Supporting Information

2,3-Difunctionalization of Quinones: A Gold-Catalyzed Cascade Approach for Trifluoromethyl-Amination or Sulfoximination

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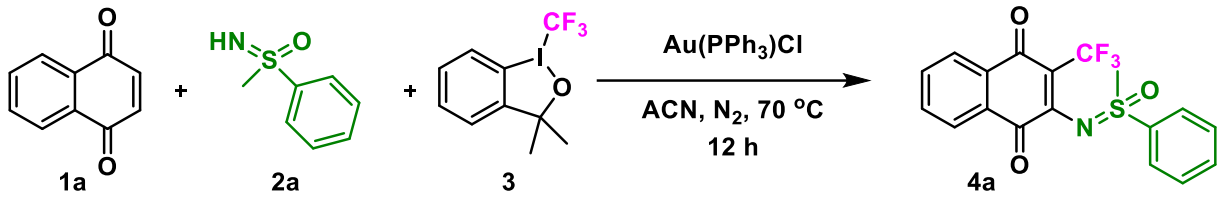
Content

General experimental section:

All reactions were performed in oven-dried glass apparatus. Solvents were distilled in the standard way, and commercial reagents were used without any purification. Analytical TLC was performed on 60 F254 plates and visualized by exposure to ultraviolet light (UV-254 nm). Column chromatography was carried out with silica gel (100-200 and 200-400 mesh) and basic alumina. NMR spectra for characterization of compounds were recorded on Bruker Advance DPX FT-NMR 400 MHz instrument (^{1}H, 2D, ^{1}H-^{1}H-COSY and ^{1}H-^{13}C HMBC, HMQC, and NOESY) at 400 MHz and (^{13}C) at 100 MHz respectively. ^{19}F NMR were recorded at 376 MHz. Chemical shifts (δ) are reported in ppm, using the residual solvent peak in $CDCl_3$ (δH = 7.26 and δC = 77.16 ppm) as internal reference and coupling constants (J) are given in hertz (Hz). The following abbreviations were used to explain the multiplicities: s = singlet, d = doublet, t = triplet, q = quartet, m = multiplet. High-Resolution Mass Spectra (HRMS) were recorded using Waters XEVO-G2-XS-Q-TOF mass spectrometer.

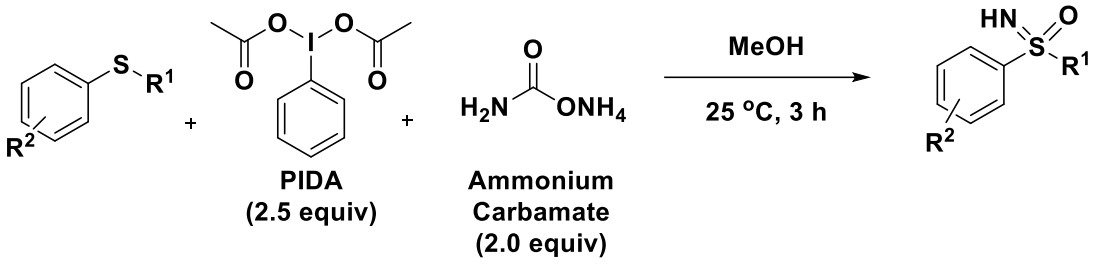
General Procedure for the synthesis of trifluoromethyl aminated derivatives



To an oven dried Schlenk tube equipped with a magnetic stir bar, was added quinone **1** (0.32 mmol, 1.0 equiv), amine/sulfoximine **2a** (0.32 mmol,1.0 equiv), Togni reagent **3** (0.63 mmol, 2.0 equiv), $Au(PPh_3)Cl$ (10 mol%) and sealed with a septum, and degassed by alternating vacuum evacuation and nitrogen backfill (three times) before acetonitrile (5 mL) was added. The reaction was then stirred at 70 °C for 12 h. After the reaction was complete, the solvent was removed under reduced

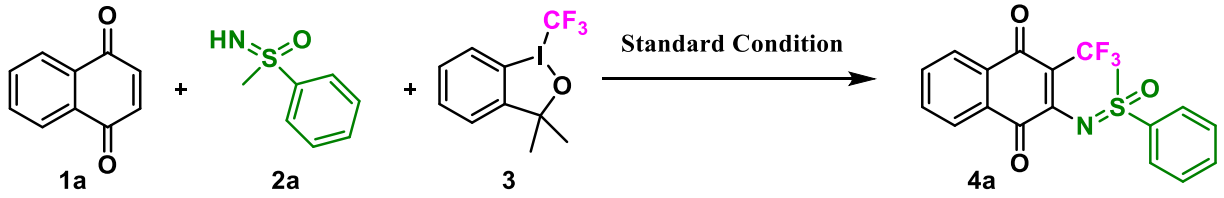
pressure with rotary evaporator. The crude residue was purified by silica gel column chromatography to afford pure product.

General Procedure for the synthesis of sulfoximines



The sulfide (1 equiv), phenyliodine(III)diacetate (PIDA) (2.5 equiv) and ammonium carbamate (2.0 equiv) were added to a flask containing a stirrer bar. MeOH was added to it and the reaction was allowed to stir at 25 ^{o}C for 3 h. After the indicated reaction time, the solvent was removed under reduced pressure and purified by column chromatography which afforded the sulfoximine product.

Optimization of the Reaction Conditions

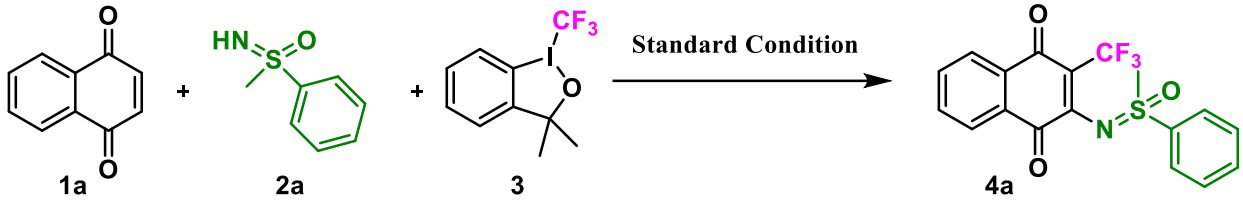


a) Table S1. Examination of Metal Catalysts other than Gold

S No.	Metal Catalyst	Solvent	Isolated Yield (%) of 4a
1	-	ACN	NR
2	CuI	ACN	7
3	CuBr	ACN	13
4	$Cu(MeCN)_4PF_6$	ACN	48

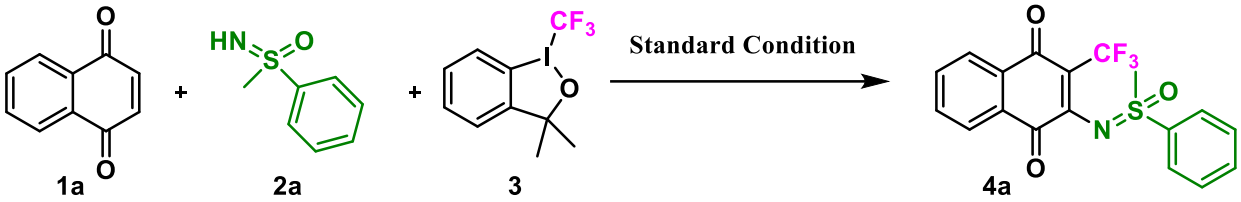
5	$Cu(MeCN)_4BF4$	ACN	42
6	$Cu(OAc)_2 . H_2O$	ACN	NR
7	$FeCl_3$	ACN	NR
8	$Pd(OAc)_2$	ACN	37
9	**$Au(PPh_3)Cl$**	**ACN**	**72**
10	$Cu(OTf)_2$	ACN	39

b) Table S2. Examination of Different Solvents



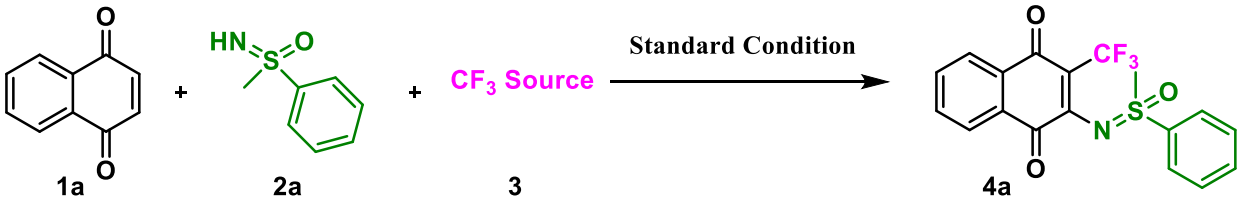
S No.	Metal Catalyst	Solvent	Isolated Yield (%) of 4a
1	$Au(PPh_3)Cl$	THF	36
2	$Au(PPh_3)Cl$	DMSO	NR
3	$Au(PPh_3)Cl$	DMF	NR
4	$Au(PPh_3)Cl$	MeOH	trace
5	$Au(PPh_3)Cl$	t-BuOH	trace
6	$Au(PPh_3)Cl$	EtOH	trace
7	$Au(PPh_3)Cl$	Chlorobenzene	NR
8	$Au(PPh_3)Cl$	$CDCl_3$	53
9	$Au(PPh_3)Cl$	Toluene	NR
10	**$Au(PPh_3)Cl$**	**ACN**	**72**
11	$Au(PPh_3)Cl$	DCM	47
12	$Au(PPh_3)Cl$	DCE	24

c) Table S3: Examination of different reaction temperatures



S No.	Temperature (° C)	Isolated Yield (%) of 4a
1	RT	NR
2	40	NR
3	70	72
4	85	57

d) Table S4: Examination of various trifluoromethylating agents



S No.	CF_3 Reagents	Isolated Yield (%) of 4a
1	Togni I reagent (1-Trifluoromethyl-3,3-dimethyl-1,2-benziodoxole)	72
2	Togni II reagent (1-Trifluoromethyl-1,2-beenziodoxol-3-(1H)-on)	15
3	Umemoto reagent (5-(Trifluoromethyl)dibenzothiophenium tetrafluoroborate)	24

Togni 1 and Sulfoximine Mutual Activation

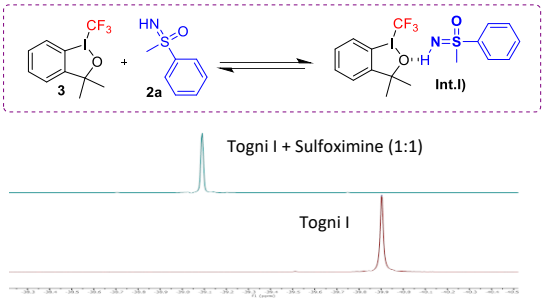


Figure S1: Chemical Shift in ^{19}F NMR of Togni I (alone) and Togni I with Sulfoximine

Job's Plot

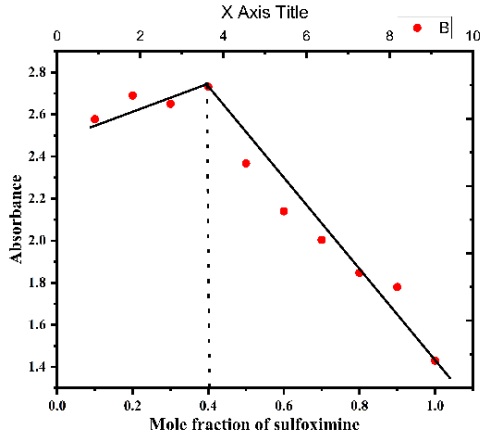


Figure S2: Job's Plot to determine the binding stoichiometry between Togni I and sulfoximine

XPS Spectra

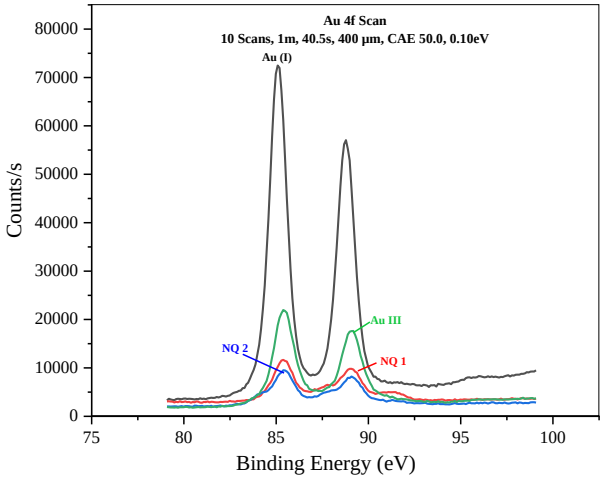
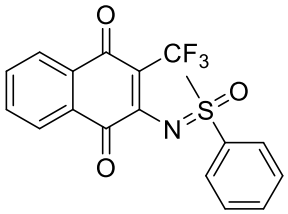


Figure S3: XPS spectra of Au(I), Au (III), NQ-1 (reaction aliquot after 3h) and NQ-2 (reaction aliquot after 6h)

Physical and Spectroscopic Characterization Data of Compounds:

2-((methyl(oxo)(phenyl)-λ^6-sulfaneylidene)amino)-3-(trifluoromethyl)naphthalene-1,4-dione (4a)



The compound **4a** was purified by column chromatography on silica gel (Eluent: EtOAc/Hexane = 2/8), 86.35 mg, 72% yield; yellow solid.

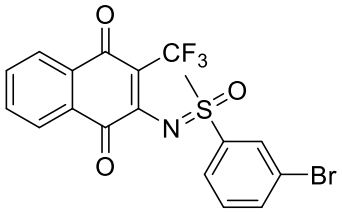
^{1}H NMR (400 MHz, $CDCl_3$): δ 8.13 – 8.09 (m, 1H), 8.03 – 7.98 (m, 2H), 7.95 – 7.92 (m, 1H), 7.74 (m, 1H), 7.67 – 7.59 (m, 4H), 3.41 (s, 3H).

^{19}F NMR (377 MHz, $CDCl_3$): δ -57.30 (s, 3F).

^{13}C {^{1}H} NMR (151 MHz, $CDCl_3$): δ 180.8, 180.3, 150.4, 141.3, 141.2, 135.1, 133.4, 132.9, 132.6, 129.7, 129.6, 127.5, 127.0, 126.9, 126.6, 126.3, 126.3, 126.2, 123.9 (q, *J* = 276.3 Hz), 116.8 (q, *J* = 27.2 Hz), 49.5.

HRMS (ESI) m/z: $[M+H]^+$ Calcd. For $C_{18}H_{13}F_3NO_3S$: 380.0568; found: 380.0566.

2-(((3-bromophenyl)(methyl)(oxo)-λ^6-sulfaneylidene)amino)-3-(trifluoromethyl)naphthalene-1,4-dione (4b)



The compound **4b** was purified by column chromatography on silica gel (Eluent: EtOAc/Hexane = 1/9), 101.45 mg, 70% yield; yellow solid.

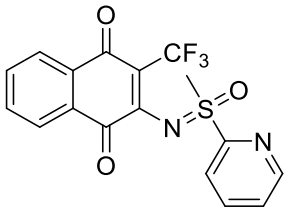
^{1}H NMR (400 MHz, $CDCl_3$): δ 8.16 (t, *J* = 1.8 Hz, 1H), 8.12 (d, *J* = 7.7 Hz, 1H), 7.95 (d, *J* = 7.7 Hz, 1H), 7.92-7.89 (m, 1H), 7.79 – 7.73 (m, 2H), 7.64 (td, *J* = 7.6, 1.0 Hz, 1H), 7.48 (t, *J* = 8.0 Hz, 1H), 3.41 (s, 3H).

^{19}F NMR (377 MHz, $CDCl_3$): δ -57.31 (s, 3F).

^{13}C {^{1}H} NMR (101 MHz, $CDCl_3$): δ 180.8, 180.3, 149.8, 143.2, 136.4, 135.3, 133.0, 132.6, 131.2, 129.5, 129.3, 127.03, 126.6, 124.8, 124.5 (q, *J* = 282.8 Hz), 123.7, 117.2 (q, *J* = 26.4 Hz), 49.4.

HRMS (ESI) m/z: $[M+H]^+$ Calcd. For $C_{18}H_{14}NO_3F_3SBr$: 459.9830; found: 459.9837.

2-((methyl(oxo)(pyridin-4-yl)-λ^6-sulfaneylidene)amino)-3-(trifluoromethyl)naphthalene-1,4-dione (4c)



The compound **4c** was purified by column chromatography on silica gel (Eluent: EtOAc/Hexane = 2/8), 87.78 mg, 73% yield; yellow solid.

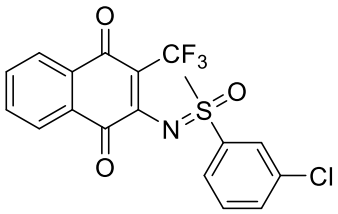
^{1}H NMR (400 MHz, $CDCl_3$): δ 8.71 – 8.67 (m, 1H), 8.38 (d, *J* = 8.0 Hz, 1H), 8.10 (dd, *J* = 7.8, 0.8 Hz, 1H), 8.06 (td, *J* = 7.8, 1.7 Hz, 1H), 7.94 (dd, *J* = 7.7, 0.9 Hz, 1H), 7.75 (td, *J* = 7.6, 1.3 Hz, 1H), 7.63 (td, *J* = 7.6, 1.2 Hz, 1H), 7.58 – 7.55 (m, 1H), 3.56 (s, 3H).

^{19}F NMR (377 MHz, $CDCl_3$): δ -57.01 (s, 3F).

^{13}C {^{1}H} NMR (101 MHz, $CDCl_3$): δ 181.2, 180.5, 158.9, 150.0, 138.7, 135.3, 133.1, 132.8, 129.7, 127.2, 127.0, 126.7, 123.4 (d, *J* = 280.7 Hz), 122.2, 117.1 (q, *J* = 26.5 Hz), 45.1.

HRMS (ESI) m/z: $[M+H]^+$ Calcd. For $C_{17}H_{12}N_2O_3F_3S$: 381.0521; found: 381.0524.

2-(((3-chlorophenyl)(methyl)(oxo)-λ^6-sulfaneylidene)amino)-3(trifluoromethyl)naphthalene-1,4-dione (4d)



The compound **4d** was purified by column chromatography on silica gel (Eluent: EtOAc/Hexane = 1/9), 98.02 mg, 75% yield; yellow solid.

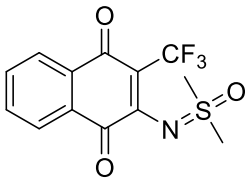
^{1}H NMR (400 MHz, $CDCl_3$): δ 8.12 (d, *J* = 7.8 Hz, 1H), 8.00 (t, *J* = 1.9 Hz, 1H), 7.95 (d, *J* = 7.6 Hz, 1H), 7.88-7.85 (m, 1H), 7.78-7.74 (m, 1H), 7.66 – 7.61 (m, 2H), 7.55 (t, *J* = 7.9 Hz, 1H), 3.41 (s, 3H).

^{19}F NMR (377 MHz, $CDCl_3$): δ -57.31 (s, 3F).

^{13}C {^{1}H} NMR (101 MHz, $CDCl_3$): δ 180.9, 180.4, 149.9, 143.2, 136.1, 135.4, 133.6, 133.2, 132.7, 131.2, 129.6, 127.1, 126.8, 126.6, 124.5, 123.32 (q, *J* = 276.4 Hz), 117.4 (q, *J* = 26.4 Hz), 49.51 (s).

HRMS (ESI) m/z: $[M+H]^+$ Calcd. For $C_{18}H_{12}NO_3F_3SCl$: 414.0179; found: 414.0176.

2-((dimethyl(oxo)- λ^{6}-sulfaneylidene)amino)-3-(trifluoromethyl)naphthalene-1,4-dione (4e)



The compound **4e** was purified by column chromatography on silica gel (Eluent: EtOAc/Hexane = 3/7), 118.95 mg, 77% yield; yellow solid.

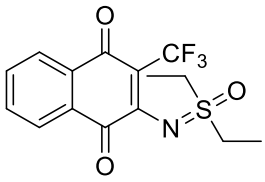
^{1}H NMR (400 MHz, $CDCl_3$): δ 8.12 (dd, *J* = 7.7, 0.9 Hz, 1H), 8.07 (dd, *J* = 7.7, 0.9 Hz, 1H), 7.78 (td, *J* = 7.6, 1.4 Hz, 1H), 7.69 (td, *J* = 7.6, 1.3 Hz, 1H), 3.46 (s, 6H).

^{19}F NMR (377 MHz, $CDCl_3$): δ -57.15 (s, 3F).

^{13}C {^{1}H} NMR (101 MHz, $CDCl_3$): δ 182.1, 180.5, 150.3, 135.4, 133.1, 132.8, 130.0, 127.0, 126.8, 123.8 (q, *J* =272.7 Hz), 116.4 (q, *J* =25.8 Hz), 46.8.

HRMS (ESI) m/z: $[M+H]^+$ Calcd. For $C_{13}H_{11}NO_3F_3S$: 318.0142; found: 318.0142.

2-((diethyl(oxo)- λ^{6}-sulfaneylidene)amino)-3-(trifluoromethyl)naphthalene-1,4-dione (4f)



The compound **4f** was purified by column chromatography on silica gel (Eluent: EtOAc/Hexane = 3/7), 81.88 mg, 75% yield; yellow solid.

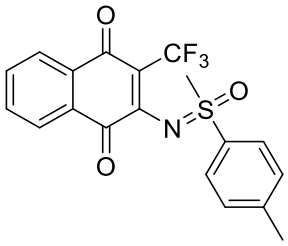
^{1}H NMR (400 MHz, $CDCl_3$): δ 8.14 – 8.10 (m, 1H), 8.05 (dd, *J* = 7.7, 0.8 Hz, 1H), 7.76 (td, *J* = 7.6, 1.2 Hz, 1H), 7.67 (td, *J* = 7.6, 1.2 Hz, 1H), 3.51 (q, *J* = 7.4 Hz, 4H), 1.48 (t, *J* = 7.4 Hz, 6H).

^{19}F NMR (377 MHz, $CDCl_3$): δ -57.13 (s, 3F).

^{13}C {^{1}H} NMR (101 MHz, $CDCl_3$): δ 182.1, 180.4, 151.7, 135.3, 133.0, 132.9, 130.1, 126.9, 126.7, 122.3 (q, *J* = 277.7 Hz), 116.1 (q, *J* = 26.0 Hz), 50.2, 7.6.

HRMS (ESI) m/z: $[M+H]^+$ Calcd. For $C_{15}H_{15}F_3NO_3S$: 346.0725; found: 346.0723.

2-((methyl(oxo)(p-tolyl)-λ^6-sulfaneylidene)amino)-3-(trifluoromethyl)naphthalene-1,4-dione (4g)



The compound **4g** was purified by column chromatography on silica gel (Eluent: EtOAc/Hexane = 2/8), 84.56 mg, 68% yield; yellow solid.

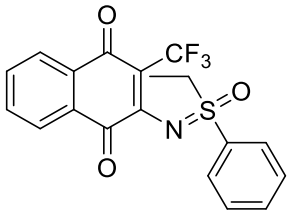
^{1}H NMR (400 MHz, $CDCl_3$): δ 8.11 (d, *J* = 7.7 Hz, 1H), 7.94 (d, *J* = 7.7 Hz, 1H), 7.87 (d, *J* = 8.2 Hz, 2H), 7.74 (t, *J* = 7.4 Hz, 1H), 7.61 (t, *J* = 7.5 Hz, 1H), 7.39 (d, *J* = 8.1 Hz, 2H), 3.39 (s, 3H), 2.45 (s, 3H).

^{19}F NMR (377 MHz, $CDCl_3$): δ -57.30 (s, 3F).

^{13}C {^{1}H} NMR (101 MHz, $CDCl_3$): δ 180.9, 180.5, 150.6, 144.5, 138.2, 135.2, 133.0, 132.8, 130.5, 129.8, 127.1, 126.7, 126.5, 122.8 (q, *J* = 141.4 Hz) 109.5 (q, *J* = 121.2 Hz), 49.7, 21.7.

HRMS (ESI) m/z: $[M+H]^+$ Calcd. For $C_{19}H_{15}F_3NO_3S$: 394.0725; found: 394.0722.

2-((ethyl(oxo)(phenyl)- λ^6-sulfaneylidene)amino)-3-(trifluoromethyl)naphthalene-1,4-dione (4h)



The compound **4h** was purified by column chromatography on silica gel (Eluent: EtOAc/Hexane = 2/8), 89.50 mg, 72% yield; yellow solid.

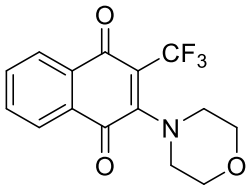
^{1}H NMR (400 MHz, $CDCl_3$): δ 8.10 (d, *J* = 7.8 Hz, 1H), 7.96 – 7.85 (m, 3H), 7.75 – 7.69 (m, 1H), 7.68 – 7.53 (m, 4H), 3.43 (dd, *J* = 7.3, 3.7 Hz, 2H), 1.36 (dd, *J* = 7.7, 7.0 Hz, 3H).

^{19}F NMR (377 MHz, $CDCl_3$): δ -57.21 (s, 3F).

^{13}C {^{1}H} NMR (101 MHz, $CDCl_3$): 180.7, 180.4, 151.0, 140.6, 139.2, 135.2, 133.4, 133.0, 132.8, 129.8, 127.0 (2C), 126.6, 123.8 (q, *J* = 277.8 Hz), 117.8 (q, *J* = 9.1 Hz), 55.8, 7.3.

HRMS (ESI) m/z: $[M+H]^+$ Calcd. For $C_{19}H_{15}F_3NO_3S$: 394.0725; found: 394.0728.

2-morpholino-3-(trifluoromethyl)naphthalene-1,4-dione (4i)



The compound **4i** was purified by column chromatography on basic alumina (Eluent: EtOAc/Hexane = 1/9), 66.92 mg, 68% yield; orange coloured solid; m.p. = 175 - 177 ^{o}C.

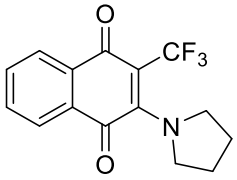
^{1}H NMR (400 MHz, $CDCl_3$): δ 8.10 (dd, *J* = 7.5, 0.9 Hz, 1H), 8.02 – 7.99 (m, 1H), 7.75 (dt, *J* = 7.6, 3.8 Hz, 1H), 7.70 (dt, *J* = 7.5, 1.4 Hz, 1H), 3.89 – 3.86 (m, 4H), 3.73 – 3.69 (m, 4H).

^{19}F NMR (377 MHz, $CDCl_3$): δ -56.77 (s, 3F).

^{13}C {^{1}H} NMR (101 MHz, $CDCl_3$): δ 183.4, 181.0, 151.9, 134.9, 133.4, 132.2, 131.7, 126.9, 126.3, 123.4 (q, *J* = 274.7 Hz), 111.4 (q, *J* = 28.5 Hz), 67.5, 54.2 (d, *J* = 2.3 Hz).

HRMS (ESI) m/z: $[M+H]^+$ Calcd. For $C_{15}H_{13}F_3NO_3$: 312.8001; found: 311.8005.

2-(pyrrolidin-1-yl)-3-(trifluoromethyl)naphthalene-1,4-dione (4j)



The compound **4j** was purified by column chromatography on basic alumina (Eluent: EtOAc/Hexane = 1/9), 59.74 mg, 64% yield; orange coloured solid.

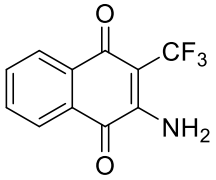
^{1}H NMR (400 MHz, $CDCl_3$): δ 8.10 (d, *J* = 7.7 Hz, 1H), 7.88 (dd, *J* = 7.6, 0.6 Hz, 1H), 7.72 (td, *J* = 7.6, 1.2 Hz, 1H), 7.61 (td, *J* = 7.6, 1.2 Hz, 1H), 3.82 (d, *J* = 0.9 Hz, 4H), 1.98 – 1.94 (m, 4H).

^{19}F NMR (377 MHz, $CDCl_3$): δ -52.73 (s, 3F).

^{13}C {^{1}H} NMR (101 MHz, $CDCl_3$): δ 184.4, 178.8, 155.2, 134.9, 133.0, 132.4, 131.2, 126.4, 125.7, 124.4 (q, *J* = 272.7 Hz), 102.6 (q, *J* = 18.5 Hz), 54.6, 25.3.

HRMS (ESI) m/z: $[M+H]^+$ Calcd. For $C_{15}H_{13}NO_2F_3$: 296.0898; found: 296.0899.

2-**amino-3-(trifluoromethyl)naphthalene-1,4-dione (4k)**



The compound **4k** was purified by column chromatography on silica gel (Eluent: EtOAc/Hexane = 1/9), 59.54 mg, 78% yield; yellow solid.

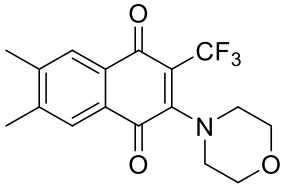
^{1}H NMR (400 MHz, $CDCl_3$): δ 8.17 (d, *J* = 7.8 Hz, 1H), 8.09 (d, *J* = 7.7 Hz, 1H), 7.83 – 7.78 (m, 1H), 7.72 – 7.66 (m, 1H), 6.52 (s, 1H), 6.07 (s, 1H).

^{19}F NMR (377 MHz, $CDCl_3$): δ -55.97 (s, 3F).

^{13}C {^{1}H} NMR (101 MHz, $CDCl_3$): δ 180.3, 179.0, 146.0, 136.0, 133.0 (d, *J* = 13.7 Hz), 129.5, 127.0, 126.8, 125.0 (q, *J* = 275.7 Hz), 102.6 (q, *J* = 27.5 Hz).

HRMS (ESI) m/z: $[M+H]^+$ Calcd. For $C_{11}H_7F_3NO_2$: 242.0429; found: 242.0424.

6,7-dimethyl-2-(piperidin-1-yl)-3-(trifluoromethyl)naphthalene-1,4-dione (4l)



The compound **4l** was purified by column chromatography on basic alumina (Eluent: EtOAc/Hexane = 1/9), 58.32 mg, 64% yield; yellow solid.

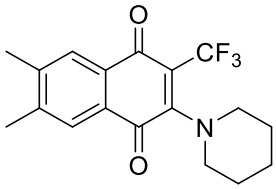
^{1}H NMR (400 MHz, $CDCl_3$): δ 7.84 (s, 1H), 7.74 (s, 1H), 3.89 – 3.86 (m, 4H), 3.71 – 3.67 (m, 4H), 2.39 (d, *J* = 4.6 Hz, 6H).

^{19}F NMR (377 MHz, $CDCl_3$): δ -56.69 (s, 3F).

^{13}C {^{1}H} NMR (101 MHz, $CDCl_3$): δ 183.4, 181.5, 151.9, 145.1, 143.1, 130.2, 129.6, 127.9, 127.2, 123.5 (q, *J* = 275.7 Hz), 111.3 (q, *J* = 28.5 Hz), 67.5, 54.2, 20.5, 20.2.

HRMS (ESI) m/z: $[M+H]^+$ Calcd. For $C_{17}H_{17}F_3NO_3$: 340.1161; found: 340.1163.

6,7-dimethyl-2-morpholino-3-(trifluoromethyl)naphthalene-1,4-dione (4m)



The compound **4m** was purified by column chromatography on basic alumina (Eluent: EtOAc/Hexane = 1/19), 56.16 mg, 62% yield; yellow solid.

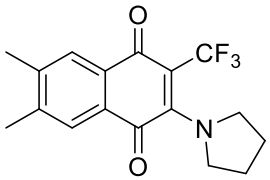
^{1}H NMR (400 MHz, $CDCl_3$): δ 7.84 (s, 2H), 7.74 (s, 2H), 3.61 (s, 8H), 2.38 (d, *J* = 4.6 Hz, 15H), 1.77 (d, *J* = 9.5 Hz, 8H), 1.59 (s, 4H).

^{19}F NMR (377 MHz, $CDCl_3$): δ -56.61 (s, 3F).

^{13}C {^{1}H} NMR (101 MHz, $CDCl_3$): δ 183.6, 181.5, 152.8, 144.7, 142.7, 130.4, 129.7, 127.8, 127.1, 123.9 (q, *J* = 275.7 Hz), 113.6 (q, *J* = 30.3 Hz), 55.2, 27.1, 24.1, 20.4, 20.2.

HRMS (ESI) m/z: $[M+H]^+$ Calcd. For $C_{18}H_{19}NO_2F_3$: 338.1368 found: 338.1370.

6,7-dimethyl-2-(pyrrolidin-1-yl)-3-(trifluoromethyl)naphthalene-1,4-dione (4n)



The compound **4n** was purified by column chromatography on basic alumina (Eluent: EtOAc/Hexane = 1/19), 52.09 mg, 60% yield; yellow solid.

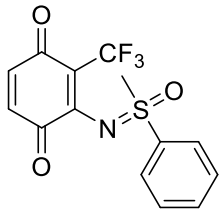
^{1}H NMR (400 MHz, $CDCl_3$): ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.84 (s, 1H), 7.64 (s, 1H), 3.82 (s, 4H), 2.37 (d, *J* = 9.0 Hz, 6H), 1.96 (t, *J* = 6.5 Hz, 4H).

^{19}F NMR (377 MHz, $CDCl_3$): δ -52.60 (s, 3F).

^{13}C {^{1}H} NMR (101 MHz, $CDCl_3$): δ 183.2, 178.1, 154.2, 143.8, 140.8, 129.8 (d, *J* = 1.2 Hz), 127.8, 126.7 (d, *J* = 3.1 Hz), 126.2, 125.7, 100.8 (q, *J* = 29.7 Hz), 53.4, 24.1, 19.3, 18.9.

HRMS (ESI) m/z: $[M+H]^+$ Calcd. For $C_{17}H_{17}F_3NO_2$: 324.1211 found: 324.1207.

2-((methyl(oxo)(phenyl)-λ^{6}-sulfaneylidene)amino)-3-(trifluoromethyl)cyclohexa-2,5-diene-1,4-dione (5a)



The compound 5**a** was purified by column chromatography on silica gel (Eluent: EtOAc/Hexane = 3/17), 118.80 mg, 78% yield; yellow solid.

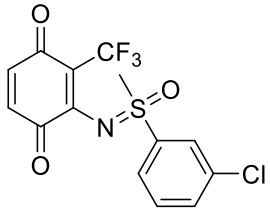
^{1}H NMR (400 MHz, CDCl3): δ 7.98-7.95 (m, 2H), 7.69 – 7.59 (m, 3H), 6.66 (q, J = 10.1 Hz, 2H), 3.38 (s, 3H).

^{19}F NMR (377 MHz, $CDCl_3$): δ -51.67 (s, 3F).

^{13}C {^{1}H} NMR (101 MHz, $CDCl_3$): δ 182.6, 182.2, 148.8, 140.9, 139.3, 133.6, 132.6, 129.9, 126.4, 123.1(q, *J* = 277.7 Hz), 115.0 (q, *J* = 27.1 Hz), 49.4.

HRMS (ESI) m/z: $[M+H]^+$ Calcd. For $C_{14}H_{11}F_3NO_3S$: 330.0412; found: 330.0410.

2-(((3-chlorophenyl)(methyl)(oxo)-λ^6-sulfaneylidene)amino)-3-(trifluoromethyl)cyclohexa-2,5-diene-1,4-dione (5b)



The compound **5b** was purified by column chromatography on silica gel (Eluent: EtOAc/Hexane = 1/9), 126.04 mg, 75% yield; yellow solid.

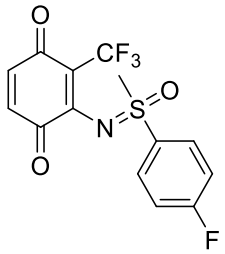
^{1}H NMR (400 MHz, $CDCl_3$): δ 7.95 (t, *J* = 1.8 Hz, 1H), 7.82 (d, *J* = 7.9 Hz, 1H), 7.63 (d, *J* = 8.7 Hz, 1H), 7.55 (t, *J* = 7.9 Hz, 1H), 6.71 – 6.64 (m, 2H), 3.38 (s, 3H).

^{19}F NMR (377 MHz, $CDCl_3$): δ -57.63 (s, 3F).

^{13}C {^{1}H} NMR (101 MHz, $CDCl_3$): δ 182.5, 182.3, 148.2, 142.9, 139.3, 136.2, 133.8, 132.7, 131.2, 126.6, 126.0 (q, *J* = 275.9 Hz), 124.5, 115.5 (q, *J* = 30.3 Hz), 49.4.

HRMS (ESI) m/z: $[M+H]^+$ Calcd. For $C_{14}H_{10}NO_3F_3ClS$: 364.0022; found: 364.0017.

2-(((4-fluorophenyl)(methyl)(oxo)-λ^6-sulfaneylidene)amino)-3-(trifluoromethyl)cyclohexa-2,5-diene-1,4-dione (5c)



The compound **5c** was purified by column chromatography on silica gel (Eluent: EtOAc/Hexane = 3/7), 101.20 mg, 63% yield; yellow solid.

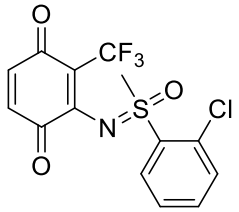
^{1}H NMR (400 MHz, $CDCl_3$): δ 8.01 – 7.96 (m, 2H), 7.31 – 7.27 (m, 2H), 6.68 (q, *J* = 10.1 Hz, 2H), 3.39 (s, 3H).

^{19}F NMR (377 MHz, $CDCl_3$): δ -57.62 (s, 3F), -103.58 (m, 1F).

^{13}C {^{1}H} NMR (101 MHz, $CDCl_3$): δ 182.5, 182.3, 165.7 (d, *J* = 256.5 Hz), 148.5, 139.3 (d, *J* = 1.1 Hz), 137.0 (d, *J* = 3.5 Hz), 132.7, 129.4 (d, *J* = 9.6 Hz), 123.0 (q, *J* = 275.7 Hz), 117.3, 117.1, 115.6 (q, *J* = 27.1 Hz), 49.52.

HRMS (ESI) m/z: $[M+H]^+$ Calcd. For $C_{14}H_{10}F_4NO_3S$: 348.0318; found: 348.0315.

2-(((2-chlorophenyl)(methyl)(oxo)-λ^6-sulfaneylidene)amino)-3-(trifluoromethyl)cyclohexa-2,5-diene-1,4-dione (5d)



The compound **5d** was purified by column chromatography on silica gel (Eluent: EtOAc/Hexane = 2/8), 100.83 mg, 60% yield; yellow solid.

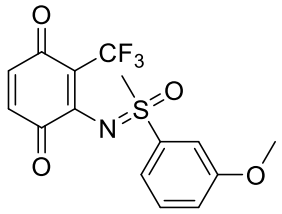
^{1}H NMR (400 MHz, $CDCl_3$): δ 8.39 – 8.35 (m, 1H), 7.60 – 7.56 (m, 2H), 7.53 – 7.50 (m, 1H), 6.67 (d, *J* = 10.0 Hz, 1H), 6.59 (d, *J* = 10.0 Hz, 1H), 3.48 (s, 3H).

^{19}F NMR (377 MHz, $CDCl_3$): δ -57.28 (s, 3F).

^{13}C {^{1}H} NMR (101 MHz, $CDCl_3$): δ 182.7, 182.0, 147.7, 139.4, 138.4, 134.4, 132.6, 132.3, 131.3, 130.8, 128.0, 122.8 (q, *J* = 277.7 Hz), 116.4 (q, *J* = 38.4 Hz), 47.2.

HRMS (ESI) m/z: $[M+H]^+$ Calcd. For $C_{14}H_{10}NO_3F_3SCl$: 364.0022; found: 364.0020.

2-(((3-methoxyphenyl)(methyl)(oxo)-λ^6-sulfaneylidene)amino)-3-(trifluoromethyl)cyclohexa-2,5-diene-1,4-dione (5e)



The compound **5e** was purified by column chromatography on silica gel (Eluent: EtOAc/Hexane = 2/8), 108.03 mg, 65% yield; yellow solid.

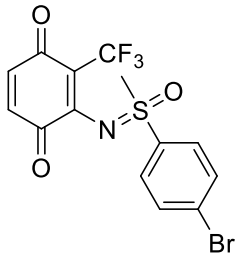
^{1}H NMR (400 MHz, $CDCl_3$): δ 7.91 – 7.85 (m, 2H), 7.07 – 7.03 (m, 2H), 6.64 (d, *J* = 6.2 Hz, 2H), 3.88 (s, 3H), 3.37 (s, 3H).

^{19}F NMR (377 MHz, $CDCl_3$): δ -57.58 (s, 3F).

^{13}C {^{1}H} NMR (101 MHz, $CDCl_3$): δ 182.6, 182.3, 163.6, 149.1, 139.2, 132.7, 132.0, 130.4, 128.7, 121.5 (q, *J* = 39.3 Hz), 114.9 (d, *J* = 12.6 Hz), 55.9, 46.7.

HRMS (ESI) m/z: $[M+H]^+$ Calcd. For $C_{15}H_{13}F_3NO_4S$: 360.0517; found: 360.0515.

2-(((4-bromophenyl)(methyl)(oxo)-λ^6-sulfaneylidene)amino)-3-(trifluoromethyl)cyclohexa-2,5-diene-1,4-dione (5f)



The compound **5f** was purified by column chromatography on silica gel (Eluent: EtOAc/Hexane = 1/9), 135.67 mg, 72% yield; yellow solid.

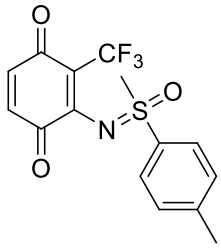
^{1}H NMR (400 MHz, $CDCl_3$): δ 7.95 (t, *J* = 1.8 Hz, 1H), 7.83 (dd, *J* = 7.8, 1.0 Hz, 1H), 7.65 – 7.61 (m, 1H), 7.55 (t, *J* = 7.9 Hz, 1H), 6.68 (q, *J* = 10.1 Hz, 2H), 3.38 (s, 3H).

^{19}F NMR (377 MHz, $CDCl_3$): δ -57.63 (s, 3F).

^{13}C {^{1}H} NMR (101 MHz, $CDCl_3$): δ 182.5, 182.3, 148.2, 142.9, 139.4, 136.2, 133.8, 132.7, 131.2, 126.6, 126.0 (q, *J* = 224.2 Hz), 124.5, 115.5 (q, *J* = 27.3 Hz), 105.1, 49.4.

HRMS (ESI) m/z: $[M+H]^+$ Calcd. For $C_{14}H_{10}F_3NO_3SBr$: 407.9517; found: 407.9519.

2-((methyl(oxo)(p-tolyl)-λ^6-sulfaneylidene)amino)-3-(trifluoromethyl)cyclohexa-2,5-diene-1,4-dione (5g)



The compound **5g** was purified by column chromatography on silica gel (Eluent: EtOAc/Hexane = 1/9), 114.33 mg, 69% yield; yellow solid.

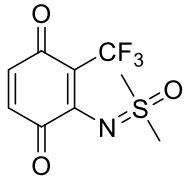
^{1}H NMR (400 MHz, $CDCl_3$): δ 7.82 (d, *J* = 8.4 Hz, 2H), 7.39 (d, *J* = 8.0 Hz, 2H), 6.63 (q, *J* = 10.1 Hz, 2H), 3.36 (s, 3H), 2.45 (s, 3H).

^{19}F NMR (377 MHz, $CDCl_3$): δ -57.5 8 (s, 3F).

^{13}C {^{1}H} NMR (101 MHz, $CDCl_3$): δ 182.7, 182.2, 149.0, 144.8, 139.2 (d, *J* = 1.1 Hz), 137.8, 132.7, 130.5, 126.4, 121.3 (q, *J* = 161.6 Hz), 114.8 (q, *J* = 27.1 Hz), 49.5, 21.7.

HRMS (ESI) m/z: $[M+H]^+$ Calcd. For $C_{15}H_{13}F_3NO_3S$: 344.0568; found: 344.0569.

2-((dimethyl(oxo)-λ^6-sulfaneylidene)amino)-3-(trifluoromethyl)cyclohexa-2,5-diene-1,4-dione (5h)



The compound **5h** was purified by column chromatography on silica gel (Eluent: EtOAc/Hexane = 2/8), 82.81 mg, 67% yield; yellow solid.

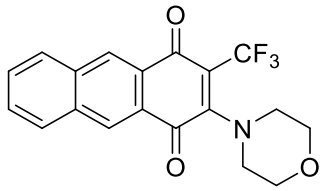
^{1}H NMR (400 MHz, $CDCl_3$): δ 6.64 (q, *J* = 10.1 Hz, 1H), 3.31 (s, 3H).

^{19}F NMR (377 MHz, $CDCl_3$): δ -57.53 (s, 3F).

^{13}C {^{1}H} NMR (101 MHz, $CDCl_3$): δ 183.5, 182.6, 148.7, 139.5, 132.9, 124.3, 121.4 (q, *J* =37.5 Hz), 46.8.

HRMS (ESI) m/z: $[M+H]^+$ Calcd. For $C_9H_9F_3N_2O_3S$: 268.0255; found: 268.0254.

2-morpholino-3-(trifluoromethyl)anthracene-1,4-dione (5i)



The compound **5i** was purified by column chromatography on basic alumina (Eluent: EtOAc/Hexane = 1/9), 55.53 mg, 64% yield; orange coloured solid.

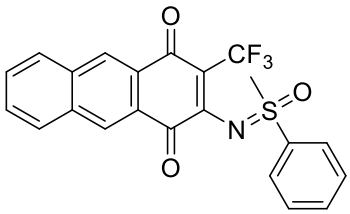
^{1}H NMR (400 MHz, $CDCl_3$): δ 8.61 (s, 1H), 8.55 (s, 1H), 8.07 – 8.02 (m, 2H), 7.72 – 7.65 (m, 2H), 3.93 – 3.89 (m, 4H), 3.79 – 3.75 (m, 4H).

^{19}F NMR (377 MHz, $CDCl_3$): δ -56.95 (s, 3F).

^{13}C {^{1}H} NMR (101 MHz, $CDCl_3$): δ 183.3, 180.9, 153.0, 135.6, 134.7, 130.2, 130.0, 129.7, 129.4, 128.3, 128.1, 123.5 (q, *J* = 274.7 Hz), 113.4 (q, *J* = 17.4 Hz), 67.5, 54.1.

HRMS (ESI) m/z: $[M+H]^+$ Calcd. For $C_{19}H_{15}NO_3F_3$: 362.1004; found: 362.1006.

2-((methyl(oxo)(phenyl)- λ^6-sulfaneylidene)amino)-3-(trifluoromethyl)anthracene-1,4-dione (5j)



The compound **5j** was purified by column chromatography on silica gel (Eluent: EtOAc/Hexane = 2/8), 59.81 mg, 58% yield; yellow solid.

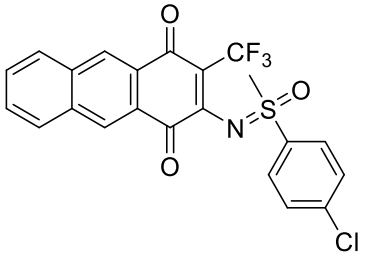
^{1}H NMR (400 MHz, $CDCl_3$): δ 8.60 (s, 1H), 8.48 (s, 1H), 8.04 – 8.00 (m, 3H), 7.93 (d, *J* = 7.9 Hz, 1H), 7.68-7.60 (m, 5H), 3.43 (s, 3H).

^{19}F NMR (377 MHz, $CDCl_3$): δ -57.35 (s, 3F).

^{13}C {^{1}H} NMR (101 MHz, $CDCl_3$): δ 180.6, 180.2, 151.6, 141.6, 135.8, 134.4, 133.4, 130.2 (2C), 130.0 (2C), 129.9, 129.4, 128.8, 128.6, 126.4, 123.6 (q, *J* = 278.7 Hz), 118.4 (q, *J* = 26.0 Hz), 49.7.

HRMS (ESI) m/z: $[M+H]^+$ Calcd. For $C_{22}H_{15}F_3NO_3S$: 430.0725; found: 430.0727.

2-(((4-chlorophenyl)(methyl)(oxo)-λ^6-sulfaneylidene)amino)-3-(trifluoromethyl)anthracene-1,4-dione (5k)



The compound **5k** was purified by column chromatography on silica gel (Eluent: EtOAc/Hexane = 3/17), 58.98 mg, 53% yield; yellow solid.

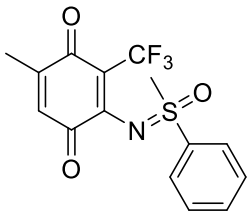
^{1}H NMR (400 MHz, $CDCl_3$): δ 8.58 (s, 1H), 8.48 (s, 1H), 8.01 (d, *J* = 8.1 Hz, 1H), 8.00 – 7.96 (m, 2H), 7.93 (d, *J* = 8.0 Hz, 1H), 7.68-7.62 (m, 2H), 7.61 – 7.58 (m, 2H), 3.44 (s, 3H).

^{19}F NMR (377 MHz, $CDCl_3$): δ -57.32 (s, 3F).

^{13}C {^{1}H} NMR (101 MHz, $CDCl_3$): δ 180.6, 180.1, 151.2, 140.1 (d, *J* = 4.4 Hz), 135.6, 134.4, 130.2 (t, *J* = 6.5 Hz), 129.4, 128.7, 127.9, 126.2, 123.4 (q, *J* = 277.7 Hz), 118.7 (q, *J* = 26.0 Hz), 49.61 (s).

.**HRMS (ESI) m/z:** $[M+H]^+$ Calcd. For $C_{22}H_{14}F_3NO_3SCl$: 464.0335; found: 464.0341.

5-methyl-2-((methyl(oxo)(phenyl)-l6-sulfaneylidene)amino)-3-(trifluoromethyl)cyclohexa-2,5-diene-1,4-dione (5l)



The compound **5l** was purified by column chromatography on silica gel (Eluent: EtOAc/Hexane = 1/9), 97.8 mg, 70% yield; yellow solid.

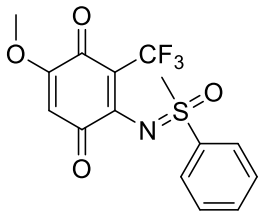
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.96 – 7.92 (m, 2H), 7.66 – 7.57 (m, 3H), 6.48 (d, *J* = 1.6 Hz, 1H), 3.35 (s, 3H), 2.05 (d, *J* = 1.6 Hz, 3H).

^{19}F NMR (377 MHz, $CDCl_3$) δ -57.50 (s).

^{13}C NMR (101 MHz, $CDCl_3$) δ 182.9, 182.1, 149.1, 148.7, 141.2, 133.5, 129.8 (d, *J* = 15.3 Hz), 126.4, 121.9, 103.3, 49.4, 16.4.

HRMS (ESI) m/z: $[M+H]^+$ Calcd. For $C_{15}H_{13}F_3NO_3S$: 344.0568; found: 344.0552.

5-methoxy-2-((methyl(oxo)(phenyl)-l6-sulfaneylidene)amino)-3-(trifluoromethyl)cyclohexa-2,5-diene-1,4-dione (5m)



The compound **5m** was purified by column chromatography on silica gel (Eluent: EtOAc/Hexane = 1/9), 94.5 mg, 73% yield; yellow solid.

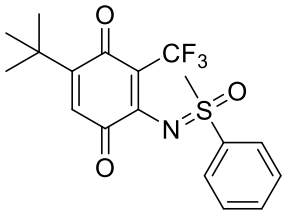
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.96 – 7.92 (m, 2H), 7.64 – 7.56 (m, 3H), 5.81 (s, 1H), 3.72 (s, 3H), 3.35 (s, 3H).

^{19}F NMR (377 MHz, $CDCl_3$) δ -57.05 (s).

^{13}C NMR (101 MHz, $CDCl_3$) δ 182.9, 178.0, 155.9, 147.1, 141.2, 133.5, 129.8, 126.4, 122.9 (q, *J* = 272.7 Hz), 114.0 (q, *J* = 27.1 Hz), 109.2 (d, *J* = 1.4 Hz), 56.5, 49.4.

HRMS (ESI) m/z: $[M+H]^+$ Calcd. For $C_{15}H_{13}F_3NO_4S$: 360.0517; found: 360.0361.

5-(tert-butyl)-2-((methyl(oxo)(phenyl)-l6-sulfaneylidene)amino)-3-(trifluoromethyl)cyclohexa-2,5-diene-1,4-dione (5n)



The compound **5n** was purified by column chromatography on silica gel (Eluent: EtOAc/Hexane = 1/9), 86.0 mg, 71% yield; yellow solid.

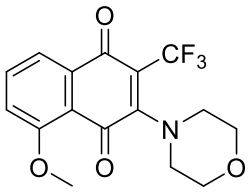
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.96 – 7.94 (m, 2H), 7.65 – 7.57 (m, 3H), 6.47 (s, 1H), 3.40 (s, 3H), 1.12 (s, 9H).

^{19}F NMR (377 MHz, $CDCl_3$) δ -57.71 (s).

^{13}C NMR (101 MHz, $CDCl_3$) δ 183.2, 182.4, 152.7, 150.5, 141.0, 134.1, 134.5, 129.8, 126.6, 123.0 (q, *J* = 282.8 Hz), 113.4 (q, *J* = 28.3 Hz), 49.3, 35.1, 28.9.

HRMS (ESI) m/z: $[M+H]^+$ Calcd. For $C_{18}H_{19}F_3NO_3S$: 386.1038; found: 386.1023.

5-methoxy-3-morpholino-2-(trifluoromethyl)naphthalene-1,4-dione (8a)



The compound **8a** was purified by column chromatography on silica gel (Eluent: EtOAc/Hexane = 1/9), 39.0 mg, 43% yield; orange coloured solid.

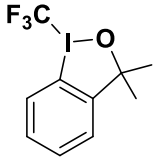
^{1}H NMR (400 MHz, $CDCl_3$): δ 8.15 – 8.09 (m, 3H), 7.92 (d, *J* = 7.6 Hz, 1H), 7.70 – 7.66 (m, 1H), 7.62 – 7.57 (m, 1H), 3.9 (m, 4H), 3.68 (m, 4H).

^{19}F NMR (377 MHz, $CDCl_3$): δ -56.38 (s, 3F).

^{13}C {^{1}H} NMR (101 MHz, $CDCl_3$): δ 180.6, 180.2, 151.6, 141.6, 135.8, 134.4, 133.4, 130.2 (2C), 130.0 (2C), 129.9, 129.4, 128.8, 128.6, 126.4, 125.0, 122.2, 118.4 (q, *J* = 26.0 Hz), 49.7.

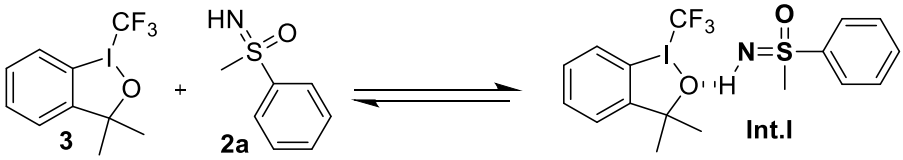
HRMS (ESI) m/z: $[M+H]^+$ Calcd. For $C_{16}H_{15}F_3NO_4$: 342.0953; found: 342.0948.

3,3-dimethyl-1-(trifluoromethyl)-1,3-dihydro-1λ^3-benzo[d][1,2]iodaoxole



^{19}F NMR (377 MHz, $CDCl_3$): δ 39.90 (s, 3F).

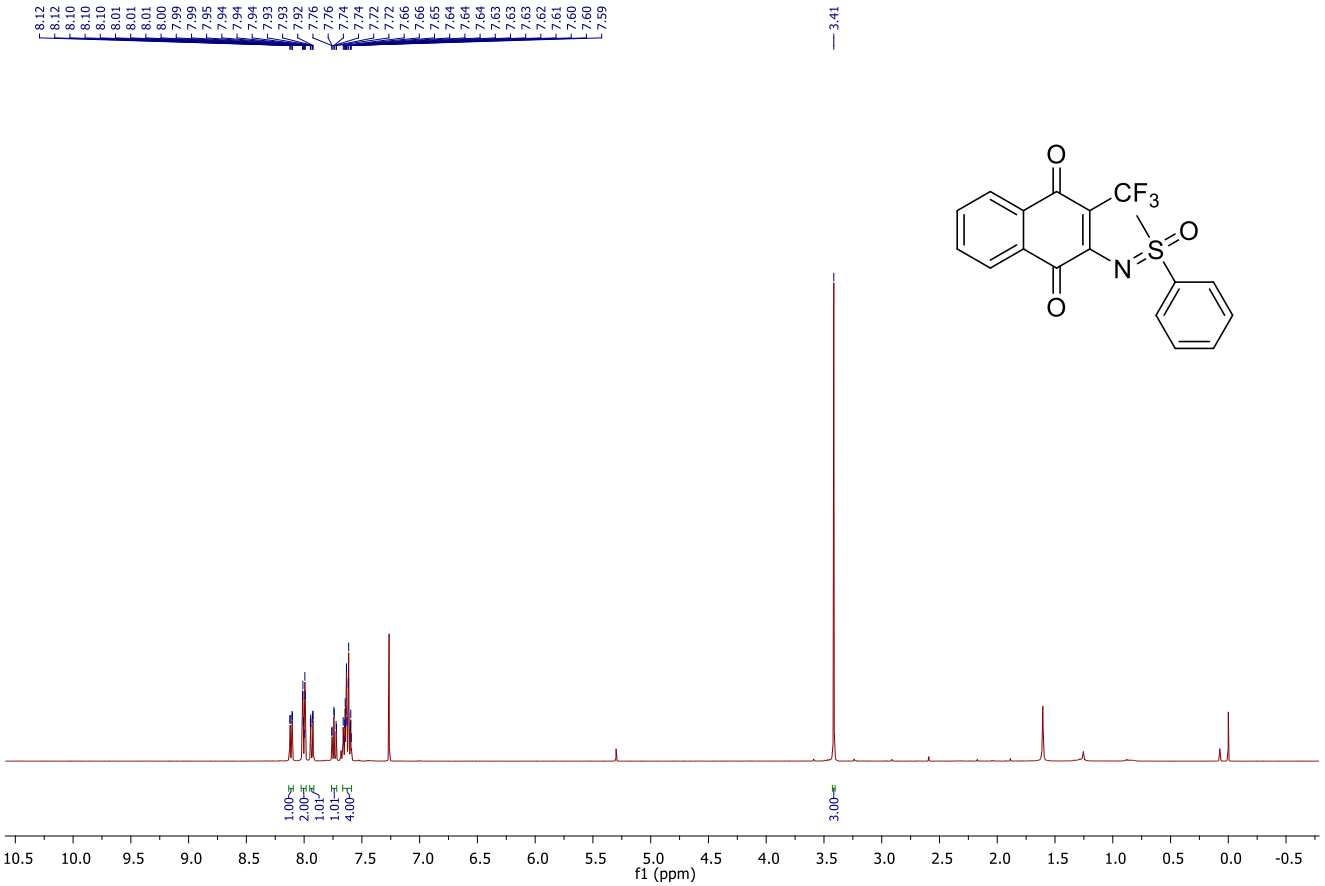
Togni-1 + Sulfoximine



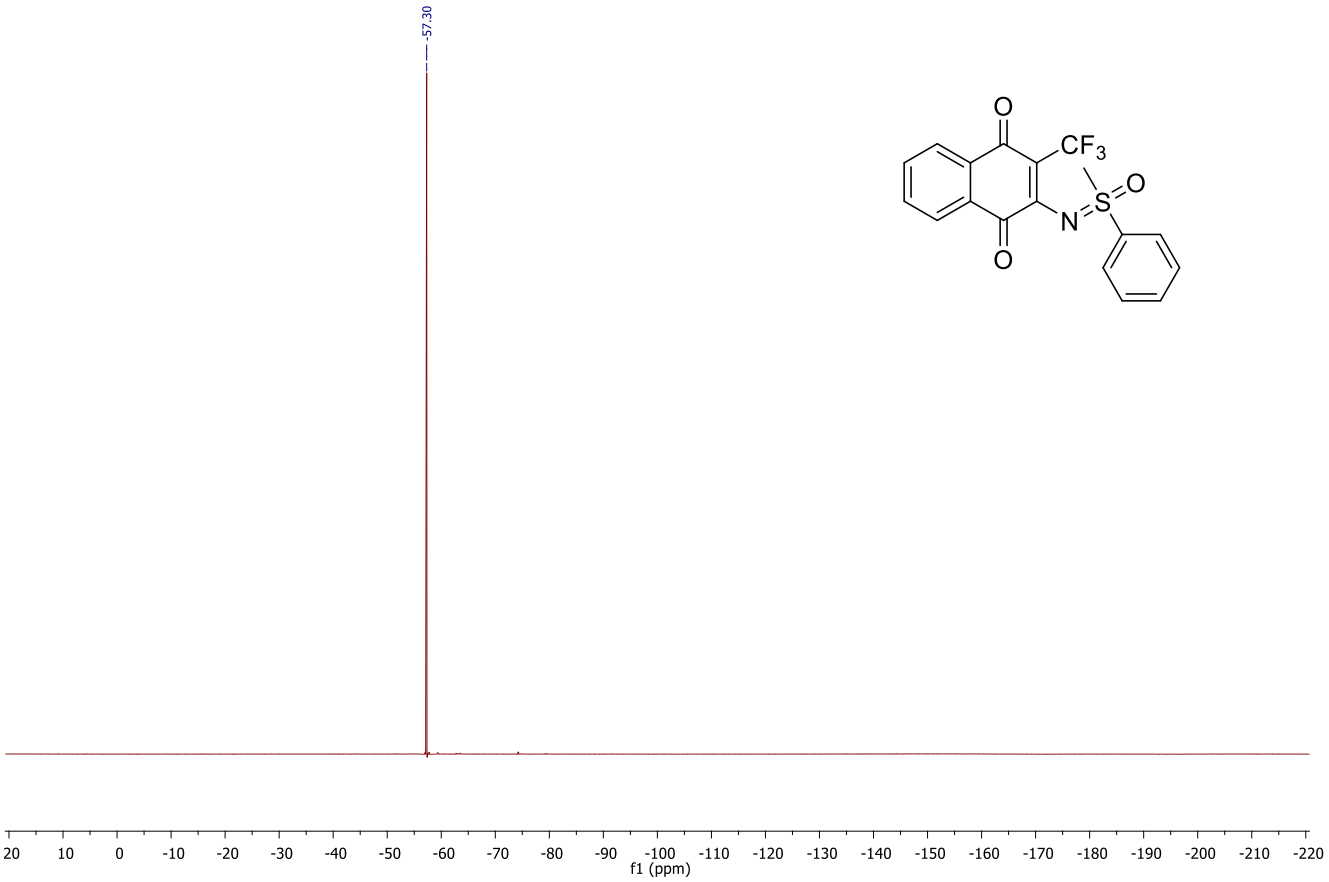
^{19}F NMR (377 MHz, $CDCl_3$): δ 39.54 (s, 3F).

^{1}H and ^{13}C $\{^{1}H\}$ NMR and HRMS Spectra

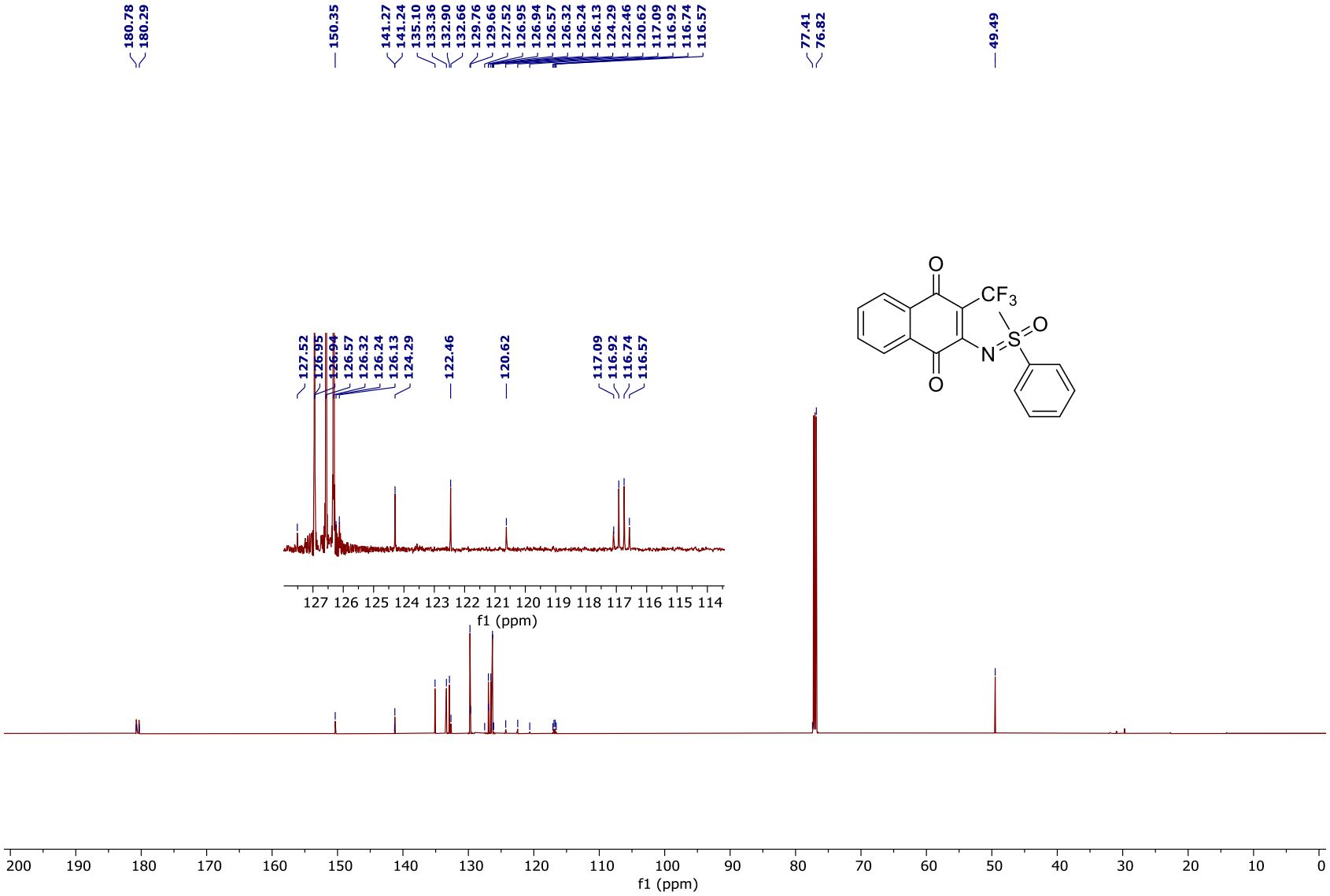
^{1}H NMR (400 MHz) of 4a in $CDCl_3$



^{19}F NMR (377 MHz) of 4a in $CDCl_3$



^{13}C {^{1}H} NMR (101 MHz) of 3a in $CDCl_3$



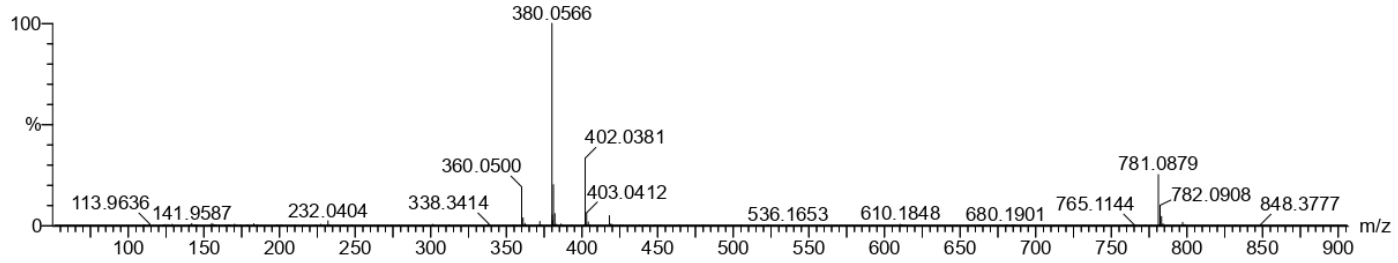
HRMS of 4a

Elemental Composition Report **Page 1**

Single Mass Analysis
Tolerance = 50.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

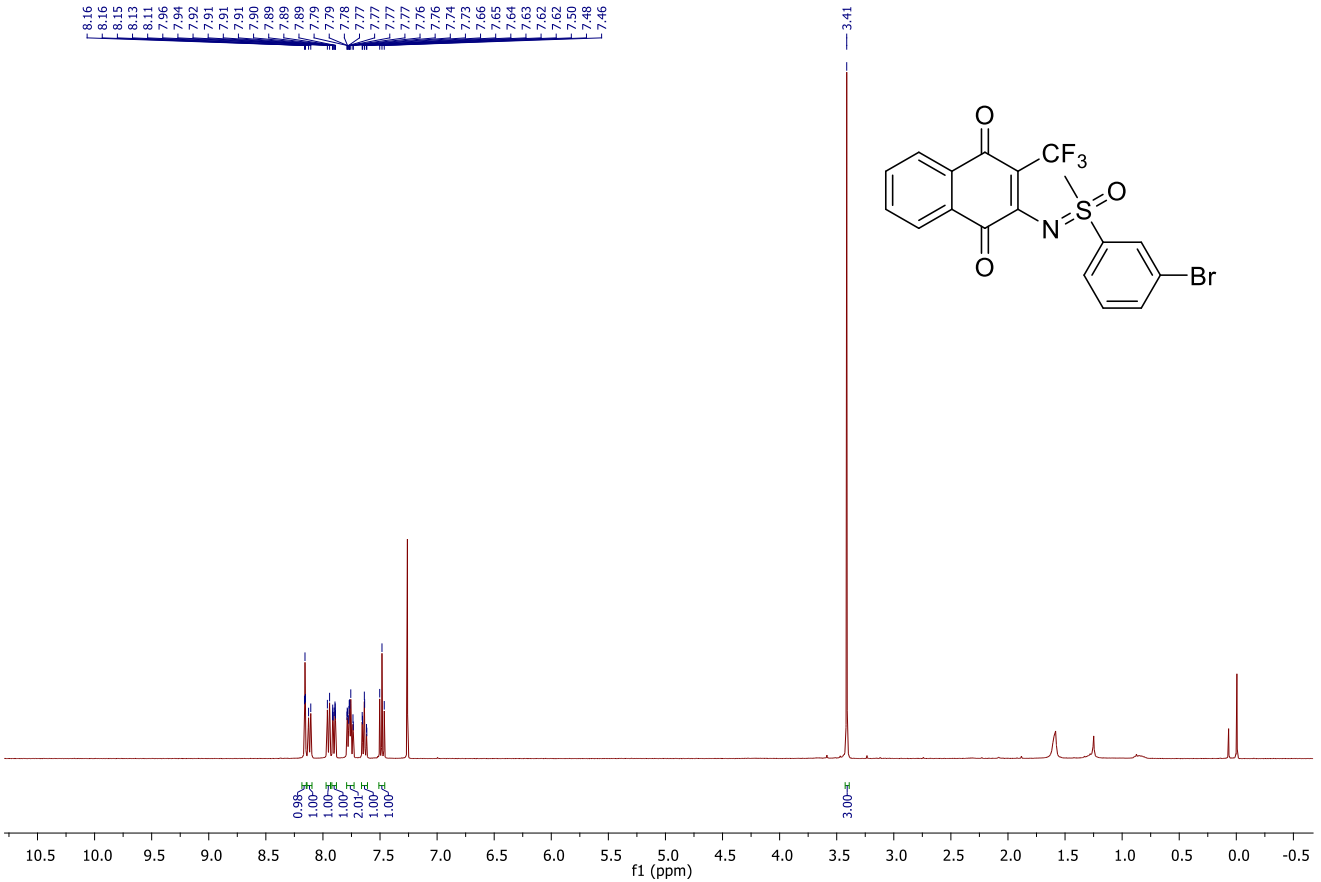
Monoisotopic Mass, Even Electron Ions
69 formula(e) evaluated with 1 results within limits (up to 3 closest results for each mass)
Elements Used:
C: 0-18 H: 0-100 N: 0-1 O: 0-3 F: 0-3 S: 0-1

NQ-1-CF3 QMI DIVISION, CSIR-IIIM JAMMU 11-Jul-2023
Xevo G2-XS QTOF YFC2015 11:58:59
110723_02 11 (0.242) 1: TOF MS ES+
1.28e+007

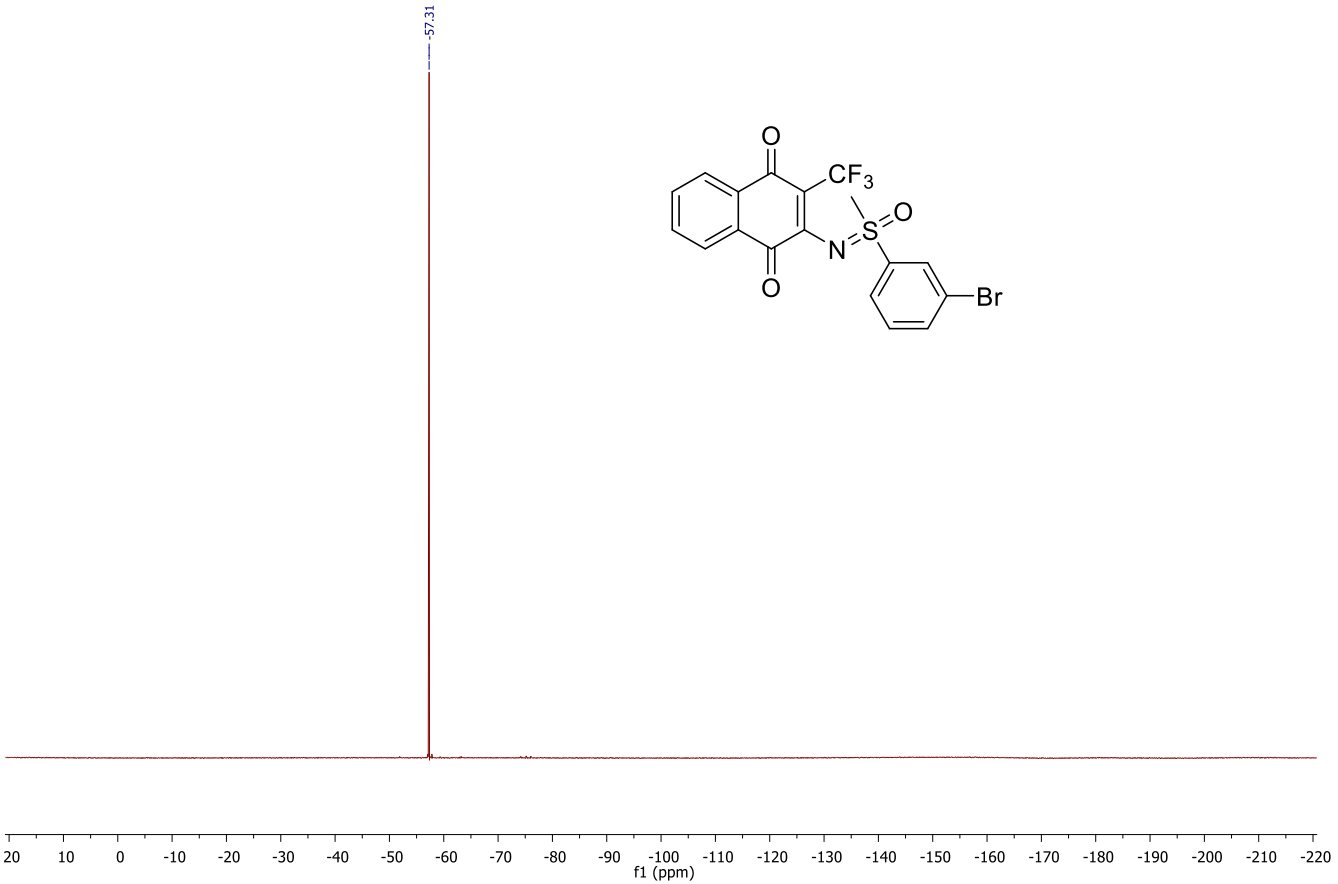


Minimum:				-1.5				
Maximum:		2.0	50.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
380.0566	380.0568	-0.2	-0.5	11.5	876.5	n/a	n/a	C18 H13 N O3 F3 S

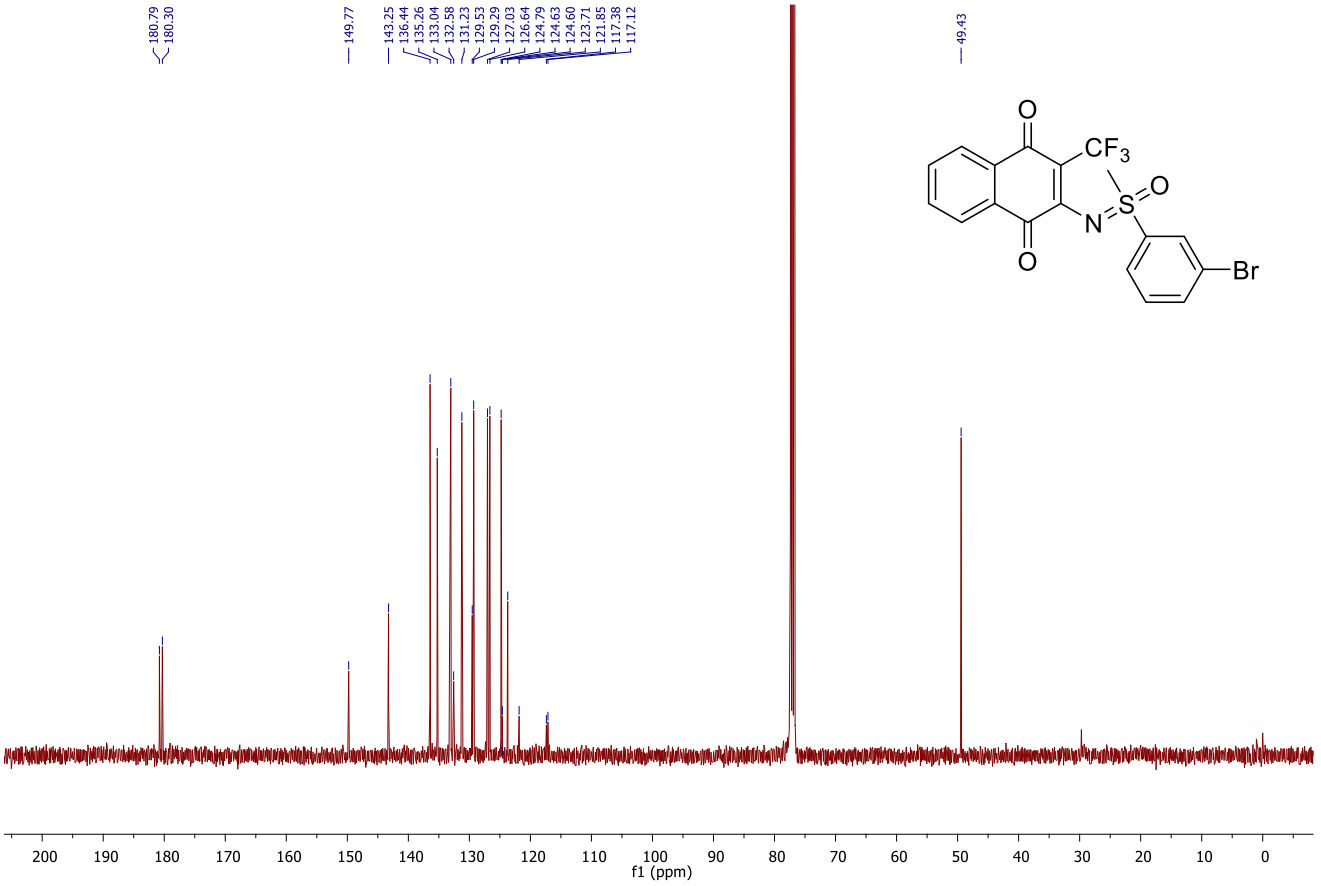
^{1}H NMR (400 MHz) of 4b in $CDCl_3$



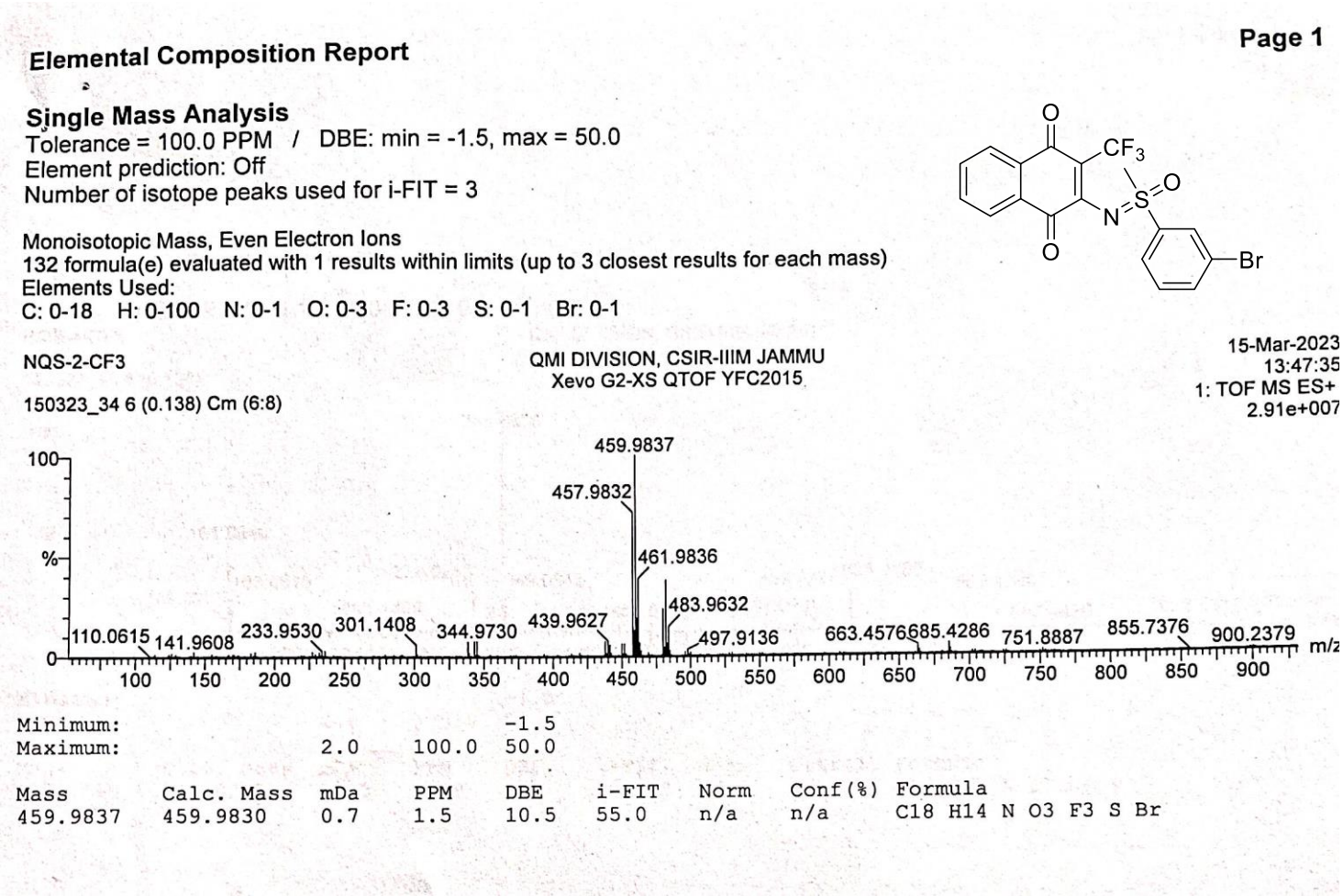
^{19}F NMR (377 MHz) of 4b in $CDCl_3$



^{13}C {^{1}H} NMR (101 MHz) of 4b in $CDCl_3$



HRMS of 4b



Elemental Composition Report

Page 1

Single Mass Analysis
Tolerance = 100.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
132 formula(e) evaluated with 1 results within limits (up to 3 closest results for each mass)
Elements Used:
C: 0-18 H: 0-100 N: 0-1 O: 0-3 F: 0-3 S: 0-1 Br: 0-1

NQS-2-CF3

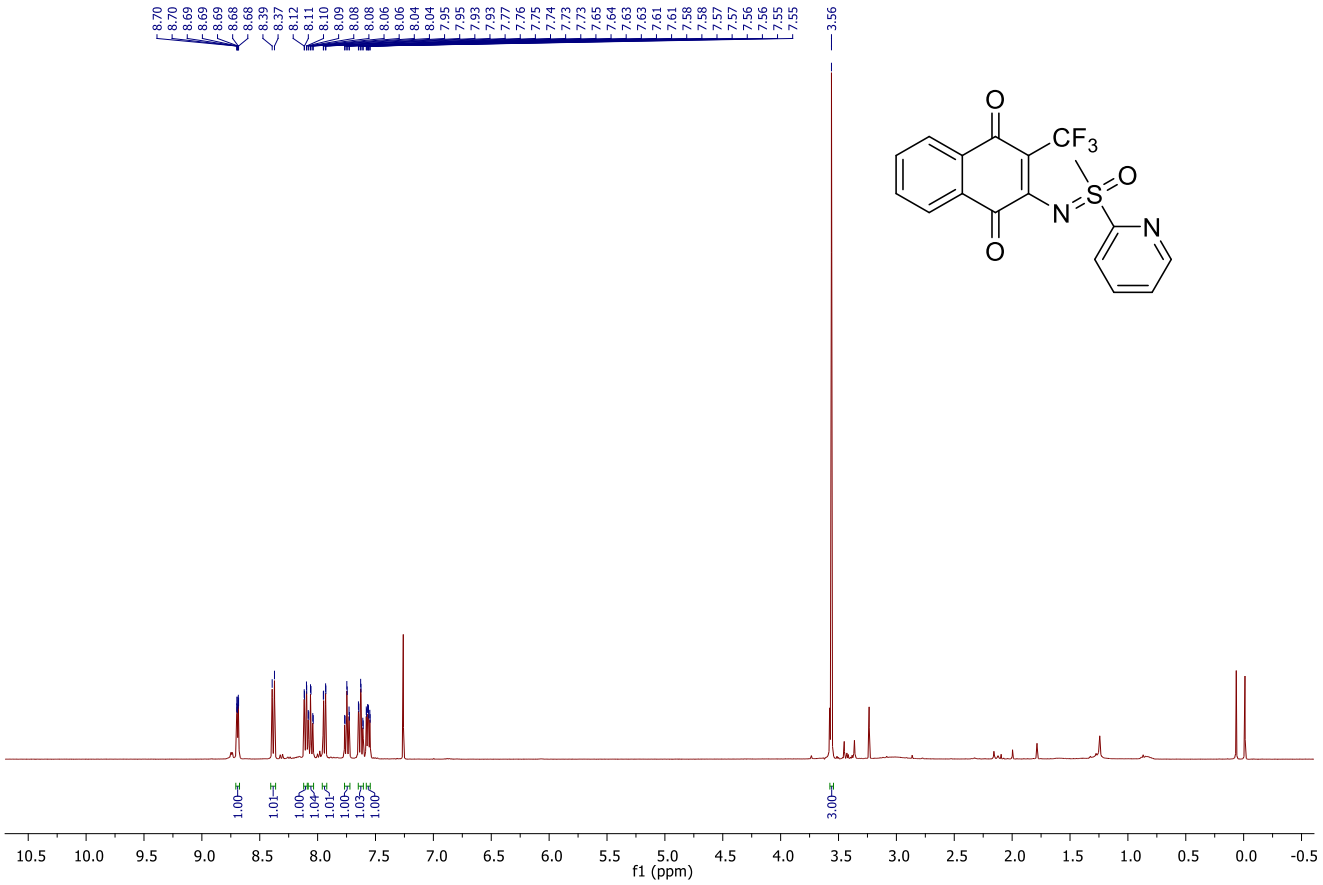
150323_34 6 (0.138) Cm (6:8)

QMI DIVISION, CSIR-IIIM JAMMU
Xevo G2-XS QTOF YFC2015

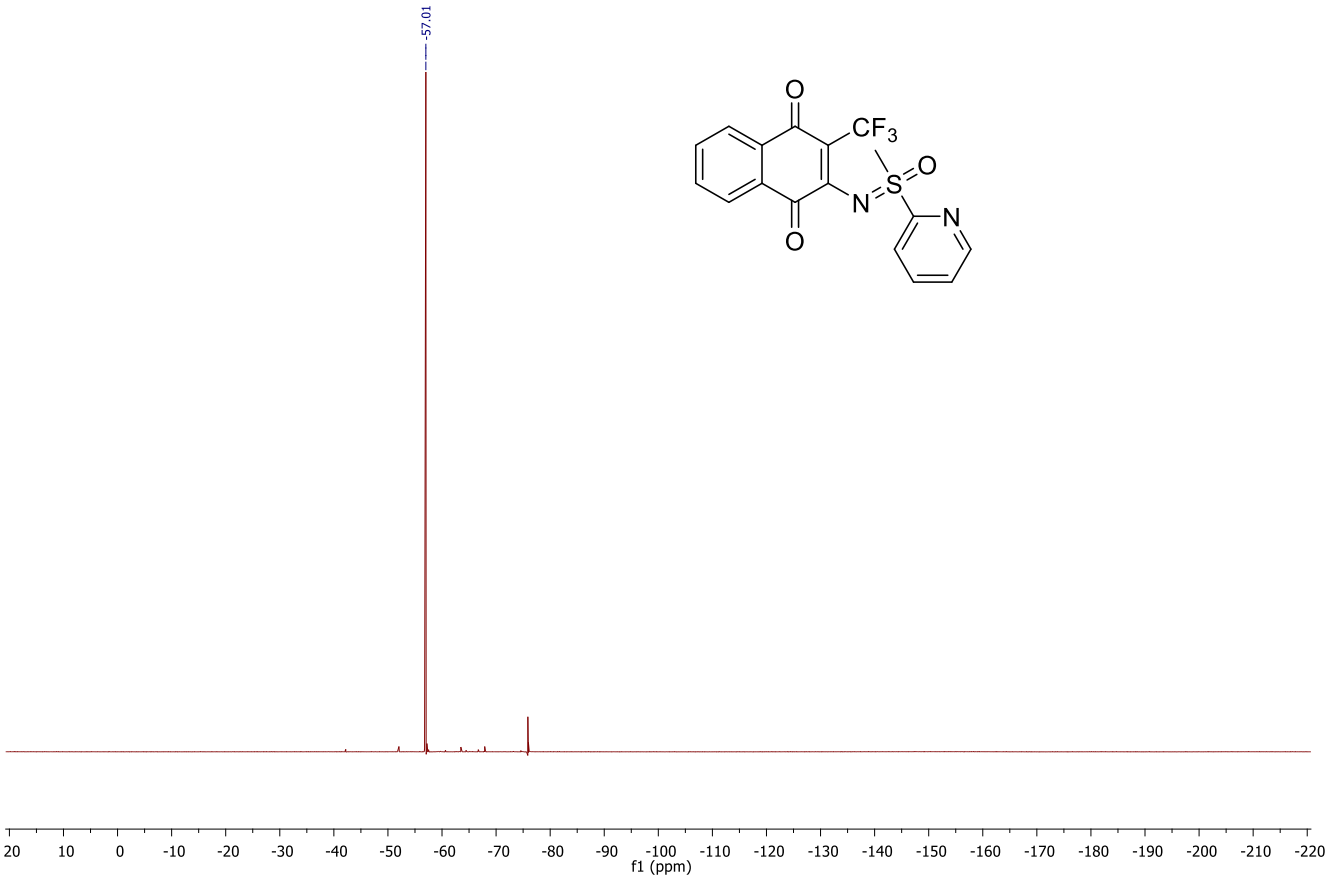
15-Mar-2023
13:47:35
1: TOF MS ES+
2.91e+007

Minimum:				-1.5				
Maximum:		2.0	100.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
459.9837	459.9830	0.7	1.5	10.5	55.0	n/a	n/a	C18 H14 N O3 F3 S Br

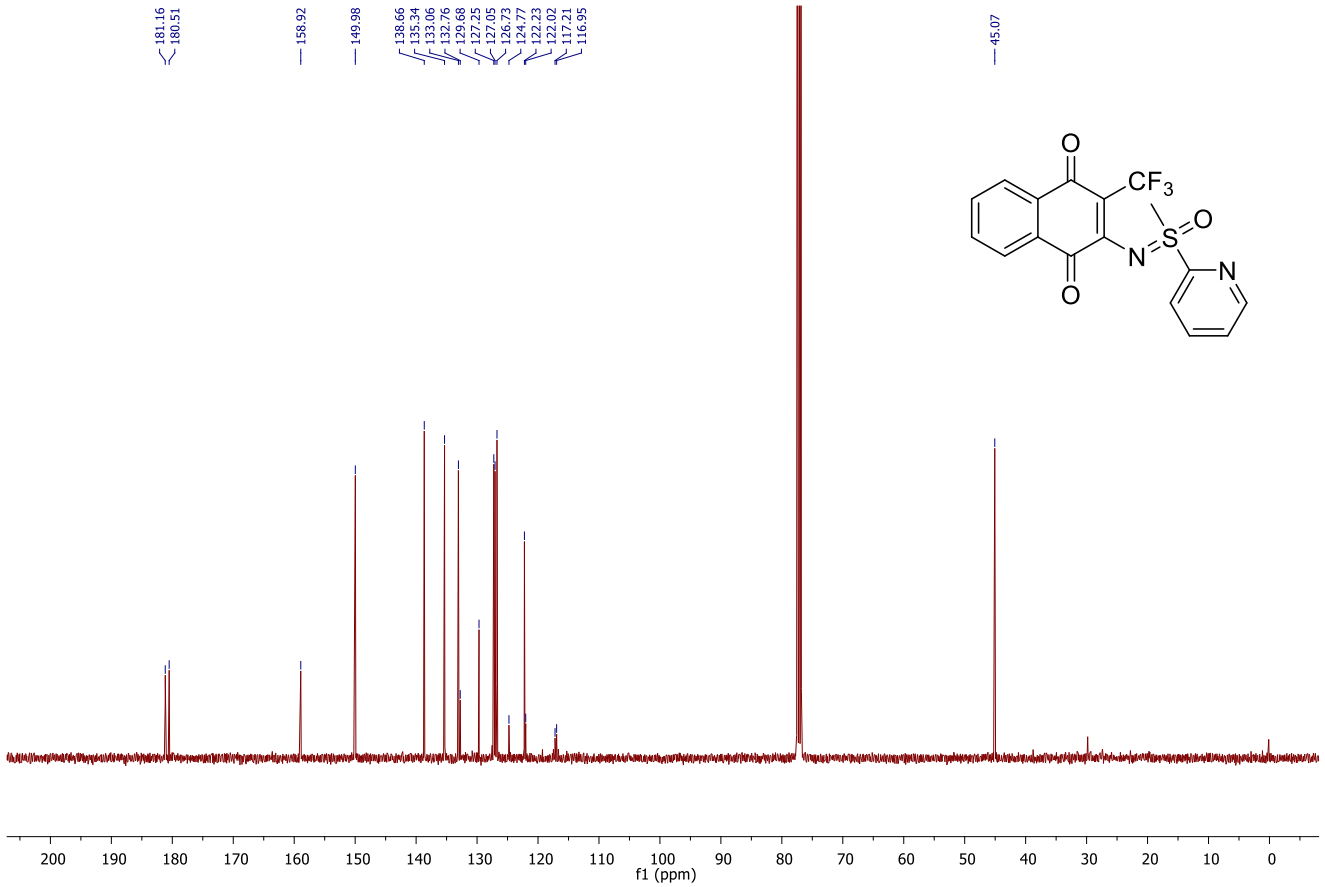
^{1}H NMR (400 MHz) of 4c in $CDCl_3$



^{19}F NMR (377 MHz) of 4c in $CDCl_3$



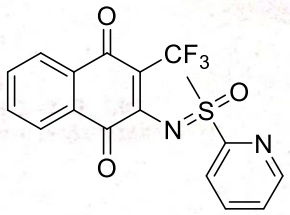
^{13}C {^{1}H} NMR (101 MHz) of 4c in $CDCl_3$



HRMS of 4c

Elemental Composition Report Page 1

Single Mass Analysis
Tolerance = 100.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

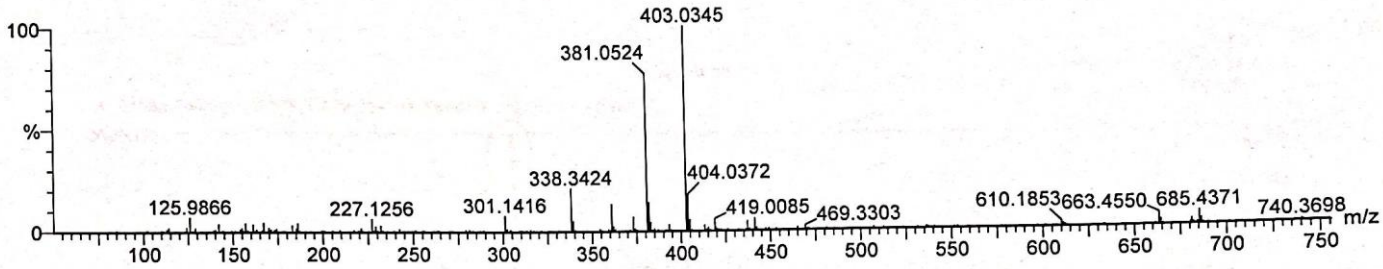


Monoisotopic Mass, Even Electron Ions
101 formula(e) evaluated with 1 results within limits (up to 3 closest results for each mass)
Elements Used:
C: 0-17 H: 0-100 N: 0-2 O: 0-3 F: 0-3 S: 0-1

NQS-3-CF3
QMI DIVISION, CSIR-IIIM JAMMU
Xevo G2-XS QTOF YFC2015

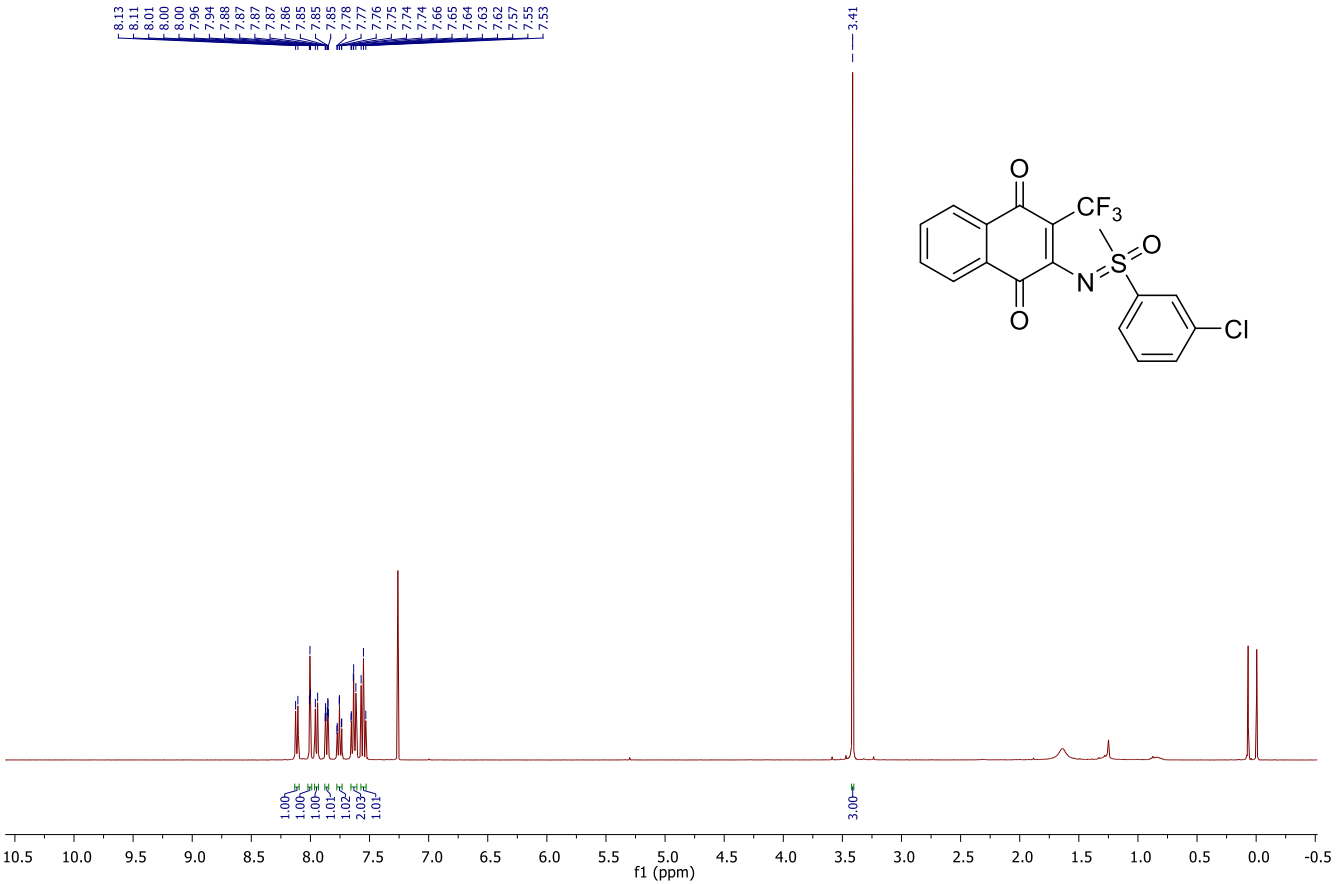
15-Mar-2023
12:42:42
1: TOF MS ES+
6.40e+006

150323_09 6 (0.138)

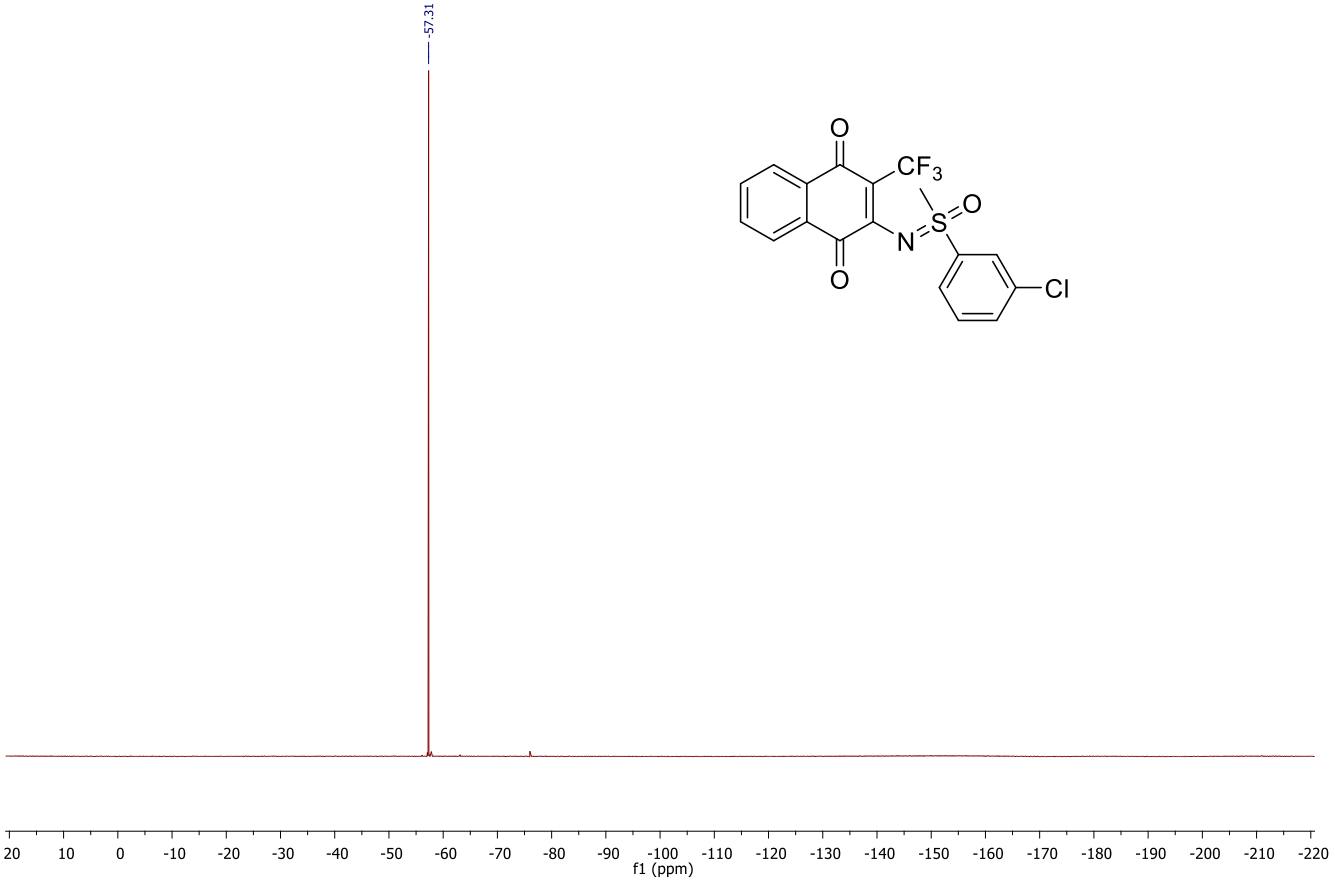


Minimum:				-1.5				
Maximum:		2.0	100.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
381.0524	381.0521	0.3	0.8	11.5	1044.7	n/a	n/a	C17 H12 N2 O3 F3 S

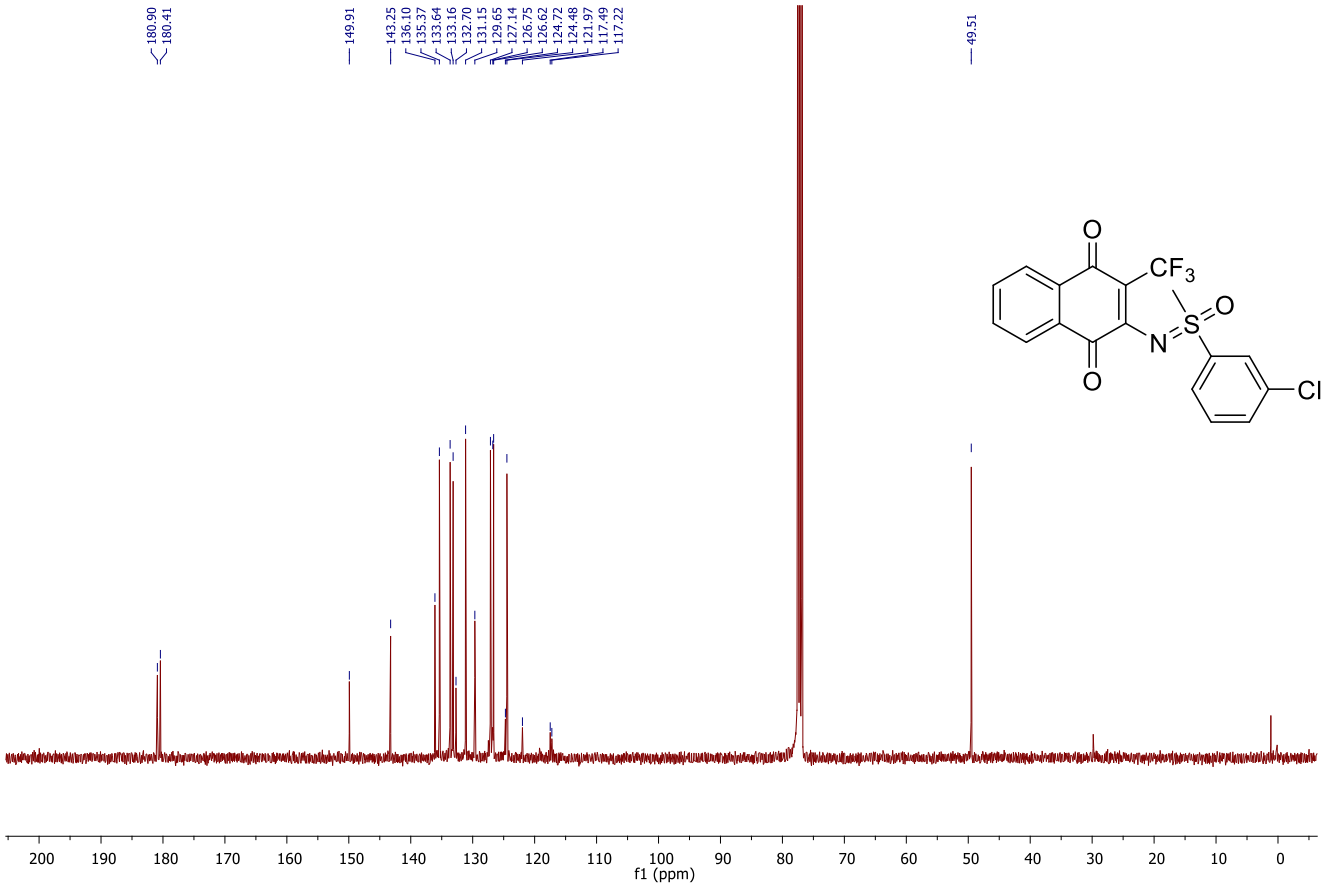
^{1}H NMR (400 MHz) of 4d in $CDCl_3$



^{19}F NMR (377 MHz) of 4d in $CDCl_3$

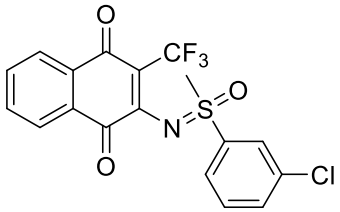


^{13}C {^{1}H} NMR (101 MHz) of 4d in $CDCl_3$



HRMS of 4d

Elemental Composition Report **Page 1**



Single Mass Analysis
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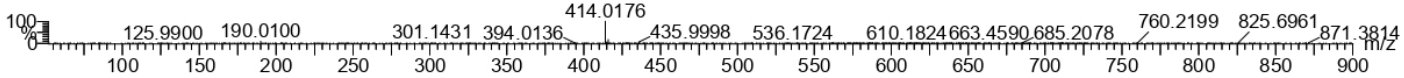
Element prediction: Off
Number of isotope peaks used for i-FIT = 4

Monoisotopic Mass, Even Electron Ions
133 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 0-18 H: 0-100 N: 0-1 O: 0-3 F: 0-3 S: 0-1 Cl: 0-1

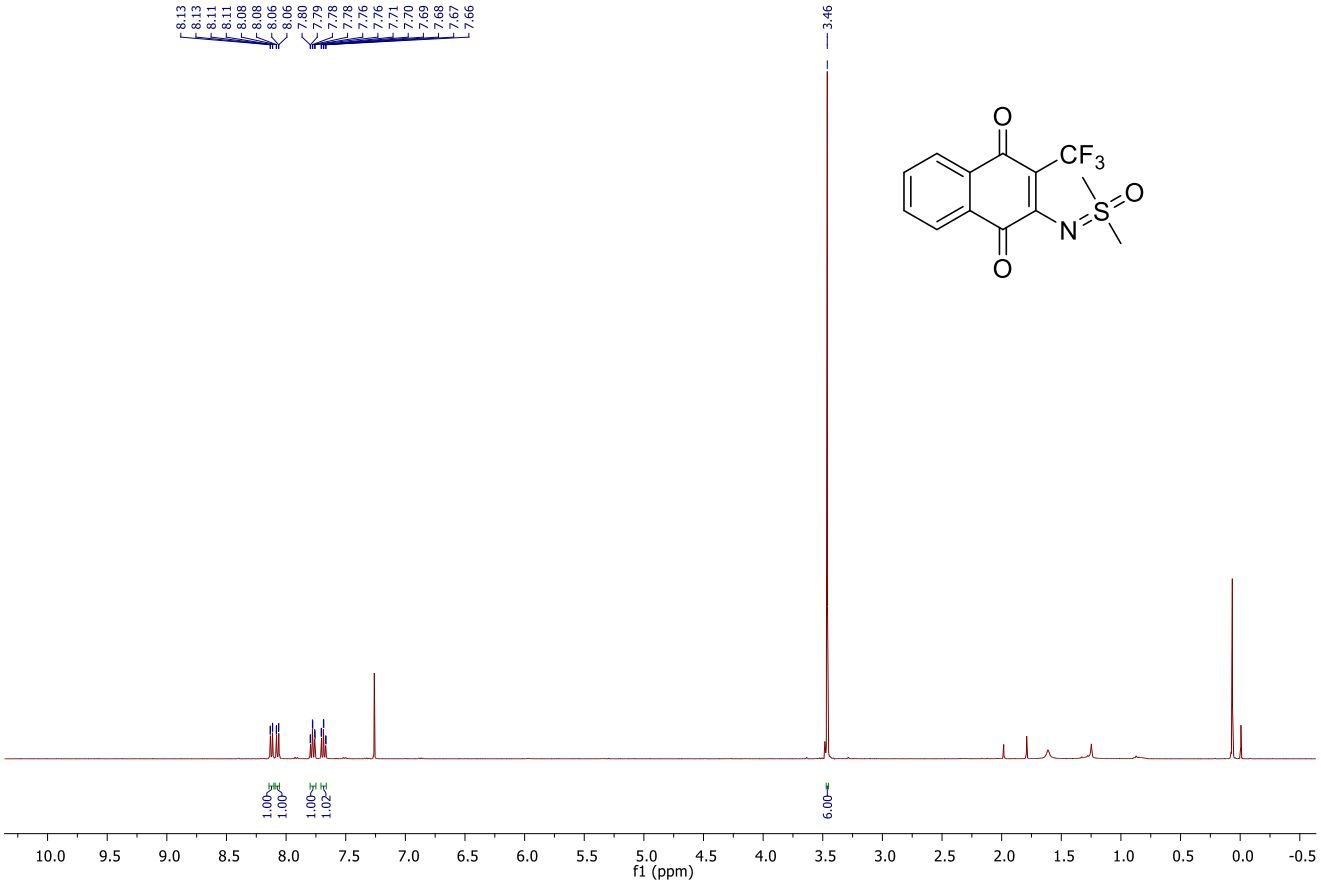
280623_03 9 (0.208)
1: TOF MS ES+

1.49e+005

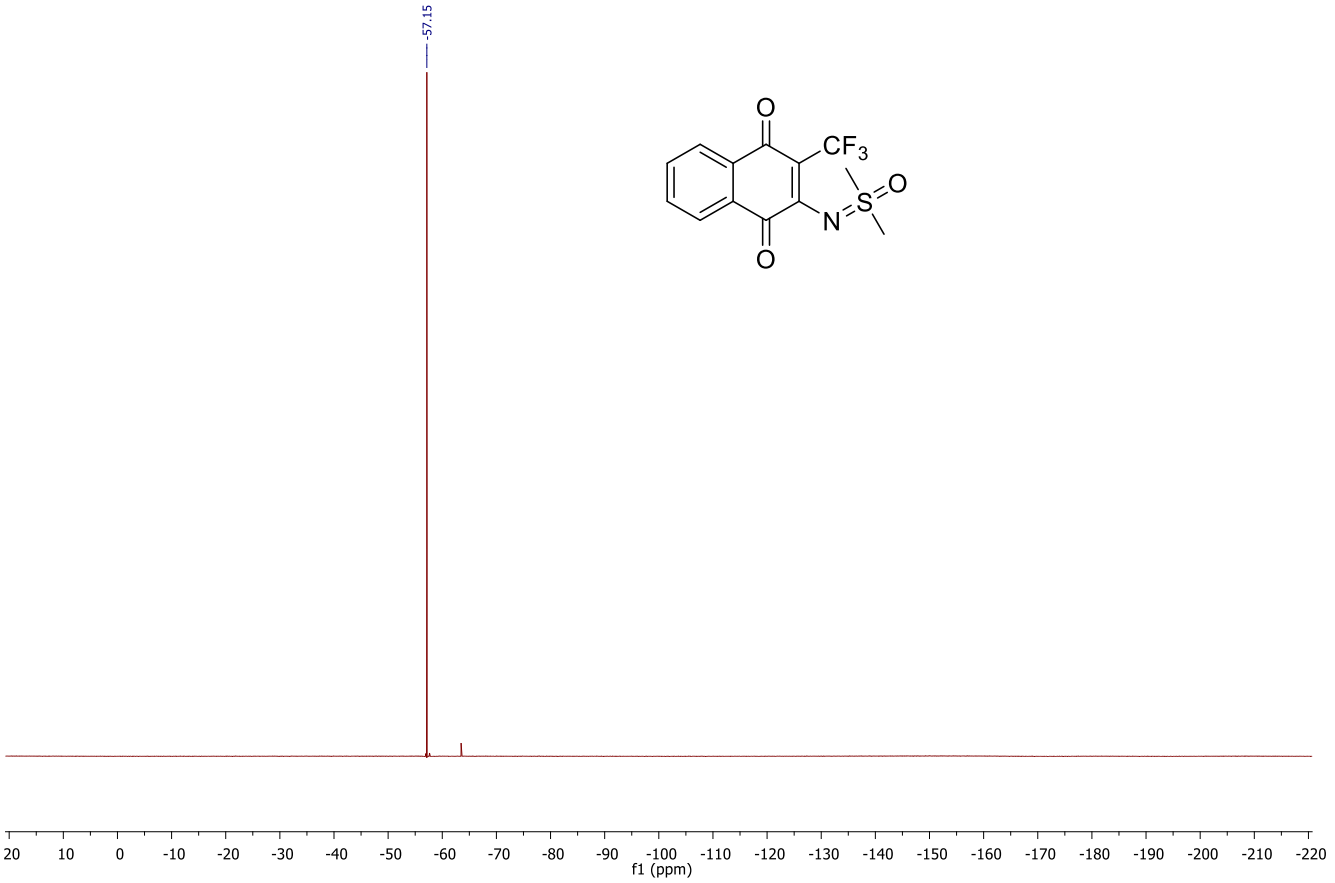


Minimum:				-1.5				
Maximum:		5.0	50.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
414.0176	414.0179	-0.3	-0.7	11.5	117.9	n/a	n/a	C18 H12 N O3 F3 S Cl

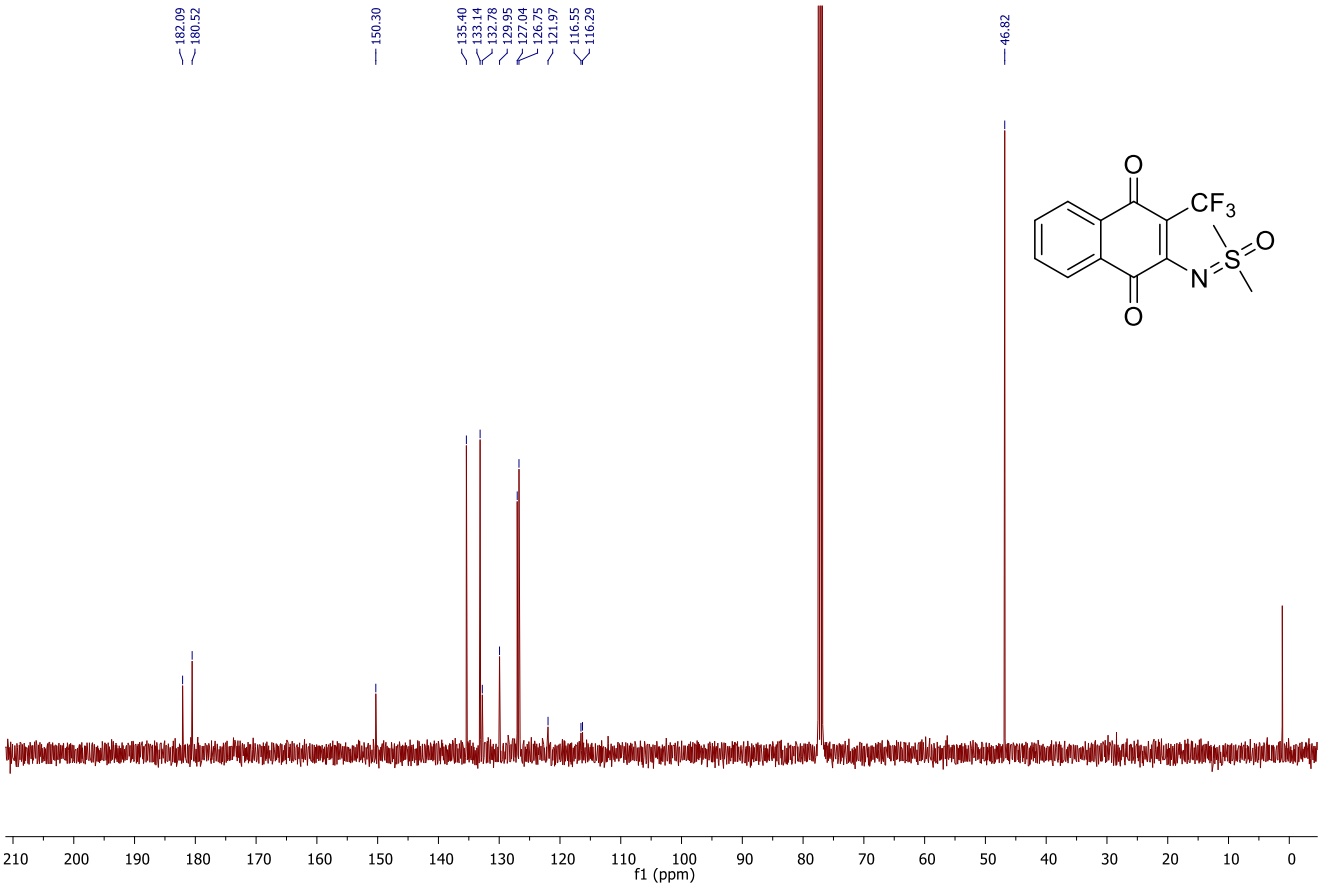
^{1}H NMR (400 MHz) of 4e in $CDCl_3$



^{19}F NMR (377 MHz) of 4e in $CDCl_3$



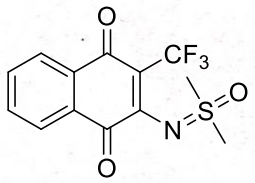
^{13}C {^{1}H} NMR (101 MHz) of 4e in $CDCl_3$



HRMS of 4e

Elemental Composition Report

Single Mass Analysis
Tolerance = 100.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3



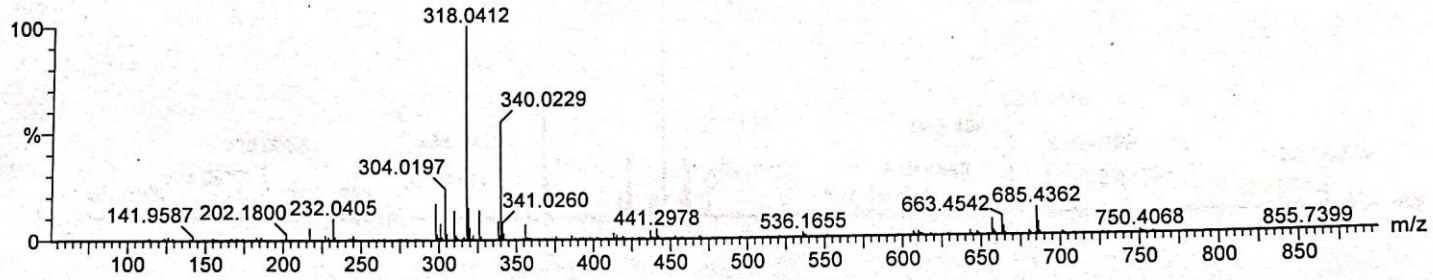
Monoisotopic Mass, Even Electron Ions
65 formula(e) evaluated with 1 results within limits (up to 3 closest results for each mass)
Elements Used:
C: 0-13 H: 0-100 N: 0-1 O: 0-3 S: 0-1 F: 0-3

NQS-6-CF3

150323_32 6 (0.138)

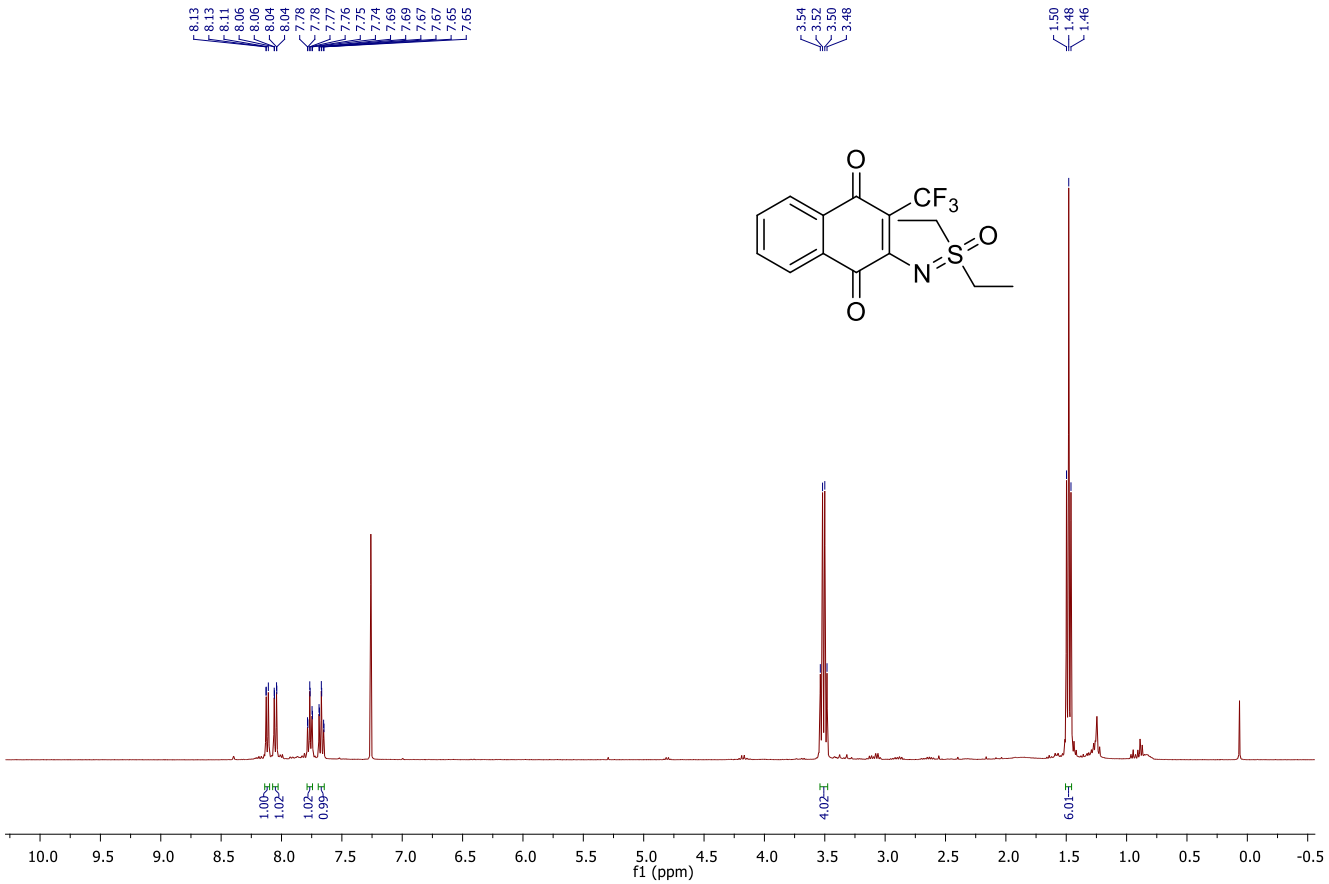
QMI DIVISION, CSIR-IIIM JAMMU
Xevo G2-XS QTOF YFC2015

15-Mar-2023
13:42:27
1: TOF MS ES+
1.28e+007

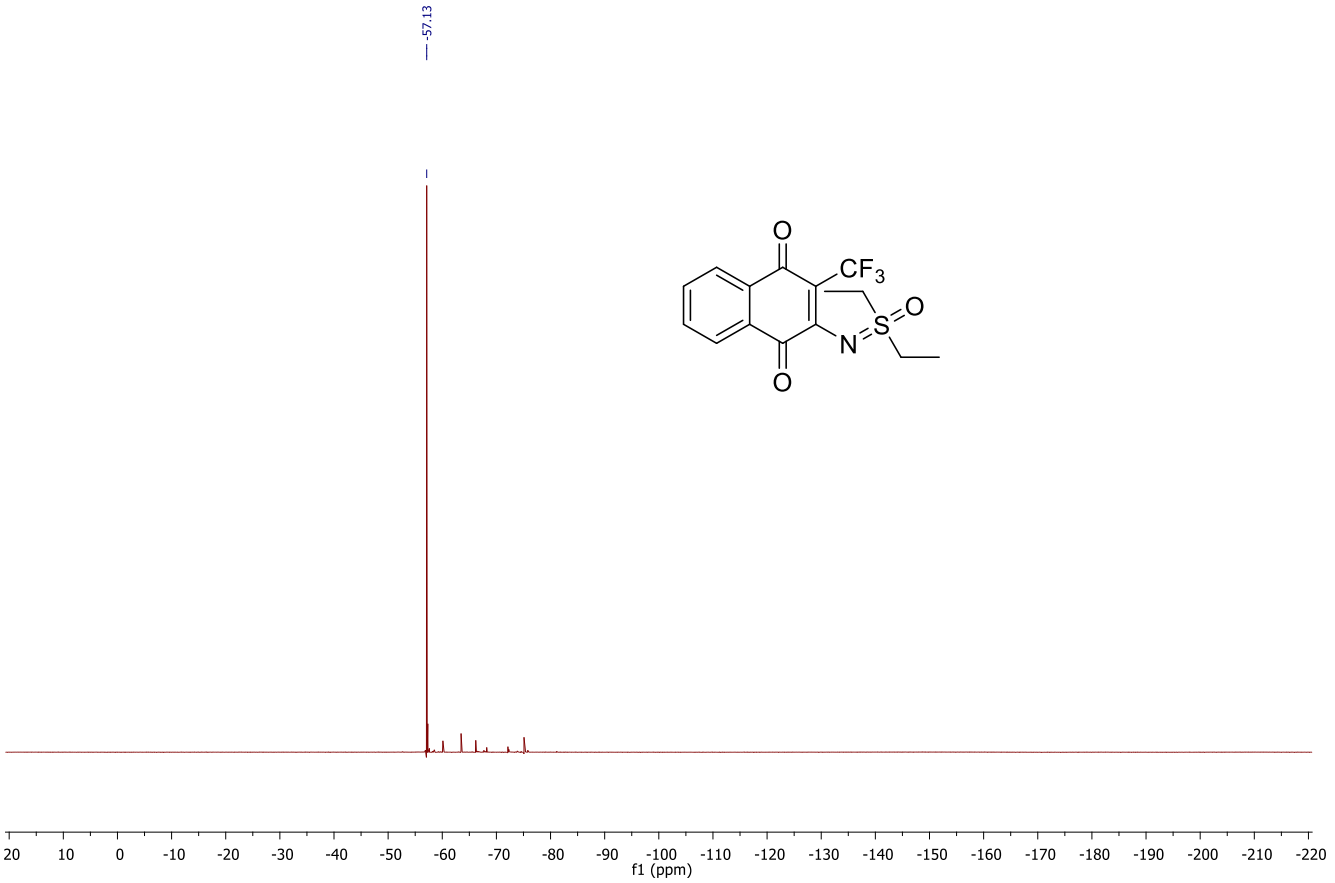


Minimum:				-1.5				
Maximum:		2.0	100.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
318.0412	318.0412	0.0	0.0	7.5	1113.3	n/a	n/a	C13 H11 N O3 S F3

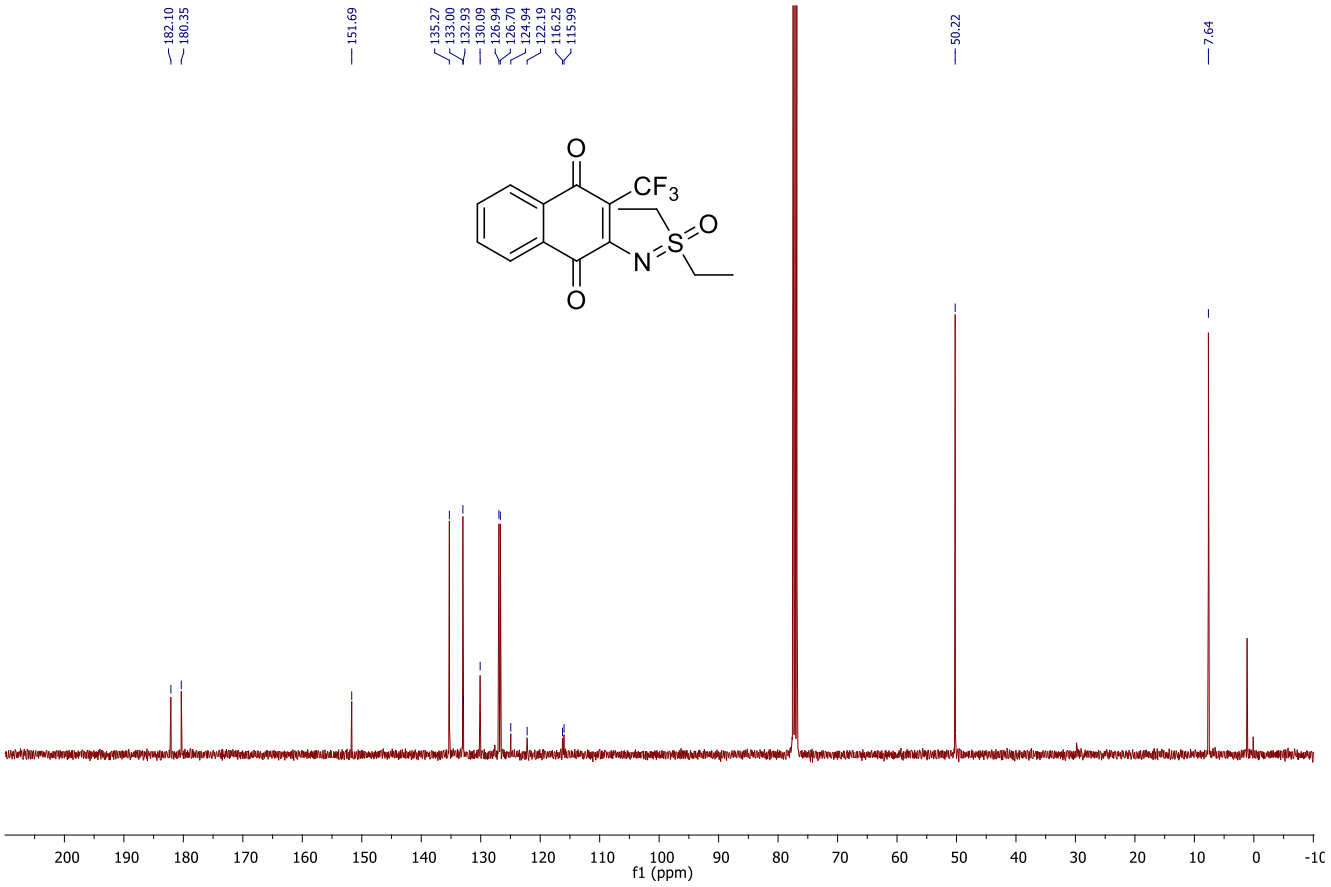
^{1}H NMR (400 MHz) of 4f in $CDCl_3$



^{19}F NMR (377 MHz) of 4f in $CDCl_3$



^{13}C {^{1}H} NMR (101 MHz) of 4f in $CDCl_3$



HRMS of 4f

Elemental Composition Report

Page 1

Single Mass Analysis
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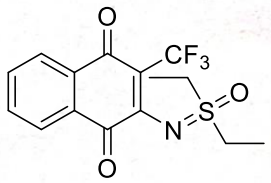
Element prediction: Off
Number of isotope peaks used for i-FIT = 3



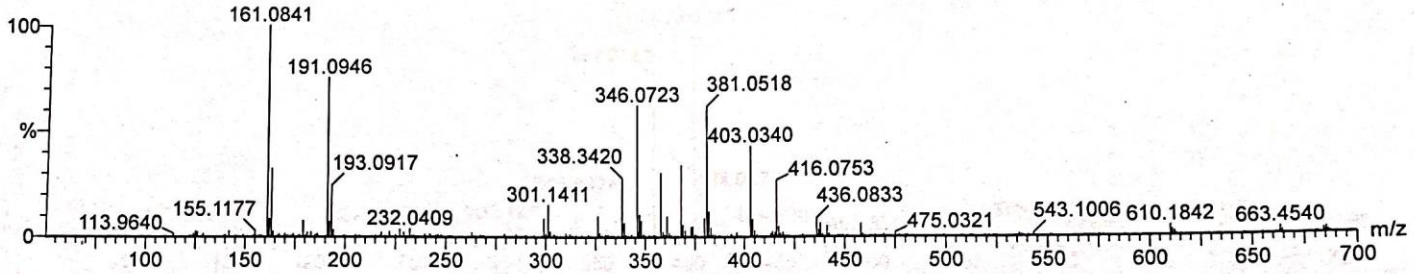
Monoisotopic Mass, Even Electron Ions
65 formula(e) evaluated with 1 results within limits (up to 3 closest results for each mass)
Elements Used:
C: 0-15 H: 0-100 N: 0-1 O: 0-3 F: 0-3 S: 0-1

NQS-7-CF3

QMI DIVISION, CSIR-IIIM JAMMU
Xevo G2-XS QTOF YFC2015

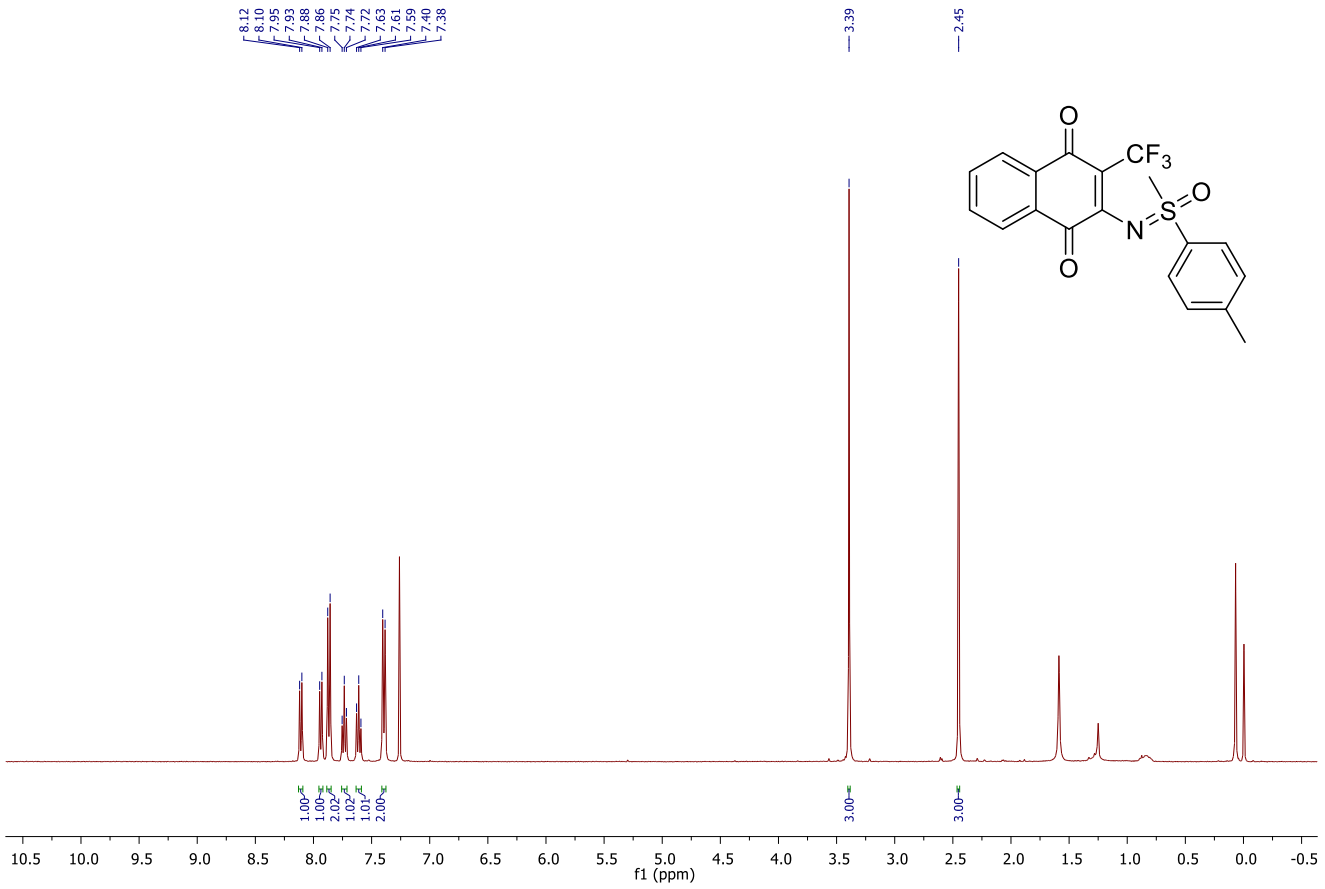
15-Mar-2023
12:39:59
1: TOF MS ES+
7.26e+006

150323_08 6 (0.138)

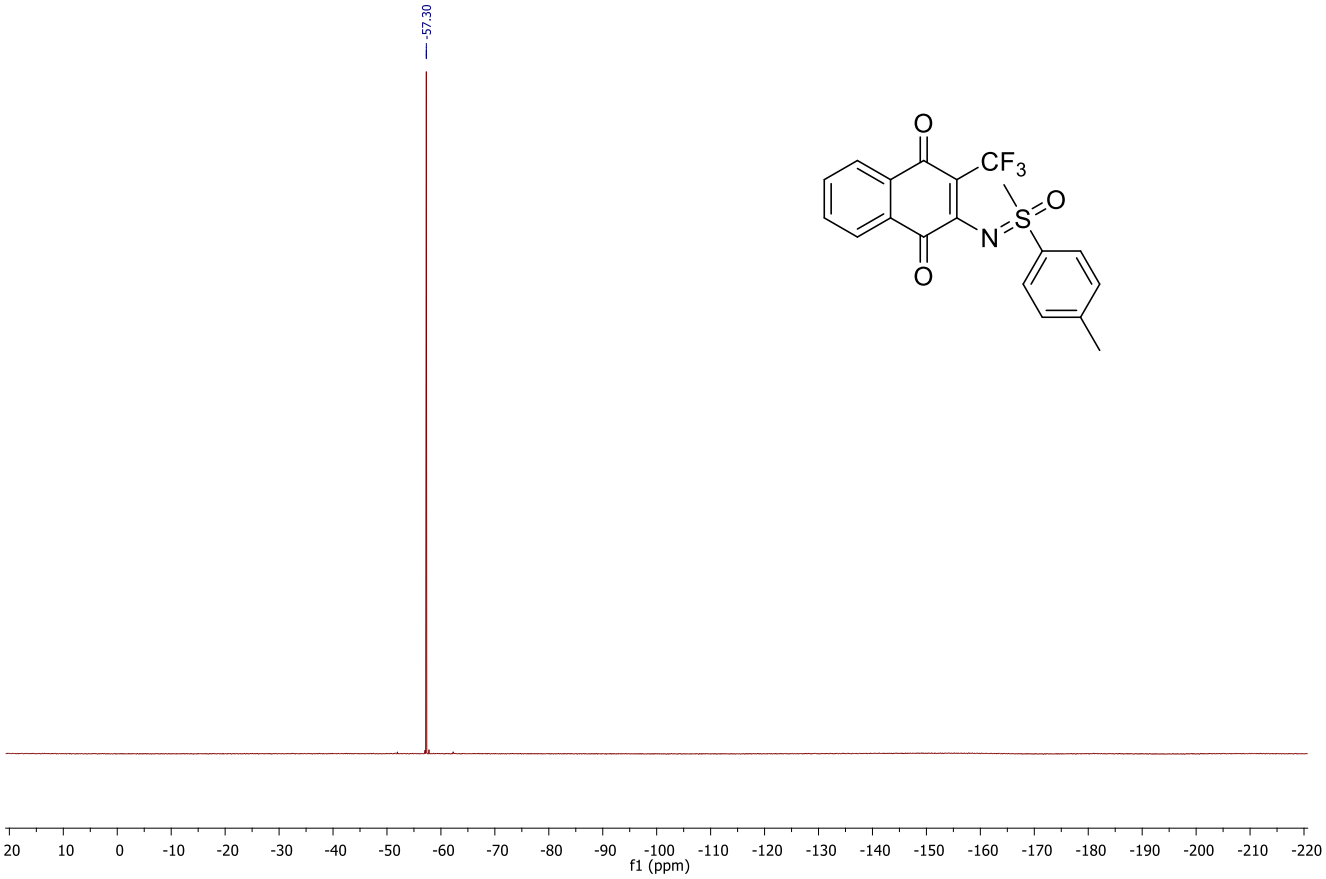


Minimum:				-1.5				
Maximum:		2.0	100.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
346.0723	346.0725	-0.2	-0.6	7.5	1166.6	n/a	n/a	C15 H15 N O3 F3 S

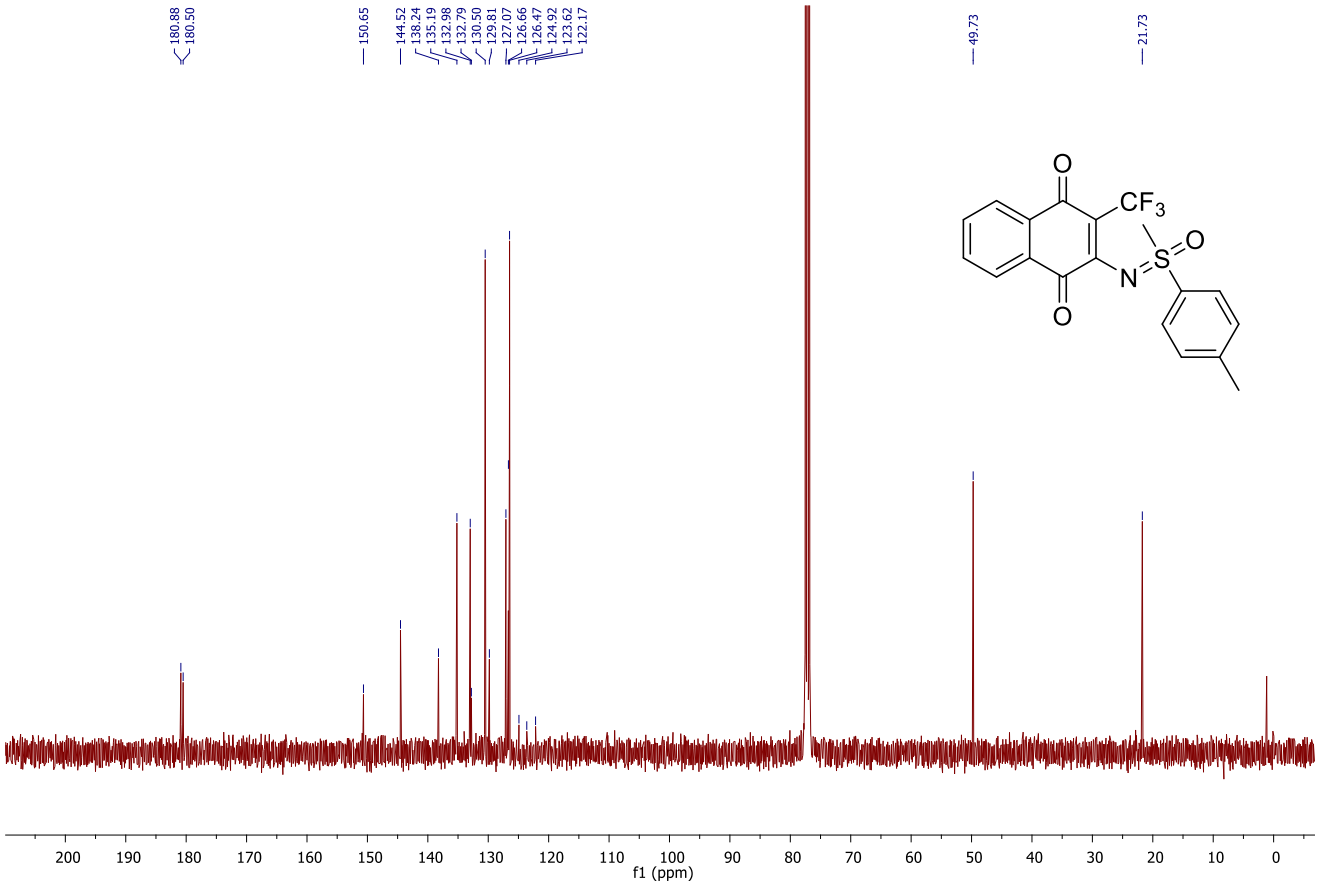
^{1}H NMR (400 MHz) of 4g in $CDCl_3$



^{19}F NMR (377 MHz) of 4g in $CDCl_3$



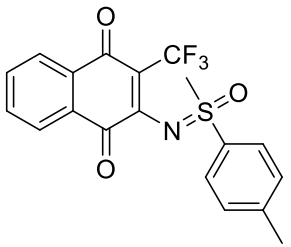
^{13}C {^{1}H} NMR (101 MHz) of 4g in $CDCl_3$



HRMS of 4g

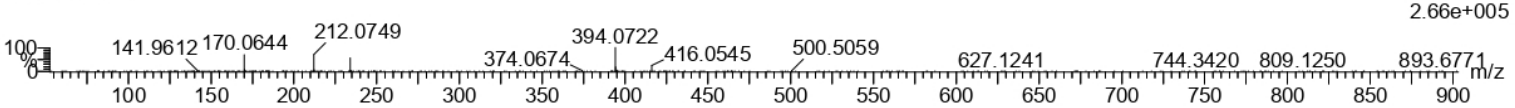
Elemental Composition Report **Page 1**

Single Mass Analysis
Tolerance = 50.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 4



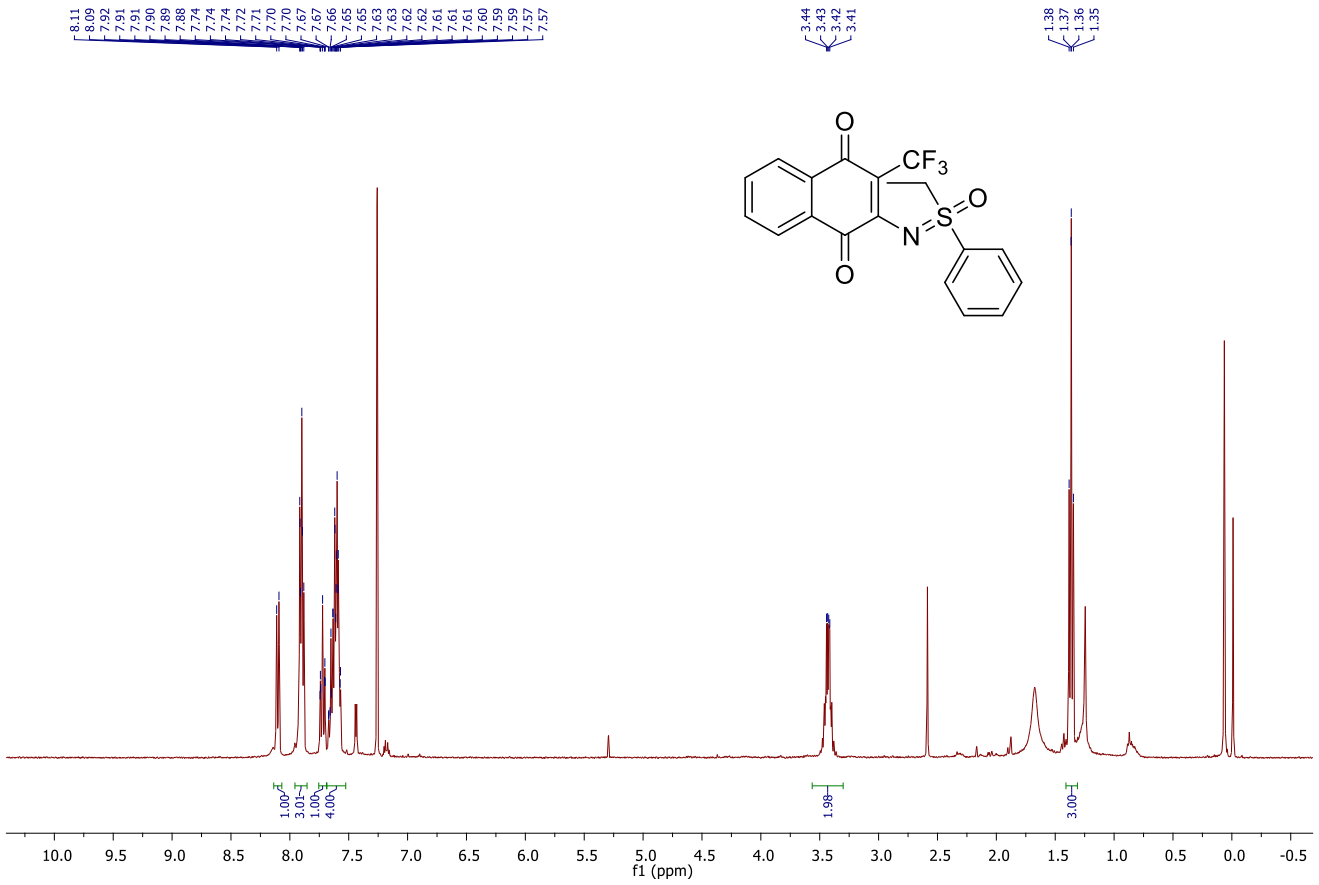
Monoisotopic Mass, Even Electron Ions
69 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 0-19 H: 0-100 N: 0-1 O: 0-3 F: 0-3 S: 0-1

280623_05 17 (0.363)
1: TOF MS ES+

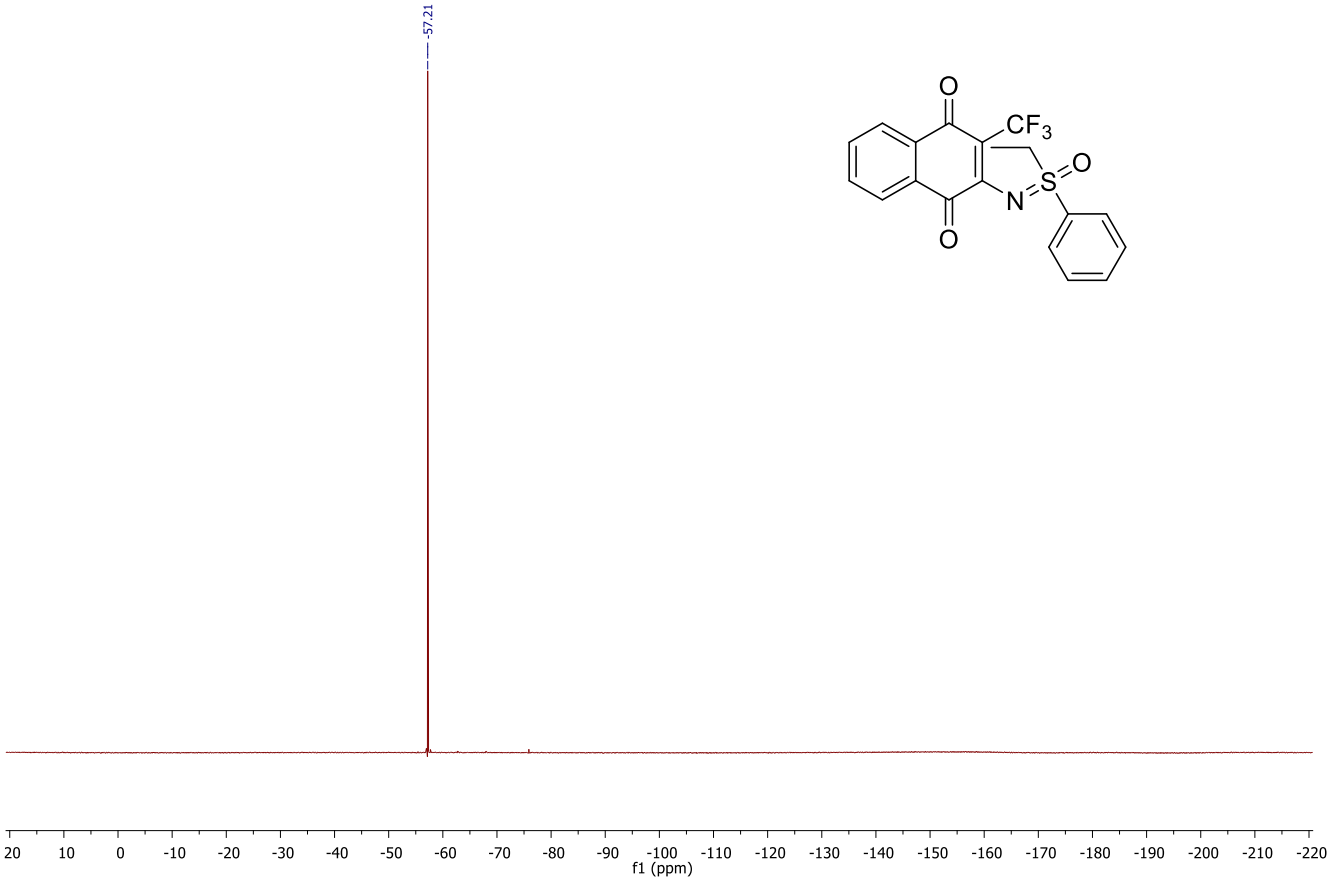


Minimum:				-1.5				
Maximum:		5.0	50.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
394.0722	394.0725	-0.3	-0.8	11.5	107.5	n/a	n/a	C19 H15 N O3 F3 S

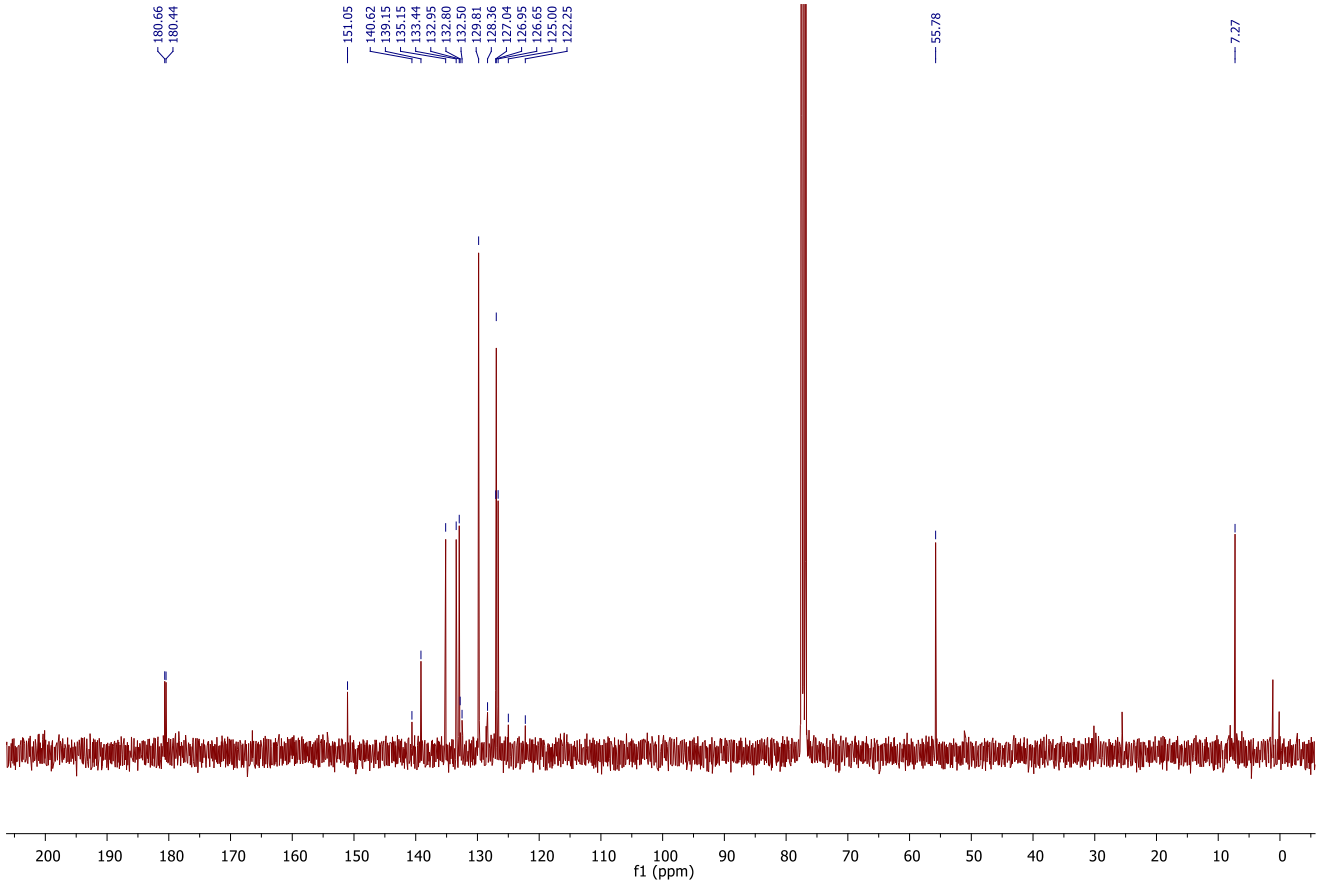
^{1}H NMR (400 MHz) of 4h in $CDCl_3$



^{19}F NMR (377 MHz) of 4h in $CDCl_3$



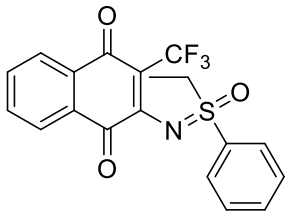
^{13}C {^{1}H} NMR (101 MHz) of 4h in $CDCl_3$



HRMS of 4h

Elemental Composition Report **Page 1**

Single Mass Analysis
Tolerance = 100.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

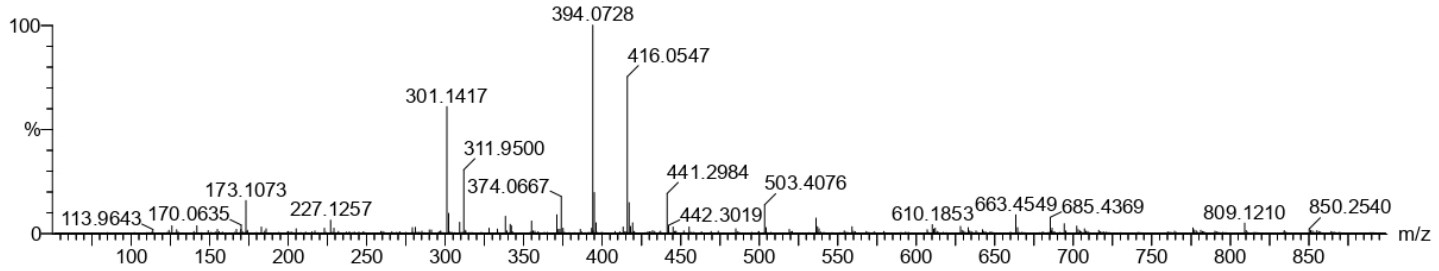


Monoisotopic Mass, Even Electron Ions
69 formula(e) evaluated with 1 results within limits (up to 3 closest results for each mass)
Elements Used:
C: 0-19 H: 0-100 N: 0-1 O: 0-3 S: 0-1 F: 0-3

NQS-10-CF3
280323_13 6 (0.138)

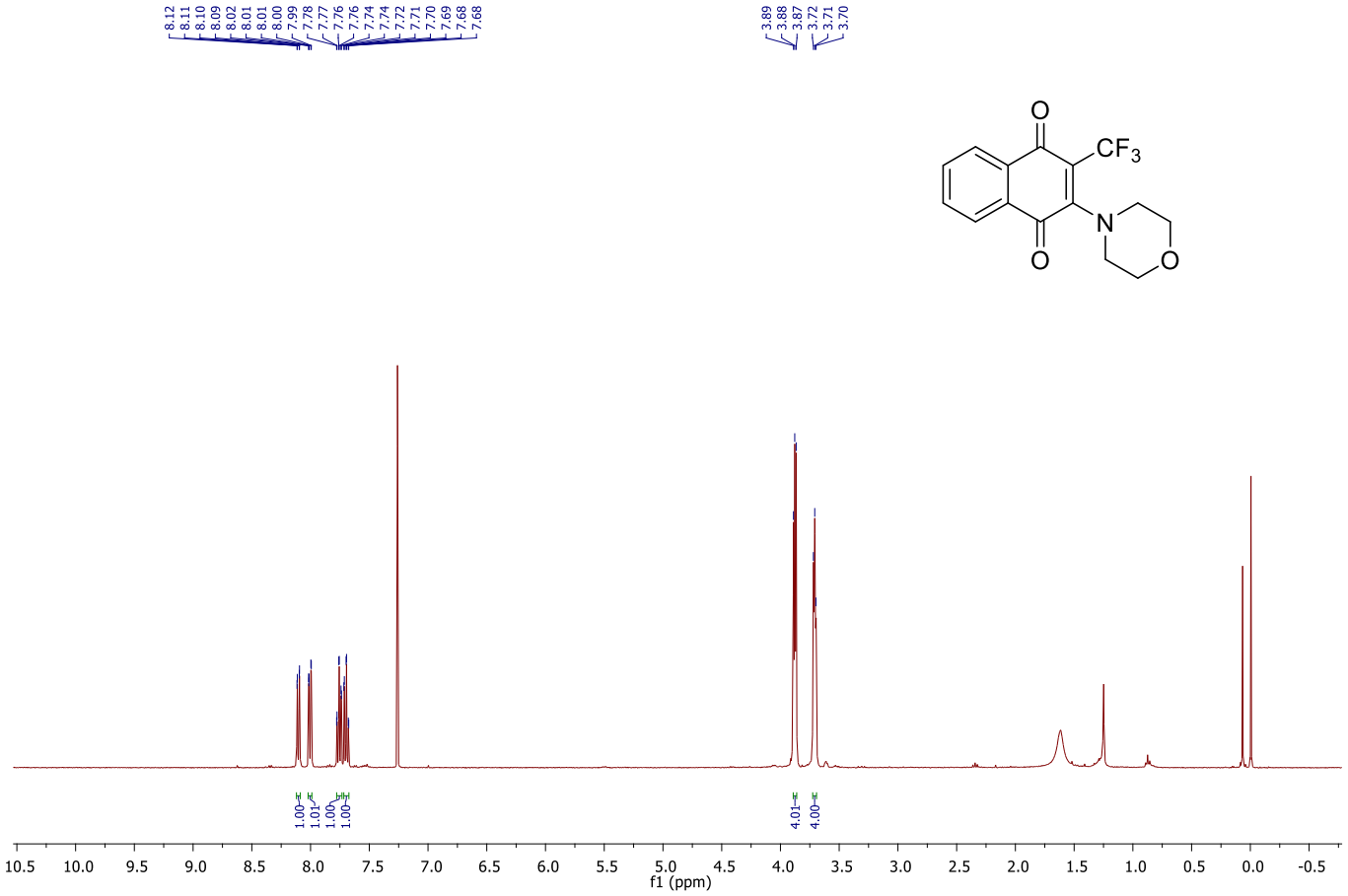
QMI DIVISION, CSIR-IIIM JAMMU
Xevo G2-XS QTOF YFC2015

28-Mar-2023
12:40:06
1: TOF MS ES+
2.49e+006

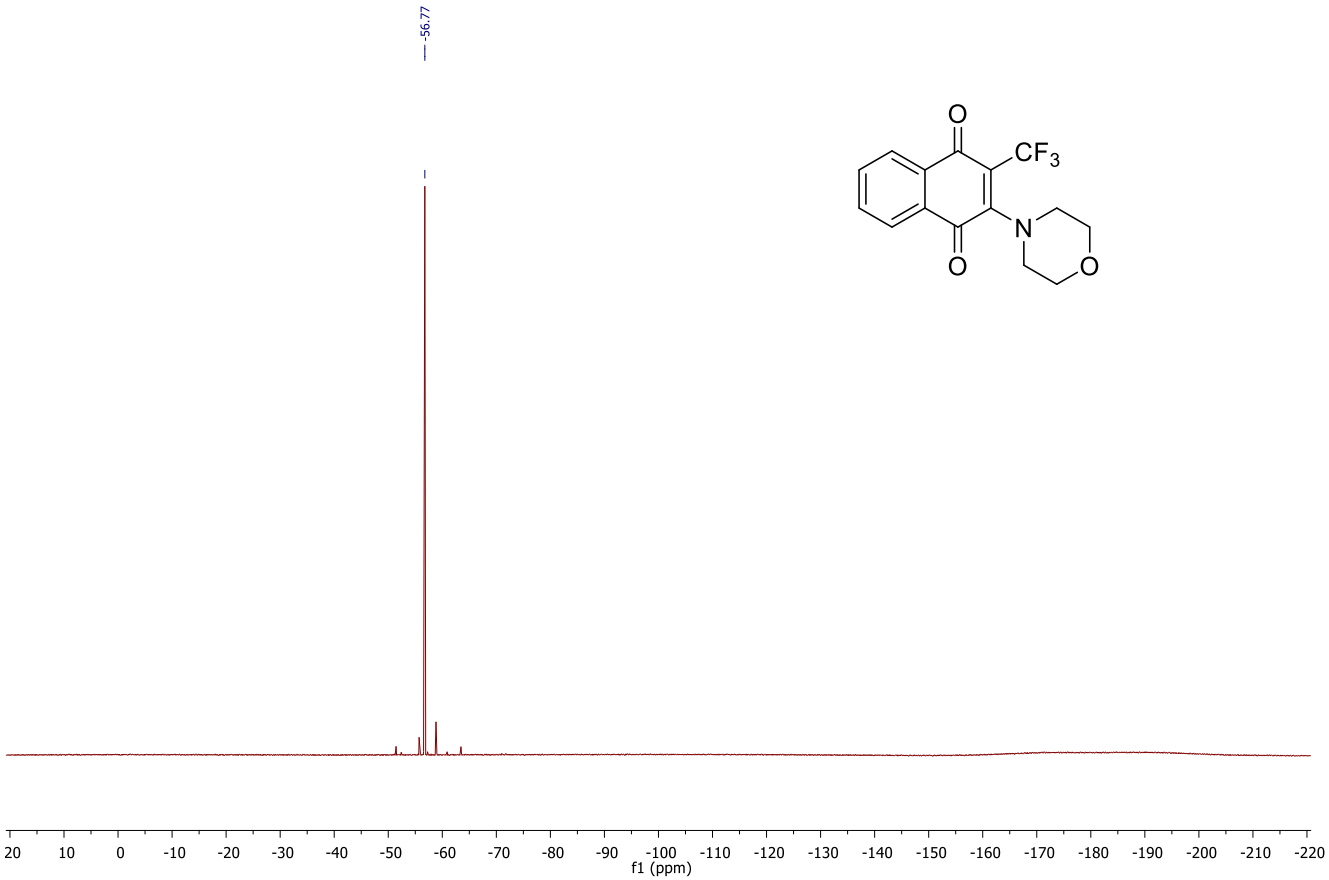


Minimum:				-1.5				
Maximum:		2.0	100.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
394.0728	394.0725	0.3	0.8	11.5	894.9	n/a	n/a	C19 H15 N O3 S F3

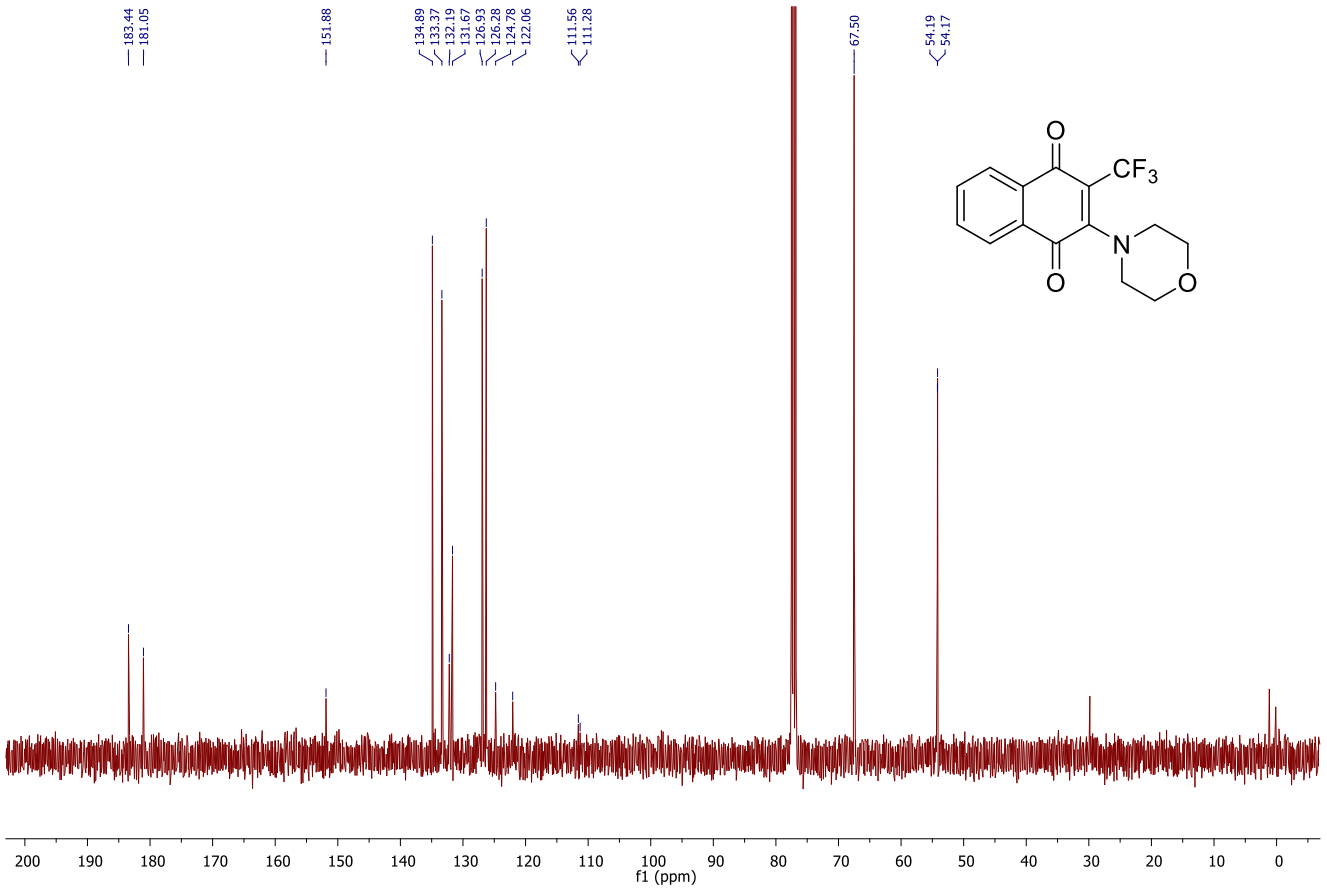
^{1}H NMR (400 MHz) of 4i in $CDCl_3$



^{19}F NMR (377 MHz) of 4i in $CDCl_3$



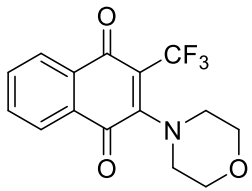
^{13}C {^{1}H} NMR (101 MHz) of 4i in $CDCl_3$



HRMS of 4i

Elemental Composition Report **Page 1**

Single Mass Analysis
Tolerance = 100.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

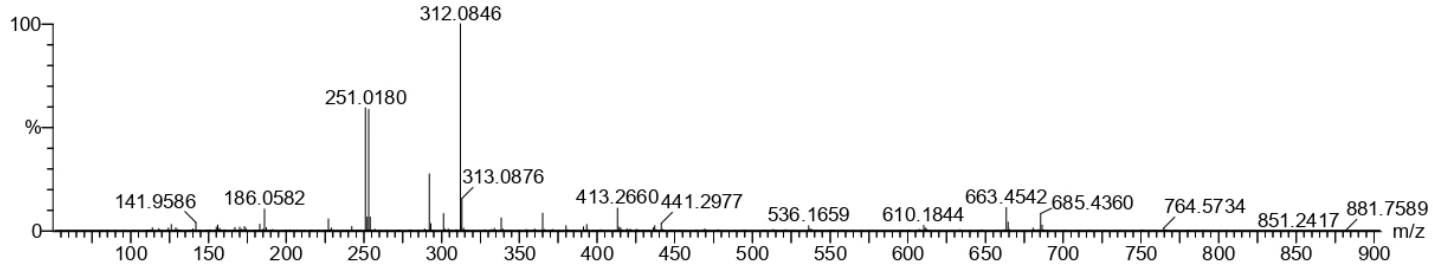


Monoisotopic Mass, Even Electron Ions
33 formula(e) evaluated with 1 results within limits (up to 3 closest results for each mass)
Elements Used:
C: 0-15 H: 0-100 N: 0-1 O: 0-3 F: 0-3

NQA-1-CF3
280323_10 6 (0.138)

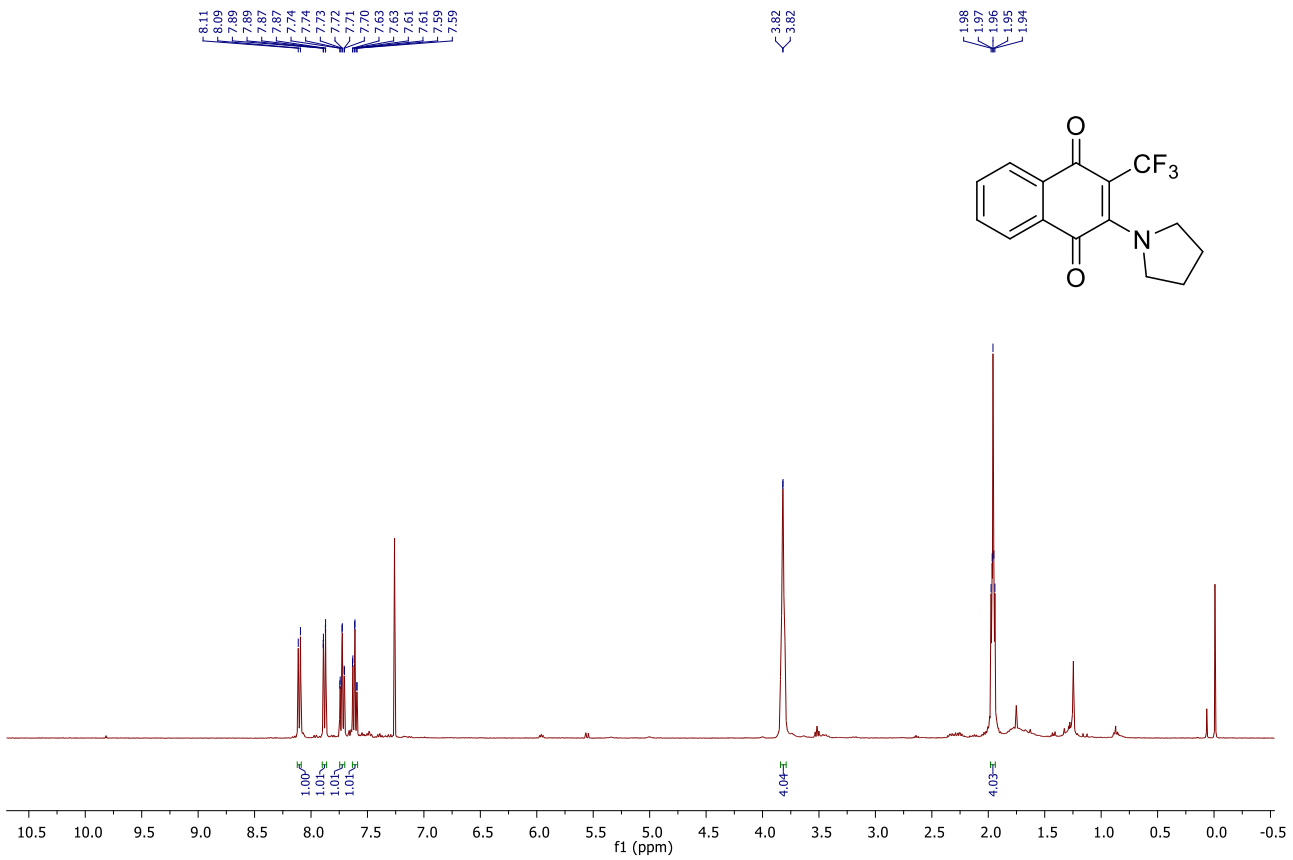
QMI DIVISION, CSIR-IIIM JAMMU
Xevo G2-XS QTOF YFC2015

28-Mar-2023
12:32:14
1: TOF MS ES+
3.28e+006

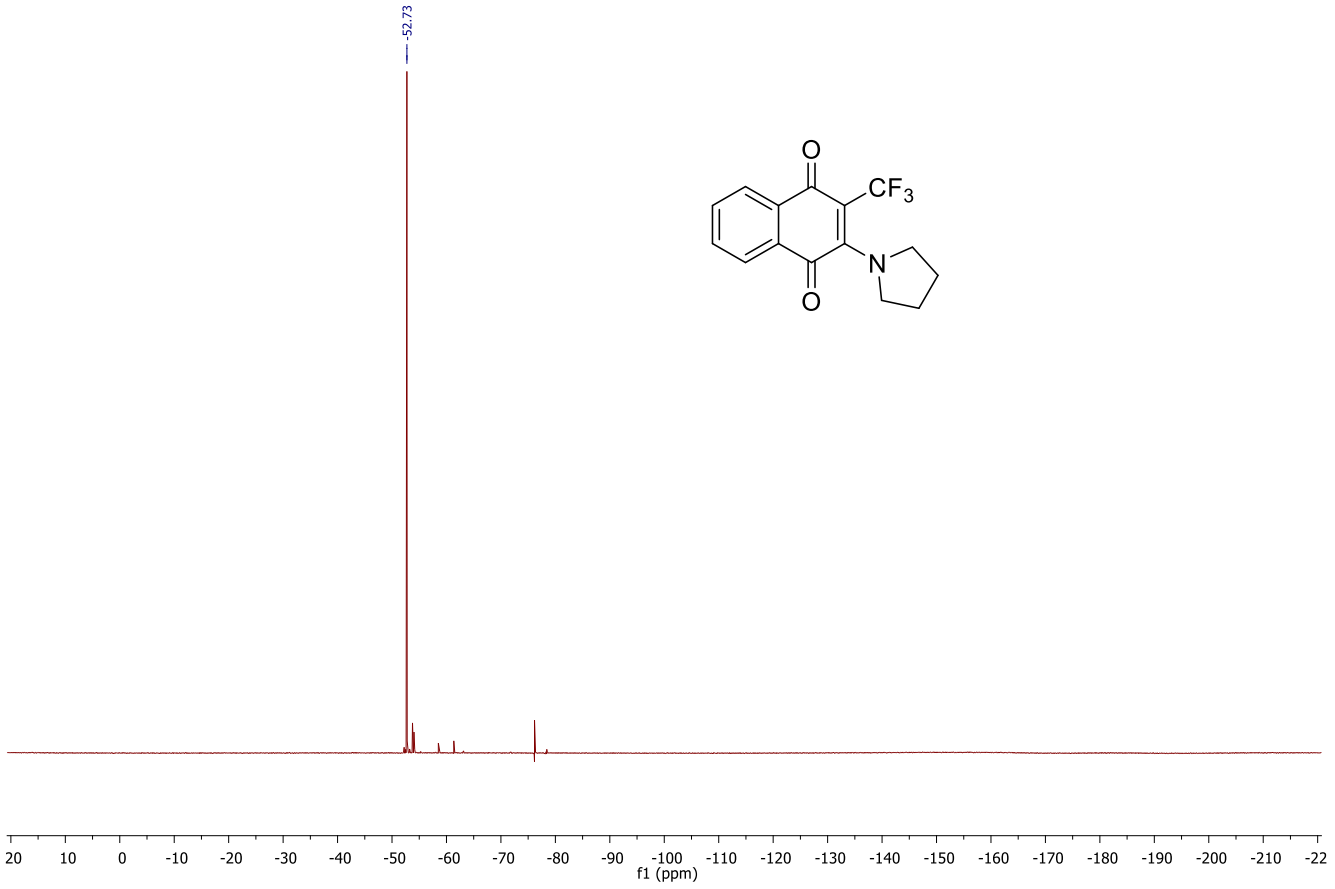


Minimum:				-1.5				
Maximum:		2.0	100.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
312.0846	312.0848	-0.2	-0.6	8.5	1004.4	n/a	n/a	C15 H13 N O3 F3

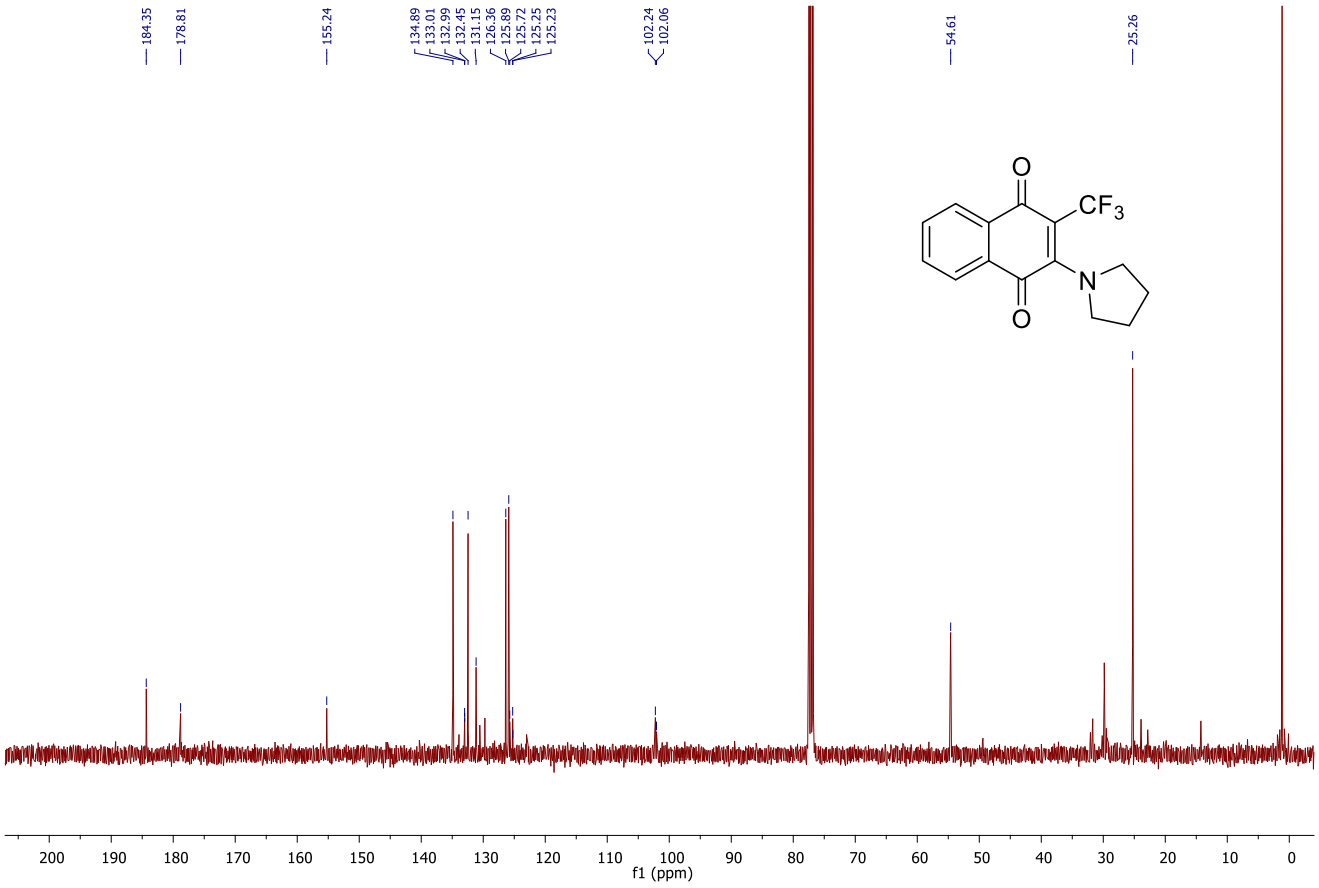
^{1}H NMR (400 MHz) of 4j in $CDCl_3$



^{19}F NMR (377 MHz) of 4j in $CDCl_3$

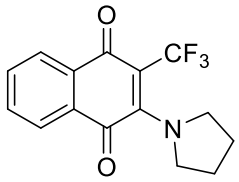


^{13}C {^{1}H} NMR (101 MHz) of 4j in $CDCl_3$



HRMS of 4j

Elemental Composition Report **Page 1**



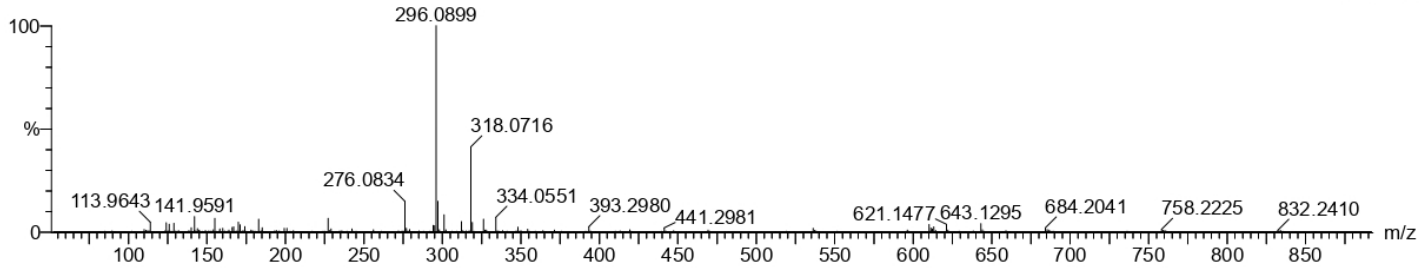
Single Mass Analysis
Tolerance = 50.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
25 formula(e) evaluated with 1 results within limits (up to 3 closest results for each mass)
Elements Used:
C: 0-15 H: 0-100 N: 0-1 O: 0-2 F: 0-3

NQA-PYRRP-CF3
120723_05 10 (0.225)

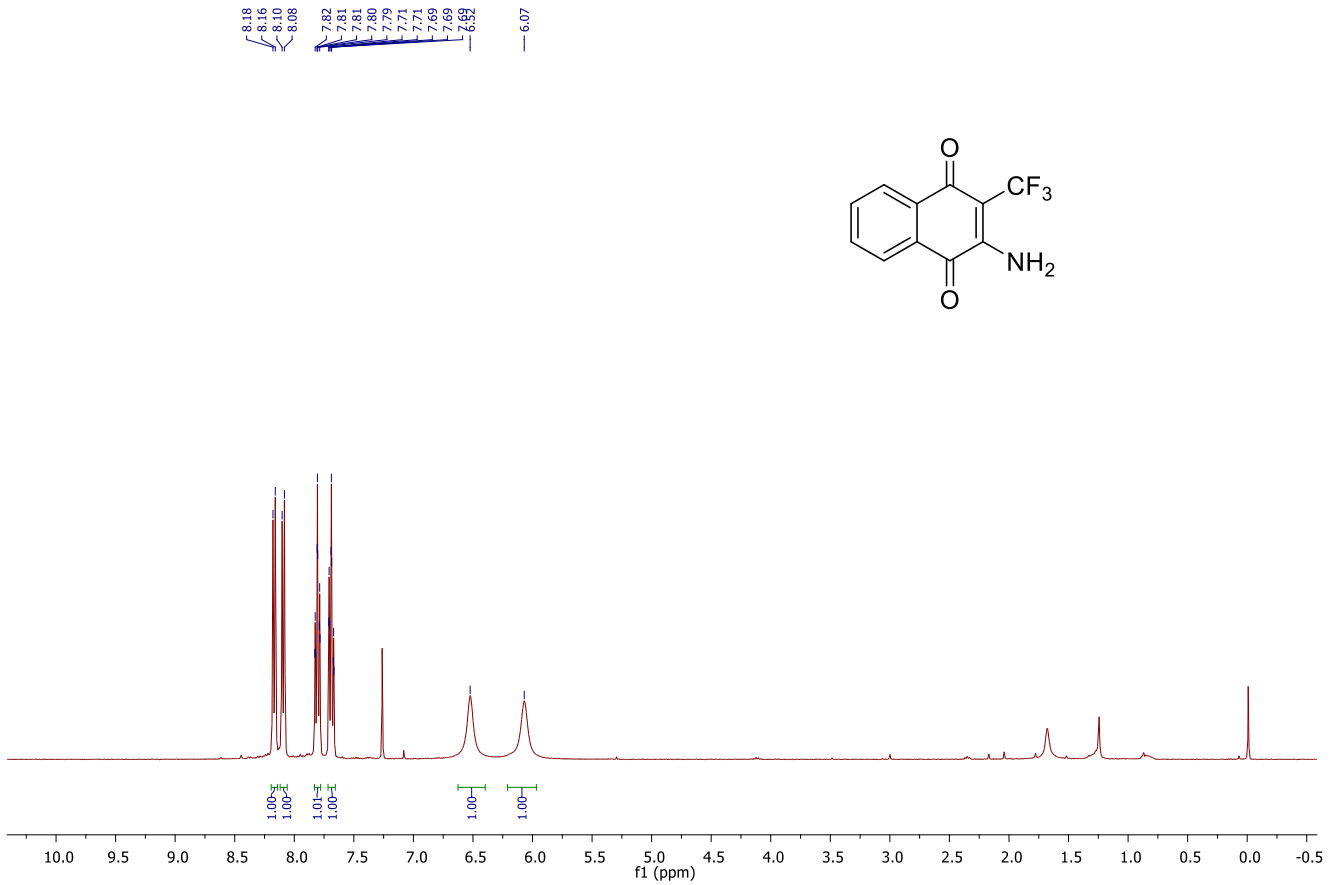
QMI DIVISION, CSIR-IIIM JAMMU
Xevo G2-XS QTOF YFC2015

12-Jul-2023
11:54:48
1: TOF MS ES+
1.59e+006

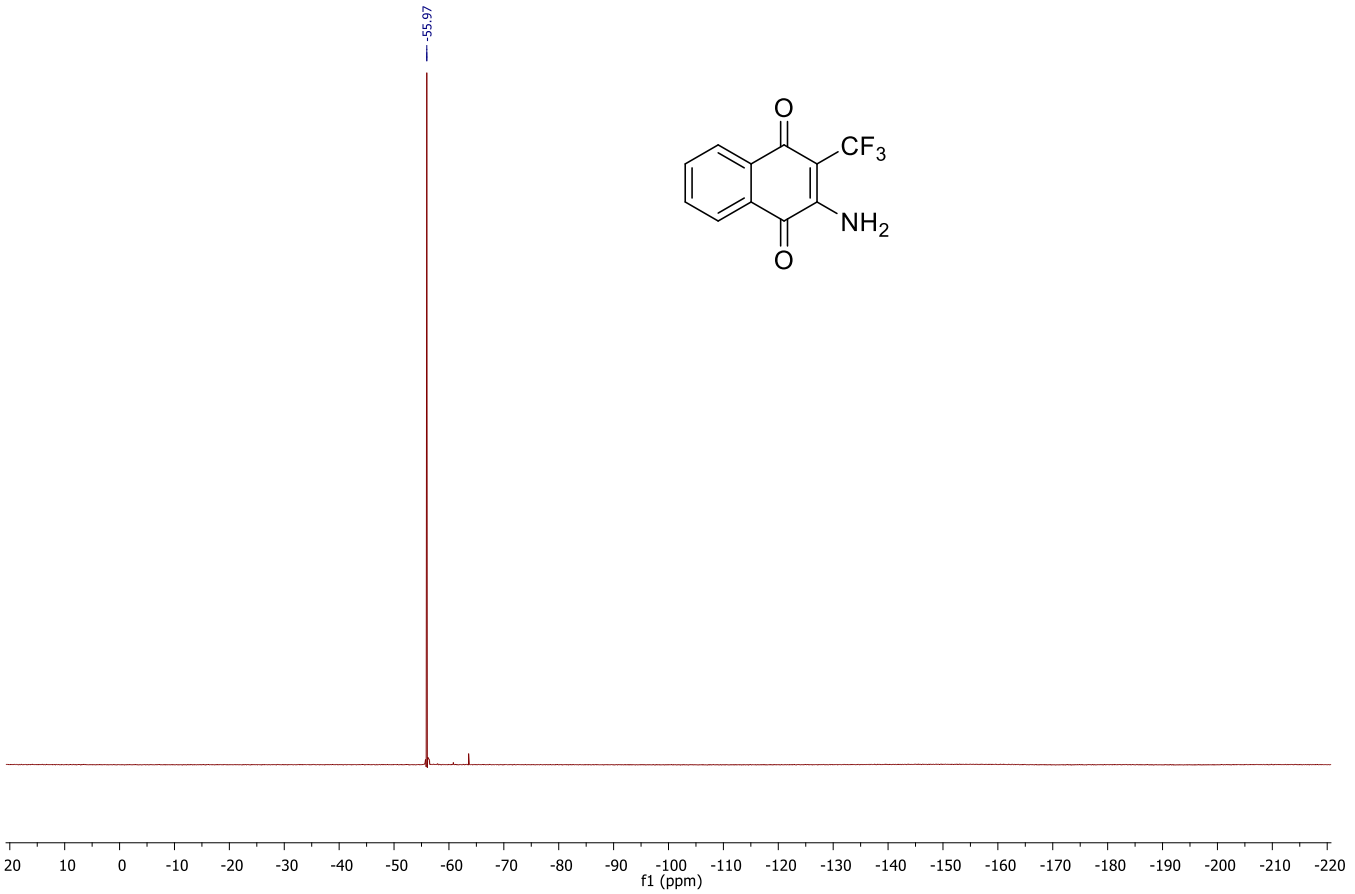


Minimum:				-1.5				
Maximum:		2.0	50.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
296.0899	296.0898	0.1	0.3	8.5	869.3	n/a	n/a	C15 H13 N O2 F3

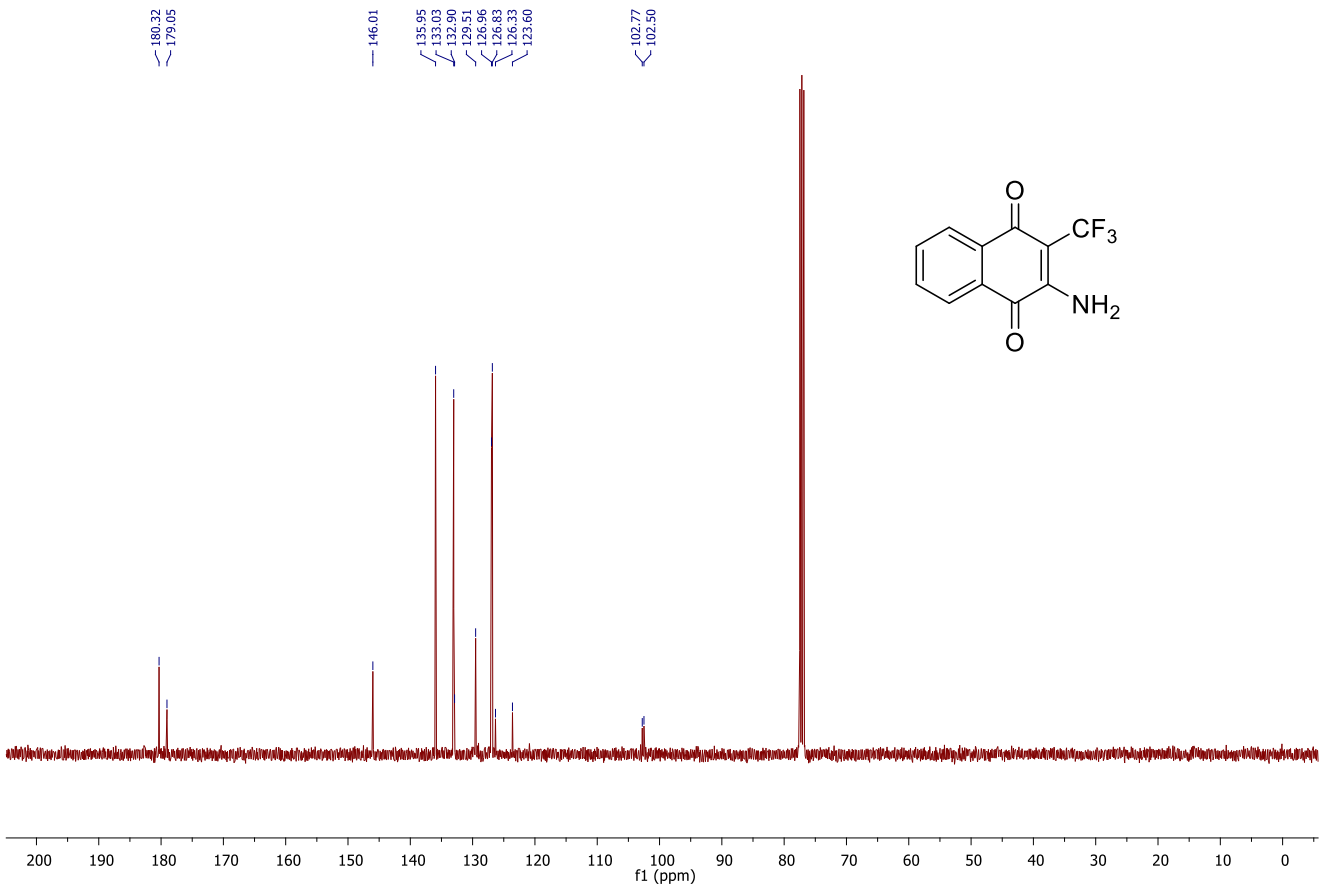
^{1}H NMR (400 MHz) of 4k in $CDCl_3$



^{19}F NMR (377 MHz) of 4k in $CDCl_3$



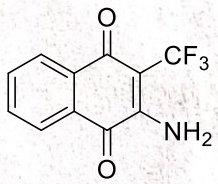
^{13}C {^{1}H} NMR (101 MHz) of 4k in $CDCl_3$



HRMS of 4k

Elemental Composition Report Page 1

Single Mass Analysis
Tolerance = 100.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3



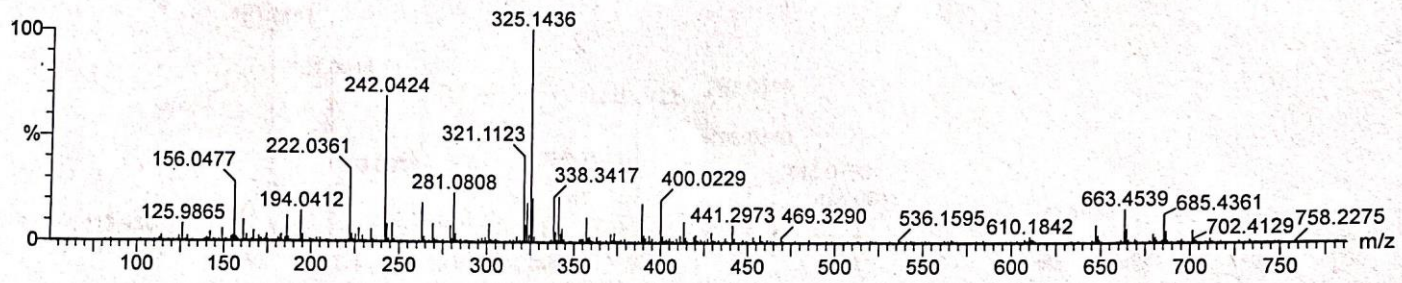
Monoisotopic Mass, Even Electron Ions
25 formula(e) evaluated with 1 results within limits (up to 3 closest results for each mass)
Elements Used:
C: 0-11 H: 0-100 N: 0-1 O: 0-2 F: 0-3

NQ-NH2-CF3

QMI DIVISION, CSIR-IIIM JAMMU
Xevo G2-XS QTOF YFC2015

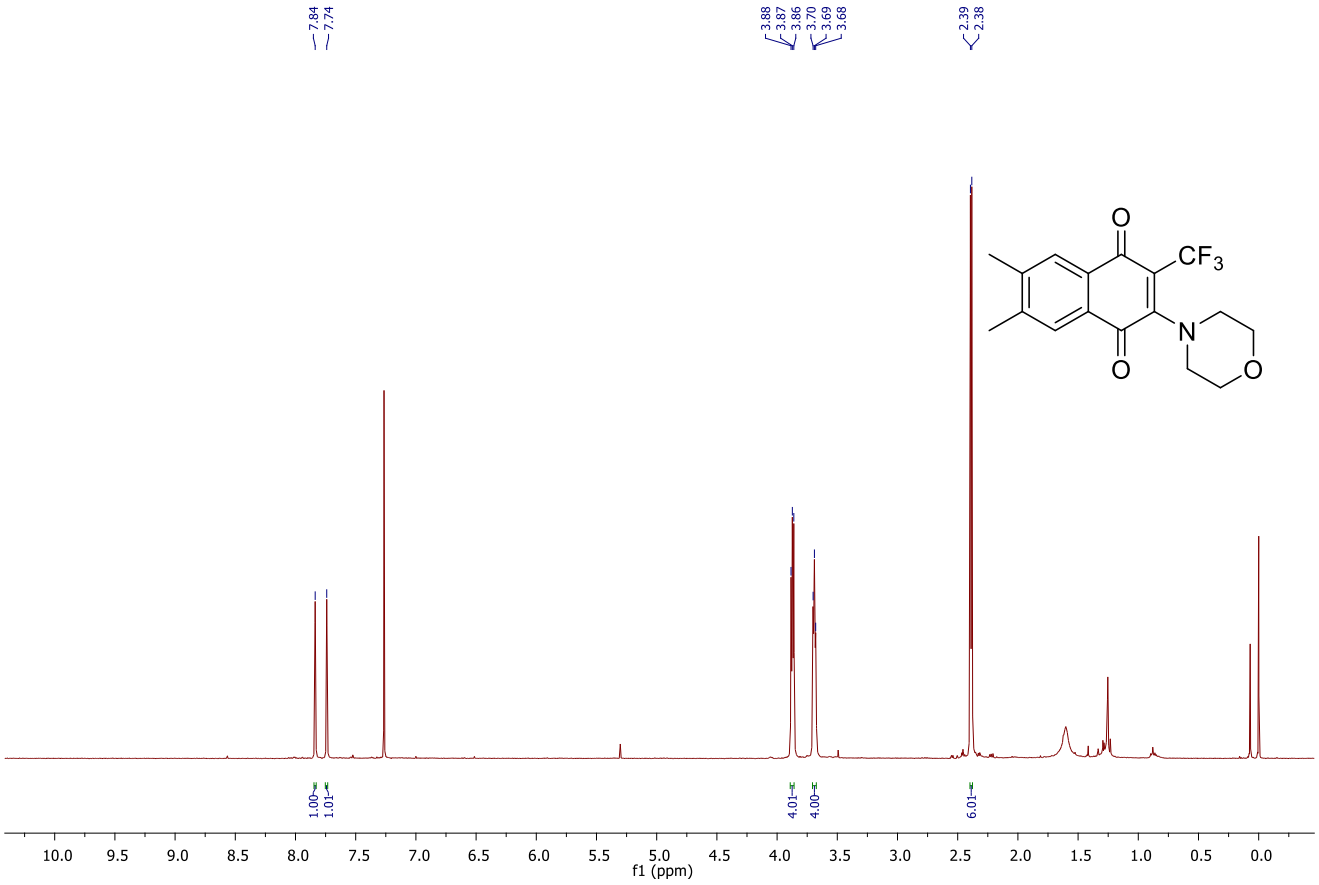
15-Mar-2023
12:34:41
1: TOF MS ES+
4.12e+006

150323_06 7 (0.155)

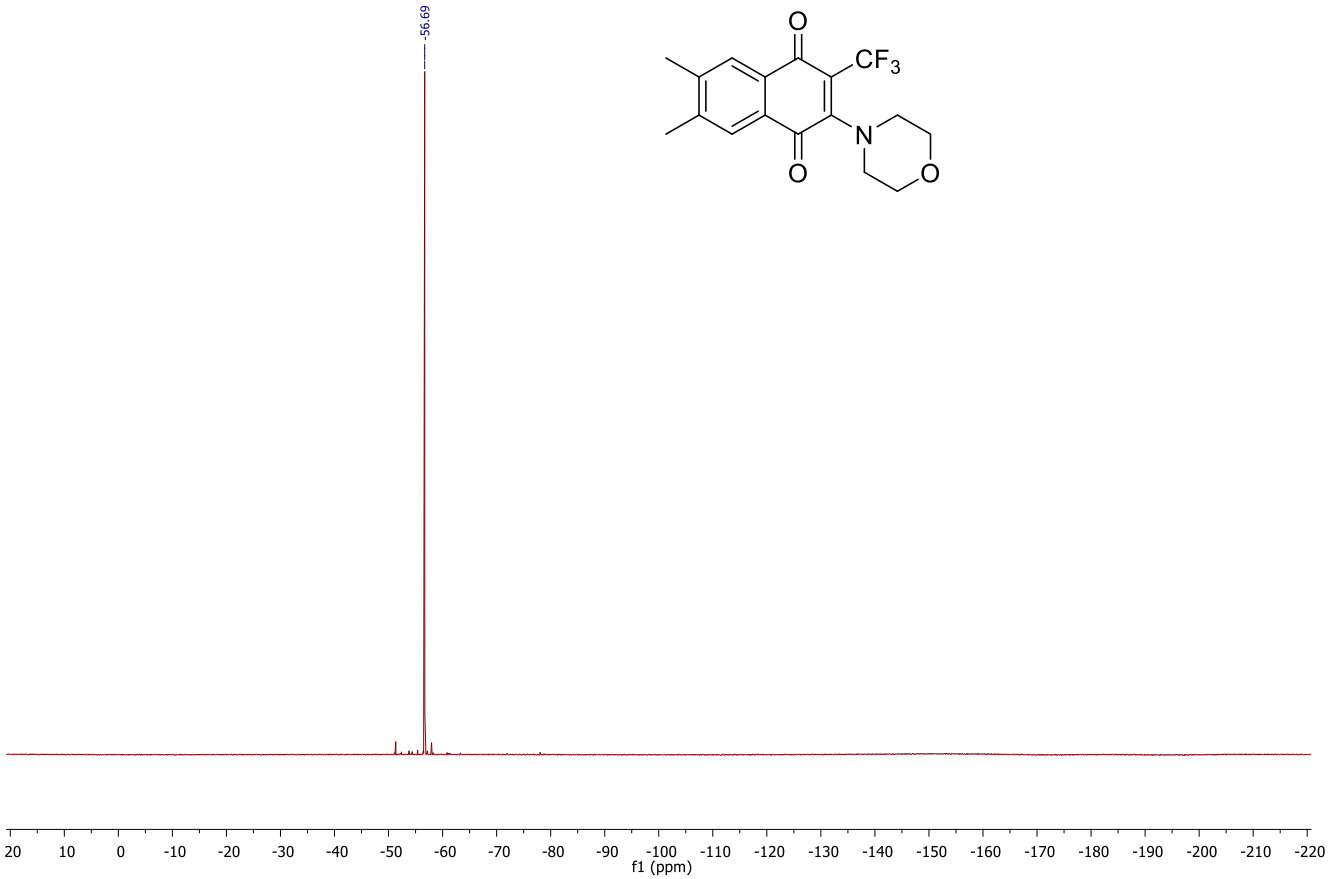


Minimum:				-1.5				
Maximum:		2.0	100.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
242.0424	242.0429	-0.5	-2.1	7.5	1391.6	n/a	n/a	C11 H7 N O2 F3

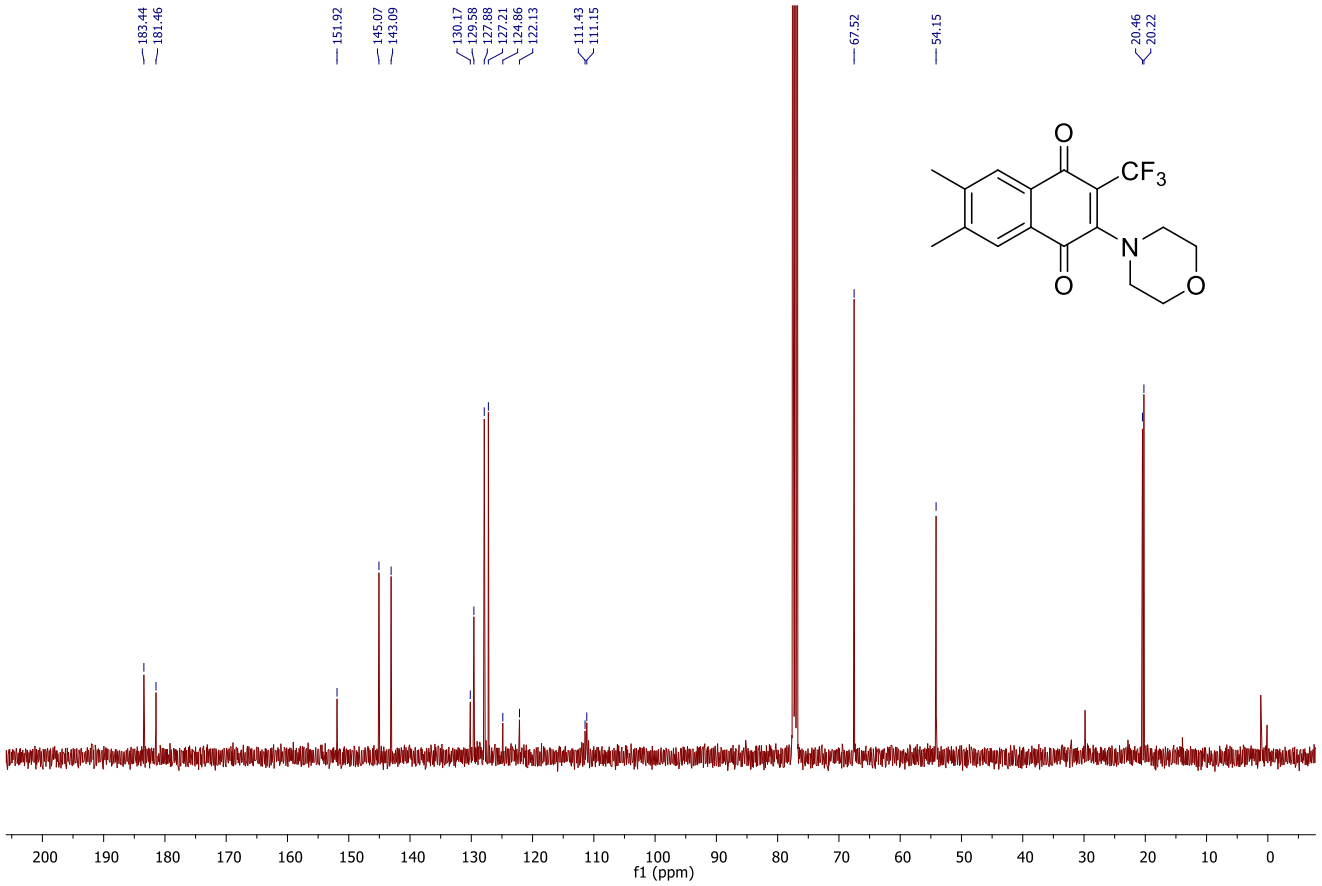
^{1}H NMR (400 MHz) of 4l in $CDCl_3$



^{19}F NMR (377 MHz) of 4l in $CDCl_3$

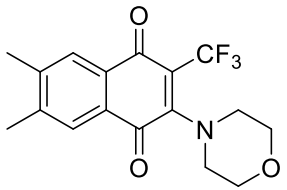


^{13}C {^{1}H} NMR (101 MHz) of 4l in $CDCl_3$



HRMS of 4l

Elemental Composition Report **Page 1**



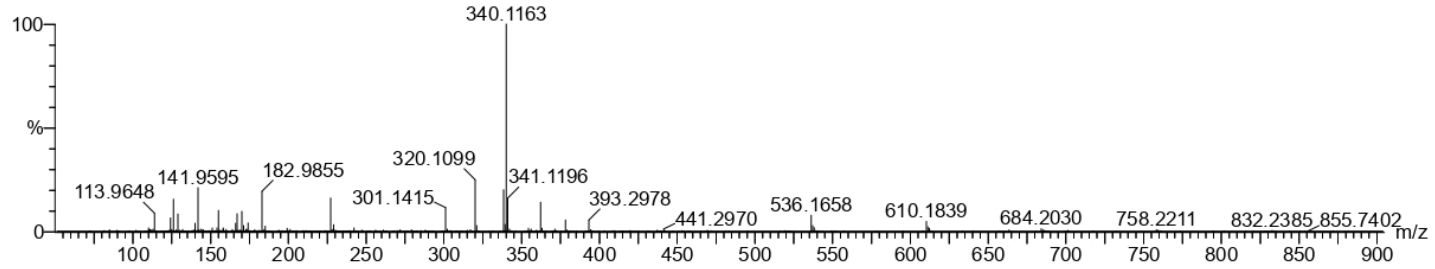
Single Mass Analysis
Tolerance = 100.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
33 formula(e) evaluated with 1 results within limits (up to 3 closest results for each mass)
Elements Used:
C: 0-17 H: 0-100 N: 0-1 O: 0-3 F: 0-3

NQDMA-1-CF3
060423_11 8 (0.172)

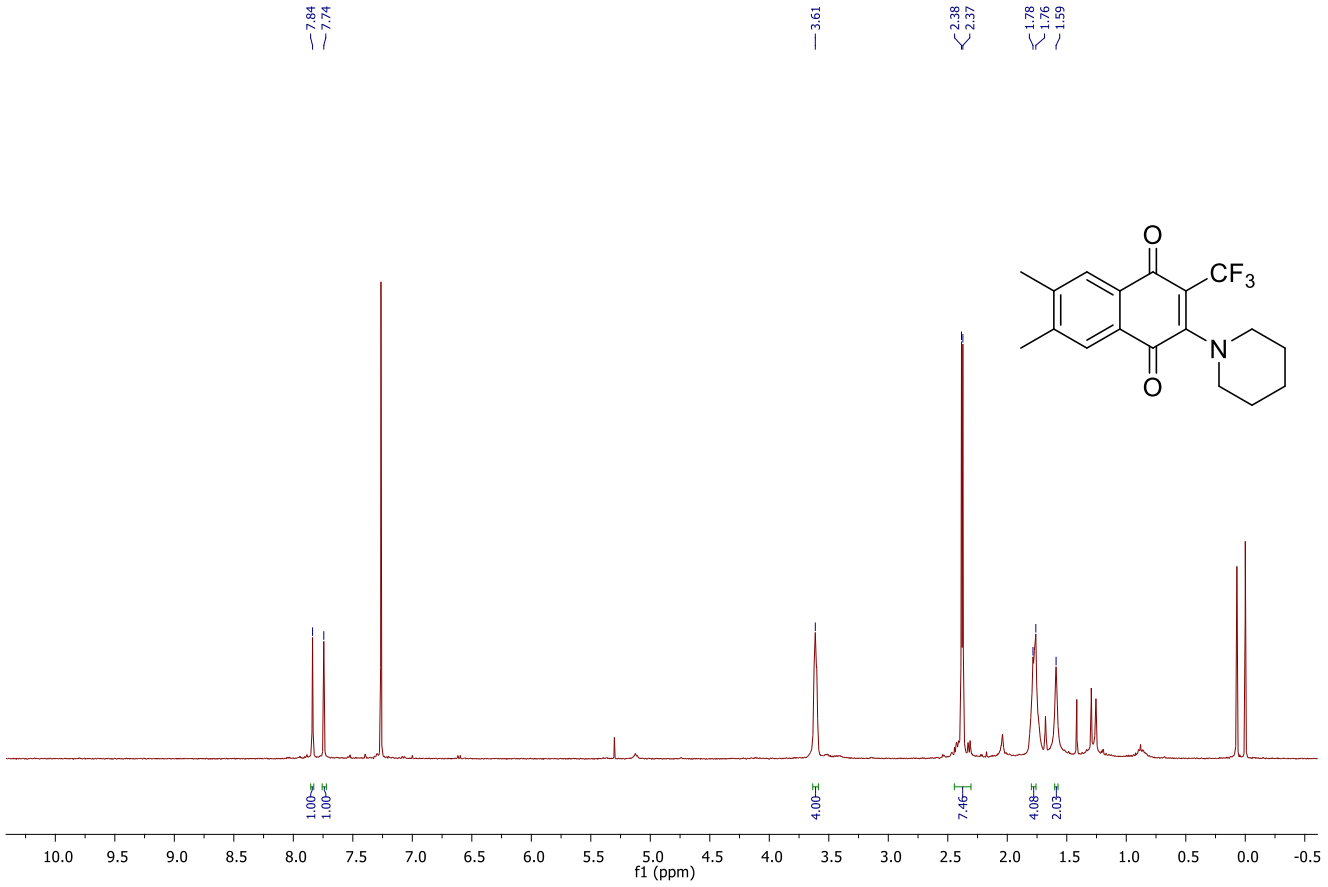
QMI DIVISION, CSIR-IIIM JAMMU
Xevo G2-XS QTOF YFC2015

06-Apr-2023
12:13:13
1: TOF MS ES+
1.19e+006

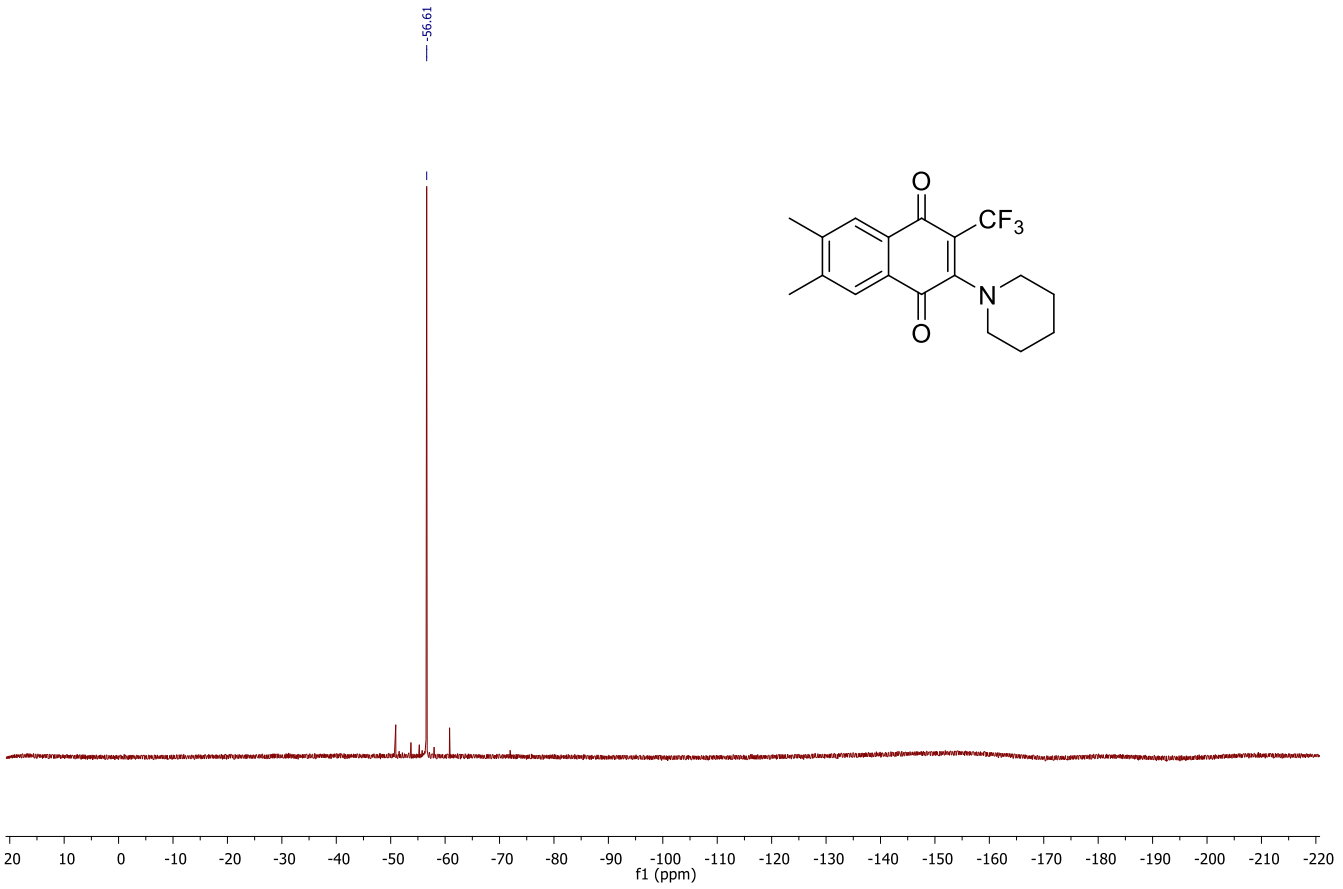


Minimum:				-1.5				
Maximum:		2.0	100.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
340.1163	340.1161	0.2	0.6	8.5	838.3	n/a	n/a	C17 H17 N O3 F3

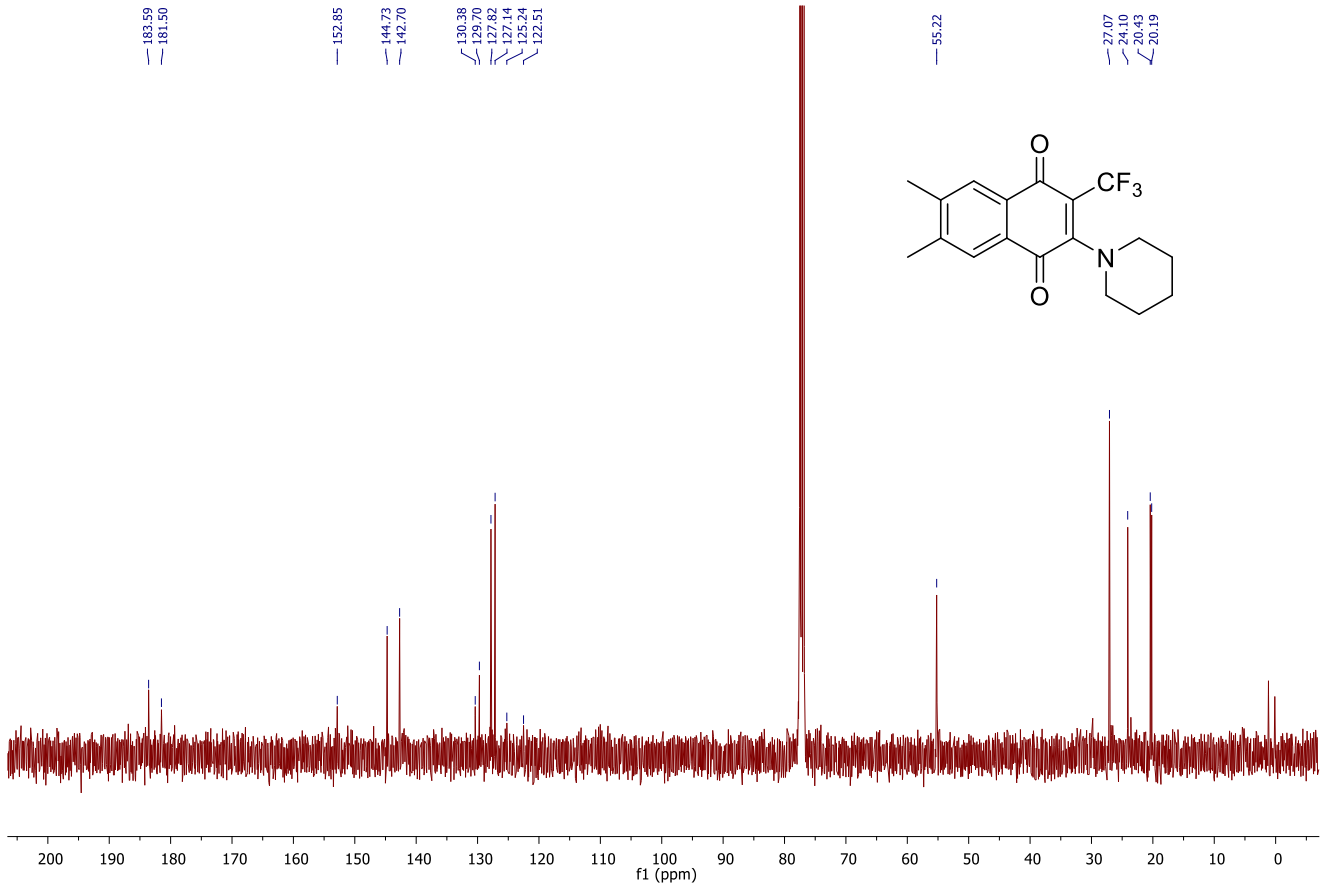
^{1}H NMR (400 MHz) of 4m in $CDCl_3$



^{19}F NMR (377 MHz) of 4m in $CDCl_3$



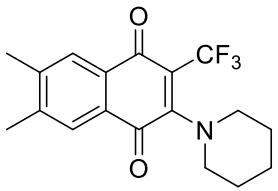
^{13}C {^{1}H} NMR (101 MHz) of 4m in $CDCl_3$



HRMS of 4m

Elemental Composition Report **Page 1**

Single Mass Analysis
Tolerance = 50.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

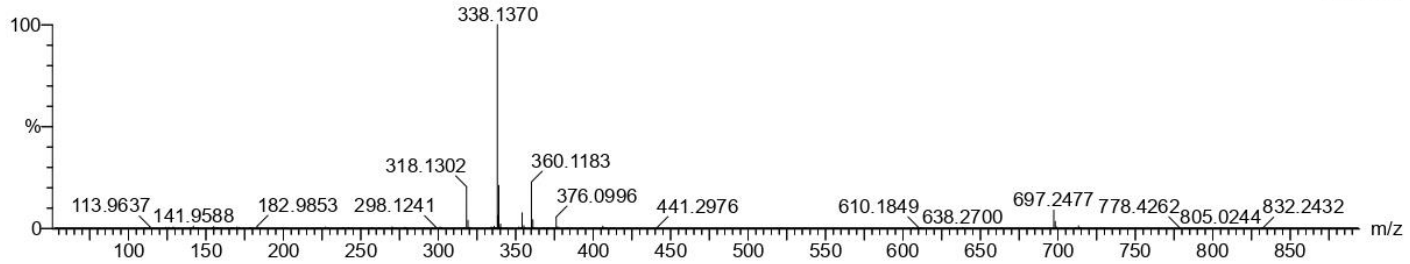


Monoisotopic Mass, Even Electron Ions
25 formula(e) evaluated with 1 results within limits (up to 3 closest results for each mass)
Elements Used:
C: 0-18 H: 0-100 N: 0-1 O: 0-2 F: 0-3

DM-NQ-1
110723_03 9 (0.208)

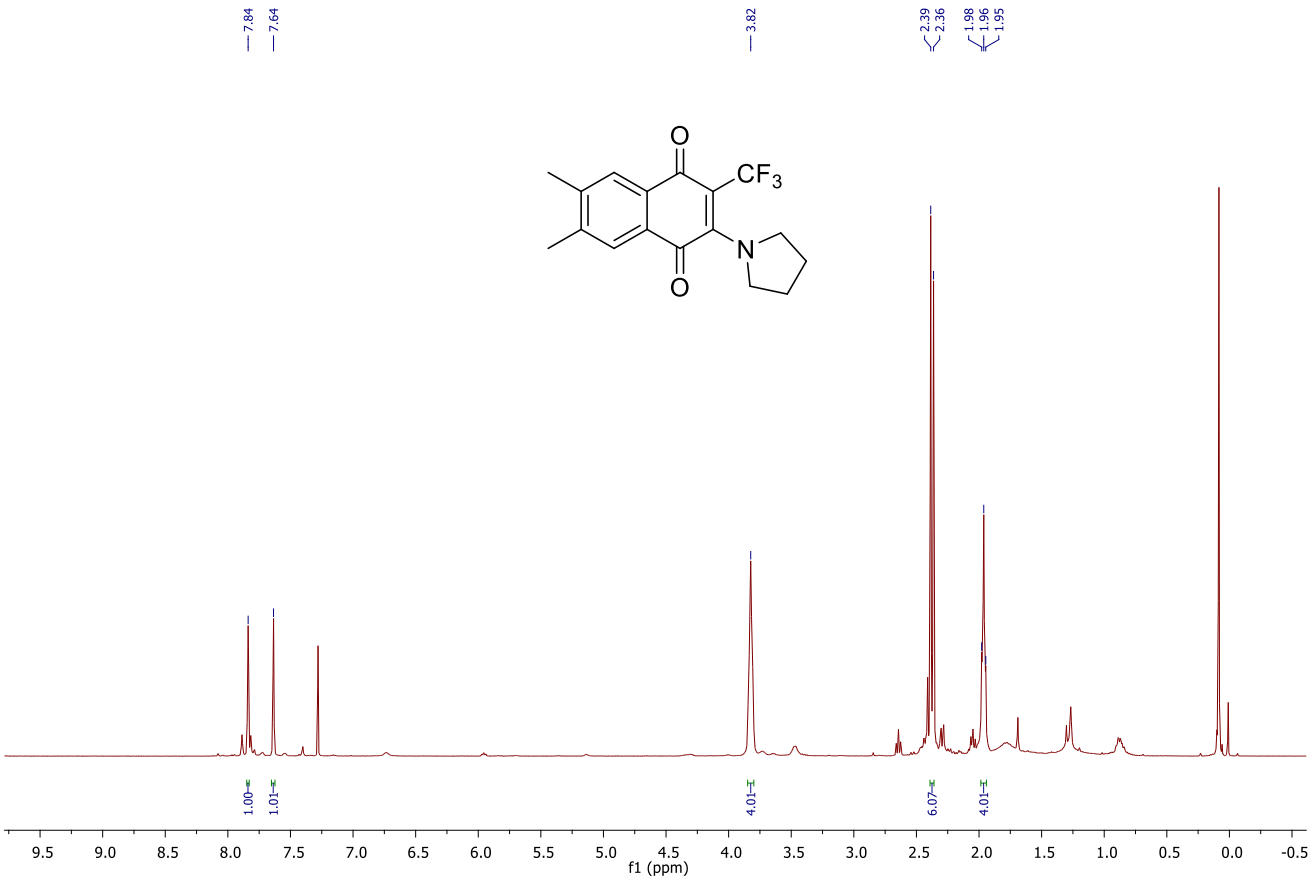
QMI DIVISION, CSIR-IIIM JAMMU
Xevo G2-XS QTOF YFC2015

11-Jul-2023
12:01:34
1: TOF MS ES+
1.39e+007

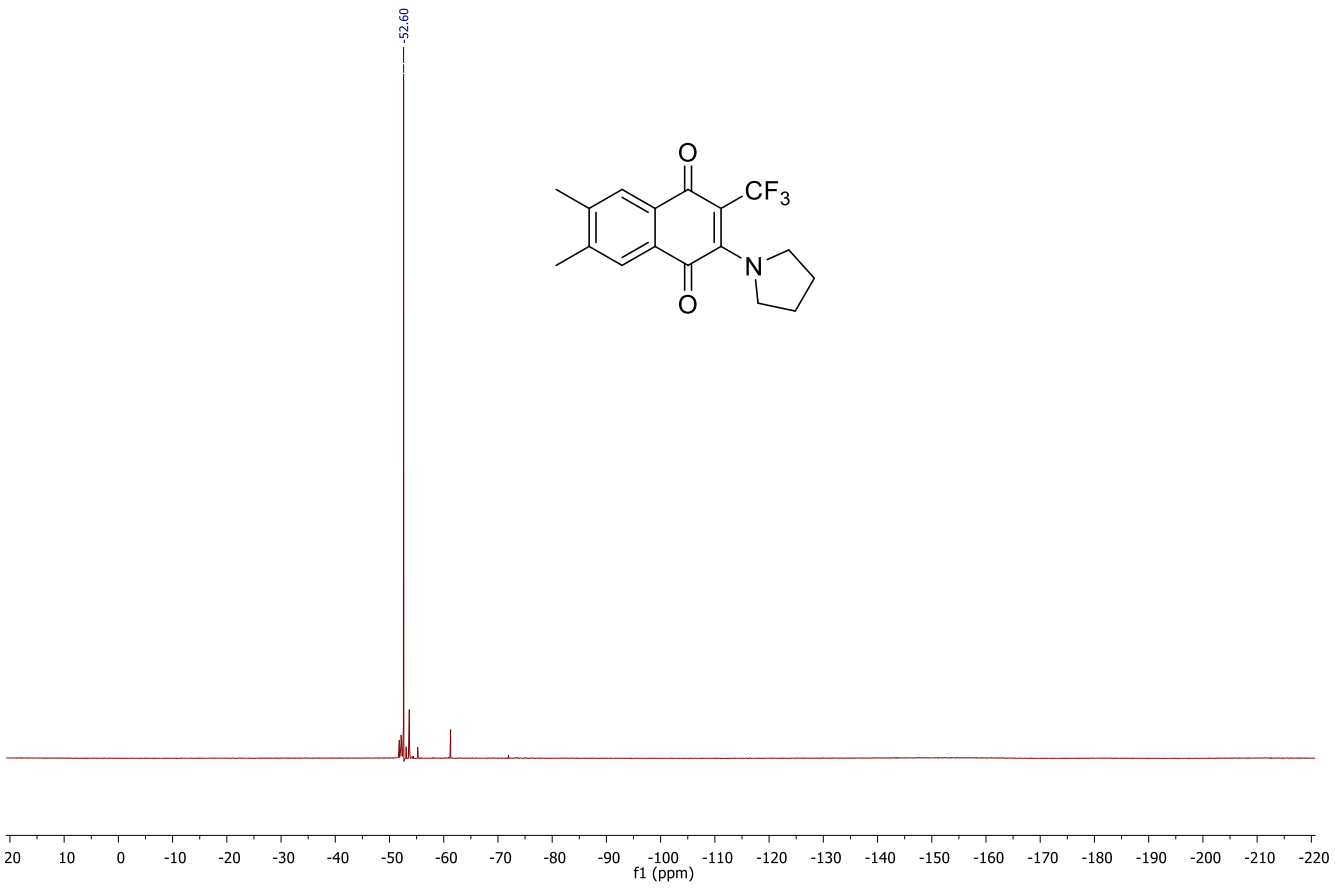


Minimum:				-1.5				
Maximum:		2.0	50.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
338.1370	338.1368	0.2	0.6	8.5	938.0	n/a	n/a	C18 H19 N O2 F3

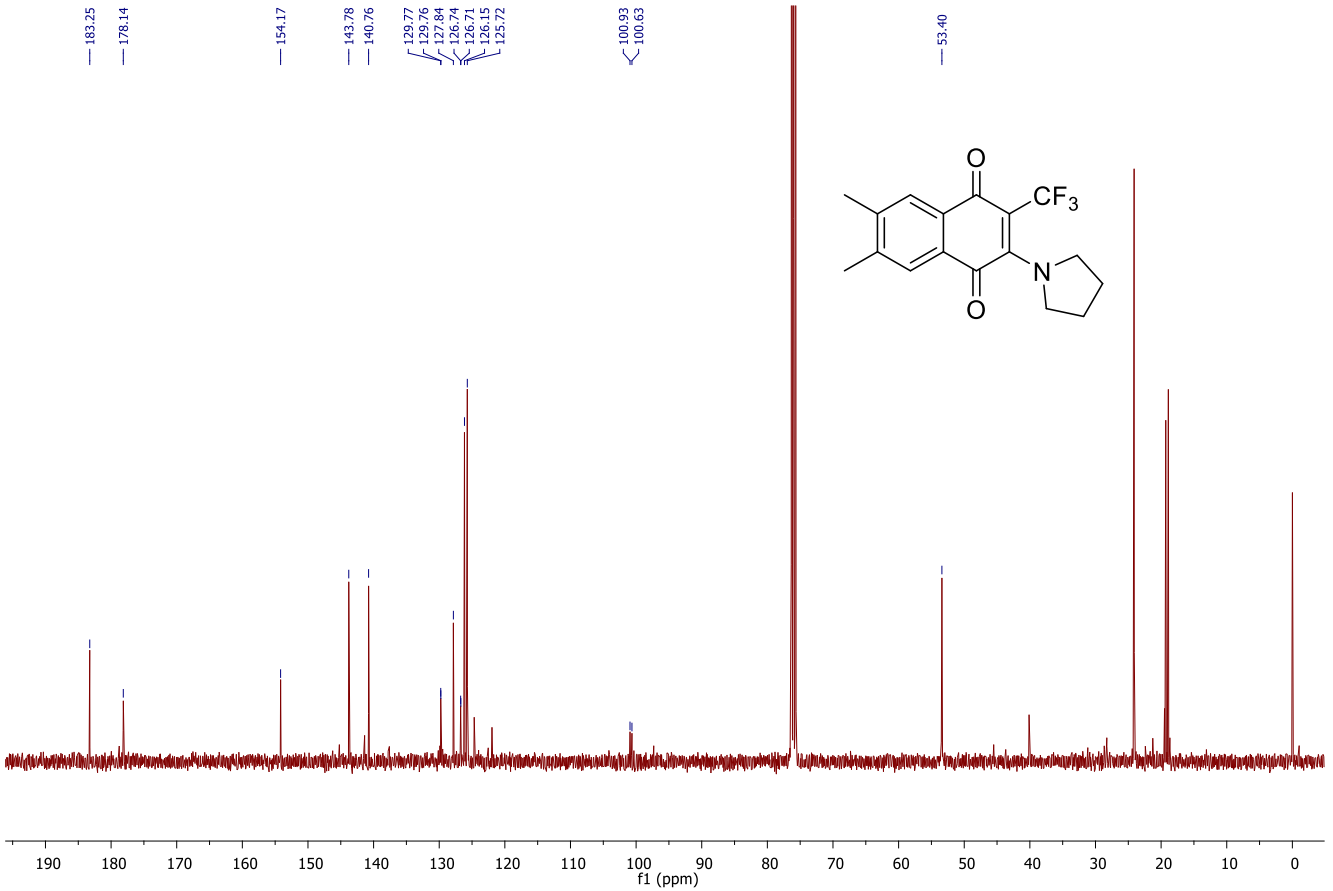
^{1}H NMR (400 MHz) of 4n in $CDCl_3$



^{19}F NMR (377 MHz) of 4n in $CDCl_3$



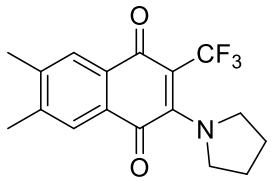
^{13}C {^{1}H} NMR (101 MHz) of 4n in $CDCl_3$



HRMS of 4n

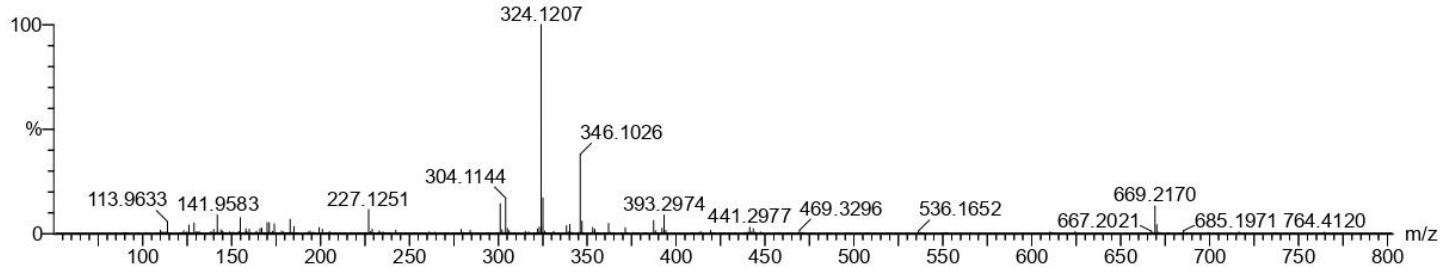
Elemental Composition Report **Page 1**

Single Mass Analysis
Tolerance = 50.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3



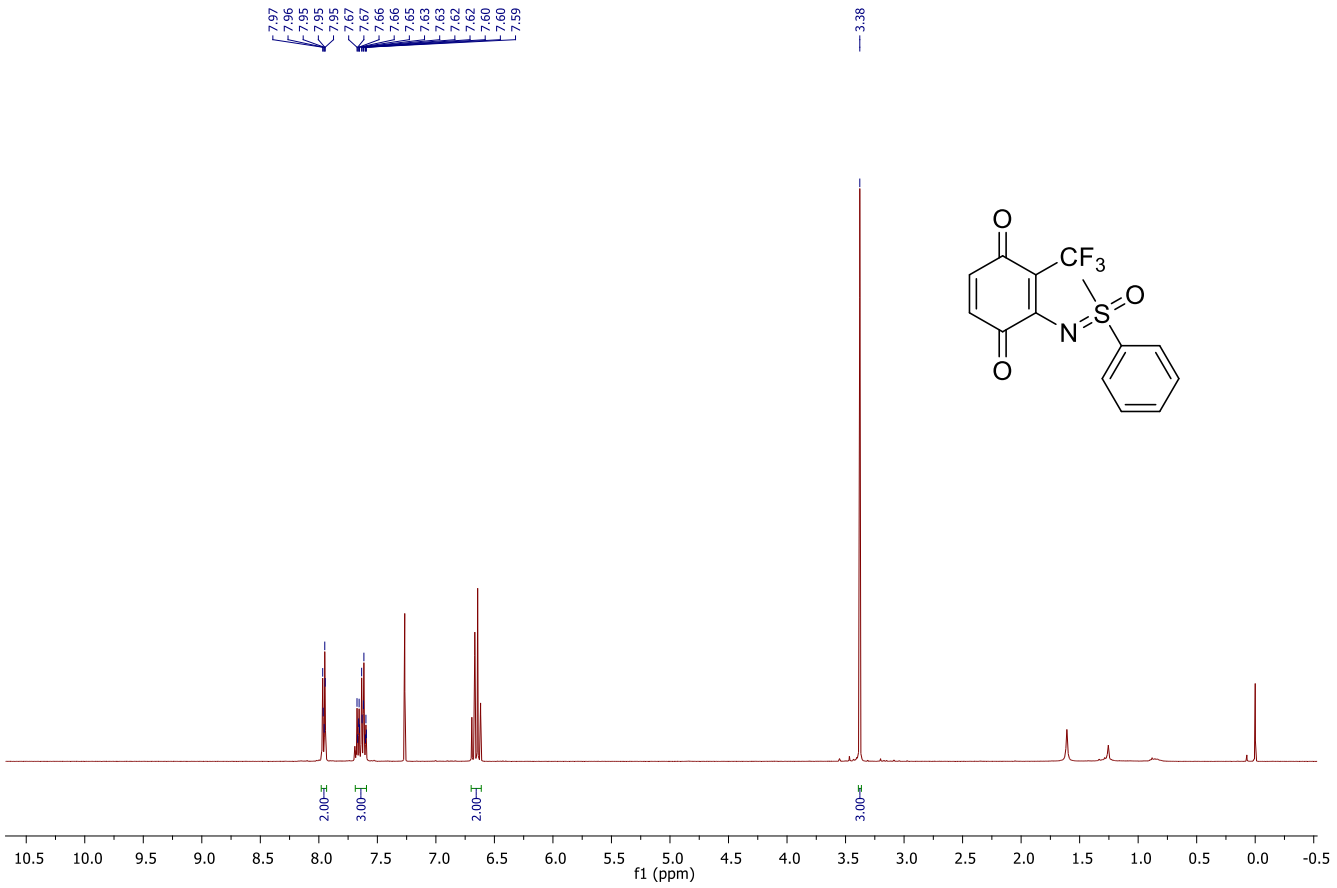
Monoisotopic Mass, Even Electron Ions
25 formula(e) evaluated with 1 results within limits (up to 3 closest results for each mass)
Elements Used:
C: 0-17 H: 0-100 N: 0-1 O: 0-2 F: 0-3

DM-NQ-2 QMI DIVISION, CSIR-IIIM JAMMU 10-Jul-2023
Xevo G2-XS QTOF YFC2015 12:58:16
100723_14 4 (0.104) 1: TOF MS ES+
1.18e+006

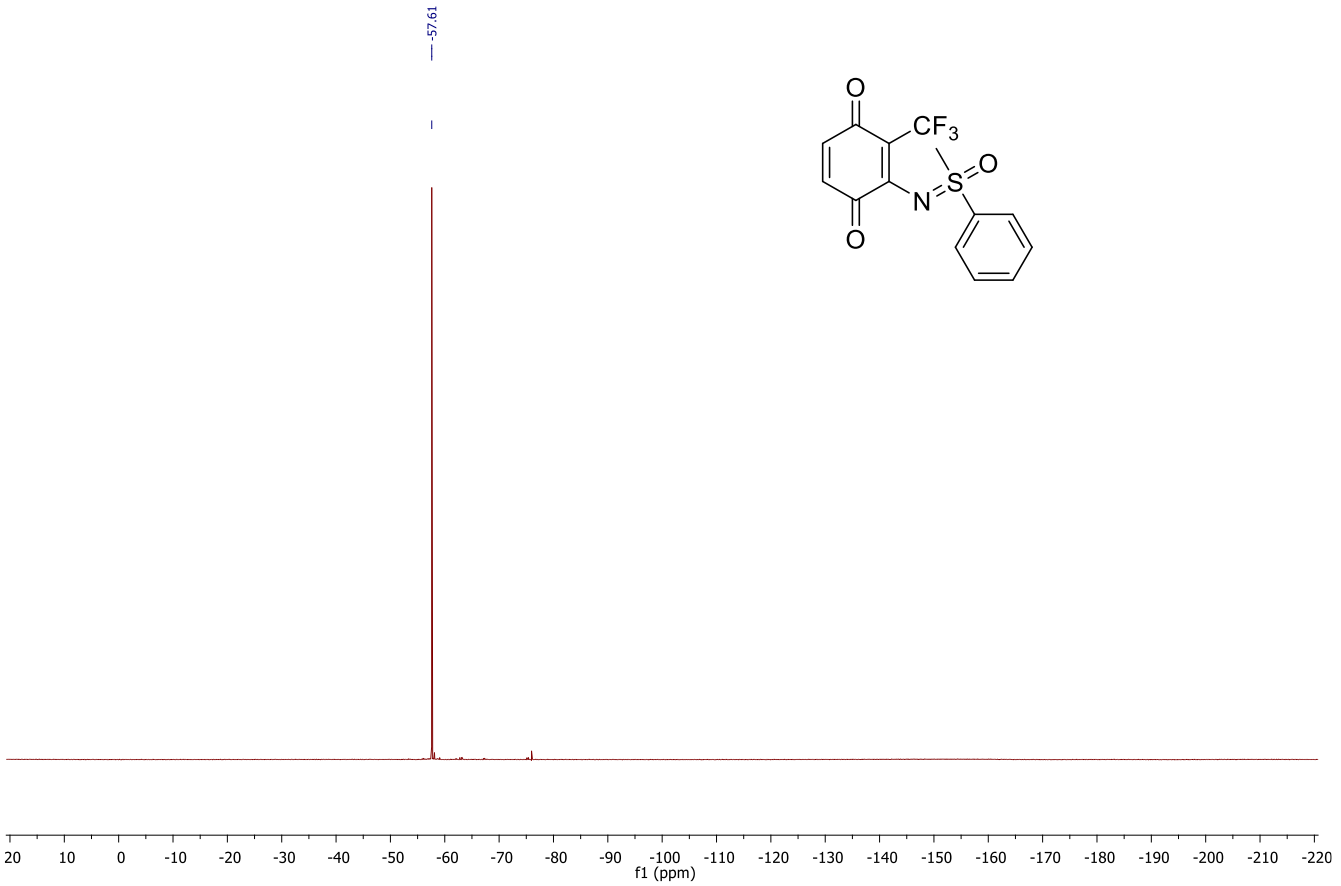


Minimum:				-1.5				
Maximum:		2.0	50.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
324.1207	324.1211	-0.4	-1.2	8.5	927.8	n/a	n/a	C17 H17 N O2 F3

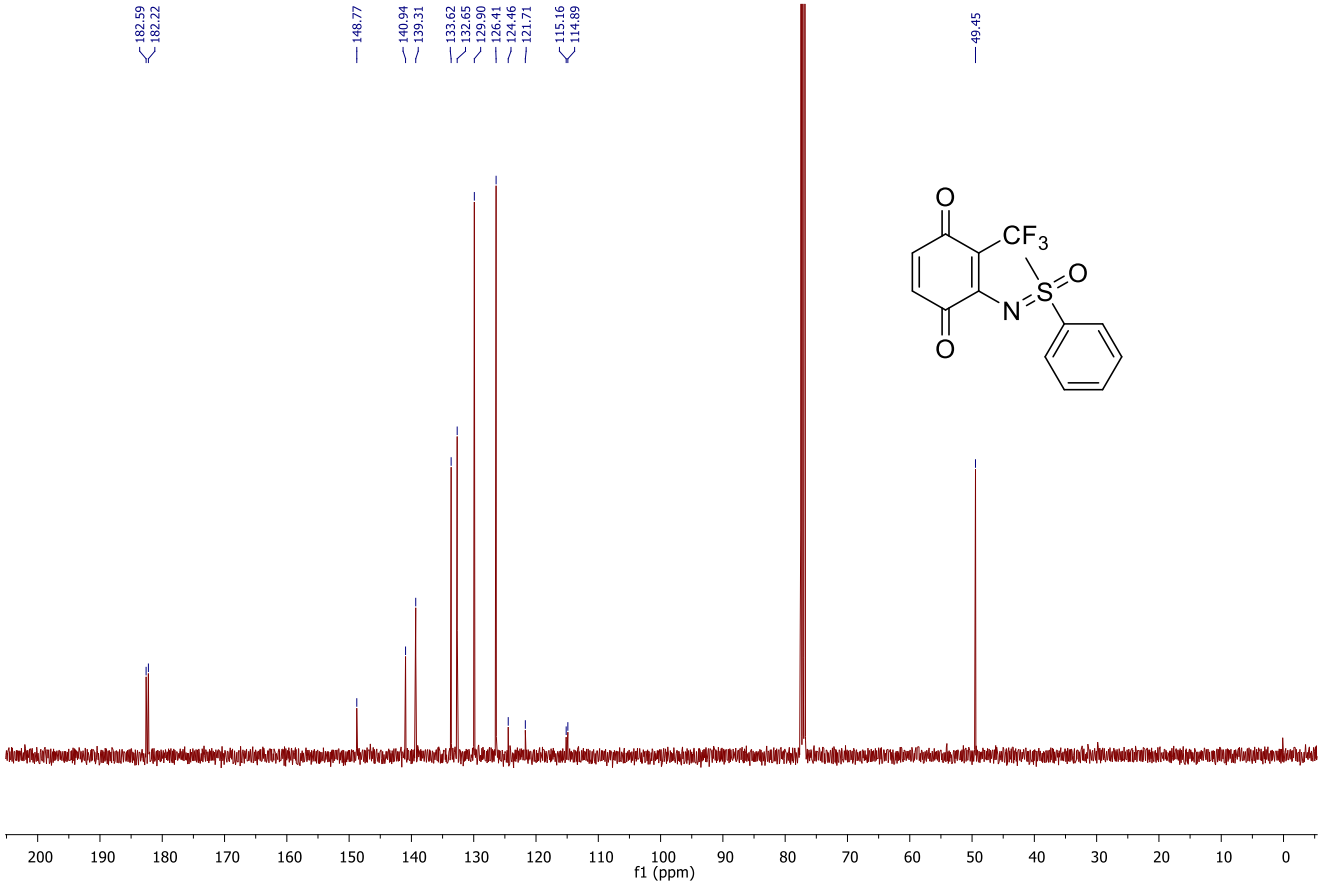
^{1}H NMR (400 MHz) of 5a in $CDCl_3$



^{19}F NMR (377 MHz) of 5a in $CDCl_3$



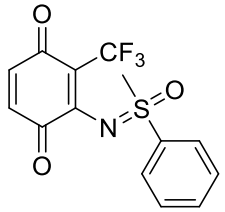
^{13}C {^{1}H} NMR (101 MHz) of 5a in $CDCl_3$



HRMS of 5a

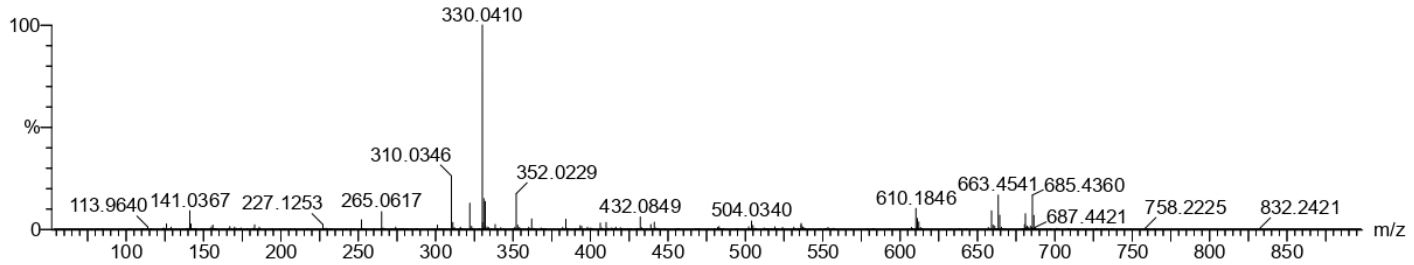
Elemental Composition Report **Page 1**

Single Mass Analysis
Tolerance = 100.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3



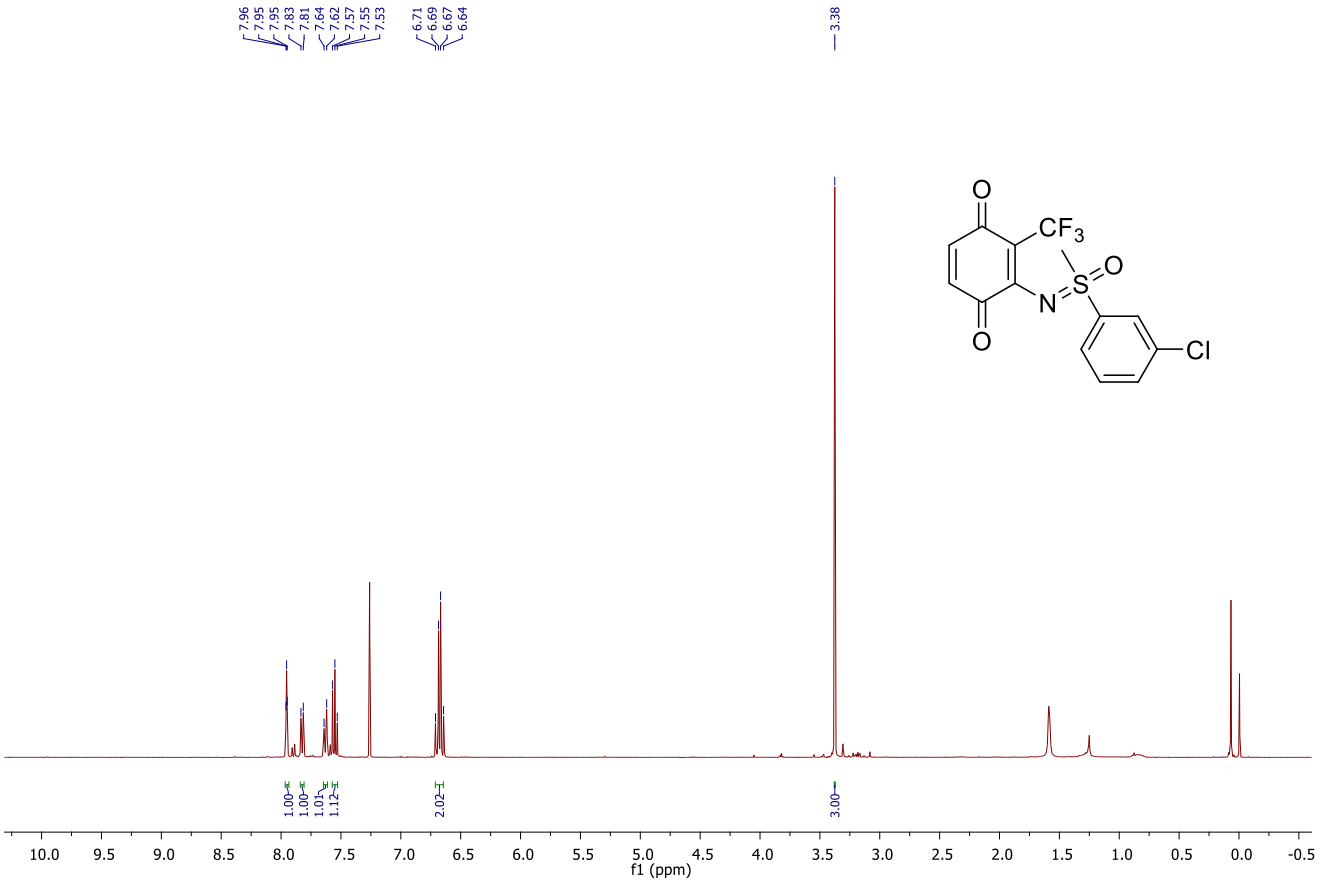
Monoisotopic Mass, Even Electron Ions
65 formula(e) evaluated with 1 results within limits (up to 3 closest results for each mass)
Elements Used:
C: 0-14 H: 0-100 N: 0-1 O: 0-3 F: 0-3 S: 0-1

BQS-1-CF3
QMI DIVISION, CSIR-IIIM JAMMU
Xevo G2-XS QTOF YFC2015
28-Mar-2023
12:29:40
280323_09 7 (0.155)
1: TOF MS ES+
5.49e+006

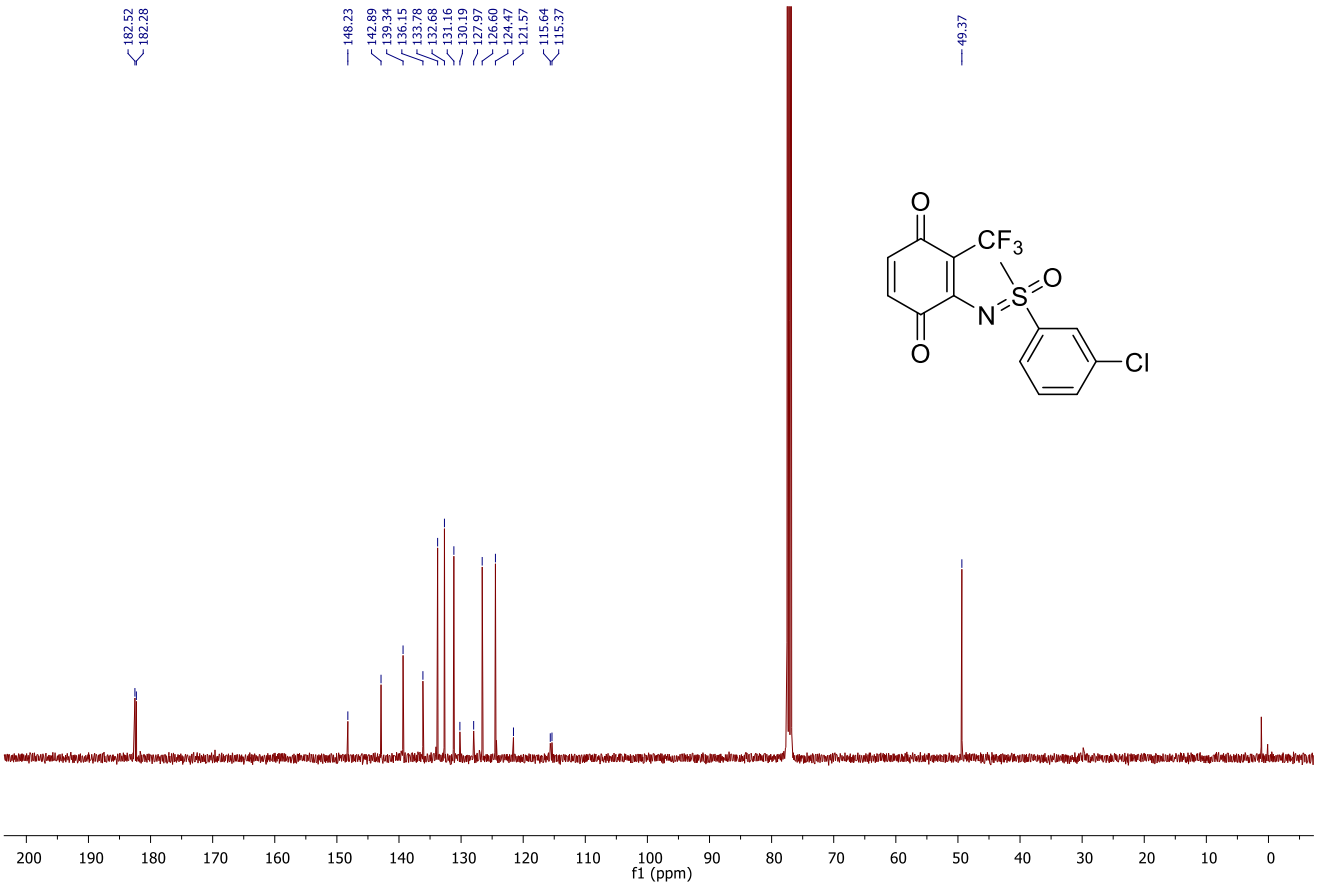


Minimum:				-1.5				
Maximum:		2.0	100.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
330.0410	330.0412	-0.2	-0.6	8.5	807.8	n/a	n/a	C14 H11 N O3 F3 S

^{1}H NMR (400 MHz) of 5b in $CDCl_3$



^{13}C {^{1}H} NMR (101 MHz) of 5b in $CDCl_3$

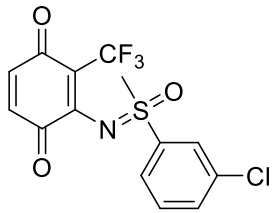


HRMS of 5b

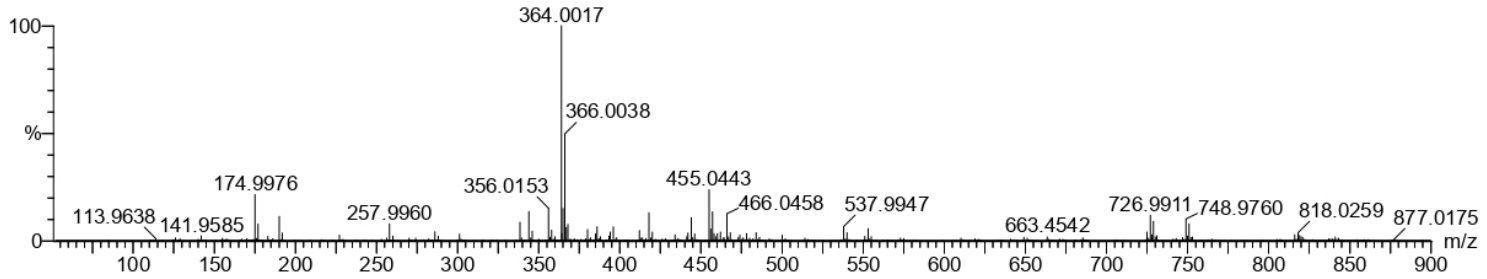
Elemental Composition Report **Page 1**

Single Mass Analysis
Tolerance = 100.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
129 formula(e) evaluated with 1 results within limits (up to 3 closest results for each mass)
Elements Used:
C: 0-14 H: 0-100 N: 0-1 O: 0-3 F: 0-3 S: 0-1 Cl: 0-1

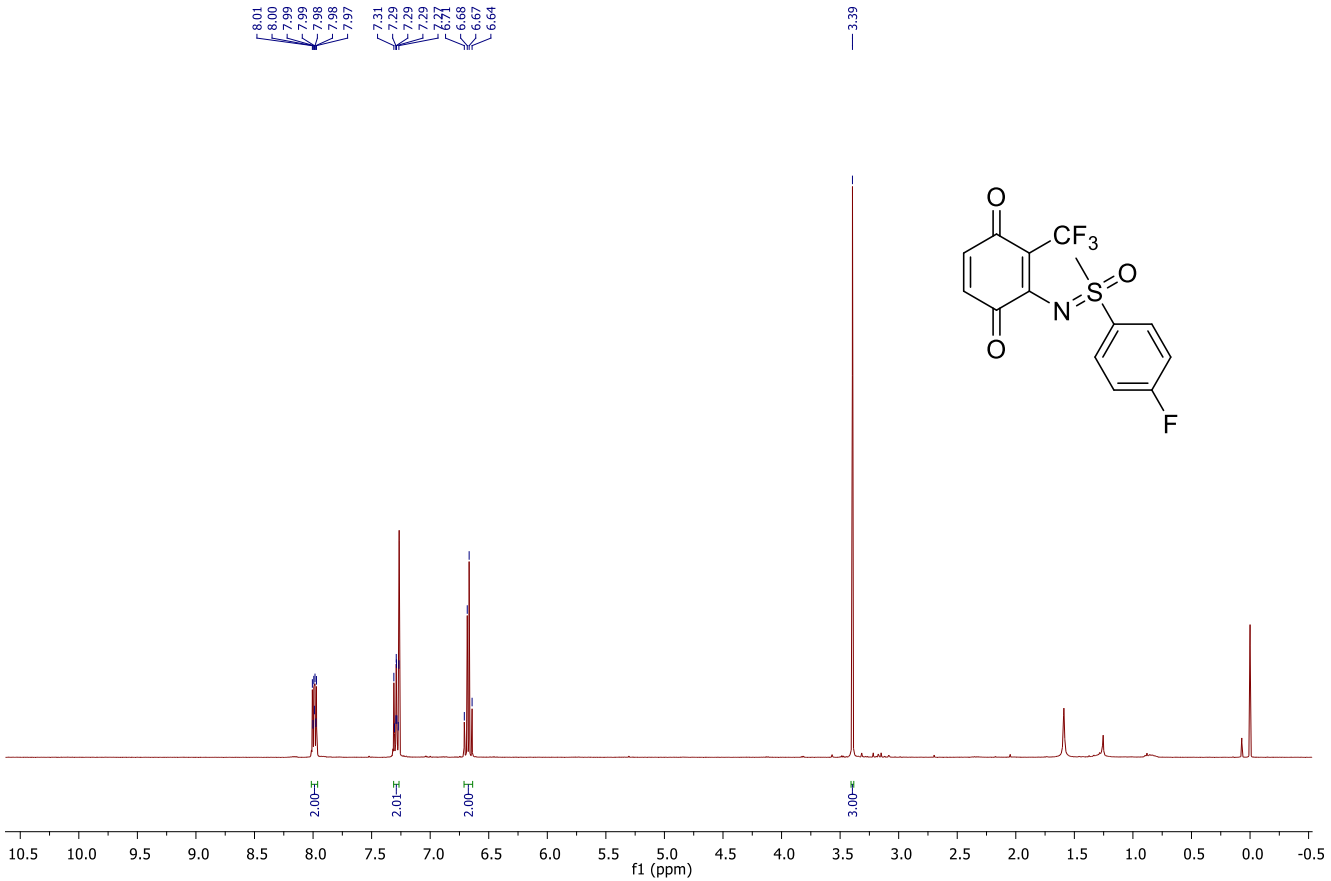


BQS-3-CF3
QMI DIVISION, CSIR-IIIM JAMMU
Xevo G2-XS QTOF YFC2015
28-Mar-2023
12:34:48
280323_11 6 (0.138)
1: TOF MS ES+
4.50e+006

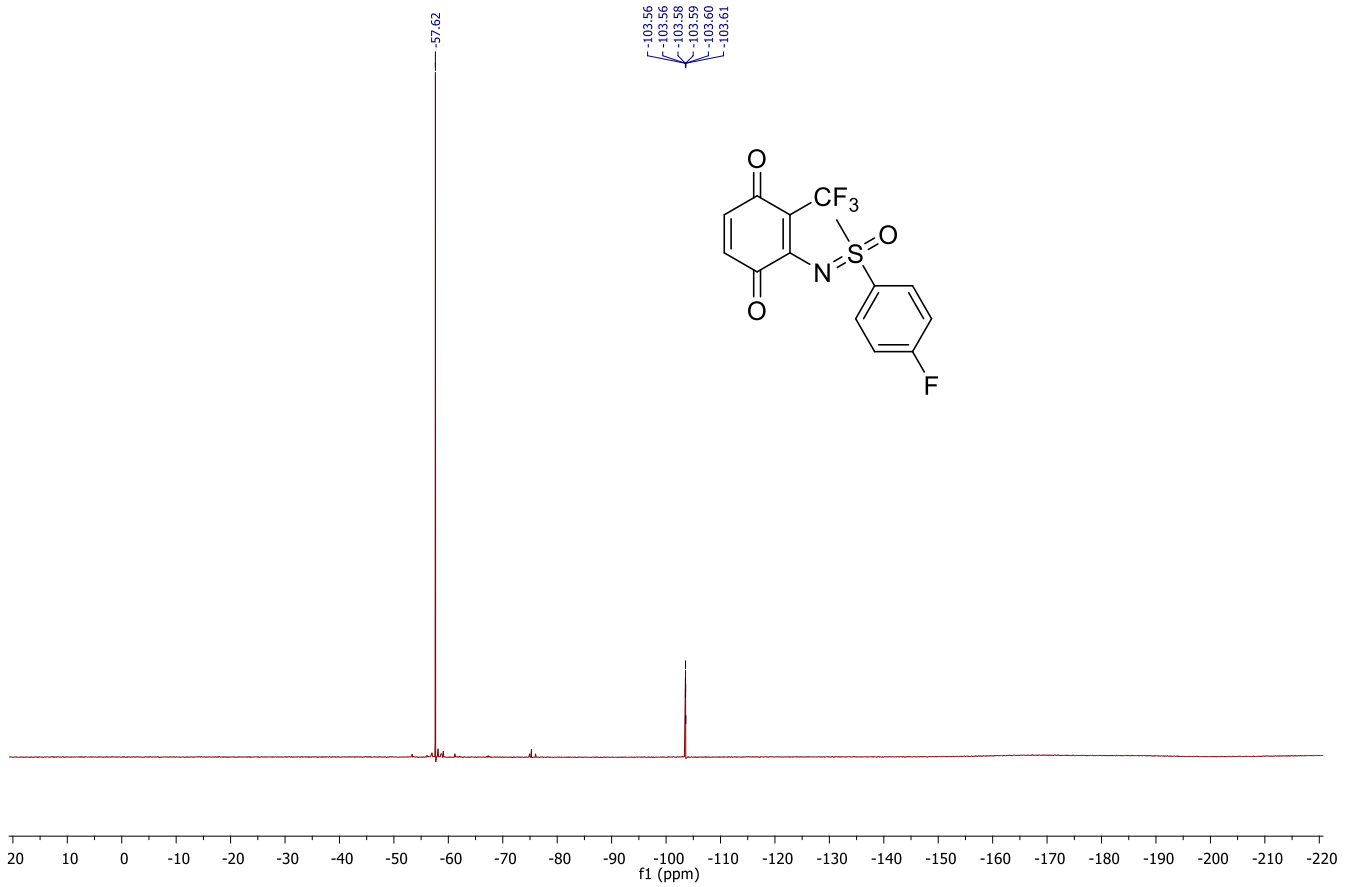


Minimum:				-1.5				
Maximum:		2.0	100.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
364.0017	364.0022	-0.5	-1.4	8.5	916.9	n/a	n/a	C14 H10 N O3 F3 S Cl

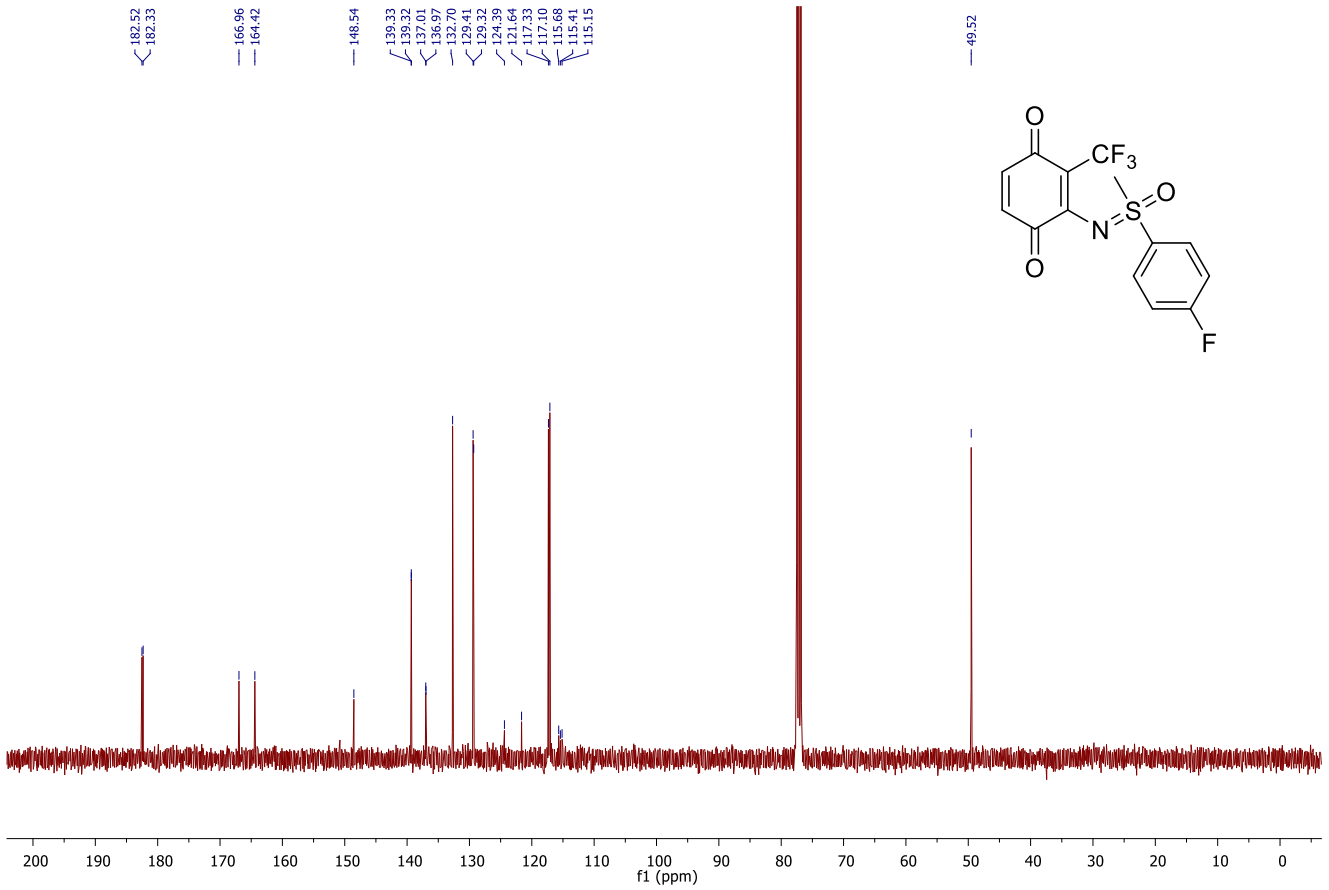
^{1}H NMR (400 MHz) of 5c in $CDCl_3$



^{19}F NMR (377 MHz) of 5c in $CDCl_3$



^{13}C {^{1}H} NMR (101 MHz) of 5c in $CDCl_3$



HRMS of 5b

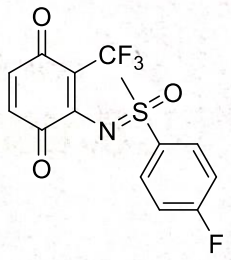
Elemental Composition Report

Page 1

Single Mass Analysis

Tolerance = 100.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

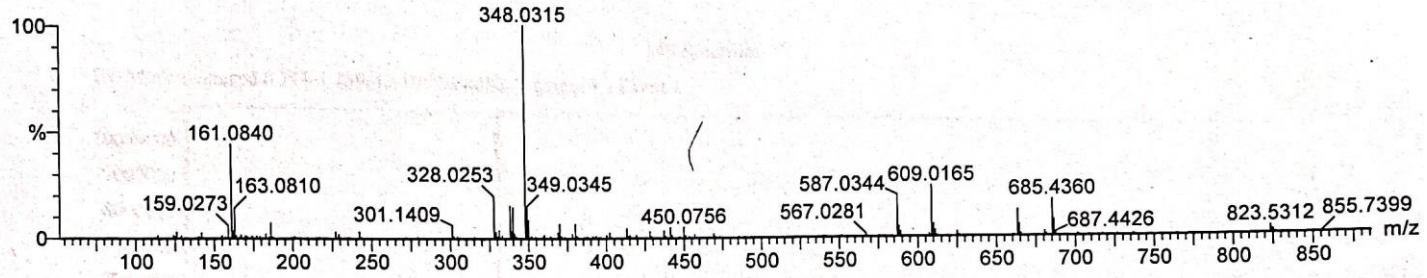
Monoisotopic Mass, Even Electron Ions
81 formula(e) evaluated with 1 results within limits (up to 3 closest results for each mass)
Elements Used:
C: 0-14 H: 0-100 N: 0-1 O: 0-3 F: 0-4 S: 0-1



BQS-4-CF3
QMI DIVISION, CSIR-IIIM JAMMU
Xevo G2-XS QTOF YFC2015

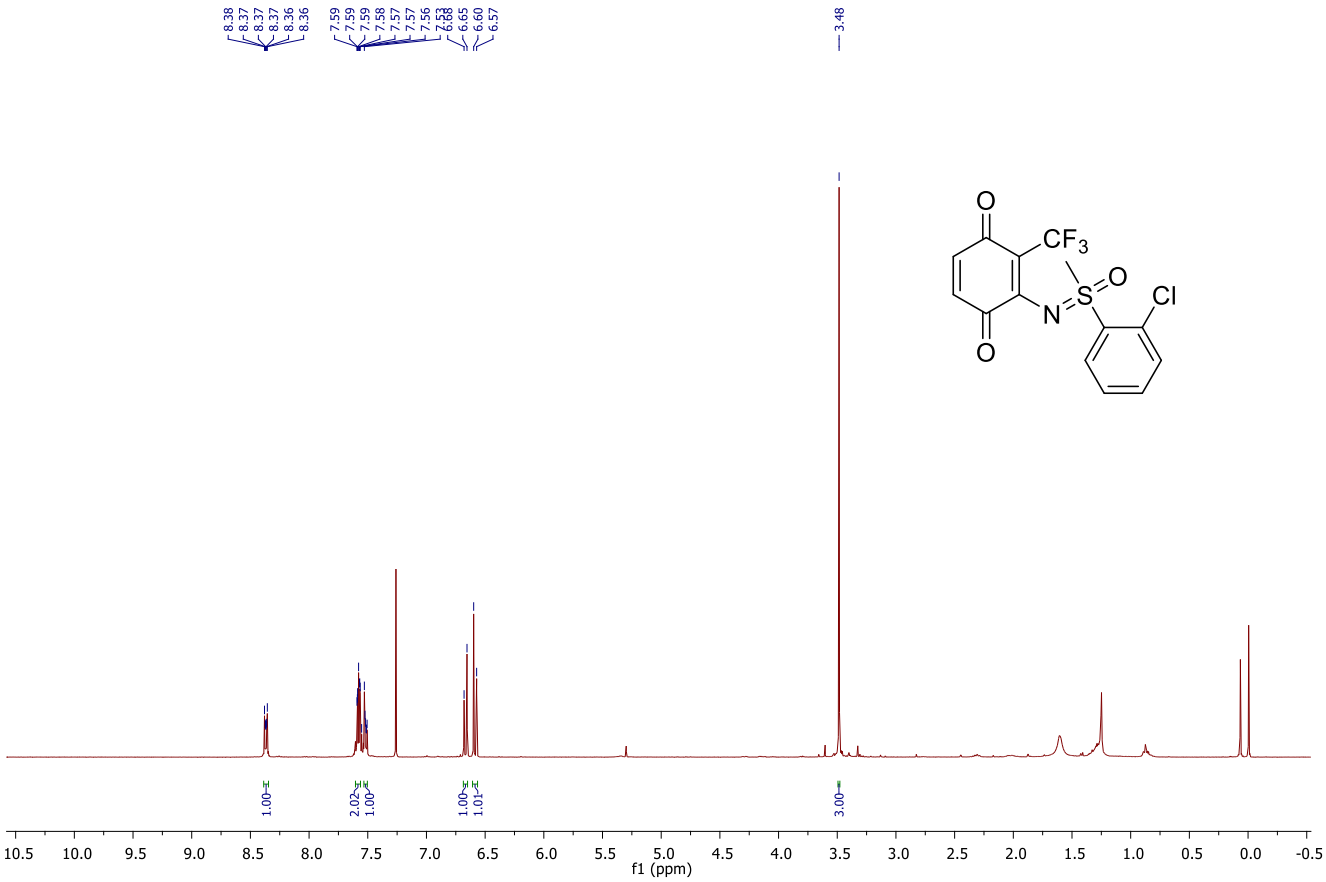
15-Mar-2023
13:50:09
1: TOF MS ES+
7.90e+006

150323_35 6 (0.138)

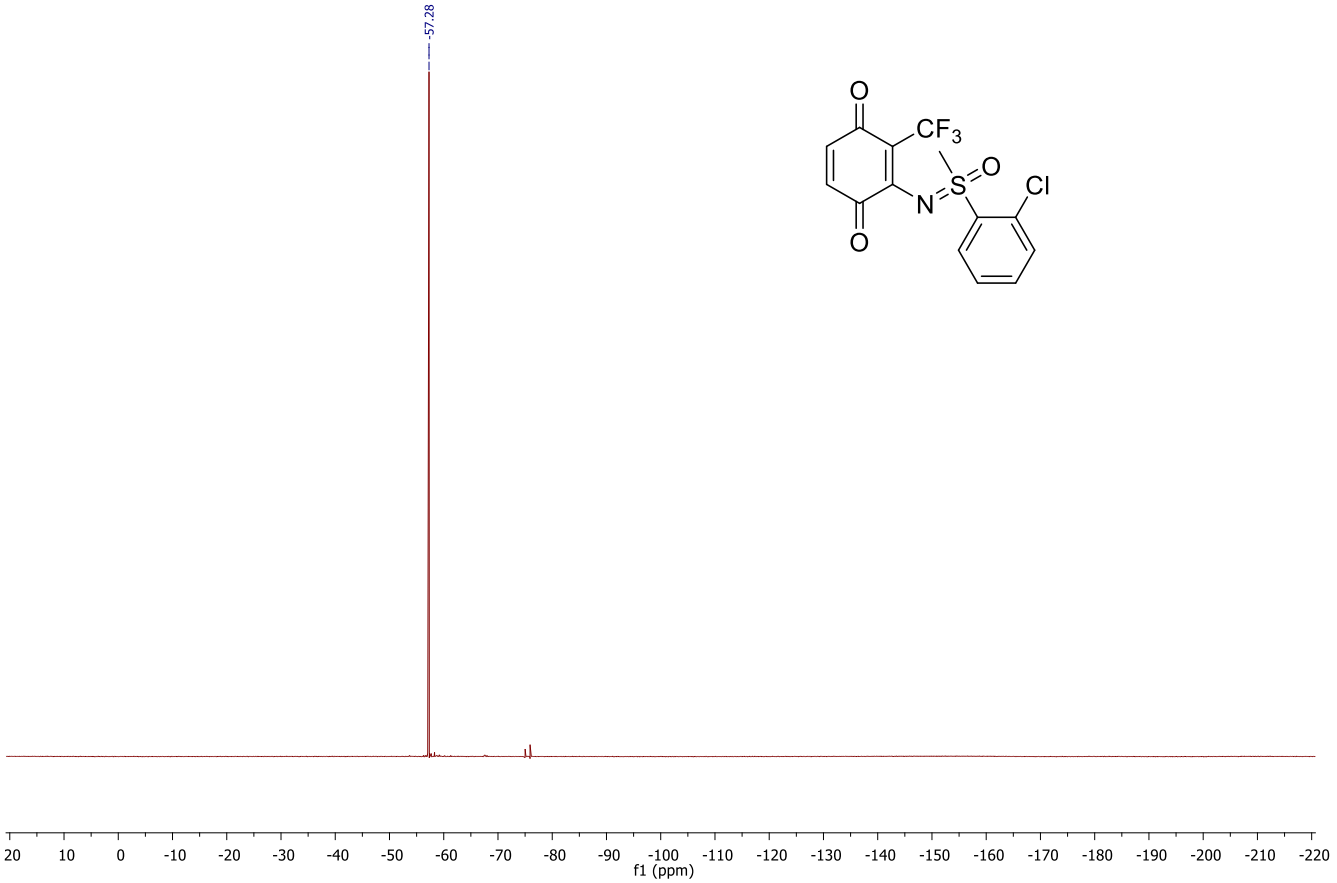


Minimum:				-1.5				
Maximum:		2.0	100.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
348.0315	348.0318	-0.3	-0.9	8.5	1058.5	n/a	n/a	C14 H10 N O3 F4 S

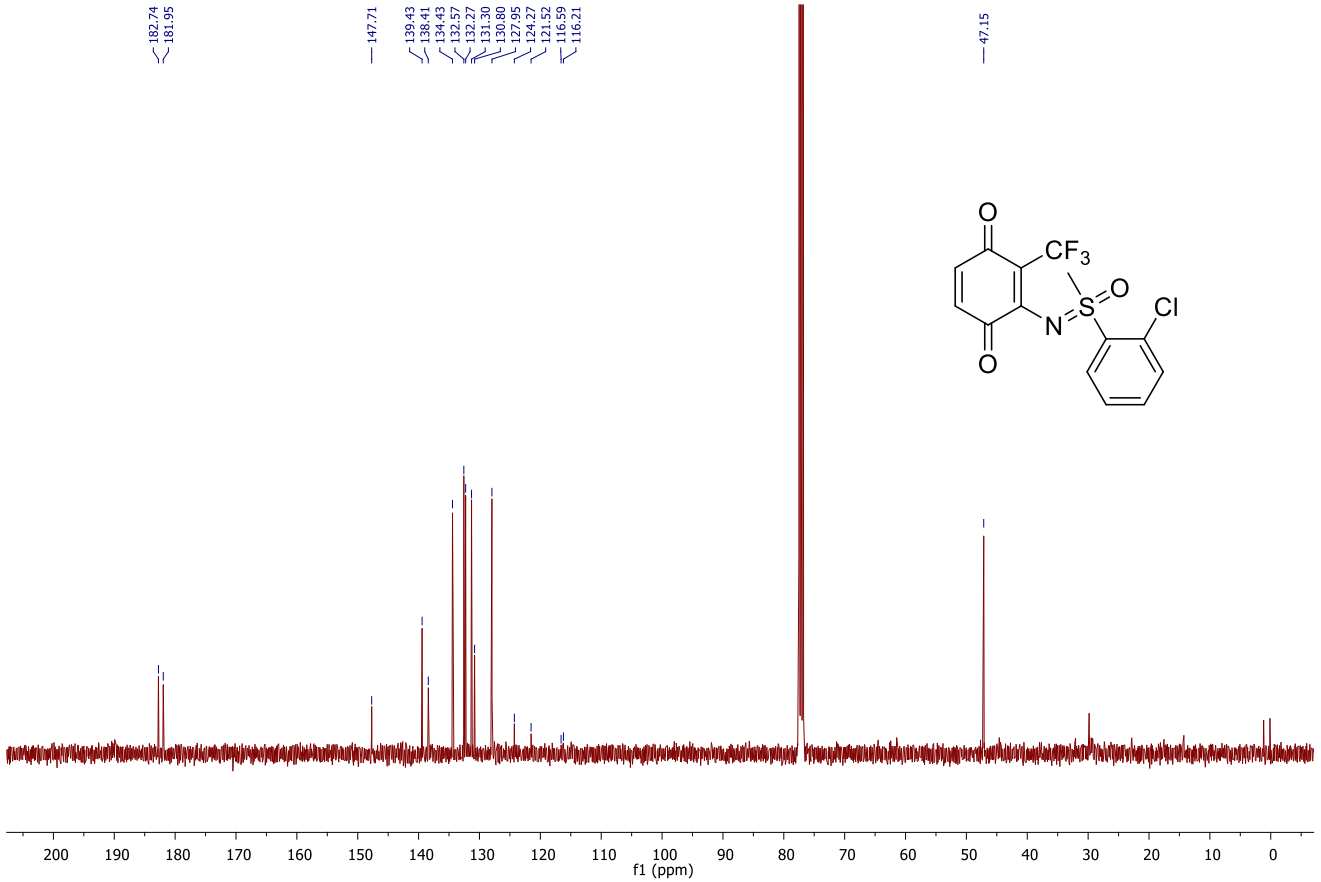
^{1}H NMR (400 MHz) of 5d in $CDCl_3$



^{19}F NMR (377 MHz) of 5d in $CDCl_3$



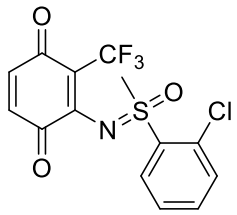
^{13}C {^{1}H} NMR (101 MHz) of 5d in $CDCl_3$



HRMS of 5d

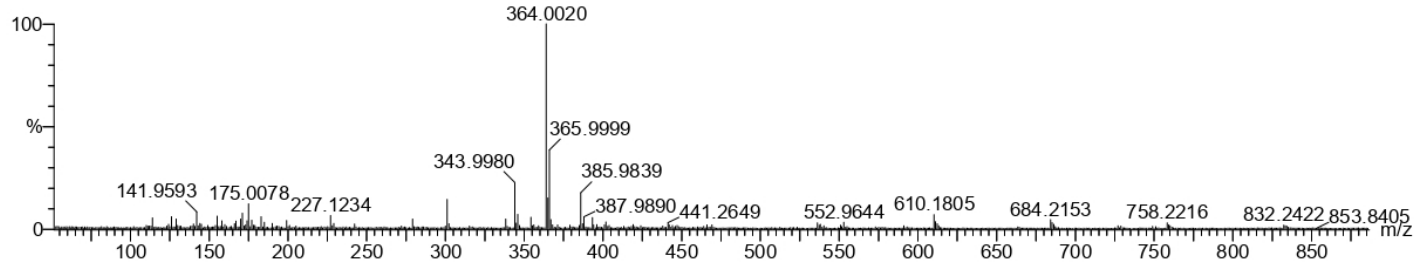
Elemental Composition Report **Page 1**

Single Mass Analysis
Tolerance = 100.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3



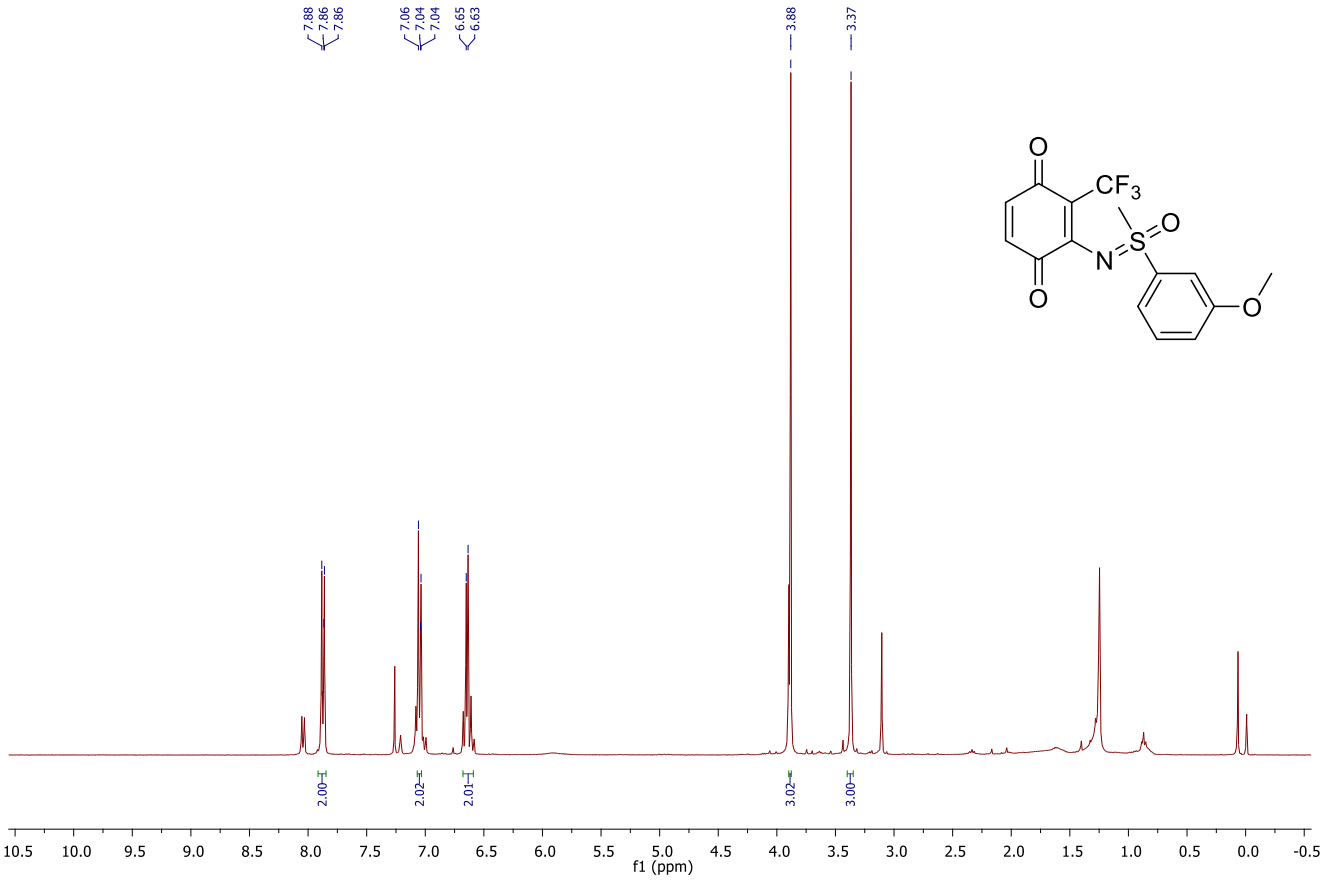
Monoisotopic Mass, Even Electron Ions
129 formula(e) evaluated with 1 results within limits (up to 3 closest results for each mass)
Elements Used:
C: 0-14 H: 0-100 N: 0-1 O: 0-3 F: 0-3 S: 0-1 Cl: 0-1

BQS-5-CF3 QMI DIVISION, CSIR-IIIM JAMMU 05-Jul-2023
Xevo G2-XS QTOF YFC2015 14:18:11
050723_04 15 (0.310) Cm (15:16) 1: TOF MS ES+
3.32e+006

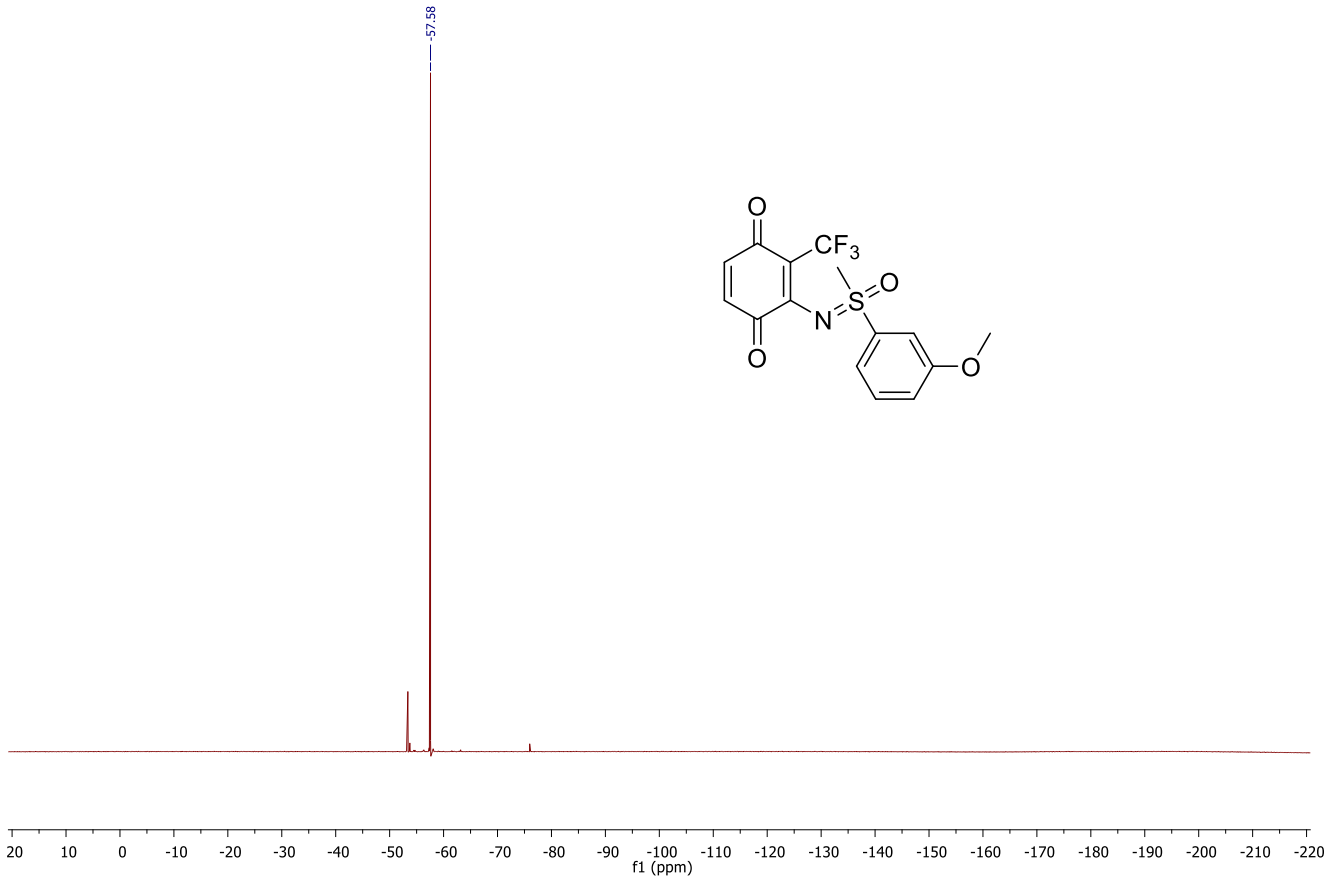


Minimum:				-1.5				
Maximum:		2.0	100.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
364.0020	364.0022	-0.2	-0.5	8.5	30.6	n/a	n/a	C14 H10 N O3 F3 S Cl

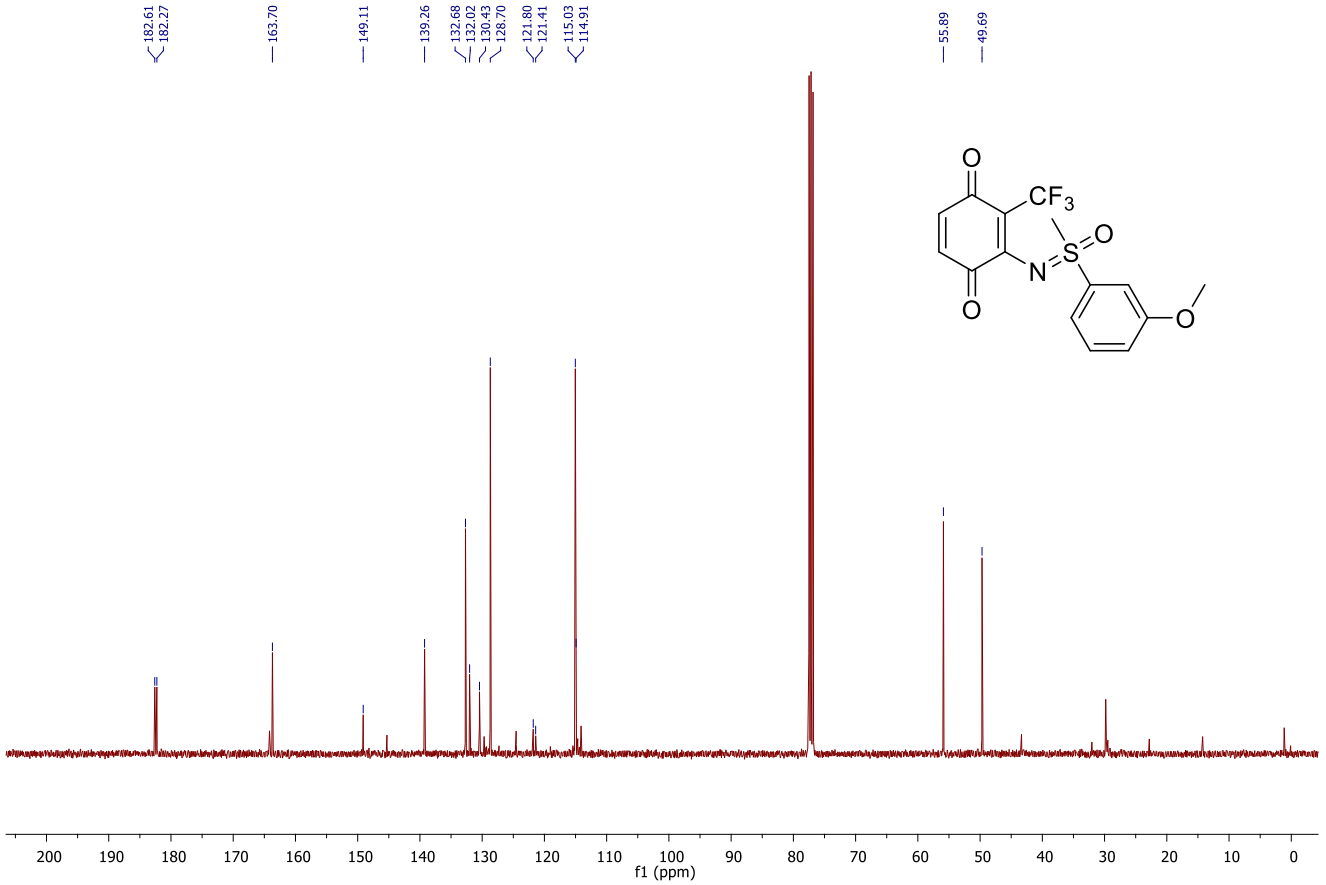
^{1}H NMR (400 MHz) of 5e in $CDCl_3$



^{19}F NMR (377 MHz) of 5e in $CDCl_3$



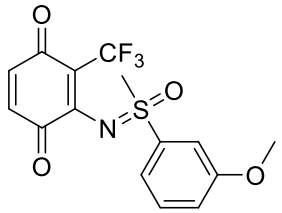
^{13}C {^{1}H} NMR (101 MHz) of 5e in $CDCl_3$



HRMS of 5e

Elemental Composition Report **Page 1**

Single Mass Analysis
Tolerance = 100.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

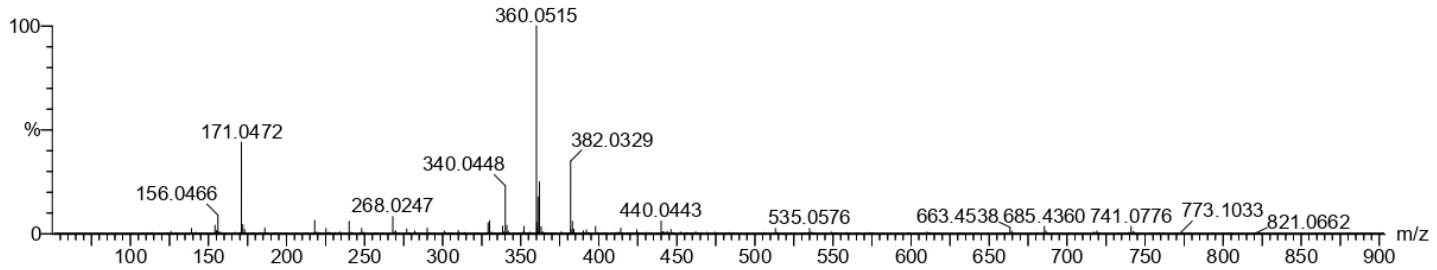


Monoisotopic Mass, Even Electron Ions
81 formula(e) evaluated with 1 results within limits (up to 3 closest results for each mass)
Elements Used:
C: 0-15 H: 0-100 N: 0-1 O: 0-4 F: 0-3 S: 0-1

BQ-OMe
050723_06 7 (0.155)

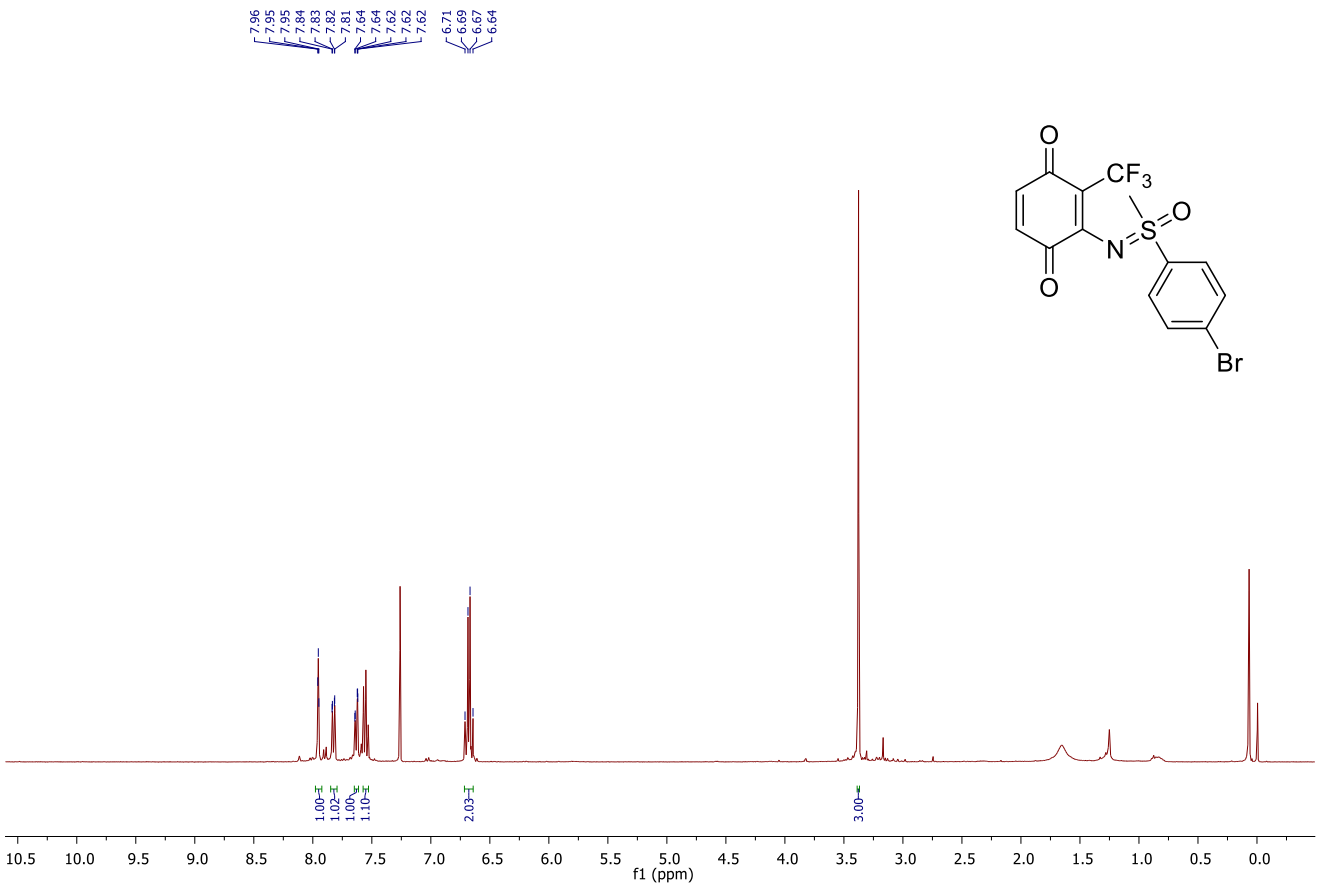
QMI DIVISION, CSIR-IIIM JAMMU
Xevo G2-XS QTOF YFC2015

05-Jul-2023
14:23:20
1: TOF MS ES+
1.50e+007

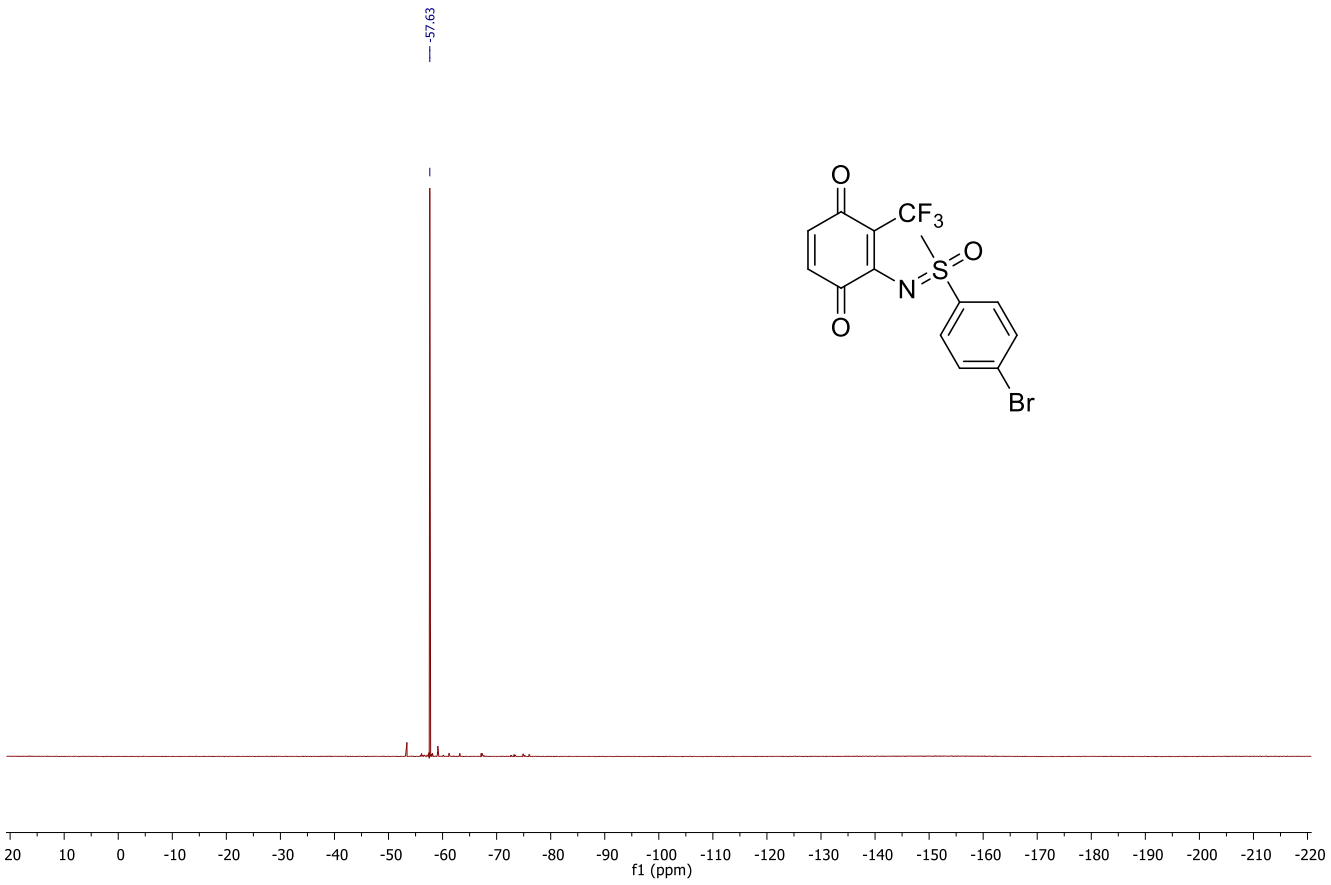


Minimum:				-1.5				
Maximum:		2.0	100.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
360.0515	360.0517	-0.2	-0.6	8.5	1038.0	n/a	n/a	C15 H13 N O4 F3 S

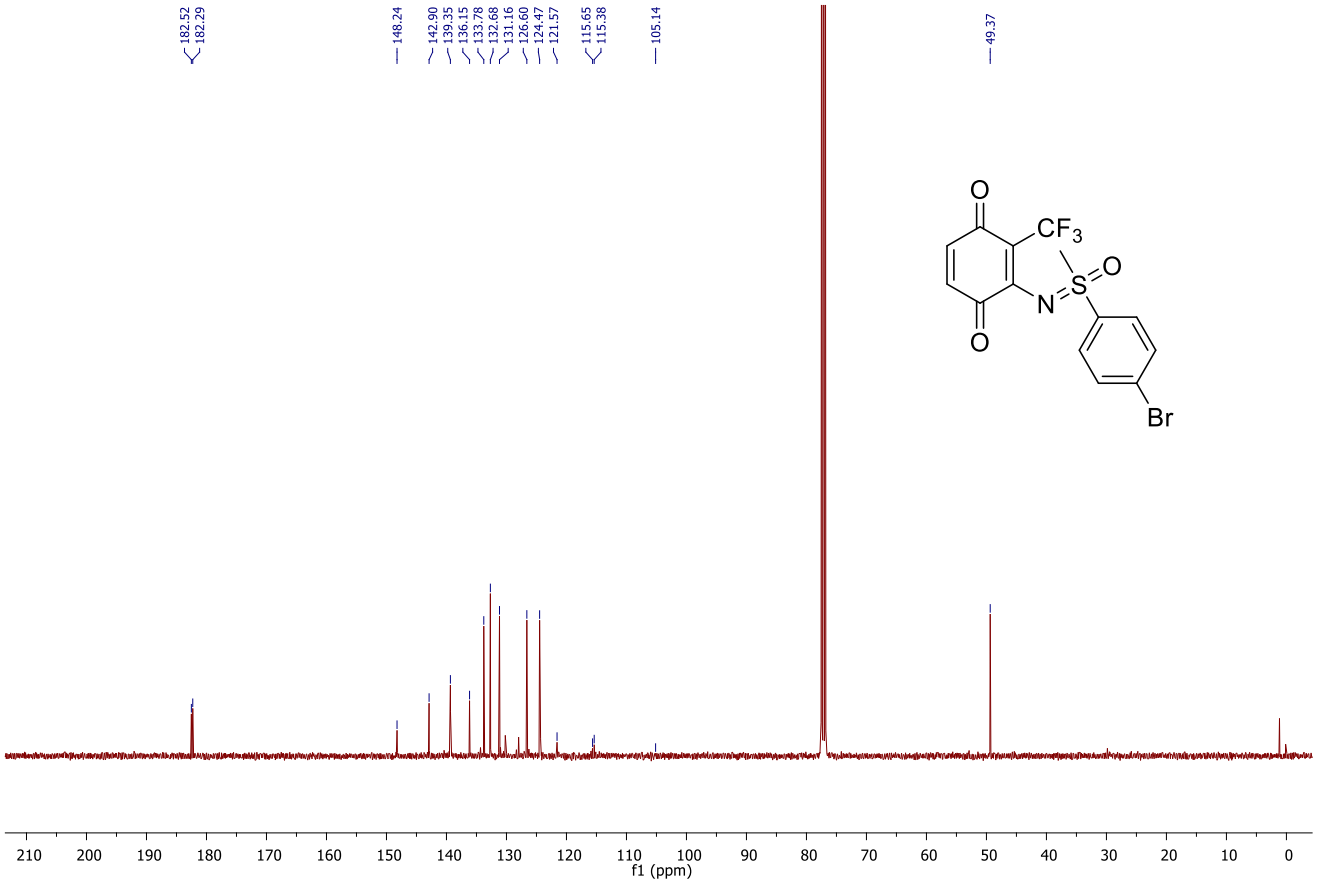
^{1}H NMR (400 MHz) of 5f in $CDCl_3$



^{19}F NMR (377 MHz) of 5f in $CDCl_3$



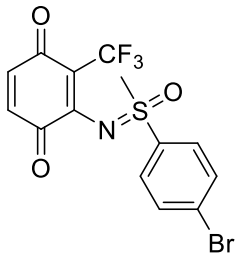
^{13}C {^{1}H} NMR (101 MHz) of 5f in $CDCl_3$



HRMS of 5f

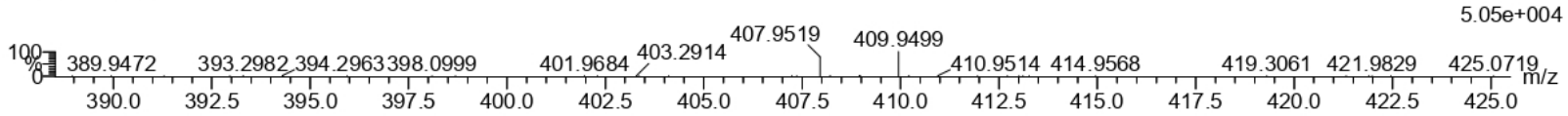
Elemental Composition Report **Page 1**

Single Mass Analysis
Tolerance = 50.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 4



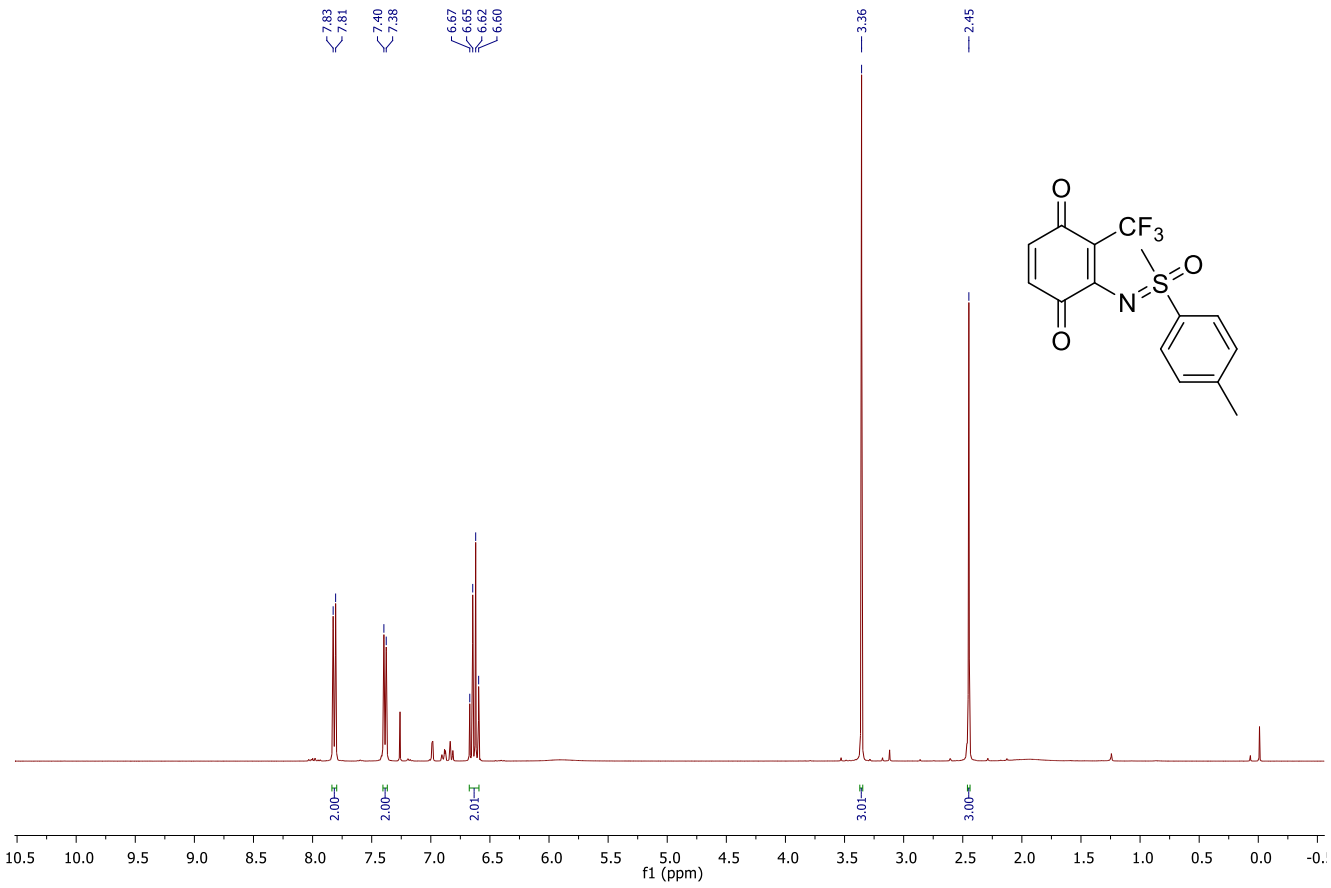
Monoisotopic Mass, Even Electron Ions
129 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 0-14 H: 0-100 N: 0-1 O: 0-3 F: 0-3 S: 0-1 Br: 0-1

280623_04 10 (0.225)
1: TOF MS ES+

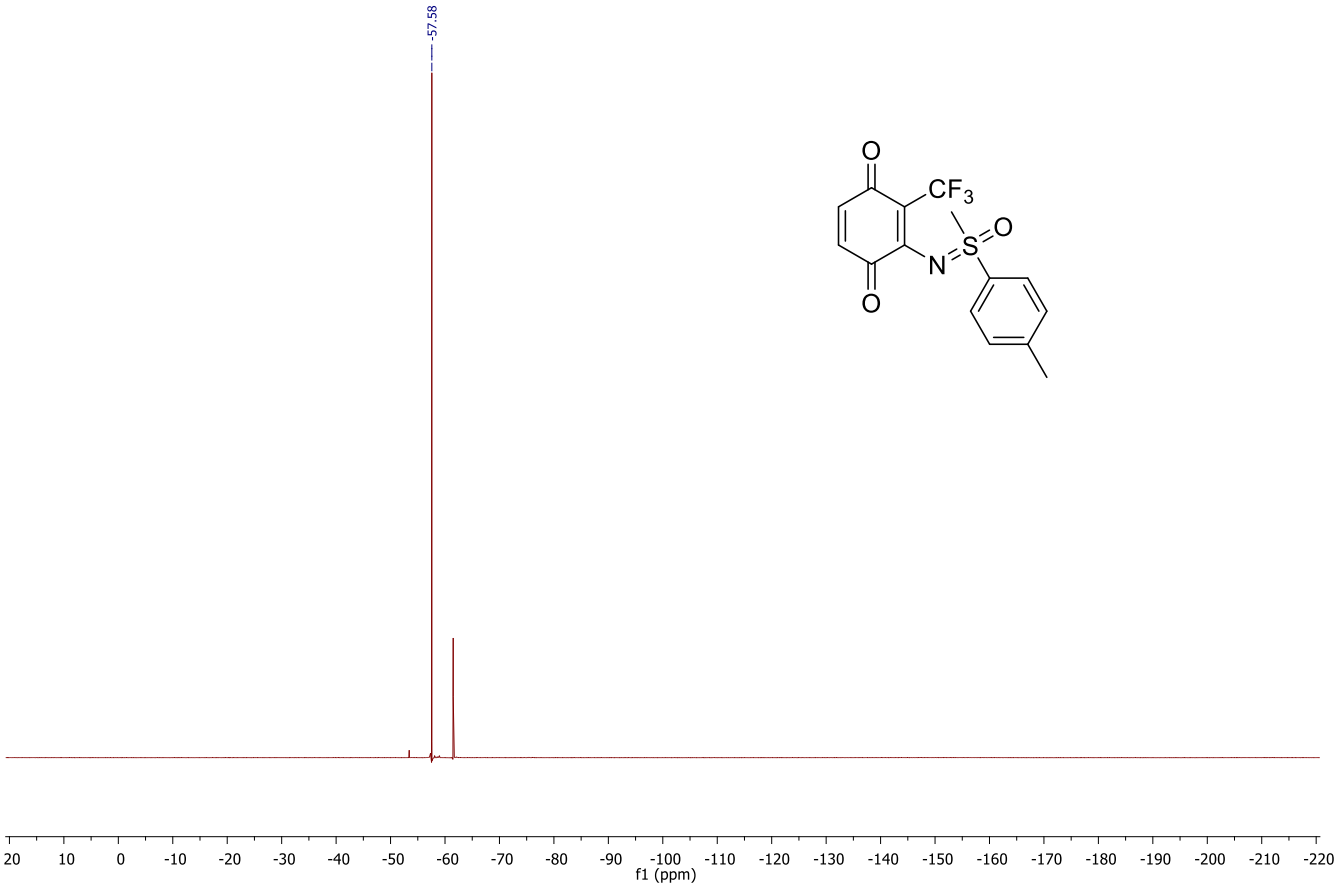


Minimum:				-1.5				
Maximum:		5.0	50.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
407.9519	407.9517	0.2	0.5	8.5	76.9	n/a	n/a	C14 H10 N O3 F3 S Br

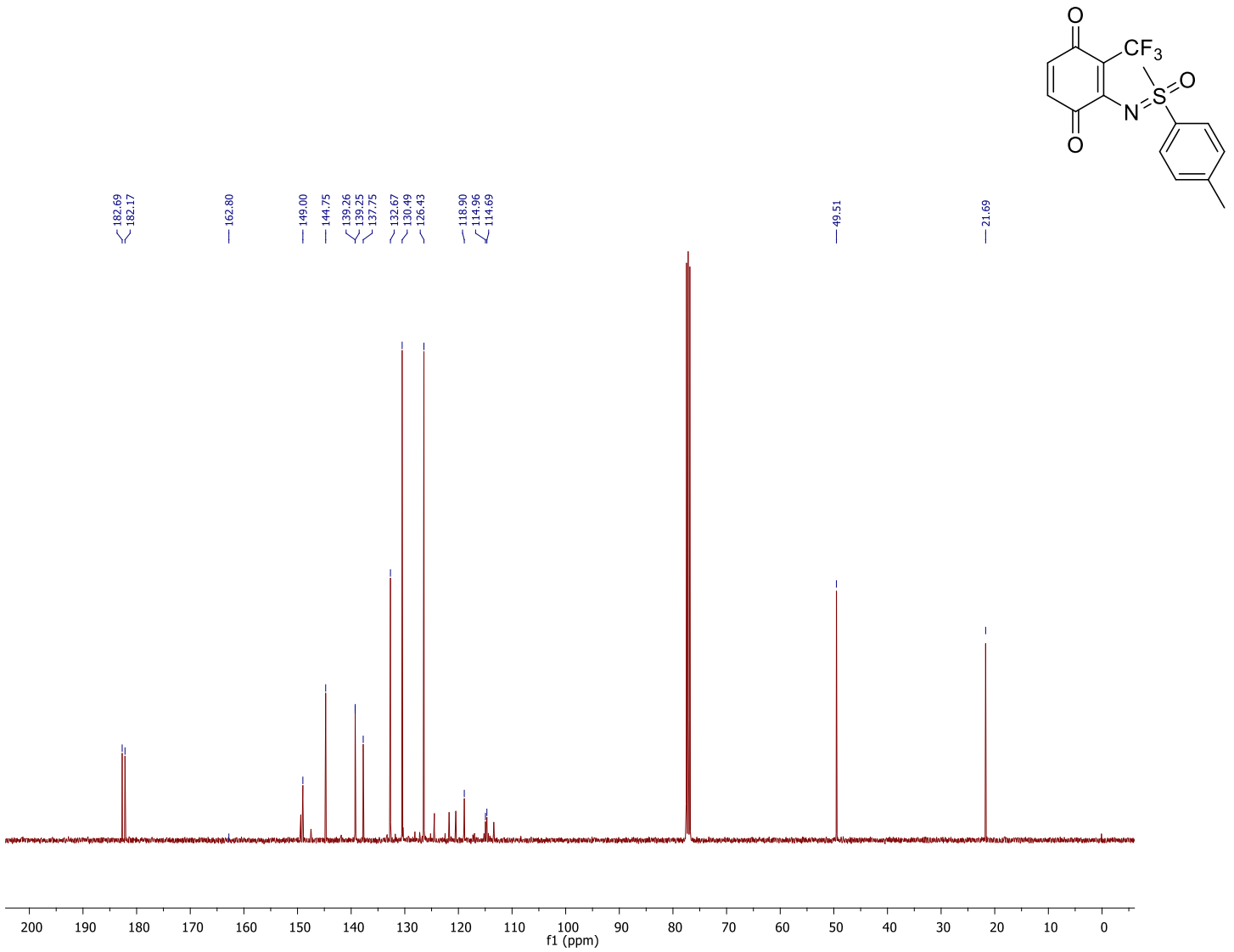
^{1}H NMR (400 MHz) of 5g in $CDCl_3$



^{19}F NMR (377 MHz) of 5g in $CDCl_3$



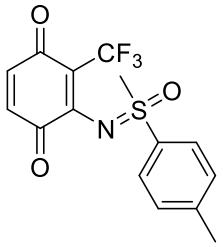
^{13}C {^{1}H} NMR (101 MHz) of 5g in $CDCl_3$



HRMS of 5g

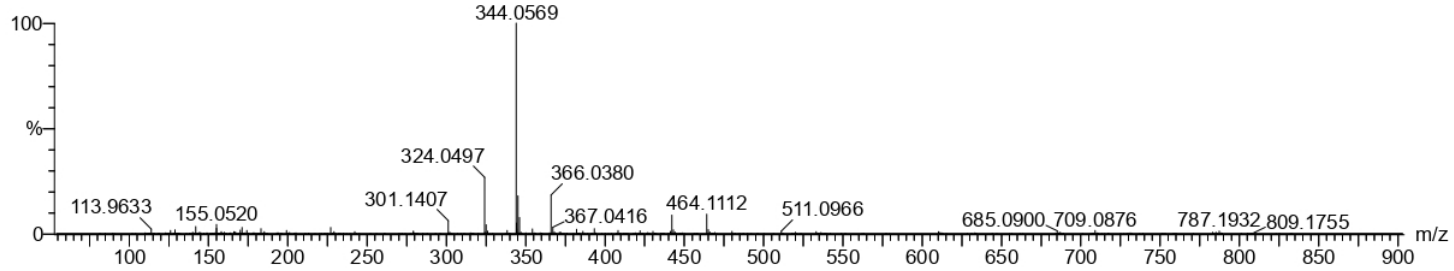
Elemental Composition Report **Page 1**

Single Mass Analysis
Tolerance = 100.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3



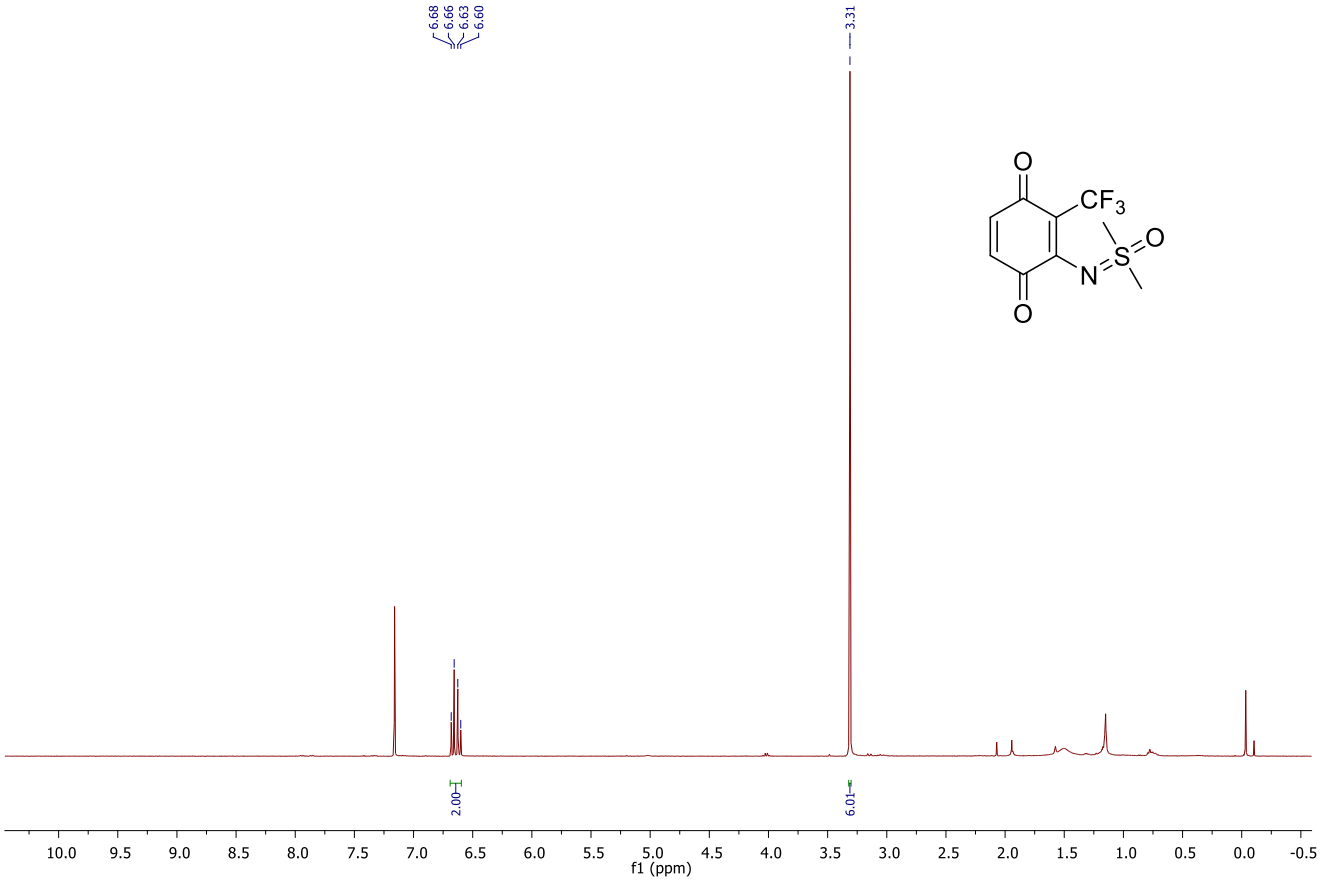
Monoisotopic Mass, Even Electron Ions
65 formula(e) evaluated with 1 results within limits (up to 3 closest results for each mass)
Elements Used:
C: 0-15 H: 0-100 N: 0-1 O: 0-3 F: 0-3 S: 0-1

BQ-4Me
QMI DIVISION, CSIR-IIIM JAMMU
Xevo G2-XS QTOF YFC2015
05-Jul-2023
14:15:28
050723_03 4 (0.104)
1: TOF MS ES+
3.77e+006

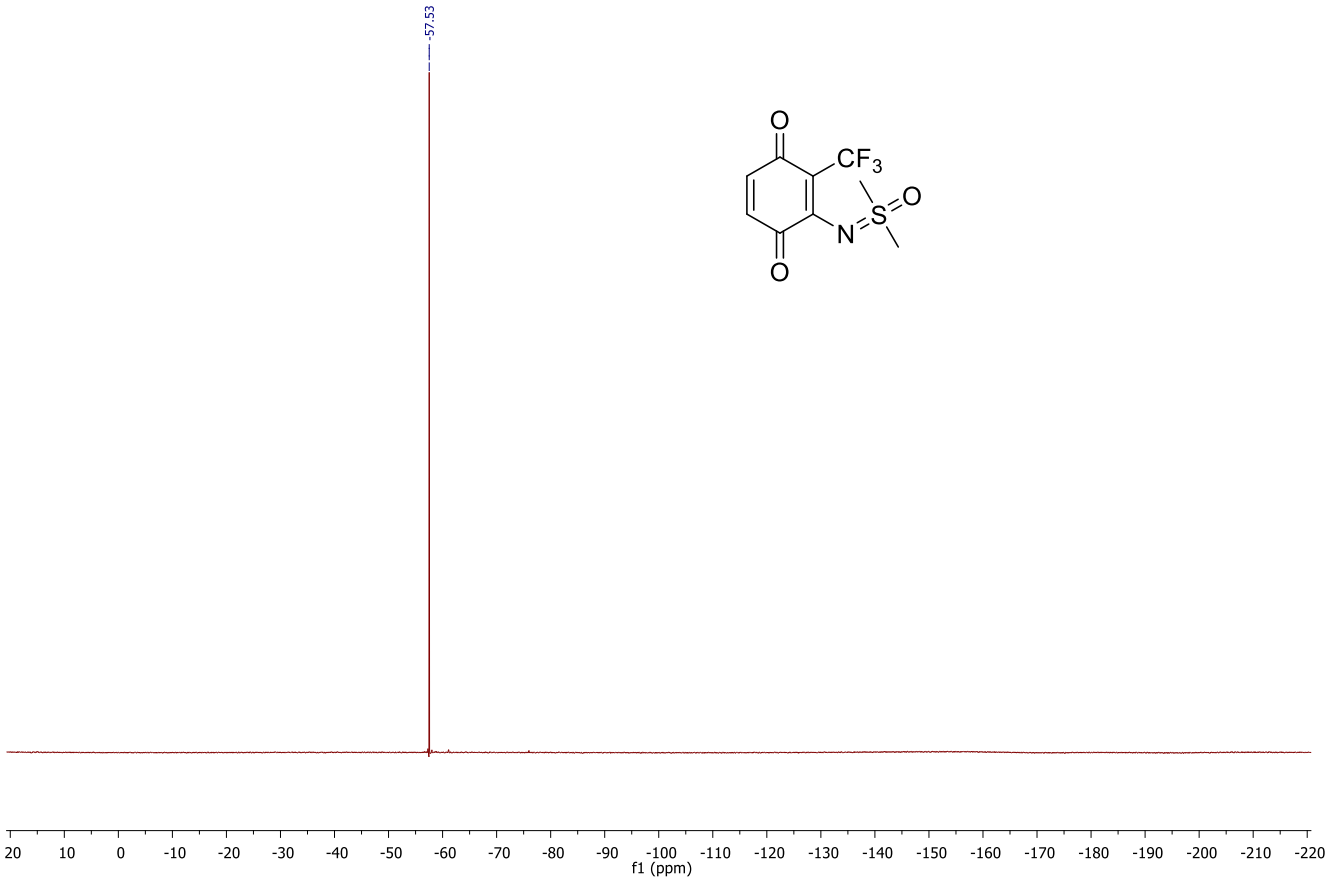


Minimum:				-1.5				
Maximum:		2.0	100.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
344.0569	344.0568	0.1	0.3	8.5	926.2	n/a	n/a	C15 H13 N O3 F3 S

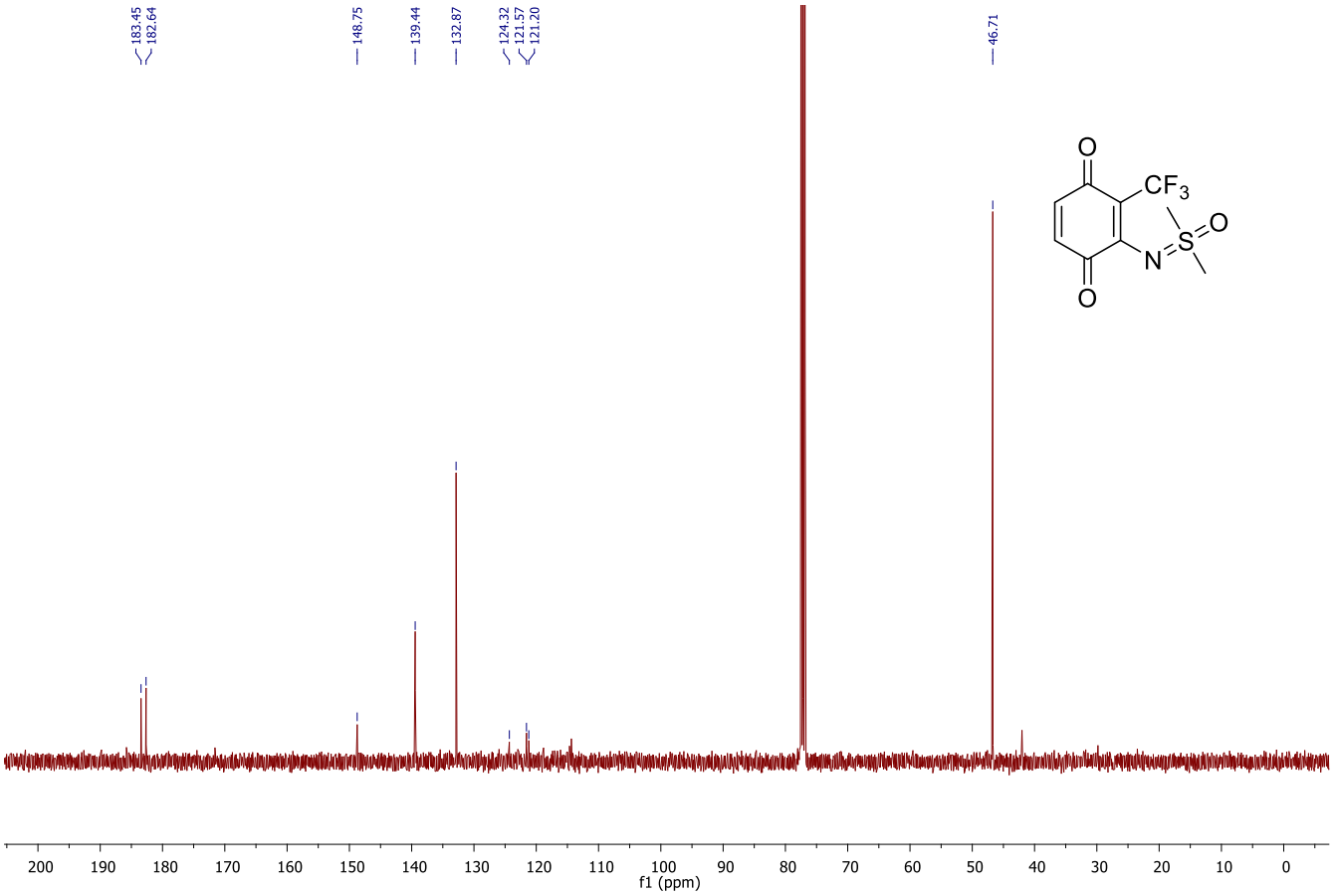
^{1}H NMR (400 MHz) of 5h in $CDCl_3$



^{19}F NMR (377 MHz) of 5h in $CDCl_3$



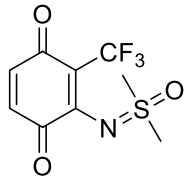
^{13}C {^{1}H} NMR (101 MHz) of 5h in $CDCl_3$



HRMS of 5h

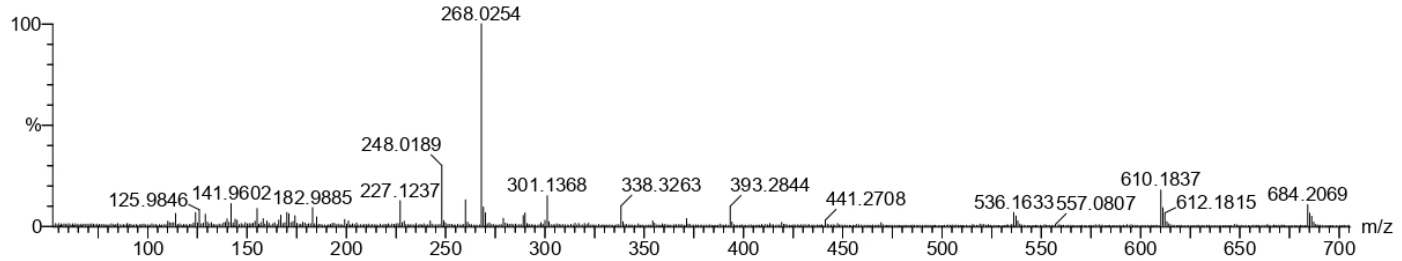
Elemental Composition Report **Page 1**

Single Mass Analysis
Tolerance = 50.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3



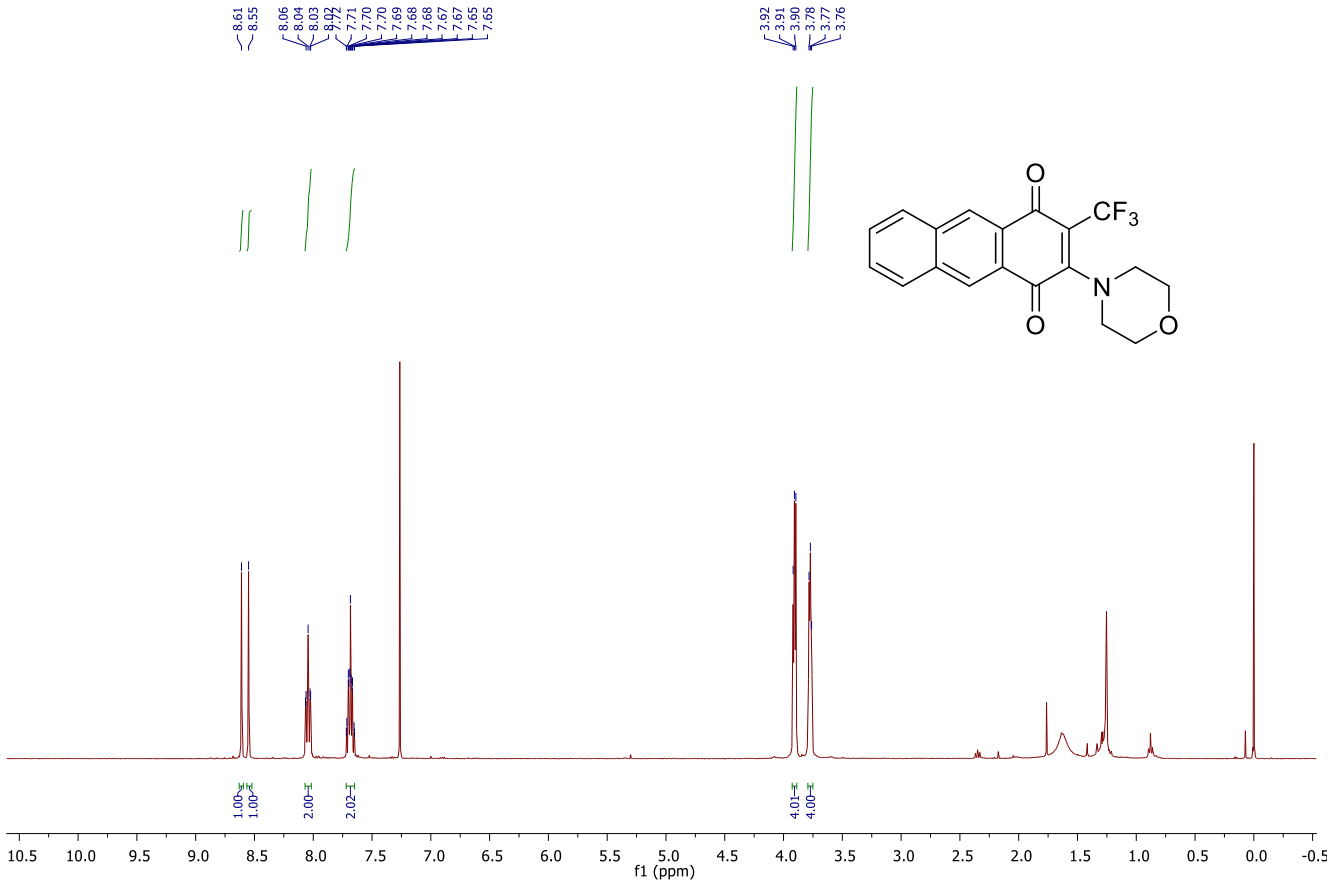
Monoisotopic Mass, Even Electron Ions
75 formula(e) evaluated with 1 results within limits (up to 3 closest results for each mass)
Elements Used:
C: 0-11 H: 0-100 N: 0-1 O: 0-3 F: 0-3 S: 0-1

BQS-9-CF3 QMI DIVISION, CSIR-IIIM JAMMU 10-Jul-2023
Xevo G2-XS QTOF YFC2015 12:32:18
100723_04 9 (0.208) Cm (9:11) 1: TOF MS ES+
3.86e+006

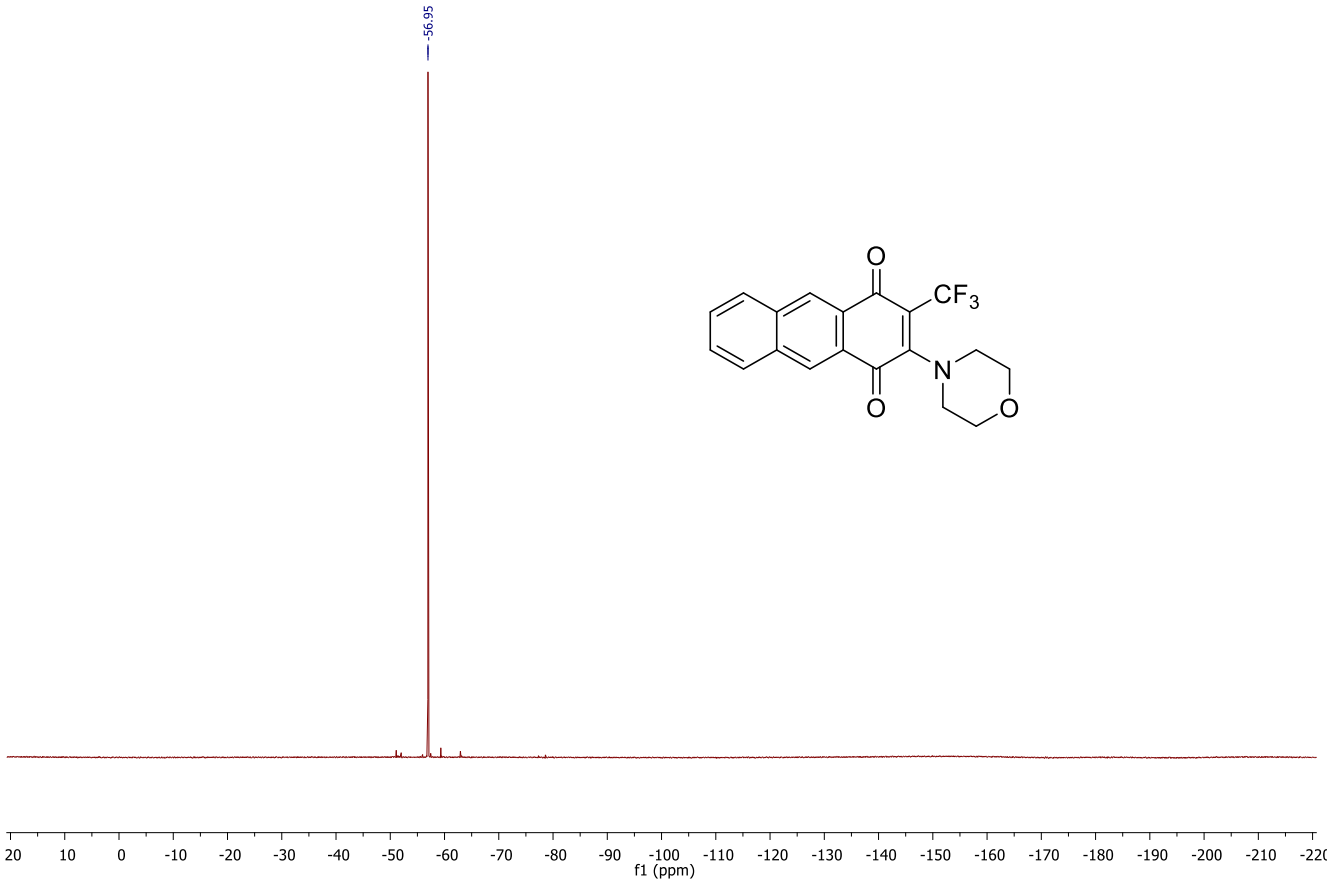


Minimum:				-1.5				
Maximum:		2.0	50.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
268.0254	268.0255	-0.1	-0.4	4.5	54.7	n/a	n/a	C9 H9 N O3 F3 S

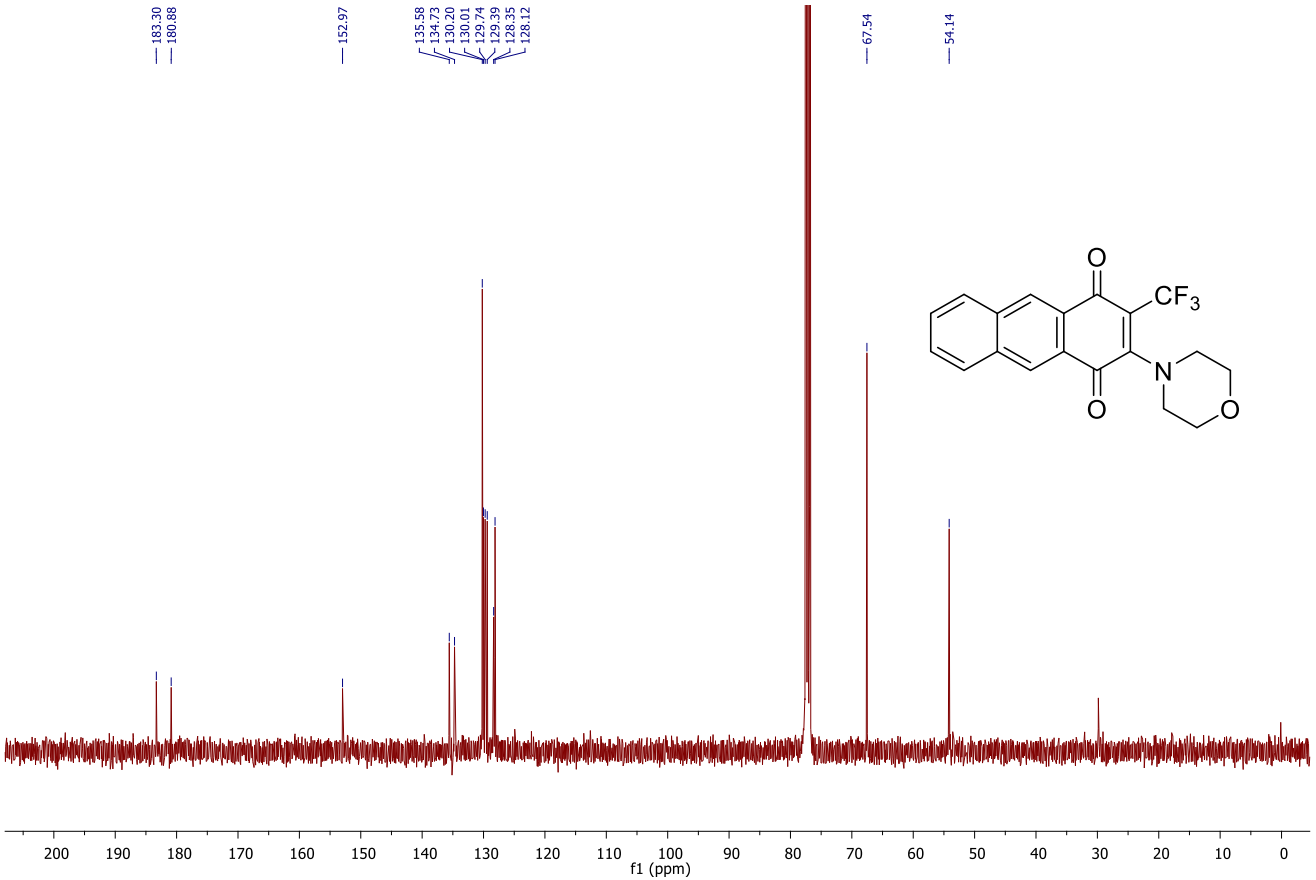
^{1}H NMR (400 MHz) of 5i in $CDCl_3$



^{19}F NMR (377 MHz) of 5i in $CDCl_3$

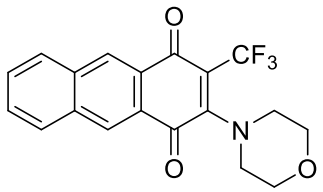


^{13}C {^{1}H} NMR (101 MHz) of 5i in $CDCl_3$



HRMS of 5i

Elemental Composition Report **Page 1**

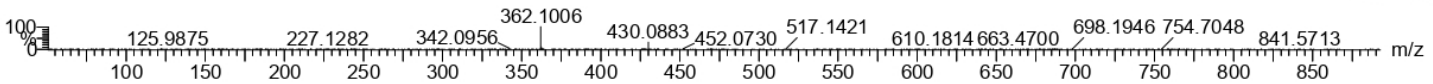


Single Mass Analysis
Tolerance = 50.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 4

Monoisotopic Mass, Even Electron Ions
37 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 0-19 H: 0-100 N: 0-1 O: 0-3 F: 0-3

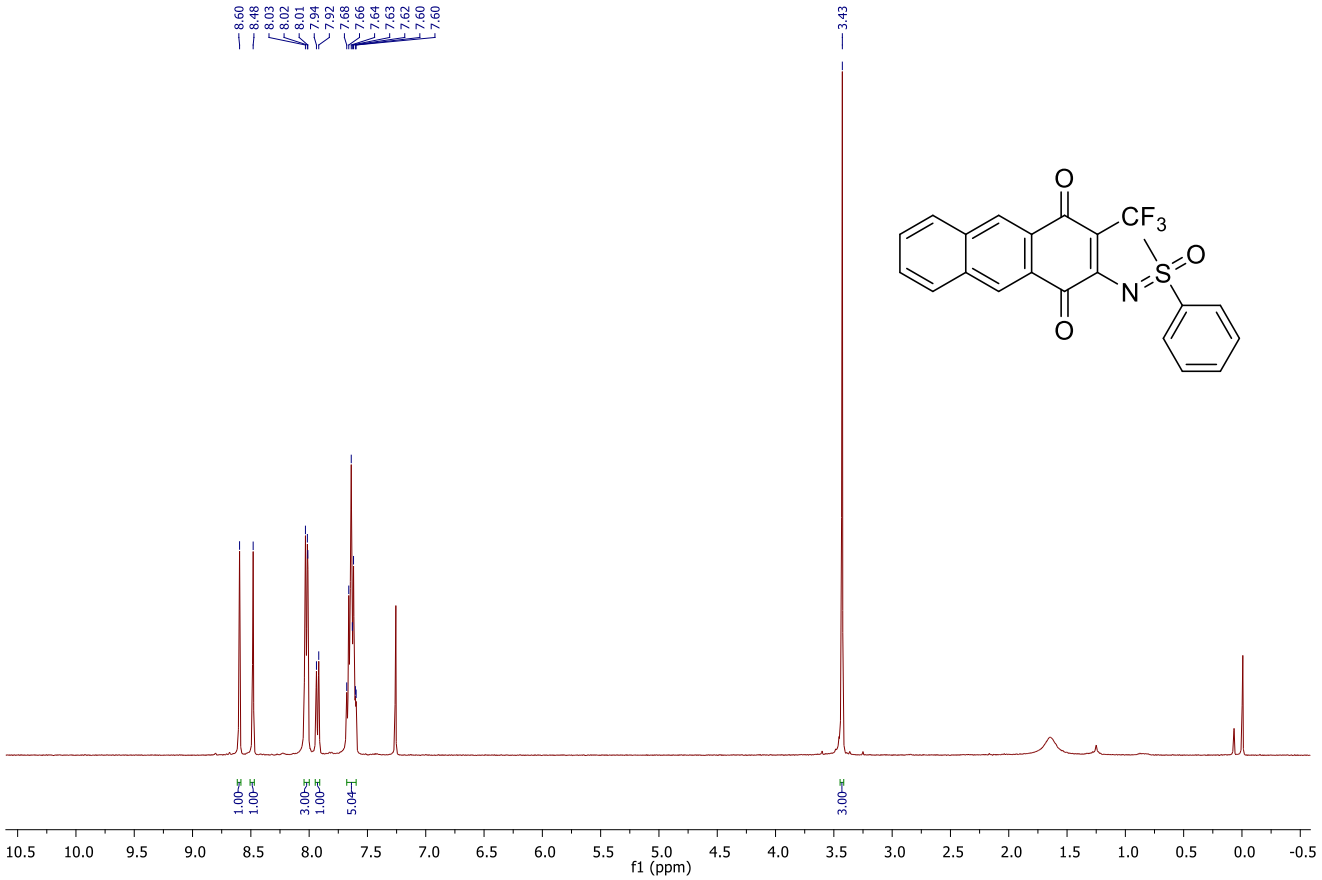
280623_02 9 (0.208)
1: TOF MS ES+

1.78e+005

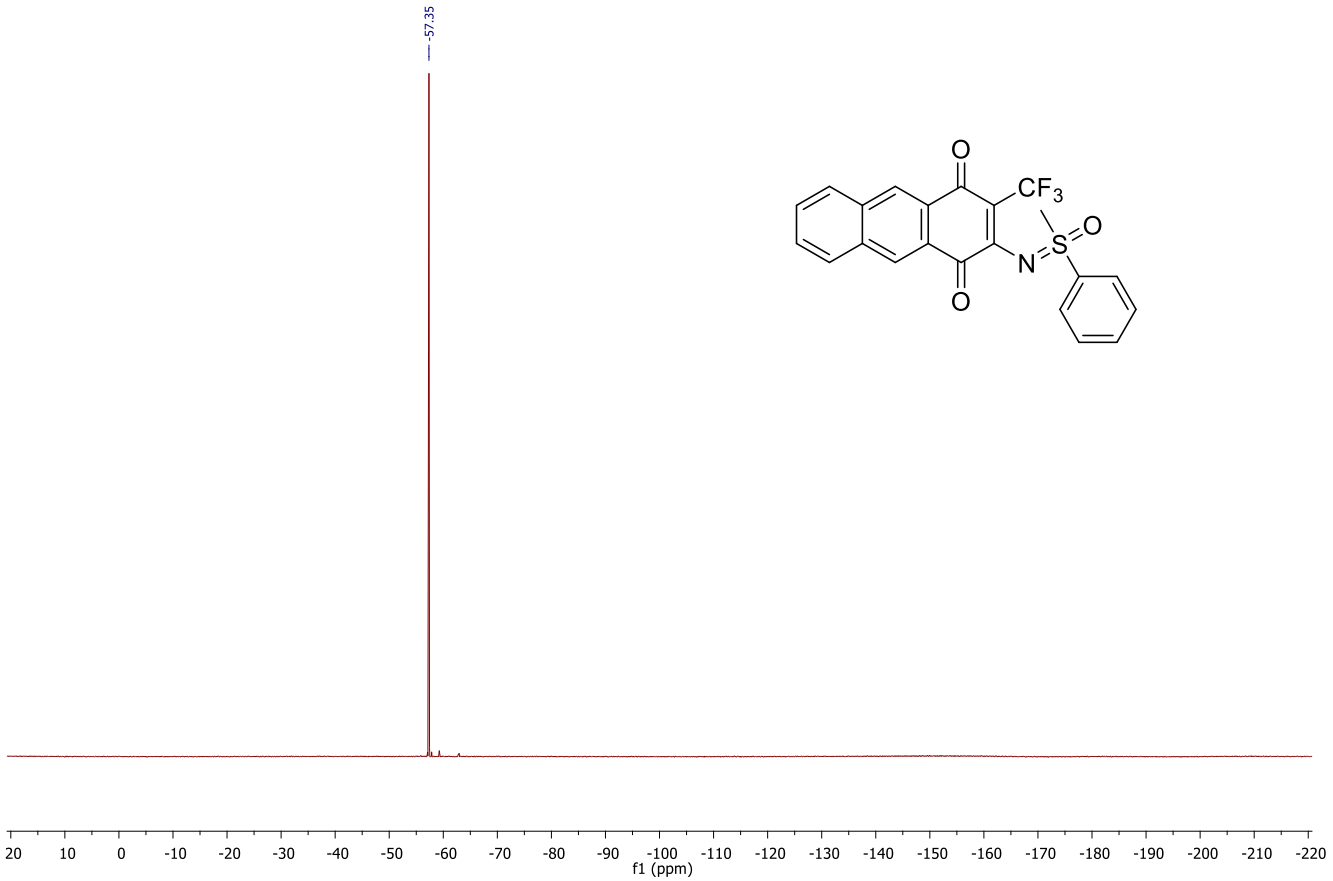


Minimum:				-1.5				
Maximum:		5.0	50.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
362.1006	362.1004	0.2	0.6	11.5	87.7	n/a	n/a	C19 H15 N O3 F3

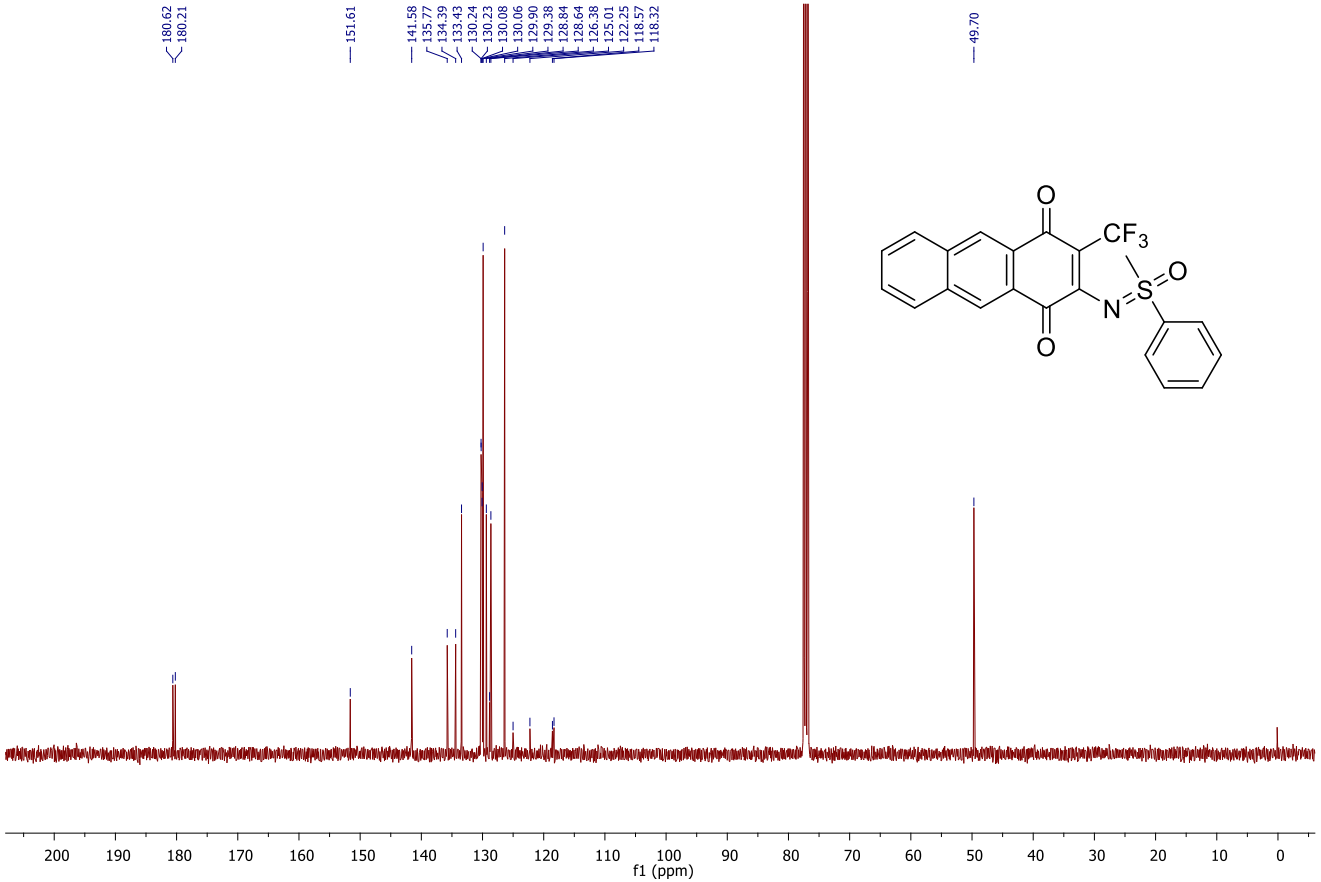
^{1}H NMR (400 MHz) of 5j in $CDCl_3$



^{19}F NMR (377 MHz) of 5j in $CDCl_3$



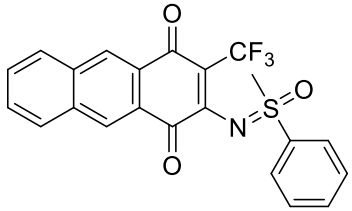
^{13}C {^{1}H} NMR (101 MHz) of 5j in $CDCl_3$



HRMS of 5j

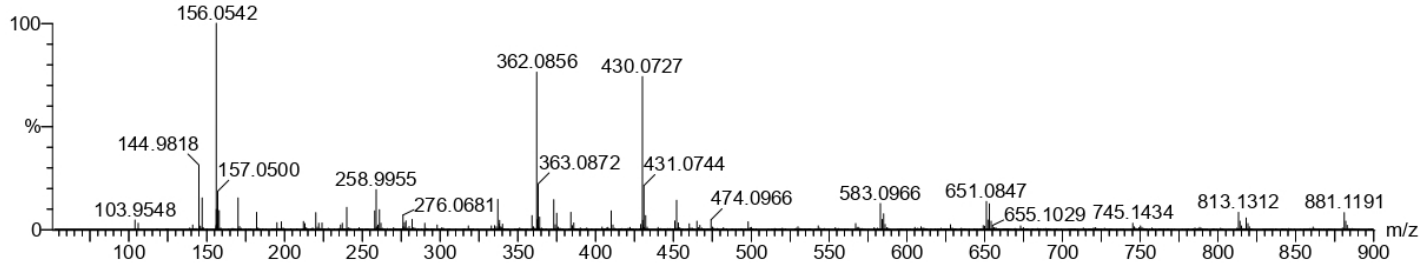
Elemental Composition Report **Page 1**

Single Mass Analysis
Tolerance = 100.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3



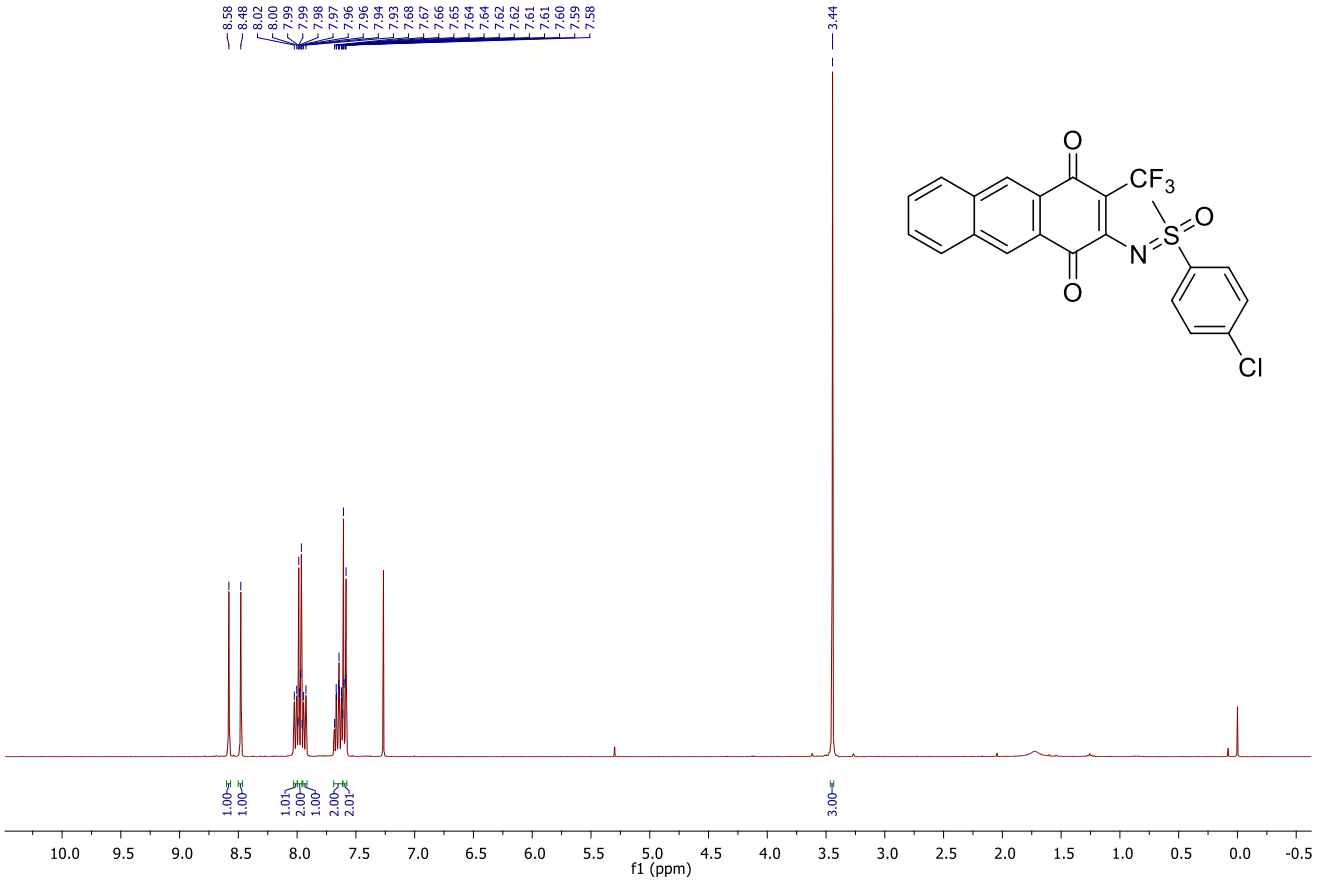
Monoisotopic Mass, Even Electron Ions
69 formula(e) evaluated with 1 results within limits (up to 3 closest results for each mass)
Elements Used:
C: 0-22 H: 0-100 N: 0-1 O: 0-3 F: 0-3 S: 0-1

AQS-CF3
QMI DIVISION, CSIR-IIIM JAMMU
Xevo G2-XS QTOF YFC2015
05-Jul-2023
14:20:46
050723_05 6 (0.138)
1: TOF MS ES+
2.59e+007

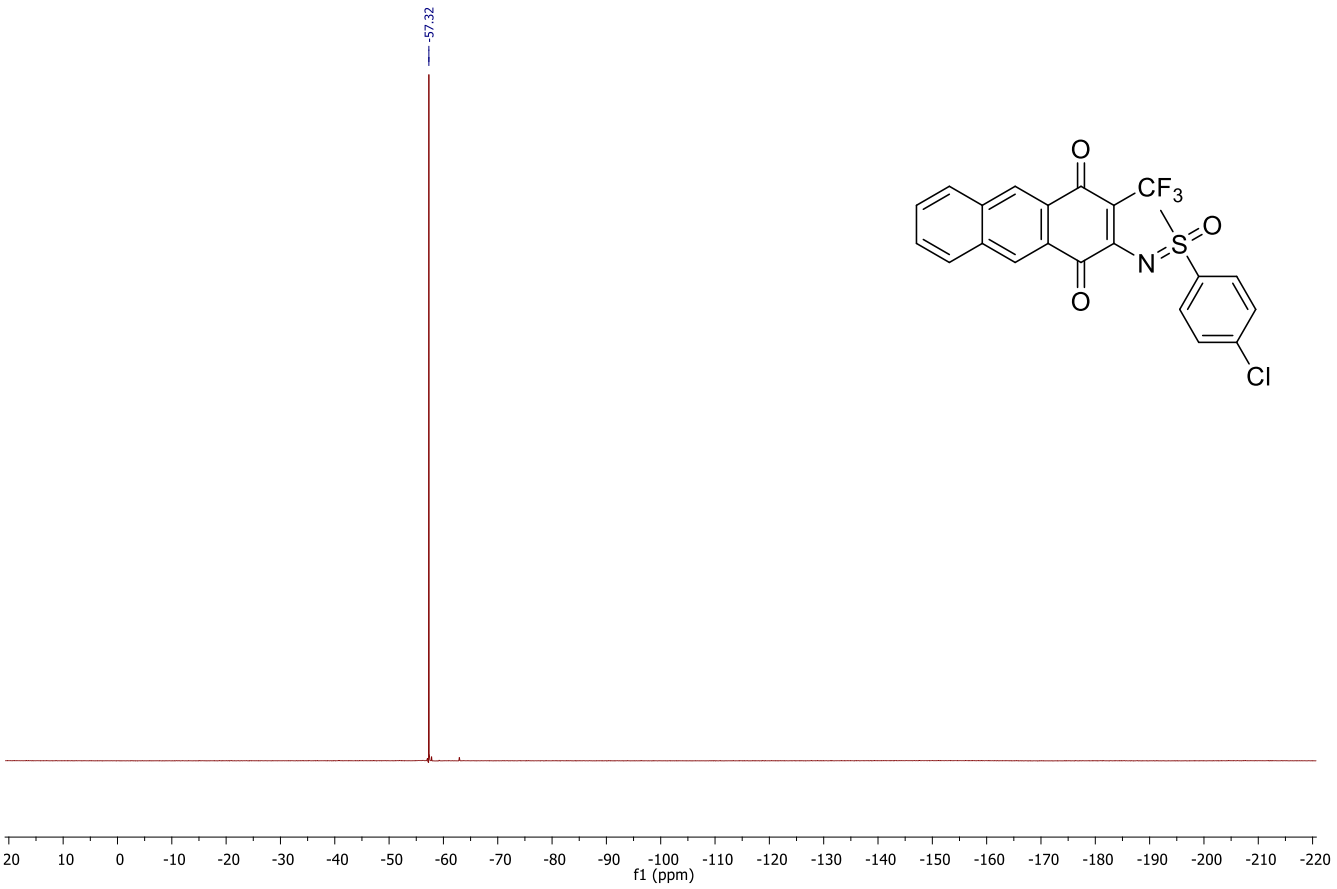


Minimum:				-1.5				
Maximum:		2.0	100.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
430.0727	430.0725	0.2	0.5	14.5	891.7	n/a	n/a	C22 H15 N O3 F3 S

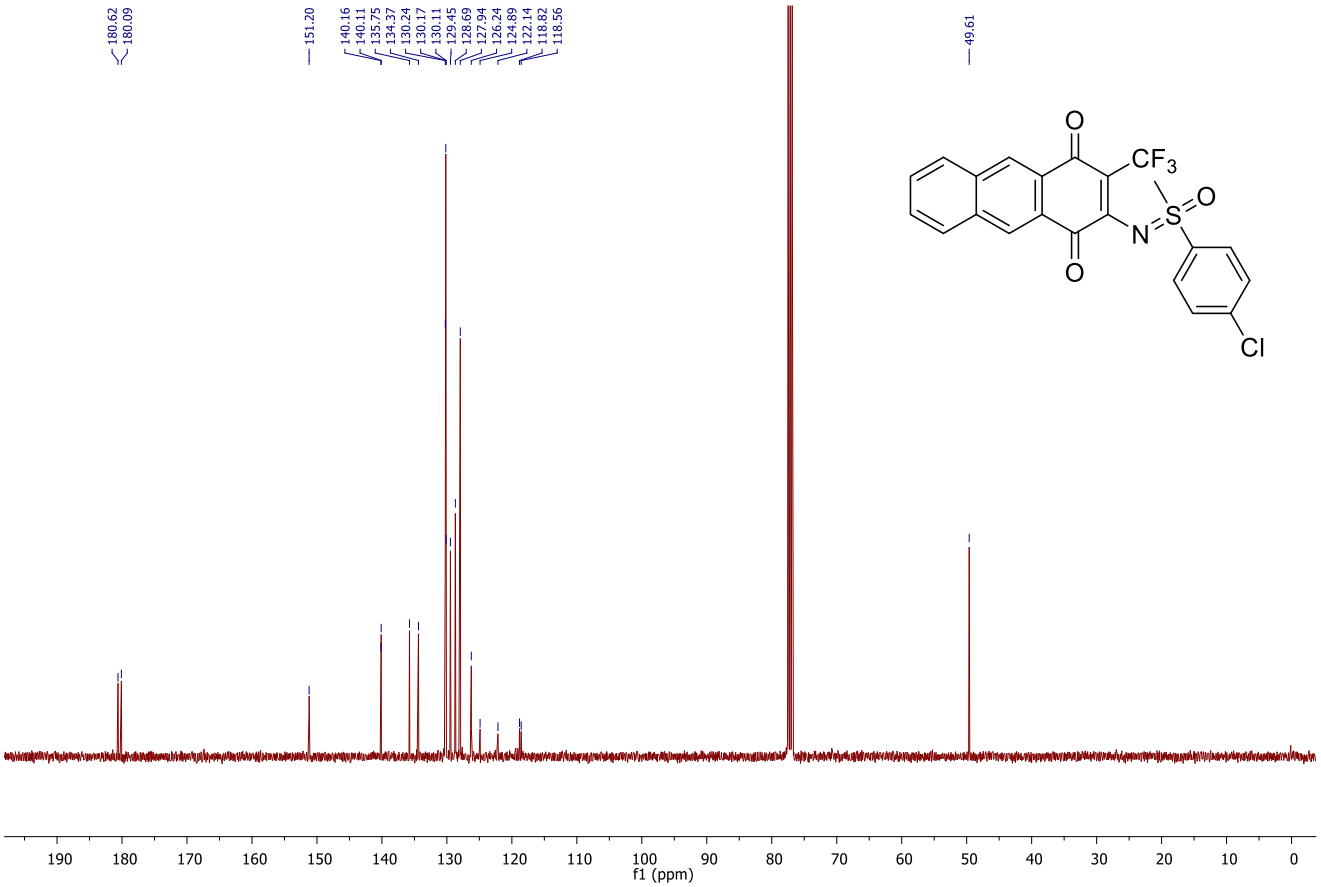
^{1}H NMR (400 MHz) of 5k in $CDCl_3$



^{19}F NMR (377 MHz) of 5k in $CDCl_3$

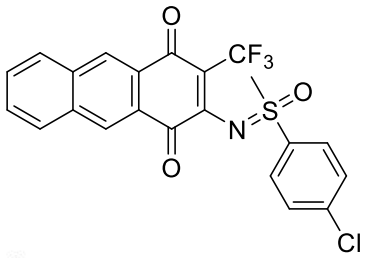


^{13}C {^{1}H} NMR (101 MHz) of 5k in $CDCl_3$



HRMS of 5k

Elemental Composition Report



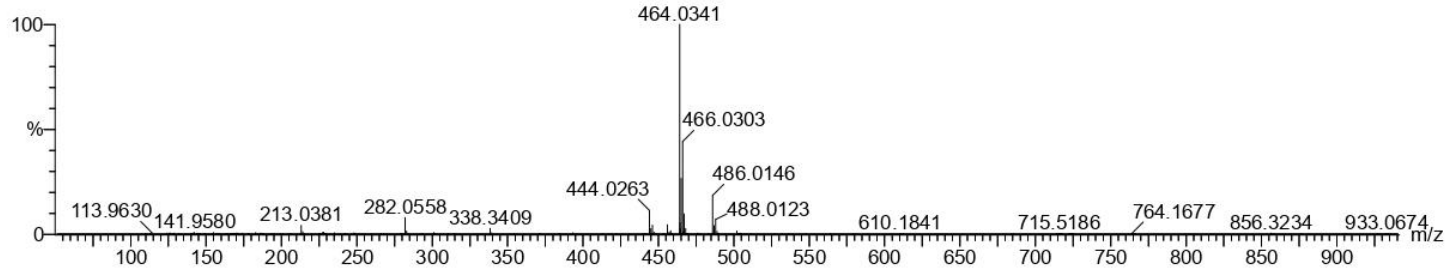
Single Mass Analysis
Tolerance = 50.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
127 formula(e) evaluated with 1 results within limits (up to 3 closest results for each mass)
Elements Used:
C: 0-22 H: 0-45 N: 0-1 O: 0-3 F: 0-3 S: 0-1 Cl: 0-1

AQS-2-CF3
100723_02 8 (0.172)

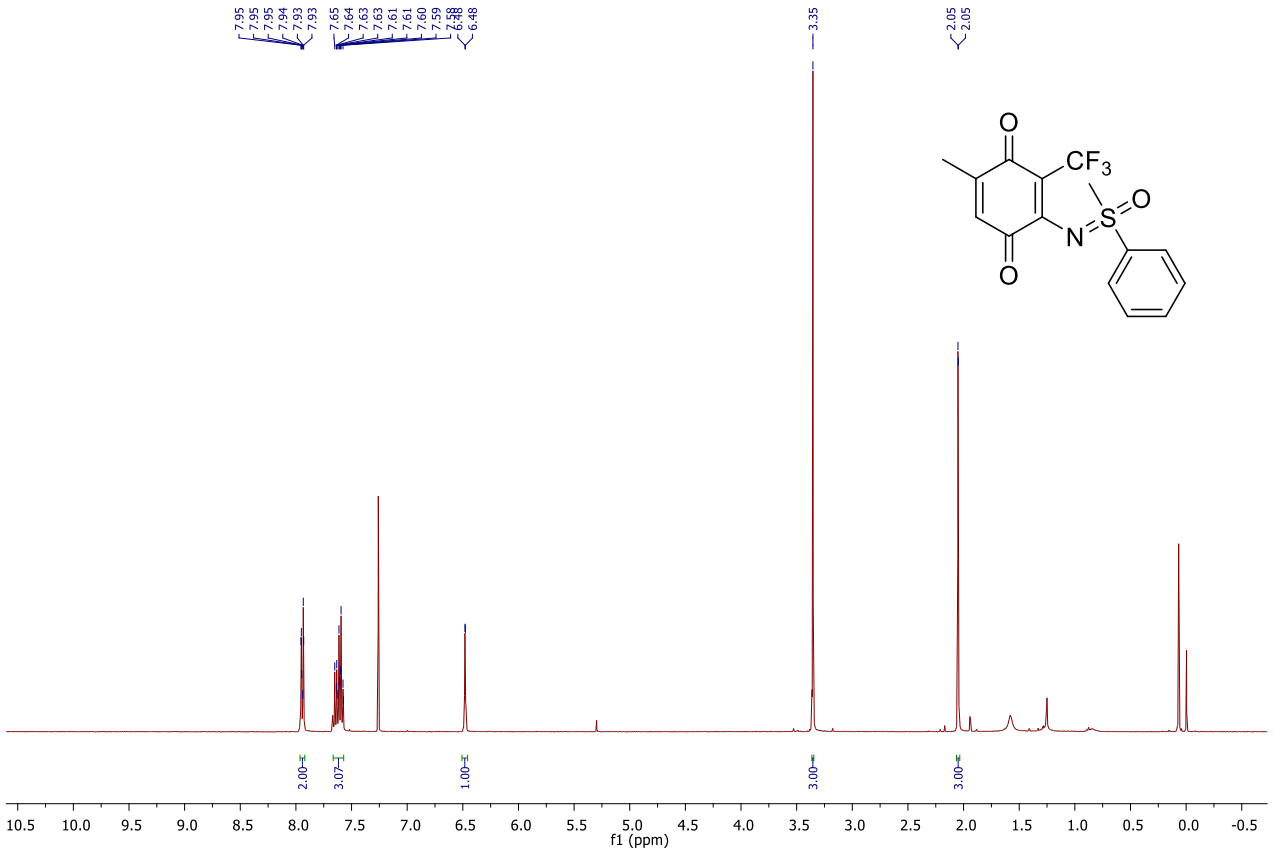
QMI DIVISION, CSIR-IIIM JAMMU
Xevo G2-XS QTOF YFC2015

10-Jul-2023
12:26:54
1: TOF MS ES+
1.47e+007

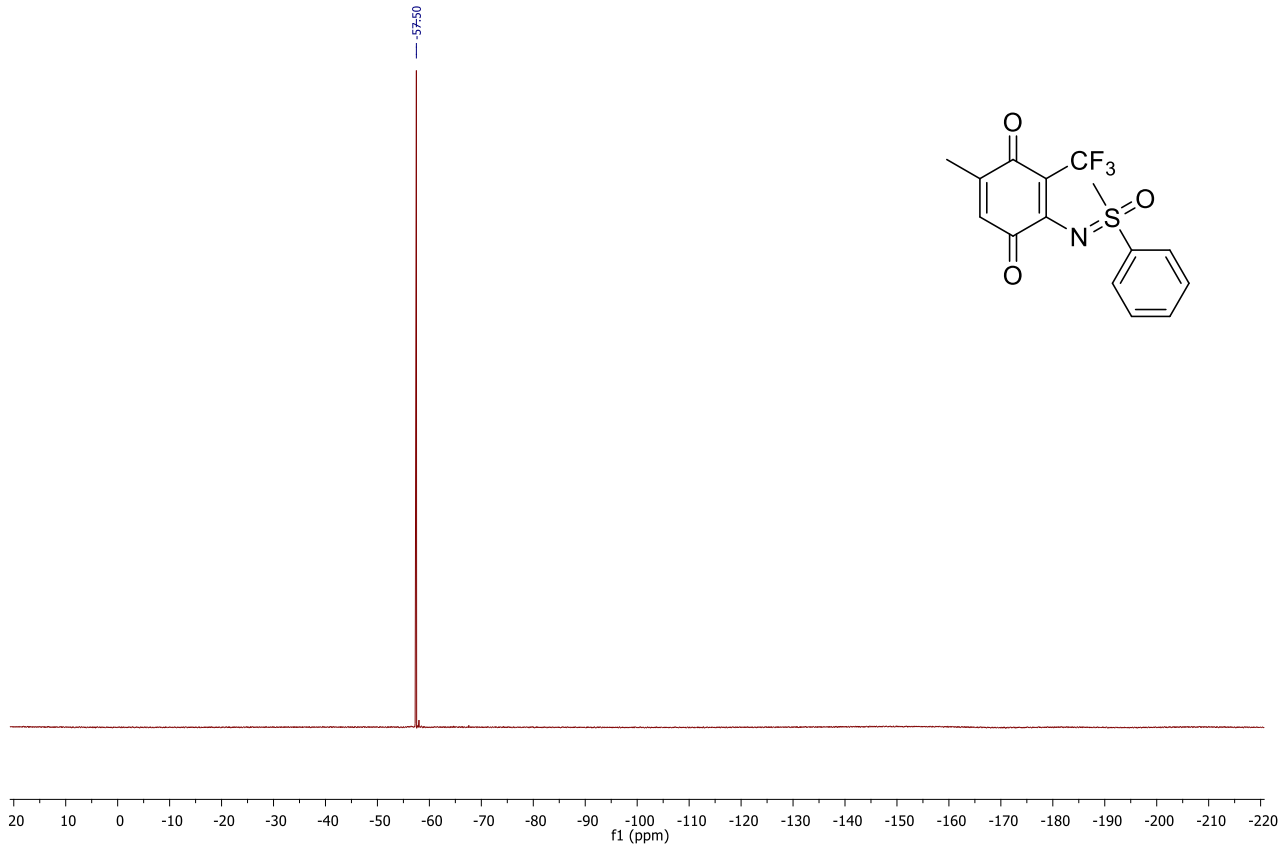


Minimum:				-1.5				
Maximum:		2.0	50.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
464.0341	464.0335	0.6	1.3	14.5	844.4	n/a	n/a	C22 H14 N O3 F3 S Cl

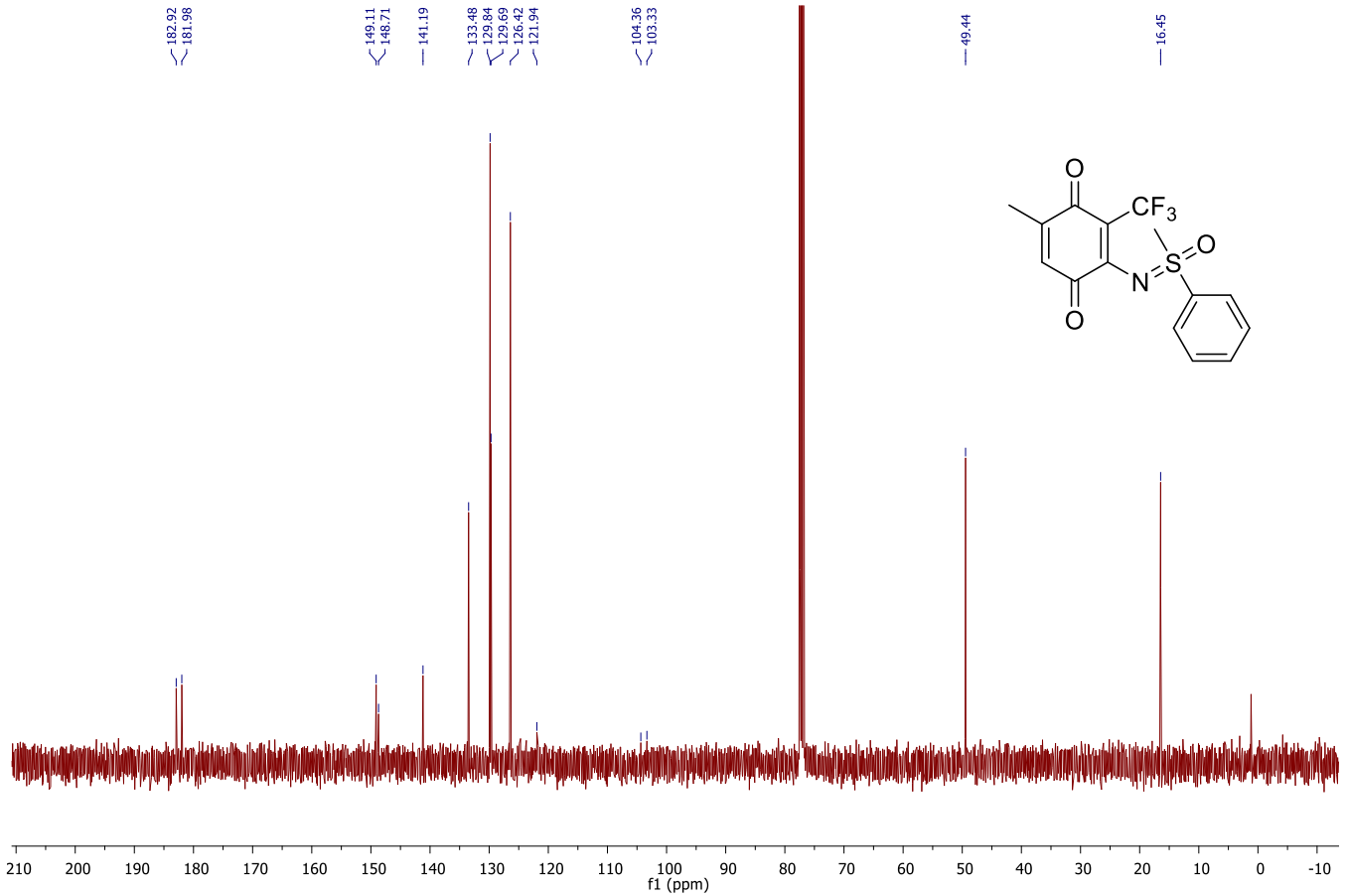
^{1}H NMR (400 MHz) of 5l in $CDCl_3$



^{19}F NMR (377 MHz) of 5l in $CDCl_3$



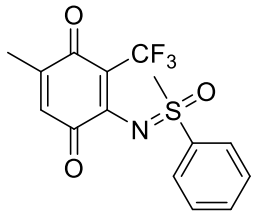
^{13}C {^{1}H} NMR (101 MHz) of 5l in $CDCl_3$



HRMS of 5l

Elemental Composition Report **Page 1**

Single Mass Analysis
Tolerance = 50.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

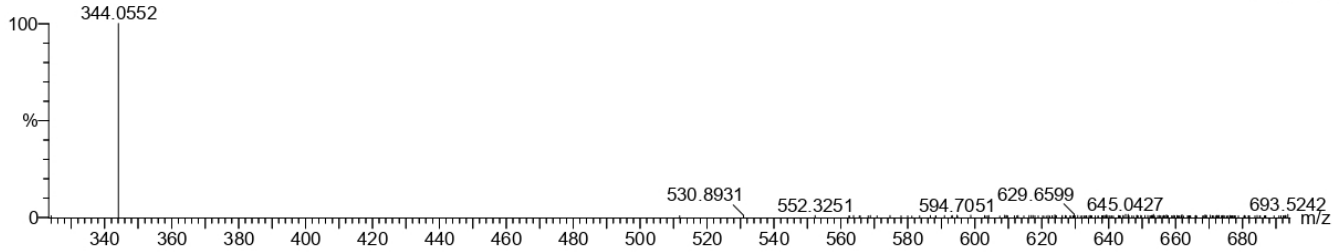


Monoisotopic Mass, Even Electron Ions
65 formula(e) evaluated with 1 results within limits (up to 3 closest results for each mass)
Elements Used:
C: 0-15 H: 0-100 N: 0-1 O: 0-3 S: 0-1 F: 0-3

Me-BQ
080823_04 4 (0.104)

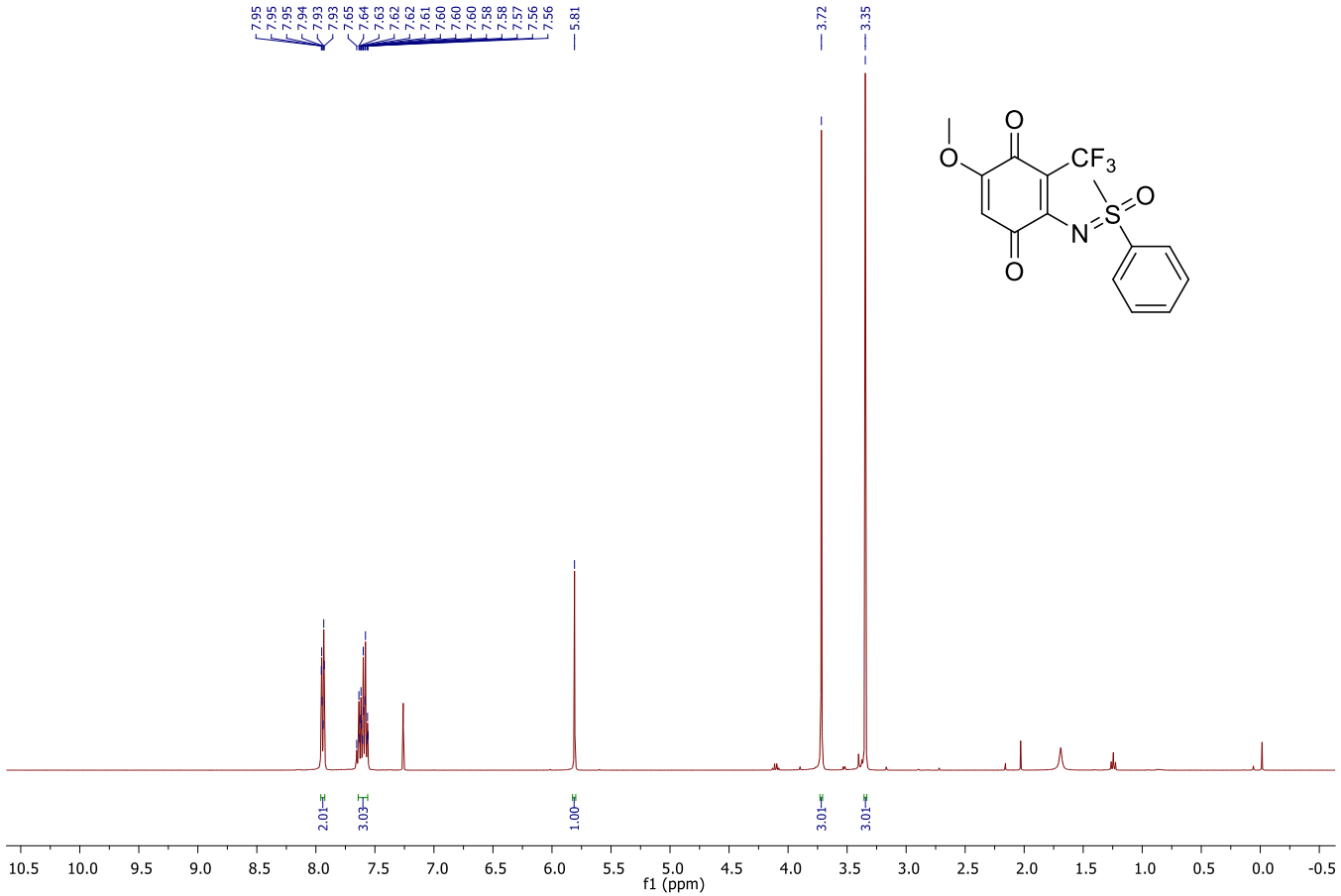
QMI DIVISION, CSIR-IIIM JAMMU
Xevo G2-XS QTOF YFC2015

08-Aug-2023
11:30:11
1: TOF MS ES+
2.88e+003

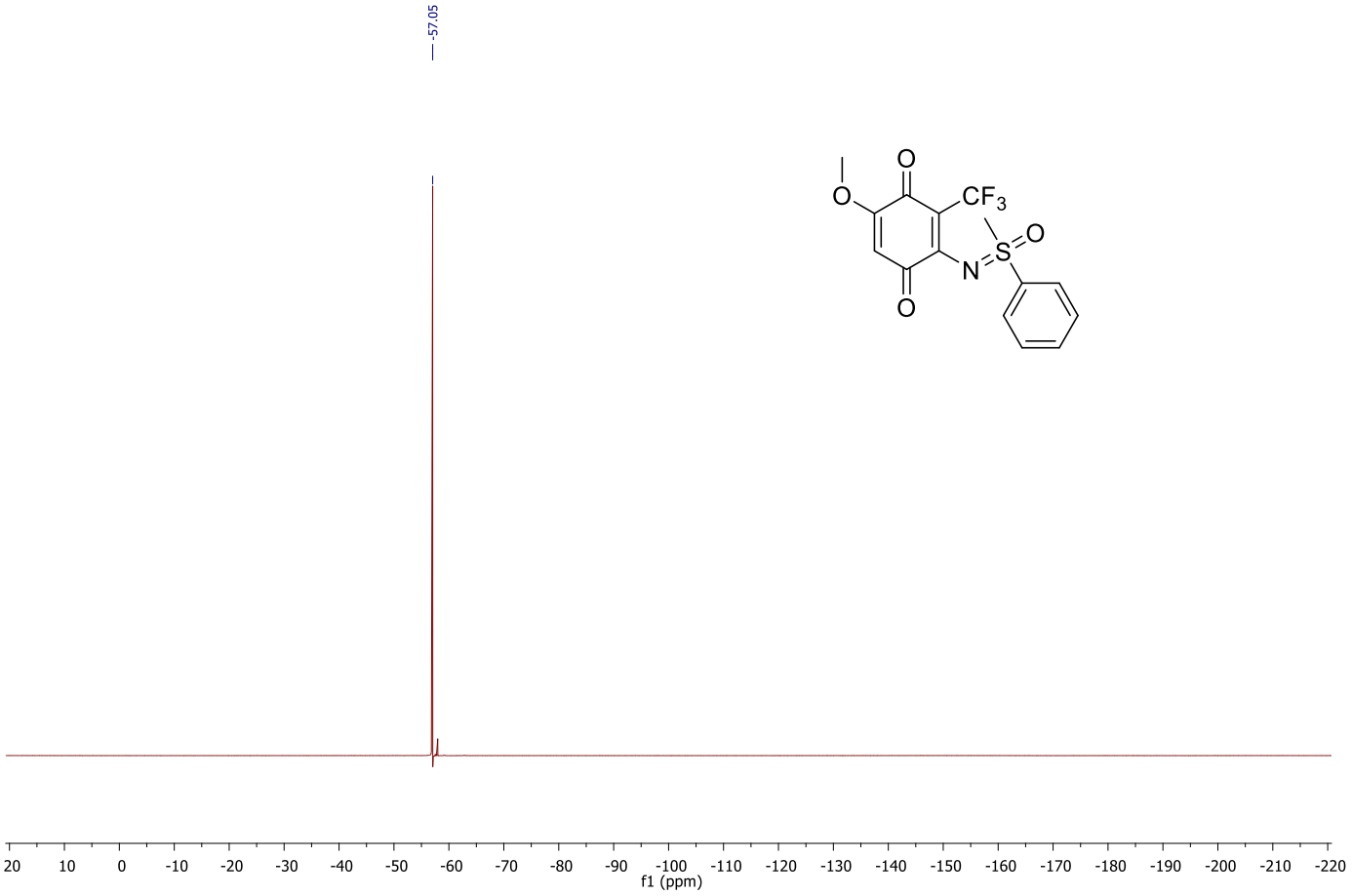


Minimum:				-1.5				
Maximum:		2.0	50.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
344.0552	344.0568	-1.6	-4.7	8.5	26.2	n/a	n/a	C15 H13 N O3 S F3

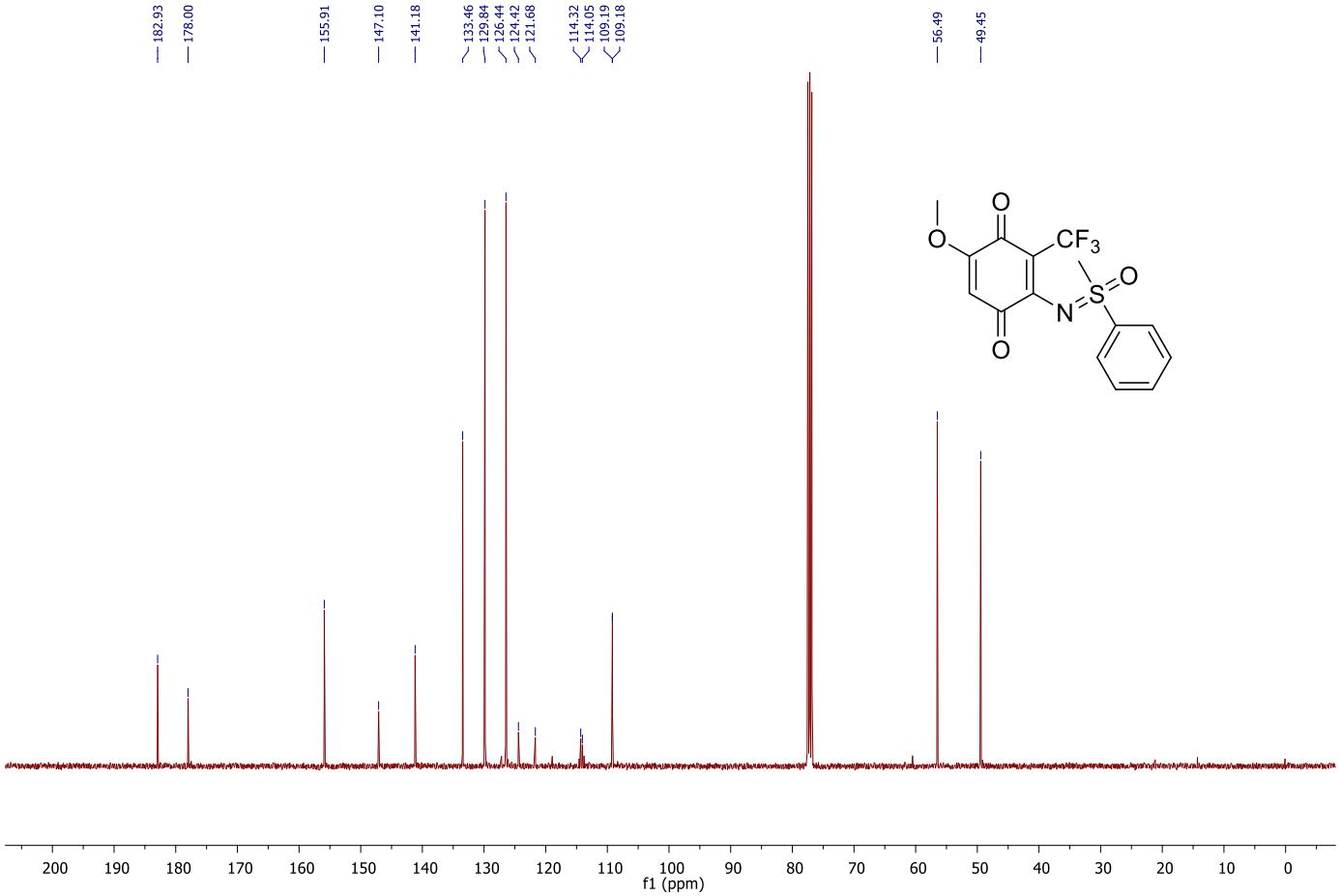
^{1}H NMR (400 MHz) of 5m in $CDCl_3$



^{19}F NMR (377 MHz) of 5m in $CDCl_3$

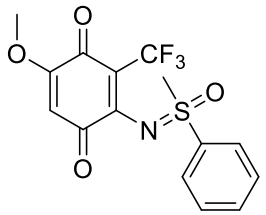


^{13}C {^{1}H} NMR (101 MHz) of 5m in $CDCl_3$



HRMS of 5m

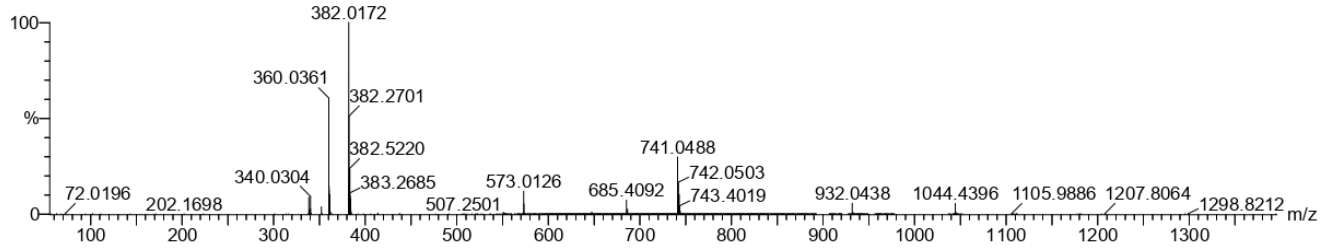
Elemental Composition Report **Page 1**



Single Mass Analysis
Tolerance = 50.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

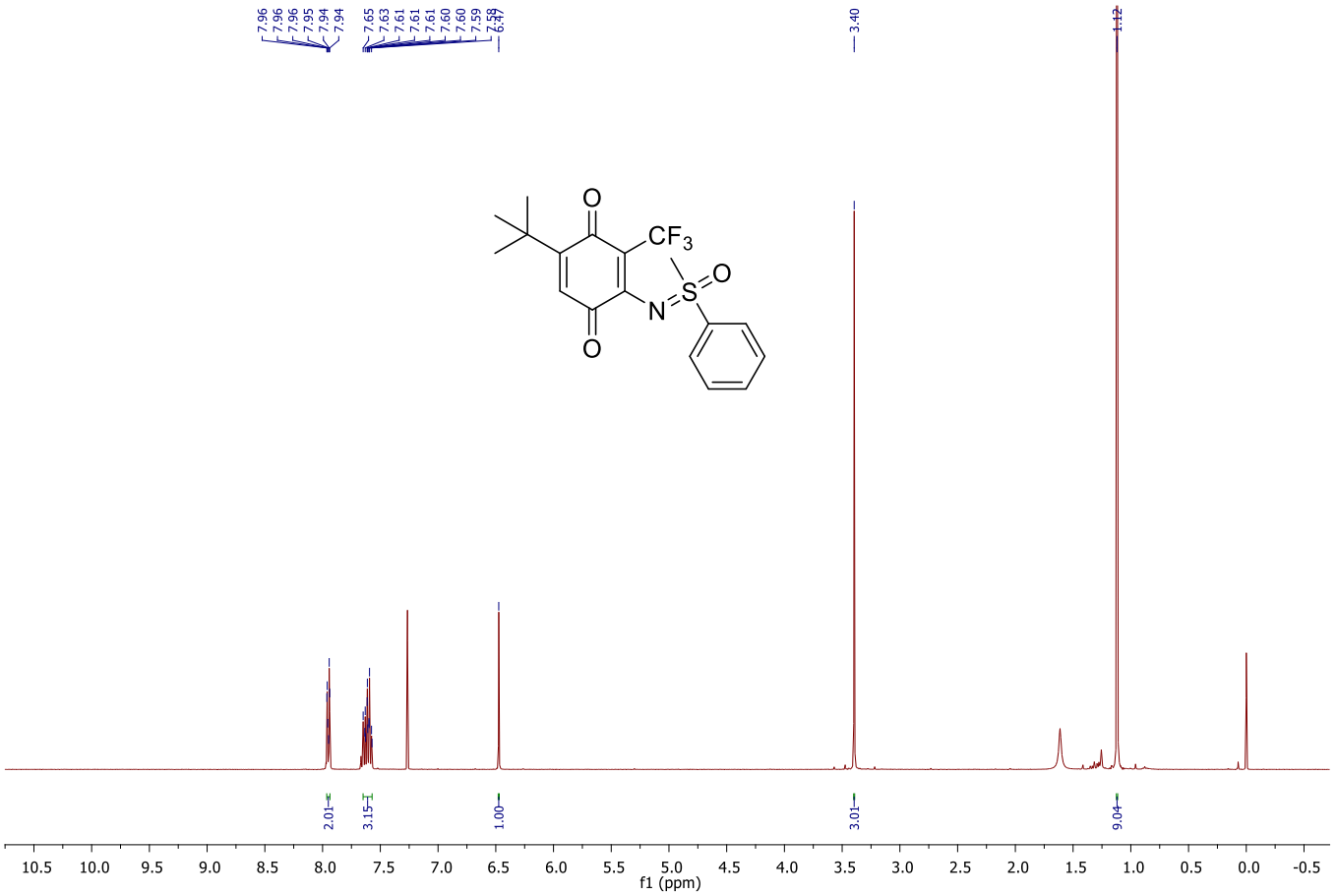
Monoisotopic Mass, Even Electron Ions
81 formula(e) evaluated with 1 results within limits (up to 3 closest results for each mass)
Elements Used:
C: 0-15 H: 0-100 N: 0-1 O: 0-4 F: 0-3 S: 0-1

OMe-BQ
QMI DIVISION, CSIR-IIIM JAMMU
Xevo G2-XS QTOF YFC2015
09-Aug-2023
16:55:49
080823_02 6 (0.138)
1: TOF MS ES+
4.40e+006

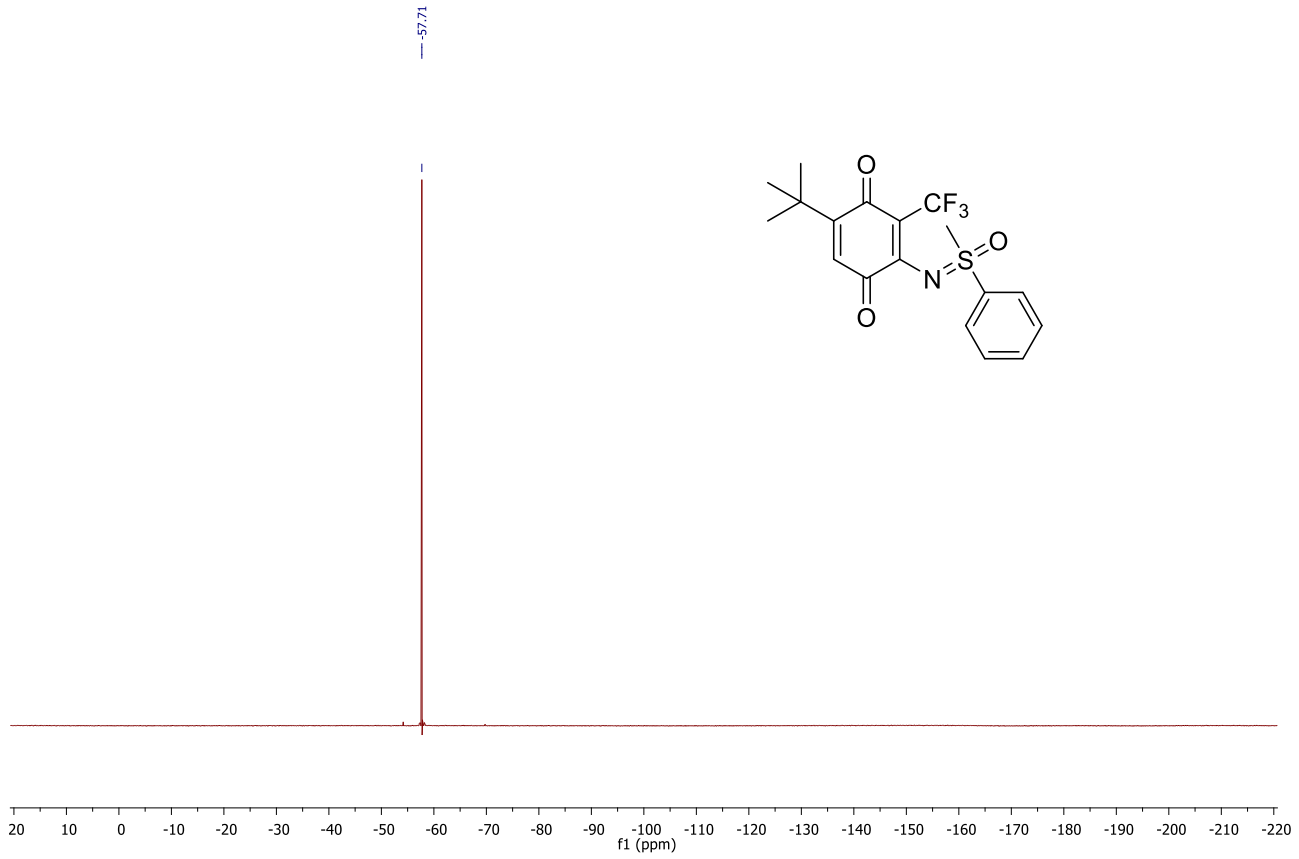


Minimum:				-1.5				
Maximum:		2.0	50.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
360.0361	360.0517	-15.6	-43.3	8.5	326.1	n/a	n/a	C15 H13 N O4 F3 S

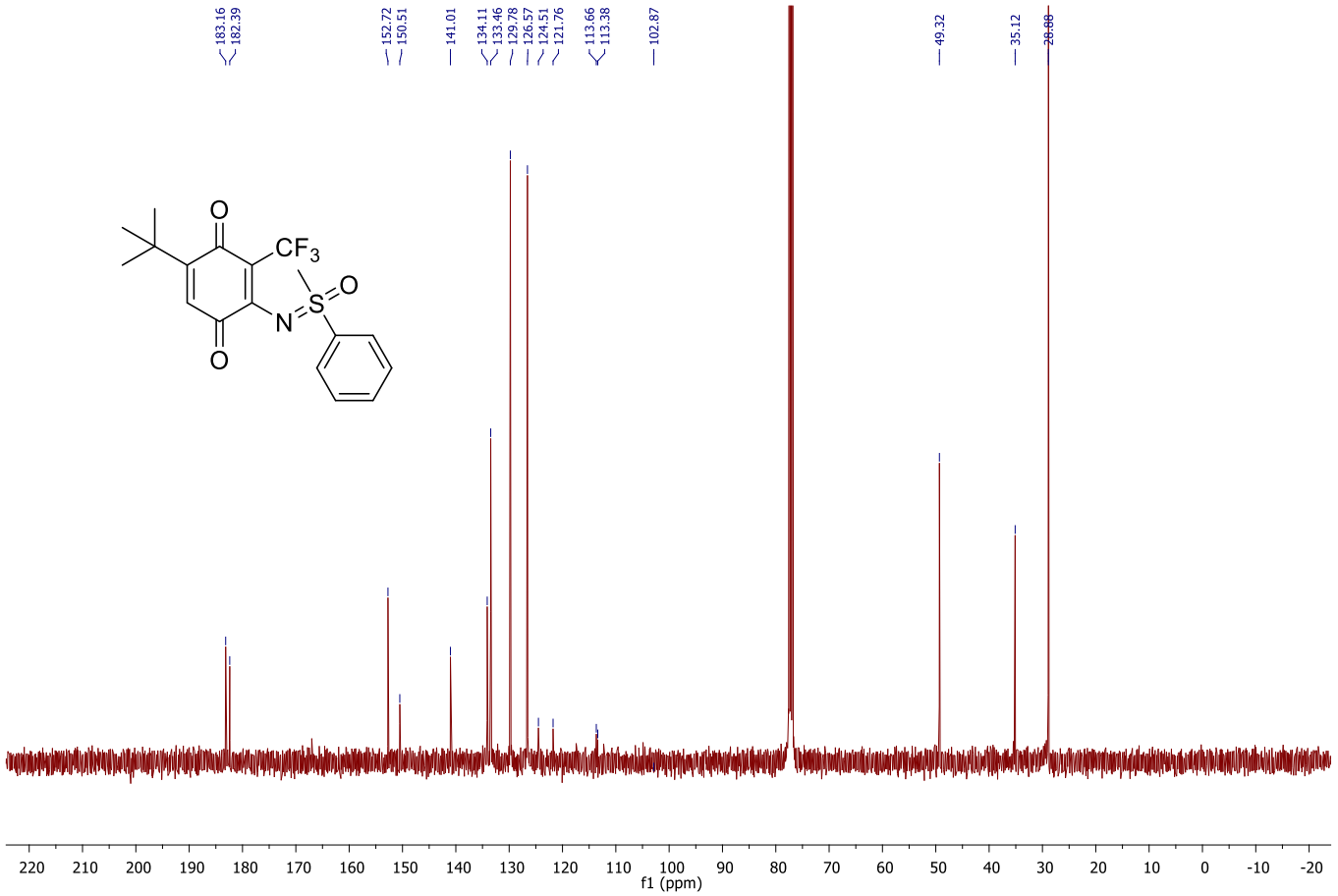
^{1}H NMR (400 MHz) of 5n in $CDCl_3$



^{19}F NMR (377 MHz) of 5n in $CDCl_3$

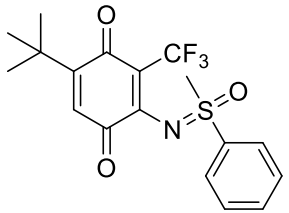


^{13}C {^{1}H} NMR (101 MHz) of 5n in $CDCl_3$



HRMS of 5n

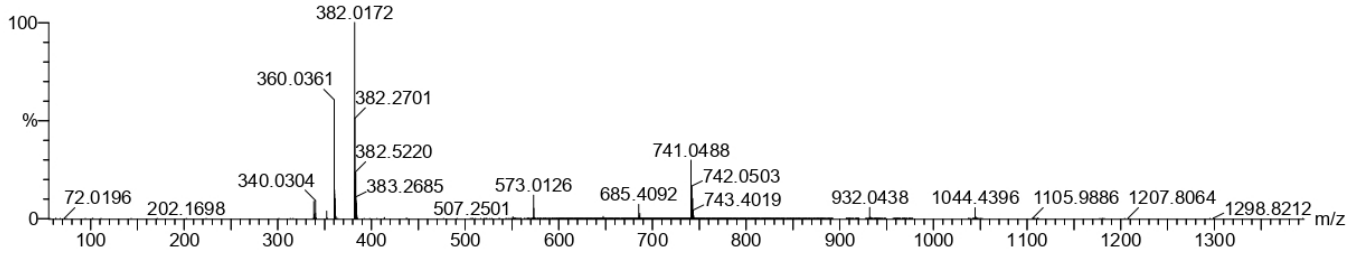
Elemental Composition Report **Page 1**



Single Mass Analysis
Tolerance = 50.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

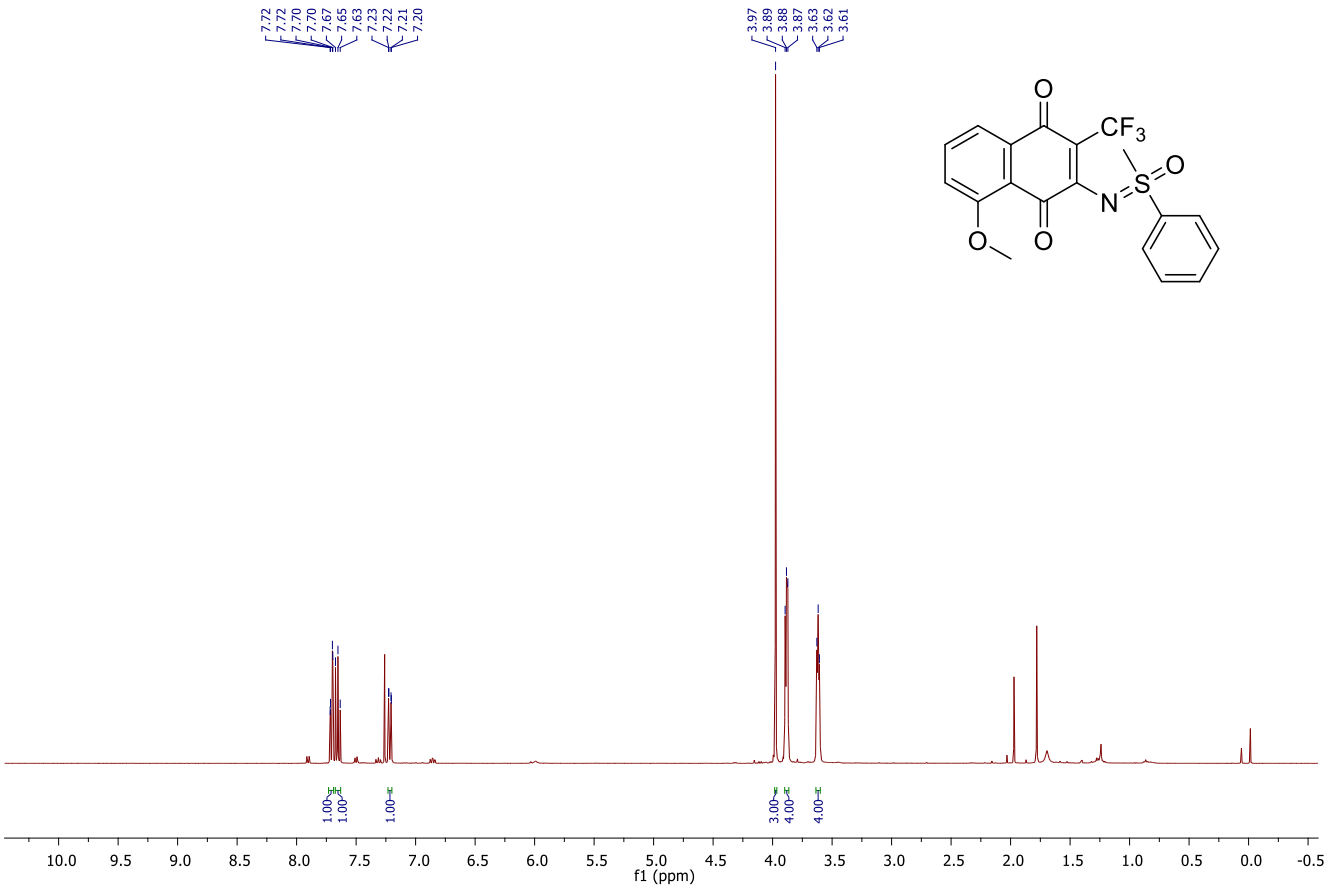
Monoisotopic Mass, Even Electron Ions
81 formula(e) evaluated with 1 results within limits (up to 3 closest results for each mass)
Elements Used:
C: 0-15 H: 0-100 N: 0-1 O: 0-4 F: 0-3 S: 0-1

OMe-BQ
QMI DIVISION, CSIR-IIIM JAMMU
Xevo G2-XS QTOF YFC2015
09-Aug-2023
16:55:49
080823_02 6 (0.138)
1: TOF MS ES+
4.40e+006

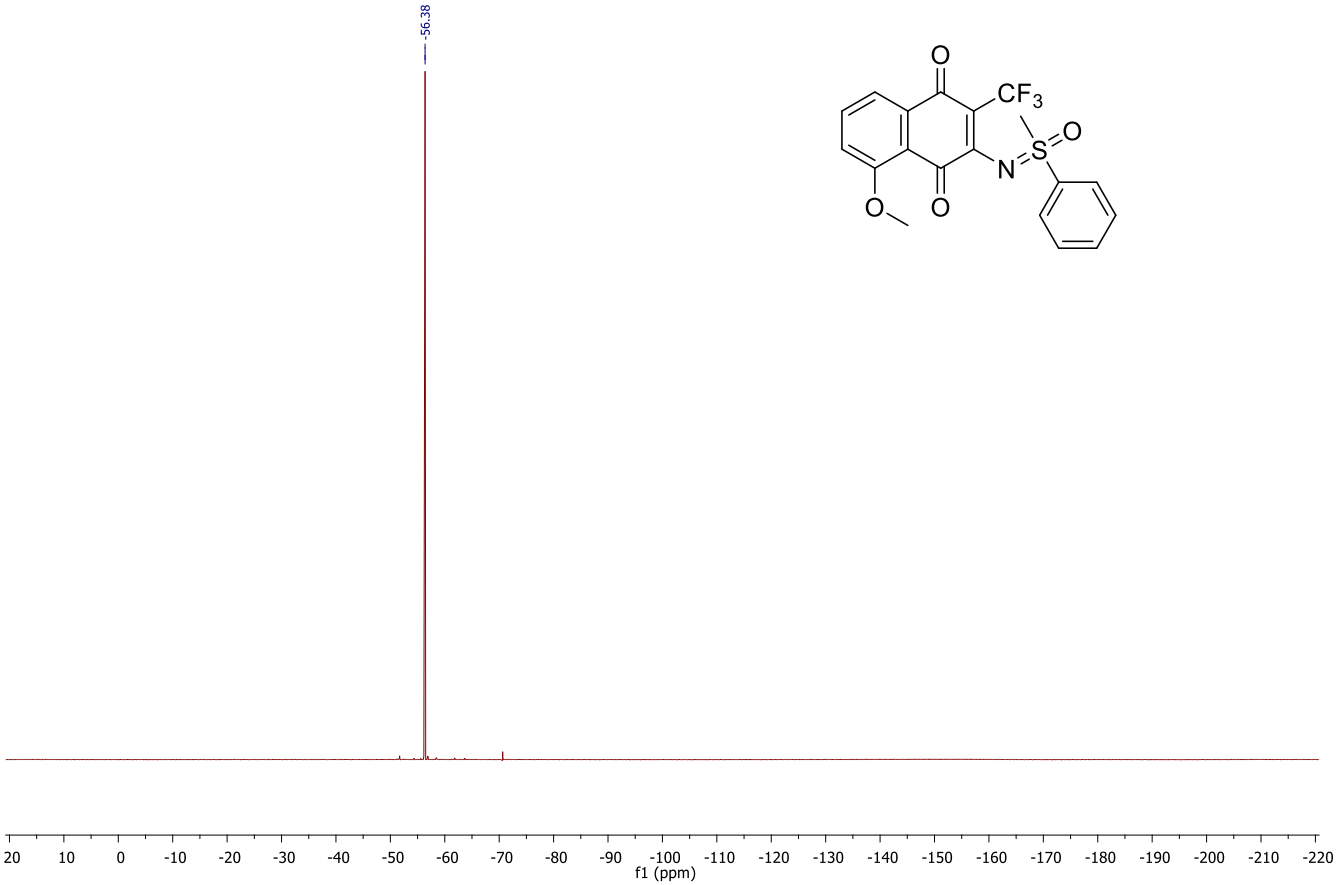


Minimum:				-1.5				
Maximum:		2.0	50.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
360.0361	360.0517	-15.6	-43.3	8.5	326.1	n/a	n/a	C15 H13 N O4 F3 S

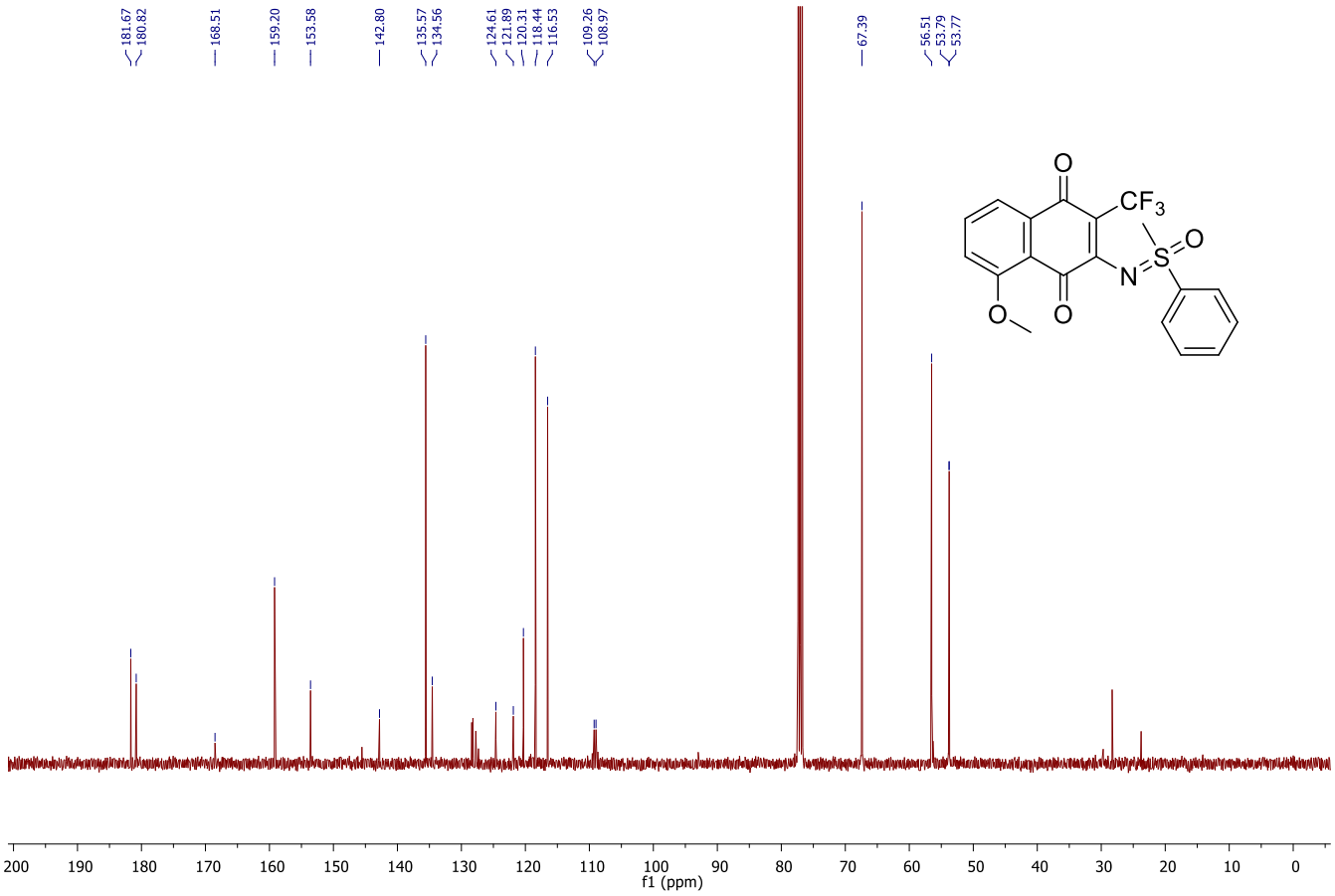
^{1}H NMR (400 MHz) of 8a in $CDCl_3$



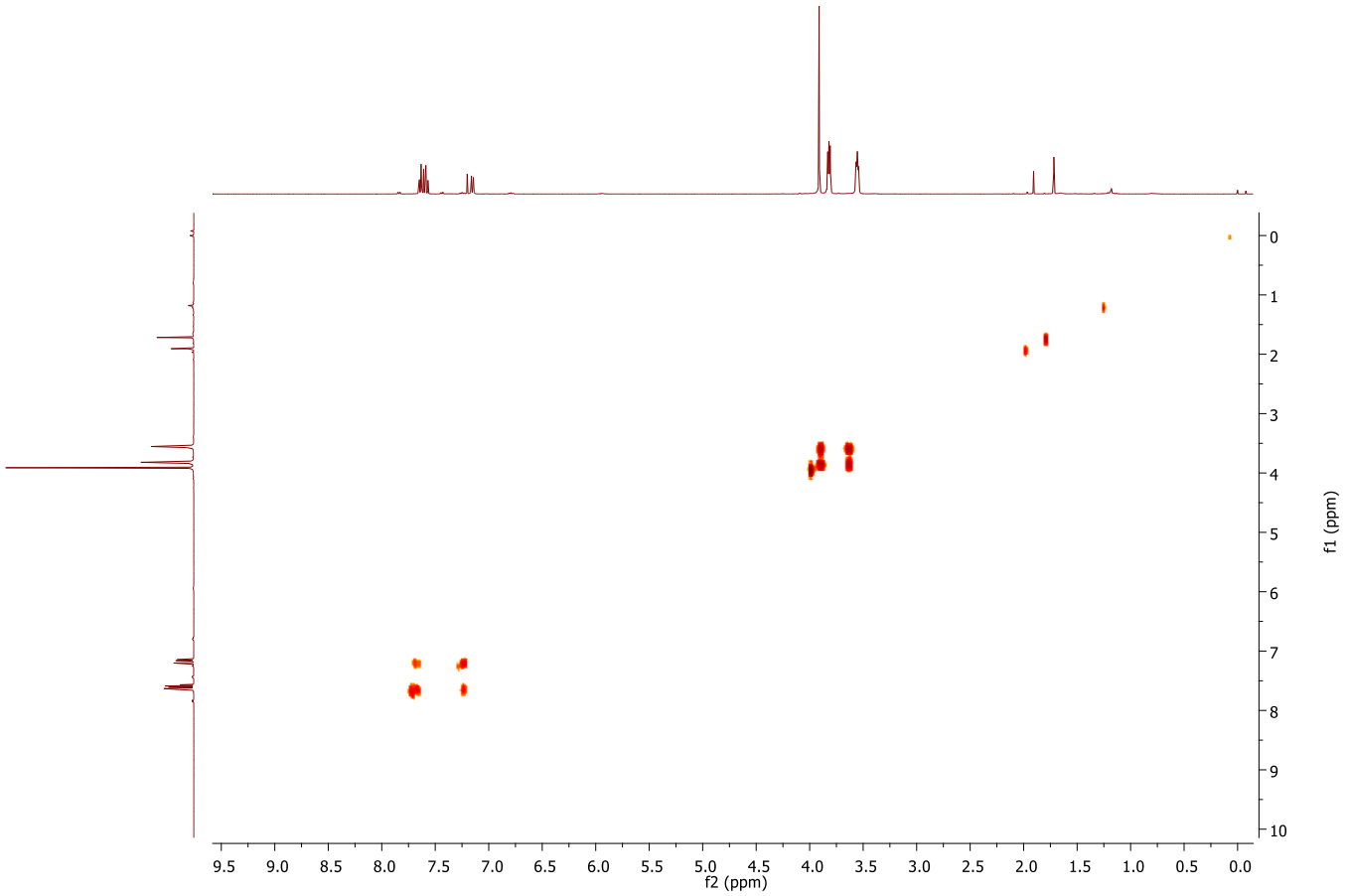
^{19}F NMR (377 MHz) of 8a in $CDCl_3$



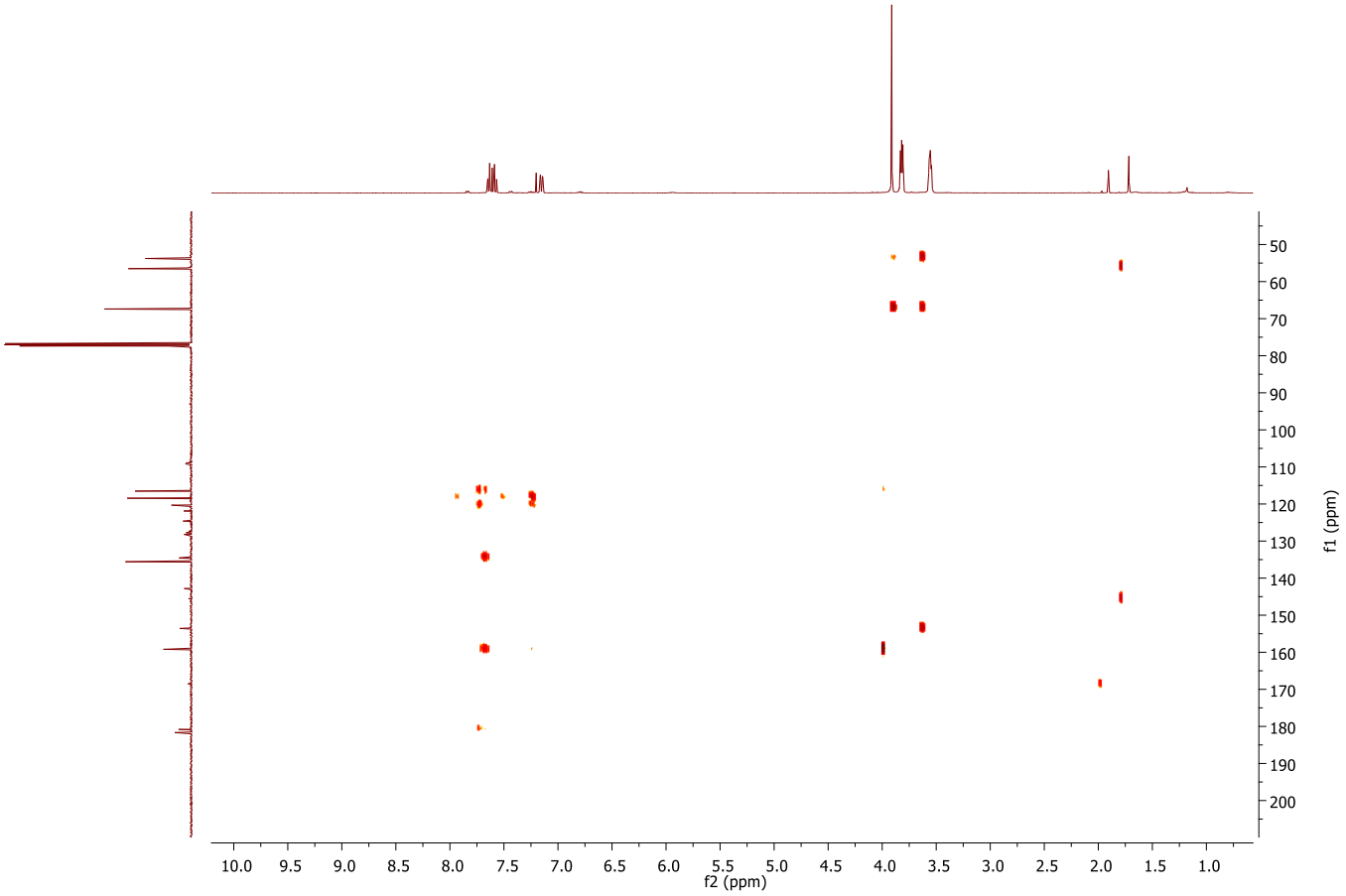
^{13}C {^{1}H} NMR (101 MHz) of 8a in $CDCl_3$



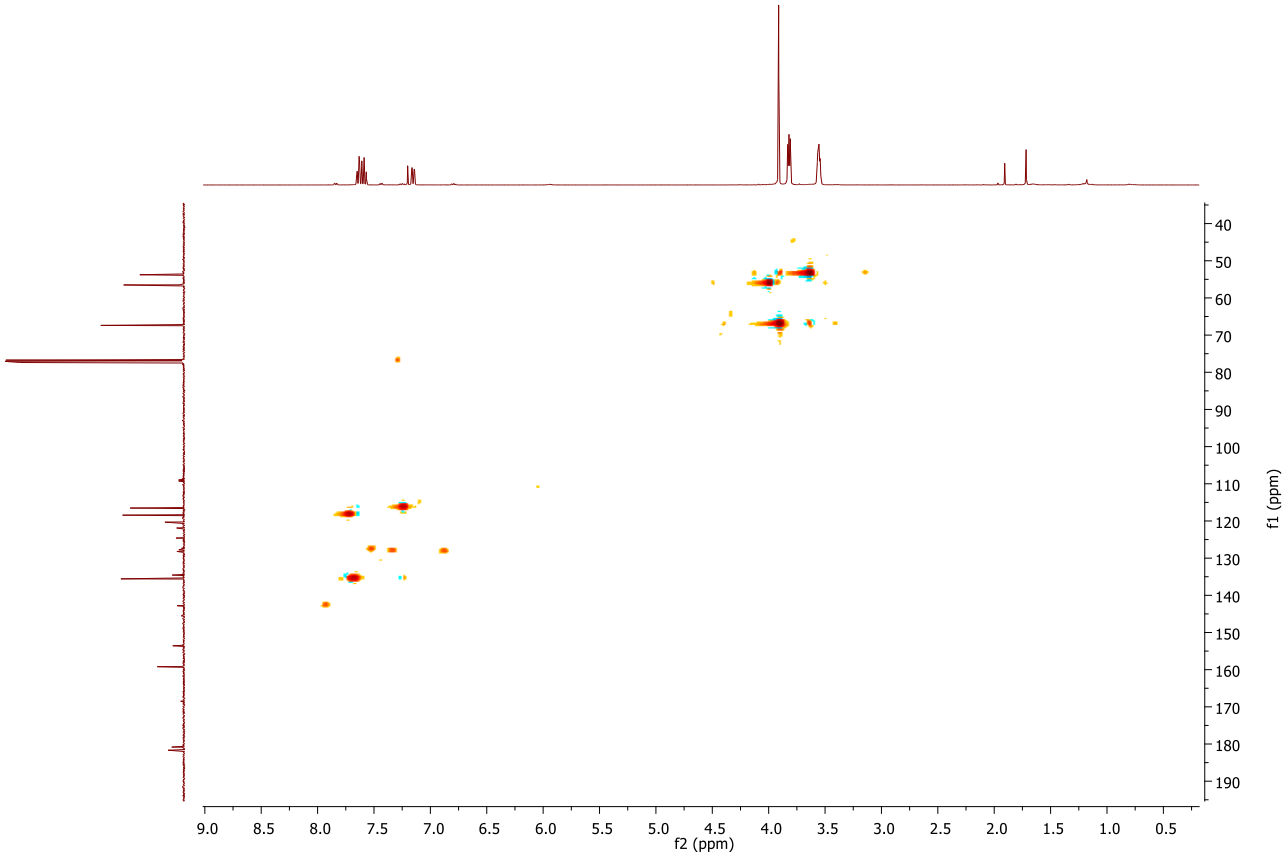
COSY NMR of 8a in $CDCl_3$



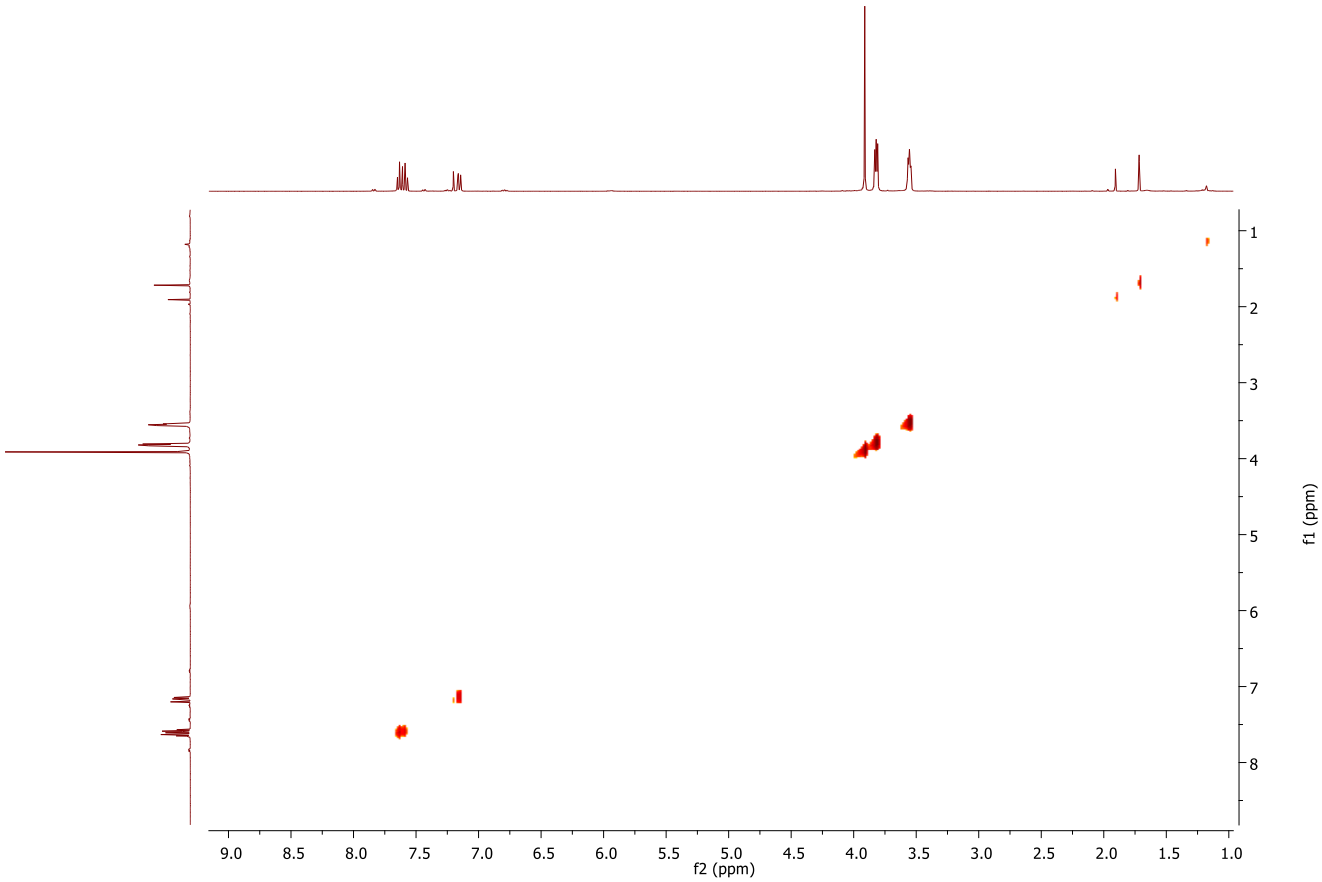
HMBC NMR of 8a in $CDCl_3$



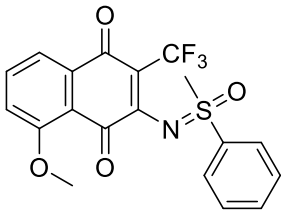
HSQC NMR of 8a in $CDCl_3$



NOESY NMR of 8a in $CDCl_3$



HRMS of 8a



Elemental Composition Report **Page 1**

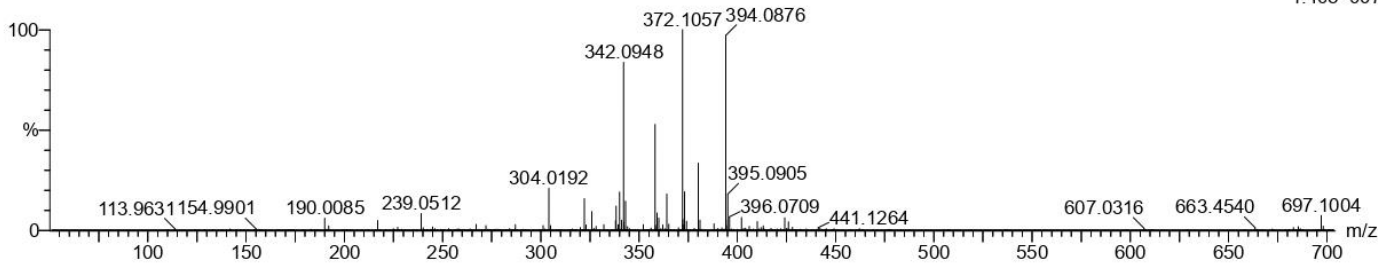
Single Mass Analysis
Tolerance = 50.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
41 formula(e) evaluated with 1 results within limits (up to 3 closest results for each mass)
Elements Used:
C: 0-16 H: 0-100 N: 0-1 O: 0-4 F: 0-3

5-OMe NQ-MOR
100723_03 6 (0.138)

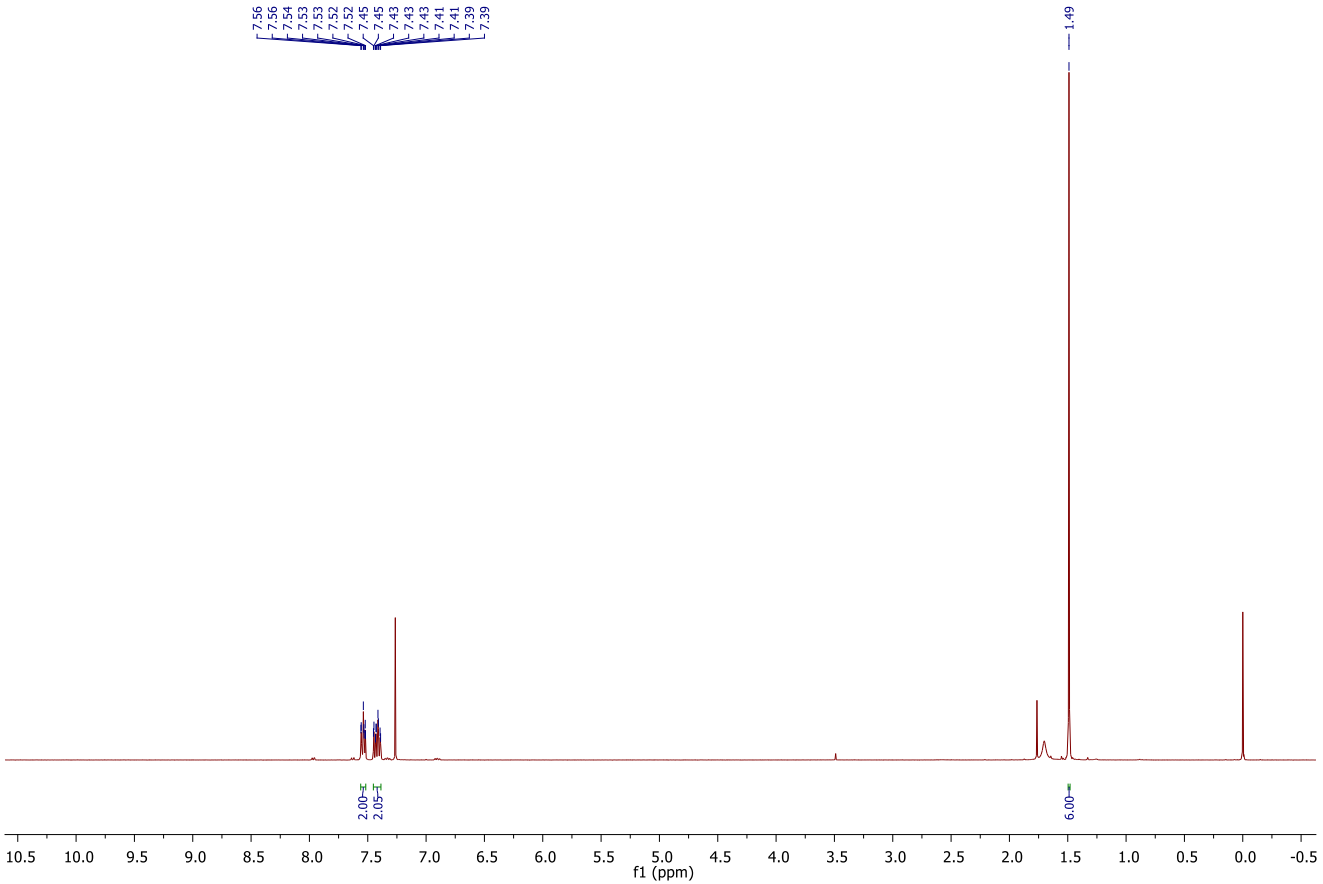
QMI DIVISION, CSIR-IIIM JAMMU
Xevo G2-XS QTOF YFC2015

10-Jul-2023
12:29:37
1: TOF MS ES+
1.40e+007

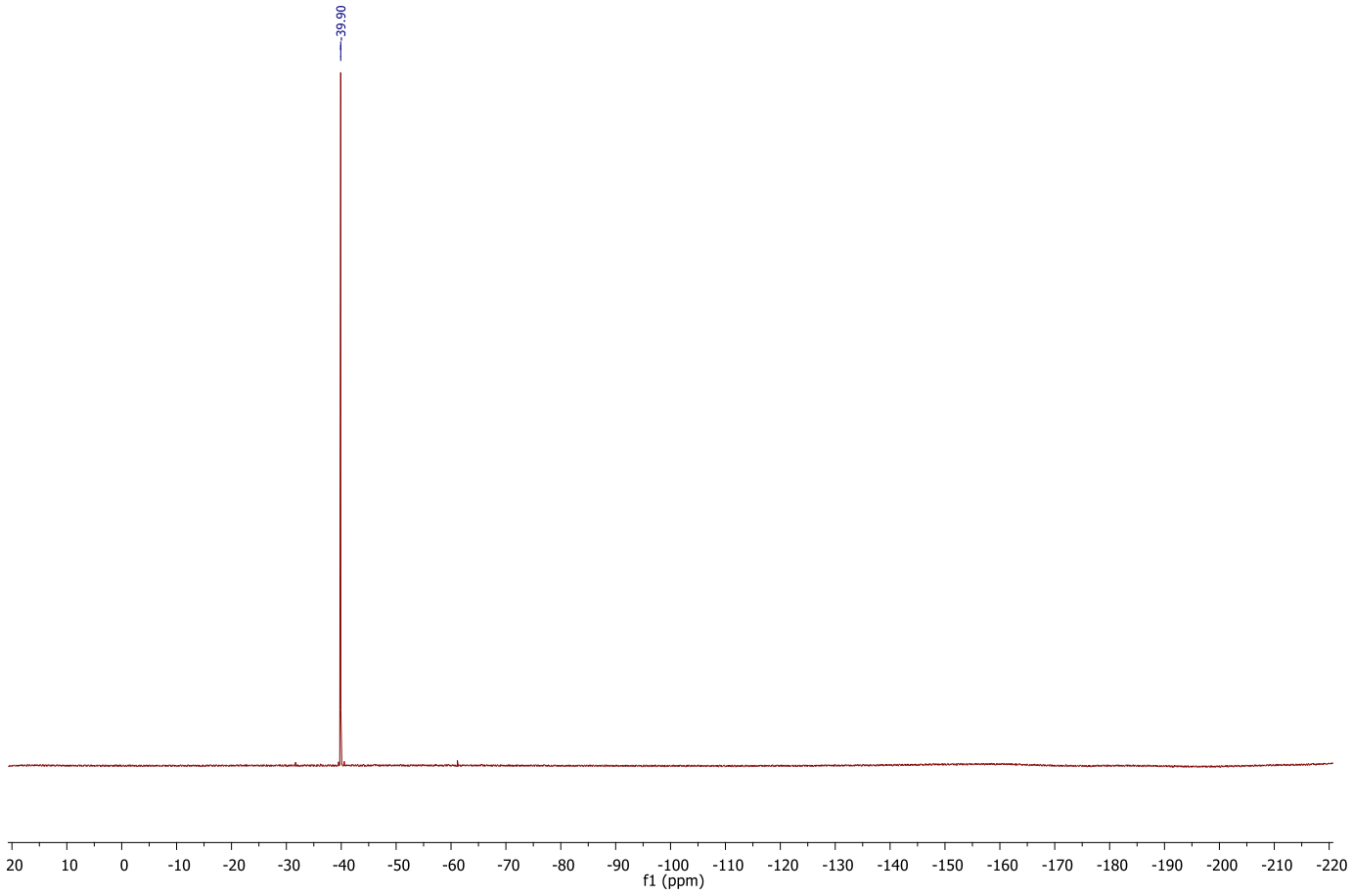


Minimum:				-1.5				
Maximum:		2.0	50.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
342.0948	342.0953	-0.5	-1.5	8.5	955.9	n/a	n/a	C16 H15 N O4 F3

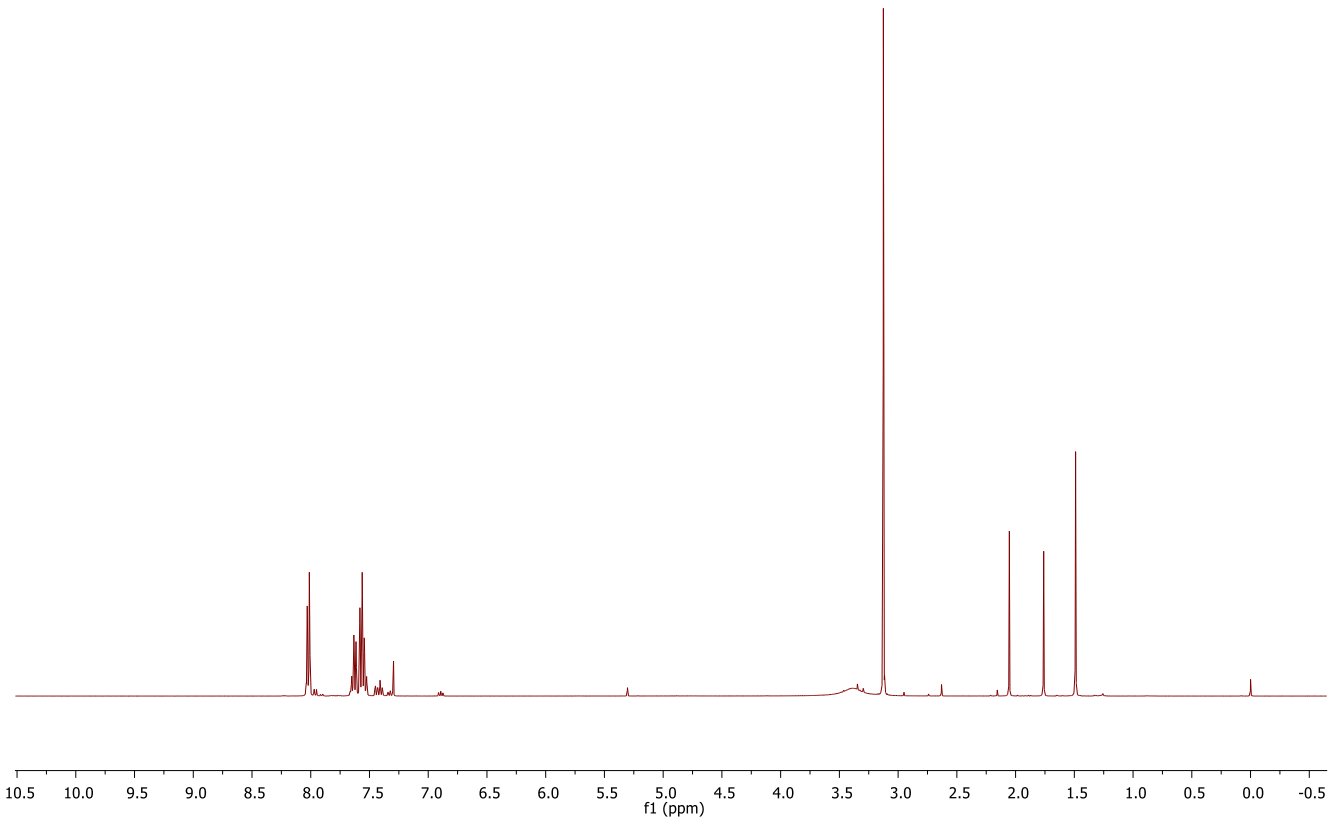
^{1}H NMR (400 MHz) of Togni-1 in $CDCl_3$



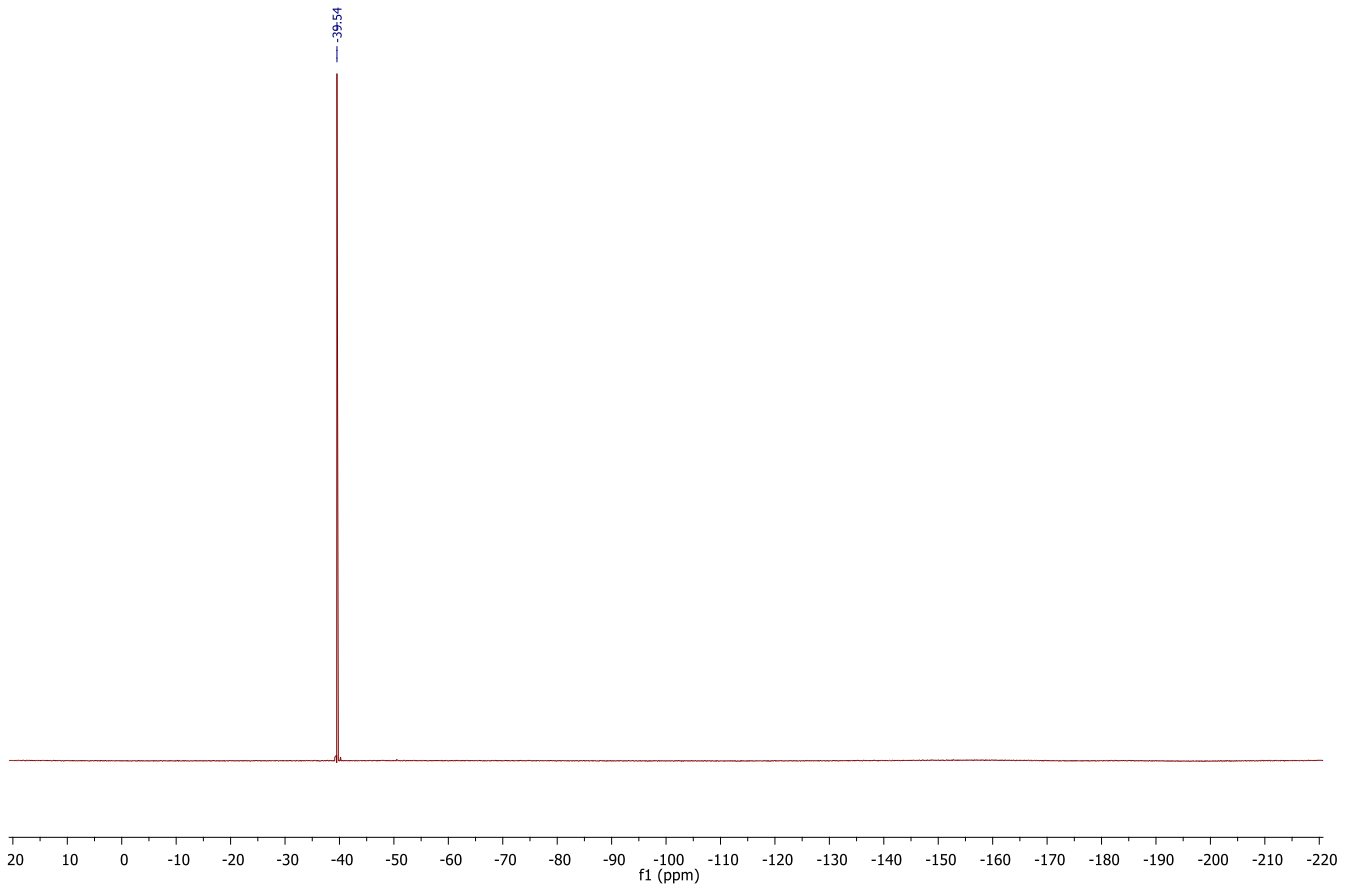
^{19}F NMR (377 MHz) of Togni-1 in $CDCl_3$



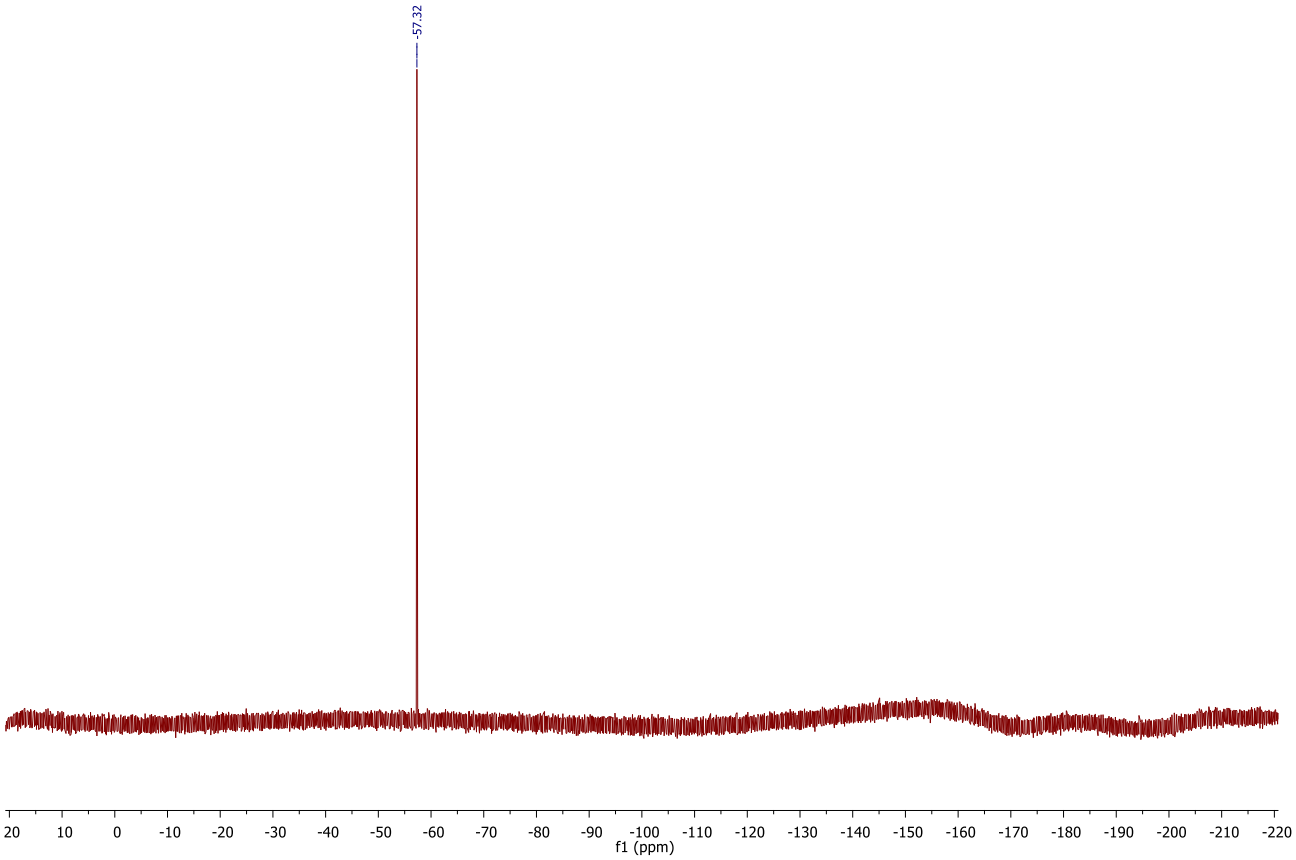
^{1}H NMR (400 MHz) of Togni-1 + Sulfoximine in $CDCl_3$



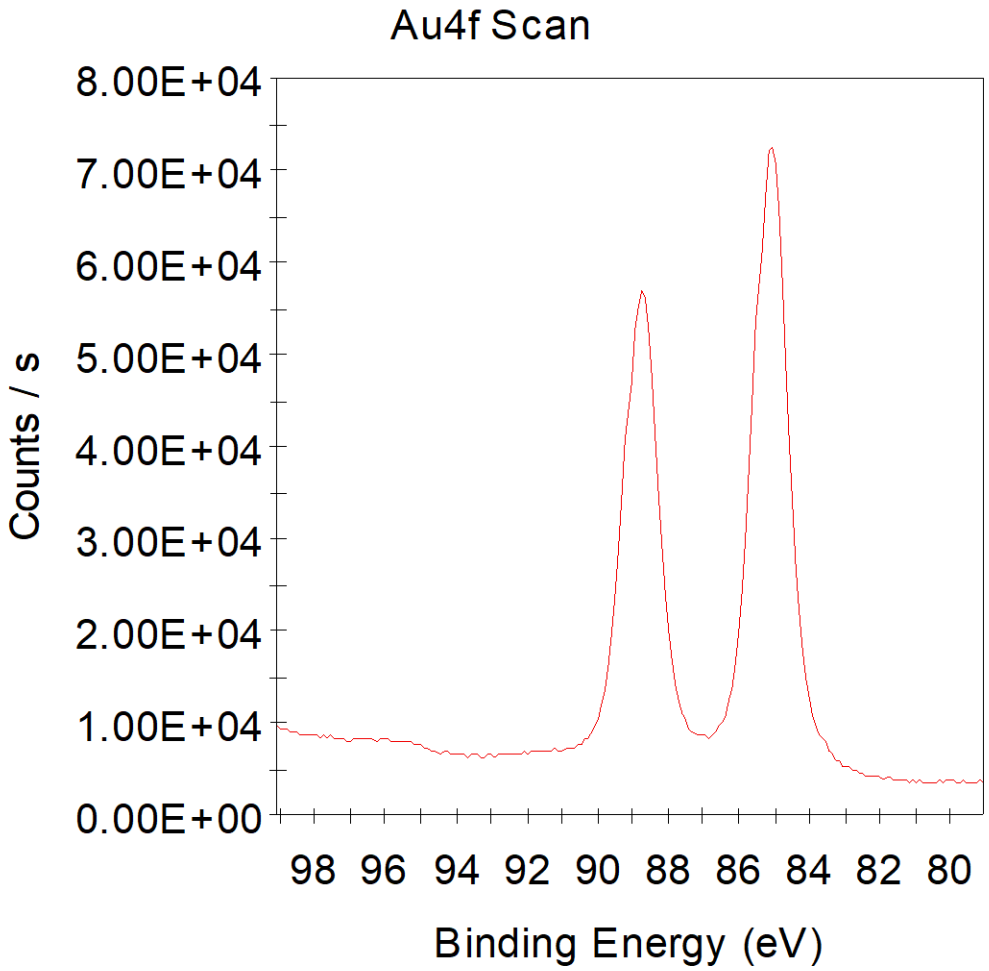
^{19}F NMR (377 MHz) of Togni-1 + Sulfoximine in $CDCl_3$



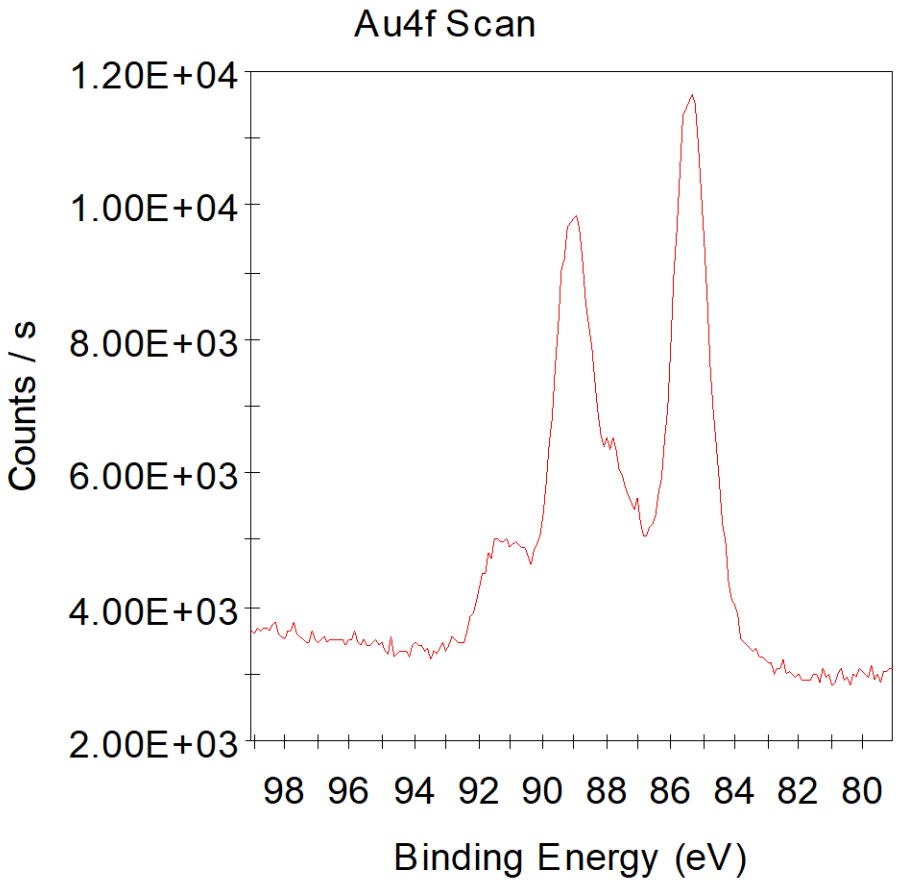
^{19}F NMR (377 MHz) of TEMPO-CF_3 adduct



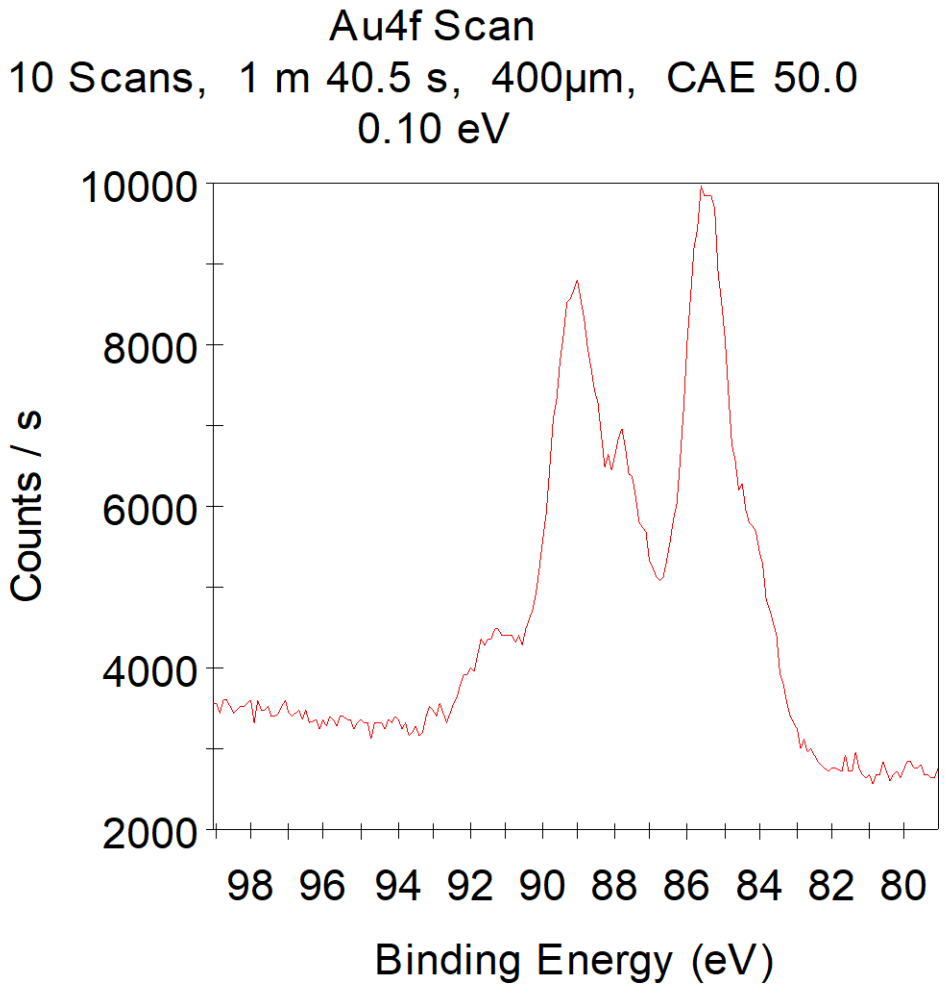
XPS Spectra of Au(I)



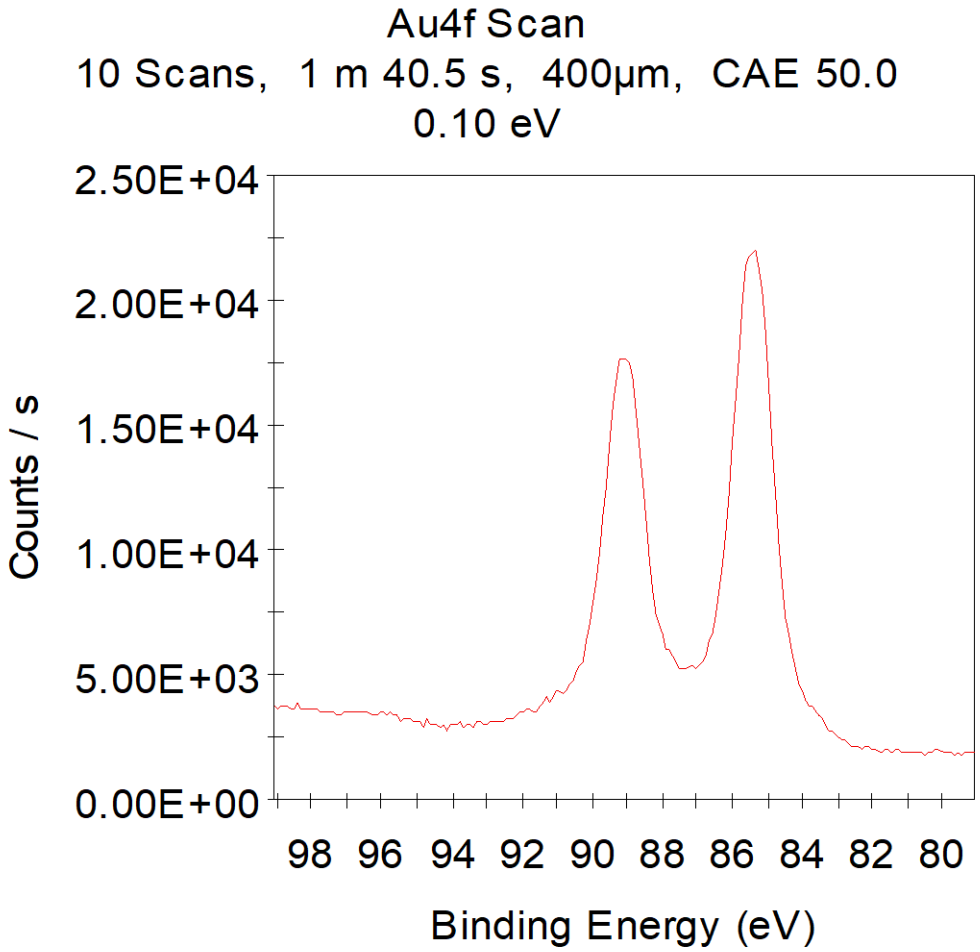
XPS Spectra of NQ-1



XPS Spectra of NQ-2

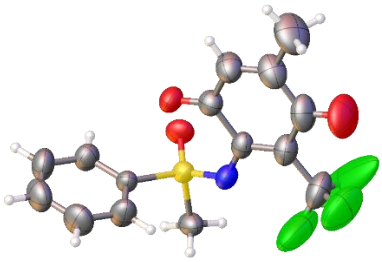


XPS Spectra of Au(III)



X-ray Crystallography Data

Table S5. Crystal data and structure refinement for 5l



Compound 5l (CCDC 2294386)

Identification code	5L
Empirical formula	$C_{15}H_{13}F_3NO_3S$
Formula weight	344.337
Temperature/K	200.00
Crystal system	monoclinic
Space group	$P2_1/n$
a/Å	5.624(4)
b/Å	25.714(14)
c/Å	11.107(5)
α/°	90
β/°	103.105(19)
γ/°	90
Volume/Å^3	1564.5(15)
Z	4
ρ_{calc}g/cm^3	1.462
μ/mm^{-1}	0.252
F(000)	709.1
Crystal size/mm^3	0.2 × 0.19 × 0.168
Radiation	Mo Kα (λ = 0.71073)
2Θ range for data collection/°	4.92 to 56.74
Index ranges	$-7 \le h \le 7$, $-34 \le k \le 34$, $-14 \le l \le 14$
Reflections collected	36690
Independent reflections	3864 [R_{int} = 0.0921, R_{sigma} = 0.0523]
Data/restraints/parameters	3864/0/210
Goodness-of-fit on F^2	1.055
Final R indexes [I>=2σ (I)]	R_1 = 0.0954, wR_2 = 0.2433
Final R indexes [all data]	R_1 = 0.1198, wR_2 = 0.2534
Largest diff. peak/hole / e Å^{-3}	0.86/-0.57