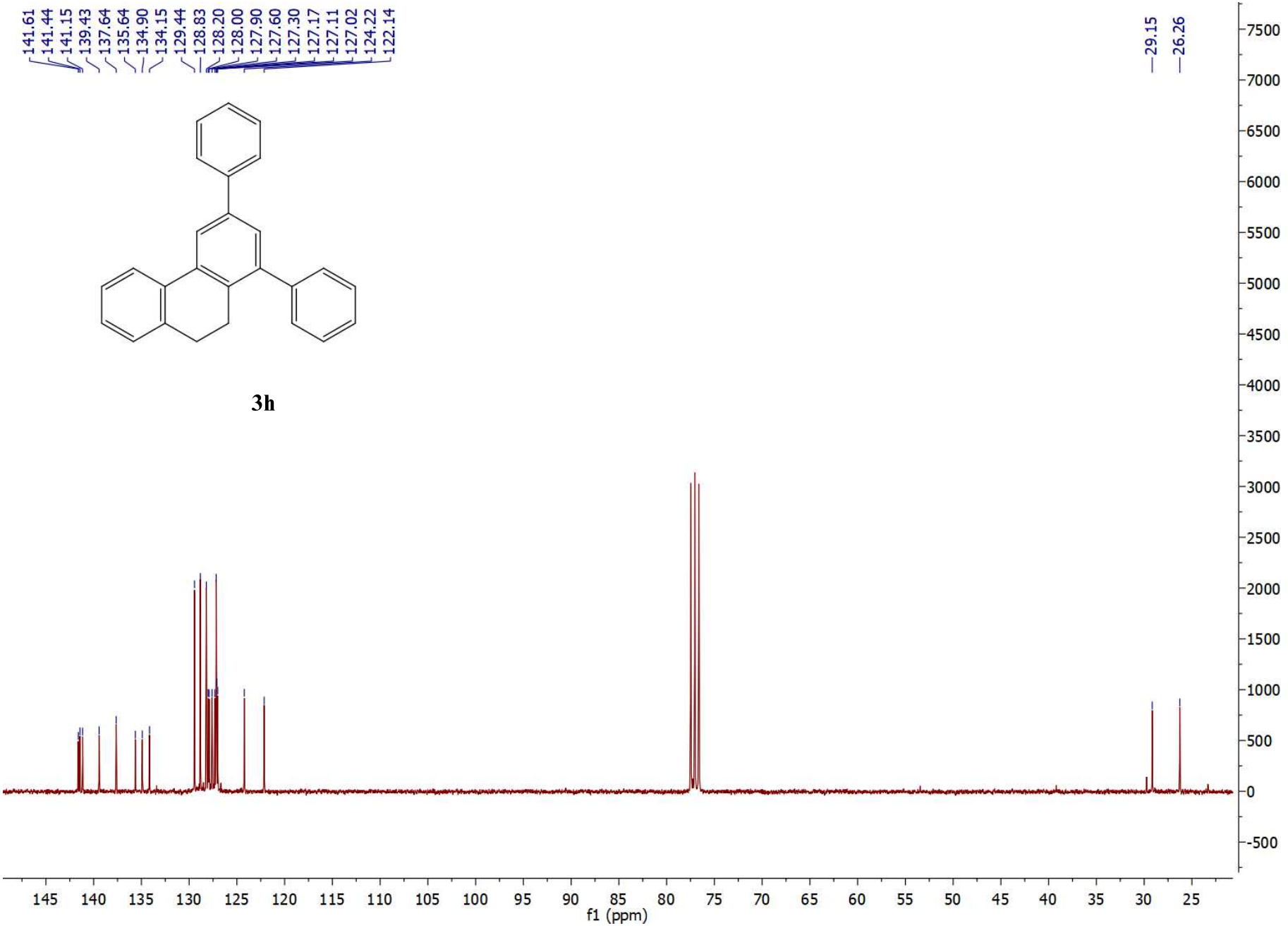

140.2
139.9
137.5
137.0
135.2
135.2
135.2
135.1
133.7
130.1
129.1
128.7
128.4
128.1
128.0
127.4
127.2
126.5
126.3
124.4
123.7
123.6
123.6
123.5
122.9
119.2
77.6 CDCl3
77.2 CDCl3
77.2 CDCl3
76.7 CDCl3
28.4
25.0
24.9
24.9
24.9
F
F
F
3g
f1 (ppm)
f1 (ppm)


-60.10
F
F
F
23000
22000
21000
20000
19000
18000
17000
16000
15000
14000
13000
12000
11000
10000
9000
8000
7000
6000
5000
4000
3000
2000
1000
0
-1000
-2000
-53
-54
-55
-56
-57
-58
-59
-60
-61
-62
-63
-64
-65
-66
-67
f1 (ppm)

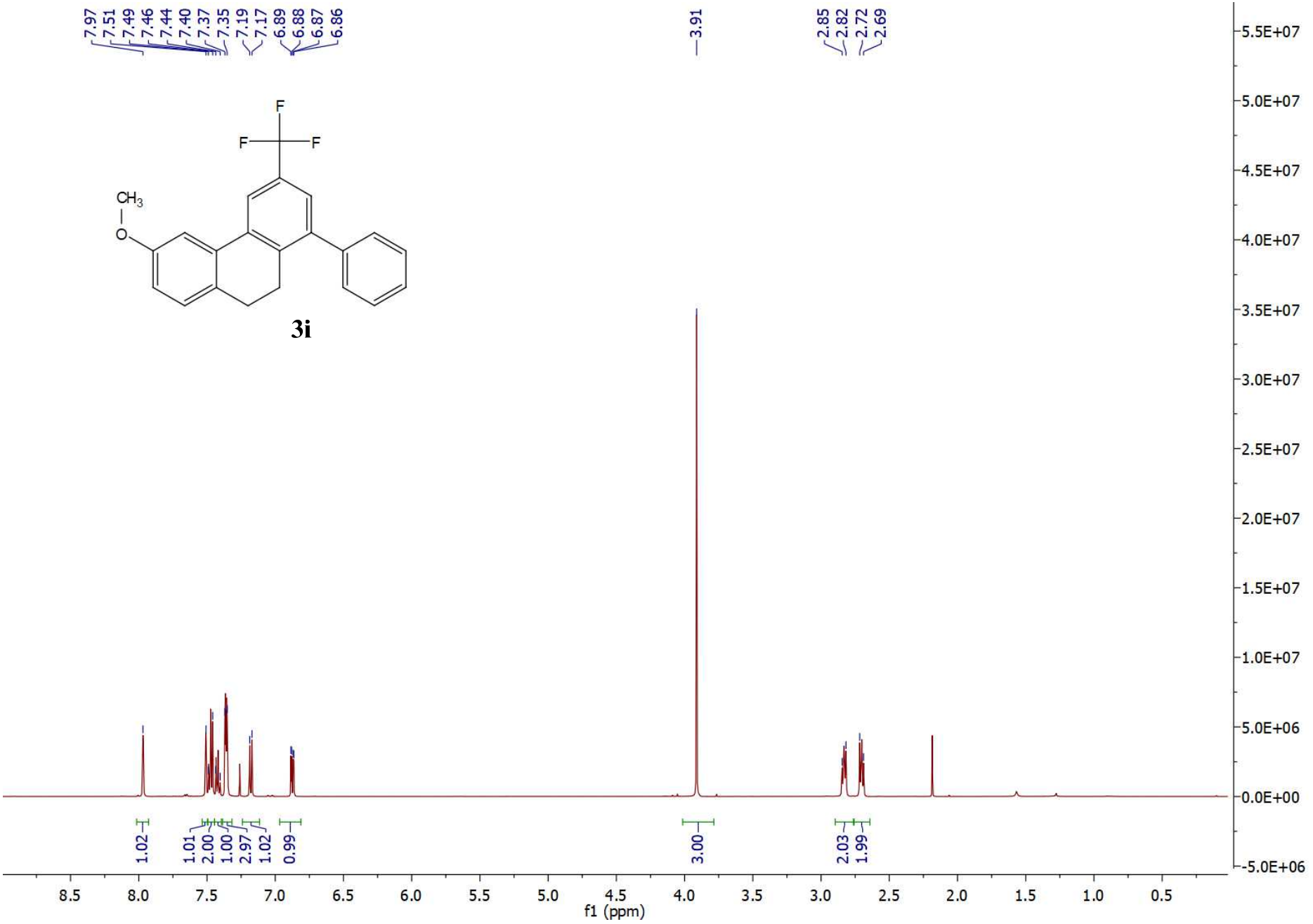
3g


7.92
7.91
7.80
7.77
7.61
7.58
7.41
7.14
2.79
2.74
2.71
2.66
38000
36000
34000
32000
30000
28000
26000
24000
22000
20000
18000
16000
14000
12000
10000
8000
6000
4000
2000
0
-2000
1.06
1.03
2.07
12.72
2.00
2.09
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

3h


141.61
141.44
141.15
139.43
137.64
135.64
134.90
134.15
129.44
128.83
128.20
128.00
127.90
127.60
127.30
127.17
127.11
127.02
124.22
122.14
29.15
26.26
7500
7000
6500
6000
5500
5000
4500
4000
3500
3000
2500
2000
1500
1000
500
0
-500
145
140
135
130
125
120
115
110
105
100
95
90
85
80
75
70
65
60
55
50
45
40
35
30
25
f1 (ppm)

3h


7.97
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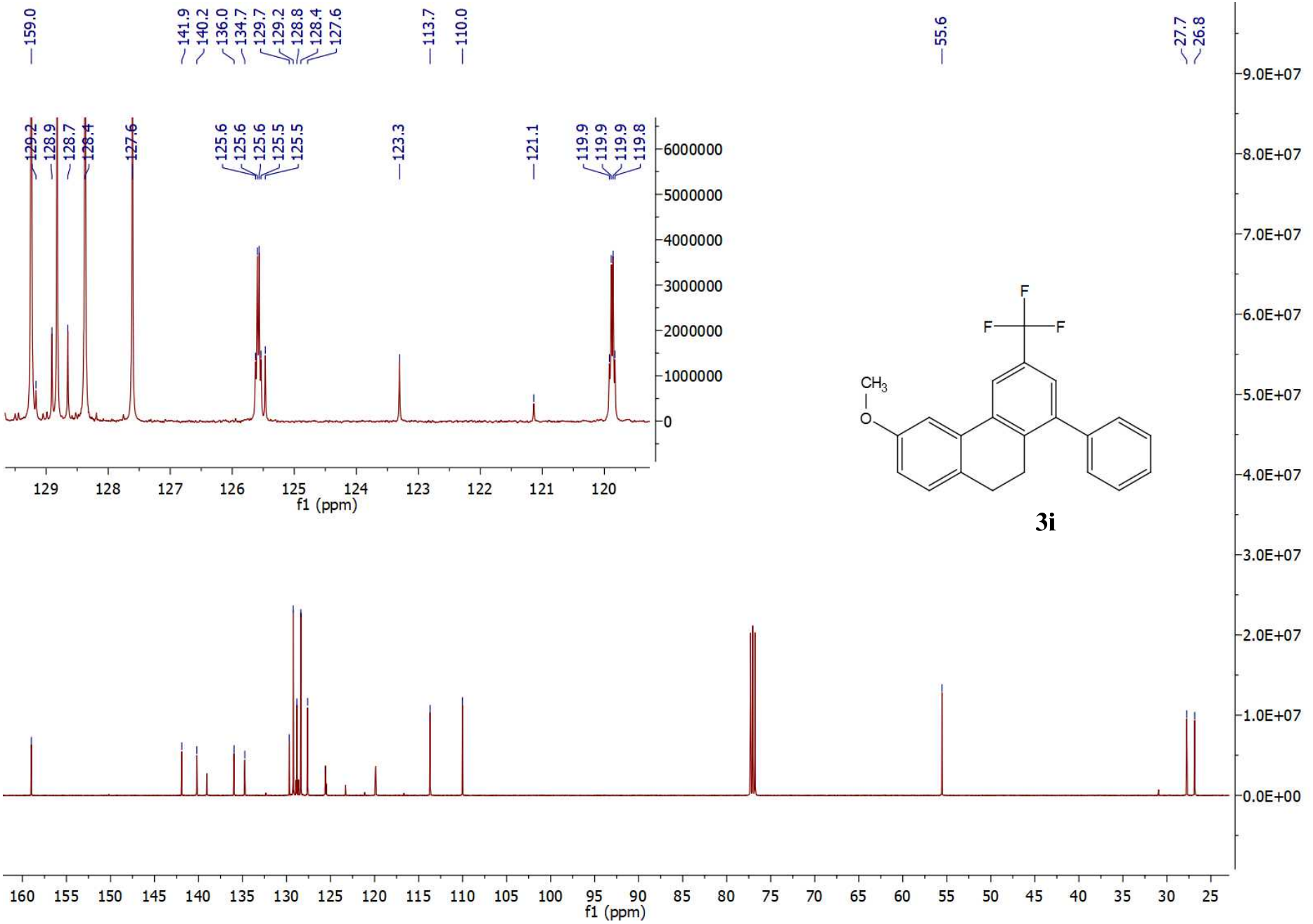
7.44
7.40
7.37
7.35
7.19
7.17
6.89
6.88
6.87
6.86
3.91
2.85
2.82
2.72
2.69
F
F
F
CH3
O
3i
1.02
1.01
2.00
1.00
2.97
1.02
0.99
3.00
2.03
1.99
f1 (ppm)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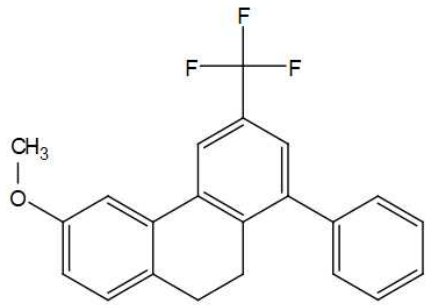
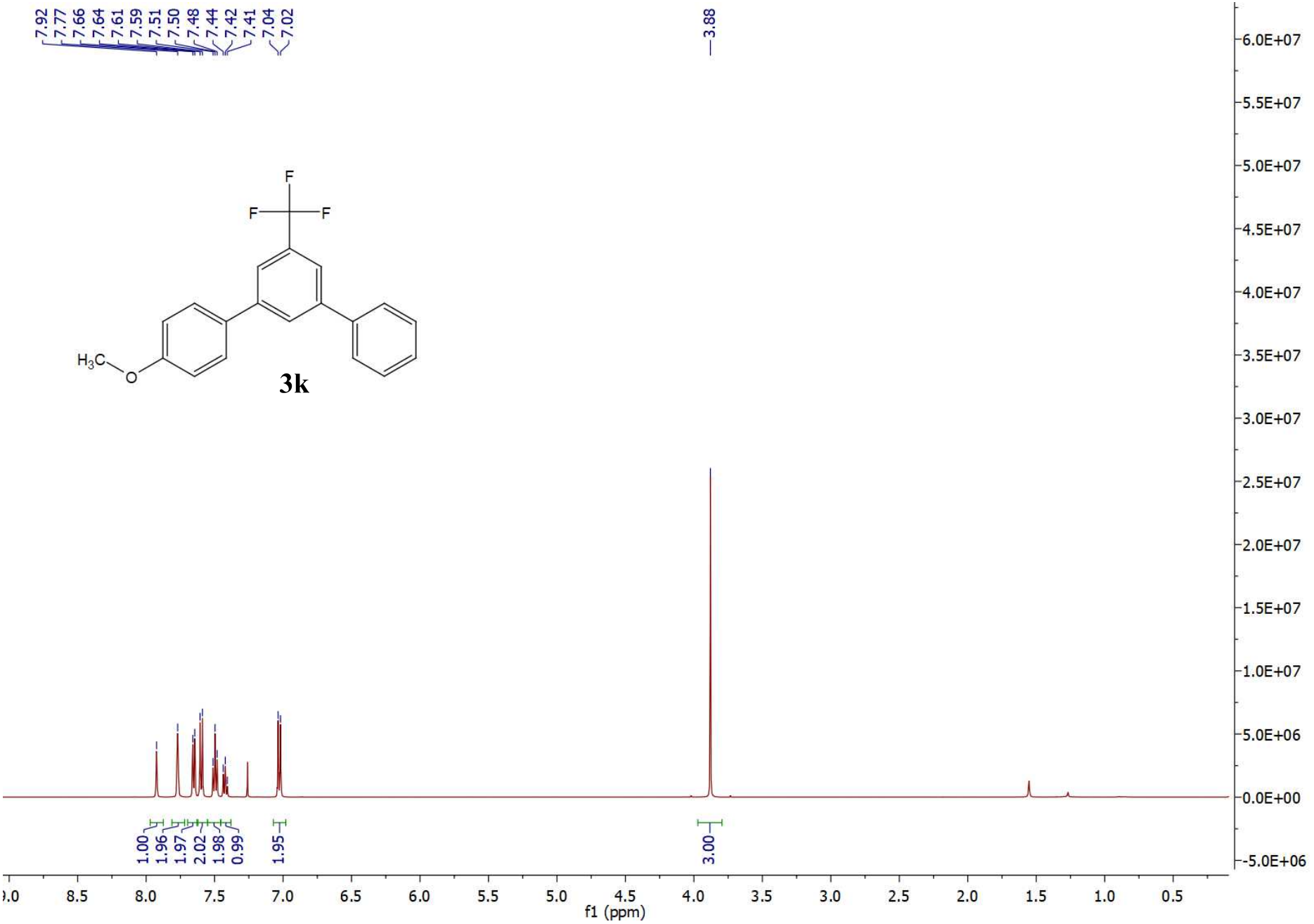
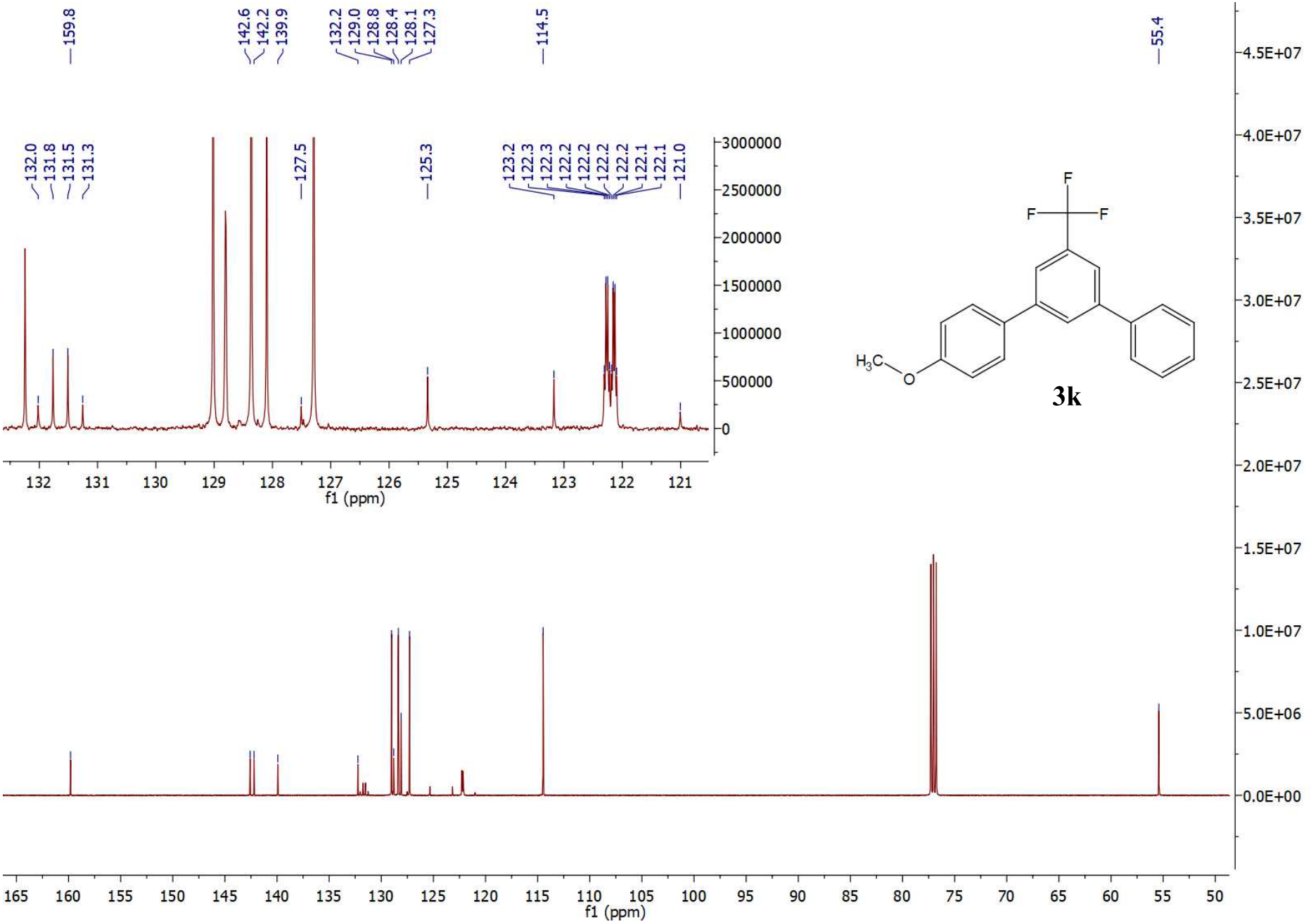
140.2
136.0
134.7
129.7
129.2
128.8
128.4
127.6
113.7
110.0
55.6
27.7
26.8
129.2
128.9
128.7
128.4
127.6
125.6
125.6
125.6
125.5
125.5
123.3
121.1
119.9
119.9
119.9
119.8
f1 (ppm)
F
F
F
CH3
O
3i
f1 (ppm)

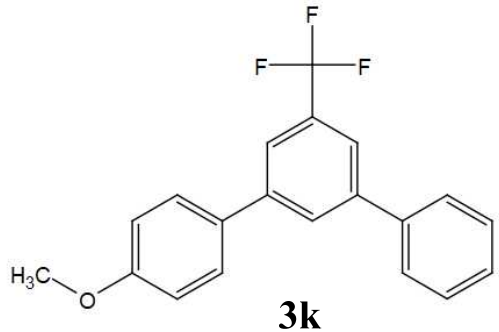

F
F
F
CH3
O

3i

-62.36
25000
20000
15000
10000
5000
0
-53
-54
-55
-56
-57
-58
-59
-60
-61
-62
-63
-64
-65
-66
-67
-68
-69
-70
-71
-72
f1 (ppm)

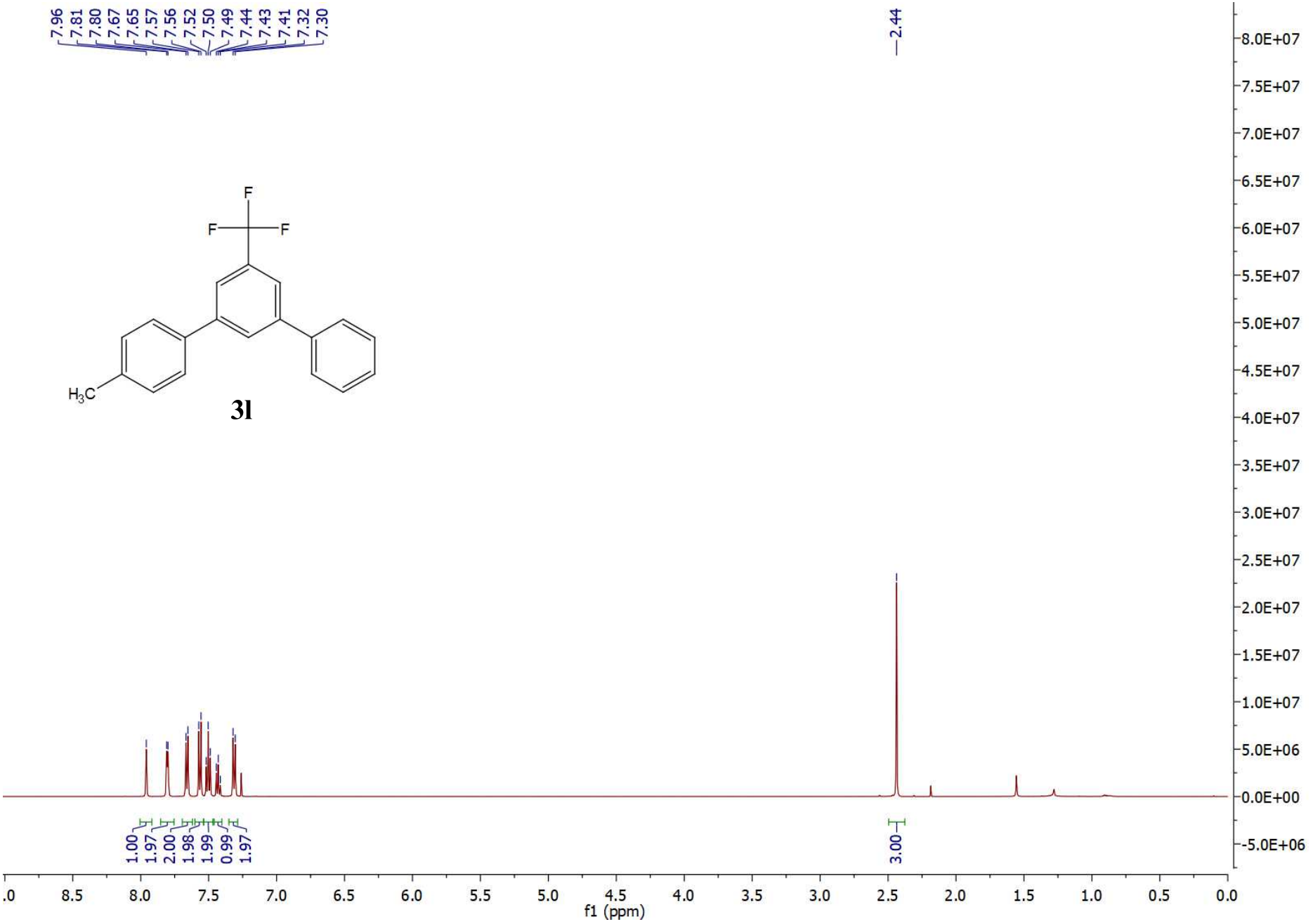

7.92
7.77
7.66
7.64
7.61
7.59
7.51
7.50
7.48
7.44
7.42
7.41
7.04
7.02
3.88
F
F
F
H3C
O
3k
6.0E+07
5.5E+07
5.0E+07
4.5E+07
4.0E+07
3.5E+07
3.0E+07
2.5E+07
2.0E+07
1.5E+07
1.0E+07
5.0E+06
0.0E+00
-5.0E+06
1.00
1.96
1.97
2.02
1.98
0.99
1.95
3.00
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
f1 (ppm)

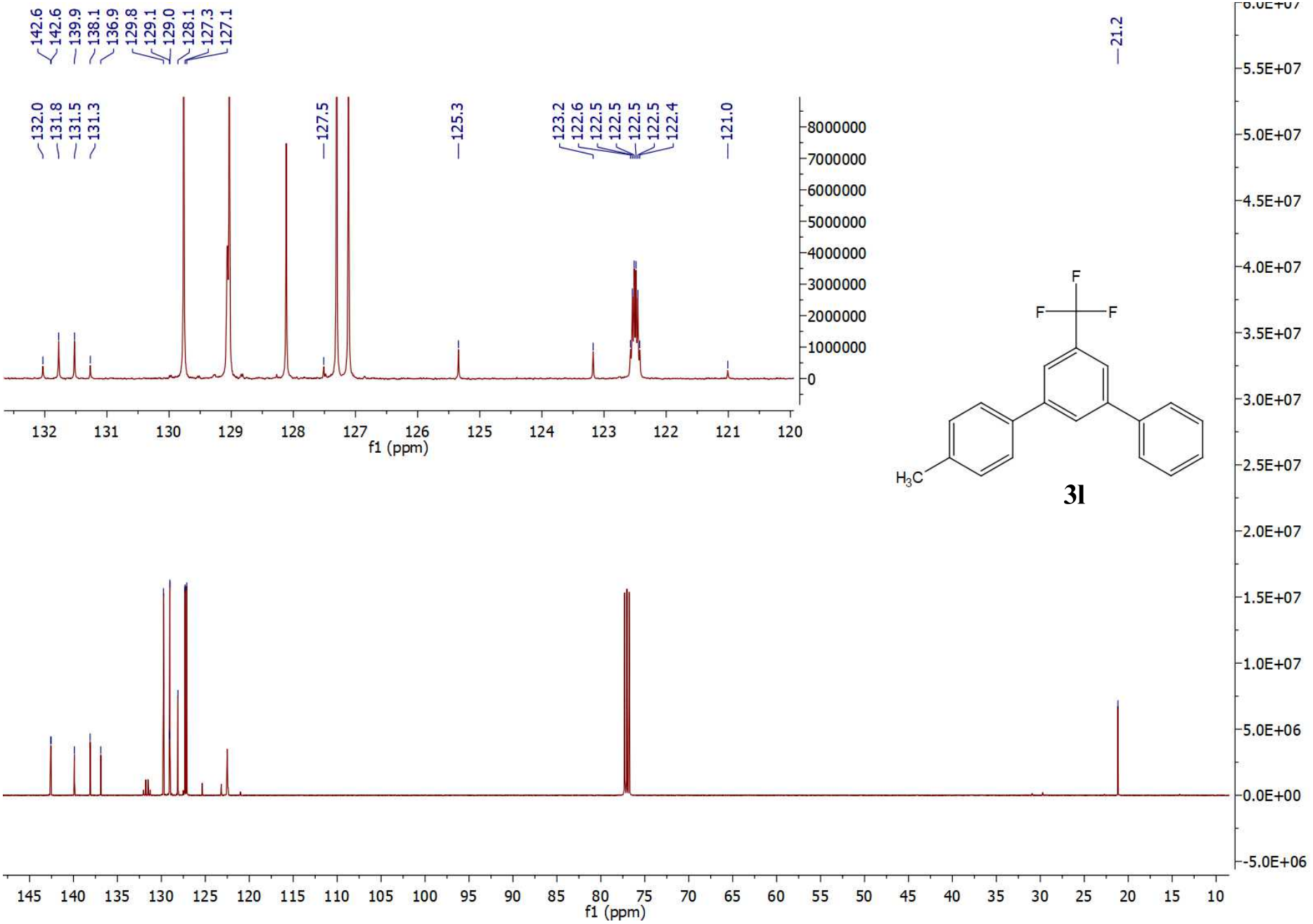

159.8
142.6
142.2
139.9
132.2
129.0
128.8
128.4
128.1
127.3
114.5
55.4
132.0
131.8
131.5
131.3
127.5
125.3
123.2
122.3
122.3
122.2
122.2
122.2
122.2
122.1
122.1
121.0
f1 (ppm)
F
F
F
H3C
O
3k

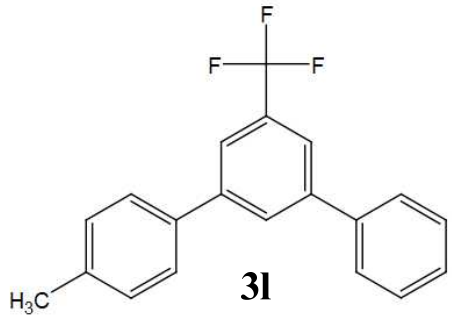

F
F
F
H3C
O

3k

-62.48
1.60E+08
1.50E+08
1.40E+08
1.30E+08
1.20E+08
1.10E+08
1.00E+08
9.00E+07
8.00E+07
7.00E+07
6.00E+07
5.00E+07
4.00E+07
3.00E+07
2.00E+07
1.00E+07
0.00E+00
-1.00E+07
-52 -53 -54 -55 -56 -57 -58 -59 -60 -61 -62 -63 -64 -65 -66 -67 -68 -69 -70 -71 -72 -73
f1 (ppm)

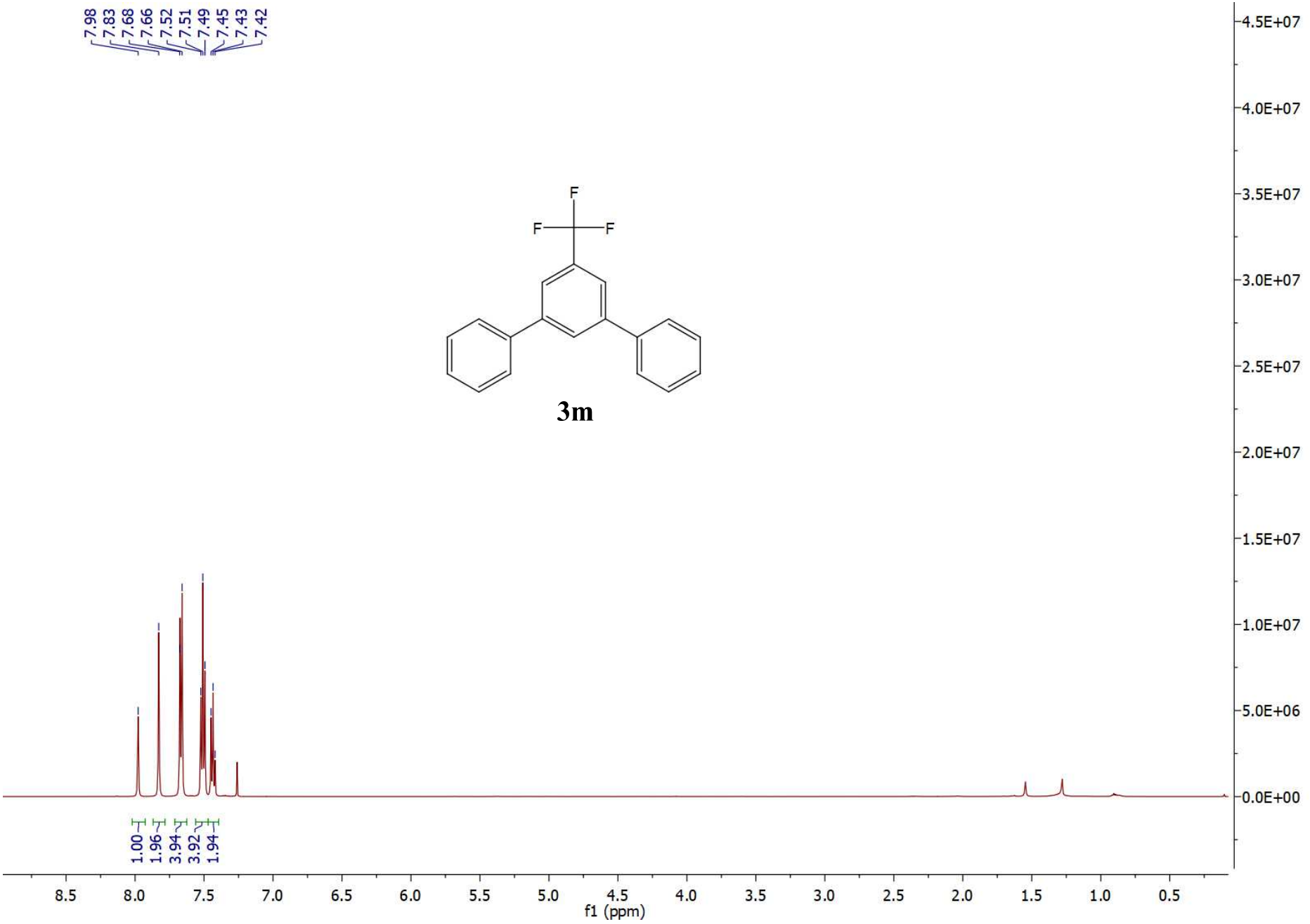

7.96
7.81
7.80
7.67
7.65
7.57
7.56
7.52
7.50
7.49
7.44
7.43
7.41
7.32
7.30
2.44
F
F
F
H3C
3l
8.0E+07
7.5E+07
7.0E+07
6.5E+07
6.0E+07
5.5E+07
5.0E+07
4.5E+07
4.0E+07
3.5E+07
3.0E+07
2.5E+07
2.0E+07
1.5E+07
1.0E+07
5.0E+06
0.0E+00
-5.0E+06
1.00
1.97
2.00
1.98
1.99
0.99
1.97
3.00
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

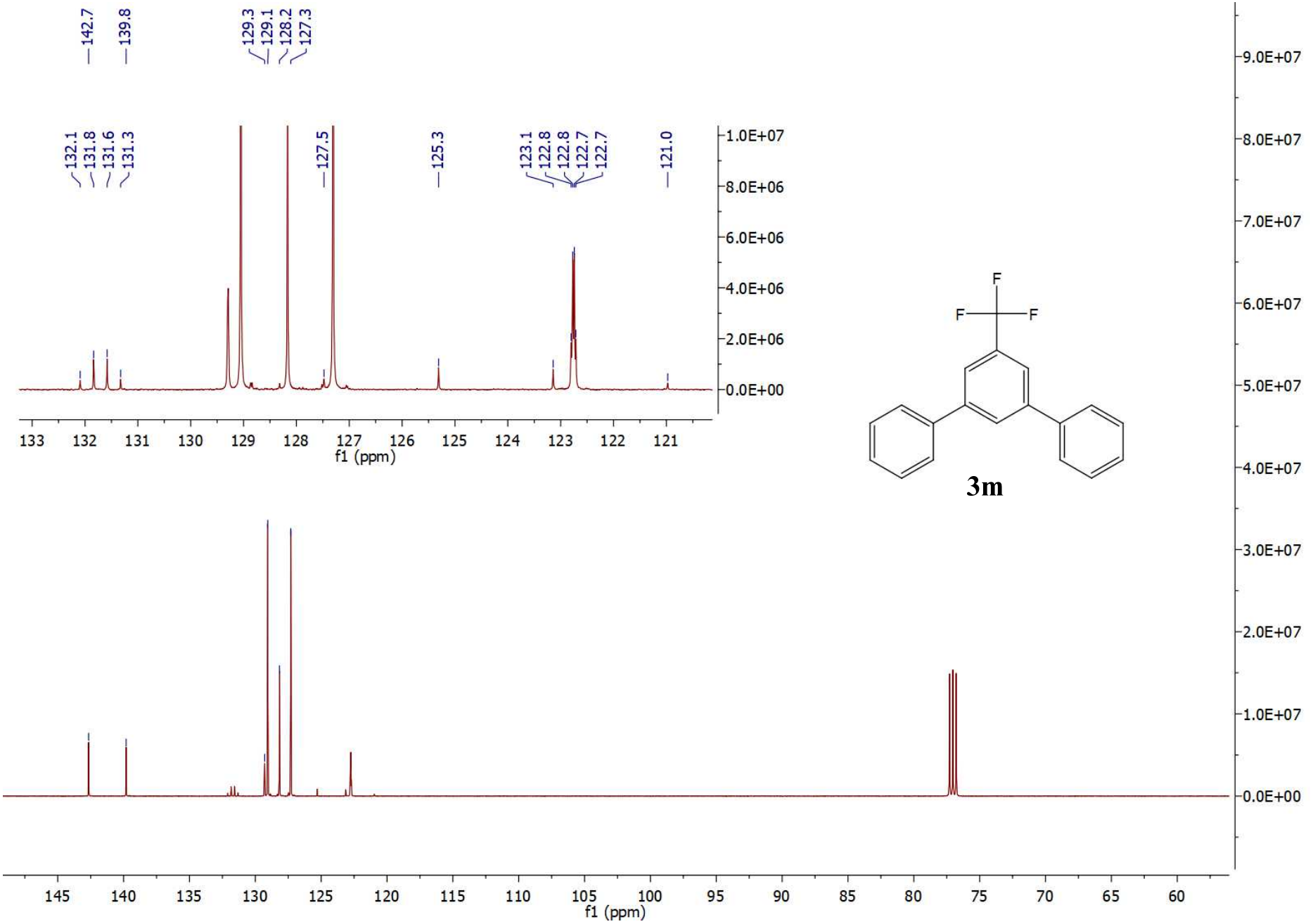

142.6
142.6
139.9
138.1
136.9
129.8
129.1
129.0
128.1
127.3
127.1
132.0
131.8
131.5
131.3
127.5
125.3
123.2
122.6
122.5
122.5
122.5
122.5
122.4
121.0
21.2
f1 (ppm)
F
F
F
H3C
3l

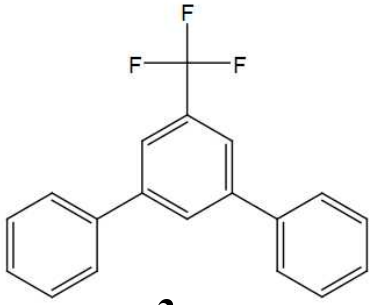

F
F
F
H3C

3l

-62.46
2.8E+08
2.6E+08
2.4E+08
2.2E+08
2.0E+08
1.8E+08
1.6E+08
1.4E+08
1.2E+08
1.0E+08
8.0E+07
6.0E+07
4.0E+07
2.0E+07
0.0E+00
-2.0E+07
-59.8
-60.2
-60.6
-61.0
-61.4
-61.8
-62.2
-62.6
-63.0
-63.4
-63.8
-64.2
-64.6
-65.0
-65.4
f1 (ppm)

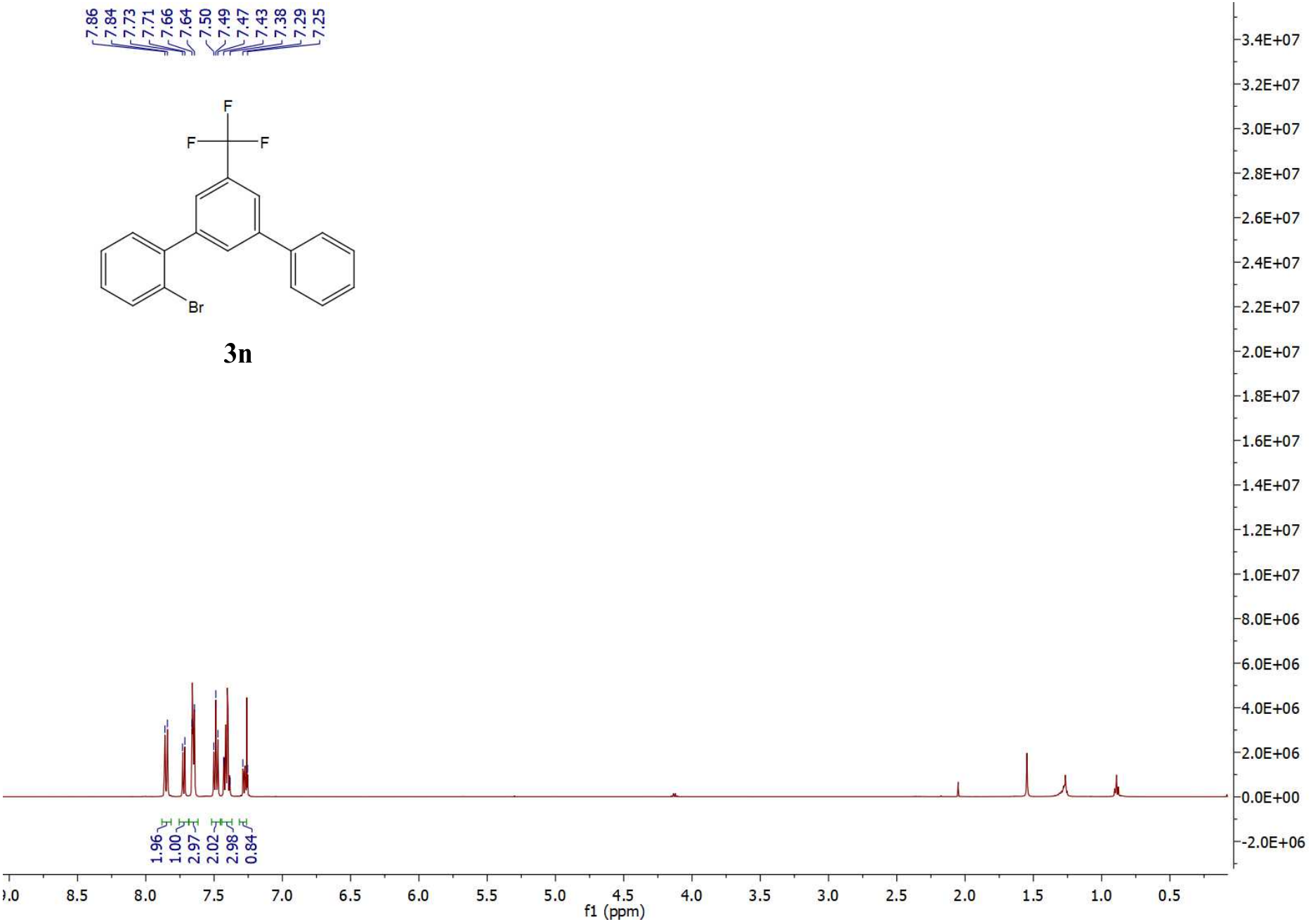

7.98
7.83
7.68
7.66
7.52
7.51
7.49
7.45
7.43
7.42
F
F
F
3m
4.5E+07
4.0E+07
3.5E+07
3.0E+07
2.5E+07
2.0E+07
1.5E+07
1.0E+07
5.0E+06
0.0E+00
1.00
1.96
3.94
3.92
1.94
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
f1 (ppm)


142.7
139.8
129.3
129.1
128.2
127.3
132.1
131.8
131.6
131.3
127.5
125.3
123.1
122.8
122.8
122.7
122.7
121.0
f1 (ppm)
F
F
F
3m
f1 (ppm)

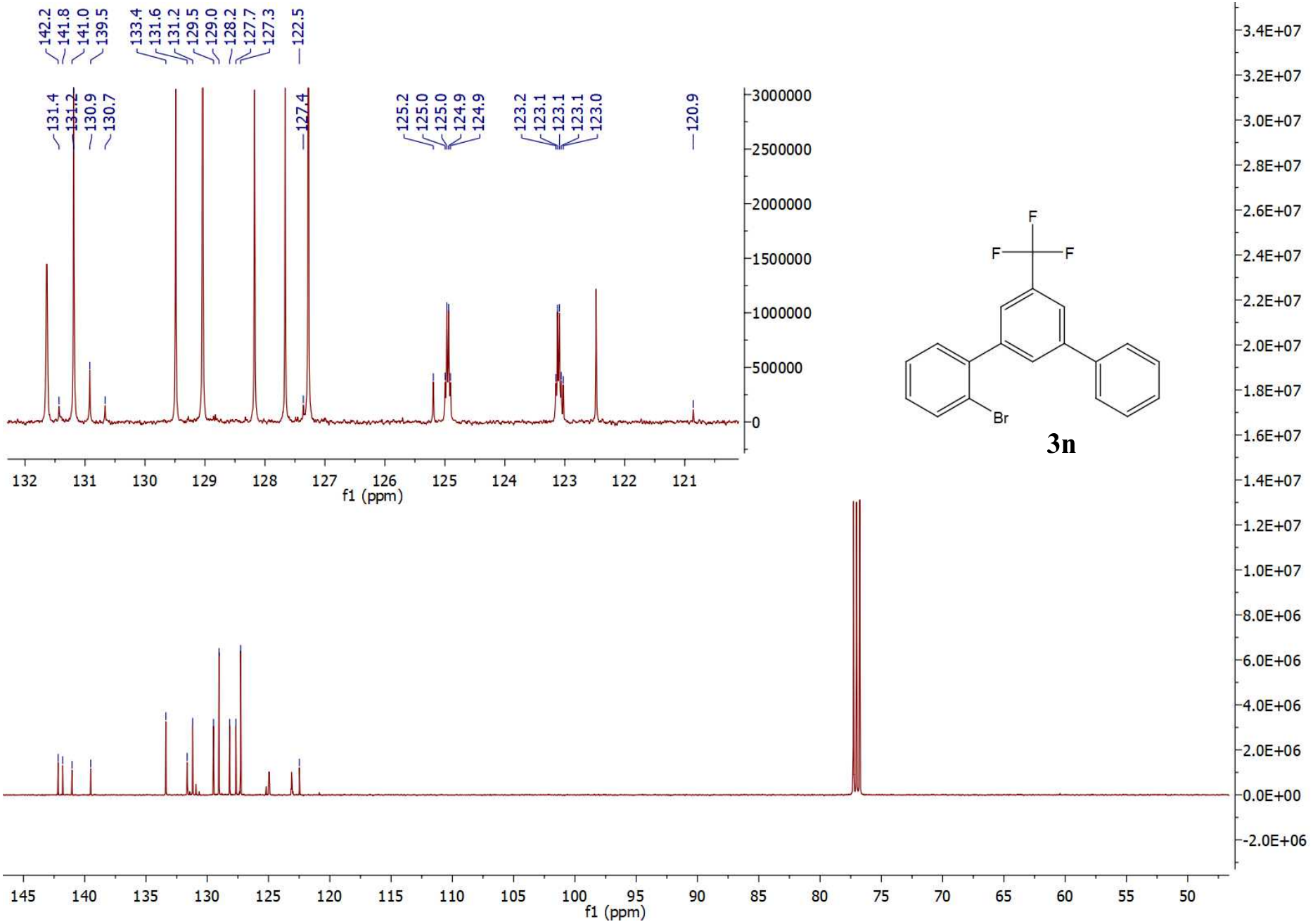

F
F
F

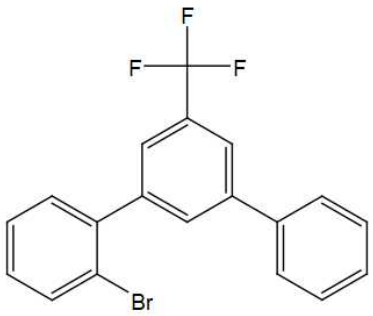
3m

-62.46
2.30E+08
2.20E+08
2.10E+08
2.00E+08
1.90E+08
1.80E+08
1.70E+08
1.60E+08
1.50E+08
1.40E+08
1.30E+08
1.20E+08
1.10E+08
1.00E+08
9.00E+07
8.00E+07
7.00E+07
6.00E+07
5.00E+07
4.00E+07
3.00E+07
2.00E+07
1.00E+07
0.00E+00
-1.00E+07
-2.00E+07
-53
-54
-55
-56
-57
-58
-59
-60
-61
-62
-63
-64
-65
-66
-67
-68
-69
-70
-71
f1 (ppm)


7.86
7.84
7.73
7.71
7.66
7.64
7.50
7.49
7.47
7.43
7.38
7.29
7.25
F
F
F
Br
1.96
1.00
2.97
2.02
2.98
0.84
f1 (ppm)

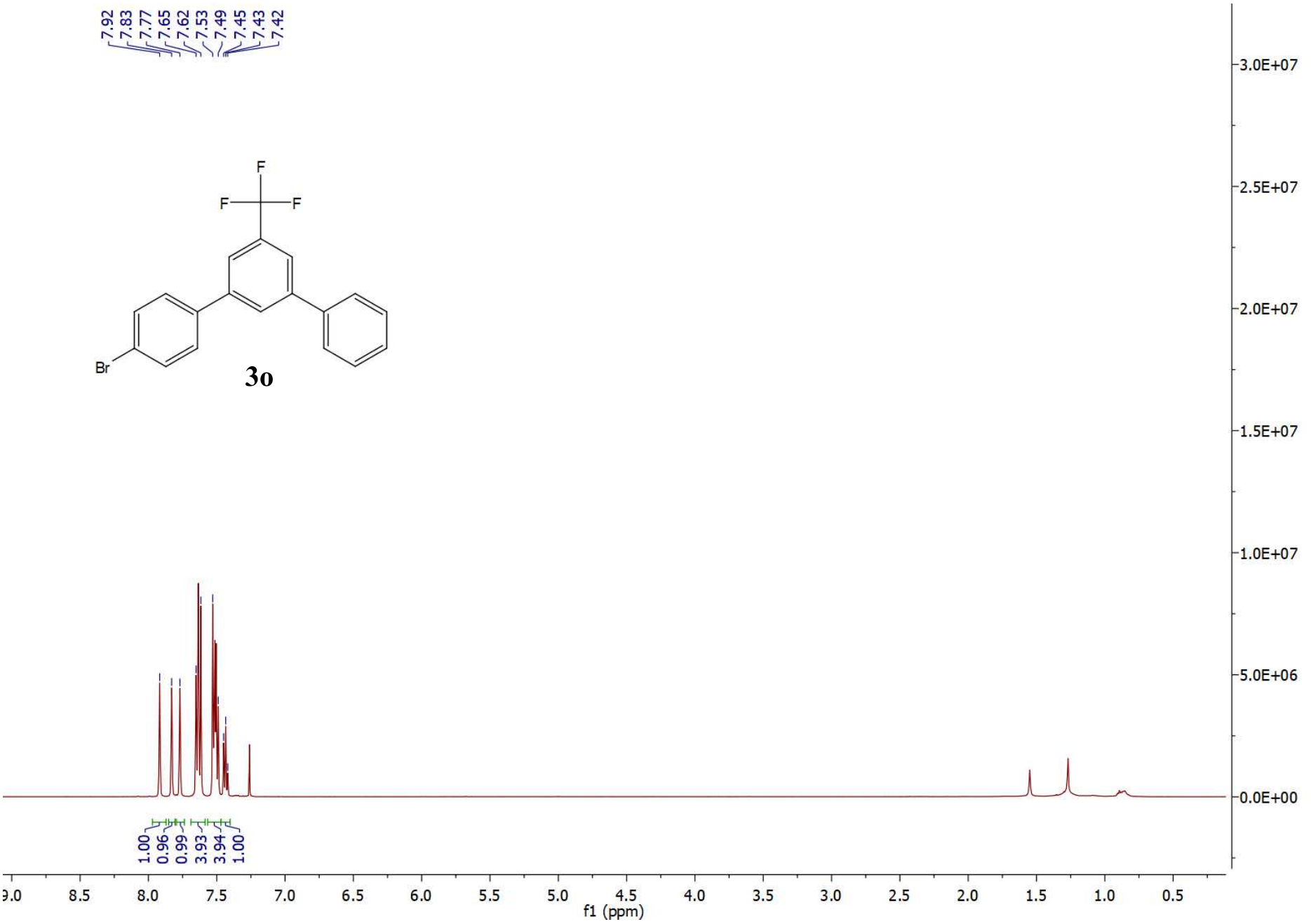
3n

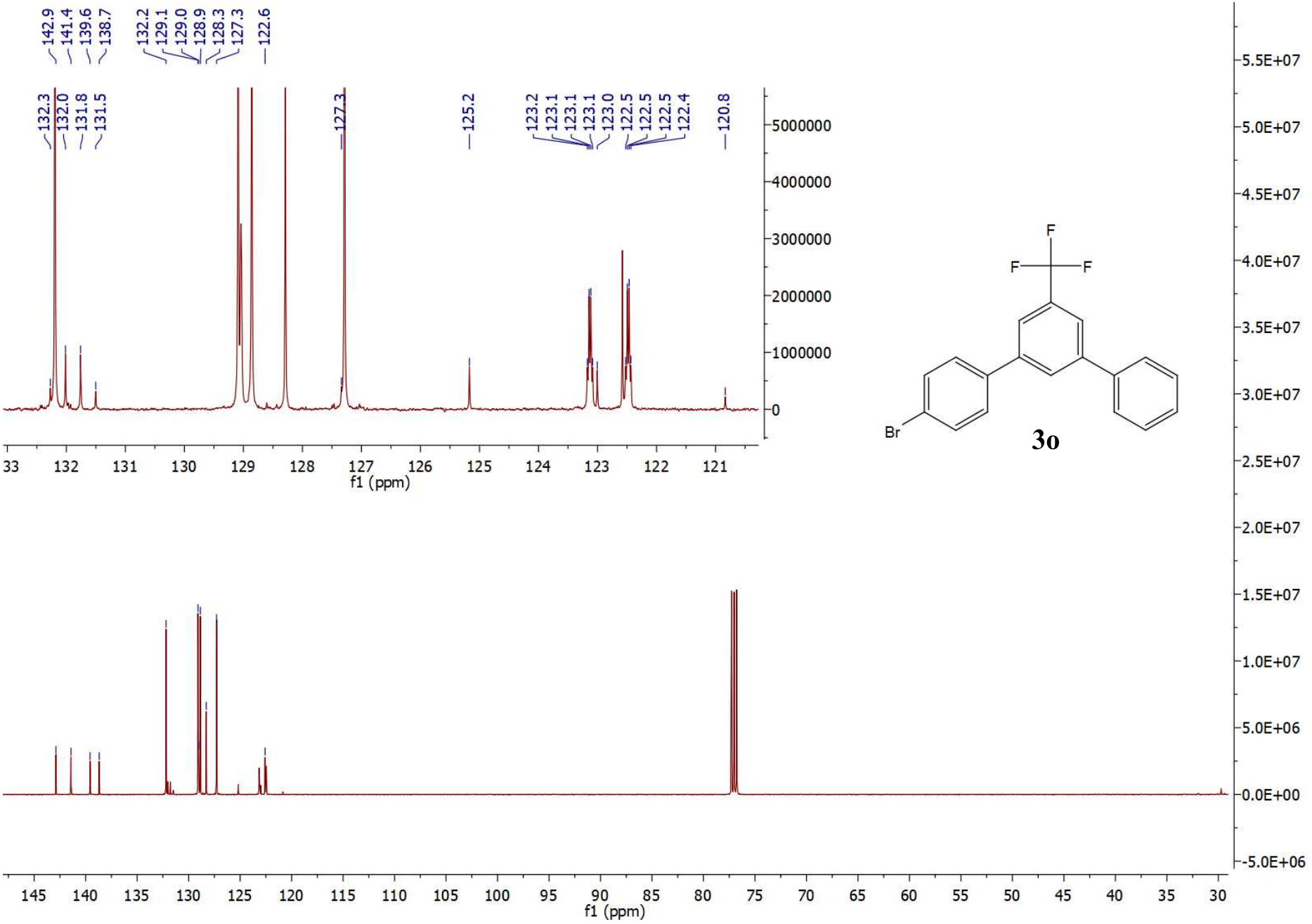

142.2
141.8
141.0
139.5
133.4
131.6
131.2
129.5
129.0
128.2
127.7
127.3
122.5
131.4
131.2
130.9
130.7
127.4
125.2
125.0
125.0
124.9
124.9
123.2
123.1
123.1
123.1
123.0
120.9
f1 (ppm)
F
F
F
Br
3n
f1 (ppm)

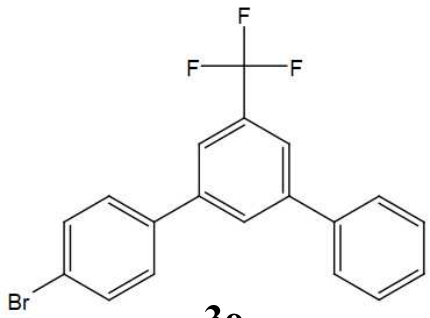

F
F
F
Br

3n

-62.44
1.00E+08
9.00E+07
8.00E+07
7.00E+07
6.00E+07
5.00E+07
4.00E+07
3.00E+07
2.00E+07
1.00E+07
0.00E+00
-53
-54
-55
-56
-57
-58
-59
-60
-61
-62
-63
-64
-65
-66
-67
-68
-69
-70
-71
-72
f1 (ppm)

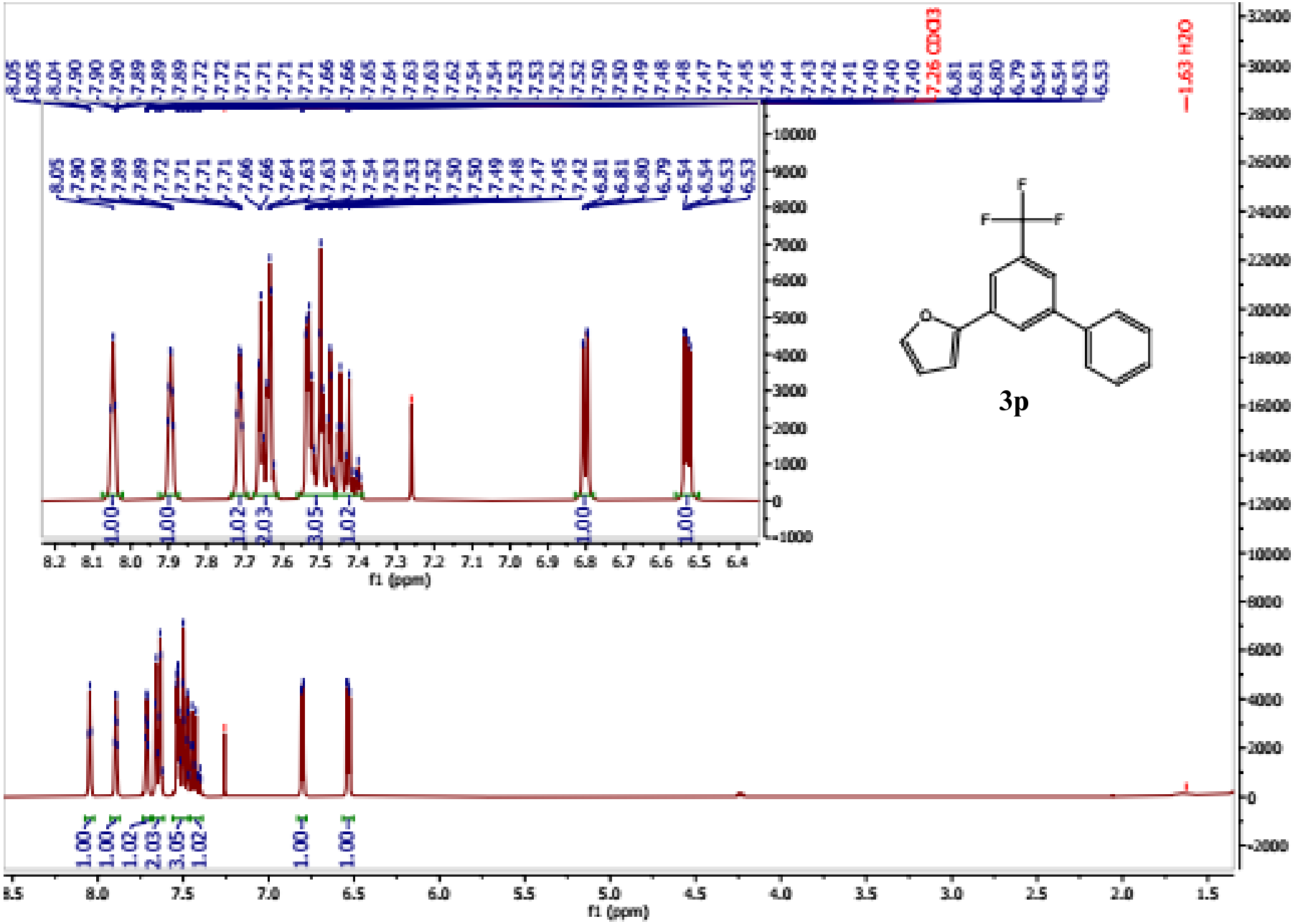

7.92
7.83
7.77
7.65
7.62
7.53
7.49
7.45
7.43
7.42
F
F
F
Br
3o
3.0E+07
2.5E+07
2.0E+07
1.5E+07
1.0E+07
5.0E+06
0.0E+00
1.00
0.96
0.99
3.93
3.94
1.00
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
f1 (ppm)

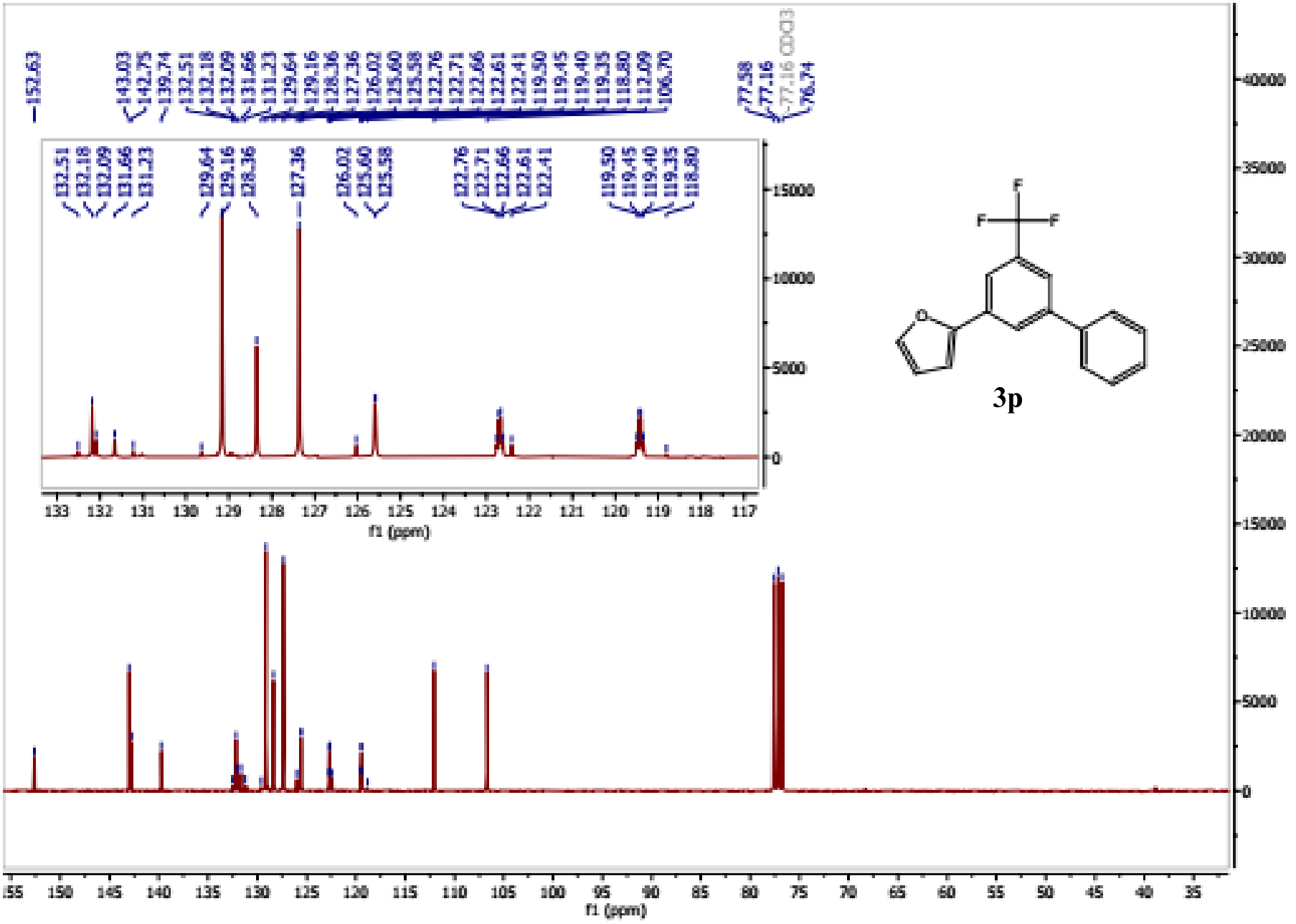

142.9
141.4
139.6
138.7
132.2
129.1
129.0
128.9
128.3
127.3
122.6
132.3
132.0
131.8
131.5
127.3
125.2
123.2
123.1
123.1
123.1
123.0
122.5
122.5
122.5
122.4
120.8
f1 (ppm)
F
F
F
Br
3o

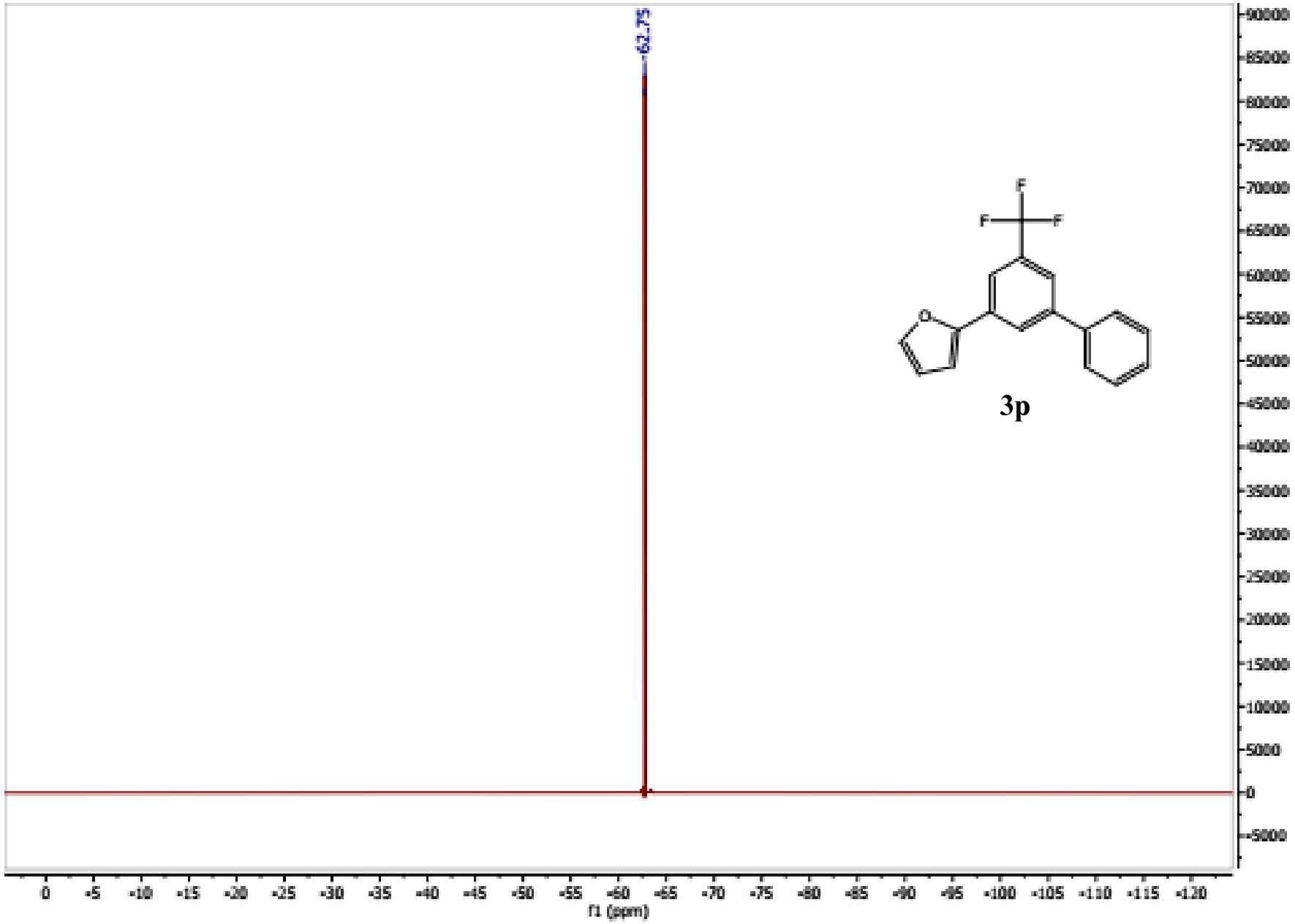

F
F
F
Br

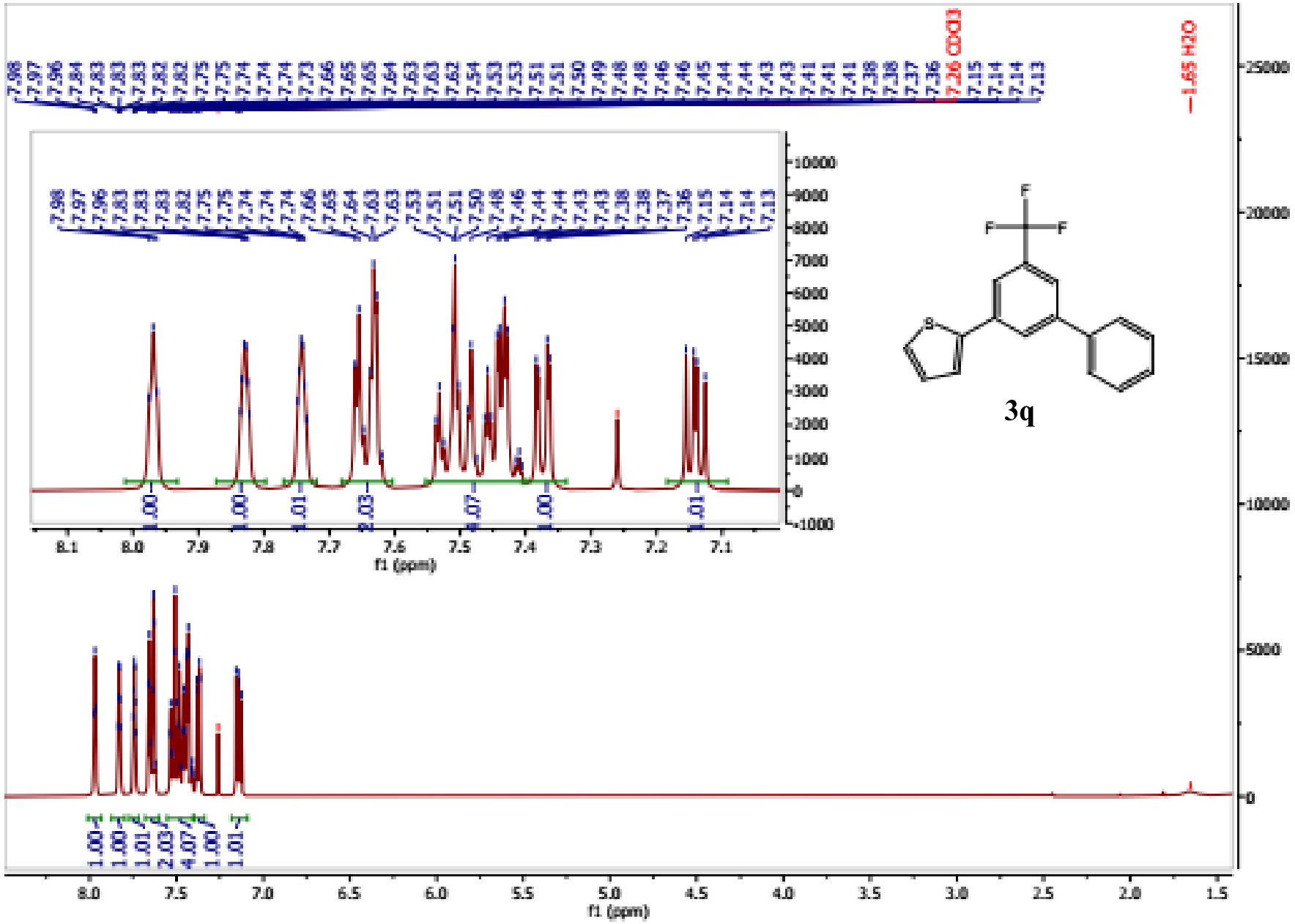
3o

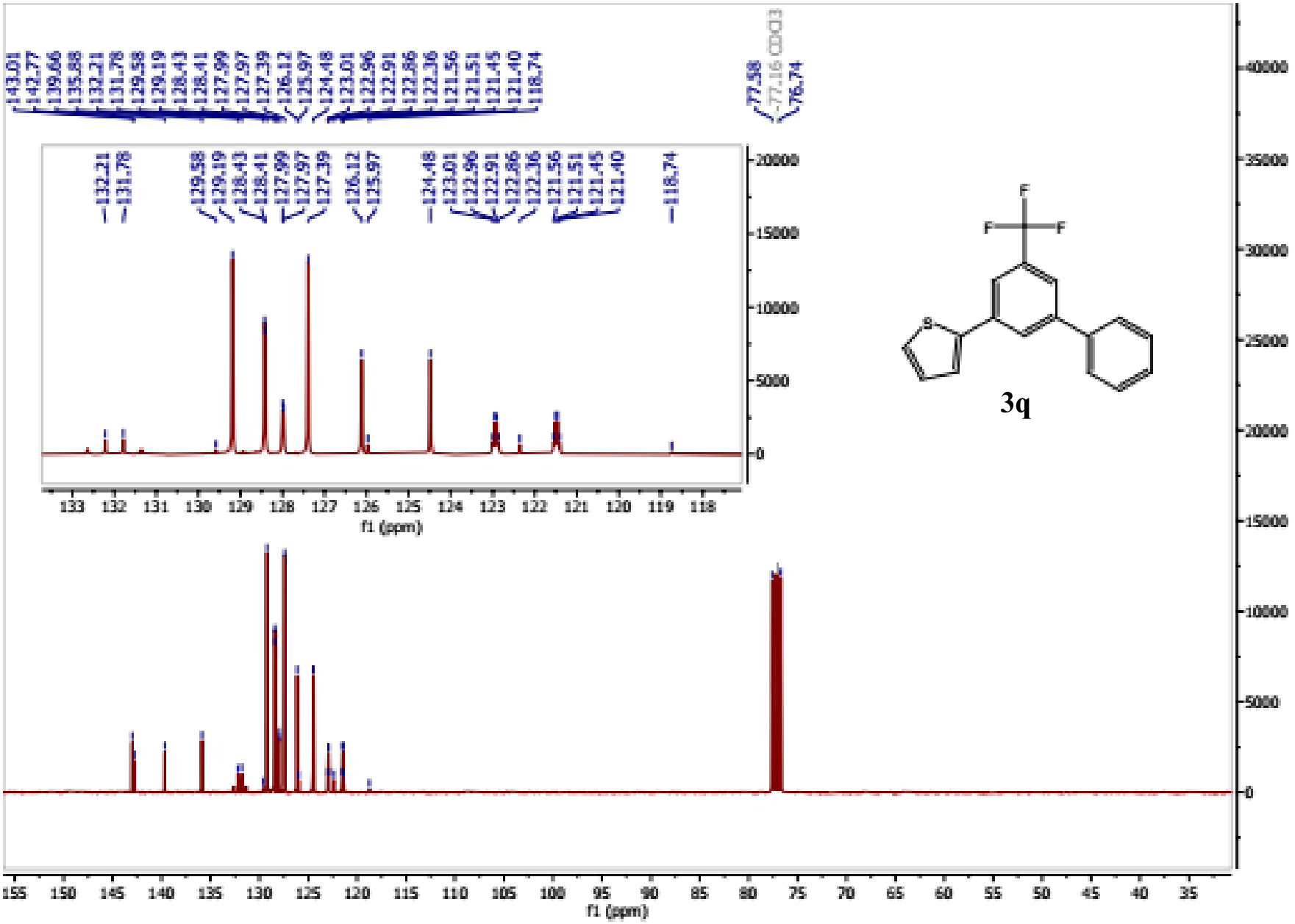
-62.51
2.4E+08
2.2E+08
2.0E+08
1.8E+08
1.6E+08
1.4E+08
1.2E+08
1.0E+08
8.0E+07
6.0E+07
4.0E+07
2.0E+07
0.0E+00
-2.0E+07
-52
-53
-54
-55
-56
-57
-58
-59
-60
-61
-62
-63
-64
-65
-66
-67
-68
-69
-70
-71
-72
f1 (ppm)

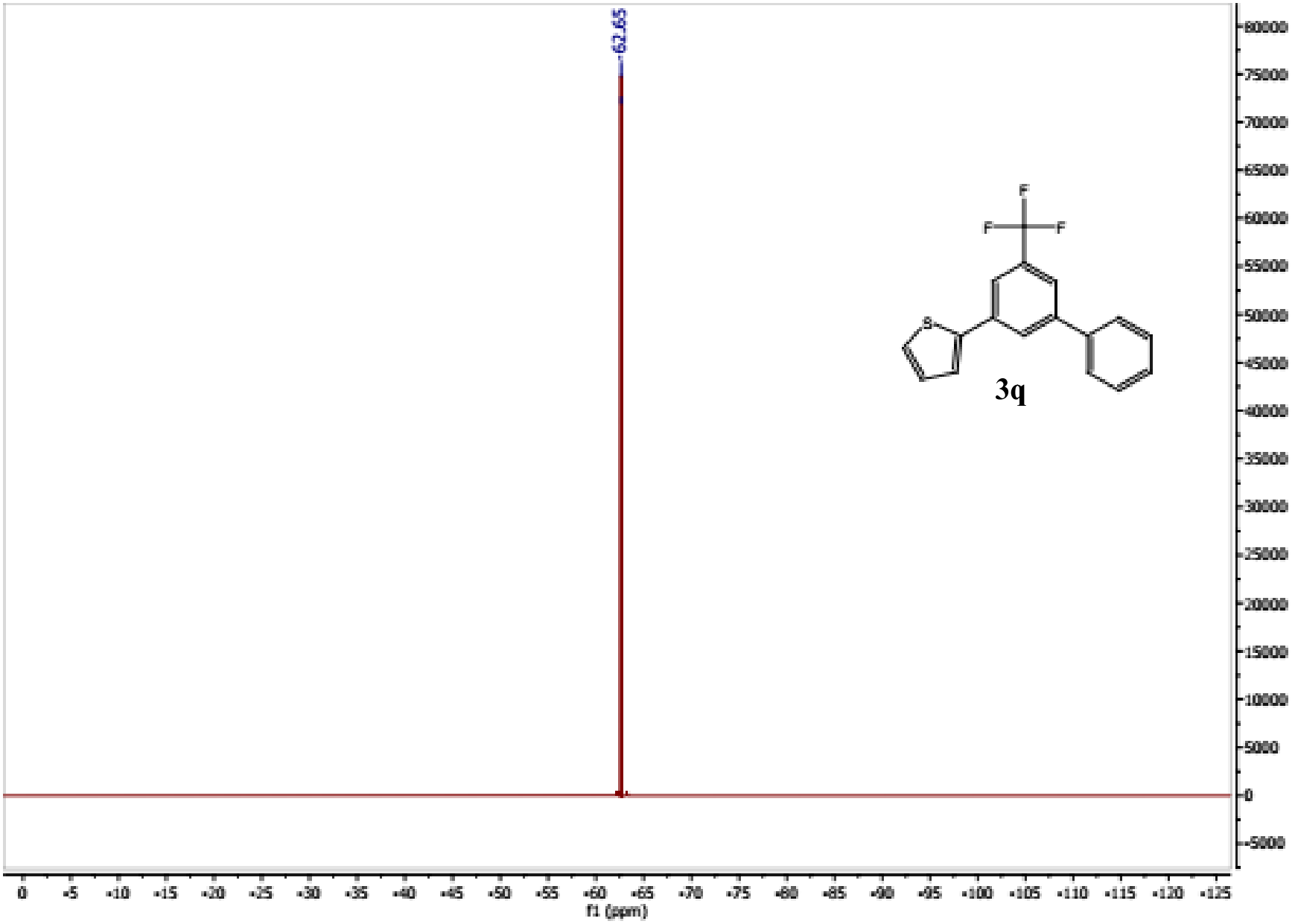

7.26 CDCl3
1.63 H2O
F
F
F
O
3p
f1 (ppm)

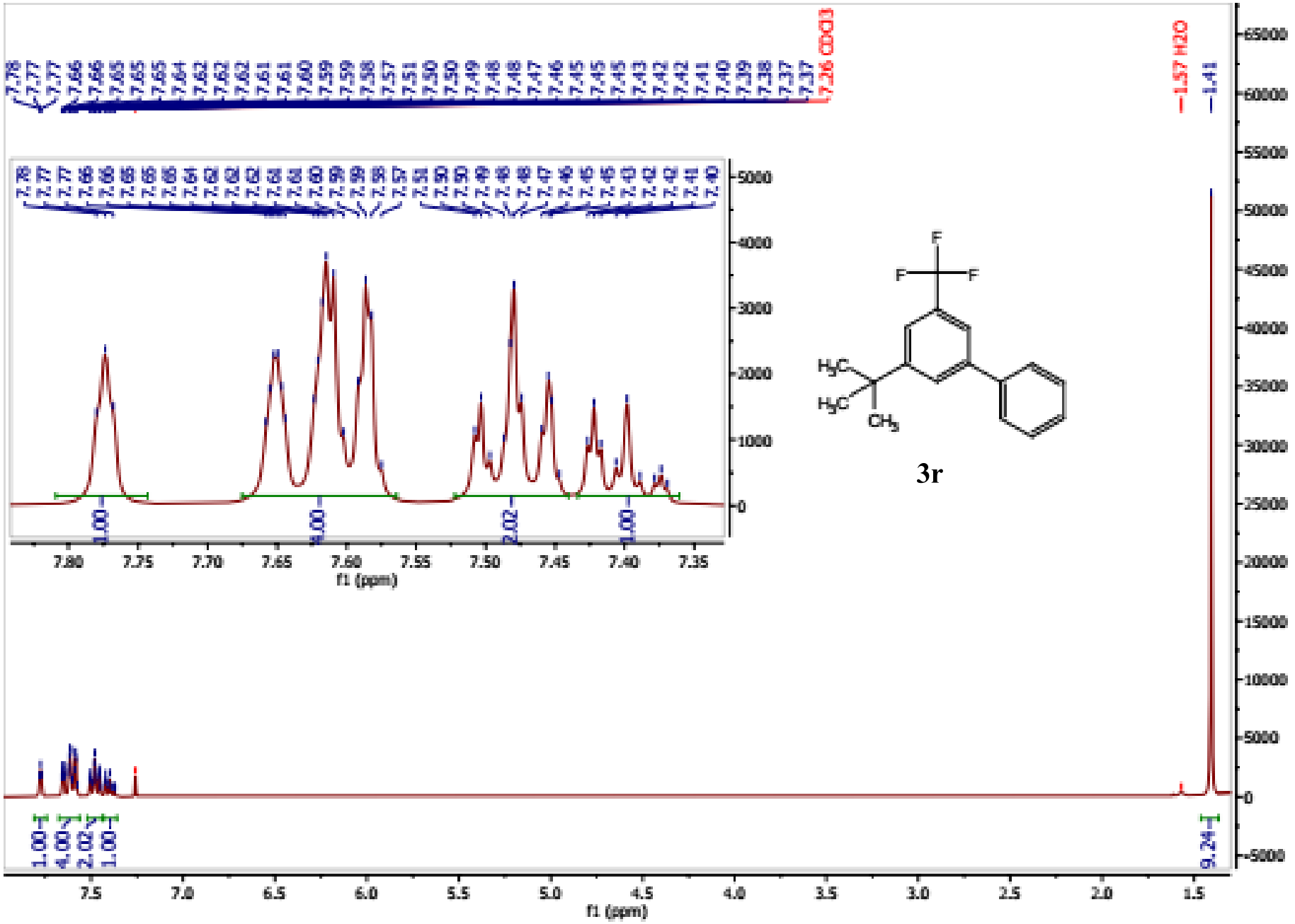

152.63
143.03
142.75
139.74
132.51
132.18
132.09
131.66
131.23
129.64
129.16
128.36
127.36
126.02
125.60
125.58
122.76
122.71
122.66
122.61
122.41
119.50
119.45
119.40
119.35
118.80
112.09
106.70
77.58
77.16
76.74
f1 (ppm)
F
F
F
O
3p


-62.75
F
F
F
O
3p
f1 (ppm)

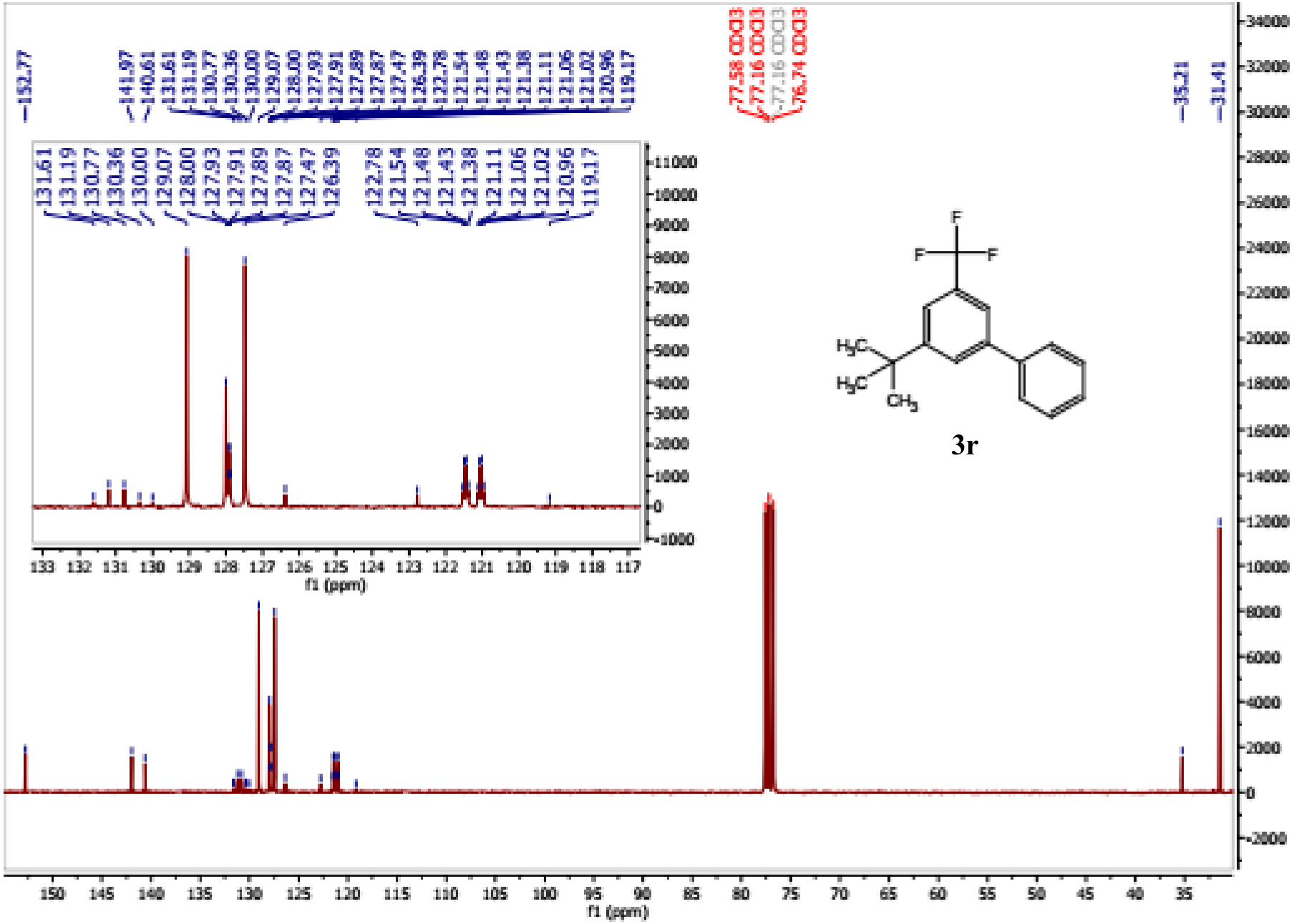

7.26 CDCl3
1.65 H2O
F
F
F
S
3q
f1 (ppm)


143.01
142.77
139.66
135.88
132.21
131.78
129.58
129.19
128.43
128.41
127.99
127.97
127.39
126.12
125.97
124.48
123.01
122.96
122.91
122.86
122.36
121.56
121.51
121.45
121.40
118.74
77.58
77.16 CDCl3
76.74
F
F
F
S
3q
f1 (ppm)
f1 (ppm)

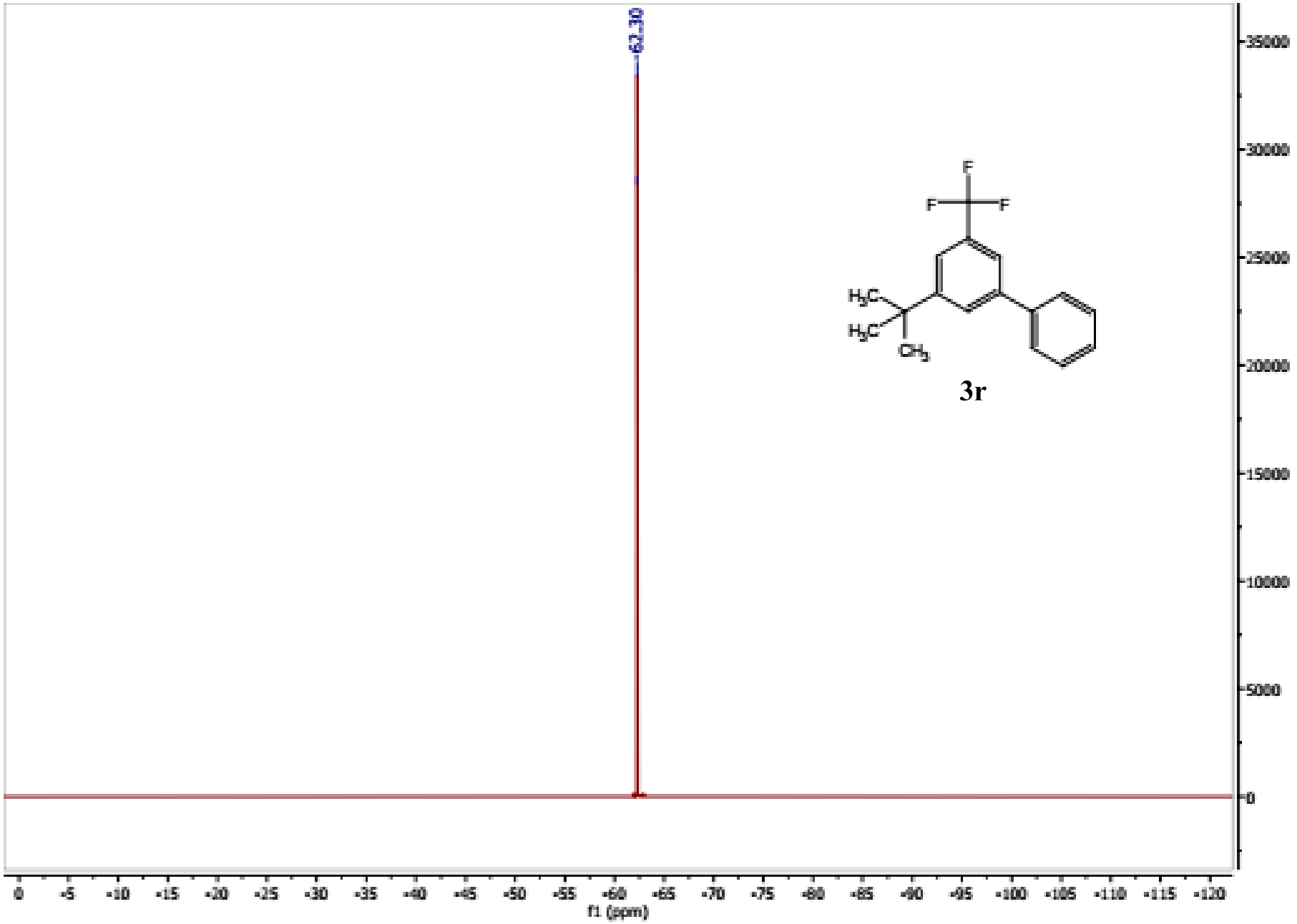

62.65
F
F
F
S
3q
80000
75000
70000
65000
60000
55000
50000
45000
40000
35000
30000
25000
20000
15000
10000
5000
0
-5000
0 5 10 15 20 25 30 35 40 45 50 55 60 65 70 75 80 85 90 95 100 105 110 115 120 125
f1 (ppm)


7.78
7.77
7.77
7.66
7.66
7.65
7.65
7.65
7.64
7.62
7.62
7.62
7.61
7.61
7.60
7.59
7.59
7.58
7.57
7.51
7.50
7.50
7.49
7.48
7.48
7.47
7.46
7.45
7.45
7.45
7.43
7.42
7.42
7.41
7.40
7.39
7.38
7.37
7.37
7.26 CDCl3
1.57 H2O
1.41
1.00
4.00
2.02
1.00
9.24
f1 (ppm)
F
F
F
H3C
H3C
CH3

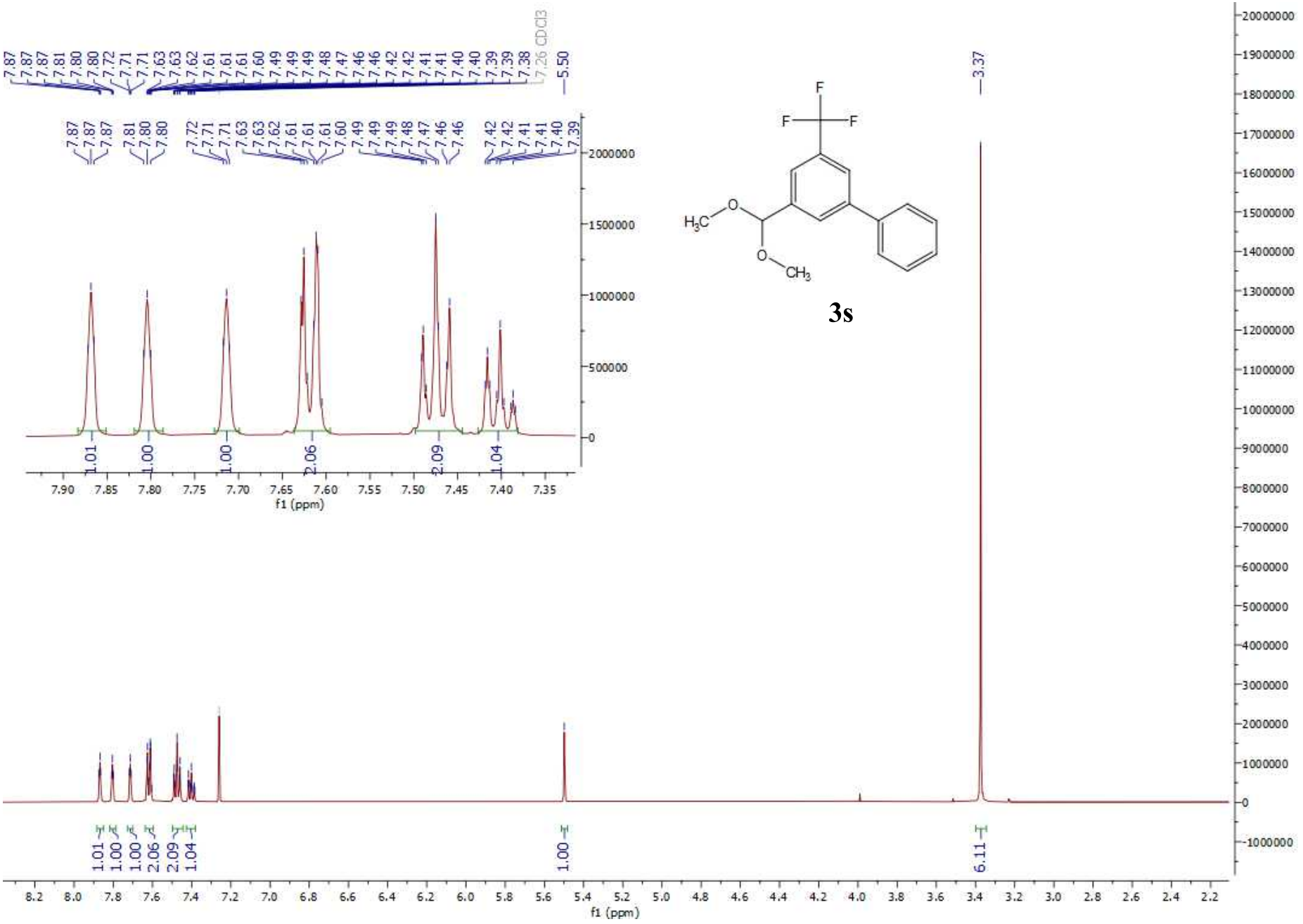
3r


152.77
141.97
140.61
131.61
131.19
130.77
130.36
130.00
129.07
128.00
127.93
127.91
127.89
127.87
127.47
126.39
122.78
121.54
121.48
121.43
121.38
121.11
121.06
121.02
120.96
119.17
77.58 CDCl3
77.16 CDCl3
76.74 CDCl3
35.21
31.41
F
F
F
H3C
H3C
CH3
f1 (ppm)

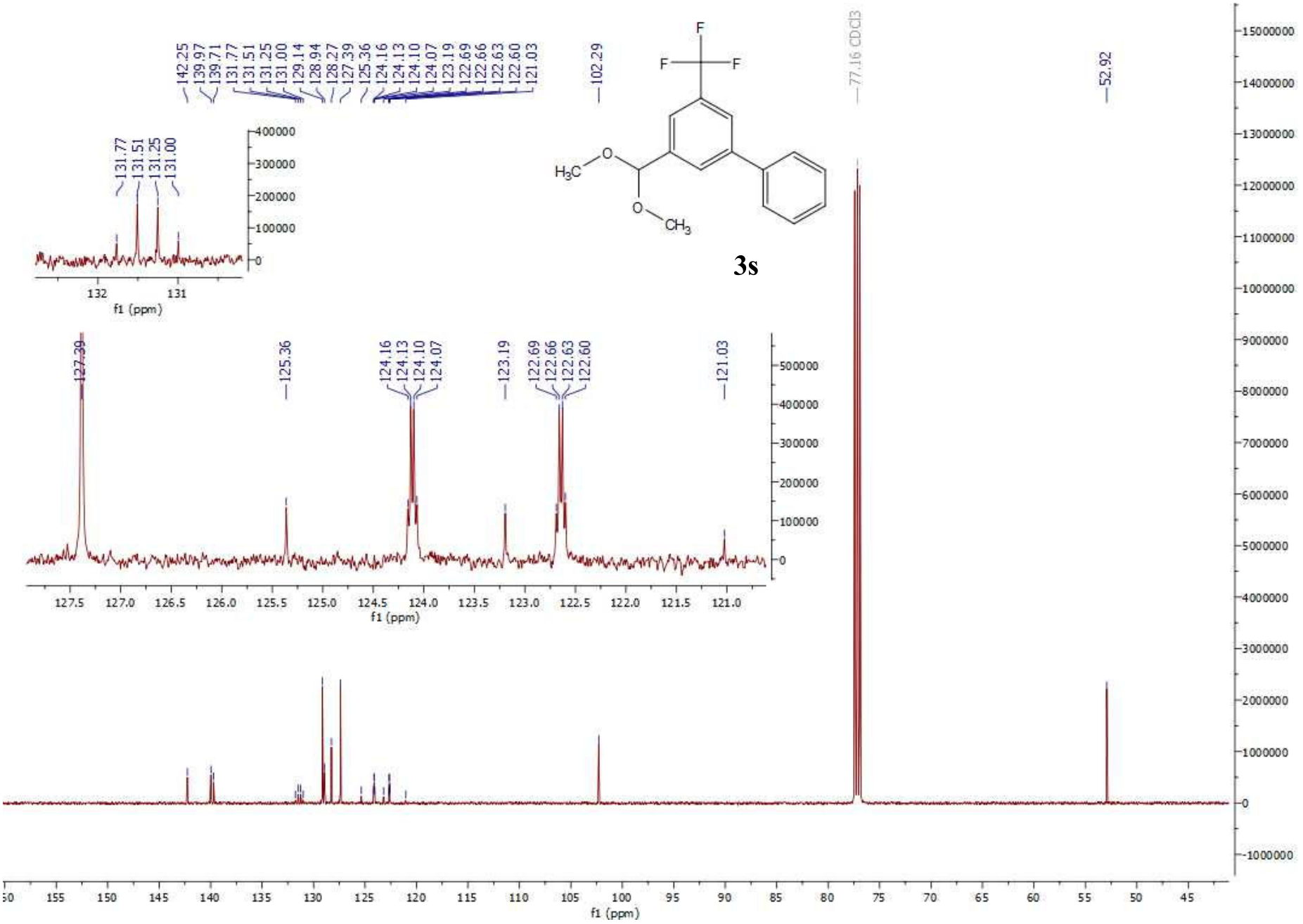
3r

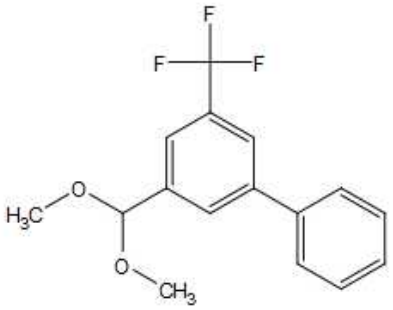

62.30
F
F
F
H3C
H3C
CH3
35000
30000
25000
20000
15000
10000
5000
0
0 -5 -10 -15 -20 -25 -30 -35 -40 -45 -50 -55 -60 -65 -70 -75 -80 -85 -90 -95 -100 -105 -110 -115 -120
f1 (ppm)

3r


7.87
7.87
7.87
7.81
7.80
7.80
7.72
7.71
7.71
7.63
7.63
7.62
7.61
7.61
7.61
7.60
7.49
7.49
7.48
7.47
7.46
7.46
7.42
7.42
7.41
7.41
7.40
7.40
7.39
7.39
7.38
7.26 CDCl3
5.50
3.37
1.01
1.00
1.00
2.06
2.09
1.04
1.00
6.11
f1 (ppm)
F
F
F
O
H3C
O
CH3

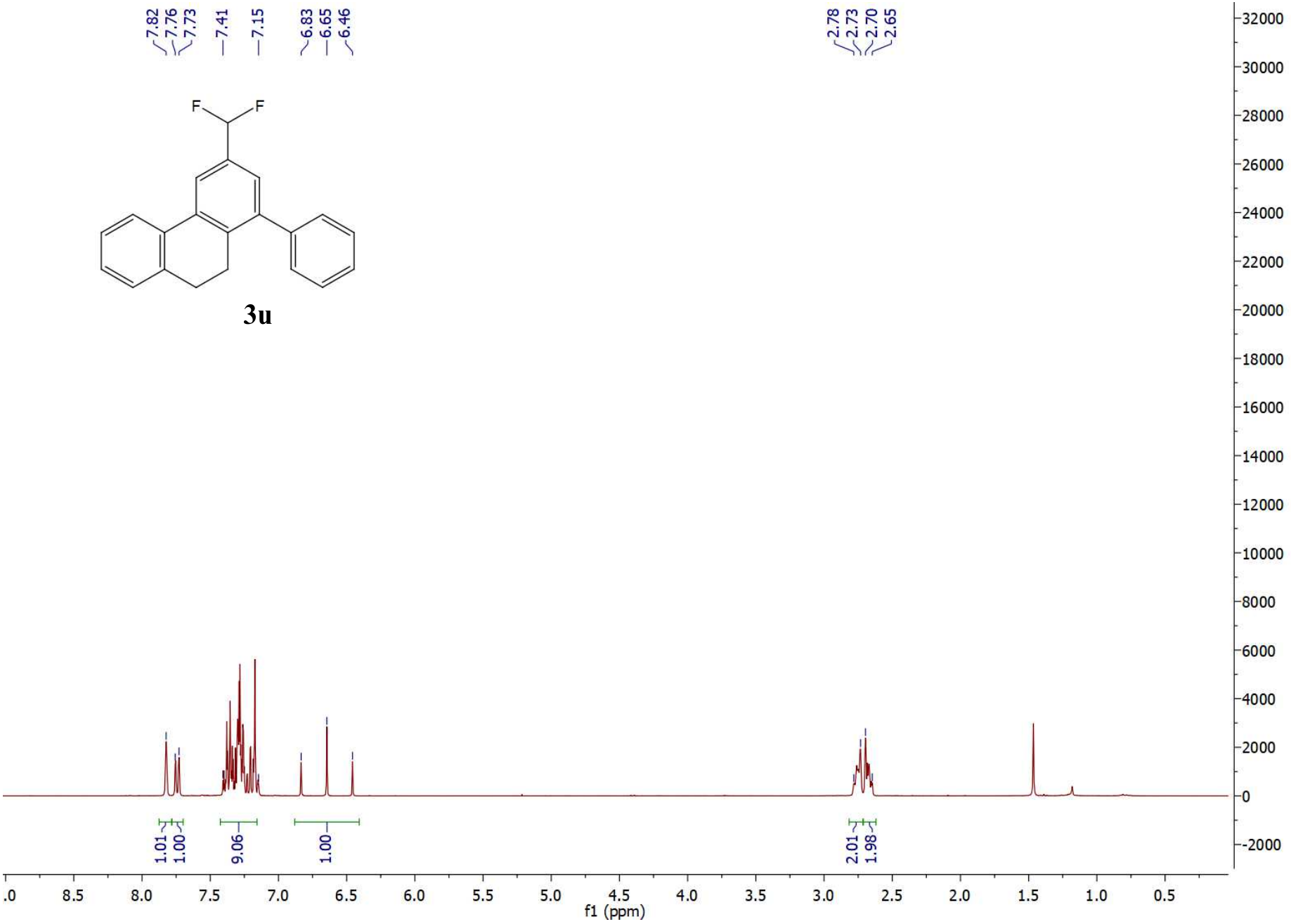
3s


142.25
139.97
139.71
131.77
131.51
131.25
131.00
129.14
128.94
128.27
127.39
125.36
124.16
124.13
124.10
124.07
123.19
122.69
122.66
122.63
122.60
121.03
102.29
77.16 CDCl3
52.92
F
F
F
O
H3C
O
CH3
3s
f1 (ppm)

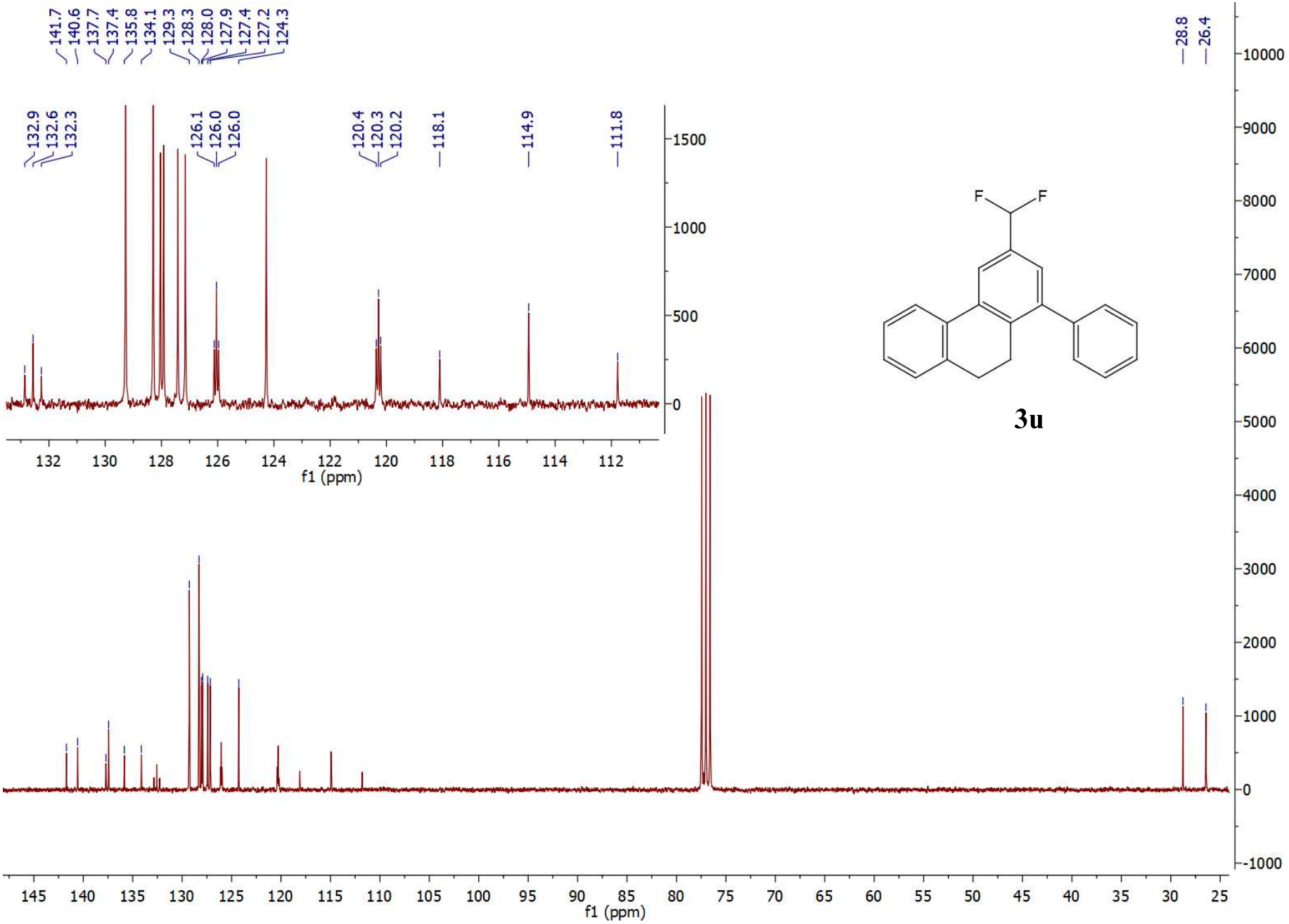

F
F
F
O
H3C
O
CH3

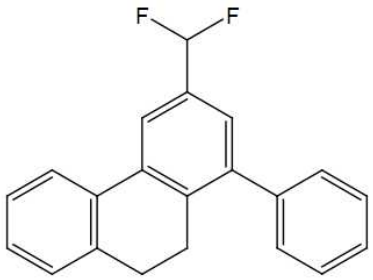
3s

-62.48
20000000
19000000
18000000
17000000
16000000
15000000
14000000
13000000
12000000
11000000
10000000
9000000
8000000
7000000
6000000
5000000
4000000
3000000
2000000
1000000
0
-1000000
-2000000
-30
-35
-40
-45
-50
-55
-60
-65
-70
-75
-80
-85
-90
-95
f1 (ppm)


7.82
7.76
7.73
7.41
7.15
6.83
6.65
6.46
2.78
2.73
2.70
2.65
F
F
1.01
1.00
9.06
1.00
2.01
1.98
f1 (ppm)

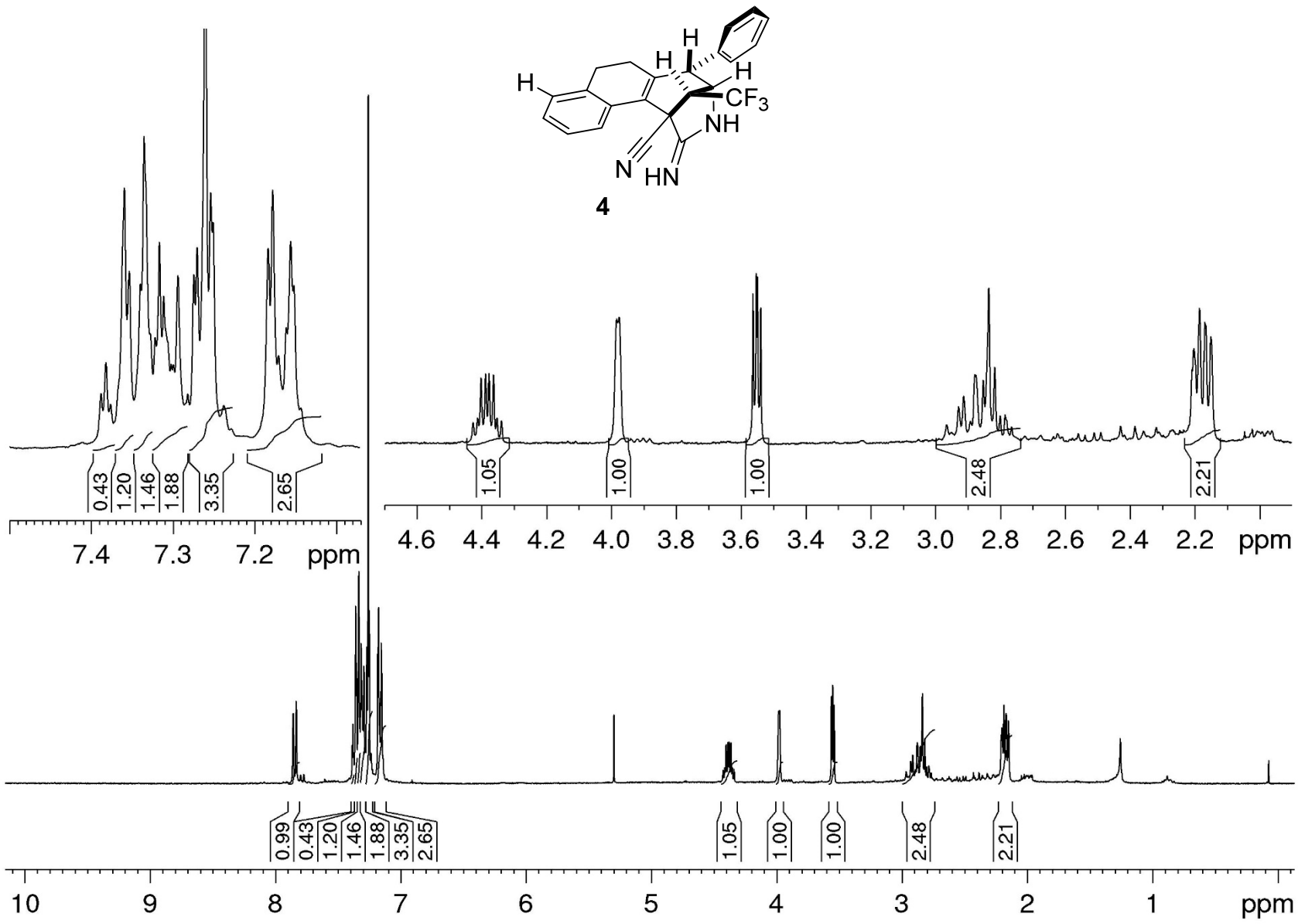
3u

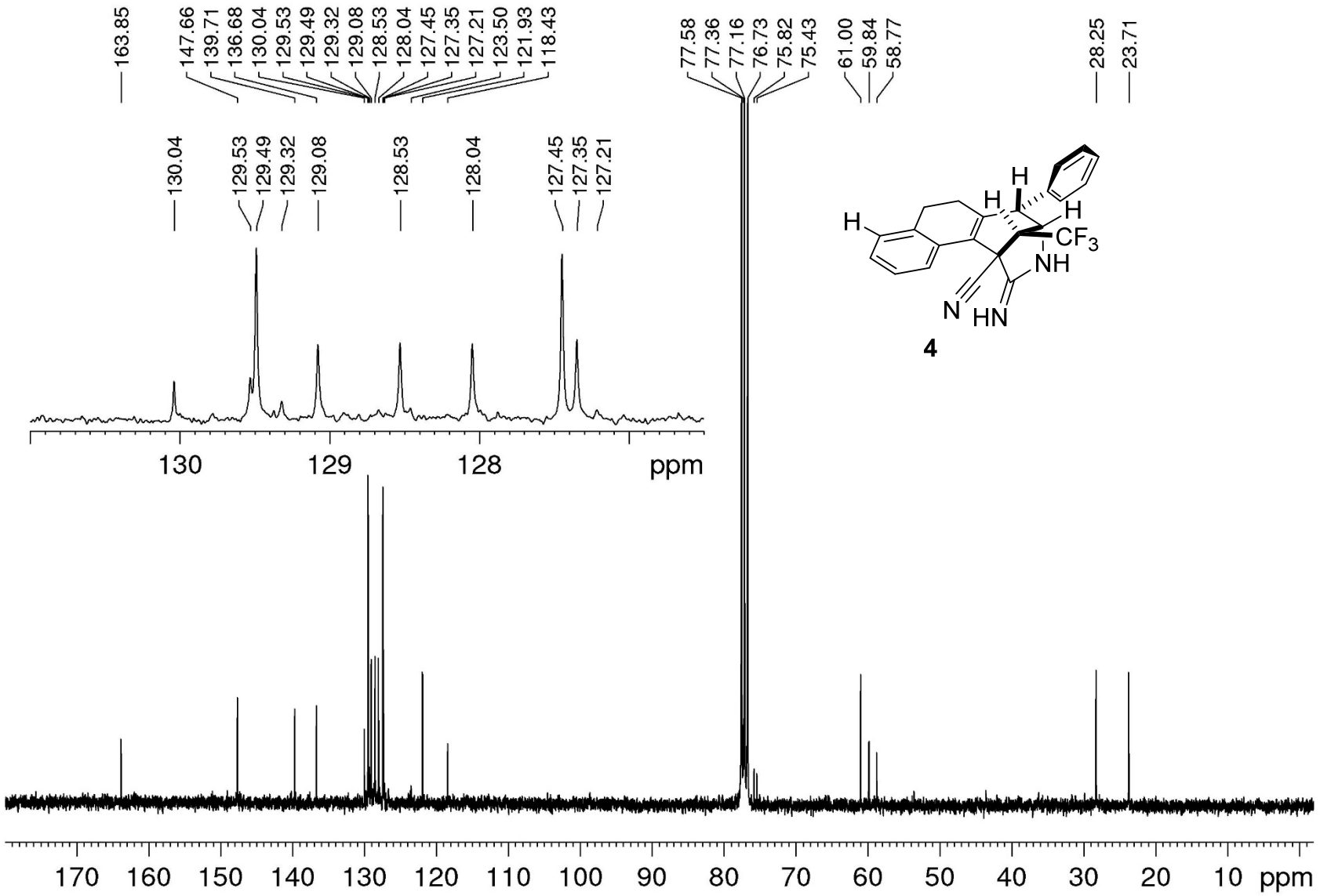

141.7
140.6
137.7
137.4
135.8
134.1
129.3
128.3
128.0
127.9
127.4
127.2
124.3
28.8
26.4
132.9
132.6
132.3
126.1
126.0
126.0
120.4
120.3
120.2
118.1
114.9
111.8
F
F
3u
f1 (ppm)
f1 (ppm)

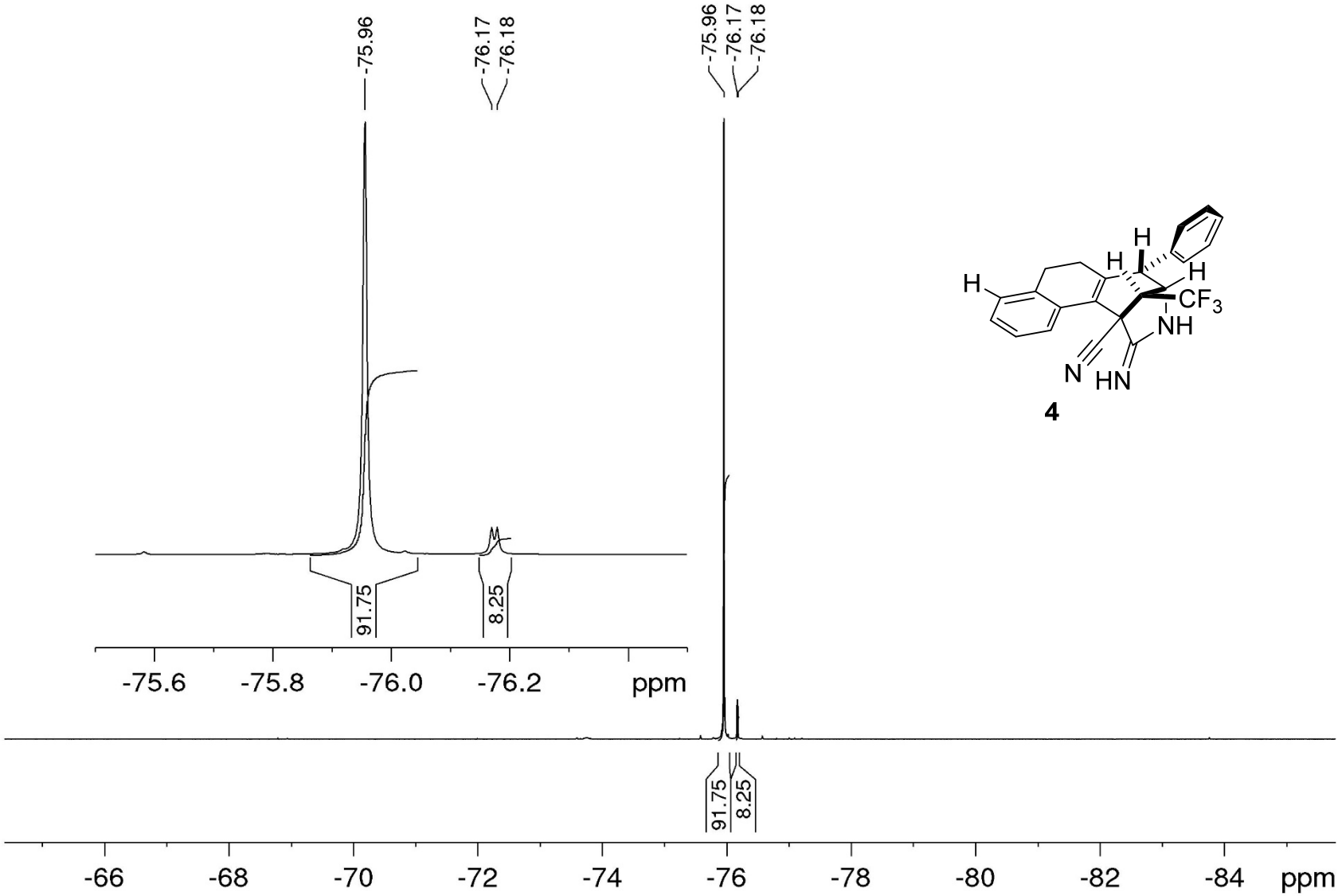

F
F

3u

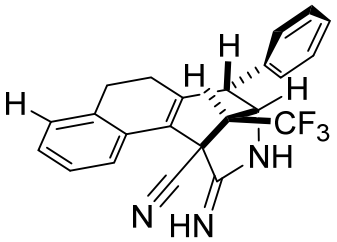
-110.04
-110.05
-110.05
-110.24
-110.25
-110.25
10000
9000
8000
7000
6000
5000
4000
3000
2000
1000
0
-1000
-106.5
-107.0
-107.5
-108.0
-108.5
-109.0
-109.5
-110.0
-110.5
-111.0
-111.5
-112.0
-112.5
-113.0
-113.5
-114.0
f1 (ppm)


H
H
H
H
CF3
NH
N
HN
4
0.43
1.20
1.46
1.88
3.35
2.65
7.4
7.3
7.2
ppm
1.05
1.00
1.00
2.48
2.21
4.6
4.4
4.2
4.0
3.8
3.6
3.4
3.2
3.0
2.8
2.6
2.4
2.2
ppm
0.99
0.43
1.20
1.46
1.88
3.35
2.65
1.05
1.00
1.00
2.48
2.21
10
9
8
7
6
5
4
3
2
1
ppm

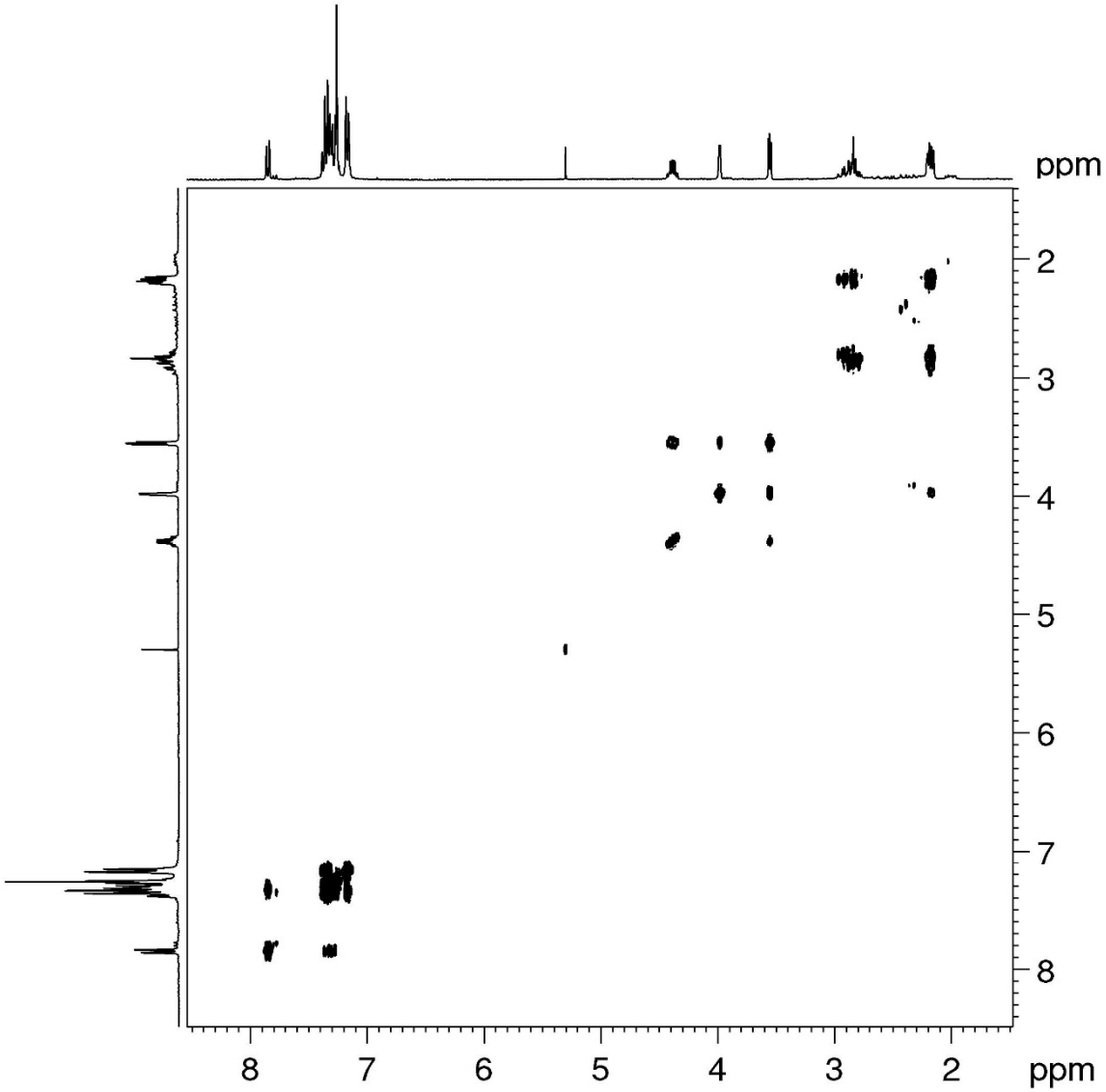

163.85
147.66
139.71
136.68
130.04
129.53
129.49
129.32
129.08
128.53
128.04
127.45
127.35
127.21
123.50
121.93
118.43
77.58
77.36
77.16
76.73
75.82
75.43
61.00
59.84
58.77
28.25
23.71
130
129
128
ppm
H
H
H
H
CF3
NH
N
HN
4
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm

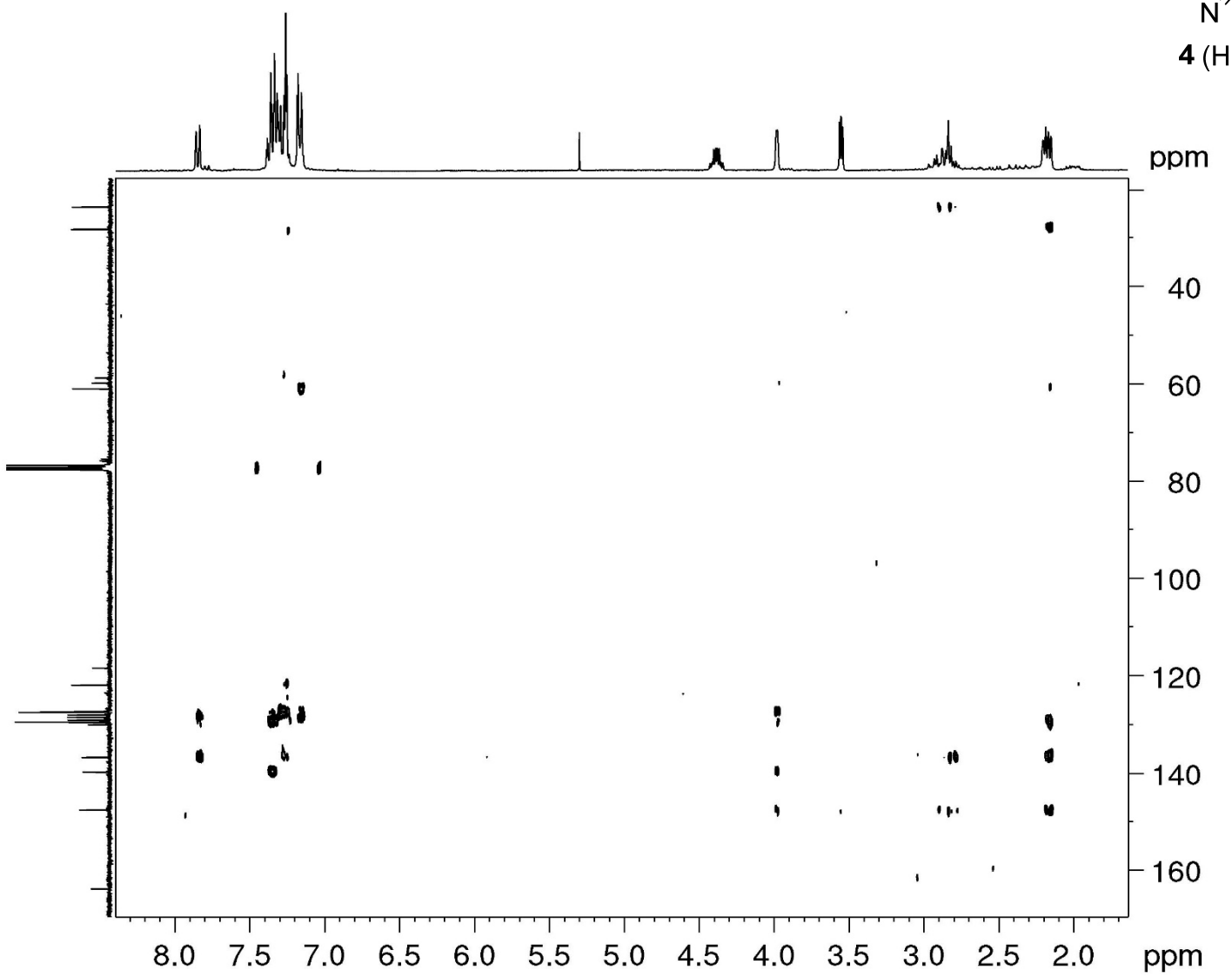

-75.96
-76.17
-76.18
-75.96
-76.17
-76.18
91.75
8.25
-75.6
-75.8
-76.0
-76.2
ppm
91.75
8.25
-66
-68
-70
-72
-74
-76
-78
-80
-82
-84
ppm
H
H
H
H
CF3
NH
N
HN

4

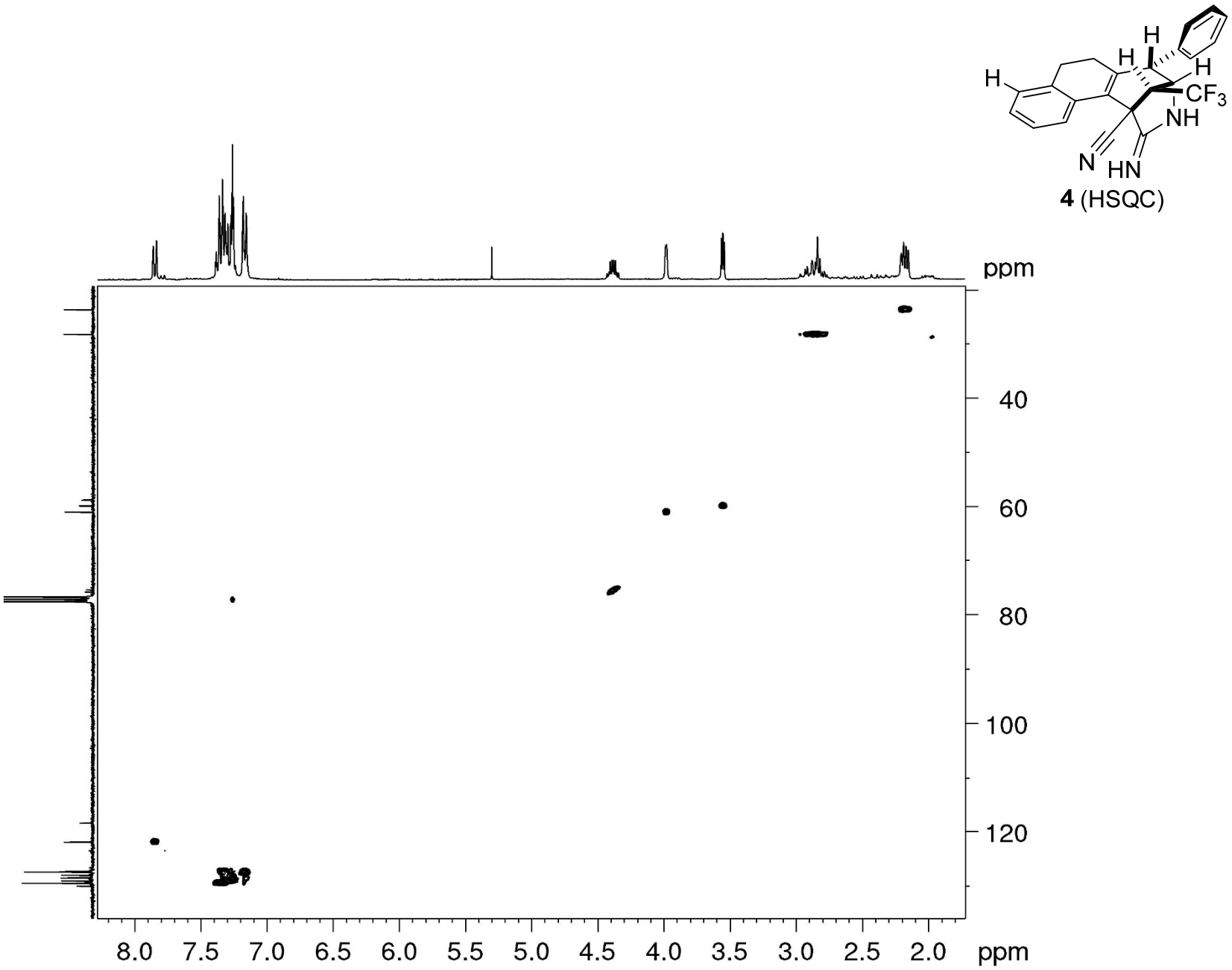


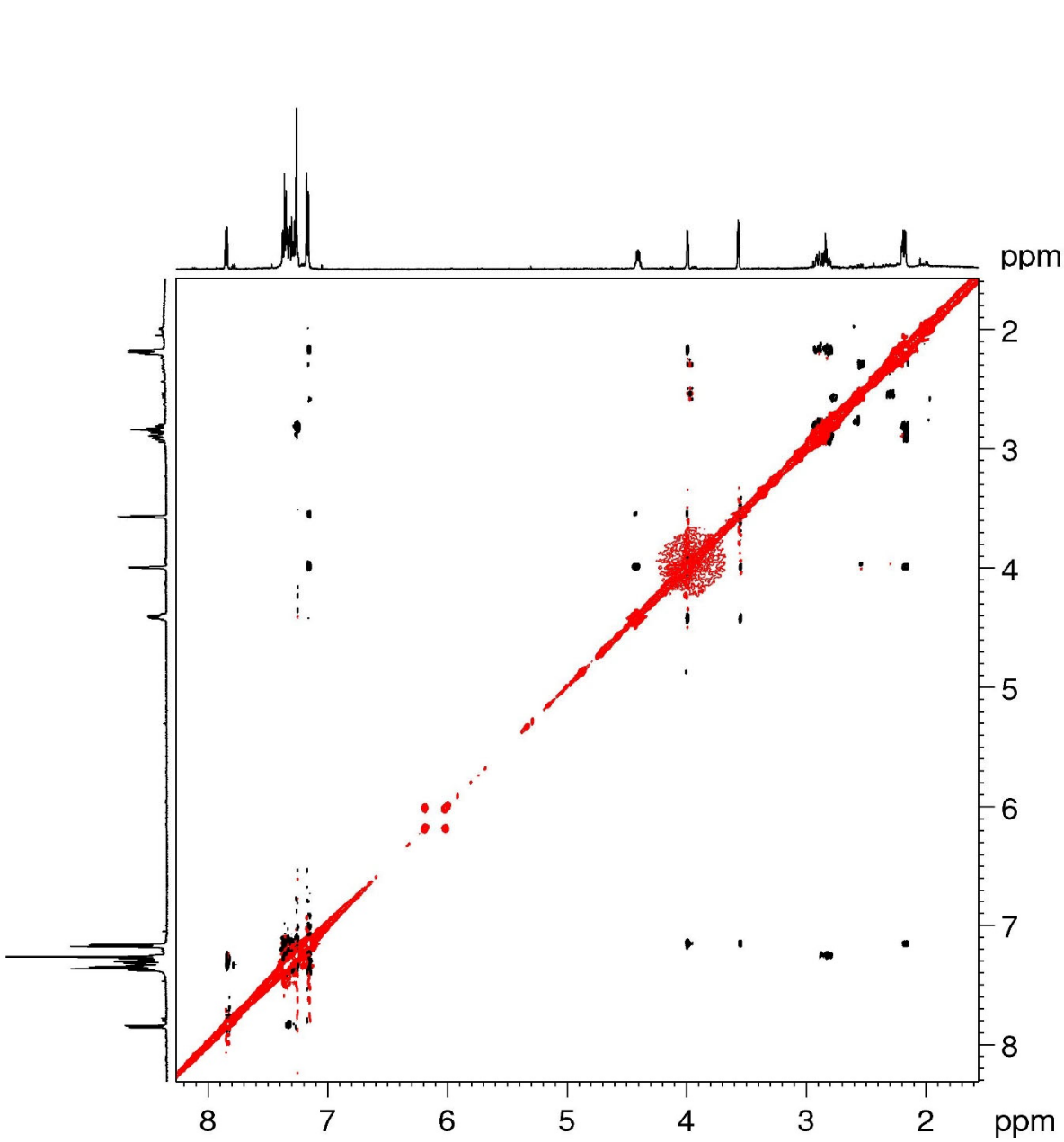
4 (COSY)

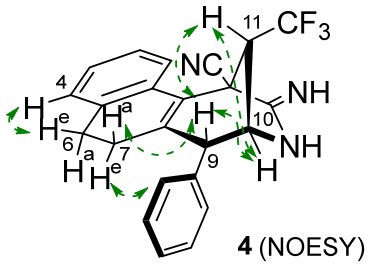



H
H
H
H
CF3
NH
N
HN
ppm
40
60
80
100
120
140
160
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
ppm

4 (HMBC)


H
H
H
H
CF3
NH
N
HN
4 (HSQC)
ppm
40
60
80
100
120
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
ppm





4 (NOESY)