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Design, synthesis, *in silico* studies, and biological evaluation of novel pyrimidine-5-carbonitrile derivatives as potential anti-proliferative agents, VEGFR-2 inhibitors and apoptotic inducers

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Content

All the reagents, chemicals, apparatus used in chemistry section.

All melting points had been concluded by open capillary system on Stuart melting point apparatus SMP30 and had been uncorrected. The IR spectra were certified on a Bruker FT/IR-ATR spectrometer and expressed in wave number (cm^{-1}). The ^{1}H NMR spectra were recorded at 400 MHz while ^{13}C NMR spectra were run at 100 MHz, on a Bruker 400 MHZ-NMR spectrophotometer. TMS was used as internal standard, coupling constant (*J*) values were given in Hertz, chemical shifts were measured in δ (ppm) and recorded relative to (DMSO-d_6) solvent. The mass spectra were acquired on Varian Mat 311-A spectrometer (70 e.v.). Progress of reactions were monitored by TLC using TLC sheets coated with UV fluorescent silica gel and were visualized using UV lamp and different developing solvent system of DCM / methanol mixtures as mobile phases. Purity of the synthesized compounds was performed using a Waters Alliance 2695 HPLC, Column Thermo HYPERSIL BDS C18.

Table S-1: Signaling ratio of each signal group for compounds **11b** and **12b.**

Compound	**Key groups**	**Total integration**	**Integration of the 1st signal (%)**	**Integration of the 2nd signal (%)**
11b	CH_3	3.13	1.76 (56.2)	1.37 (43.8)
	SCH_3	3.20	1.93 (60.3)	1.27 (39.7)
	NH	1.20	0.59 (57.85)	0.43 (42.15)
	CONH	1.30	0.60	0.43

			(58.25)	(41.75)
12b	CH_3	2.94	1.95 (66.32)	0.99 (33.67)
	SCH_3	3.11	2.01 (64.63)	1.10 (35.36)
	NH	0.86	0.53 (61.62)	0.33 (38.37)
	CONH	0.74	0.43 (58.10)	0.31 (41.89)

Biological testing

1. *In vitro* anti-proliferative activity

MTT assay protocol was applied as described previously to assess the anti-proliferative activity of the synthesized compounds. Two human cancer cell lines (HCT-116 and MCF-7 **)** were used in this test. At first, the cell lines were cultured in RPMI-1640 medium with 10% fetal bovine serum. Antibiotics (100 unit's/ml penicillin and100 µg/ml streptomycin) were added at 37ºC in a 5% CO_2 incubator. The cell lines were seeded in a 96-well plate at a density of 1.0 x 10^4 cells / well at 37º C for 24 h under 5% CO_2. After incubation, the cells were treated with different concentrations of the synthesized compounds and incubated for 48 h. After 48 h of drug treatment, 20 µl of MTT solution at 5mg/ml was added and incubated for 4 h. Dimethyl sulfoxide (DMSO) in volume of 100 µl was added into each well to dissolve the purple formazan formed. The colorimetric assay was measured and recorded at absorbance of 570 nm using a plate reader (EXL 800, USA). The relative cell viability in percentage was calculated as (A570 of treated samples/A570 of untreated sample) X 100. The half maximal inhibitory concentration (IC_{50}) values are presented using non-linear regression analysis of the data set from three experiments with three plate wells were used for an individual concentration.

2. *In vitro* VEGFR-2 TK assay

The most active derivatives (**9d, 11b, 11c, 11d, 11e, 12b, 12c,** and **12d**) that exhibited promising antiproliferative activities against HCT-116 and MCF-7 cell lines were tested for its inhibitory activity against VEGFR-2 TK. Human VEGFR-2 TK ELISA kit (Enzyme-Linked

Immunosorbent Assay) was utilized in this test. At first, specific antibody for VEGFR-2 TK was seeded on a 96-well plate and 100 µL of the standard solution or the tested compound was added, all were incubated at room temperature for 2.5 h. Then washed, 100 µL of the prepared biotin antibody was added, then incubated at room temperature for an additional 1 h. and washed. Then, 100 µL of streptavidin solution was added and incubated for 45 min. at room temperature and washed again, 100 µL of TMB Substrate reagent was added and incubated for 30 min. at room temperature. 50 µL of the stop solution was added, then was read at 450 nm immediately. The standard curve was drawn, concentrations on the X-axis and the absorbance on the Y-axis.

3. **Flow cytometry analysis for cell cycle**

To investigate the effect of the synthesized compounds on the various phases of the cell cycle in HCT-116 cells, flow cytometric analysis of cell cycle was performed using Epics XL-MCL™ Flow Cytometer according to flow cytometric analysis technique.

Flow Cytometry Kit for Cell Cycle Analysis (ab139418_Propidium Iodide Flow Cytometry Kit/BD) was used in this test. HCT-116 cells were treated with compound **11e** (1.14±0.01 µM) for 24 h. Then, the cells were fixed in 70% ethanol at 4 °C for 12 h. After that, the cells were washed with cold PBS, incubated with 100 µl RNase A at 37 °C for 30 min, and stained with 400 µl PI in the dark at room temperature for a further 30 min. The stained cells were measured using Epics XL-MCL™ Flow Cytometer (Beckman Coulter), and the data were analyzed using Flowing software (version 2.5.1, Turku Center for Biotechnology, Turku, Finland).

4. Flow cytometry analysis for apoptosis

Flow cytometry cell apoptosis analysis was used to investigate the apoptotic effect of the synthesized compounds. HCT-116 cells were treated with compound **11e** (1.14±0.01 µM) for 24 h, collected by trypsin, centrifuged, washed two successive times with PBS, suspended in 500 µl binding buffer, and double stained with 5 µl Annexin V-FITC and 5 µl PI in the dark at room temperature for 15 min. The stained cells were measured using Epics XL-MCL™ Flow Cytometer and analyzed using Flowing software.

5. ***In vitro* immunomodulatory assay of TNF-α and IL-6.**

The effects of compound **11e** on the expression of TNF-α and IL-6 were determined using qRTPCR technique. The quantity of immunomodulatory proteins (TNF-α and IL-6) in control and compound **11e** (at the IC_{50} concentration)-treated HCT-116 cells was assessed by qRTPCR (reference). Total RNA from vehicle-treated control (0.01% DMSO) and 10k-treated HCT-116 cells were extracted as-per the manufacturer instructions (RNeasy mini kit, Qiagen, Germany). After RNA extraction, cDNA was prepared using the Revert Aid First Strand cDNA Synthesis kit (Thermo Scientific, USA). Amplification of target cDNA for apoptosis markers and GAPDH [as a normalization (housekeeping) gene] was done using one-step RT-PCR SYBR® Green kit Master Mix (Bio-Rad Laboratories, USA) on Rotor-Gene Q real-time PCR thermal cycler instrument. cDNA (2 µl aliquots) was mixed with 1 µl of forward primer, 1 µl reverse primer, 10 µl master mixture, and the reaction volume was completed to 20 µl with nuclease-free water. All experiments were performed in triplicates.

6. **Statistical analysis**

Graph Pad Prism 6 software was used for statistical evaluation of the grouped data. Values are expressed as the mean ± SEM of the triplicates of each experiment. p value of less than 0.05 was accepted as statistically significant.

Molecular docking studies and molecular dynamic simulation

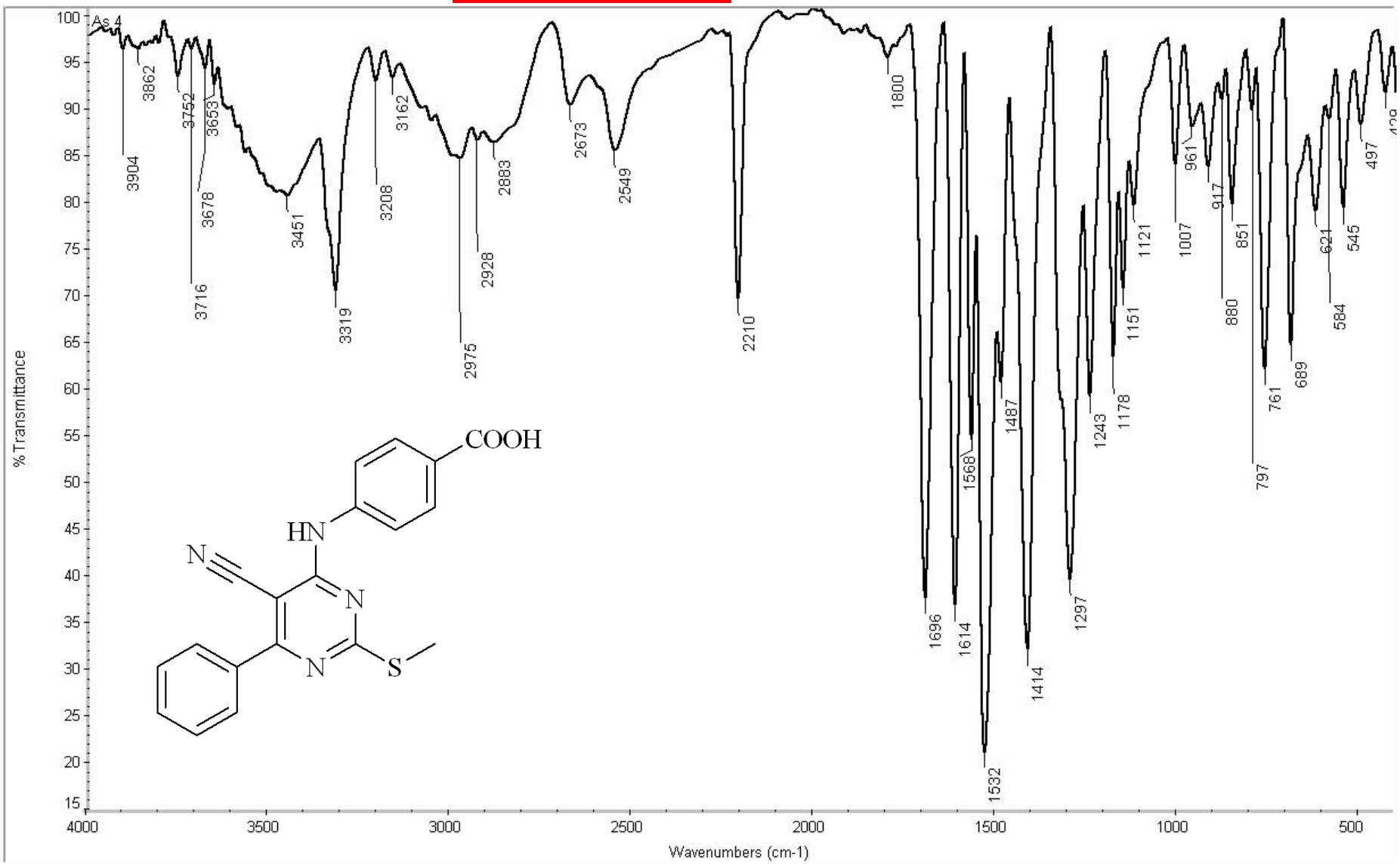
MOE 19.0102 software was used in the docking studies, where the binding affinities of target compounds against the ATP binding site of VEGFR-2 TK were evaluated. The 3D crystal structure of VEGFR-2 TK was downloaded from the Protein Data Bank, http://www.rcsb.org/pdb (PDB ID: 1YWN: 1.71 Å). At first, water molecules were deleted from the downloaded protein molecule. Energy minimization was performed by applying CHARMm and MMFF94 force fields. The active binding site was identified and prepared for docking protocol. The 2D structures of thalidomide and the target compounds were drawn using ChemBioDraw Ultra 14.0 and saved in MDL-SD file format. The re-docking of the co-crystallized ligand (4-amino-furo[2,3-d]pyrimidine) molecule into the ATP binding site of VEGFR-2 TK validated the docking process. The re-docked pose overlaid with the original one and had the same binding mode which was consistent with the reported mode (**Fig. XXX& XXX**). The re-docked pose had root mean square deviation (RMSD) 0.49 Å and docking score of -10.90 kcal/mol. After opening of the SD file and protonation of the 3D structures, energy was minimized. Preparation of the target structures was

done through optimization of the parameters. The docking process was done using the MOE 19.0102 software and Sorafenib was used as reference. A maximum of 15 conformers was considered for each molecule in the docking analysis. Then, the docking scores of the most ideal pose for each of the docked molecules were recorded **(Table xxx)**.

On the other hand, Molecular dynamics simulation of the protein-ligand complexes was performed using GROMACS[1] 2021.1 version and Linux 5.4 package. The GROMOS96 54a7 forcefield was selected as the force field for proteins and the ligand topologies were generated from the PRODRG[2] server. All the complexes were solvated using simple point charge (SPC) water molecules in a rectangular box. To make the simulation system electrically neutral, the required number of Na+ and Cl− ions were added while 0.15 mol/L salt concentrations were set in all the systems. Using the steepest descent method, all the solvated systems were subjected to energy minimization for 5000 steps. Afterwards, NVT (constant number of particles, volume, and temperature) series, NPT (constant number of particles, pressure, and temperature) series, and the production run were conducted in the MD simulation. The NVT and the NPT series were conducted at a 300 K temperature and 1 atm pressure for the duration of 300 ps. V-rescale thermostat and Parrinello-Rahman barostat were selected for the performed simulation. Finally, the production run was performed at 300 K for a duration of 100 ns (nanoseconds). Thereafter, a comparative analysis was performed measuring root mean square deviation (RMSD), root mean square fluctuation (RMSF), radius of gyration (Rg), solvent accessible surface area (SASA) and hydrogen bonds to analyze their stability. The Xmgrace program was used to represent the analyses in the form of plots.

Spectral data of intermediate and final target compounds **(3, 4, 5, 6, 8, 9a-d, 11a-e, and 12a-g)**

Compound 4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70
65
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55
50
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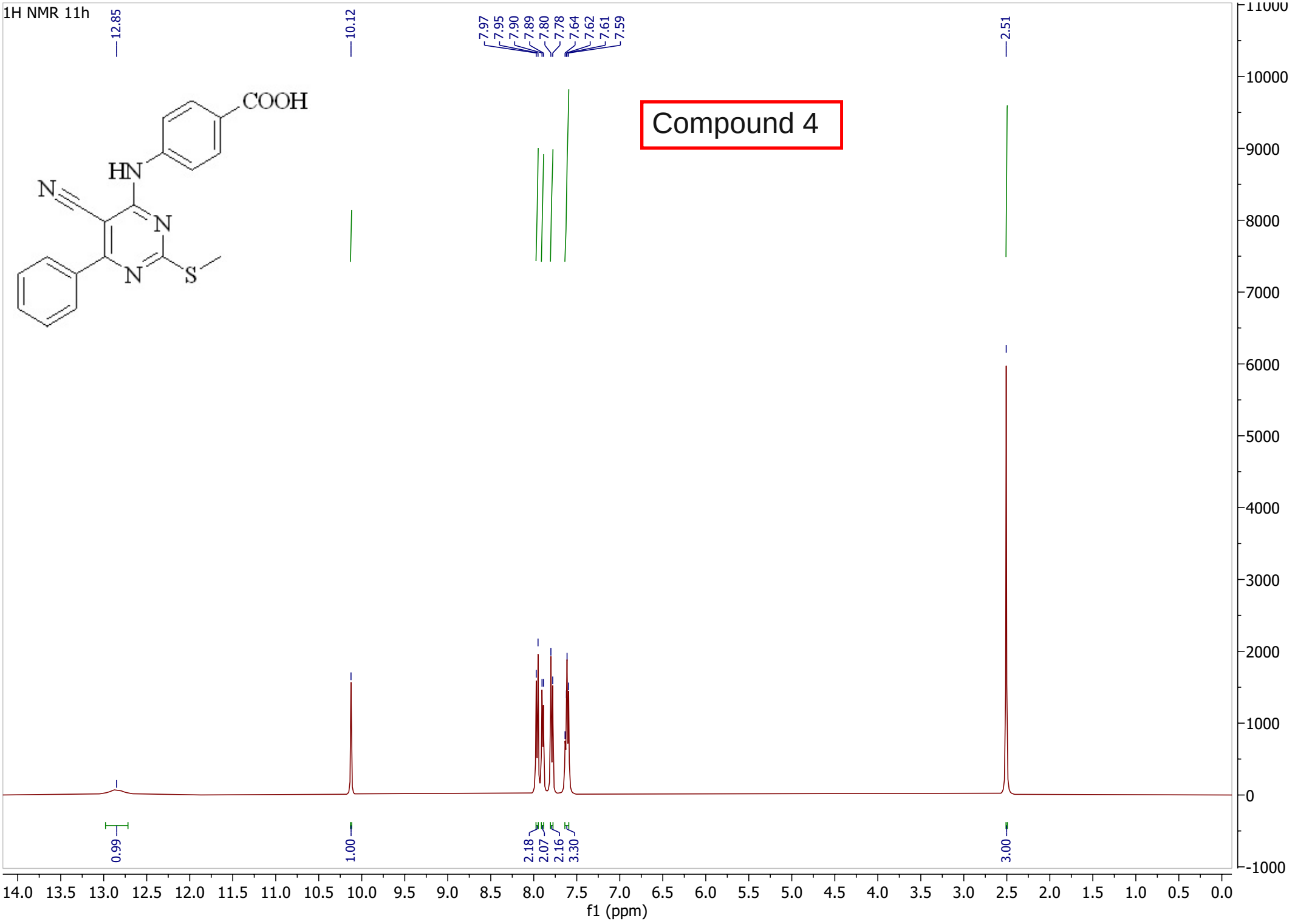
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10.12
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7.90
7.89
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7.78
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7.62
7.61
7.59
2.51
COOH
HN
N
N
N
S
Compound 4
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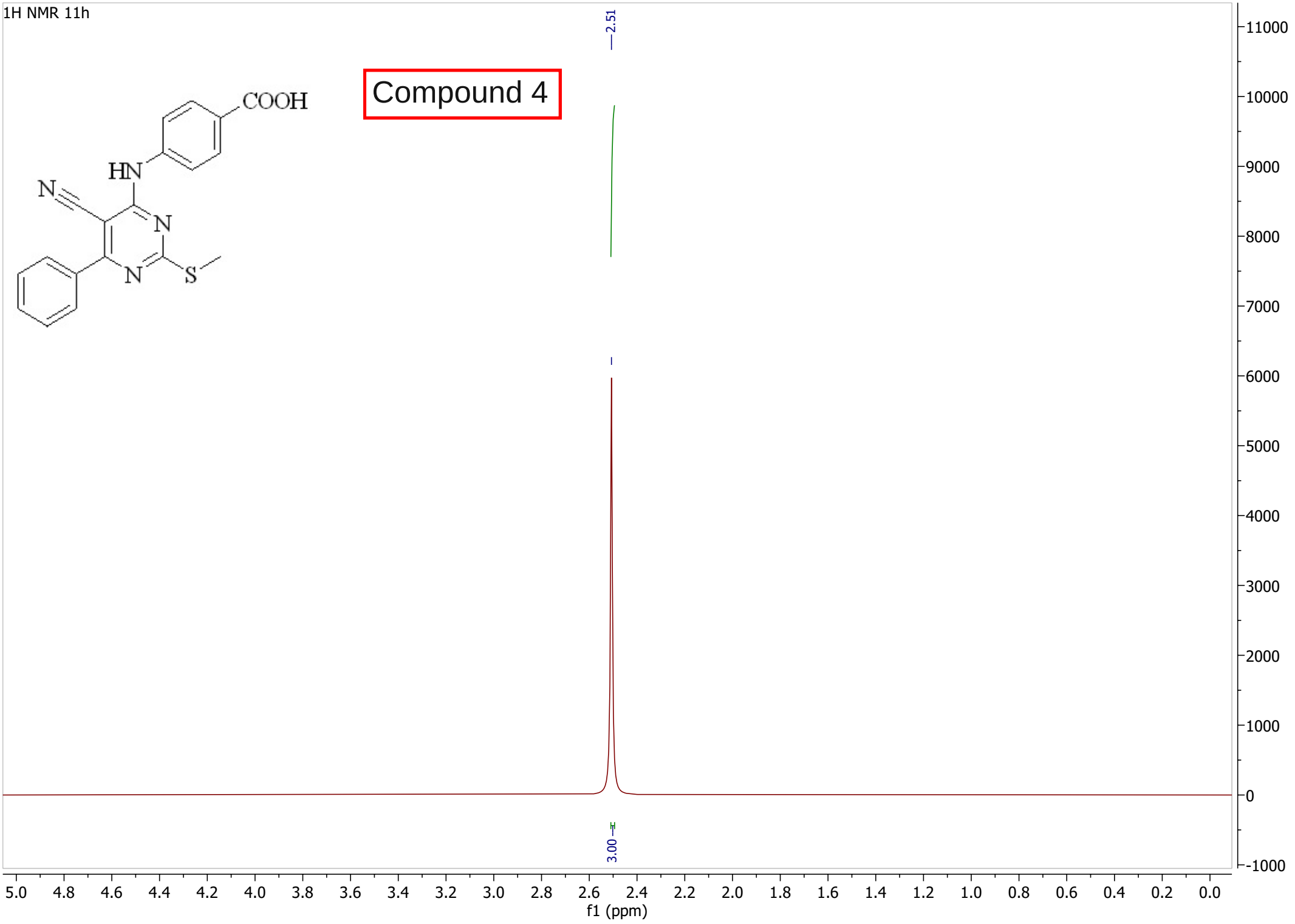
f1 (ppm)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Compound 4
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S
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5000
4000
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4.6
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4.2
4.0
3.8
3.6
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3.2
3.0
2.8
2.6
2.4
2.2
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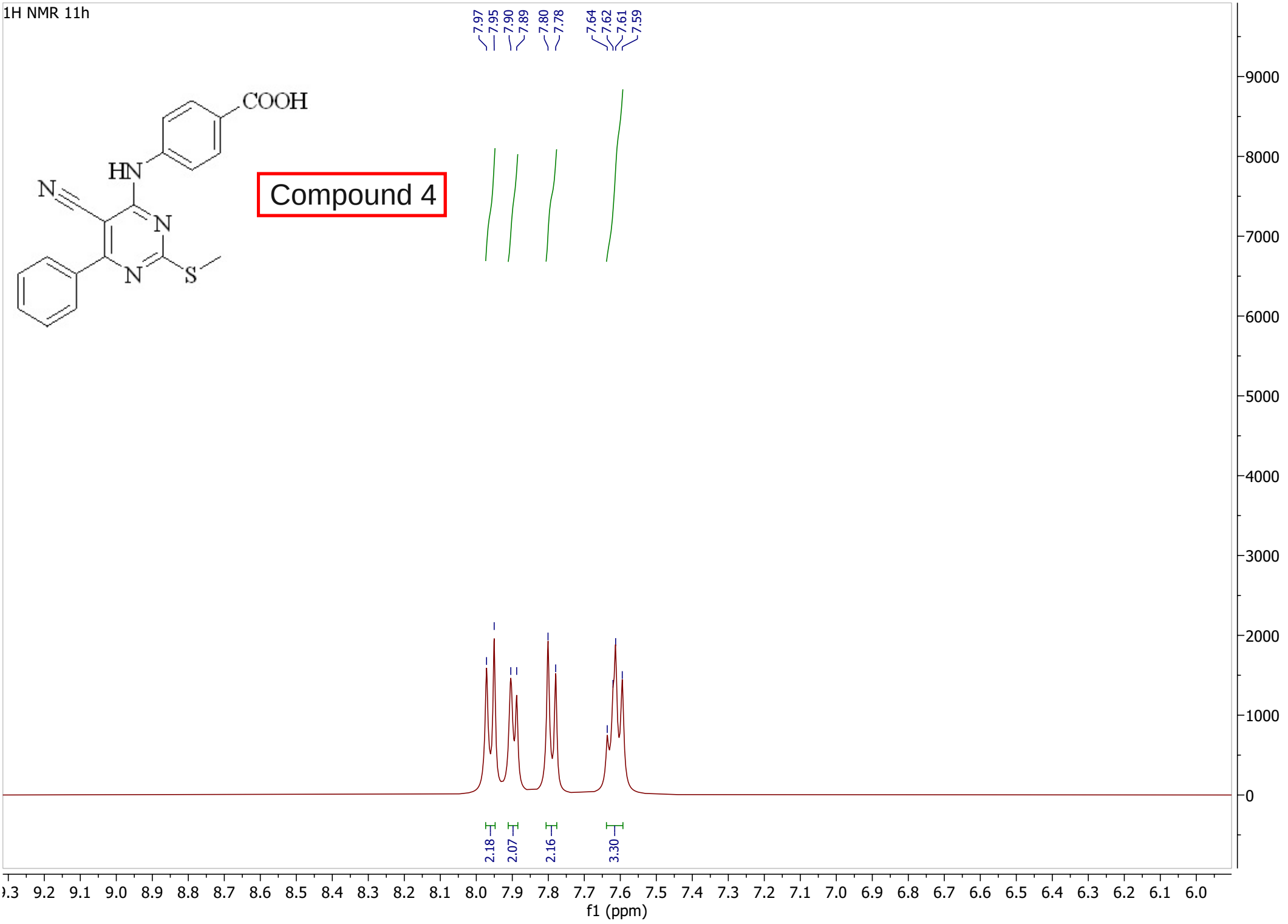
f1 (ppm)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7.59
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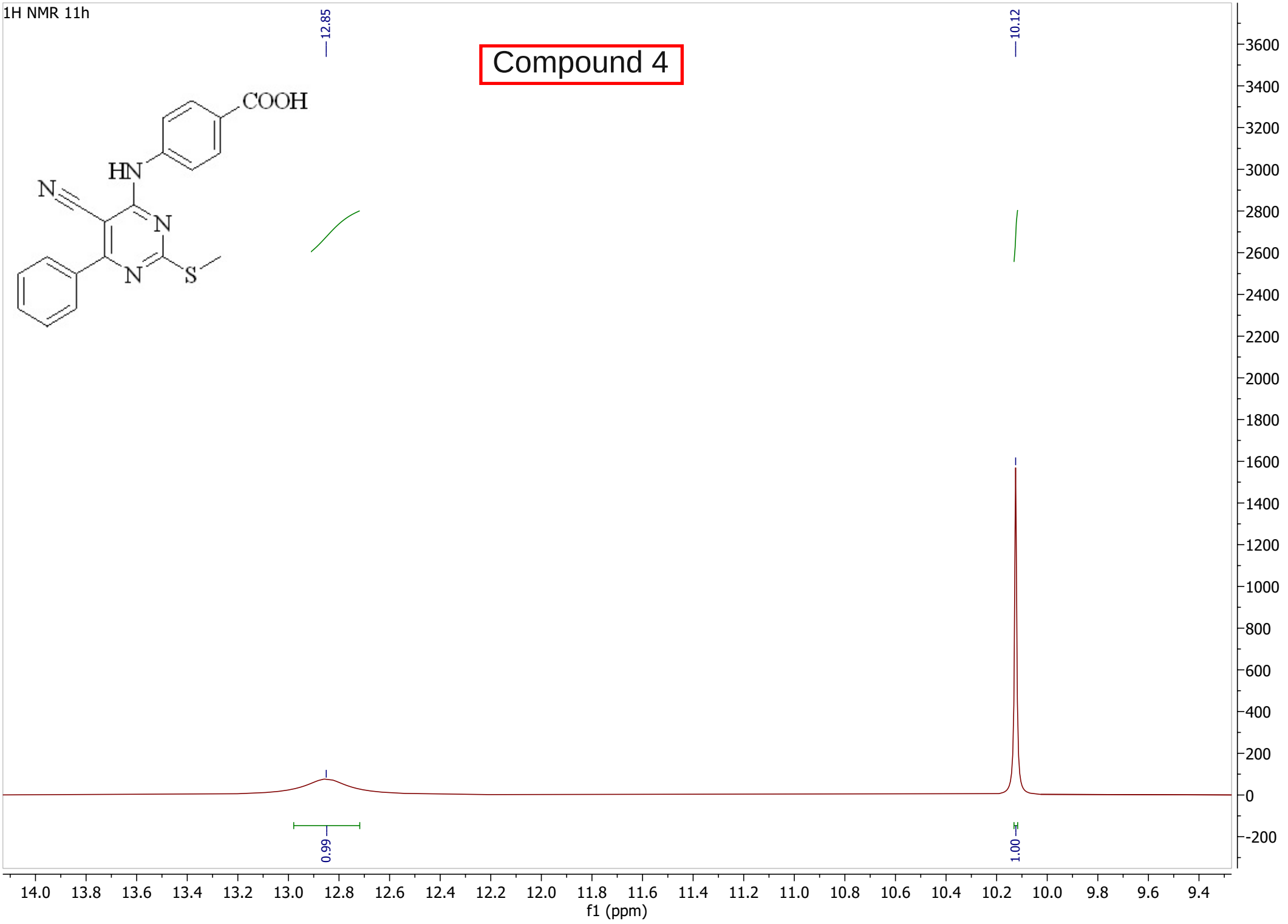
N
N
N
S
Compound 4
2.18
2.07
2.16
3.30
9000
8000
7000
6000
5000
4000
3000
2000
1000
0
9.3 9.2 9.1 9.0 8.9 8.8 8.7 8.6 8.5 8.4 8.3 8.2 8.1 8.0 7.9 7.8 7.7 7.6 7.5 7.4 7.3 7.2 7.1 7.0 6.9 6.8 6.7 6.6 6.5 6.4 6.3 6.2 6.1 6.0
f1 (ppm)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1800
1600
1400
1200
1000
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600
400
200
0
-200
0.99
1.00
14.0
13.8
13.6
13.4
13.2
13.0
12.8
12.6
12.4
12.2
12.0
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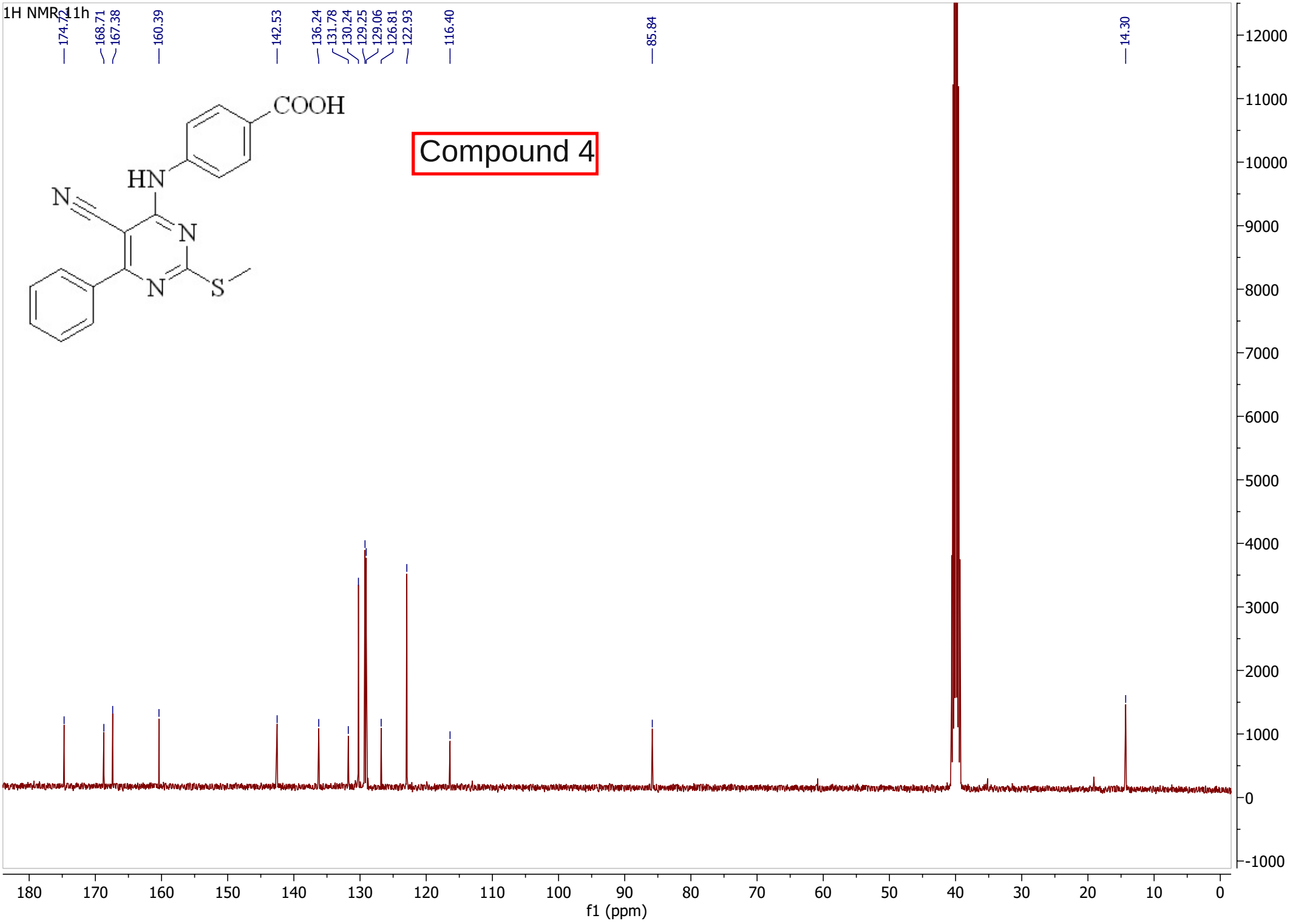
f1 (ppm)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136.24
131.78
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126.81
122.93
116.40
85.84
14.30
COOH
HN
N
N
N
S
Compound 4
12000
11000
10000
9000
8000
7000
6000
5000
4000
3000
2000
1000
0
-1000
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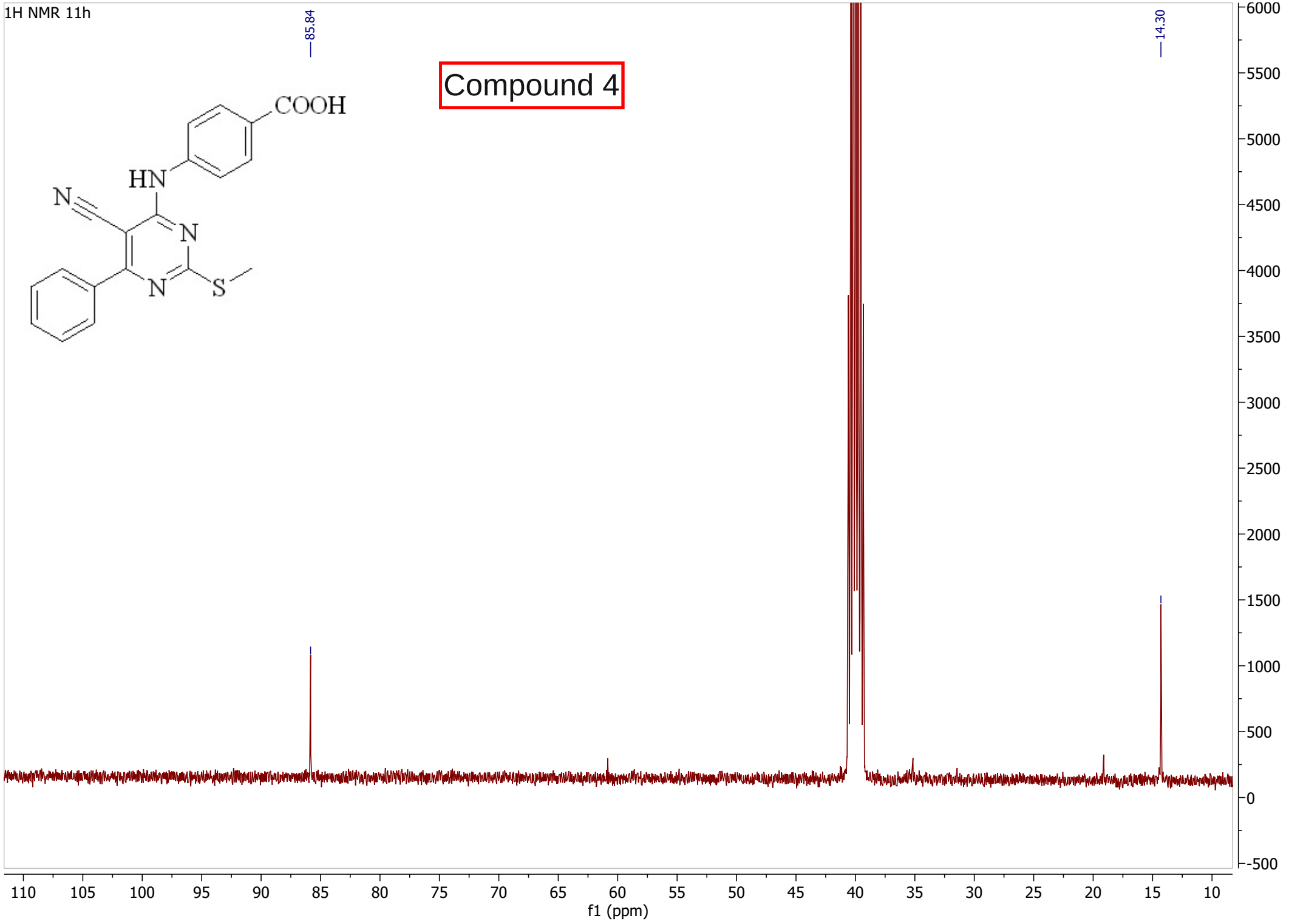
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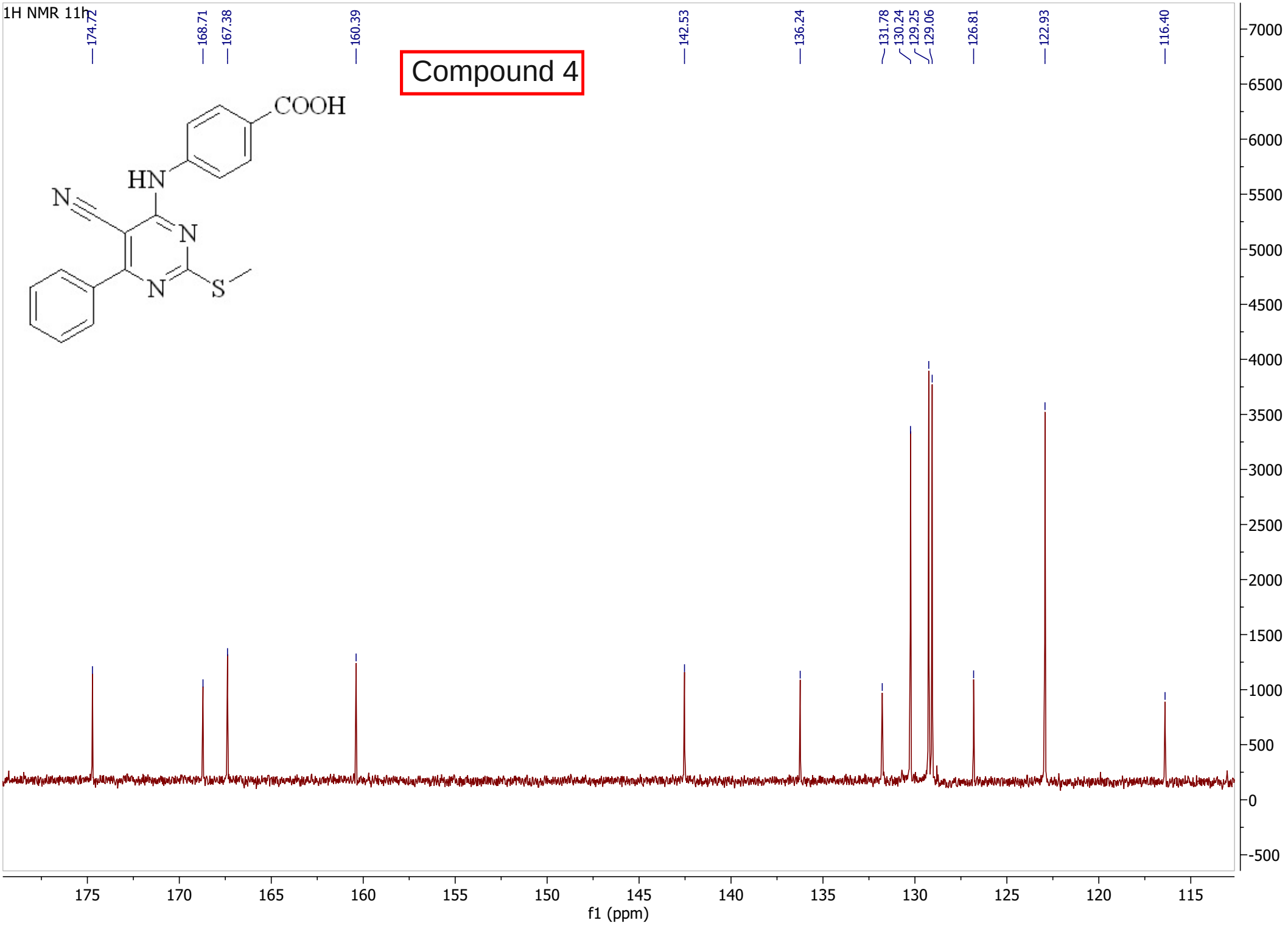
f1 (ppm)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167.38
160.39
142.53
136.24
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126.81
122.93
116.40
Compound 4
COOH
HN
N
N
N
S
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6500
6000
5500
5000
4500
4000
3500
3000
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2000
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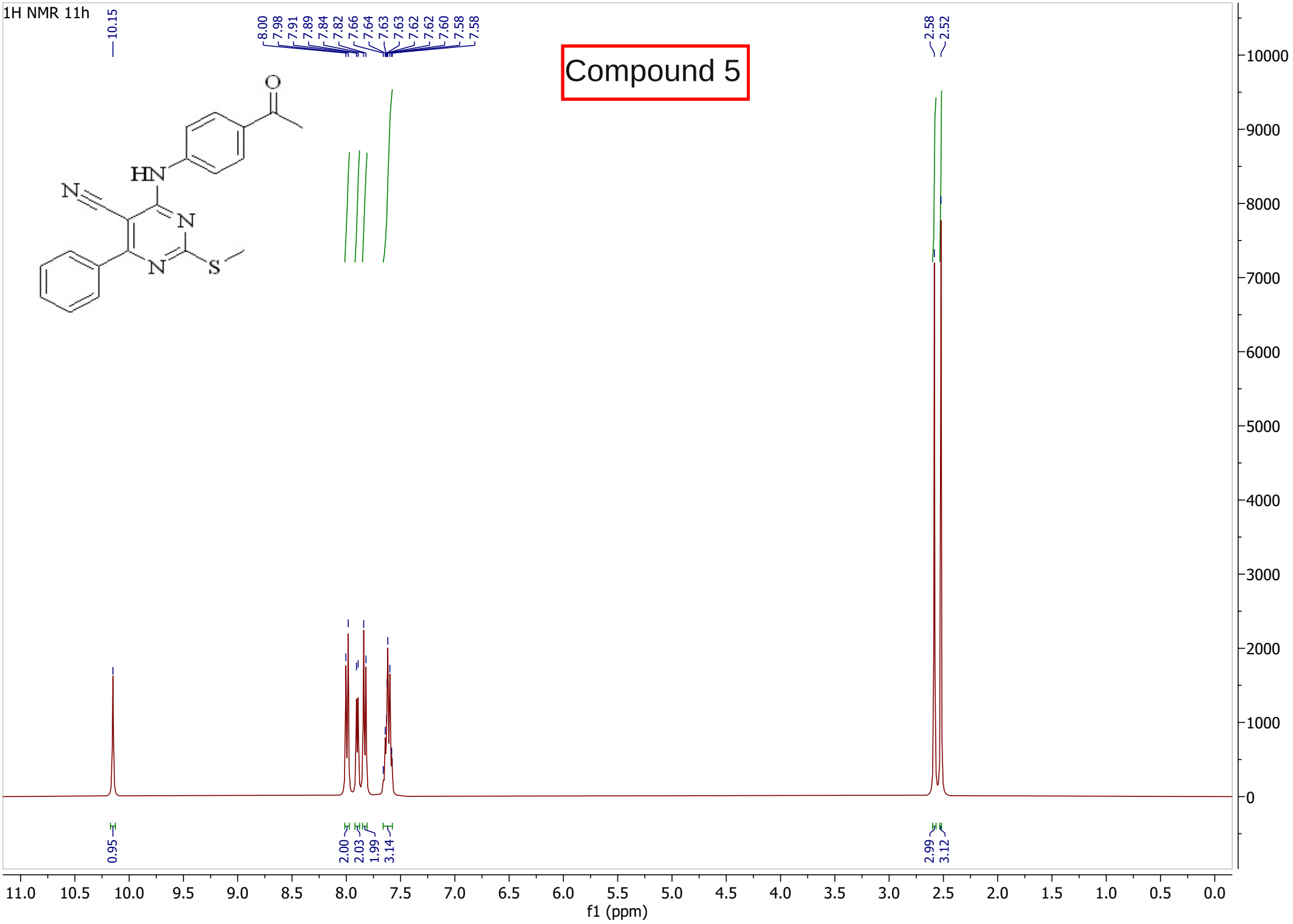
f1 (ppm)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7.89
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7.63
7.62
7.62
7.60
7.58
7.58
2.58
2.52
HN
N
N
N
S
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2.99
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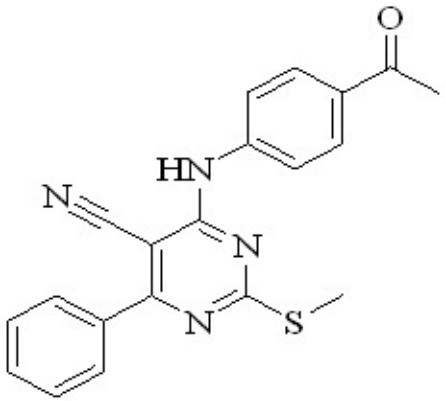
f1 (ppm)

1H NMR 11h



Compound 5

2.58
2.52

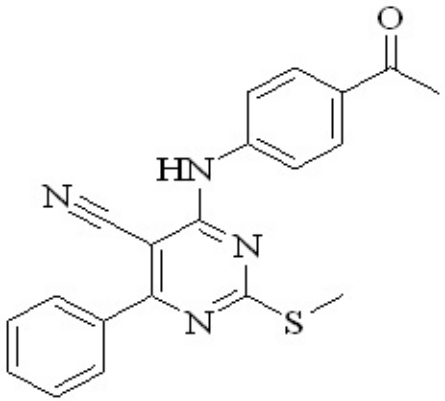
2.99
3.12

10000
9000
8000
7000
6000
5000
4000
3000
2000
1000
0

6.0 5.8 5.6 5.4 5.2 5.0 4.8 4.6 4.4 4.2 4.0 3.8 3.6 3.4 3.2 3.0 2.8 2.6 2.4 2.2 2.0 1.8 1.6 1.4 1.2 1.0 0.8 0.6 0.4 0.2 0.0

f1 (ppm)

1H NMR 11h



Compound 5

8.00
7.98
7.91
7.89
7.84
7.82
7.66
7.64
7.63
7.63
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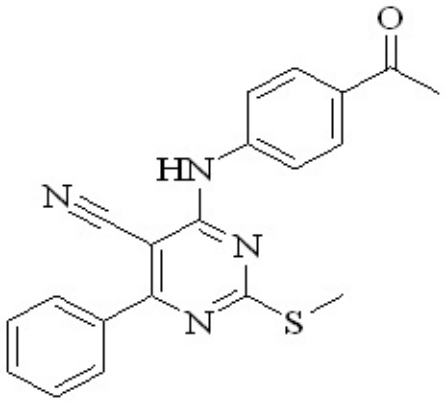
2.03
1.99
3.14

f1 (ppm)

1H NMR 11h



Compound 5

10.15

0.95

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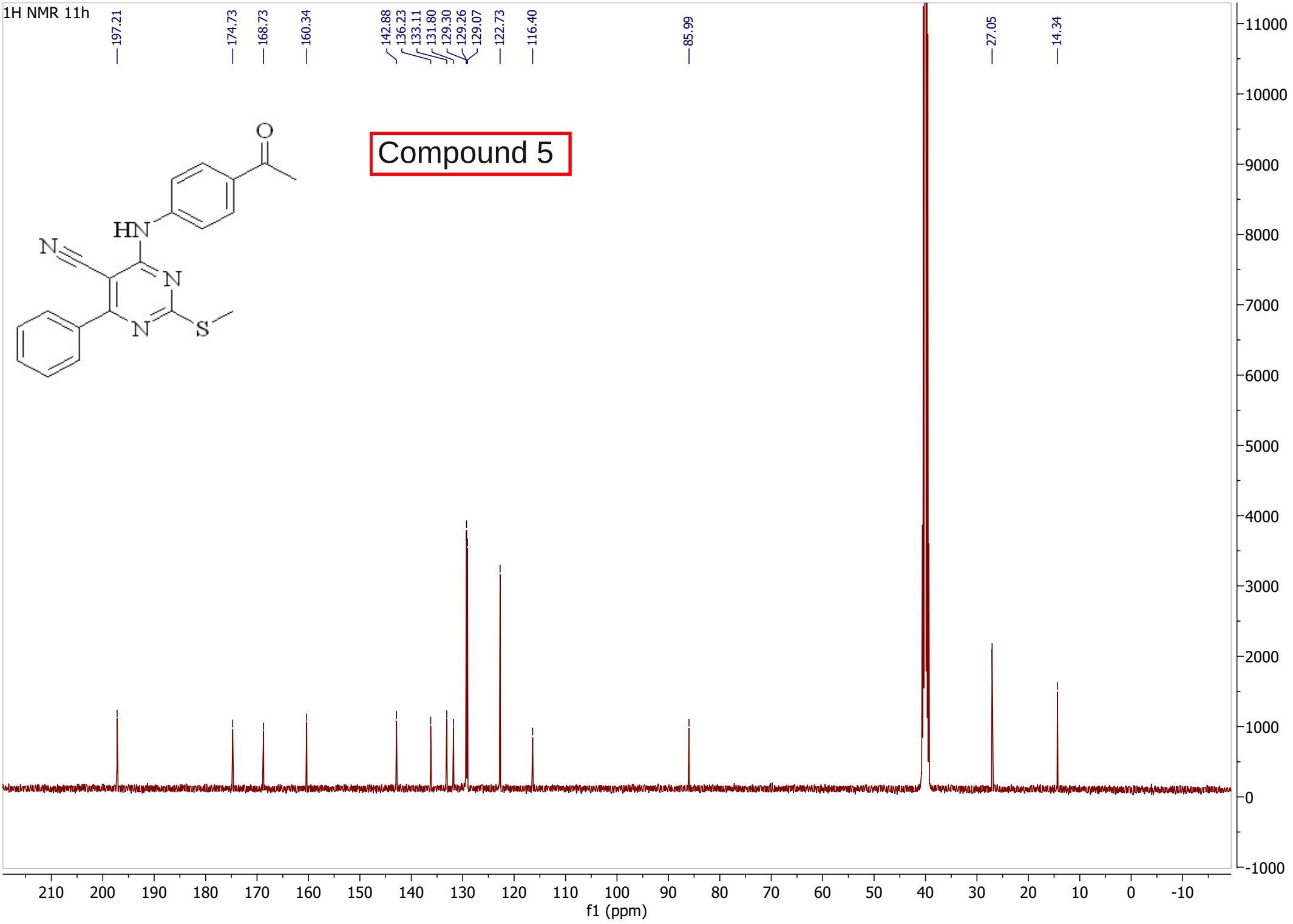
6500
6000
5500
5000
4500
4000
3500
3000
2500
2000
1500
1000
500
0
-500

10.75 10.70 10.65 10.60 10.55 10.50 10.45 10.40 10.35 10.30 10.25 10.20 10.15 10.10 10.05 10.00 9.95 9.90 9.85 9.80 9.75 9.70 9.65 9.60

f1 (ppm)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197.21
174.73
168.73
160.34
142.88
136.23
133.11
131.80
129.30
129.26
129.07
122.73
116.40
85.99
27.05
14.34
Compound 5
O
HN
N
N
N
S
11000
10000
9000
8000
7000
6000
5000
4000
3000
2000
1000
0
-1000
210
200
190
180
170
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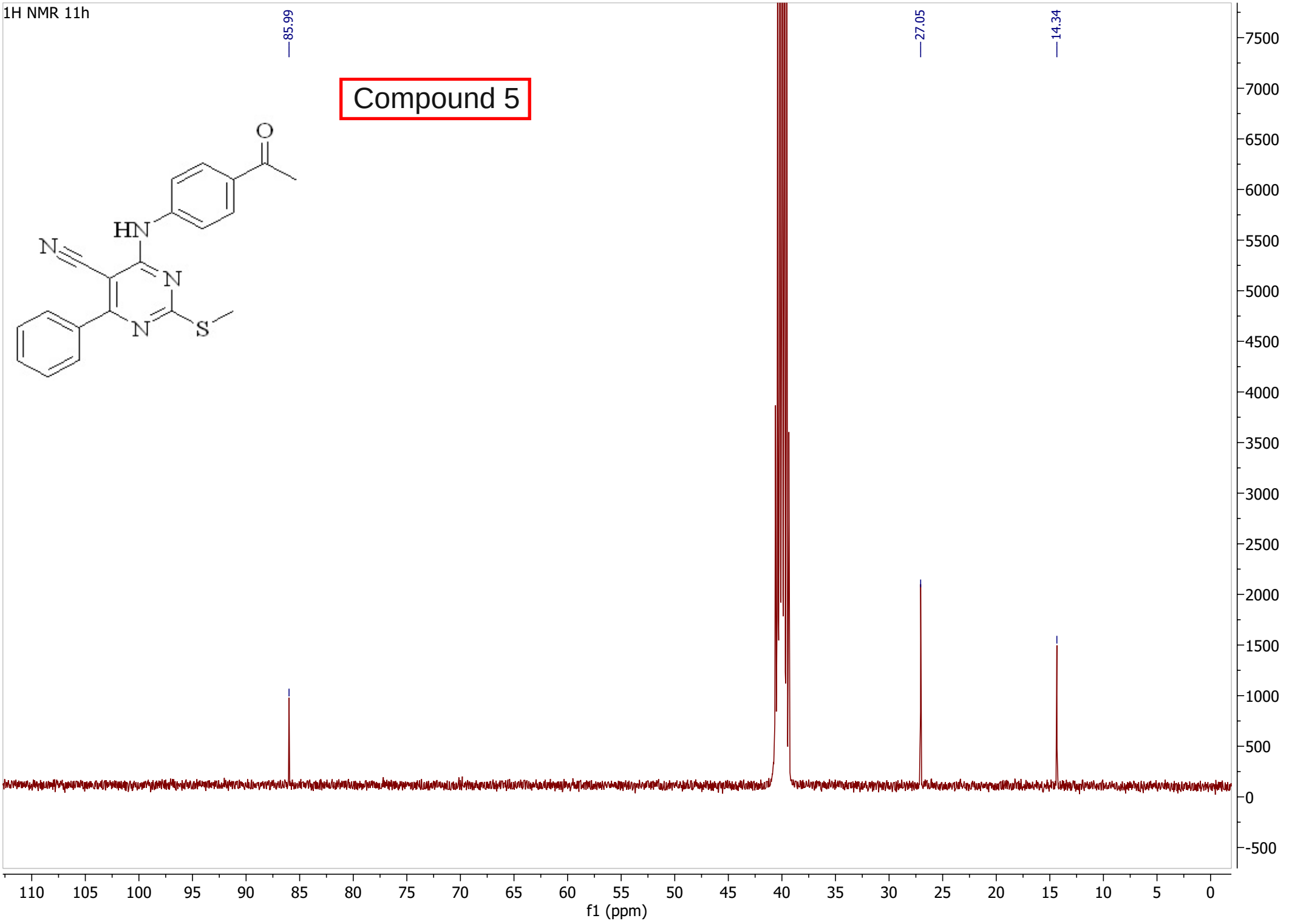
0
-10
f1 (ppm)


1H NMR 11h
85.99
27.05
14.34
Compound 5
O
HN
N
N
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4500
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500
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100
95
90
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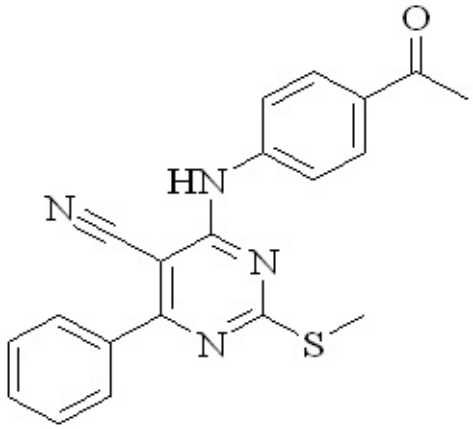
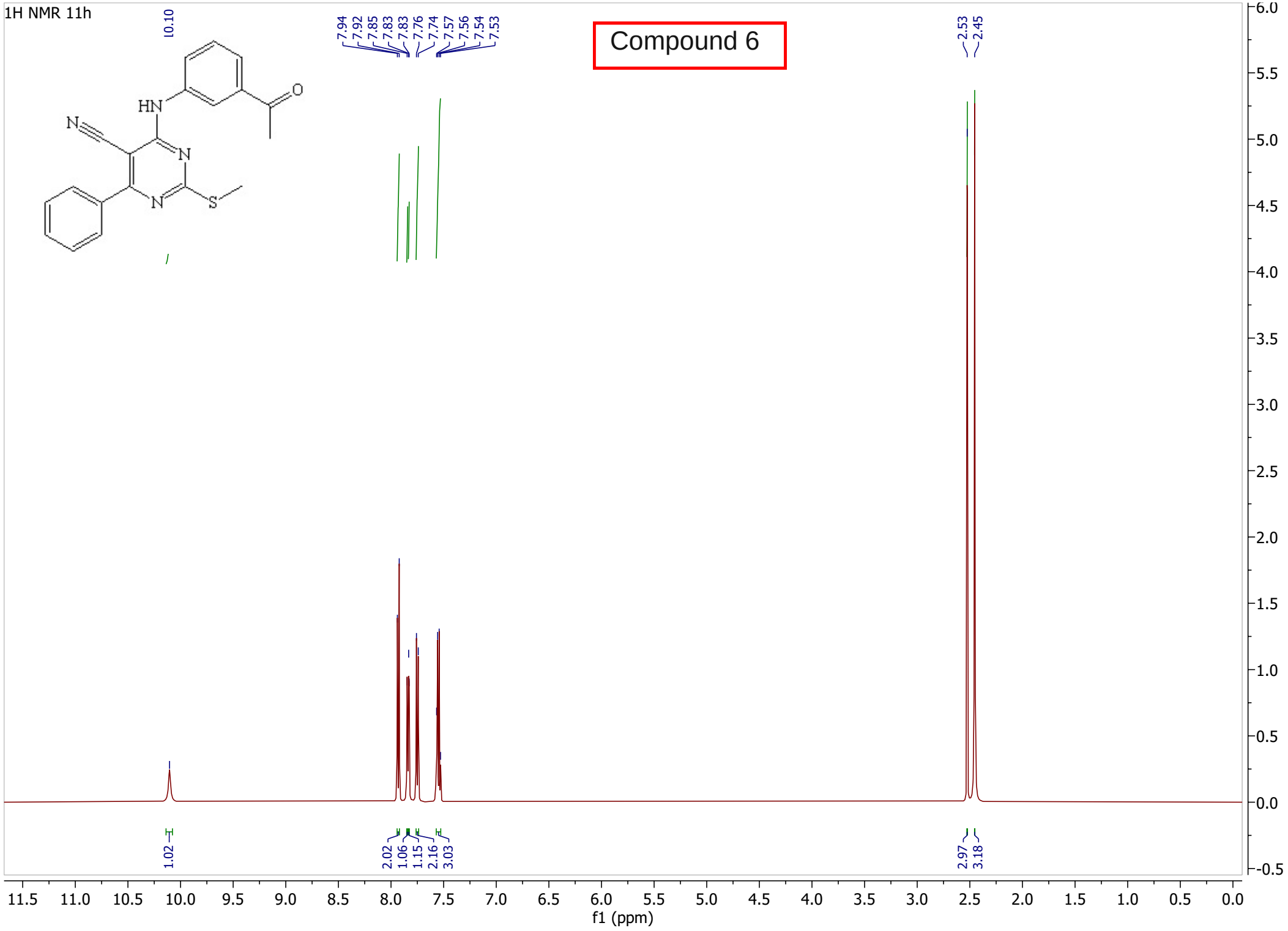
f1 (ppm)

1H NMR 11h



Compound 5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Compound 6
10.10
7.94
7.92
7.85
7.83
7.83
7.76
7.74
7.57
7.56
7.54
7.53
2.53
2.45
HN
O
N
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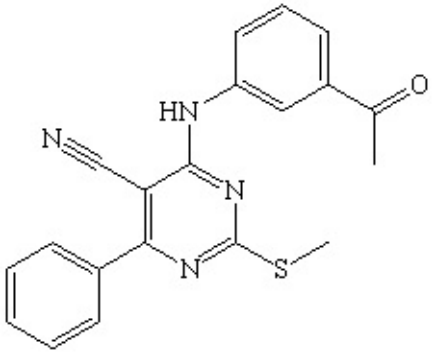
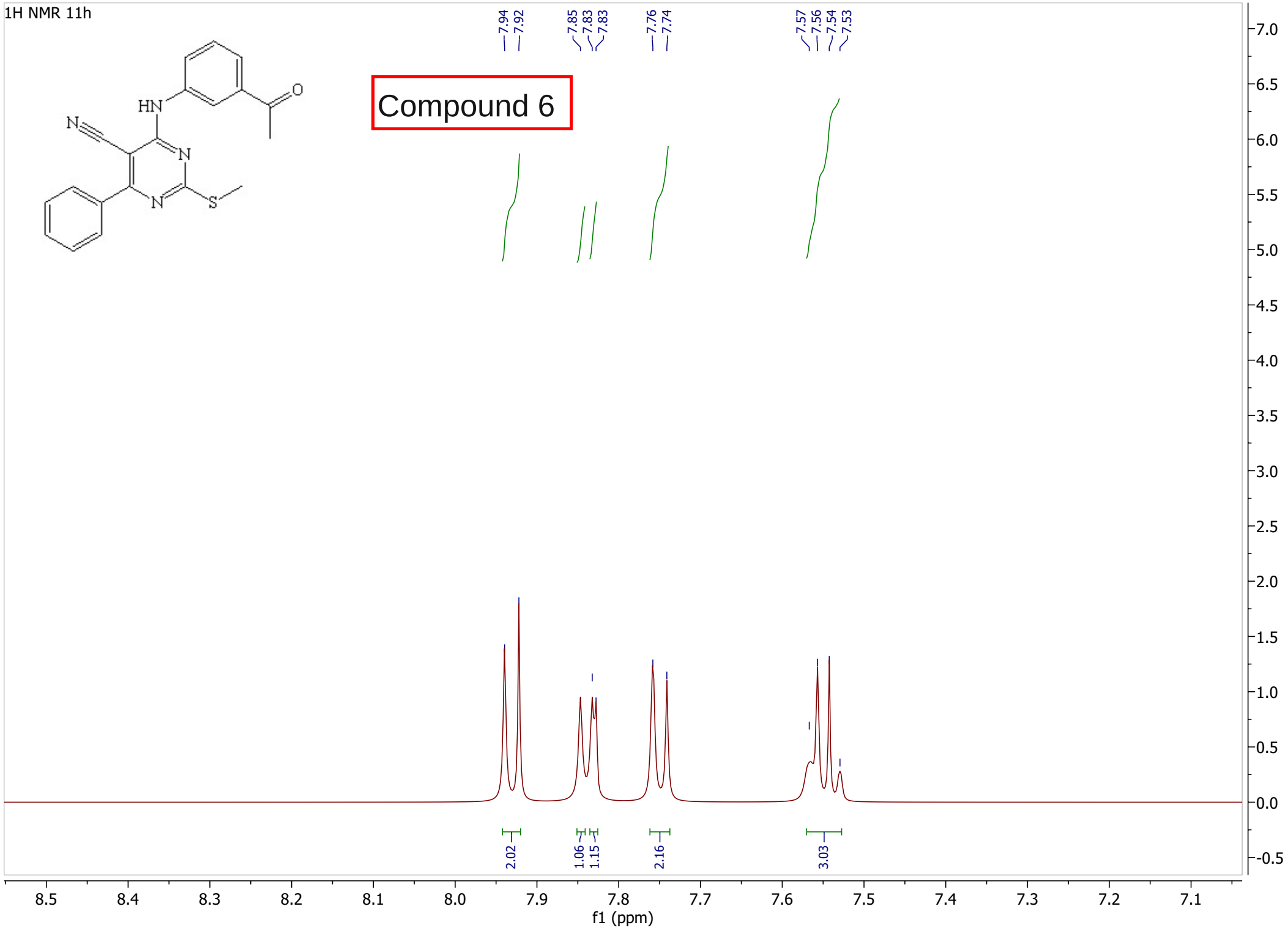
3.03
2.97
3.18
f1 (ppm)

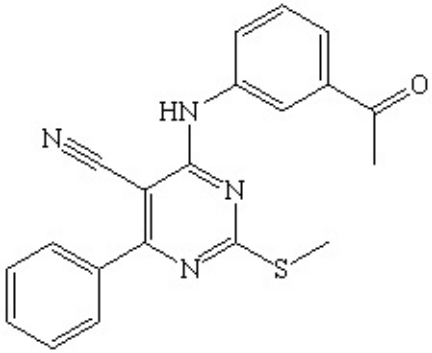
1H NMR 11h



Compound 6


1H NMR 11h
Compound 6
7.94
7.92
7.85
7.83
7.83
7.76
7.74
7.57
7.56
7.54
7.53
HN
O
N
N
N
S
2.02
1.06
1.15
2.16
3.03
f1 (ppm)

1H NMR 11h



Compound 6

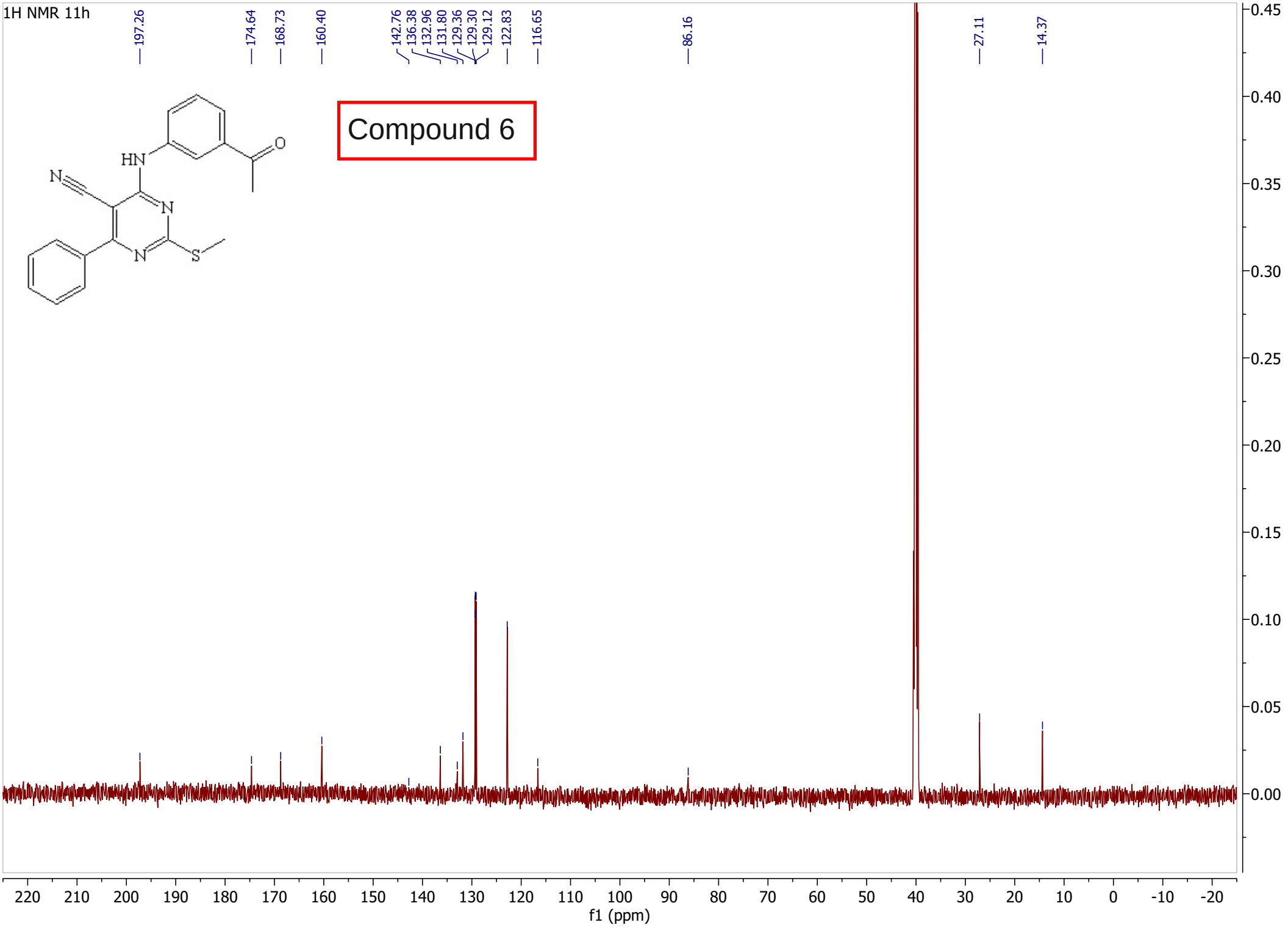
10.10

1.02

11.2 11.1 11.0 10.9 10.8 10.7 10.6 10.5 10.4 10.3 10.2 10.1 10.0 9.9 9.8 9.7 9.6 9.5 9.4 9.3 9.2 9.1 9.0 8.9 8.8

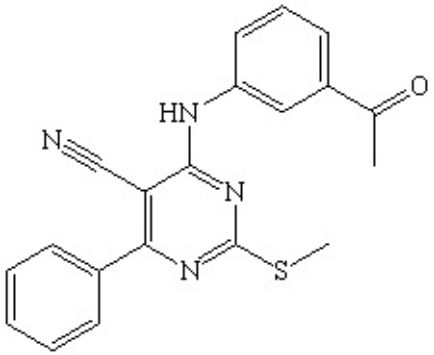
f1 (ppm)

2.1 2.0 1.9 1.8 1.7 1.6 1.5 1.4 1.3 1.2 1.1 1.0 0.9 0.8 0.7 0.6 0.5 0.4 0.3 0.2 0.1 0.0 -0.1


1H NMR 11h
197.26
174.64
168.73
160.40
142.76
136.38
132.96
131.80
129.36
129.30
129.12
122.83
116.65
86.16
27.11
14.37
Compound 6
HN
O
N
N
N
S
0.45
0.40
0.35
0.30
0.25
0.20
0.15
0.10
0.05
0.00
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20
f1 (ppm)

1H NMR 11h

Compound 6



86.16

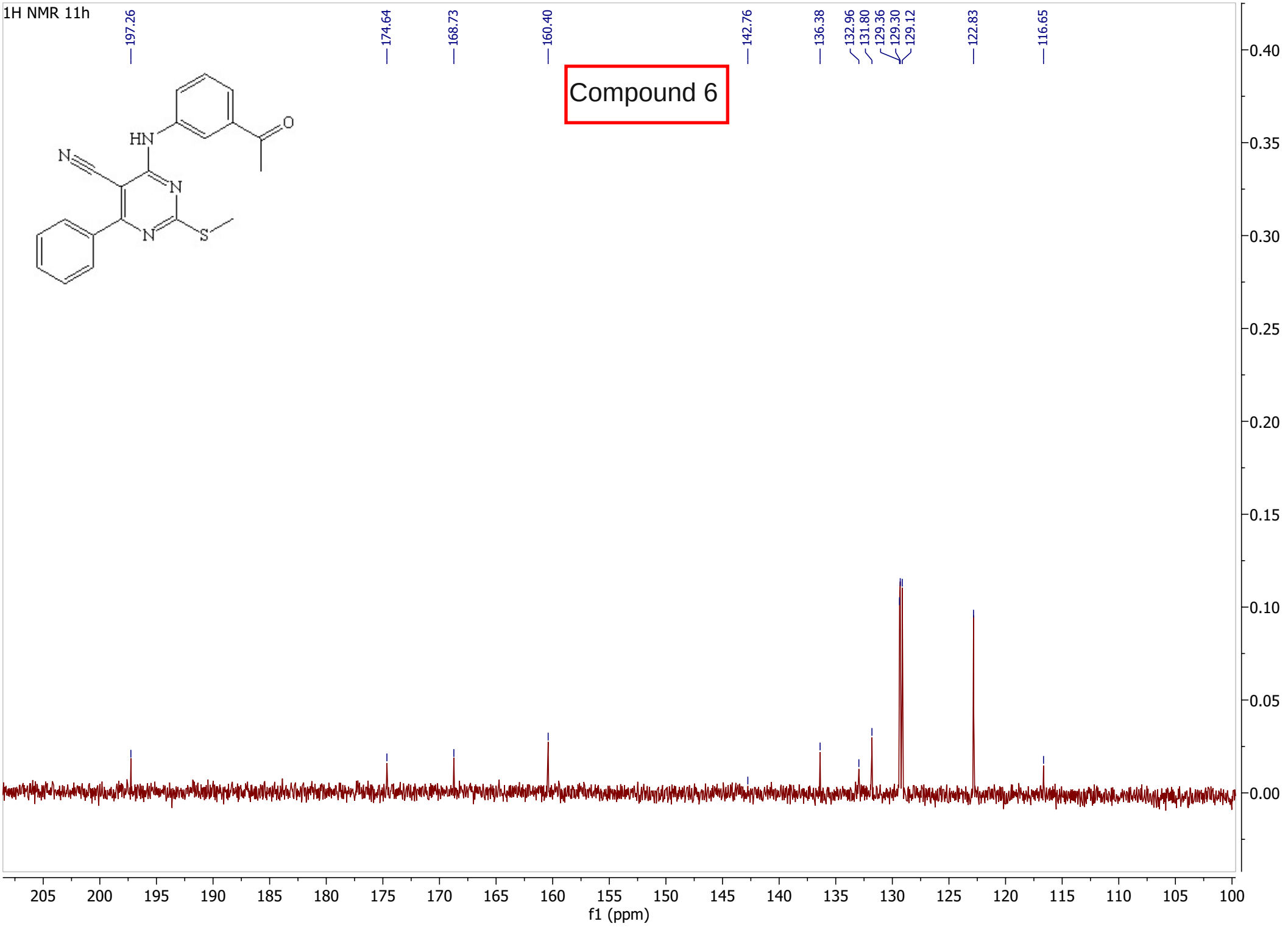
27.11

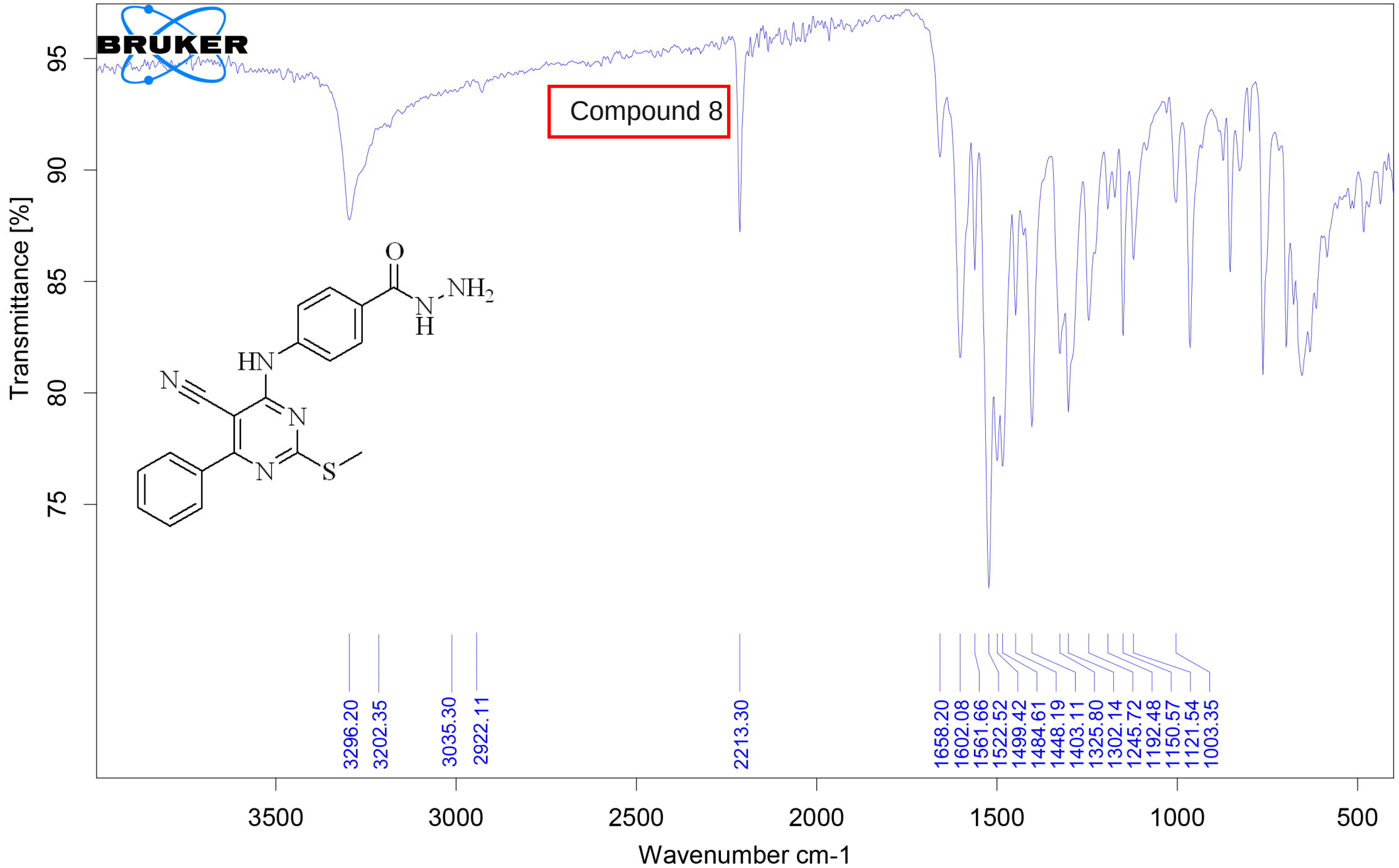
14.37

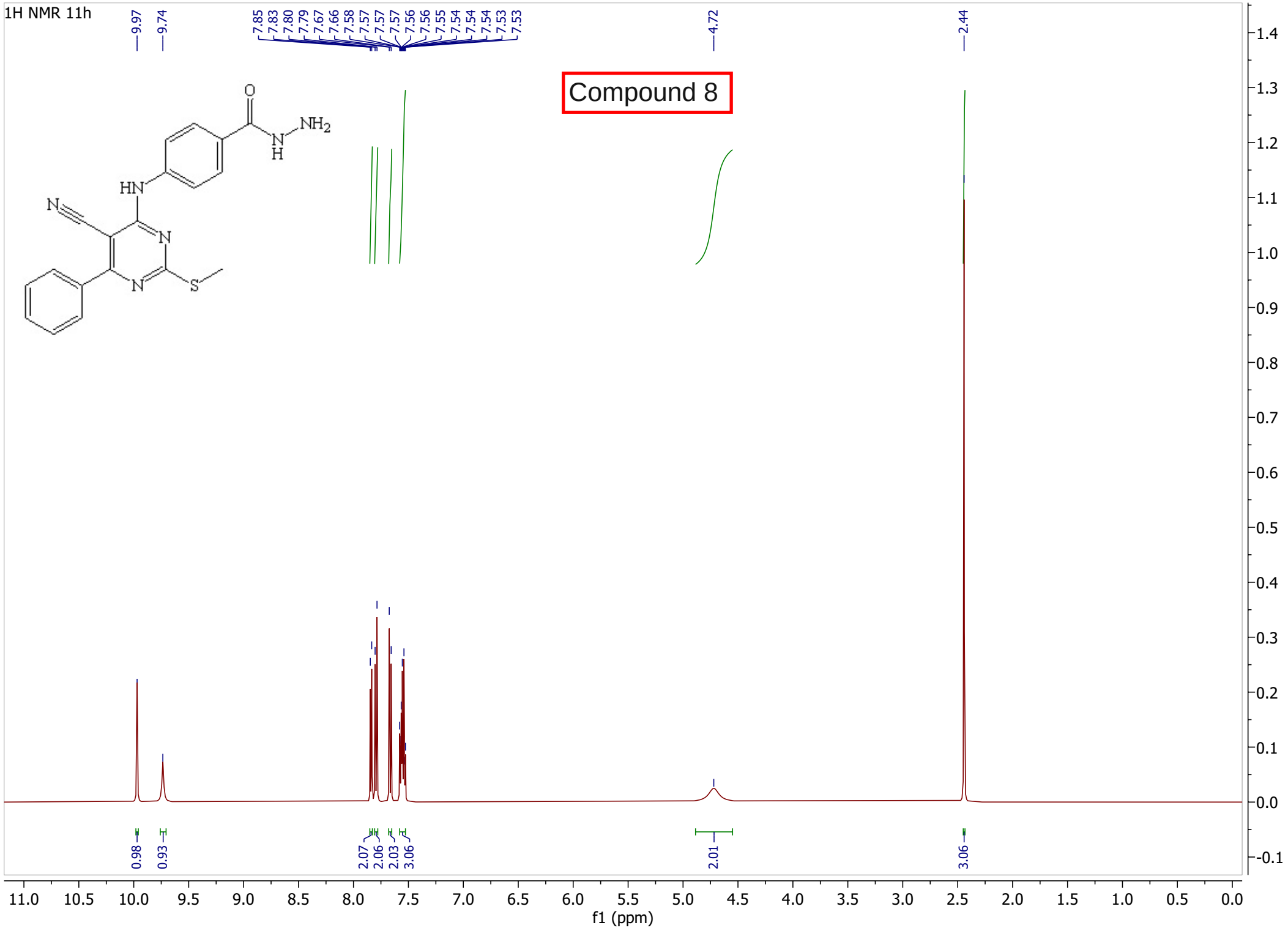
0.50
0.45
0.40
0.35
0.30
0.25
0.20
0.15
0.10
0.05
0.00
-0.05

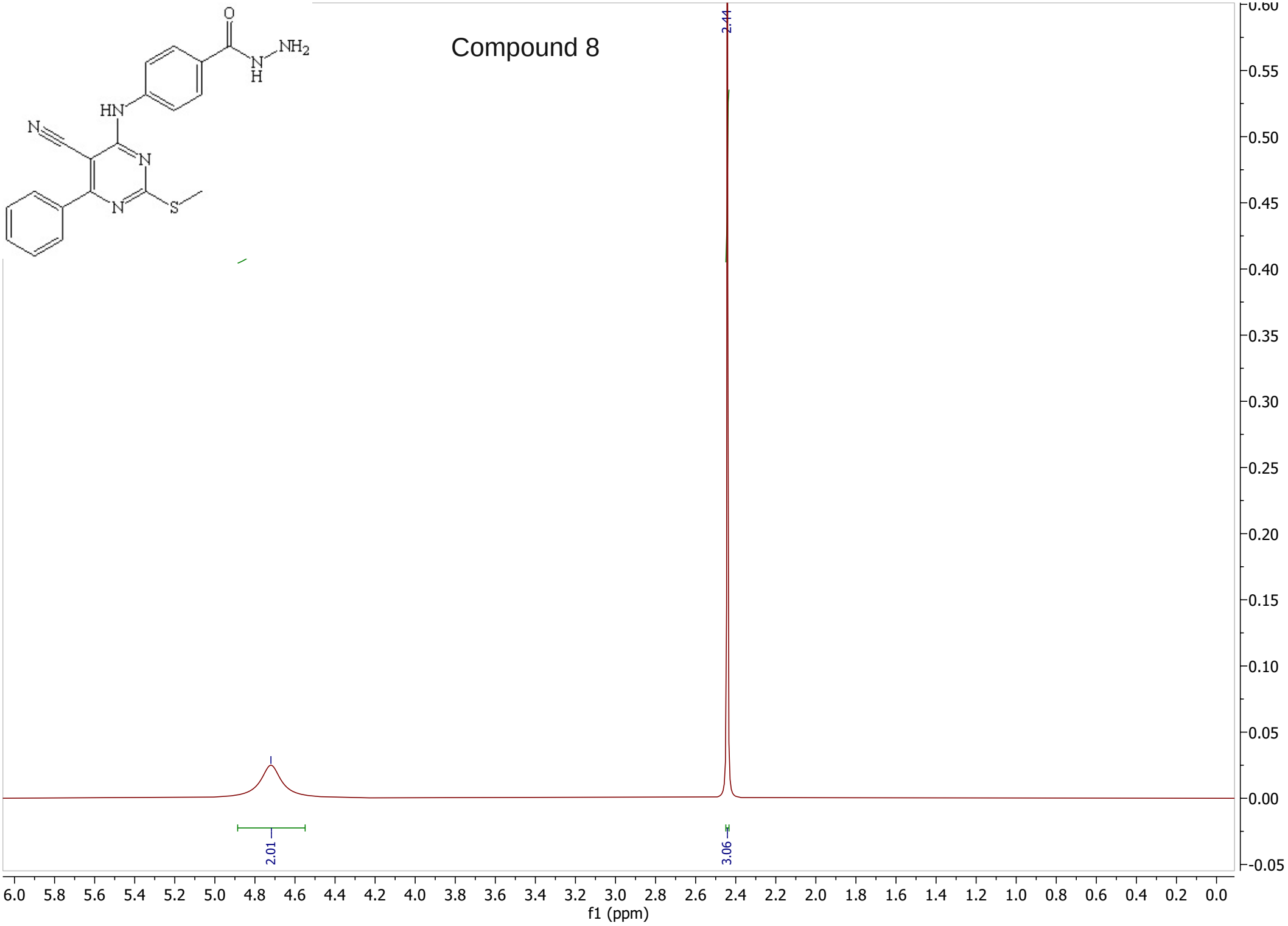
95 90 85 80 75 70 65 60 55 50 45 40 35 30 25 20 15 10 5

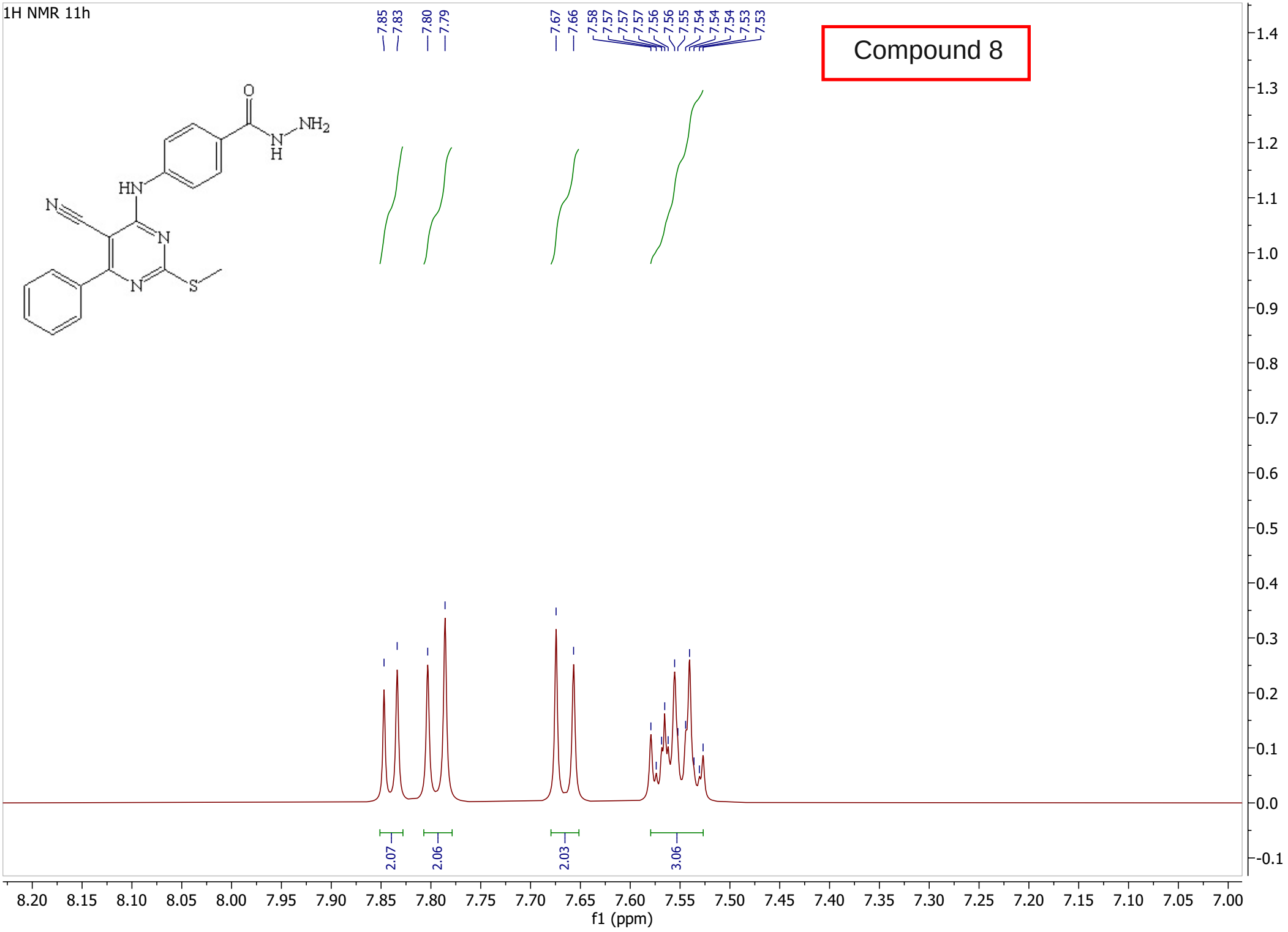
f1 (ppm)

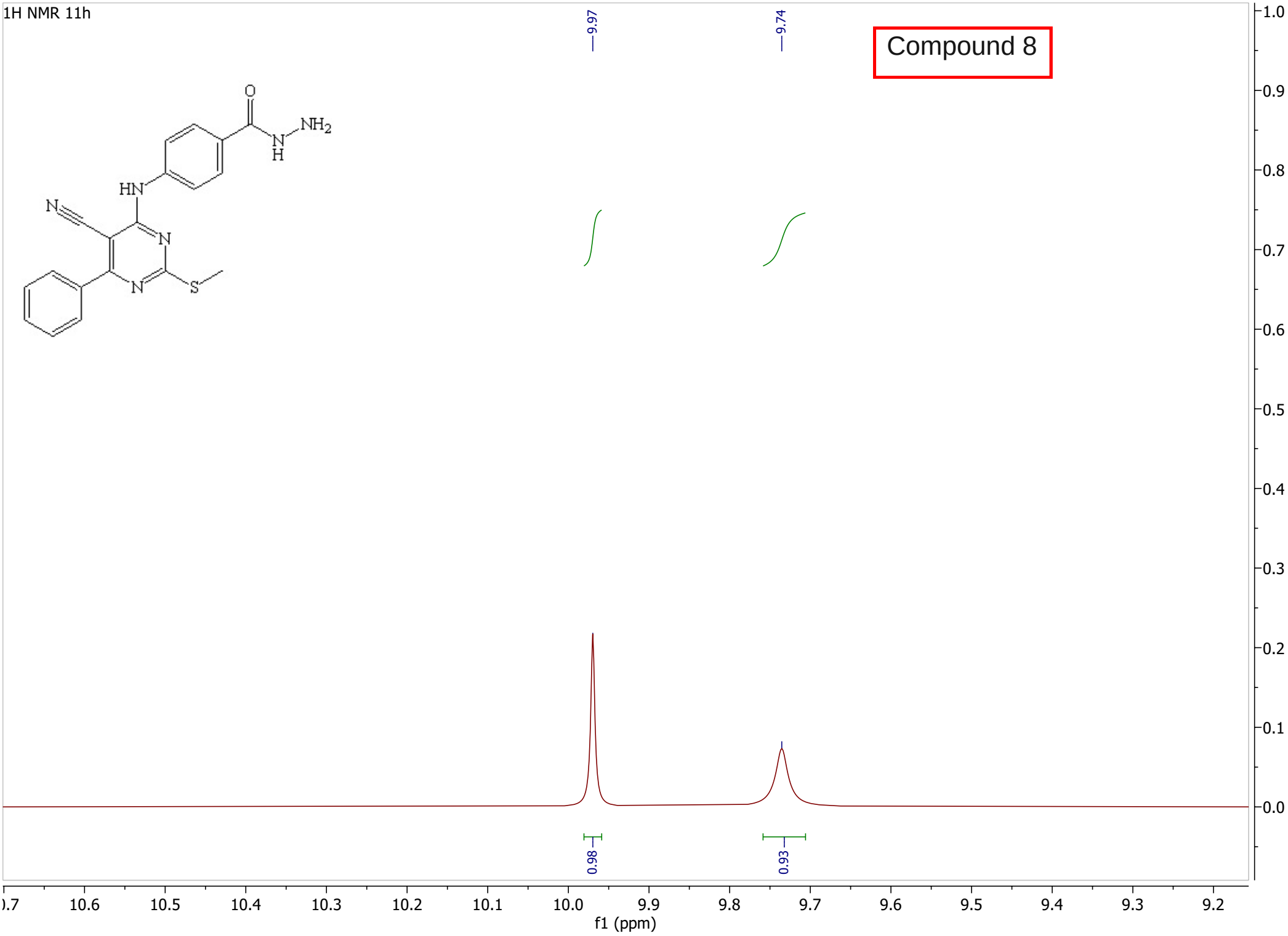

1H NMR 11h
197.26
174.64
168.73
160.40
142.76
136.38
132.96
131.80
129.36
129.30
129.12
122.83
116.65
Compound 6
HN
O
N
N
N
S
0.40
0.35
0.30
0.25
0.20
0.15
0.10
0.05
0.00
205
200
195
190
185
180
175
170
165
160
155
150
145
140
135
130
125
120
115
110
105
100
f1 (ppm)

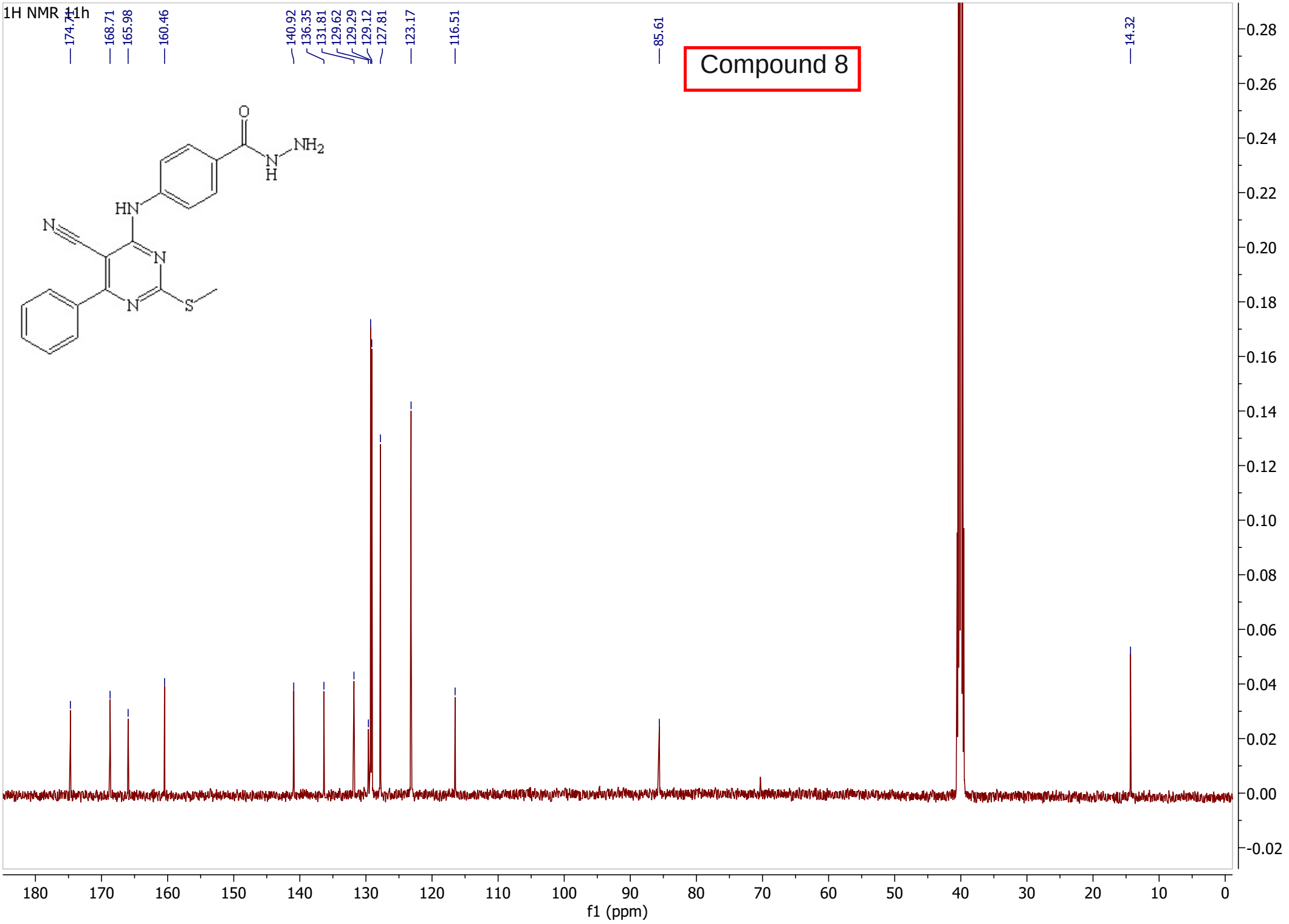

BRUKER
Compound 8
Transmittance [%]
95
90
85
80
75
3296.20
3202.35
3035.30
2922.11
2213.30
1658.20
1602.08
1561.66
1522.52
1499.42
1484.61
1448.19
1403.11
1325.80
1302.14
1245.72
1192.48
1150.57
1121.54
1003.35
3500
3000
2500
2000
1500
1000
500
Wavenumber cm-1

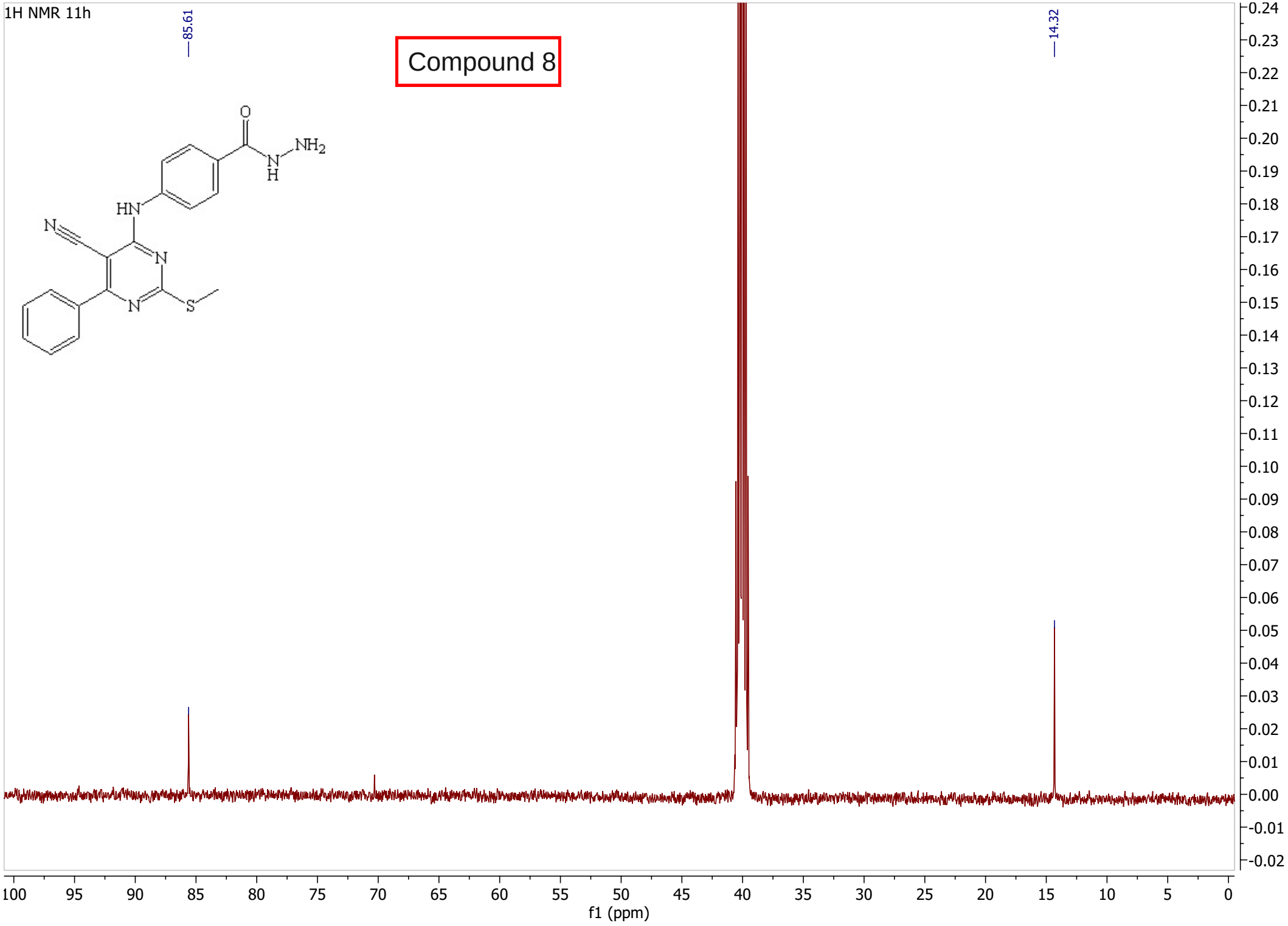

1H NMR 11h
9.97
9.74
7.85
7.83
7.80
7.79
7.67
7.66
7.58
7.57
7.57
7.57
7.56
7.56
7.55
7.54
7.54
7.54
7.53
7.53
4.72
2.44
Compound 8
O
NH2
N
H
HN
N
N
N
S
0.98
0.93
2.07
2.06
2.03
3.06
2.01
3.06
f1 (ppm)

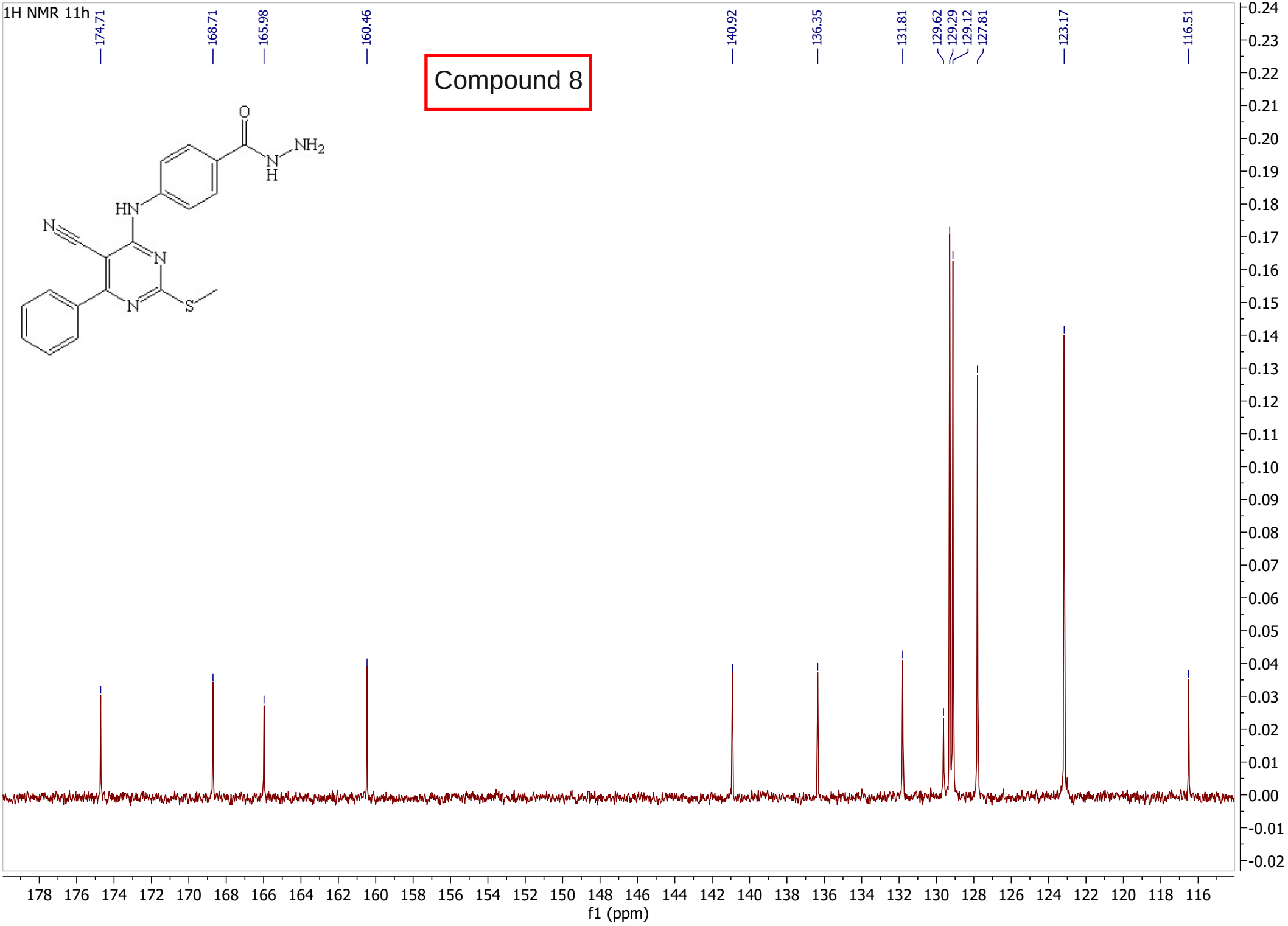

Compound 8
O
NH2
N
H
HN
N
N
N
S
2.41
2.01
3.06
0.60
0.55
0.50
0.45
0.40
0.35
0.30
0.25
0.20
0.15
0.10
0.05
0.00
-0.05
6.0 5.8 5.6 5.4 5.2 5.0 4.8 4.6 4.4 4.2 4.0 3.8 3.6 3.4 3.2 3.0 2.8 2.6 2.4 2.2 2.0 1.8 1.6 1.4 1.2 1.0 0.8 0.6 0.4 0.2 0.0
f1 (ppm)

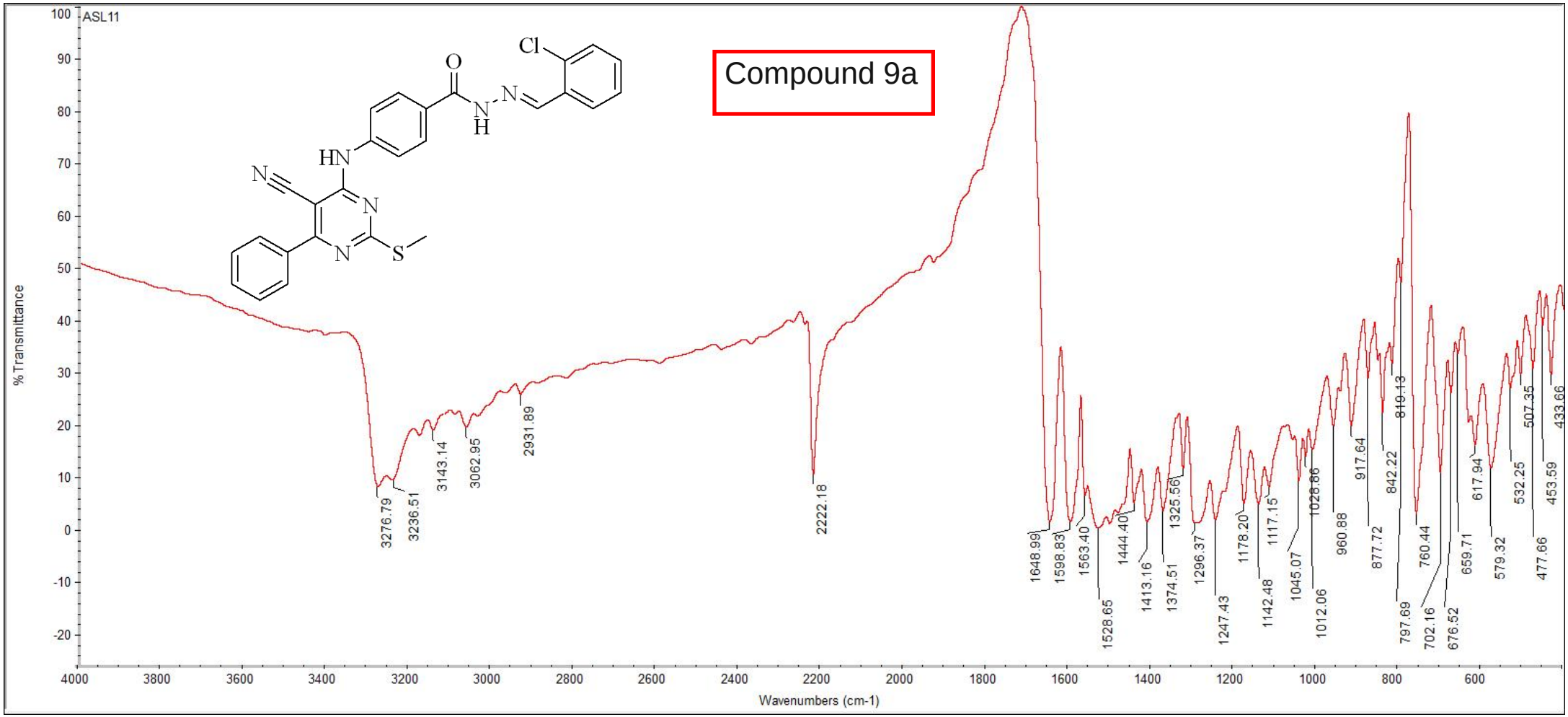

1H NMR 11h
Compound 8
7.85
7.83
7.80
7.79
7.67
7.66
7.58
7.57
7.57
7.57
7.56
7.56
7.55
7.54
7.54
7.54
7.53
7.53
O
NH2
N
H
HN
N
N
N
S
2.07
2.06
2.03
3.06
f1 (ppm)

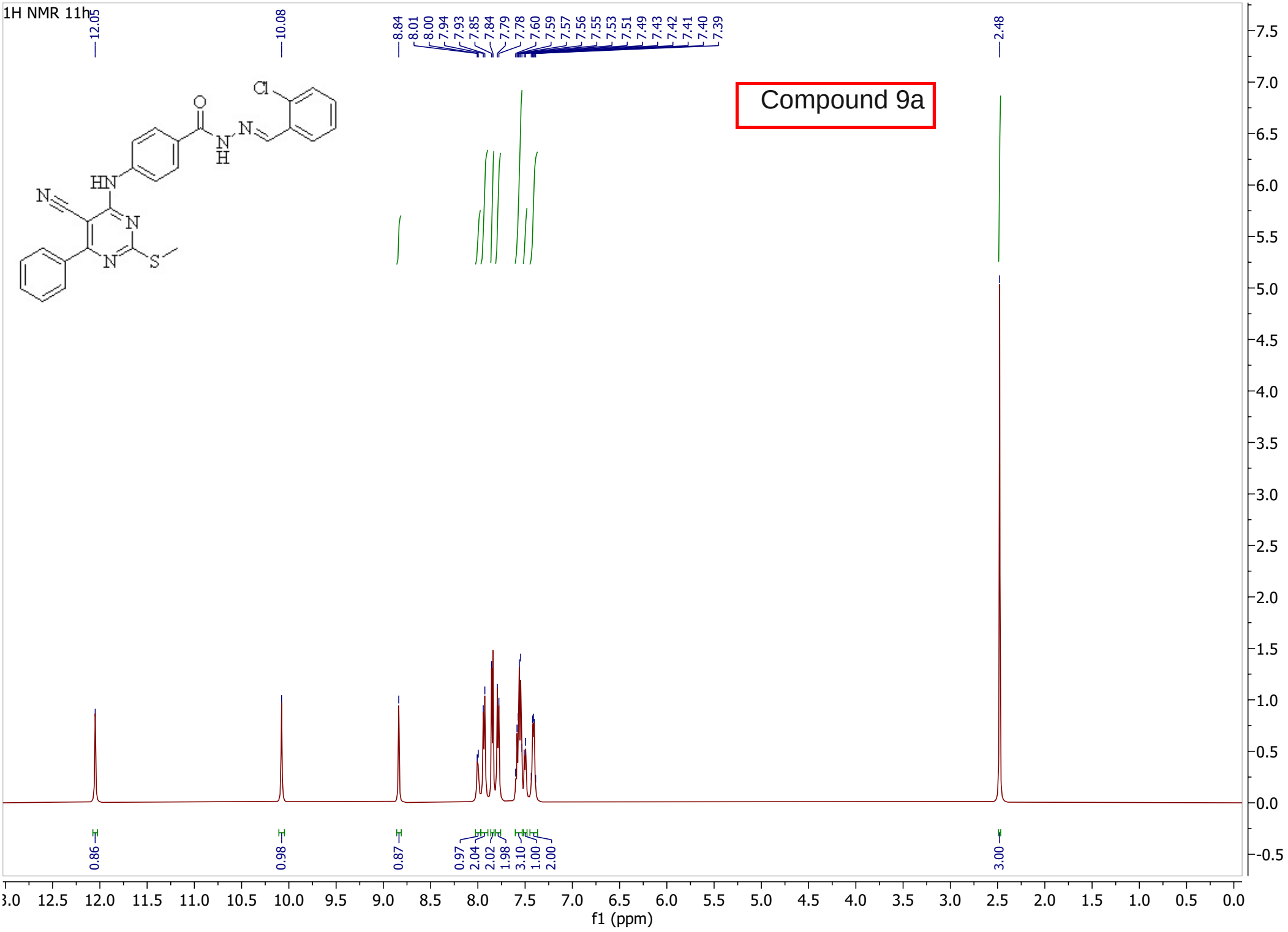

1H NMR 11h
9.97
9.74
Compound 8
O
NH2
N
H
HN
N
N
N
S
0.98
0.93
1.0
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0.0
10.6
10.5
10.4
10.3
10.2
10.1
10.0
9.9
9.8
9.7
9.6
9.5
9.4
9.3
9.2
f1 (ppm)


1H NMR 11h
174.77
168.71
165.98
160.46
140.92
136.35
131.81
129.62
129.29
129.12
127.81
123.17
116.51
85.61
14.32
Compound 8
O
NH2
N
H
HN
N
N
N
S
0.28
0.26
0.24
0.22
0.20
0.18
0.16
0.14
0.12
0.10
0.08
0.06
0.04
0.02
0.00
-0.02
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

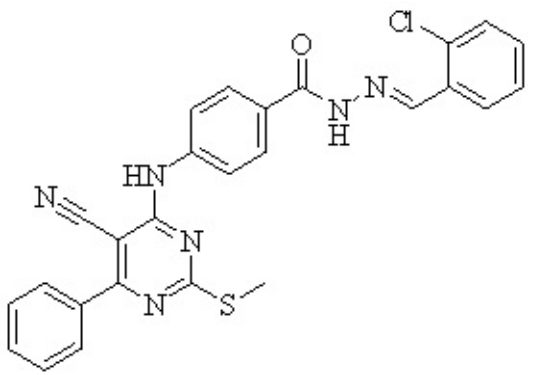

1H NMR 11h
85.61
14.32
Compound 8
O
NH2
N
H
HN
N
N
N
S
0.24
0.23
0.22
0.21
0.20
0.19
0.18
0.17
0.16
0.15
0.14
0.13
0.12
0.11
0.10
0.09
0.08
0.07
0.06
0.05
0.04
0.03
0.02
0.01
0.00
-0.01
-0.02
100
95
90
85
80
75
70
65
60
55
50
45
40
35
30
25
20
15
10
5
0
f1 (ppm)


1H NMR 11h
174.71
168.71
165.98
160.46
140.92
136.35
131.81
129.62
129.29
129.12
127.81
123.17
116.51
Compound 8
O
NH2
N
H
HN
N
N
N
S
f1 (ppm)


ASL11
Compound 9a
% Transmittance
Wavenumbers (cm-1)
3276.79
3236.51
3143.14
3062.95
2931.89
2222.18
1648.99
1598.83
1563.40
1528.65
1444.40
1413.16
1374.51
1325.56
1296.37
1247.43
1178.20
1142.48
1117.15
1045.07
1028.86
1012.06
960.88
917.64
877.72
842.22
819.13
797.69
760.44
702.16
676.52
659.71
617.94
579.32
532.25
507.35
477.66
453.59
433.66
Cl
O
N
H
HN
N
N
N
S


1H NMR 11h
12.05
10.08
8.84
8.01
8.00
7.94
7.93
7.85
7.84
7.79
7.78
7.60
7.59
7.57
7.56
7.55
7.53
7.51
7.49
7.43
7.42
7.41
7.40
7.39
2.48
Compound 9a
Cl
O
N
N
H
HN
N
N
N
S
0.86
0.98
0.87
0.97
2.04
2.02
1.98
3.10
1.00
2.00
3.00
f1 (ppm)

1H NMR 11h

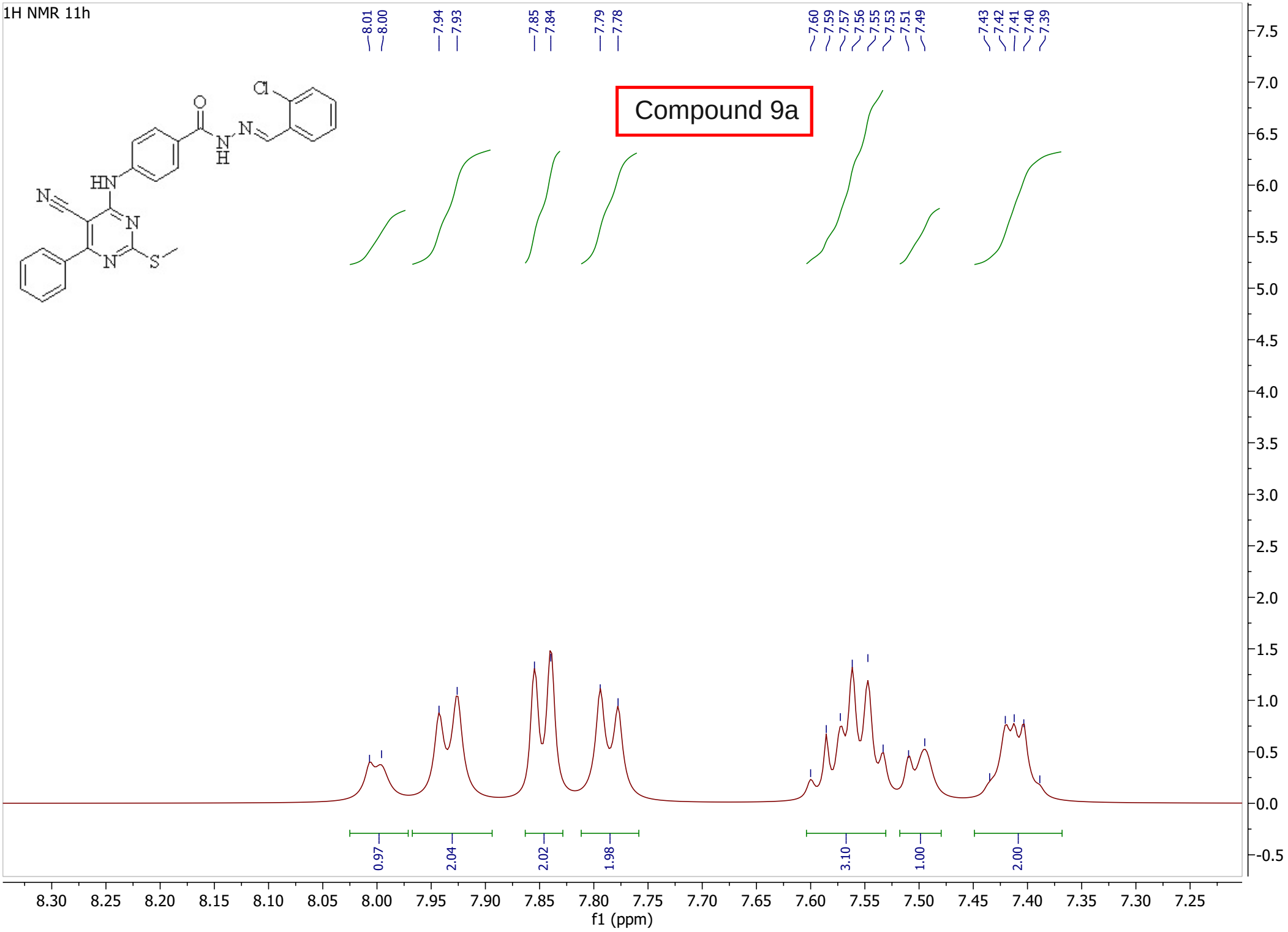


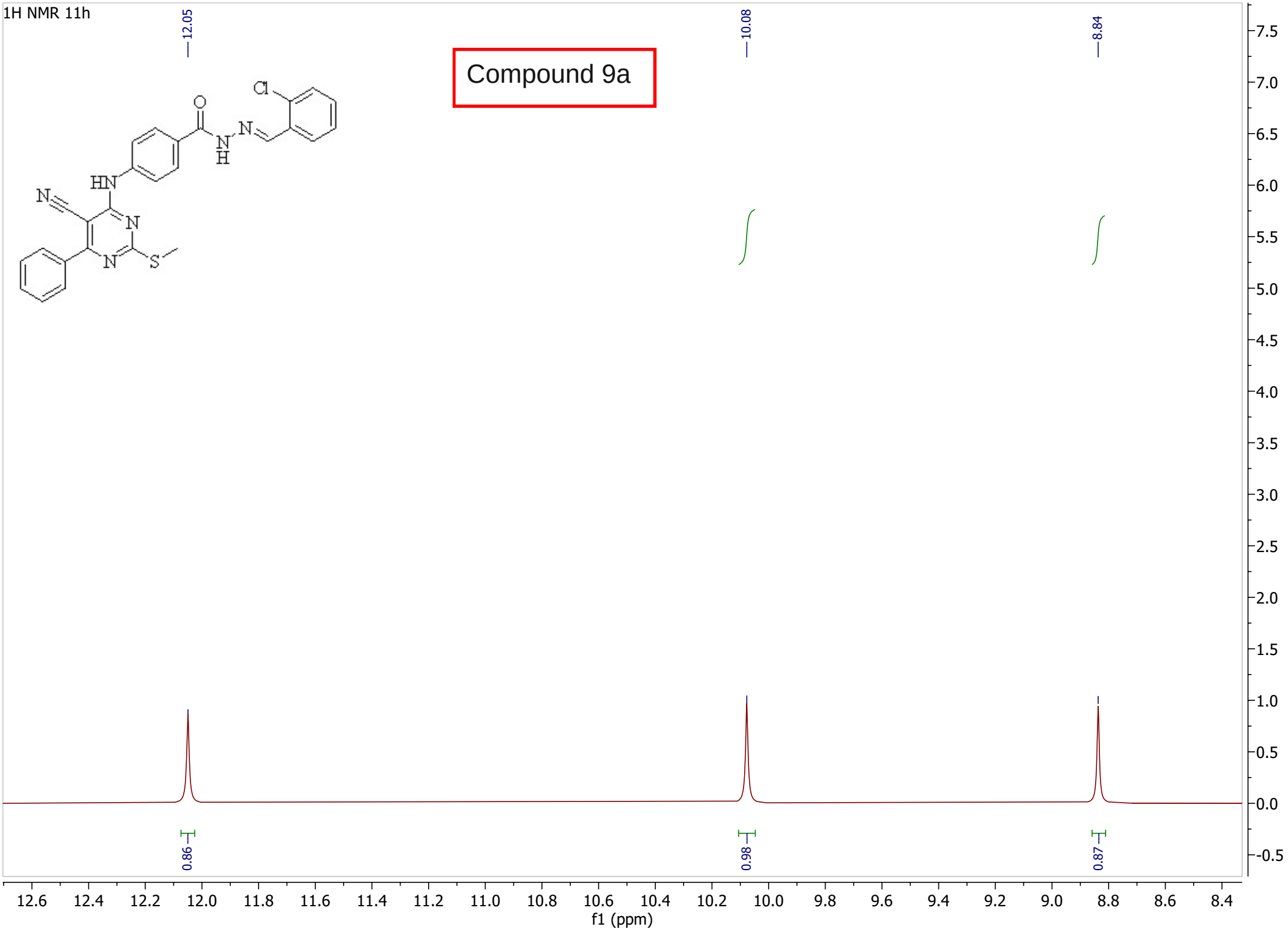
Compound 9a

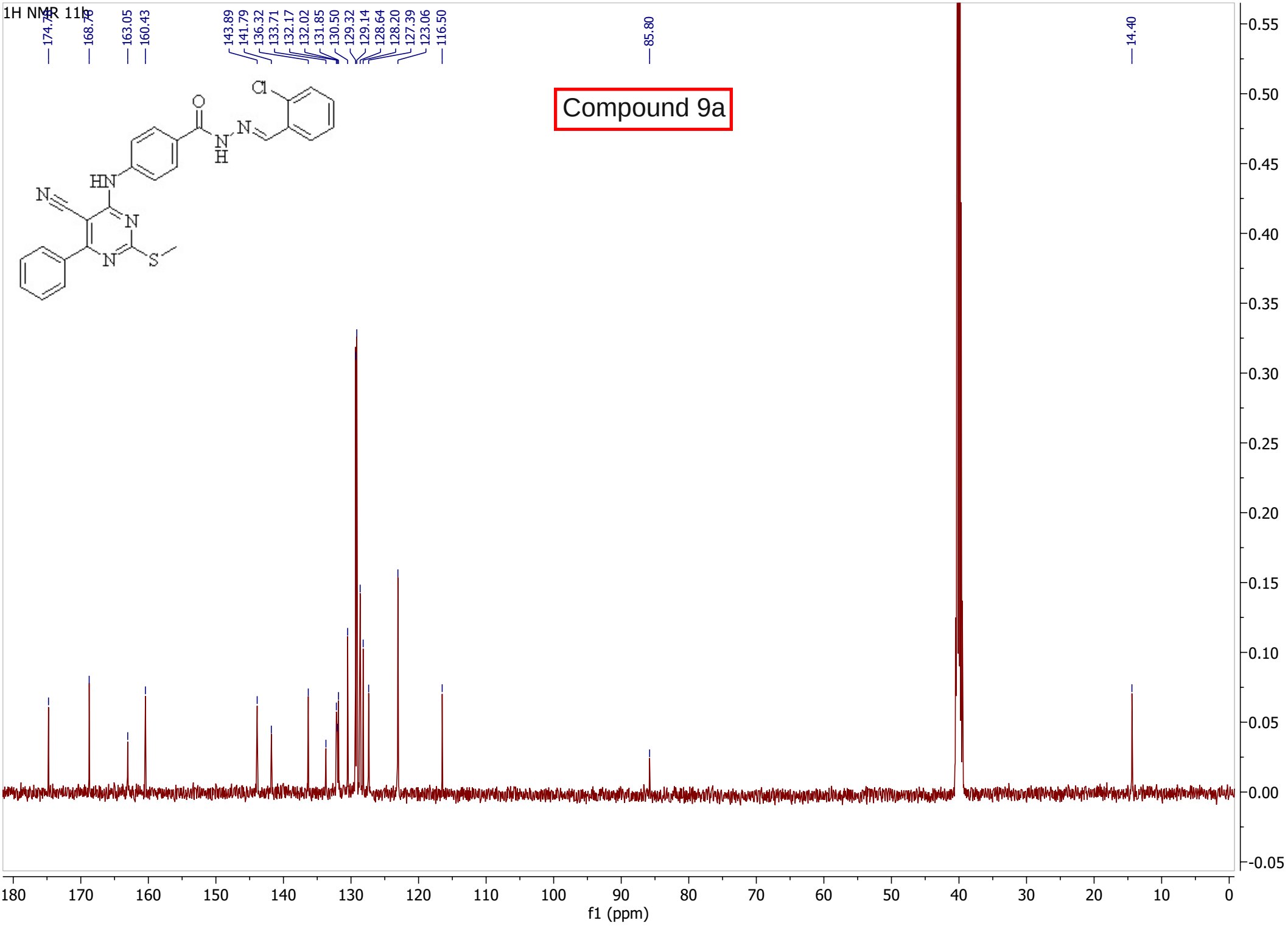
2.48

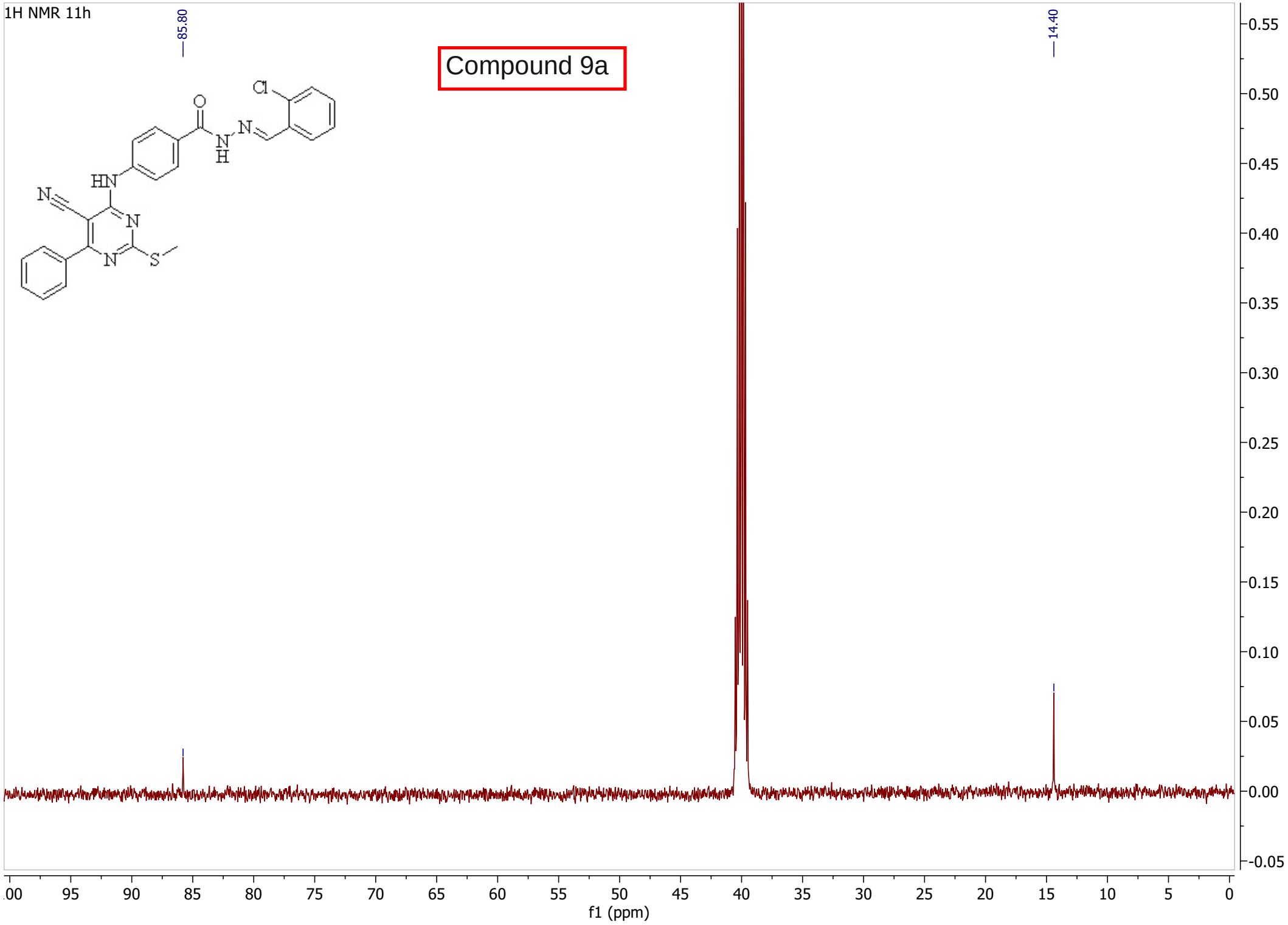
3.00

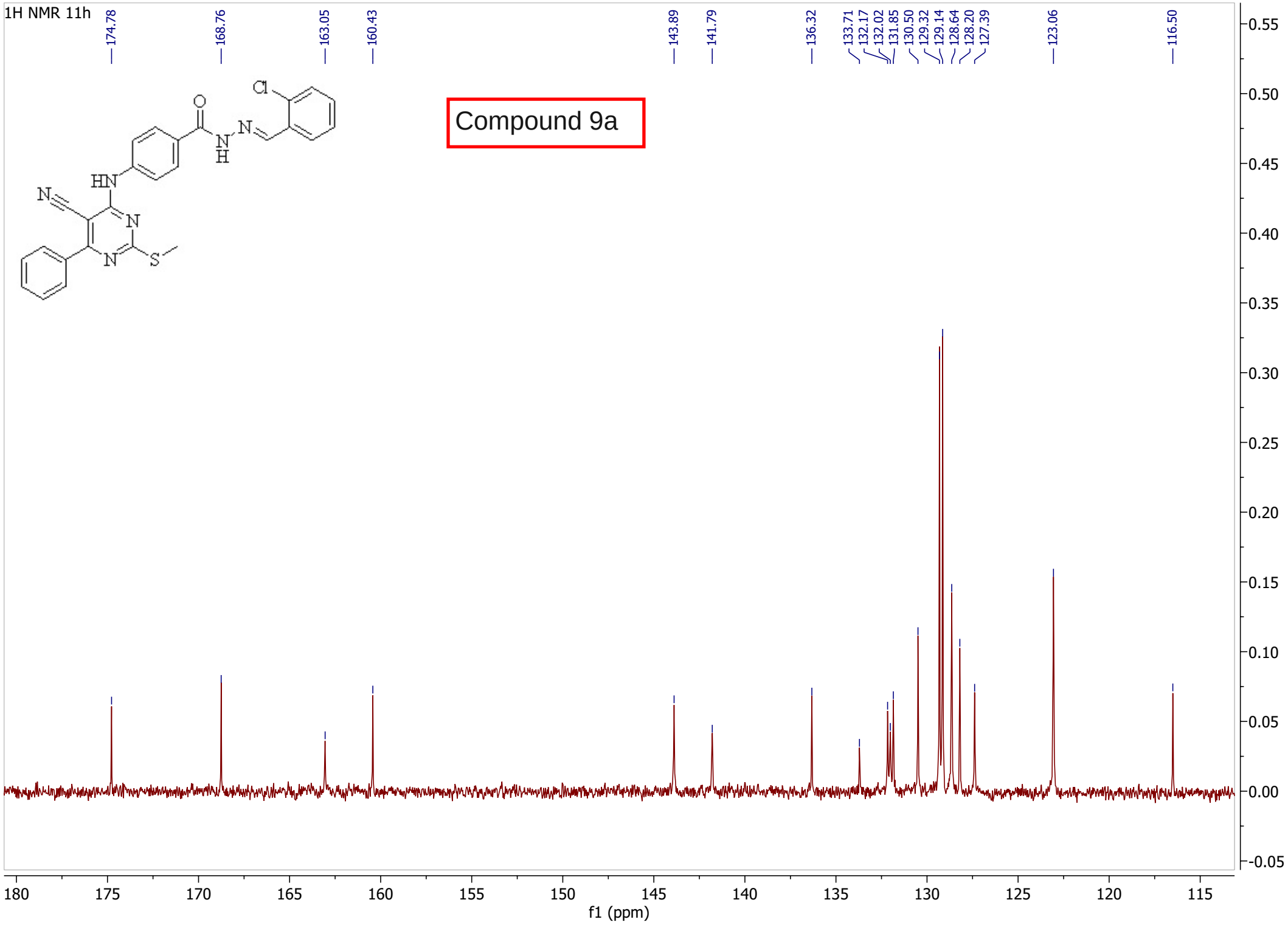
f1 (ppm)


1H NMR 11h
8.01
8.00
7.94
7.93
7.85
7.84
7.79
7.78
7.60
7.59
7.57
7.56
7.55
7.53
7.51
7.49
7.43
7.42
7.41
7.40
7.39
Compound 9a
Cl
O
N
H
N
HN
N
N
N
S
0.97
2.04
2.02
1.98
3.10
1.00
2.00
f1 (ppm)


1H NMR 11h
12.05
10.08
8.84
Compound 9a
Cl
O
N
N
H
HN
N
N
N
S
0.86
0.98
0.87
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
12.6
12.4
12.2
12.0
11.8
11.6
11.4
11.2
11.0
10.8
10.6
10.4
10.2
10.0
9.8
9.6
9.4
9.2
9.0
8.8
8.6
8.4
f1 (ppm)

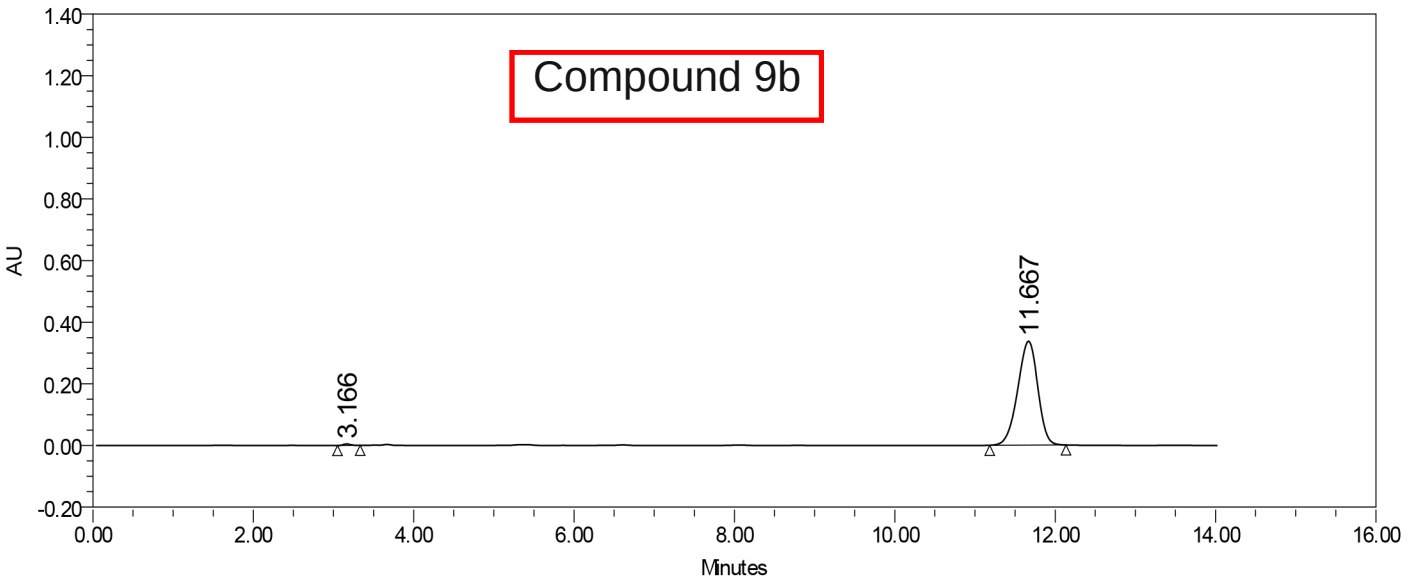

1H NMR 11b
174.77
168.78
163.05
160.43
143.89
141.79
136.32
133.71
132.17
132.02
131.85
130.50
129.32
129.14
128.64
128.20
127.39
123.06
116.50
85.80
14.40
Compound 9a
Cl
O
N
N
H
HN
N
N
N
S
0.55
0.50
0.45
0.40
0.35
0.30
0.25
0.20
0.15
0.10
0.05
0.00
-0.05
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


1H NMR 11h
85.80
14.40
Compound 9a
Cl
O
N
N
H
HN
N
N
N
S
0.55
0.50
0.45
0.40
0.35
0.30
0.25
0.20
0.15
0.10
0.05
0.00
-0.05
00
95
90
85
80
75
70
65
60
55
50
45
40
35
30
25
20
15
10
5
0
f1 (ppm)

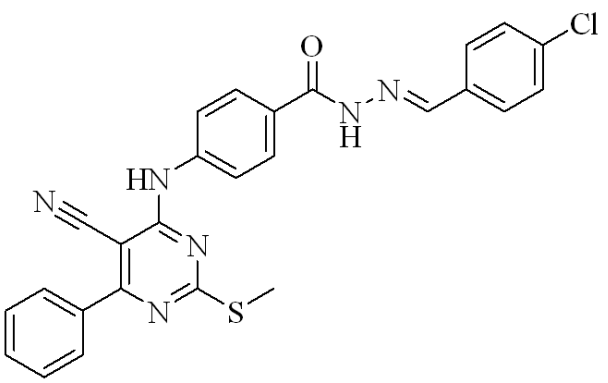

1H NMR 11h
174.78
168.76
163.05
160.43
143.89
141.79
136.32
133.71
132.17
132.02
131.85
130.50
129.32
129.14
128.64
128.20
127.39
123.06
116.50
Compound 9a
Cl
O
N
N
H
HN
N
N
N
S
0.55
0.50
0.45
0.40
0.35
0.30
0.25
0.20
0.15
0.10
0.05
0.00
-0.05
180
175
170
165
160
155
150
145
140
135
130
125
120
115
f1 (ppm)

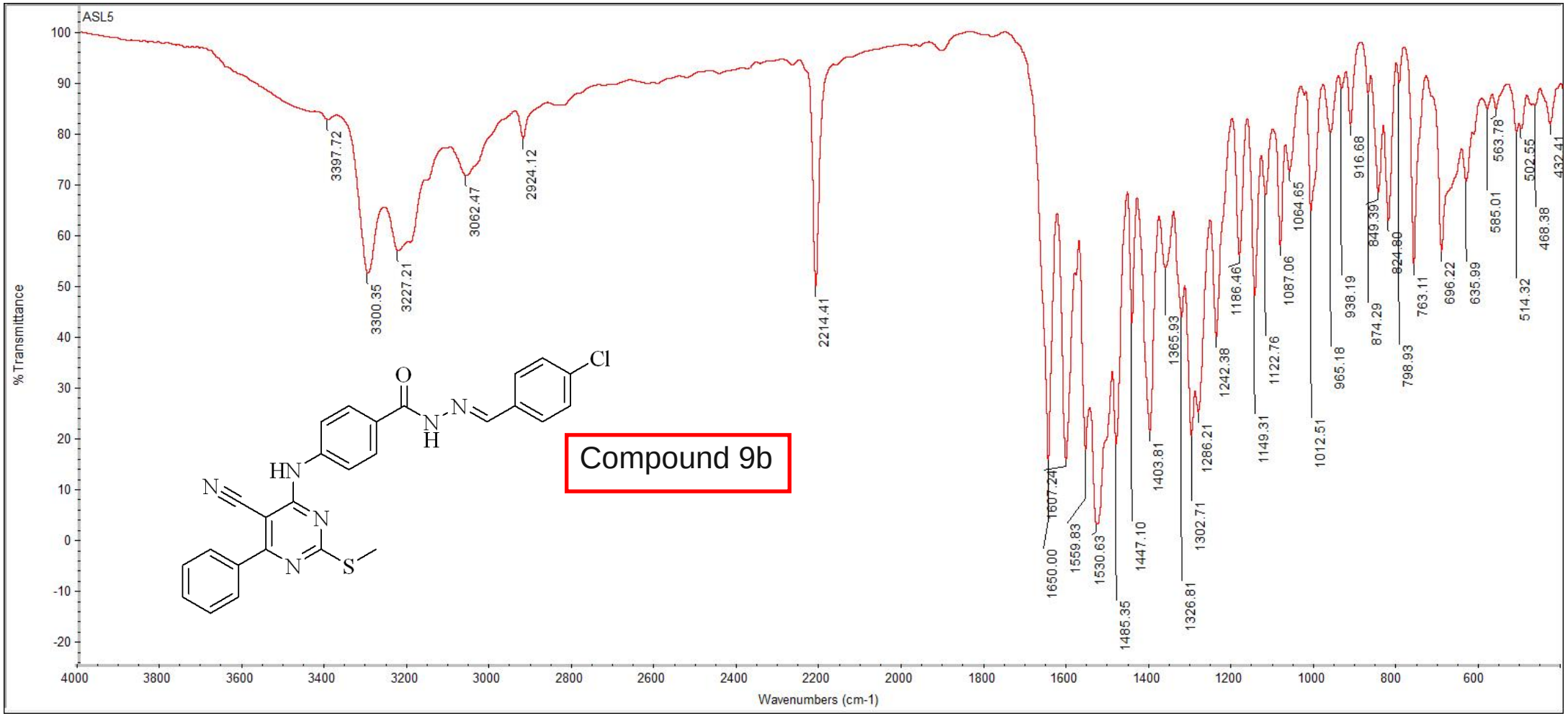
SAMPLE INFORMATION

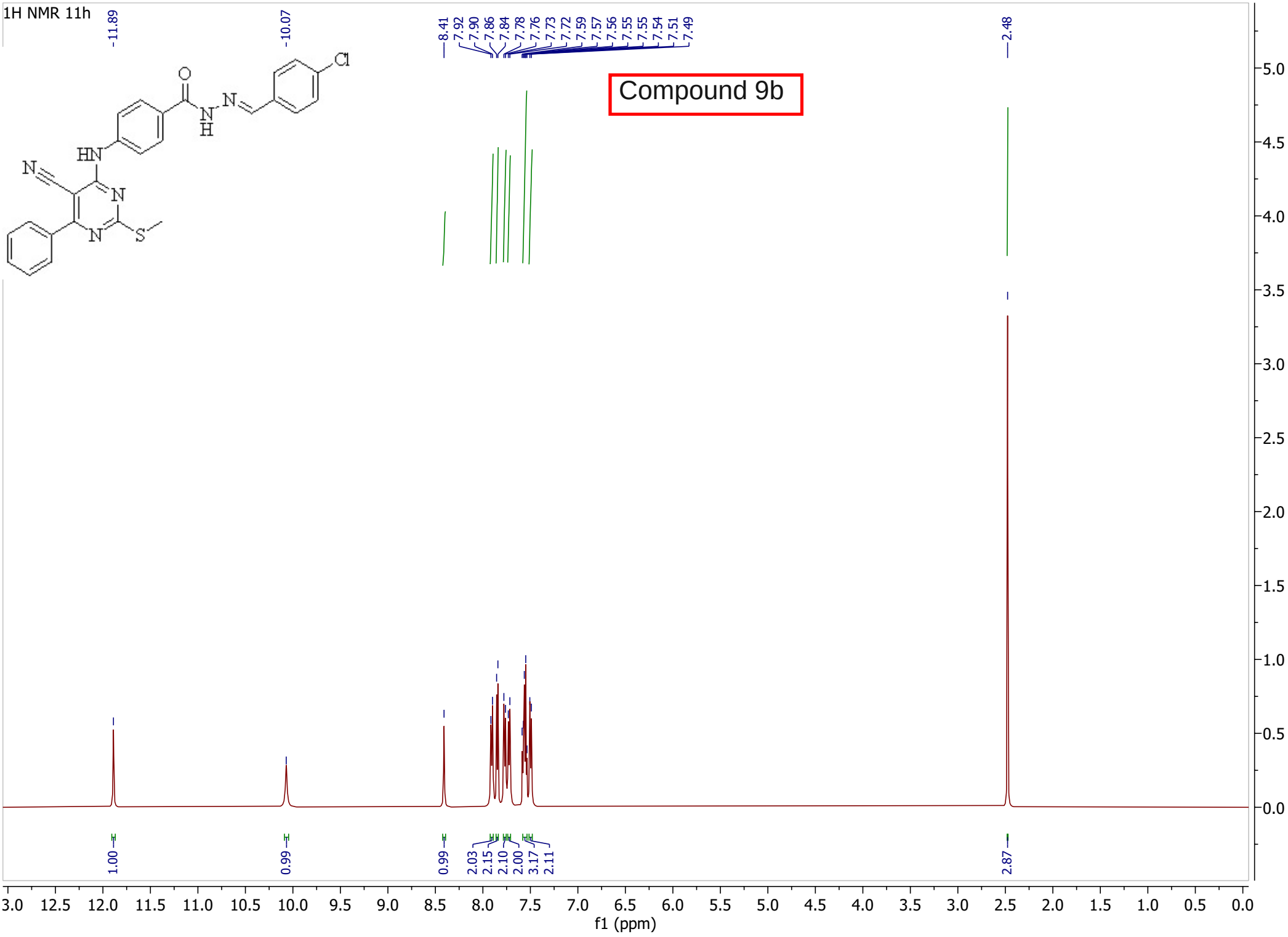
Sample Name:	ASL5 Compound 9b	Acquired By:	System
Sample Type:	Unknown	Sample Set Name:	
Vial:	14	Acq. Method Set:	Organic
Injection #:	1	Processing Method:	Default
Injection Volume:	2.00 ul	Channel Name:	320.0nm
Run Time:	14.0 Minutes	Proc. Chnl. Descr.:	W2996 PDA 320.0 nm (PDA 190.0 to
Date Acquired:	11/6/2022 5:18:18 AM EET		
Date Processed:	11/6/2022 5:33:06 AM EET		

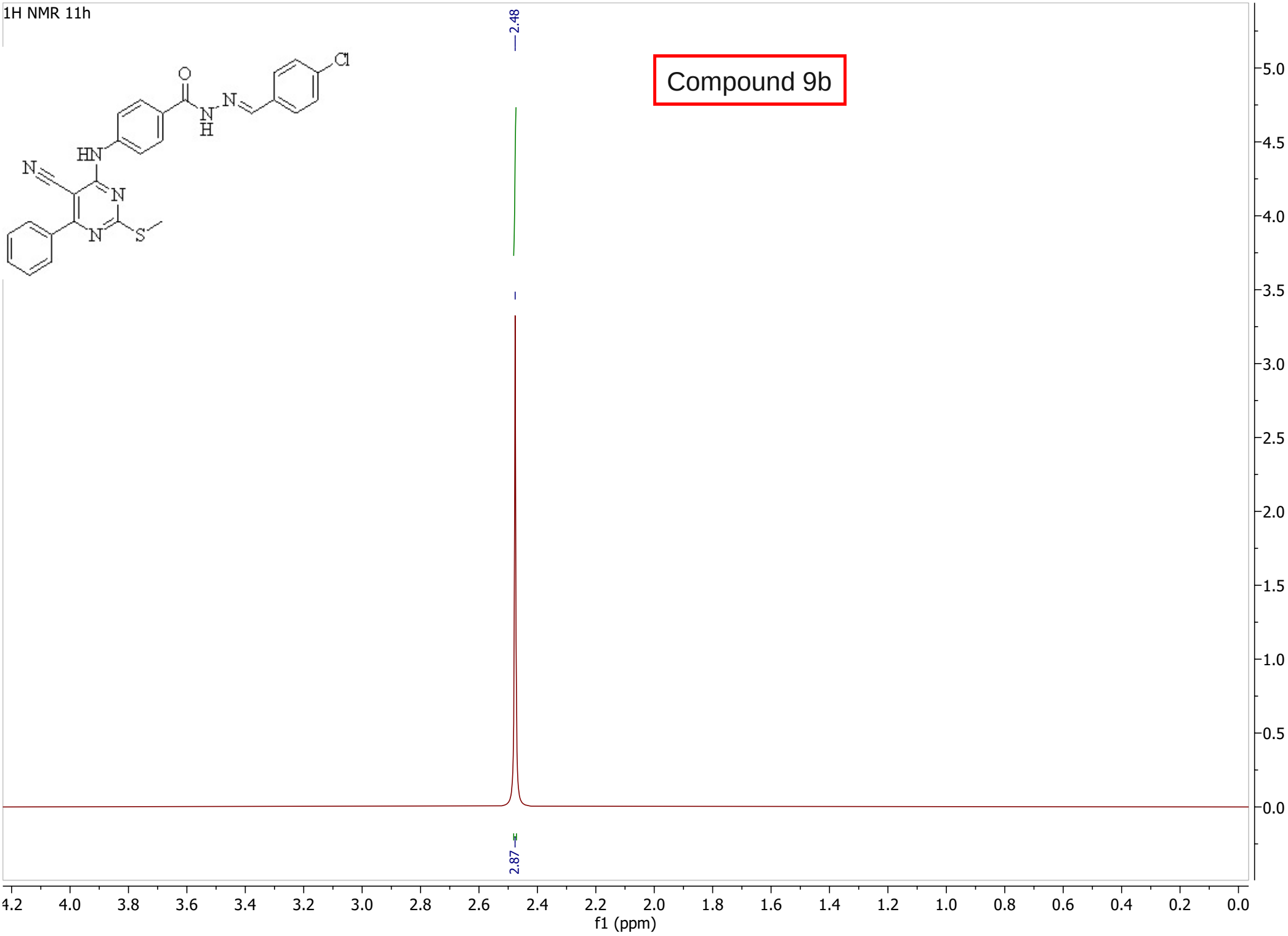


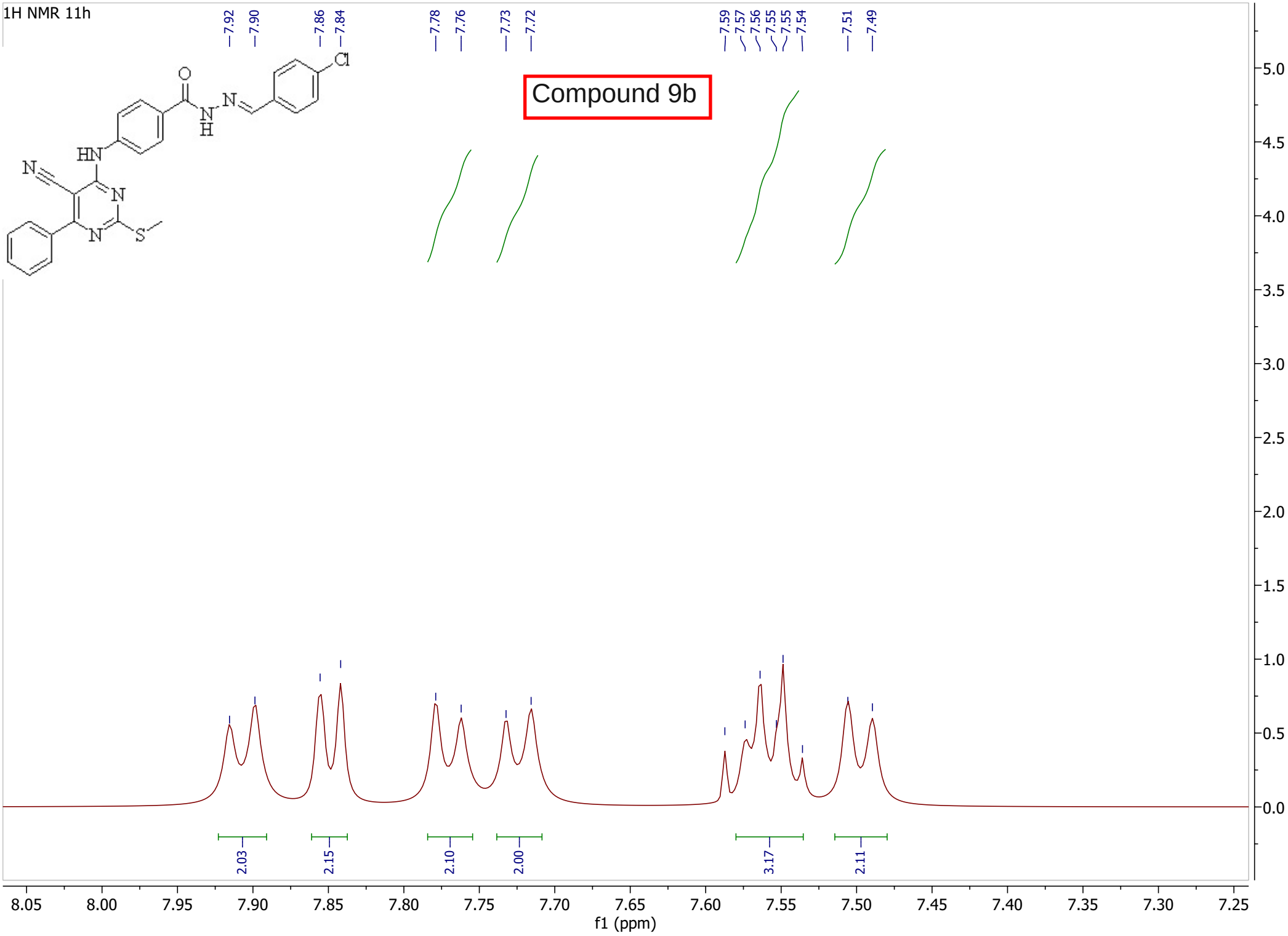
	RT	Area	% Area	Height
1	3.166	27922	0.47	4657
2	11.667	5852346	99.53	337582

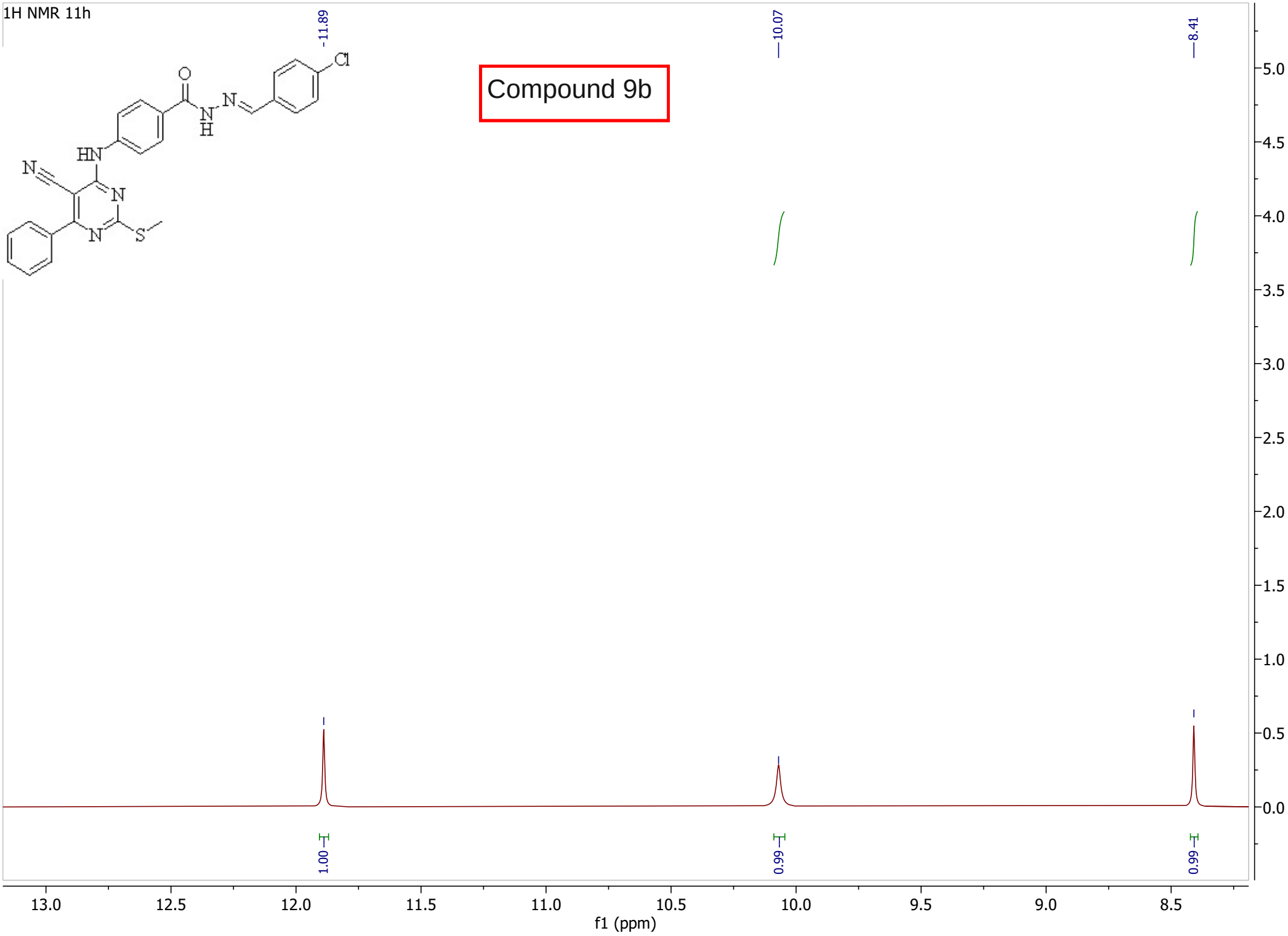


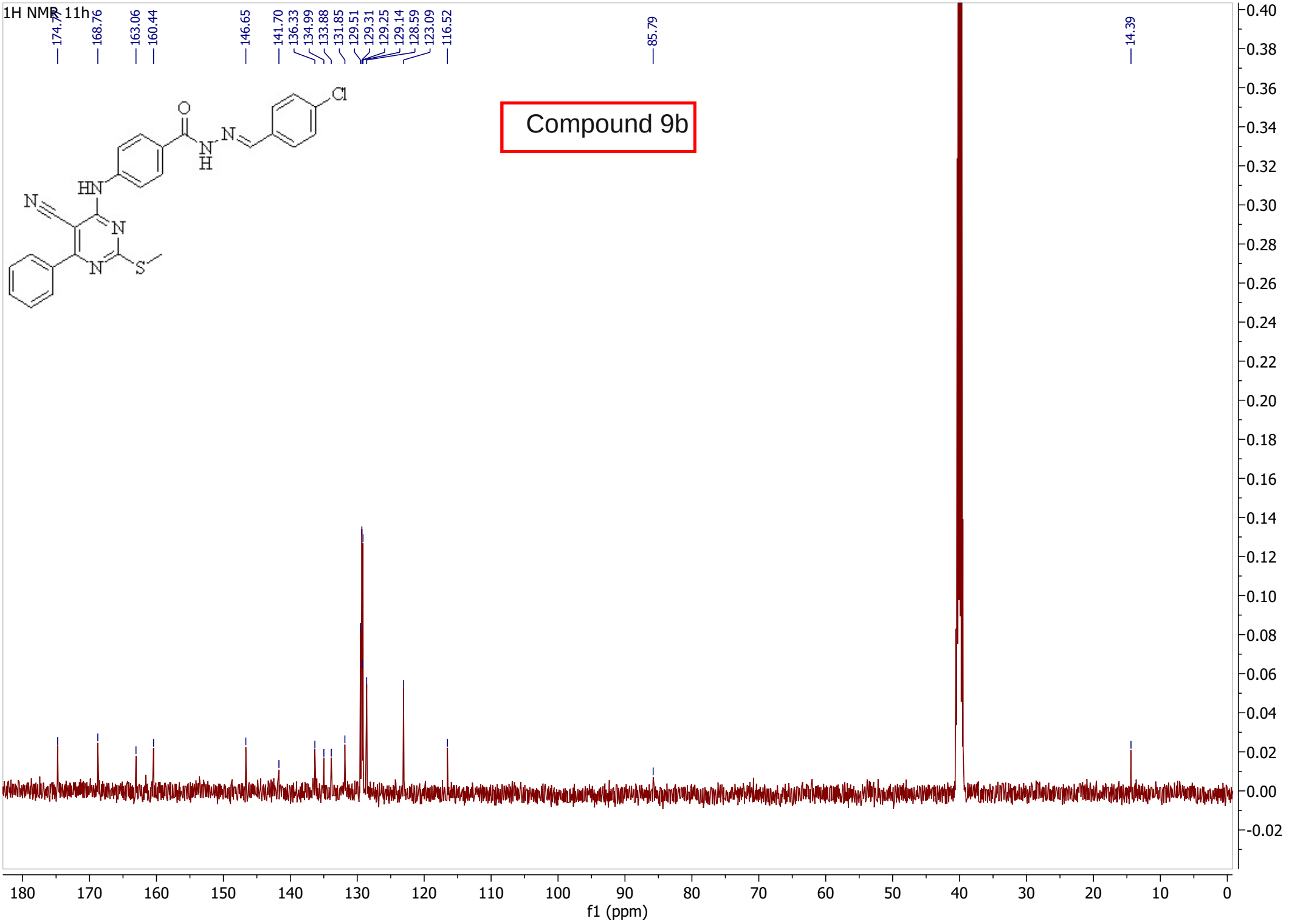

ASL5
% Transmittance
Wavenumbers (cm-1)
3397.72
3300.35
3227.21
3062.47
2924.12
2214.41
1650.00
1607.24
1559.83
1530.63
1485.35
1447.10
1403.81
1365.93
1326.81
1302.71
1286.21
1242.38
1186.46
1149.31
1122.76
1087.06
1064.65
1012.51
965.18
938.19
916.68
874.29
849.39
824.80
798.93
763.11
696.22
635.99
585.01
563.78
514.32
502.55
468.38
432.41
Compound 9b

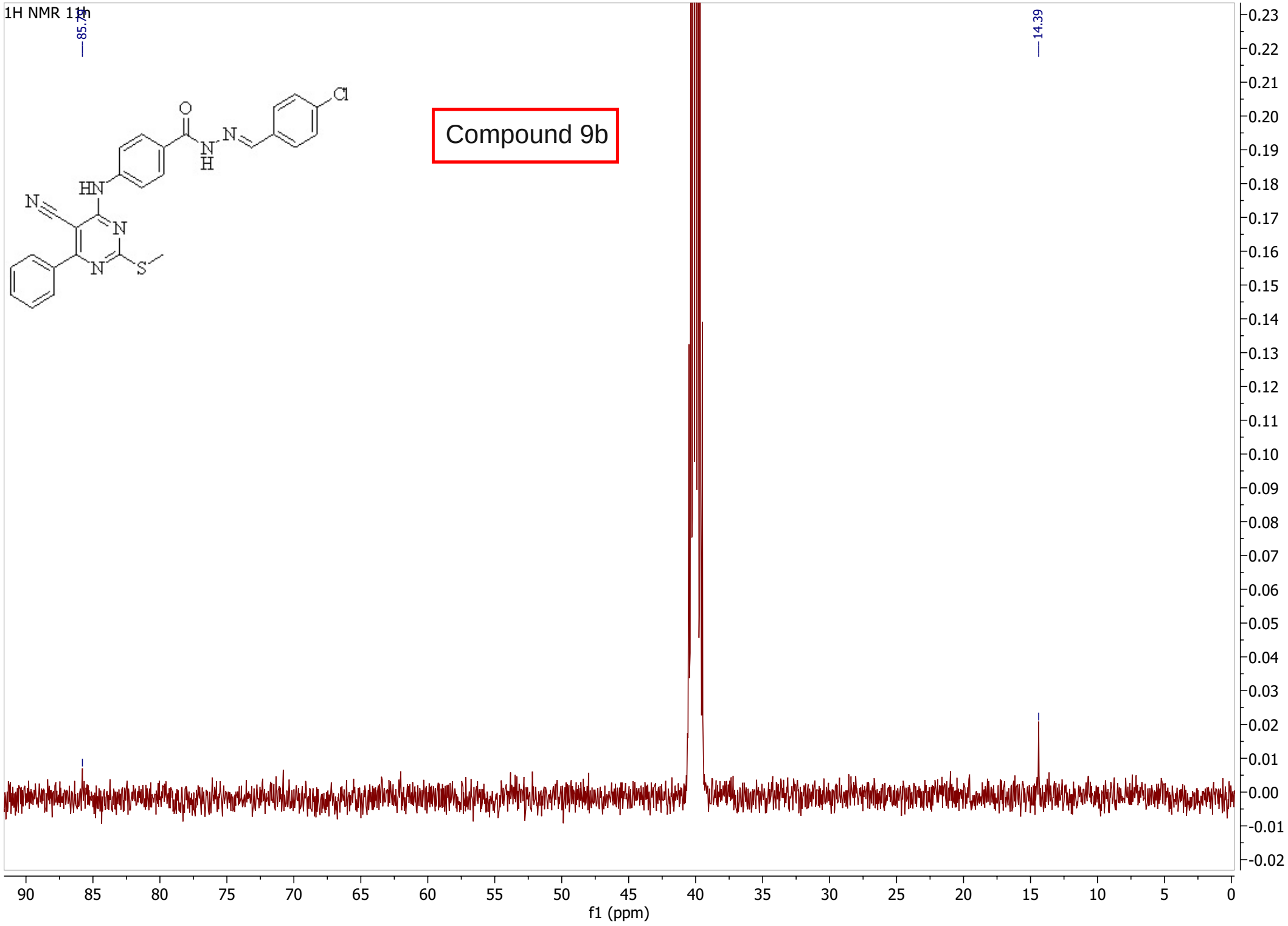

1H NMR 11h
-11.89
-10.07
8.41
7.92
7.90
7.86
7.84
7.78
7.76
7.73
7.72
7.59
7.57
7.56
7.55
7.55
7.54
7.51
7.49
2.48
Compound 9b
Cl
O
N
N
H
HN
N
N
N
S
1.00
0.99
0.99
2.03
2.15
2.10
2.00
3.17
2.11
2.87
f1 (ppm)

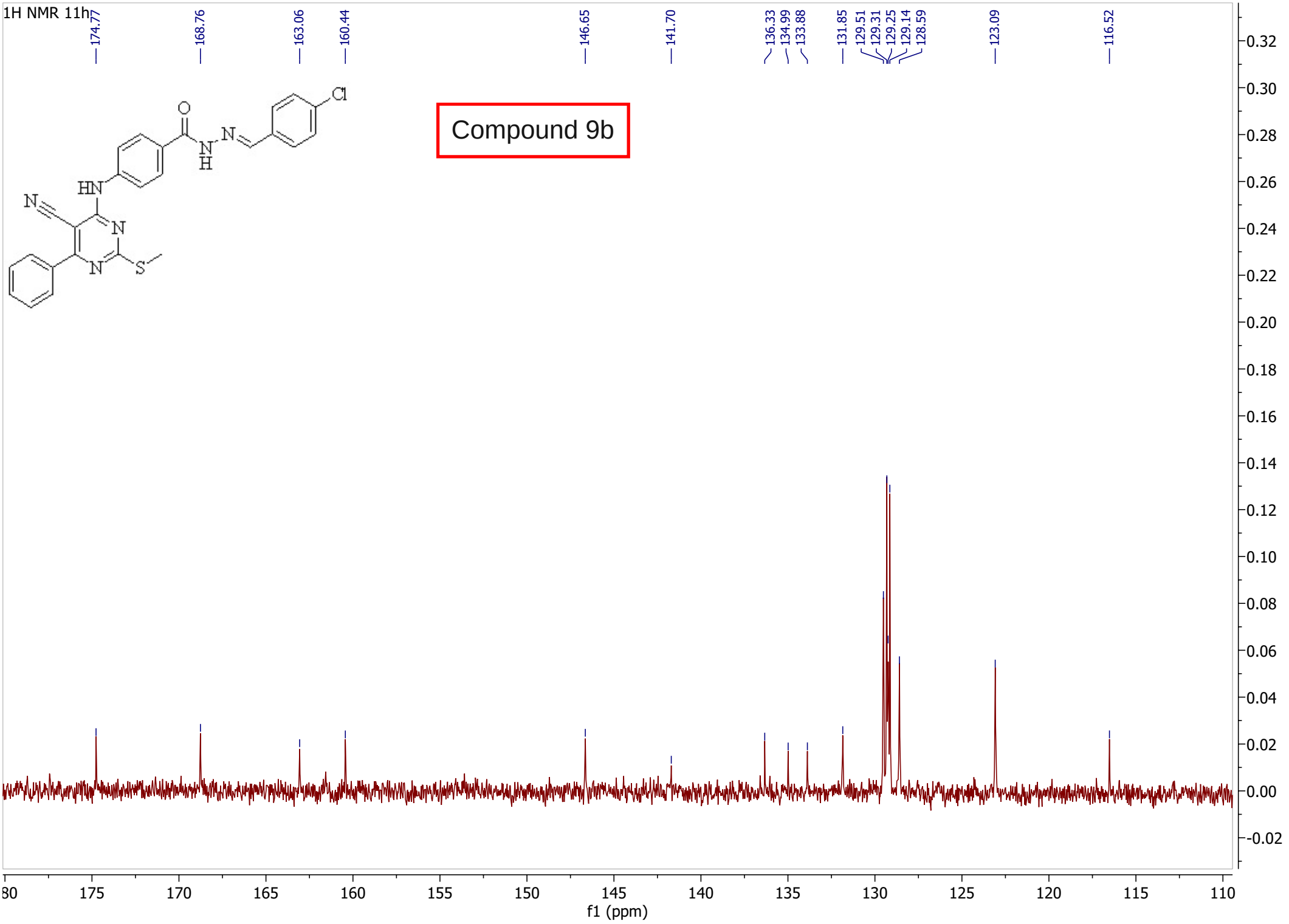

1H NMR 11h
2.48
Compound 9b
Cl
O
N
N
H
HN
N
N
N
S
2.87
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
4.2
4.0
3.8
3.6
3.4
3.2
3.0
2.8
2.6
2.4
2.2
2.0
1.8
1.6
1.4
1.2
1.0
0.8
0.6
0.4
0.2
0.0
f1 (ppm)


1H NMR 11h
7.92
7.90
7.86
7.84
7.78
7.76
7.73
7.72
7.59
7.57
7.56
7.55
7.55
7.54
7.51
7.49
Compound 9b
Cl
O
N
H
N
HN
N
N
N
S
2.03
2.15
2.10
2.00
3.17
2.11
8.05
8.00
7.95
7.90
7.85
7.80
7.75
7.70
7.65
7.60
7.55
7.50
7.45
7.40
7.35
7.30
7.25
f1 (ppm)
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0


1H NMR 11h
Compound 9b
11.89
10.07
8.41
1.00
0.99
0.99
13.0
12.5
12.0
11.5
11.0
10.5
10.0
9.5
9.0
8.5
f1 (ppm)
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0


1H NMR 11h
174.77
168.76
163.06
160.44
146.65
141.70
136.33
134.99
133.88
131.85
129.51
129.31
129.25
129.14
128.59
123.09
116.52
85.79
14.39
Compound 9b
Cl
O
N
H
HN
N
N
N
S
0.40
0.38
0.36
0.34
0.32
0.30
0.28
0.26
0.24
0.22
0.20
0.18
0.16
0.14
0.12
0.10
0.08
0.06
0.04
0.02
0.00
-0.02
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


1H NMR 11h
85.72
14.39
Compound 9b
Cl
O
N
N
H
HN
N
N
N
S
0.23
0.22
0.21
0.20
0.19
0.18
0.17
0.16
0.15
0.14
0.13
0.12
0.11
0.10
0.09
0.08
0.07
0.06
0.05
0.04
0.03
0.02
0.01
0.00
-0.01
-0.02
90
85
80
75
70
65
60
55
50
45
40
35
30
25
20
15
10
5
0
f1 (ppm)


1H NMR 11h
174.77
168.76
163.06
160.44
146.65
141.70
136.33
134.99
133.88
131.85
129.51
129.31
129.25
129.14
128.59
123.09
116.52
Compound 9b
Cl
O
N
H
HN
N
N
N
S
0.32
0.30
0.28
0.26
0.24
0.22
0.20
0.18
0.16
0.14
0.12
0.10
0.08
0.06
0.04
0.02
0.00
-0.02
180
175
170
165
160
155
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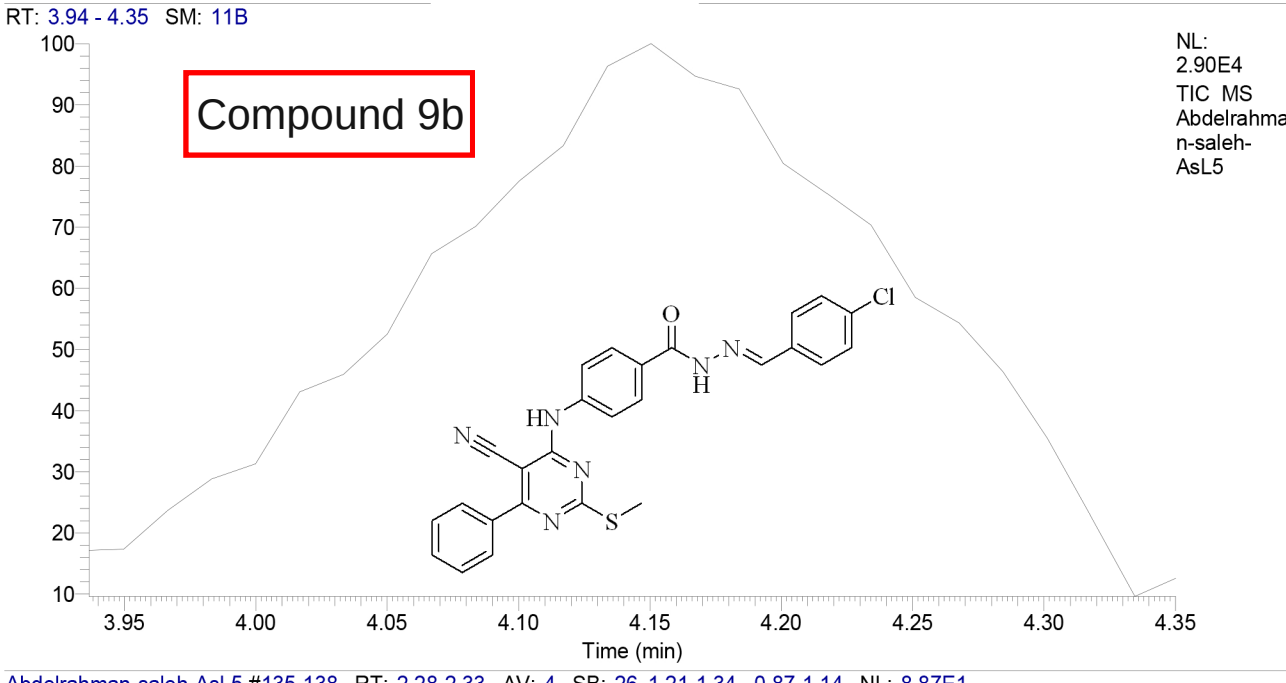
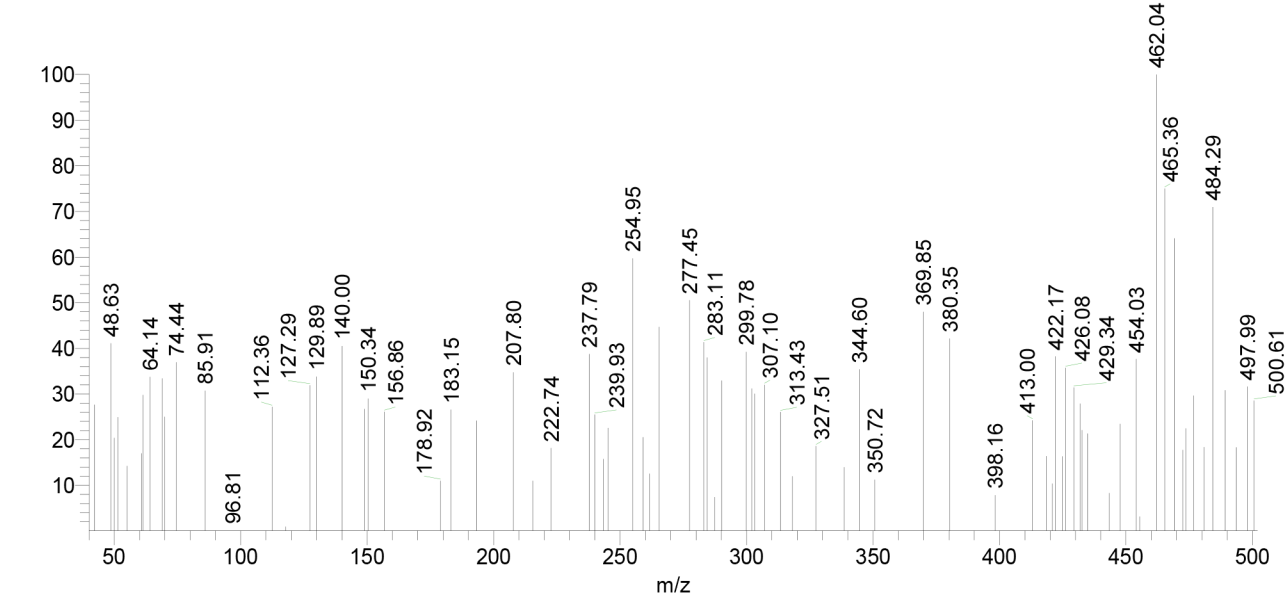
140
135
130
125
120
115
110
f1 (ppm)

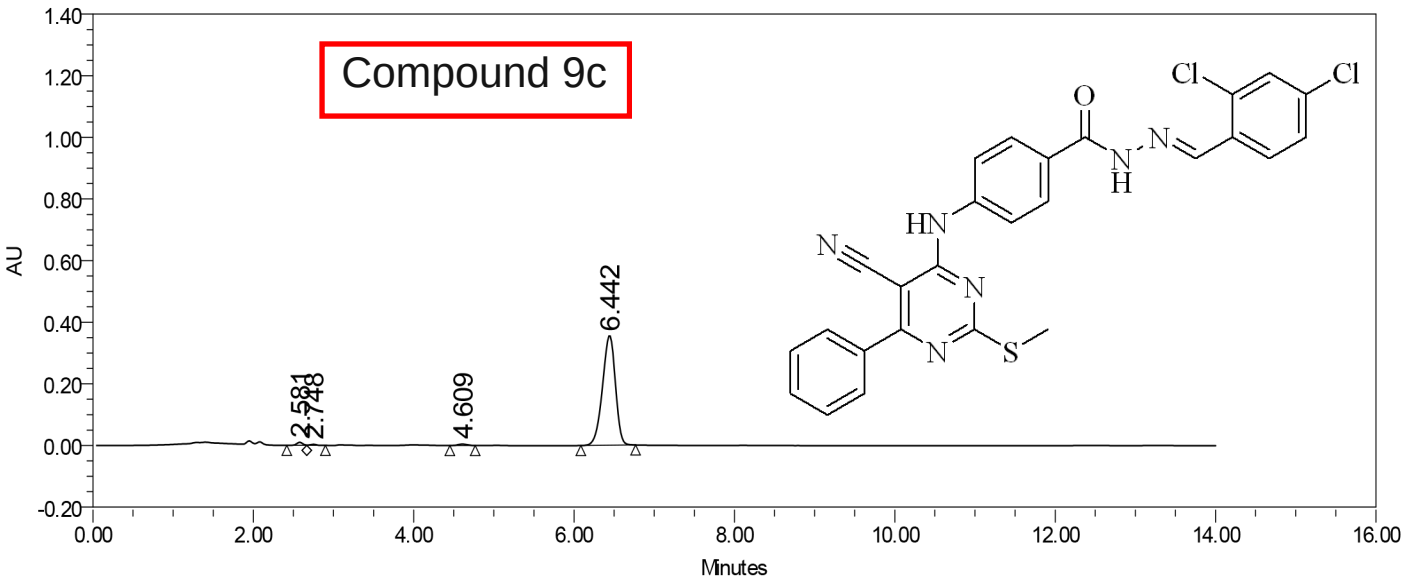


Abdelrahman-saleh-AsL5 #135-138 RT: 2.28-2.33 AV: 4 SB: 26 1.21-1.34 , 0.87-1.14 NL: 8.87E1
T: + c EI Full ms [40.00-1000.00]

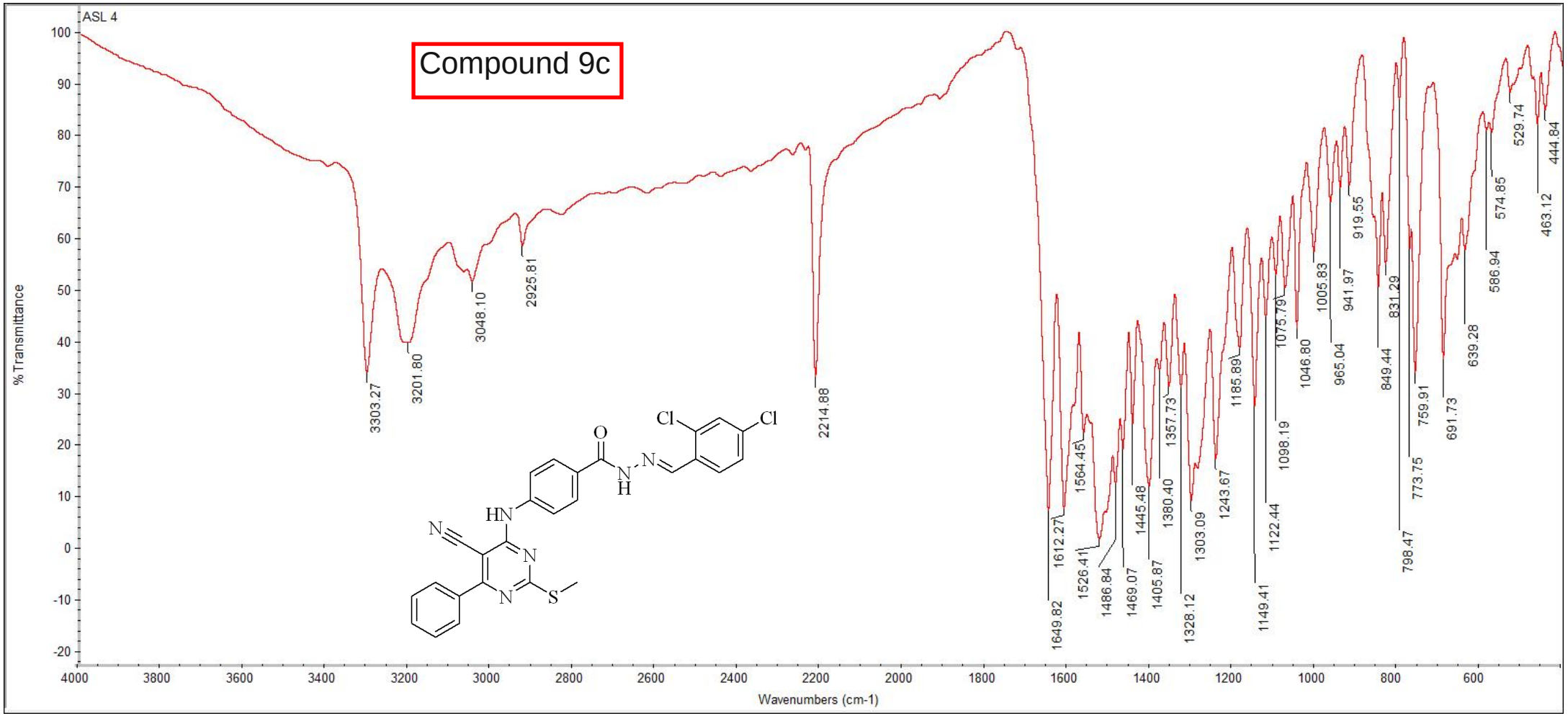


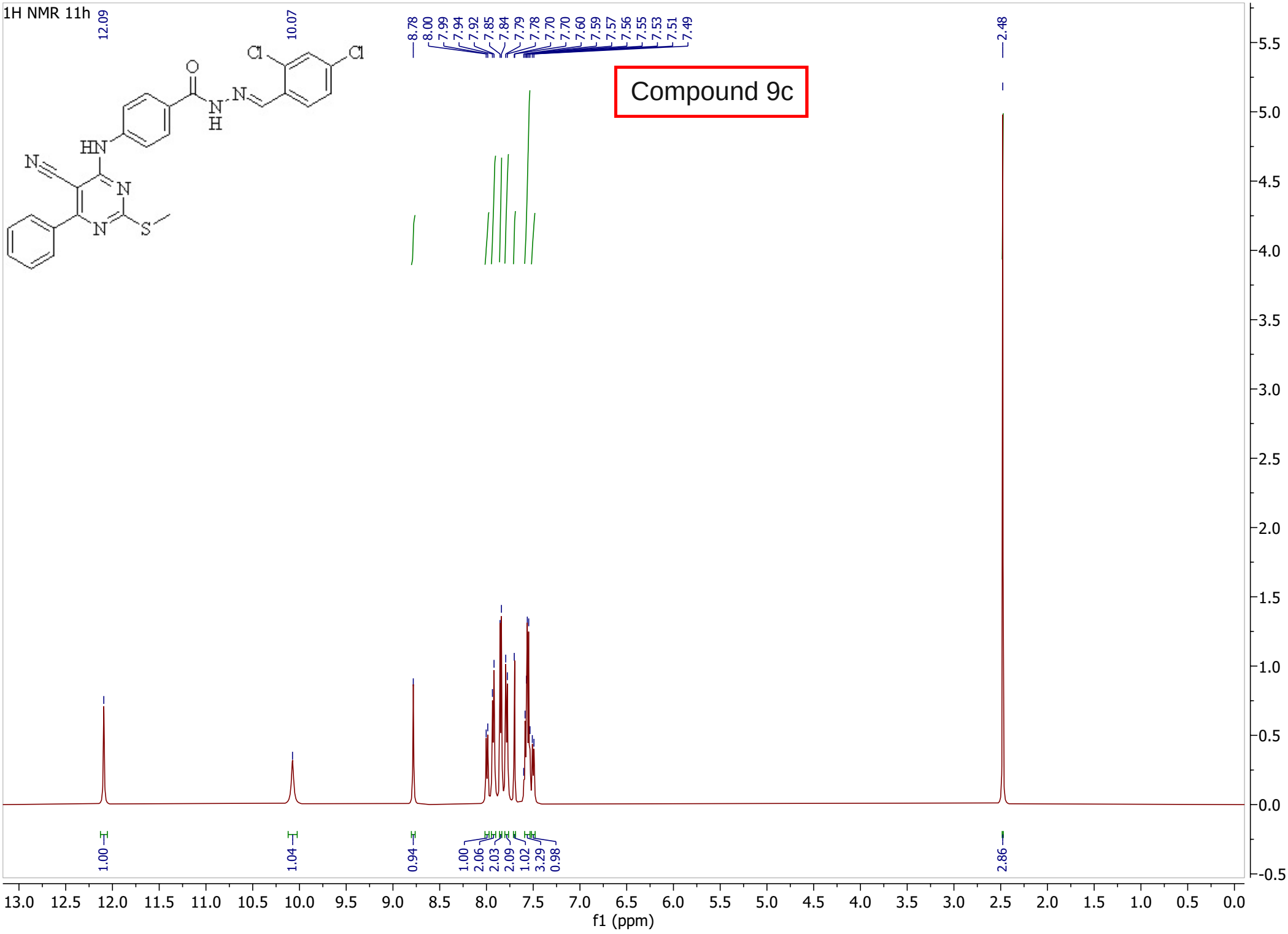
SAMPLE INFORMATION

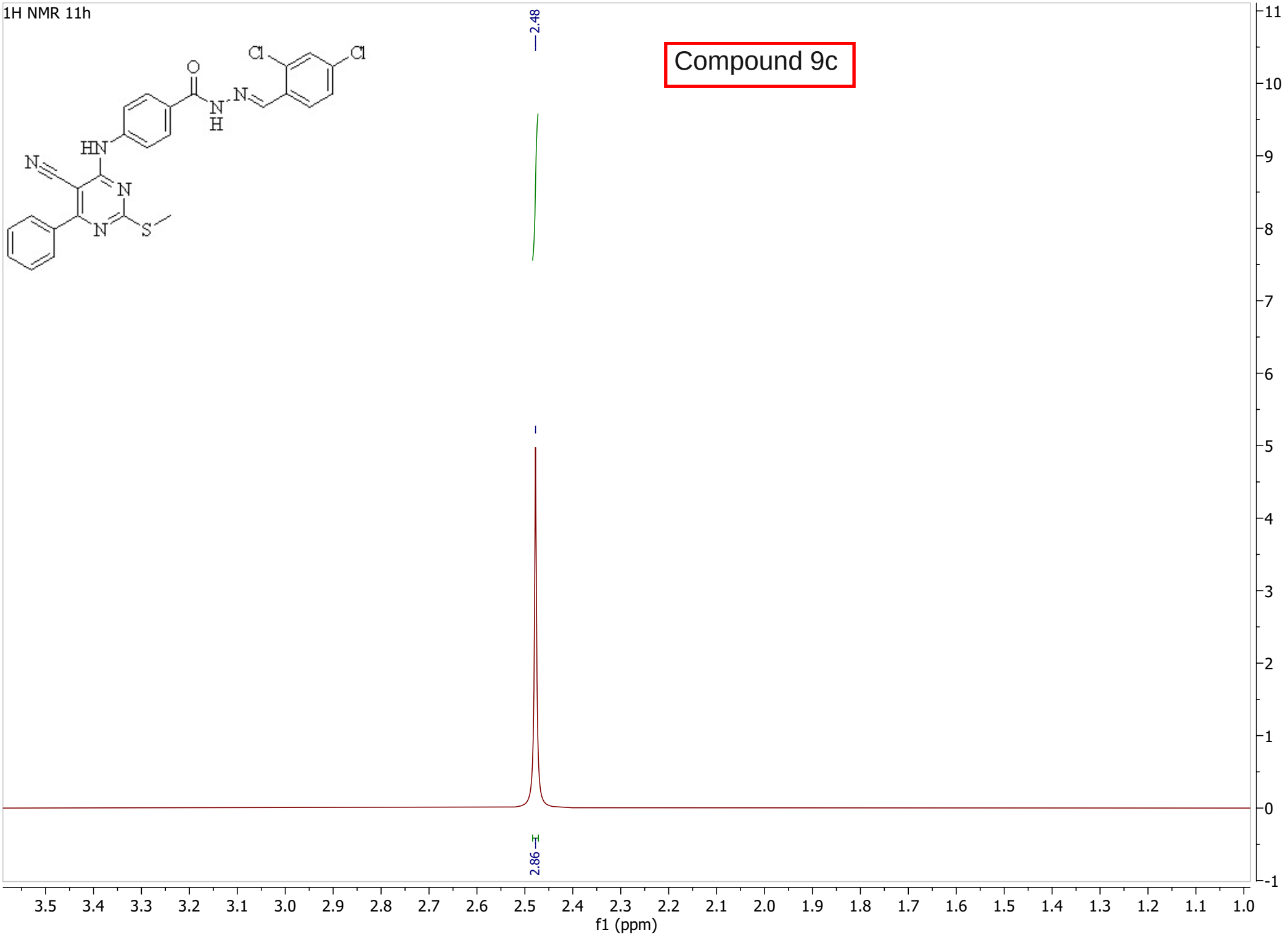
Sample Name:	ASL4	Compound 9c	Acquired By:	System
Sample Type:	Unknown		Sample Set Name:	
Vial:	13		Acq. Method Set:	Organic
Injection #:	1		Processing Method:	Default
Injection Volume:	2.00 ul		Channel Name:	261.4nm
Run Time:	14.0 Minutes		Proc. Chnl. Descr.:	W2996 PDA 261.4 nm (PDA 190.0 to
Date Acquired:	11/6/2022 6:18:22 AM EET			
Date Processed:	11/6/2022 6:33:43 AM EET			

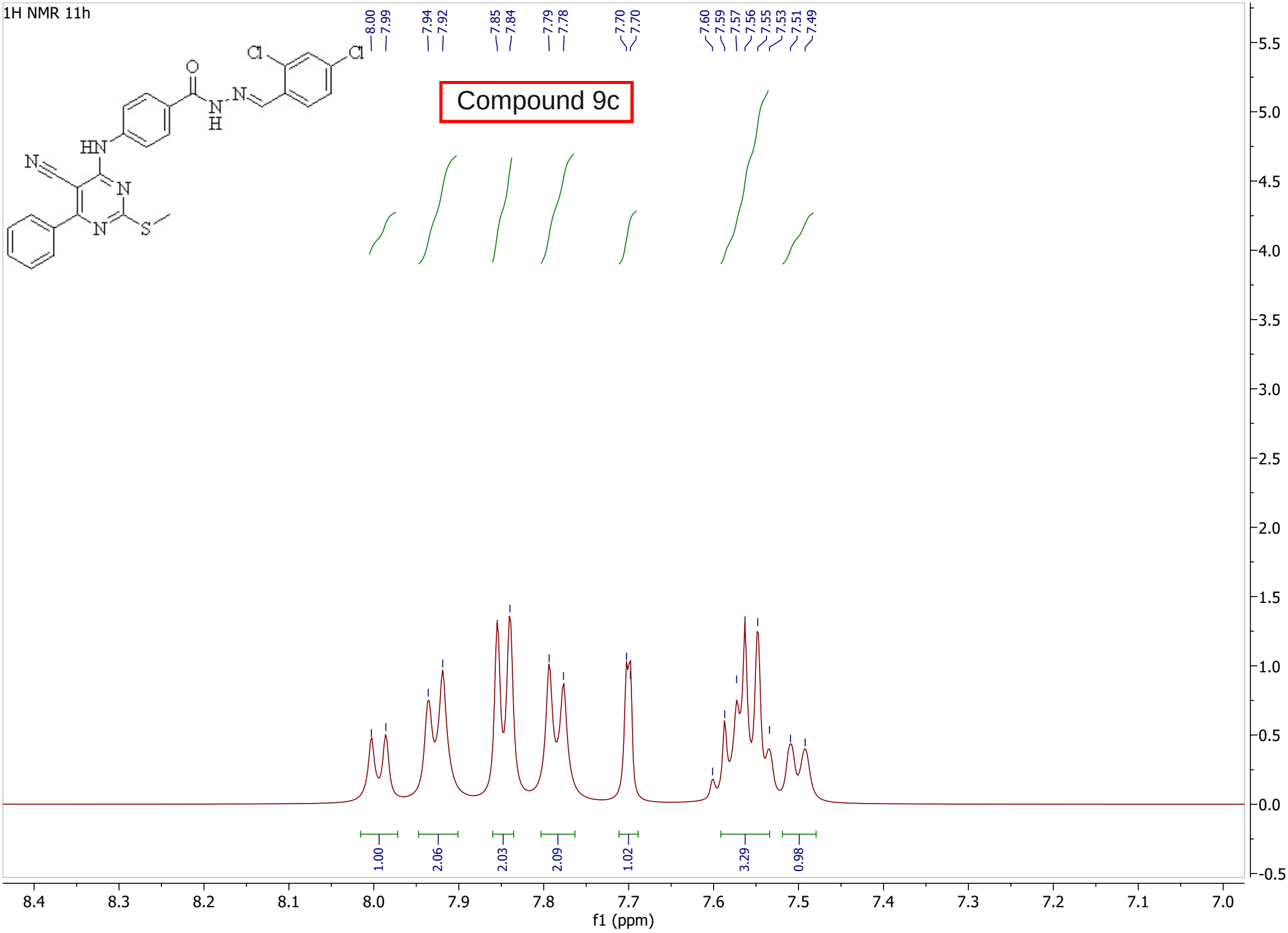


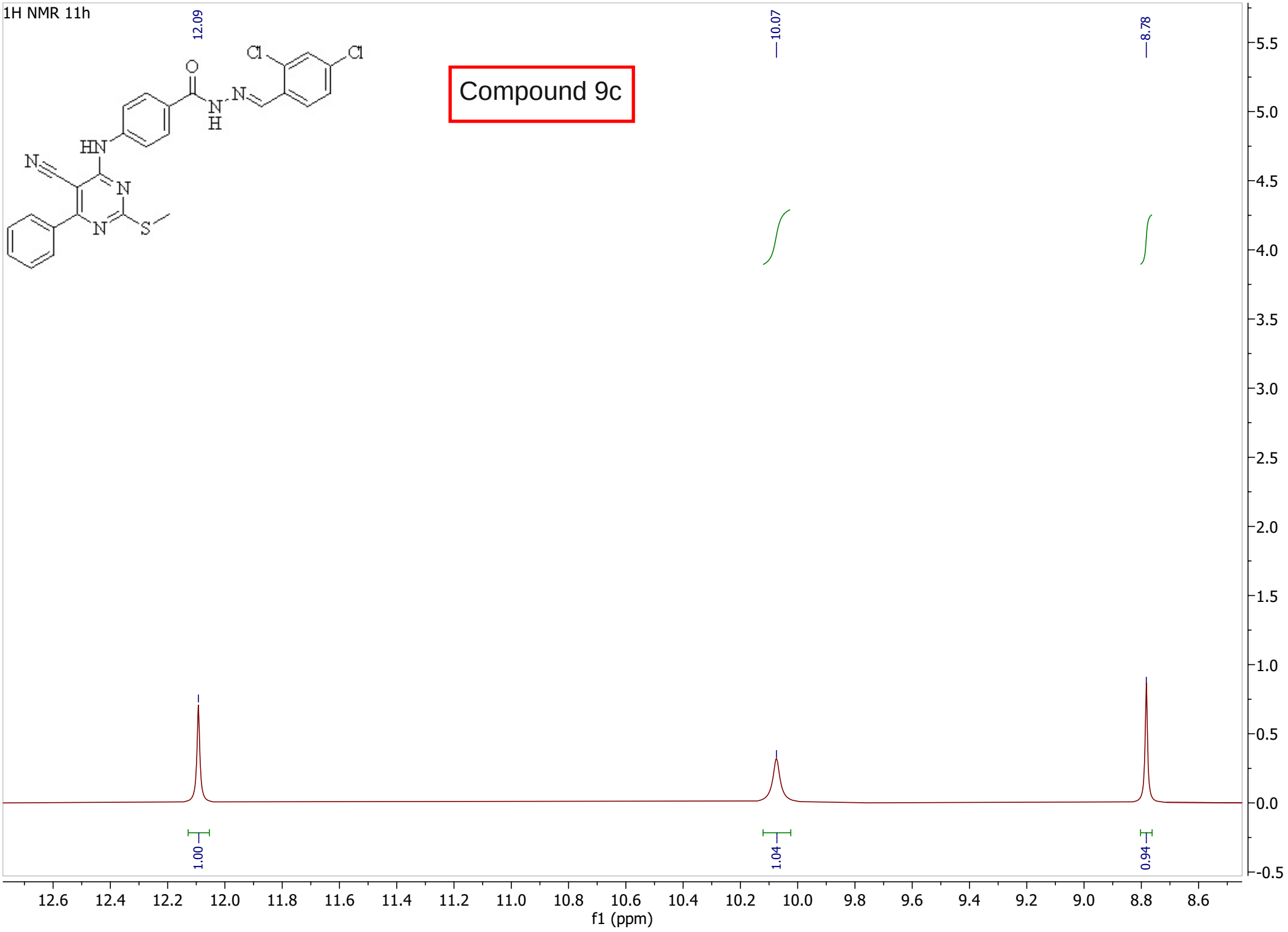
	RT	Area	% Area	Height
1	2.581	50406	1.23	9675
2	2.748	17187	0.42	3193
3	4.609	36709	0.89	4451
4	6.442	3997303	97.46	355748

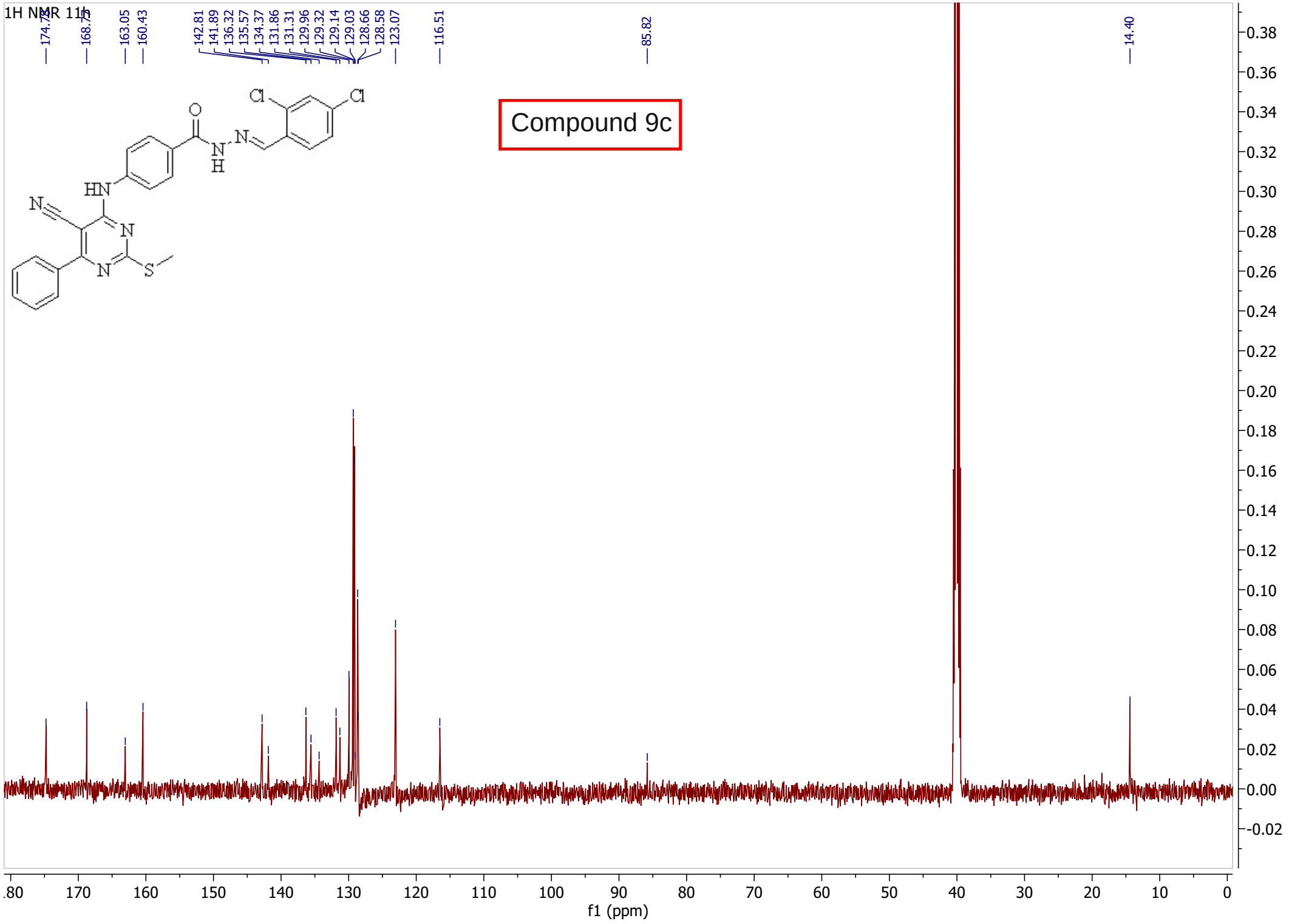

ASL 4
Compound 9c
% Transmittance
Wavenumbers (cm-1)
3303.27
3201.80
3048.10
2925.81
2214.88
1649.82
1612.27
1564.45
1526.41
1486.84
1469.07
1445.48
1405.87
1380.40
1357.73
1328.12
1303.09
1243.67
1185.89
1149.41
1122.44
1098.19
1075.79
1046.80
1005.83
965.04
941.97
919.55
849.44
831.29
798.47
773.75
759.91
691.73
639.28
586.94
574.85
529.74
463.12
444.84
Cl
Cl
O
N
H
N
HN
N
N
S

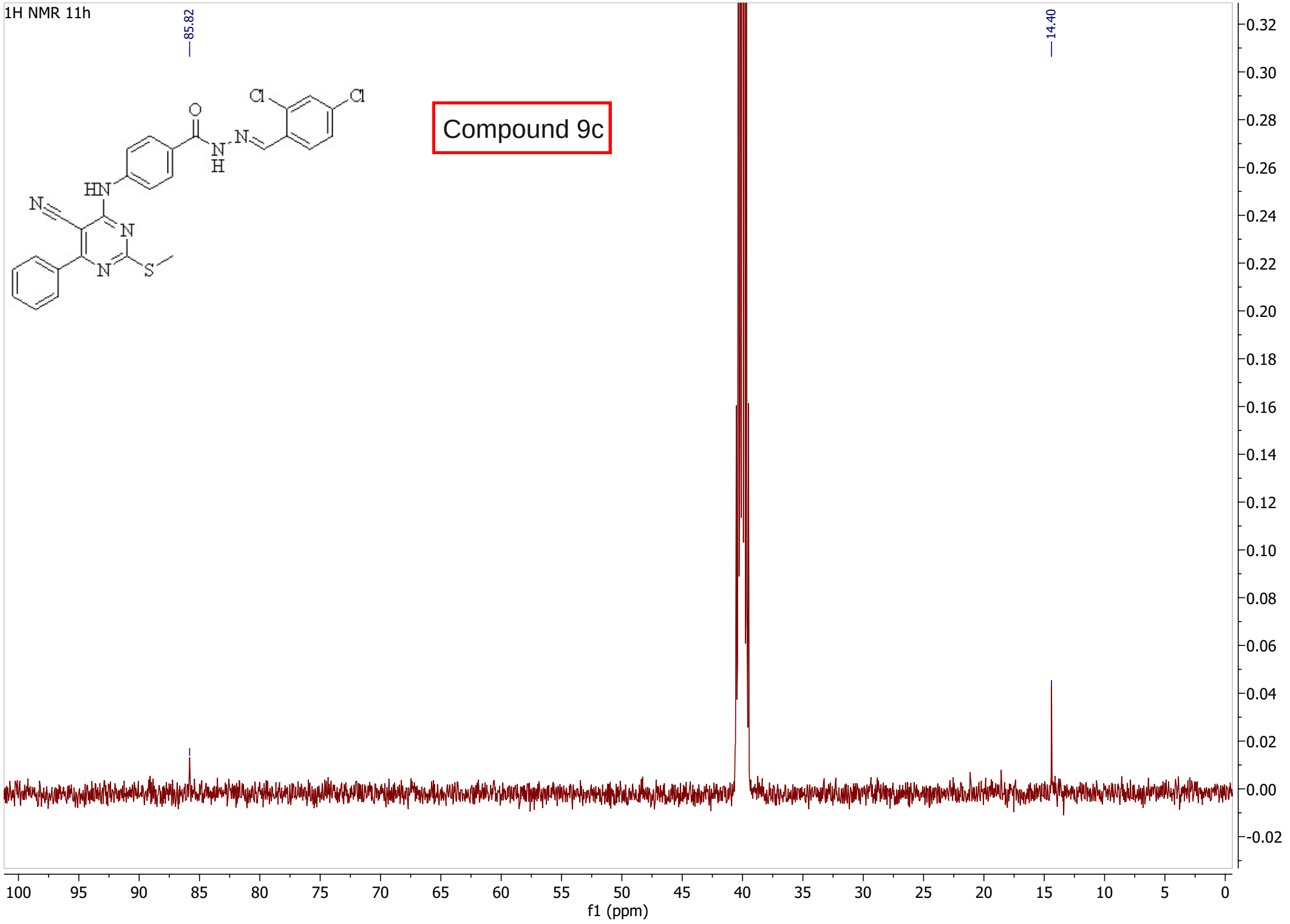

1H NMR 11h
Compound 9c
12.09
10.07
8.78
8.00
7.99
7.94
7.92
7.85
7.84
7.79
7.78
7.70
7.70
7.60
7.59
7.57
7.56
7.55
7.53
7.51
7.49
2.48
1.00
1.04
0.94
1.00
2.06
2.03
2.09
1.02
3.29
0.98
2.86
f1 (ppm)

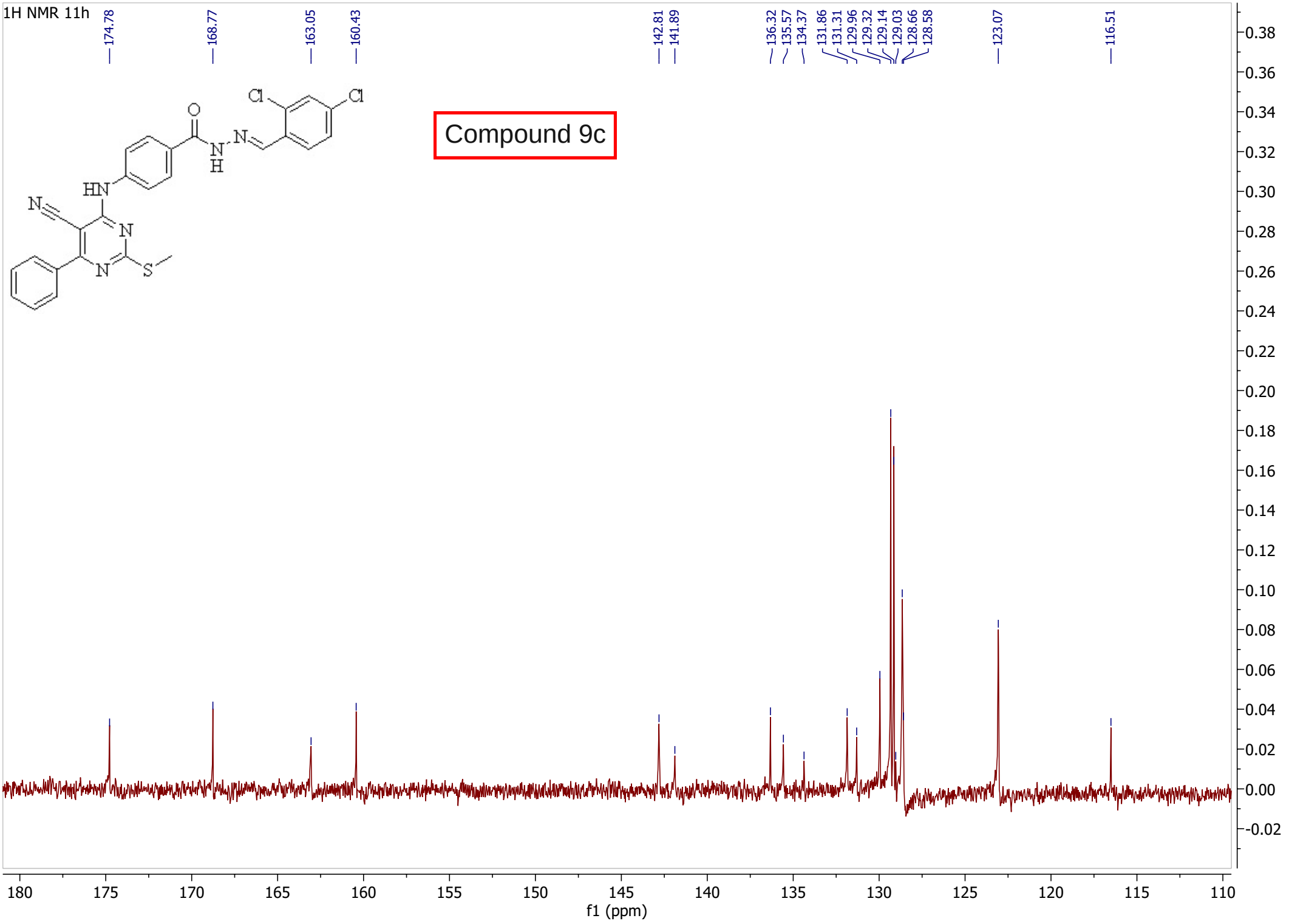

1H NMR 11h
Compound 9c
2.48
2.86
f1 (ppm)

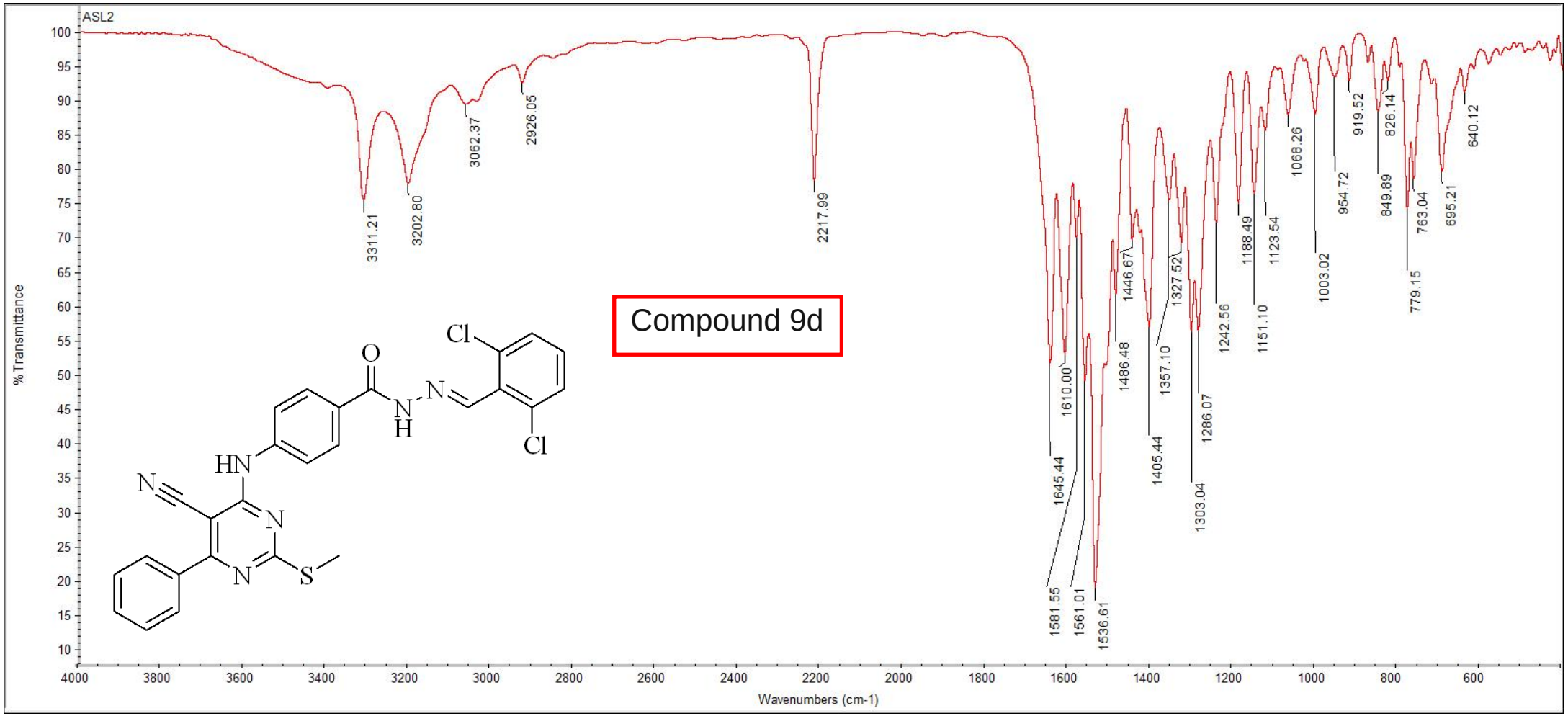

1H NMR 11h
Compound 9c
8.00
7.99
7.94
7.92
7.85
7.84
7.79
7.78
7.70
7.70
7.60
7.59
7.57
7.56
7.55
7.53
7.51
7.49
1.00
2.06
2.03
2.09
1.02
3.29
0.98
f1 (ppm)

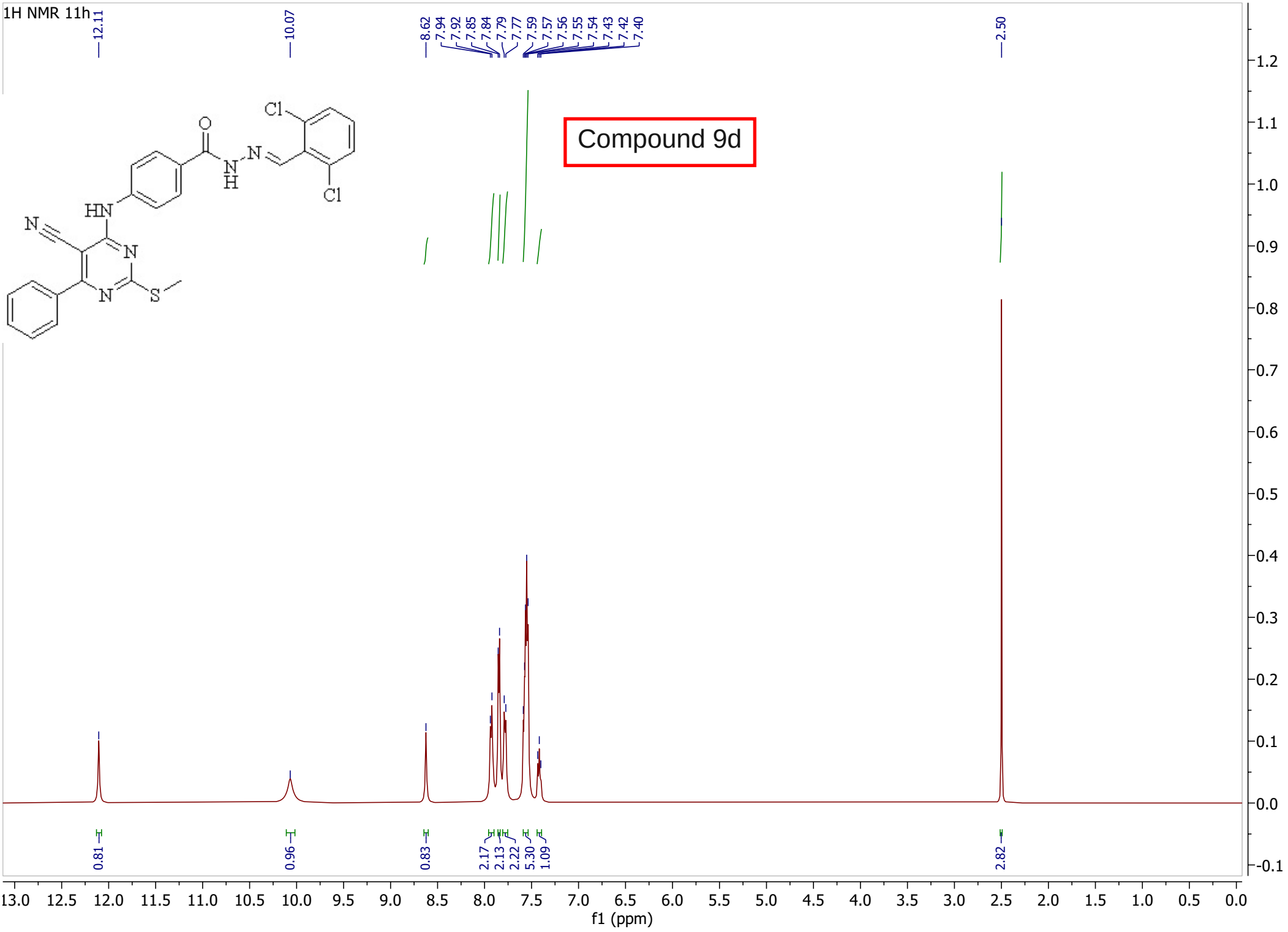

1H NMR 11h
12.09
10.07
8.78
Compound 9c
Cl
Cl
O
N
H
N
HN
N
N
N
S
1.00
1.04
0.94
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
12.6
12.4
12.2
12.0
11.8
11.6
11.4
11.2
11.0
10.8
10.6
10.4
10.2
10.0
9.8
9.6
9.4
9.2
9.0
8.8
8.6
f1 (ppm)

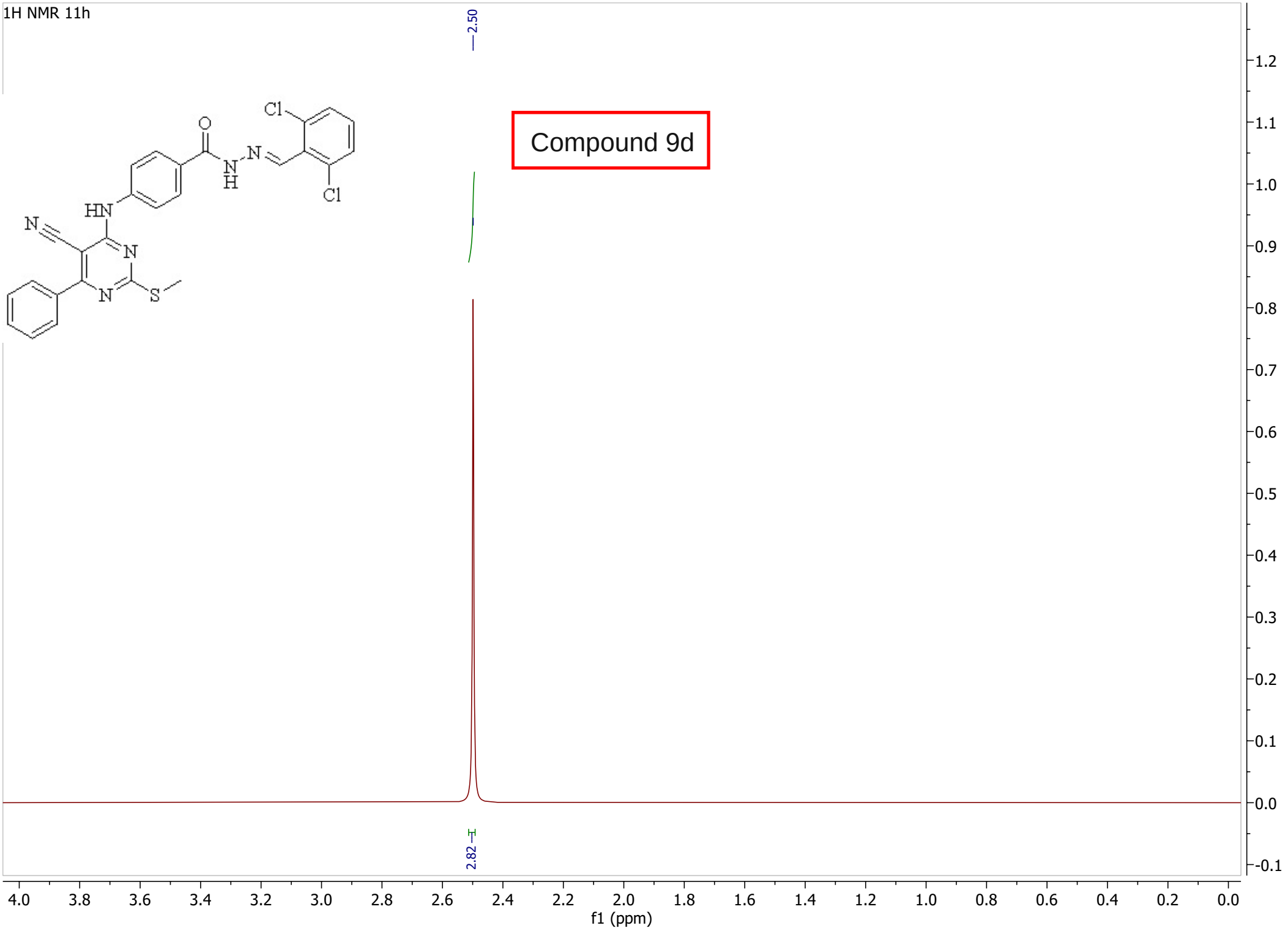

1H NMR 11h
174.75
168.72
163.05
160.43
142.81
141.89
136.32
135.57
134.37
131.86
131.31
129.96
129.32
129.14
129.03
128.66
128.58
123.07
116.51
85.82
14.40
Compound 9c
Cl
Cl
O
N
H
N
HN
N
N
N
S
0.38
0.36
0.34
0.32
0.30
0.28
0.26
0.24
0.22
0.20
0.18
0.16
0.14
0.12
0.10
0.08
0.06
0.04
0.02
0.00
-0.02
.80
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

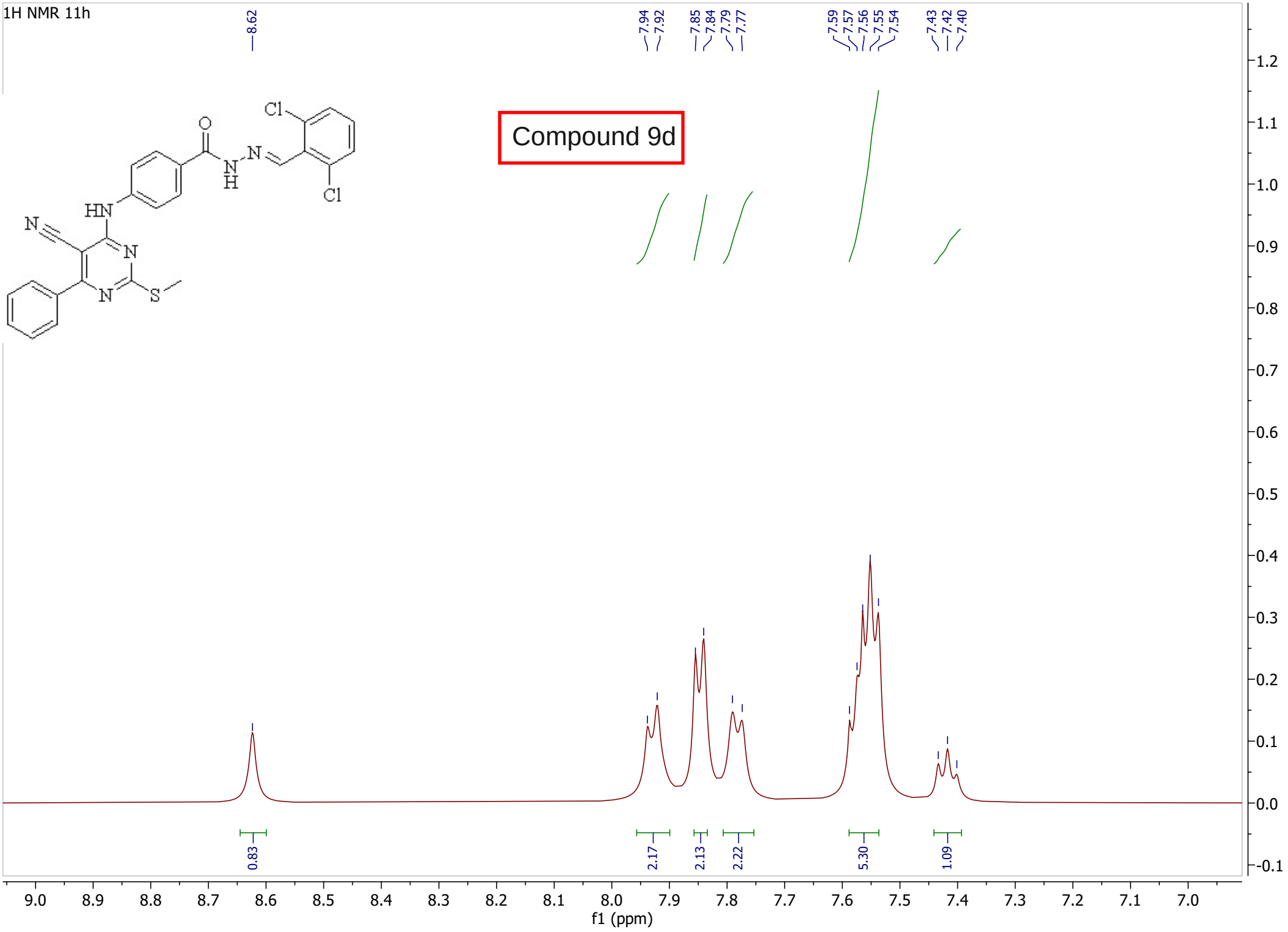

1H NMR 11h
85.82
14.40
Compound 9c
Cl
Cl
O
N
H
N
HN
N
N
N
S
0.32
0.30
0.28
0.26
0.24
0.22
0.20
0.18
0.16
0.14
0.12
0.10
0.08
0.06
0.04
0.02
0.00
-0.02
100
95
90
85
80
75
70
65
60
55
50
45
40
35
30
25
20
15
10
5
0
f1 (ppm)


1H NMR 11h
174.78
168.77
163.05
160.43
142.81
141.89
136.32
135.57
134.37
131.86
131.31
129.96
129.32
129.14
129.03
128.66
128.58
123.07
116.51
Compound 9c
Cl
Cl
O
N
H
N
HN
N
N
N
S
0.38
0.36
0.34
0.32
0.30
0.28
0.26
0.24
0.22
0.20
0.18
0.16
0.14
0.12
0.10
0.08
0.06
0.04
0.02
0.00
-0.02
180
175
170
165
160
155
150
145
140
135
130
125
120
115
110
f1 (ppm)

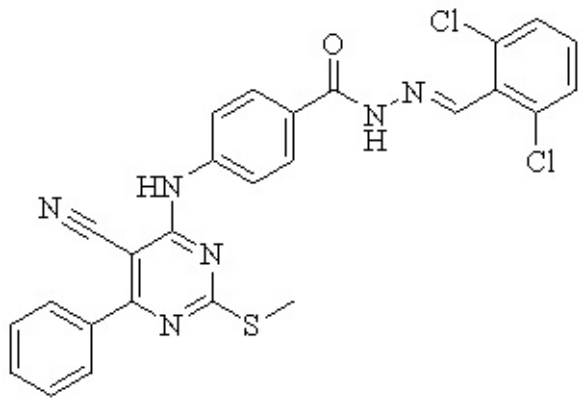

ASL2
% Transmittance
Wavenumbers (cm-1)
3311.21
3202.80
3062.37
2926.05
2217.99
1645.44
1610.00
1581.55
1561.01
1536.61
1486.48
1446.67
1405.44
1357.10
1327.52
1303.04
1286.07
1242.56
1188.49
1151.10
1123.54
1068.26
1003.02
954.72
919.52
849.89
826.14
779.15
763.04
695.21
640.12
Compound 9d
Cl
O
N
H
N
HN
N
N
S
Cl


1H NMR 11h
12.11
10.07
8.62
7.94
7.92
7.85
7.84
7.79
7.77
7.59
7.57
7.56
7.55
7.54
7.43
7.42
7.40
2.50
Compound 9d
Cl
Cl
O
N
H
N
HN
N
N
N
S
0.81
0.96
0.83
2.17
2.13
2.22
5.30
1.09
2.82
f1 (ppm)


1H NMR 11h
2.50
Compound 9d
2.82
f1 (ppm)


1H NMR 11h
8.62
7.94
7.92
7.85
7.84
7.79
7.77
7.59
7.57
7.56
7.55
7.54
7.43
7.42
7.40
Compound 9d
0.83
2.17
2.13
2.22
5.30
1.09
f1 (ppm)

1H NMR 11h



Compound 9d

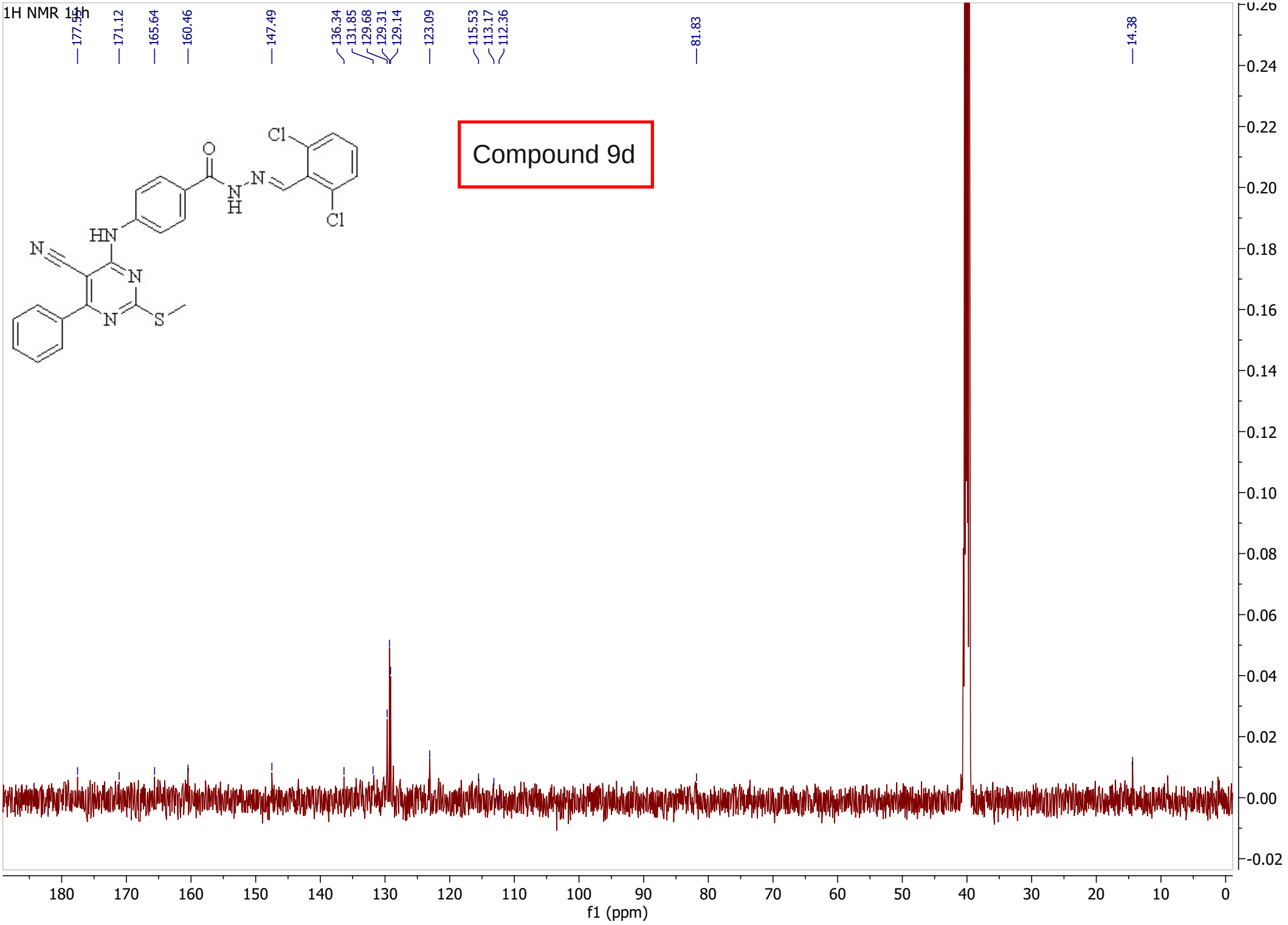
12.11

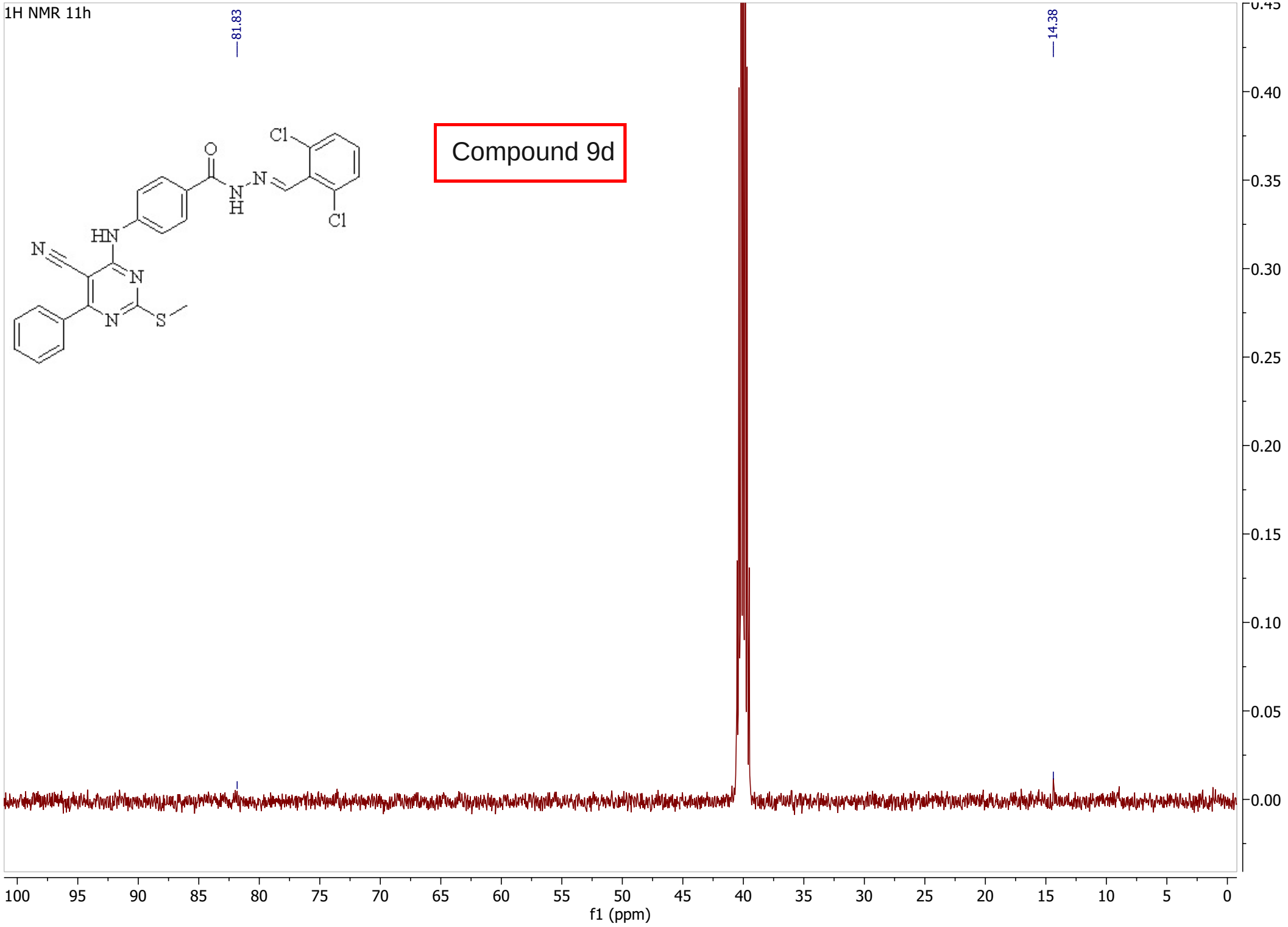
10.07

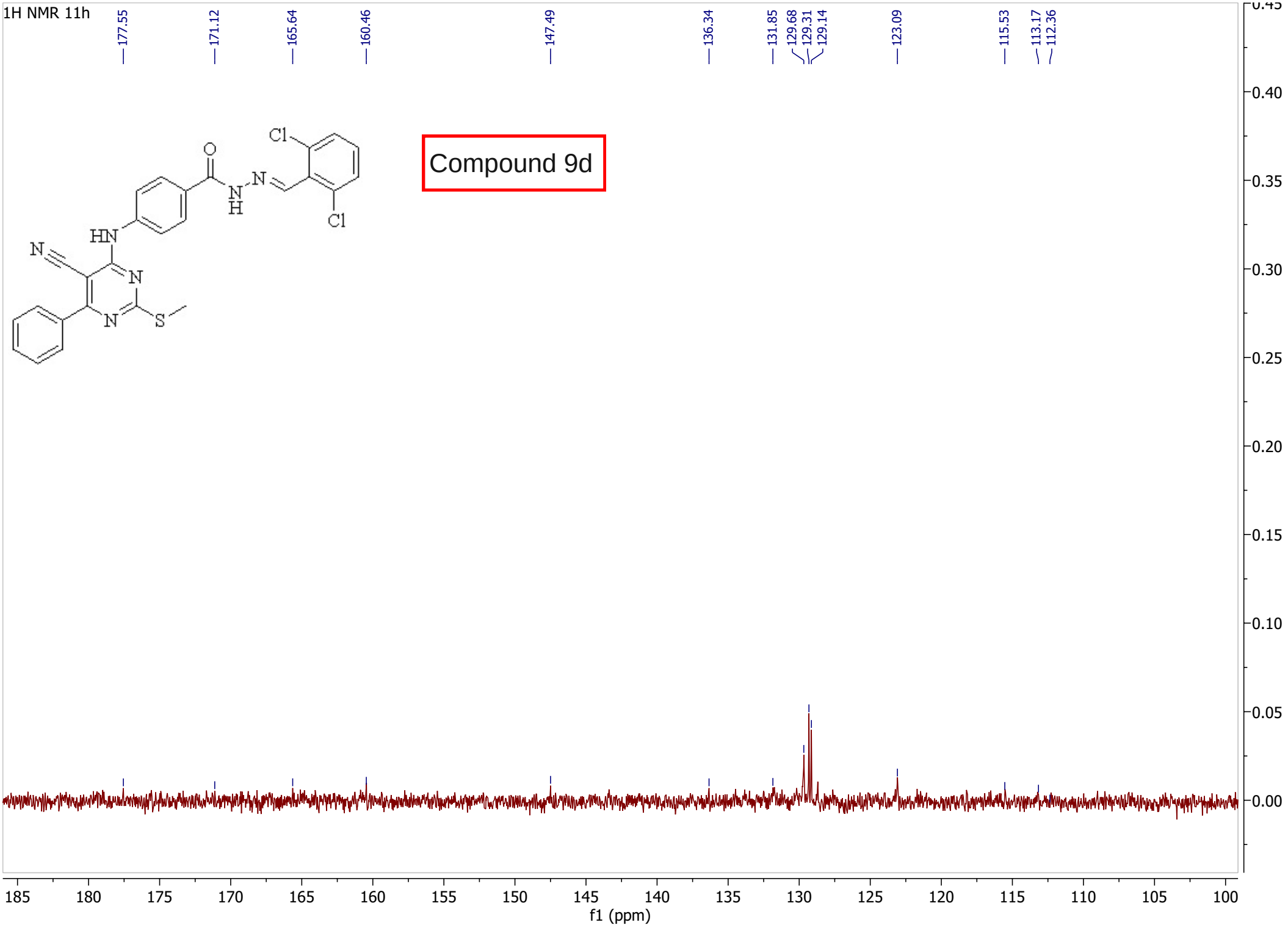
0.81

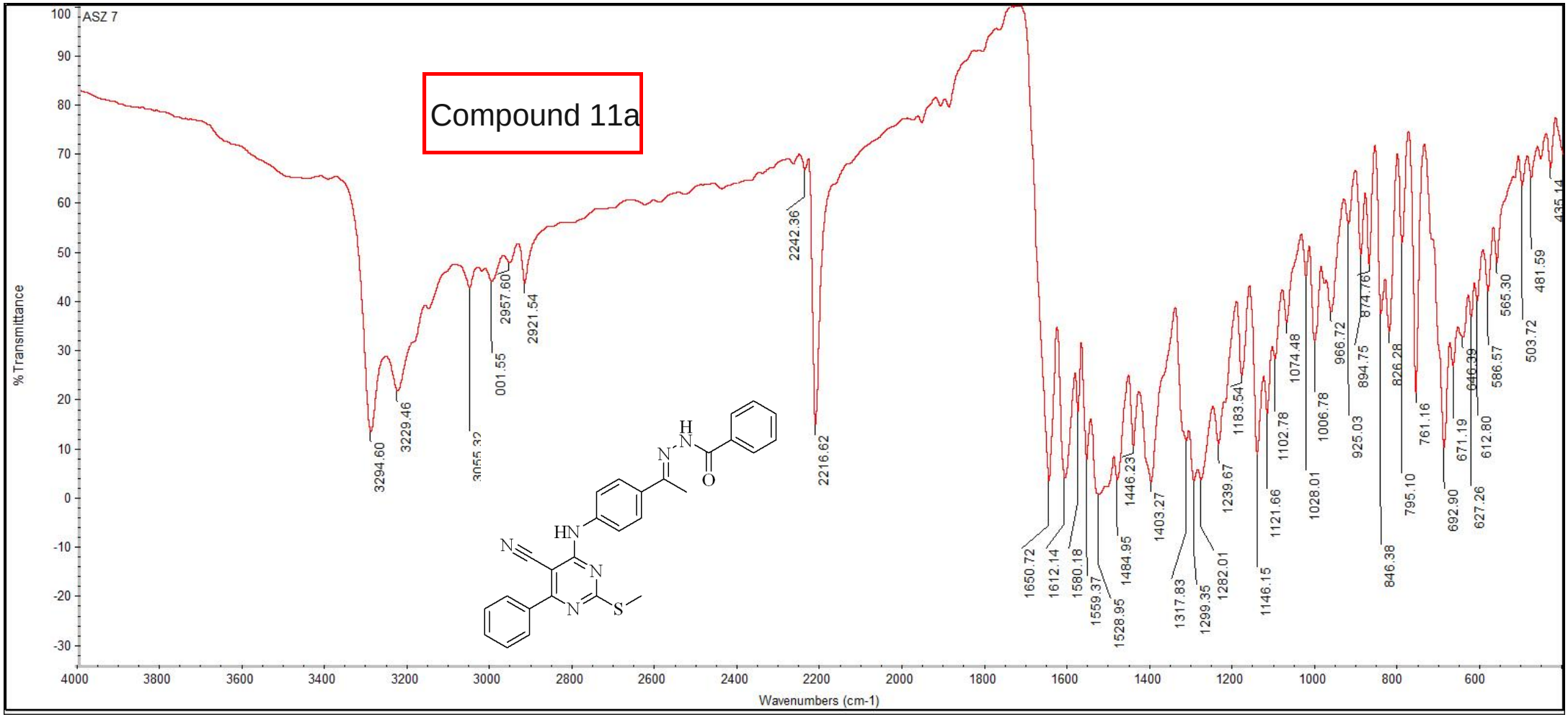
0.96

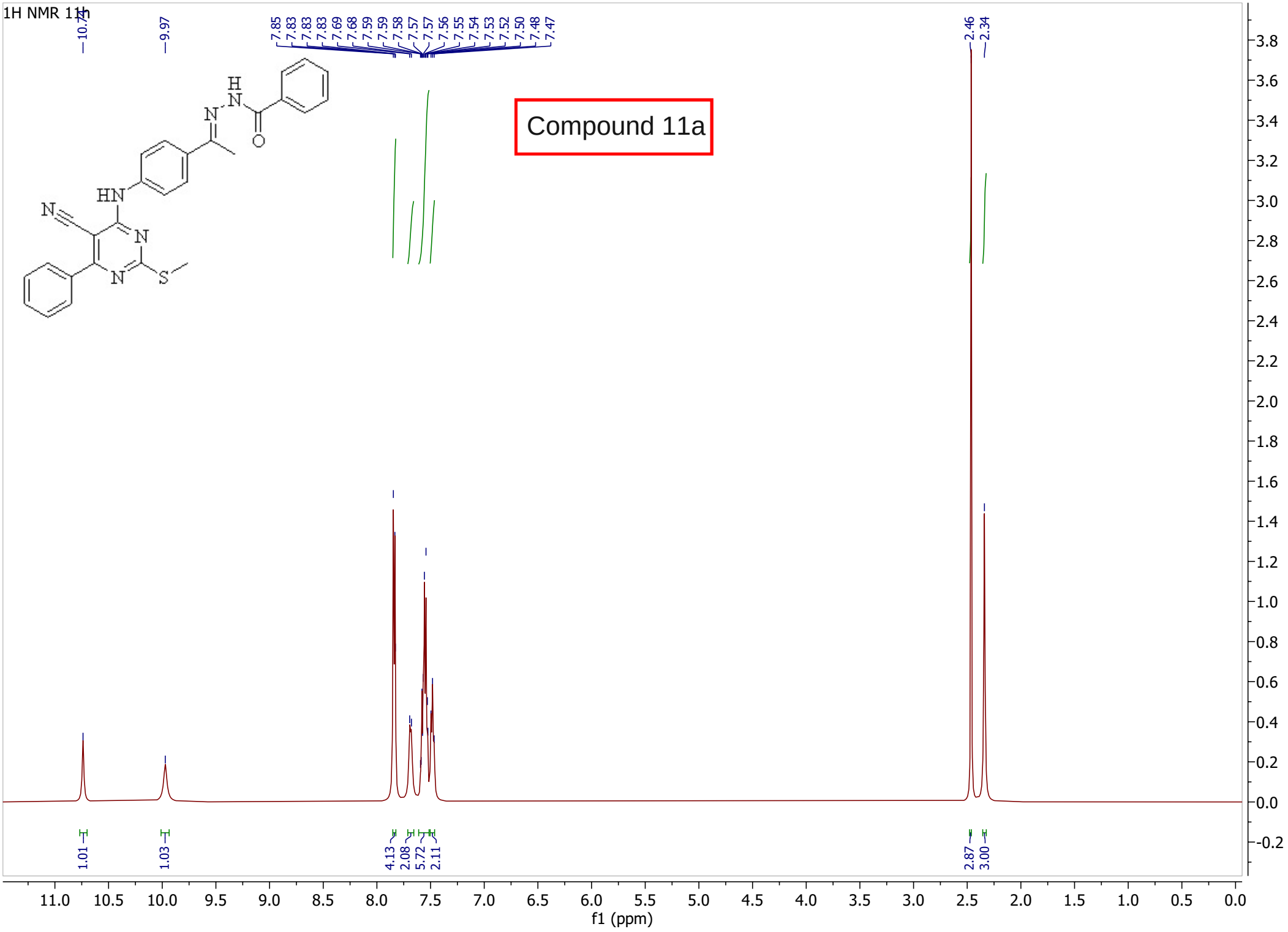
f1 (ppm)

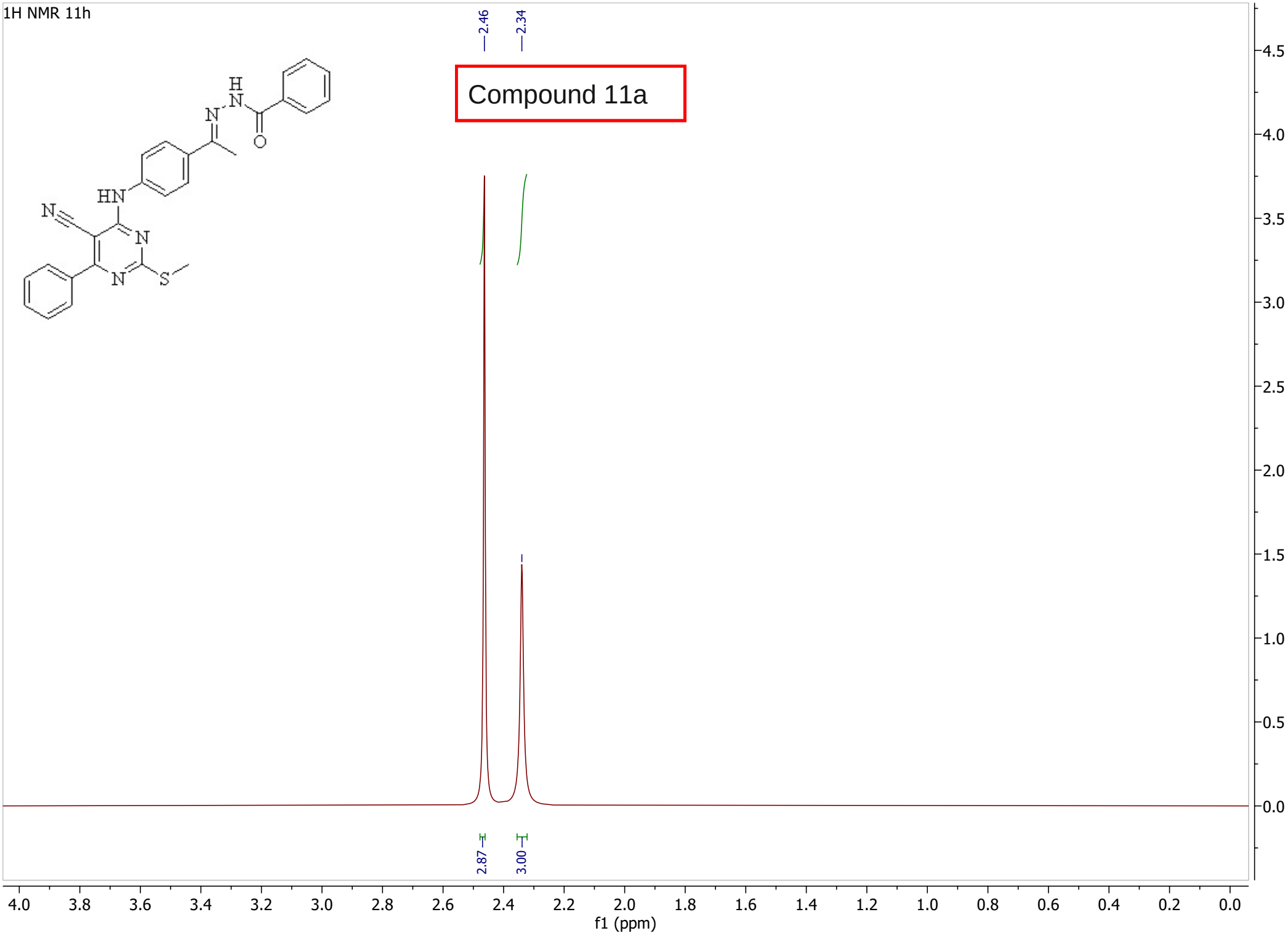

1H NMR 1h
177.55
171.12
165.64
160.46
147.49
136.34
131.85
129.68
129.31
129.14
123.09
115.53
113.17
112.36
81.83
14.38
Compound 9d
Cl
Cl
O
N
N
H
HN
N
N
N
S
0.26
0.24
0.22
0.20
0.18
0.16
0.14
0.12
0.10
0.08
0.06
0.04
0.02
0.00
-0.02
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

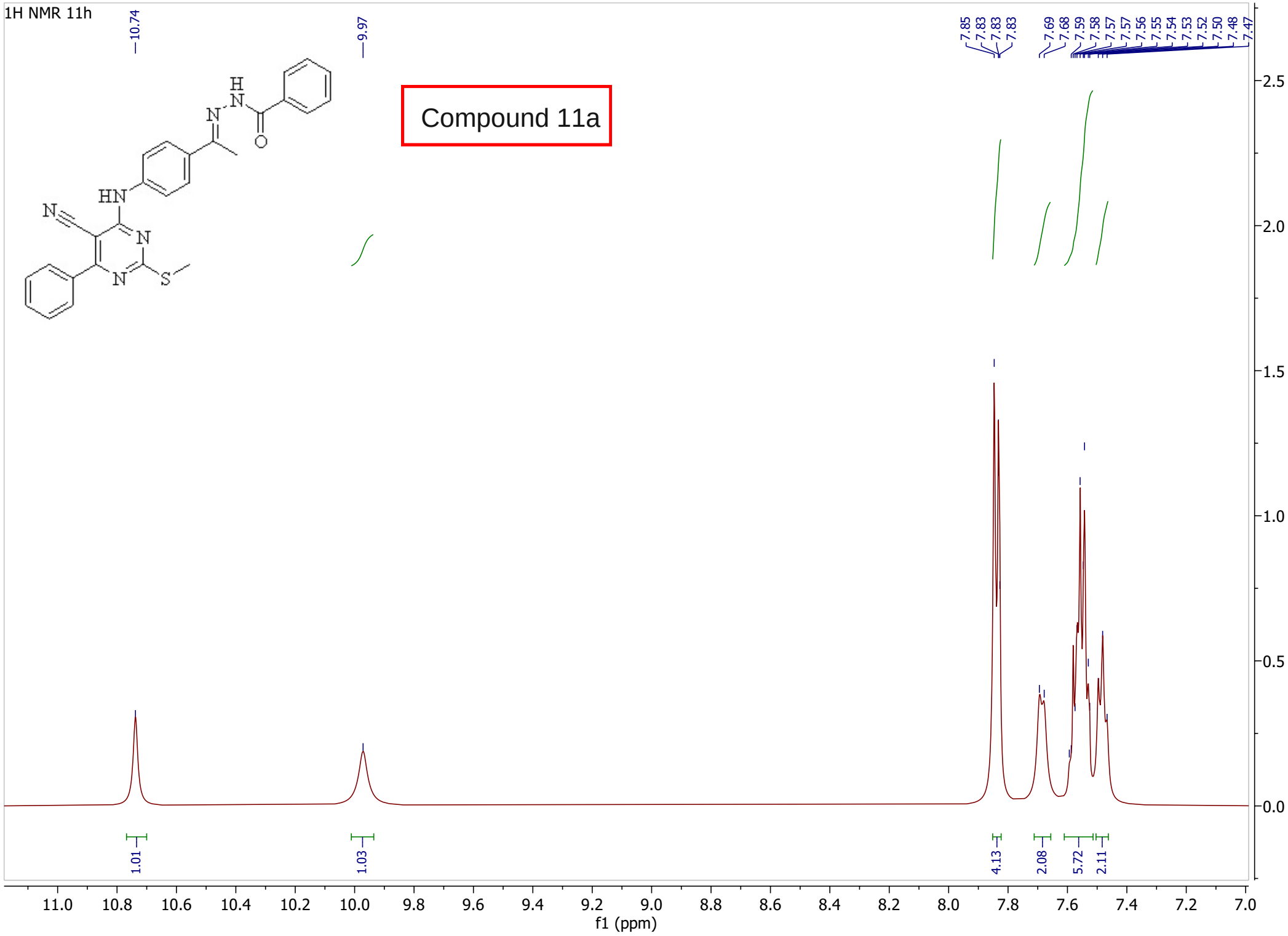

1H NMR 11h
81.83
14.38
Compound 9d
Cl
Cl
O
N
N
H
HN
N
N
N
S
0.40
0.35
0.30
0.25
0.20
0.15
0.10
0.05
0.00
100
95
90
85
80
75
70
65
60
55
50
45
40
35
30
25
20
15
10
5
0
f1 (ppm)

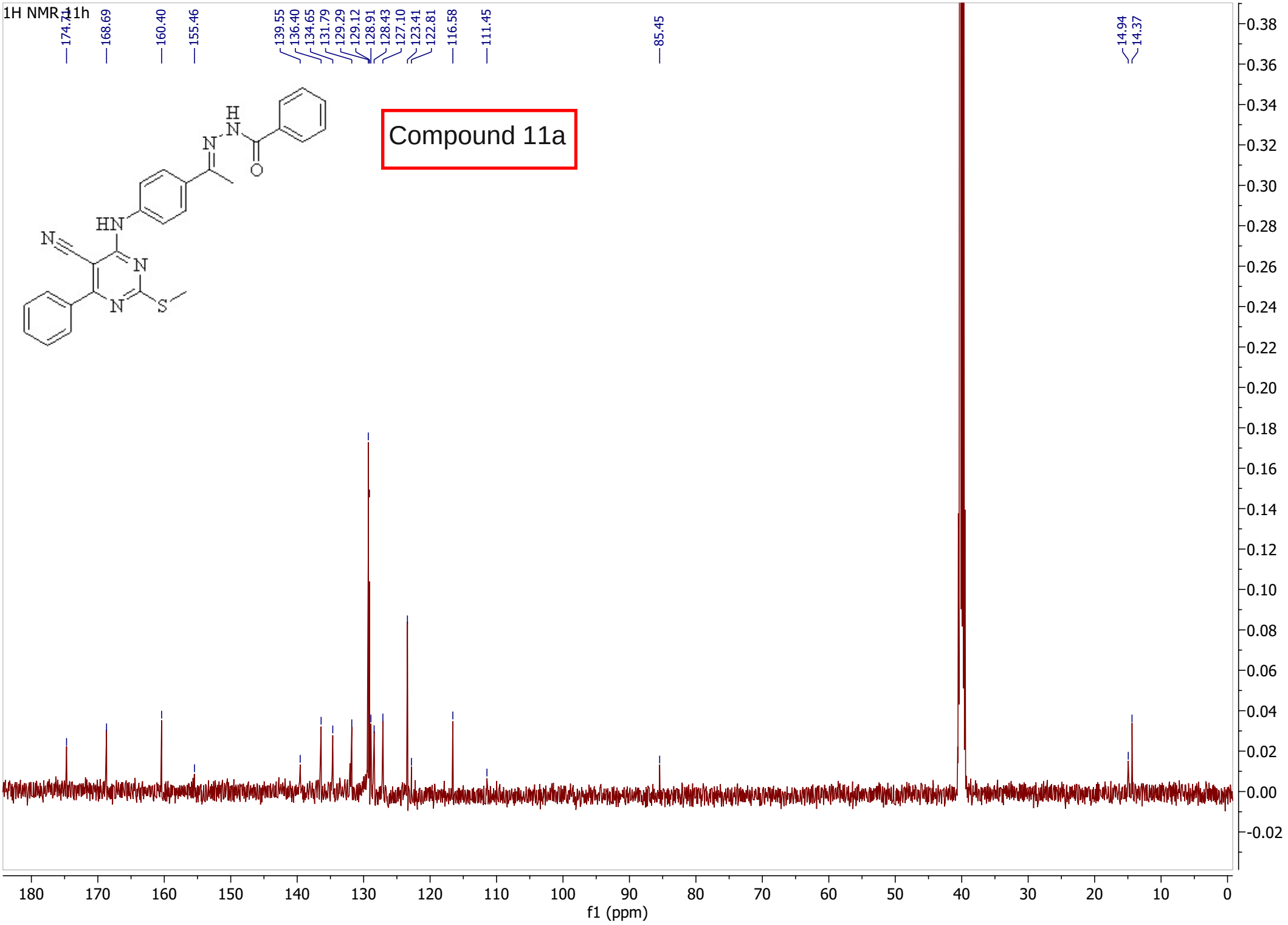

1H NMR 11h
177.55
171.12
165.64
160.46
147.49
136.34
131.85
129.68
129.31
129.14
123.09
115.53
113.17
112.36
Compound 9d
Cl
O
N
N
H
HN
N
N
S
Cl
0.40
0.35
0.30
0.25
0.20
0.15
0.10
0.05
0.00
185
180
175
170
165
160
155
150
145
140
135
130
125
120
115
110
105
100
f1 (ppm)

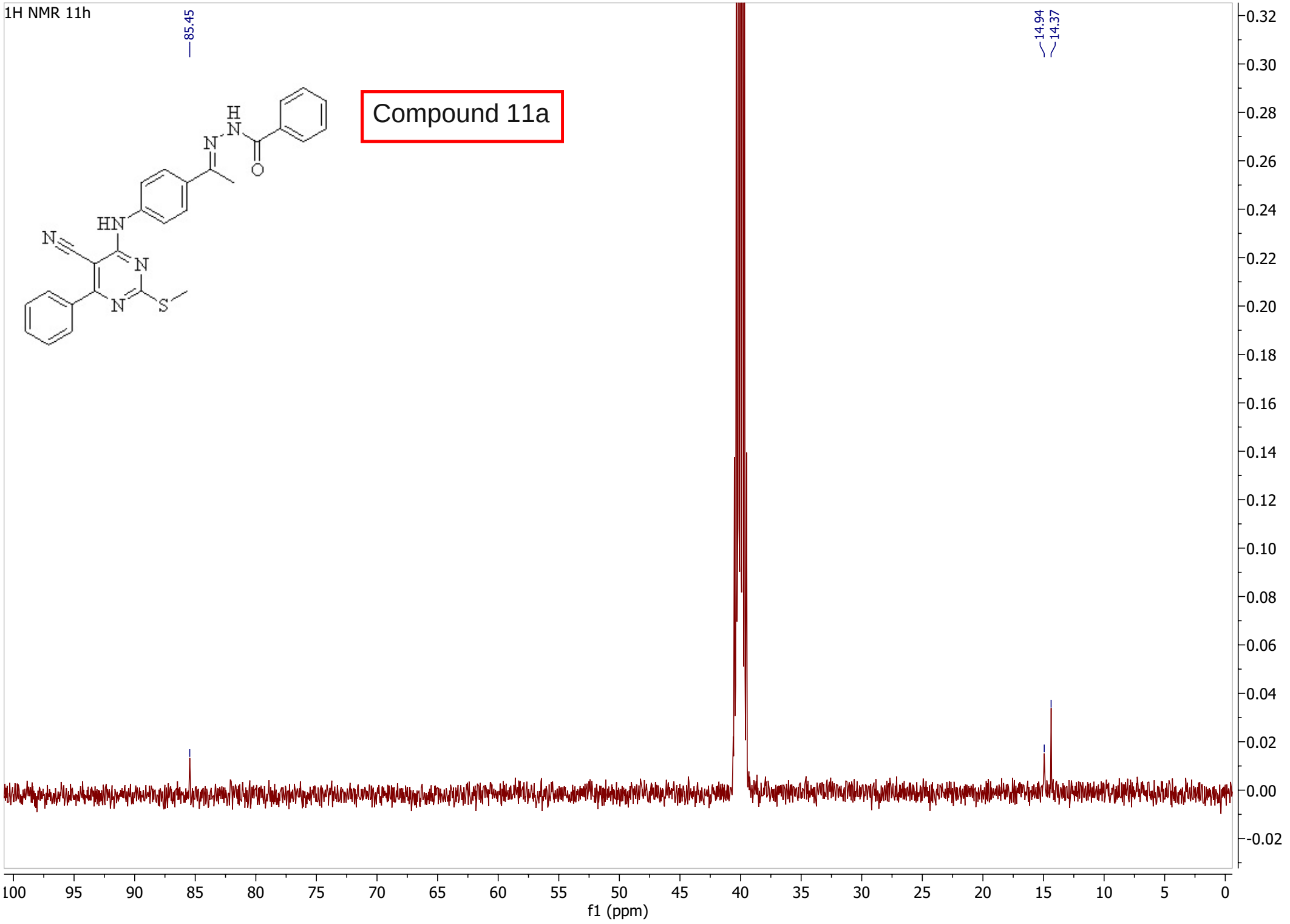

ASZ 7
Compound 11a
% Transmittance
Wavenumbers (cm-1)
3294.60
3229.46
3055.32
3001.55
2957.60
2921.54
2242.36
2216.62
1650.72
1612.14
1580.18
1559.37
1528.95
1484.95
1446.23
1403.27
1317.83
1299.35
1282.01
1239.67
1183.54
1146.15
1121.66
1102.78
1074.48
1028.01
1006.78
966.72
925.03
894.75
874.76
846.38
826.28
795.10
761.16
692.90
671.19
646.39
627.26
612.80
586.57
565.30
503.72
481.59
HN
N
O
S

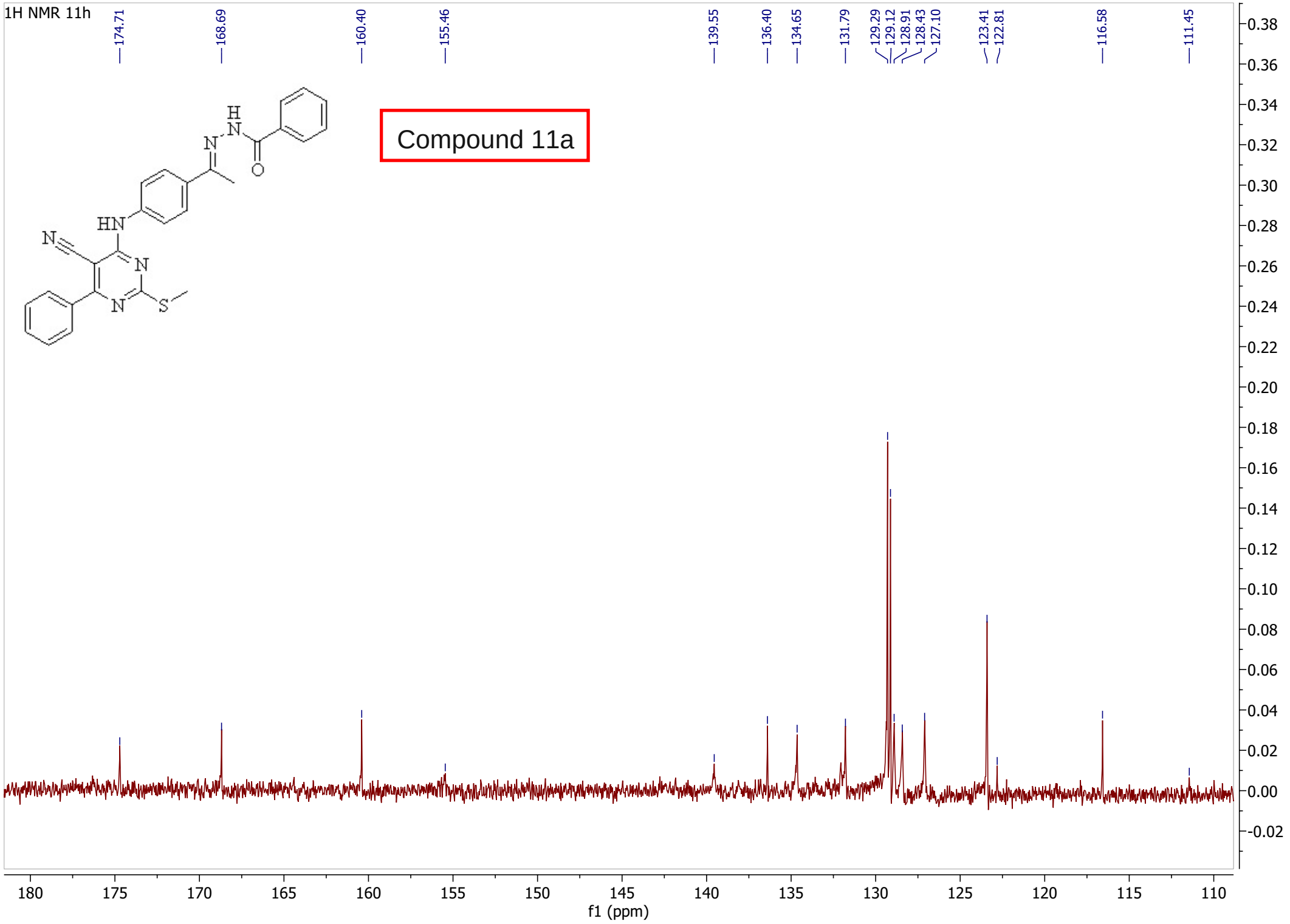

1H NMR 11h
10.77
9.97
7.85
7.83
7.83
7.83
7.69
7.68
7.59
7.59
7.58
7.57
7.57
7.56
7.55
7.54
7.53
7.52
7.50
7.48
7.47
2.46
2.34
Compound 11a
1.01
1.03
4.13
2.08
5.72
2.11
2.87
3.00
f1 (ppm)


1H NMR 11h
2.46
2.34
Compound 11a
2.87
3.00
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
4.0 3.8 3.6 3.4 3.2 3.0 2.8 2.6 2.4 2.2 2.0 1.8 1.6 1.4 1.2 1.0 0.8 0.6 0.4 0.2 0.0
f1 (ppm)


1H NMR 11h
Compound 11a
10.74
9.97
7.85
7.83
7.83
7.83
7.69
7.68
7.59
7.58
7.57
7.57
7.56
7.55
7.54
7.53
7.52
7.50
7.48
7.47
1.01
1.03
4.13
2.08
5.72
2.11
f1 (ppm)

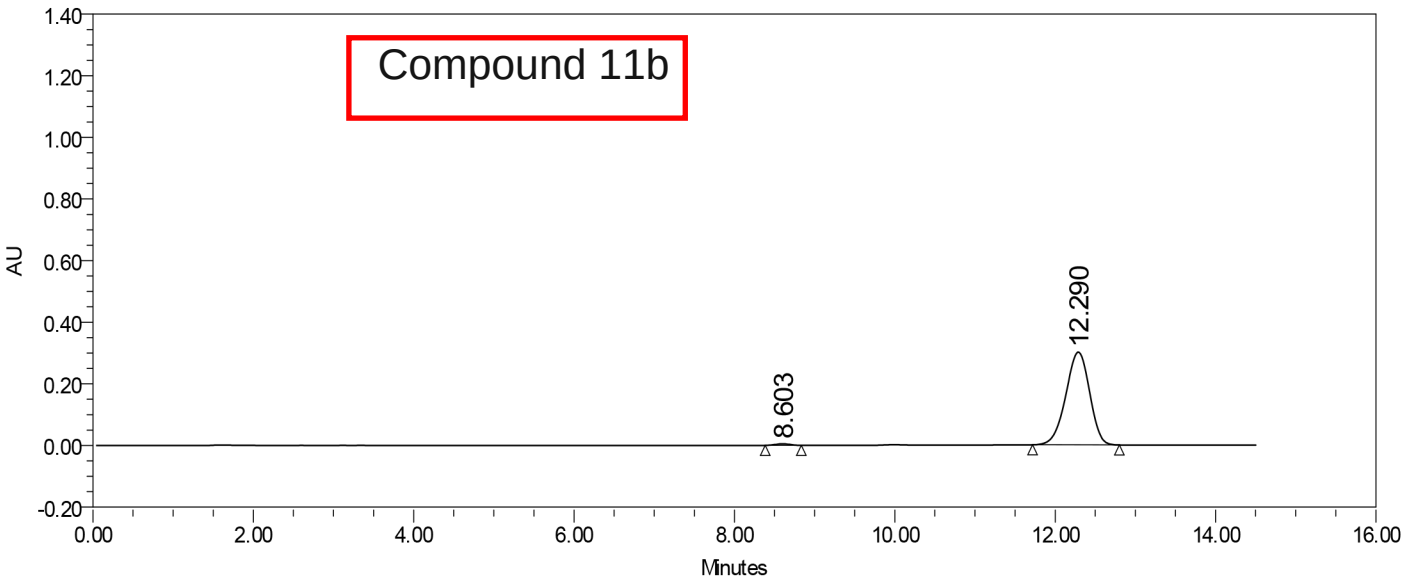

1H NMR 11h
174.71
168.69
160.40
155.46
139.55
136.40
134.65
131.79
129.29
129.12
128.91
128.43
127.10
123.41
122.81
116.58
111.45
85.45
14.94
14.37
Compound 11a
f1 (ppm)


1H NMR 11h
85.45
14.94
14.37
Compound 11a
f1 (ppm)


1H NMR 11h
174.71
168.69
160.40
155.46
139.55
136.40
134.65
131.79
129.29
129.12
128.91
128.43
127.10
123.41
122.81
116.58
111.45
Compound 11a
0.38
0.36
0.34
0.32
0.30
0.28
0.26
0.24
0.22
0.20
0.18
0.16
0.14
0.12
0.10
0.08
0.06
0.04
0.02
0.00
-0.02
180
175
170
165
160
155
150
145
140
135
130
125
120
115
110
f1 (ppm)

SAMPLE INFORMATION

Sample Name:	ASZ3 Compound 11b	Acquired By:	System
Sample Type:	Unknown	Sample Set Name:	1
Vial:	6	Acq. Method Set:	Organic
Injection #:	1	Processing Method:	Default
Injection Volume:	2.00 ul	Channel Name:	278.9nm
Run Time:	14.5 Minutes	Proc. Chnl. Descr.:	W2996 PDA 278.9 nm (PDA 190.0 to
Date Acquired:	11/5/2022 11:30:47 PM EET		
Date Processed:	11/6/2022 5:22:27 AM EET		



	RT	Area	% Area	Height
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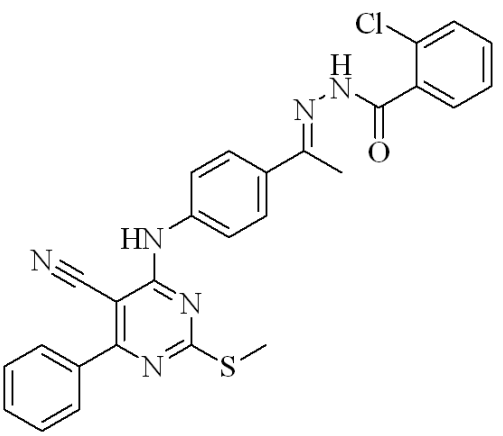
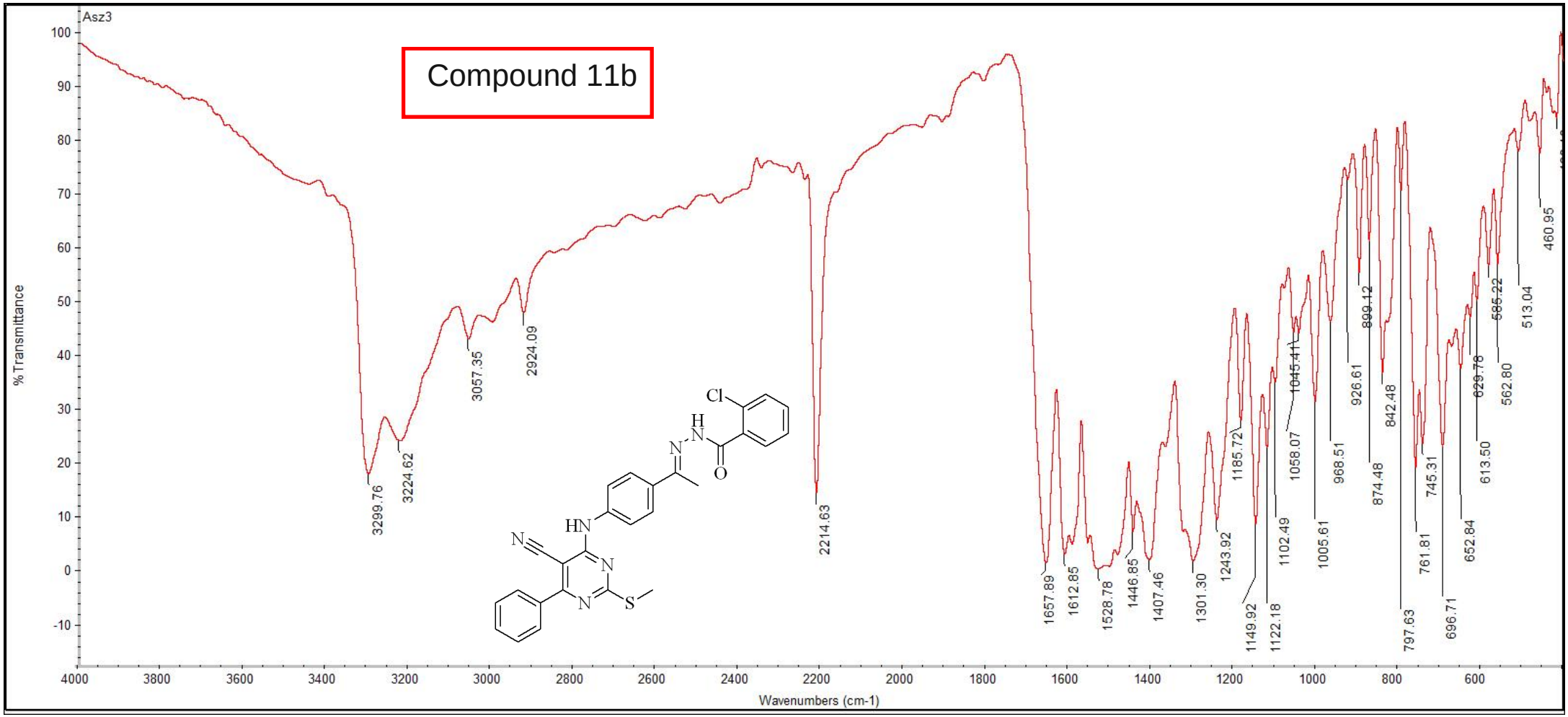
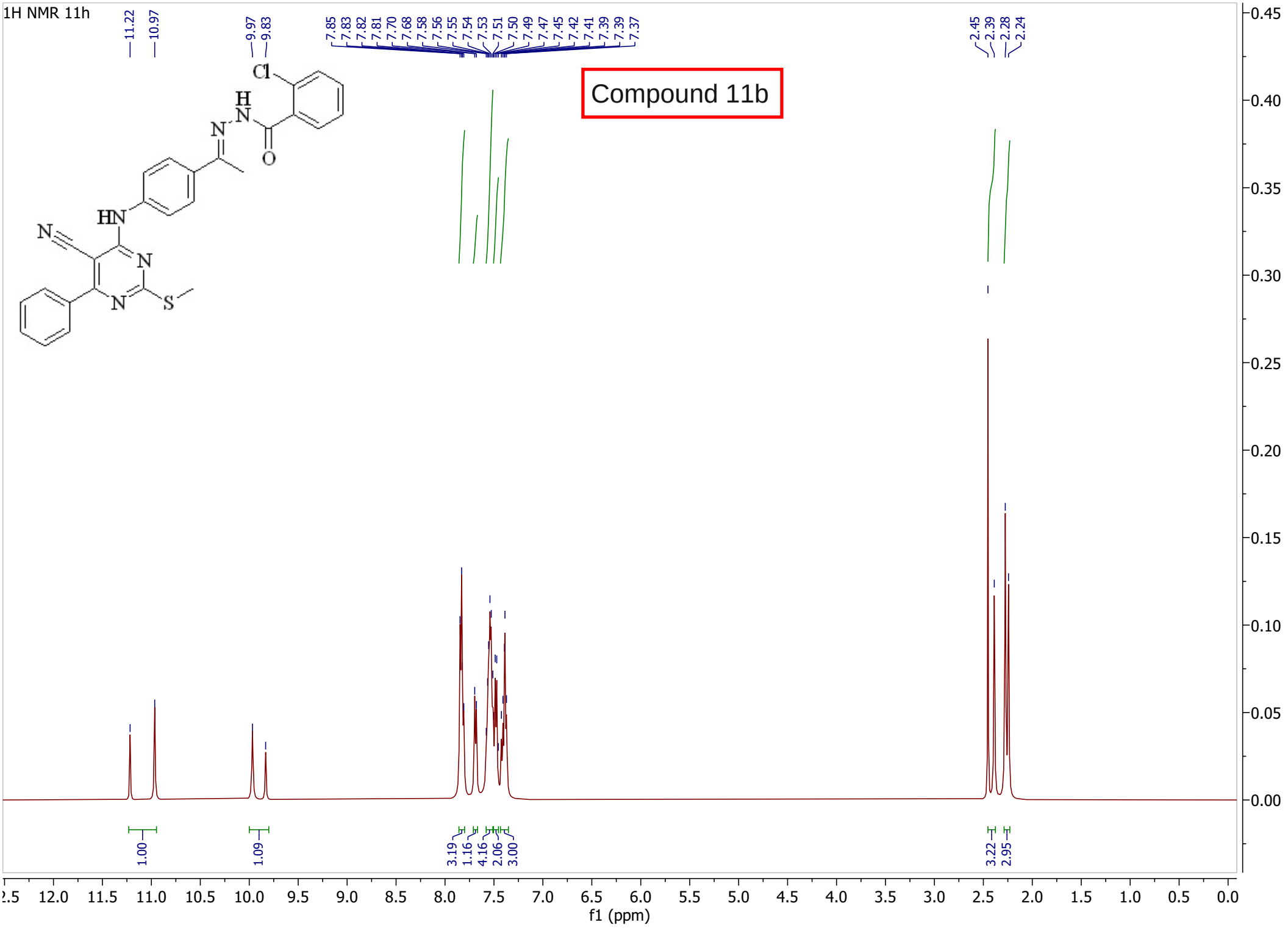
2	12.290	6208543	99.01	301317




Asz3
Compound 11b
% Transmittance
Wavenumbers (cm-1)
3299.76
3224.62
3057.35
2924.09
2214.63
1657.89
1612.85
1528.78
1446.85
1407.46
1301.30
1243.92
1185.72
1149.92
1122.18
1102.49
1058.07
1045.41
1005.61
968.51
926.61
899.12
874.48
842.48
797.63
761.81
745.31
696.71
652.84
629.78
613.50
585.22
562.80
513.04
460.95
Cl
H
N
O
HN
N
S


1H NMR 11h
Compound 11b
11.22
10.97
9.97
9.83
7.85
7.83
7.82
7.81
7.70
7.68
7.58
7.56
7.55
7.54
7.53
7.51
7.50
7.49
7.47
7.45
7.42
7.41
7.39
7.39
7.37
2.45
2.39
2.28
2.24
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1.09
3.19
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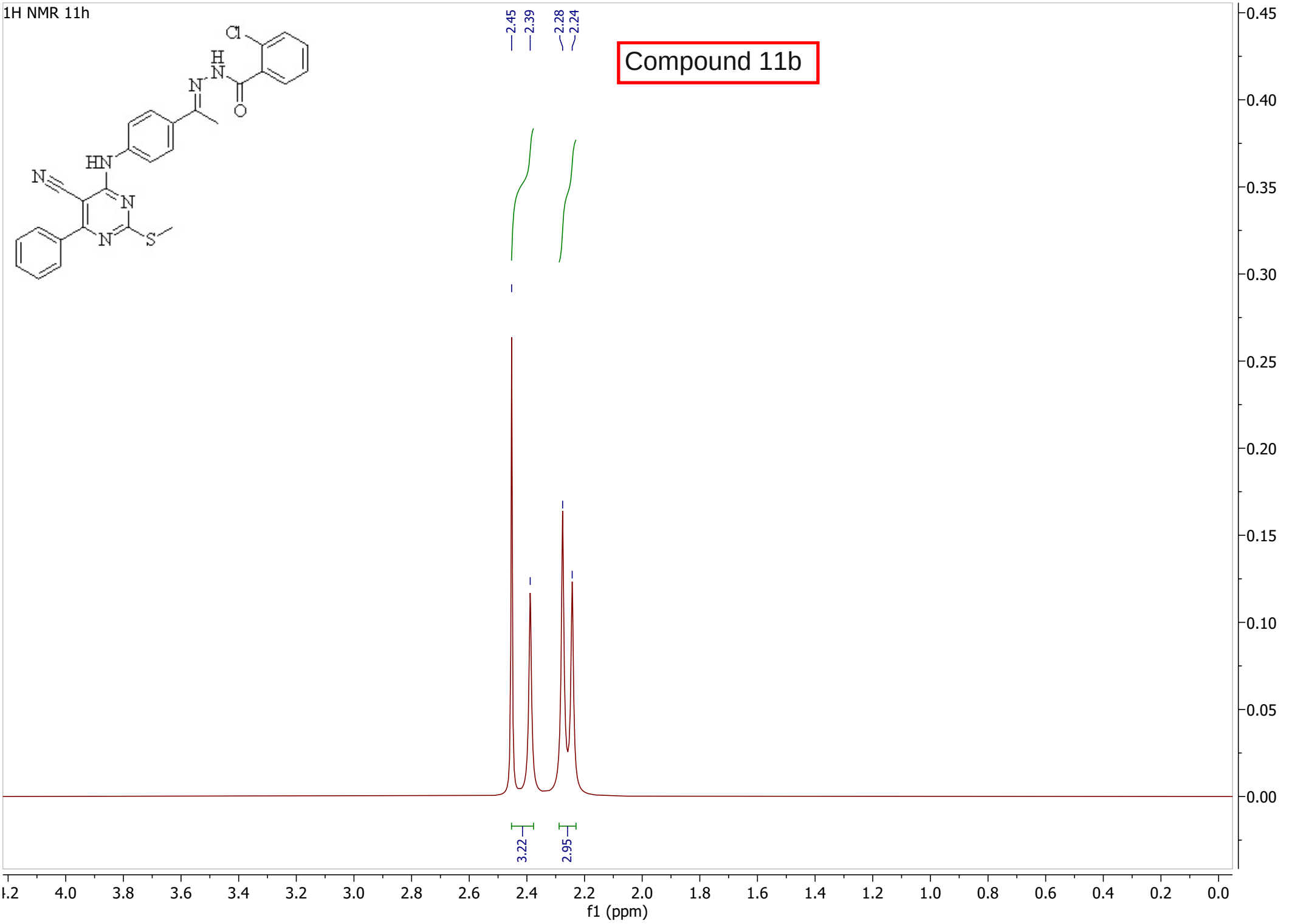
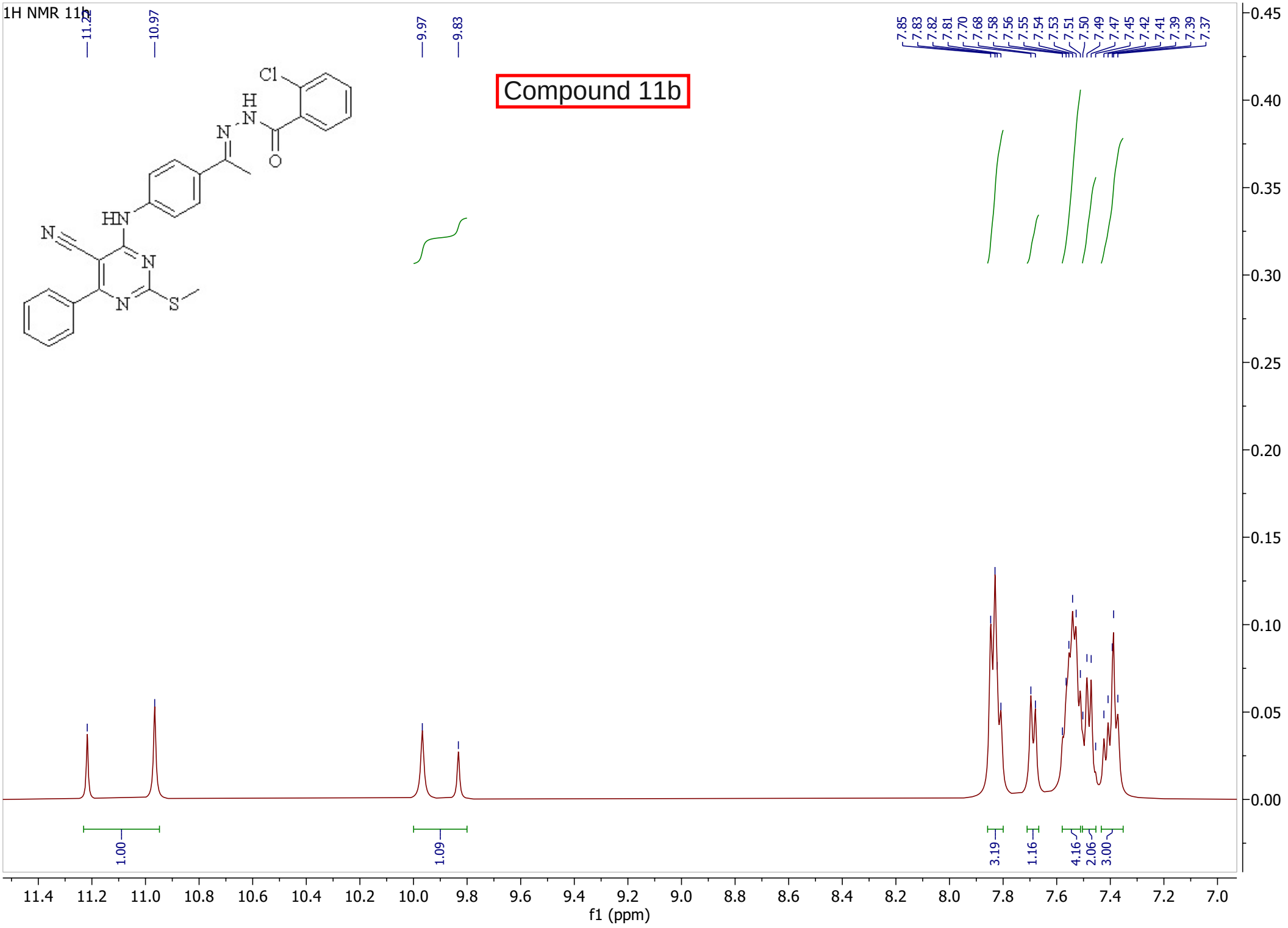
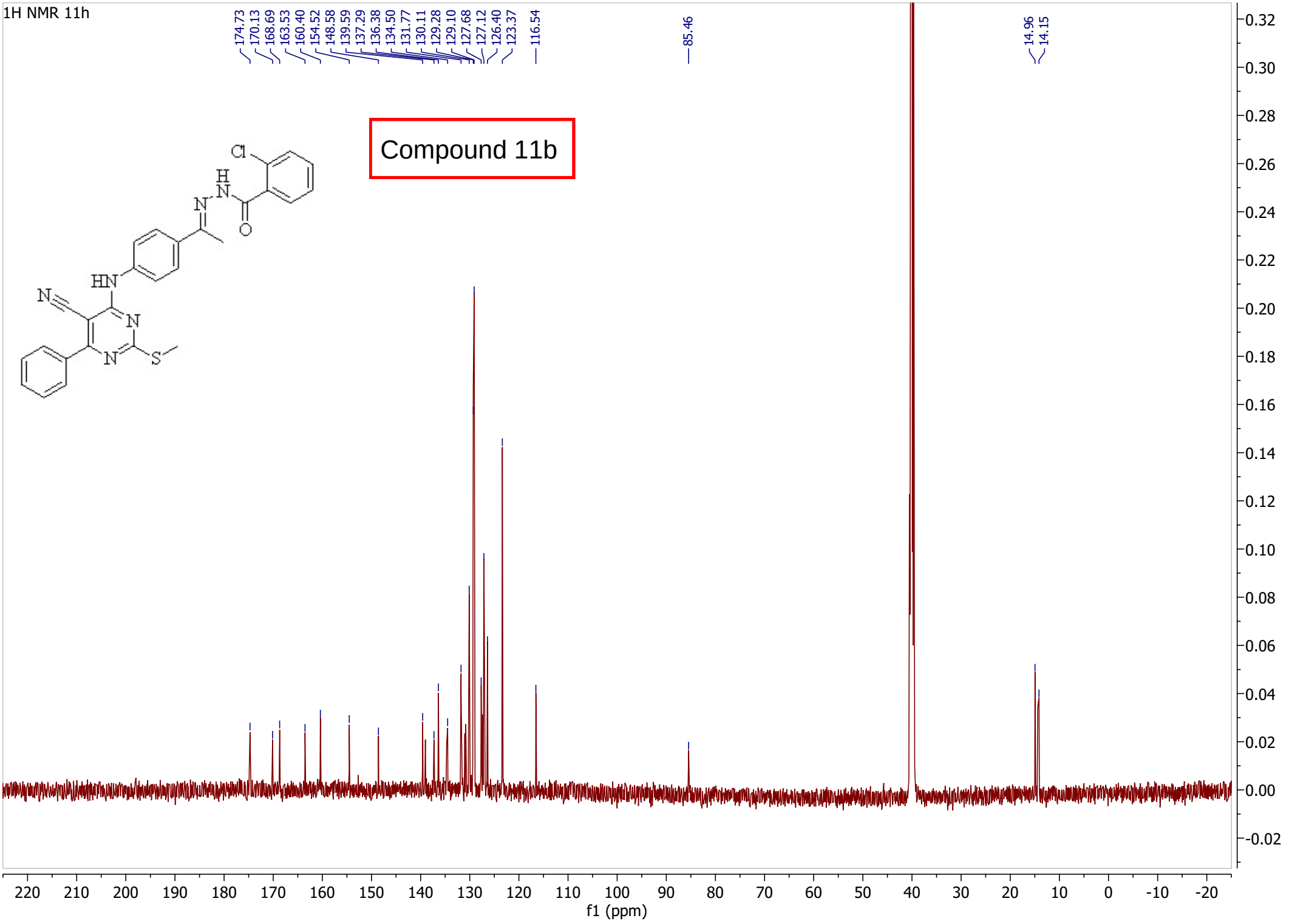
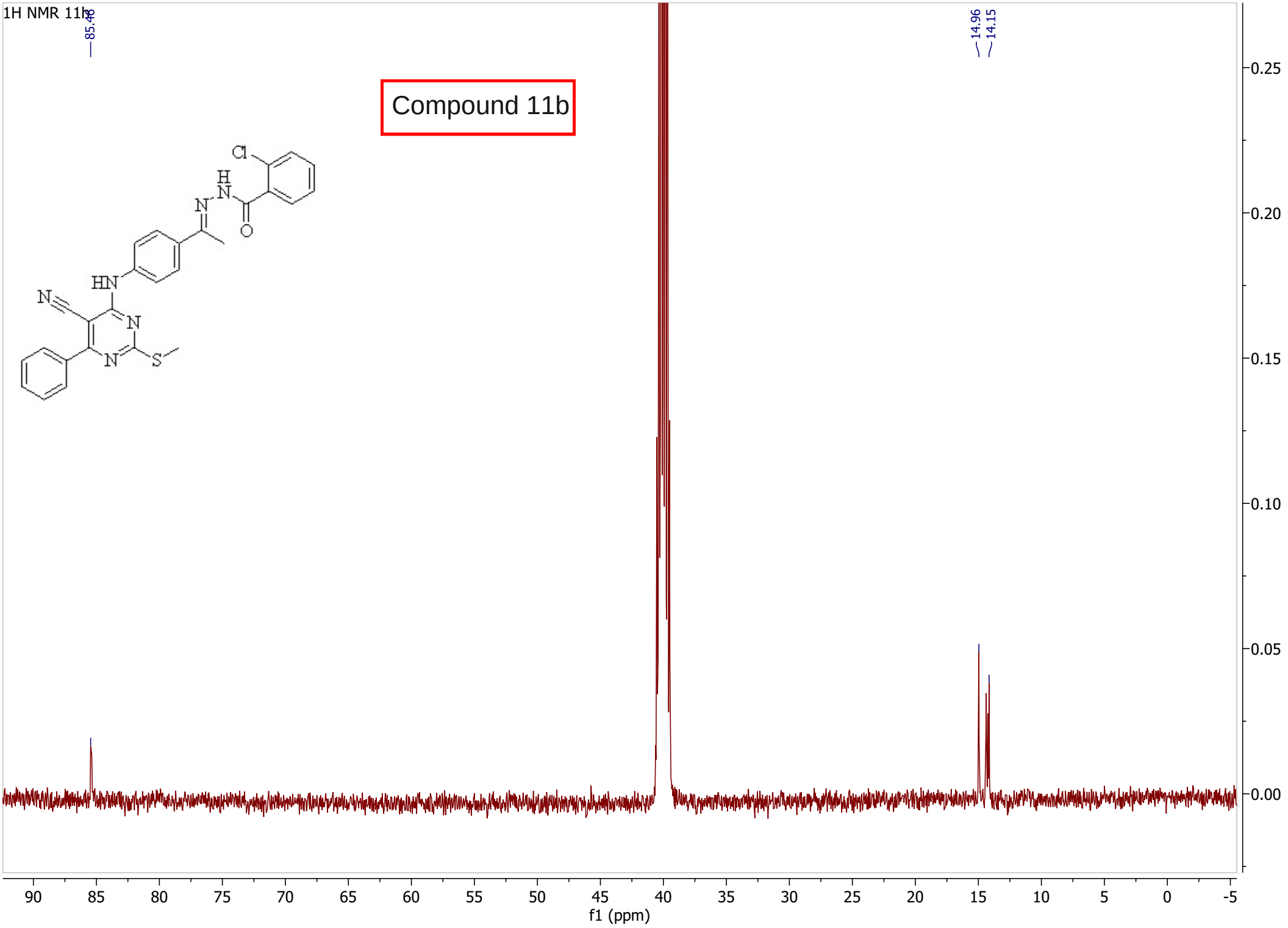
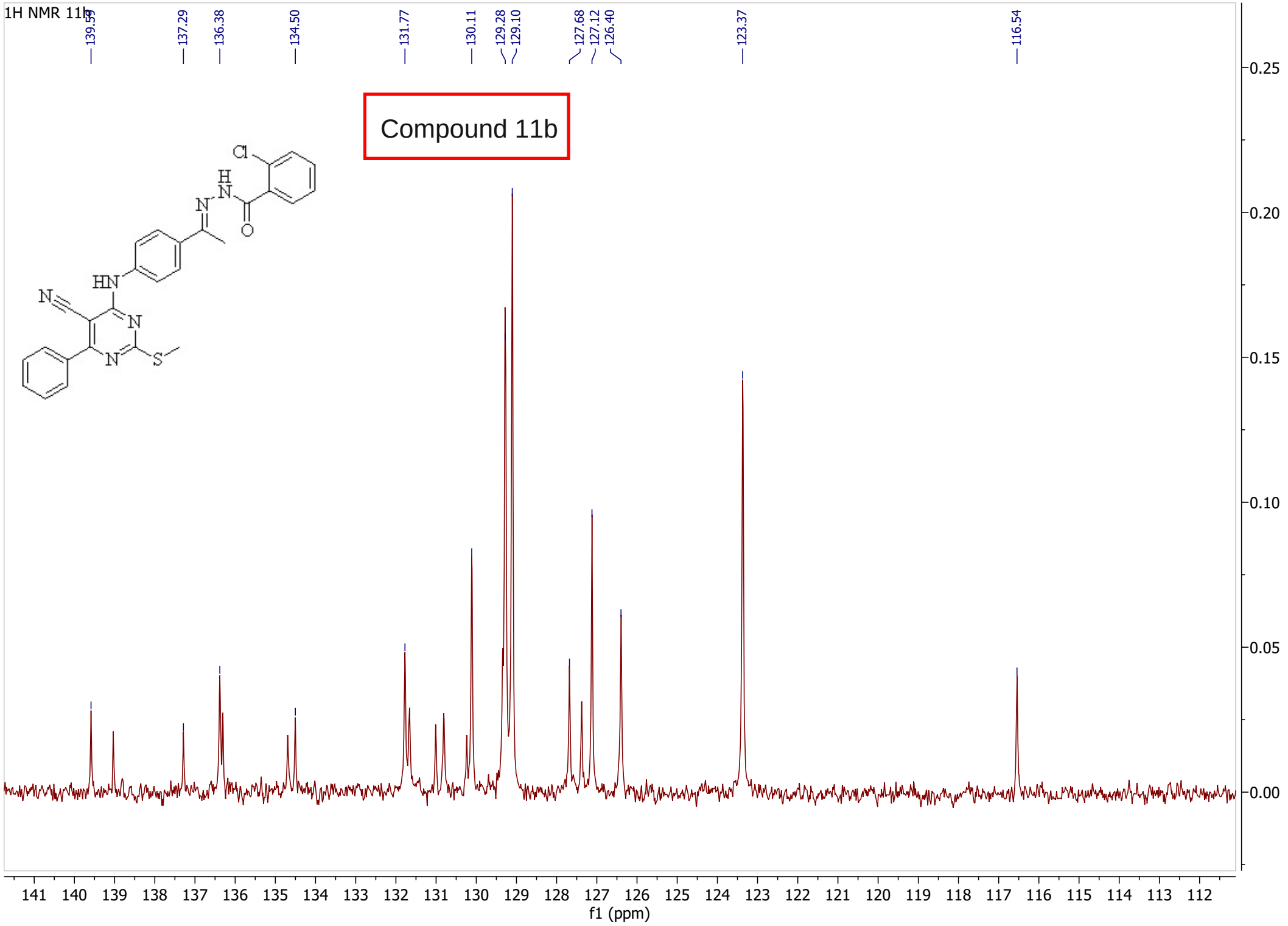
4.16
2.06
3.00
3.22
2.95
f1 (ppm)

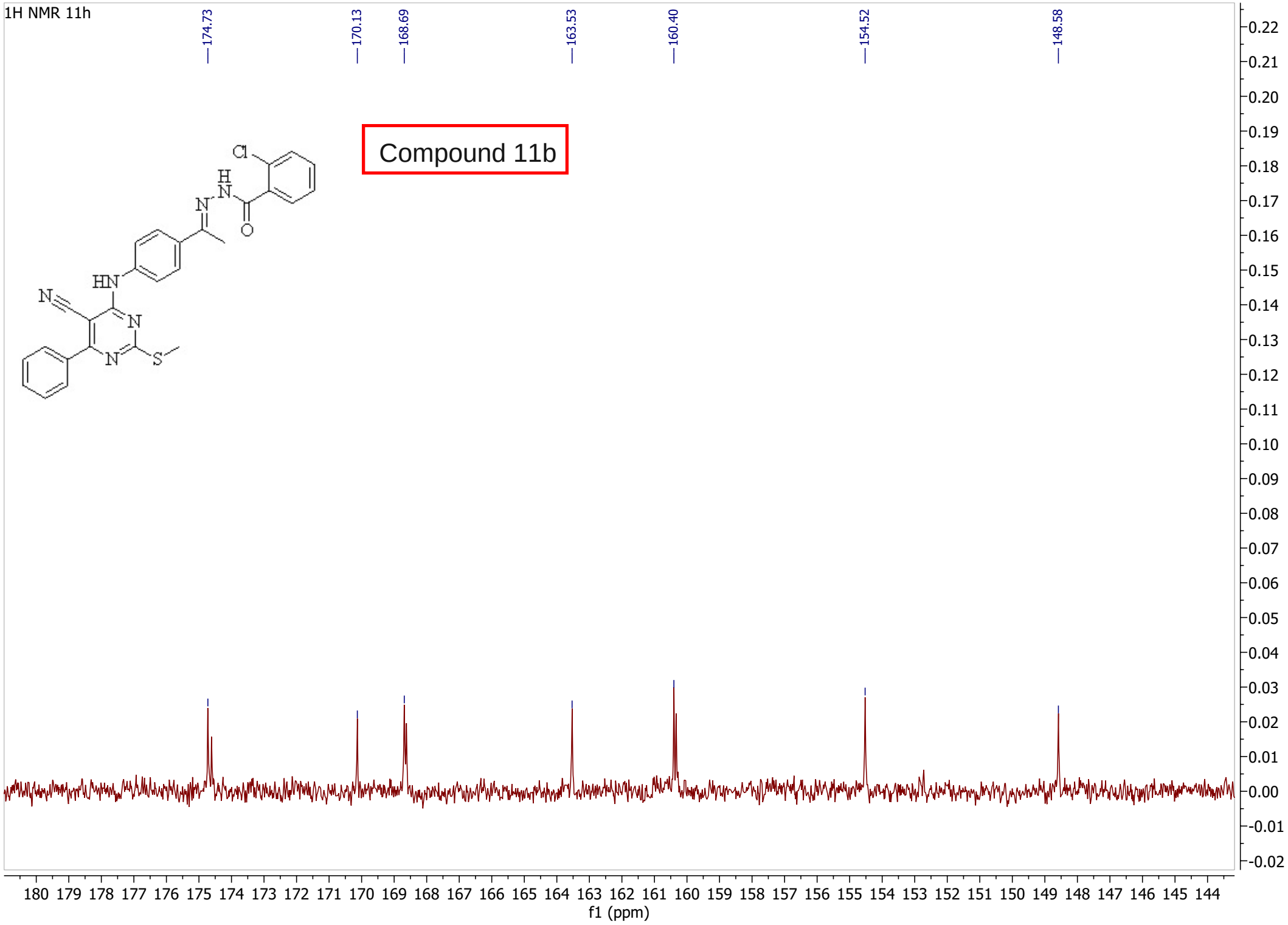

1H NMR 11h
Compound 11b
2.45
2.39
2.28
2.24
3.22
2.95
f1 (ppm)

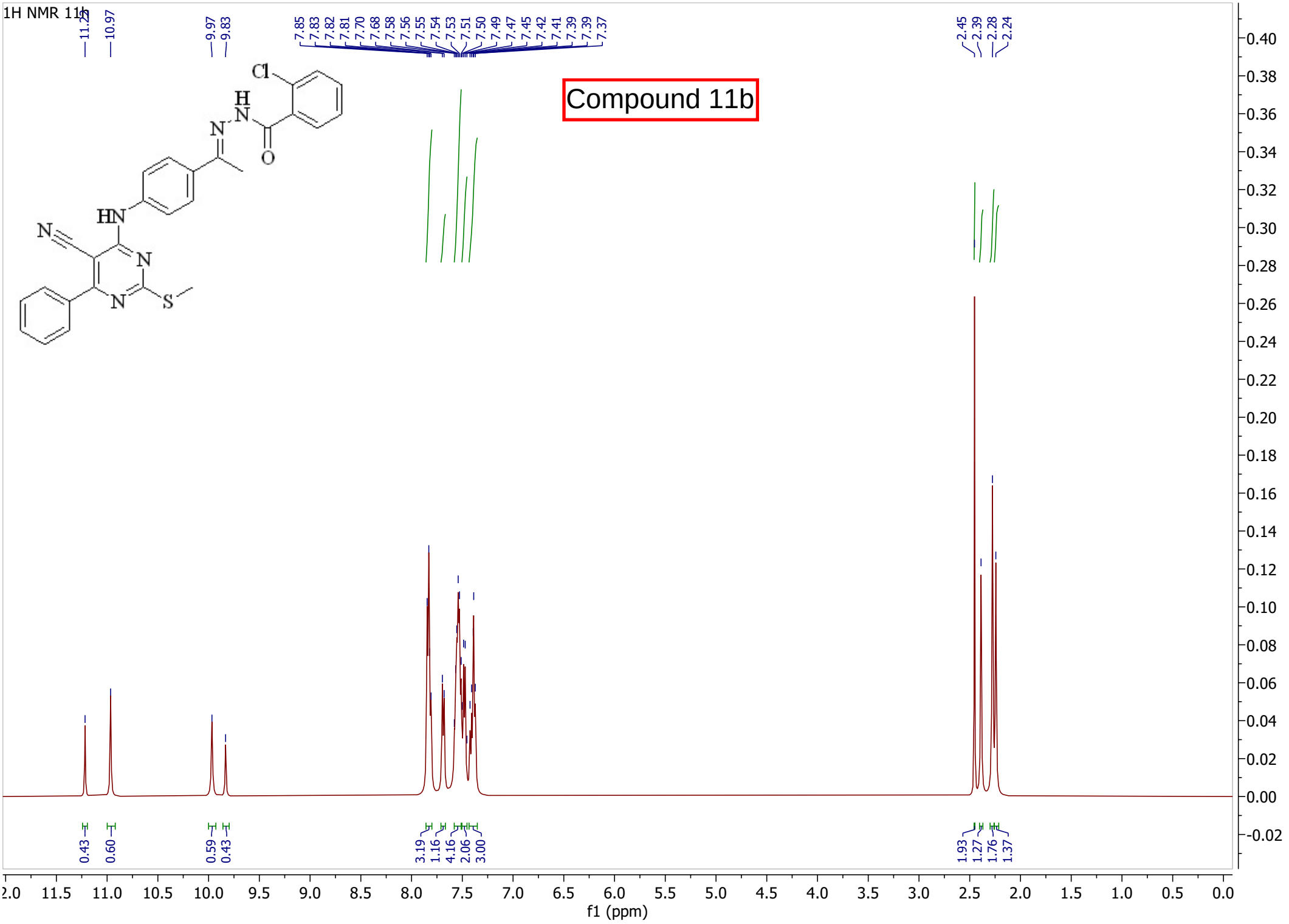

1H NMR 11b
Compound 11b
11.22
10.97
9.97
9.83
7.85
7.83
7.82
7.81
7.70
7.68
7.58
7.56
7.55
7.54
7.53
7.51
7.50
7.49
7.47
7.45
7.42
7.41
7.39
7.39
7.37
Cl
H
N
N
O
HN
N
N
N
N
S
1.00
1.09
3.19
1.16
4.16
2.06
3.00
0.45
0.40
0.35
0.30
0.25
0.20
0.15
0.10
0.05
0.00
11.4
11.2
11.0
10.8
10.6
10.4
10.2
10.0
9.8
9.6
9.4
9.2
9.0
8.8
8.6
8.4
8.2
8.0
7.8
7.6
7.4
7.2
7.0
f1 (ppm)

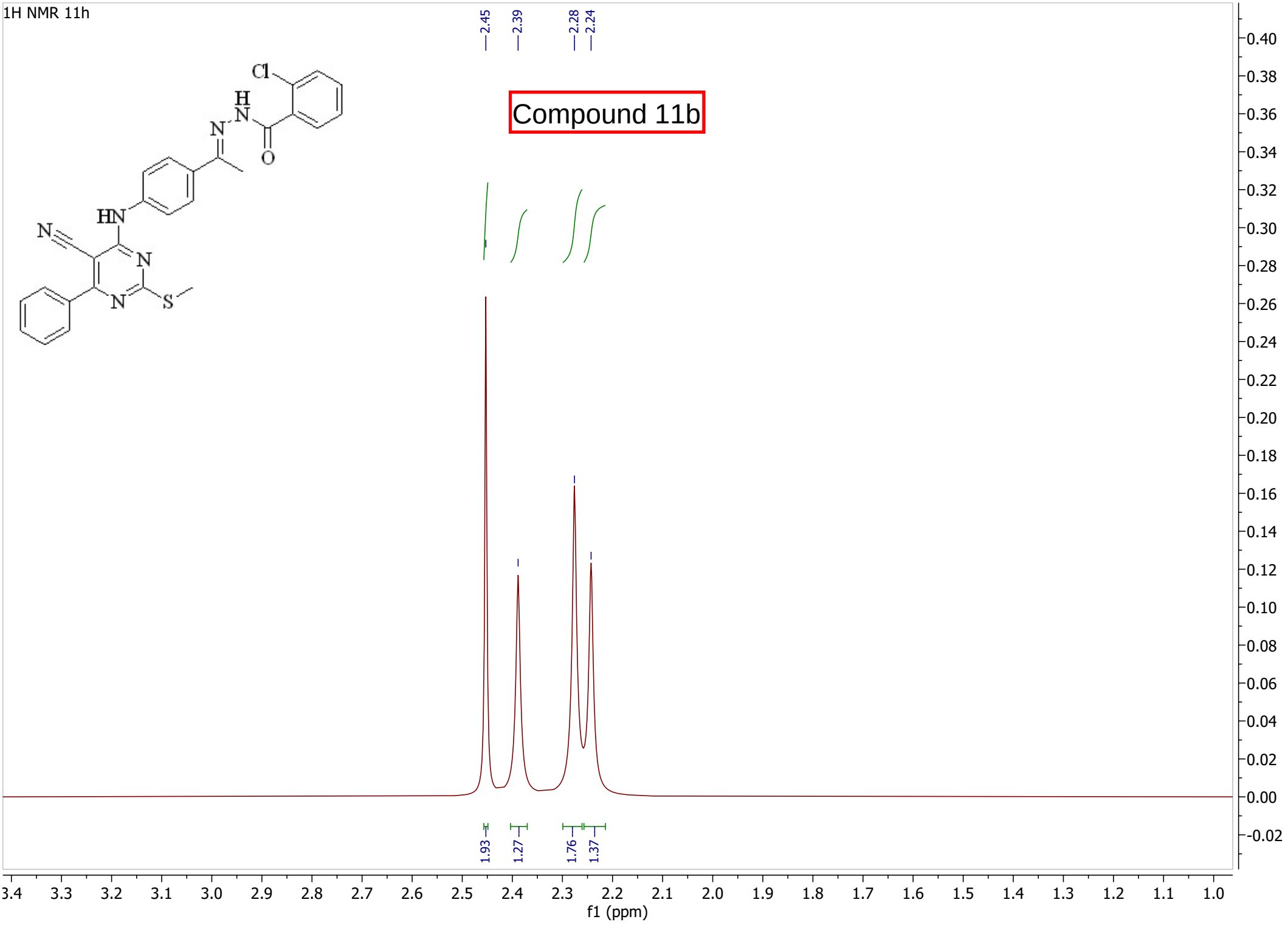

1H NMR 11h
174.73
170.13
168.69
163.53
160.40
154.52
148.58
139.59
137.29
136.38
134.50
131.77
130.11
129.28
129.10
127.68
127.12
126.40
123.37
116.54
85.46
14.96
14.15
Compound 11b
Cl
H
N
N
O
HN
N
N
N
S
0.32
0.30
0.28
0.26
0.24
0.22
0.20
0.18
0.16
0.14
0.12
0.10
0.08
0.06
0.04
0.02
0.00
-0.02
220
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
-20
f1 (ppm)

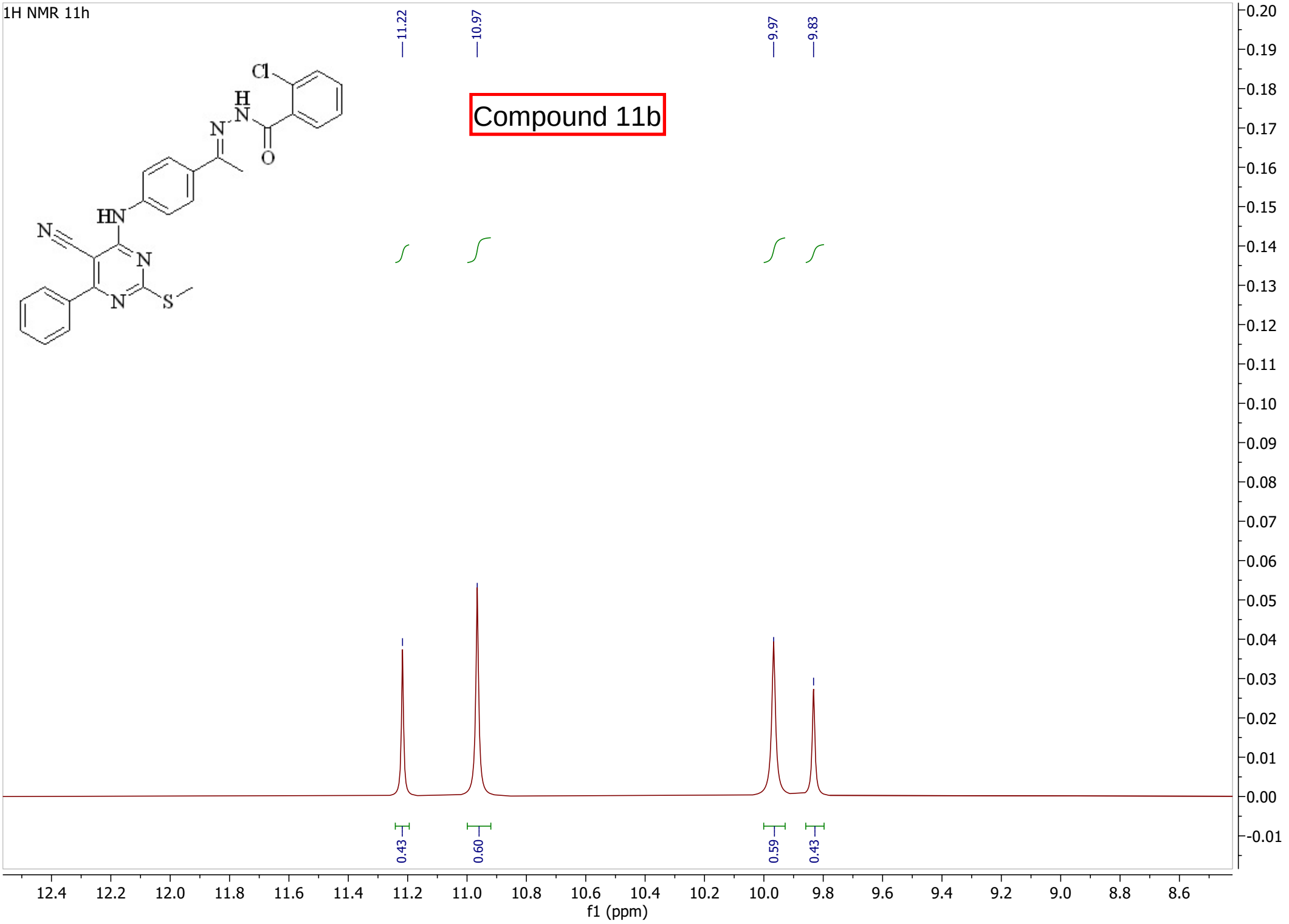

1H NMR 11b
85.46
14.96
14.15
Compound 11b
Cl
H
N
N
O
HN
N
N
N
S
0.25
0.20
0.15
0.10
0.05
0.00
90
85
80
75
70
65
60
55
50
45
40
35
30
25
20
15
10
5
0
-5
f1 (ppm)


1H NMR 11b
139.59
137.29
136.38
134.50
131.77
130.11
129.28
129.10
127.68
127.12
126.40
123.37
116.54
Compound 11b
Cl
H
N
N
O
HN
N
N
N
S
0.25
0.20
0.15
0.10
0.05
0.00
141 140 139 138 137 136 135 134 133 132 131 130 129 128 127 126 125 124 123 122 121 120 119 118 117 116 115 114 113 112
f1 (ppm)


1H NMR 11h
174.73
170.13
168.69
163.53
160.40
154.52
148.58
Compound 11b
Cl
H
N
N
O
HN
N
N
N
S
0.22
0.21
0.20
0.19
0.18
0.17
0.16
0.15
0.14
0.13
0.12
0.11
0.10
0.09
0.08
0.07
0.06
0.05
0.04
0.03
0.02
0.01
0.00
-0.01
-0.02
180 179 178 177 176 175 174 173 172 171 170 169 168 167 166 165 164 163 162 161 160 159 158 157 156 155 154 153 152 151 150 149 148 147 146 145 144
f1 (ppm)

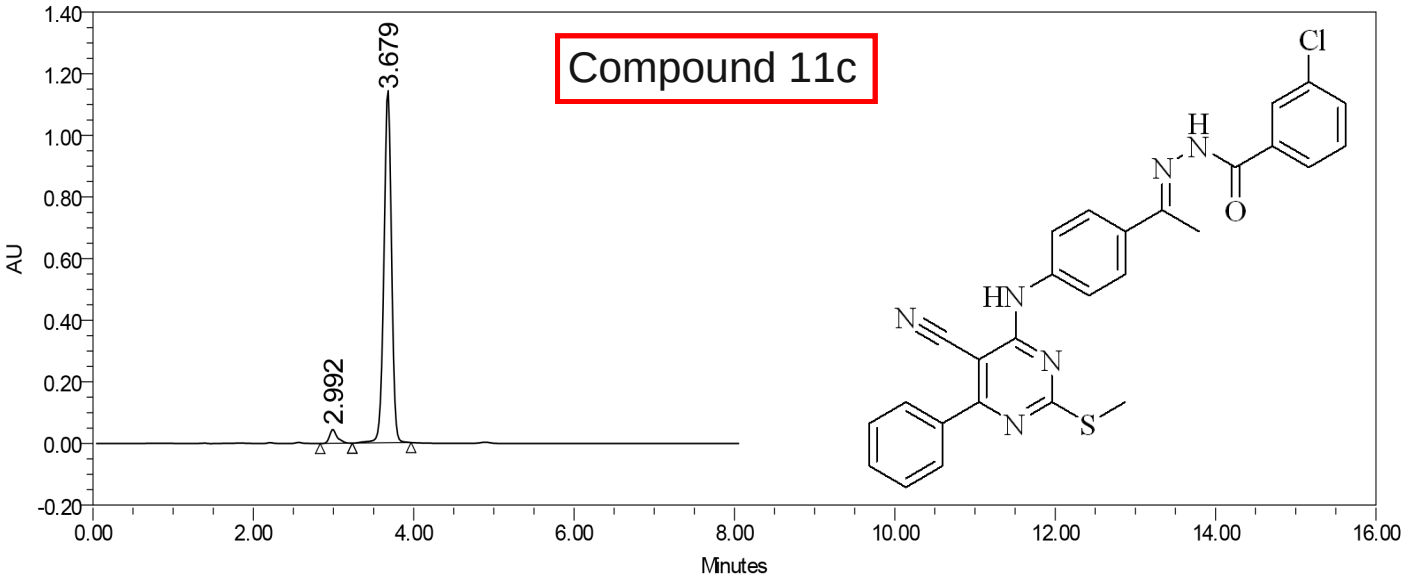

1H NMR 11b
Compound 11b
11.22
10.97
9.97
9.83
7.85
7.83
7.82
7.81
7.70
7.68
7.58
7.56
7.55
7.54
7.53
7.51
7.50
7.49
7.47
7.45
7.42
7.41
7.39
7.39
7.37
2.45
2.39
2.28
2.24
0.43
0.60
0.59
0.43
3.19
1.16
4.16
2.06
3.00
1.93
1.27
1.76
1.37
f1 (ppm)


1H NMR 11h
2.45
2.39
2.28
2.24
Compound 11b
Cl
H
N
N
O
HN
N
N
N
S
1.93
1.27
1.76
1.37
f1 (ppm)

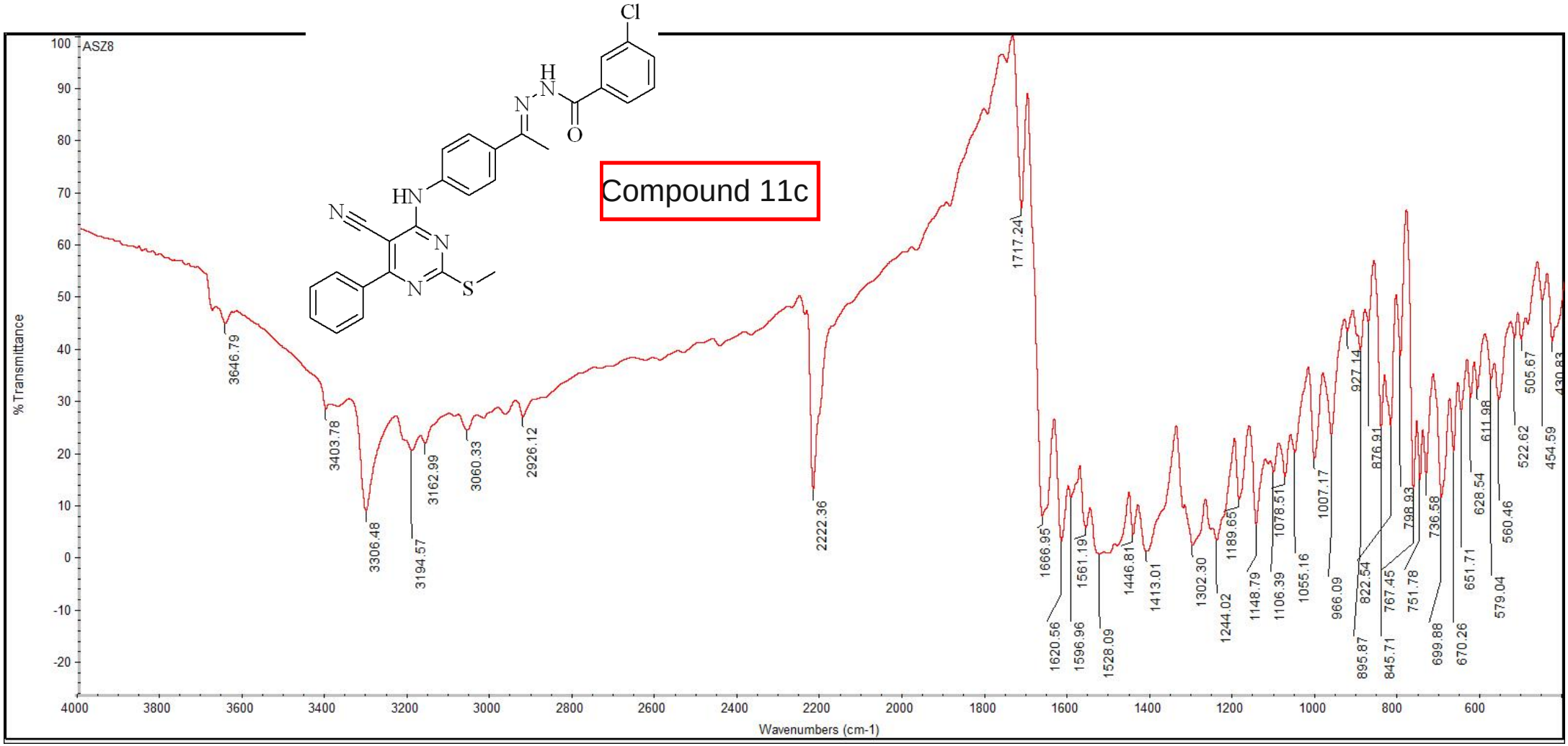

1H NMR 11h
11.22
10.97
9.97
9.83
Compound 11b
Cl
H
N
N
O
HN
N
N
N
S
0.43
0.60
0.59
0.43
12.4
12.2
12.0
11.8
11.6
11.4
11.2
11.0
10.8
10.6
10.4
10.2
10.0
9.8
9.6
9.4
9.2
9.0
8.8
8.6
f1 (ppm)
0.20
0.19
0.18
0.17
0.16
0.15
0.14
0.13
0.12
0.11
0.10
0.09
0.08
0.07
0.06
0.05
0.04
0.03
0.02
0.01
0.00
-0.01

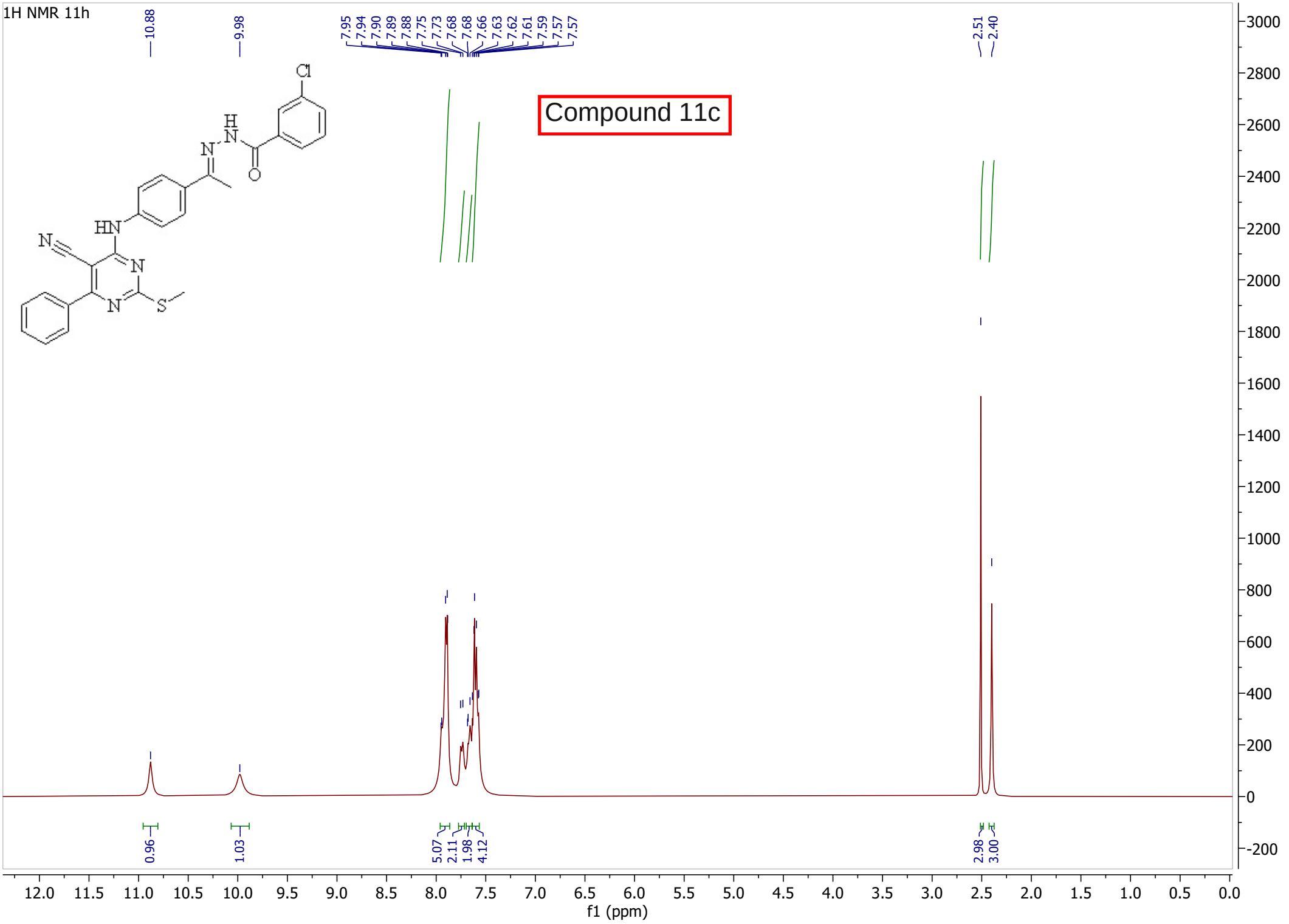
SAMPLE INFORMATION

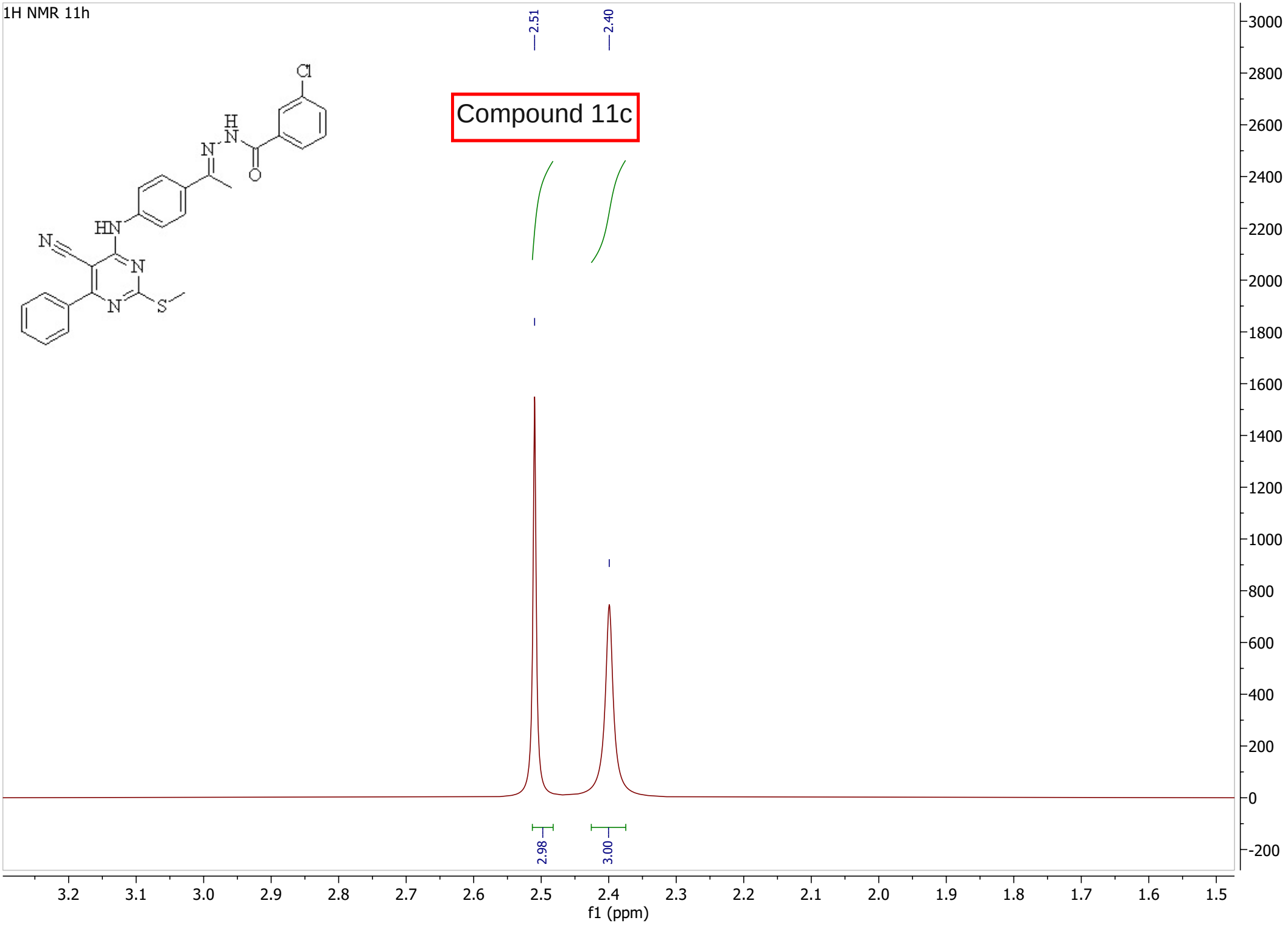
Sample Name:	ASZ8 Compound 11c	Acquired By:	System
Sample Type:	Unknown	Sample Set Name:	
Vial:	10	Acq. Method Set:	Organic
Injection #:	1	Processing Method:	Default
Injection Volume:	2.00 ul	Channel Name:	320.0nm@1
Run Time:	14.0 Minutes	Proc. Chnl. Descr.:	W2996 PDA 320.0 nm (PDA 190.0 to
Date Acquired:	11/6/2022 5:39:21 AM EET		
Date Processed:	11/6/2022 5:48:29 AM EET		

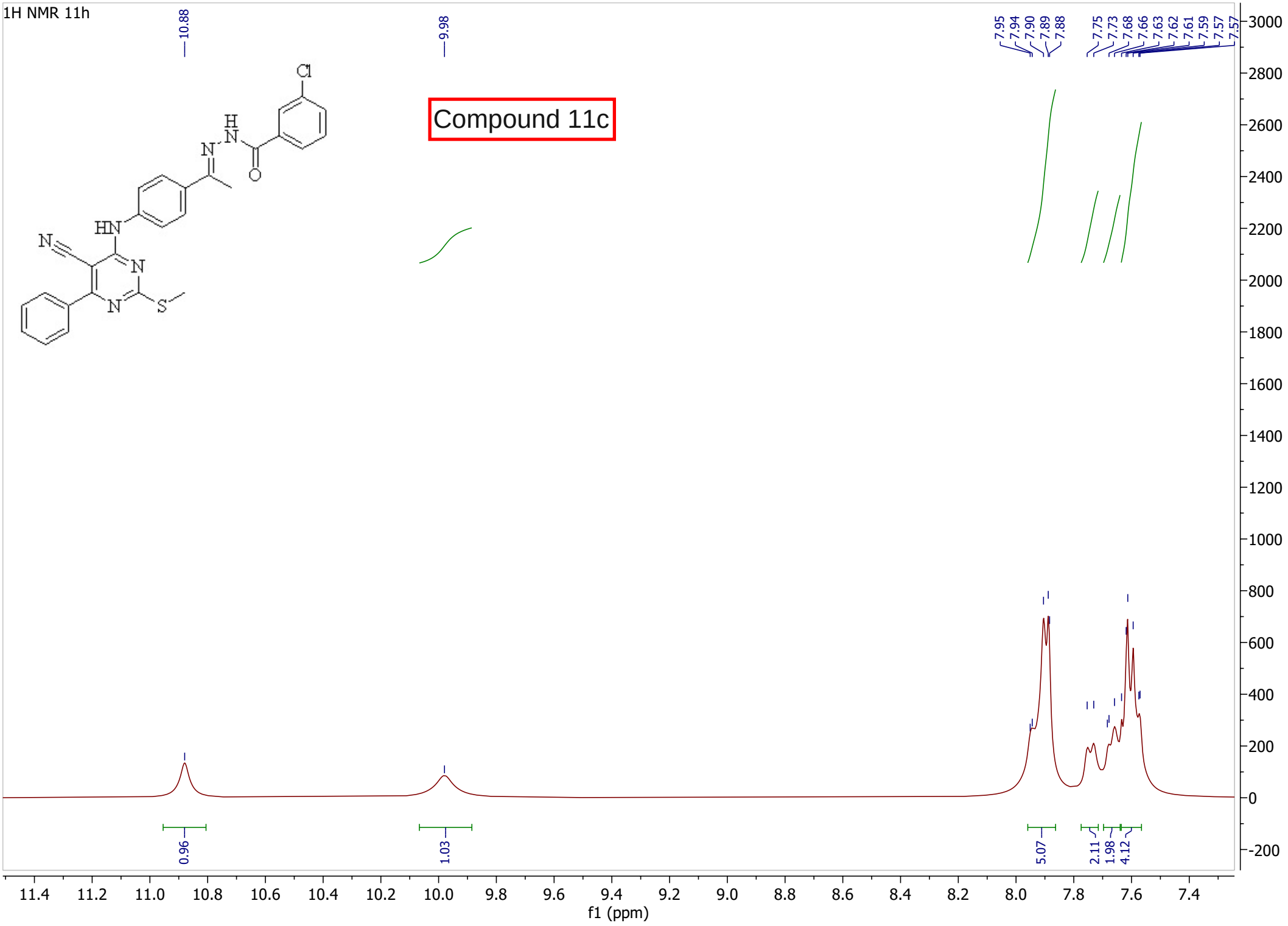


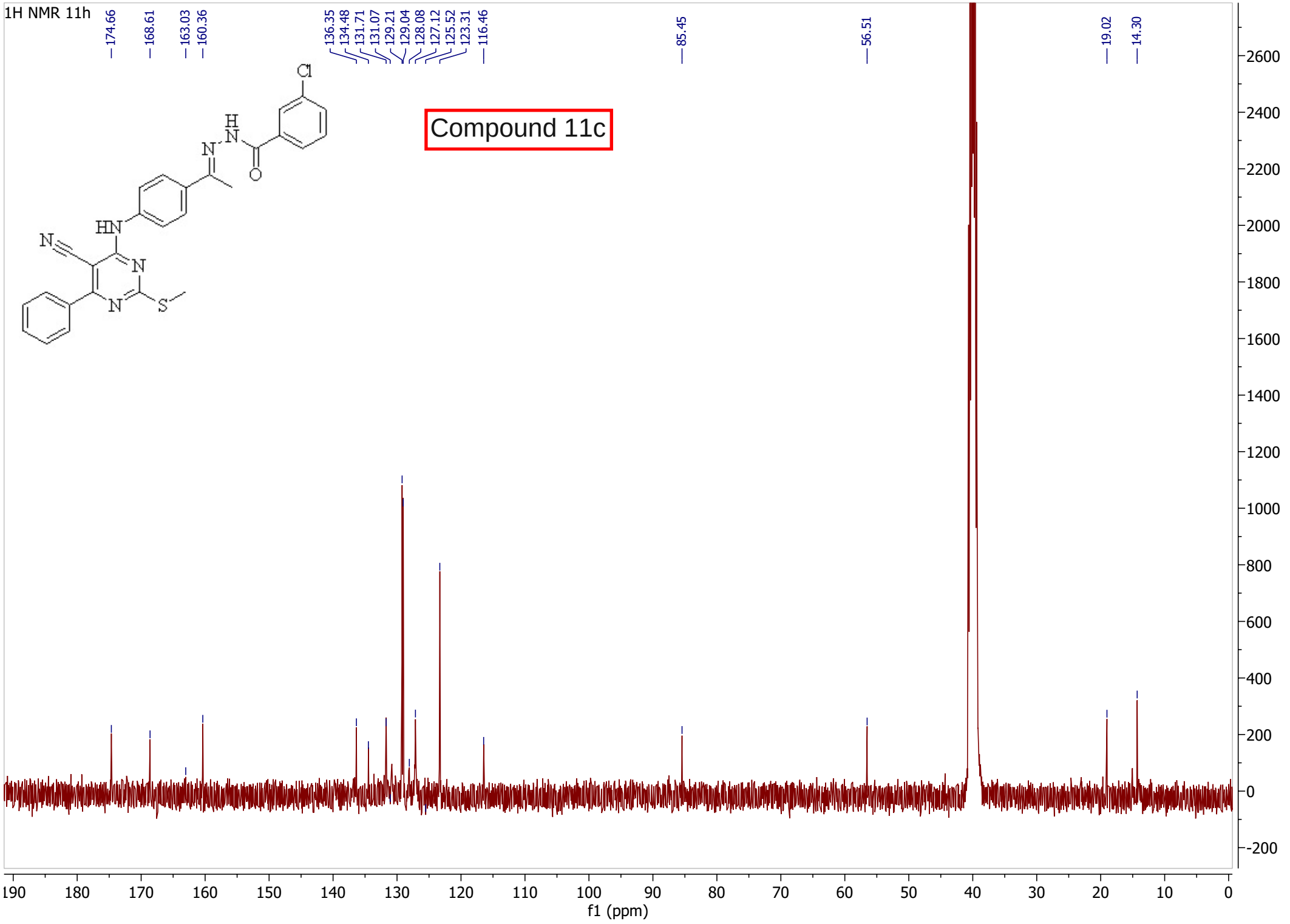
	RT	Area	% Area	Height
1	2.992	297834	3.75	44622
2	3.679	7639522	96.25	1142412

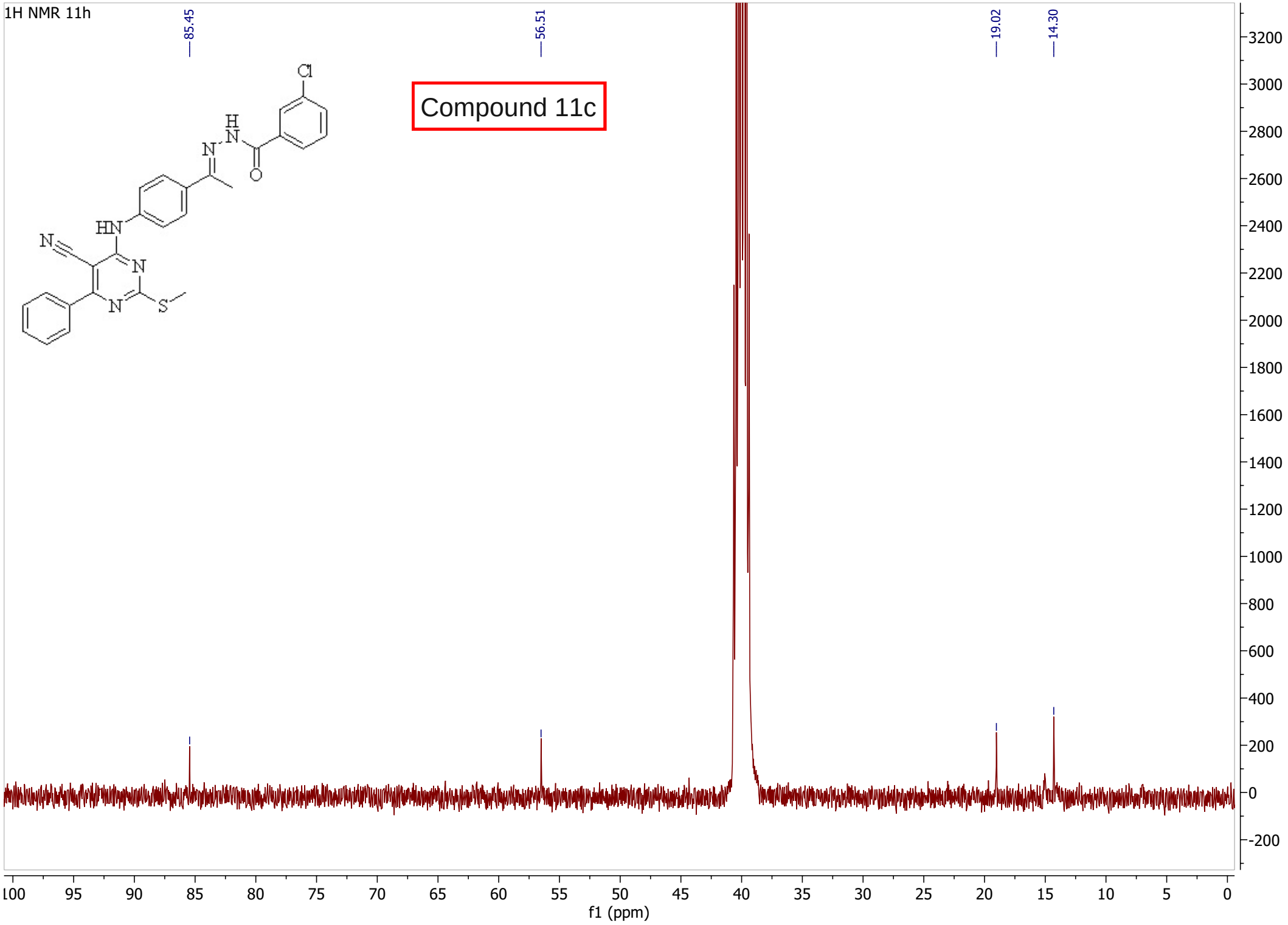

ASZ8
Compound 11c
% Transmittance
Wavenumbers (cm-1)
3646.79
3403.78
3306.48
3194.57
3162.99
3060.33
2926.12
2222.36
1717.24
1666.95
1620.56
1596.96
1561.19
1528.09
1446.81
1413.01
1302.30
1244.02
1189.65
1148.79
1106.39
1078.51
1055.16
1007.17
966.09
927.14
895.87
876.91
845.71
822.54
798.93
767.45
751.78
736.58
699.88
670.26
651.71
628.54
611.98
579.04
560.46
522.62
505.67
454.59

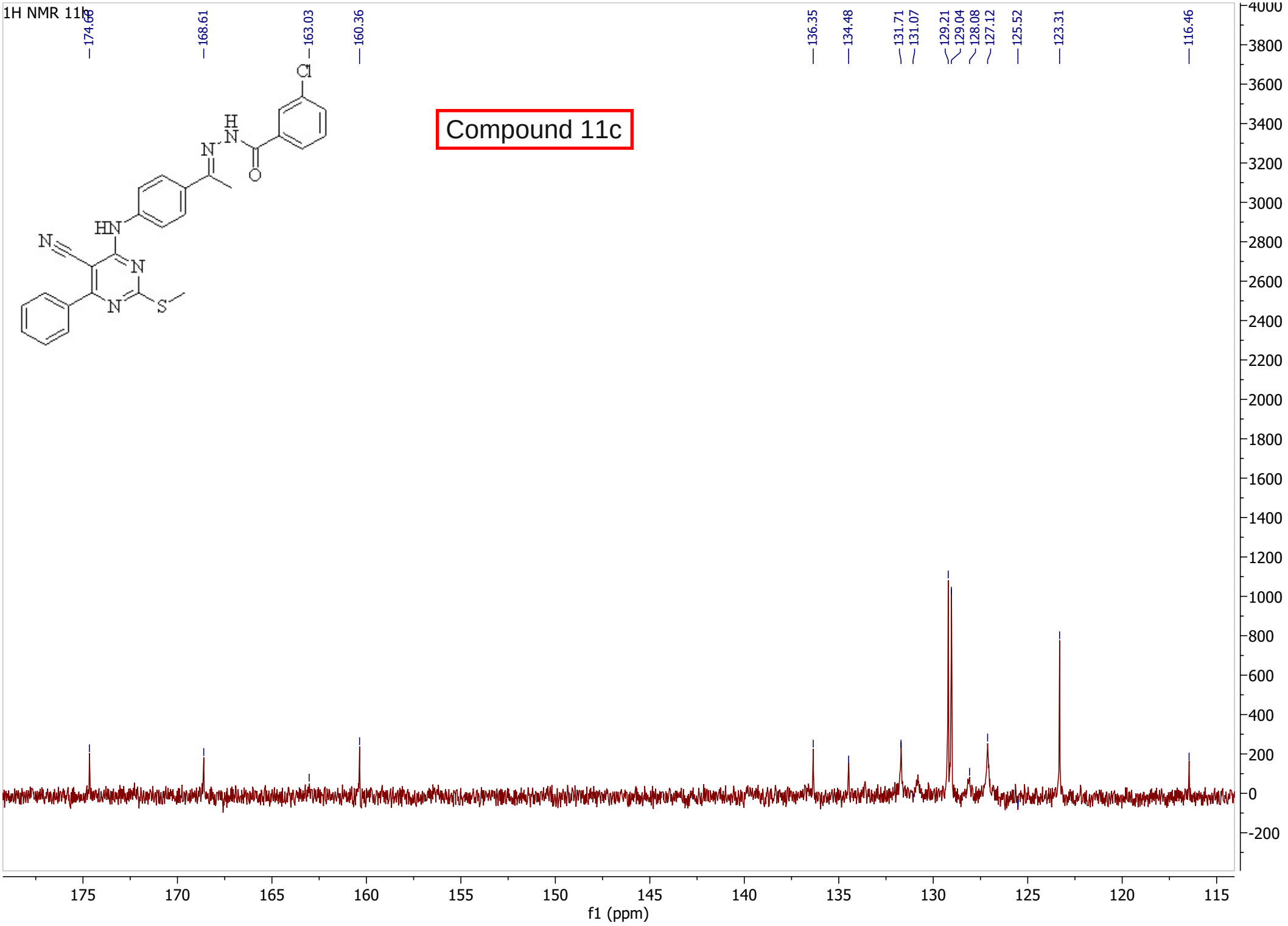

1H NMR 11h
10.88
9.98
7.95
7.94
7.90
7.89
7.88
7.75
7.73
7.68
7.68
7.66
7.63
7.62
7.61
7.59
7.57
7.57
2.51
2.40
Compound 11c
Cl
H
N
N
O
HN
N
N
N
S
0.96
1.03
5.07
2.11
1.98
4.12
2.98
3.00
f1 (ppm)


1H NMR 11h
2.51
2.40
Compound 11c
Cl
H
N
N
O
HN
N
N
N
S
2.98
3.00
3000
2800
2600
2400
2200
2000
1800
1600
1400
1200
1000
800
600
400
200
0
-200
3.2
3.1
3.0
2.9
2.8
2.7
2.6
2.5
2.4
2.3
2.2
2.1
2.0
1.9
1.8
1.7
1.6
1.5
f1 (ppm)


1H NMR 11h
10.88
9.98
7.95
7.94
7.90
7.89
7.88
7.75
7.73
7.68
7.66
7.63
7.62
7.61
7.59
7.57
7.57
Compound 11c
Cl
H
N
N
O
HN
N
N
N
N
S
0.96
1.03
5.07
2.11
1.98
4.12
f1 (ppm)

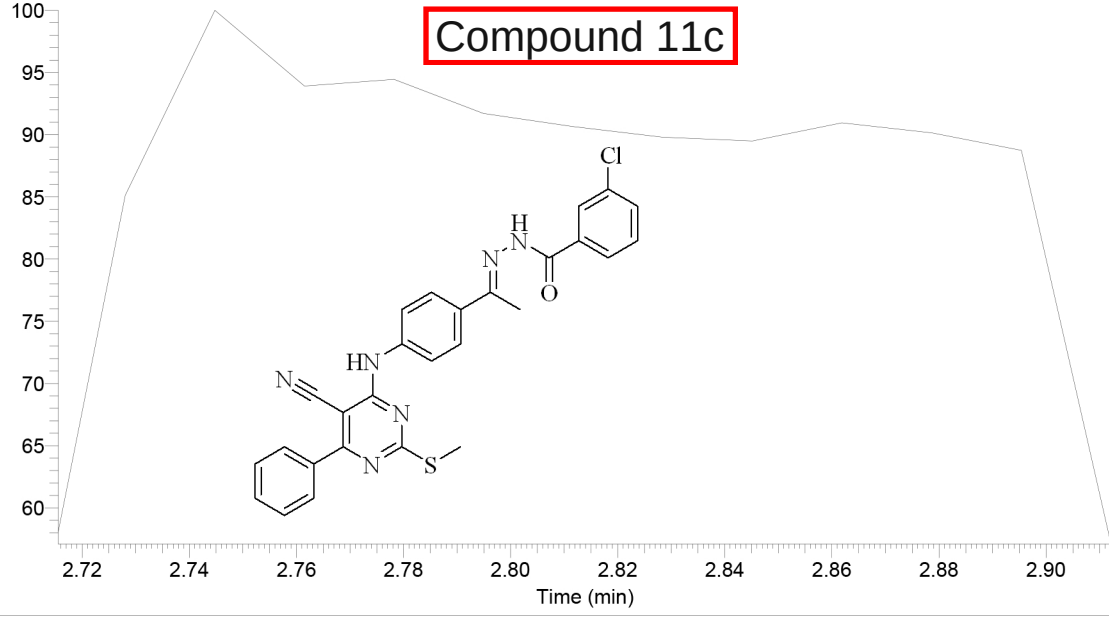

1H NMR 11h
174.66
168.61
163.03
160.36
136.35
134.48
131.71
131.07
129.21
129.04
128.08
127.12
125.52
123.31
116.46
85.45
56.51
19.02
14.30
Compound 11c
Cl
H
N
N
O
HN
N
N
N
S
2600
2400
2200
2000
1800
1600
1400
1200
1000
800
600
400
200
0
-200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


1H NMR 11h
85.45
56.51
19.02
14.30
Compound 11c
Cl
H
N
N
O
HN
N
N
N
S
3200
3000
2800
2600
2400
2200
2000
1800
1600
1400
1200
1000
800
600
400
200
0
-200
100
95
90
85
80
75
70
65
60
55
50
45
40
35
30
25
20
15
10
5
0
f1 (ppm)

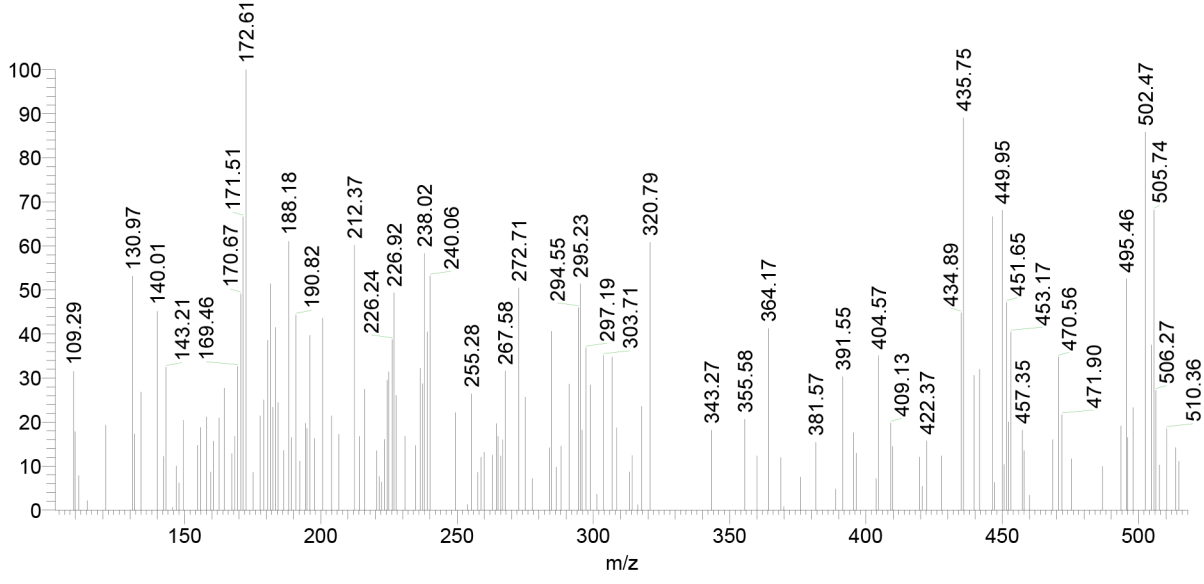

1H NMR 11b
174.68
168.61
163.03
160.36
136.35
134.48
131.71
131.07
129.21
129.04
128.08
127.12
125.52
123.31
116.46
Compound 11c
Cl
H
N
N
O
HN
N
N
N
S
4000
3800
3600
3400
3200
3000
2800
2600
2400
2200
2000
1800
1600
1400
1200
1000
800
600
400
200
0
-200
175
170
165
160
155
150
145
140
135
130
125
120
115
f1 (ppm)

RT: 2.72 - 2.91 SM: 11B

Compound 11c

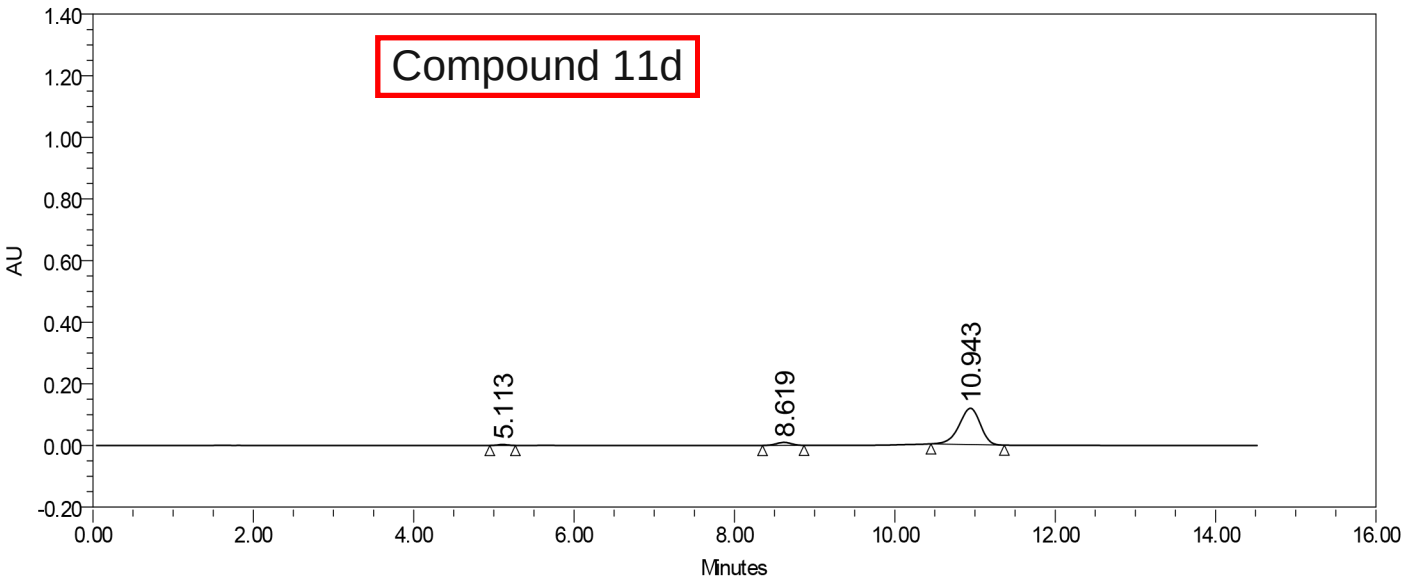


Abdelrahman-saleh-Asz8 #217-220 RT: 3.65-3.70 AV: 4 SB: 26 1.21-1.34 , 0.87-1.14 NL: 1.09E2
T: + c EI Full ms [40.00-1000.00]

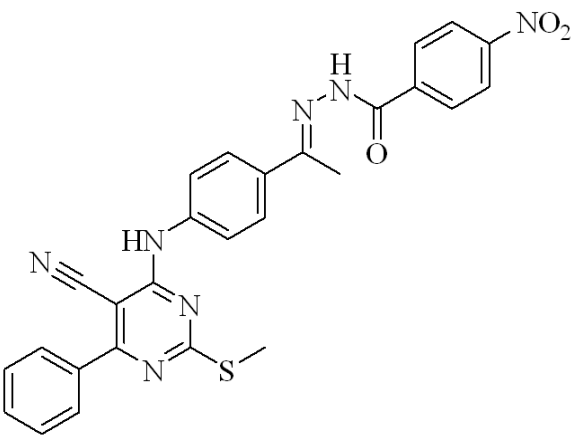


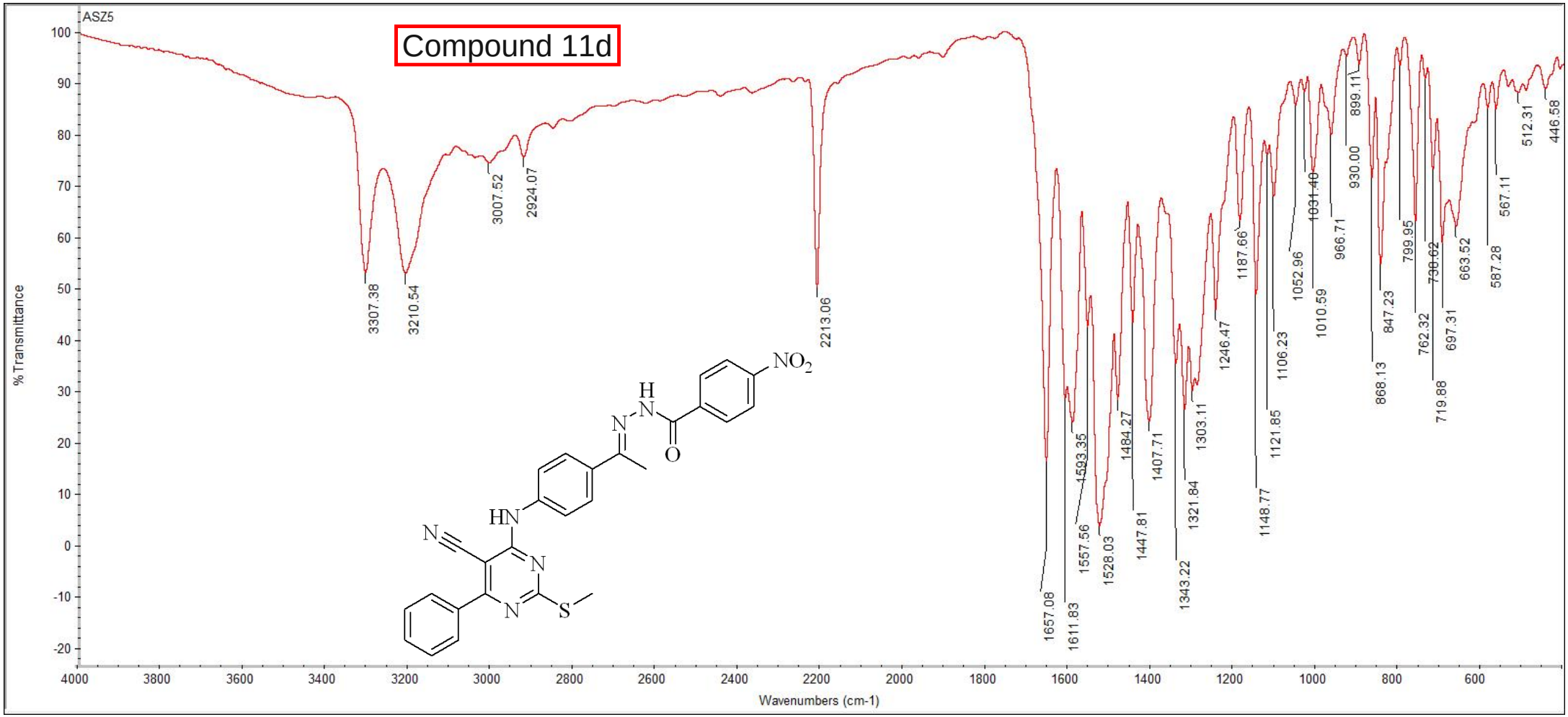
SAMPLE INFORMATION

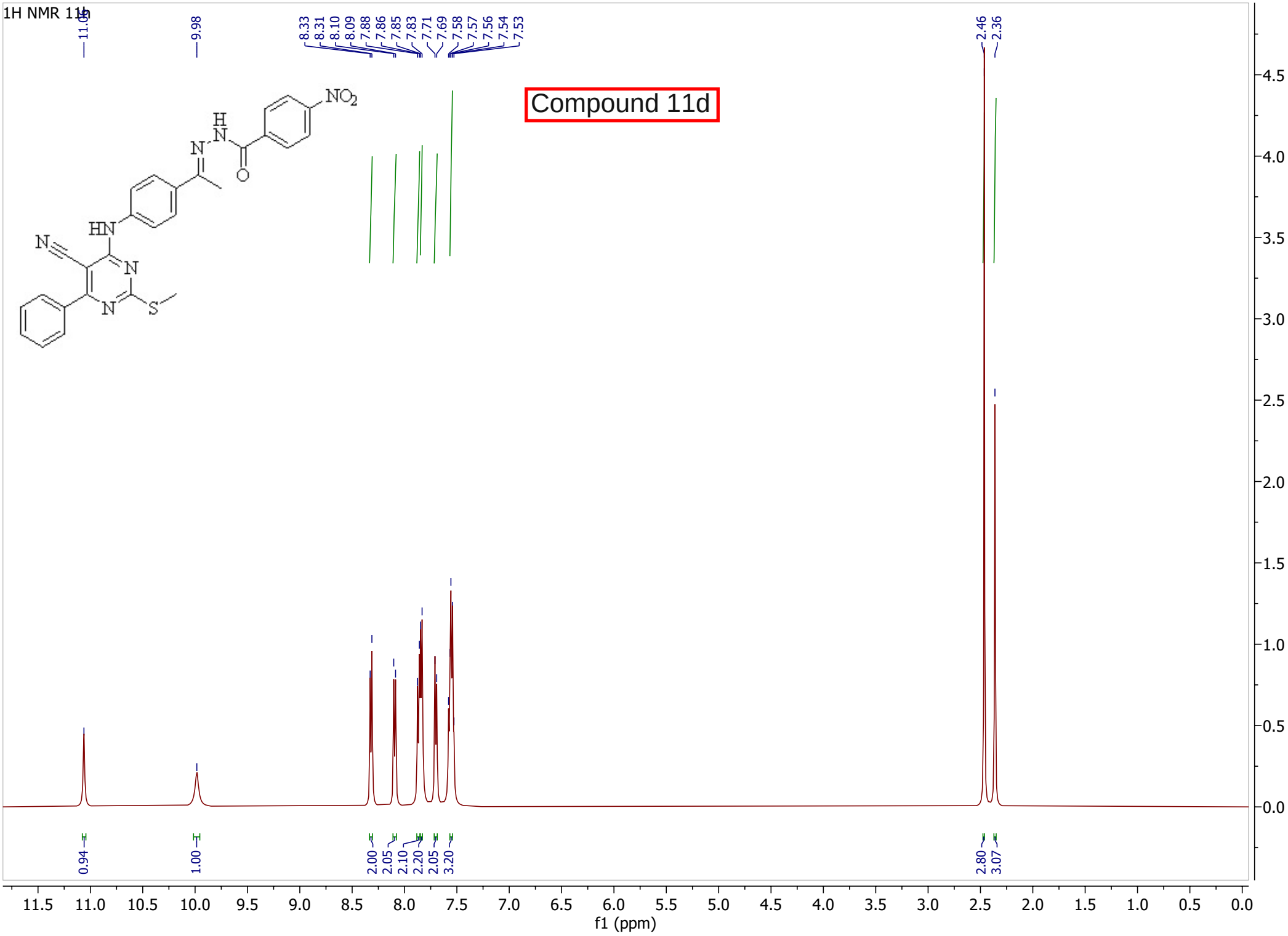
Sample Name:	ASZ5 Compound 11d	Acquired By:	System
Sample Type:	Unknown	Sample Set Name:	1
Vial:	8	Acq. Method Set:	Organic
Injection #:	1	Processing Method:	Default
Injection Volume:	2.00 ul	Channel Name:	318.0nm
Run Time:	14.5 Minutes	Proc. Chnl. Descr.:	W2996 PDA 318.0 nm (PDA 190.0 to
Date Acquired:	11/6/2022 12:01:19 AM EET		
Date Processed:	11/6/2022 5:21:16 AM EET		

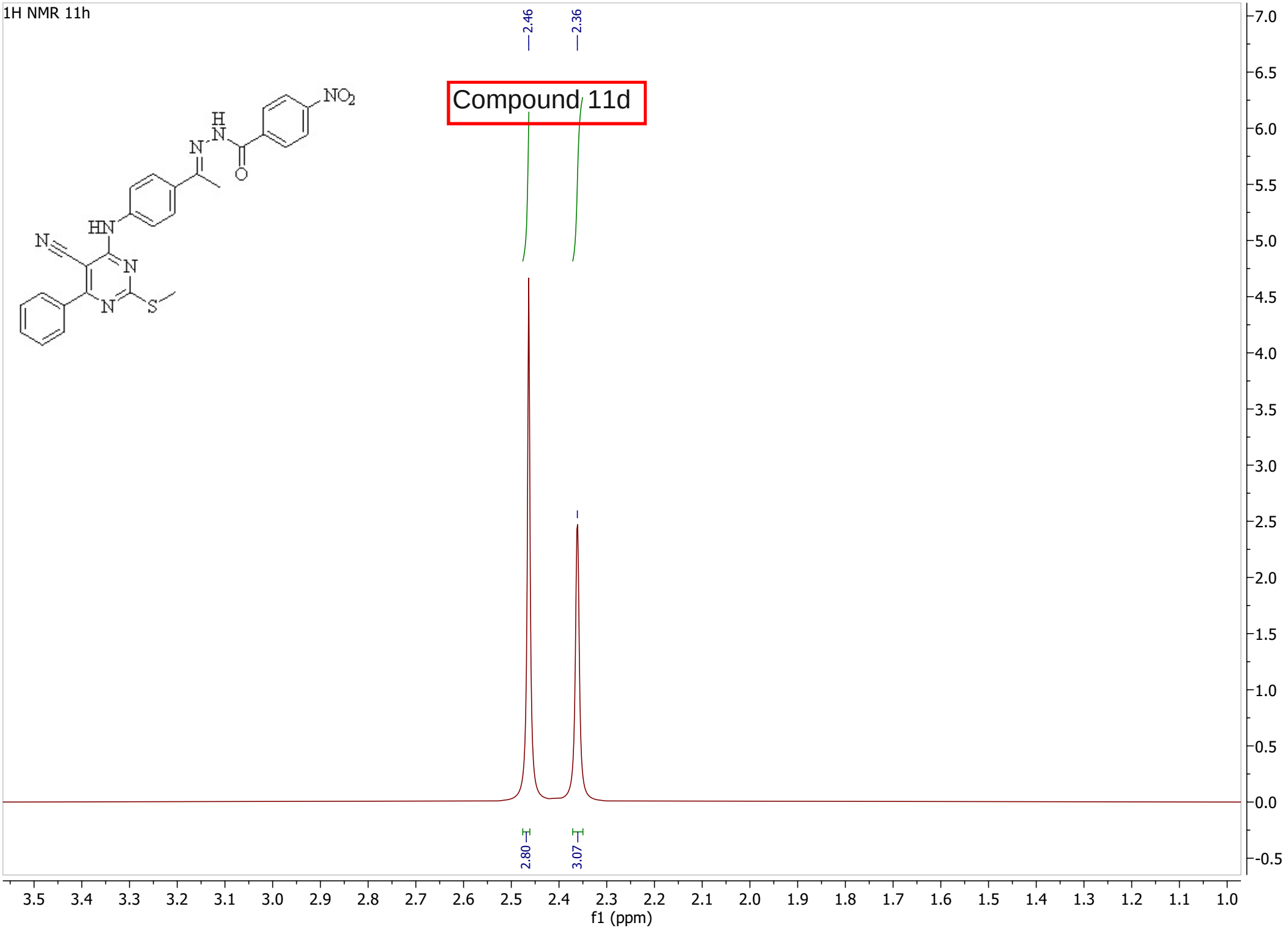


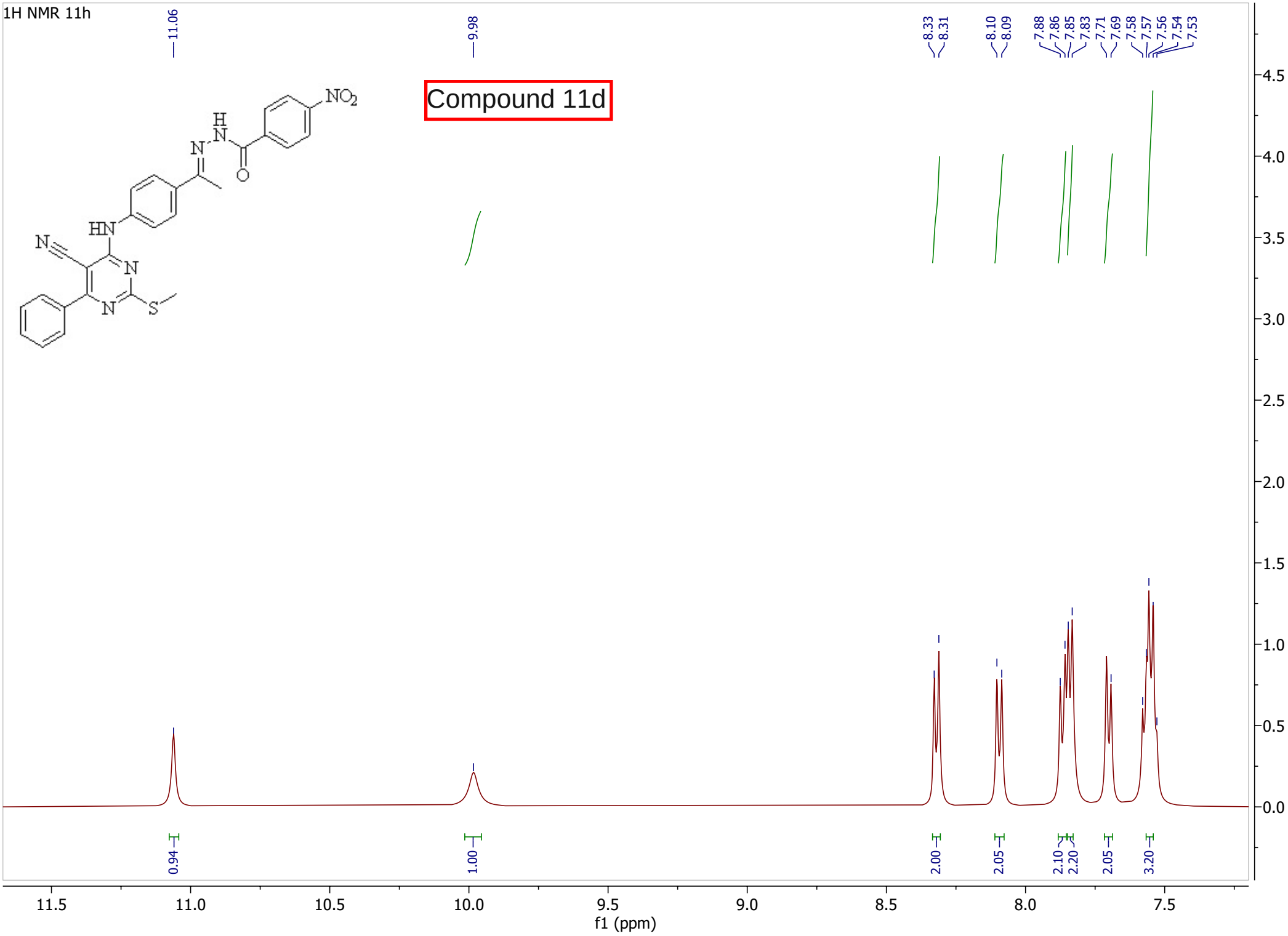
	RT	Area	% Area	Height
1	5.113	26989	1.16	3282
2	8.619	125681	5.42	9731
3	10.943	2164478	93.41	117977

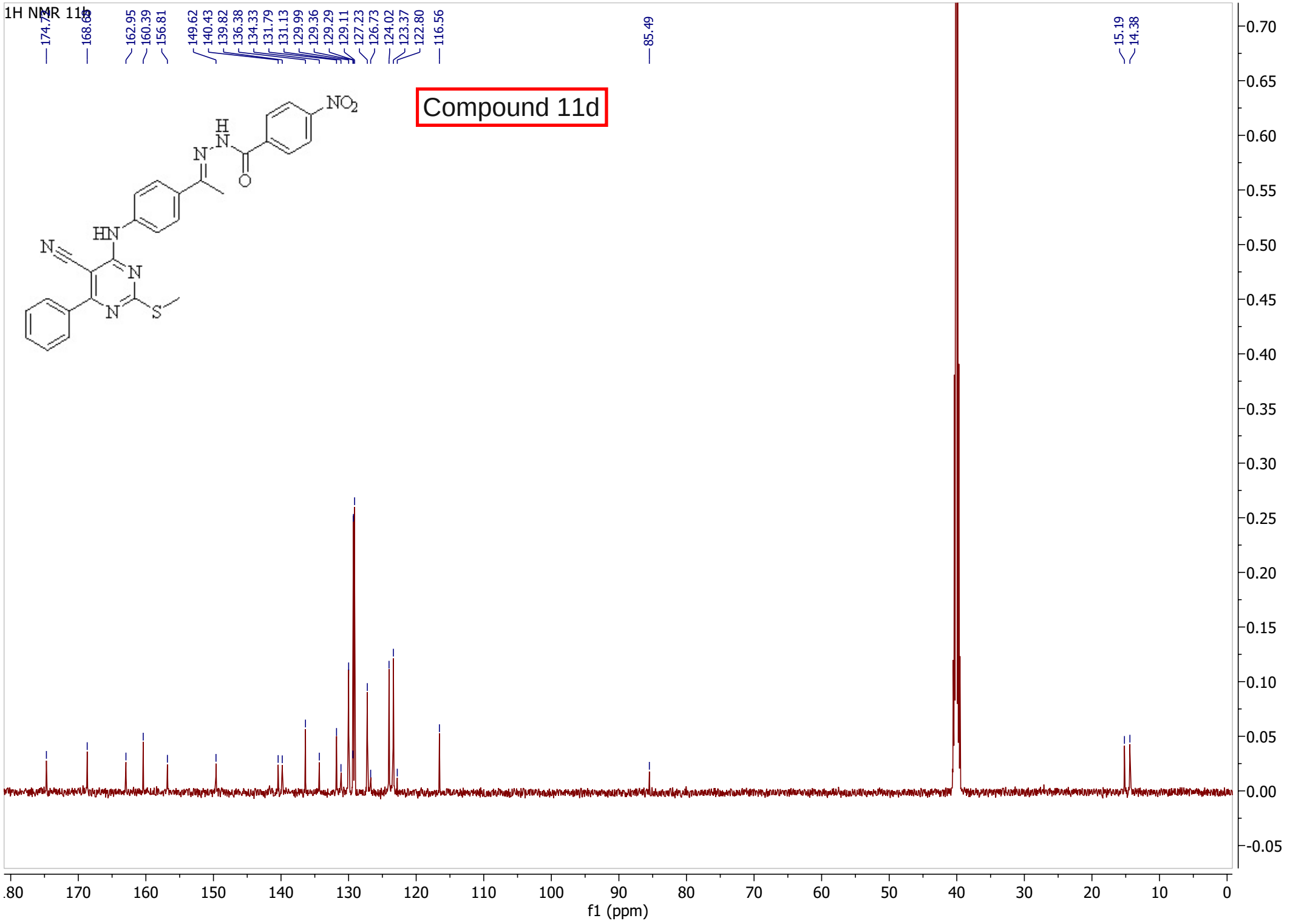


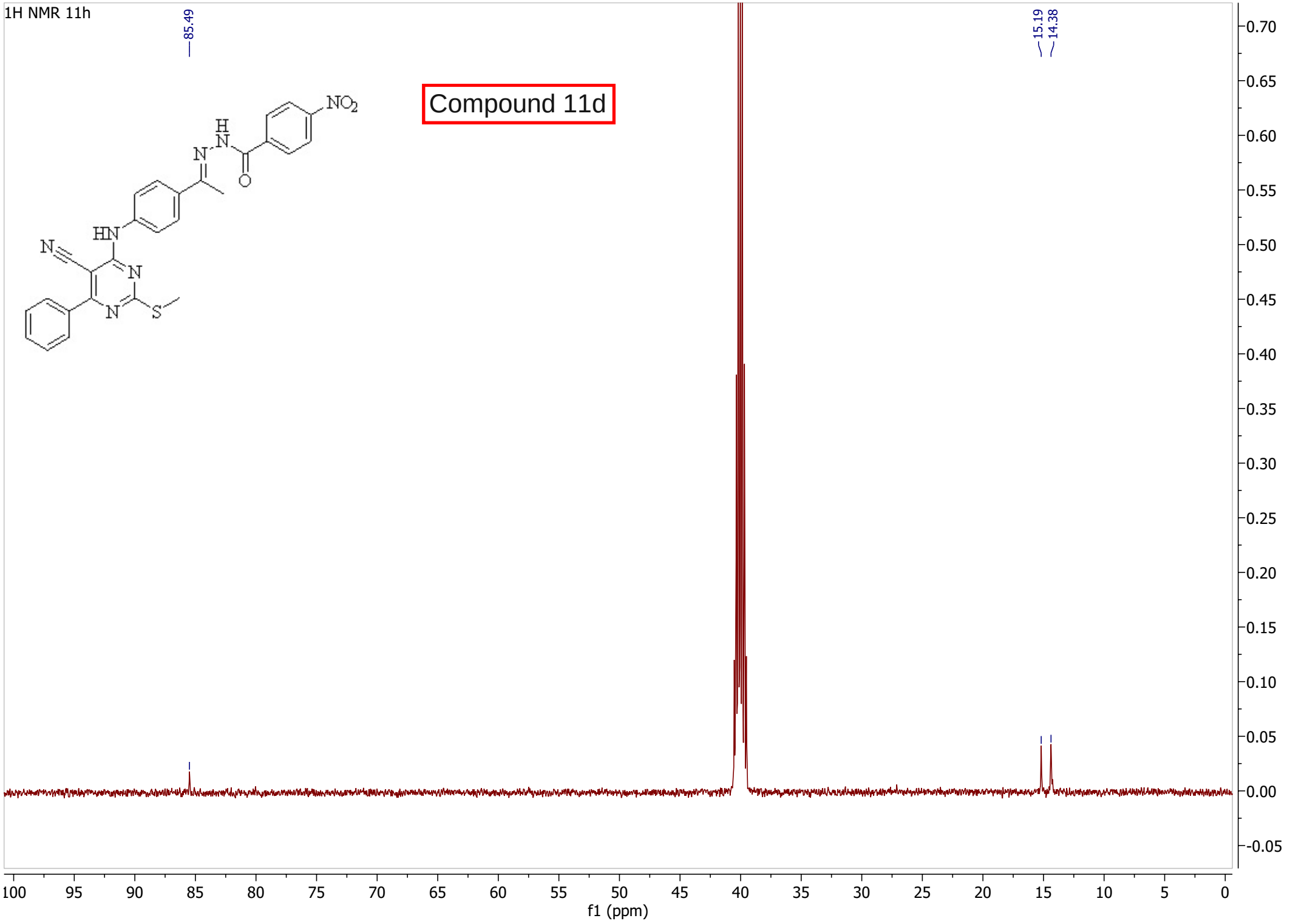

ASZ5
Compound 11d
% Transmittance
Wavenumbers (cm-1)
3307.38
3210.54
3007.52
2924.07
2213.06
1657.08
1611.83
1557.56
1528.03
1593.35
1484.27
1447.81
1407.71
1343.22
1321.84
1303.11
1246.47
1187.66
1148.77
1121.85
1106.23
1052.96
1031.40
1010.59
966.71
930.00
899.11
868.13
847.23
799.95
762.32
730.62
719.88
697.31
663.52
587.28
567.11
512.31
446.58
NO2
H
N
HN
O
S

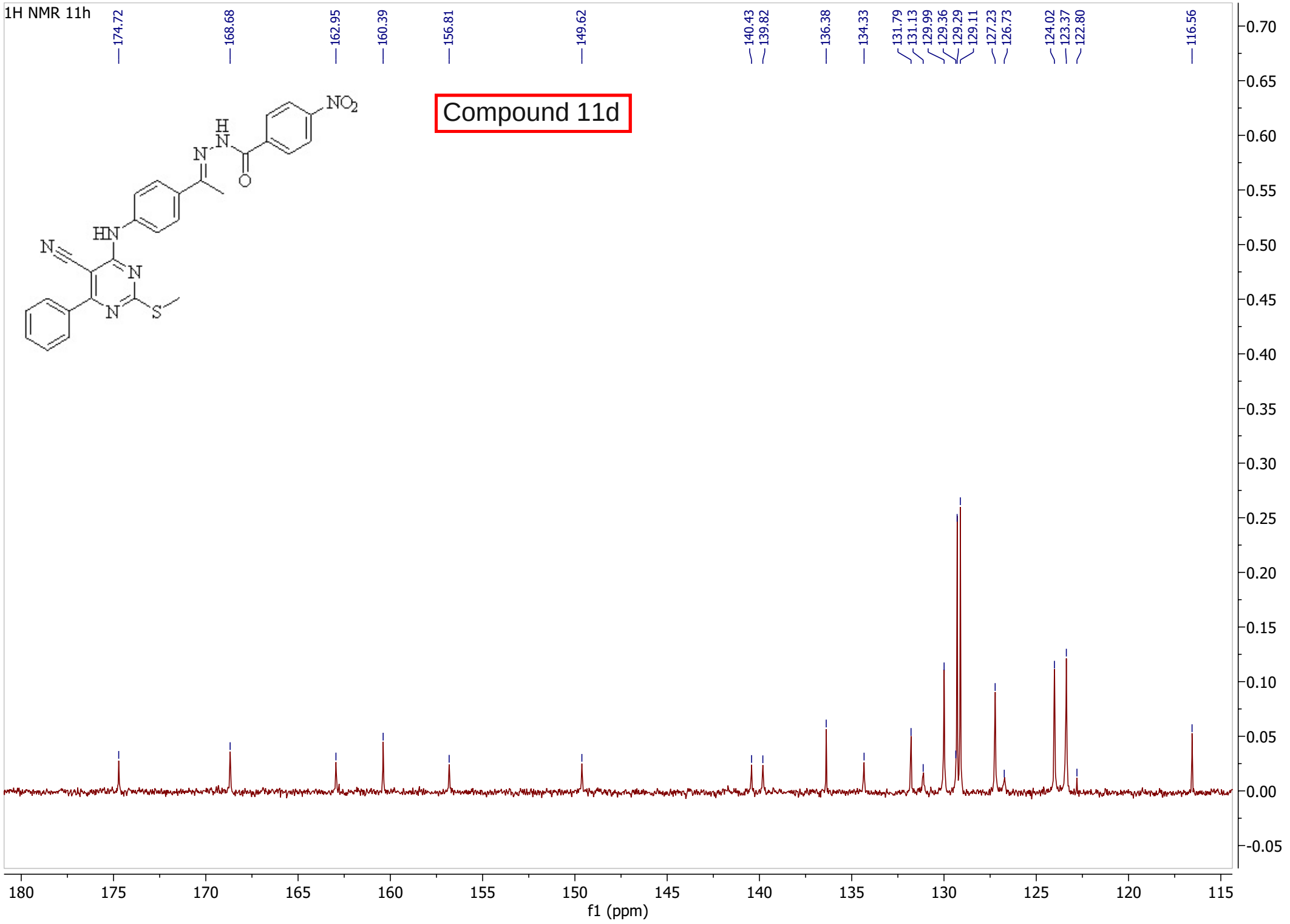

1H NMR 11d
11.03
9.98
8.33
8.31
8.10
8.09
7.88
7.86
7.85
7.83
7.71
7.69
7.58
7.57
7.56
7.54
7.53
2.46
2.36
Compound 11d
NO2
H
N
N
O
HN
N
N
N
S
0.94
1.00
2.00
2.05
2.10
2.20
2.05
3.20
2.80
3.07
f1 (ppm)

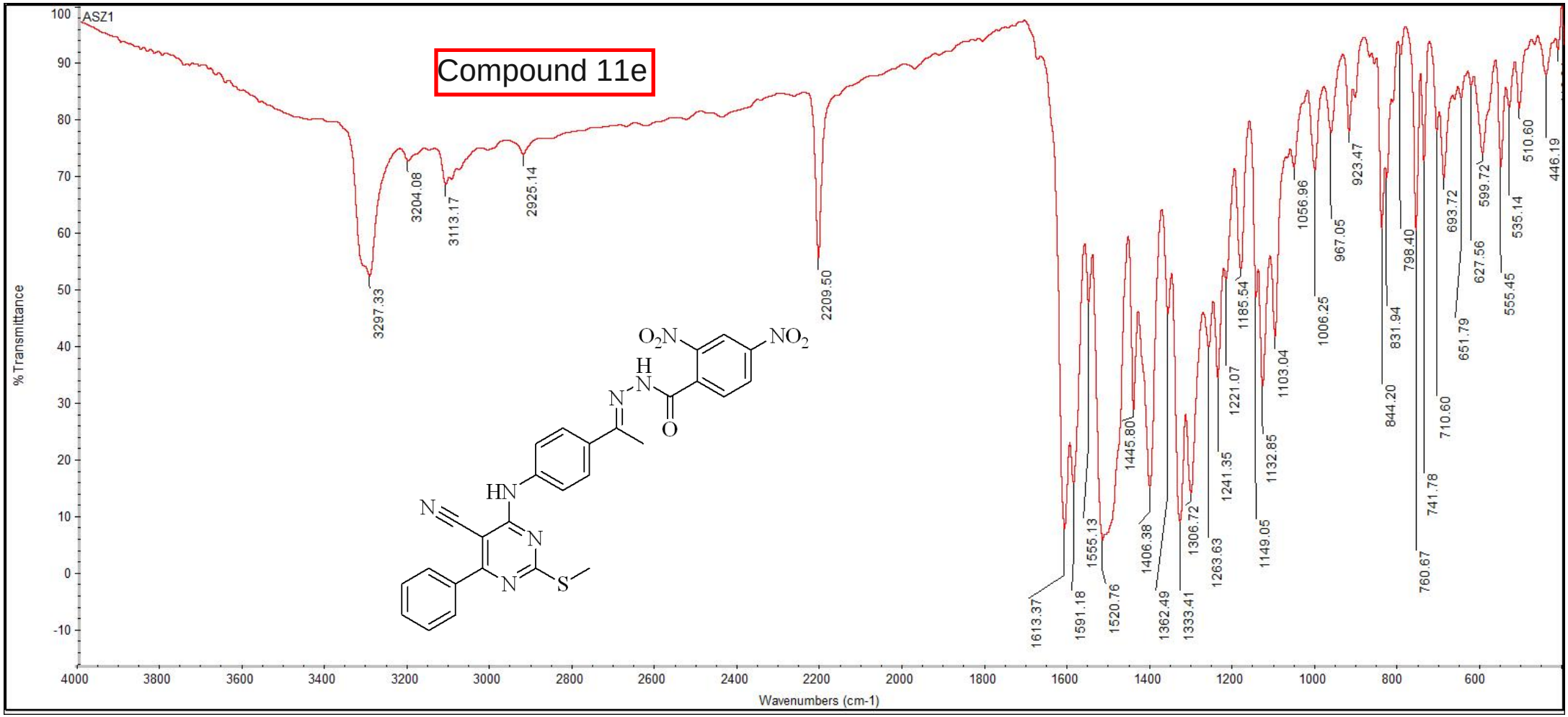

1H NMR 11h
2.46
2.36
Compound 11d
NO2
H
N
N
O
HN
N
N
N
S
2.80
3.07
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
3.5 3.4 3.3 3.2 3.1 3.0 2.9 2.8 2.7 2.6 2.5 2.4 2.3 2.2 2.1 2.0 1.9 1.8 1.7 1.6 1.5 1.4 1.3 1.2 1.1 1.0
f1 (ppm)

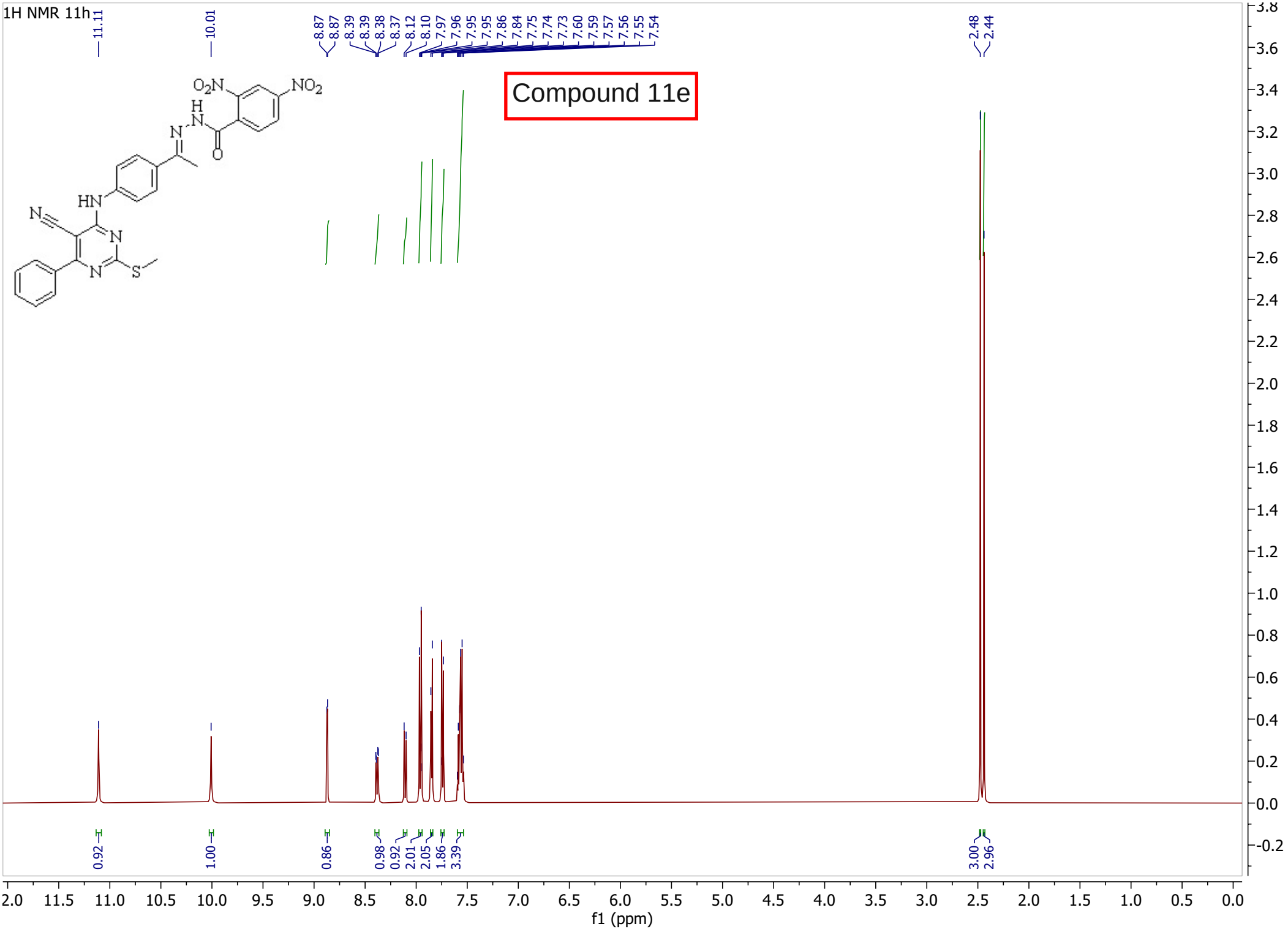

1H NMR 11h
11.06
9.98
8.33
8.31
8.10
8.09
7.88
7.86
7.85
7.83
7.71
7.69
7.58
7.57
7.56
7.54
7.53
Compound 11d
NO2
H
N
N
O
HN
N
N
N
S
0.94
1.00
2.00
2.05
2.10
2.20
2.05
3.20
11.5
11.0
10.5
10.0
9.5
9.0
8.5
8.0
7.5
f1 (ppm)
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0


1H NMR 11d
174.75
168.69
162.95
160.39
156.81
149.62
140.43
139.82
136.38
134.33
131.79
131.13
129.99
129.36
129.29
129.11
127.23
126.73
124.02
123.37
122.80
116.56
85.49
15.19
14.38
Compound 11d
NO2
H
N
N
O
HN
N
N
N
S
0.70
0.65
0.60
0.55
0.50
0.45
0.40
0.35
0.30
0.25
0.20
0.15
0.10
0.05
0.00
-0.05
.80
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

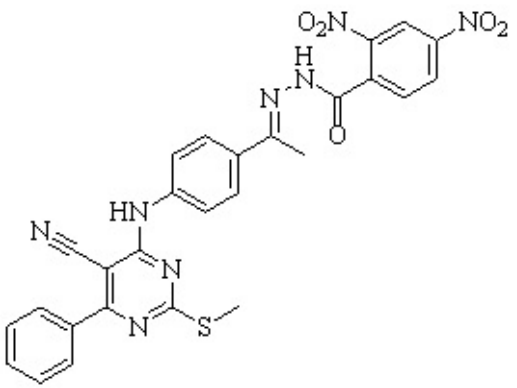

1H NMR 11h
85.49
15.19
14.38
Compound 11d
NO2
H
N
N
O
HN
N
N
N
S
0.70
0.65
0.60
0.55
0.50
0.45
0.40
0.35
0.30
0.25
0.20
0.15
0.10
0.05
0.00
-0.05
100
95
90
85
80
75
70
65
60
55
50
45
40
35
30
25
20
15
10
5
0
f1 (ppm)


1H NMR 11h
174.72
168.68
162.95
160.39
156.81
149.62
140.43
139.82
136.38
134.33
131.79
131.13
129.99
129.36
129.29
129.11
127.23
126.73
124.02
123.37
122.80
116.56
Compound 11d
NO2
H
N
N
HN
N
N
N
S
0.70
0.65
0.60
0.55
0.50
0.45
0.40
0.35
0.30
0.25
0.20
0.15
0.10
0.05
0.00
-0.05
180
175
170
165
160
155
150
145
140
135
130
125
120
115
f1 (ppm)

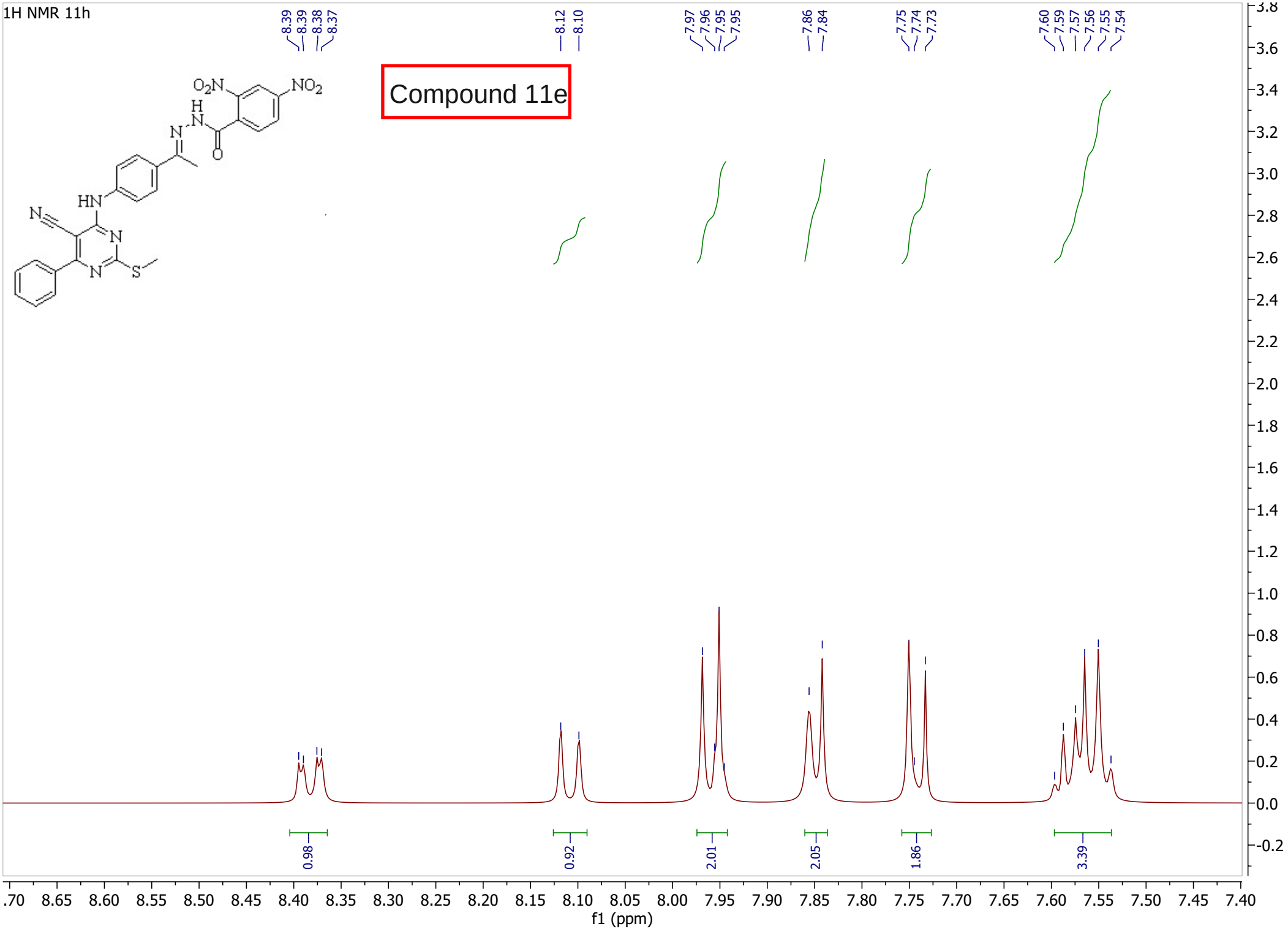

ASZ1
Compound 11e
% Transmittance
Wavenumbers (cm-1)
3297.33
3204.08
3113.17
2925.14
2209.50
1613.37
1591.18
1555.13
1520.76
1445.80
1406.38
1362.49
1333.41
1306.72
1263.63
1241.35
1221.07
1185.54
1149.05
1132.85
1103.04
1056.96
1006.25
967.05
923.47
844.20
831.94
798.40
760.67
741.78
710.60
693.72
651.79
627.56
599.72
555.45
535.14
510.60
446.19
O2N
NO2
H
N
N
O
HN
N
N
N
S

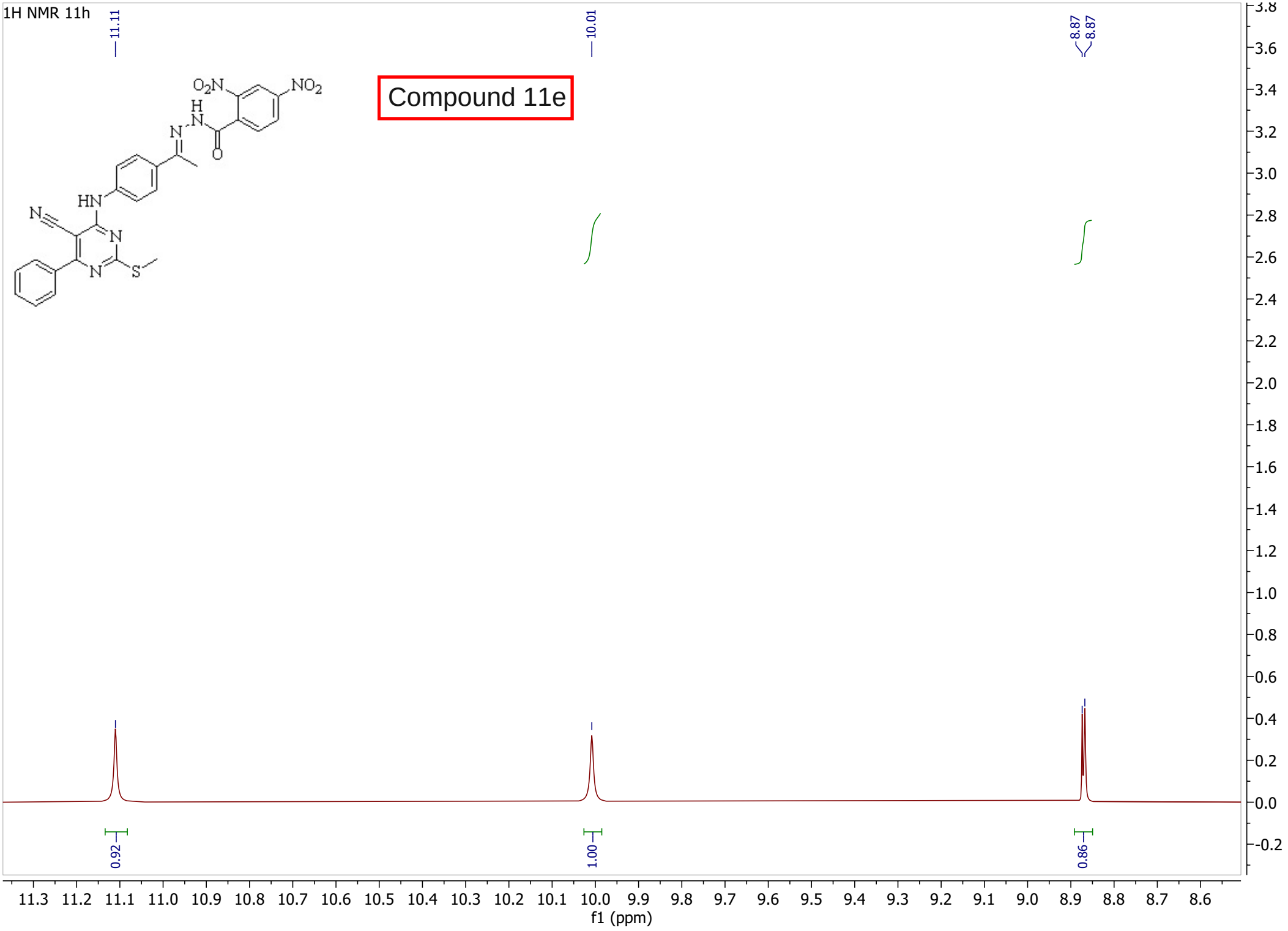

1H NMR 11h
Compound 11e
11.11
10.01
8.87
8.87
8.39
8.39
8.38
8.37
8.12
8.10
7.97
7.96
7.95
7.95
7.86
7.84
7.75
7.74
7.73
7.60
7.59
7.57
7.56
7.55
7.54
2.48
2.44
0.92
1.00
0.86
0.98
0.92
2.01
2.05
1.86
3.39
3.00
2.96
f1 (ppm)

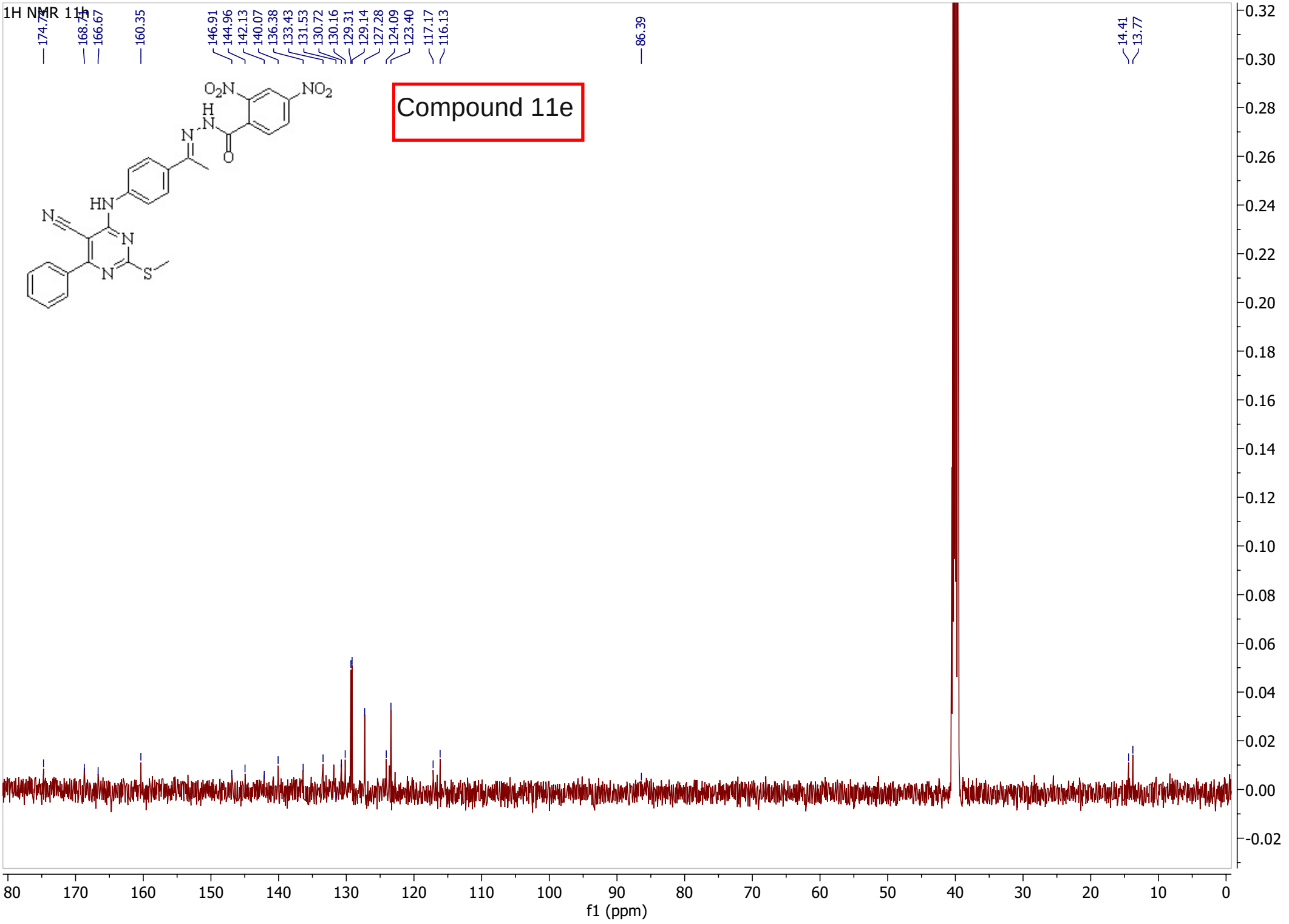
1H NMR 11h

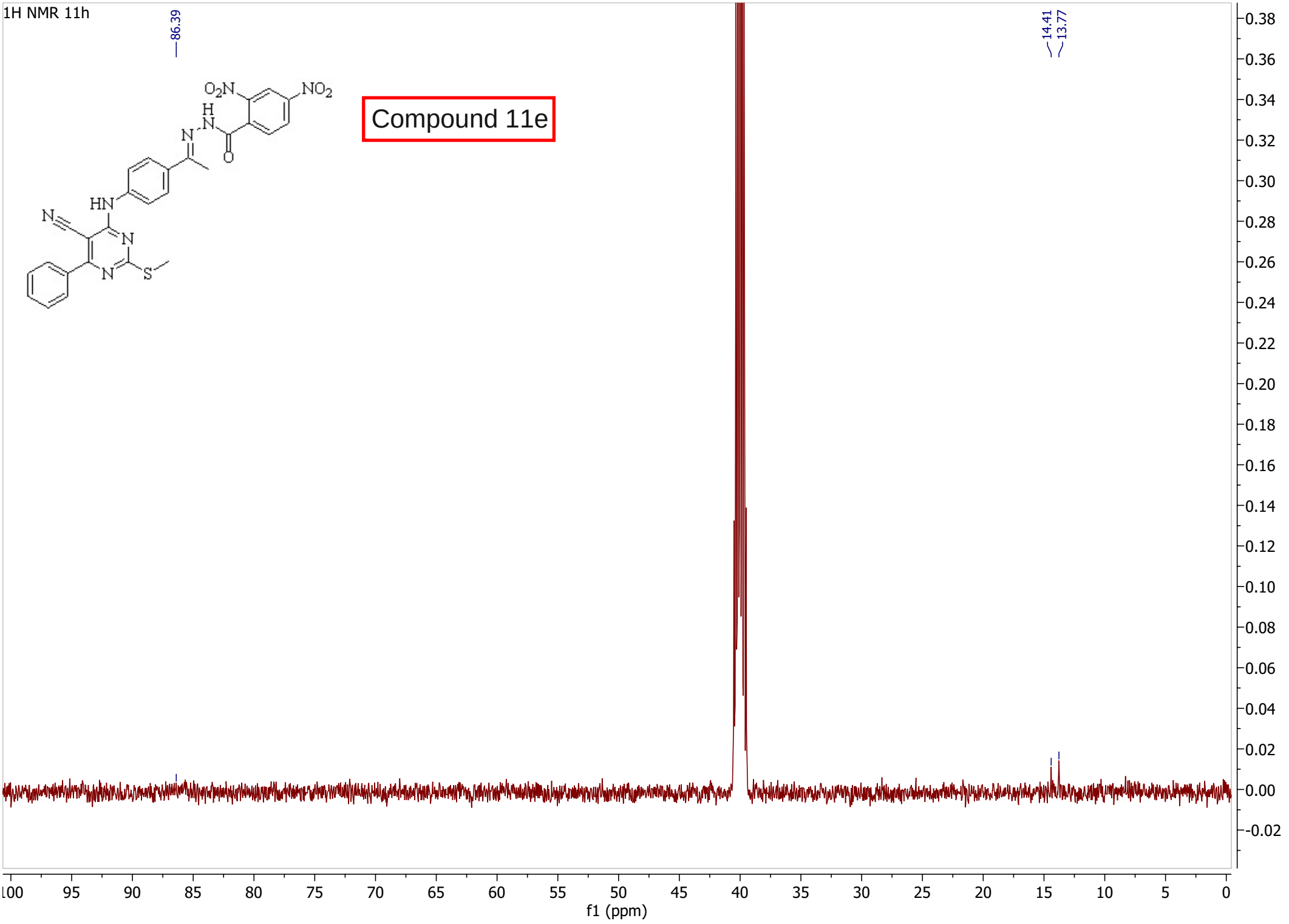


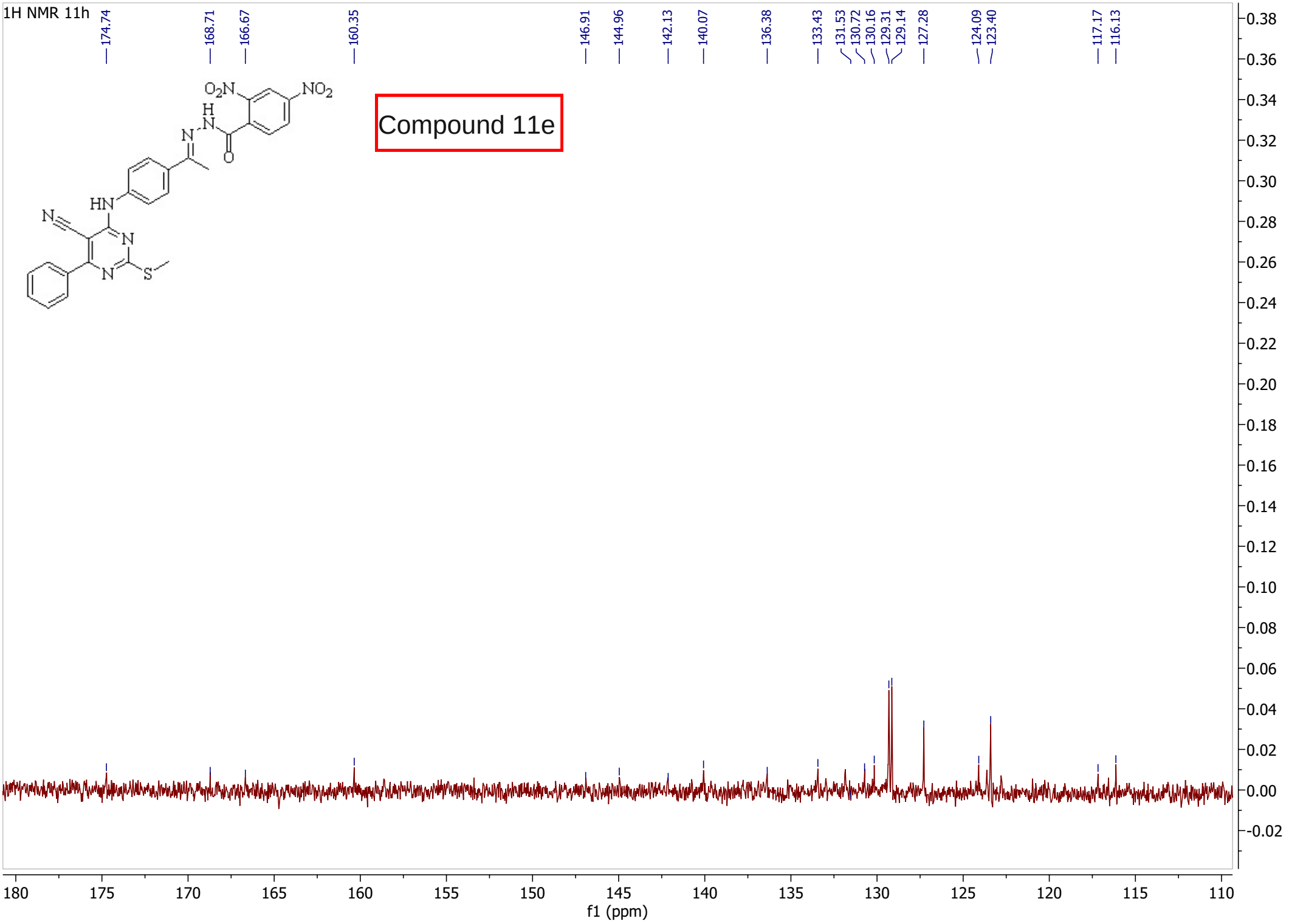
Compound 11e


1H NMR 11h
Compound 11e
8.39
8.39
8.38
8.37
8.12
8.10
7.97
7.96
7.95
7.95
7.86
7.84
7.75
7.74
7.73
7.60
7.59
7.57
7.56
7.55
7.54
0.98
0.92
2.01
2.05
1.86
3.39
f1 (ppm)


1H NMR 11h
11.11
10.01
8.87
8.87
Compound 11e
0.92
1.00
0.86
f1 (ppm)

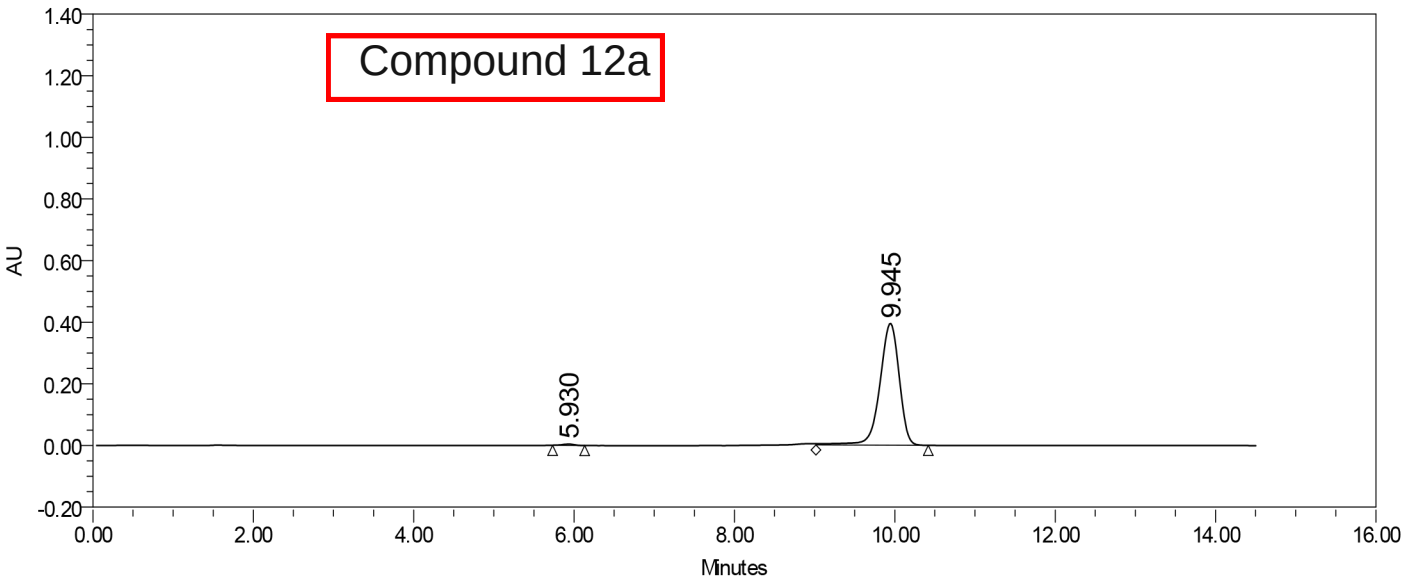

1H NMR 11h
174.73
168.77
166.67
160.35
146.91
144.96
142.13
140.07
136.38
133.43
131.53
130.72
130.16
129.31
129.14
127.28
124.09
123.40
117.17
116.13
86.39
14.41
13.77
Compound 11e
f1 (ppm)


1H NMR 11h
86.39
14.41
13.77
Compound 11e
f1 (ppm)

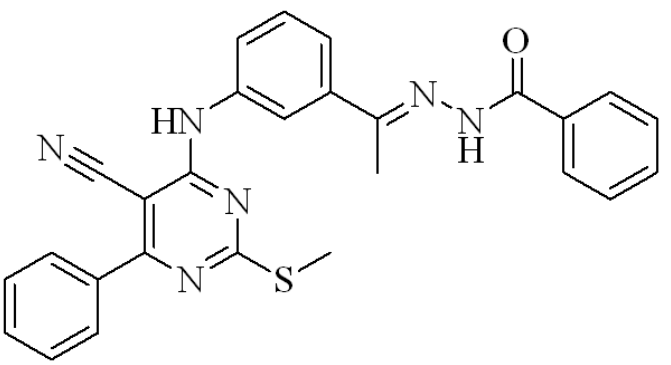

1H NMR 11h
174.74
168.71
166.67
160.35
146.91
144.96
142.13
140.07
136.38
133.43
131.53
130.72
130.16
129.31
129.14
127.28
124.09
123.40
117.17
116.13
Compound 11e
O2N
NO2
H
N
N
O
HN
N
N
N
S
0.38
0.36
0.34
0.32
0.30
0.28
0.26
0.24
0.22
0.20
0.18
0.16
0.14
0.12
0.10
0.08
0.06
0.04
0.02
0.00
-0.02
180
175
170
165
160
155
150
145
140
135
130
125
120
115
110
f1 (ppm)

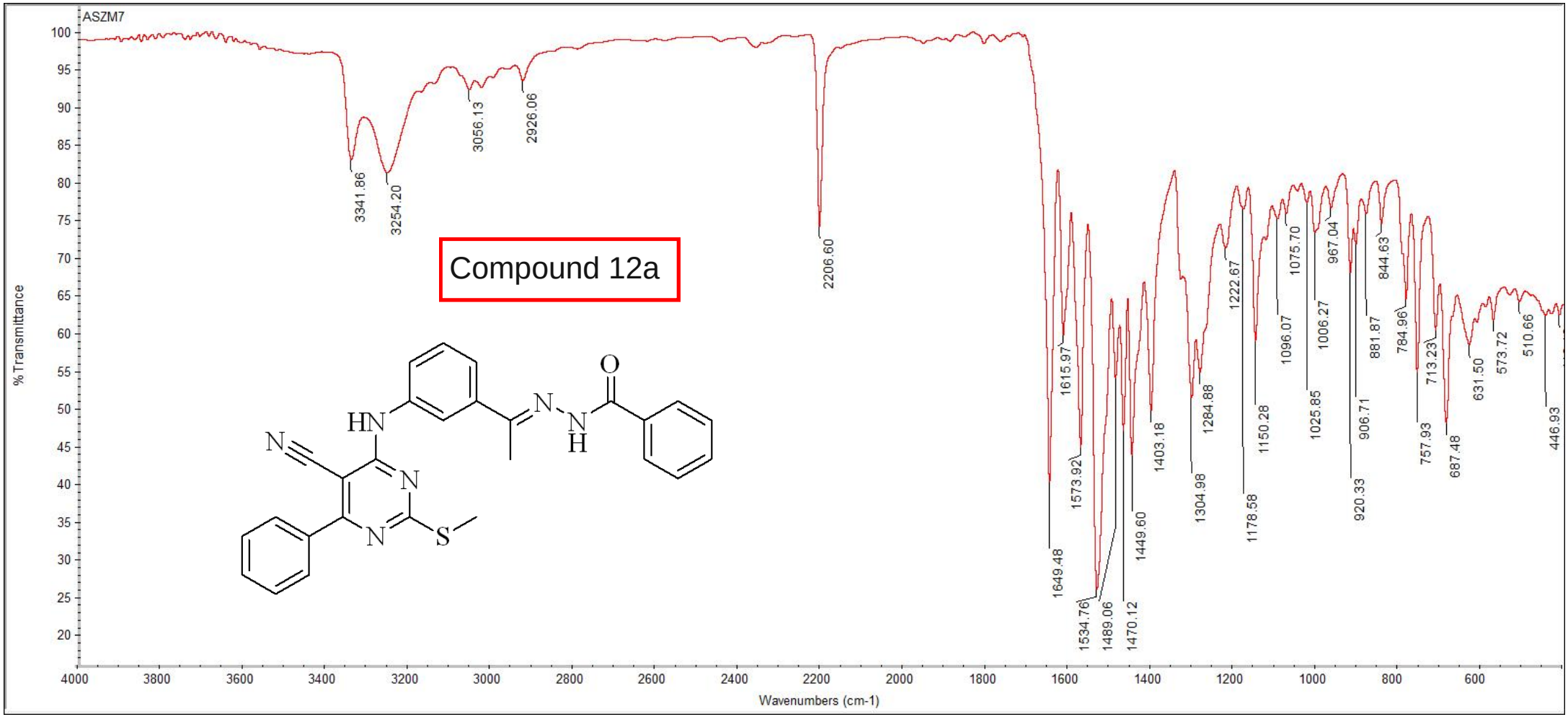
SAMPLE INFORMATION

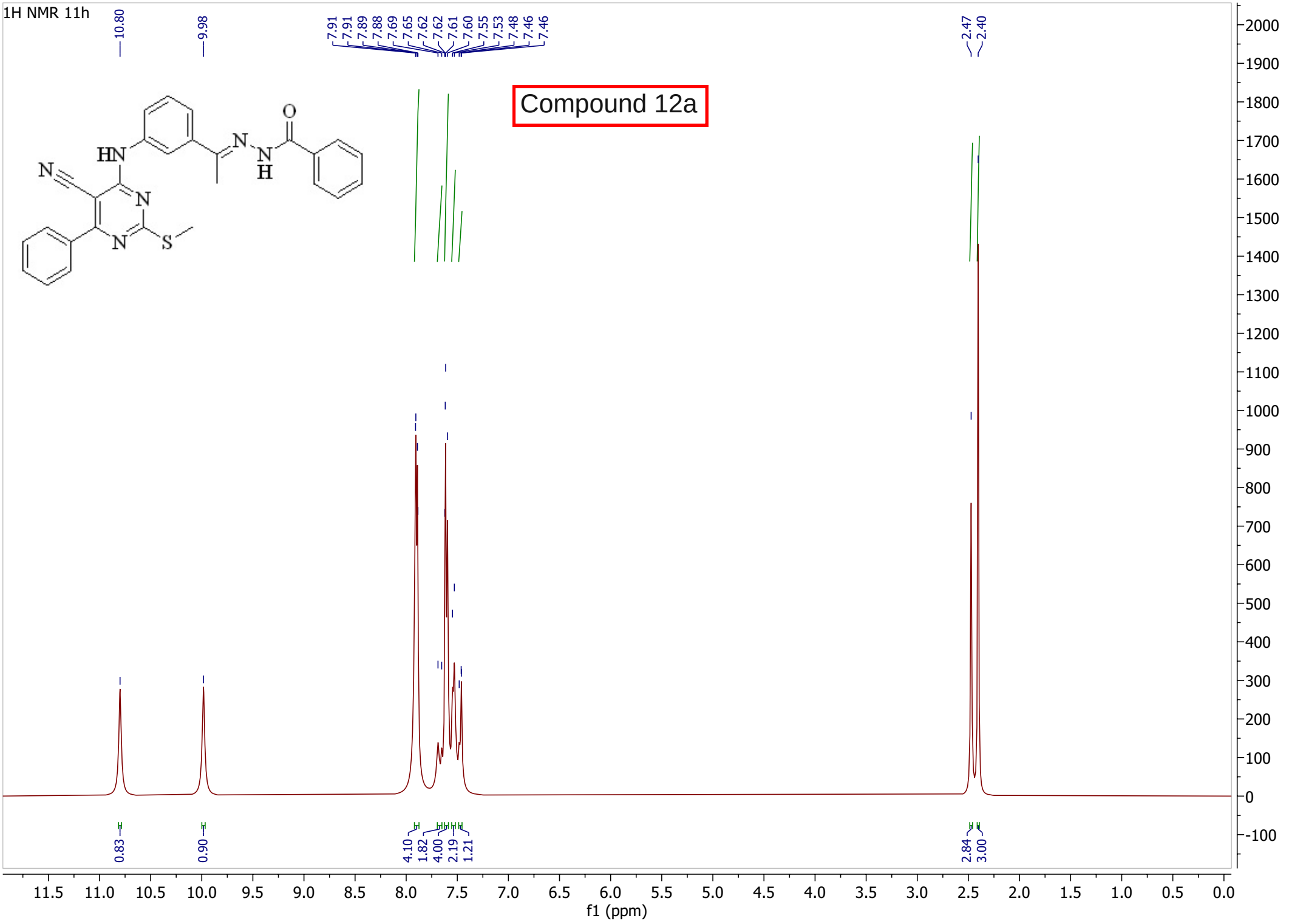
Sample Name:	ASZM7 Compound 12a	Acquired By:	System
Sample Type:	Unknown	Sample Set Name:	1
Vial:	17	Acq. Method Set:	Organic1
Injection #:	1	Processing Method:	Default1
Injection Volume:	2.00 ul	Channel Name:	280.0nm
Run Time:	14.5 Minutes	Proc. Chnl. Descr.:	W2996 PDA 280.0 nm (PDA 190.0 to
Date Acquired:	11/6/2022 2:34:04 AM EET		
Date Processed:	11/6/2022 5:08:35 AM EET		



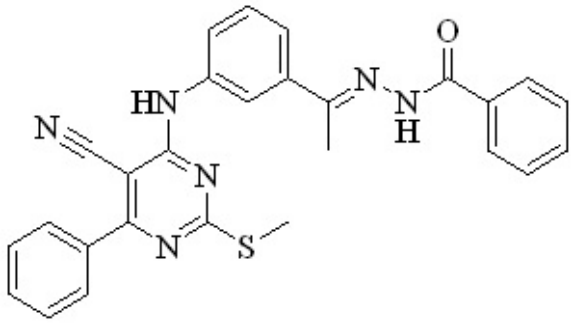
	RT	Area	% Area	Height
1	5.930	40958	0.62	4091
2	9.945	6609864	99.38	395628




ASZM7
% Transmittance
Wavenumbers (cm-1)
Compound 12a
3341.86
3254.20
3056.13
2926.06
2206.60
1649.48
1615.97
1573.92
1534.76
1489.06
1470.12
1449.60
1403.18
1304.98
1284.88
1222.67
1178.58
1150.28
1096.07
1075.70
1025.85
1006.27
967.04
920.33
906.71
881.87
844.63
784.96
757.93
713.23
687.48
631.50
573.72
510.66
446.93


1H NMR 11h
10.80
9.98
7.91
7.91
7.89
7.88
7.69
7.65
7.62
7.62
7.61
7.60
7.55
7.53
7.48
7.46
7.46
2.47
2.40
Compound 12a
HN
N
N
H
O
N
N
N
S
0.83
0.90
4.10
1.82
4.00
2.19
1.21
2.84
3.00
f1 (ppm)

1H NMR 11h

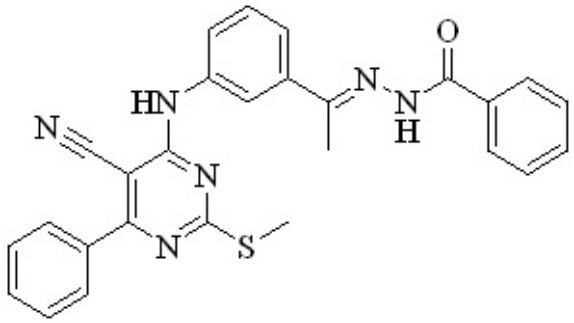


Compound 12a

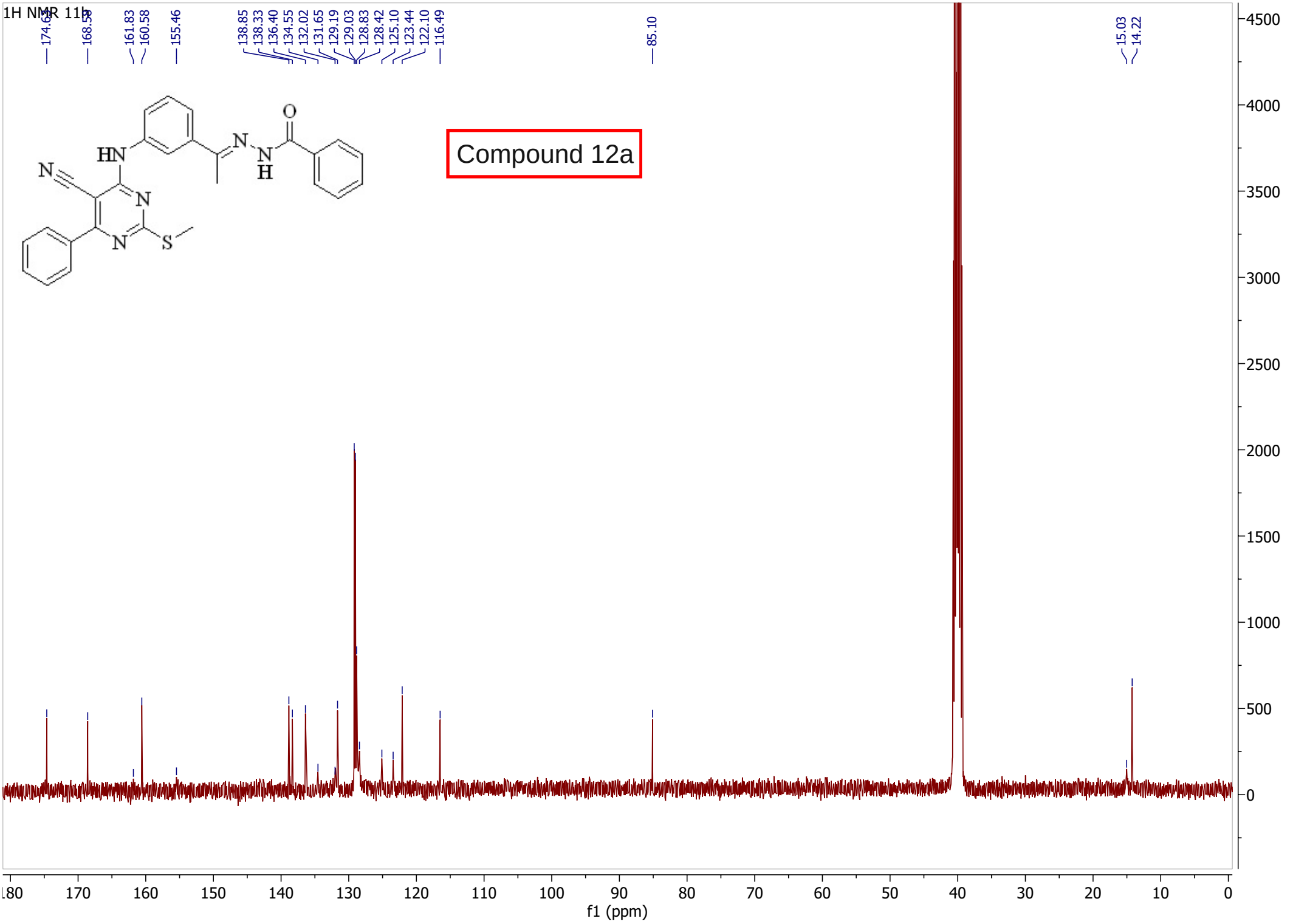
2.47
2.40
2.84
3.00

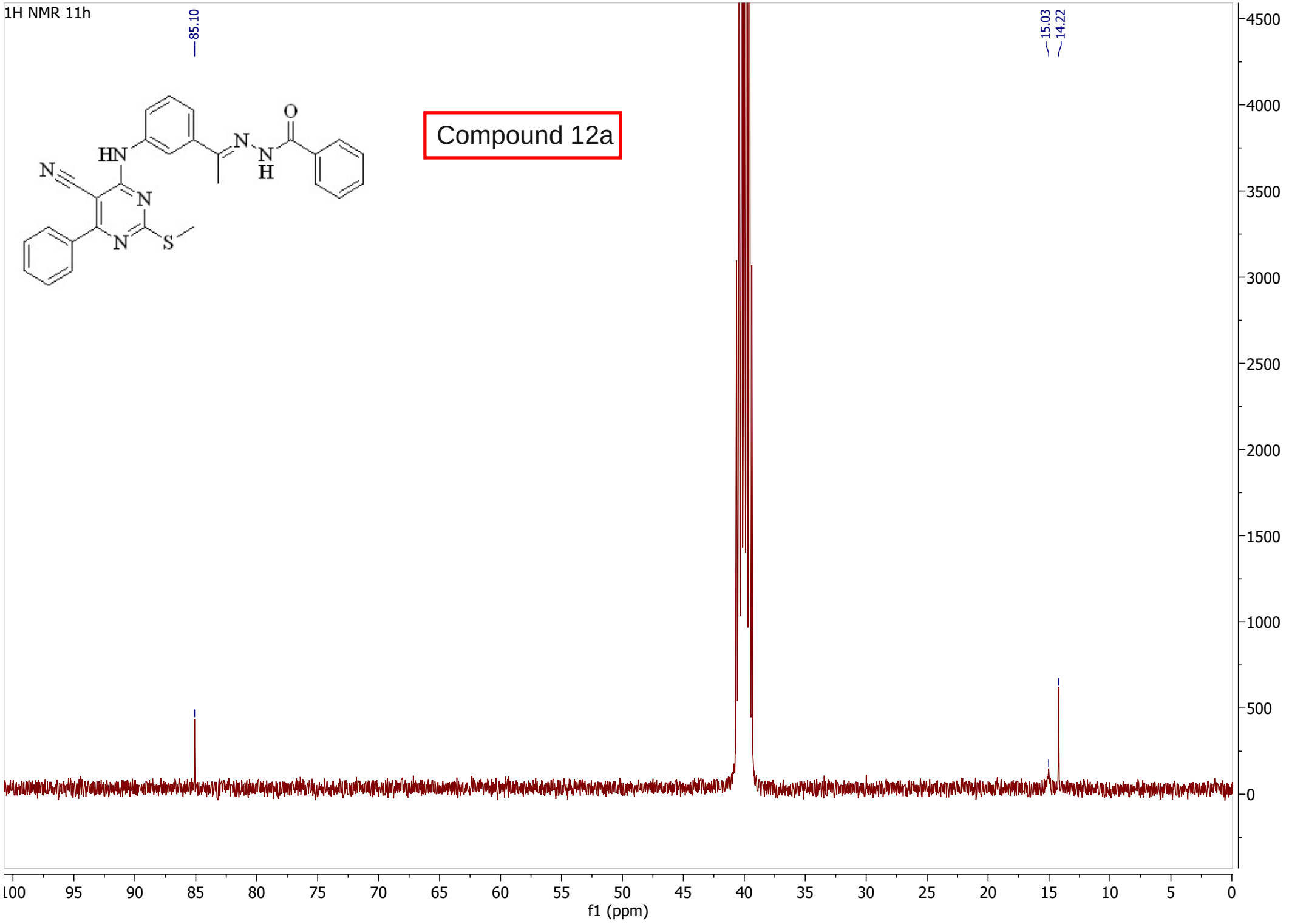
f1 (ppm)

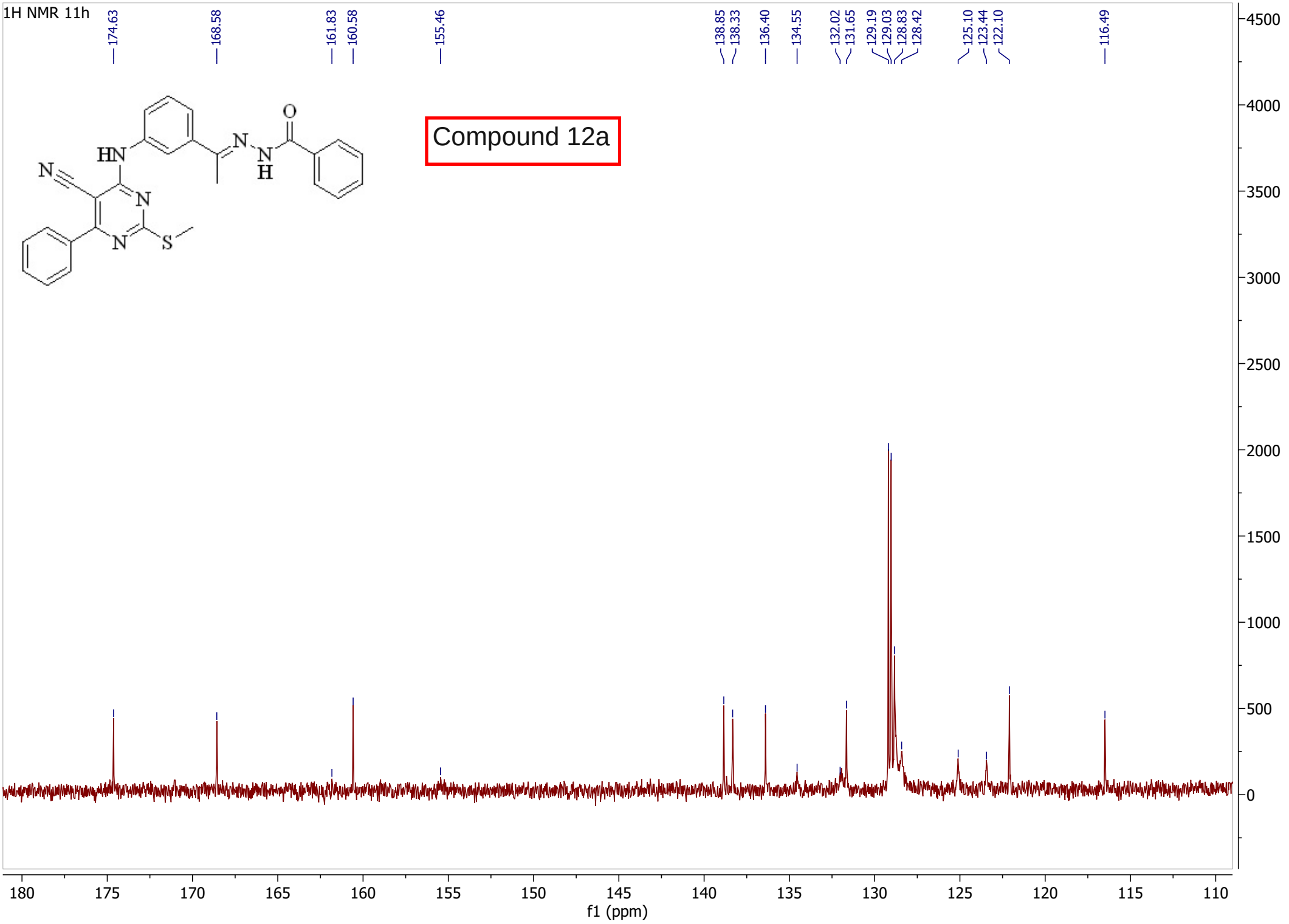
1H NMR 11h

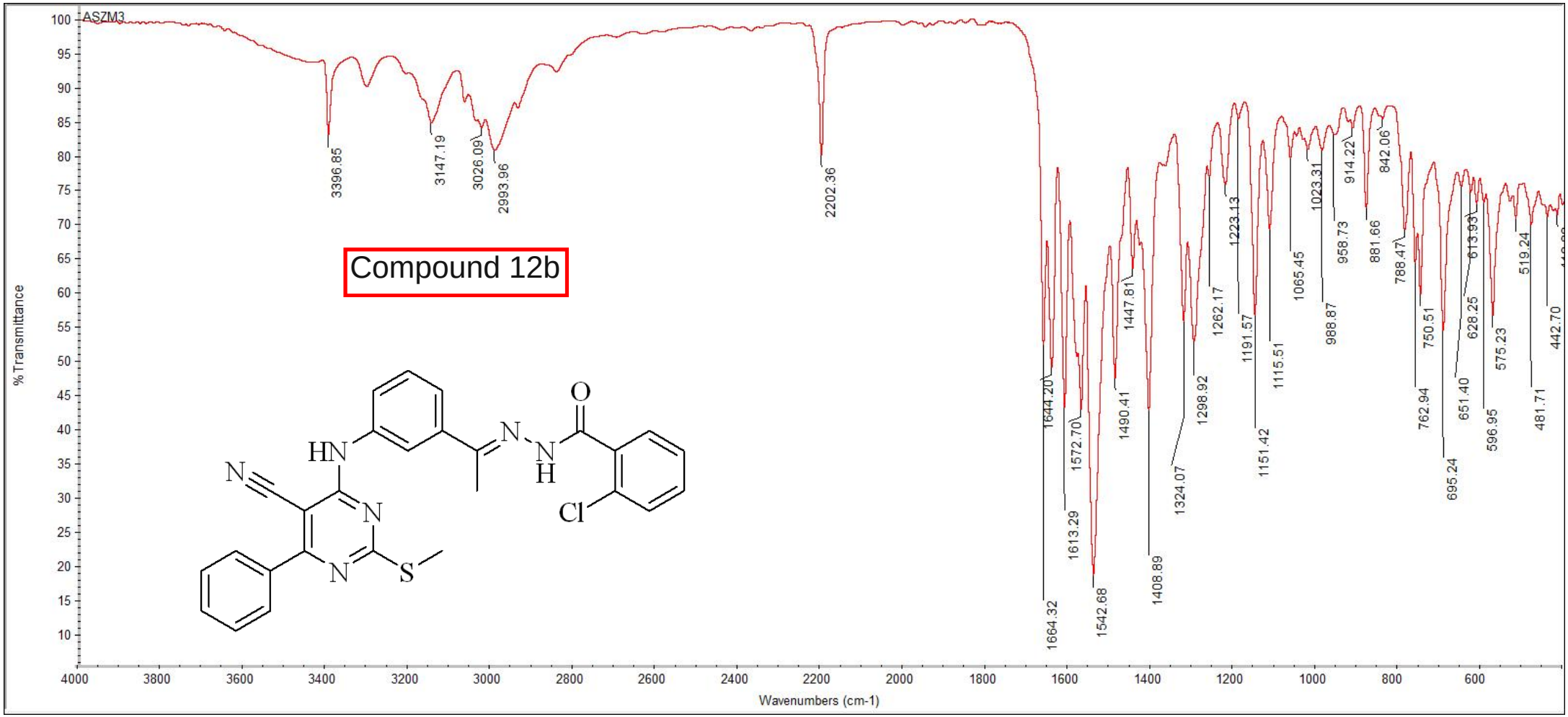


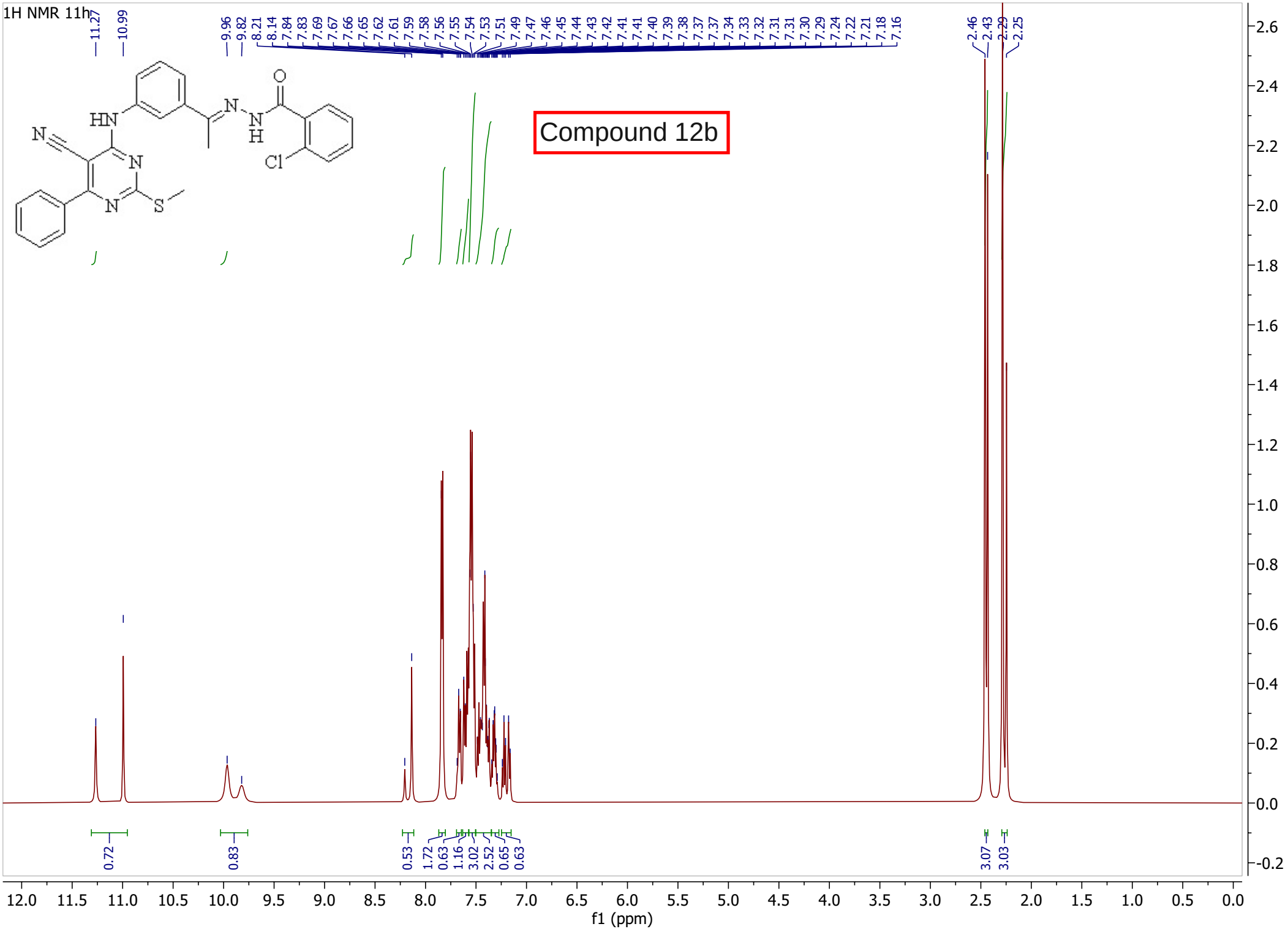
Compound 12a


1H NMR 11b
174.62
168.56
161.83
160.58
155.46
138.85
138.33
136.40
134.55
132.02
131.65
129.19
129.03
128.83
128.42
125.10
123.44
122.10
116.49
85.10
15.03
14.22
Compound 12a
HN
N
N
H
O
N
N
N
S
4500
4000
3500
3000
2500
2000
1500
1000
500
0
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

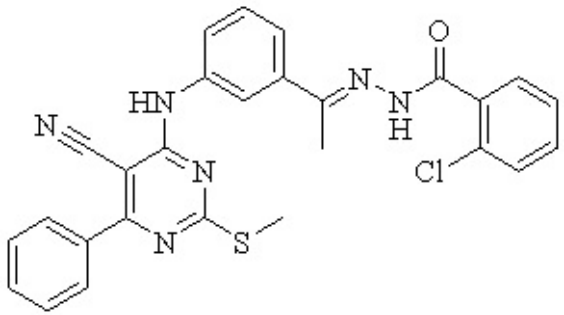

1H NMR 11h
85.10
15.03
14.22
Compound 12a
HN
N
N
H
O
N
N
N
S
4500
4000
3500
3000
2500
2000
1500
1000
500
0
100
95
90
85
80
75
70
65
60
55
50
45
40
35
30
25
20
15
10
5
0
f1 (ppm)


1H NMR 11h
174.63
168.58
161.83
160.58
155.46
138.85
138.33
136.40
134.55
132.02
131.65
129.19
129.03
128.83
128.42
125.10
123.44
122.10
116.49
Compound 12a
HN
N
N
H
O
N
N
N
S
4500
4000
3500
3000
2500
2000
1500
1000
500
0
180
175
170
165
160
155
150
145
140
135
130
125
120
115
110
f1 (ppm)


ASZM3
% Transmittance
Wavenumbers (cm-1)
Compound 12b
3396.85
3147.19
3026.09
2993.96
2202.36
1664.32
1644.20
1613.29
1572.70
1542.68
1490.41
1447.81
1408.89
1324.07
1298.92
1262.17
1223.13
1191.57
1151.42
1115.51
1065.45
1023.31
988.87
958.73
914.22
881.66
842.06
788.47
762.94
750.51
695.24
651.40
628.25
613.93
596.95
575.23
519.24
481.71
442.70


1H NMR 11h
Compound 12b
f1 (ppm)

1H NMR 11h

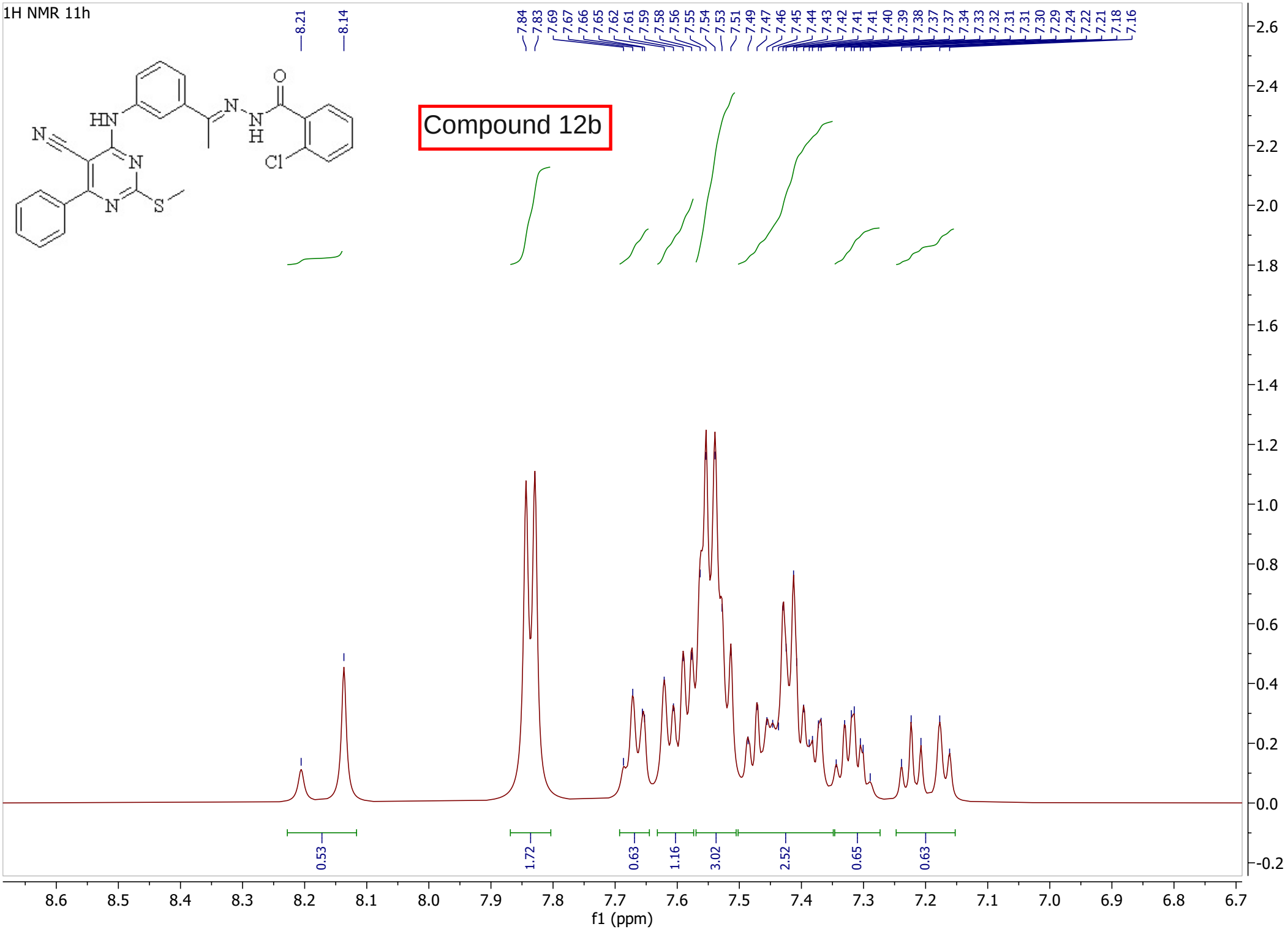


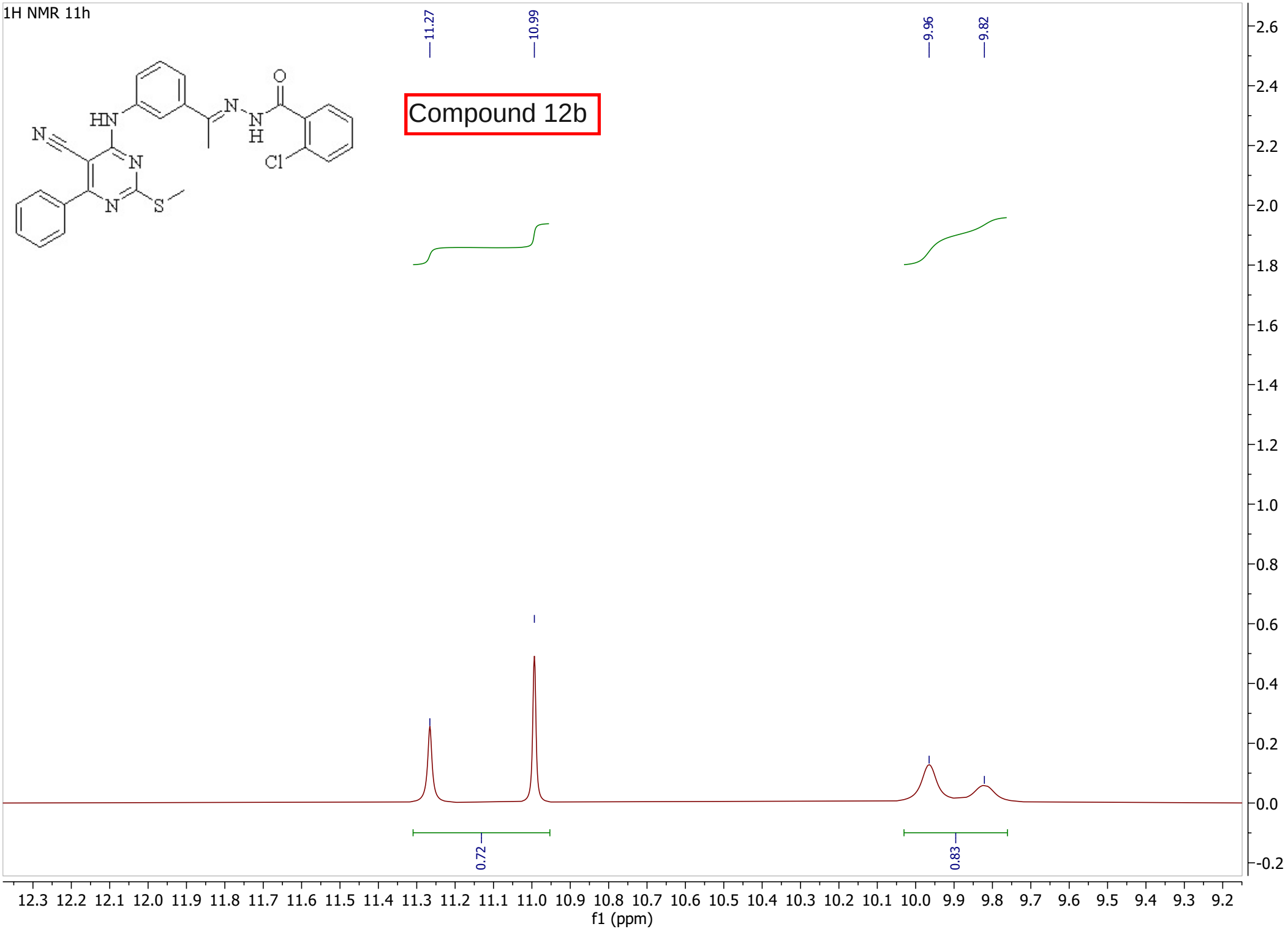
Compound 12b

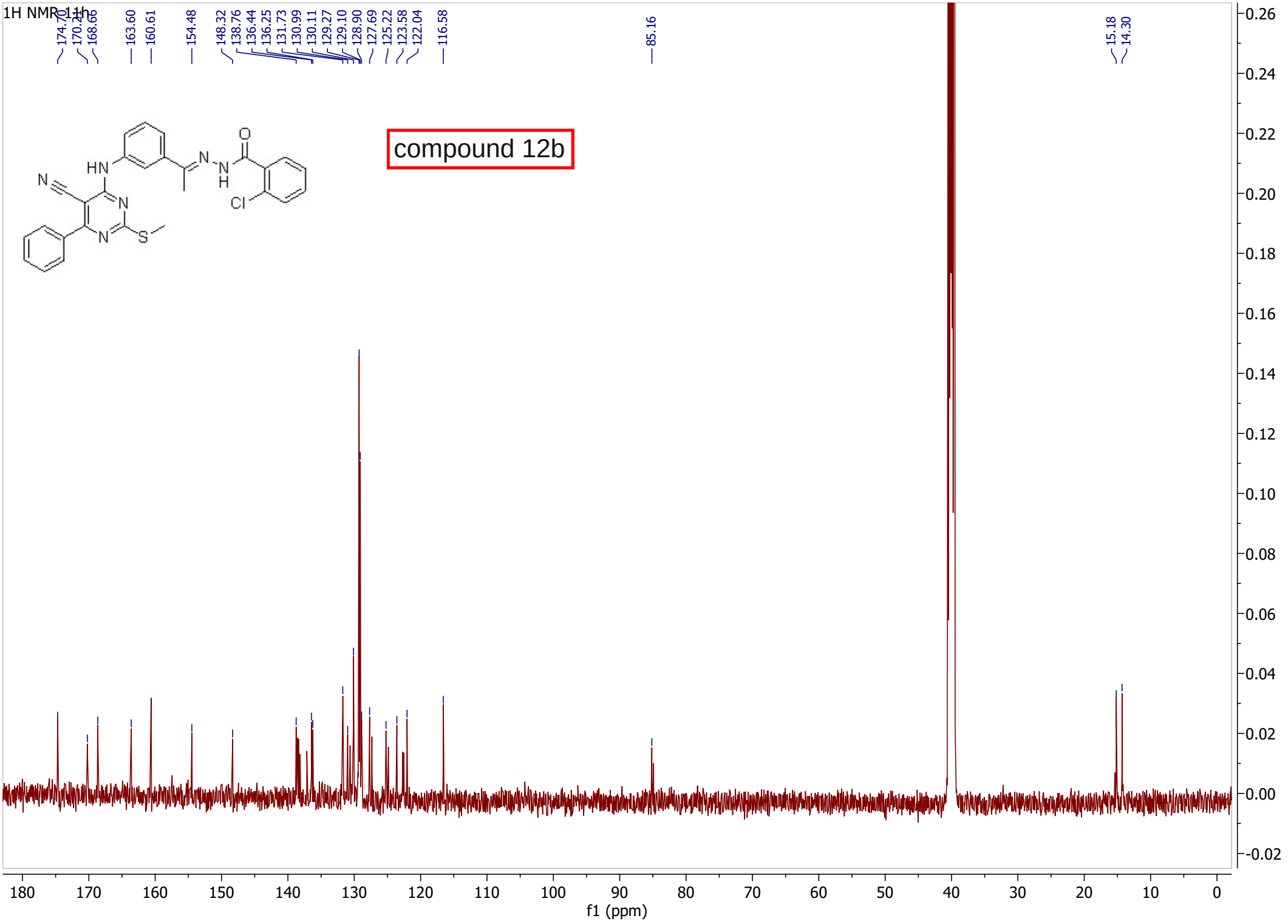
2.46
2.43
2.29
2.25

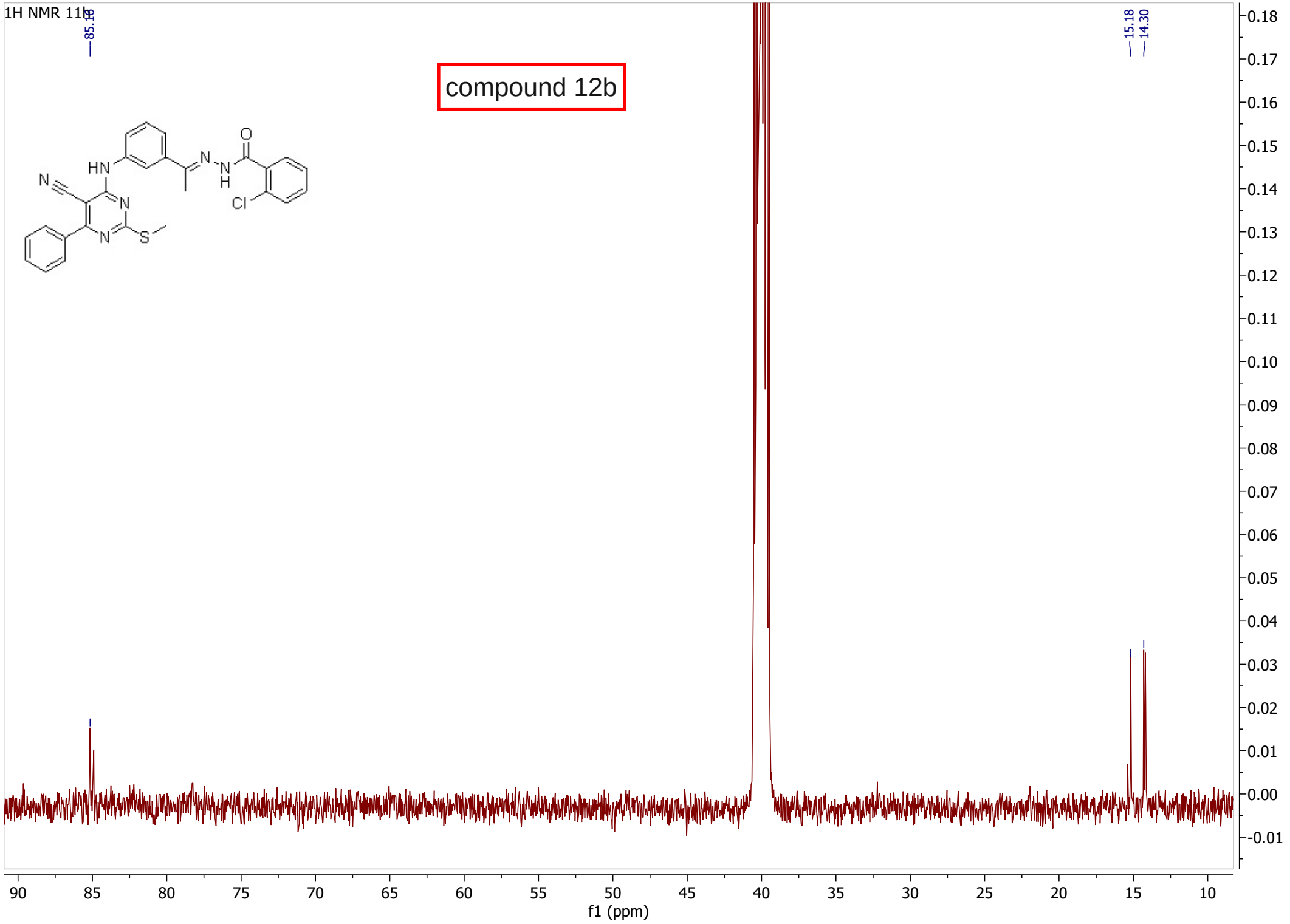
3.07
3.03

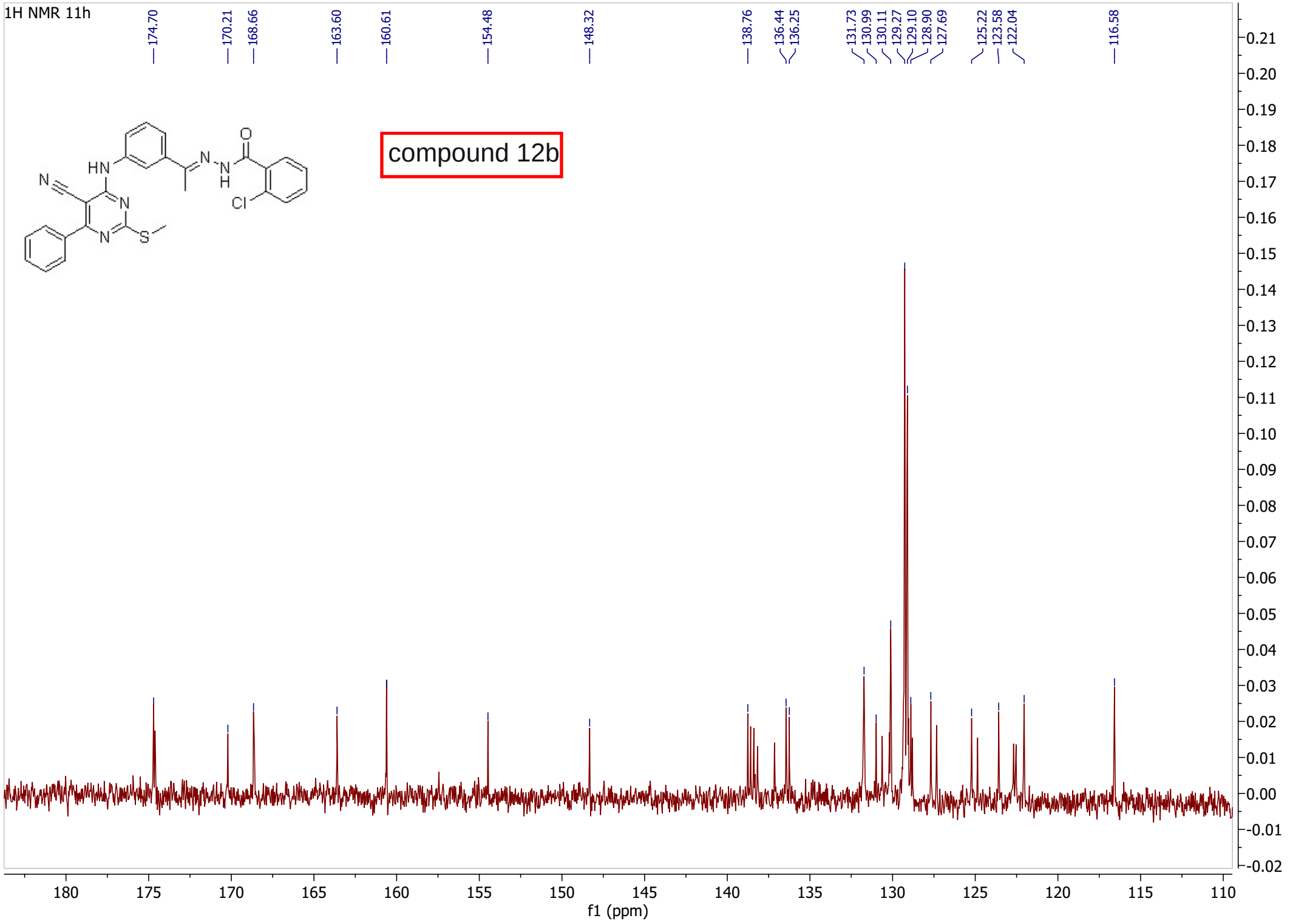
f1 (ppm)

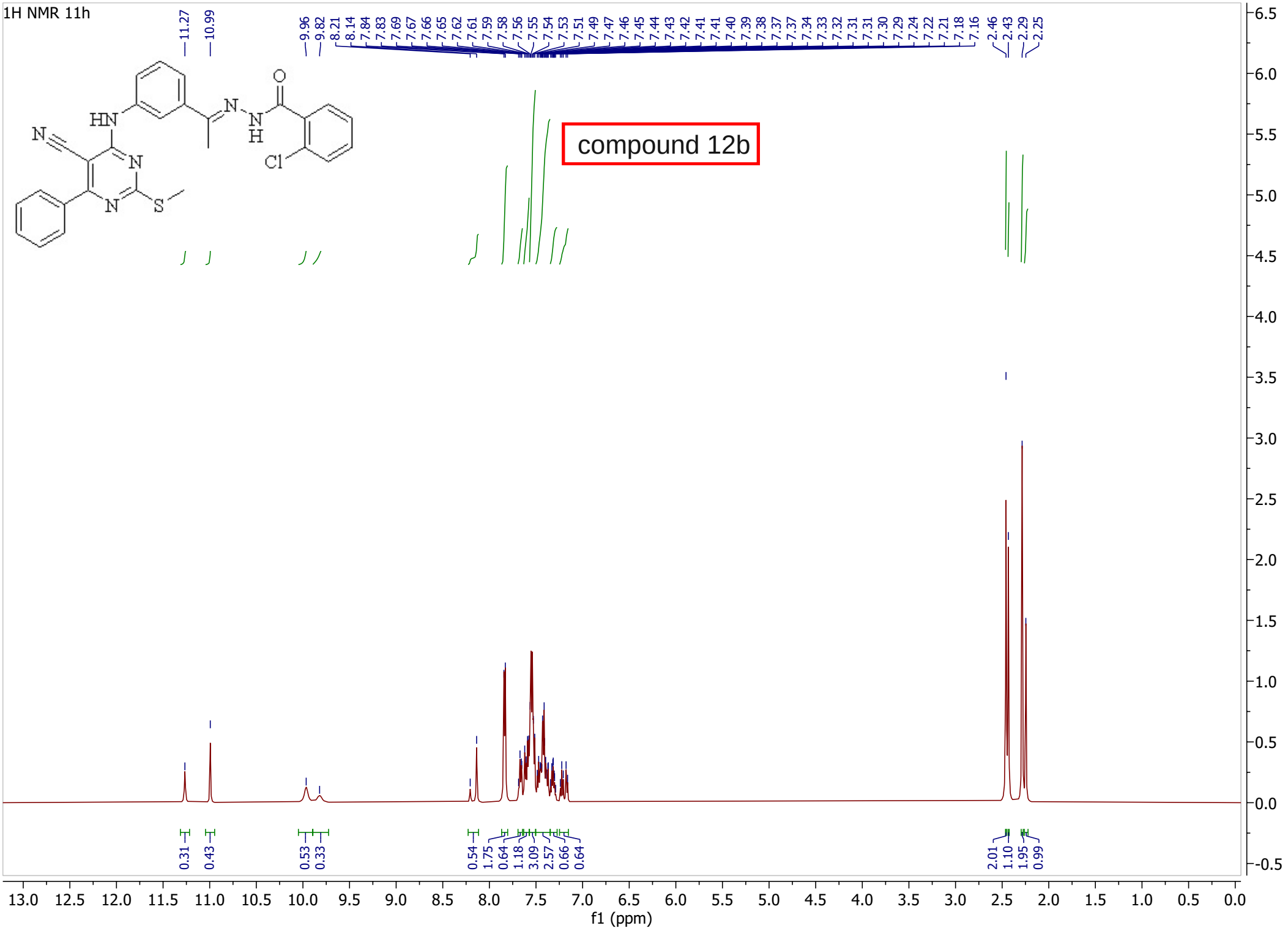

1H NMR 11h
Compound 12b
8.21
8.14
7.84
7.83
7.69
7.67
7.66
7.65
7.62
7.61
7.59
7.58
7.56
7.55
7.54
7.53
7.51
7.49
7.47
7.46
7.45
7.44
7.43
7.42
7.41
7.41
7.40
7.39
7.38
7.37
7.37
7.34
7.33
7.32
7.31
7.31
7.30
7.29
7.24
7.22
7.21
7.18
7.16
0.53
1.72
0.63
1.16
3.02
2.52
0.65
0.63
f1 (ppm)

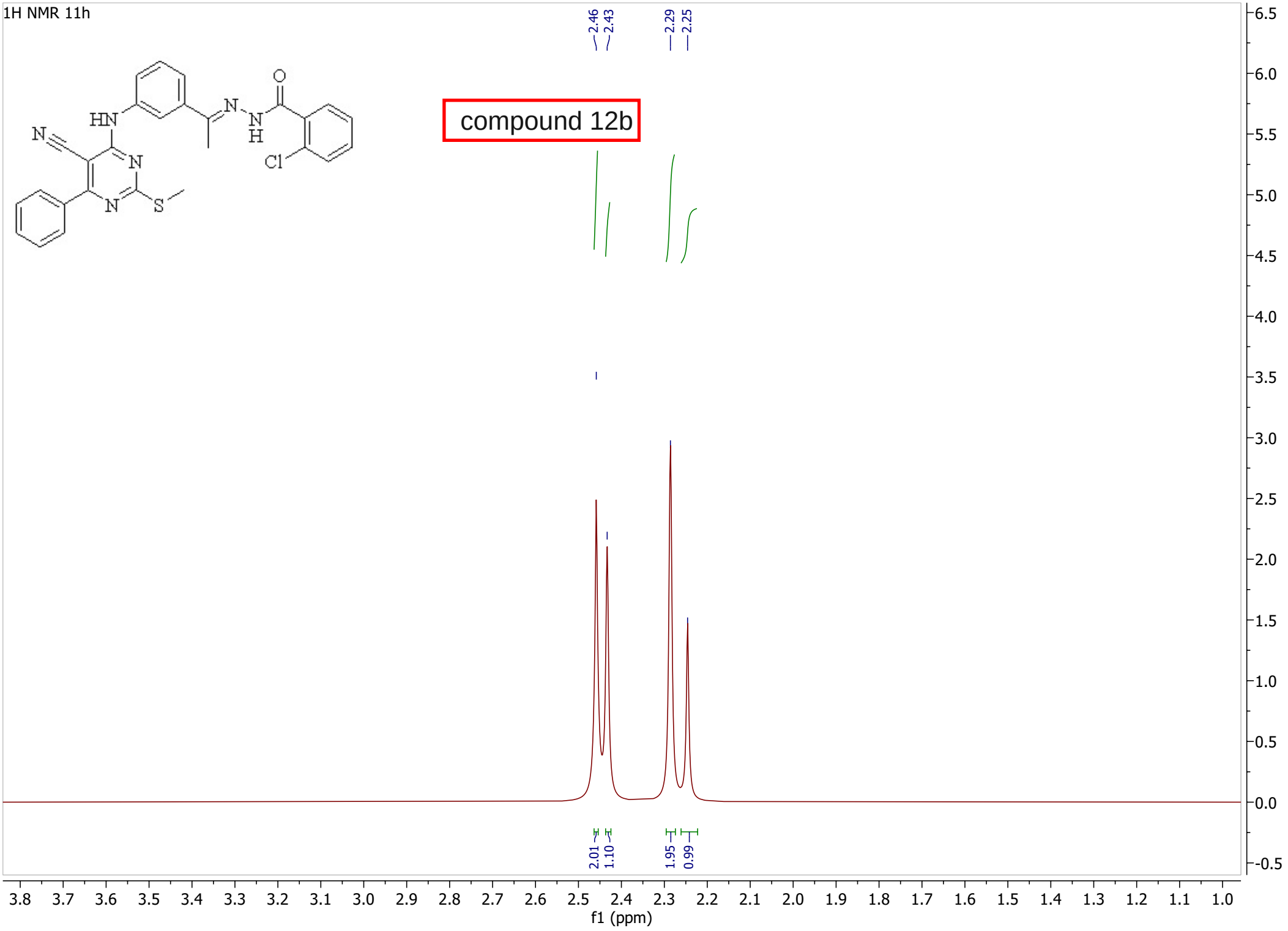

1H NMR 11h
11.27
10.99
9.96
9.82
Compound 12b
HN
N
N
H
Cl
N
N
N
S
0.72
0.83
2.6
2.4
2.2
2.0
1.8
1.6
1.4
1.2
1.0
0.8
0.6
0.4
0.2
0.0
-0.2
12.3 12.2 12.1 12.0 11.9 11.8 11.7 11.6 11.5 11.4 11.3 11.2 11.1 11.0 10.9 10.8 10.7 10.6 10.5 10.4 10.3 10.2 10.1 10.0 9.9 9.8 9.7 9.6 9.5 9.4 9.3 9.2
f1 (ppm)

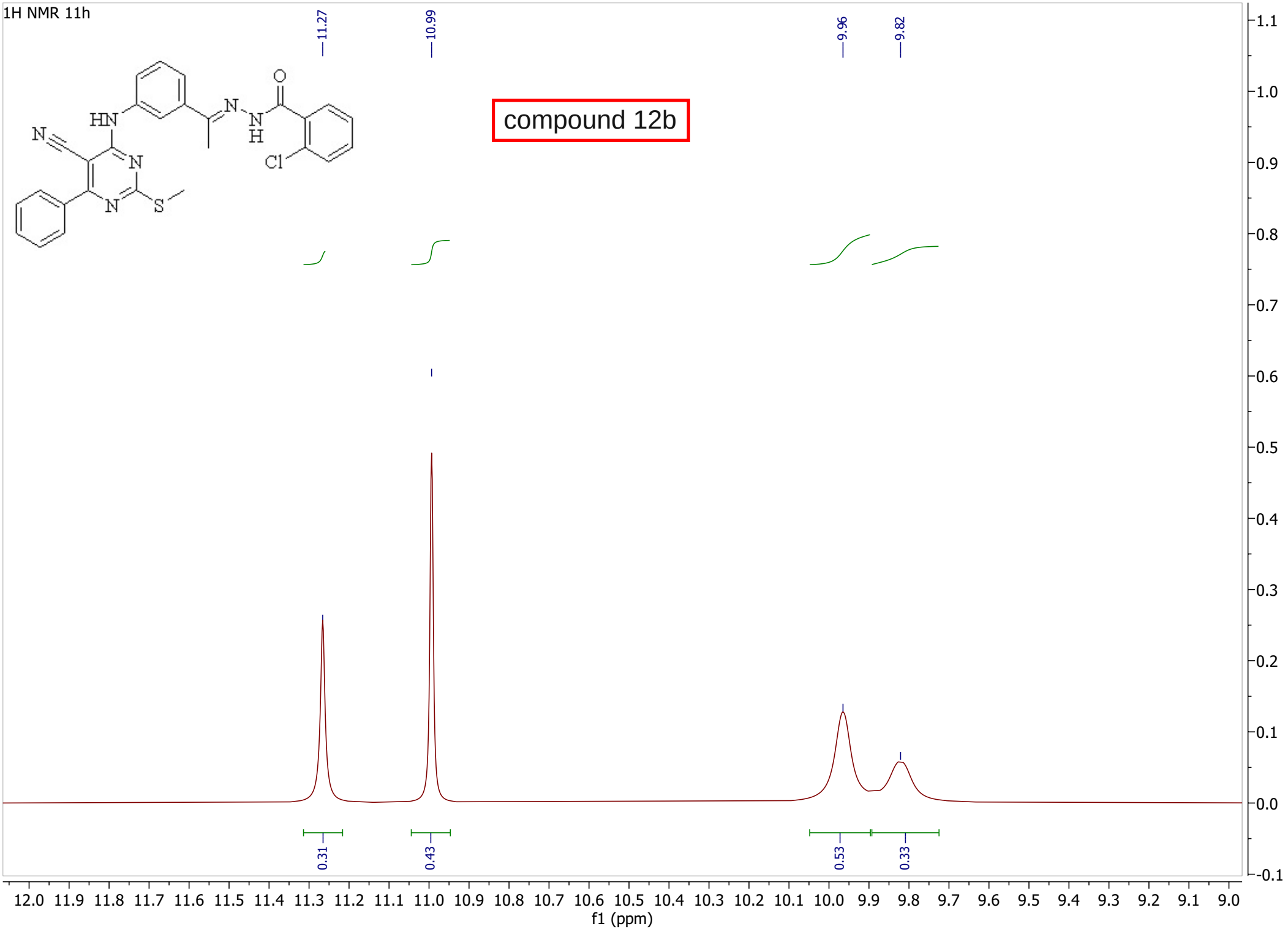

1H NMR 11h
174.70
170.21
168.66
163.60
160.61
154.48
148.32
138.76
136.44
136.25
131.73
130.99
130.11
129.27
129.10
128.90
127.69
125.22
123.58
122.04
116.58
85.16
15.18
14.30
compound 12b
HN
N
N
N
S
O
N
H
Cl
0.26
0.24
0.22
0.20
0.18
0.16
0.14
0.12
0.10
0.08
0.06
0.04
0.02
0.00
-0.02
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


1H NMR 11b
85.18
15.18
14.30
compound 12b
HN
N
N
N
S
N
N
H
O
Cl
0.18
0.17
0.16
0.15
0.14
0.13
0.12
0.11
0.10
0.09
0.08
0.07
0.06
0.05
0.04
0.03
0.02
0.01
0.00
-0.01
90
85
80
75
70
65
60
55
50
45
40
35
30
25
20
15
10
f1 (ppm)


1H NMR 11h
174.70
170.21
168.66
163.60
160.61
154.48
148.32
138.76
136.44
136.25
131.73
130.99
130.11
129.27
129.10
128.90
127.69
125.22
123.58
122.04
116.58
compound 12b
HN
N
N
N
S
N
H
O
Cl
f1 (ppm)

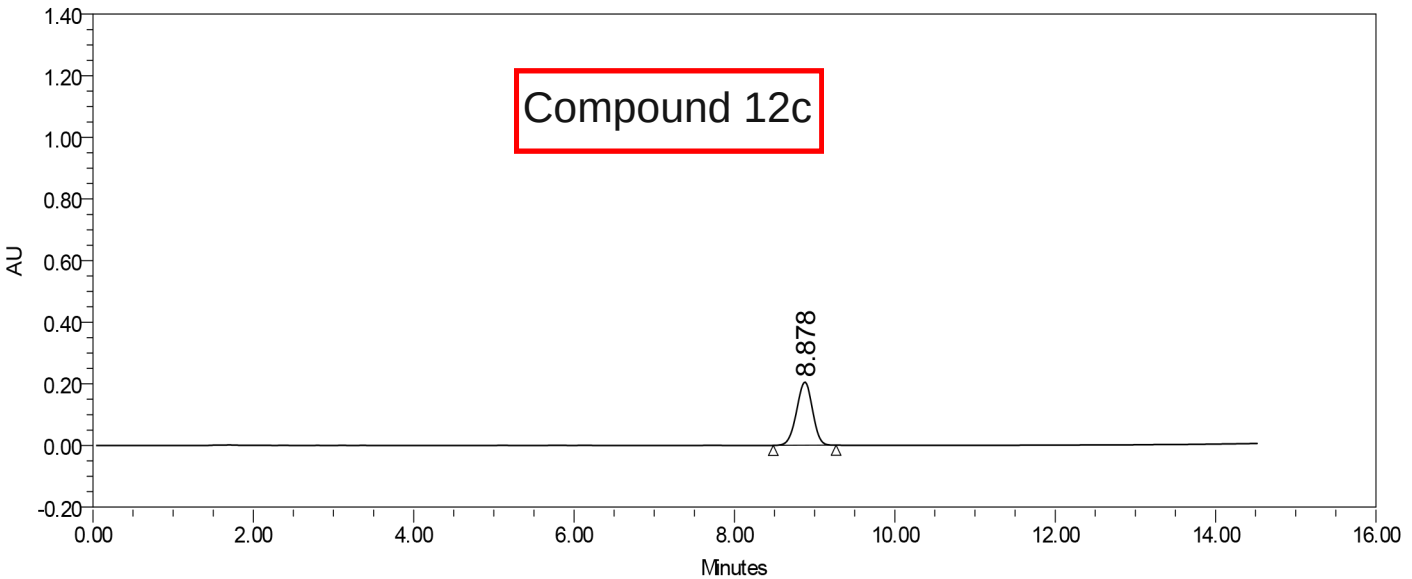

1H NMR 11h
compound 12b
f1 (ppm)


1H NMR 11h
compound 12b
2.46
2.43
2.29
2.25
2.01
1.10
1.95
0.99
f1 (ppm)


1H NMR 11h
11.27
10.99
9.96
9.82
compound 12b
HN
N
N
H
Cl
N
N
N
S
0.31
0.43
0.53
0.33
1.1
1.0
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0.0
-0.1
12.0 11.9 11.8 11.7 11.6 11.5 11.4 11.3 11.2 11.1 11.0 10.9 10.8 10.7 10.6 10.5 10.4 10.3 10.2 10.1 10.0 9.9 9.8 9.7 9.6 9.5 9.4 9.3 9.2 9.1 9.0
f1 (ppm)

SAMPLE INFORMATION

Sample Name:	ASZM8 Compound 12c	Acquired By:	System
Sample Type:	Unknown	Sample Set Name:	1
Vial:	20	Acq. Method Set:	Organic1
Injection #:	1	Processing Method:	Default
Injection Volume:	2.00 ul	Channel Name:	275.0nm
Run Time:	14.5 Minutes	Proc. Chnl. Descr.:	W2996 PDA 275.0 nm (PDA 190.0 to
Date Acquired:	11/5/2022 9:59:08 PM EET		
Date Processed:	11/6/2022 5:29:15 AM EET		



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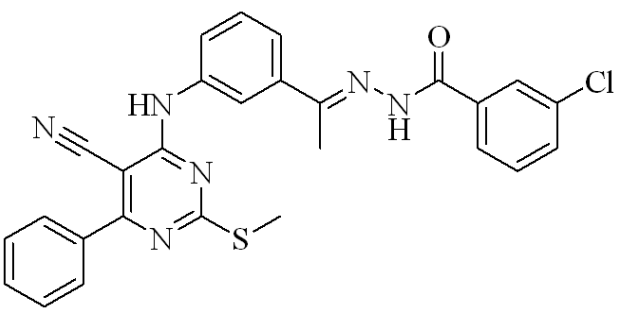
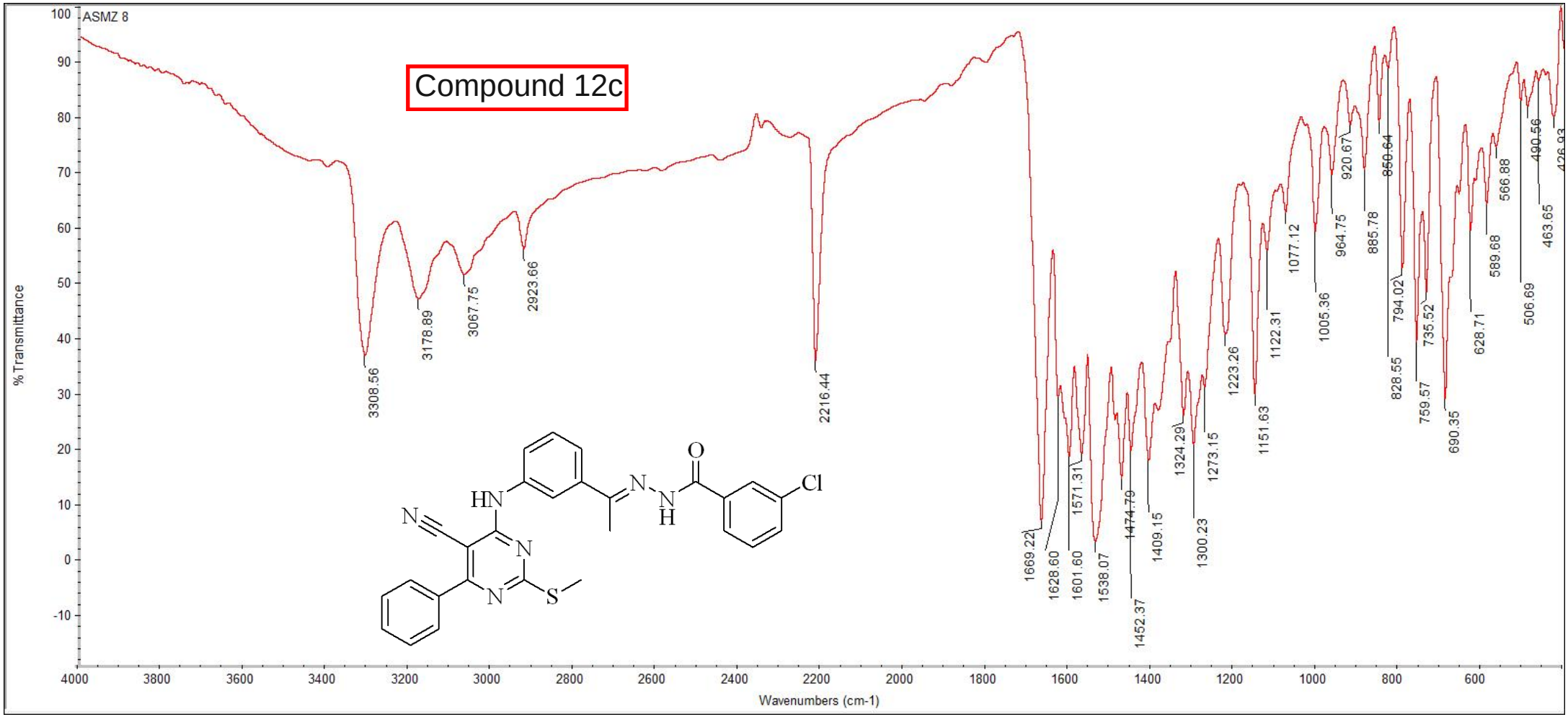
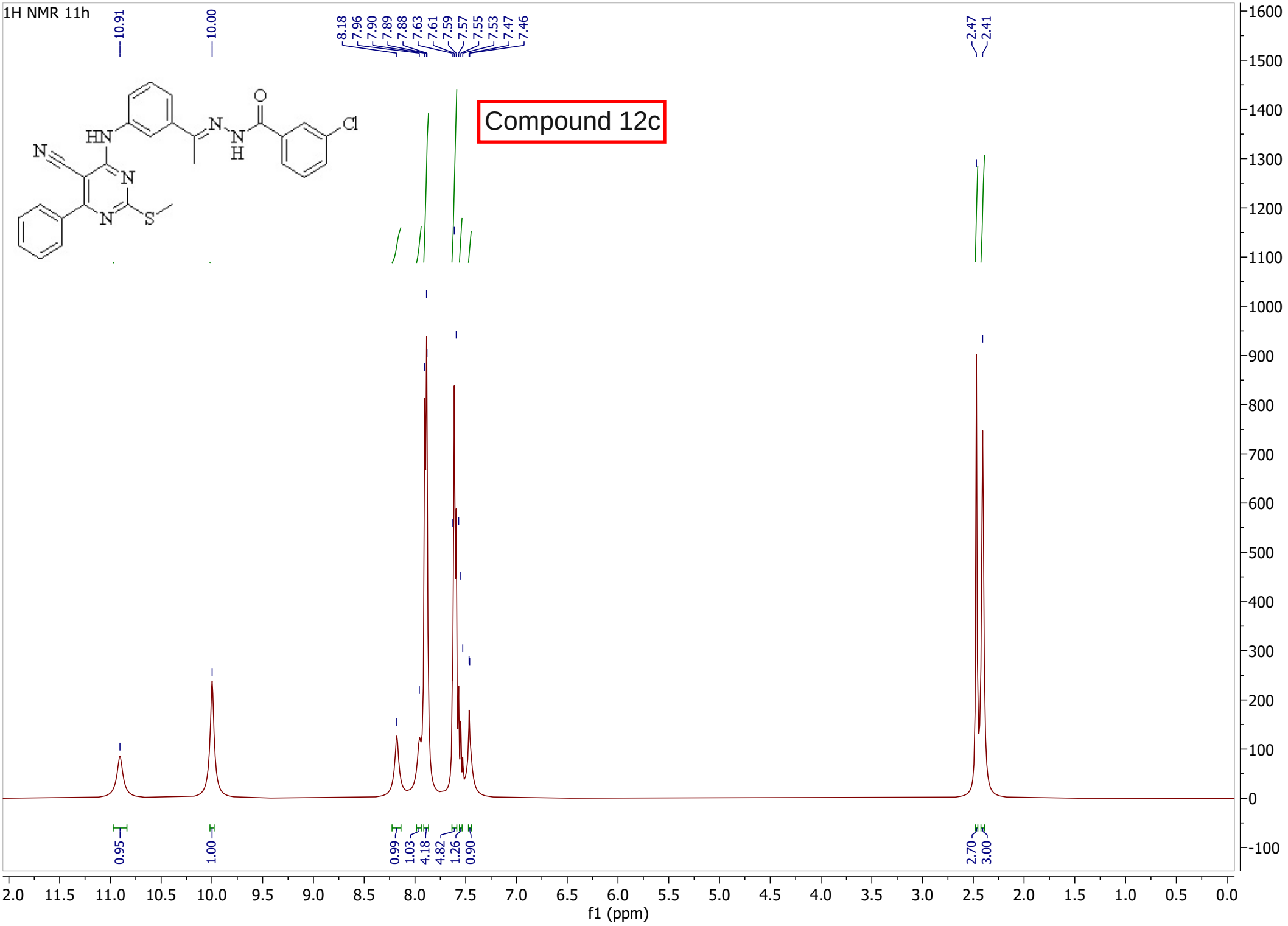
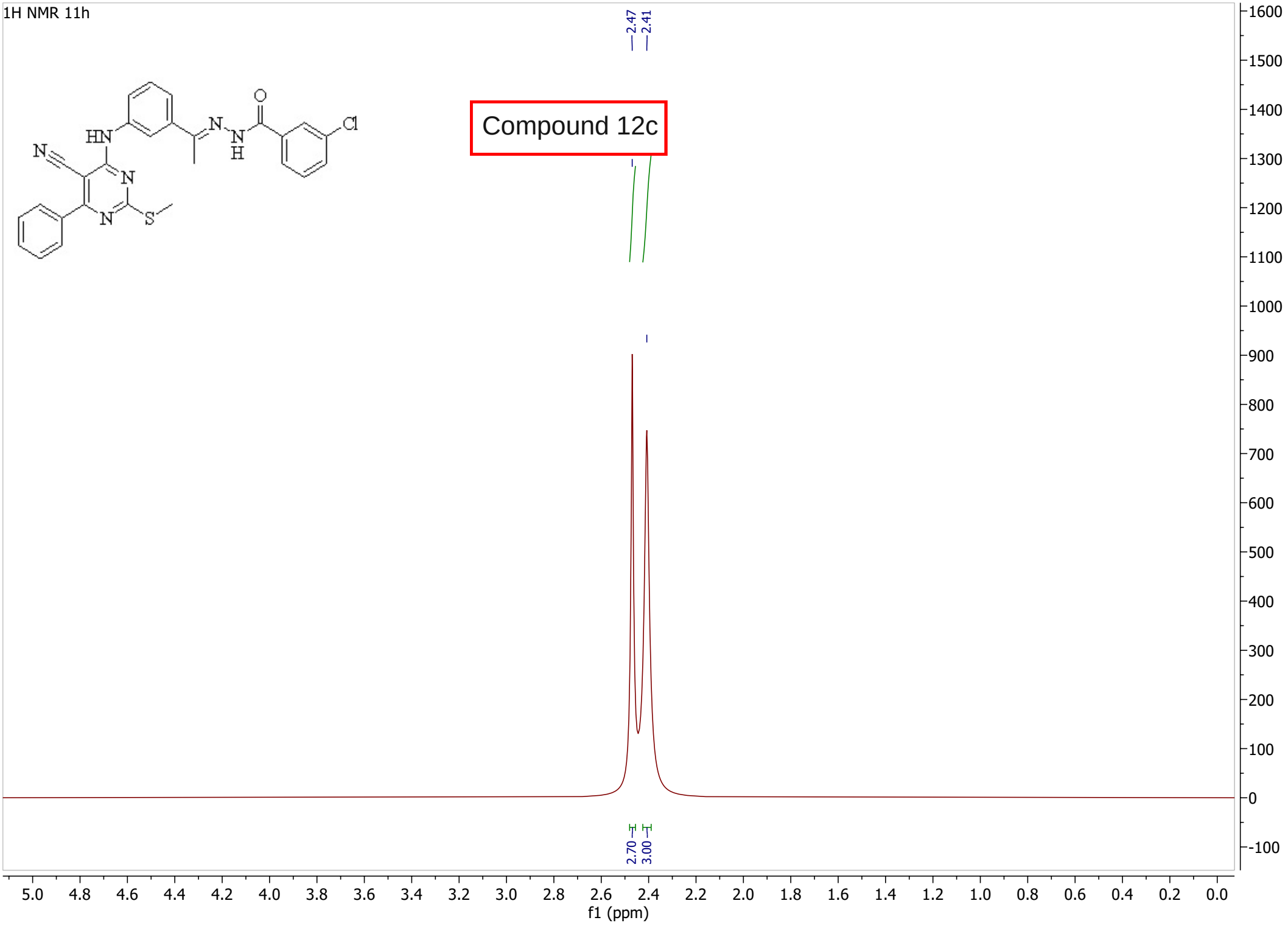
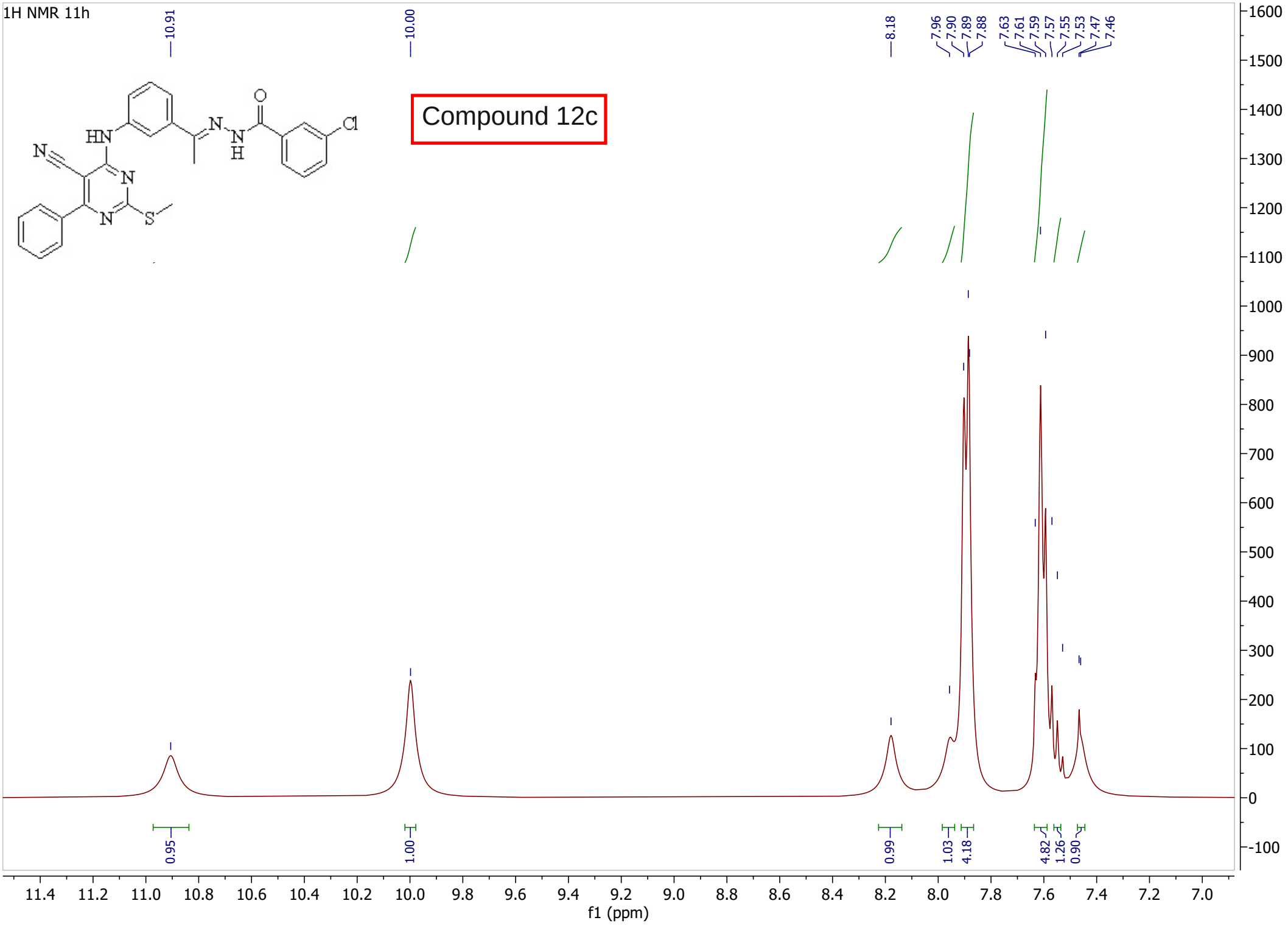
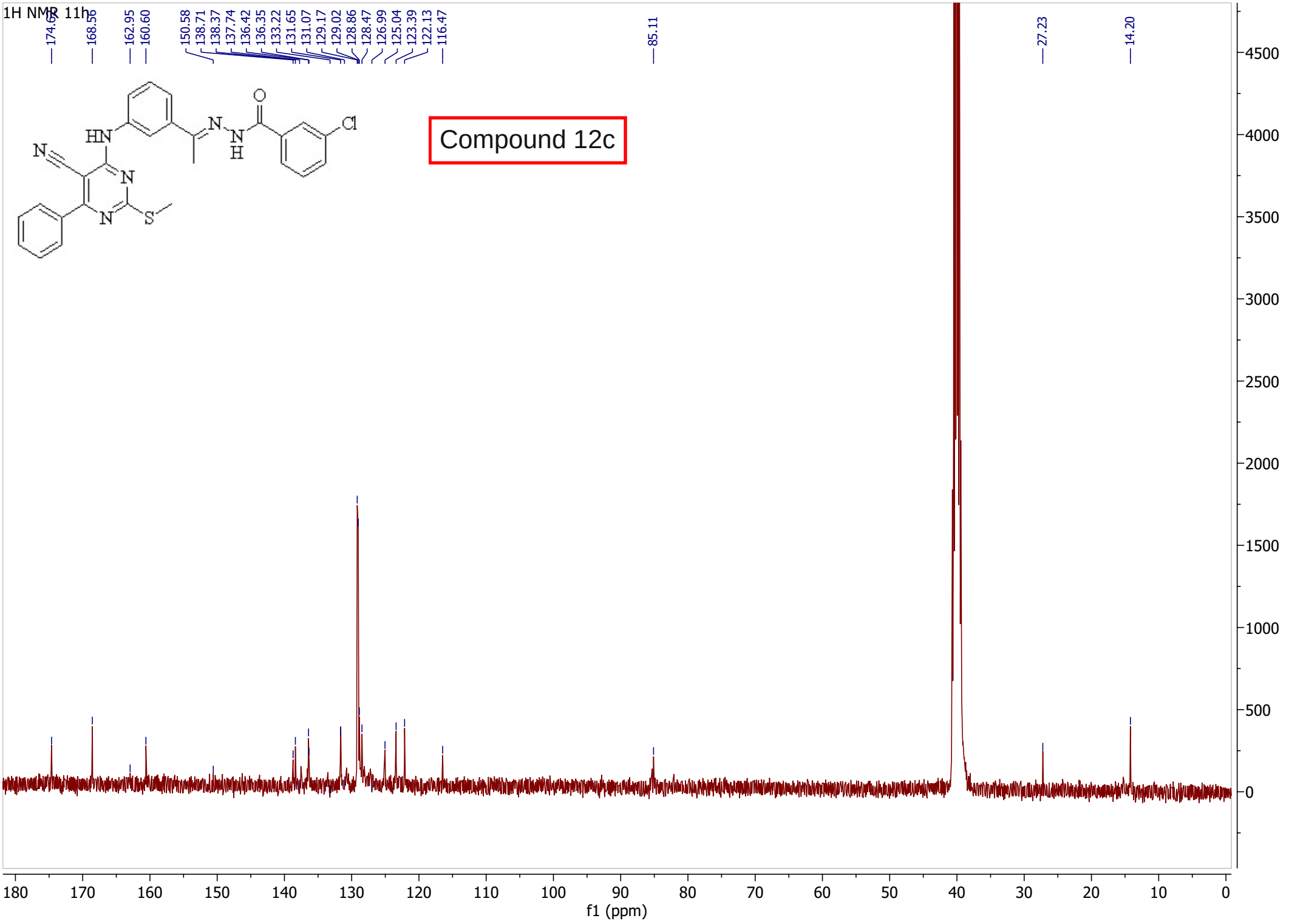


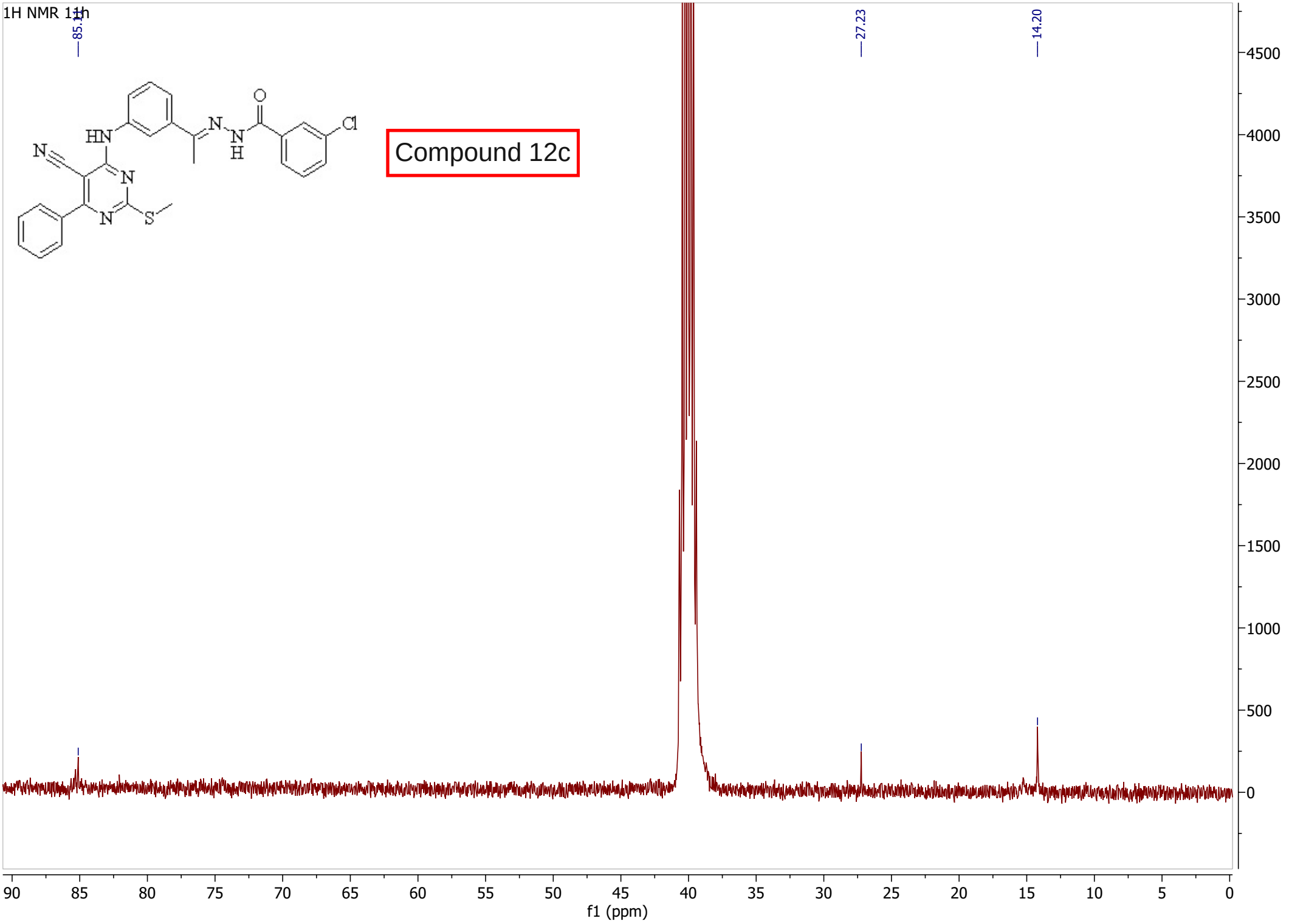

ASMZ 8
Compound 12c
% Transmittance
Wavenumbers (cm-1)
3308.56
3178.89
3067.75
2923.66
2216.44
1669.22
1628.60
1601.60
1571.31
1538.07
1474.79
1452.37
1409.15
1324.29
1300.23
1273.15
1223.26
1151.63
1122.31
1077.12
1005.36
964.75
920.67
885.78
850.64
828.55
794.02
759.57
735.52
690.35
628.71
589.68
566.88
506.69
490.56
463.65
HN
N
N
N
H
O
Cl
S

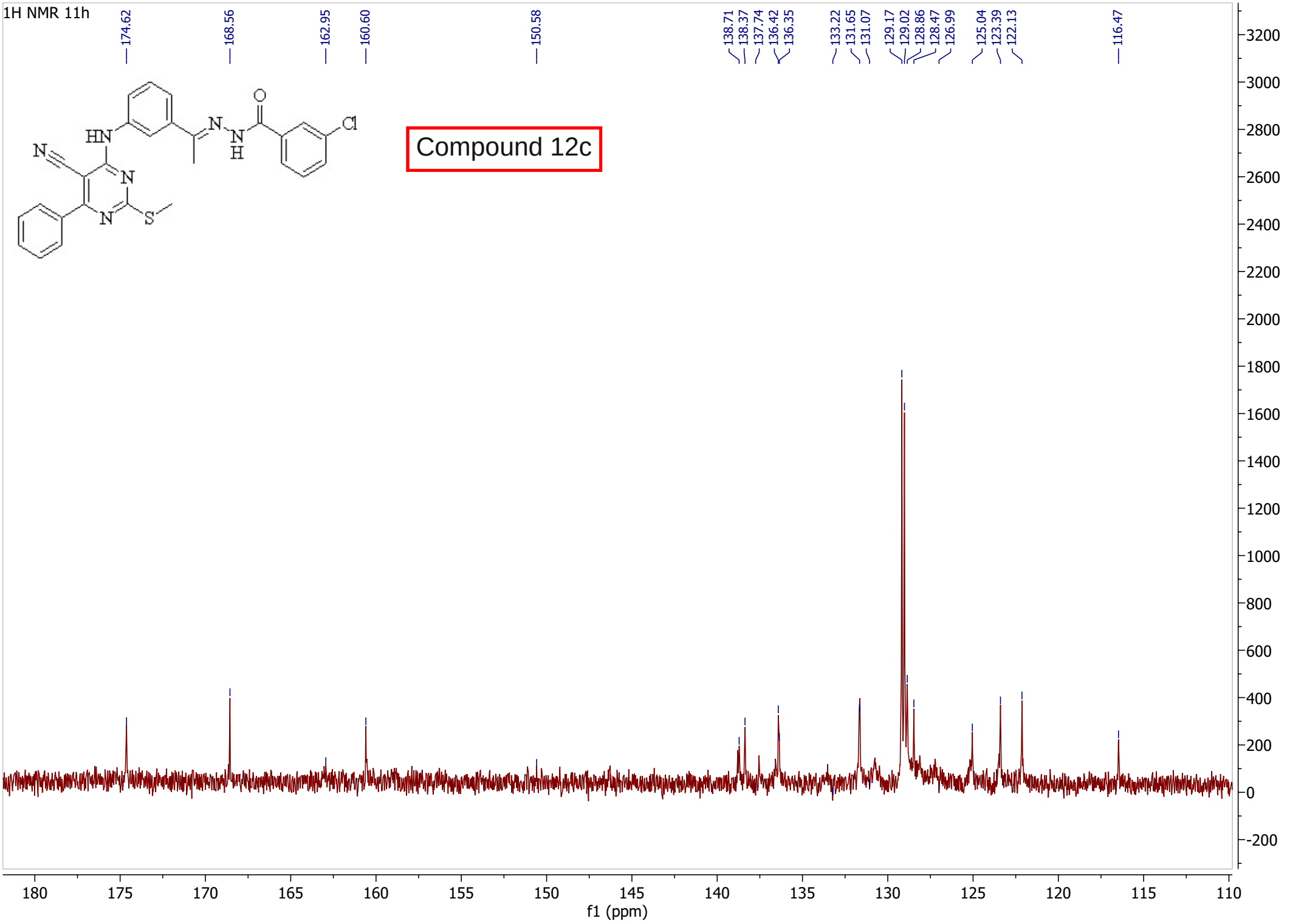

1H NMR 11h
10.91
10.00
8.18
7.96
7.90
7.89
7.88
7.63
7.61
7.59
7.57
7.55
7.53
7.47
7.46
2.47
2.41
Compound 12c
HN
N
N
H
Cl
N
N
N
S
0.95
1.00
0.99
1.03
4.18
4.82
1.26
0.90
2.70
3.00
f1 (ppm)

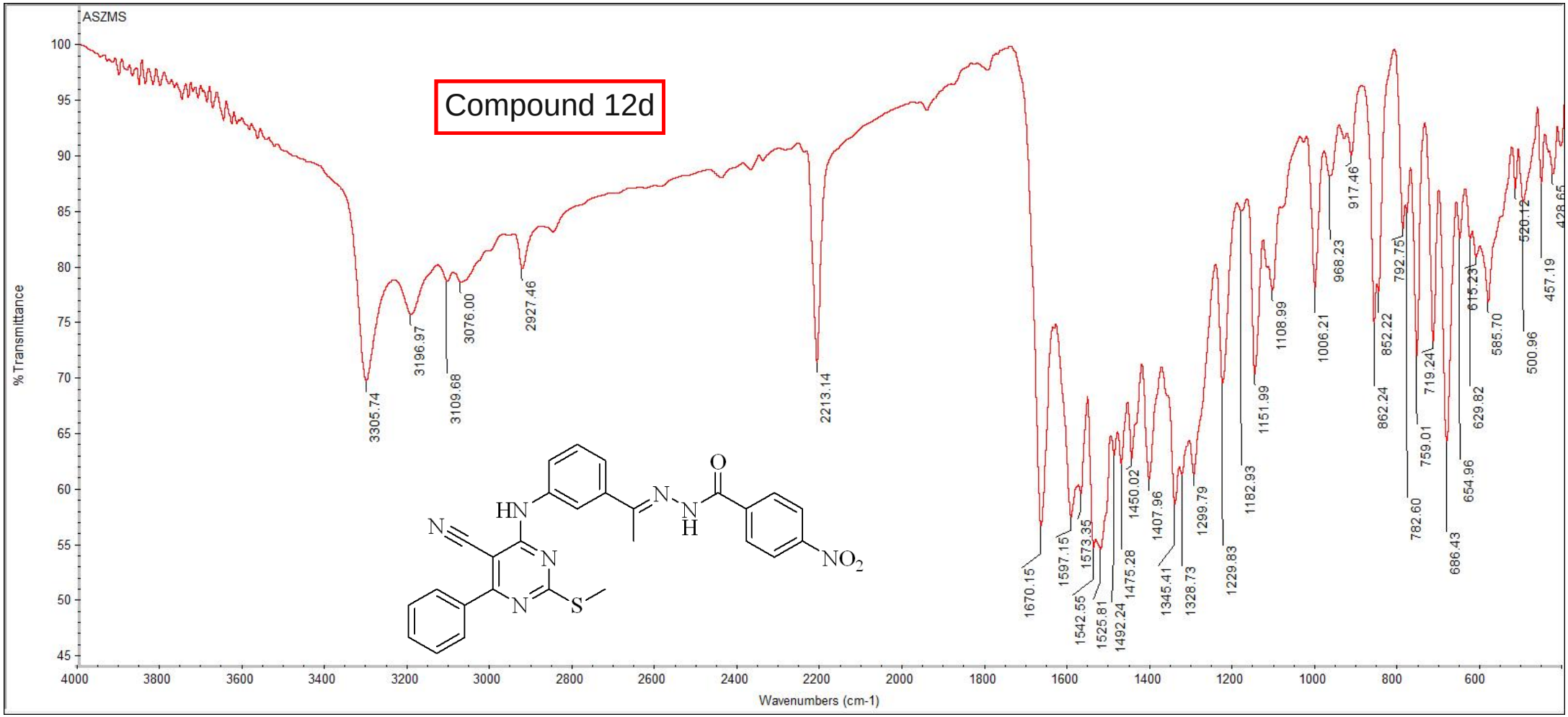

1H NMR 11h
Compound 12c
2.47
2.41
2.70
3.00
f1 (ppm)

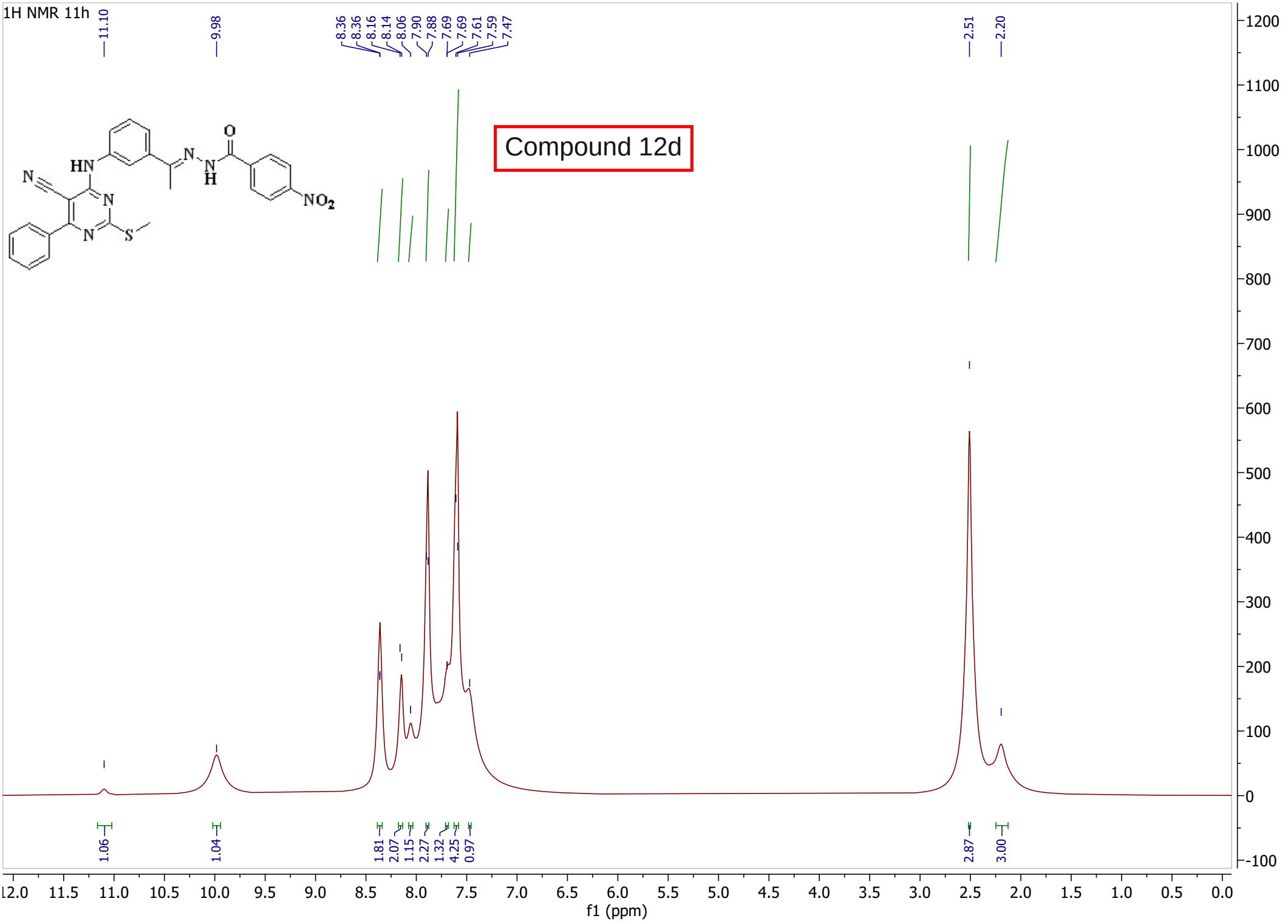

1H NMR 11h
10.91
10.00
8.18
7.96
7.90
7.89
7.88
7.63
7.61
7.59
7.57
7.55
7.53
7.47
7.46
Compound 12c
HN
N
N
H
Cl
N
N
N
S
0.95
1.00
0.99
1.03
4.18
4.82
1.26
0.90
f1 (ppm)


1H NMR 11h
174.65
168.56
162.95
160.60
150.58
138.71
138.37
137.74
136.42
136.35
133.22
131.65
131.07
129.17
129.02
128.86
128.47
126.99
125.04
123.39
122.13
116.47
85.11
27.23
14.20
Compound 12c
HN
N
N
H
Cl
N
N
N
S
O
4500
4000
3500
3000
2500
2000
1500
1000
500
0
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

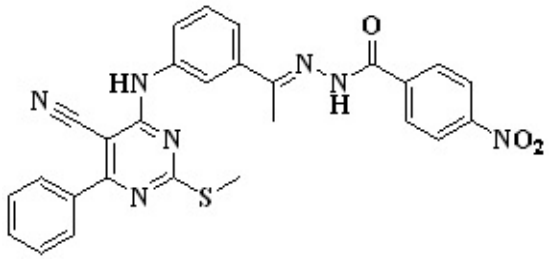

1H NMR 11h
85.11
27.23
14.20
Compound 12c
HN
N
N
H
Cl
N
N
N
S
4500
4000
3500
3000
2500
2000
1500
1000
500
0
90
85
80
75
70
65
60
55
50
45
40
35
30
25
20
15
10
5
0
f1 (ppm)


1H NMR 11h
174.62
168.56
162.95
160.60
150.58
138.71
138.37
137.74
136.42
136.35
133.22
131.65
131.07
129.17
129.02
128.86
128.47
126.99
125.04
123.39
122.13
116.47
Compound 12c
HN
N
N
H
Cl
N
N
N
S
3200
3000
2800
2600
2400
2200
2000
1800
1600
1400
1200
1000
800
600
400
200
0
-200
180
175
170
165
160
155
150
145
140
135
130
125
120
115
110
f1 (ppm)

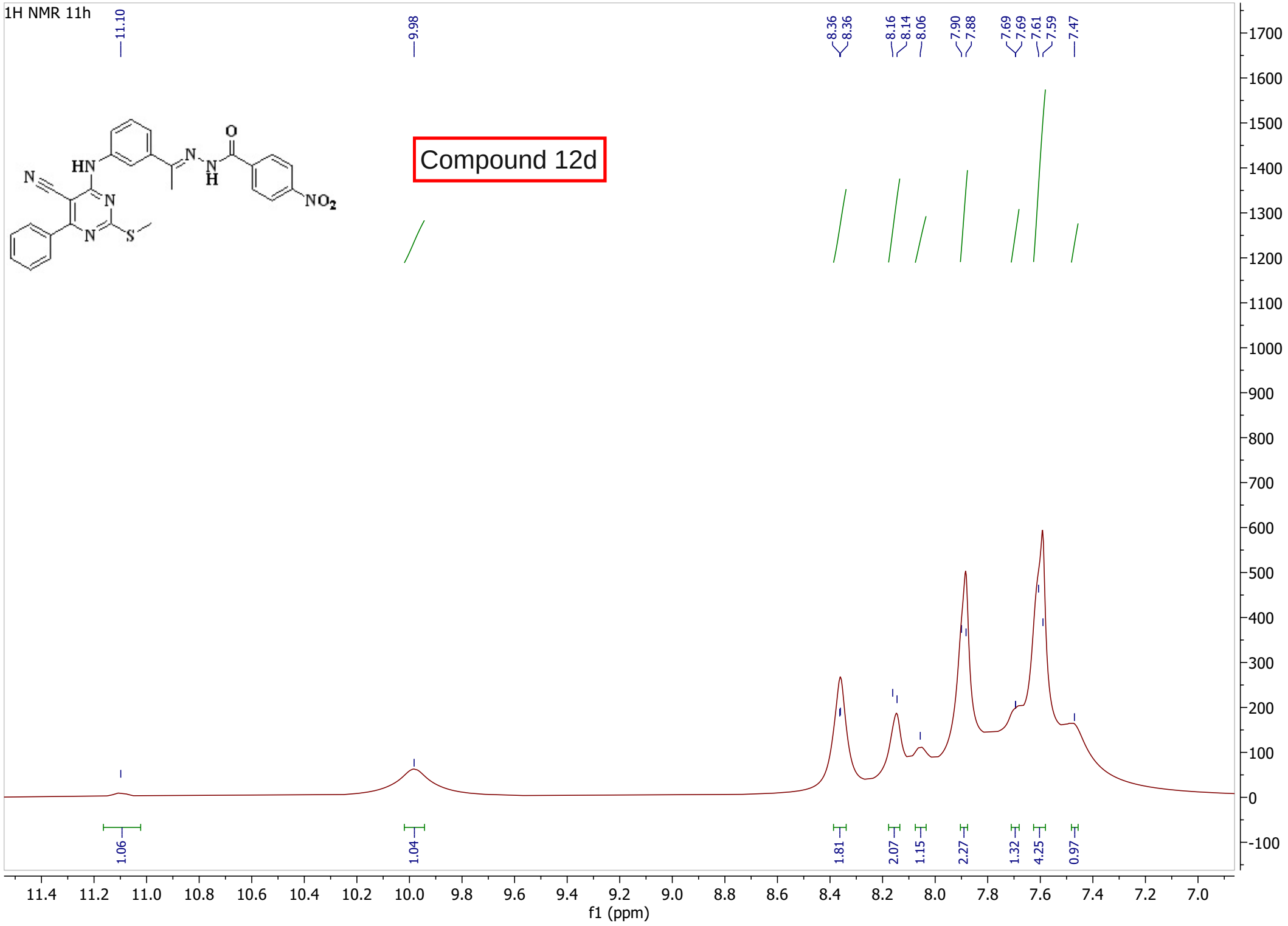

ASZMS
Compound 12d
% Transmittance
Wavenumbers (cm-1)
3305.74
3196.97
3109.68
3076.00
2927.46
2213.14
1670.15
1597.15
1573.35
1542.55
1525.81
1492.24
1475.28
1450.02
1407.96
1345.41
1328.73
1299.79
1229.83
1182.93
1151.99
1108.99
1006.21
968.23
917.46
862.24
852.22
792.75
782.60
759.01
719.24
686.43
654.96
629.82
615.23
585.70
526.12
500.96
457.19
HN
N
N
N
H
O
NO2
S

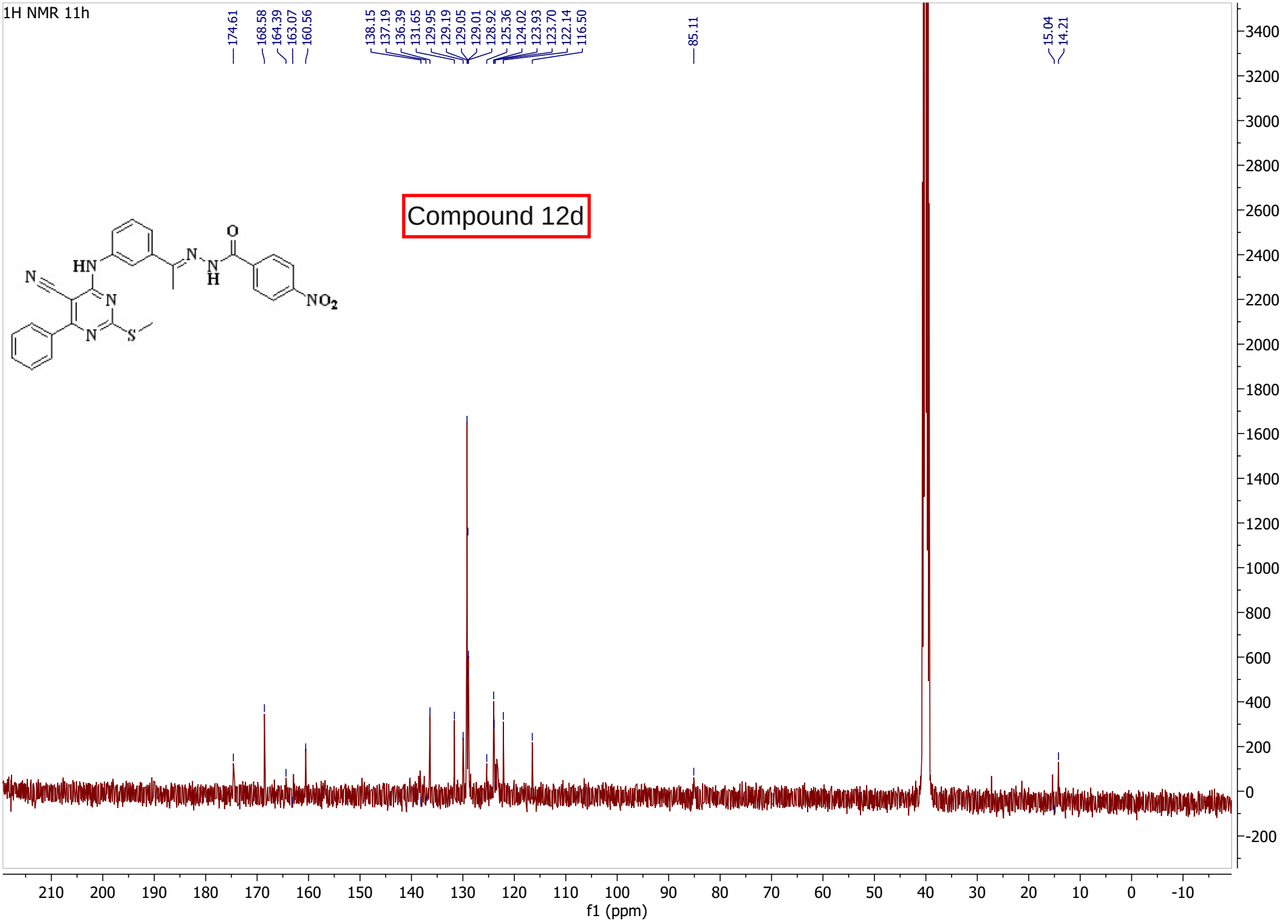

1H NMR 11h
11.10
9.98
8.36
8.36
8.16
8.14
8.06
7.90
7.88
7.69
7.69
7.61
7.59
7.47
2.51
2.20
Compound 12d
HN
N
N
N
S
N
H
O
NO2
1.06
1.04
1.81
2.07
1.15
2.27
1.32
4.25
0.97
2.87
3.00
f1 (ppm)

1H NMR 11h

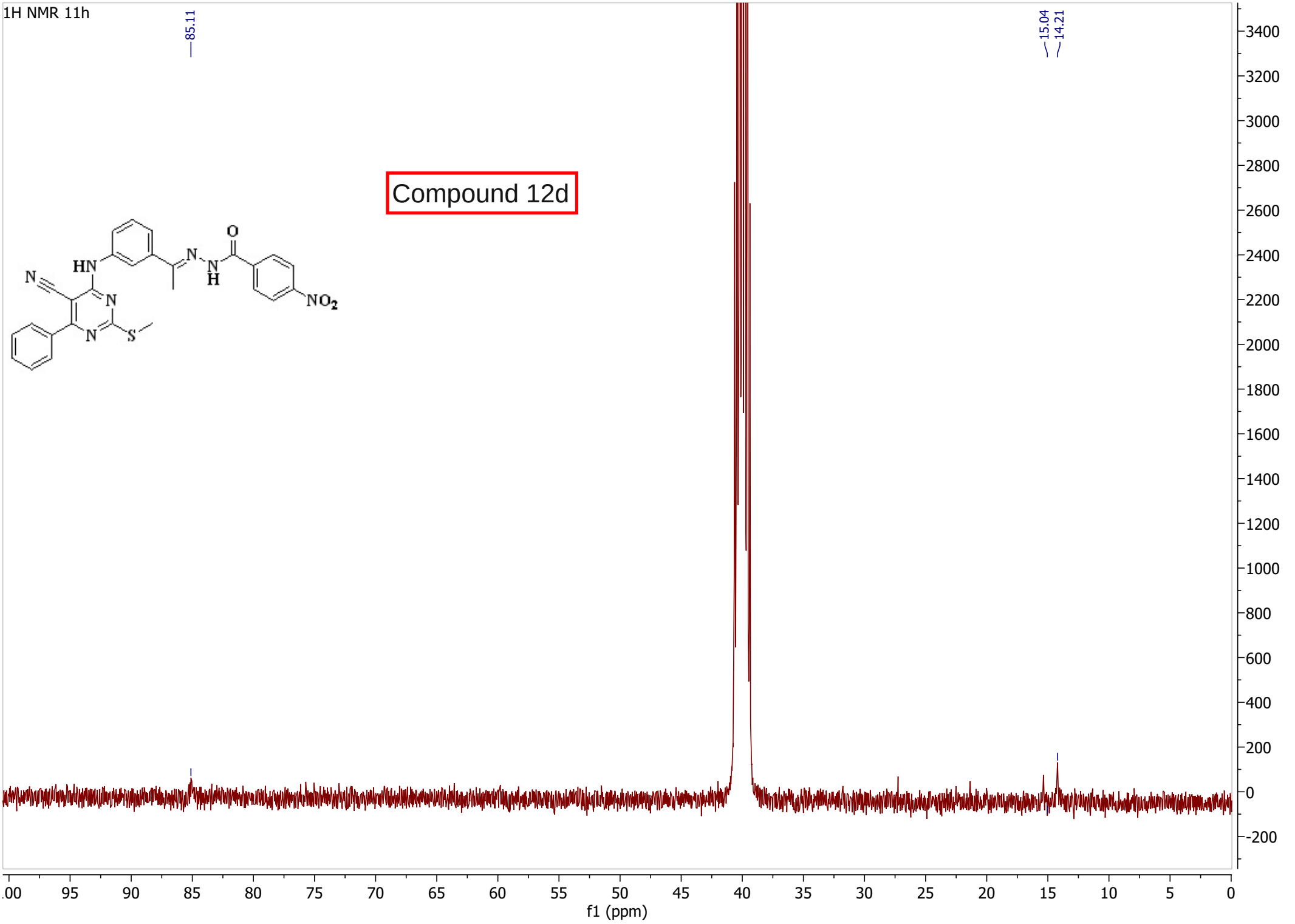


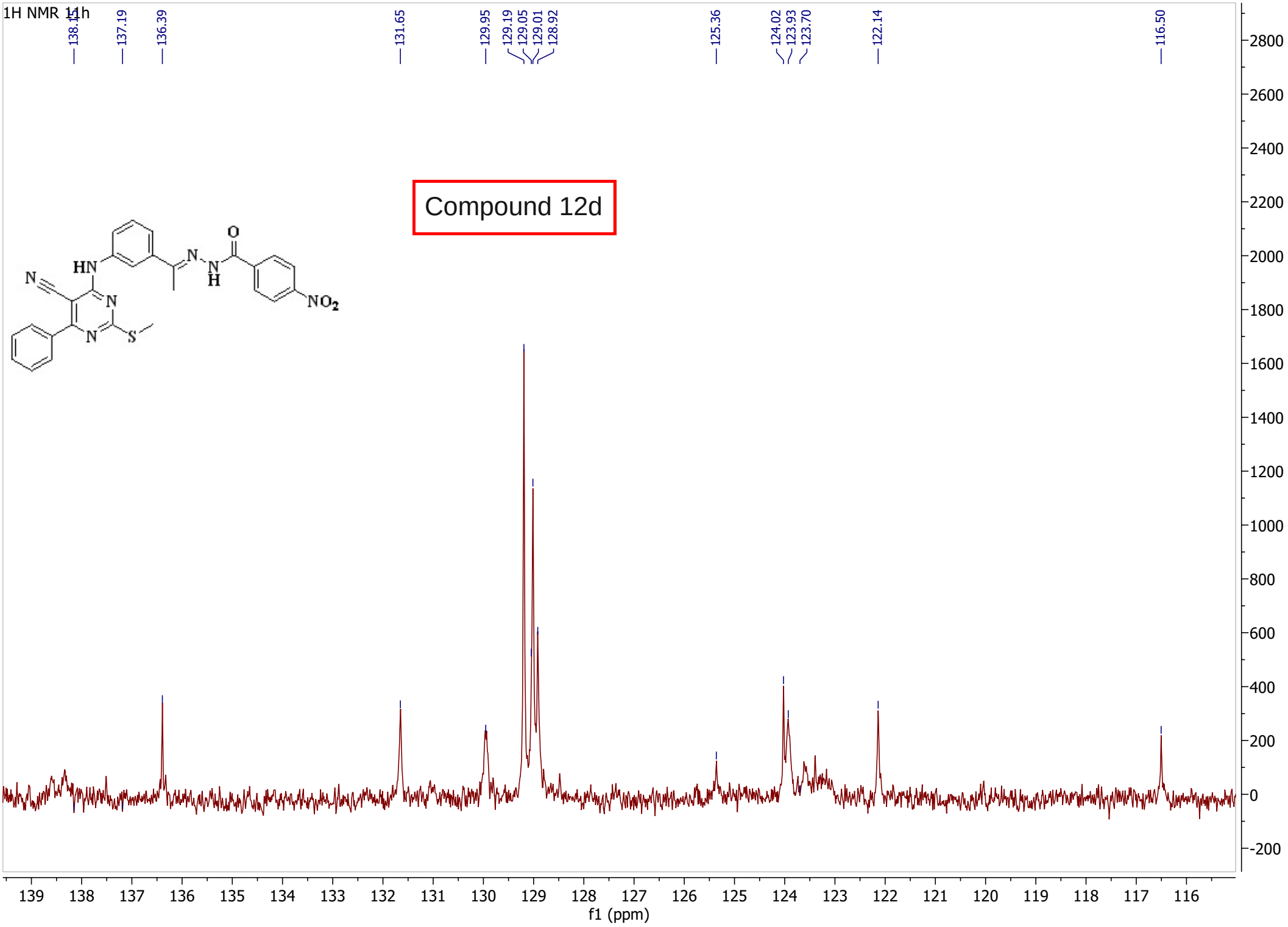
Compound 12d


1H NMR 11h
11.10
9.98
8.36
8.36
8.16
8.14
8.06
7.90
7.88
7.69
7.69
7.61
7.59
7.47
Compound 12d
HN
N
N
N
S
N
H
O
NO2
1.06
1.04
1.81
2.07
1.15
2.27
1.32
4.25
0.97
f1 (ppm)

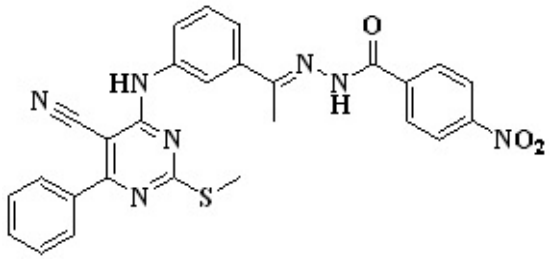

1H NMR 11h
174.61
168.58
164.39
163.07
160.56
138.15
137.19
136.39
131.65
129.95
129.19
129.05
129.01
128.92
125.36
124.02
123.93
123.70
122.14
116.50
85.11
15.04
14.21
Compound 12d
HN
N
N
H
O
N
N
S
NO2
f1 (ppm)

1H NMR 11h

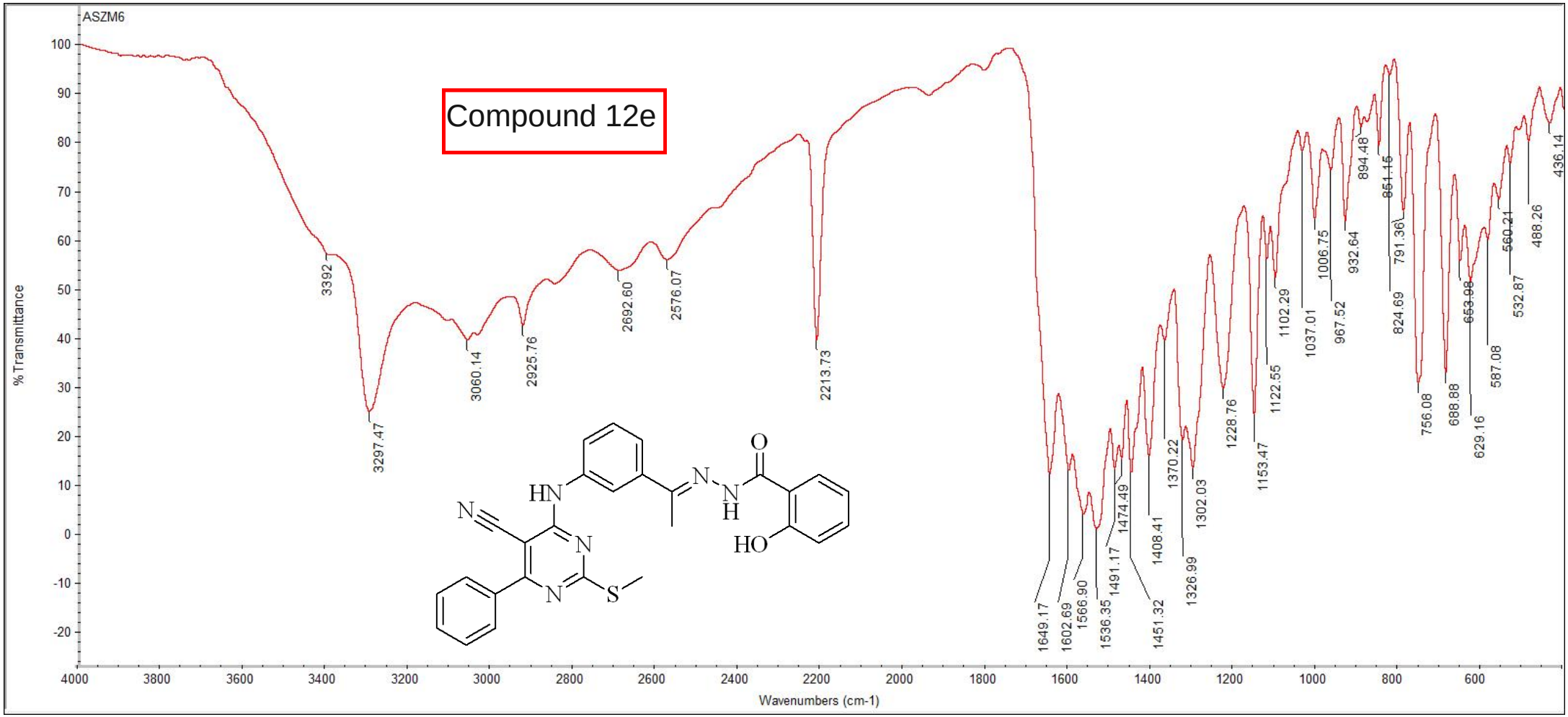

85.11
15.04
14.21
Compound 12d
HN
N
N
H
O
N
N
S
NO2
3400
3200
3000
2800
2600
2400
2200
2000
1800
1600
1400
1200
1000
800
600
400
200
0
-200
.00
95
90
85
80
75
70
65
60
55
50
45
40
35
30
25
20
15
10
5
0
f1 (ppm)

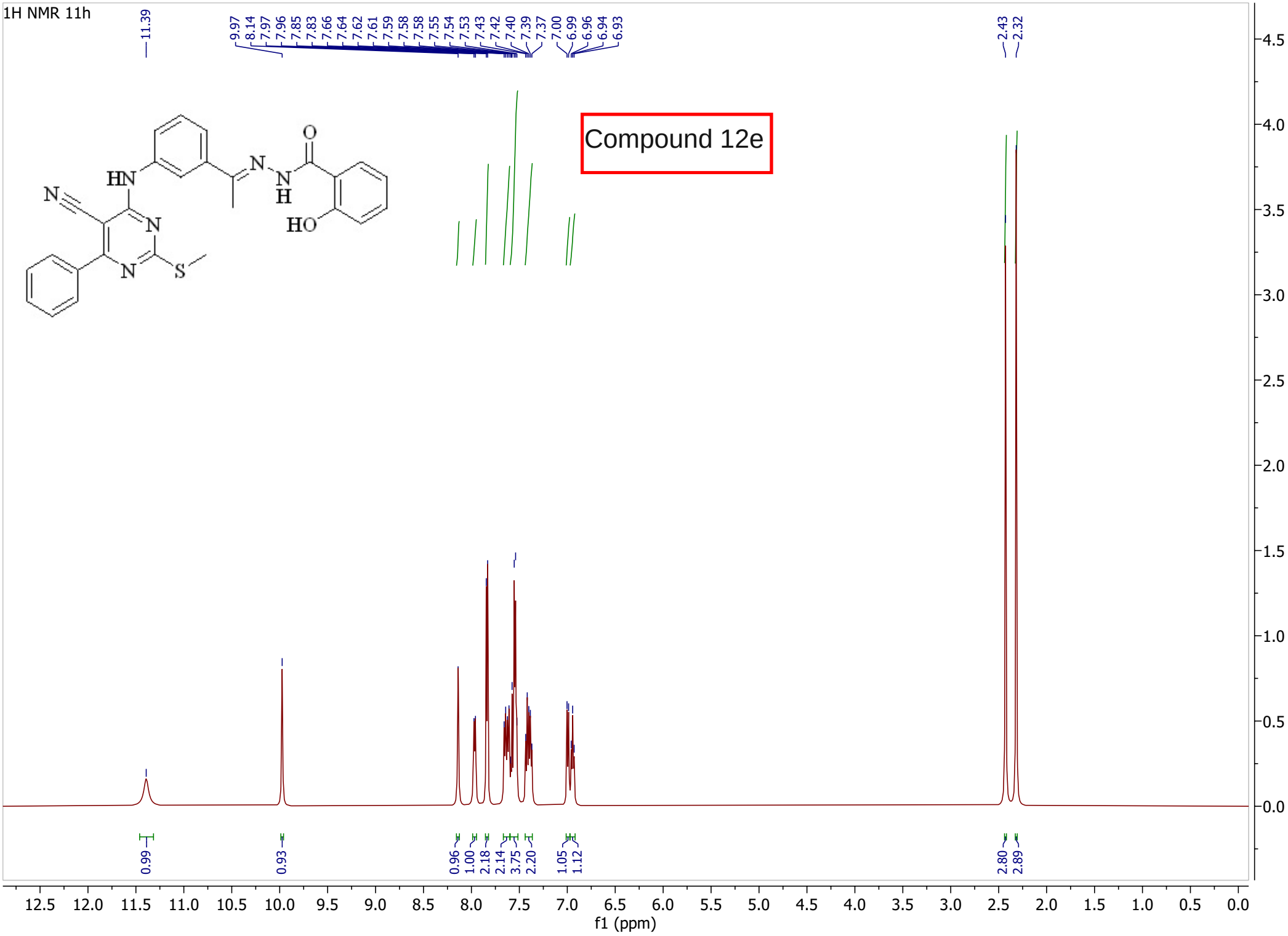

1H NMR 11h
138.11
137.19
136.39
131.65
129.95
129.19
129.05
129.01
128.92
125.36
124.02
123.93
123.70
122.14
116.50
Compound 12d
HN
N
N
H
O
N
N
S
NO2
2800
2600
2400
2200
2000
1800
1600
1400
1200
1000
800
600
400
200
0
-200
139
138
137
136
135
134
133
132
131
130
129
128
127
126
125
124
123
122
121
120
119
118
117
116
f1 (ppm)

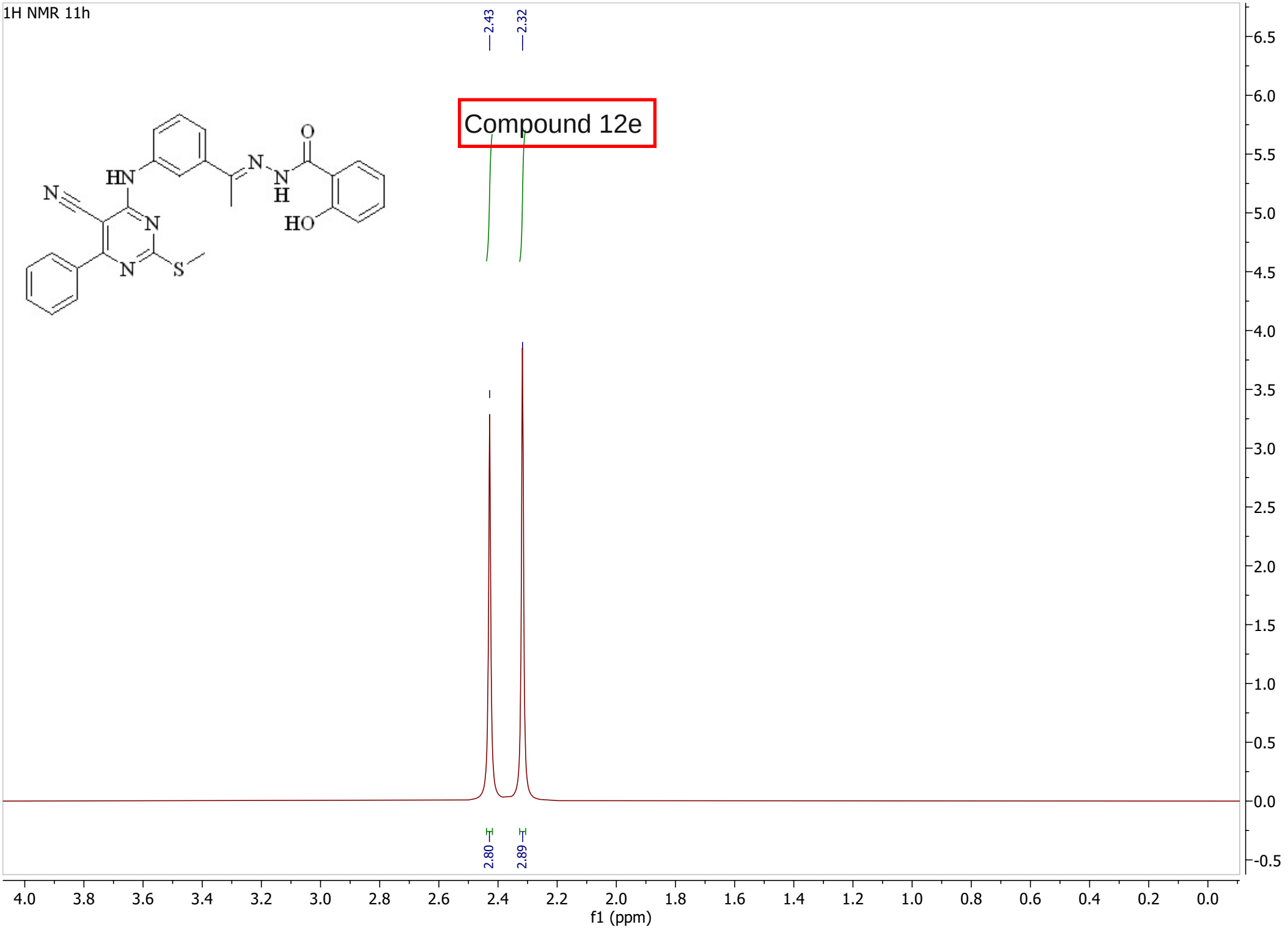
1H NMR 11h

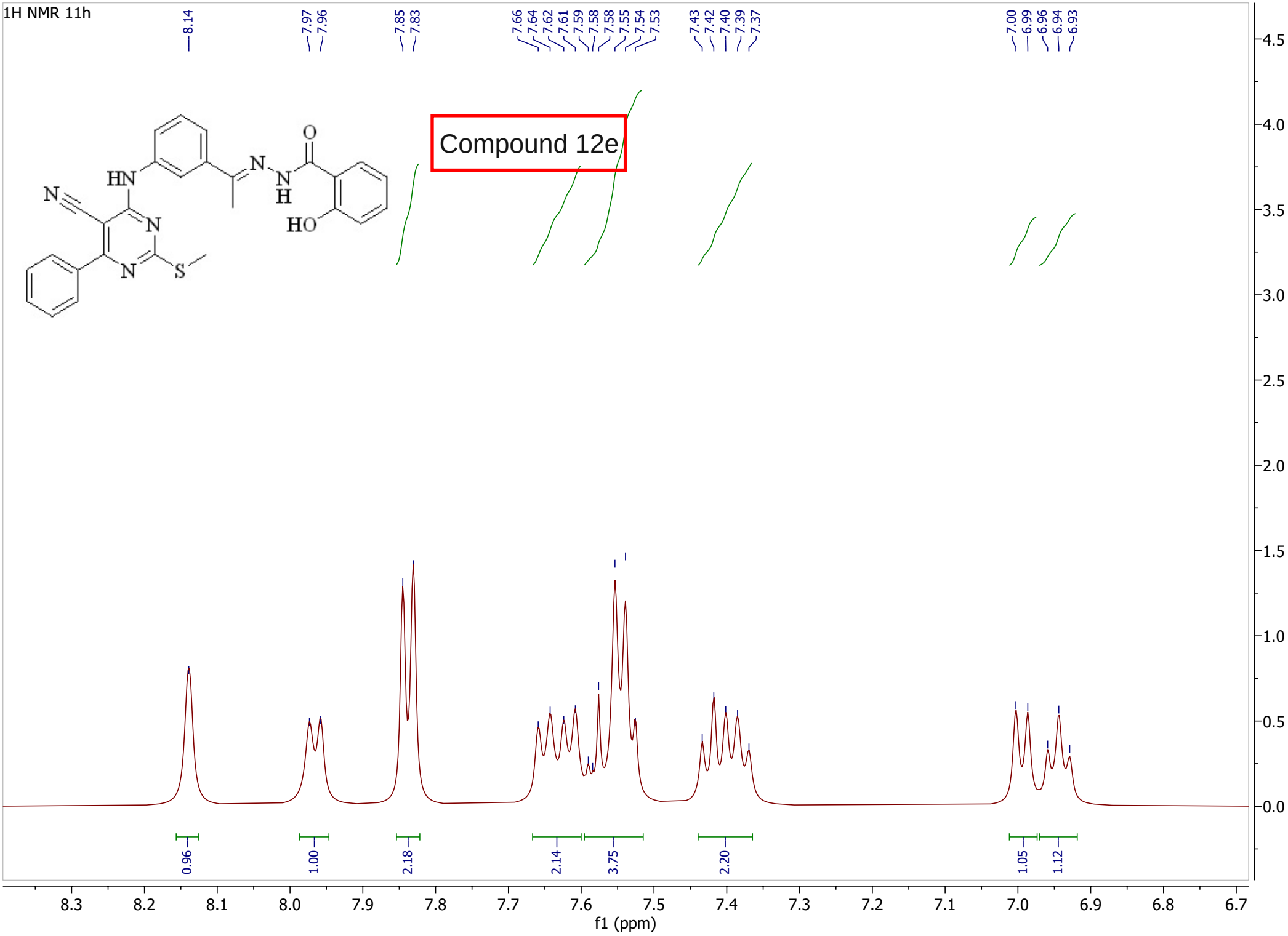


Compound 12d

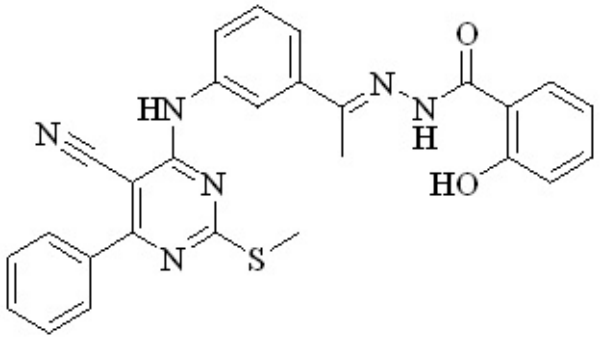

ASZM6
Compound 12e
% Transmittance
Wavenumbers (cm-1)
3392
3297.47
3060.14
2925.76
2692.60
2576.07
2213.73
1649.17
1602.69
1566.90
1536.35
1491.17
1474.49
1451.32
1408.41
1370.22
1326.99
1302.03
1228.76
1153.47
1122.55
1102.29
1037.01
1006.75
967.52
932.64
894.48
851.15
824.69
791.36
756.08
688.88
653.98
629.16
587.08
560.21
532.87
488.26
436.14
HN
N
N
N
S
O
N
H
HO


1H NMR 11h
11.39
9.97
8.14
7.97
7.96
7.85
7.83
7.66
7.64
7.62
7.61
7.59
7.58
7.58
7.55
7.54
7.53
7.43
7.42
7.40
7.39
7.37
7.00
6.99
6.96
6.94
6.93
2.43
2.32
Compound 12e
HN
N
N
H
O
HO
N
N
S
0.99
0.93
0.96
1.00
2.18
2.14
3.75
2.20
1.05
1.12
2.80
2.89
f1 (ppm)


1H NMR 11h
2.43
2.32
Compound 12e
HN
N
N
H
O
HO
N
N
S
2.80
2.89
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
4.0
3.8
3.6
3.4
3.2
3.0
2.8
2.6
2.4
2.2
2.0
1.8
1.6
1.4
1.2
1.0
0.8
0.6
0.4
0.2
0.0
f1 (ppm)


1H NMR 11h
8.14
7.97
7.96
7.85
7.83
7.66
7.64
7.62
7.61
7.59
7.58
7.58
7.55
7.54
7.53
7.43
7.42
7.40
7.39
7.37
7.00
6.99
6.96
6.94
6.93
Compound 12e
HN
N
N
H
O
HO
N
N
S
0.96
1.00
2.18
2.14
3.75
2.20
1.05
1.12
f1 (ppm)

1H NMR 11h



Compound 12e

11.39

9.97

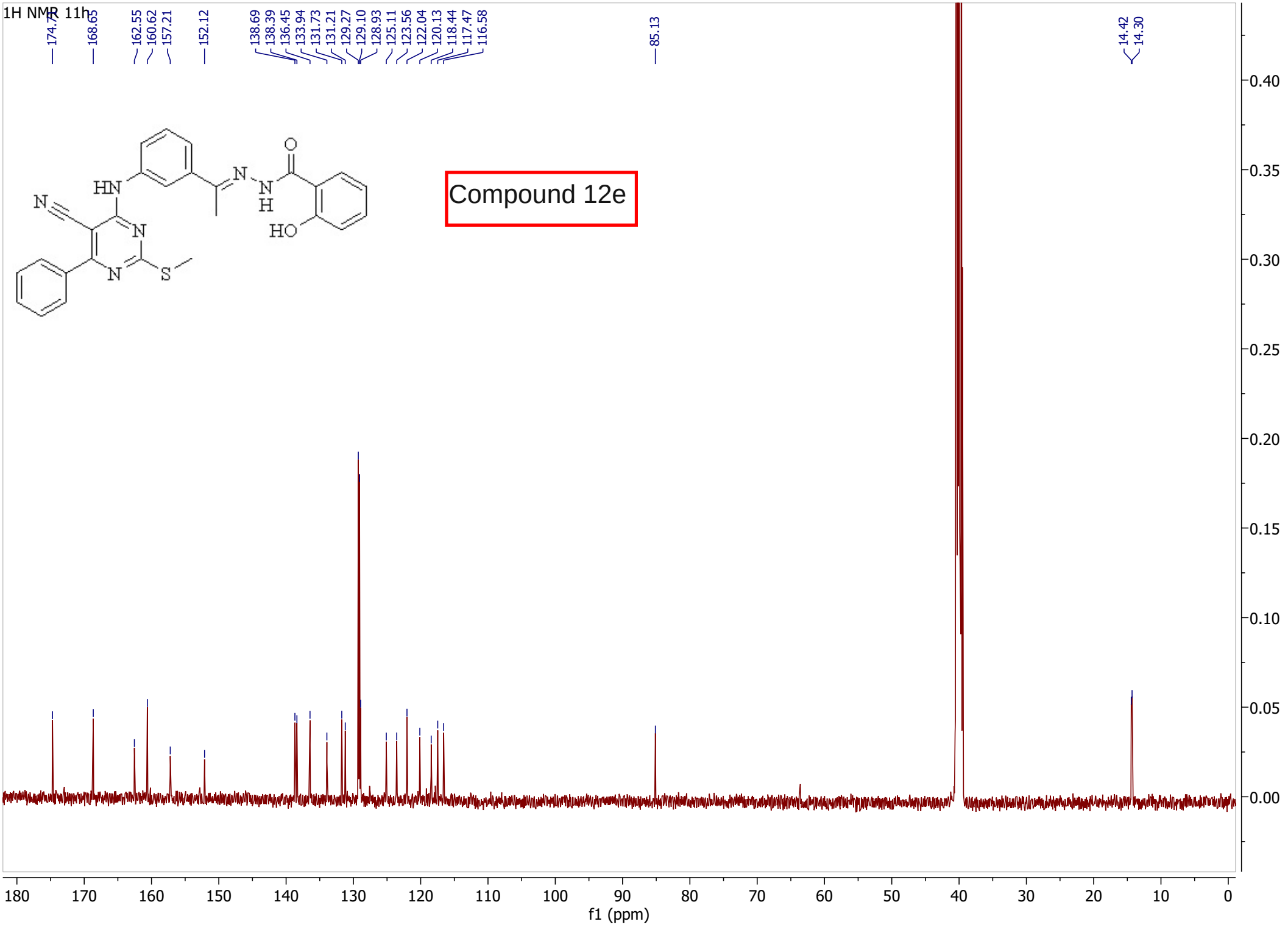
0.99

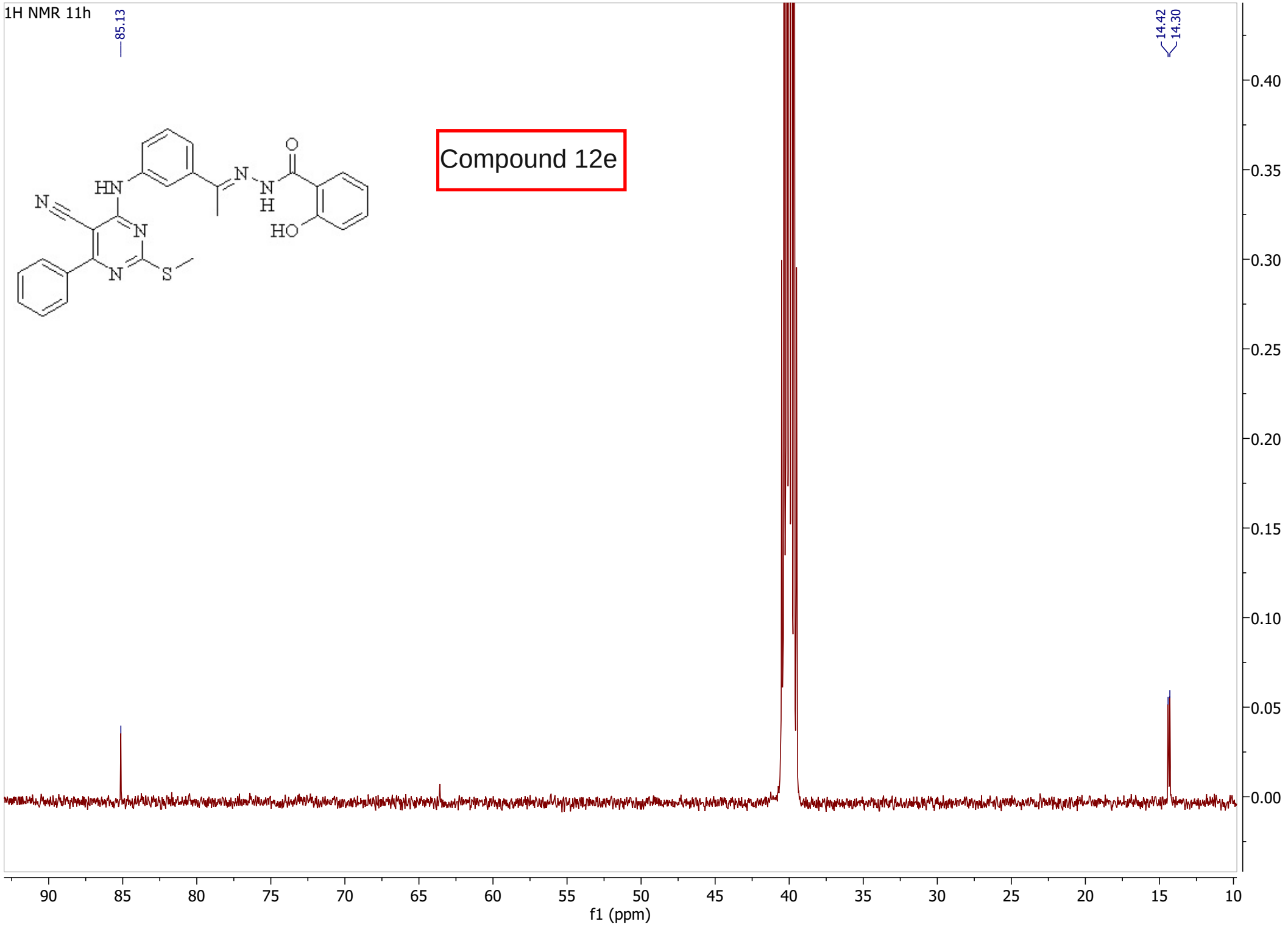
0.93

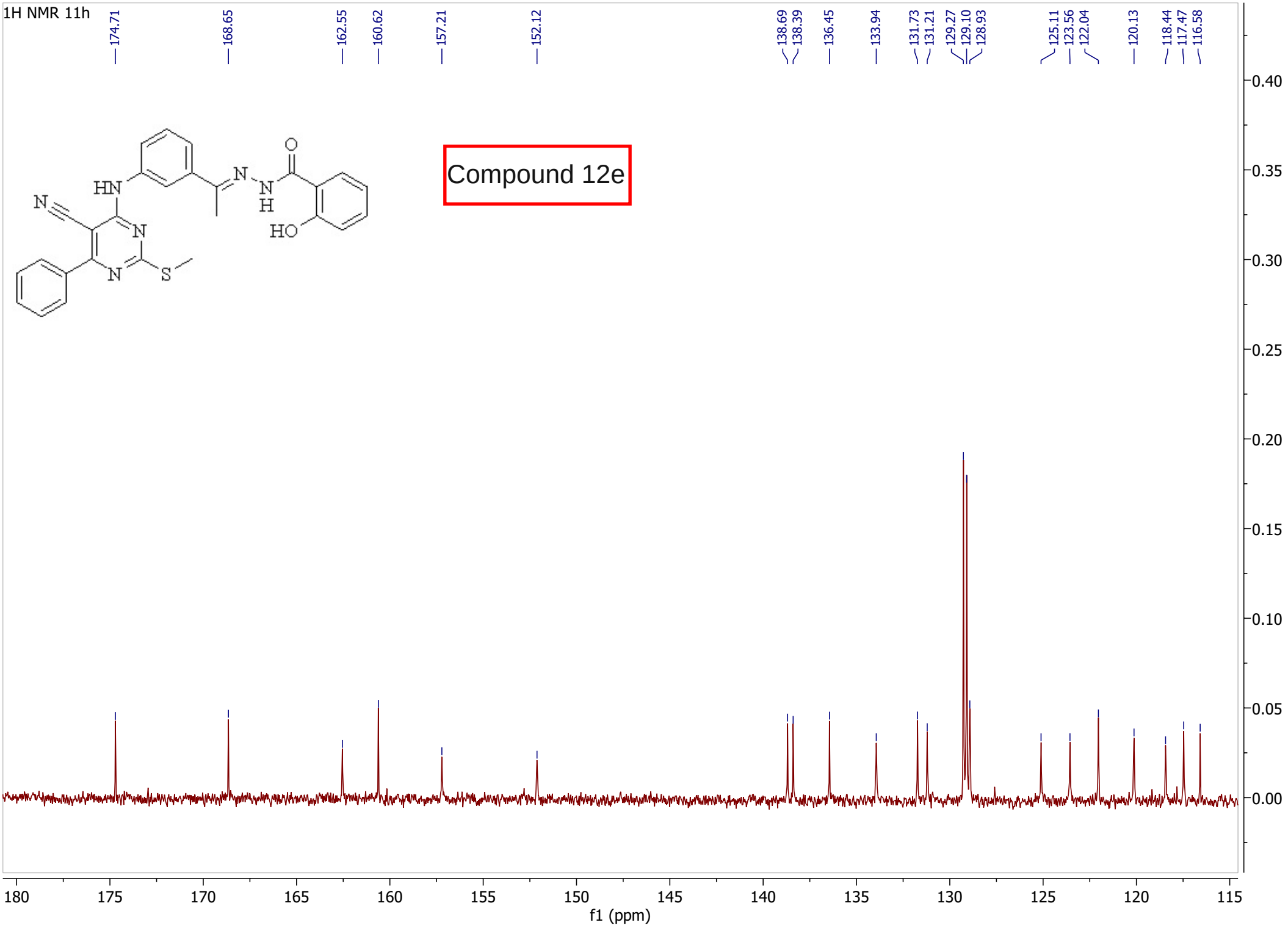
4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0

13.0 12.8 12.6 12.4 12.2 12.0 11.8 11.6 11.4 11.2 11.0 10.8 10.6 10.4 10.2 10.0 9.8 9.6 9.4 9.2 9.0

f1 (ppm)

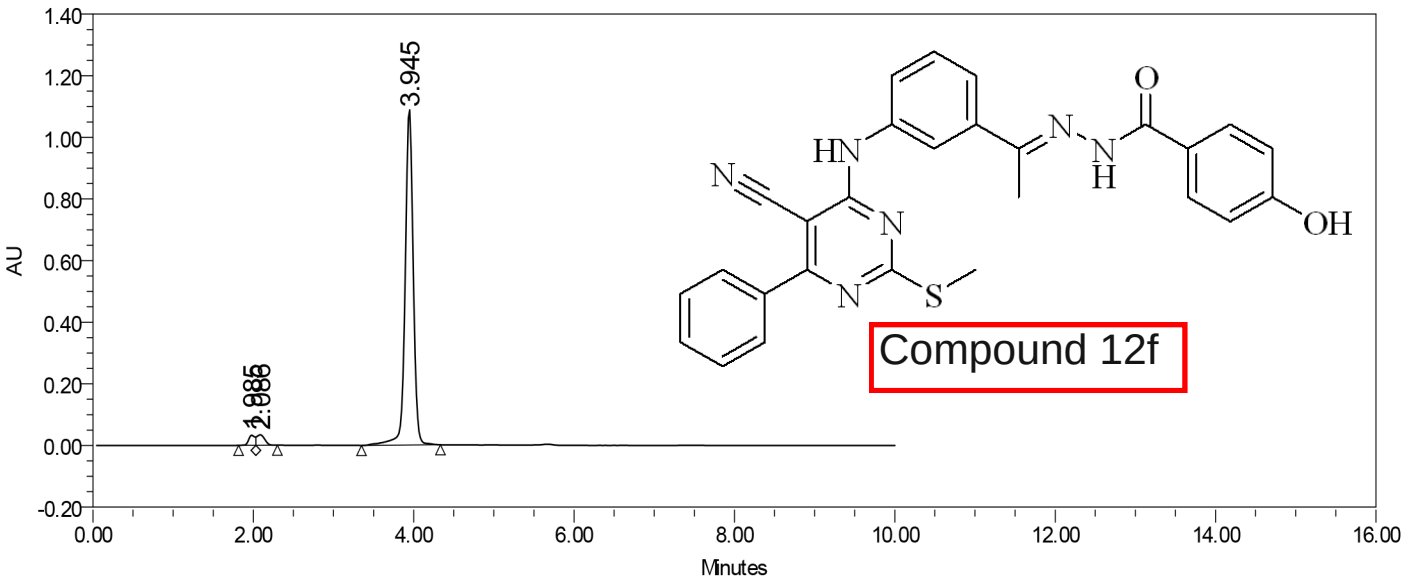

1H NMR 11h
174.74
168.65
162.55
160.62
157.21
152.12
138.69
138.39
136.45
133.94
131.73
131.21
129.27
129.10
128.93
125.11
123.56
122.04
120.13
118.44
117.47
116.58
85.13
14.42
14.30
Compound 12e
HN
N
N
N
H
HO
N
N
S
0.40
0.35
0.30
0.25
0.20
0.15
0.10
0.05
0.00
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


1H NMR 11h
85.13
14.42
14.30
Compound 12e
HN
N
N
H
HO
N
N
N
S
0.40
0.35
0.30
0.25
0.20
0.15
0.10
0.05
0.00
90
85
80
75
70
65
60
55
50
45
40
35
30
25
20
15
10
f1 (ppm)

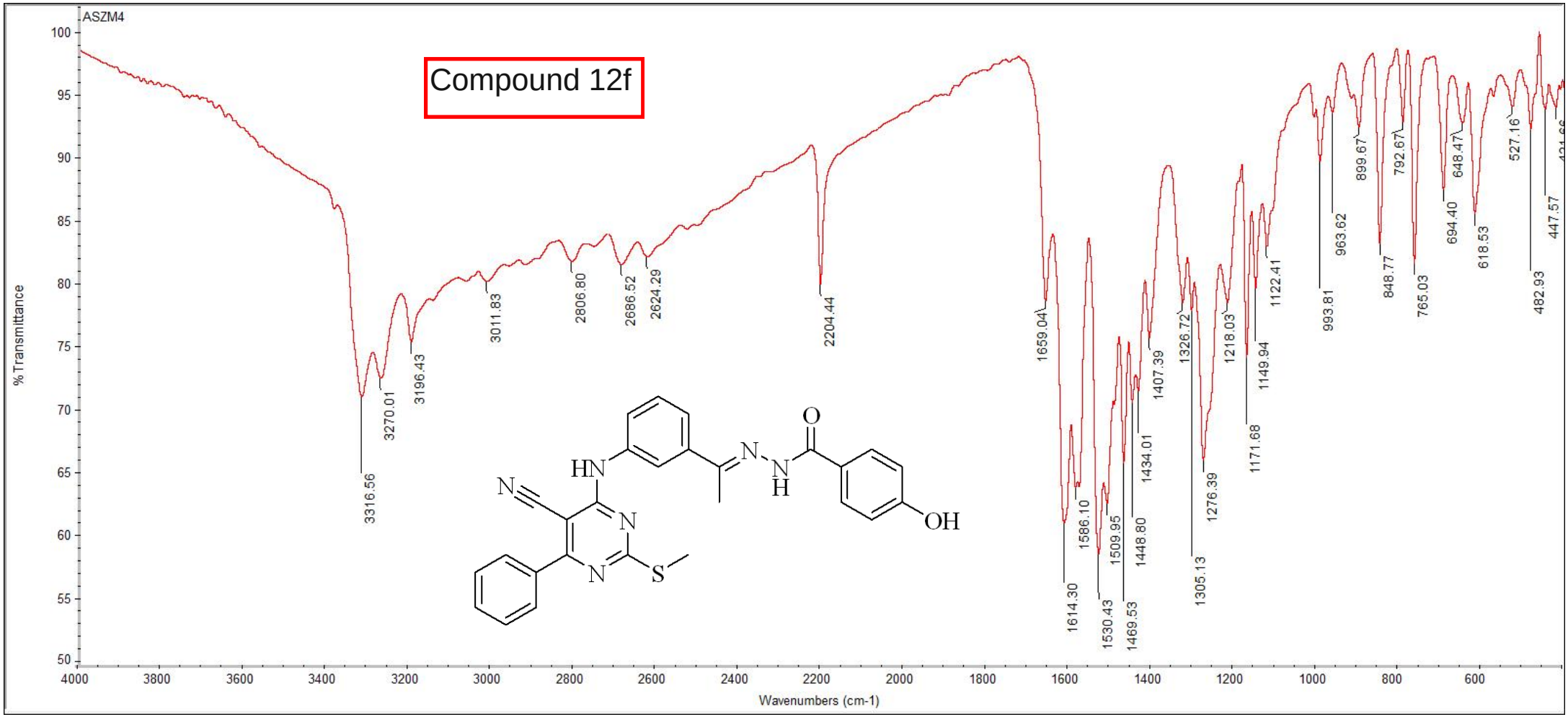

1H NMR 11h
174.71
168.65
162.55
160.62
157.21
152.12
138.69
138.39
136.45
133.94
131.73
131.21
129.27
129.10
128.93
125.11
123.56
122.04
120.13
118.44
117.47
116.58
Compound 12e
HN
N
N
H
HO
N
N
N
S
O
0.40
0.35
0.30
0.25
0.20
0.15
0.10
0.05
0.00
180
175
170
165
160
155
150
145
140
135
130
125
120
115
f1 (ppm)

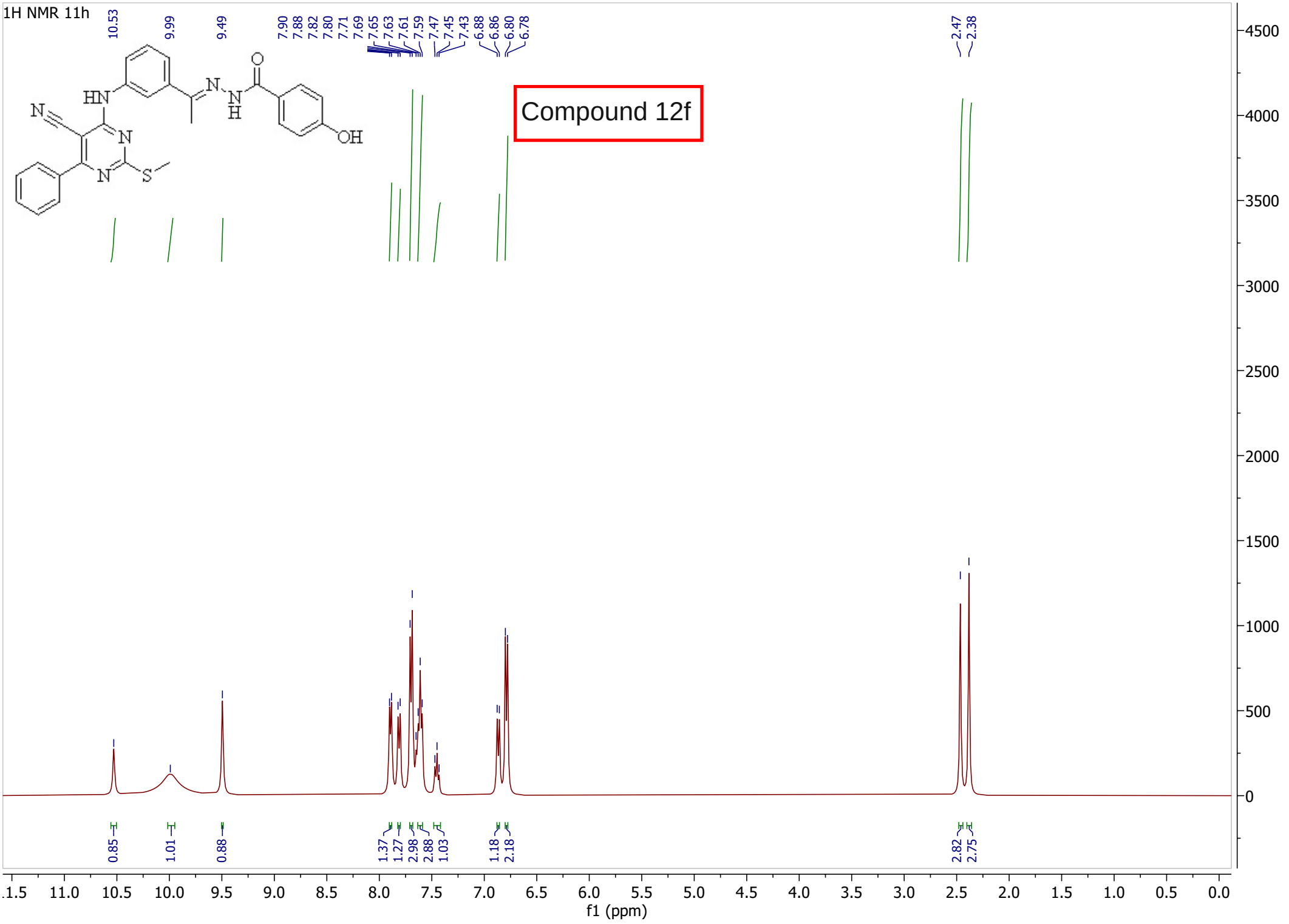
SAMPLE INFORMATION

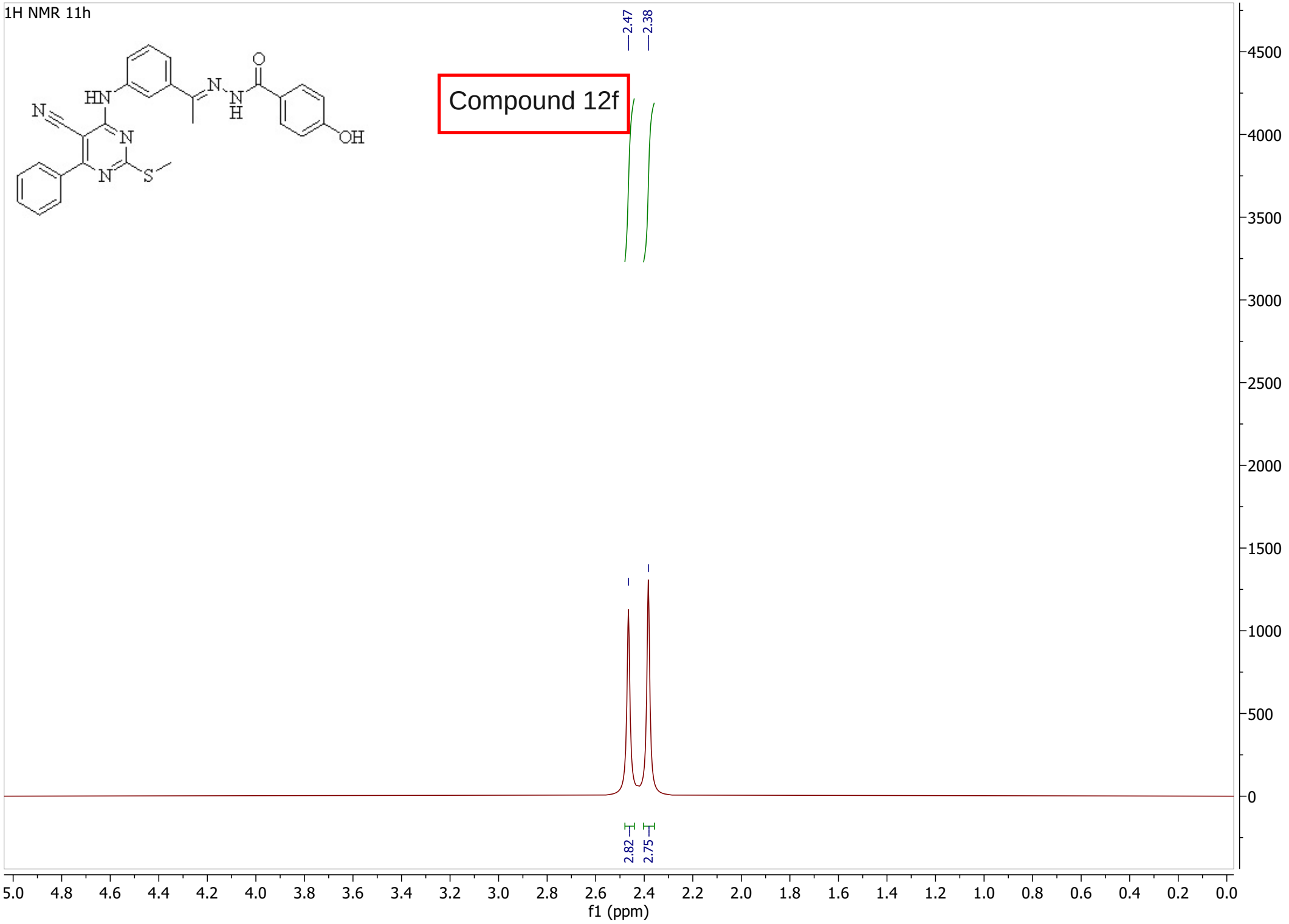
Sample Name:	ASZM4 Compound 12f	Acquired By:	System
Sample Type:	Unknown	Sample Set Name:	1
Vial:	19	Acq. Method Set:	Organic1
Injection #:	1	Processing Method:	Default
Injection Volume:	2.00 ul	Channel Name:	286.0nm
Run Time:	10.0 Minutes	Proc. Chnl. Descr.:	W2996 PDA 286.0 nm (PDA 190.0 to
Date Acquired:	11/6/2022 7:47:03 AM EET		
Date Processed:	11/6/2022 10:26:57 AM EET		

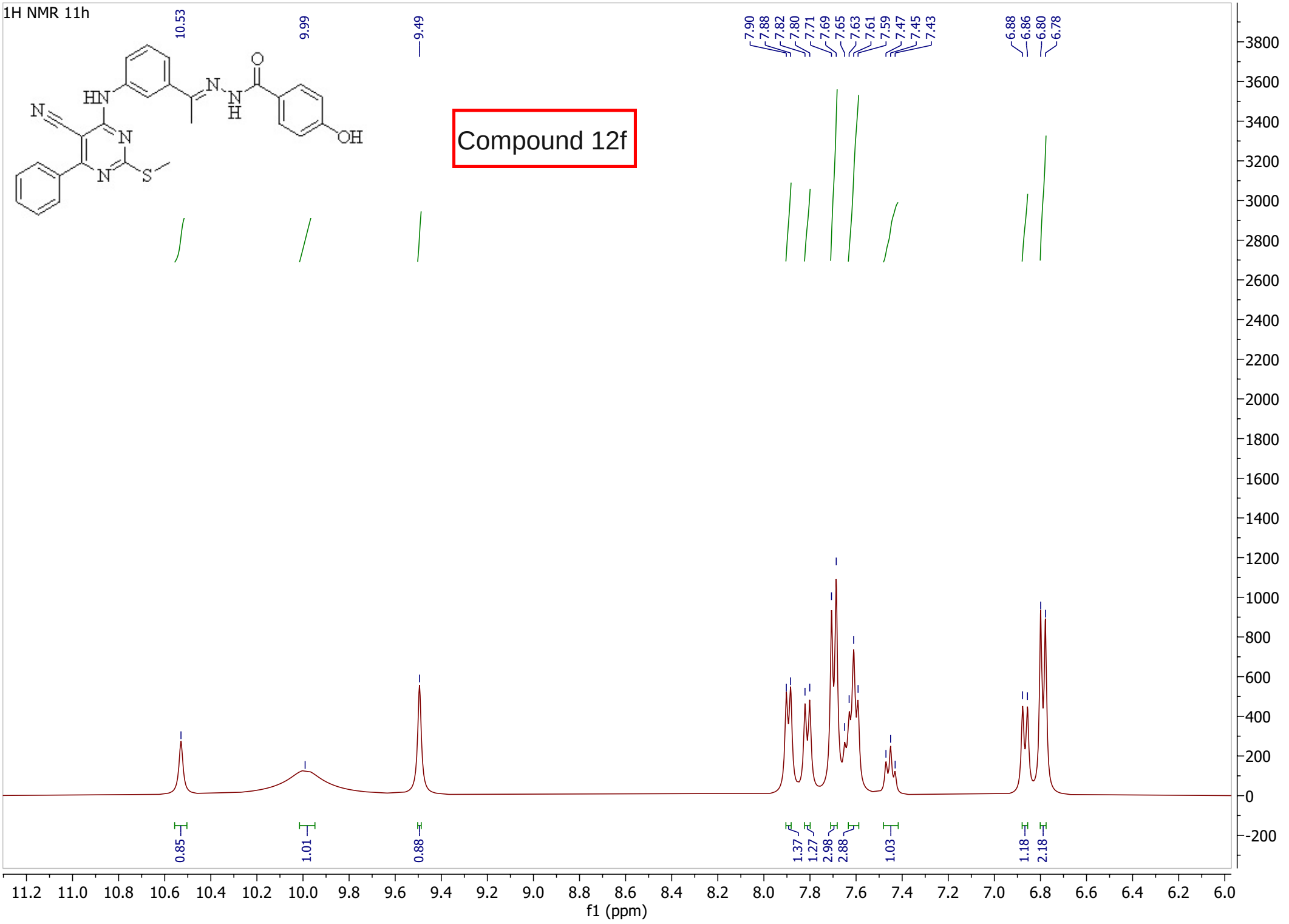


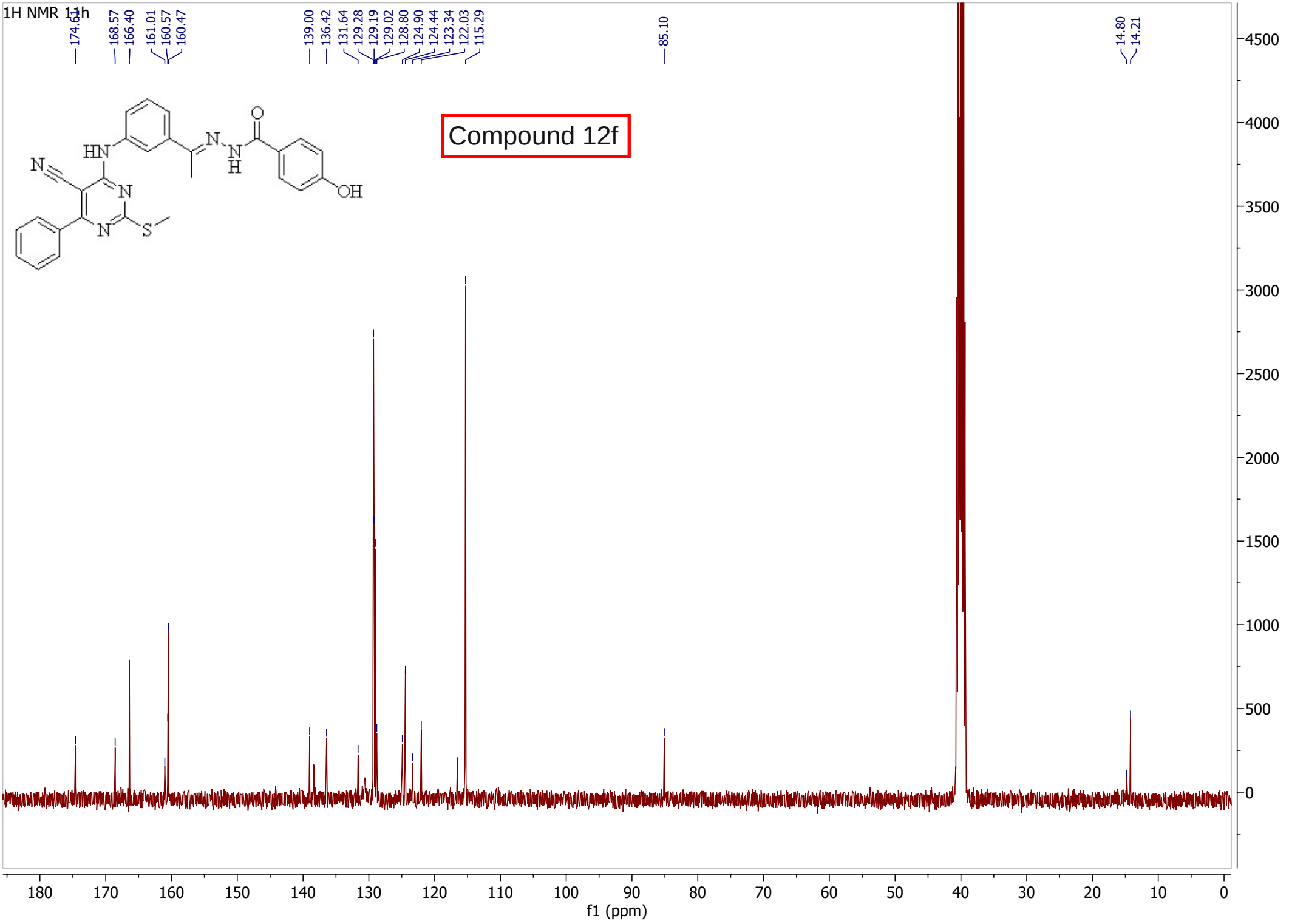
	RT	Area	% Area	Height
1	1.985	179325	2.24	32588
2	2.086	230882	2.88	33692
3	3.945	7599646	94.88	1088143

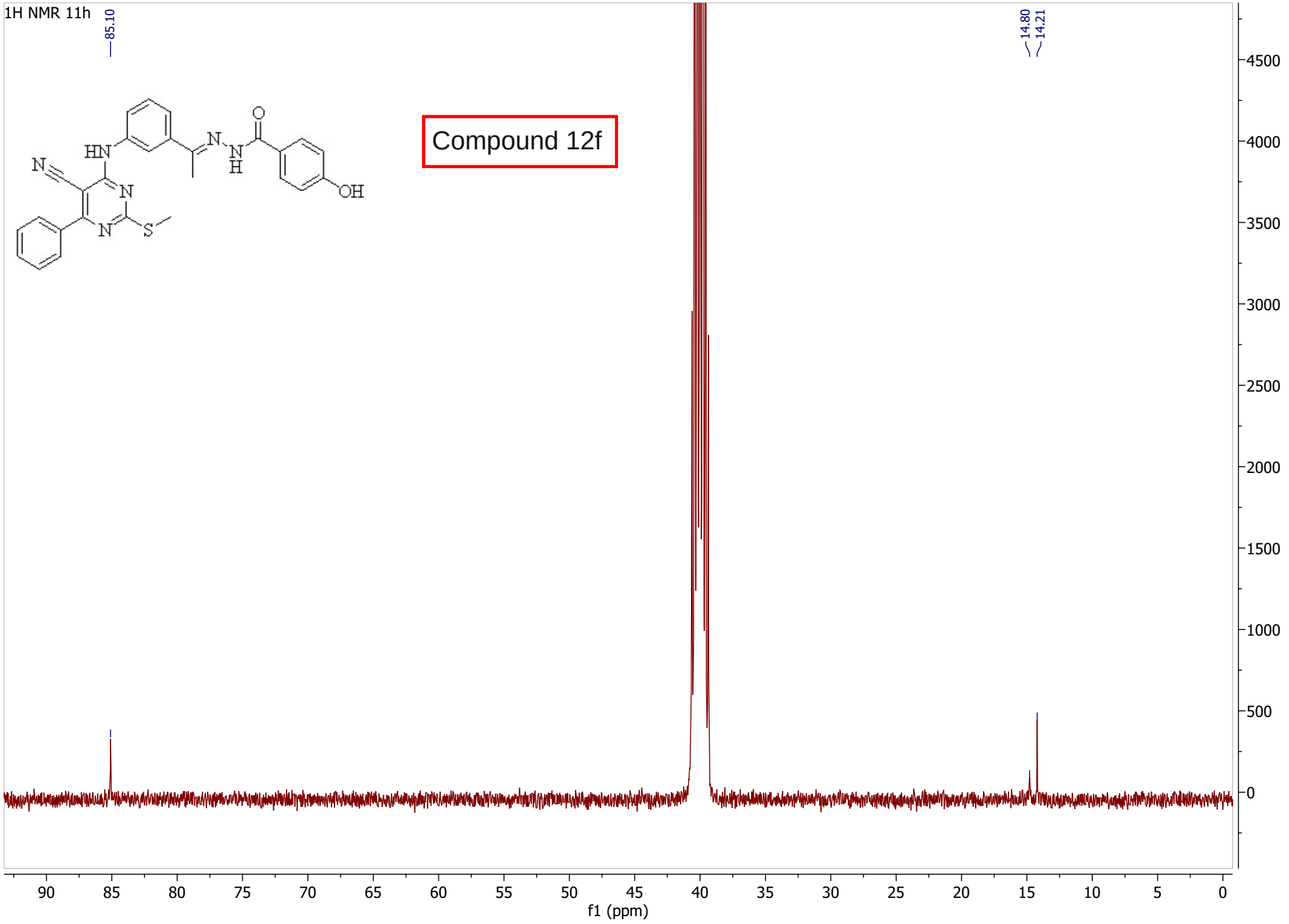

ASZM4
Compound 12f
% Transmittance
Wavenumbers (cm-1)
3316.56
3270.01
3196.43
3011.83
2806.80
2686.52
2624.29
2204.44
1659.04
1614.30
1586.10
1530.43
1509.95
1469.53
1448.80
1434.01
1407.39
1326.72
1305.13
1276.39
1218.03
1171.68
1149.94
1122.41
993.81
963.62
899.67
848.77
792.67
765.03
694.40
648.47
618.53
527.16
482.93
447.57
HN
N
N
S
N
N
H
O
OH

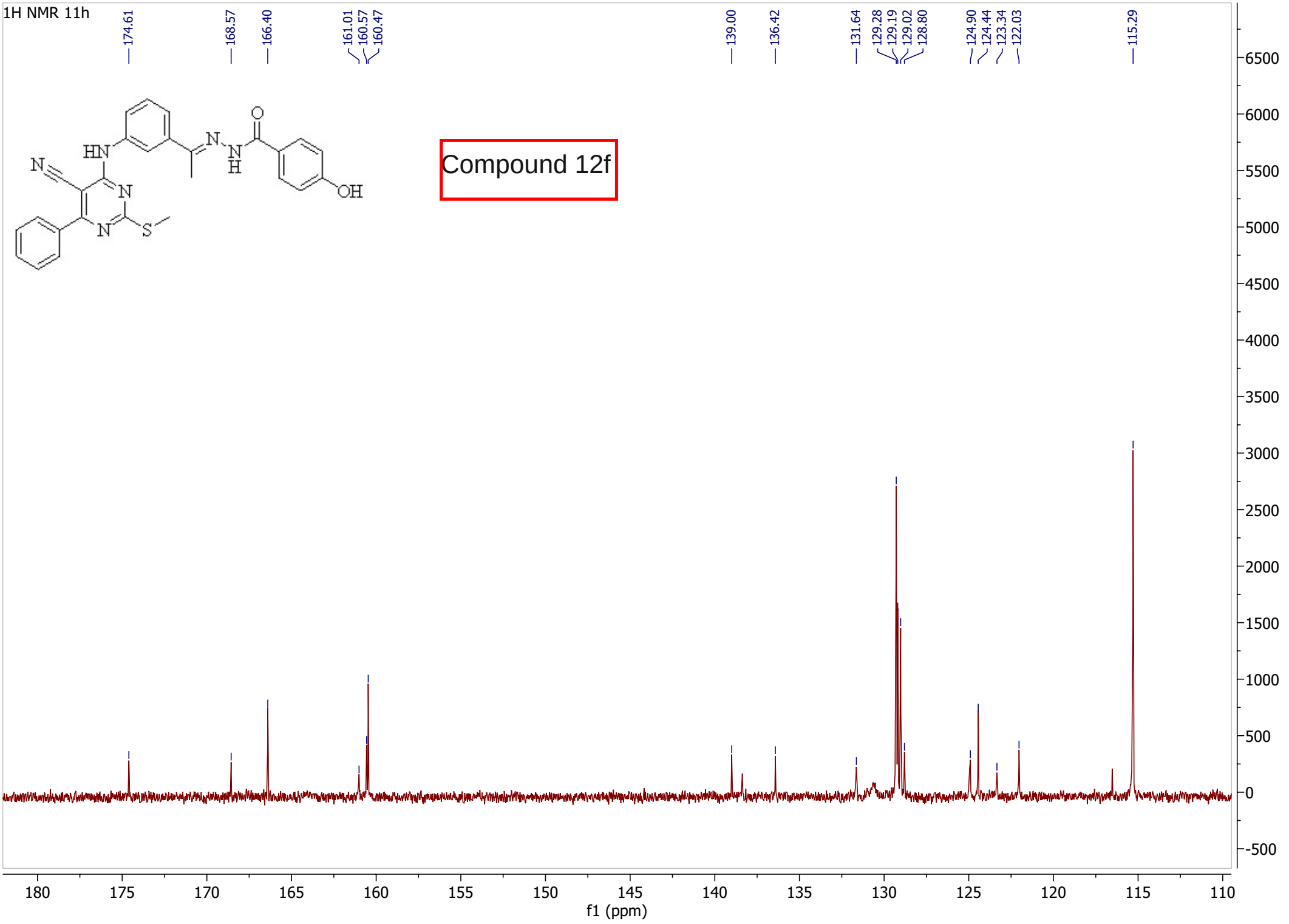

1H NMR 11h
Compound 12f
10.53
9.99
9.49
7.90
7.88
7.82
7.80
7.71
7.69
7.65
7.63
7.61
7.59
7.47
7.45
7.43
6.88
6.86
6.80
6.78
2.47
2.38
HN
N
N
H
N
N
S
OH
0.85
1.01
0.88
1.37
1.27
2.98
2.88
1.03
1.18
2.18
2.82
2.75
f1 (ppm)

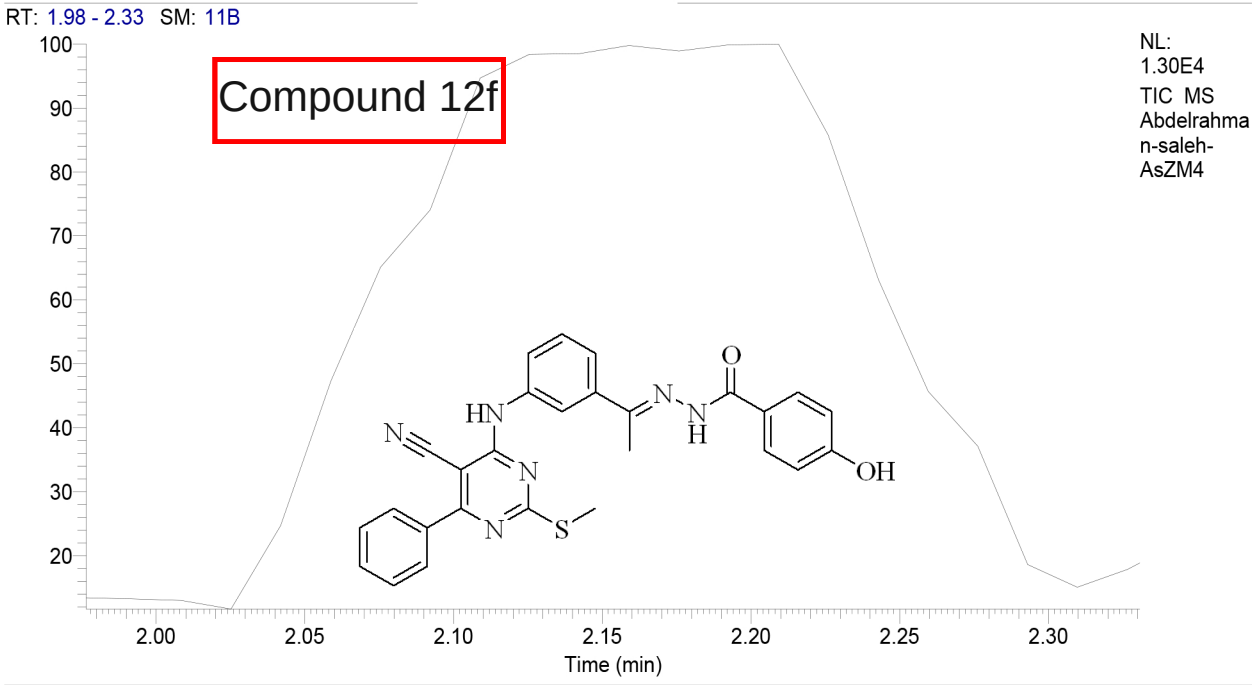

1H NMR 11h
Compound 12f
2.47
2.38
2.82
2.75
4500
4000
3500
3000
2500
2000
1500
1000
500
0
5.0 4.8 4.6 4.4 4.2 4.0 3.8 3.6 3.4 3.2 3.0 2.8 2.6 2.4 2.2 2.0 1.8 1.6 1.4 1.2 1.0 0.8 0.6 0.4 0.2 0.0
f1 (ppm)

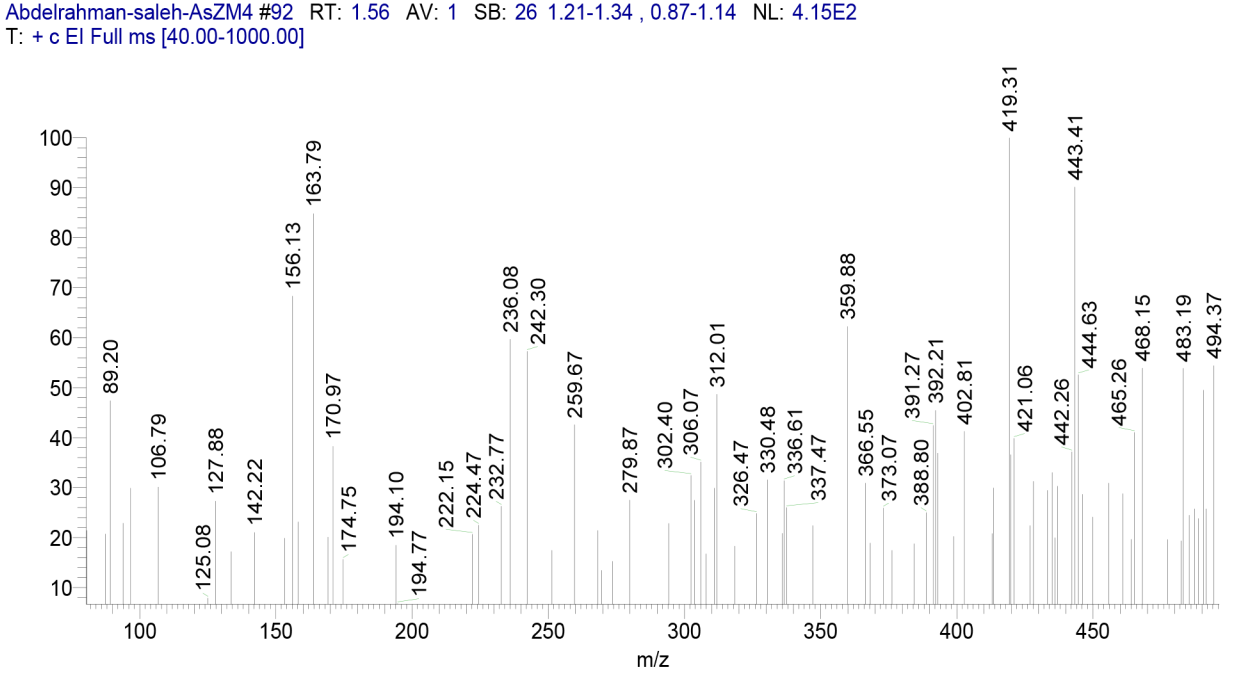

1H NMR 11h
Compound 12f
10.53
9.99
9.49
7.90
7.88
7.82
7.80
7.71
7.69
7.65
7.63
7.61
7.59
7.47
7.45
7.43
6.88
6.86
6.80
6.78
0.85
1.01
0.88
1.37
1.27
2.98
2.88
1.03
1.18
2.18
f1 (ppm)

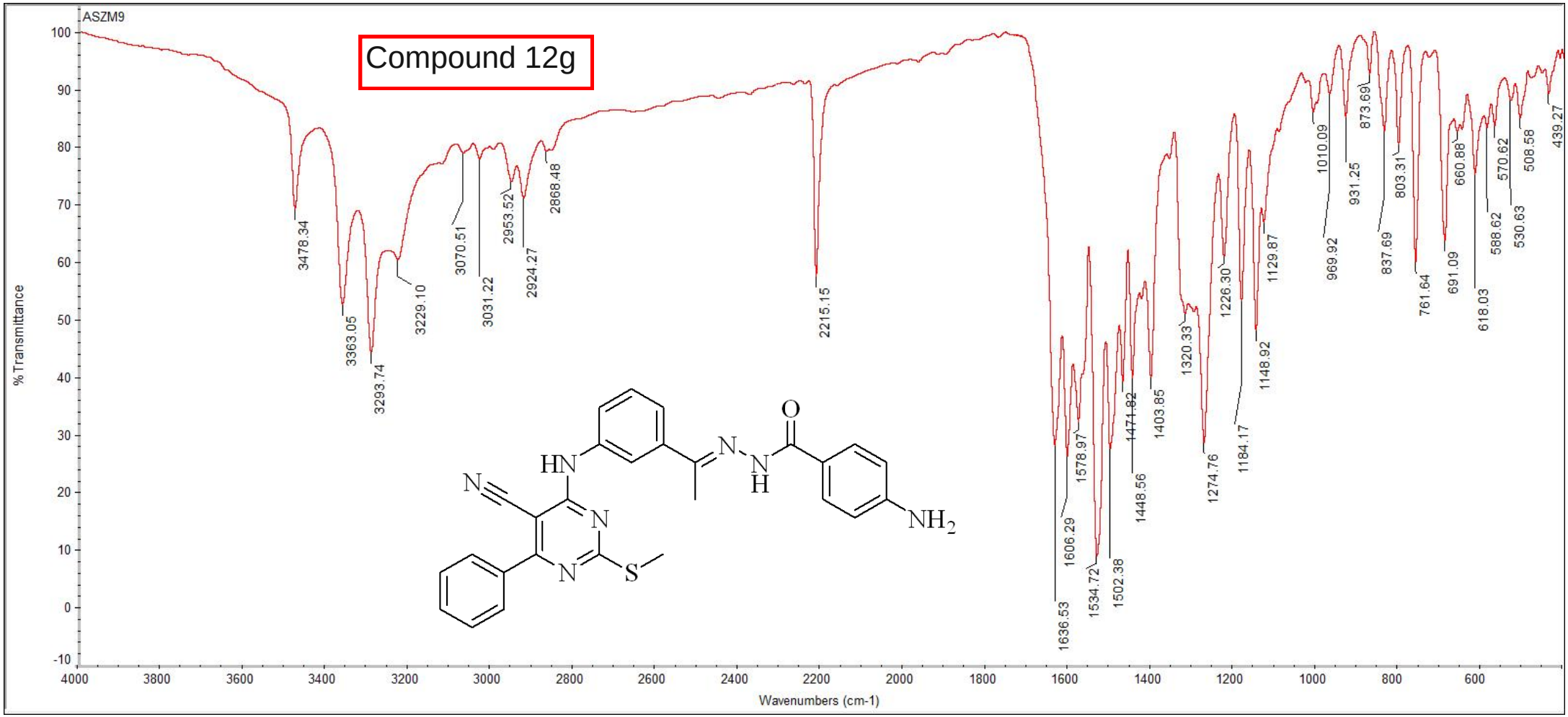

1H NMR 11h
174.64
168.57
166.40
161.01
160.57
160.47
139.00
136.42
131.64
129.28
129.19
129.02
128.80
124.90
124.44
123.34
122.03
115.29
85.10
14.80
14.21
Compound 12f
HN
N
N
H
OH
N
N
S
4500
4000
3500
3000
2500
2000
1500
1000
500
0
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

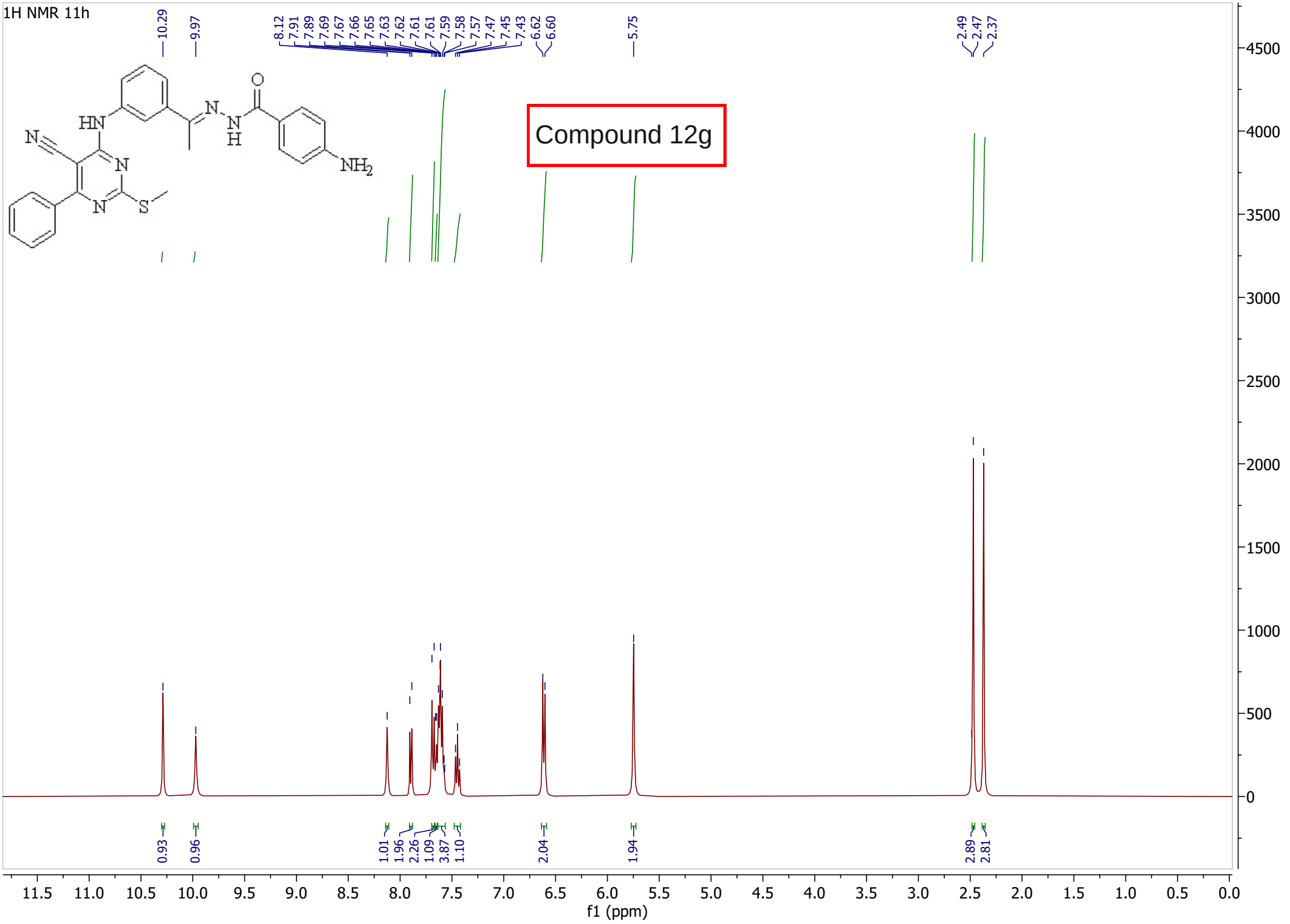

1H NMR 11h
85.10
14.80
14.21
Compound 12f
HN
N
N
H
N
N
N
S
OH
4500
4000
3500
3000
2500
2000
1500
1000
500
0
90
85
80
75
70
65
60
55
50
45
40
35
30
25
20
15
10
5
0
f1 (ppm)

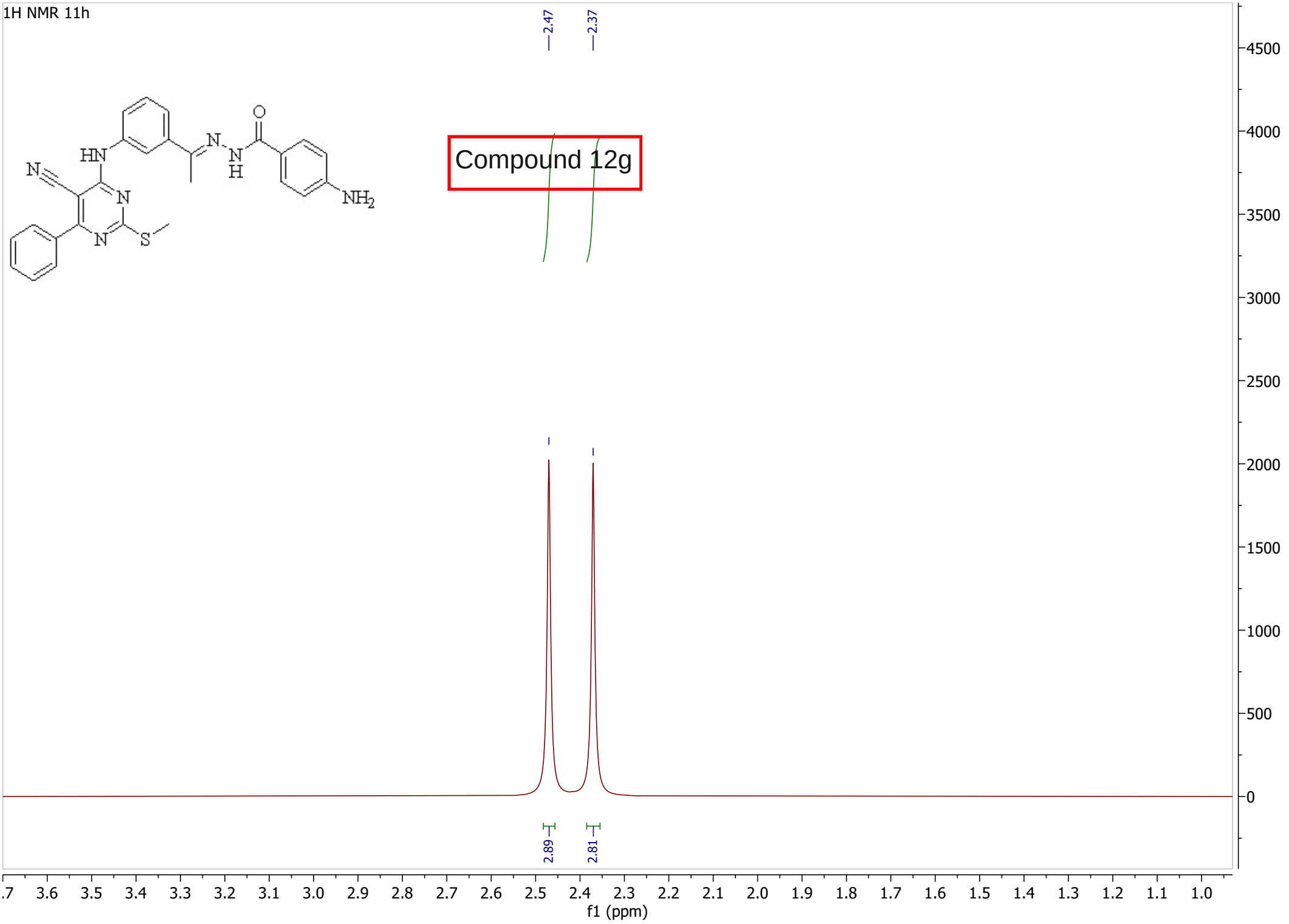

1H NMR 11h
174.61
168.57
166.40
161.01
160.57
160.47
139.00
136.42
131.64
129.28
129.19
129.02
128.80
124.90
124.44
123.34
122.03
115.29
Compound 12f
HN
N
N
H
O
OH
N
N
S
6500
6000
5500
5000
4500
4000
3500
3000
2500
2000
1500
1000
500
0
-500
180
175
170
165
160
155
150
145
140
135
130
125
120
115
110
f1 (ppm)

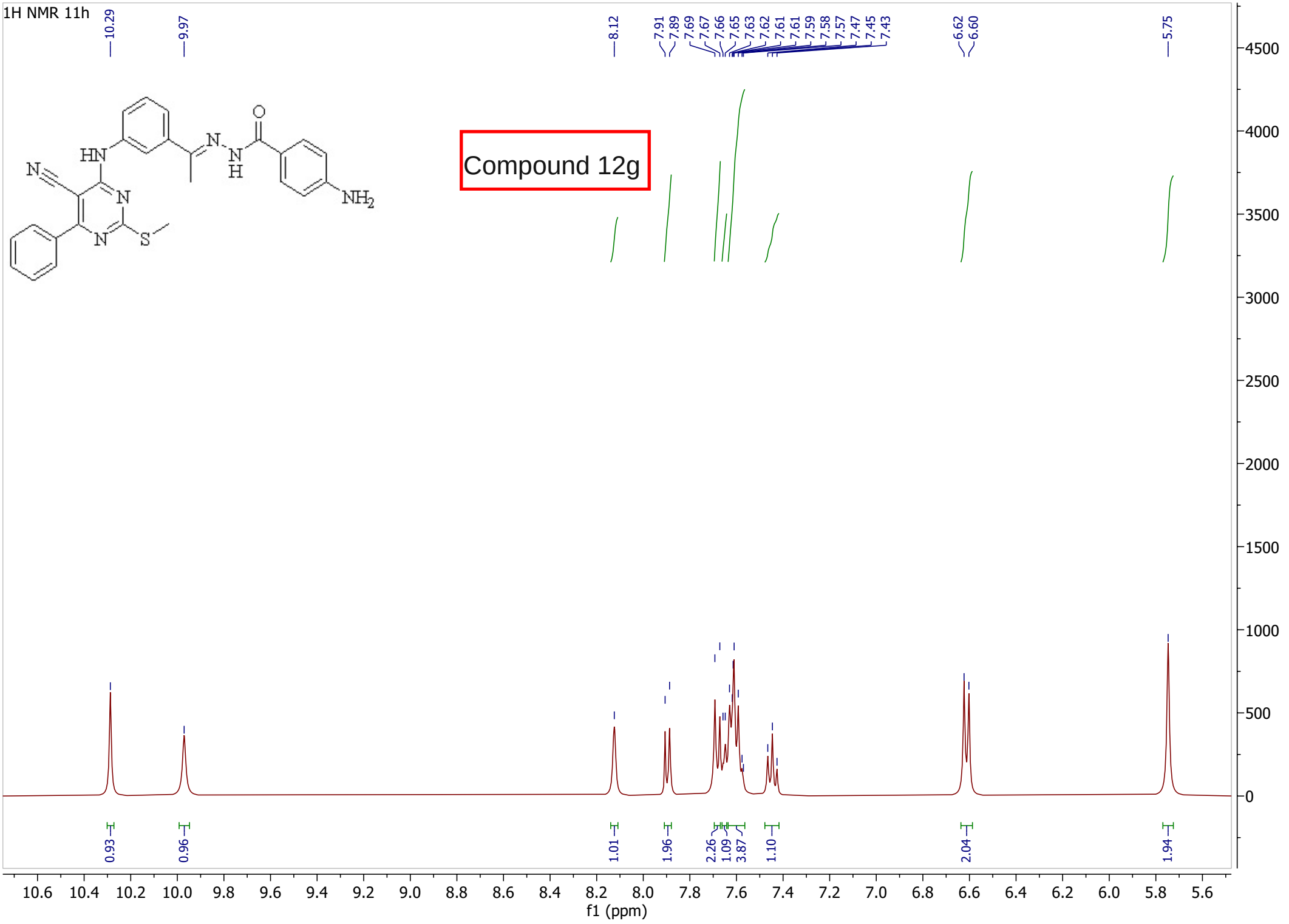

RT: 1.98 - 2.33 SM: 11B
Compound 12f
NL:
1.30E4
TIC MS
Abdelrahma
n-saleh-
AsZM4
100
90
80
70
60
50
40
30
20
2.00
2.05
2.10
2.15
2.20
2.25
2.30
Time (min)
HN
N
N
N
S
N
H
O
OH

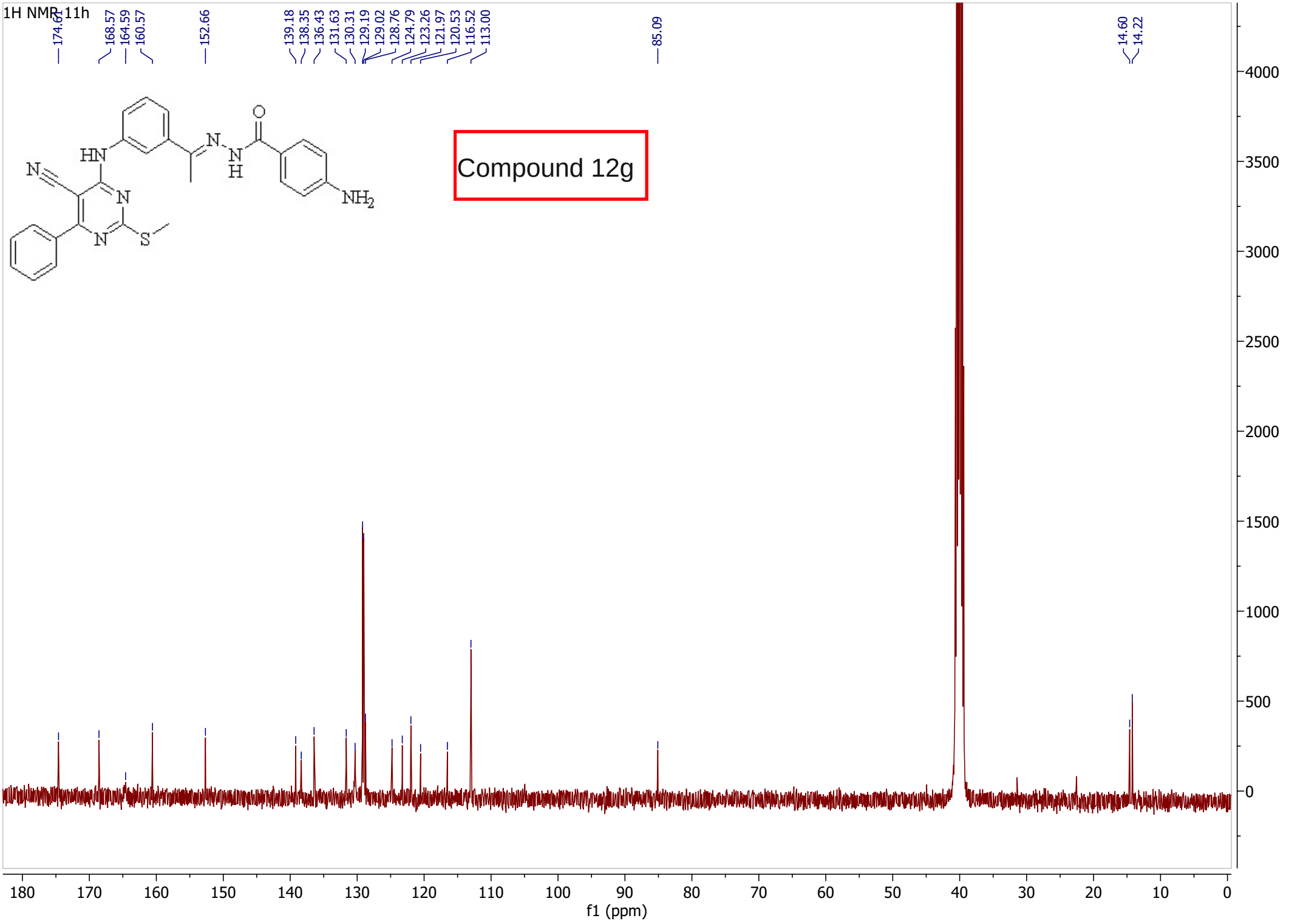

Abdelrahman-saleh-AsZM4 #92 RT: 1.56 AV: 1 SB: 26 1.21-1.34 , 0.87-1.14 NL: 4.15E2
T: + c EI Full ms [40.00-1000.00]
100
90
80
70
60
50
40
30
20
10
100
150
200
250
300
350
400
450
m/z
89.20
106.79
125.08
127.88
142.22
156.13
163.79
170.97
174.75
194.10
194.77
222.15
224.47
232.77
236.08
242.30
259.67
279.87
302.40
306.07
312.01
326.47
330.48
336.61
337.47
359.88
366.55
373.07
388.80
391.27
392.21
402.81
419.31
421.06
442.26
443.41
444.63
465.26
468.15
483.19
494.37

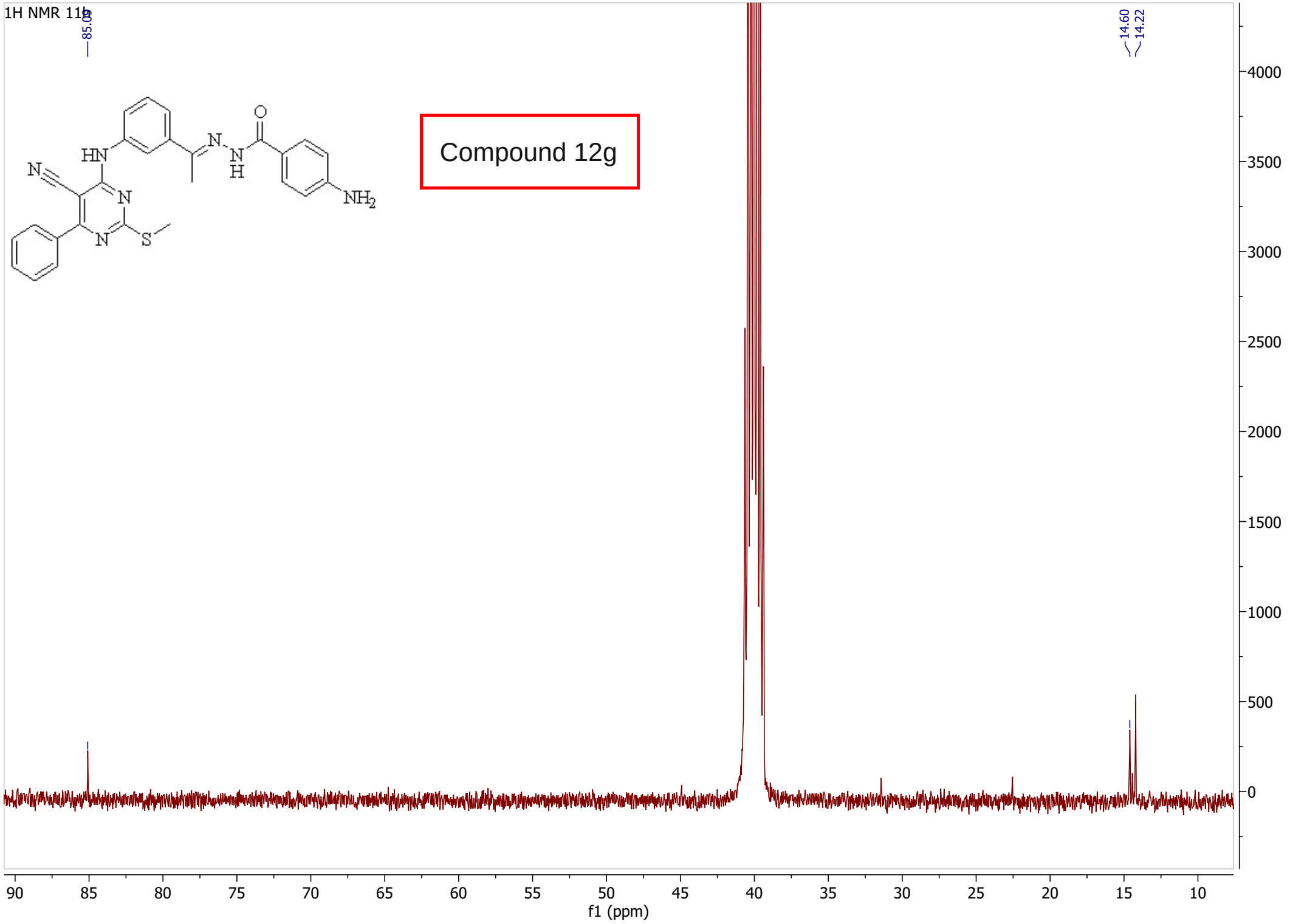

ASZM9
Compound 12g
% Transmittance
Wavenumbers (cm-1)
3478.34
3363.05
3293.74
3229.10
3070.51
3031.22
2953.52
2924.27
2868.48
2215.15
1636.53
1606.29
1578.97
1534.72
1502.38
1471.82
1448.56
1403.85
1320.33
1274.76
1226.30
1184.17
1148.92
1129.87
1010.09
969.92
931.25
873.69
837.69
803.31
761.64
691.09
660.88
618.03
588.62
570.62
530.63
508.58
439.27
HN
N
N
S
N
H
O
NH2

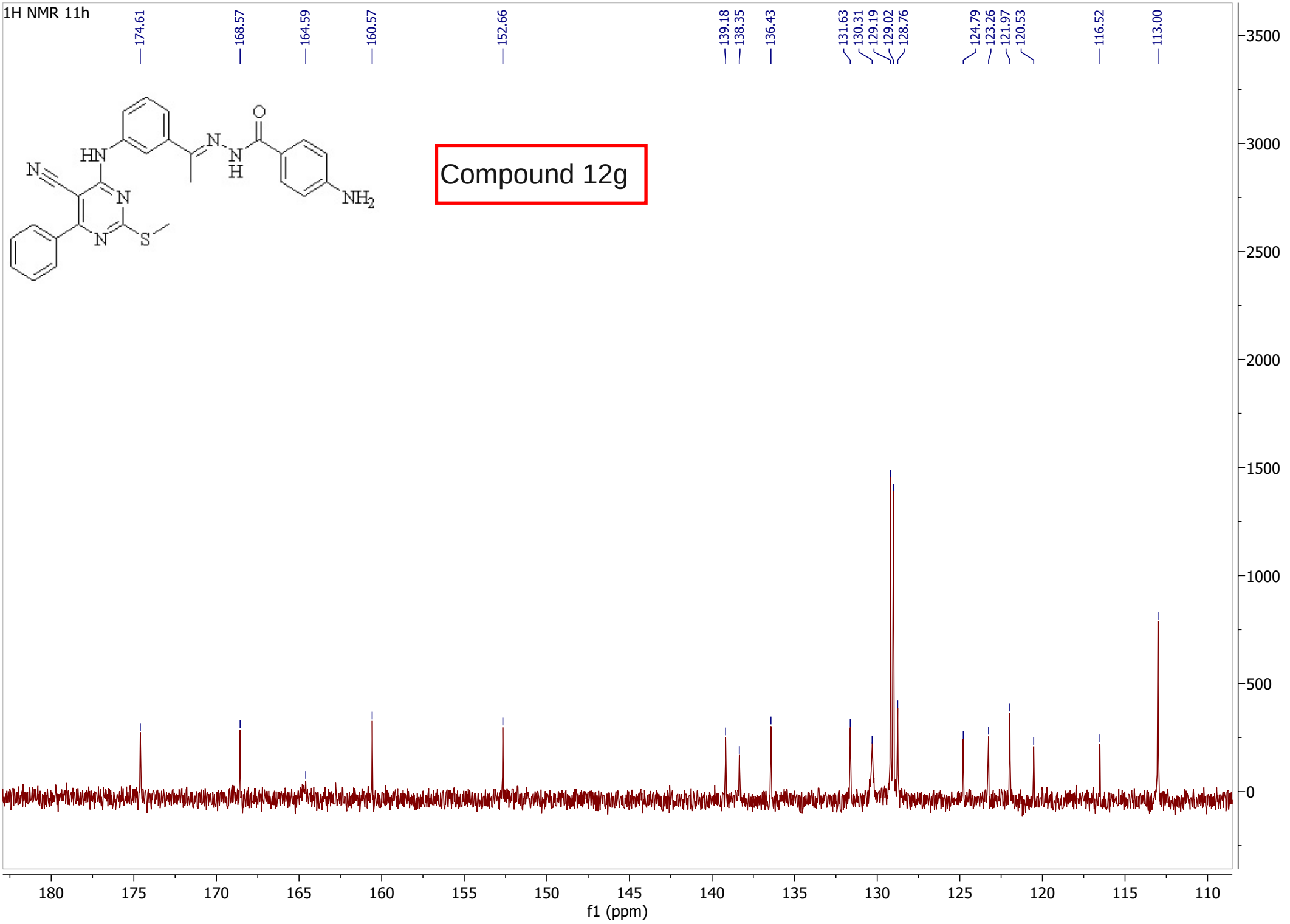

1H NMR 11h
10.29
9.97
8.12
7.91
7.89
7.69
7.67
7.66
7.65
7.63
7.62
7.61
7.61
7.59
7.58
7.57
7.47
7.45
7.43
6.62
6.60
5.75
2.49
2.47
2.37
Compound 12g
HN
N
N
H
N
N
S
NH2
0.93
0.96
1.01
1.96
2.26
1.09
3.87
1.10
2.04
1.94
2.89
2.81
f1 (ppm)


1H NMR 11h
2.47
2.37
Compound 12g
HN
N
N
H
N
N
S
NH2
2.89
2.81
4500
4000
3500
3000
2500
2000
1500
1000
500
0
3.6
3.5
3.4
3.3
3.2
3.1
3.0
2.9
2.8
2.7
2.6
2.5
2.4
2.3
2.2
2.1
2.0
1.9
1.8
1.7
1.6
1.5
1.4
1.3
1.2
1.1
1.0
f1 (ppm)


1H NMR 11h
10.29
9.97
8.12
7.91
7.89
7.69
7.67
7.66
7.65
7.63
7.62
7.61
7.61
7.59
7.58
7.57
7.47
7.45
7.43
6.62
6.60
5.75
Compound 12g
HN
N
N
H
N
N
N
S
NH2
4500
4000
3500
3000
2500
2000
1500
1000
500
0
0.93
0.96
1.01
1.96
2.26
1.09
3.87
1.10
2.04
1.94
10.6
10.4
10.2
10.0
9.8
9.6
9.4
9.2
9.0
8.8
8.6
8.4
8.2
8.0
7.8
7.6
7.4
7.2
7.0
6.8
6.6
6.4
6.2
6.0
5.8
5.6
f1 (ppm)


1H NMR 11h
174.61
168.57
164.59
160.57
152.66
139.18
138.35
136.43
131.63
130.31
129.19
129.02
128.76
124.79
123.26
121.97
120.53
116.52
113.00
85.09
14.60
14.22
Compound 12g
HN
N
N
H
N
N
S
N
NH2
4000
3500
3000
2500
2000
1500
1000
500
0
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


1H NMR 11g
85.09
14.60
14.22
Compound 12g
HN
N
N
H
N
N
N
S
NH2
4000
3500
3000
2500
2000
1500
1000
500
0
90
85
80
75
70
65
60
55
50
45
40
35
30
25
20
15
10
f1 (ppm)


1H NMR 11h
174.61
168.57
164.59
160.57
152.66
139.18
138.35
136.43
131.63
130.31
129.19
129.02
128.76
124.79
123.26
121.97
120.53
116.52
113.00
Compound 12g
HN
N
N
H
N
N
S
NH2
3500
3000
2500
2000
1500
1000
500
0
180
175
170
165
160
155
150
145
140
135
130
125
120
115
110
f1 (ppm)