Electronic Supporting Information

Oxidative Cross Coupling Reaction of 4-Hydroxydithiocoumarin and Amines/Thiols Using a Combination of I_2 and TBHP: Access to Lead Molecules for Bio-medical Applications

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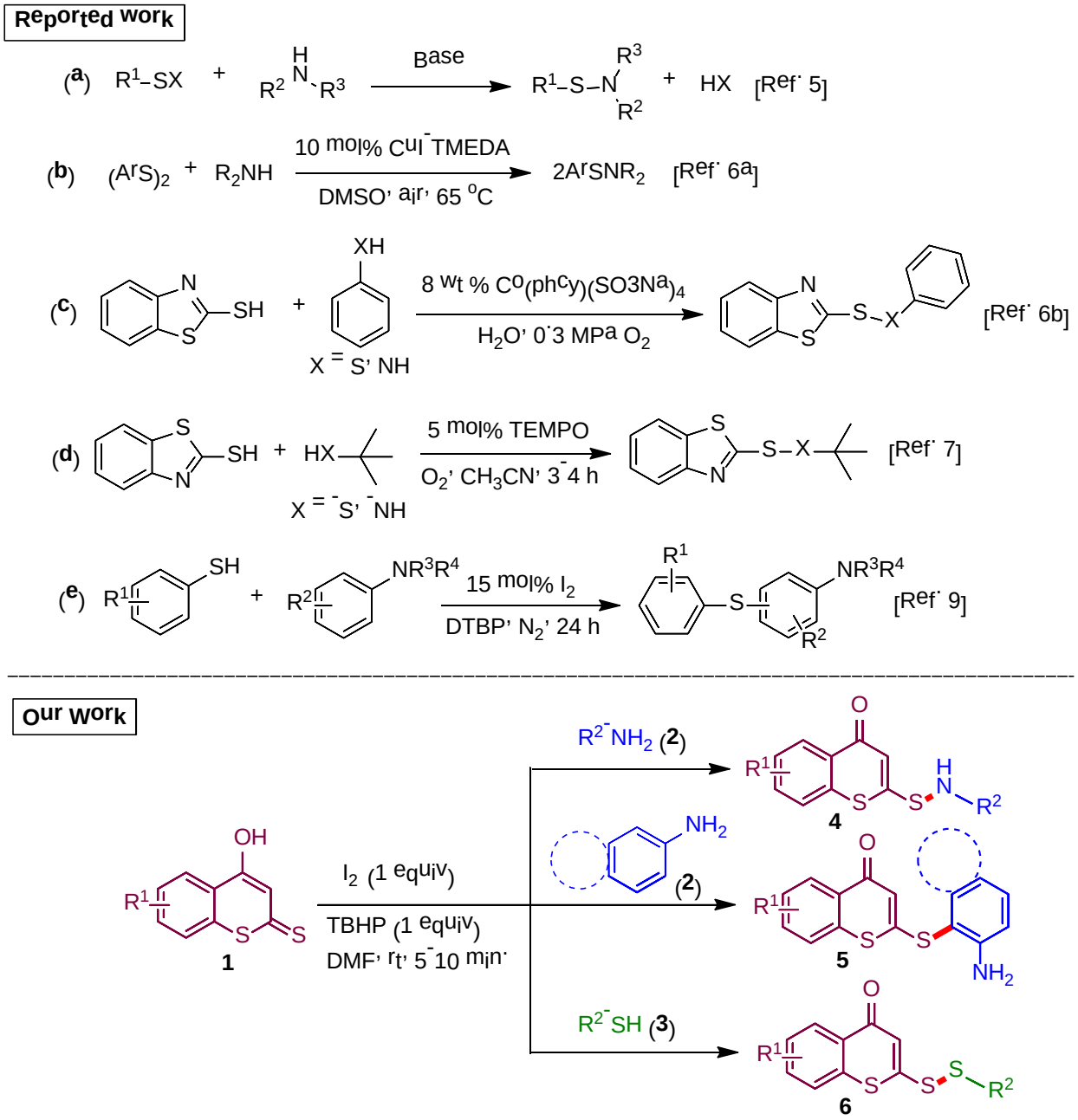
Content

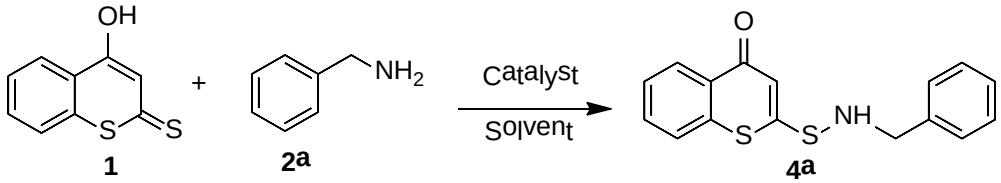
l. General Information and Methods

^{1}H and ^{13}C NMR spectra were recorded on 300 MHz, 400 MHz, 600 MHz and 75 MHz, 100 MHz, 150 MHz spectrometer TMS as internal reference; chemical shifts (δ scale) are reported in parts per million (ppm). ^{1}H NMR Spectra are reported in the order: multiplicity, coupling constant (*J*value) in hertz (Hz) and no of protons; signals were characterized as s (singlet), d (doublet), t (triplet) and m (multiplet). IR spectra were recorded in KBr. HRMS spectra were recorded using ESI and APCI (TOF) mode. The X-ray crystal structures were determined with a diffractometer. Complete crystallographic data of **4q** (CCDC no. 1572814), **5a** (CCDC no. 1583530) and **7a** (CCDC no. 1583531) for the structural analysis have been deposited with the Cambridge Crystallographic Data Centre, Copies of this information may be obtained free of charge from the Director, Cambridge Crystallographic Data Centre, 12 Union Road, Cambridge CB2 1EZ, UK, (fax: +44-1223-336033, e-mail: deposit@ccdc.cam.ac.uk or via: www.ccdc.cam.ac.uk).



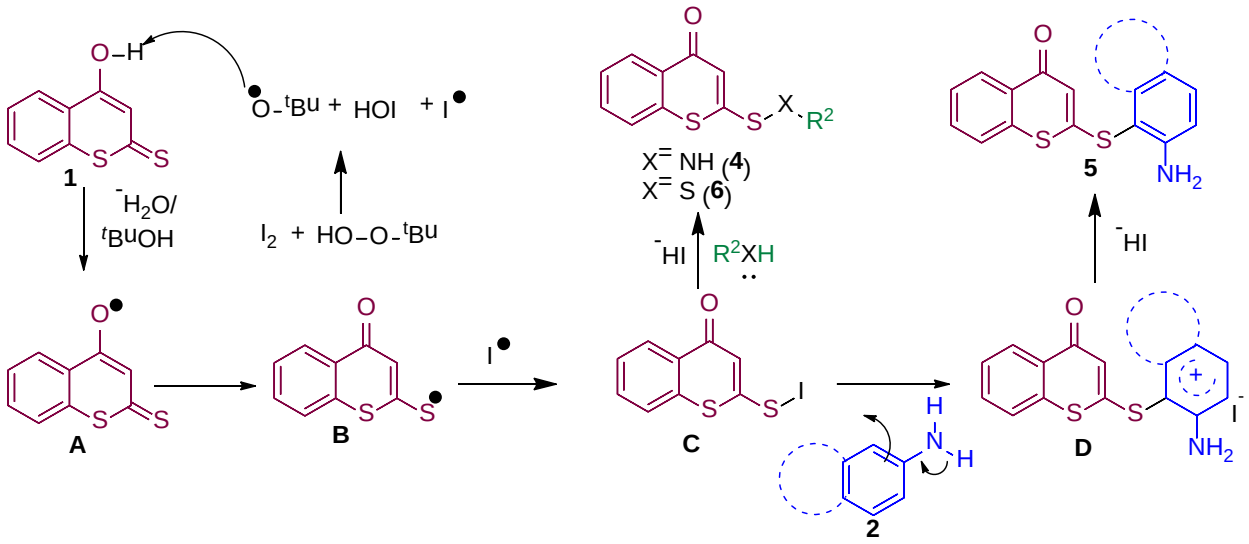
Scheme 1. Various examples for the synthesis of sulfenamides, sulfanes and disulfides through new S-N, S-C and S-S bonds formation

Table S1. Optimization of the reaction conditions[a,b]



Entry	I_2 (equiv.)	aq. TBHP (equiv.)	Solvent	Time/min	Yield (%)[b]
01	-	-	DMF	24 h	NR
02	0.3	1	DMF	2 h	NR
03	0.5	1	DMF	30	50
04	**1**	**1**	**DMF**	**5**	**95**
05	1.5	1	DMF	15	90
06	2	2	DMF	20	85
07	1	1	DMSO	40	81
08	1	1	CH_3CN	50	70
09	1	1	EtOH	50	68
10	1	1	MeOH	60	65
11	1	1	DCE	40	72
12	1	1	H_2O	8 h	20
13	1	1	THF	6 h	40
14	1	-	DMF	24 h	NR
15	-	1	DMF	24 h	NR

[a]All the reactions were carried out using 4-hydroxydithiocoumarin **1** (1 mmol), benzylamine **2** (1 mmol) in 1ml of solvent at room temperature. [b]Isolated yield.



Scheme 2. Proposed mechanism for the formation of sulfenamide, sulfanes and disulfide

3. General Experimental Procedure

3. I. General procedure for the synthesis of compounds (1)

The key starting material 4-hydroxydithiocoumarin (**1**) was prepared by following the previous reported procedure mentioned in the paper J. E. Andersonmckay and A. J. Liepa, *Aust. J. Chem*., 1987, **40**, 1179.

3. II. General Procedure for the Synthesis of 2-((benzylamino)thio)-4H-thiochromen-4-one (4), 2-((2-aminophenyl)thio)-4H-thiochromen-4-one derivatives (5) and 2-(phenyldisulfanyl)-4H-thiochromen-4-one derivatives (6)

To a stirred solution of 4-hydroxydithiocoumarin (1 equiv, **1**) and amine/thiol (1 equiv, **2/3**) in DMF (1 mL) at room temperature was added 1 equiv. of I_2 along with 1 equiv. of aq. TBHP. The reaction mixture was stirred at room temperature, and the progress of the reaction was monitored by TLC analysis. The completion of the reaction (marked by the disappearance of starting material and formation of new spot) was observed by TLC of ethyl acetate and hexane (1:4 for **4**, 2:3 for **5**, 1:49 for **6**). After completion of the reaction, I_2 was quenched with a saturated aqueous solution of $Na_2S_2O_3.6H_2O$ and followed by the extraction with ethyl acetate. The organic phase was separated, dried over anhydrous Na_2SO_4, and evaporated to give a crude residue. It was purified by the silica gel column chromatography using hexane and ethyl acetate as eluent to give the desired product **4**/**5**/**6**.

3. III. General Procedure for the Synthesis of N-benzyl-4-oxo-4H-thiochromene-2-sulfonamide (7a)

This reaction was conducted maintaining the procedure mentioned in the following paper, A. A. Dar, N. Enjamuri, M. Shadab, N. Ali, A. T. Khan, *ACS Comb. Sci*. 2015, **17**, 671.

Materials

Dulbecco's Modified Eagle's medium (DMEM) from Sigma-Aldrich, Fetal Bovine Serum (FBS) from Gibco ThermoFisher Scientific, (3-[4,5-dimethylthiazol-2-yl]-2,5 diphenyltetrazolium bromide) (MTT) from Himedia, Tissue culture dishes from Eppendorf, MCF7 cell line was procured from National Centre for Cell Science (NCCS), Pune, India.

Method

Cell Viability Assay

Breast cancer cell line MCF7 seeded in 96 well plates at a density of 7000 cells per well in DMEM media supplemented with 10% FBS was allowed to attach overnight in CO_2 incubator maintained at 37˚C supplied with 5% CO_2. Following attachment, media was discarded and fresh serum media containing varying concentrations of the compounds were added to the seeded cells. After 48 h incubation, serum media containing 5 µl of 5 mg/ml MTT solution was added to each well and the plates were incubated in the CO_2 incubator. MTT is converted to purple formazan crystals by dehydrogenase enzyme in the mitochondria of the viable cells. Subsequently, the media was discarded and DMSO was added to dissolve the formazan crystals formed by enzymatic conversion by the live cells. The product was measured by absorbance at 570 nm along with background measurement at 690 nm using multiplate reader (Tecan, Infinite M200PRO). The experiment was also performed with DMSO as control to eliminate any possibility of its effect in cell viability. Cell viability (%) relative to the control untreated cells was calculated using the following formula:

$$Cell\ viability\ (\%) = \frac{(Abs\ 570 - Abs\ 690)\ Sample}{(Abs\ 570 - Abs\ 690)\ Control} X\ 100$$

Where, Abs570 is the absorbance of formazan at 570 nm and Abs690 is the background absorbance which is subtracted from all treated and untreated sample

4. X-ray Structure of Compounds 4q, 5a and 7a

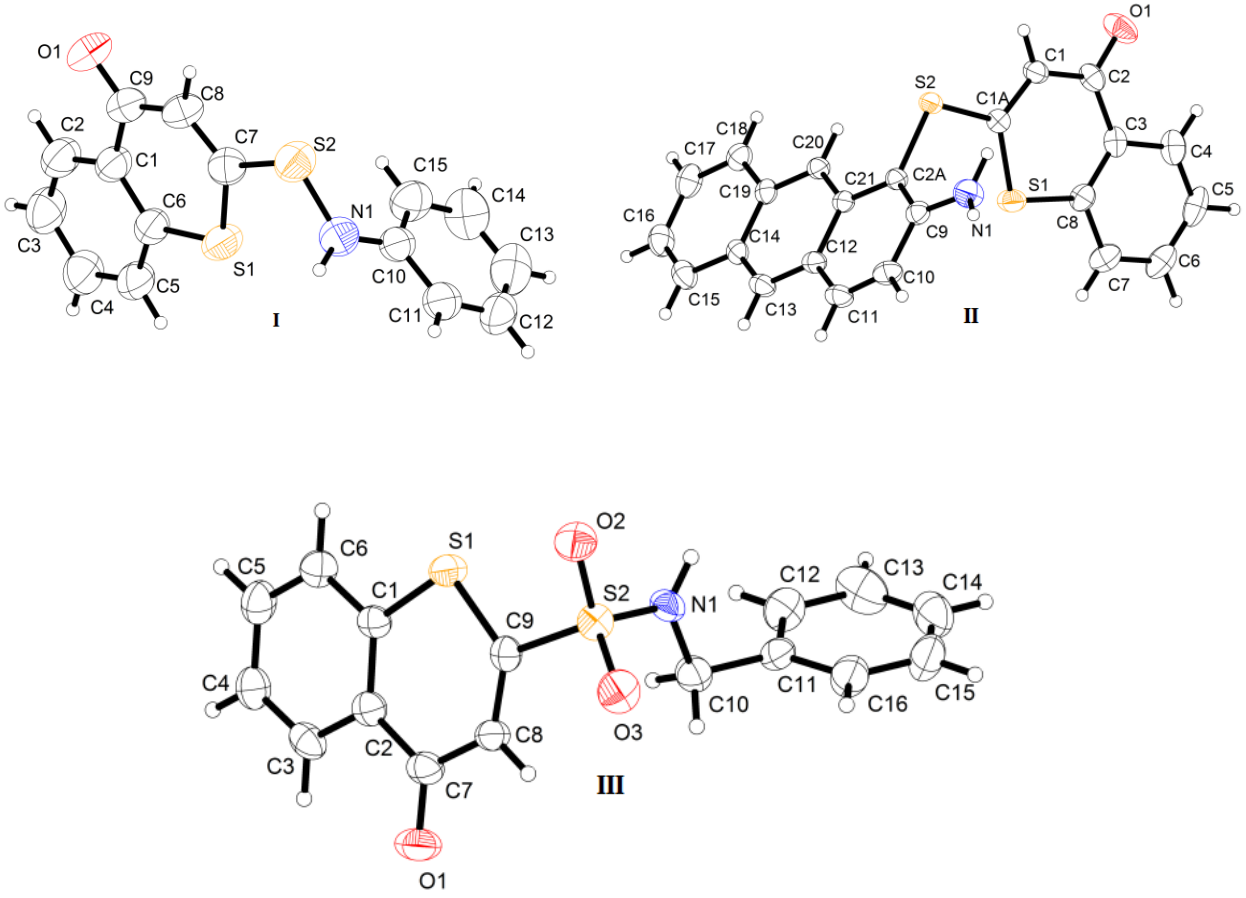


Figure 1. 40% probability of ORTEP ellipsoids of compounds **4q (I)** (CCDC 1572814), **5a (II)** (CCDC 1583530) and **7a (III)** (CCDC 1583531)

5. Crystal Data and Structure Refinement for Compound 4q, 5a and 7a

Table S2 Data collection and refinement statistics for the compounds 4q, 5a and 7a

Entry	Identification code	Compound 4q	Compound 5a	Compound 7a
01	Empirical formula	$C_{15}H_{11}NOS_2$	C23 H17 N O2 S2	C16 H13 N O3 S2
02	Formula weight	285.37	403.50	331.39
03	Temperature	296(2) K	296(2) K	293(2) K
04	Wavelength	0.71073	0.71073	0.71073
05	Radiation type	Mo K\a	Mo K\a	Mo K\a
06	Radiation source	Fine-focus sealed tube	Fine-focus sealed tube	Fine-focus sealed tube
07	Crystal system	Monoclinic	Monoclinic	Monoclinic
08	Space group	$P2_1/c$	$P2_1/c$	$P2_1$
09	Cell length	a 10.837(4) b 10.802(4) c 11.707(5)	a 16.5683(9) b 13.2261(7) c 8.5713(4)	a 10.3912(7) b 5.6999(3) c 12.8081(9)
10	Cell Angle	α 90 β 93.41(3) δ 90	α 90 β 95.047(3) δ 90	α 90.00 β 102.459(7) δ 90.00
11	Cell Volume	1367.9(9)	1870.98(17)	740.75(8)
12	Density	1.386	1.432	1.486
13	Completeness to theta	24.99°/ 99.80%	25.05°/ 99.60 %	24.99°/ 99.60 %
14	Absorption correction	multi-scan	multi-scan	multi-scan

15	Refinement method	Full-matrix least-squares on F2	Full-matrix least-squares on F2	Full-matrix least-squares on F2
16	Index ranges	-12<=h<=12, -8<=k<=12, -13<=l<=13	-19<=h<=16, -12<=k<=15, -8<=l<=10	-12<=h<=10, -6<=k<=6, 15<=l<=10
17	Reflection number	10953	9261	2197
18	Theta range	2.568- 24.998	2.84-28.73	3.26-24.99
19	Cell formula units Z	4	4	2
20	CCDC no	1572814	1583530	1583531

6. Characterization of products

2-((benzylamino)thio)-4H-thiochromen-4-one (4a): Yellow semi-solid, ^{1}H NMR (600 MHz, $CDCl_3$): δ 3.32-3.34 (m, 1H), 4.19 (d, *J* = 6.0 Hz, 2H), 6.87 (s, 1H), 7.30-7.34 (m, 1H), 7.37-7.39 (m, 4H), 7.49-7.51 (m, 1H), 7.54-7.58 (m, 2H), 8.46 (d, *J* = 12.0 Hz, 1H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 57.0, 116.4, 126.4, 127.8, 128.2, 128.5, 128.6, 128.9, 129.1, 131.2, 131.3, 137.6, 138.4, 162.8, 178.7; IR $(KBr)_{vmax}$ 1120, 1145, 1267, 1320, 1325, 1450, 1459, 1514, 1579, 2856, 2928, 2969, 3012, 3069, 3321 cm^{-1}; HRMS (ESI) Calcd For $C_{16}H_{14}NOS_2$ 300.0512 ($M + H^+$); Found 300.0509.

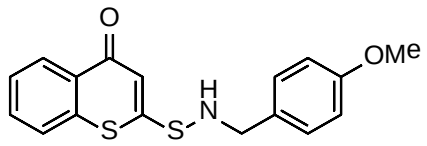
2-(((4-methylbenzyl)amino)thio)-4H-thiochromen-4-one (4b): Yellow solid, Mp 80-81˚C, ^{1}H NMR (600 MHz, $CDCl_3$): δ 2.30 (s, 3H), 3.37 (t, *J* = 6.0 Hz, 1H), 4.10 (d, *J* = 6.0 Hz, 2H), 6.81 (s, 1H), 7.12 (d, *J* = 6.0 Hz, 2H), 7.20-7.22 (m, 2H), 7.43-7.46 (m, 1H), 7.50-7.52 (m, 2H), 8.41 (d, *J* = 6.0 Hz, 1H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 21.3, 56.7, 116.3, 126.3, 127.8, 128.4, 128.8, 129.6, 131.1, 131.3, 135.4, 137.6, 137.9, 162.9, 178.6; IR $(KBr)_{vmax}$ 1131, 1166, 1237, 1317, 1338, 1436, 1458, 1514, 1586, 2853, 2923, 2967, 3012, 3050, 3356 cm^{-1}; HRMS (ESI) Calcd For $C_{17}H_{16}NOS_2$ 314.0668 ($M + H^+$); Found 314.0675.

2-(((4-chlorobenzyl)amino)thio)-4H-thiochromen-4-one (4c): Yellow solid, Mp 70-71˚C, ^{1}H NMR (600 MHz, $CDCl_3$): δ 3.37-3.38 (m, 1H), 4.16 (d, *J* = 6.0 Hz, 2H), 6.86 (s, 1H), 7.29-7.30 (m, 2H), 7.32-7.34 (m, 2H), 7.49-7.52 (m, 1H), 7.56-7.57 (m, 2H), 8.45 (d, *J* = 6.0 Hz, 1H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 56.1, 116.6, 126.4, 127.9, 128.9, 129.1, 129.9, 131.1, 131.4, 136.8, 137.5, 162.2, 178.7; IR $(KBr)_{vmax}$ 1110, 1125, 1245, 1370, 1460, 1489, 1524, 1589, 2865, 2930, 2974, 3198 cm^{-1}; HRMS (ESI) Calcd For $C_{16}H_{13}ClNOS_2$ 334.0122 ($M + H^+$); Found 334.0129.

2-(((2-chlorobenzyl)amino)thio)-4H-thiochromen-4-one (4d): Yellow semi-solid, ^{1}H NMR (400 MHz, $CDCl_3$): δ 3.59 (t, *J* = 4.0 Hz, 1H), 4.28 (d, *J* = 4.0 Hz, 2H), 6.85 (s, 1H), 7.24-7.25 (m, 2H), 7.36-7.40 (m, 2H), 7.46-7.51 (m, 1H), 7.53-7.54 (m, 2H), 8.44 (d, *J* = 8.0 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 54.8, 116.2, 126.4, 127.2, 127.8, 128.8,

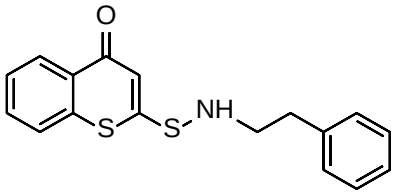
129.7, 129.9, 130.8, 131.3, 135.9, 163.1, 178.7; IR $(KBr)_{vmax}$ 1121, 1141, 1281, 1356, 1385, 1447, 1488, 1567, 1589, 1604, 2858, 2933, 2967, 3248 cm^{-1}; HRMS (ESI) Calcd For $C_{16}H_{13}ClNOS_2$ 334.0122 ($M + H^+$); Found 334.0121.

2-(((4-methoxybenzyl)amino)thio)-4H-thiochromen-4-one (4e): Yellow semi-solid, ^1H NMR



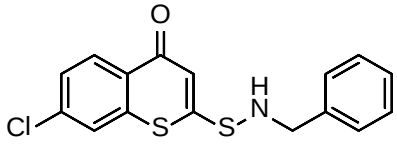
(600 MHz, $CDCl_3$): δ 3.26 (s, 1H), 3.80 (s, 3H), 4.11 (d, *J* = 6.0 Hz, 2H), 6.86 (s, 1H), 6.88 (s, 1H), 6.89 (s, 1H), 7.28 (d, *J* = 6.0 Hz, 2H), 7.48-7.51 (m, 1H), 7.54-7.57 (m, 2H), 8.46 (d, *J* = 12.0 Hz, 1H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 55.5, 56.4, 114.3, 116.3, 126.4, 127.8, 128.8, 129.9, 130.5, 131.2, 131.3, 137.6, 159.6, 162.9, 178.7; IR $(KBr)_{vmax}$ 1101, 1176, 1249, 1323, 1339, 1383, 1436, 1460, 1512, 1587, 1609, 2854, 2925, 2959, 3050, 3212 cm^{-1}; HRMS (ESI) Calcd For $C_{17}H_{16}NO_2S_2$ 330.0617 ($M + H^+$); Found 330.0615

2-((phenethylamino)thio)-4H-thiochromen-4-one (4f): Yellow semi-solid, ^1H NMR (600



MHz, $CDCl_3$): δ 2.91 (t, *J* = 6.0 Hz, 2H), 2.95 (t, *J* = 6.0 Hz, 1H), 3.31-3.34 (m, 2H), 6.82 (s, 1H), 7.21-7.22 (m, 2H), 7.23-7.25 (m, 1H), 7.30-7.34 (m, 2H), 7.48-7.57 (m, 3H), 8.44-8.45 (m, 1H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 36.9, 54.1, 116.0, 124.3, 126.4, 127.6, 127.8, 128.6, 128.9, 129.1, 131.3, 132.5, 137.6, 138.5, 163.3, 178.6; IR $(KBr)_{vmax}$ 1165, 1333, 1403, 1455, 1503, 1610, 2870, 2930, 2955, 3246 cm^{-1}; HRMS (ESI) Calcd For $C_{17}H_{16}NOS_2$ 314.0668 ($M + H^+$); Found 314.0670.

2-((benzylamino)thio)-7-chloro-4H-thiochromen-4-one (4g): Yellow semi-solid, ^1H NMR



(600 MHz, $CDCl_3$): δ 3.26 (t, *J* = 6.0 Hz, 1H), 4.20 (d, *J* = 6.0 Hz, 2H), 6.84 (s, 1H), 7.32-7.35 (m, 1H), 7.36-7.40 (m, 4H), 7.44-7.46 (m, 1H), 7.58 (s, 1H), 8.39 (d, *J* = 6.0 Hz, 1H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 57.1, 114.3, 116.4, 125.8, 128.4, 128.5, 129.0, 129.6, 130.5, 138.0, 138.3, 138.9, 139.5, 162.9, 177.8; IR $(KBr)_{vmax}$ 1120, 1167, 1398, 1325, 1459, 1586, 1598, 2856, 2928, 2969, 3221 cm^{-1}; HRMS (ESI) Calcd For $C_{16}H_{13}ClNOS_2$ 334.0122 ($M + H^+$); Found 334.0119.

7-chloro-2-(((2-chlorobenzyl)amino)thio)-4H-thiochromen-4-one (4h): Yellow solid, Mp 104-105˚C, ^{1}H NMR (600 MHz, $CDCl_3$): δ 3.54 (t, *J* = 6.0 Hz, 1H), 4.26 (d, *J* = 6.0 Hz, 2H), 6.79 (s, 1H), 7.24-7.25 (m, 2H), 7.35-7.38 (m, 2H), 7.40-7.42 (m, 1H), 7.51 (s, 1H), 8.34 (d, *J* = 12.0 Hz, 1H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 54.9, 116.2, 125.7, 127.3, 128.4, 129.5, 129.8, 130.0, 130.4, 130.9, 134.1, 135.9, 137.9, 138.9, 162.9, 177.8; IR $(KBr)_{vmax}$ 1145, 1232, 1251, 1435, 1460, 1589, 1610, 2852, 2920, 2952, 3175 cm^{-1}; HRMS (ESI) Calcd For $C_{16}H_{12}Cl_2NOS_2$ 367.9732 ($M + H^+$); Found 367.9732.

7-chloro-2-(((4-fluorobenzyl)amino)thio)-4H-thiochromen-4-one (4i): White solid, Mp 133-134˚C, ^{1}H NMR (400 MHz, $CDCl_3$): δ 3.23-3.26 (m, 1H), 4.16 (d, *J* = 4.0 Hz, 2H), 6.83 (s, 1H), 7.04-7.09 (m, 2H), 7.32-7.36 (m, 2H), 7.44-7.47 (m, 1H), 7.58 (m, 1H), 8.39 (d, *J* = 8.0 Hz, 1H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 56.2, 115.8, 115.9, 116.5, 125.7, 128.5, 129.5, 130.3, 130.3, 130.5, 133.9, 133.9, 138.1, 138.9, 161.9, 162.4, 163.6, 177.8; IR $(KBr)_{vmax}$ cm^{-1}; HRMS (ESI) Calcd For $C_{16}H_{12}ClFNOS_2$ 351.9628 ($M + H^+$); Found 351.9627.

7-chloro-2-(((2,4-dimethoxybenzyl)amino)thio)-4H-thiochromen-4-one (4j): White solid, Mp 142-143˚C, ^{1}H NMR (400 MHz, $CDCl_3$): δ 3.48-3.51 (m, 1H), 3.17 (s, 3H), 3.18 (s, 3H), 4.08 (d, *J* = 4.0 Hz, 2H), 6.44-6.47 (m, 2H), 6.87 (s, 1H), 7.15 (d, *J* = 8.0 Hz, 1H), 7.44 (d, *J* = 8.0 Hz, 1H), 7.88 (s, 1H), 8.38 (d, *J* = 8.0 Hz, 1H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 52.8, 55.5, 55.6, 98.8, 104.0, 116.0, 119.3, 125.7, 128.3, 129.6, 130.4, 131.2, 137.8, 139.3, 158.8, 161.3, 163.8, 177.8; IR $(KBr)_{vmax}$ 1158, 1210, 1263, 1286, 1320, 1383, 1419, 1452, 1507, 1582, 1607, 2922, 3232 cm^{-1}; HRMS (ESI) Calcd For $C_{18}H_{17}ClNO_3S_2$ 394.0333 ($M + H^+$); Found 394.0356.

7-chloro-2-((cyclohexylamino)thio)-4H-thiochromen-4-one (4k): Yellow semi-solid, ^{1}H NMR (600 MHz, $CDCl_3$): δ 1.13-1.31 (m, 7H), 1.60-1.63 (m, 1H), 1.75-1.78 (m, 2H), 2.04-2.06 (m, 2H), 2.79-2.83 (m, 1H), 2.88-2.89 (m, 1H), 6.83 (s, 1H), 7.42-7.44 (m, 1H), 7.56 (s, 1H), 8.37 (d, *J* = 12.0 Hz, 1H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 25.0, 25.8, 33.7, 60.4, 115.6, 125.8, 128.3, 129.6, 130.4, 137.8, 139.1, 164.8, 177.8; IR $(KBr)_{vmax}$ 1153,

1348, 1475, 1589, 1609, 2845, 2952, 2974 cm^{-1}; HRMS (ESI) Calcd For $C_{16}H_{19}ClNOS_2$ 340.0535 ($M + H^+$); Found 340.0525.

7-chloro-2-(((1-phenylethyl)amino)thio)-4H-thiochromen-4-one (4l): Yellow semi-solid, ^1H NMR (600 MHz, $CDCl_3$): δ 1.54 (d, *J* = 6.0 Hz, 3H), 3.47 (d, *J* = 6.0 Hz, 1H), 4.14-4.18 (m, 1H), 6.80 (s, 1H), 7.28-7.31 (m, 1H), 7.33-7.38 (m, 4H), 7.40-7.42 (m, 1H), 7.54 (s, 1H), 8.35 (d, *J* = 6.0 Hz, 1H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 22.5, 61.0, 116.1, 125.7, 126.7, 126.8, 128.1, 128.3, 128.9, 129.4, 130.3, 137.8, 138.9, 143.4, 163.5, 177.7; IR $(KBr)_{vmax}$ 1108, 1231, 1282, 1347, 1354, 1487, 1530, 1571, 1589, 2873, 2954, 2965, 3235 cm^{-1}; HRMS (ESI) Calcd For $C_{17}H_{15}ClNOS_2$ 348.0278 ($M + H^+$); Found 348.0279.

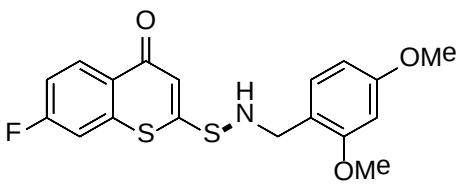
5-chloro-2-(((4-chlorobenzyl)amino)thio)-4H-thiochromen-4-one (4m): Yellow solid, Mp 116-117˚C, ^1H NMR (600 MHz, $CDCl_3$): δ 3.34-3.35 (m, 1H), 4.14 (d, *J* = 6.0 Hz, 2H), 6.77 (s, 1H), 7.28-7.29 (m, 2H), 7.32-7.33 (m, 2H), 7.37-7.40 (m, 1H), 7.45-7.48 (m, 2H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 56.2, 118.2, 125.6, 127.8, 129.1, 129.9, 130.8, 131.8, 134.1, 136.3, 136.7, 140.5, 158.8, 178.2; IR $(KBr)_{vmax}$ 1178, 1269, 1384, 1439, 1470, 1529, 1578, 1597, 2859, 2910, 2952, 3272 cm^{-1}; HRMS (ESI) Calcd For $C_{16}H_{12}Cl_2NOS_2$ 368.9732 ($M + H^+$); Found 367.9738.

2-((benzylamino)thio)-6-(trifluoromethyl)-4H-thiochromen-4-one (4n): Yellow solid, Mp 138-139˚C, ^1H NMR (400 MHz, $CDCl_3$): δ 3.30 (t, *J* = 8.0 Hz, 1H), 4.21 (d, *J* = 4.0 Hz, 2H), 6.89 (s, 1H), 7.33-7.41 (m, 5H), 7.68-7.71 (m, 1H), 7.76-7.78 (m, 1H), 8.74 (s, 1H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 57.2, 116.2, 121.0 ($^1J_{C\text{-}F}$ = 270 Hz), 122.8, 124.6, 126.2 ($^2J_{C\text{-}F}$ = 3 Hz), 126.3 (3), 126.4, 127.3 (2), 127.4 (2) ($^3J_{C\text{-}F}$ = 3 Hz), 128.4, 128.5, 129.0, 129.9 ($^4J_{C\text{-}F}$ = 33 Hz), 130.1, 130.3, 130.5, 131.3, 138.2, 141.2, 163.8, 177.5; IR $(KBr)_{vmax}$ 1129, 1169, 132, 1269, 1305, 1339, 1384, 1418, 1454, 1515, 1587, 1622, 2854, 2924, 3034, 3280 cm^{-1}; HRMS (ESI) Calcd For $C_{17}H_{13}F_3NOS_2$ 368.0385 ($M + H^+$); Found 368.0386.

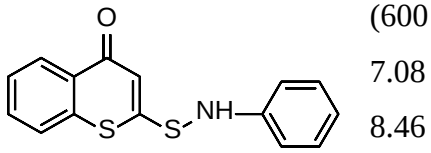
2-(((4-methoxybenzyl)amino)thio)-6-(trifluoromethyl)-4H-thiochromen-4-one (4o): Yellow solid, Mp 108-109˚C, ^1H NMR (400 MHz, $CDCl_3$): δ 3.23-3.26 (m, 1H), 3.81 (s, 3H), 4.14 (d, *J* = 8.0 Hz,

2H), 6.89-6.91(m, 3H), 7.29 (d, J = 6.0 Hz, 2H), 7.68-7.71 (m, 1H), 7.75-7.78 (m, 1H), 8.74 (s, 1H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 55.5, 56.5, 114.4, 116.2, 121.0 ($^1J_{C\text{-}F}$ = 271.5 Hz), 122.8, 124.6, 125.4, 126.2 ($^2J_{C\text{-}F}$ = 3Hz), 126.3 (4), 126.5, 127.3 (2) ($^3J_{C\text{-}F}$ = 3Hz), 127.4 (2), 129.8, 129.9, 130.1(2), 130.3(2) ($^4J_{C\text{-}F}$ = 33Hz), 130.5, 130.7, 130.9, 131.3, 141.2, 159.7, 163.9, 177.5; IR $(KBr)_{vmax}$ 1132, 1179, 1132, 1269, 1310, 1345, 1389, 1419, 1460, 1520, 1586, 1601, 2834, 2920, 3024, 3268 cm^{-1}; HRMS (ESI) Calcd For $C_{18}H_{15}F_3NO_2S_2$ 398.0491 ($M + H^+$); Found 398.0464.

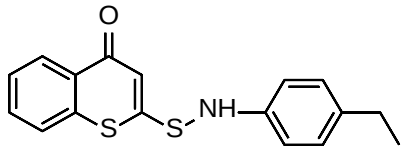
2-(((2,4-dimethoxybenzyl)amino)thio)-7-fluoro-4H-thiochromen-4-one (4p): White solid, Mp 133-134˚C, ^{1}H NMR (600 MHz, $CDCl_3$): δ 3.52 (t, J = 6.0 Hz, 1H), 3.80 (s, 3H), 3.86 (s, 3H), 4.08 (d, J = 6.0 Hz, 2H), 6.43-6.46 (m, 2H), 6.85 (s, 1H), 7.14 (d, J = 6.0 Hz, 1H), 7.18-7.20 (m, 1H), 7.23-7.25 (m, 1H), 8.45-8.47 (m, 1H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 52.8, 55.5, 55.6, 98.3, 103.9, 112.2, 112.4, 115.9, 116.0, 116.2, 119.3, 127.7, 127.8, 131.2, 131.7, 131.8, 138.9, 158.8, 161.2, 162.9, 163.6, 164.6, 177.7; IR $(KBr)_{vmax}$ cm^{-1}; HRMS (ESI) Calcd For $C_{18}H_{17}FNO_3S_2$ 378.0629 ($M + H^+$); Found 378.0630.



2-((phenylamino)thio)-4H-thiochromen-4-one (4q): Yellow solid, Mp 190-191˚C, ^{1}H NMR (600 MHz, $CDCl_3$): δ 5.37 (s, 1H), 6.93 (s,1H), 6.96-6.99 (m, 1H), 7.08 (d, J = 12.0 Hz, 1H), 7.27-7.30 (m, 2H), 7.47-7.55 (m, 4H), 8.46 (d, J = 8.0 Hz, 1H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 115.3, 116.6, 122.1, 126.4, 128.0, 128.9, 129.7, 131.1, 131.5, 137.2, 145.2, 161.6, 178.7; IR $(KBr)_{vmax}$ 1103, 1132, 1174, 1225, 1284, 1336, 1384, 1419, 1437, 1494, 1518, 1557, 1583, 1597, 2853, 2922, 2959, 3184 cm^{-1}; HRMS (ESI) Calcd For $C_{15}H_{12}NOS_2$ 286.0355 ($M + H^+$); Found 286.0361.



2-(((4-ethylphenyl)amino)thio)-4H-thiochromen-4-one (4r): Brown semi-solid, ^{1}H NMR (600 MHz, $CDCl_3$): δ 1.20 (t, J = 12.0 Hz, 3H), 2.57-2.61 (m, 2H), 5.20 (s, 1H), 6.92 (s, 1H), 7.00 (d, J = 12.0 Hz, 2H), 7.11 (d, J = 12.0 Hz, 2H), 7.48-7.51 (m, 2H), 7.52-7.55 (m, 1H), 8.45-8.47 (m, 1H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 15.9, 28.2, 114.3, 115.3, 116.4, 126.4, 127.9, 128.8, 128.9, 131.1, 131.4, 137.3, 138.1, 142.9, 162.2, 178.7; IR $(KBr)_{vmax}$ 1101, 1128, 1229,



1331, 1377, 1438, 1462, 1509, 1525, 1561, 1586, 1607, 2955, 2924, 2955, 3191 cm^{-1}; HRMS (ESI) Calcd For $C_{17}H_{16}NOS_2$ 314.0668 ($M + H^+$); Found 314.0668.

2-(((4-chlorophenyl)amino)thio)-4H-thiochromen-4-one (4s): Brown solid, Mp 70-71˚C, ^1H NMR (600 MHz, $CDCl_3$): δ 5.59 (s, 1H), 6.90 (s, 1H), 7.00-7.02 (d, *J* = 12.0 Hz, 2H), 7.22 (d, *J* = 6.0 Hz, 2H), 7.47-7.51 (m, 2H), 7.53-7.56 (m, 1H), 8.45 (d, *J* = 12.0 Hz, 1H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 116.5, 116.8, 126.4, 128.1, 128.9, 131.1, 129.6, 131.6, 137.0, 143.9, 160.7, 178.6; IR $(KBr)_{\nu max}$ 1131, 1171, 1231, 1281, 1326, 1382, 1437, 1466, 1488, 1527, 1559, 1584, 1604, 2853, 2923, 2957, 3054, 3198 cm^{-1}; HRMS (ESI) Calcd For $C_{15}H_{11}ClNOS_2$ 319.9965 ($M + H^+$); Found 319.9964.

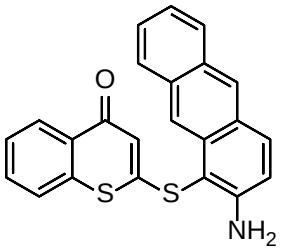
2-(((4-bromophenyl)amino)thio)-4H-thiochromen-4-one (4t): Yellow solid, Mp 105-106˚C, ^1H NMR (600 MHz, $CDCl_3$): δ 5.71 (s, 1H), 6.90 (s, 1H), 6.96 (d, *J* = 12.0 Hz, 2H), 7.34 (d, *J* = 12.0 Hz, 2H), 7.46-7.54 (m, 3H), 8.45-8.46 (m, 1H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 114.3, 116.8, 116.9, 126.4, 128.1, 128.9, 131.1, 131.6, 132.5, 137.0, 144.4, 160.8, 178.7; IR $(KBr)_{\nu max}$ 1129, 1221, 12832, 1334, 1384, 1437, 1466, 1520, 1557, 1587, 2853, 2924, 2955, 3066, 3199 cm^{-1}; HRMS (ESI) Calcd For $C_{15}H_{11}BrNOS_2$ 363.9460 ($M + H^+$); Found 363.9452.

2-(((4-fluorophenyl)amino)thio)-4H-thiochromen-4-one (4u): Yellow solid, Mp 154-155˚C, ^1H NMR (600 MHz, $CDCl_3$): δ 5.6 (s, 1H), 6.91 (s, 1H), 6.95-6.98 (m, 2H), 7.00-7.03 (m, 2H), 7.47-7.51 (m, 2H), 7.52-7.55 (m, 1H), 8.45-8.46 (m, 1H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 116.2, 116.4, 116.5, 116.6, 126.4, 128.1, 128.9, 131.1, 131.6, 137.1, 157.6, 159.2, 161.4, 178.7; IR $(KBr)_{\nu max}$ 1153, 1221, 1278, 1345, 1398, 1458, 1478, 1565, 1587, 2865, 2928, 2945, 3051, 3231 cm^{-1}; HRMS (ESI) Calcd For $C_{15}H_{11}FNOS_2$ 304.0261 ($M + H^+$); 304.0261.

2-(((3-chlorophenyl)amino)thio)-4H-thiochromen-4-one (4v): Yellow solid, Mp 158-159˚C, ^1H NMR (600 MHz, $CDCl_3$): δ 5.78 (s, 1H), 6.91 (s, 1H), 6.93-6.96 (m, 1H), 7.08 (s, 1H), 7.17 (t, *J* = 6.0 Hz, 1H), 7.47-7.55 (m, 3H), 8.45-8.47 (m, 1H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 113.5, 115.3, 116.7, 122.2, 126.4, 128.1, 128.9, 130.7, 131.1, 131.6,

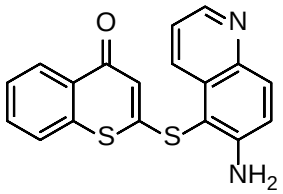
135.5, 137.0, 146.6, 160.8, 178.7; IR $(KBr)_{vmax}$ 1129, 1221, 12832, 1334, 1384, 1437, 1466, 1520, 1557, 1587, 2853, 2924, 2955, 3066, 3199 cm^{-1}; HRMS (ESI) Calcd For $C_{15}H_{11}ClNOS_2$ 319.9965 $(M + H^+)$; Found 319.9959.

2-((2-aminoanthracen-1-yl)thio)-4H-thiochromen-4-one (5a): Yellow solid, Mp 118-119˚C,



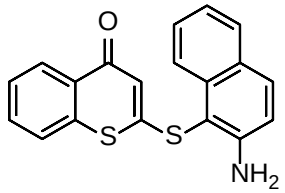
^1H NMR (600 MHz, $CDCl_3$): δ 4.97 (s, 2H), 6.99 (s, 1H), 7.07 (d, *J* = 12.0 Hz, 1H), 7.29-7.31 (m, 1H), 7.38-7.46 (m, 4H), 7.94 (t, *J* = 6.0 Hz, 2H), 8.01 (d, *J* = 12.0 Hz, 1H), 8.33 (s, 1H), 8.40-8.42 (m, 1H), 8.64 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): 119.1, 121.1, 121.7, 124.9, 125.9, 126.5, 127.8, 128.0, 128.2, 128.3, 128.9, 131.3, 134.5, 137.8, 149.8, 149.9, 155.4, 178.9; IR $(KBr)_{vmax}$ 1101, 1134, 1169, 1237, 1277, 1325, 1342, 1384, 1436, 1462, 1478, 1505, 1544, 1568, 1579, 1630, 2853, 2924, 3049, 3302, 3461 cm^{-1}; HRMS (ESI) Calcd For $C_{23}H_{16}NOS_2$ 386.0668 $(M + H^+)$; Found 386.0667.

2-((6-aminoquinolin-5-yl)thio)-4H-thiochromen-4-one (5b): Brown solid, Mp 142-143˚C, ^1H



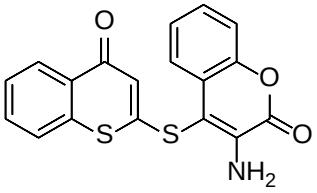
NMR (600 MHz, $CDCl_3$): δ 5.11 (s, 2H), 6.84 (s, 1H), 7.28 (s, 1H), 7.34-7.39 (m, 2H), 8.06 (d, *J* = 6.0 Hz, 1H), 8.29 (d, *J* = 6.0 Hz, 1H), 8.42 (d, *J* = 6.0 Hz, 1H), 8.68 (s, 1H); ^{13}C NMR (75 MHz, $CDCl_3$): 121.2, 121.8, 123.2, 125.9, 128.0, 128.9, 130.7, 131.6, 131.5, 132.3, 135.2, 137.7, 147.1, 150.2, 154.6, 178.9; IR $(KBr)_{vmax}$ 1245, 1370, 1520, 1590, 2845, 2930, 3025, 3325, 3482 cm^{-1}; HRMS (ESI) Calcd For $C_{18}H_{12}ClN_2OS_2$ 337.0464 $(M + H^+)$; Found 337.0461.

2-((2-aminonaphthalen-1-yl)thio)-4H-thiochromen-4-one (5c): Off-white solid, Mp 145-

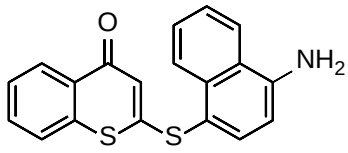


146˚C, ^1H NMR (400 MHz, $CDCl_3$): δ 4.83 (s, 2H), 6.86-6.87 (m, 1H), 7.01-7.03 (m, 1H), 7.24-7.30 (m, 2H), 7.41-7.47 (m, 3H), 7.71 (d, *J* = 8.0 Hz, 1H), 7.79 (d, *J* = 12.0 Hz, 1H), 8.16 (d, *J* = 8.0 Hz, 1H), 8.37-8.40 (m, 1H); ^{13}C NMR (75 MHz, $CDCl_3$): δ 99.1, 117.8, 121.3, 123.2, 123.4, 125.8, 127.8, 128.4, 128.6, 128.7, 128.8, 130.8, 131.3, 133.9, 136.6, 137.9, 149.9, 155.7, 178.9; IR $(KBr)_{vmax}$ 1102, 1127, 1210, 1328, 1384, 1403, 1428, 1469, 1512, 1554, 1581, 1605, 2855, 2923, 2954, 3054, 3374, 3468 cm^{-1}; HRMS (ESI) Calcd For $C_{19}H_{14}NOS_2$ 336.0512 $(M + H^+)$; Found 336.0516.

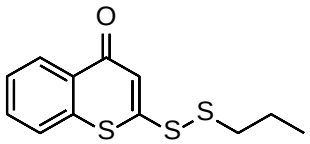
3-amino-4-((4-oxo-4H-thiochromen-2-yl)thio)-2H-chromen-2-one (5d): White solid, Mp 186-187˚C, ^{1}H NMR (400 MHz, $CDCl_3$): δ 5.42 (s, 2H), 6.99 (s, 1H), 7.27-7.31 (m, 1H), 7.33-7.36 (m, 2H), 7.39-7.41 (m, 1H), 7.47-7.56 (m, 2H), 7.73-7.74 (m, 1H), 8.43 (d, *J* = 8.0 Hz, 1H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 103.9, 116.8, 121.3, 123.4, 123.9, 125.7, 125.9, 127.6, 128.3, 129.0, 131.9, 137.4, 138.7, 147.8, 150.6, 157.2, 178.9; IR $(KBr)_{vmax}$ 1102, 1127, 1210, 1328, 1384, 1403, 1428, 1469, 1512, 1554, 1581, 1610, 2964, 3024, 3364, 3468 cm^{-1}; HRMS (ESI) Calcd For $C_{18}H_{12}NO_3S_2$ 354.0253 ($M + H^+$); Found 354.0254.



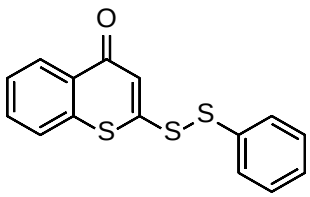
2-((4-aminonaphthalen-1-yl)thio)-4H-thiochromen-4-one (5e): Brown solid, Mp ^{1}H NMR (400 MHz, $CDCl_3$): δ 6.78-6.80 (m, 2H), 7.30-7.32 (m, 1H), 7.40-7.47 (m, 2H), 7.49-7.57 (m, 2H), 7.74 (d, *J* = 8.0 Hz, 1H), 7.86 (d, *J* = 8.0 Hz, 1H), 8.32 (d, *J* = 8.0 Hz, 1H), 8.38-8.40 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 111.3, 120.8, 121.7, 124.2, 125.8, 125.9, 126.2, 127.7, 128.2, 128.7, 130.7, 131.3, 135.8, 137.9, 138.7, 146.7, 158.8, 178.9; IR $(KBr)_{vmax}$ 1154, 1210, 1328, 1384, 1403, 1428, 1469, 1512, 1554, 1581, 1605, 2855, 2923, 2954, 3054, 3360, 3450 cm^{-1}; HRMS (ESI) Calcd For $C_{19}H_{14}NOS_2$ 336.0512 ($M + H^+$); Found 336.0517.



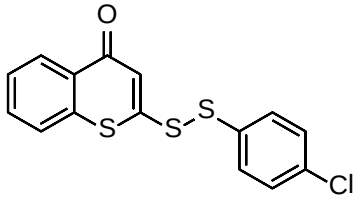
2-(propyldisulfanyl)-4H-thiochromen-4-one (6a): Yellow semi-solid, ^{1}H NMR (400 MHz, $CDCl_3$): δ 1.01 (t, *J* = 8.0 Hz, 3H), 1.70-1.79 (m, 2H), 2.38 (t, *J* = 8.0 Hz, 2H), 7.16 (s, 1H), 7.47-7.52 (m, 1H), 7.54-7.57 (m, 2H), 8.44 (d, *J* = 8.0 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 13.2, 22.3, 41.9, 113.3, 122.3, 126.2, 127.9, 128.9, 131.6, 137.7, 178.9; IR $(KBr)_{vmax}$ 1123, 1225, 1261, 1324, 1379, 1423, 1451, 1464, 1551, 1574, 1590, 1618, 2853, 2923, 2957 cm^{-1}; HRMS (ESI) Calcd For $C_{12}H_{13}OS_3$ 269.0123 ($M + H^+$); Found 269.0125.



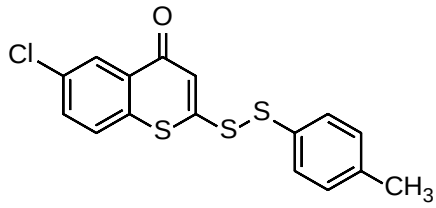
2-(phenyldisulfanyl)-4H-thiochromen-4-one (6b): Yellow semi-solid, ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.08 (s, 1H), 7.20-7.33 (m, 3H), 7.38-7.48 (m, 5H), 8.36 (d, *J* = 8.0 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 111.7, 123.3, 126.2, 128.1, 128.8, 128.9, 129.4, 129.6, 130.8, 131.7, 178.8; IR $(KBr)_{vmax}$ 1136, 1189, 1268, 1289, 1369, 1384, 1400, 1468, 1510, 1538, 1572, 1610, 2850, 2967 cm^{-1}; HRMS (ESI) Calcd For $C_{15}H_{11}OS_3$ 302.9967 ($M + H^+$); Found 302.9969.



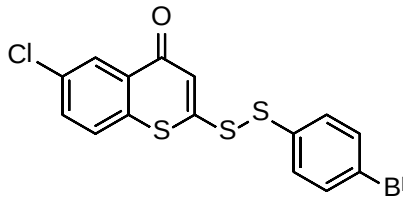
2-((4-chlorophenyl)disulfanyl)-4H-thiochromen-4-one (6c): Yellow semi-solid, ^{1}H NMR (600 MHz, $CDCl_3$): δ 7.16 (s, 1H), 7.24-7.40 (m, 2H), 7.49-7.60 (m, 5H), 8.44-8.46 (m, 1H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 123.4, 126.3, 128.3, 129.0, 129.5, 129.9, 130.6, 130.8, 131.9, 133.8, 135.2, 137.6, 154.2, 178.9; IR $(KBr)_{vmax}$ 1101, 1161, 1245, 1256, 1371, 1391, 1456, 1478, 1521, 1540, 1561, 1610, 2825, 2934 cm^{-1}; HRMS (APCI) Calcd For $C_{15}H_9ClOS_3$ 336.9577 $(M + H^+)$; Found 336.9578.



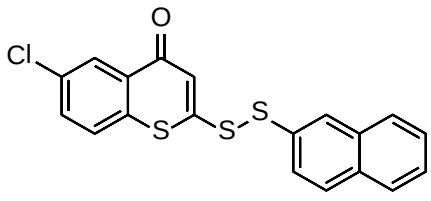
6-chloro-2-(p-tolyldisulfanyl)-4H-thiochromen-4-one (6d): Yellow solid, Mp 120-121˚C, ^{1}H NMR (600 MHz, $CDCl_3$): δ 2.34 (s, 3H), 7.15-7.17 (m, 3H), 7.46-7.47 (m, 2H), 7.50-7.51 (m, 1H), 7.53-7.55 (m, 1H), 8.42 (d, *J* = 6.0 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 21.3, 123.0, 127.7, 128.6, 130.4, 130.5, 132.1, 134.7, 135.9, 139.7, 177.7; IR $(KBr)_{vmax}$ 1104, 1142, 1181, 1260, 1281, 1312, 1384, 1397, 1451, 1490, 1507, 1527, 1582, 1610, 2853, 2923, 2955, 3024, 3086 cm^{-1}; HRMS (ESI) Calcd For $C_{16}H_{12}ClOS_3$ 350.9734 $(M + H^+)$; Found 350.9733.



2-((4-bromophenyl)disulfanyl)-6-chloro-4H-thiochromen-4-one (6e): Yellow solid, Mp 141-142˚C, ^{1}H NMR (600 MHz, $CDCl_3$): δ 7.13 (s, 1H), 7.40-7.41 (m, 2H), 7.45-7.47 (m, 3H), 7.51-7.53 (m, 1H), 8.38 (d, *J* = 6.0 Hz, 1H); ^{13}C NMR (75 MHz, $CDCl_3$): δ 122.8, 123.2, 127.7, 128.5, 130.8, 131.6, 132.2, 132.7, 134.1, 134.7, 135.5, 154.6, 177.5; IR $(KBr)_{vmax}$ 1105, 1142, 1175, 1260, 1282, 1312, 1284, 1397, 1451, 1470, 1508, 1583, 1610, 1682, 1900, 2853, 2923, 2897, 3024, 3080 cm^{-1}; HRMS (ESI) Calcd For $C_{15}H_9BrClOS_3$ 414.8682 $(M + H^+)$; Found 414.8684.



6-chloro-2-(naphthalen-2-yldisulfanyl)-4H-thiochromen-4-one (6f): Yellow semi-solid, ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.21 (s, 1H), 7.40-7.53 (m, 4H), 7.60-7.66 (m, 1H), 7.78-7.84 (m, 3H), 8.03-8.04 (m, 1H), 8.41 (d, *J* = 4.0 Hz, 1H); ^{13}C NMR (75 MHz, $CDCl_3$): δ 114.3, 122.8, 126.3, 127.2, 127.3, 127.7, 127.9, 128.1, 128.6,



128.7, 129.8, 132.1, 133.5, 134.7, 135.8, 139.4, 155.5, 177.7; IR $(KBr)_{vmax}$ 1108, 1235, 1260, 1320, 1380, 1445, 1532, 1575, 1610, 2843, 2935, 2965 cm^{-1}; HRMS (ESI) Calcd For $C_{19}H_{12}ClOS_3$ 386.9734 ($M + H^+$); Found 386.9733.

7-chloro-2-((2-chlorophenyl)disulfanyl)-4H-thiochromen-4-one (6g): Yellow semi-solid, ^1H NMR (400 MHz, $CDCl_3$): δ 7.08-7.11 (m, 1H), 7.17-7.24 (m, 2H), 7.36-7.44 (m, 2H), 7.50 (s,1H), 7.60 (d, *J* = 8.0 Hz, 1H), 8.30 (d, *J* = 8.0 Hz, 1H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 123.6, 125.7, 128.0, 128.9, 129.0, 129.5, 130.4, 130.5, 133.3, 133.5, 138.7, 138.9, 153.8, 178.1; IR $(KBr)_{vmax}$ 1146, 1263, 1286, 1314, 1377, 1401, 1463, 1522, 1583, 1618, 2853, 2924, 2955 cm^{-1}; HRMS (ESI) Calcd For $C_{15}H_9Cl_2OS_3$ 370.9187 ($M + H^+$); Found 370.9191.

7-chloro-2-((2-chlorobenzyl)disulfanyl)-4H-thiochromen-4-one (6h): Yellow semi-solid, ^1H NMR (600 MHz, $CDCl_3$): δ 4.09 (s, 2H), 6.93 (s, 1H), 7.07-7.08 (m, 2H), 7.21-7.25 (m, 2H), 7.35-7.37 (m, 1H), 7.42 (s, 1H), 8.26 (d, *J* = 12.0 Hz, 1H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 41.9, 122.6, 125.4, 126.9, 128.6, 128.8, 129.8, 129.9, 130.3, 131.9, 133.2, 134.7, 138.4, 138.9, 155.4, 177.8; IR $(KBr)_{vmax}$ 1104, 1142, 1181, 1260, 1281, 1312, 1384, 1397, 1451, 1490, 1507, 1527, 1582, 1610, 2853, 2923, 2955, 3024, 3086 cm^{-1}; HRMS (ESI) Calcd For $C_{16}H_{11}Cl_2OS_3$ 384.9344 ($M + H^+$); Found 384.9328.

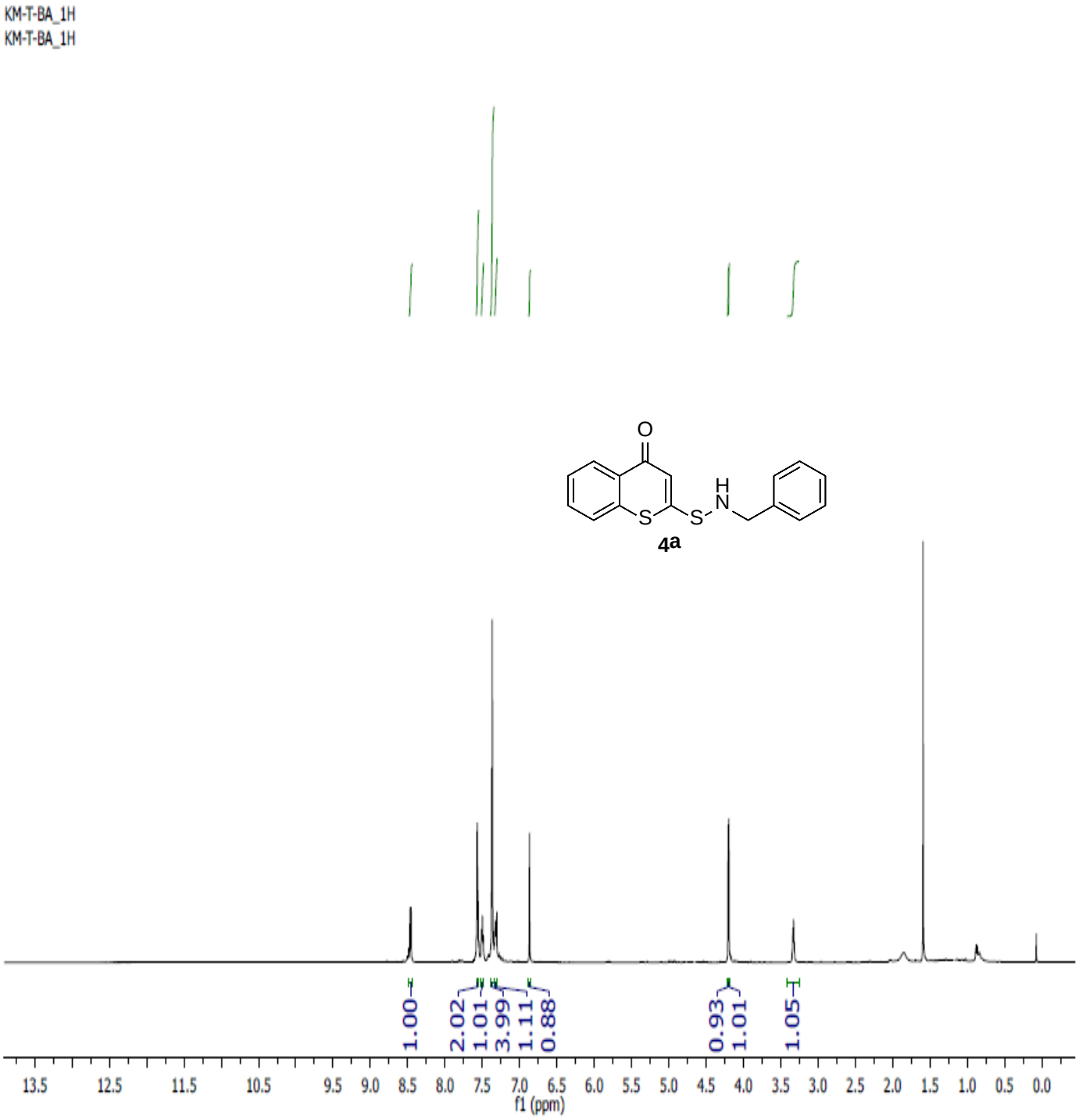
2-((2-bromophenyl)disulfanyl)-6-(trifluoromethyl)-4H-thiochromen-4-one (6i): Yellow semi-solid, ^1H NMR (400 MHz, $CDCl_3$): δ 7.14-7.17 (m, 1H), 7.21-7.22 (m, 1H), 7.32-7.35 (m, 1H), 7.56-7.58 (m, 1H), 7.64 (d, *J* = 8.0 Hz, 2H), 7.76-7.77 (m, 1H), 8.70 (s,1H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 120.8 ($^1J_{C\text{-}F}$ = 271.5 Hz), 122.5, 122.6, 123.5, 124.4, 126.0, 126.2, 126.3 ($^2J_{C\text{-}F}$ = 3 Hz), 126.4 (3), 127.3, 127.8 ($^3J_{C\text{-}F}$ = 3 Hz), 127.9 (3), 128.4, 128.7, 129.5, 130.2 ($^4J_{C\text{-}F}$ = 33 Hz), 130.4, 130.6, 130.7, 130.9, 133.6, 135.3, 141.0, 154.5, 177.7; IR $(KBr)_{vmax}$ 1110, 1139, 1171, 1252, 1284, 1332, 1389, 1397, 1461, 1496, 1510, 1522, 1598, 1602, 2843, 2930, 2965, 3029, 3091 cm^{-1}; HRMS (ESI) Calcd For $C_{16}H_9BrF_3OS_3$ 448.8946 ($M + H^+$); Found 448.8937.

2-((2-bromophenyl)disulfanyl)-7-fluoro-4H-thiochromen-4-one (6j): Yellow semi-solid, ^{1}H NMR (600 MHz, $CDCl_3$): δ 7.11-7.21 (m, 4H), 7.31-7.35 (m, 1H), 7.55-7.64 (m, 2H), 8.42-8.46 (m, 1H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 112.3, 112.4, 116.6, 116.8, 122.3, 123.5, 127.2, 128.3, 128.6, 129.3, 131.9 (2), 133.5, 135.4, 139.6, 139.7, 153.4, 163.3, 164.9, 177.8, 177.9; IR $(KBr)_{vmax}$ 1156, 1229, 12865, 1323, 1389, 1401, 1476, 1519, 1587, 1616, 2859, 2930, 2965 cm^{-1}; HRMS (ESI) Calcd For $C_{15}H_9BrFOS_3$ 398.8978 ($M + H^+$); Found 398.8984.

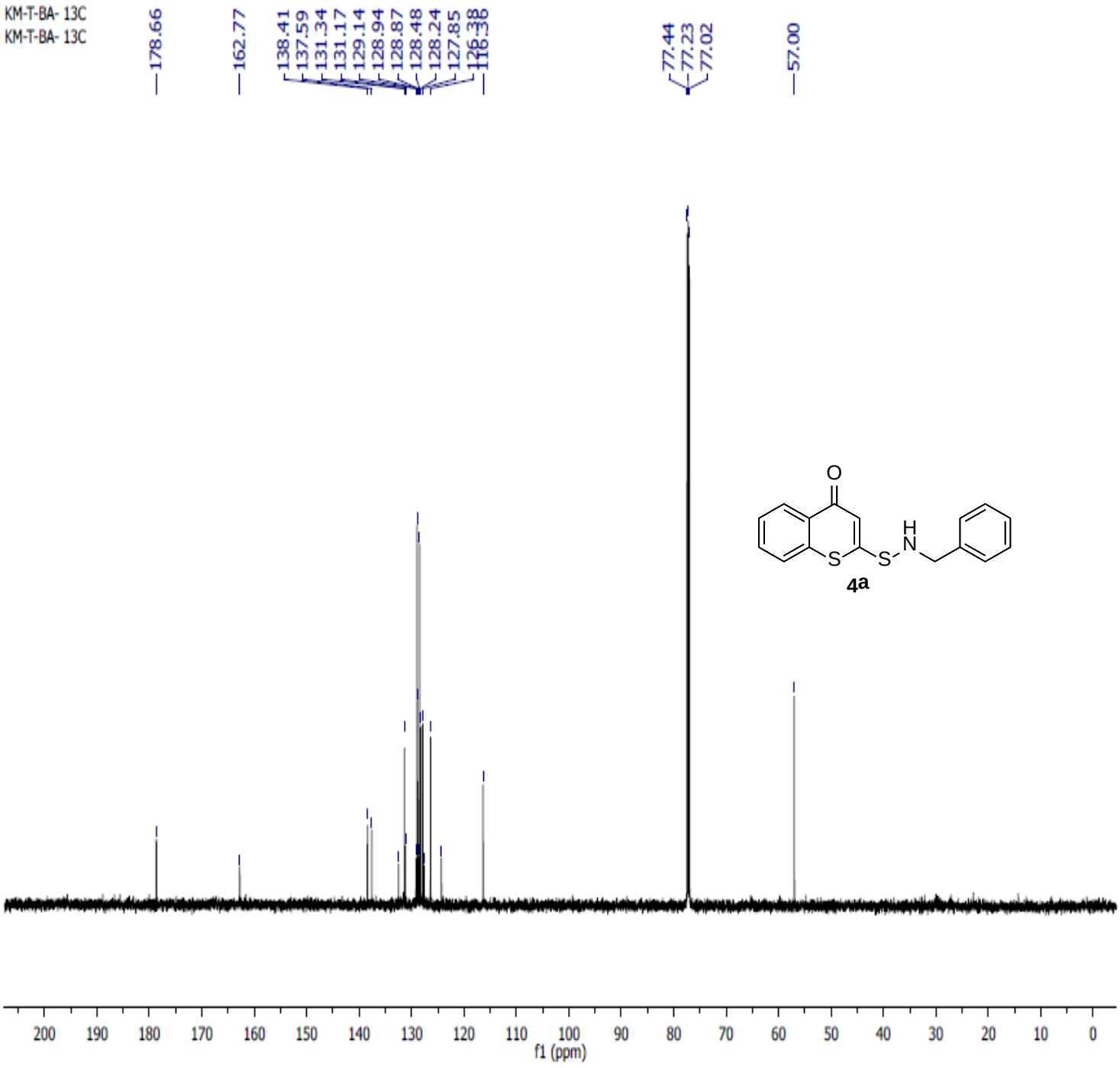
N-benzyl-4-oxo-4H-thiochromene-2-sulfonamide (7a): White solid, Mp 175-176˚C, ^{1}H NMR (600 MHz, $CDCl_3$): δ 4.05 (d, *J* = 6.0 Hz, 2H), 6.96-6.98 (m, 1H), 7.03 (d, *J* = 6.0 Hz, 2H), 7.09-7.11 (m, 2H), 7.23-7.24 (m, 1H), 7.40 (t, *J* = 6.0 Hz, 1H), 7.47-7.52 (m, 2H), 8.24 (d, *J* = 12.0 Hz, 1H), 8.45 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 47.3, 125.6, 127.1, 127.6, 127.8, 128.2, 128.3, 128.4, 132.3, 136.2, 153.6, 180.0; IR $(KBr)_{vmax}$ 1002, 1025, 1128, 1320, 1340, 1435, 1455, 1587, 1630, 1636, 2921, 3265 cm^{-1}; HRMS (ESI) Calcd For $C_{16}H_{14}NO_3S_2$ 332.0410 ($M + H^+$); Found 332.0419.

7. **Copies of ^{1}H NMR, ^{13}C NMR and HRMS spectra of all Compounds**

^{1}HNMR spectra of compound: 4a

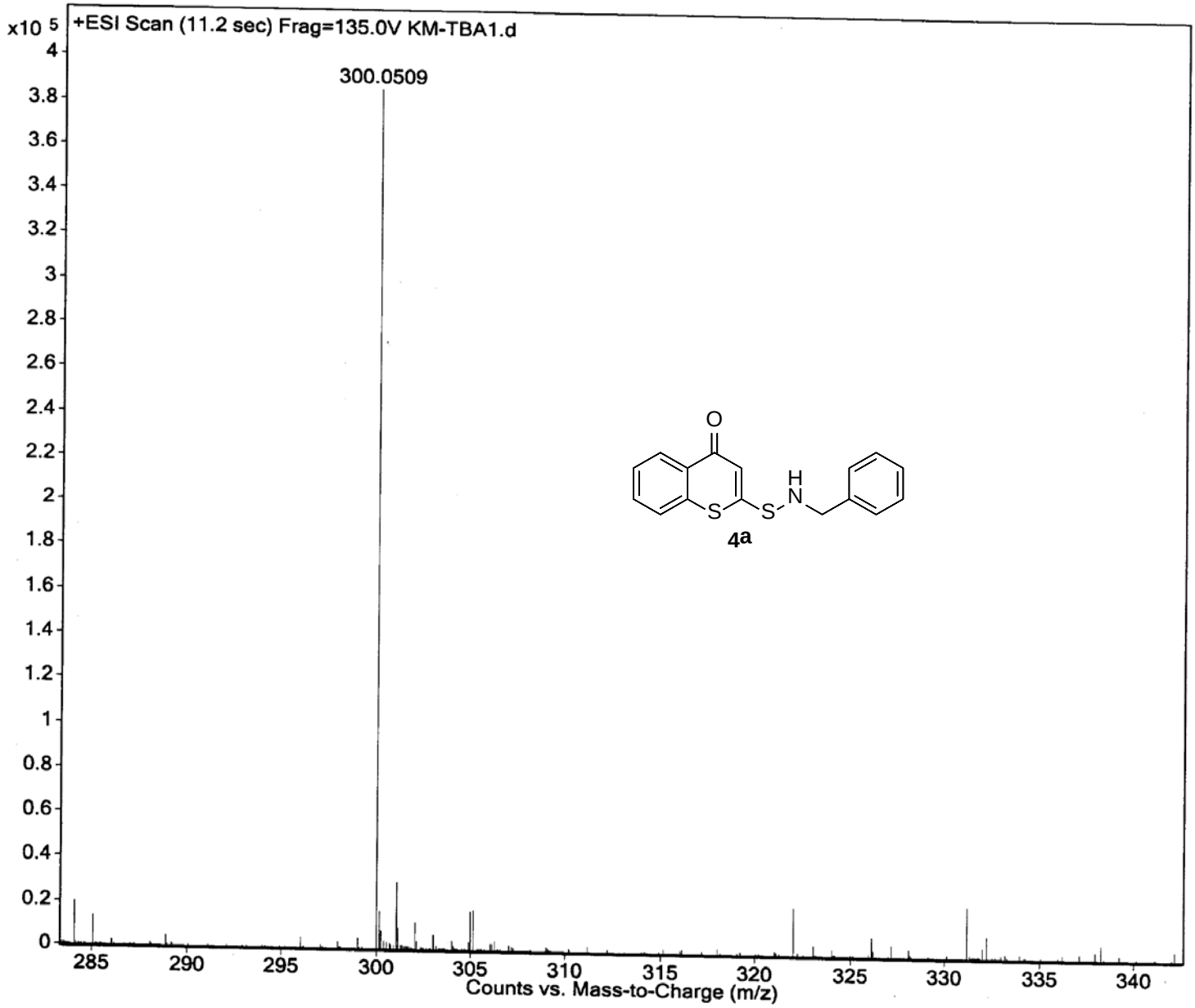


^{13}CNMR spectra of compound: 4a



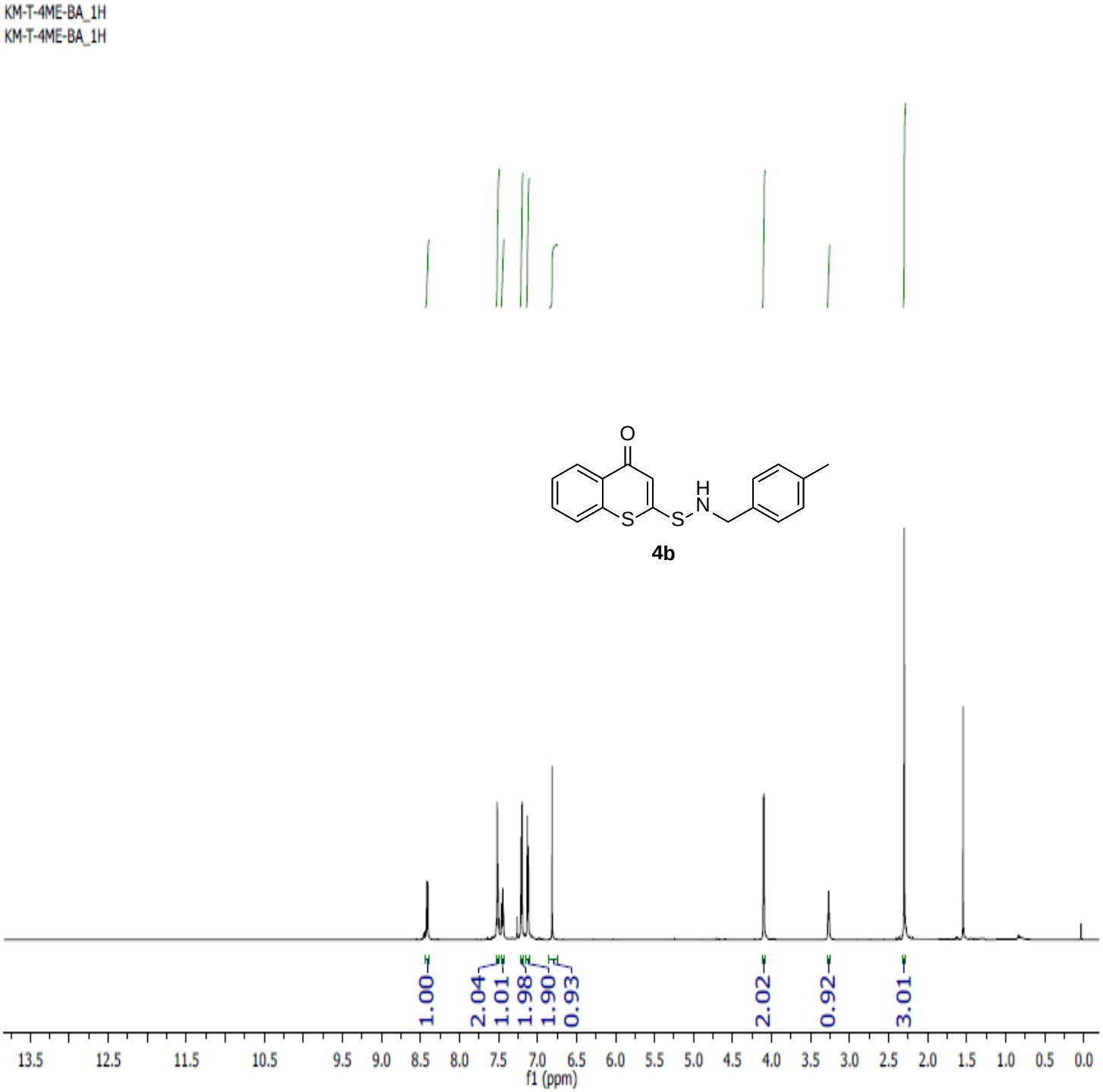
HRMS spectra of compound: 4a

Sample Name	Unavailable	**Position**	Unavailable	**Instrument Name**	Unavailable	**User Name**	Unavailable
Inj Vol	Unavailable	**InjPosition**	Unavailable	**SampleType**	Unavailable	**IRM Calibration Status**	All Ions Missed
Data Filename	KM-TBA1.d	**ACQ Method**		**Comment**	Sample information is unavailable	**Acquired Time**	Unavailable

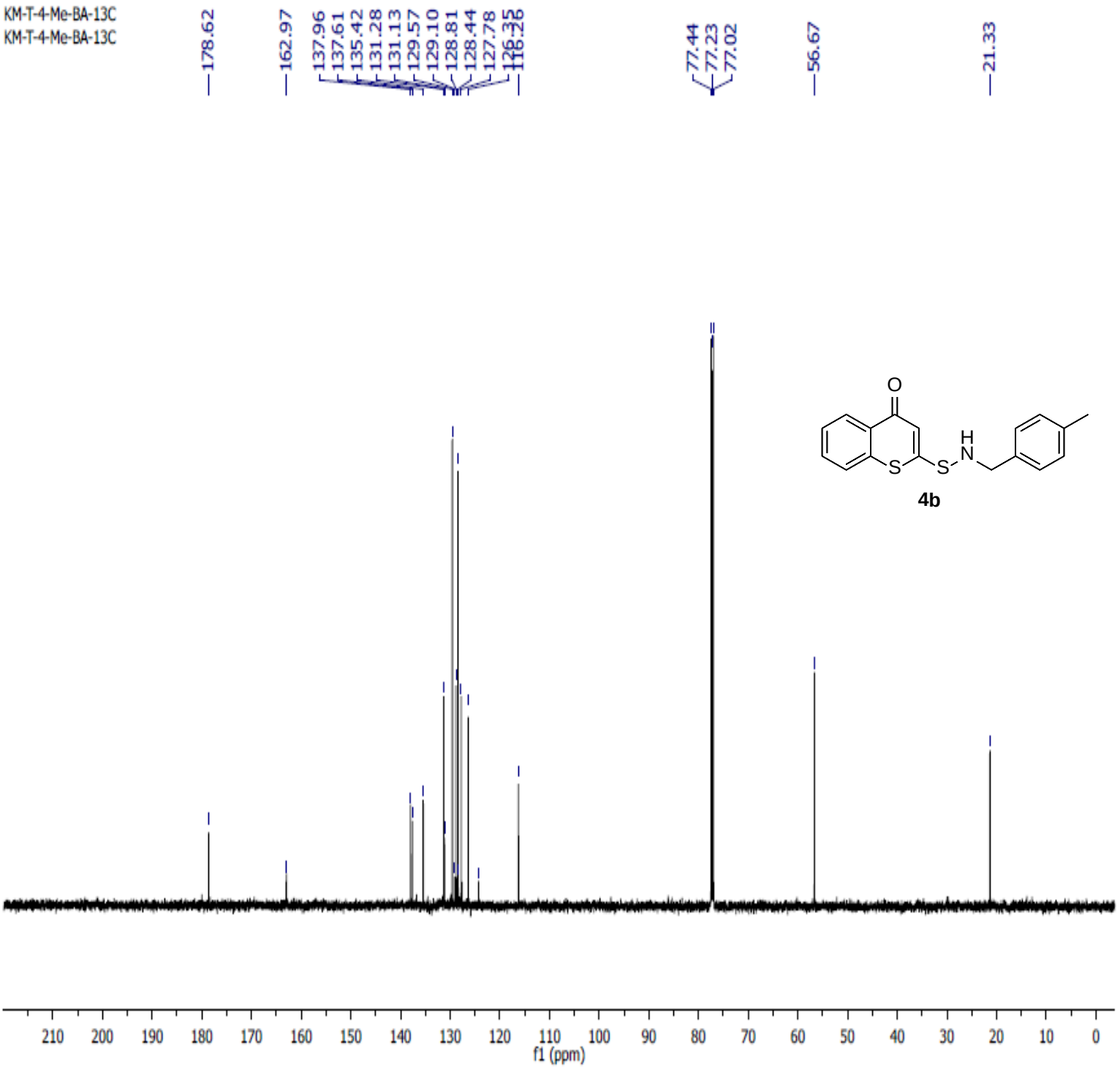


4a

^{1}HNMR spectra of compound: 4b

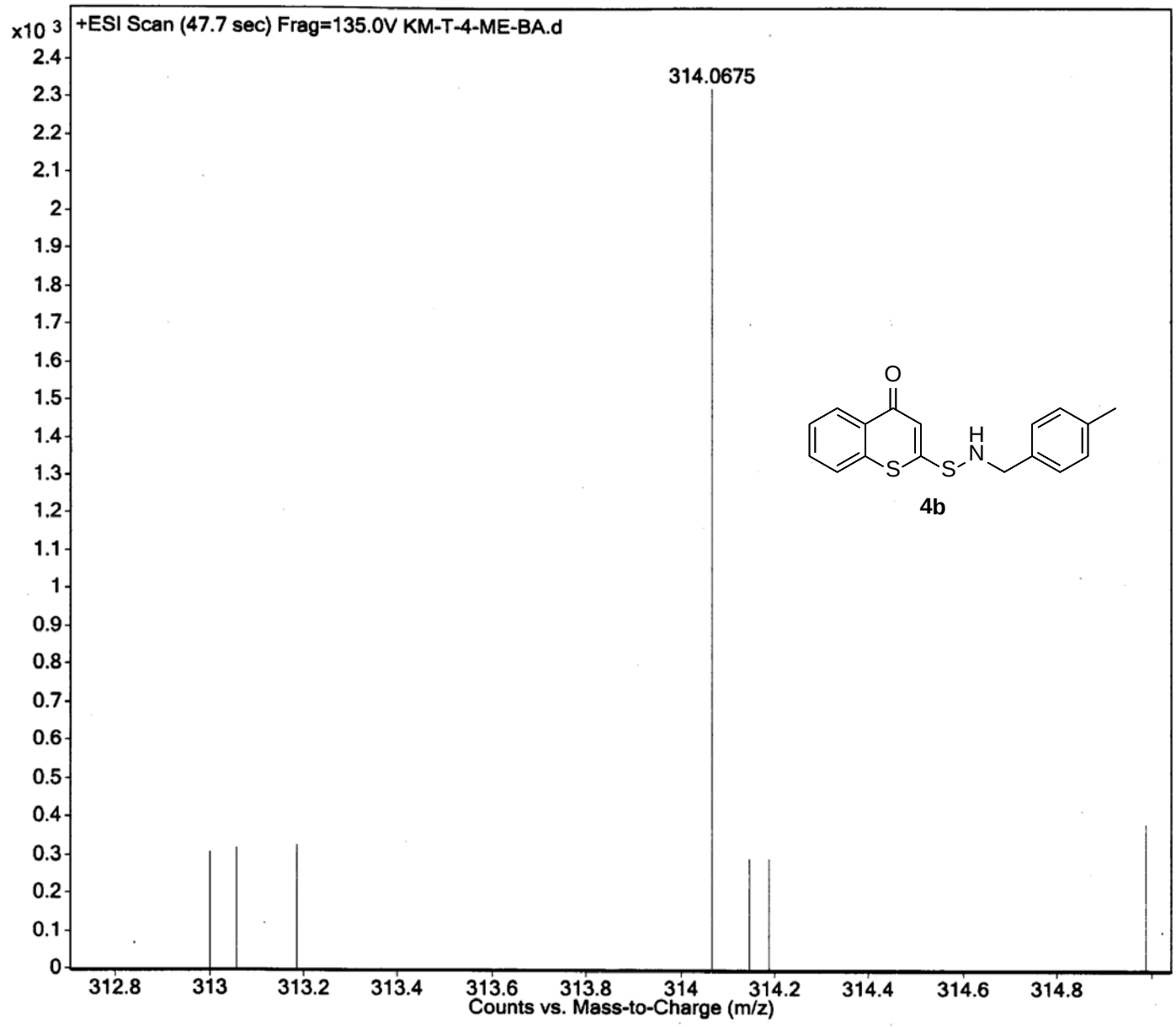


^{13}CNMR spectra of compound: 4b

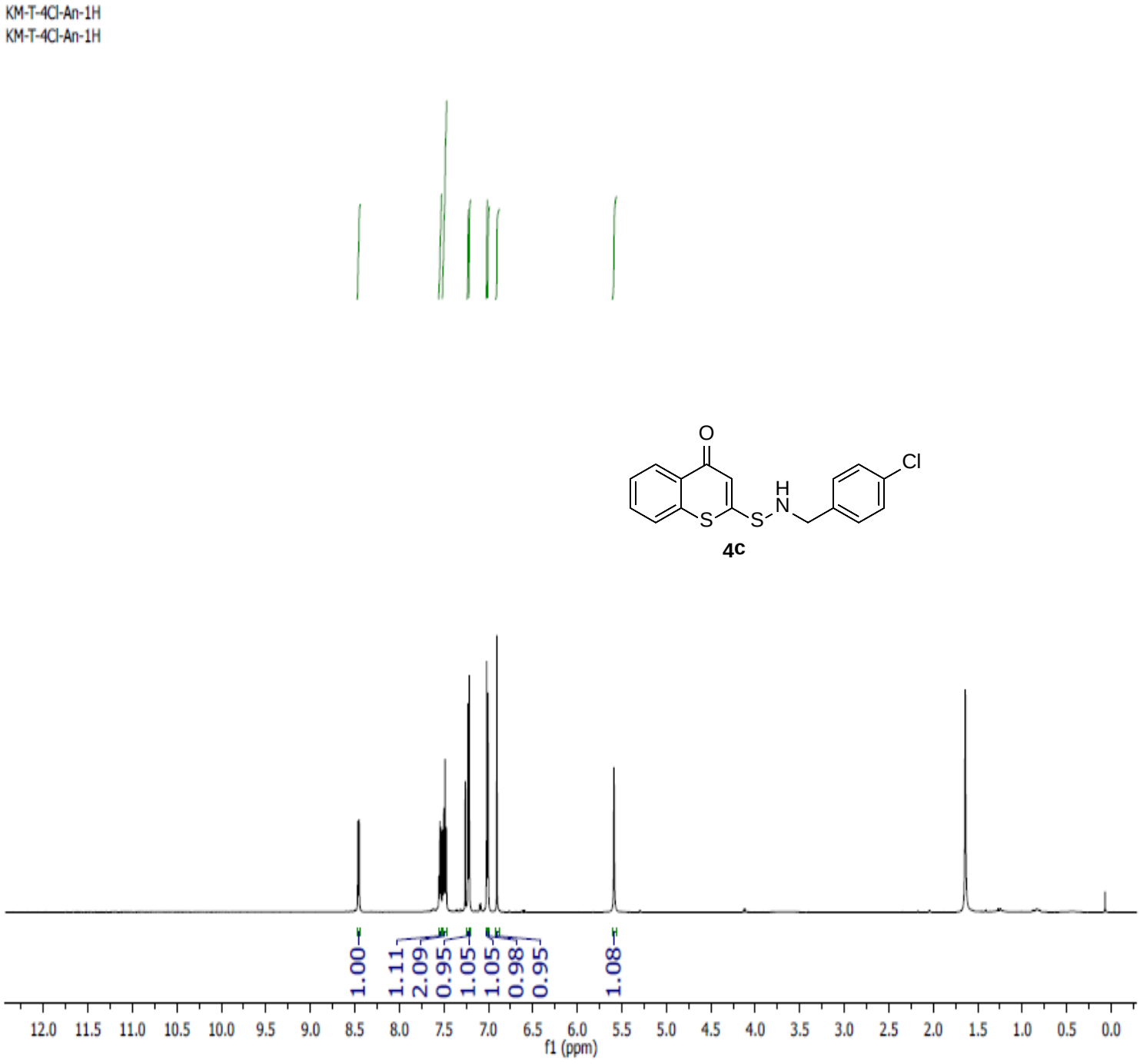


HRMS spectra of compound: 4b

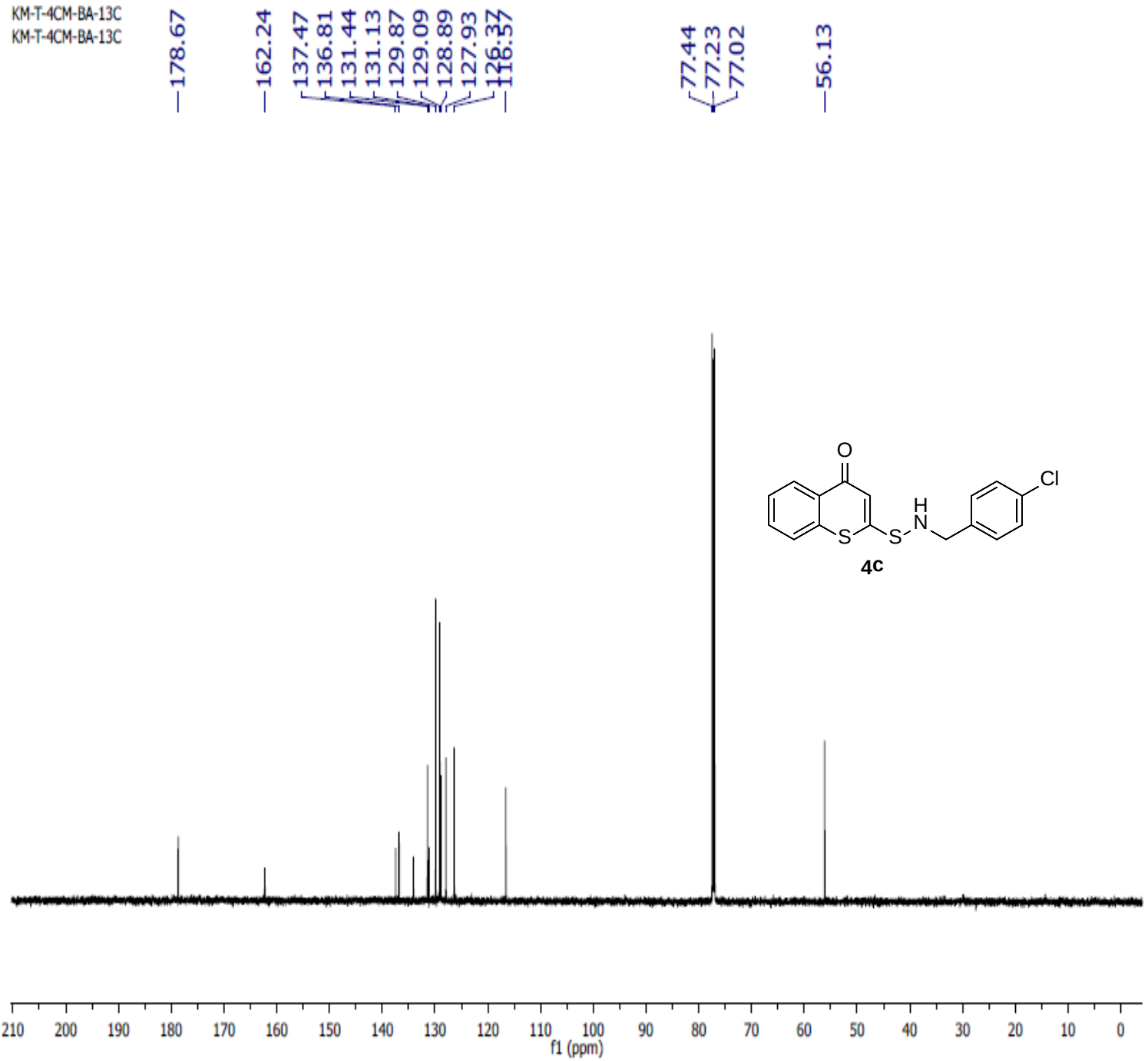
Sample Name	KM-T-4-ME-BA	**Position**	Vial 1	**Instrument Name**	Instrument 1	**User Name**	
Inj Vol	0	**InjPosition**		**SampleType**	Sample	**IRM Calibration Status**	All Ions Missed
Data Filename	KM-T-4-ME-BA.d	**ACQ Method**		**Comment**		**Acquired Time**	1/6/2017 4:21:33 PM



[1]HNMR spectra of compound: 4c

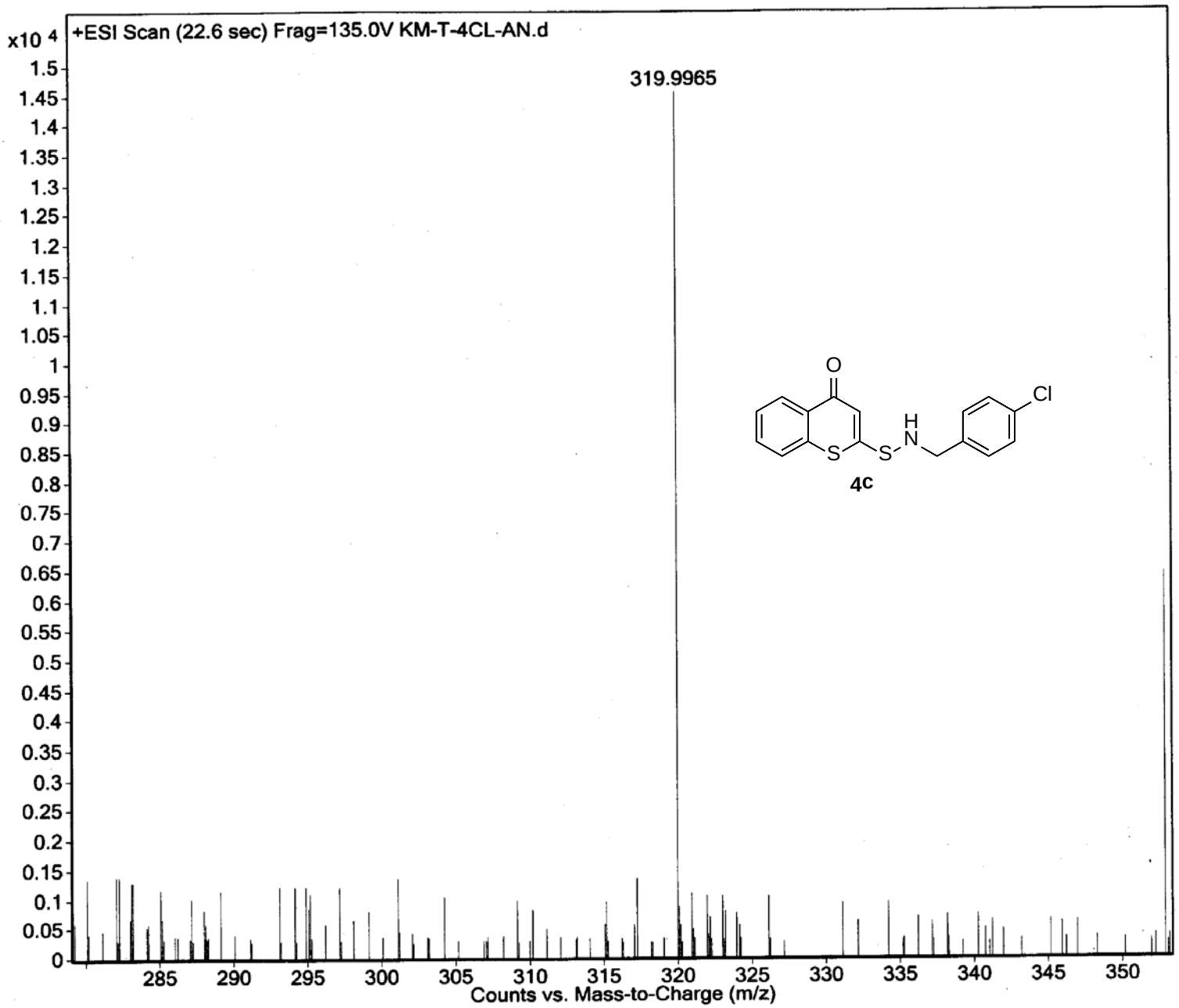


^{13}CNMR spectra of compound: 4c



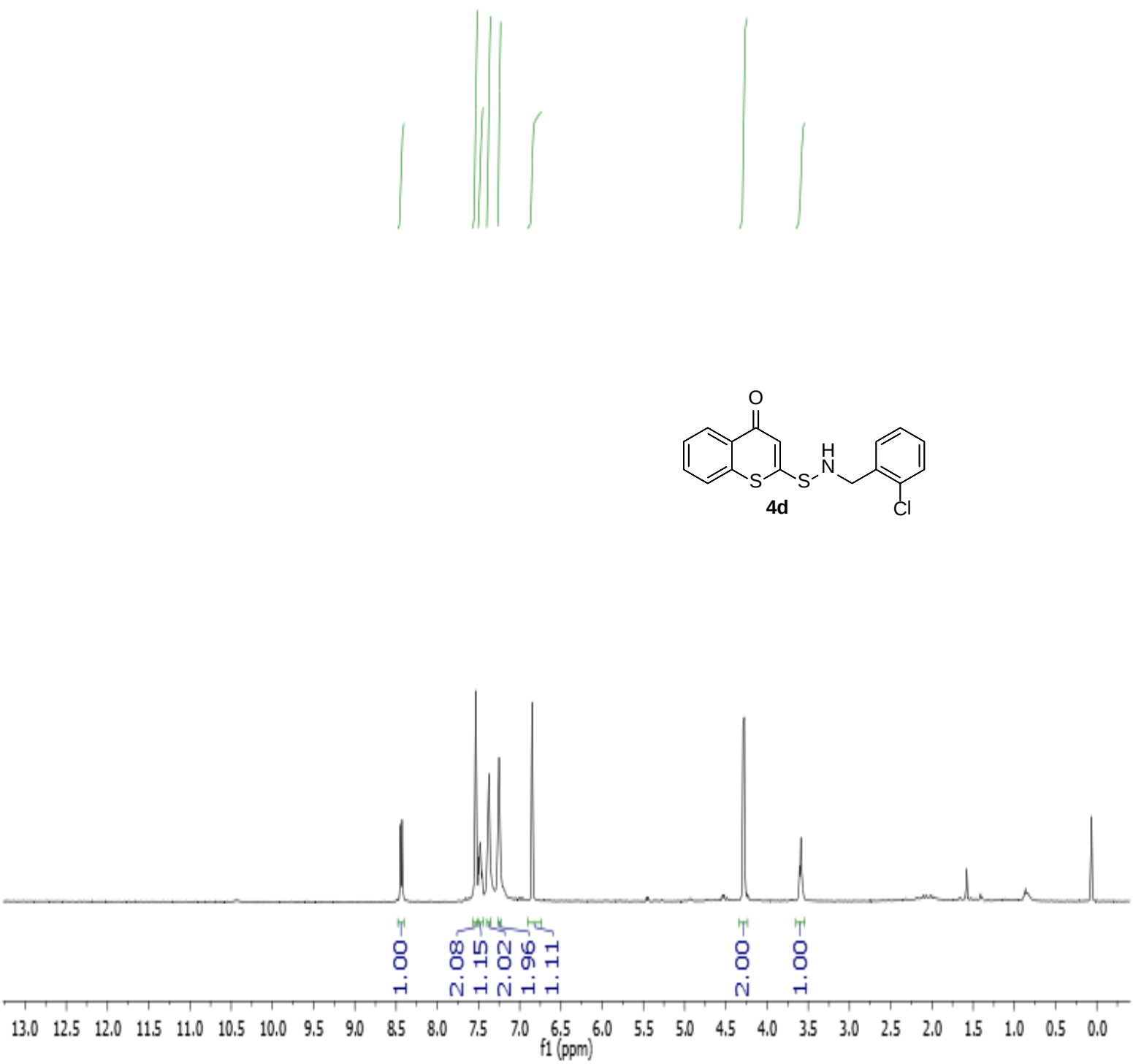
HRMS spectra of compound: 4c

Sample Name	Unavailable	**Position**	Unavailable	**Instrument Name**	Unavailable	**User Name**	Unavailable
Inj Vol	Unavailable	**InjPosition**	Unavailable	**SampleType**	Unavailable	**IRM Calibration Status**	All Ions Missed
Data Filename	KM-T-4CL-AN.d	**ACQ Method**		**Comment**	Sample information is unavailable	**Acquired Time**	Unavailable

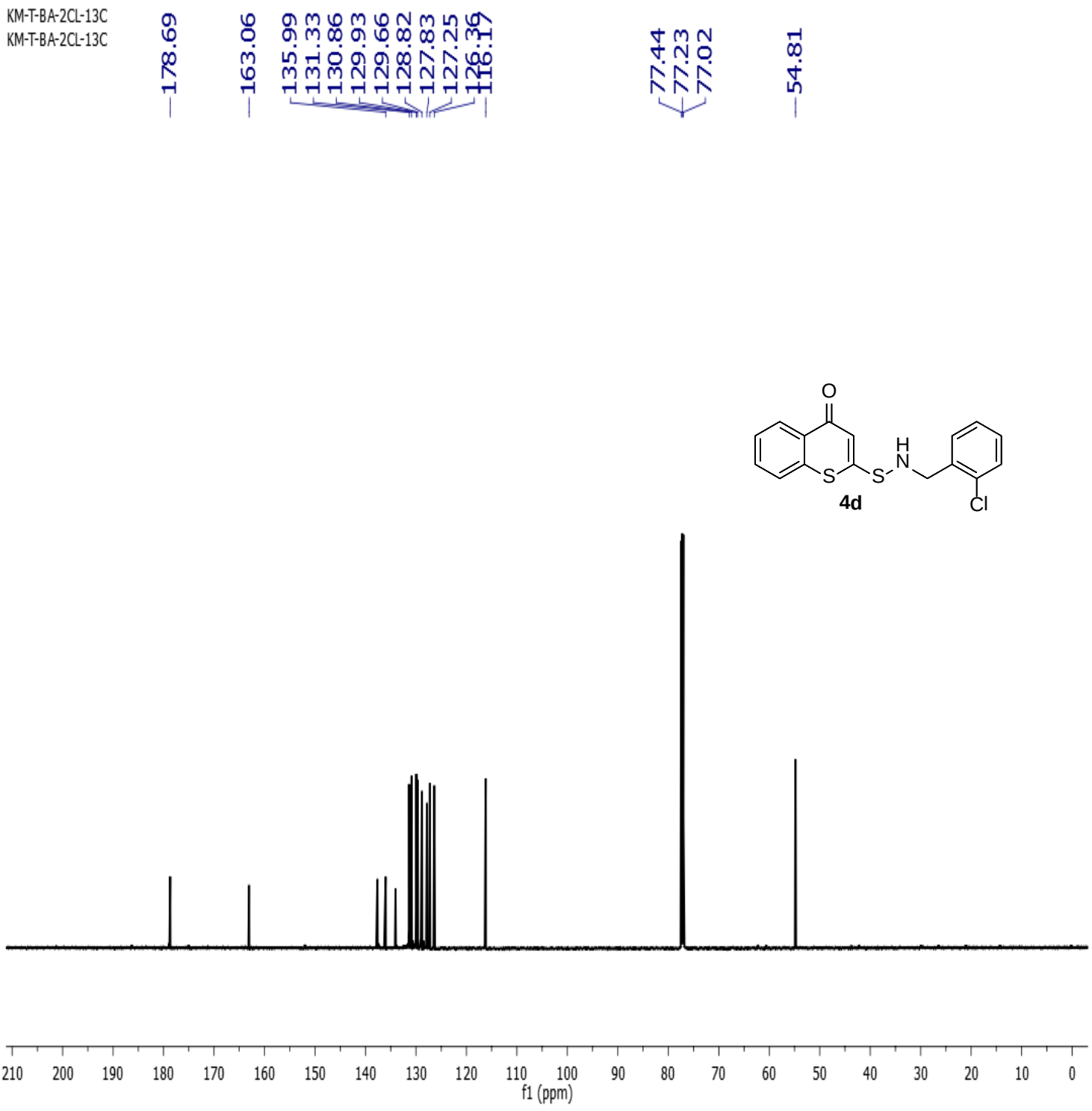


[1]HNMR spectra of compound: 4d

KM-T-2Cl-BA-1H
KM-T-2Cl-BA-1H

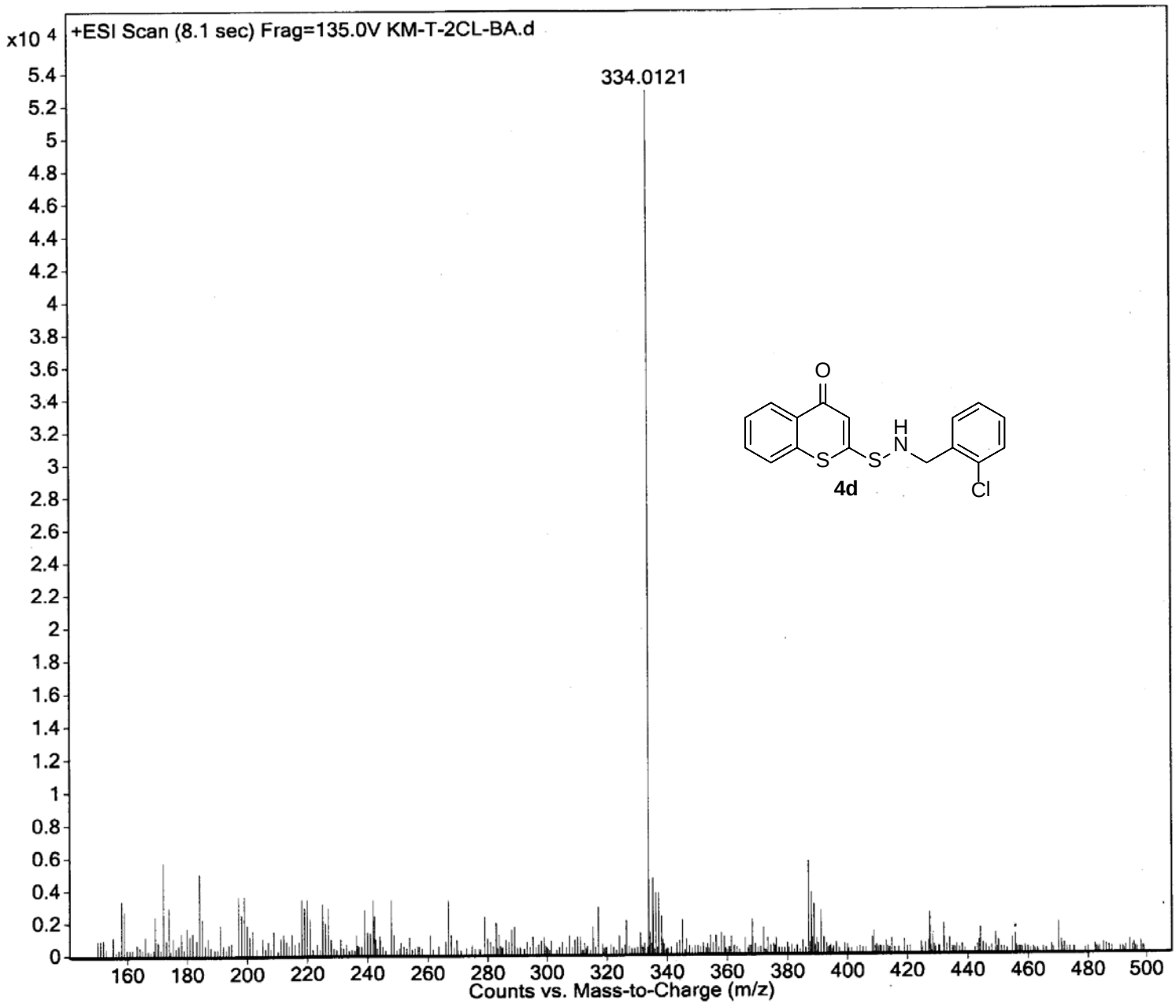


^{13}CNMR spectra of compound: 4d

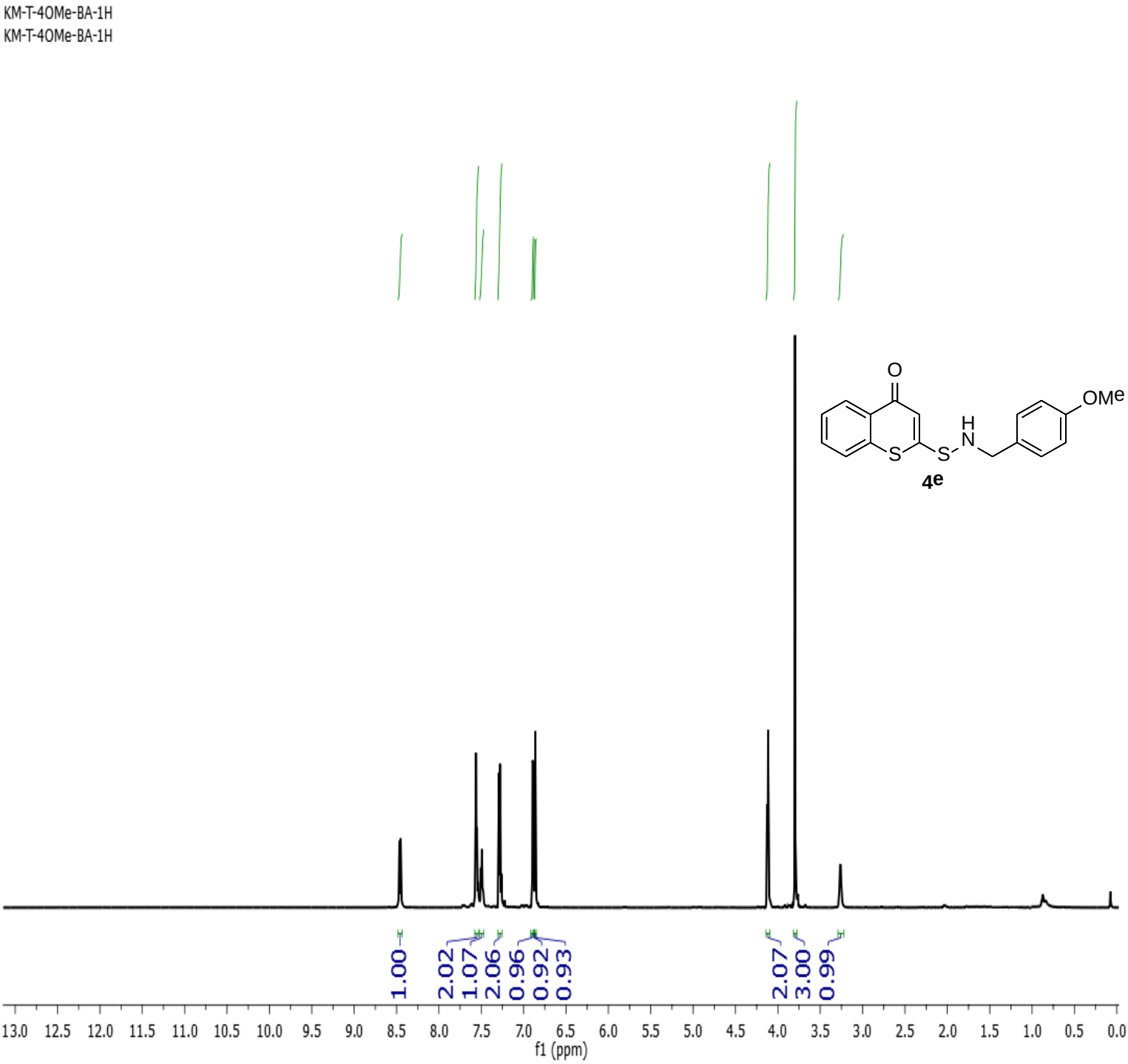


HRMS spectra of compound: 4d

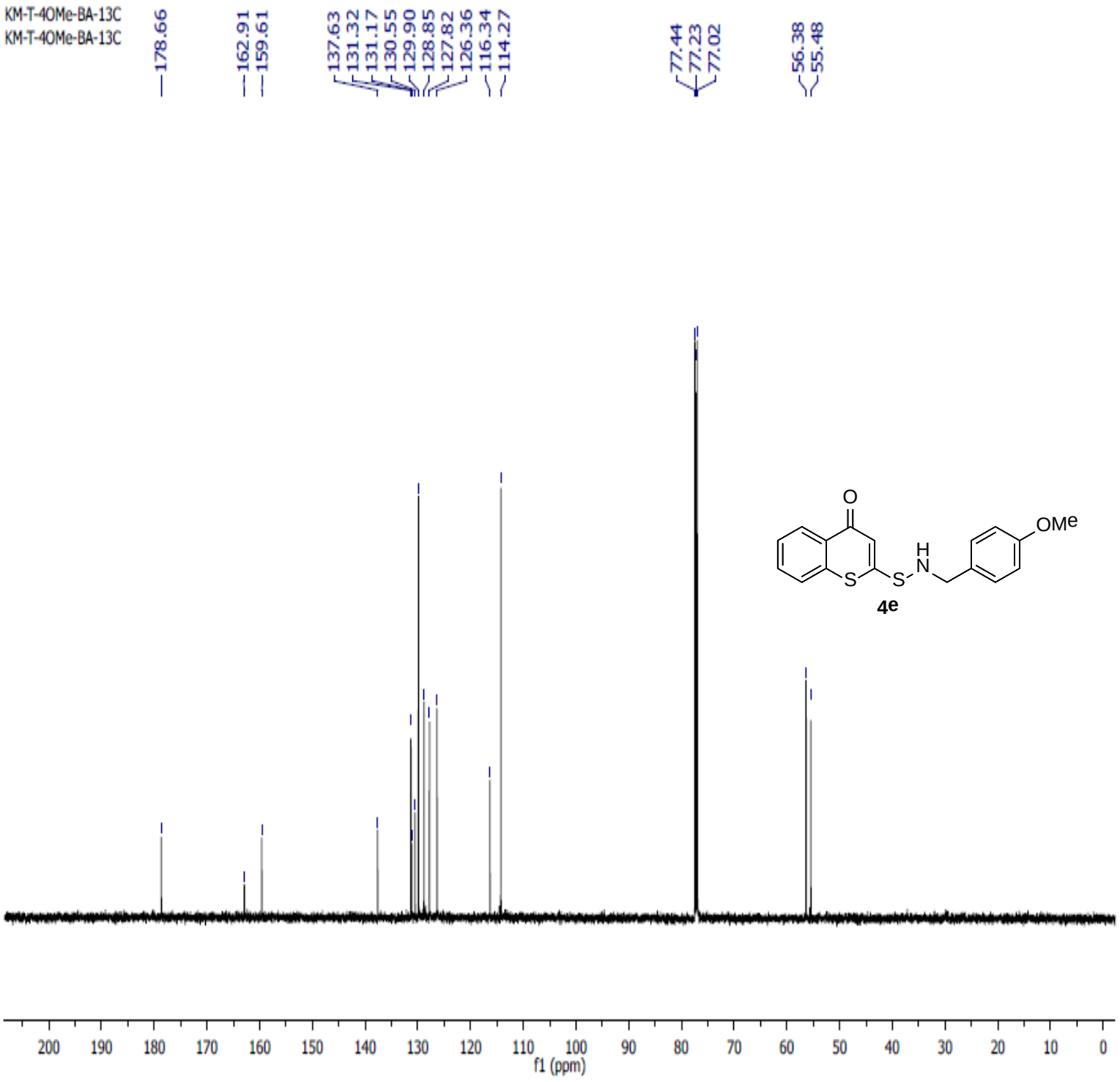
Sample Name	Unavailable	**Position**	Unavailable	**Instrument Name**	Unavailable	**User Name**	Unavailable
Inj Vol	Unavailable	**InjPosition**	Unavailable	**SampleType**	Unavailable	**IRM Calibration Status**	All Ions Missed
Data Filename	KM-T-2CL-BA.d	**ACQ Method**		**Comment**	Sample information is unavailable	**Acquired Time**	Unavailable



[1]HNMR spectra of compound: 4e

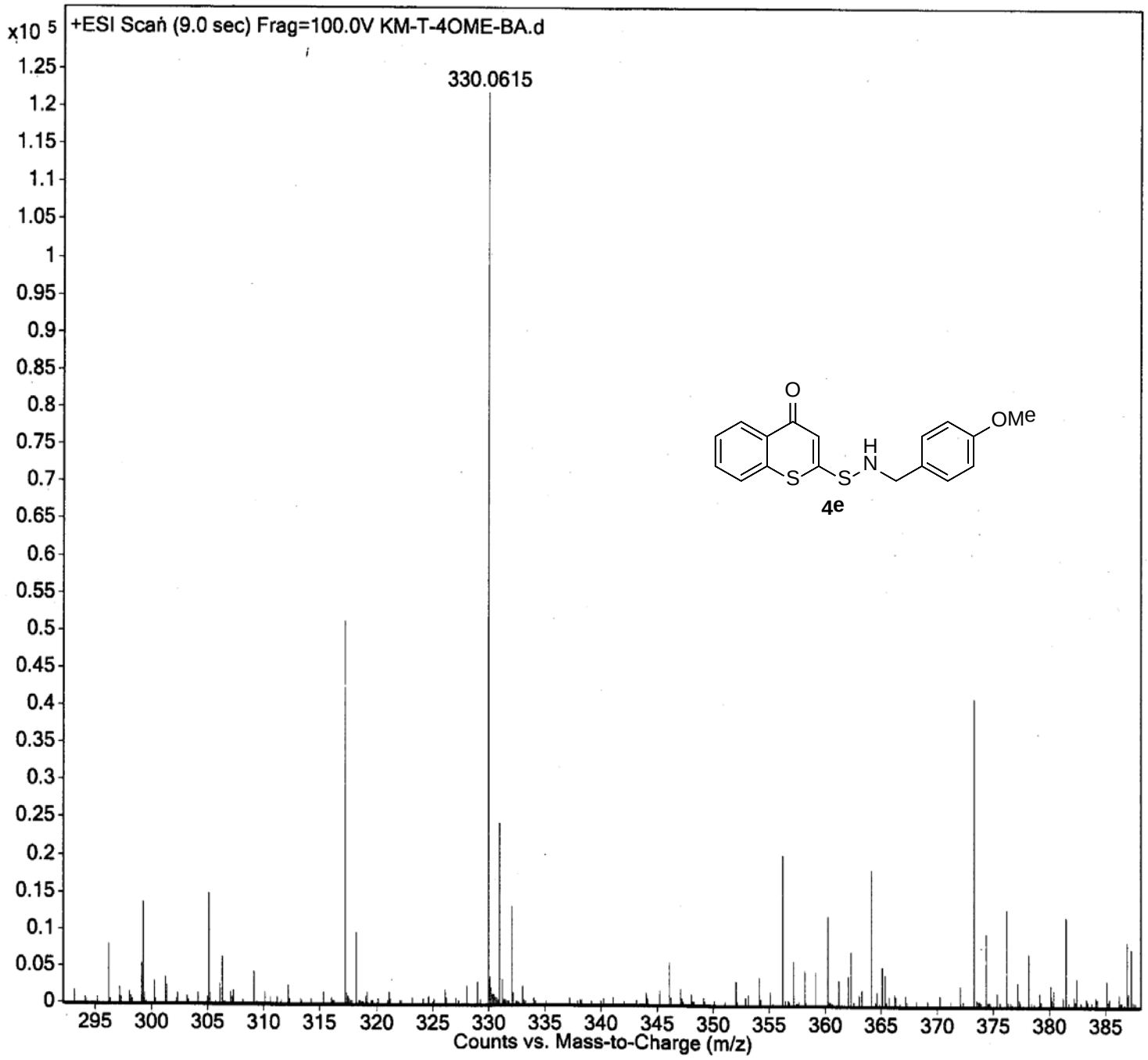


^{13}CNMR spectra of compound: 4e

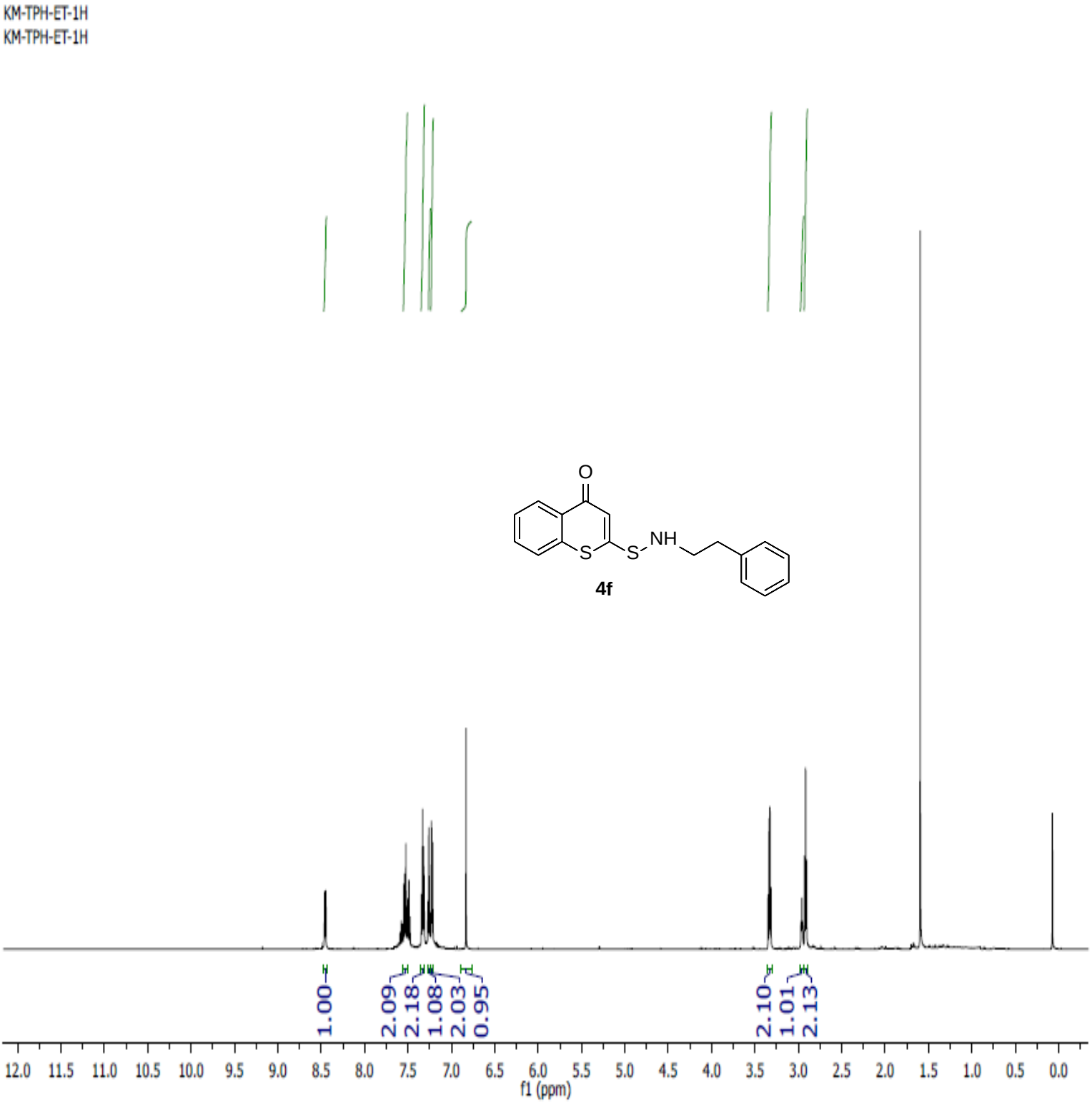


HRMS spectra of compound: 4e

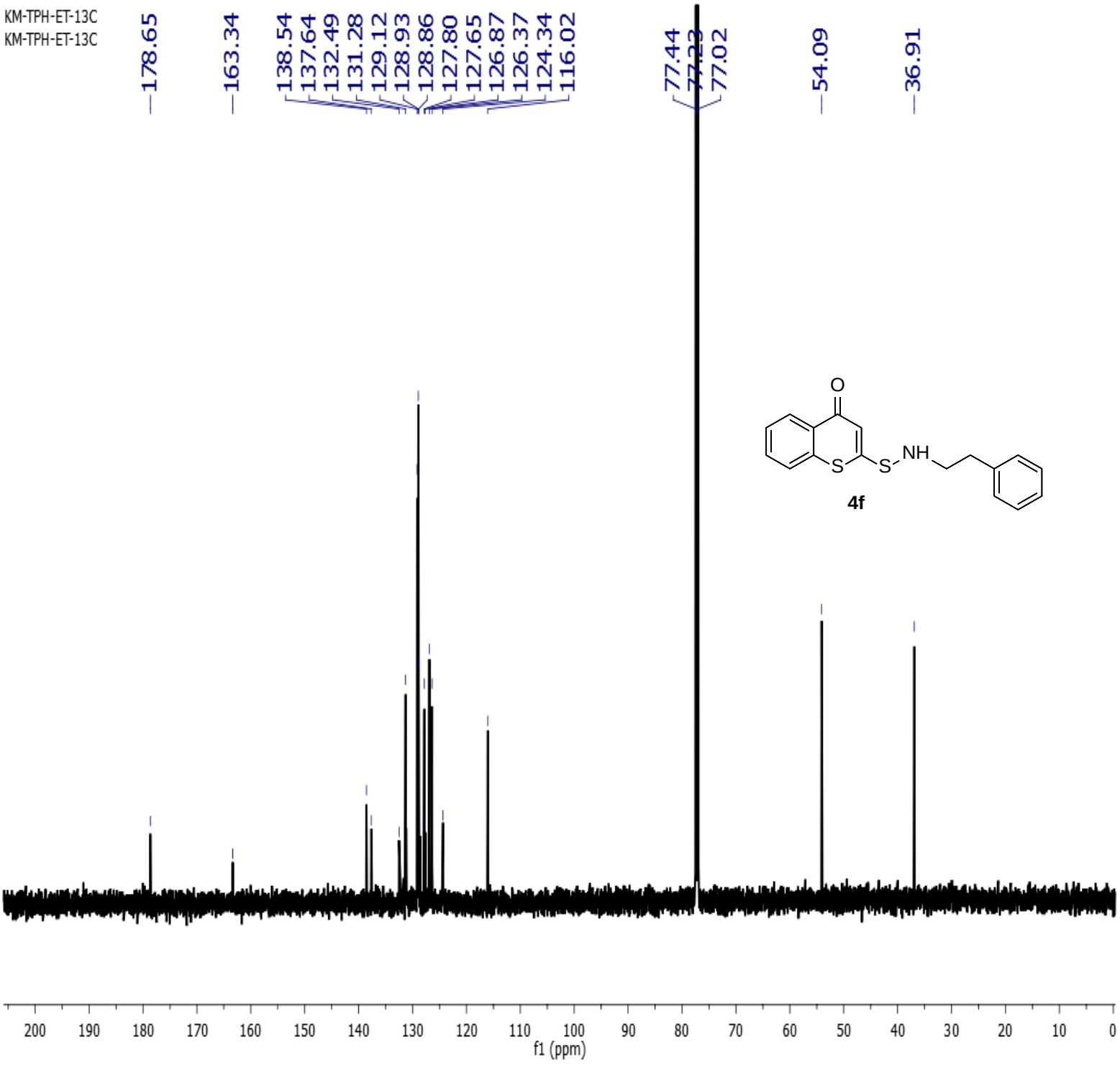
Sample Name	KM-T-4OME-BA	**Position**	Vial 1	**Instrument Name**	Instrument 1	**User Name**	
Inj Vol	0	**InjPosition**		**SampleType**	Sample	**IRM Calibration Status**	Success
Data Filename	KM-T-4OME-BA.d	**ACQ Method**		**Comment**		**Acquired Time**	9/4/2017 4:09:59 PM



[1]HNMR spectra of compound: 4f

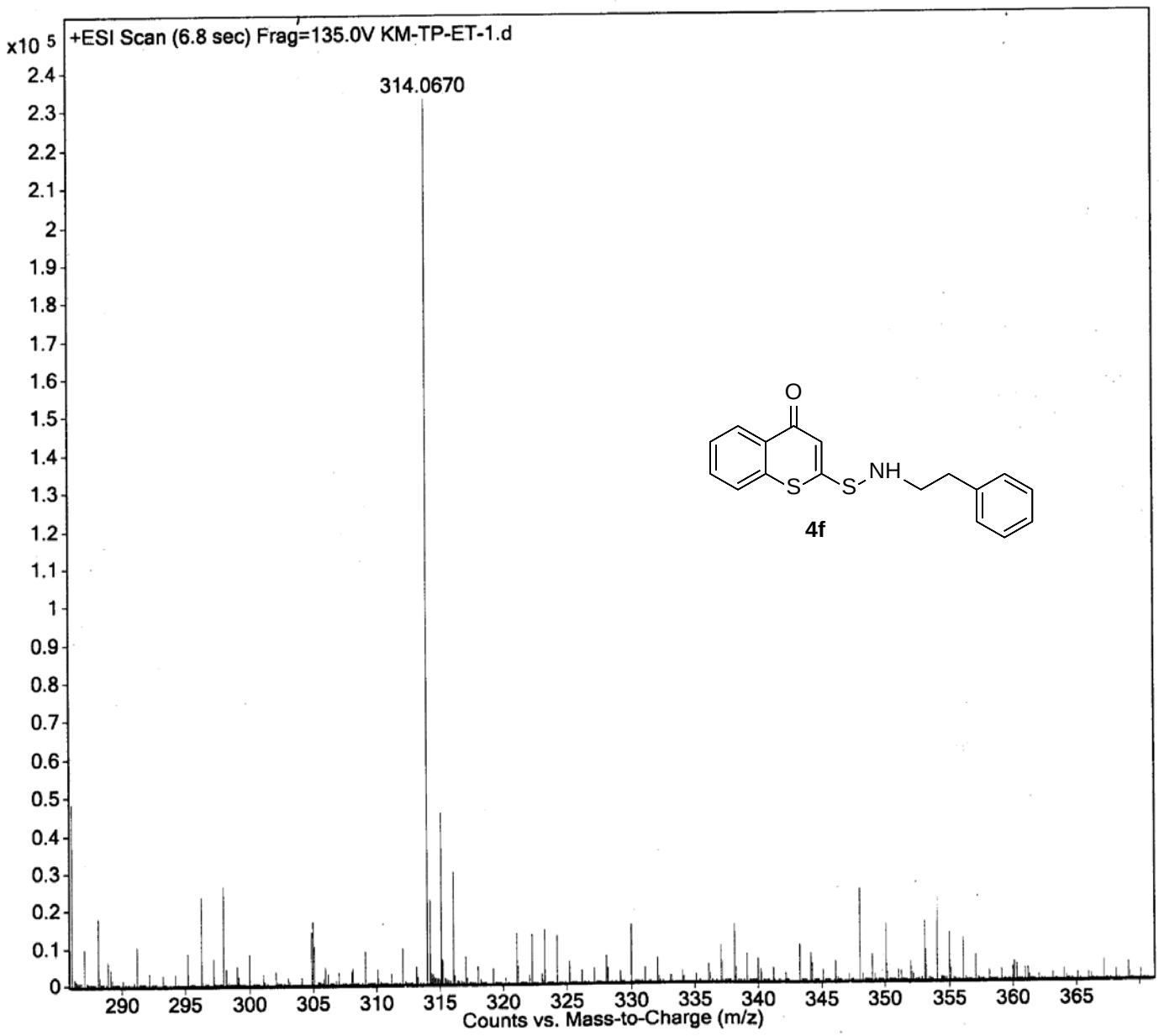


^{13}CNMR spectra of compound: 4f



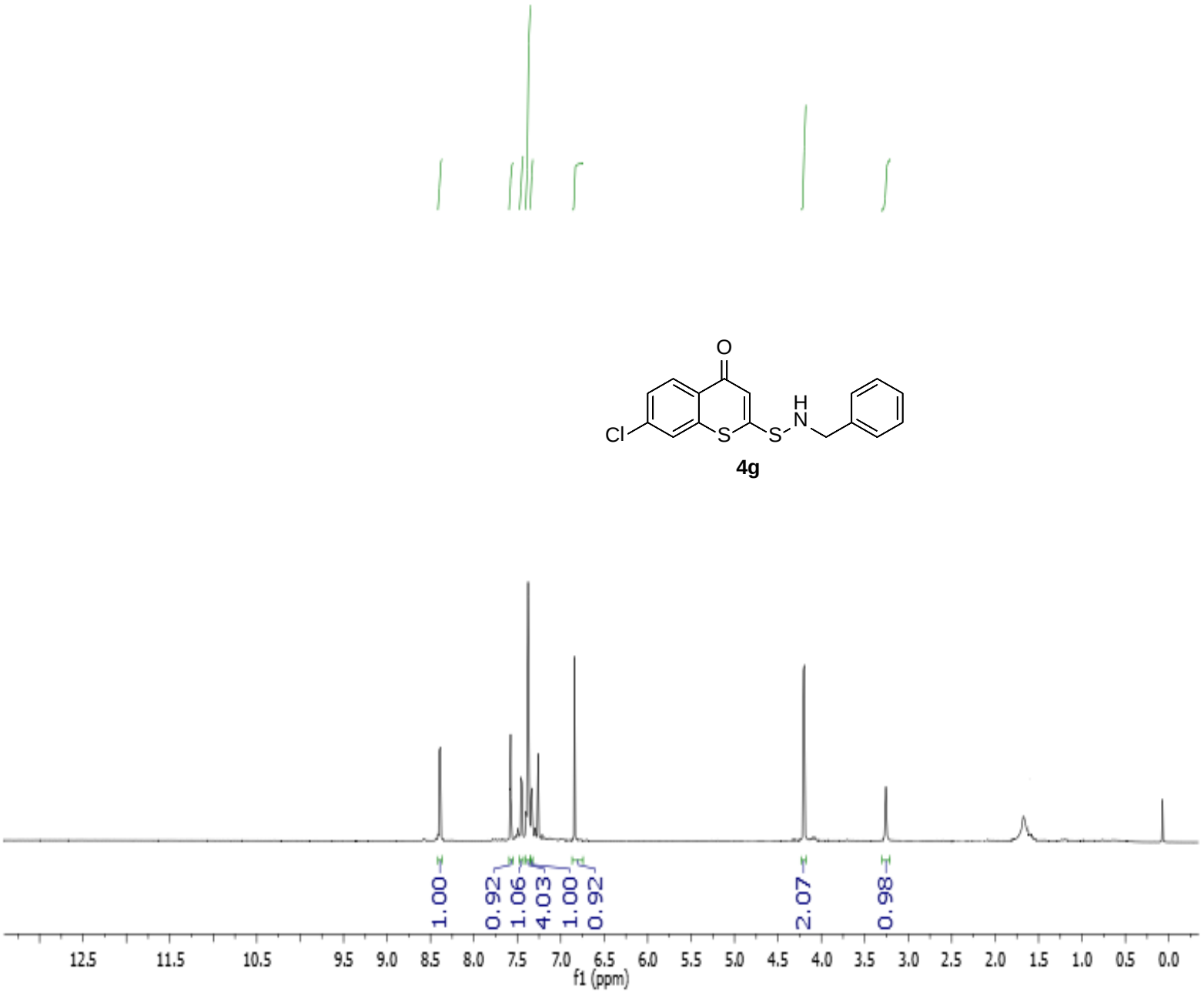
HRMS spectra of compound: 4f

Sample Name	Unavailable	**Position**	Unavailable	**Instrument Name**	Unavailable	**User Name**	Unavailable
Inj Vol	Unavailable	**InjPosition**	Unavailable	**SampleType**	Unavailable	**IRM Calibration Status**	Success
Data Filename	KM-TP-ET-1.d	**ACQ Method**		**Comment**	Sample information is unavailable	**Acquired Time**	Unavailable



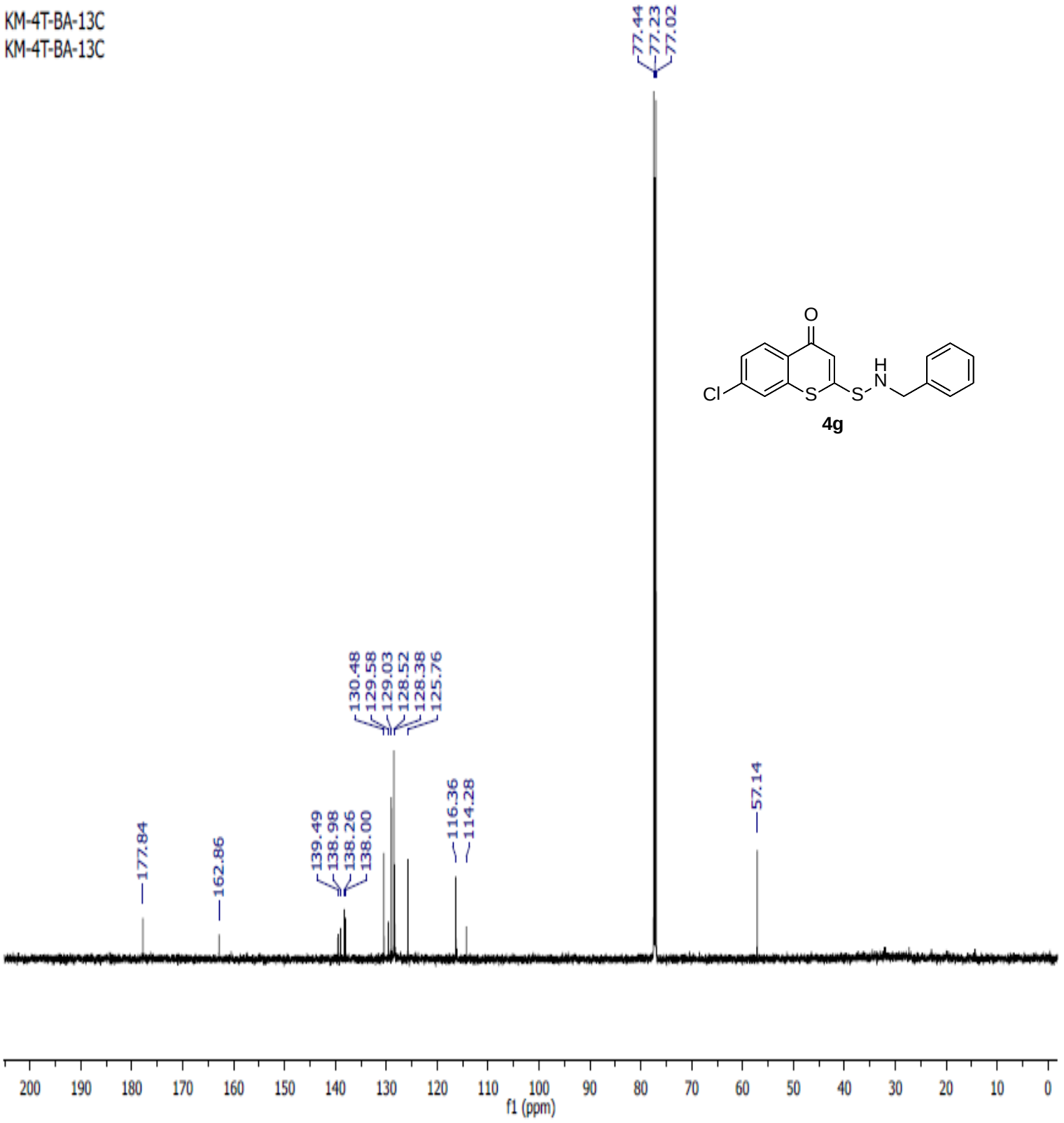
[1]HNMR spectra of compound: 4g

KM-4T-BA-1H
KM-4T-BA-1H



4g

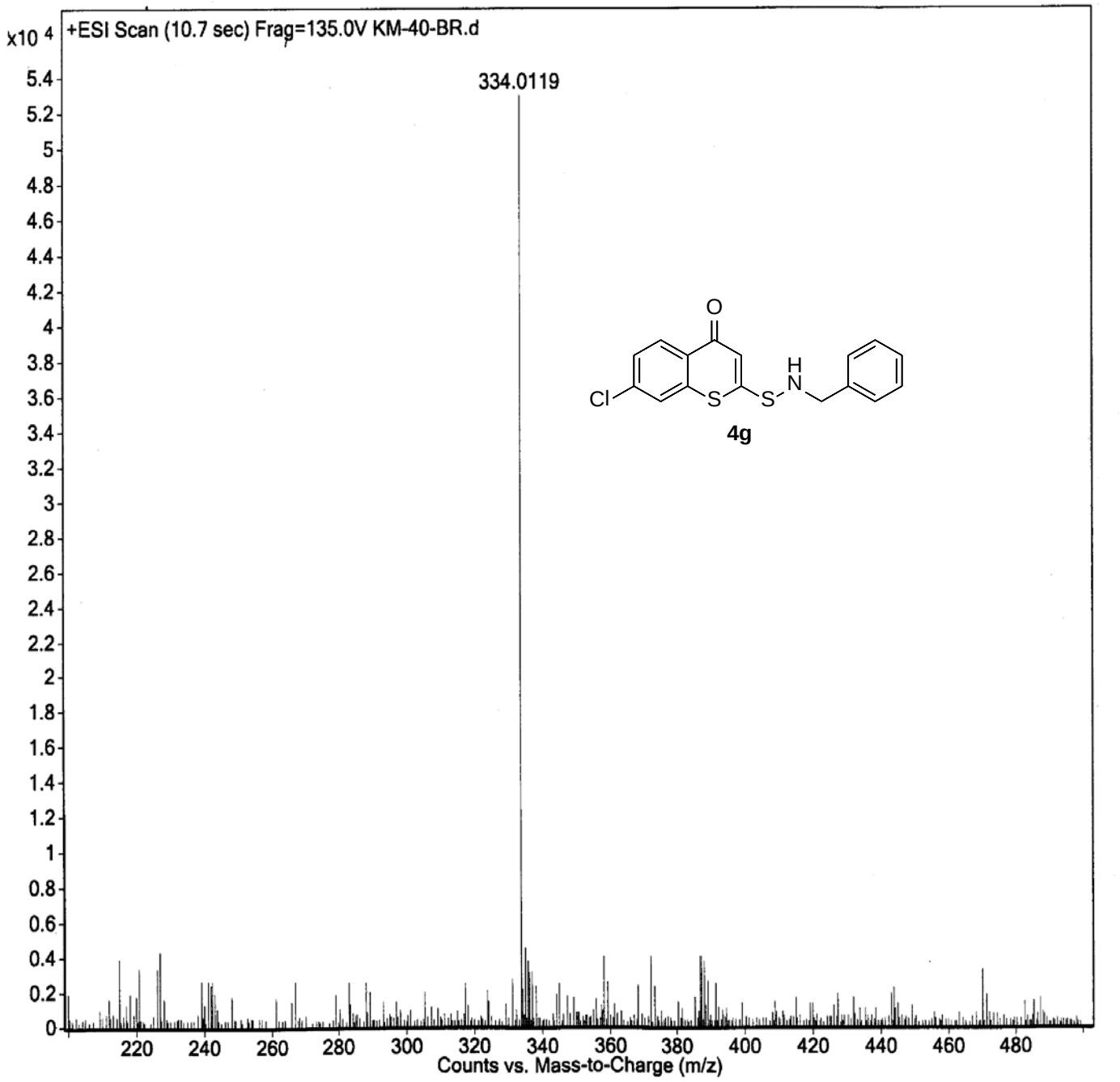
^{13}CNMR spectra of compound: 4g



4g

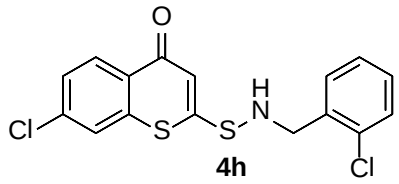
HRMS spectra of compound: 4g

Sample Name	KM-40-BR	**Position**	Vial 1	**Instrument Name**	Instrument 1	**User Name**	
Inj Vol	0	**InjPosition**		**SampleType**	Sample	**IRM Calibration Status**	All Ions Missed
Data Filename	KM-40-BR.d	**ACQ Method**		**Comment**		**Acquired Time**	8/28/2017 4:27:37 PM

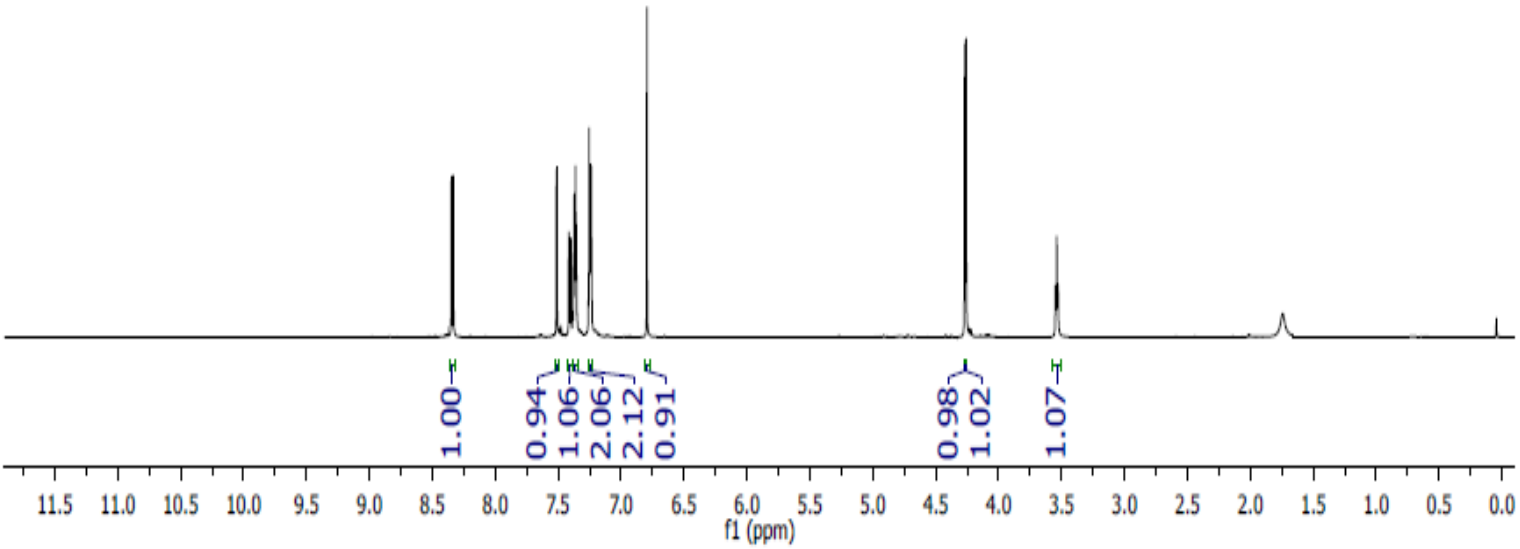


[1]HNMR spectra of compound: 4h

KM-4T-2CL-BA-1H
KM-4T-2CL-BA-1H

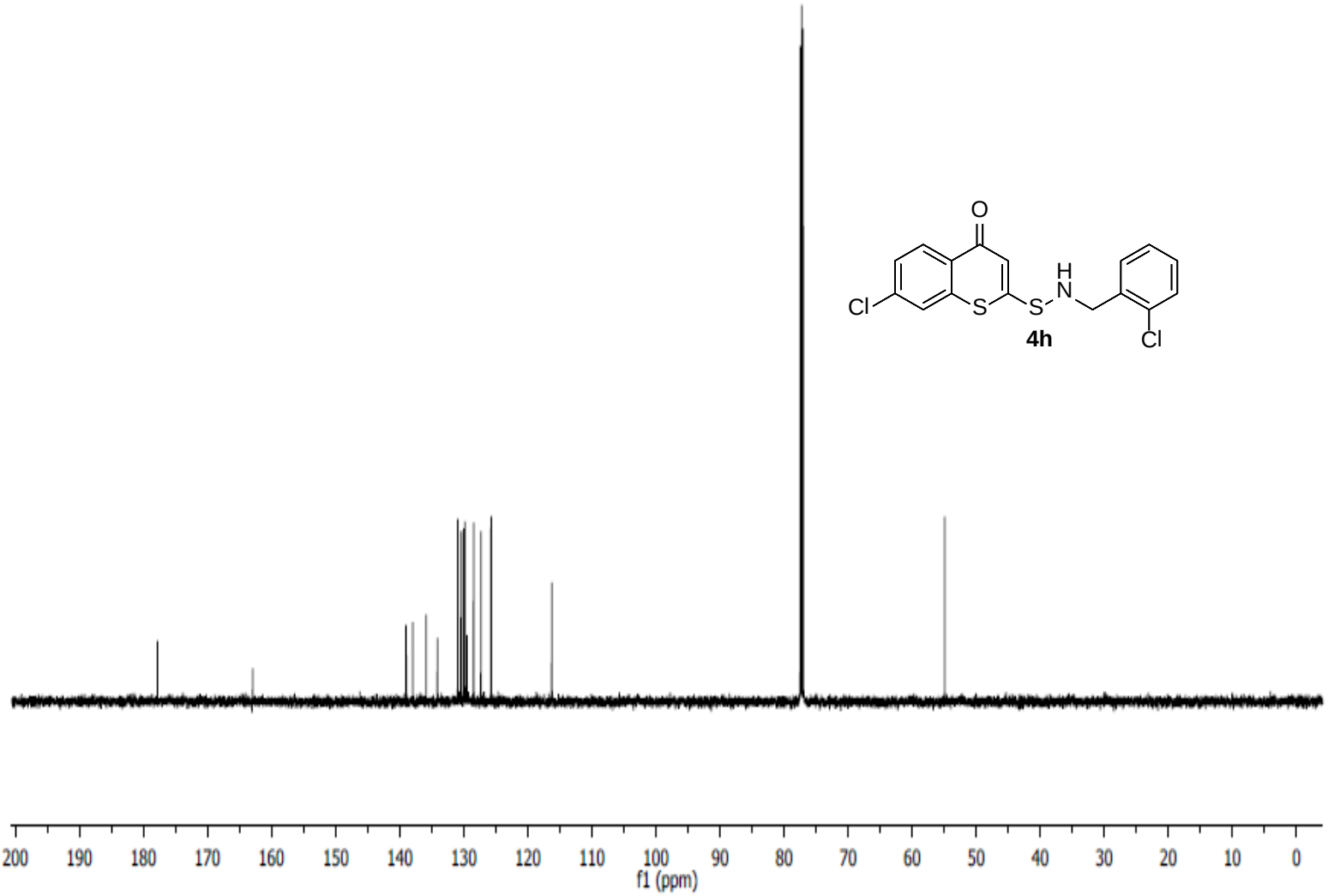


4h



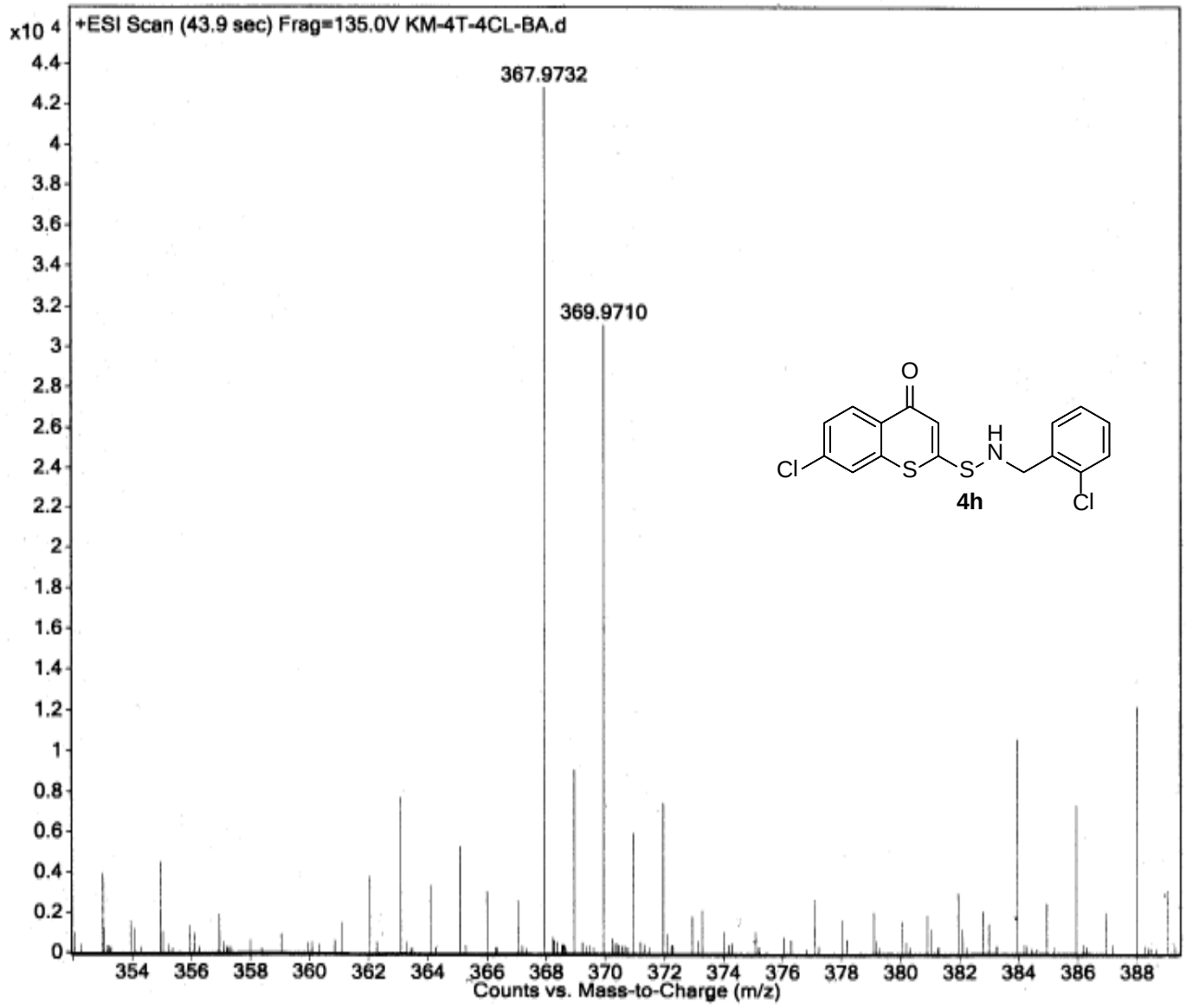
^{13}CNMR spectra of compound: 4h

4h



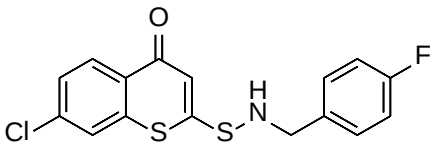
HRMS spectra of compound: 4h

Sample Name	KM-4T-4CL-BA	**Position**	Vial 1	**Instrument Name**	Instrument 1	**User Name**	
Inj Vol	0	**InjPosition**		**SampleType**	Sample	**IRM Calibration Status**	Success
Data Filename	KM-4T-4CL-BA.d	**ACQ Method**		**Comment**		**Acquired Time**	10/23/2017 4:39:20 PM

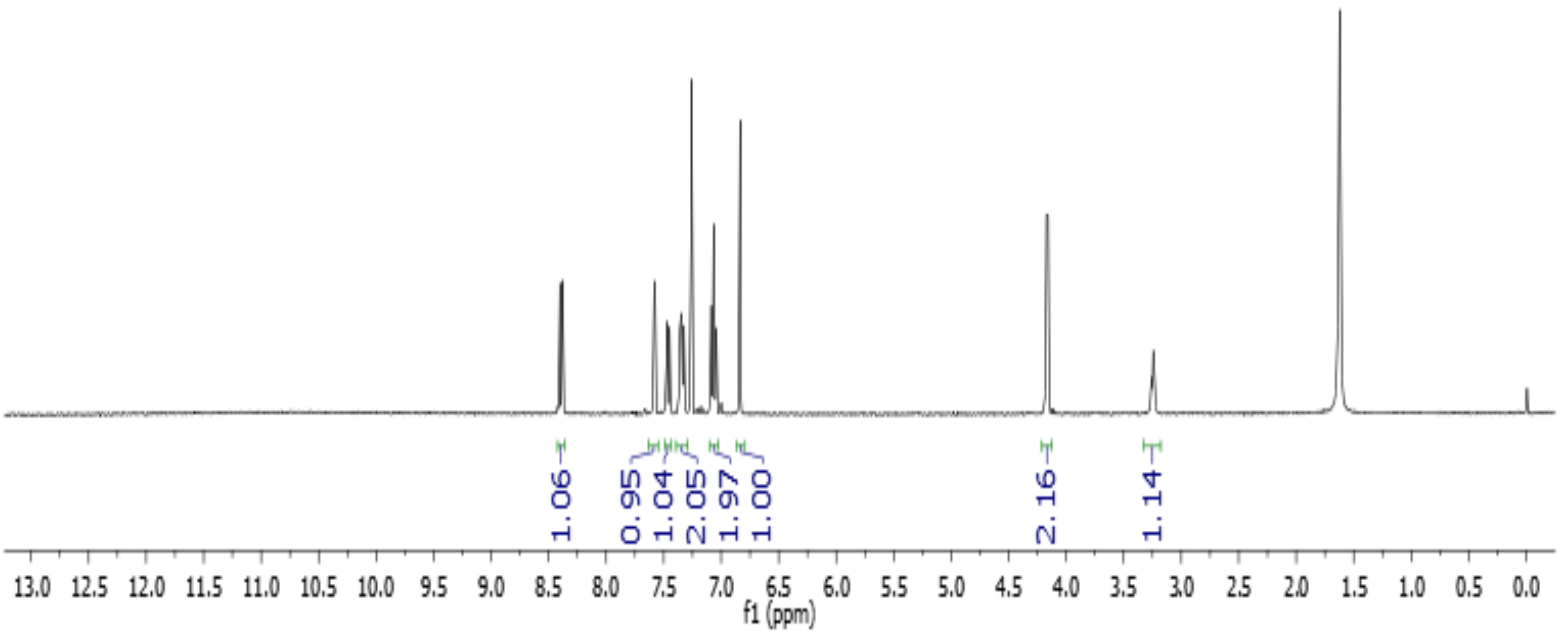


[1]HNMR spectra of compound: 4i

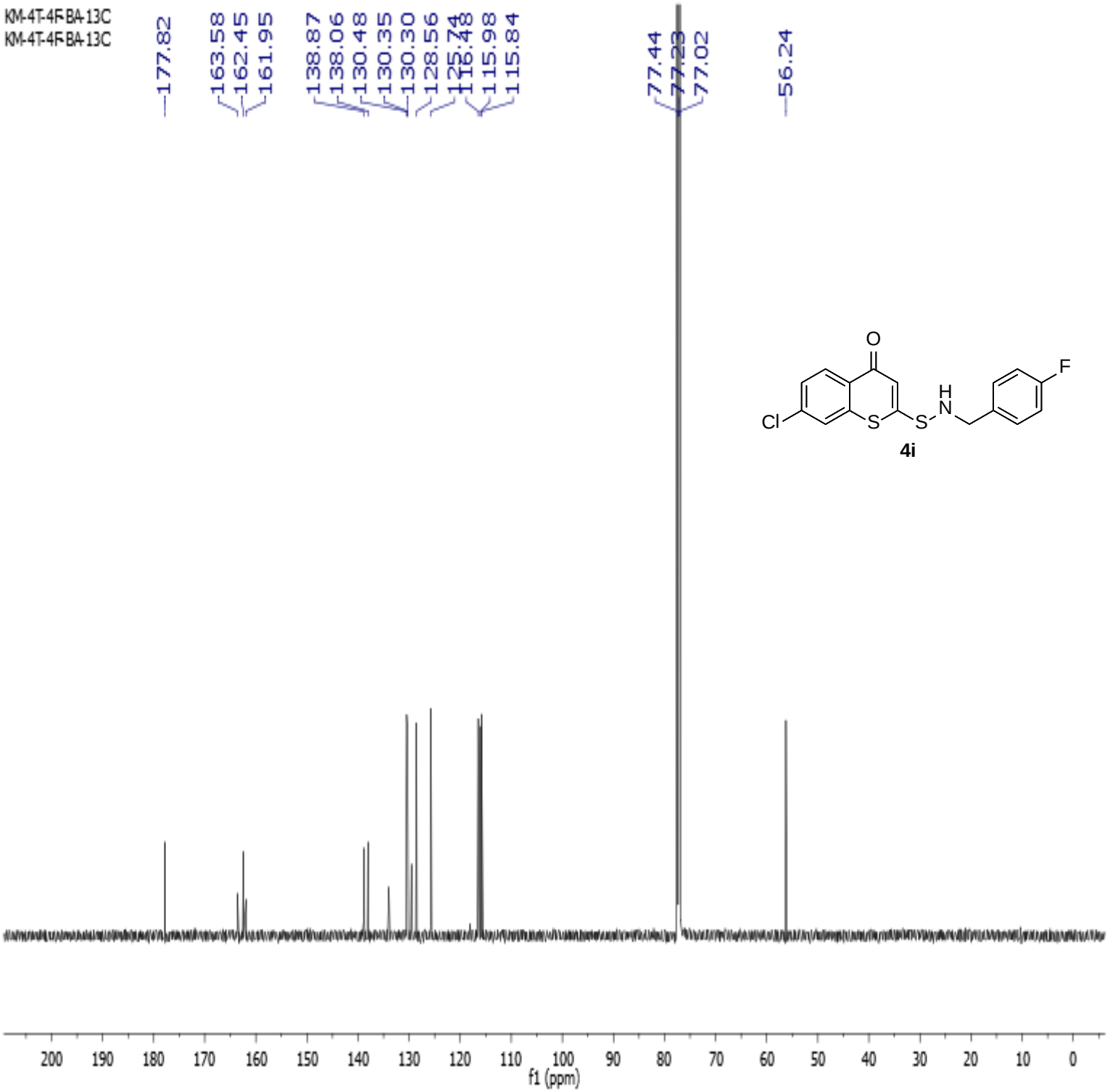
KM-4T-4F-BA-1H
KM-4T-4F-BA-1H



4i

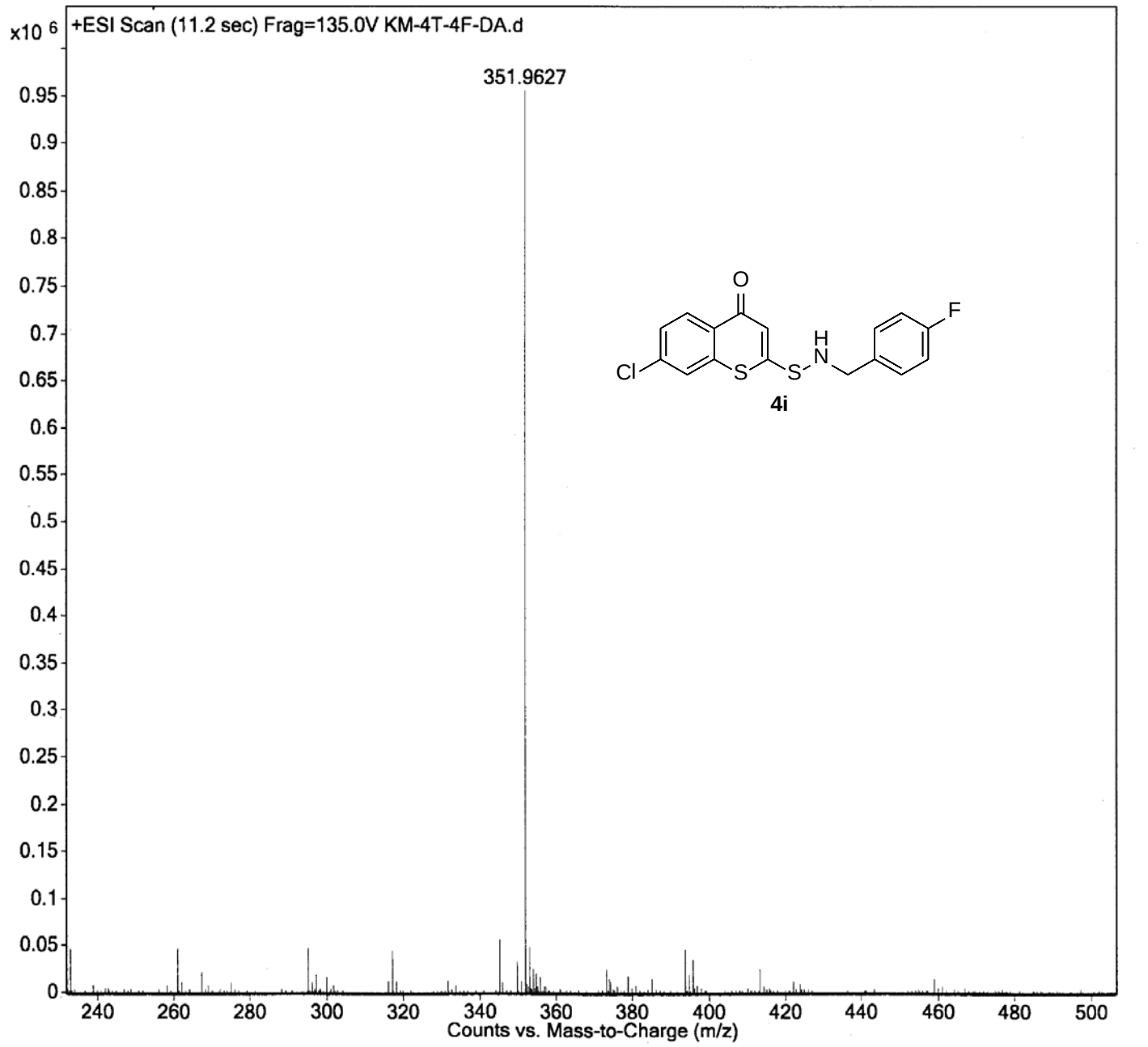


^{13}CNMR spectra of compound: 4i



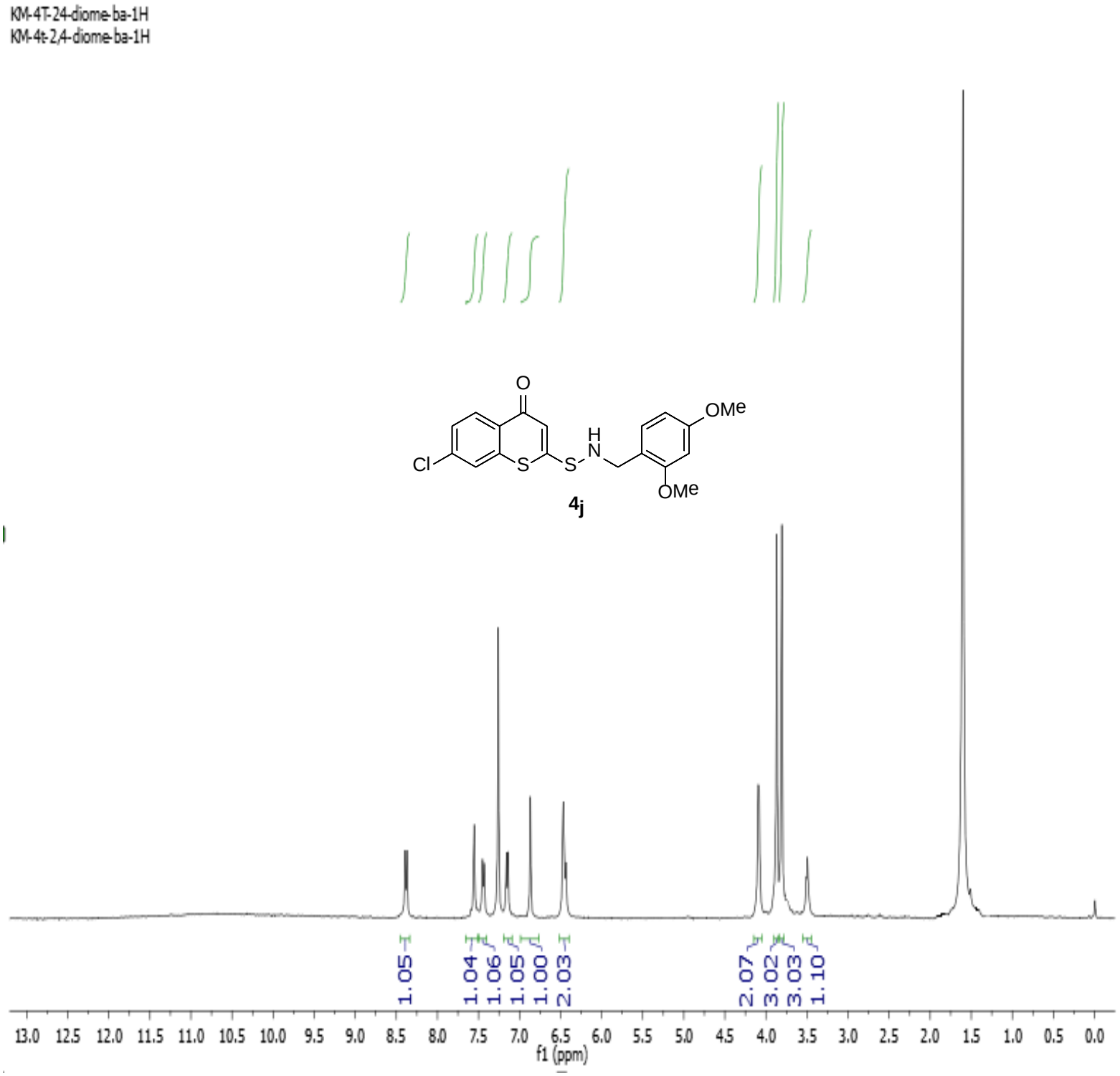
HRMS spectra of compound: 4i

Sample Name	KM-4T-4F-DA	**Position**	Vial 1	**Instrument Name**	Instrument 1	**User Name**	
Inj Vol	0	**InjPosition**		**SampleType**	Sample	**IRM Calibration Status**	Some Ions Missed
Data Filename	KM-4T-4F-DA.d	**ACQ Method**		**Comment**		**Acquired Time**	9/12/2017 4:20:38 PM

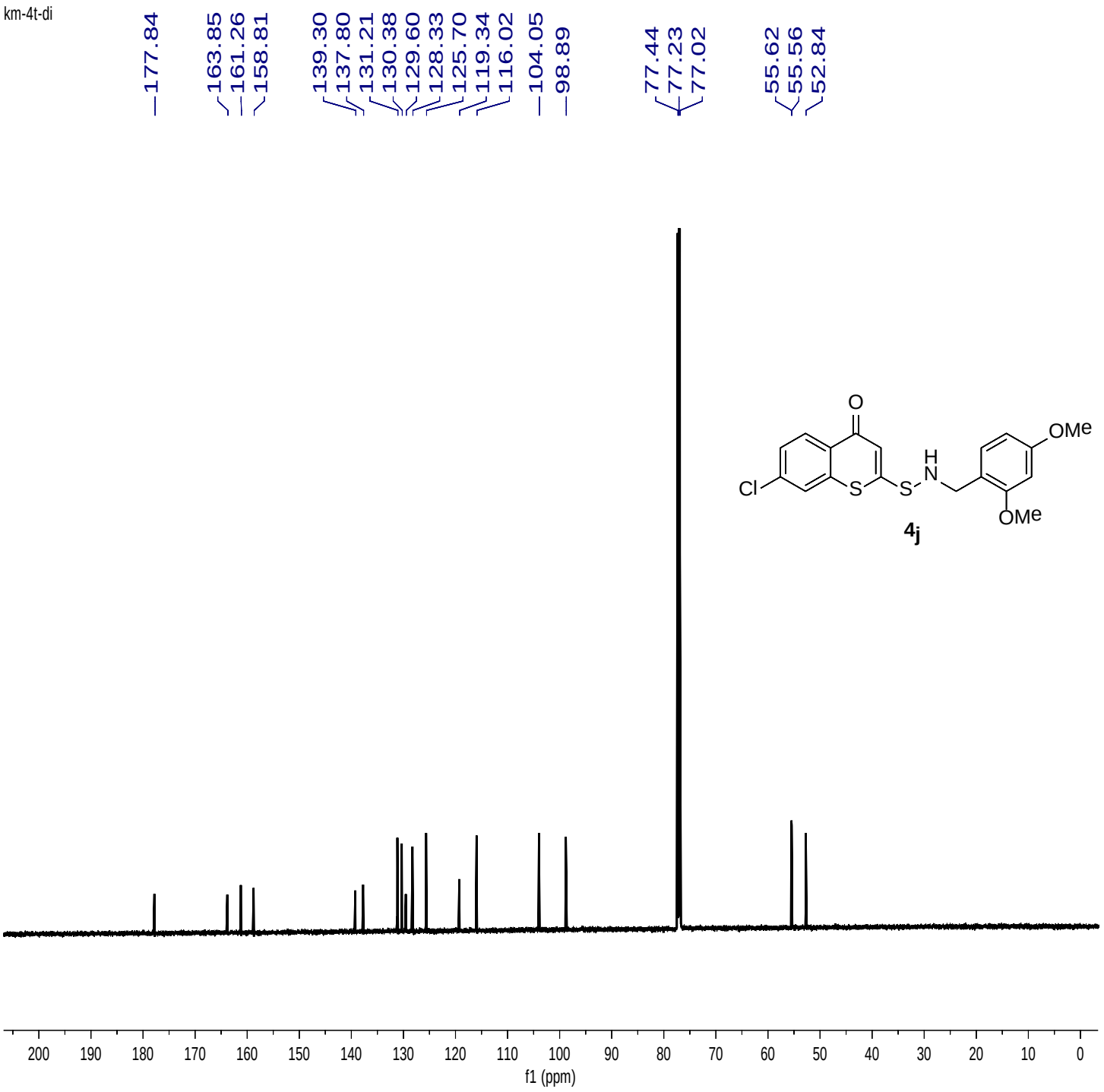


4i

[1]HNMR spectra of compound: 4j

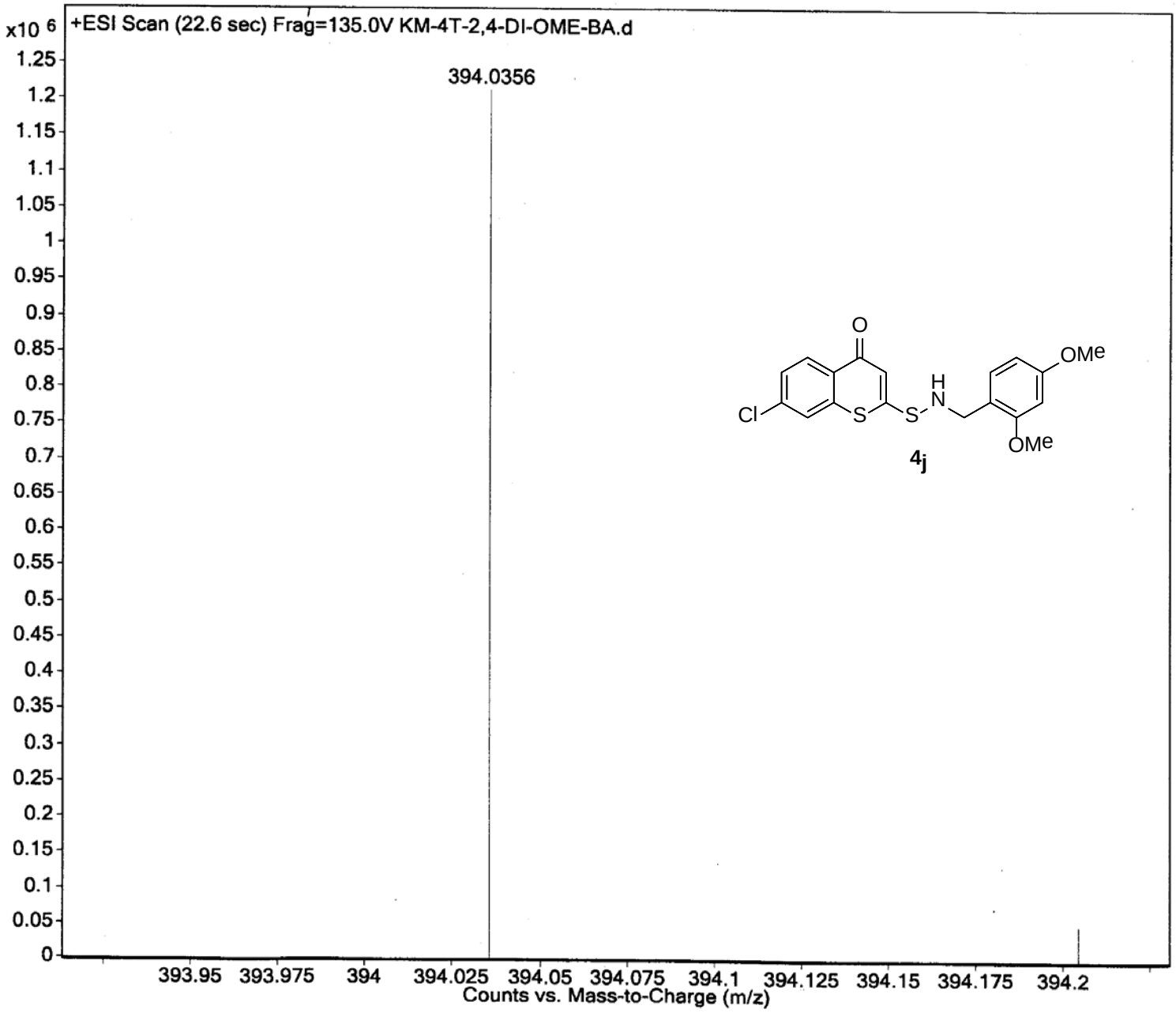


^{13}CNMR spectra of compound: 4j



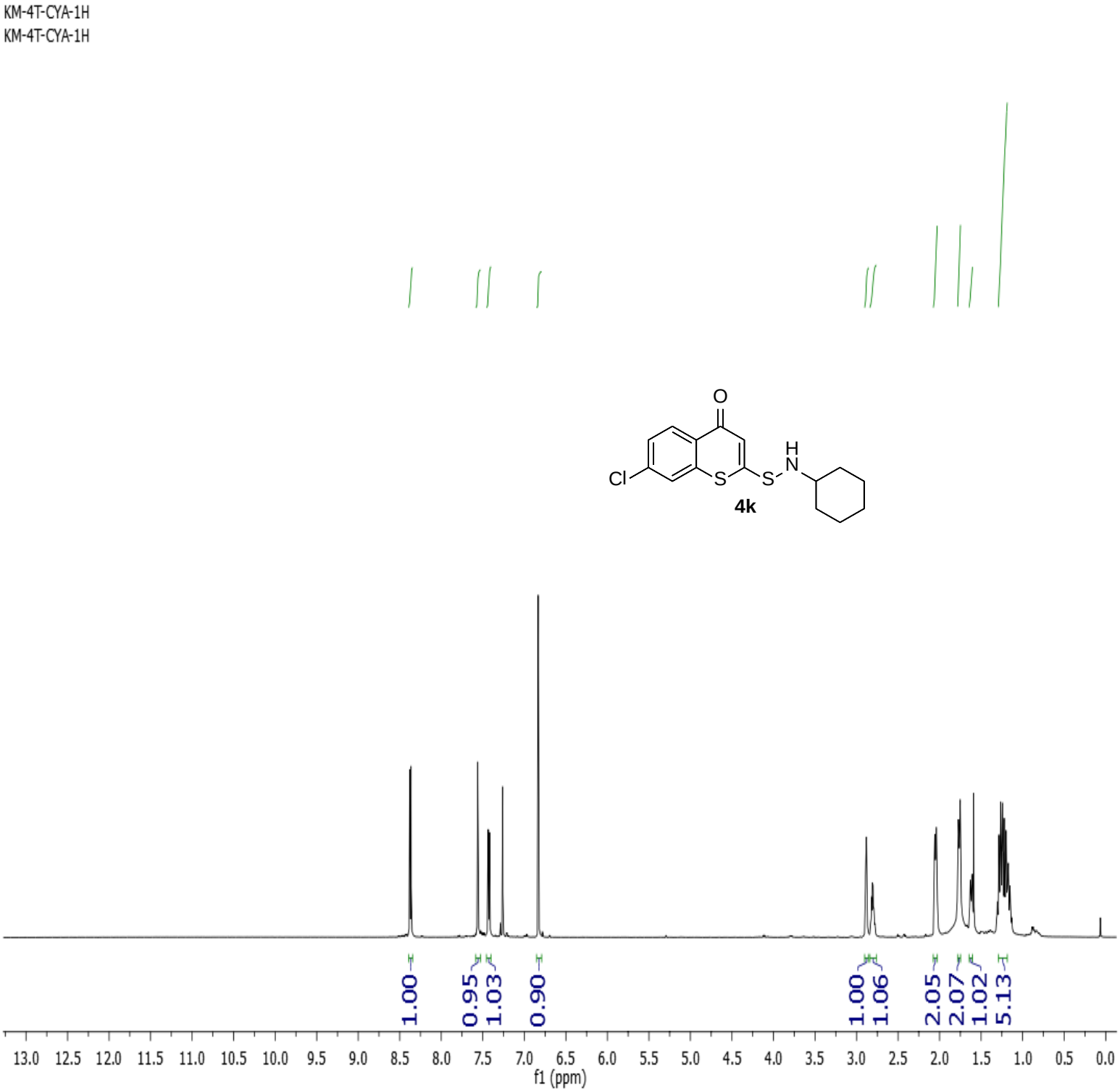
HRMS spectra of compound: 4j

Sample Name	Unavailable	**Position**	Unavailable	**Instrument Name**	Unavailable	**User Name**	Unavailable
Inj Vol	Unavailable	**InjPosition**	Unavailable	**SampleType**	Unavailable	**IRM Calibration Status**	Some Ions Missed
Data Filename	KM-4T-2,4-DI-OME-BA.	**ACQ Method**		**Comment**	Sample information is unavailable	**Acquired Time**	Unavailable

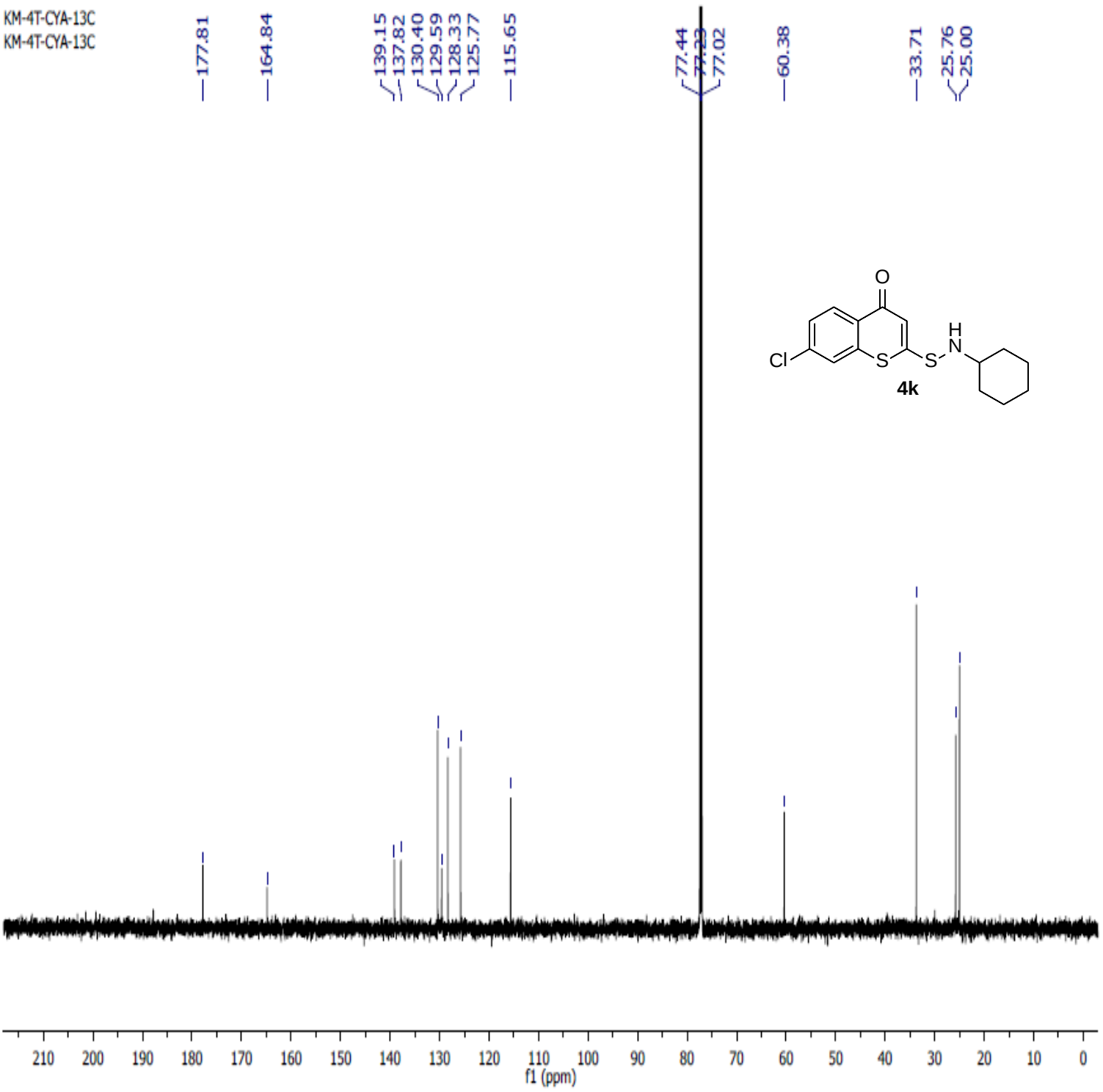


4j

[1]HNMR spectra of compound: 4k

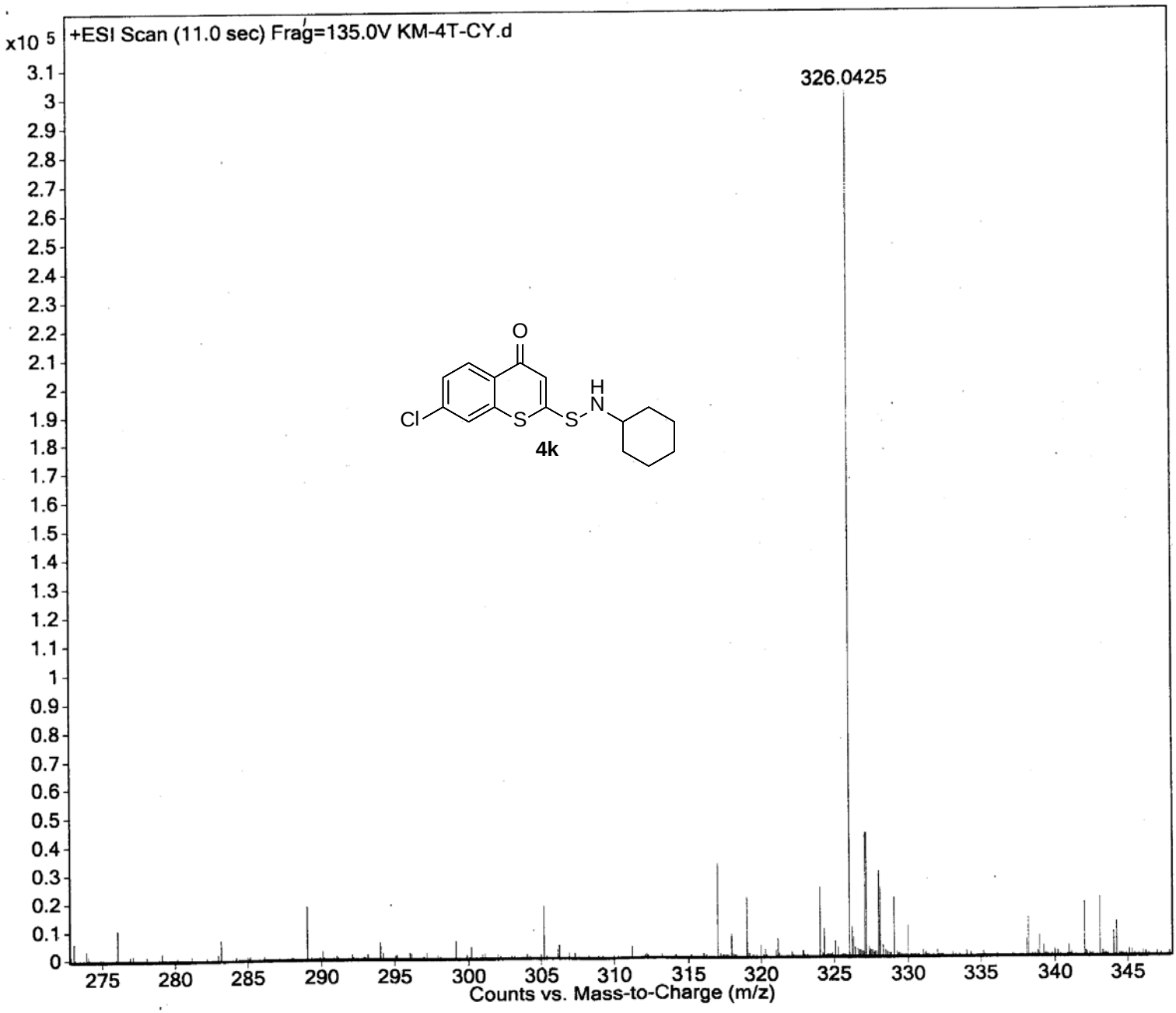


^{13}CNMR spectra of compound: 4k

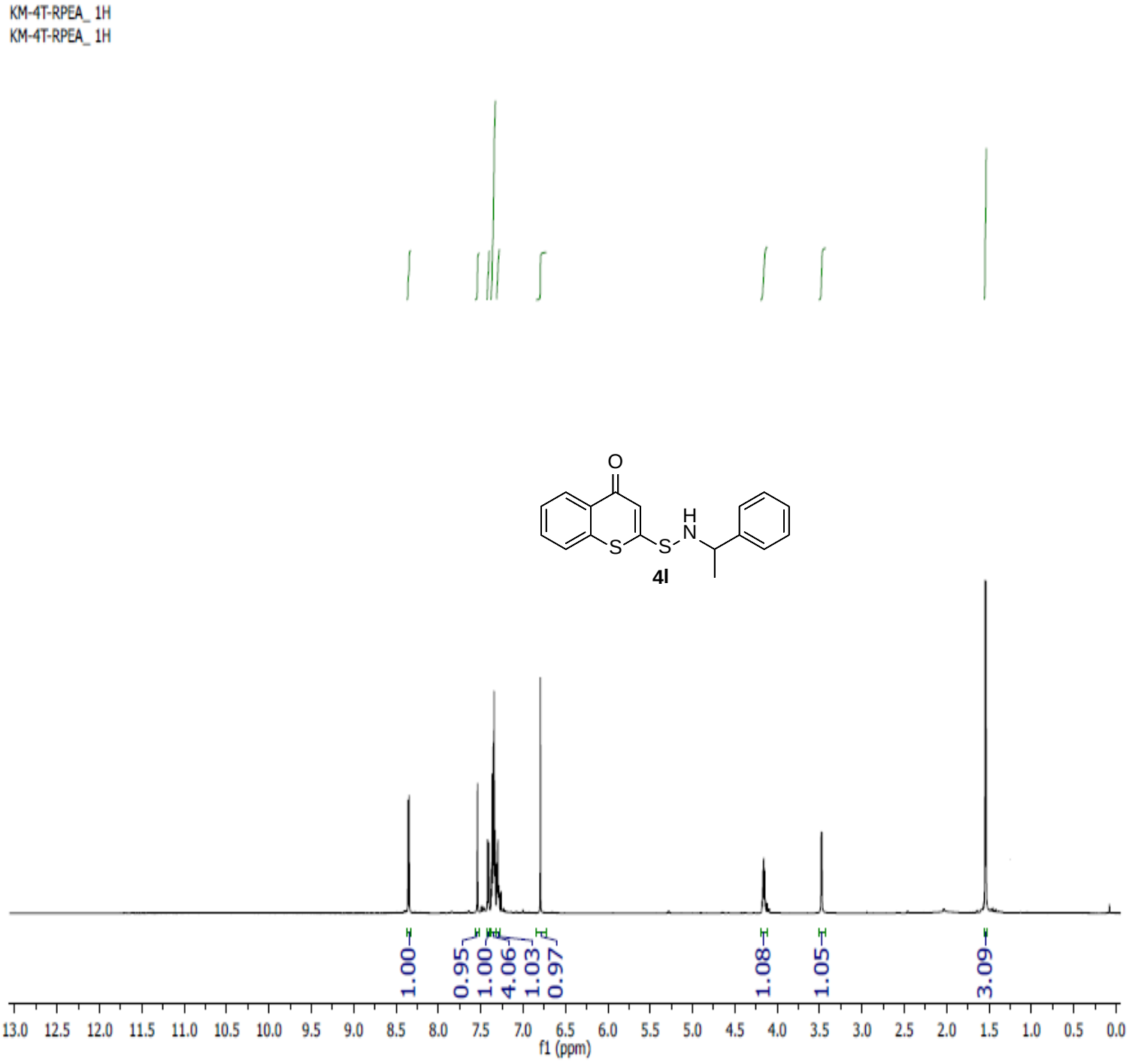


HRMS spectra of compound: 4k

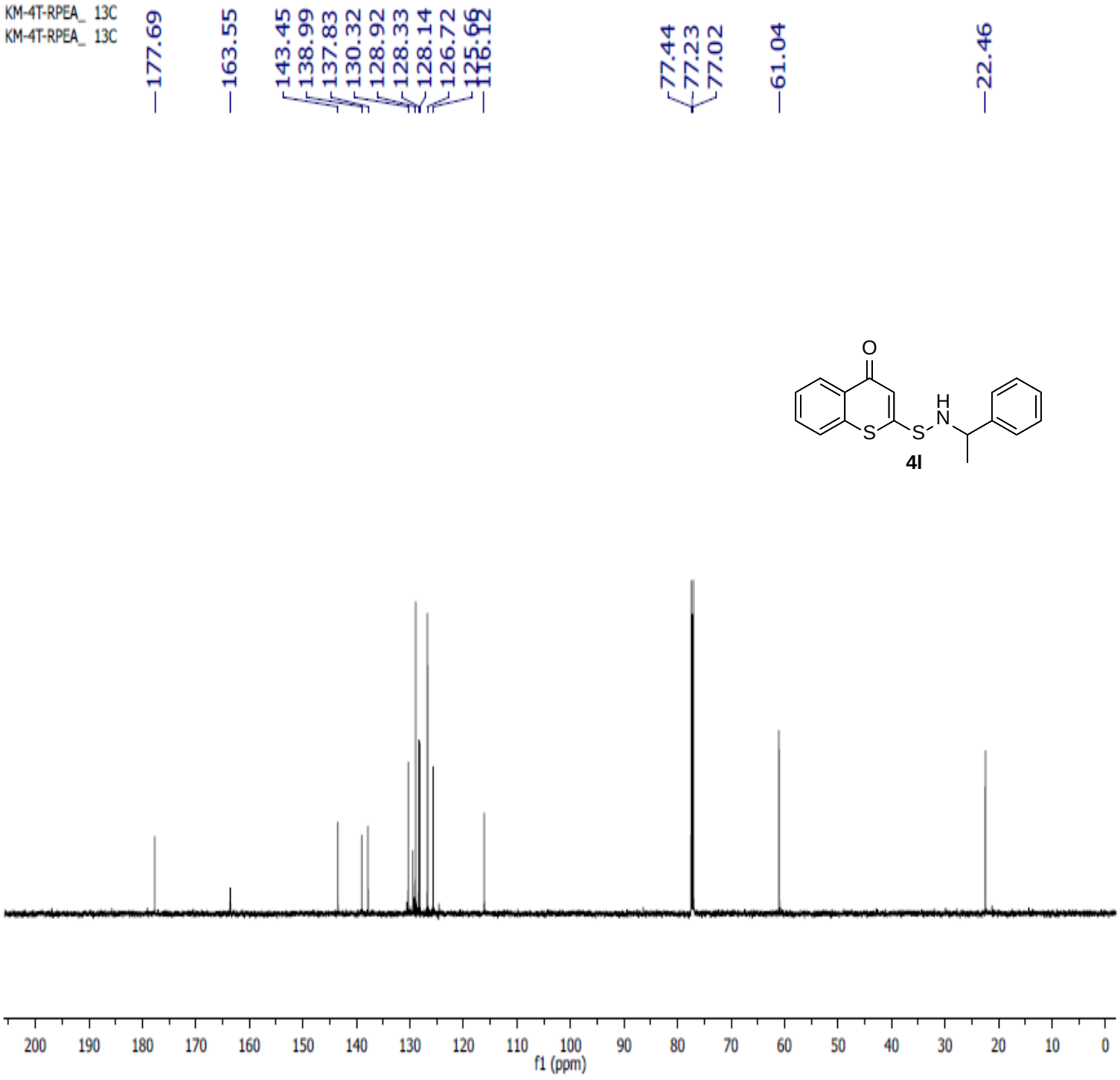
Sample Name	Unavailable	**Position**	Unavailable	**Instrument Name**	Unavailable	**User Name**	Unavailable
Inj Vol	Unavailable	**InjPosition**	Unavailable	**SampleType**	Unavailable	**IRM Calibration Status**	All Ions Missed
Data Filename	KM-4T-CY.d	**ACQ Method**		**Comment**	Sample information is unavailable	**Acquired Time**	Unavailable



[1]HNMR spectra of compound: 4l

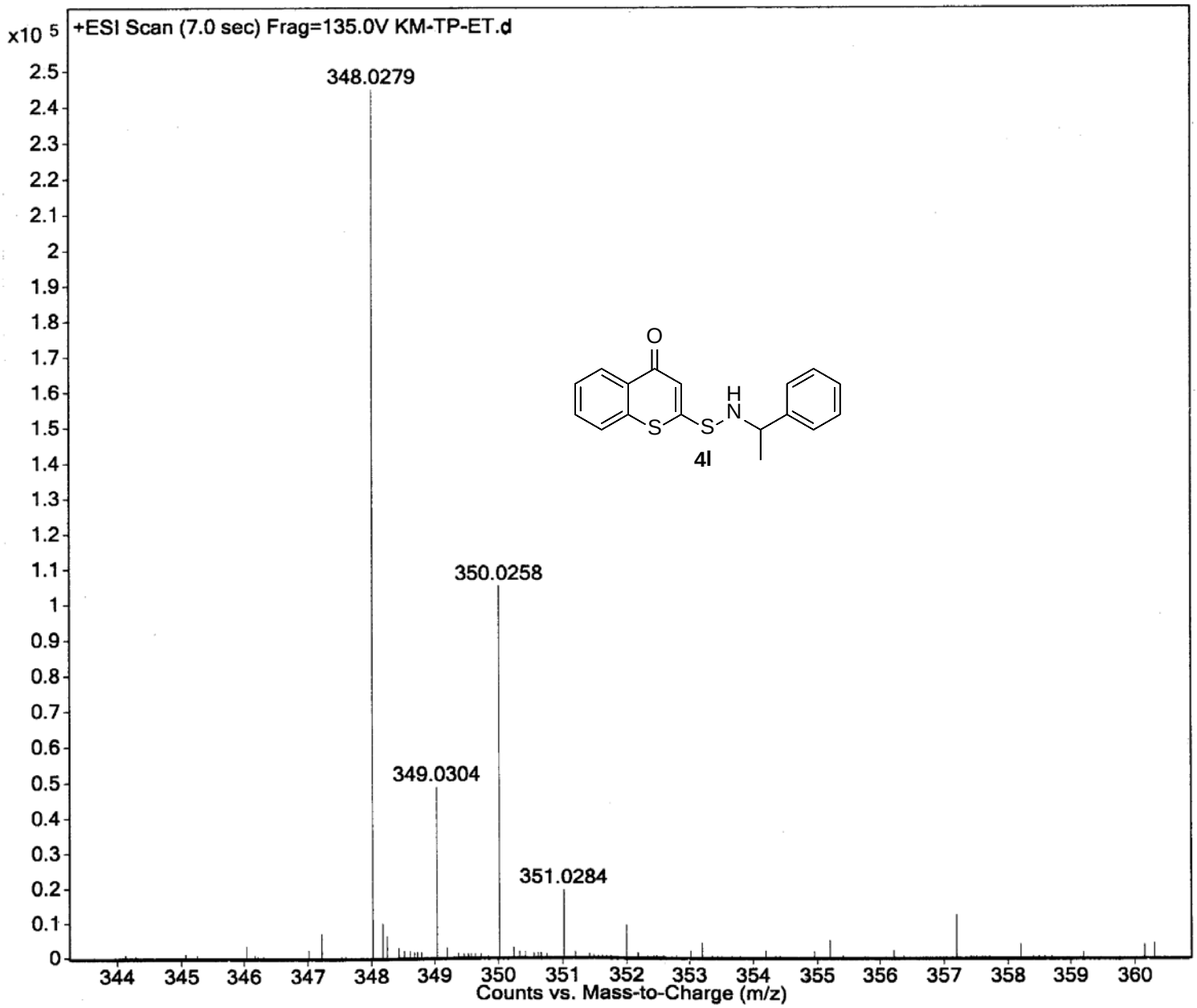


^{13}CNMR spectra of compound: 4l



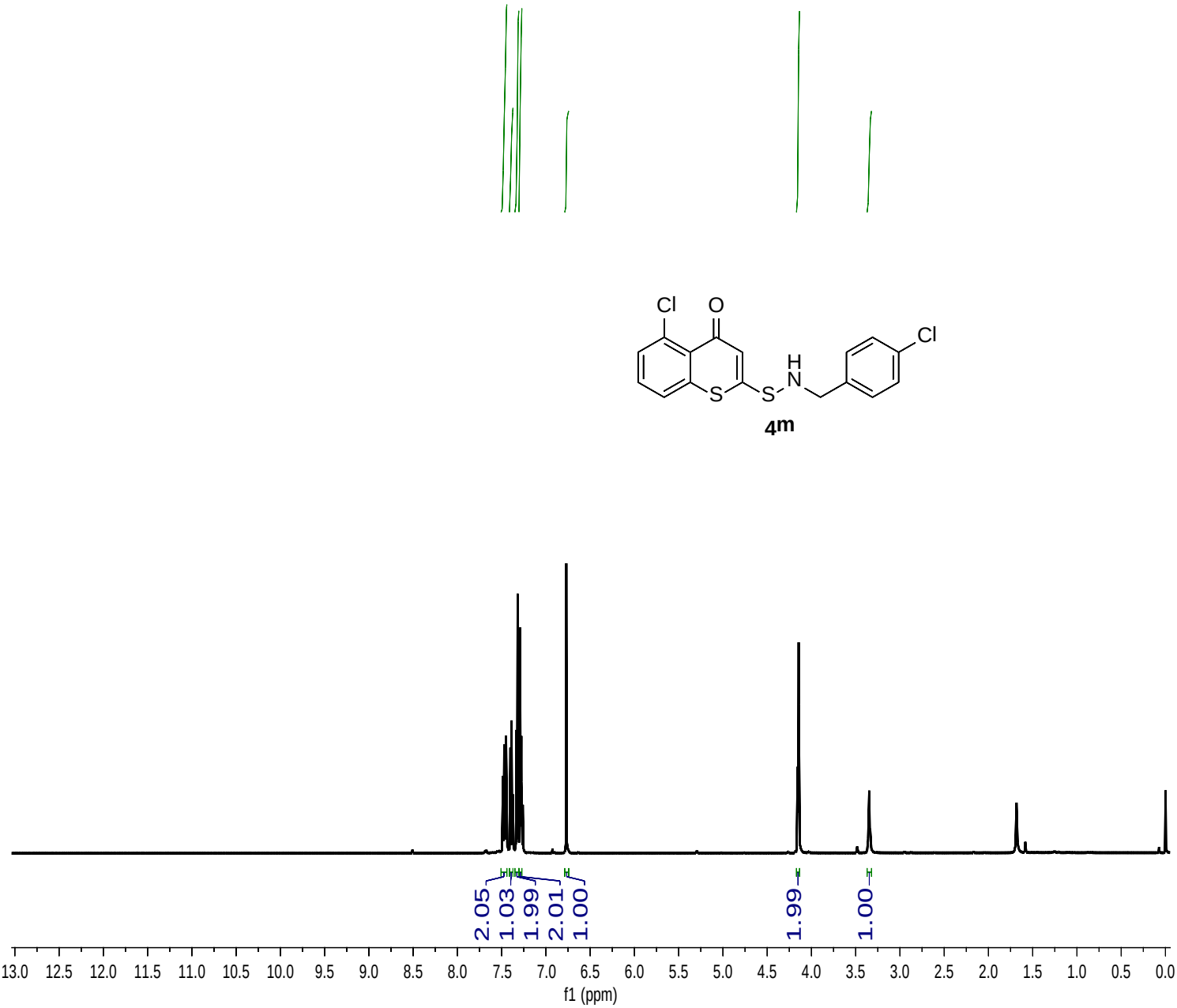
HRMS spectra of compound: 4l

Sample Name	Unavailable	**Position**	Unavailable	**Instrument Name**	Unavailable	**User Name**	Unavailable
Inj Vol	Unavailable	**InjPosition**	Unavailable	**SampleType**	Unavailable	**IRM Calibration Status**	Success
Data Filename	KM-TP-ET.d	**ACQ Method**		**Comment**	Sample information is unavailable	**Acquired Time**	Unavailable



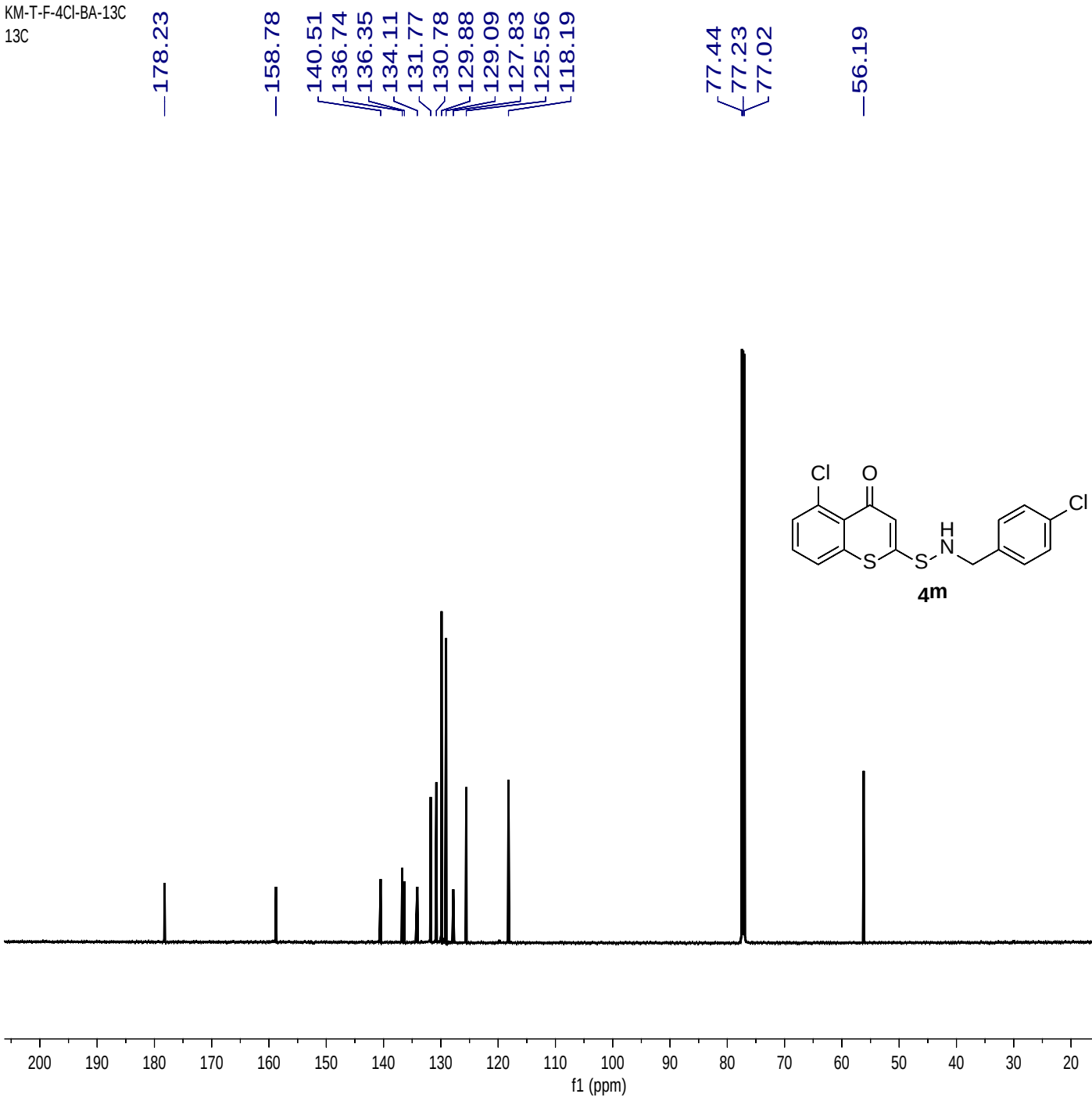
^{1}HNMR spectra of compound: 4m

KM-T-F-4Cl-BA-1H
1H



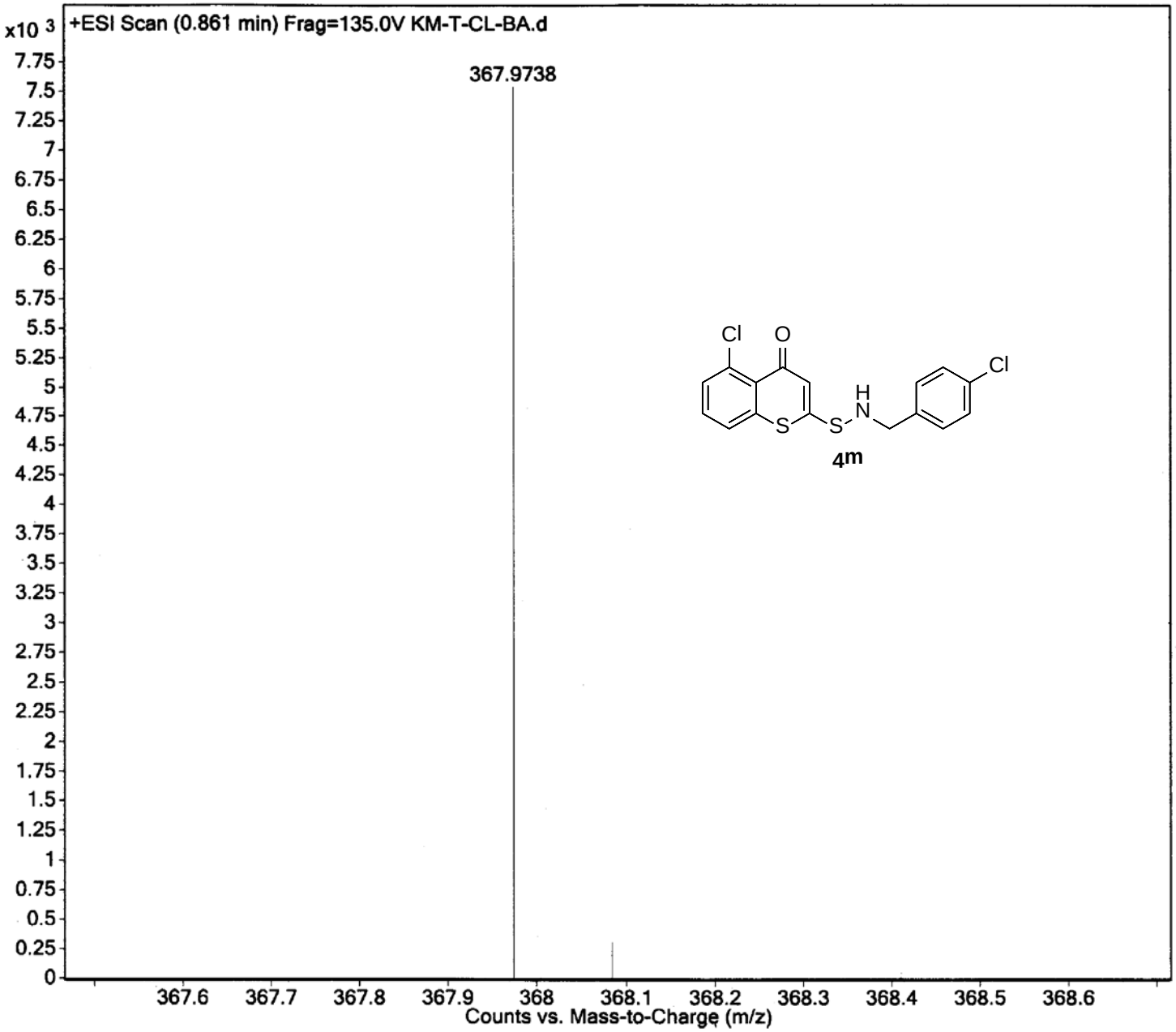
4m

^{13}CNMR spectra of compound: 4m



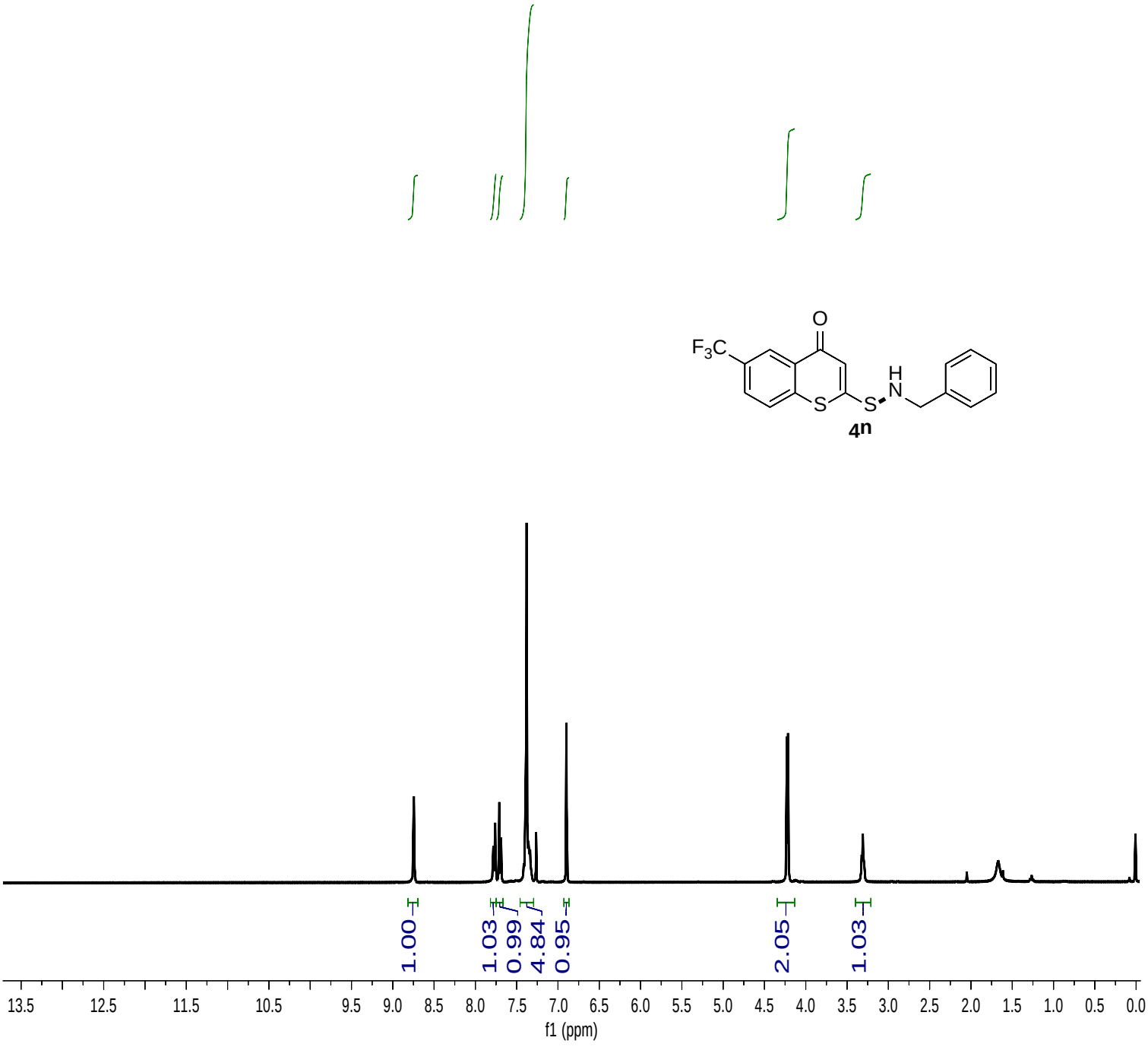
HRMS spectra of compound: 4m

Sample Name	KM-T-CL-BA	**Position**	Vial 1	**Instrument Name**	Instrument 1	**User Name**	
Inj Vol	-1	**InjPosition**		**SampleType**	Sample	**IRM Calibration Status**	Success
Data Filename	KM-T-CL-BA.d	**ACQ Method**		**Comment**		**Acquired Time**	12/26/2017 5:45:45 PM



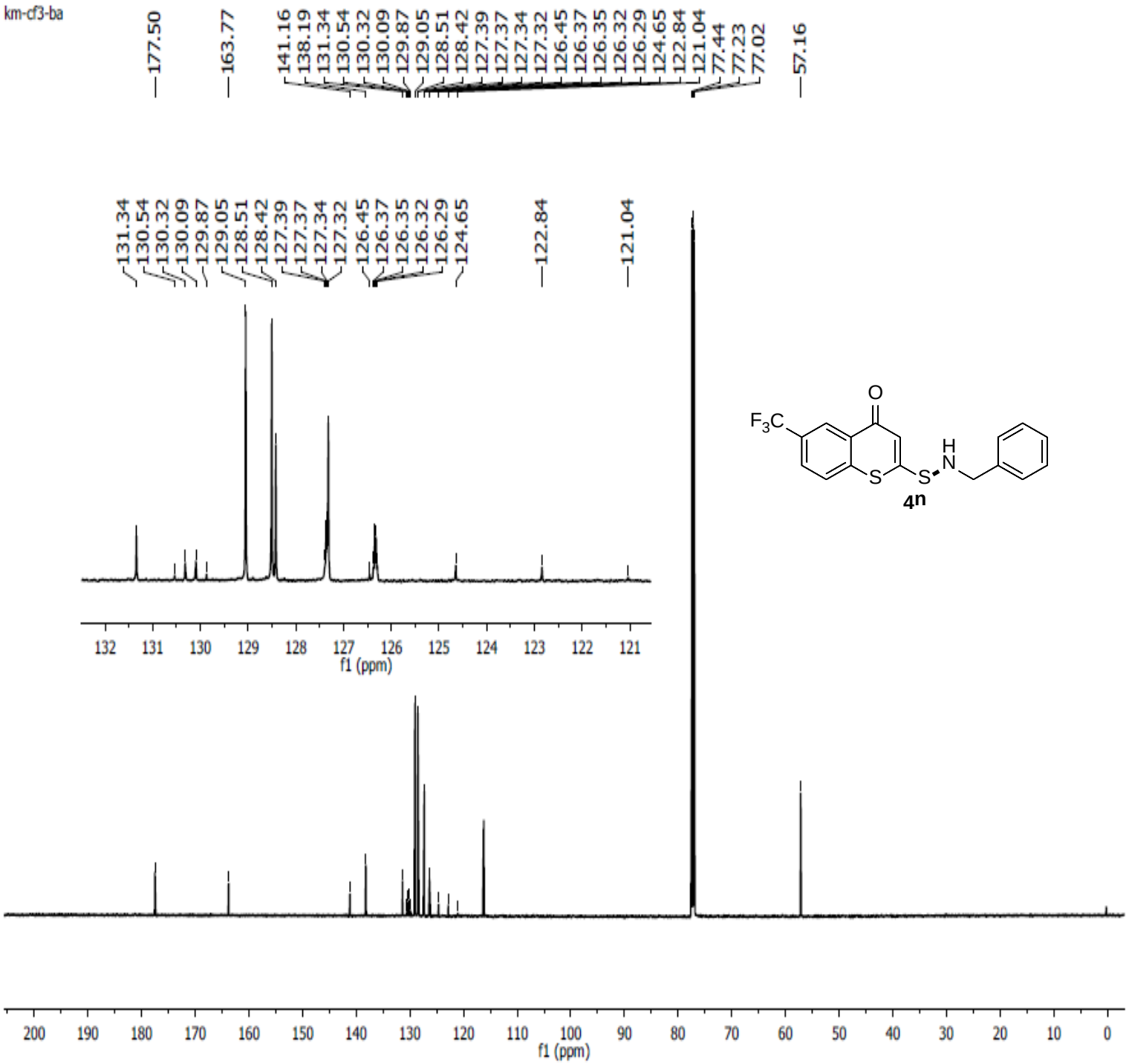
^{1}HNMR spectra of compound: 4n

KM-CF3-T-B-AM-1H
KM-CF3-T-B-AM-1H



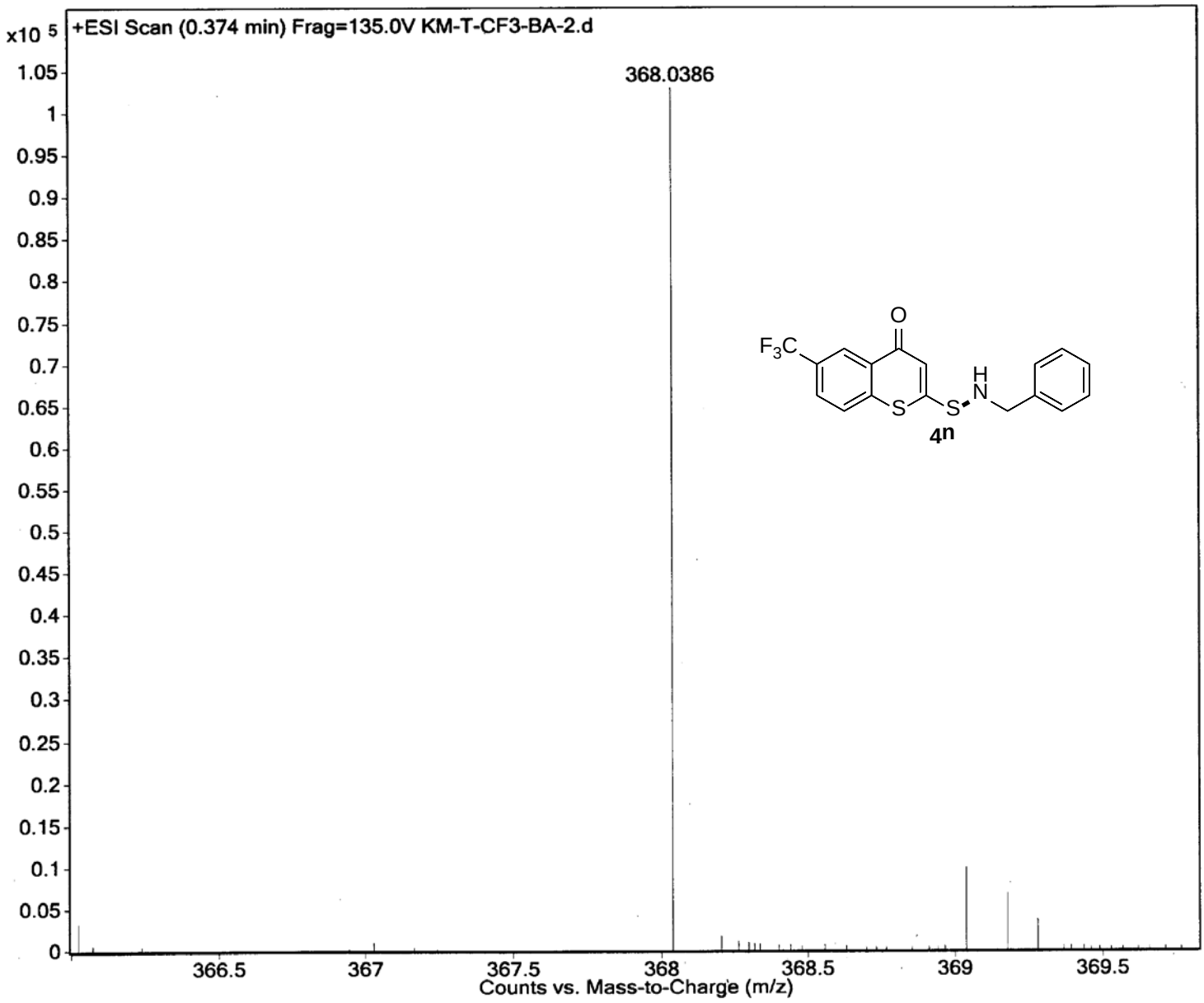
4n

^{13}CNMR spectra of compound: 4n



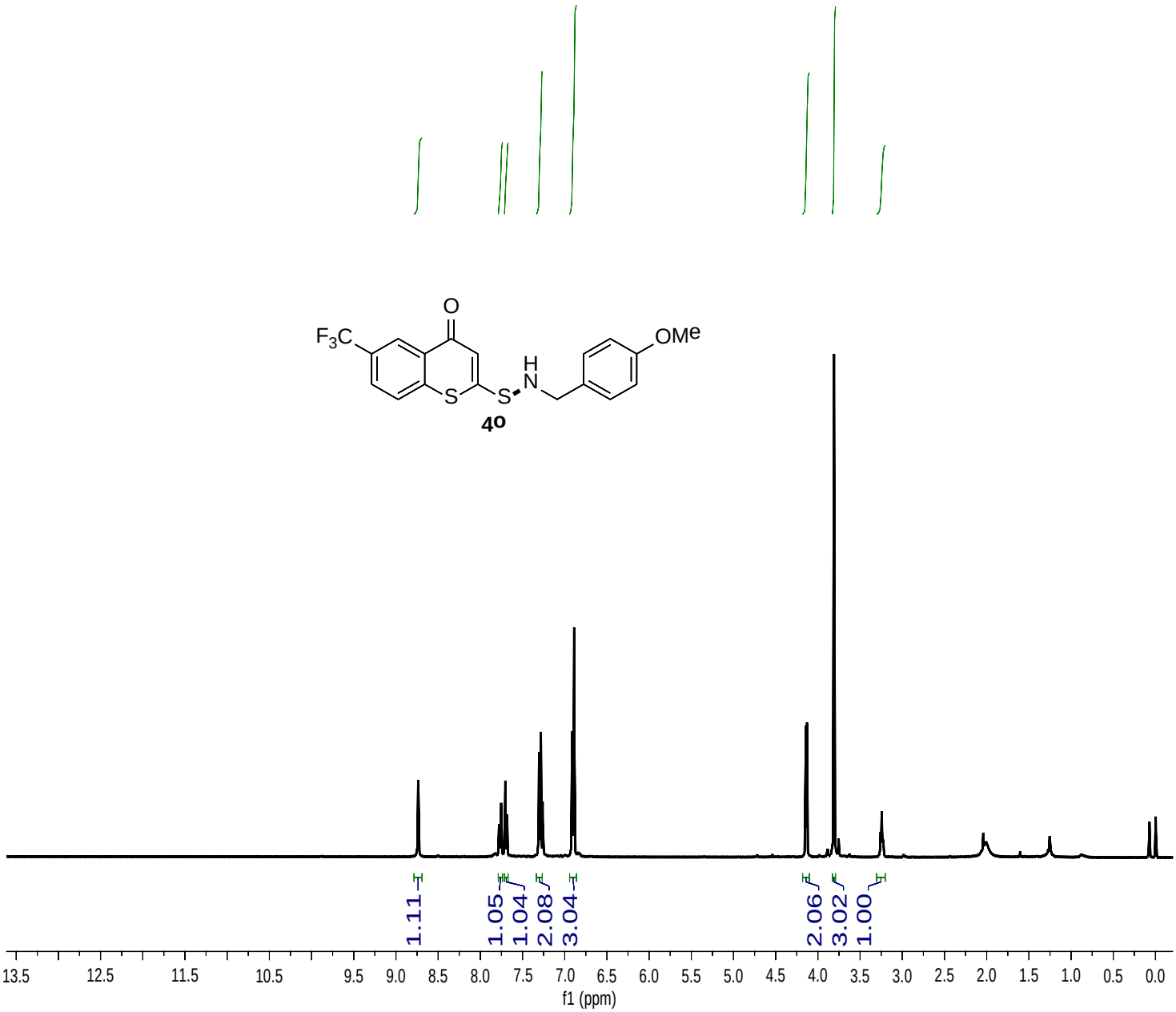
HRMS spectra of compound: 4n

Sample Name	KM-T-CF3-BA-2	**Position**	Vial 1	**Instrument Name**	Instrument 1	**User Name**	
Inj Vol	-1	**InjPosition**		**SampleType**	Sample	**IRM Calibration Status**	Success
Data Filename	KM-T-CF3-BA-2.d	**ACQ Method**		**Comment**		**Acquired Time**	12/26/2017 5:35:45 PM

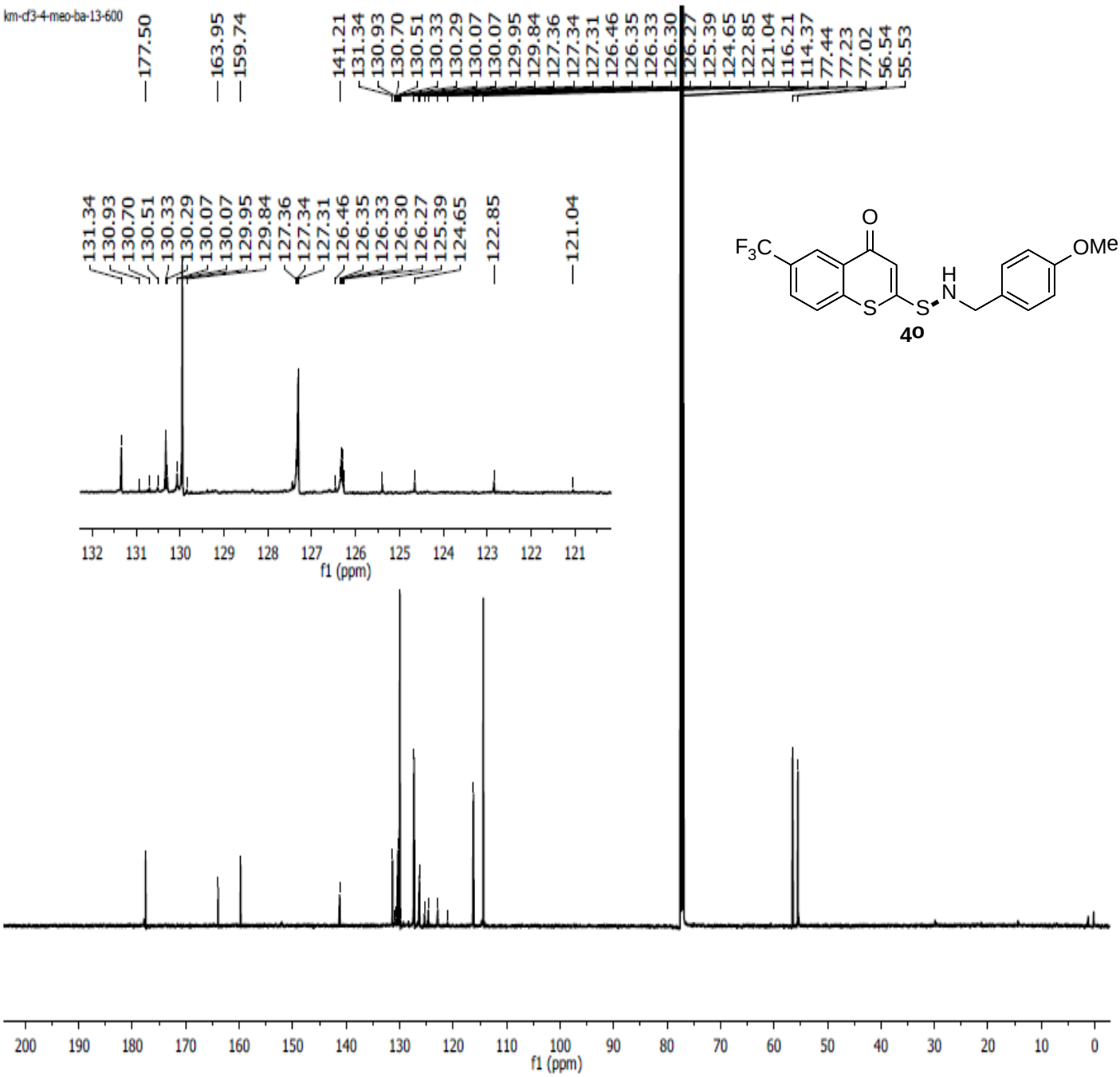


^{1}HNMR spectra of compound: 4o

KM-CF3-T-4MEO-AM-1H
KM-CF3-T-4MEO-AM-1H

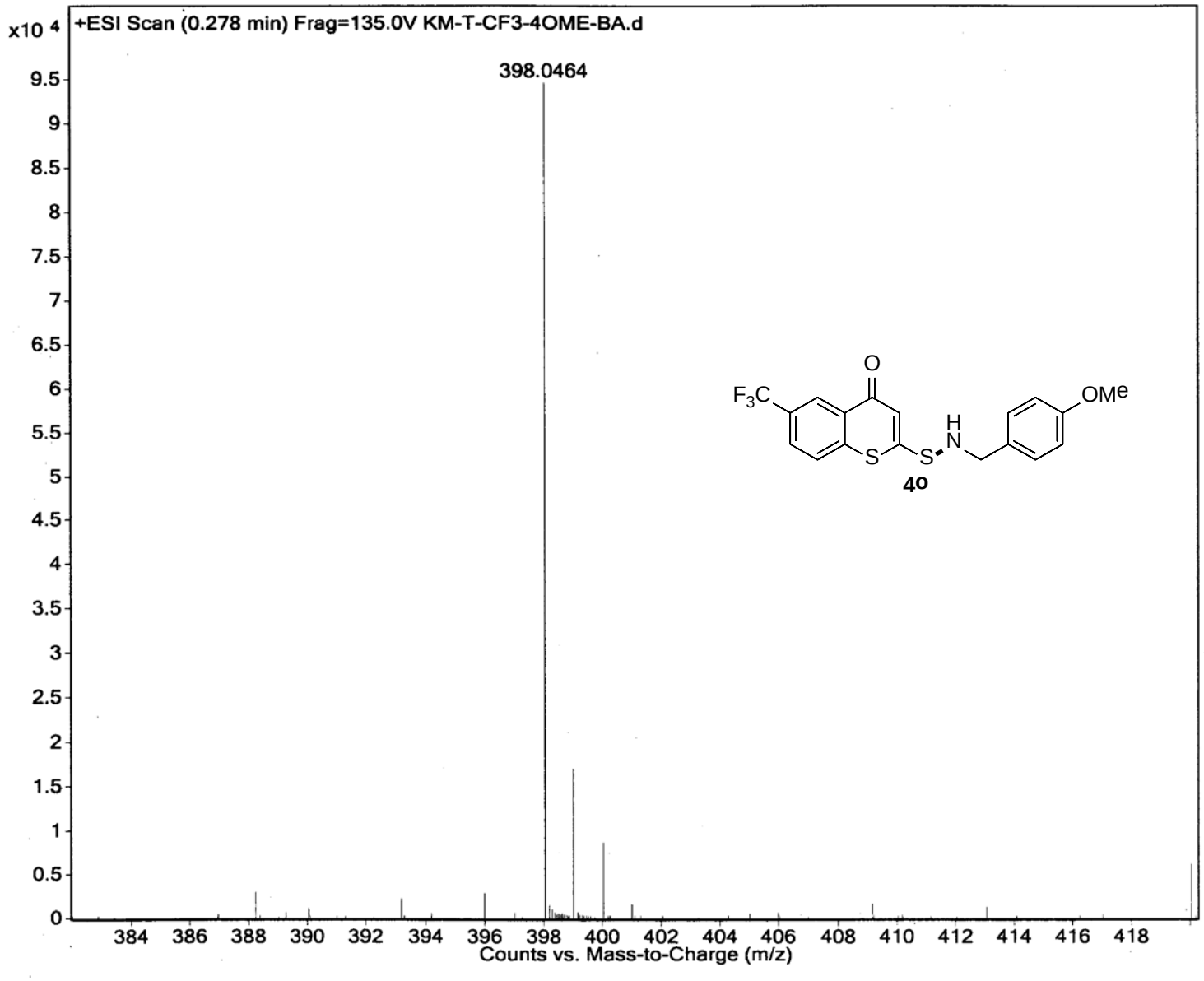


^{13}CNMR spectra of compound: 4o



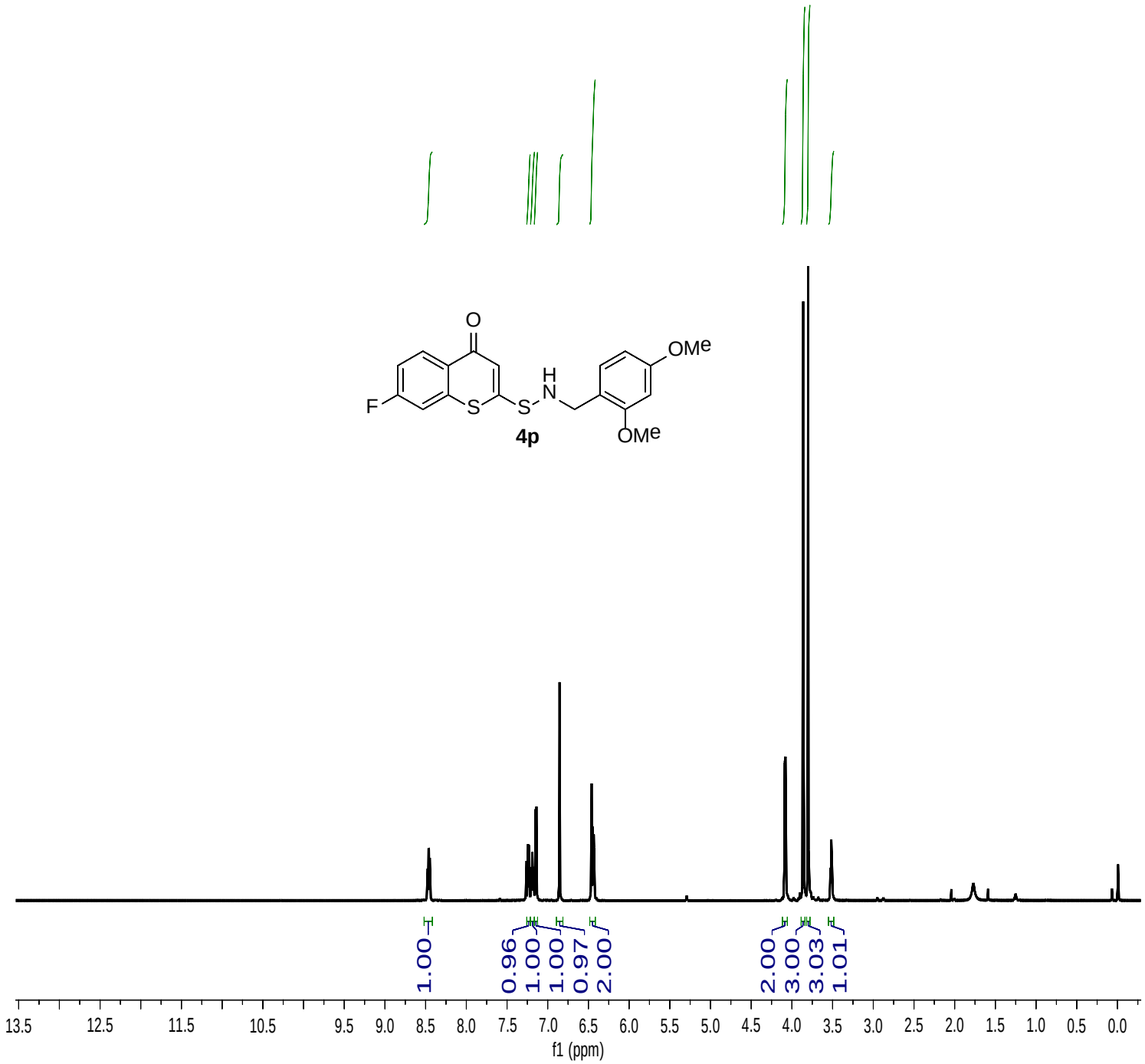
HRMS spectra of compound: 4o

Sample Name	KM-T-CF3-4OME-BA	**Position**	Vial 1	**Instrument Name**	Instrument 1	**User Name**	
Inj Vol	-1	**InjPosition**		**SampleType**	Sample	**IRM Calibration Status**	Success
Data Filename	KM-T-CF3-4OME-BA.d	**ACQ Method**		**Comment**		**Acquired Time**	12/26/2017 12:16:17 PM

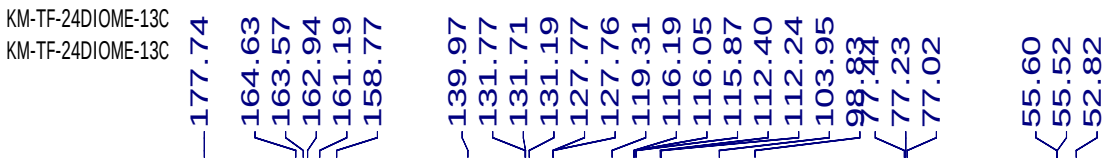


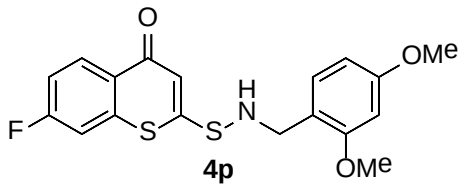
^{1}HNMR spectra of compound: 4p

KM-TF-24DIOME-1H
KM-TF-24DIOME-1H

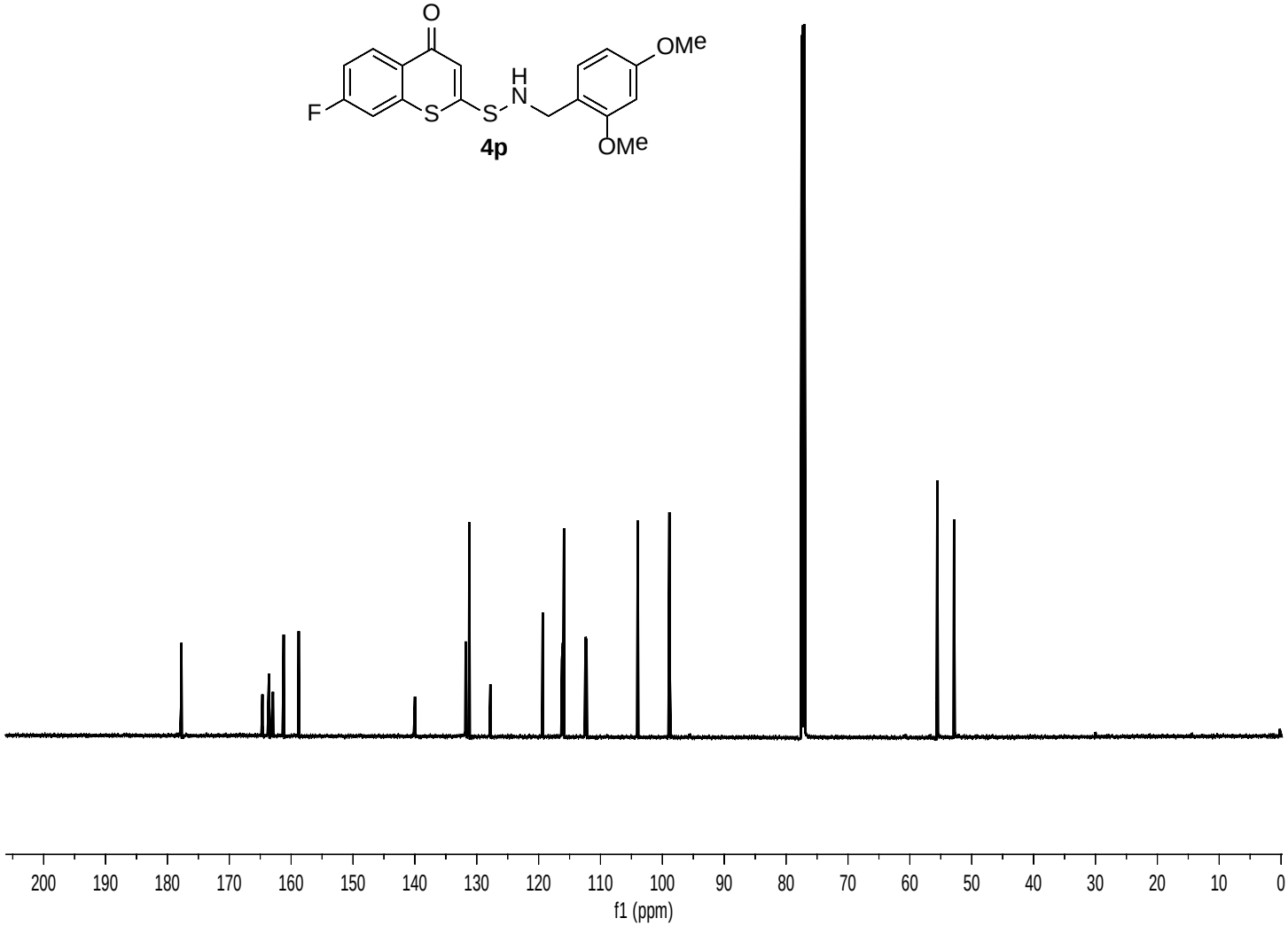


^{13}C NMR spectra of compound: 4p



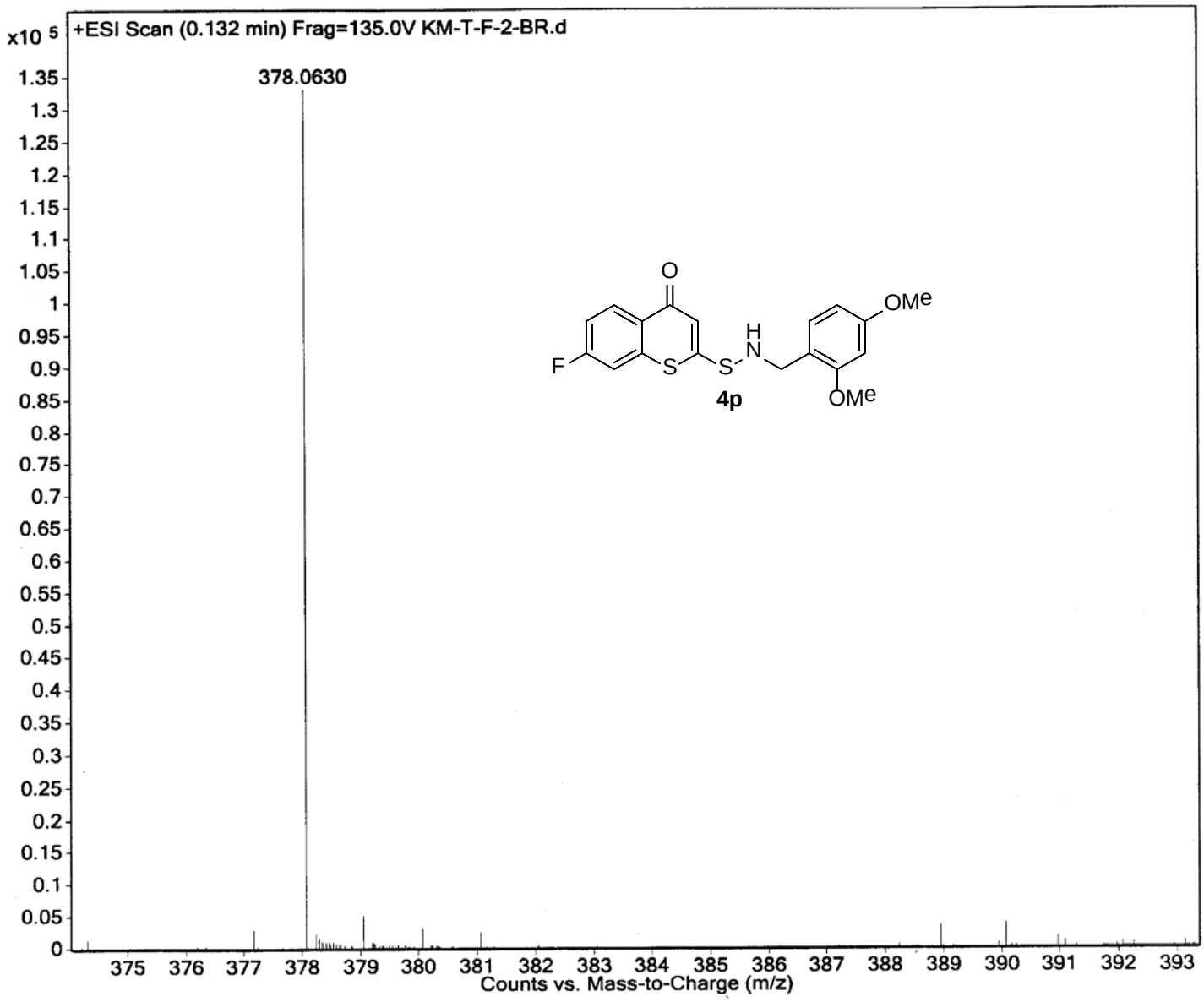


4p

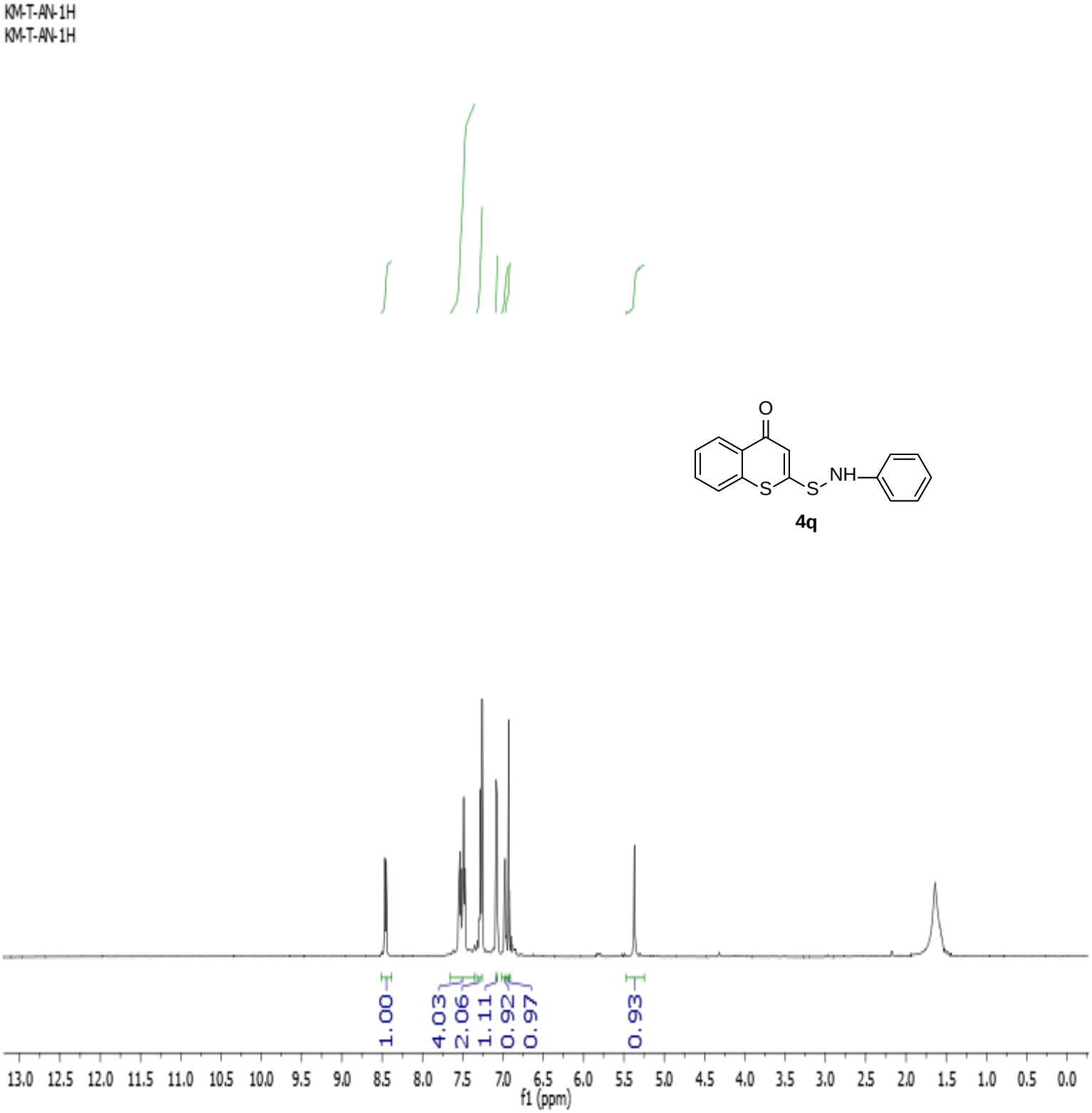


HRMS spectra of compound: 4p

Sample Name	KM-T-F-2-BR	**Position**	Vial 1	**Instrument Name**	Instrument 1	**User Name**	
Inj Vol	-1	**InjPosition**		**SampleType**	Sample	**IRM Calibration Status**	All Ions Missed
Data Filename	KM-T-F-2-BR.d	**ACQ Method**		**Comment**		**Acquired Time**	12/28/2017 11:53:12 AM

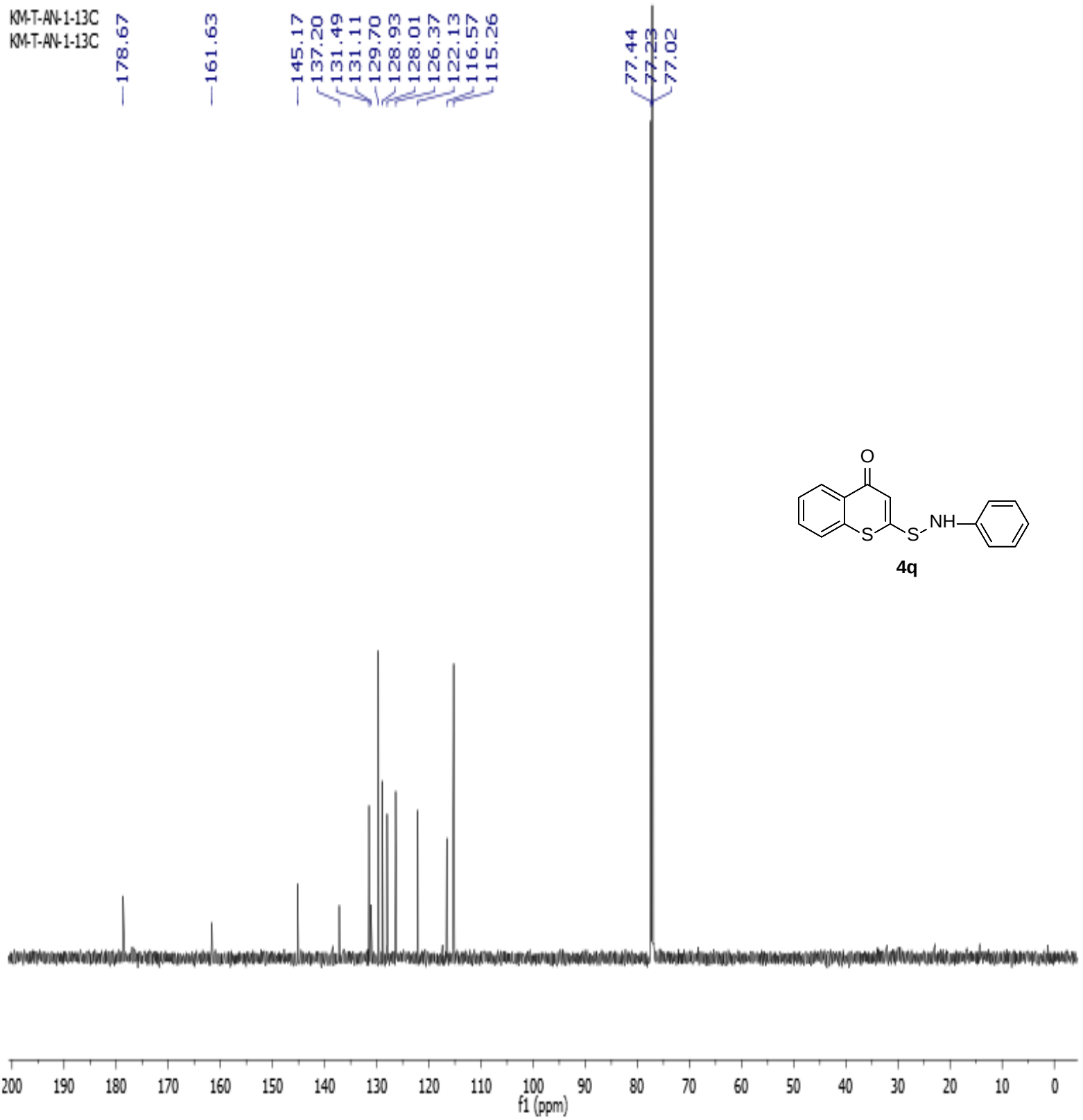


[1]HNMR spectra of compound: 4q



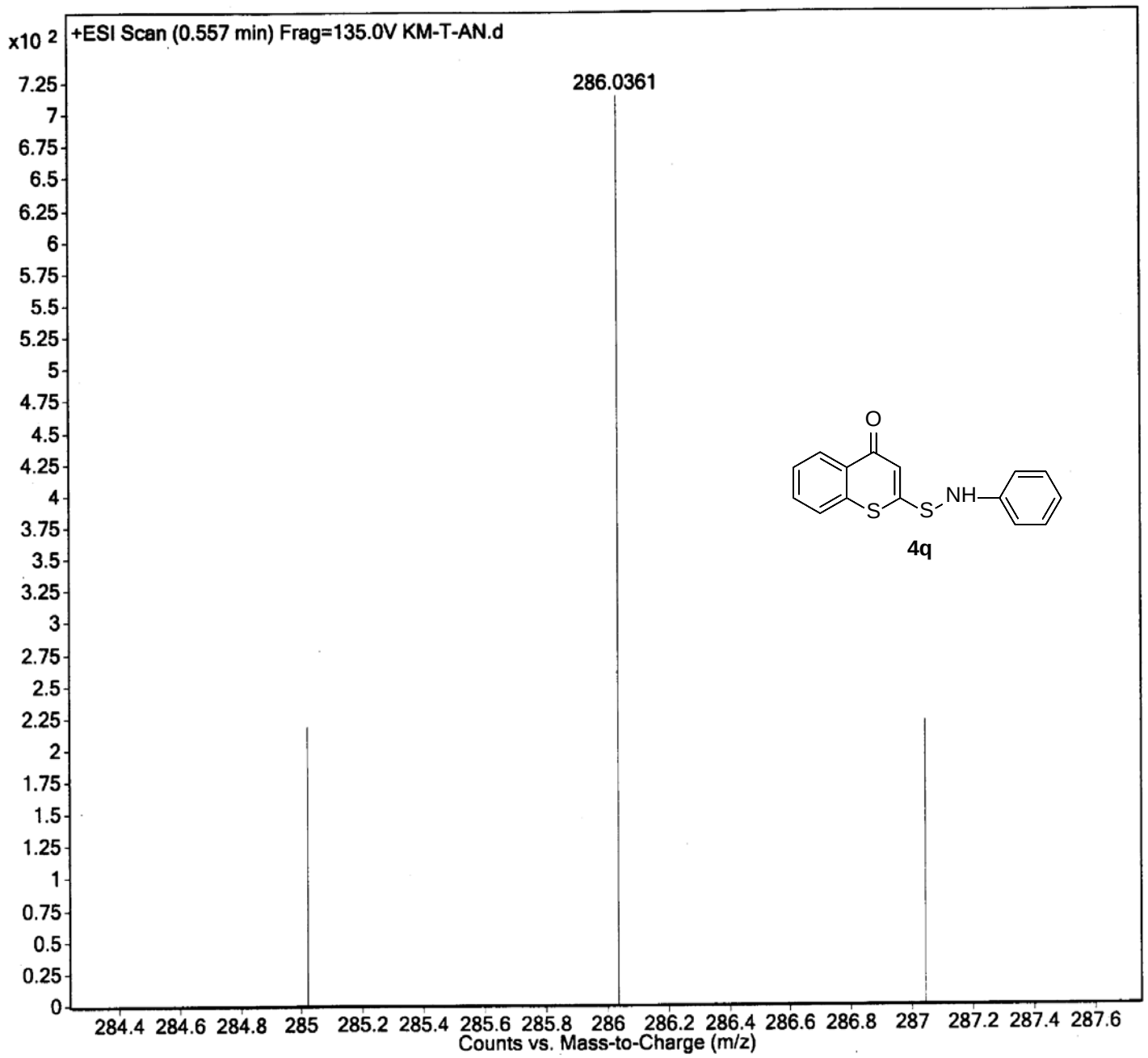
4q

^{13}C NMR spectra of compound: 4q

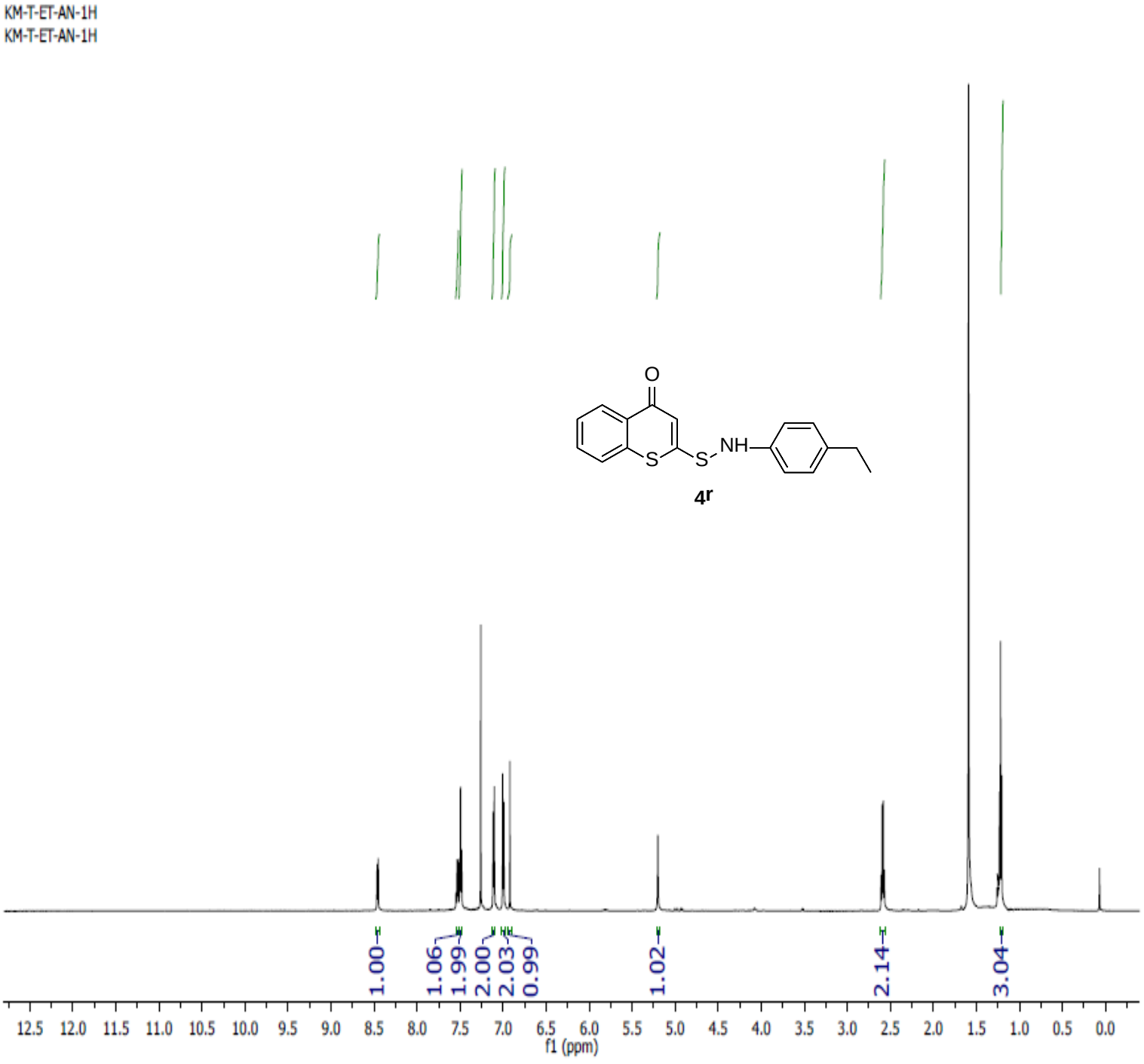


HRMS spectra of compound: 4q

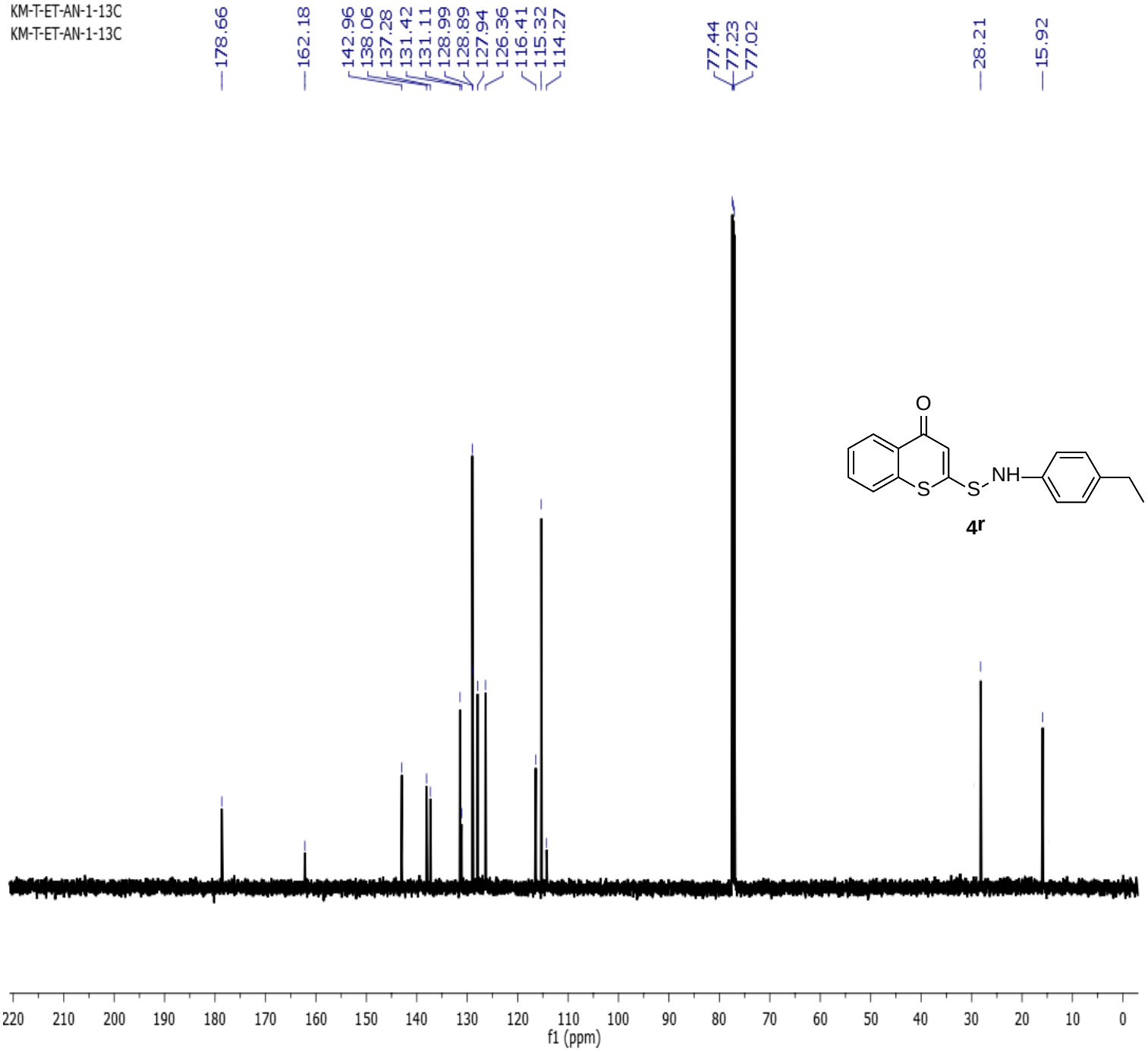
Sample Name	KM-T-AN	**Position**	Vial 1	**Instrument Name**	Instrument 1	**User Name**	
Inj Vol	-1	**InjPosition**		**SampleType**	Sample	**IRM Calibration Status**	All Ions Missed
Data Filename	KM-T-AN.d	**ACQ Method**		**Comment**		**Acquired Time**	1/3/2018 3:53:46 PM



^{1}HNMR spectra of compound: 4r

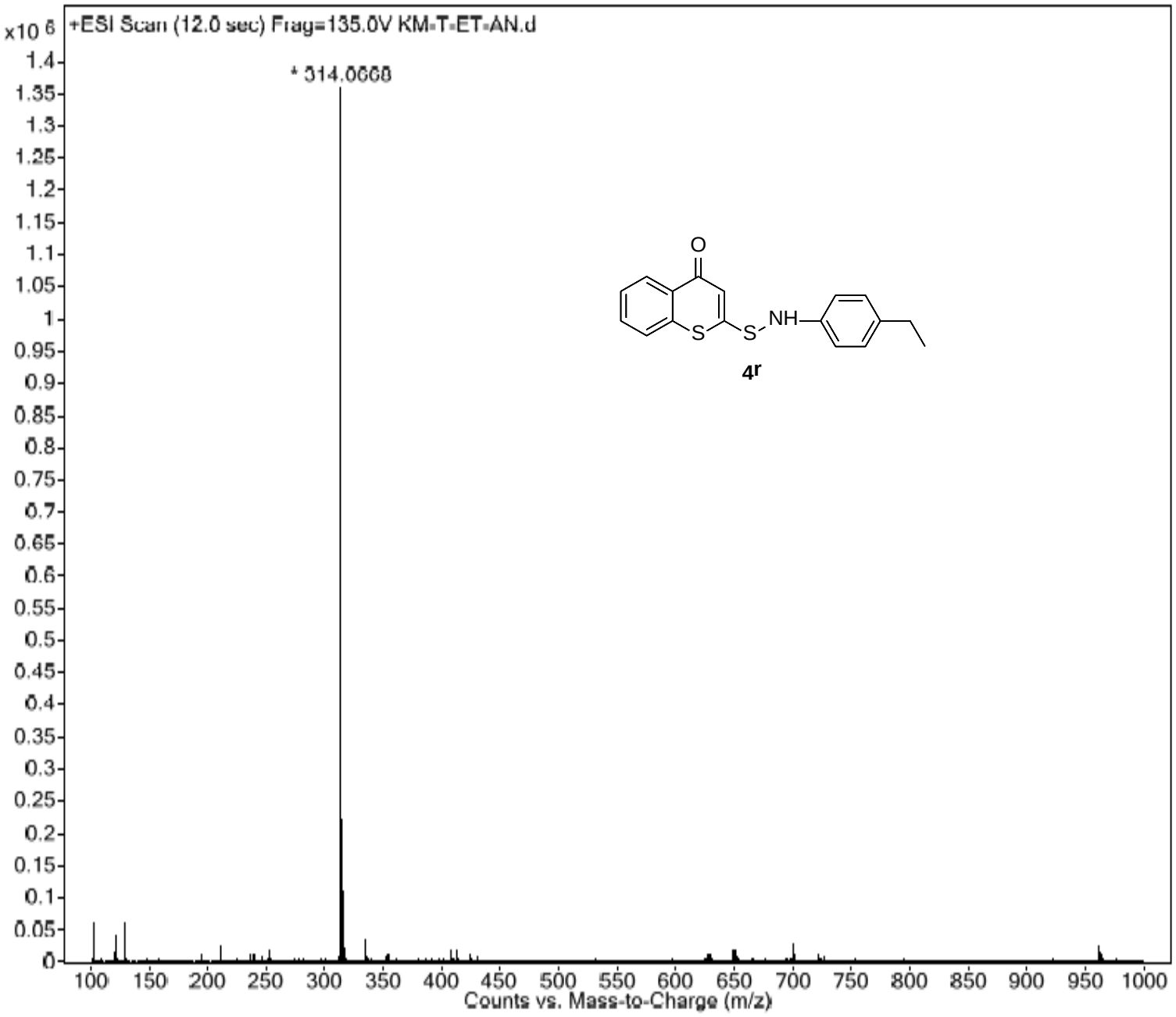


^{13}CNMR spectra of compound: 4n



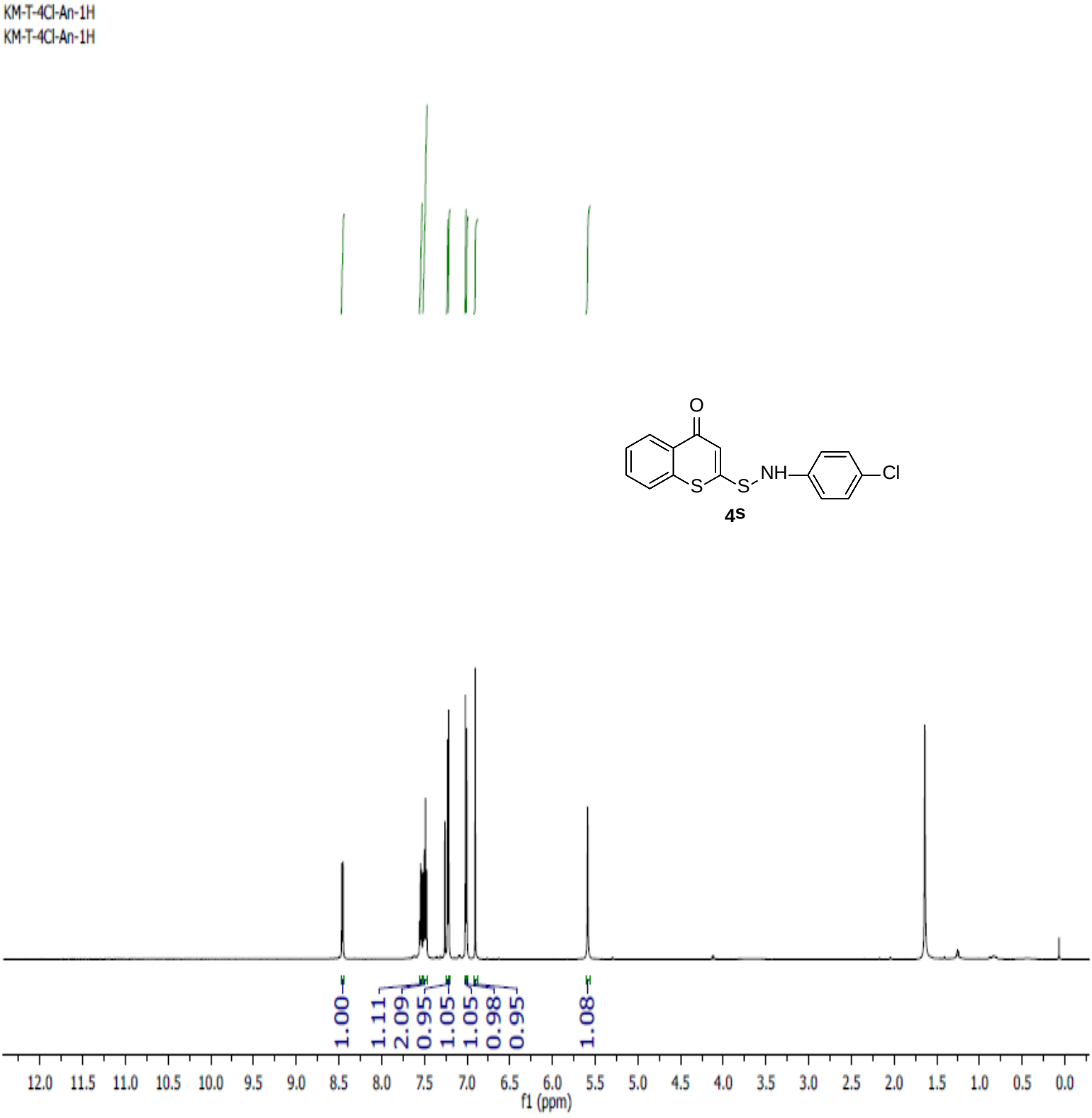
HRMS spectra of compound: 4n

Sample Name	KM-T-ET-AN	**Position**	Vial 1	**Instrument Name**	Instrument 1	**User Name**	
Inj Vol	0	**InjPosition**		**SampleType**	Sample	**IRM Calibration Status**	Some Ions Missed
Data Filename	KM-T-ET-AN.d	**ACQ Method**		**Comment**		**Acquired Time**	3/31/2017 5:02:27 PM

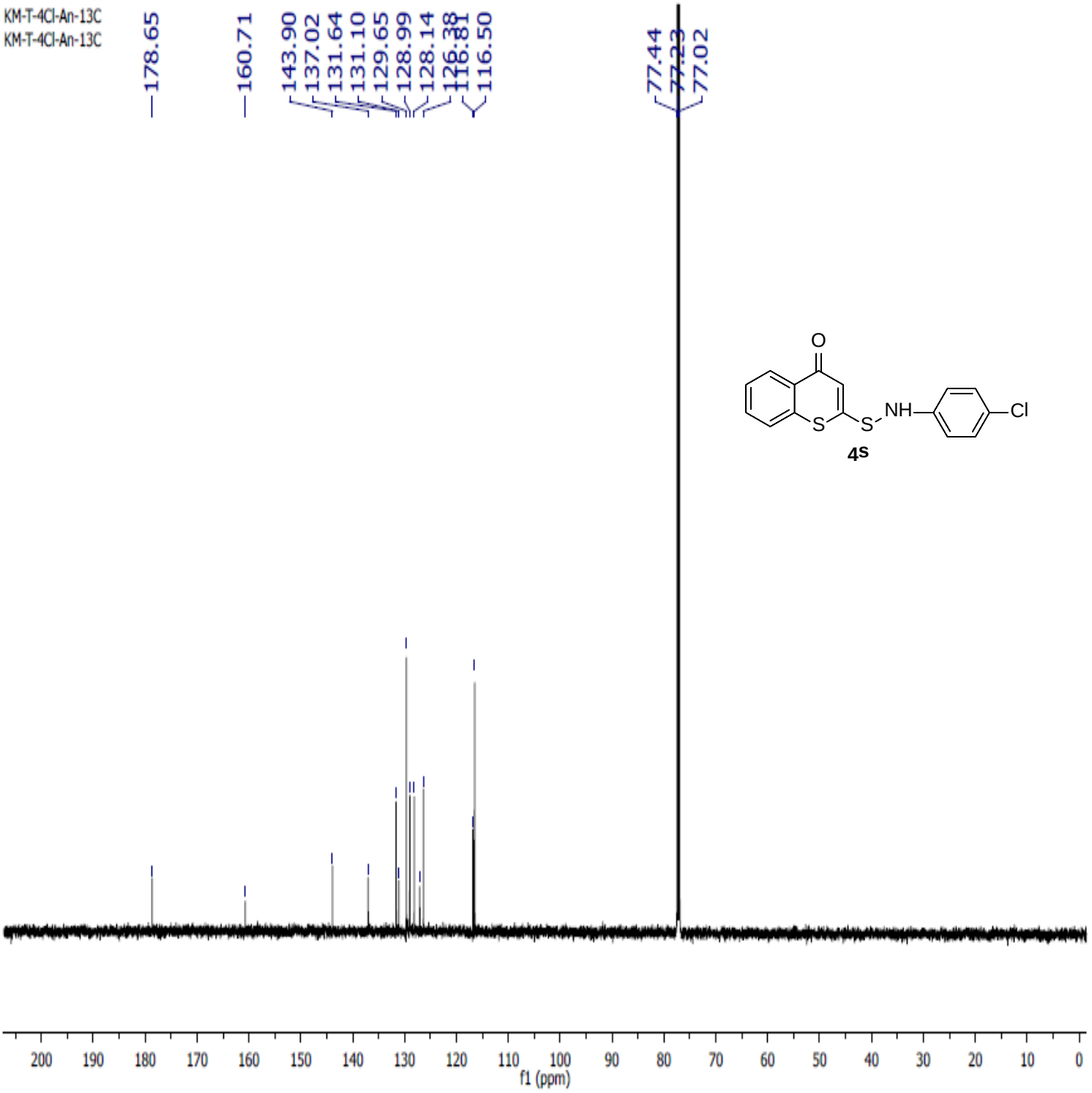


4r

[1]HNMR spectra of compound: 4s

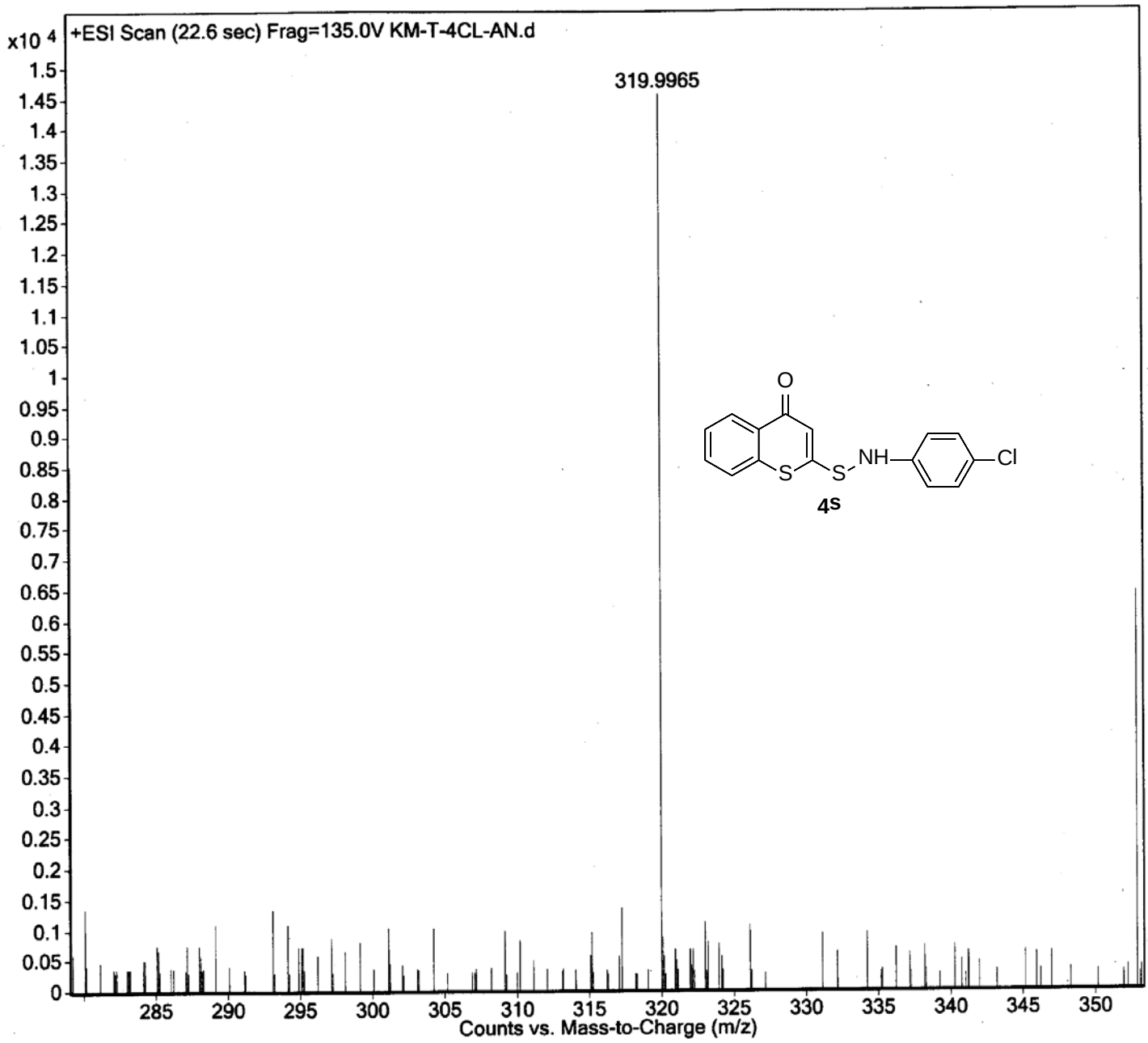


^{13}CNMR spectra of compound: 4s

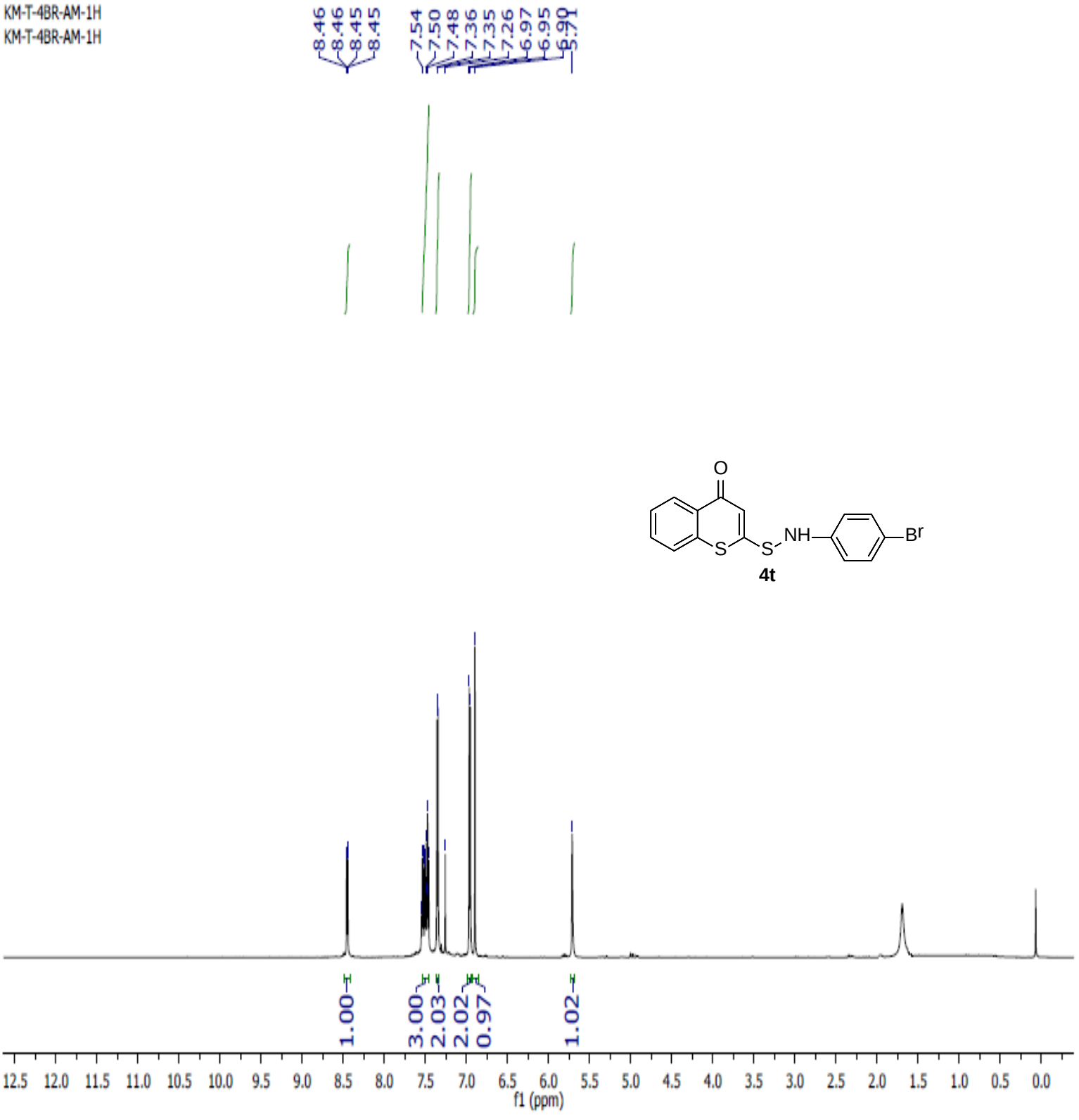


HRMS spectra of compound: 4o

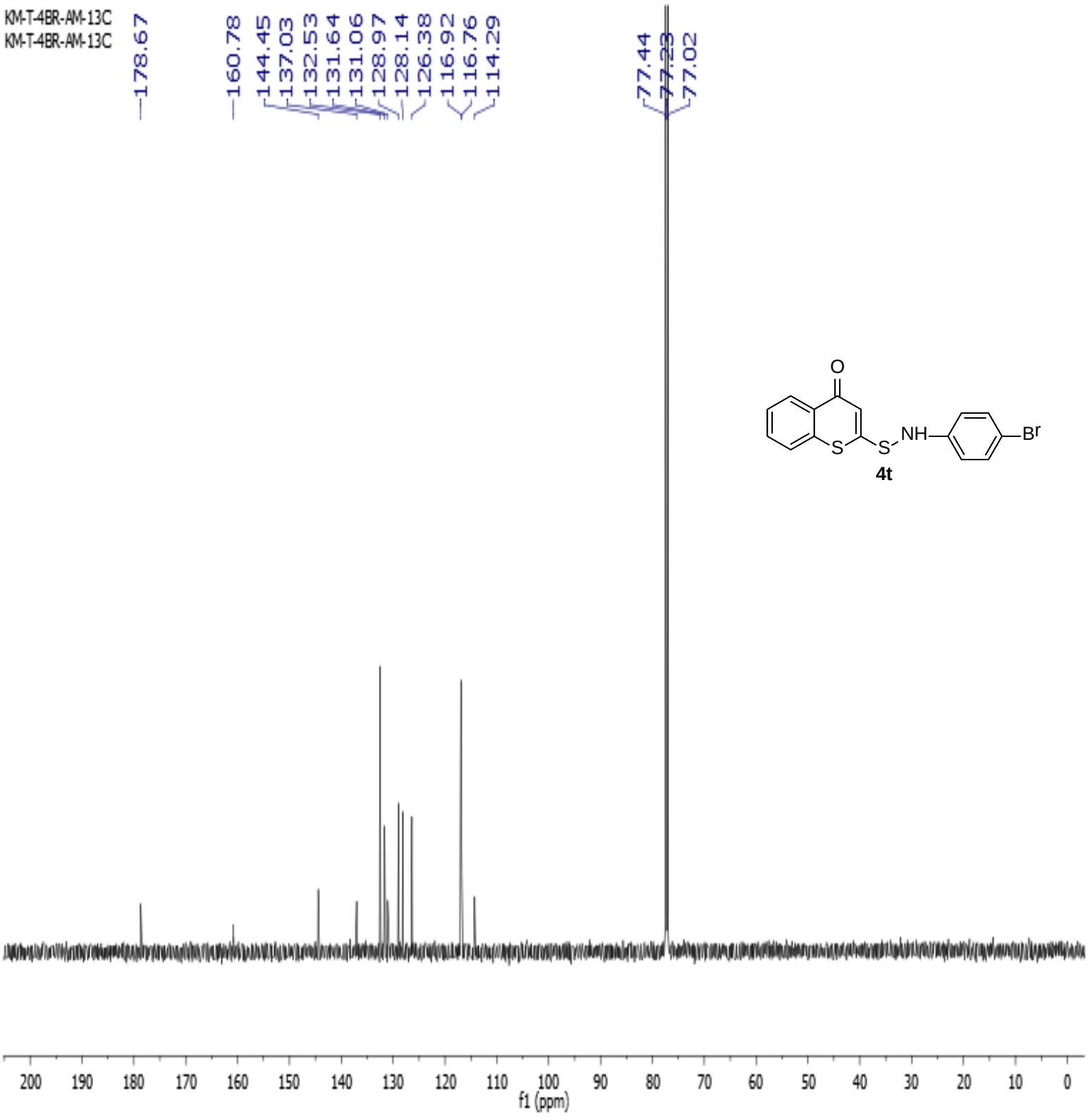
Sample Name	Unavailable	**Position**	Unavailable	**Instrument Name**	Unavailable	**User Name**	Unavailable
Inj Vol	Unavailable	**InjPosition**	Unavailable	**SampleType**	Unavailable	**IRM Calibration Status**	All Ions Missed
Data Filename	KM-T-4CL-AN.d	**ACQ Method**		**Comment**	Sample information is unavailable	**Acquired Time**	Unavailable



[1]HNMR spectra of compound: 4t

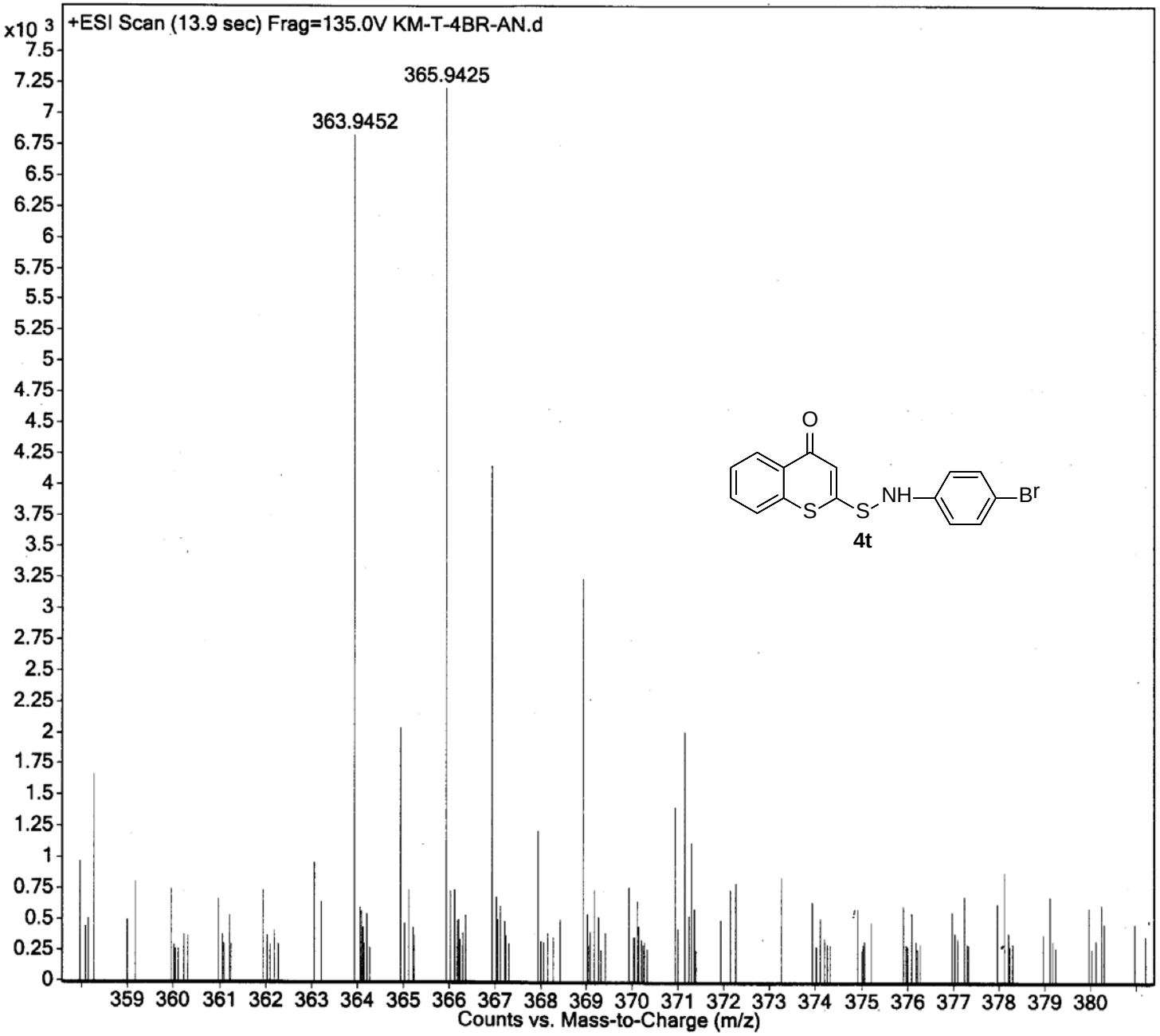


^{13}CNMR spectra of compound: 4p

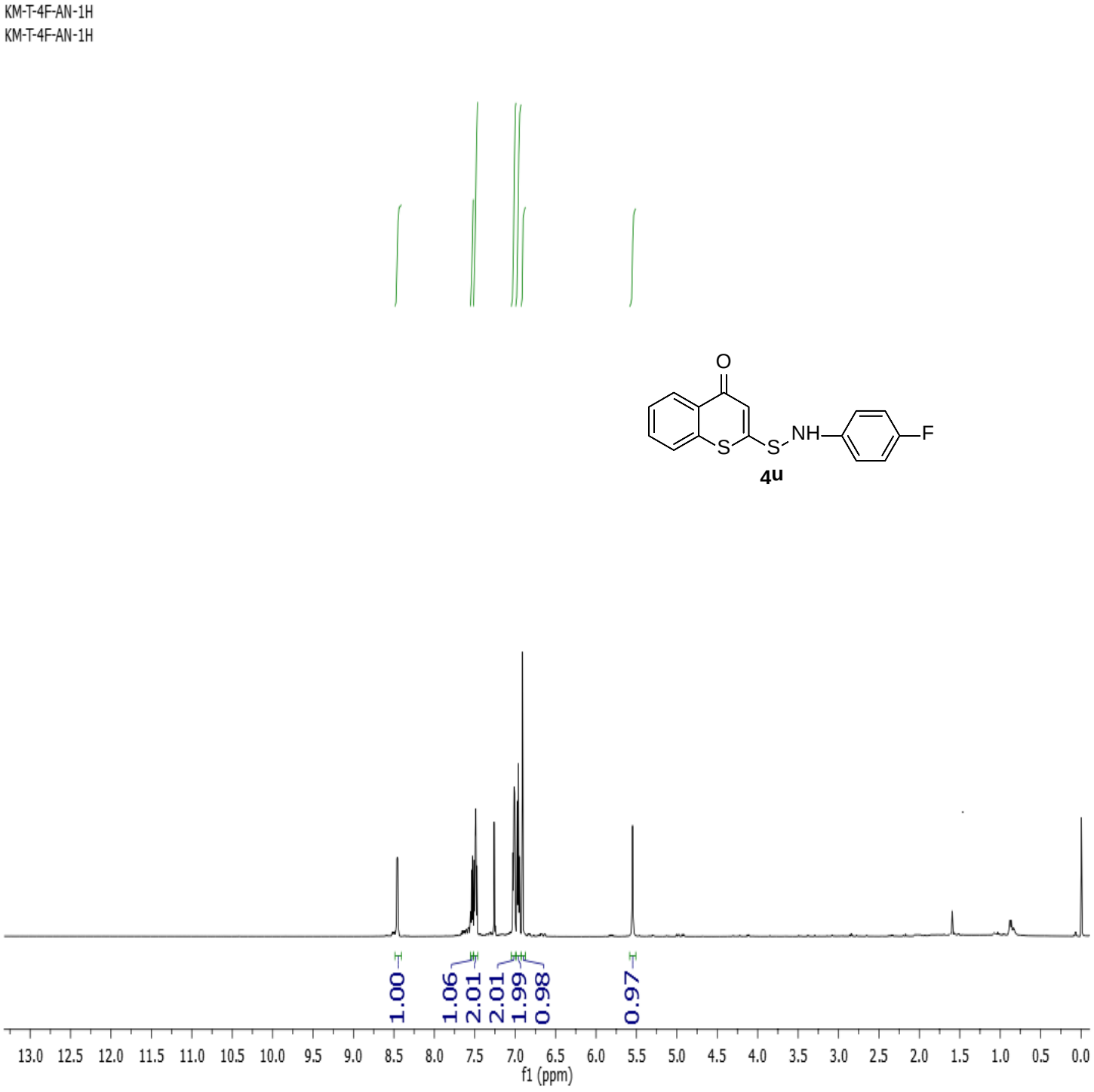


HRMS spectra of compound: 4p

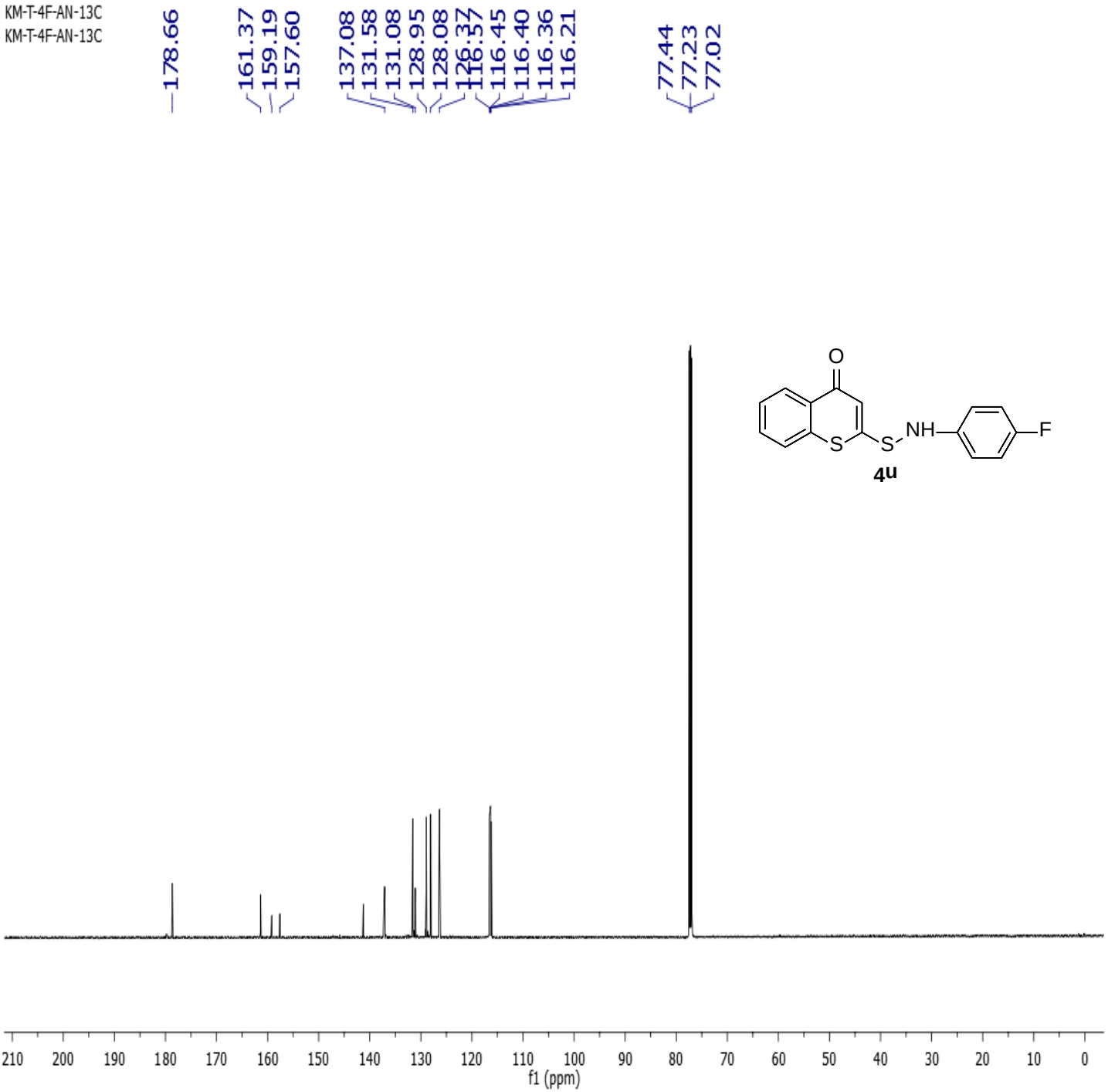
Sample Name	Unavailable	**Position**	Unavailable	**Instrument Name**	Unavailable	**User Name**	Unavailable
Inj Vol	Unavailable	**InjPosition**	Unavailable	**SampleType**	Unavailable	**IRM Calibration Status**	All Ions Missed
Data Filename	KM-T-4BR-AN.d	**ACQ Method**		**Comment**	Sample information is unavailable	**Acquired Time**	Unavailable



[1]HNMR spectra of compound: 4u

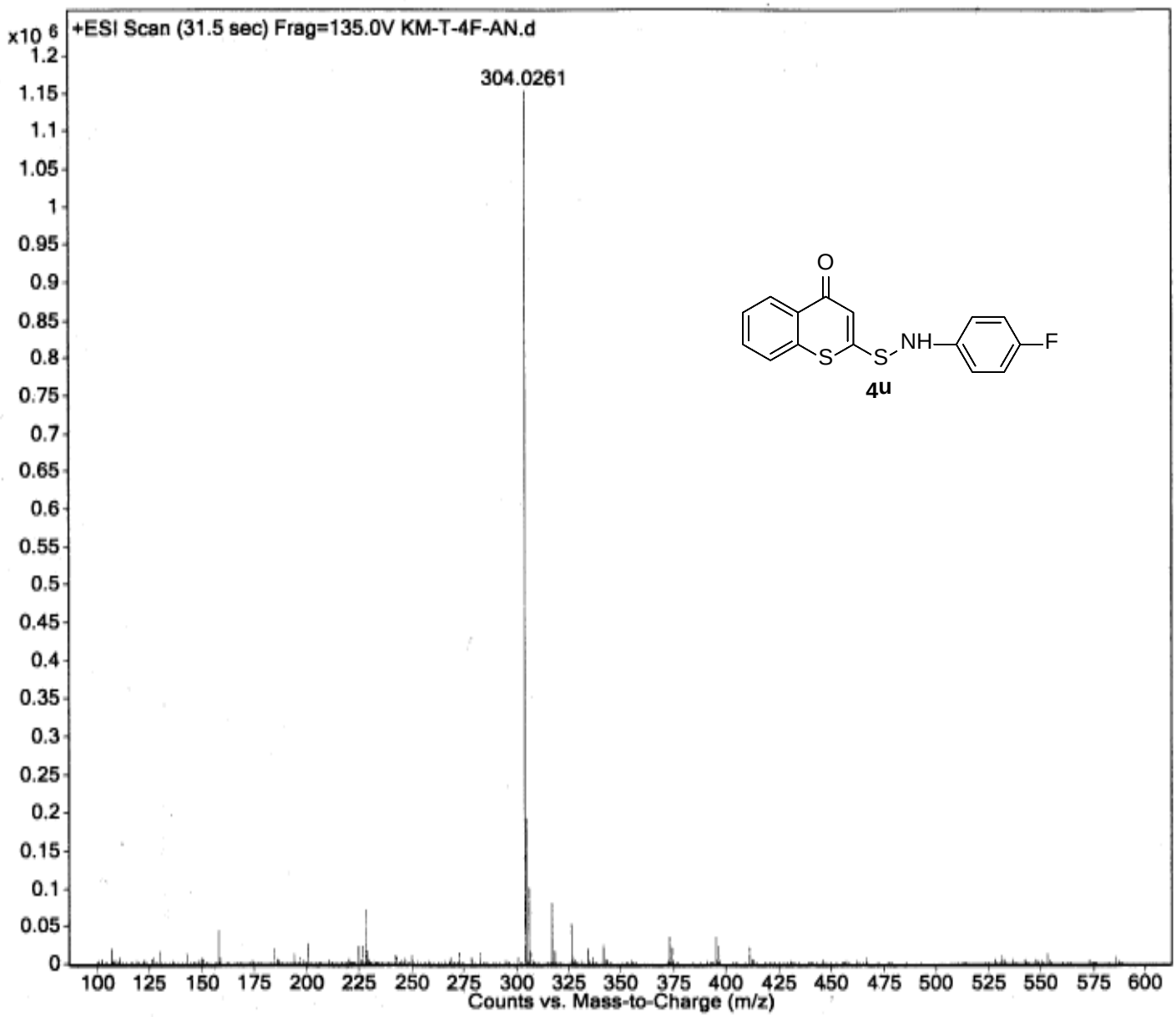


^{13}CNMR spectra of compound: 4u

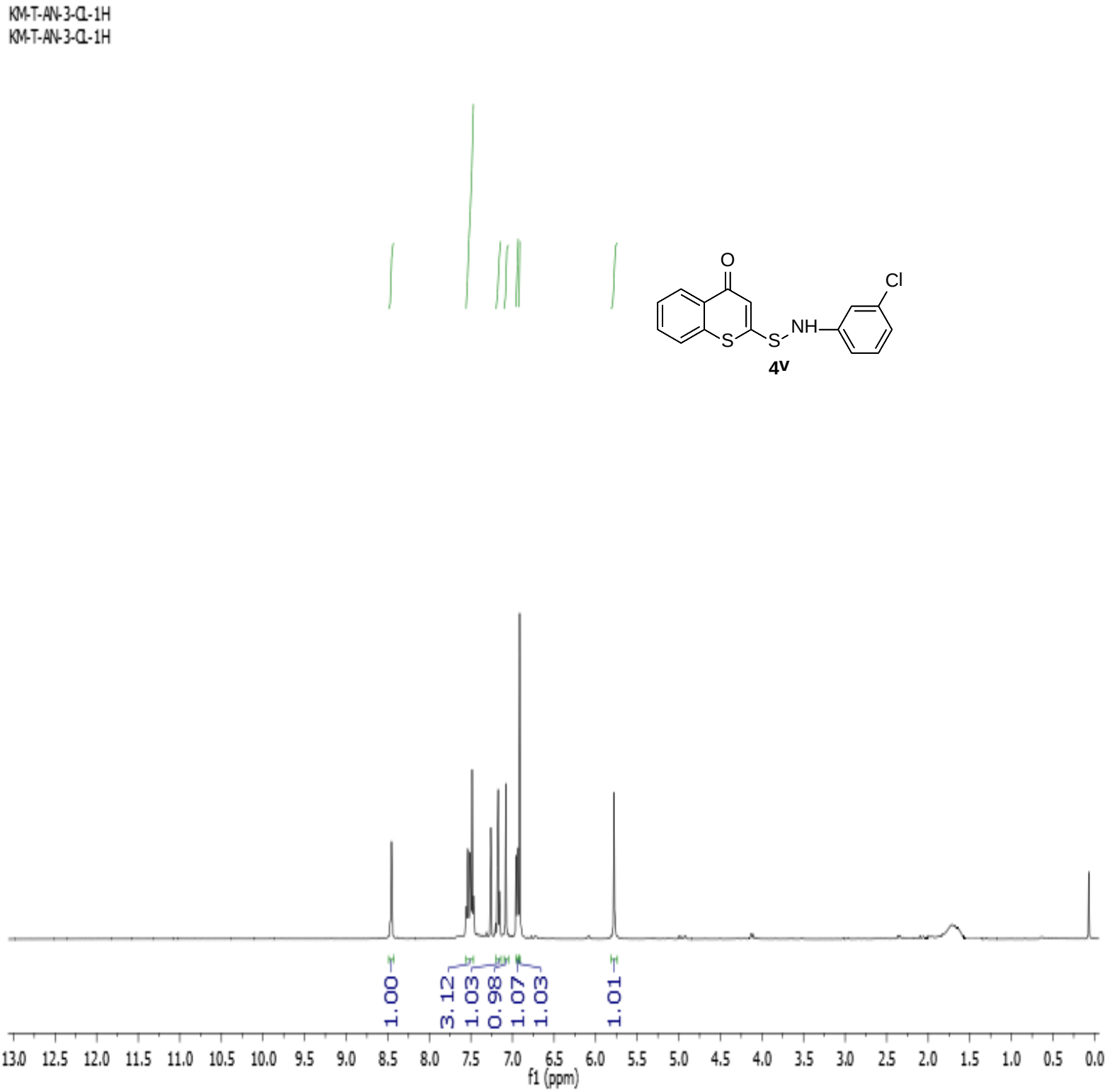


HRMS spectra of compound: 4u

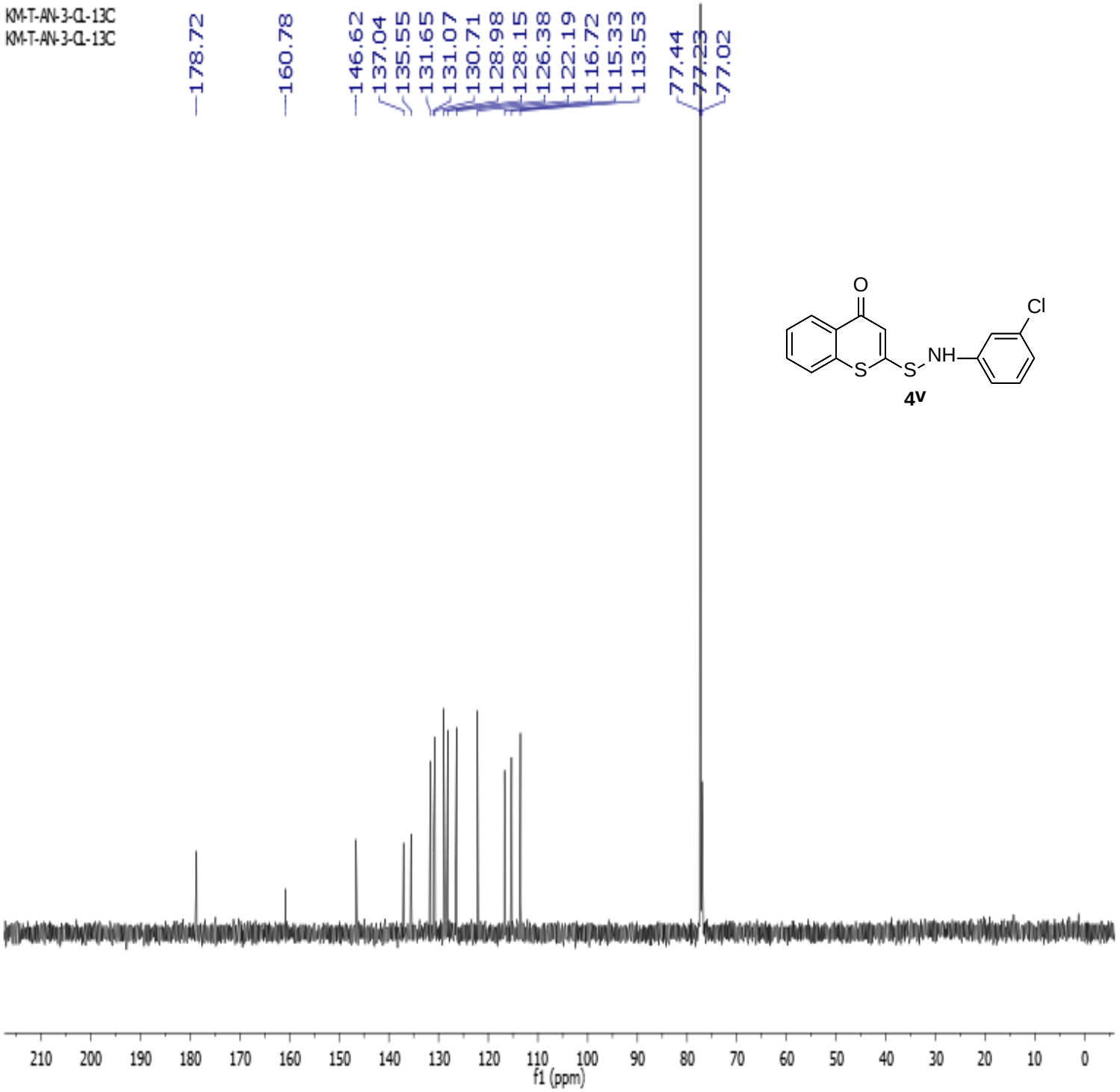
Sample Name	KM-T-4F-AN	**Position**	Vial 1	**Instrument Name**	Instrument 1	**User Name**	
Inj Vol	0	**InjPosition**		**SampleType**	Sample	**IRM Calibration Status**	Success
Data Filename	KM-T-4F-AN.d	**ACQ Method**		**Comment**		**Acquired Time**	10/23/2017 4:35:42 PM



[1]HNMR spectra of compound: 4v

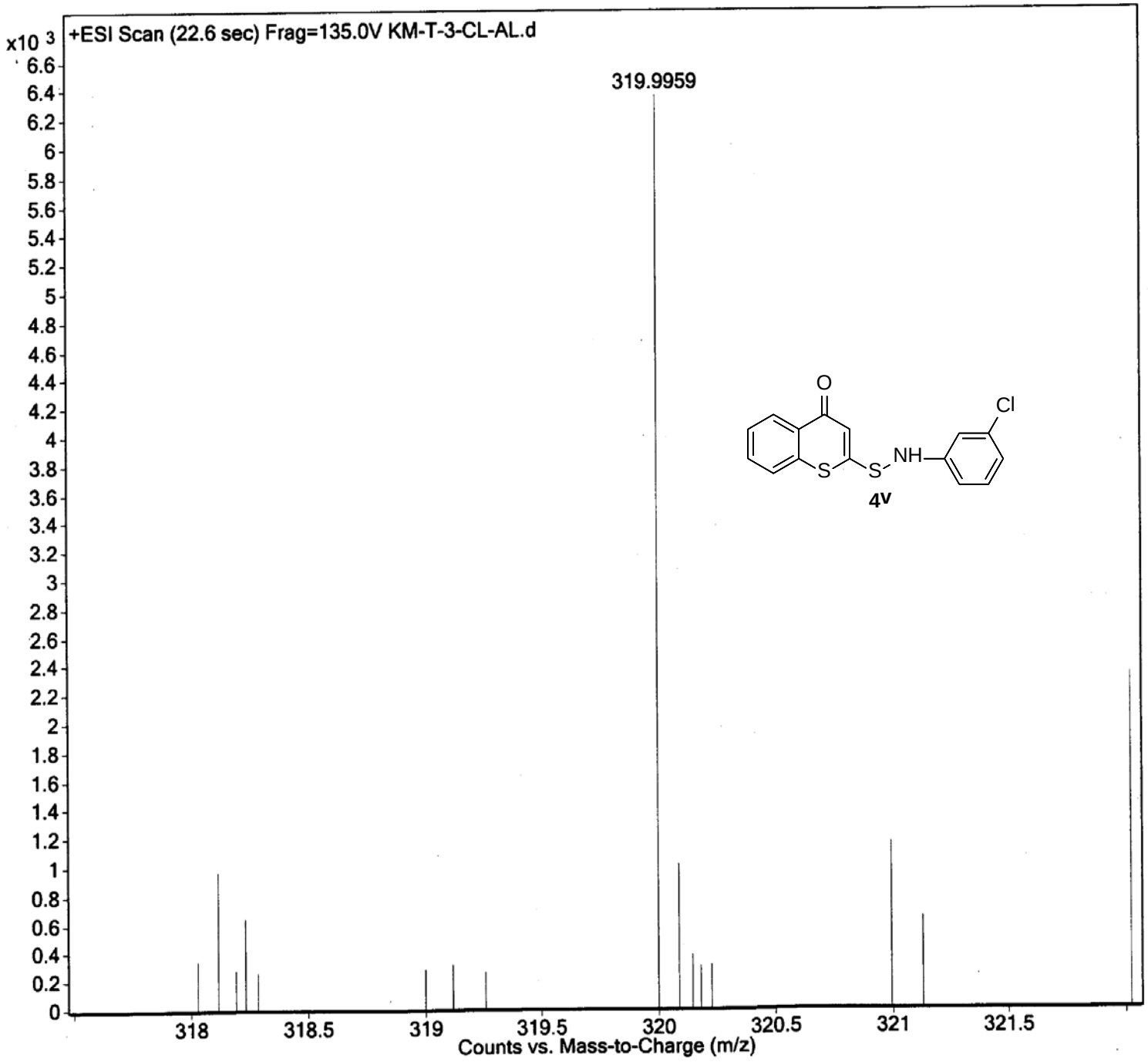


^{13}CNMR spectra of compound: 4r

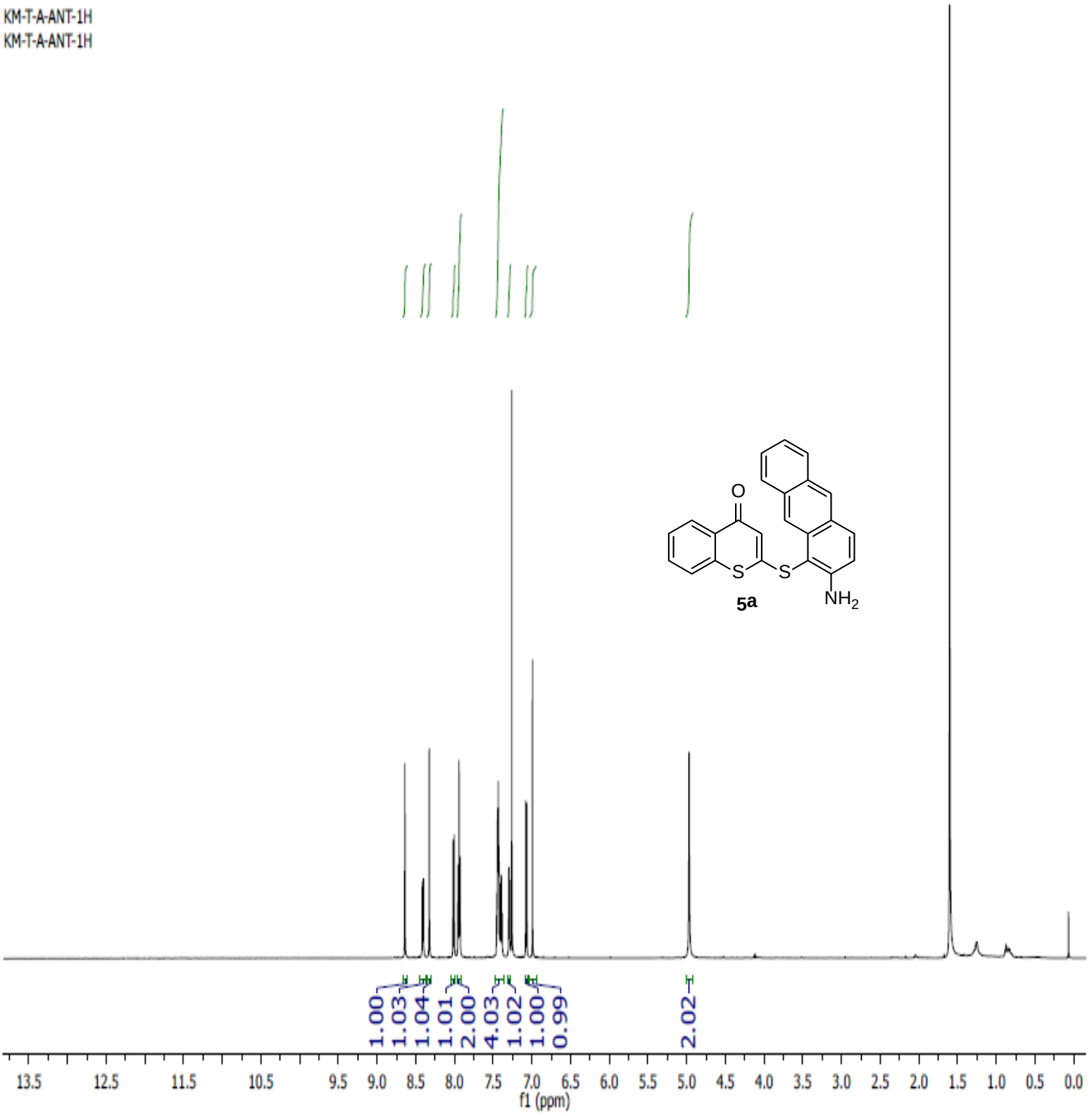


HRMS spectra of compound: 4r

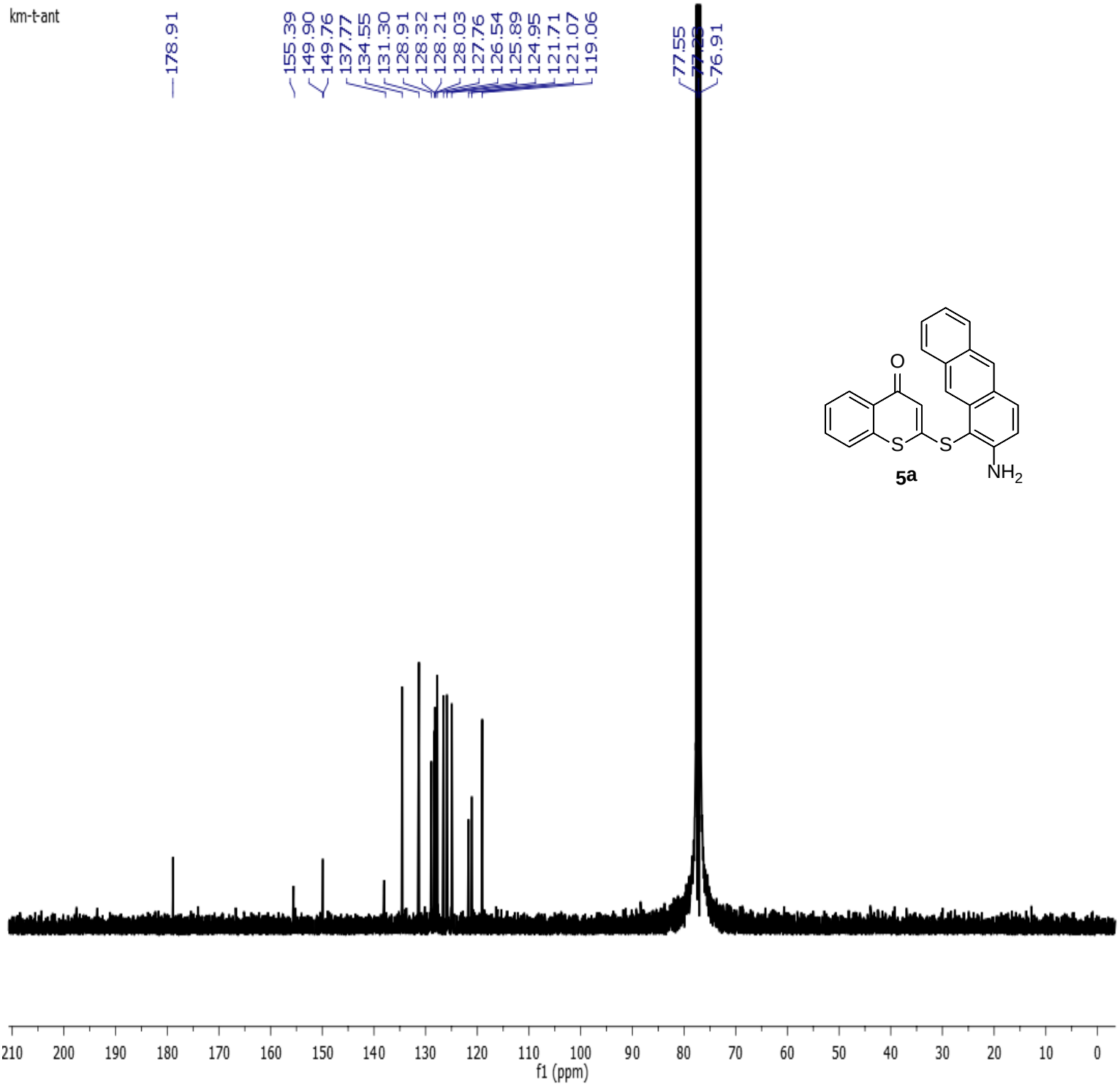
Sample Name	KM-T-3-CL-AL	**Position**	Vial 1	**Instrument Name**	Instrument 1	**User Name**	
Inj Vol	0	**InjPosition**		**SampleType**	Sample	**IRM Calibration Status**	All Ions Missed
Data Filename	KM-T-3-CL-AL.d	**ACQ Method**		**Comment**		**Acquired Time**	1/6/2017 4:17:21 PM



[1]HNMR spectra of compound: 5a

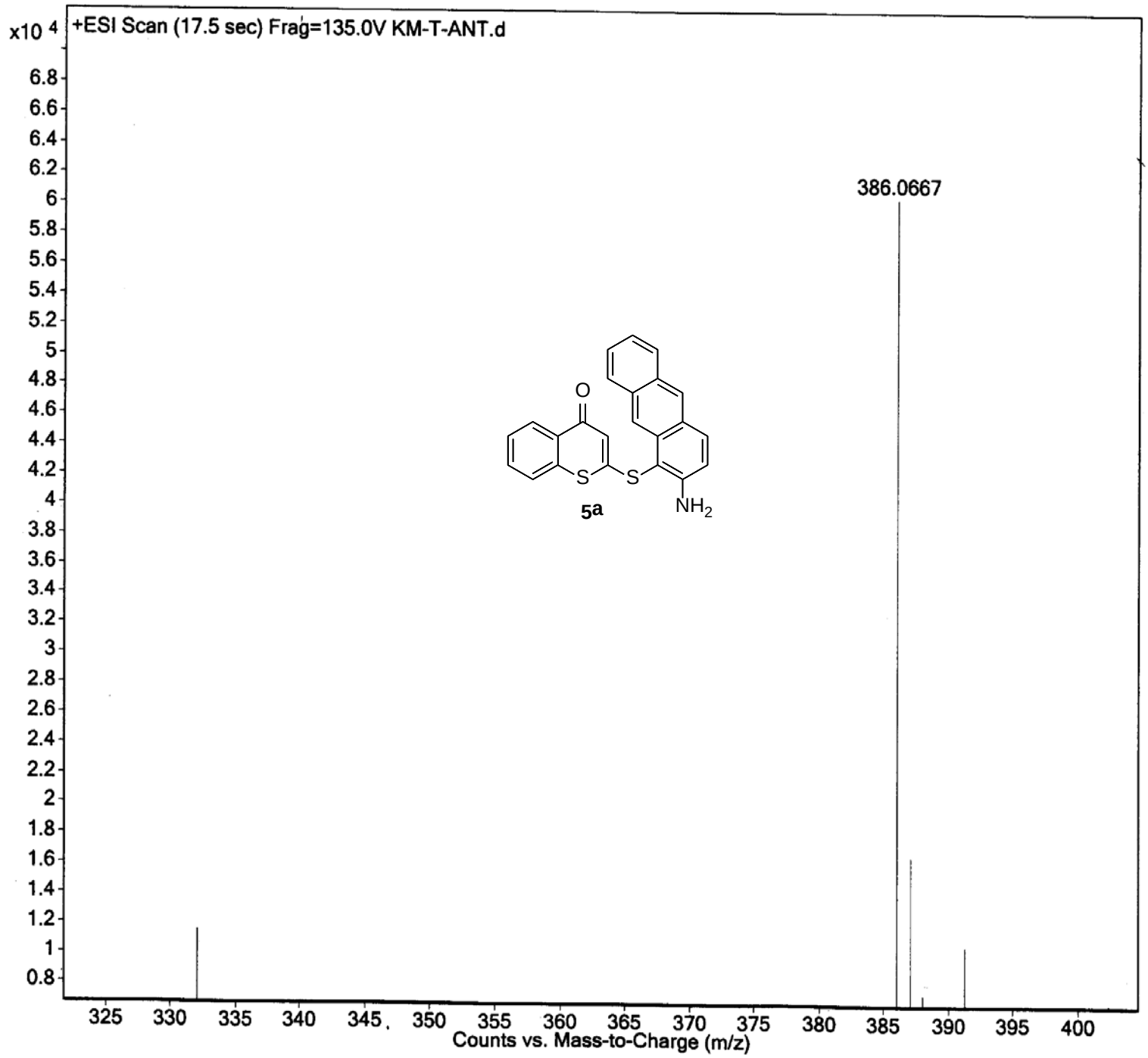


^{13}CNMR spectra of compound: 5a



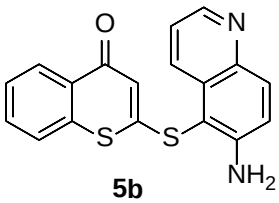
HRMS spectra of compound: 5a

Sample Name	Unavailable	**Position**	Unavailable	**Instrument Name**	Unavailable	**User Name**	Unavailable
Inj Vol	Unavailable	**InjPosition**	Unavailable	**SampleType**	Unavailable	**IRM Calibration Status**	Some Ions Missed
Data Filename	KM-T-ANT.d	**ACQ Method**		**Comment**	Sample information is unavailable	**Acquired Time**	Unavailable

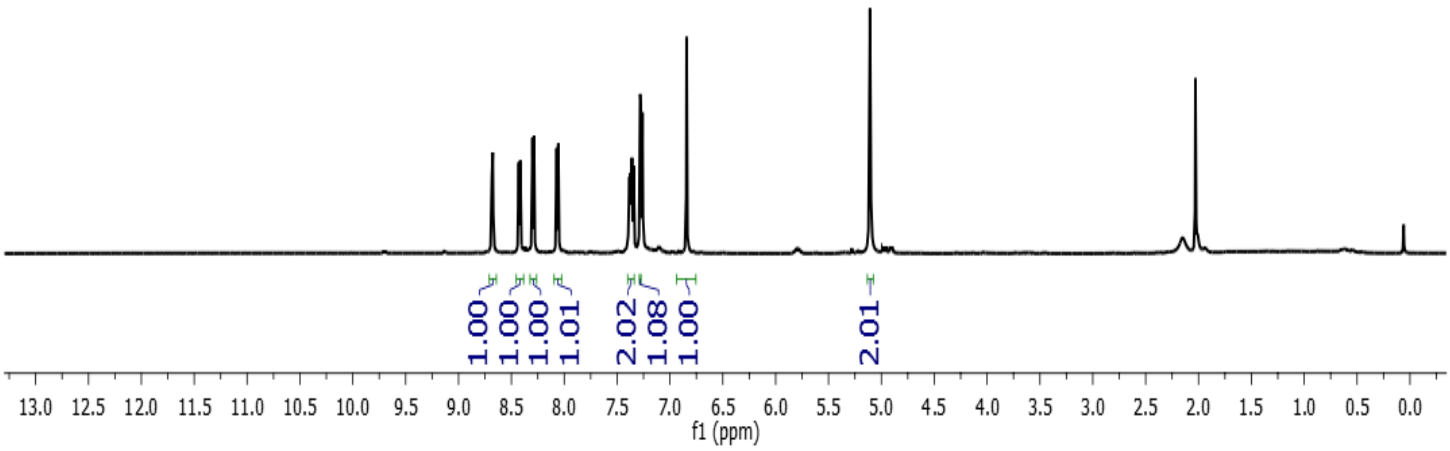


[1]HNMR spectra of compound: 5b

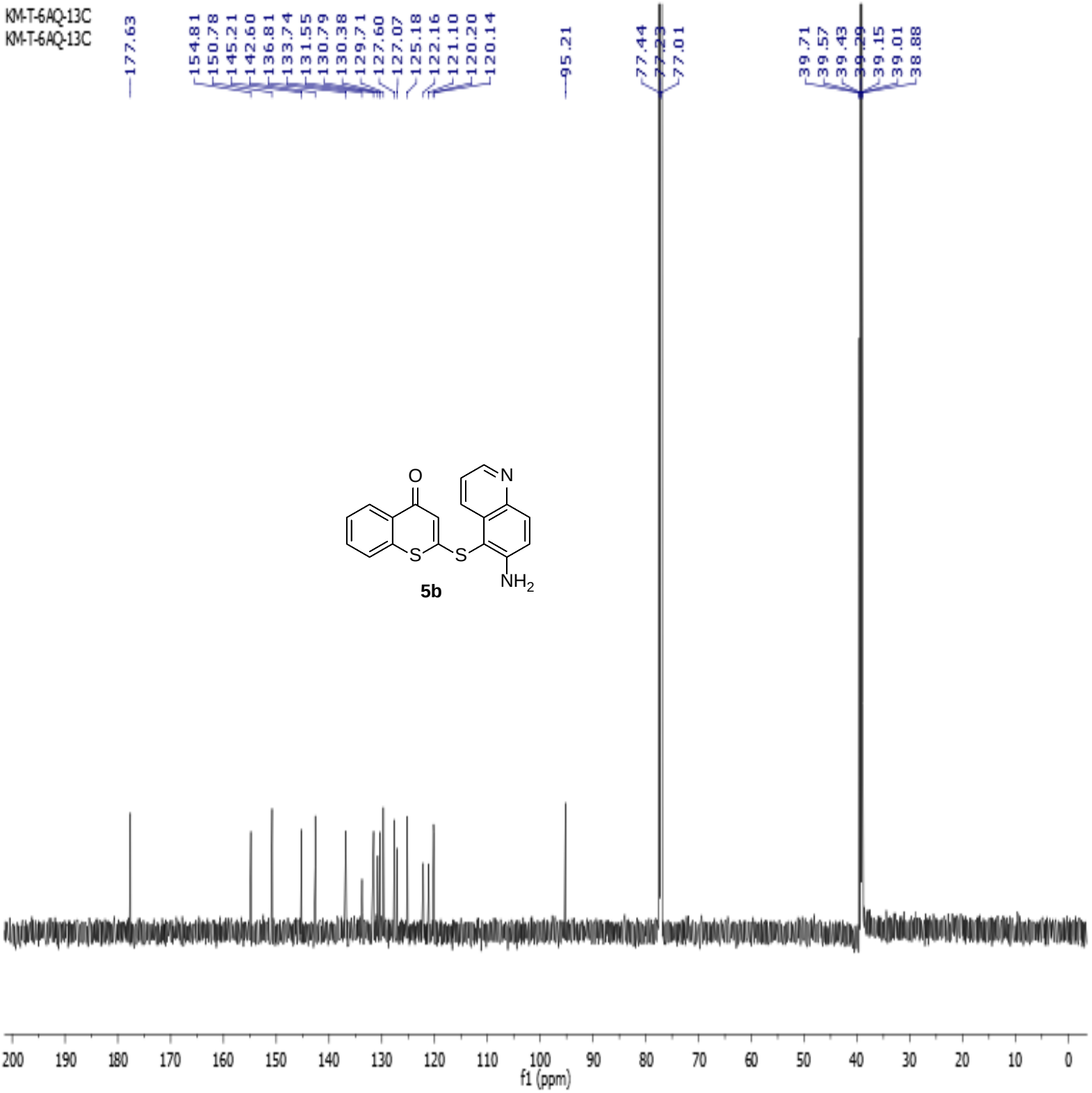
KM-4T-6AQ-1H
KM-4T-6AQ-1H



5b

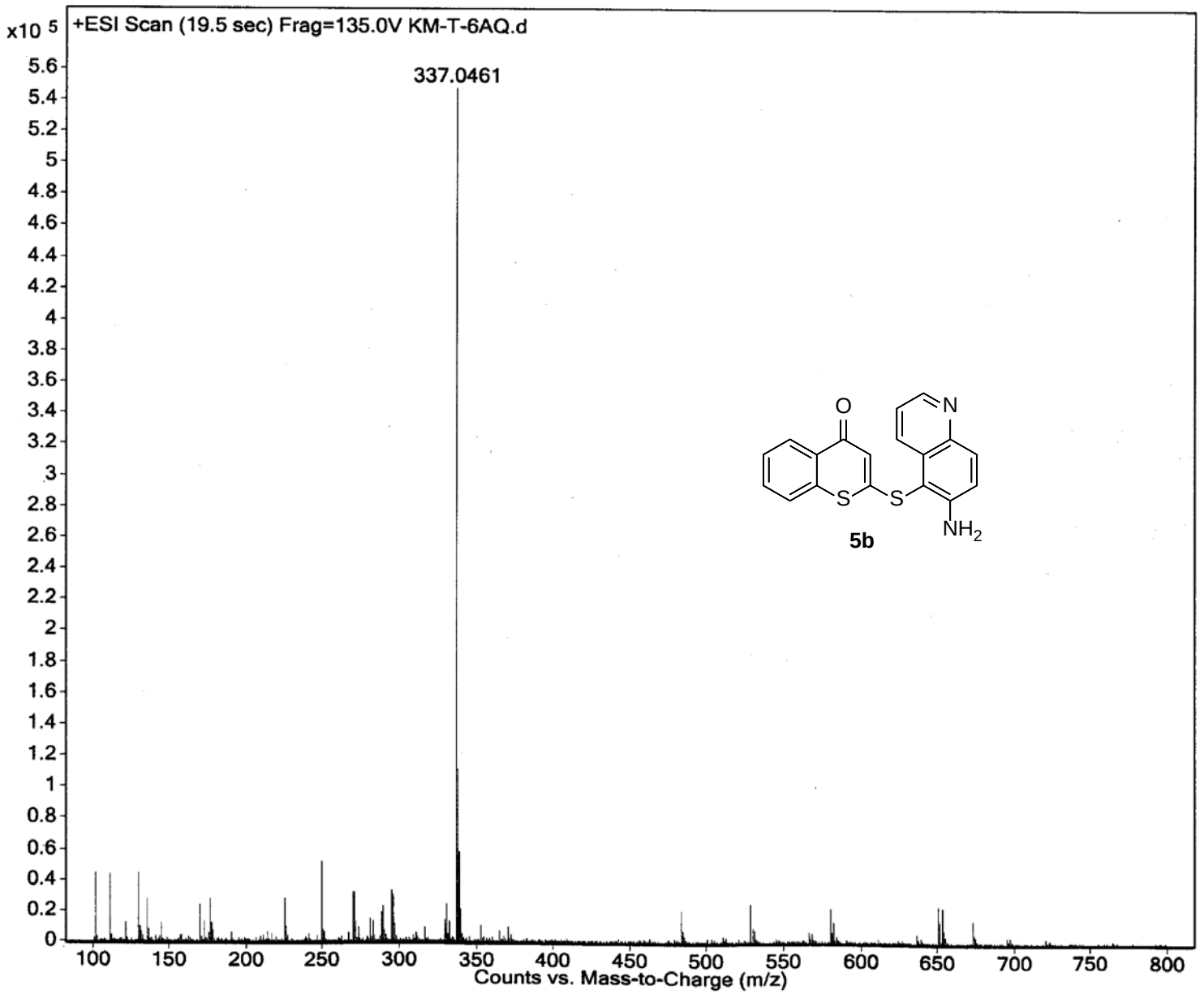


^{13}CNMR spectra of compound: 5b

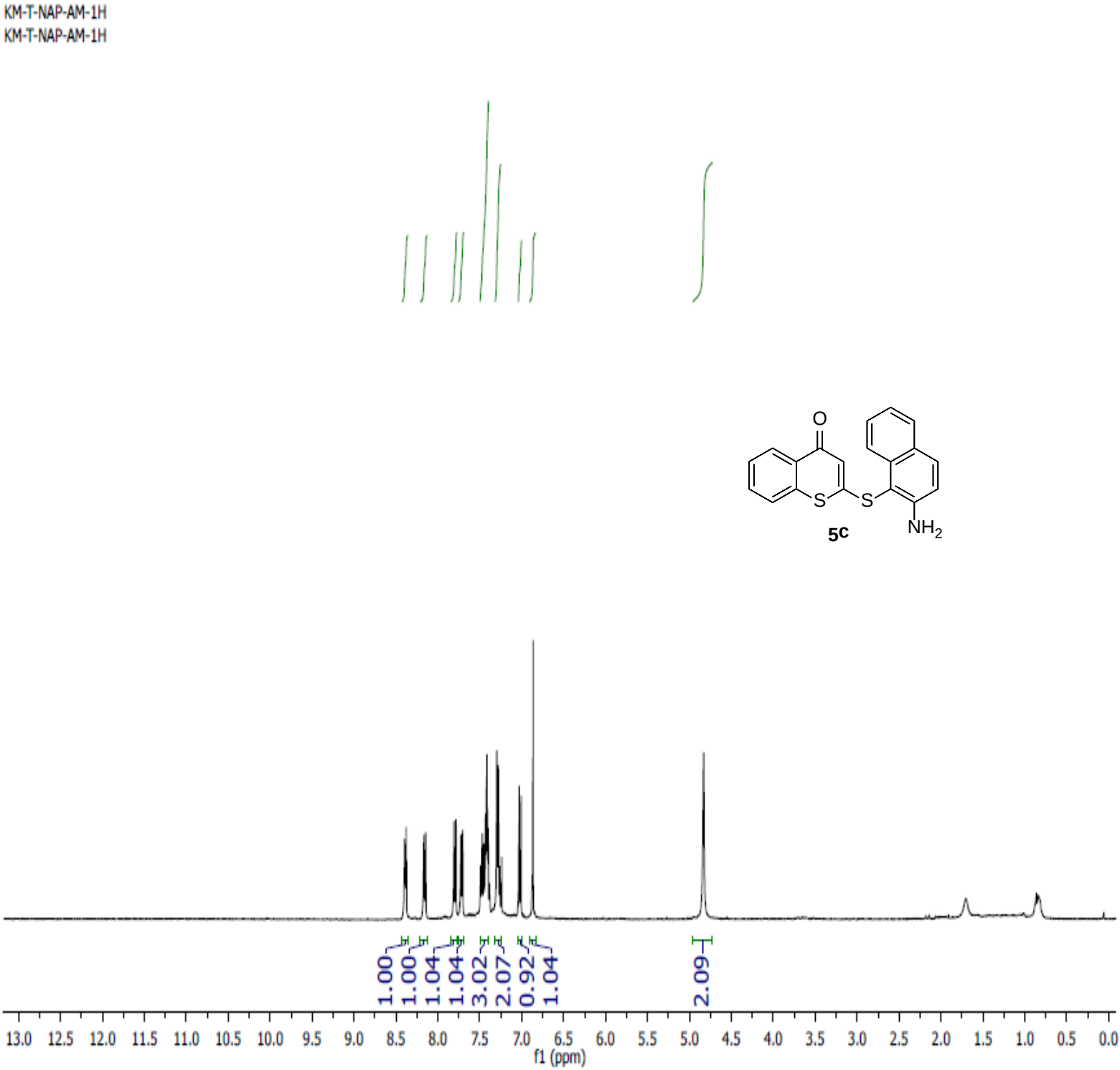


HRMS spectra of compound: 5b

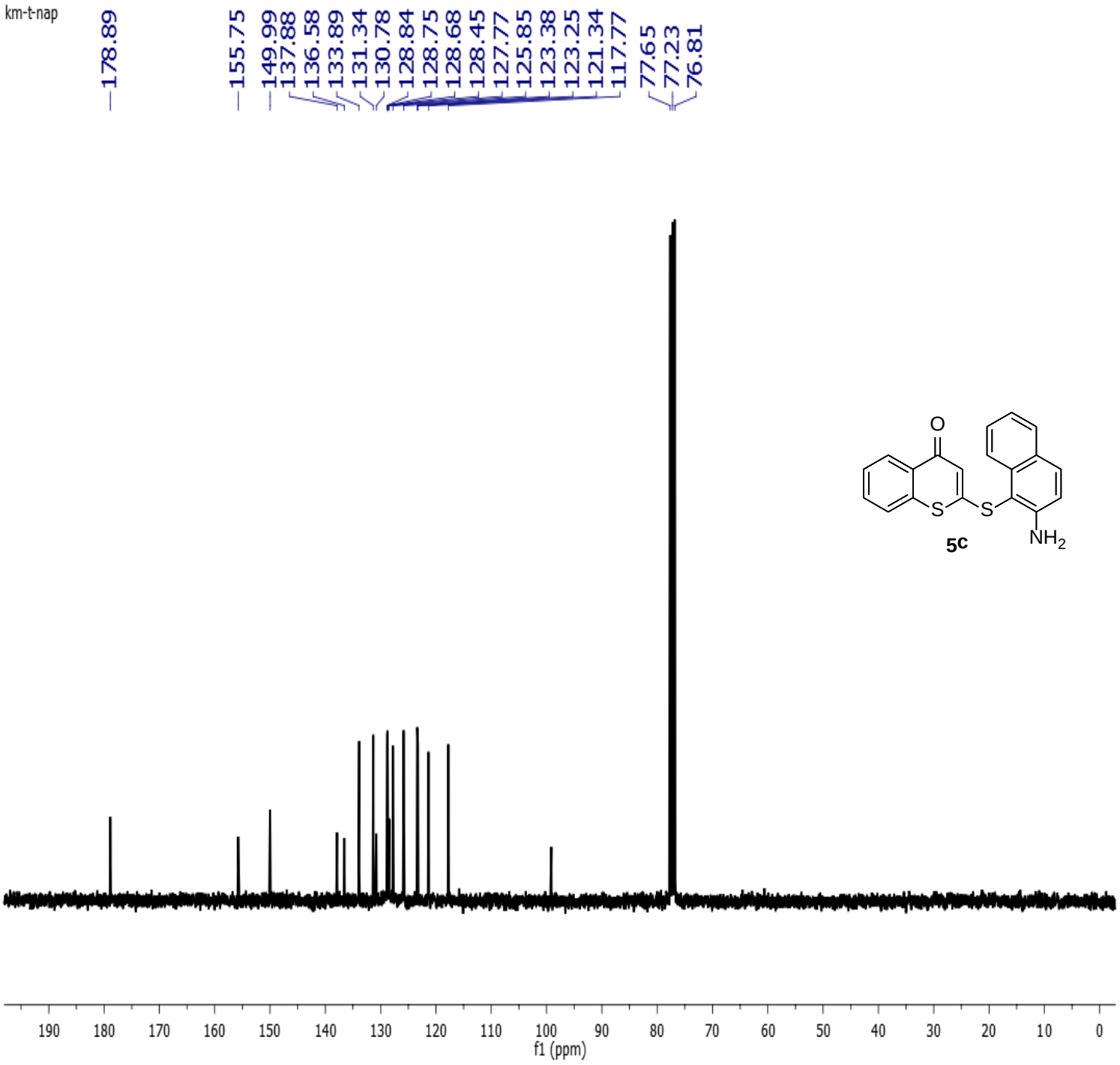
Sample Name	KM-T-6AQ	**Position**	Vial 1	**Instrument Name**	Instrument 1	**User Name**	
Inj Vol	0	**InjPosition**		**SampleType**	Sample	**IRM Calibration Status**	All Ions Missed
Data Filename	KM-T-6AQ.d	**ACQ Method**		**Comment**		**Acquired Time**	8/25/2017 4:33:21 PM



[1]HNMR spectra of compound: 5c

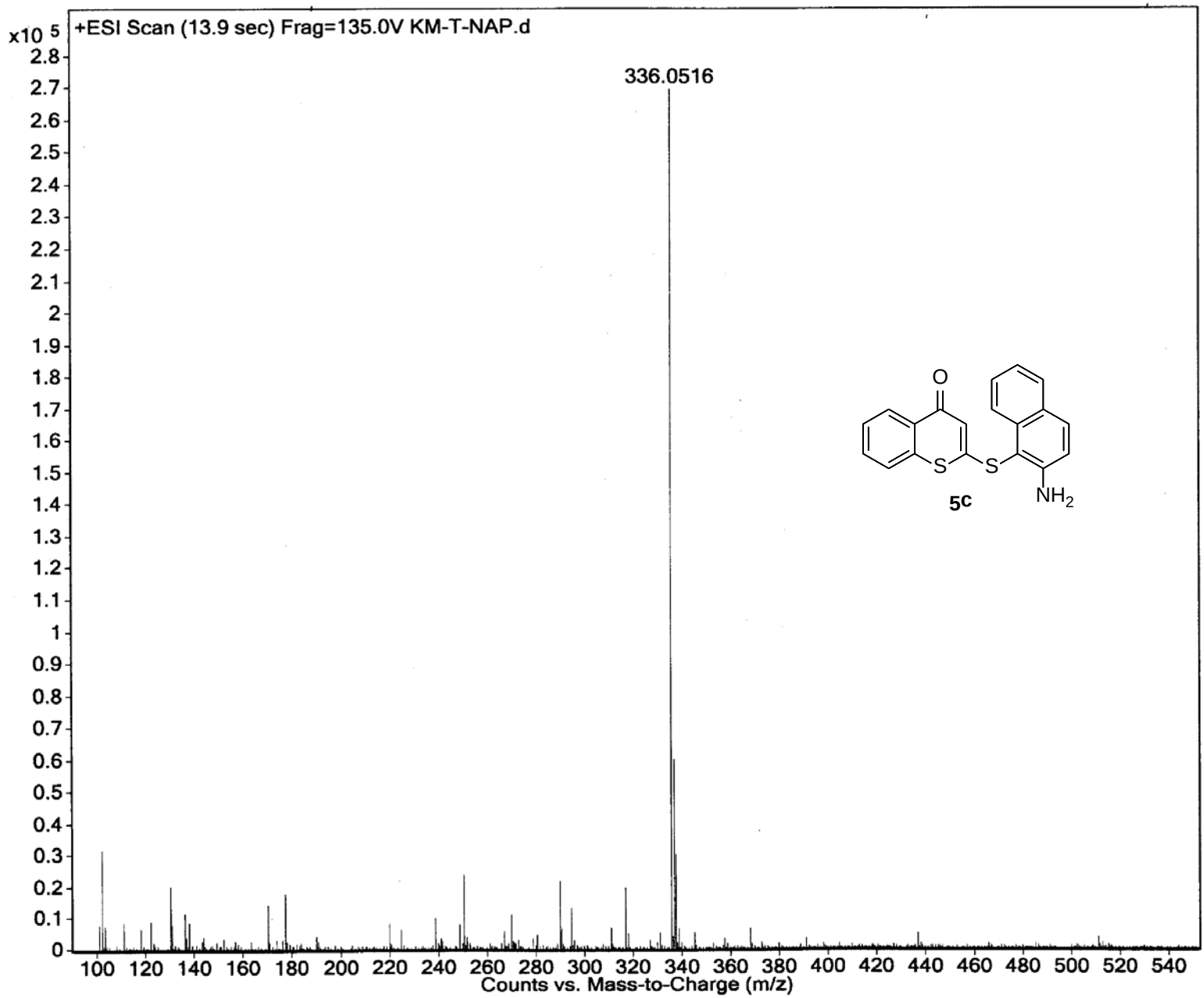


^{13}CNMR spectra of compound: 5c



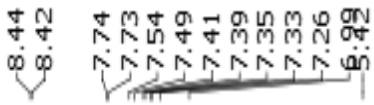
HRMS spectra of compound: 5c

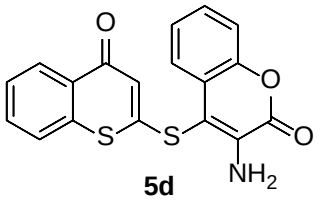
Sample Name	Unavailable	**Position**	Unavailable	**Instrument Name**	Unavailable	**User Name**	Unavailable
Inj Vol	Unavailable	**InjPosition**	Unavailable	**SampleType**	Unavailable	**IRM Calibration Status**	All Ions Missed
Data Filename	KM-T-NAP.d	**ACQ Method**		**Comment**	Sample information is unavailable	**Acquired Time**	Unavailable



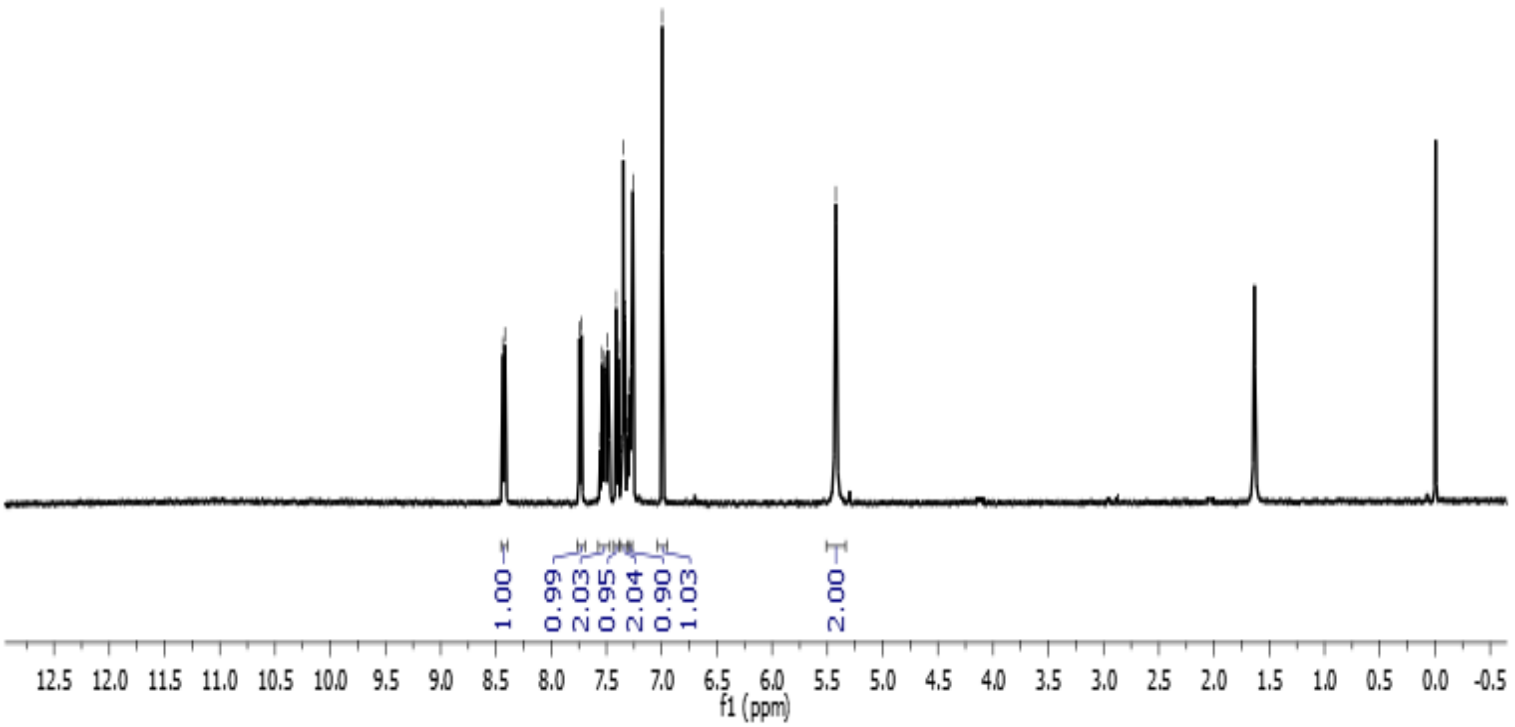
[1]HNMR spectra of compound: 5d

km-t-ac-1h
km-t-ac-1h

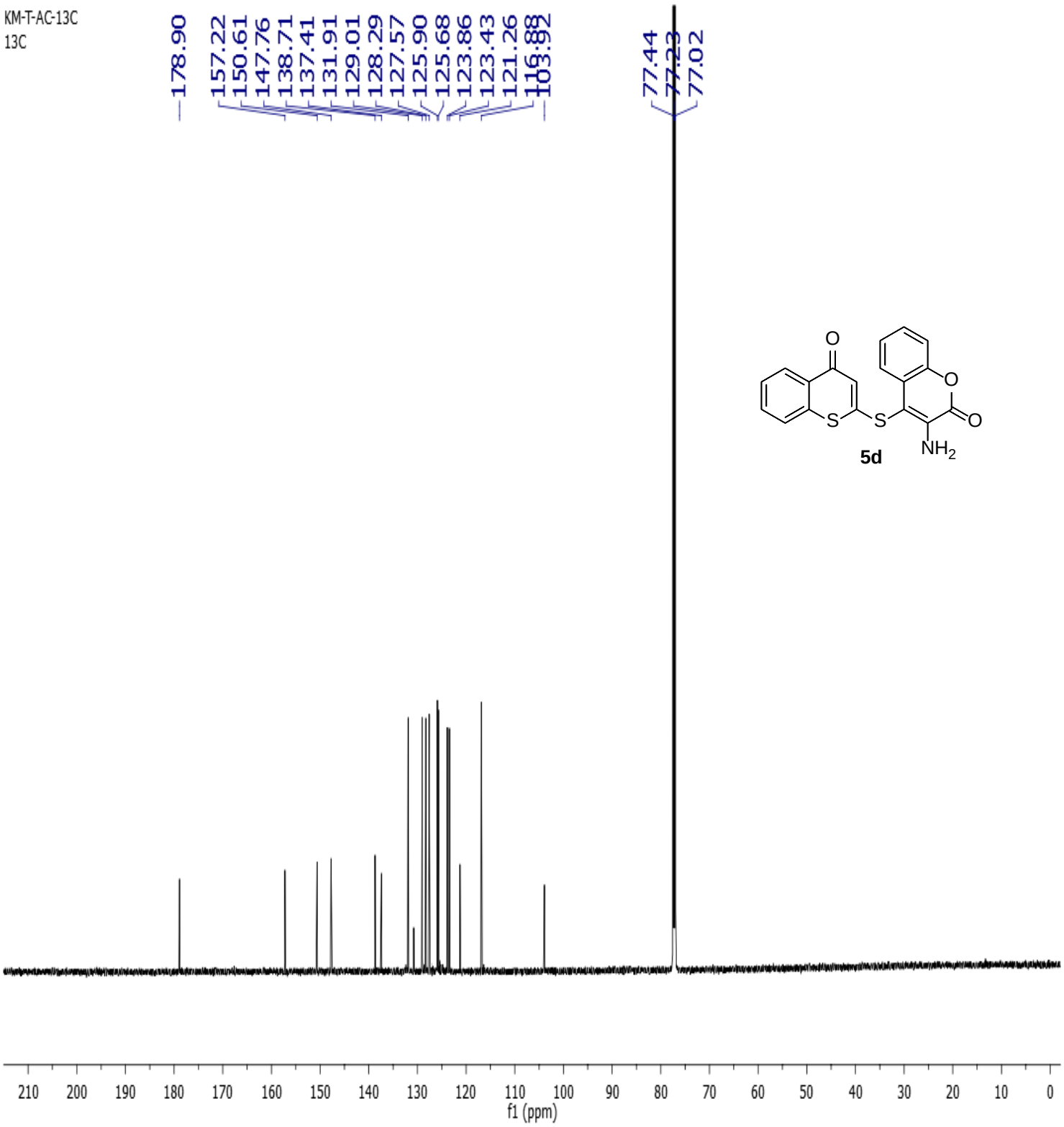




5d

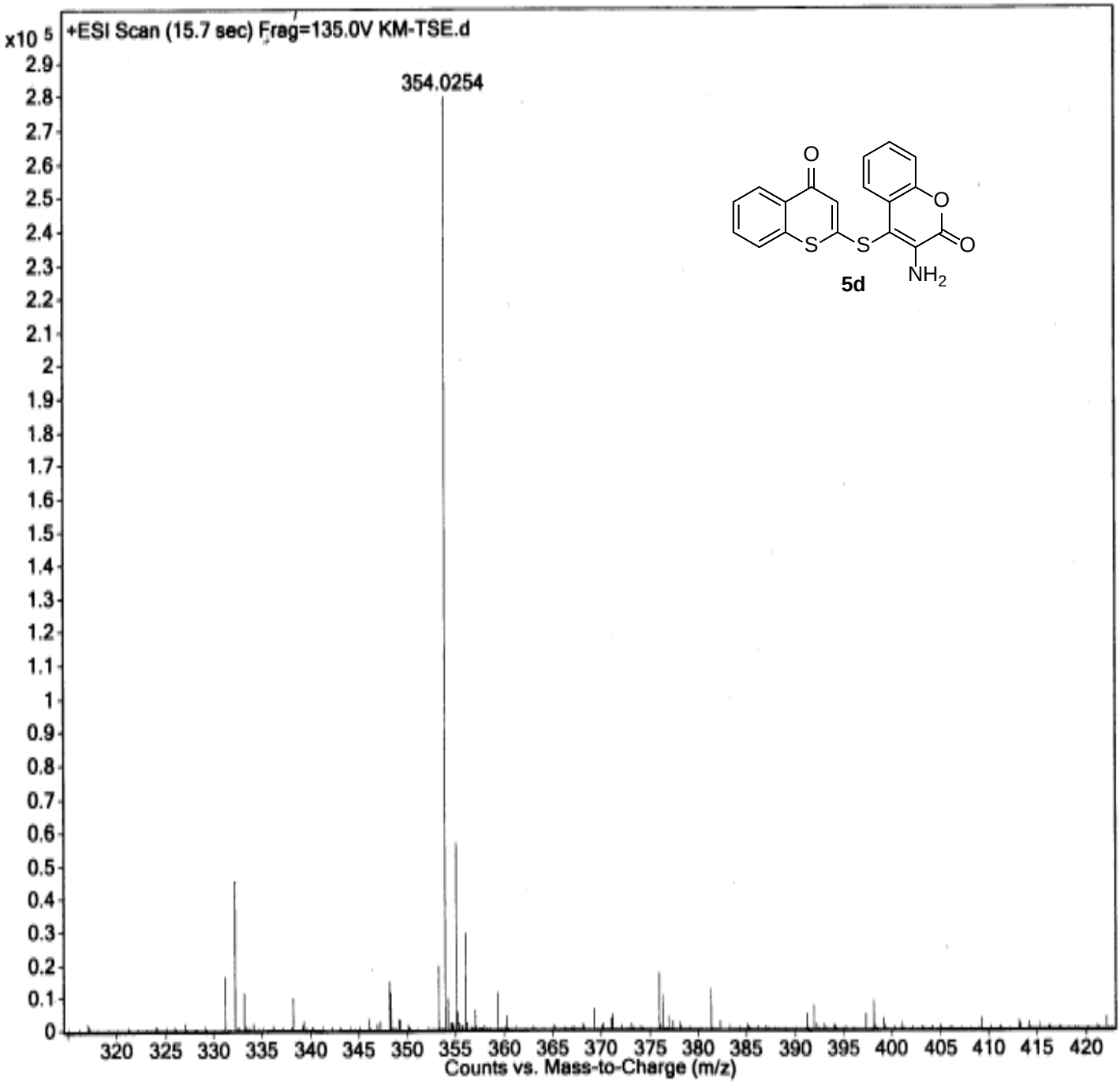


^{13}CNMR spectra of compound: 5d

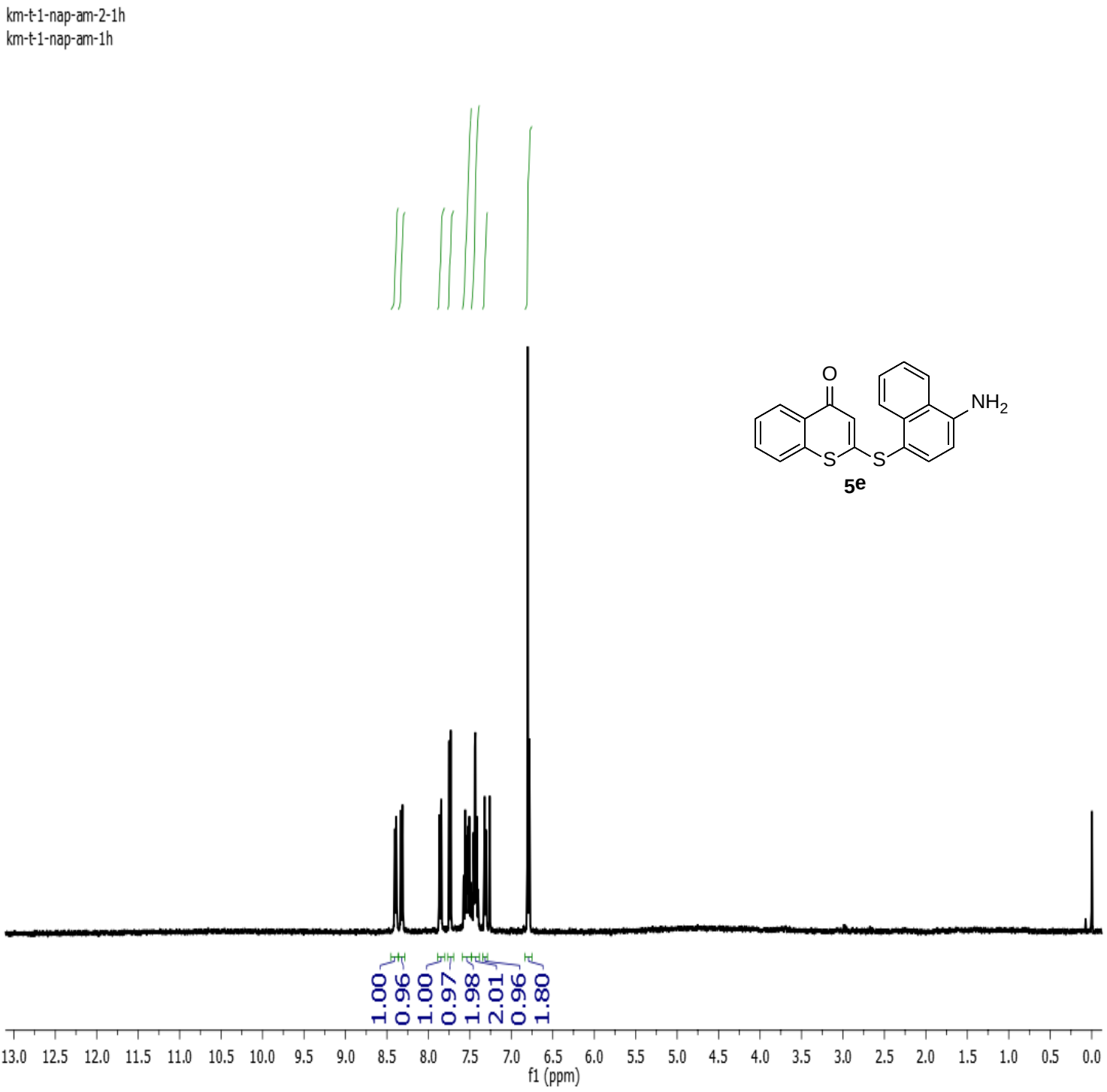


HRMS spectra of compound: 5d

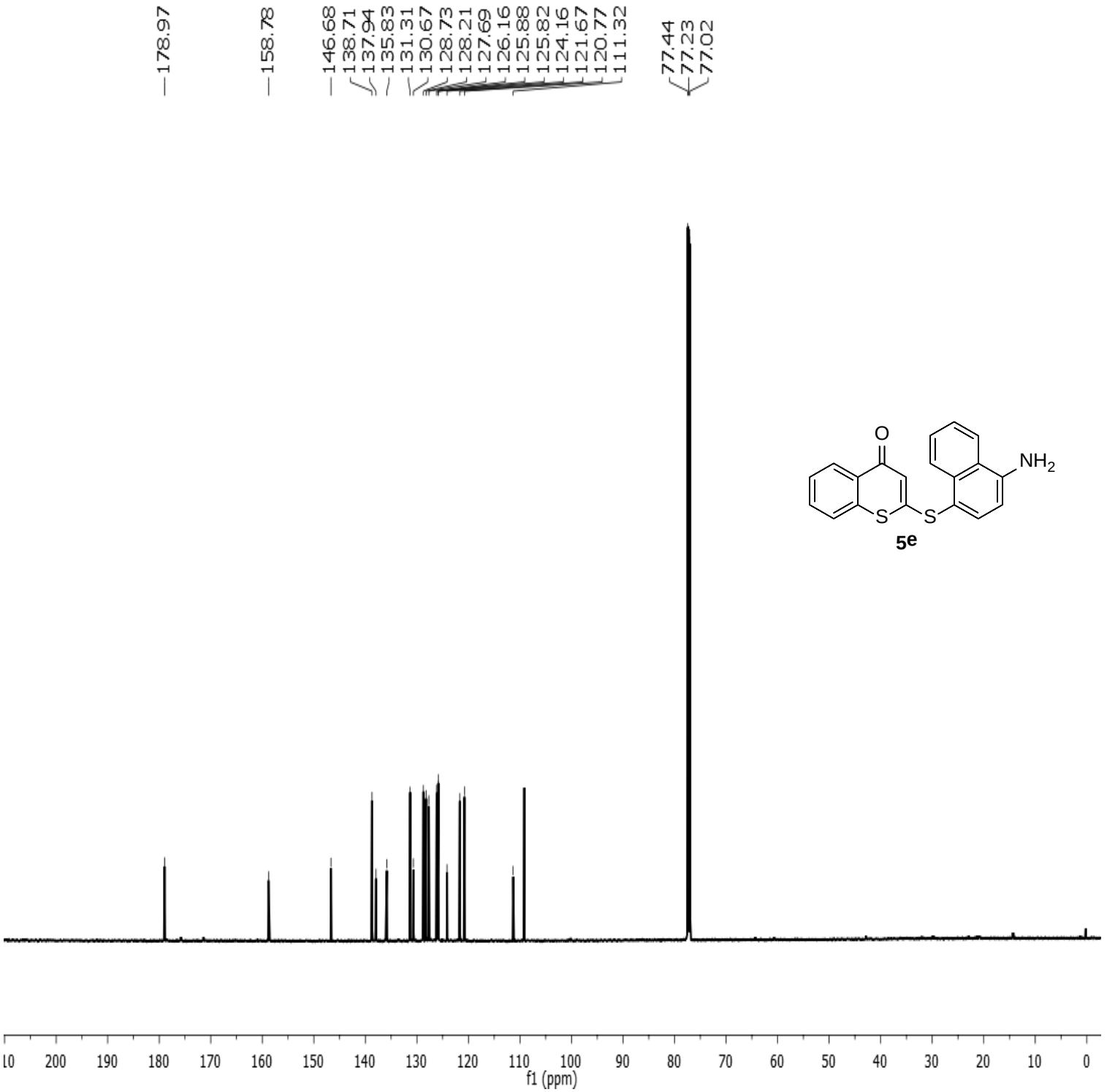
Sample Name	KM-TSE	**Position**	Vial 1	**Instrument Name**	Instrument 1	**User Name**	
Inj Vol	0	**InjPosition**		**SampleType**	Sample	**IRM Calibration Status**	Success
Data Filename	KM-TSE.d	**ACQ Method**		**Comment**		**Acquired Time**	10/17/2017 11:42:14 AM



[1]HNMR spectra of compound: 5e

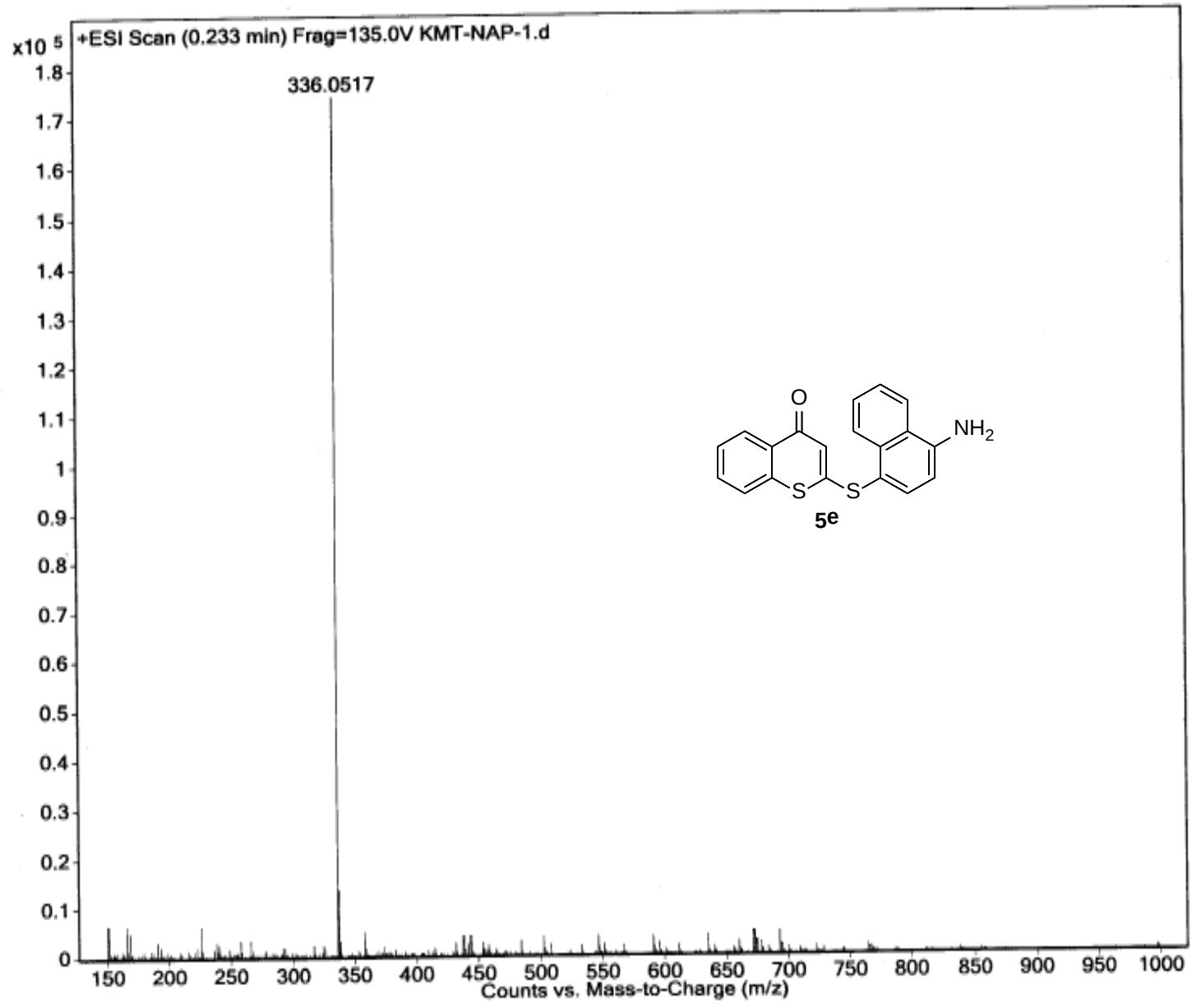


^{13}CNMR spectra of compound: 5e



HRMS spectra of compound: 5e

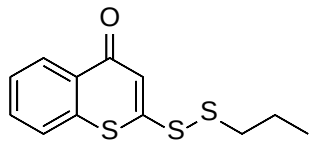
Sample Name	KMT-NAP-1	**Position**	Vial 1	**Instrument Name**	Instrument 1	**User Name**	
Inj Vol	-1	**InjPosition**		**SampleType**	Sample	**IRM Calibration Status**	Success
Data Filename	KMT-NAP-1.d	**ACQ Method**		**Comment**		**Acquired Time**	12/1/2017 6:33:19 PM



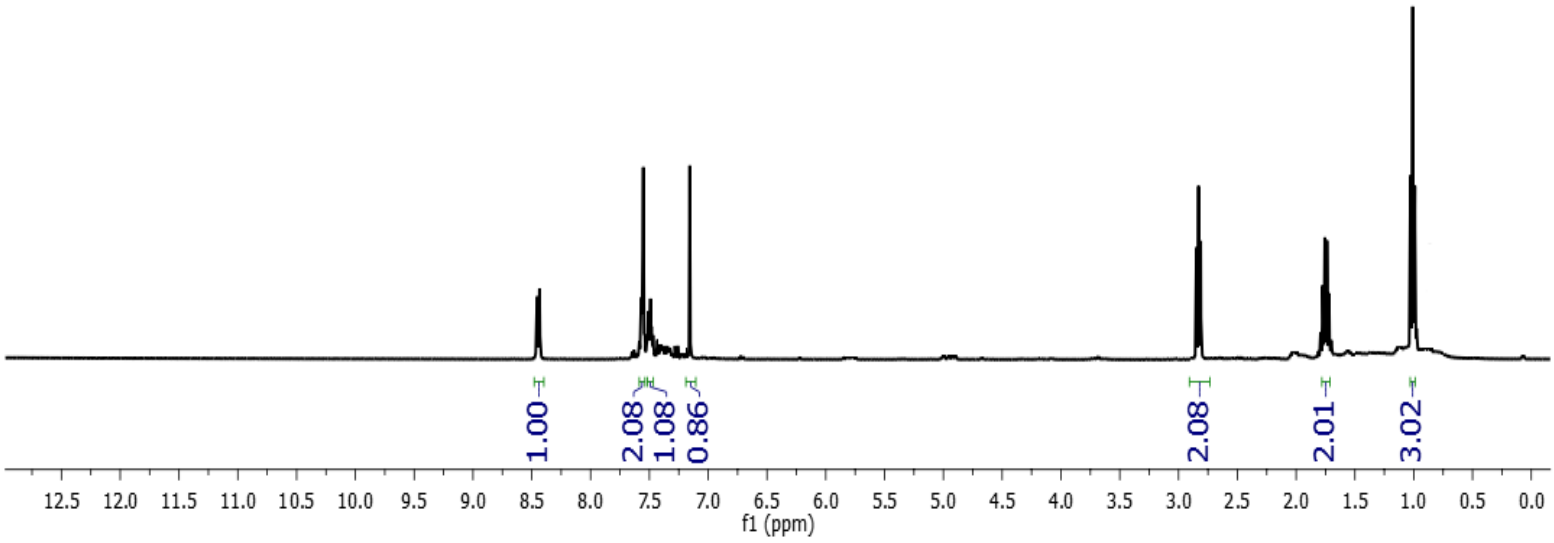
5e

[1]HNMR spectra of compound: 6a

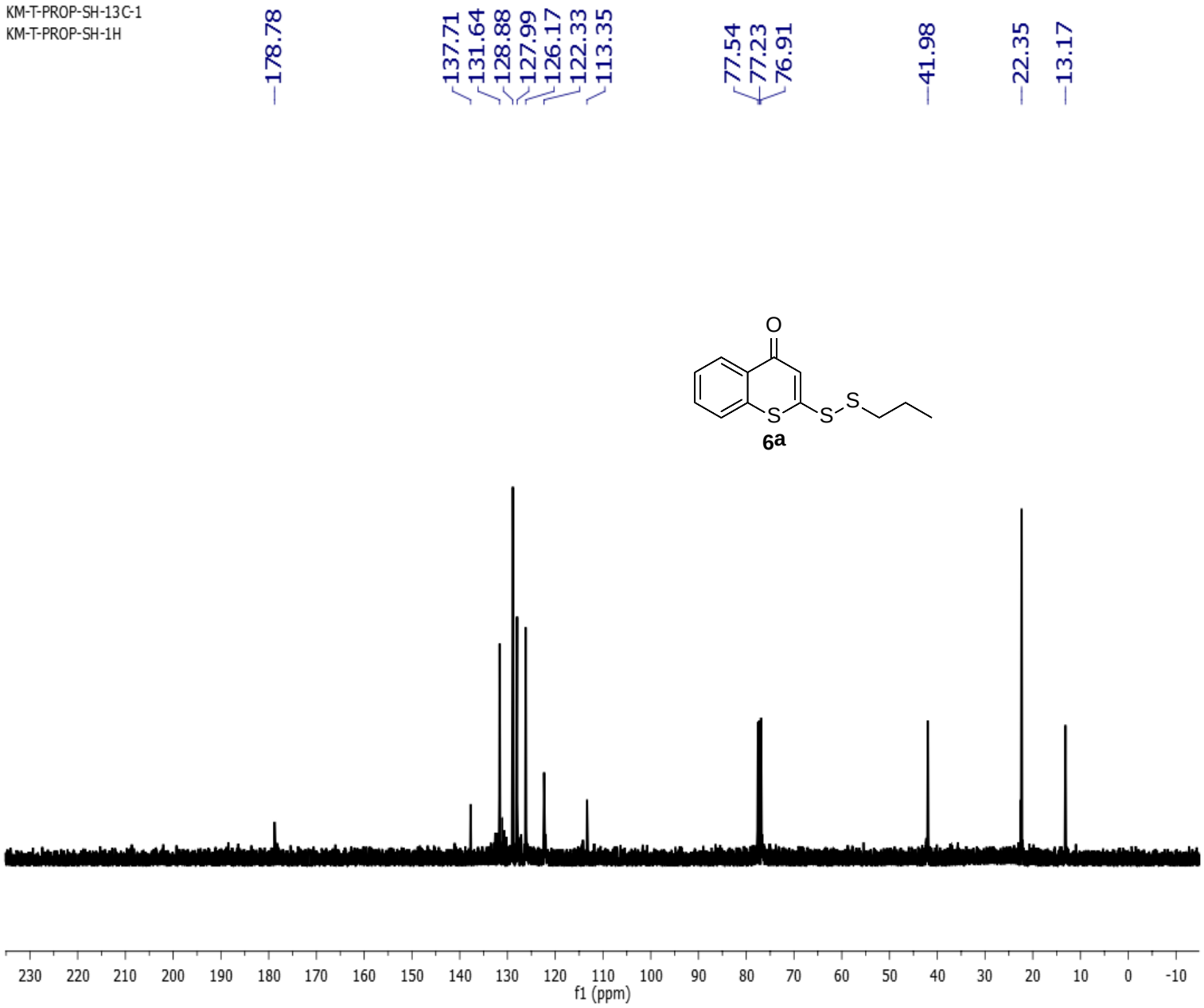
KM-T-PROP-SH-1H
KM-T-PROP-SH-1H



6a

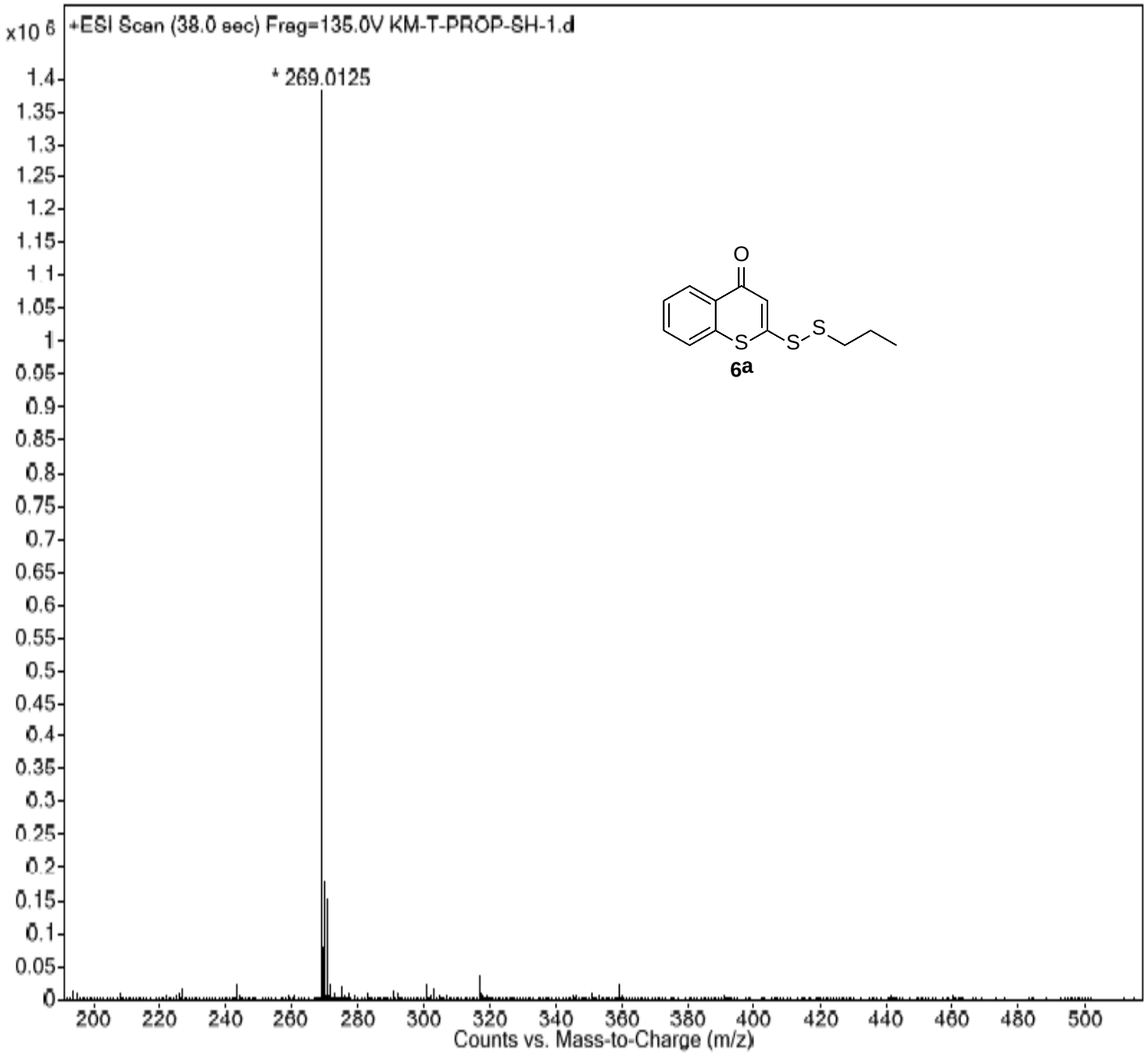


^{13}CNMR spectra of compound: 6a



HRMS spectra of compound: 6a

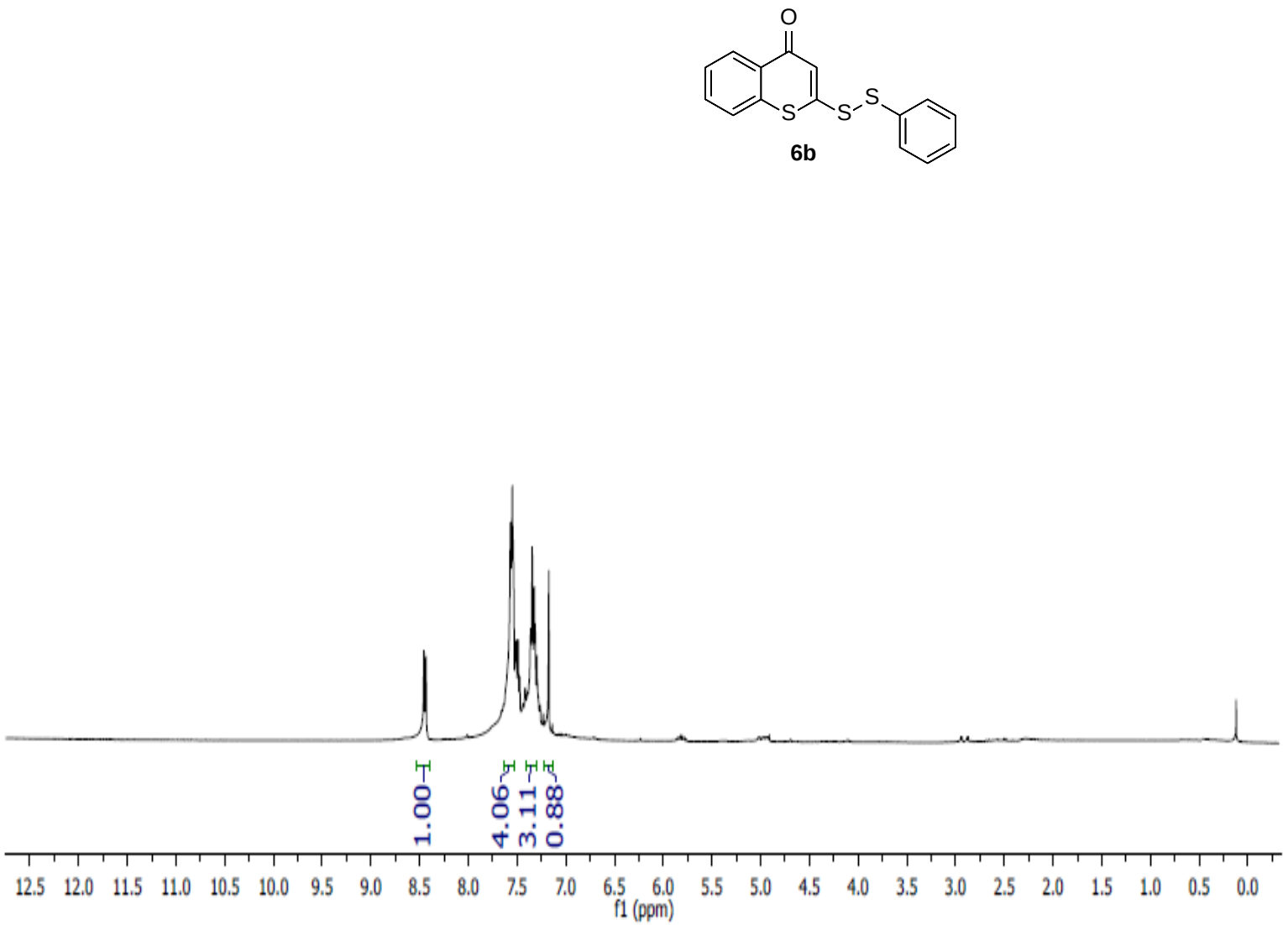
Sample Name	KM-T-PROP-SH-1	**Position**	Vial 1	**Instrument Name**	Instrument 1	**User Name**	
Inj Vol	0	**InjPosition**		**SampleType**	Sample	**IRM Calibration Status**	All Ions Missed
Data Filename	KM-T-PROP-SH-1.d	**ACQ Method**		**Comment**		**Acquired Time**	3/29/2017 4:49:55 PM



6a

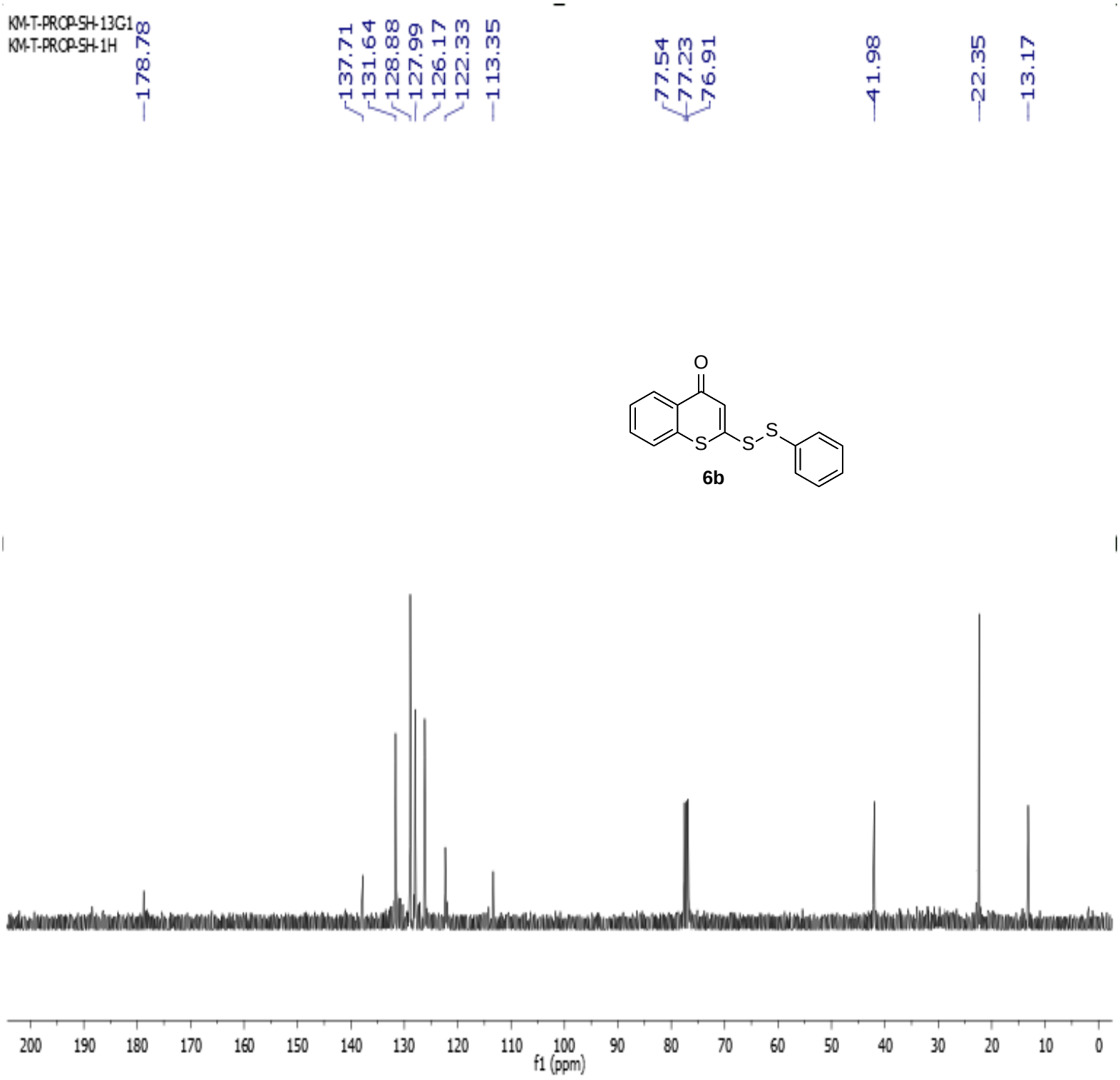
[1]HNMR spectra of compound: 6b

KM-T-P-SH-1H
KM-T-P-SH-1H



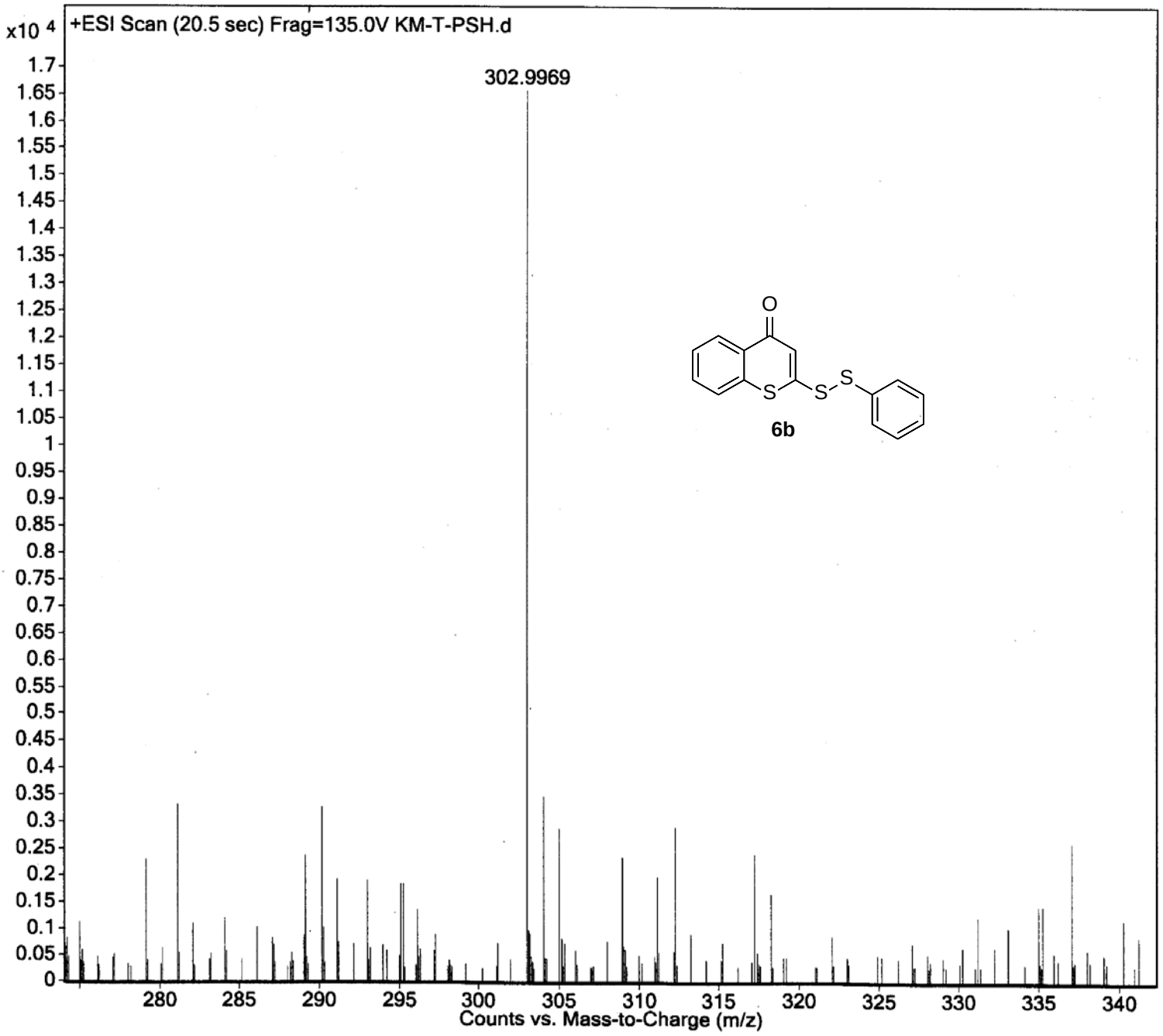
6b

^{13}CNMR spectra of compound: 6b

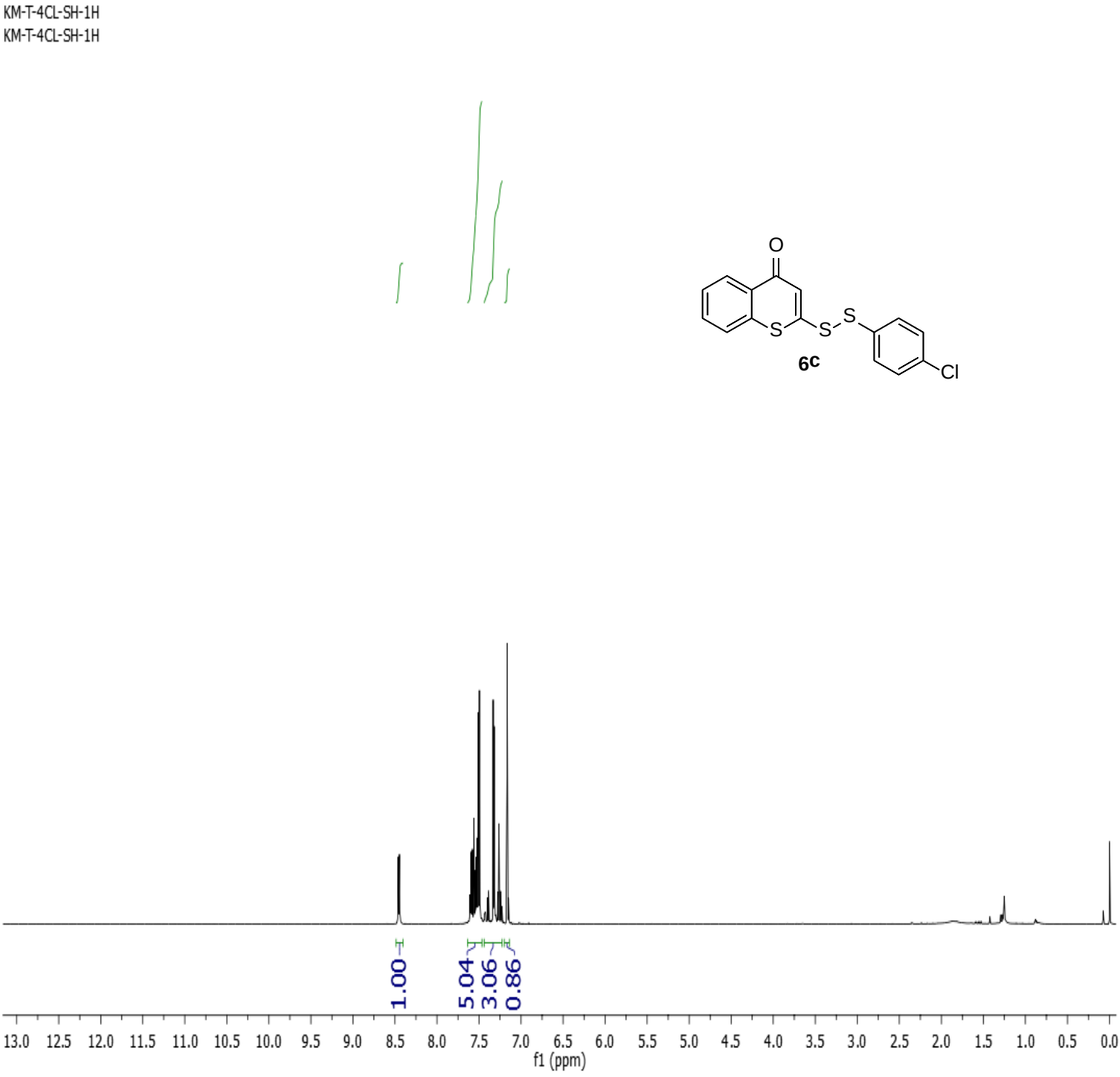


HRMS spectra of compound: 6b

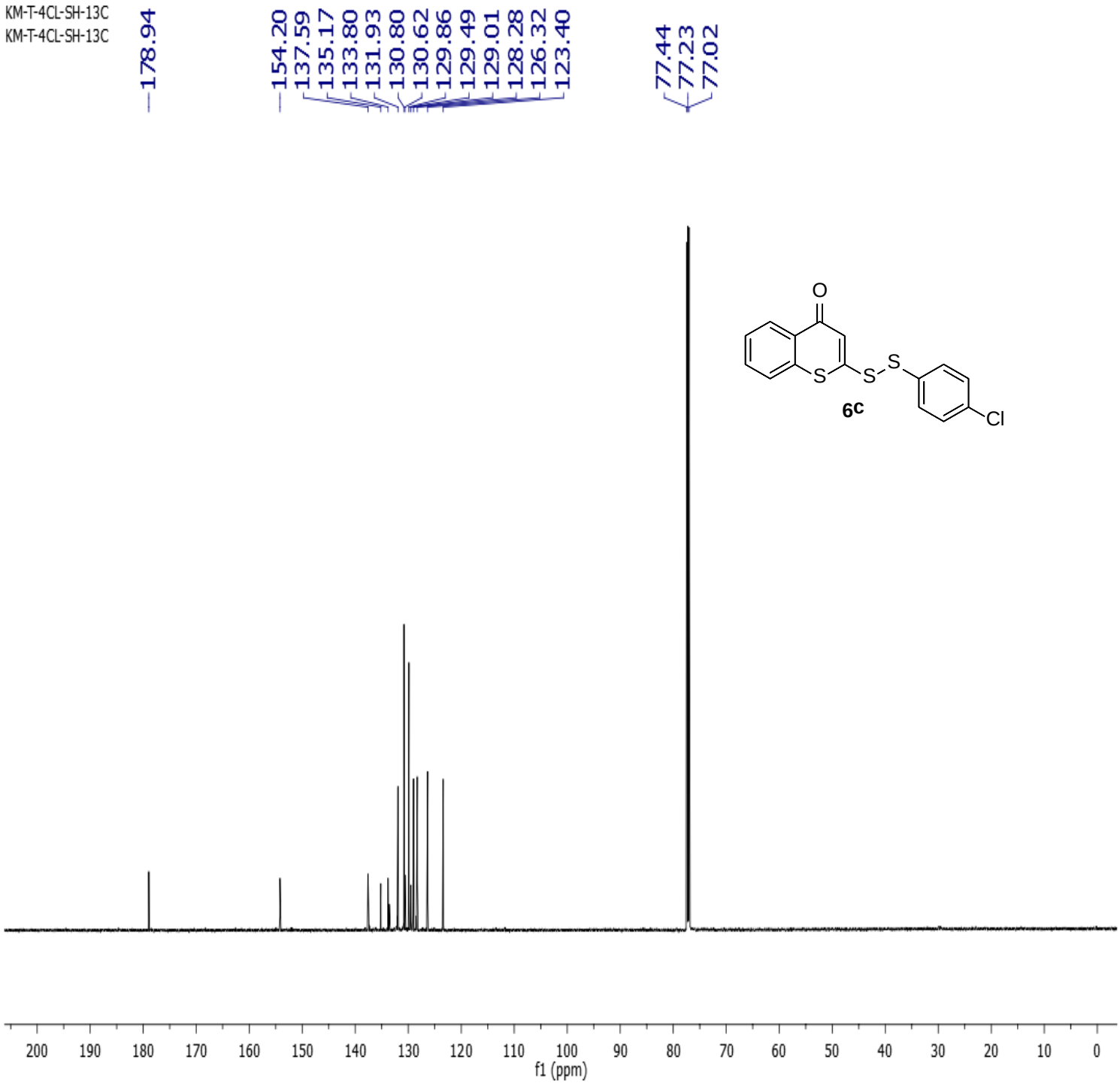
Sample Name	Unavailable	**Position**	Unavailable	**Instrument Name**	Unavailable	**User Name**	Unavailable
Inj Vol	Unavailable	**InjPosition**	Unavailable	**SampleType**	Unavailable	**IRM Calibration Status**	All Ions Missed
Data Filename	KM-T-PSH.d	**ACQ Method**		**Comment**	Sample information is unavailable	**Acquired Time**	Unavailable



[1]HNMR spectra of compound: 6c

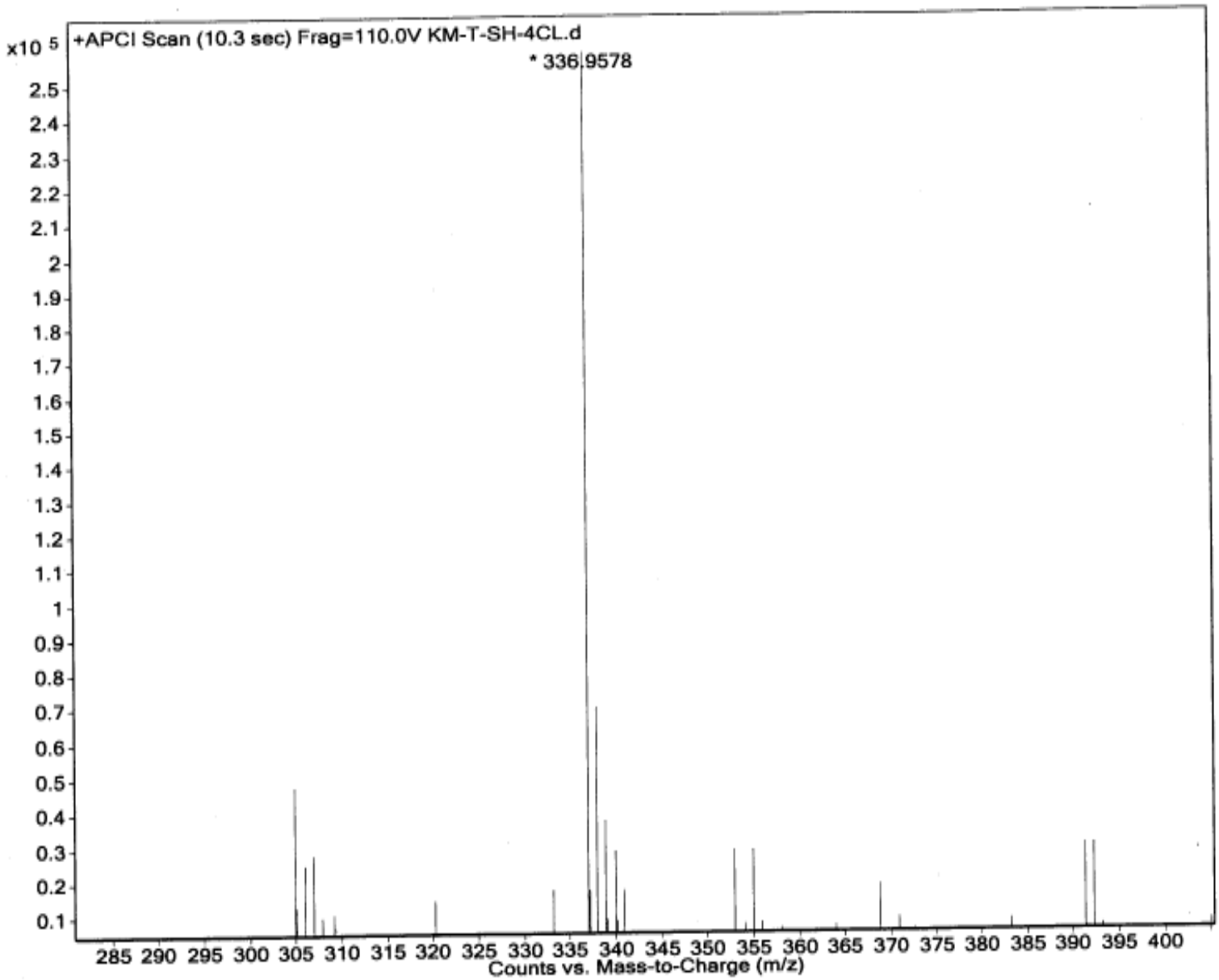


^{13}CNMR spectra of compound: 6c

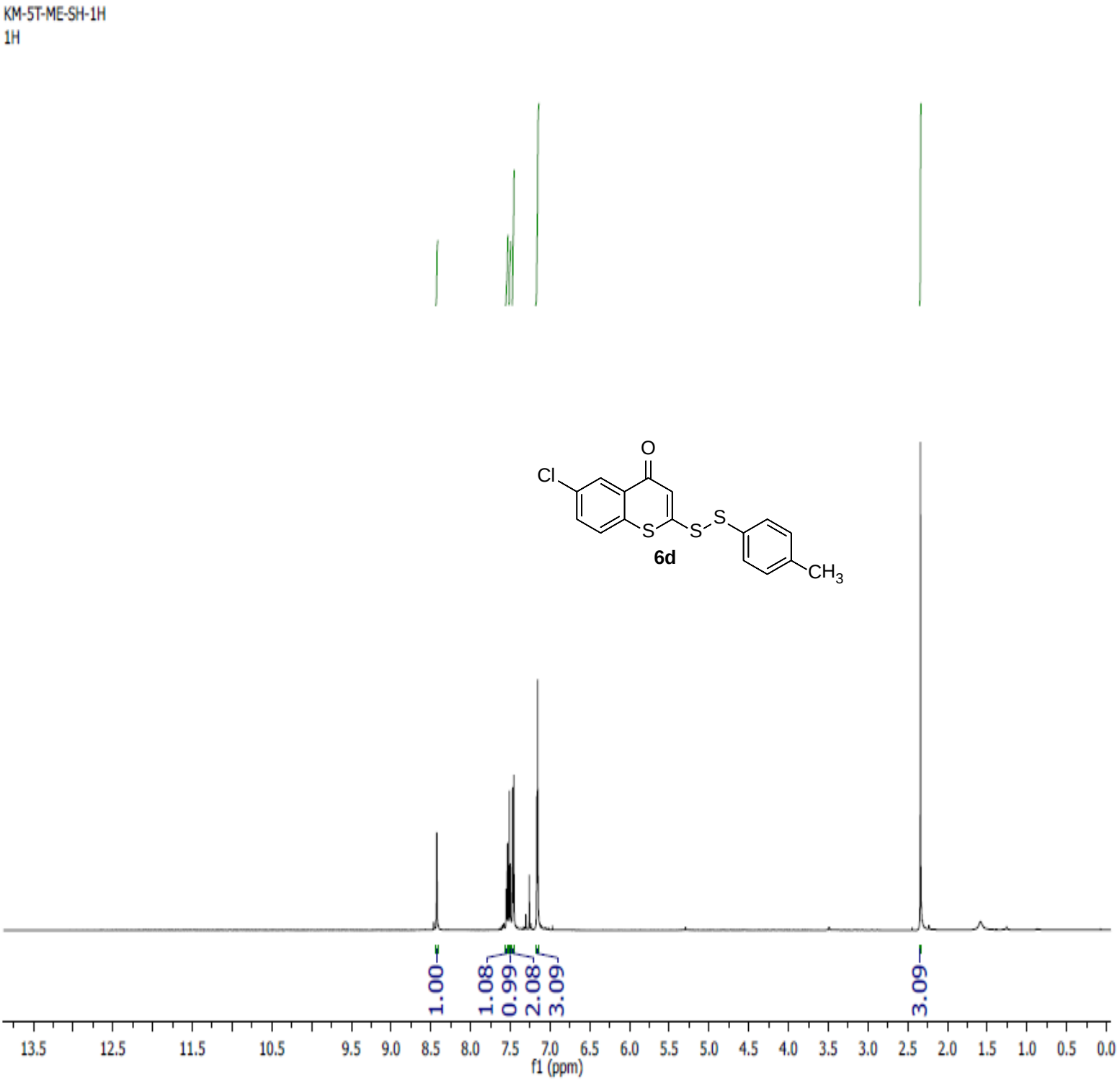


HRMS spectra of compound: 6c

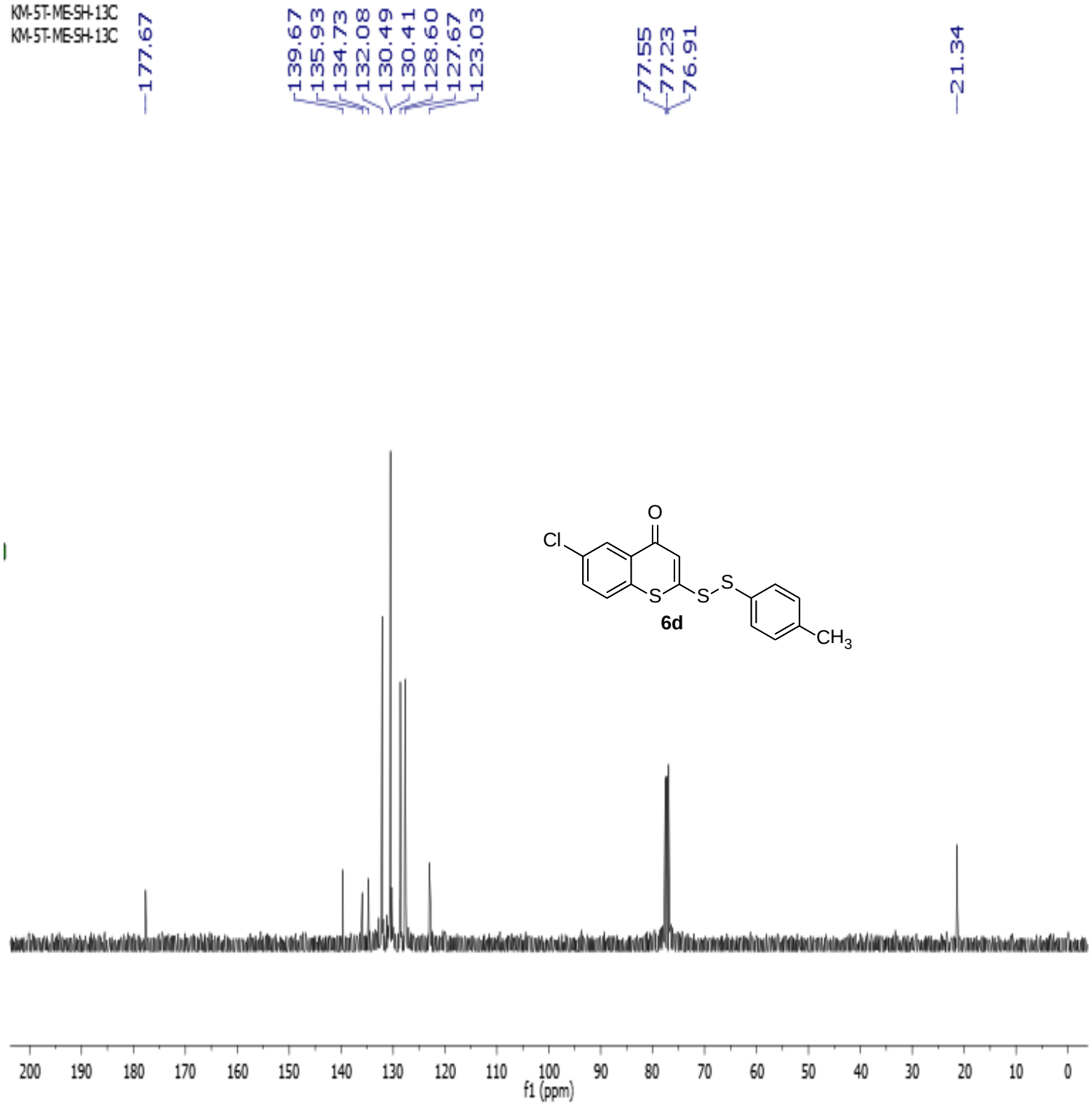
Sample Name	Unavailable	**Position**	Unavailable	**Instrument Name**	Unavailable	**User Name**	Unavailable
Inj Vol	Unavailable	**InjPosition**	Unavailable	**SampleType**	Unavailable	**IRM Calibration Status**	Success
Data Filename	KM-T-SH-4CL.d	**ACQ Method**		**Comment**	Sample information is unavailable	**Acquired Time**	Unavailable



^{1}HNMR spectra of compound: 6d

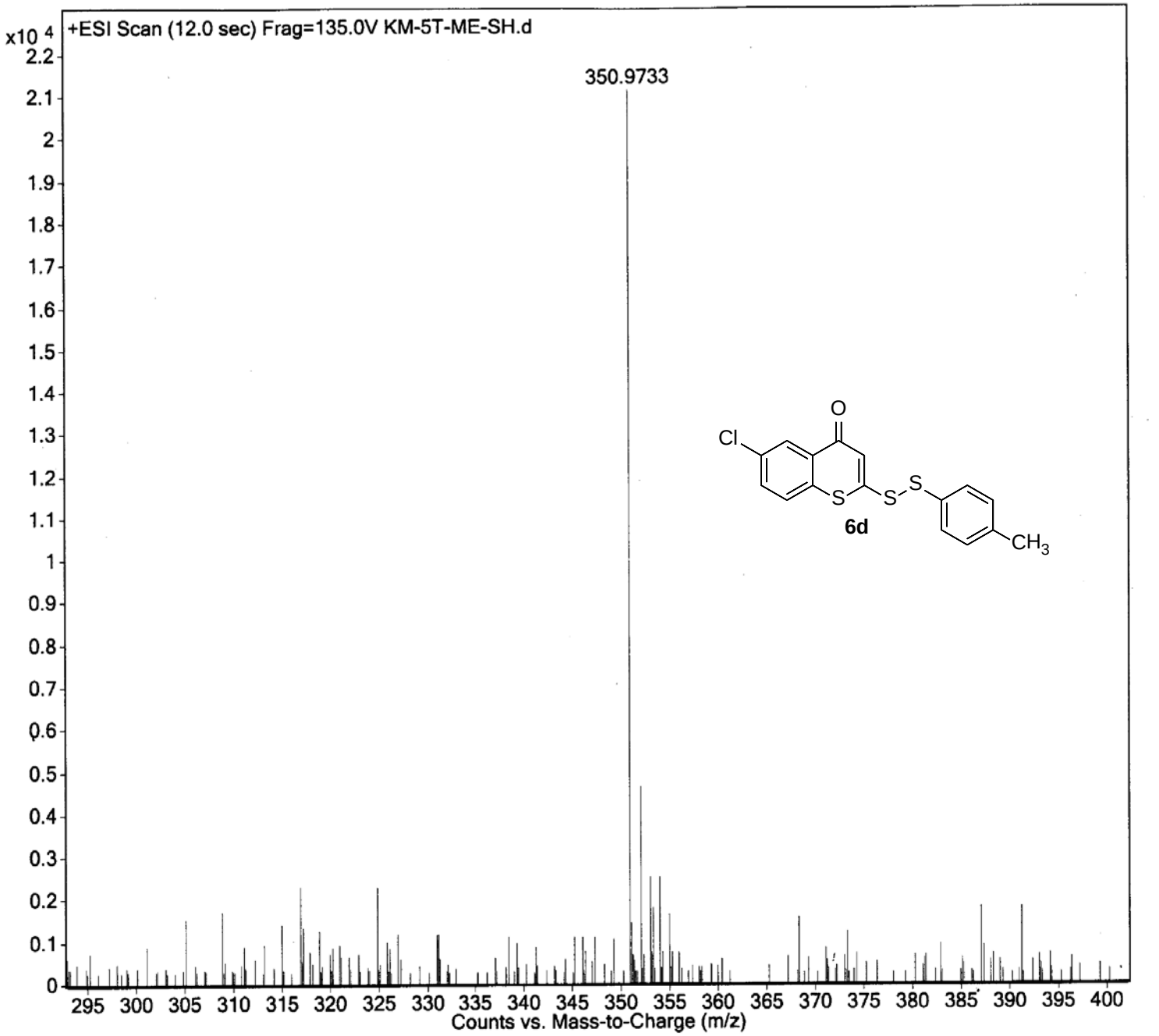


^{13}CNMR spectra of compound: 6c

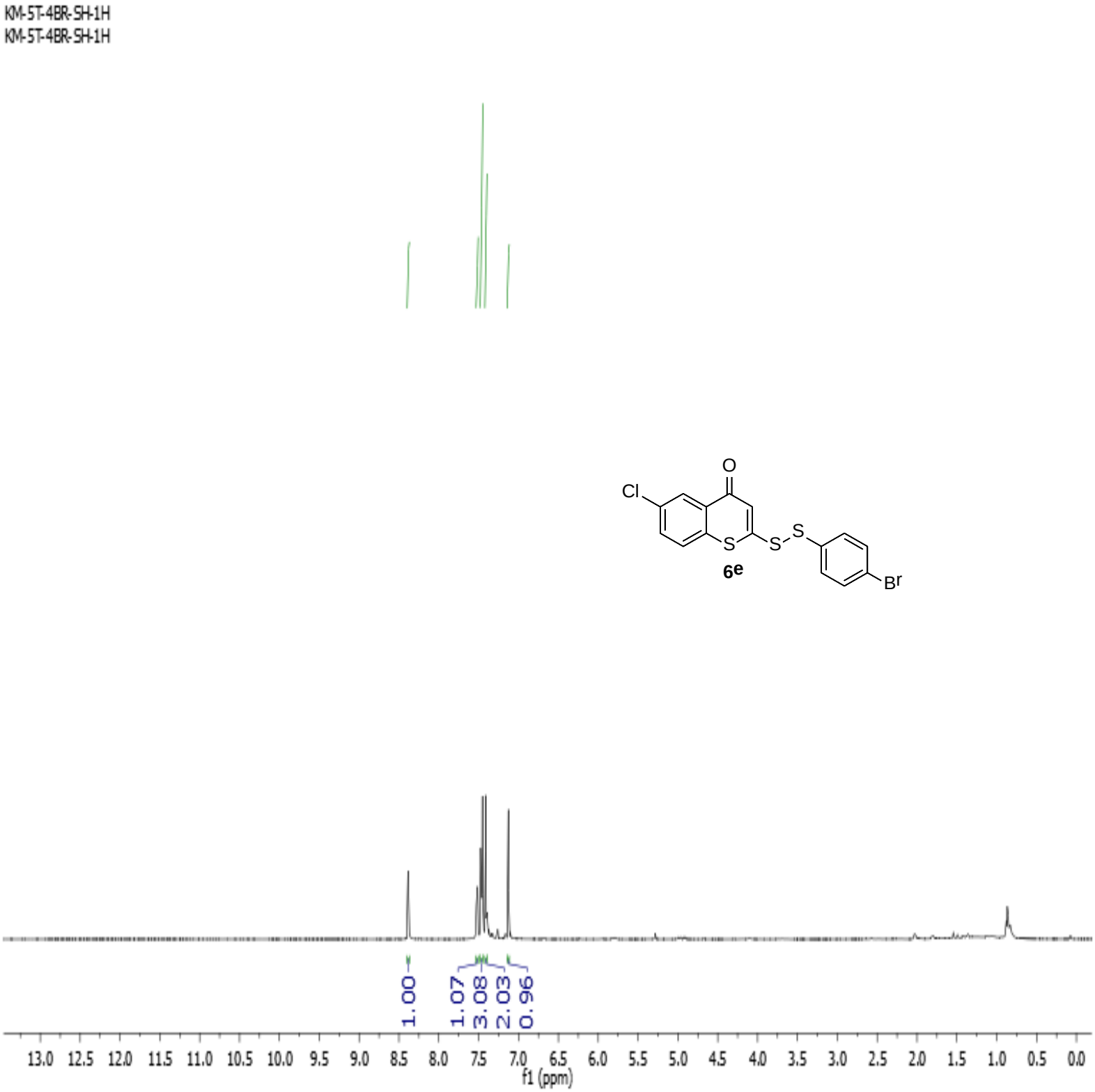


HRMS spectra of compound: 6c

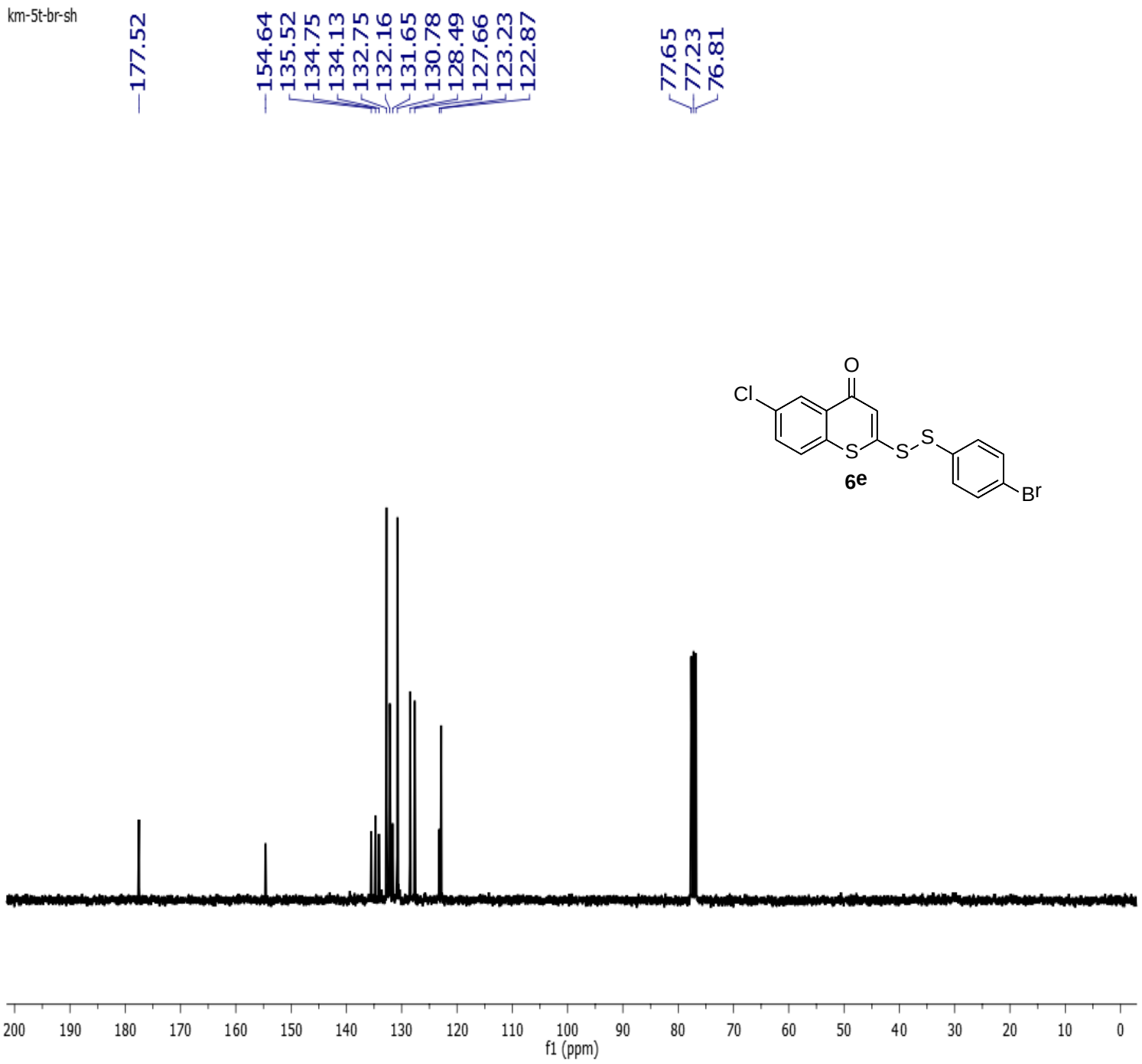
Sample Name	KM-5T-ME-SH	**Position**	Vial 1	**Instrument Name**	Instrument 1	**User Name**	
Inj Vol	0	**InjPosition**		**SampleType**	Sample	**IRM Calibration Status**	All Ions Missed
Data Filename	KM-5T-ME-SH.d	**ACQ Method**		**Comment**		**Acquired Time**	8/28/2017 4:22:04 PM



[1]HNMR spectra of compound: 6e

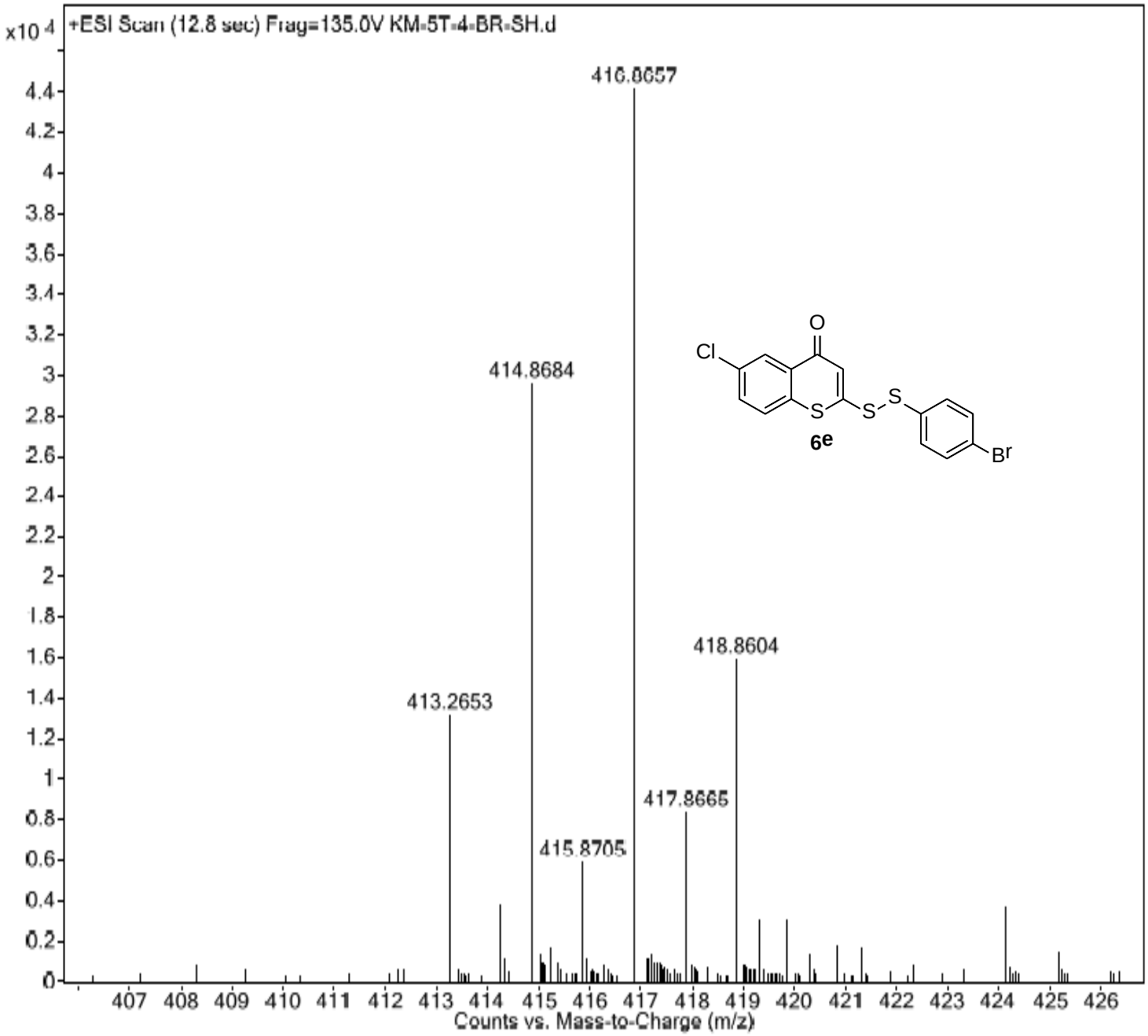


^{13}CNMR spectra of compound: 6e



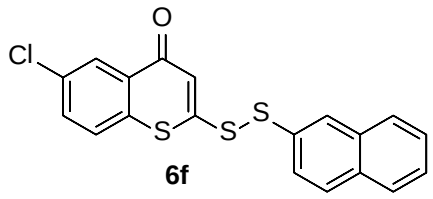
HRMS spectra of compound: 6e

Sample Name	KM-5T-4-BR-SH	**Position**	Vial 1	**Instrument Name**	Instrument 1	**User Name**	
Inj Vol	0	**InjPosition**		**SampleType**	Sample	**IRM Calibration Status**	Some Ions Missed
Data Filename	KM-5T-4-BR-SH.d	**ACQ Method**		**Comment**		**Acquired Time**	3/31/2017 5:08:58 PM

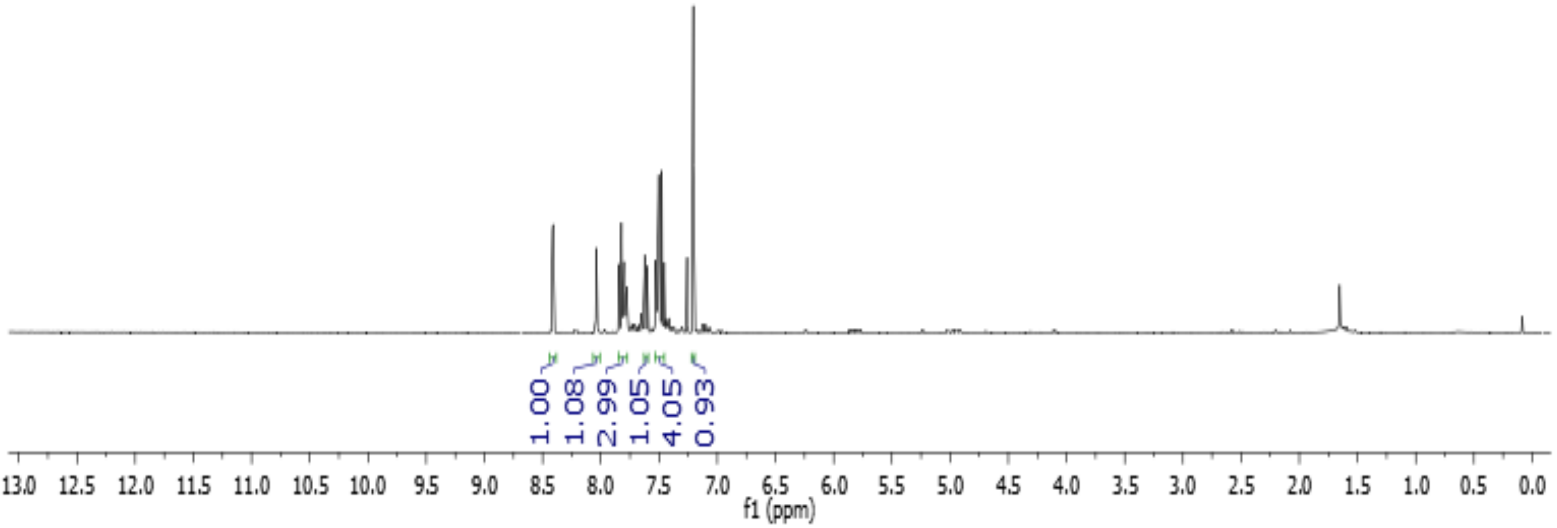


[1]HNMR spectra of compound: 6f

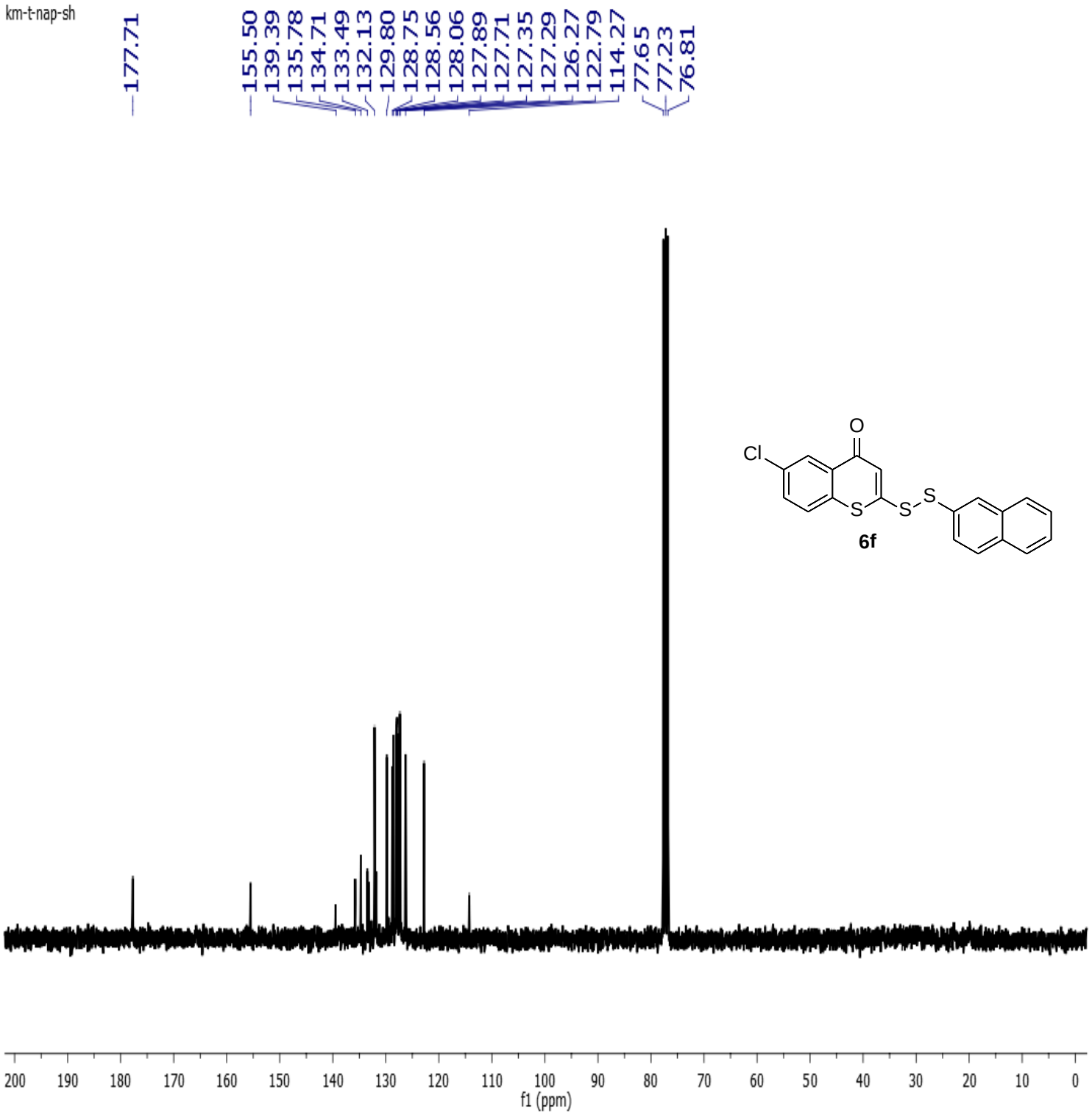
KM-5T-2-NAP-SH-1HA
KM-5T-2-NAP-SH-1H



6f

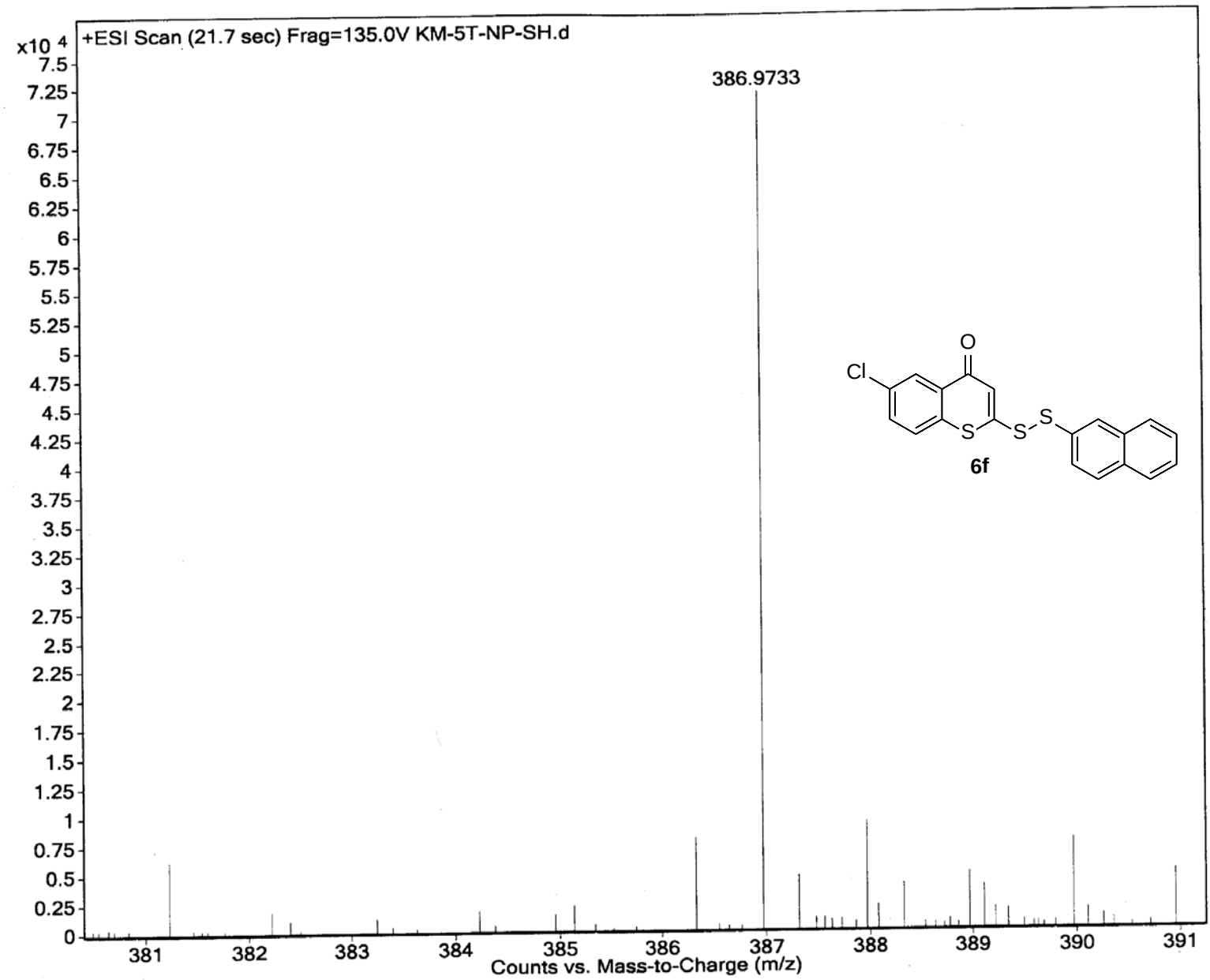


^{13}CNMR spectra of compound: 6f

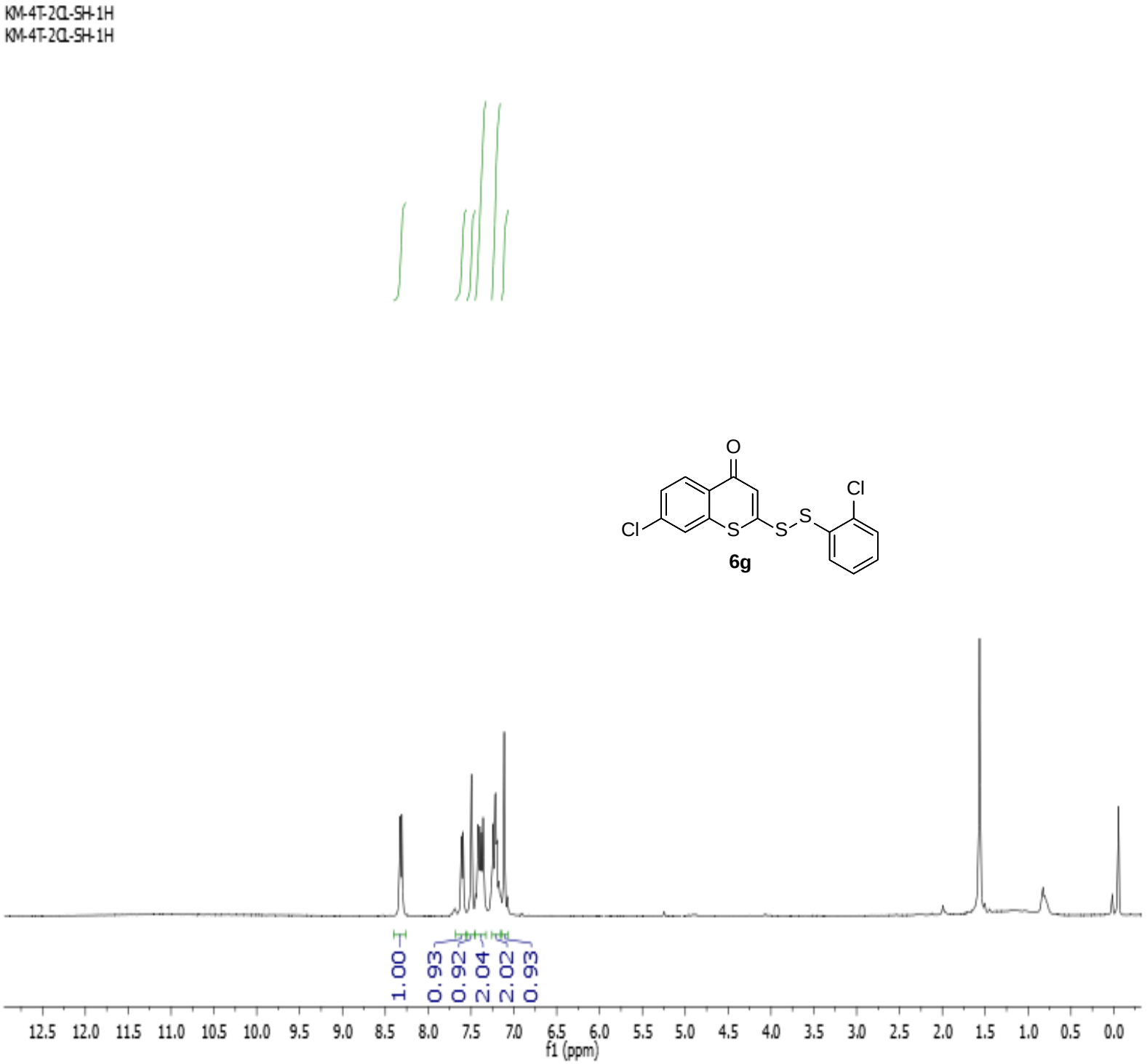


HRMS spectra of compound: 6f

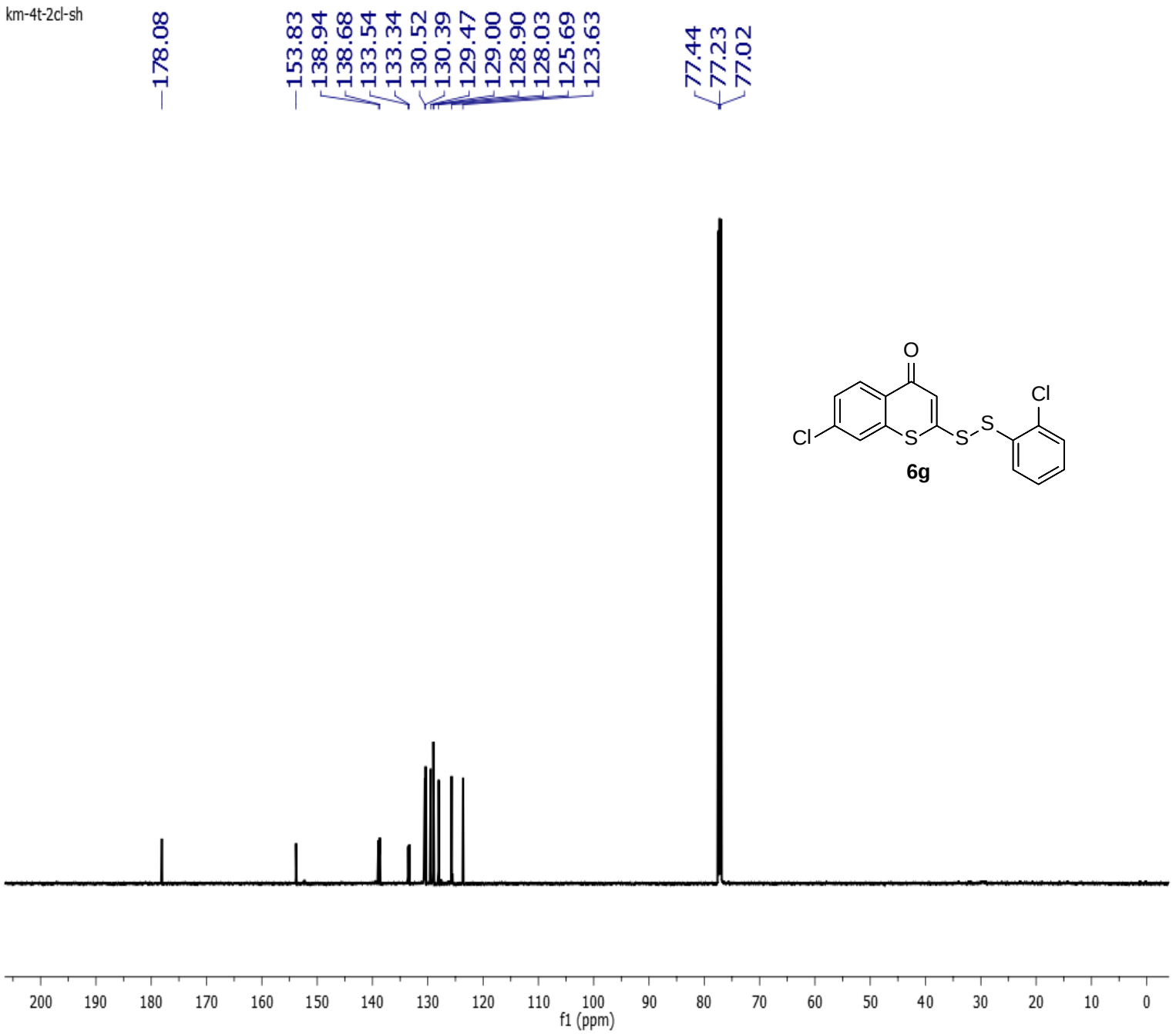
Sample Name	Unavailable	**Position**	Unavailable	**Instrument Name**	Unavailable	**User Name**	Unavailable
Inj Vol	Unavailable	**InjPosition**	Unavailable	**SampleType**	Unavailable	**IRM Calibration Status**	Success
Data Filename	KM-5T-NP-SH.d	**ACQ Method**		**Comment**	Sample information is unavailable	**Acquired Time**	Unavailable



[1]HNMR spectra of compound: 6g

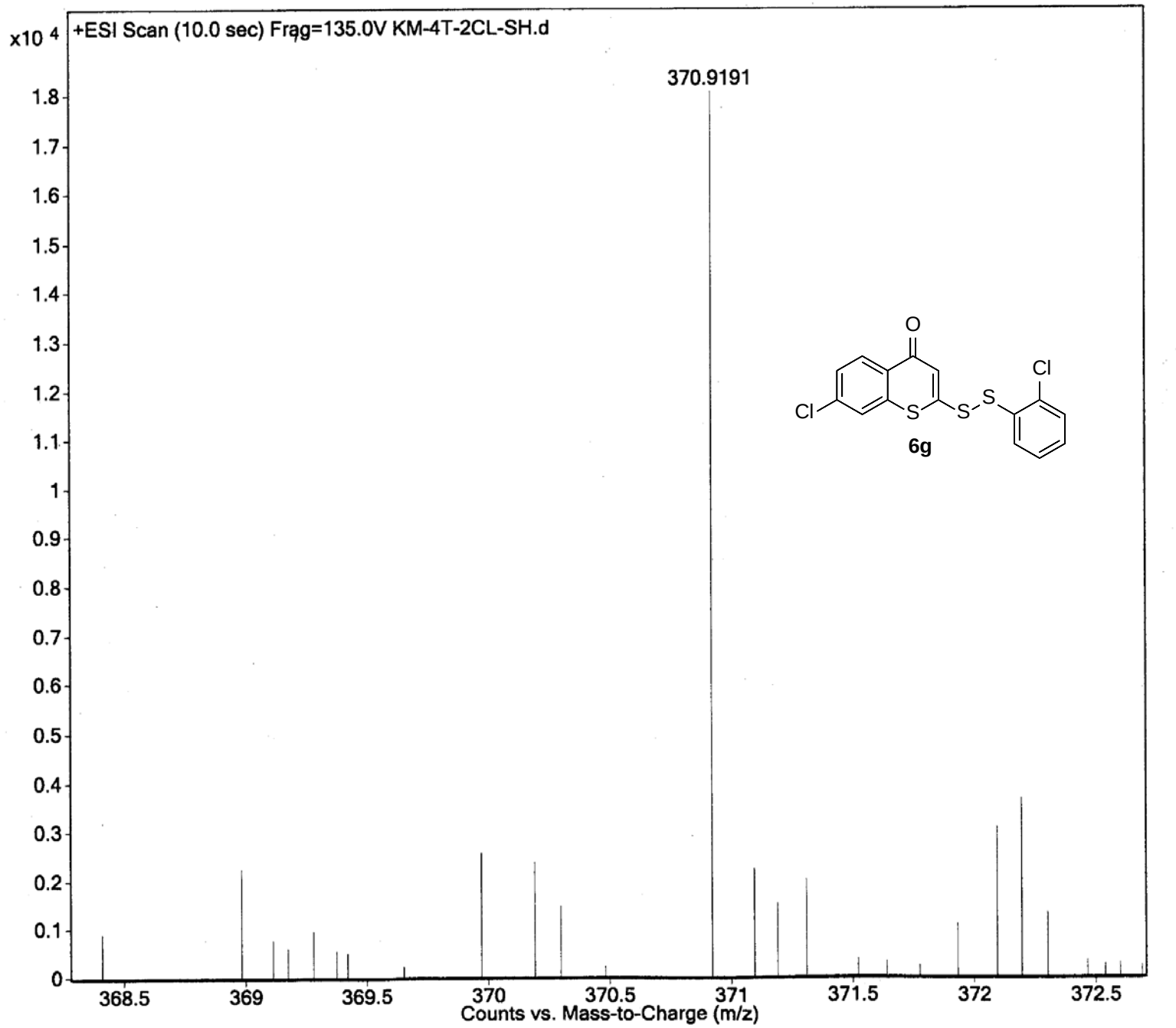


^{13}CNMR spectra of compound: 6g



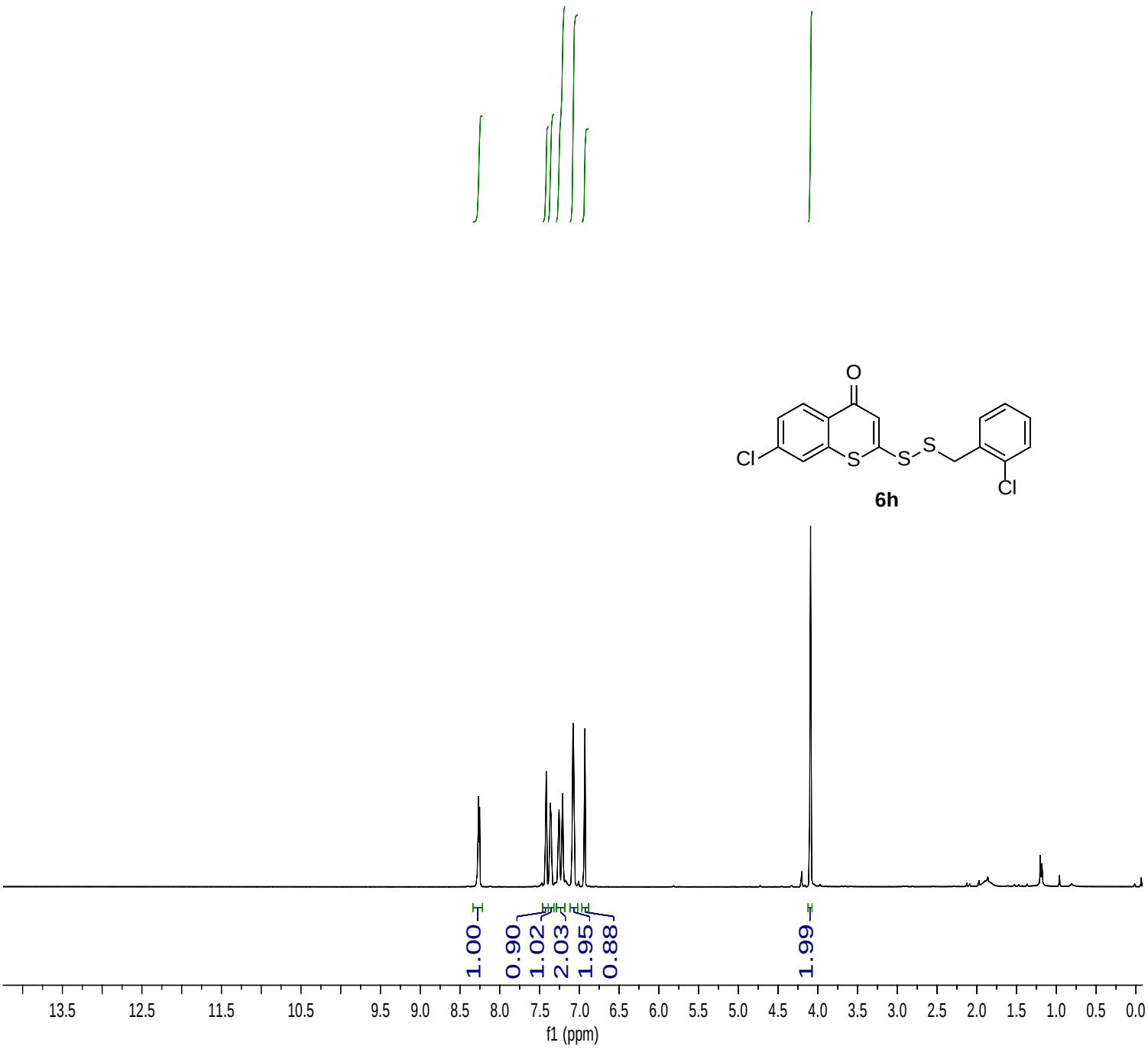
HRMS spectra of compound: 6g

Sample Name	KM-4T-2CL-SH	**Position**	Vial 1	**Instrument Name**	Instrument 1	**User Name**	
Inj Vol	0	**InjPosition**		**SampleType**	Sample	**IRM Calibration Status**	Success
Data Filename	KM-4T-2CL-SH.d	**ACQ Method**		**Comment**		**Acquired Time**	10/4/2017 4:44:37 PM

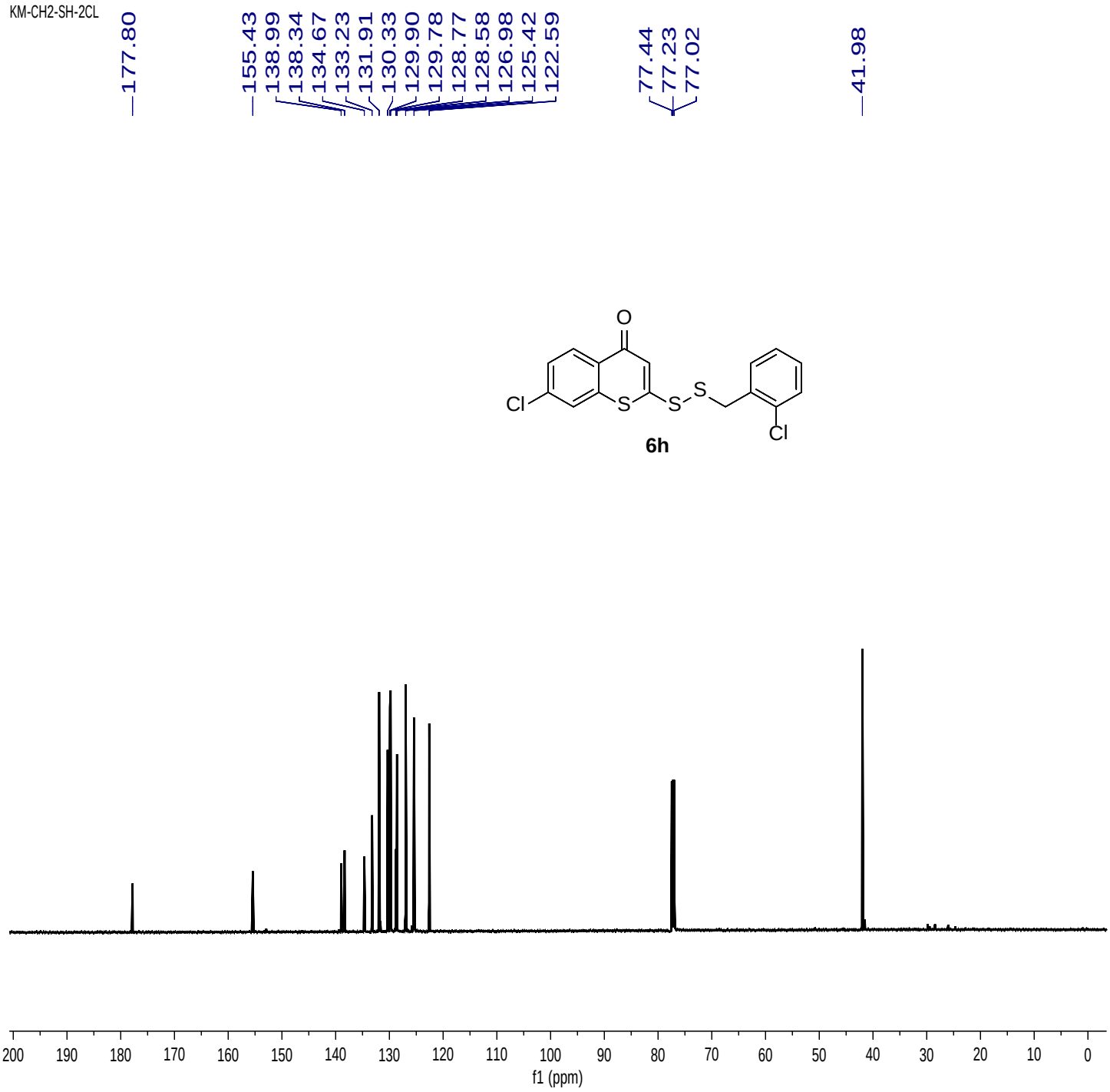


^{1}HNMR spectra of compound: 6h

KM-4T-CH2-2CL_1H
KM-4T-CH2-2CL_1

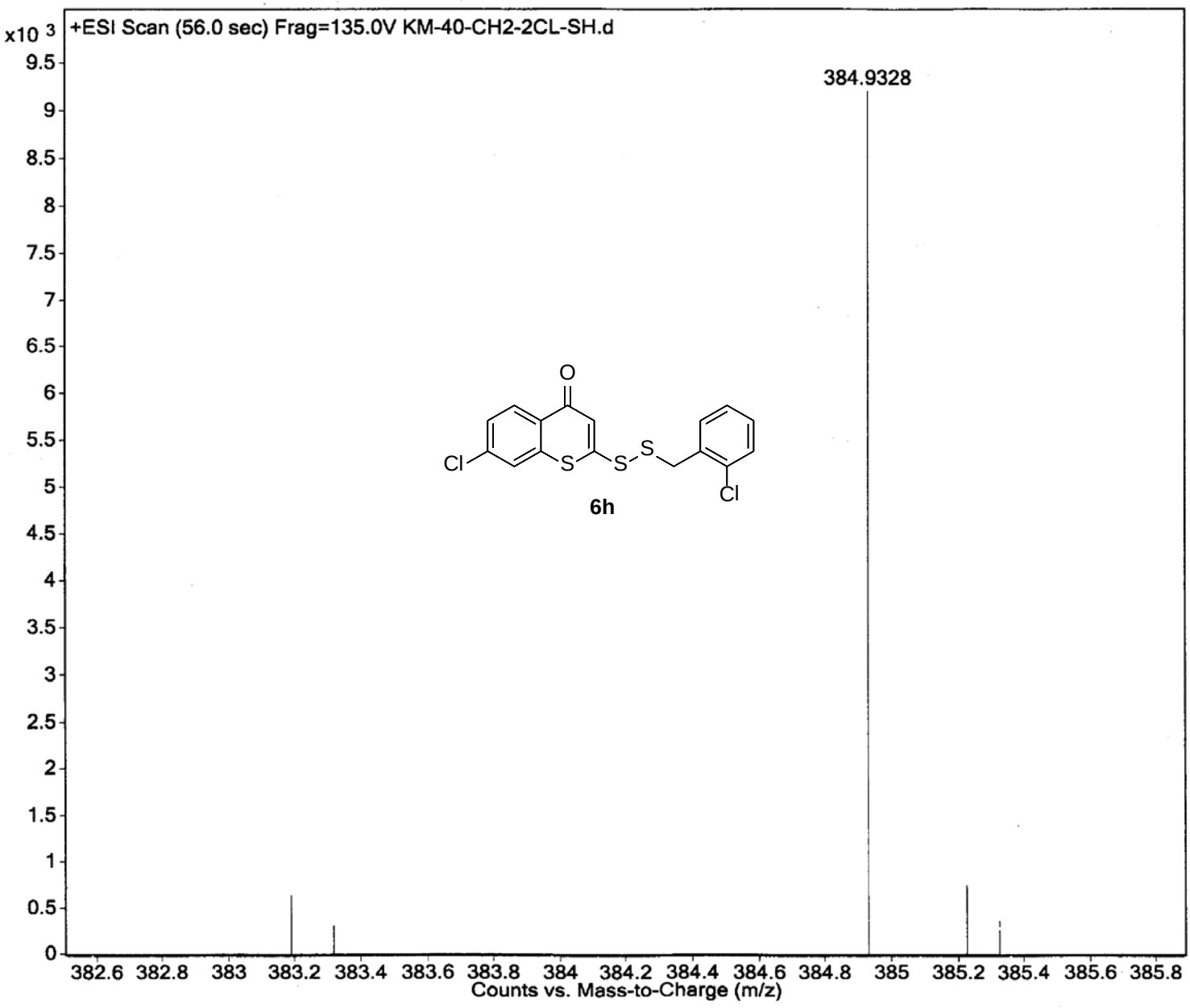


^{13}CNMR spectra of compound: 6h



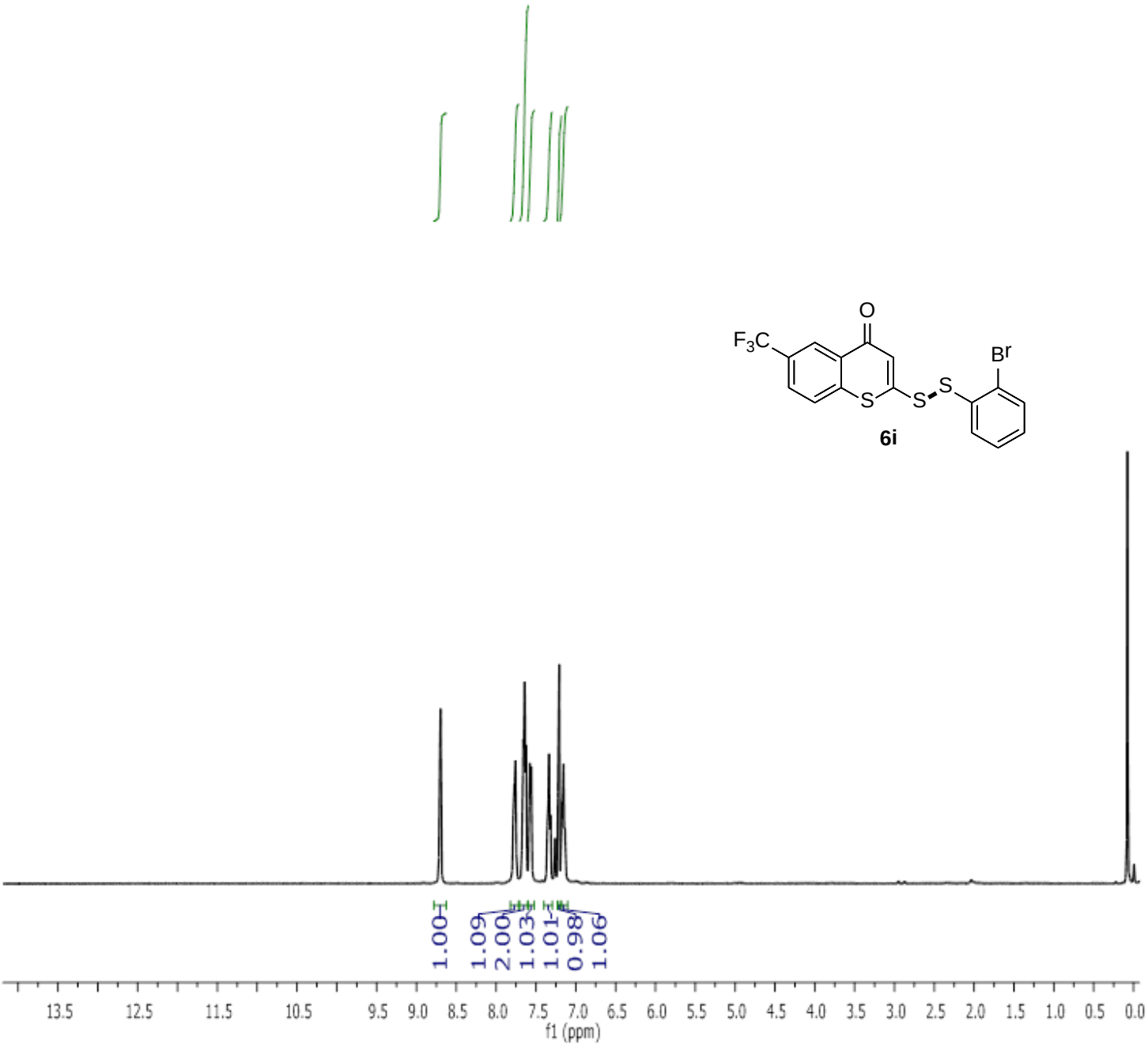
HRMS spectra of compound: 6h

Sample Name	KM-40-CH2-2CL-SH	**Position**	Vial 1	**Instrument Name**	Instrument 1	**User Name**	
Inj Vol	0	**InjPosition**		**SampleType**	Sample	**IRM Calibration Status**	All Ions Missed
Data Filename	KM-40-CH2-2CL-SH.d	**ACQ Method**		**Comment**		**Acquired Time**	9/18/2017 5:09:18 PM

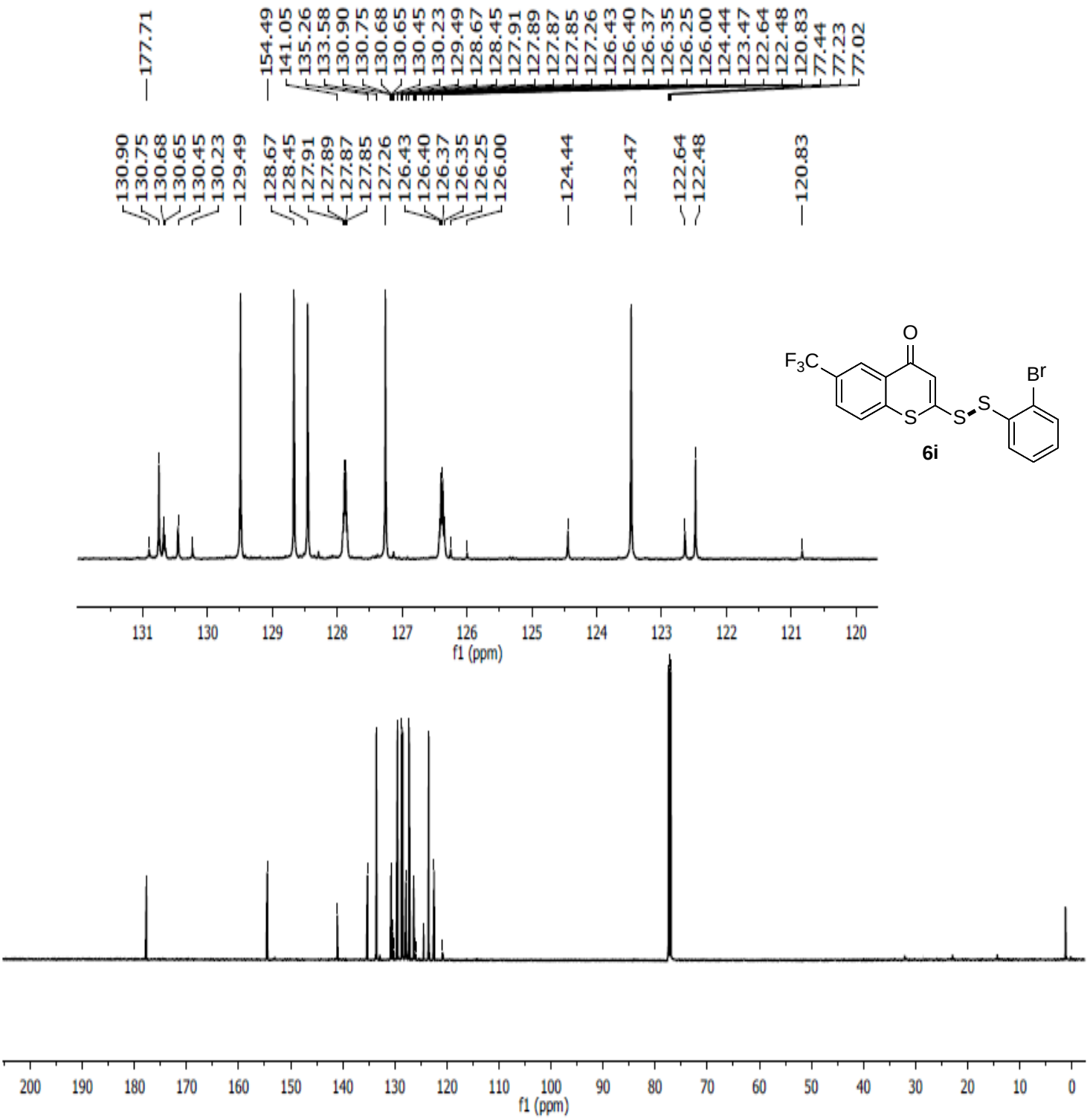


[1]HNMR spectra of compound: 6i

KM-CF3-T-2Br-SH-1H
KM-CF3-T-2Br-SH

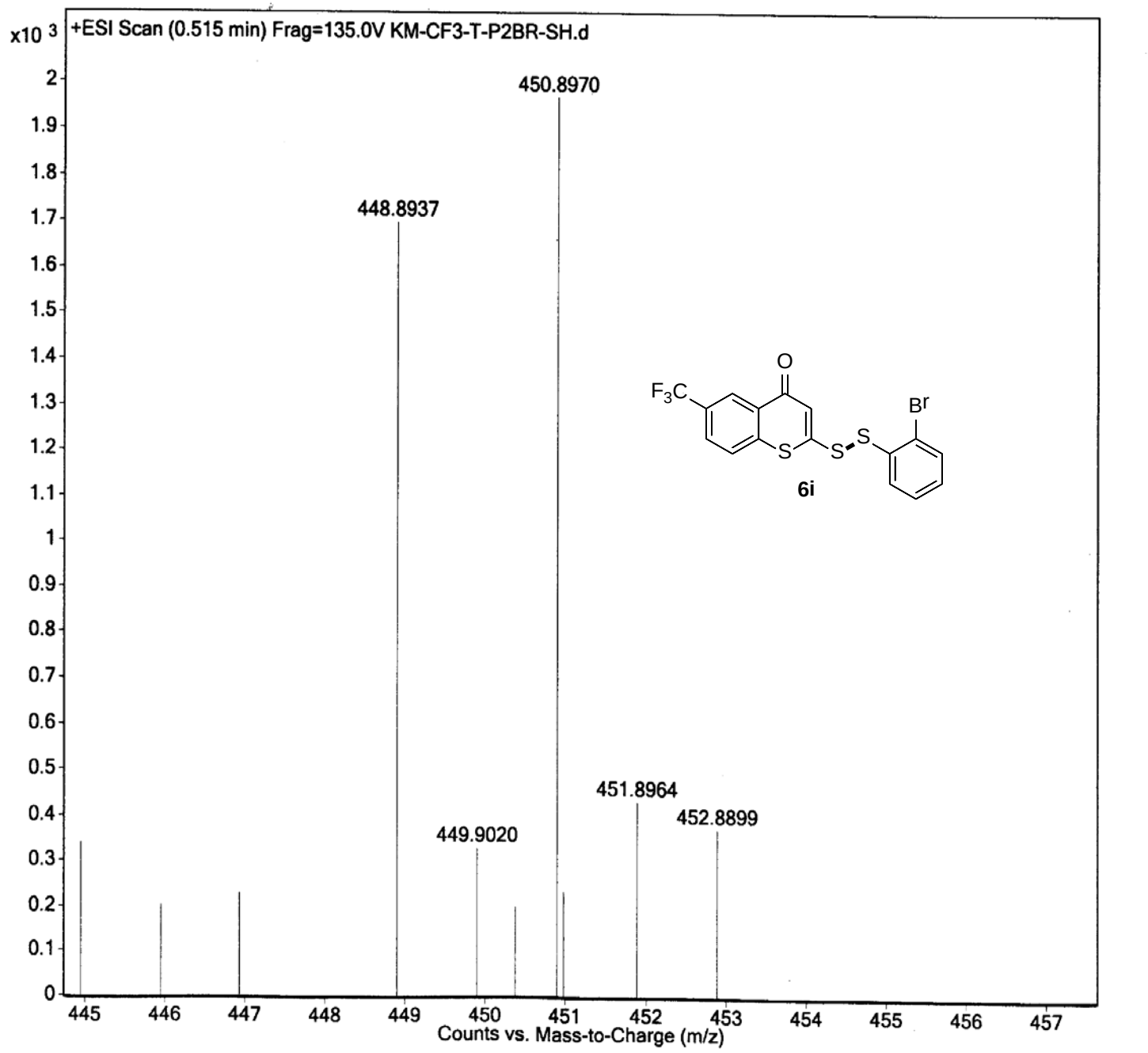


^{13}CNMR spectra of compound: 6i



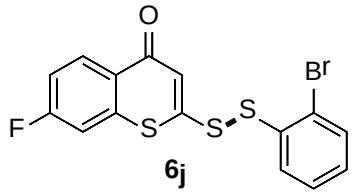
HRMS spectra of compound: 6i

Sample Name	KM-CF3-T-P2BR-SH	**Position**	Vial 1	**Instrument Name**	Instrument 1	**User Name**	
Inj Vol	-1	**InjPosition**		**SampleType**	Sample	**IRM Calibration Status**	Success
Data Filename	KM-CF3-T-P2BR-SH.d	**ACQ Method**		**Comment**		**Acquired Time**	12/21/2017 11:40:20 AM

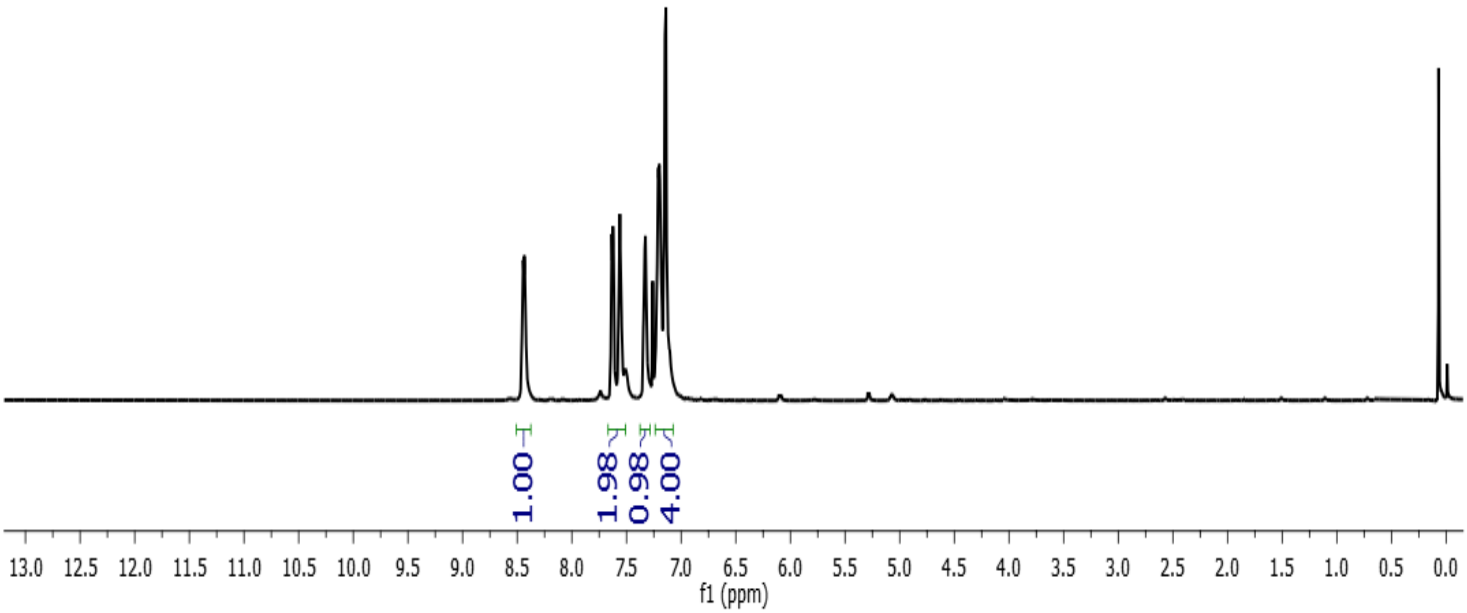


[1]HNMR spectra of compound: 6j

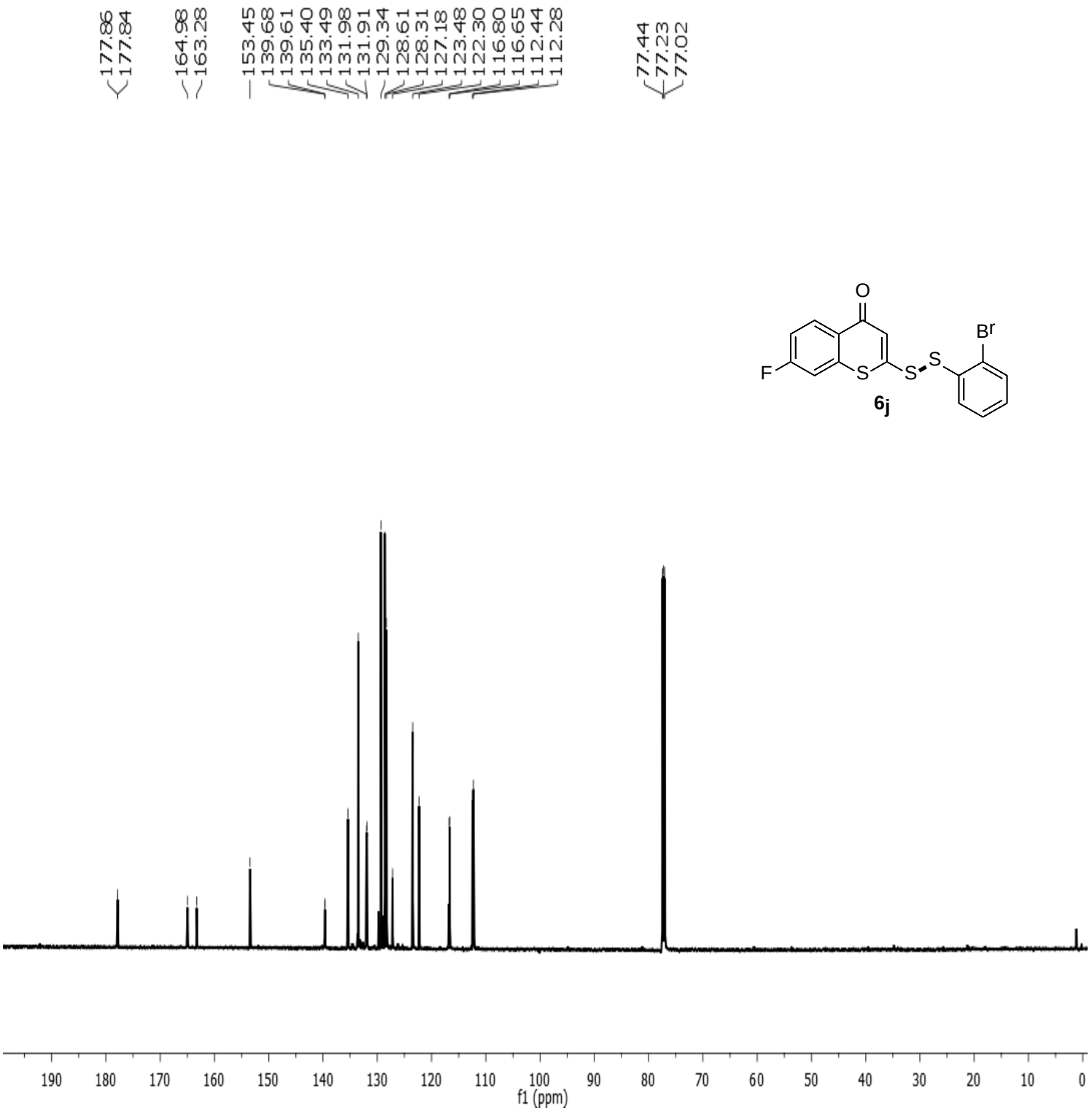
KM-TF-2BR-SH-1H
KM-TF-2BR-SH-1H



6j

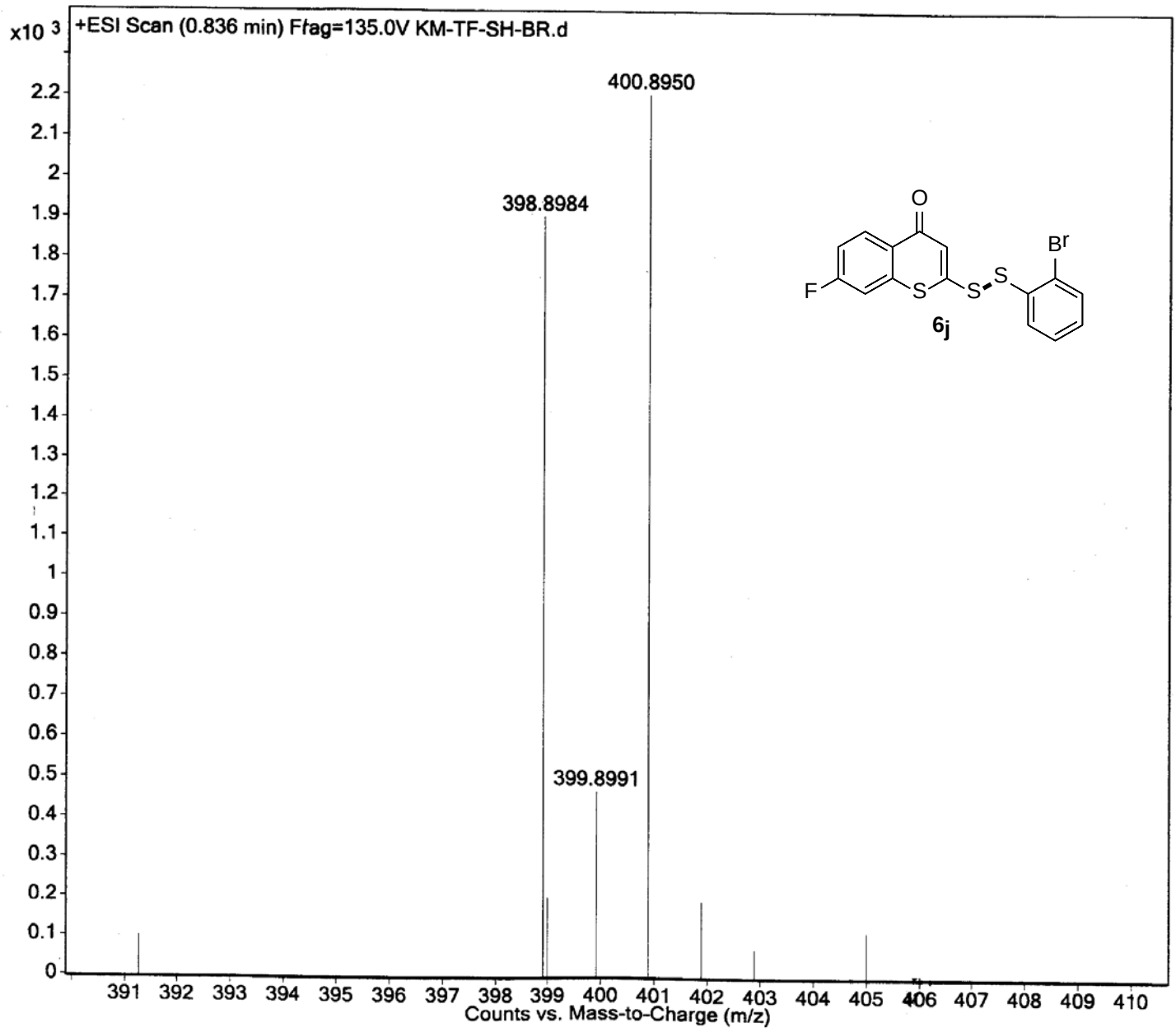


^{13}CNMR spectra of compound: 6j



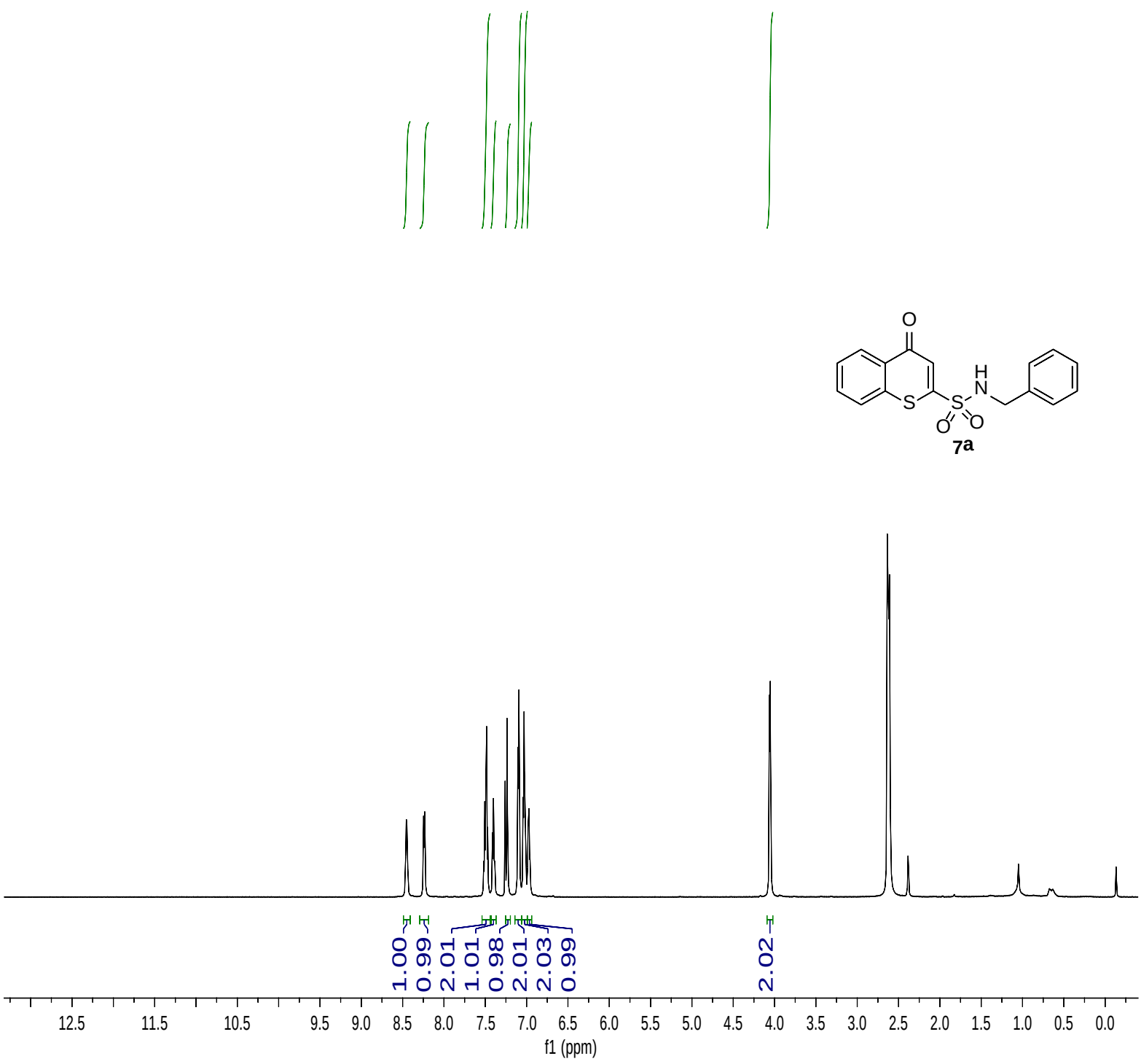
HRMS spectra of compound: 6j

Sample Name	KM-TF-SH-BR	**Position**	Vial 1	**Instrument Name**	Instrument 1	**User Name**	
Inj Vol	-1	**InjPosition**		**SampleType**	Sample	**IRM Calibration Status**	All Ions Missed
Data Filename	KM-TF-SH-BR.d	**ACQ Method**		**Comment**		**Acquired Time**	12/28/2017 12:07:56 PM

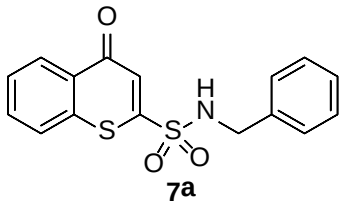


[1]HNMR spectra of compound: 7a

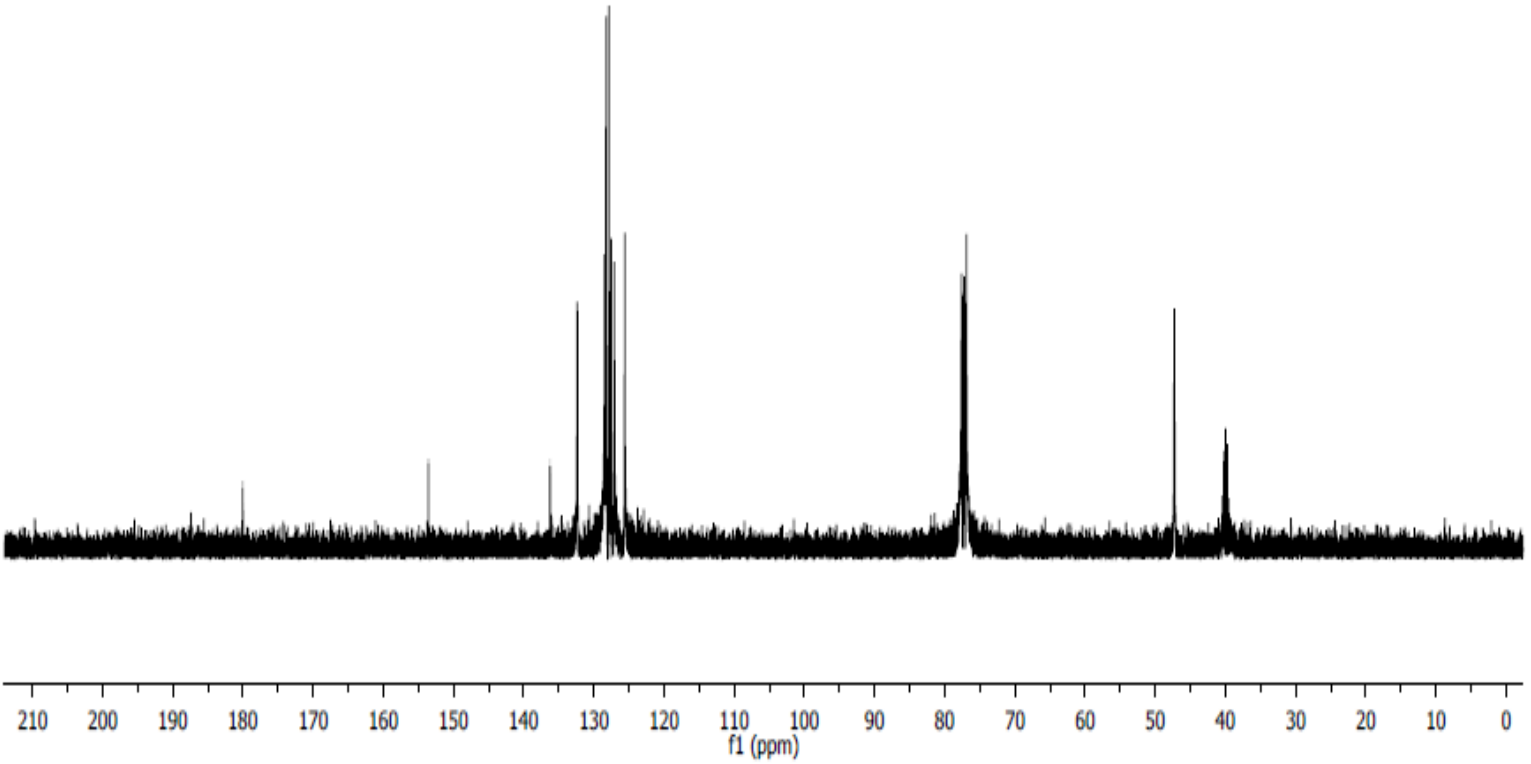
KM-T-BA-SO-1-1H
KM-T-BA-SO-1-1H



^{13}CNMR spectra of compound: 7a



7a



HRMS spectra of compound: 7a

Sample Name	Unavailable	**Position**	Unavailable	**Instrument Name**	Unavailable	**User Name**	Unavailable
Inj Vol	Unavailable	**InjPosition**	Unavailable	**SampleType**	Unavailable	**IRM Calibration Status**	All Ions Missed
Data Filename	KM-T-BA-SO.d	**ACQ Method**		**Comment**	Sample information is unavailable	**Acquired Time**	Unavailable