

Supporting Information

An Efficient Copper-Catalysed Synthesis of Symmetrical Bis(N-Arylbenzamide) Selenides and Their Conversion to Hypervalent Spiroselenuranes and Hydroxy Congeners

Rahul Kadu,[‡] Monojit Batabyal,[‡] Heena Kadyan, Apurba Lal Koner, Sangit Kumar*

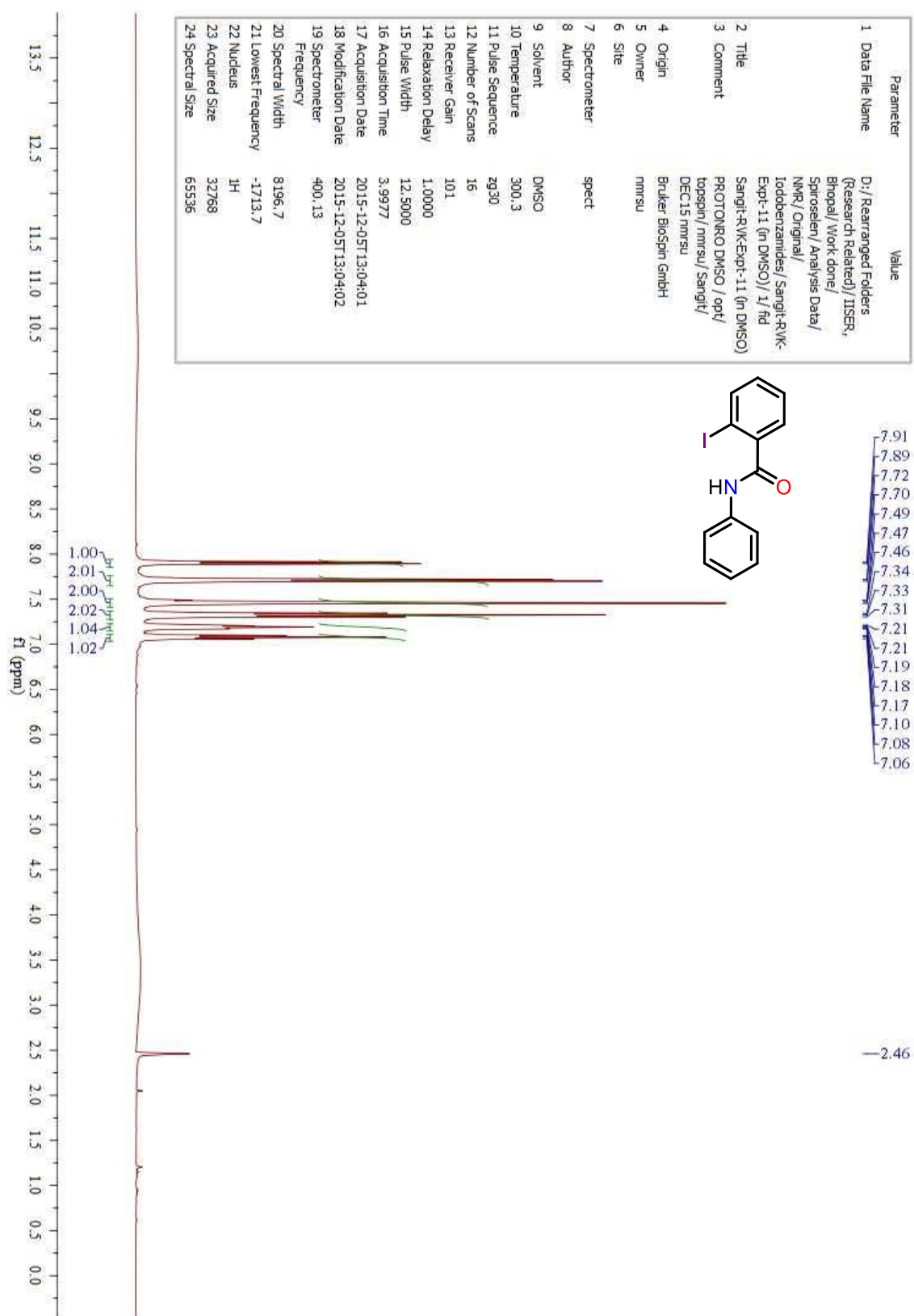
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[‡]Both authors contributed equally

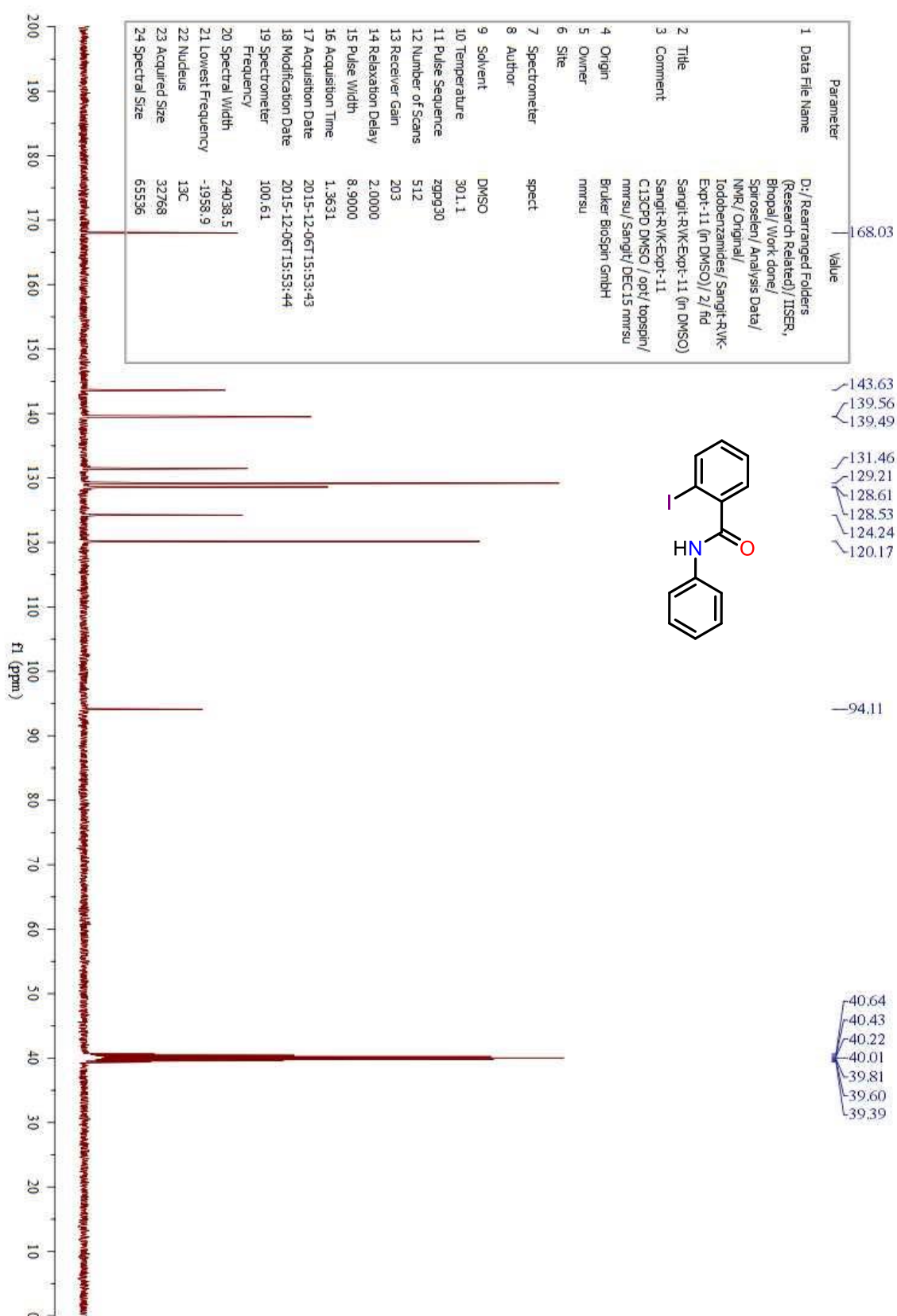
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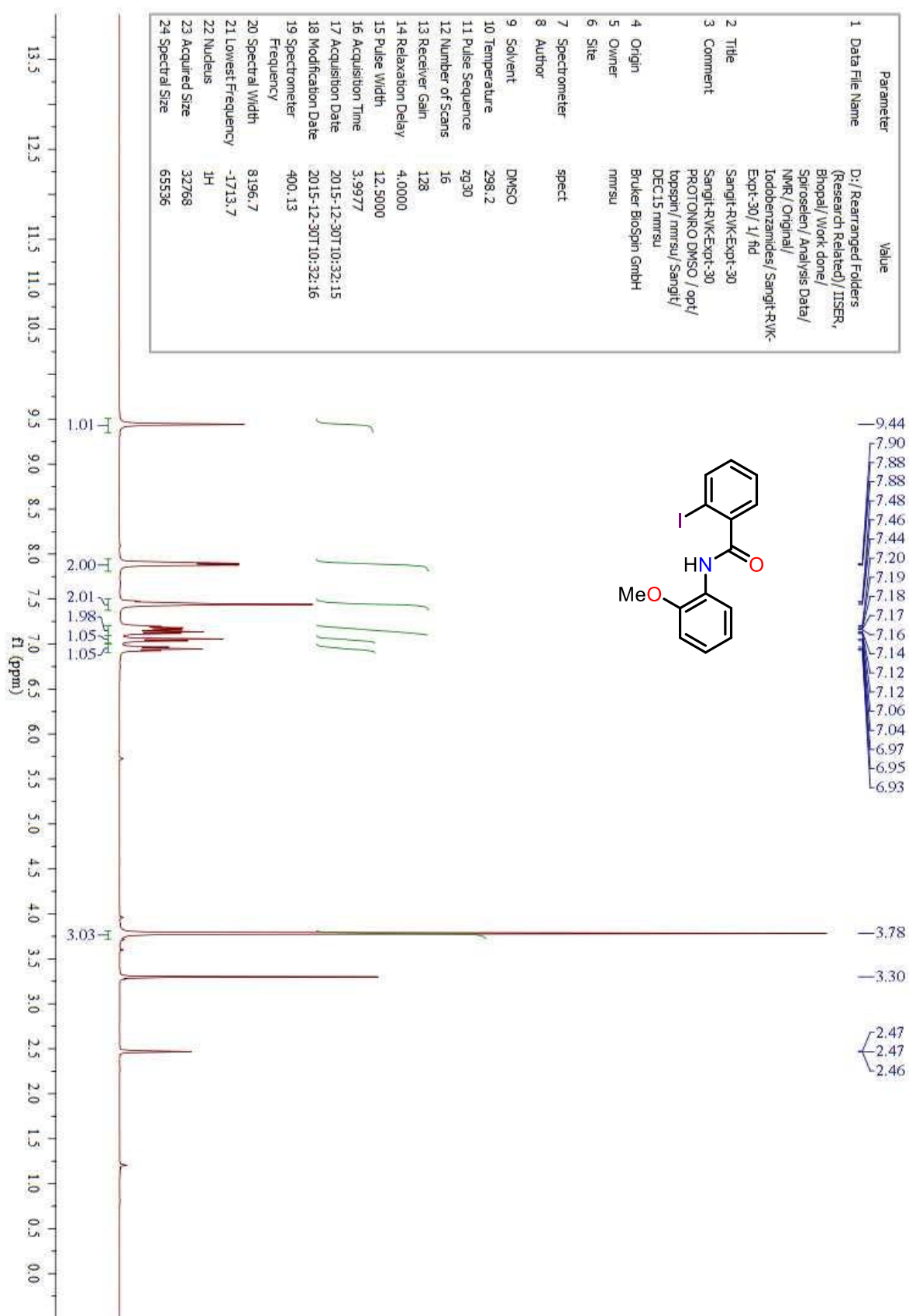
¹H NMR of 31



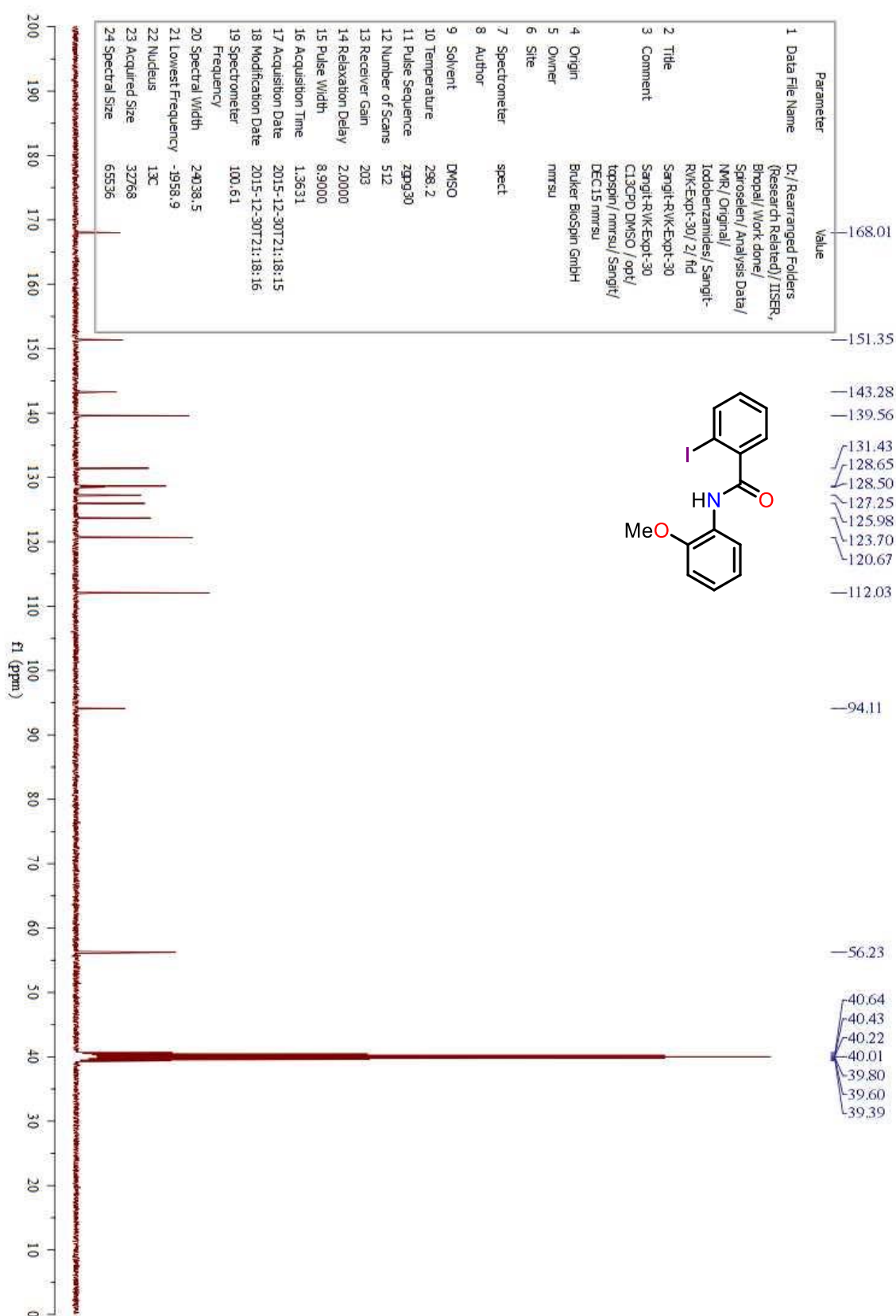
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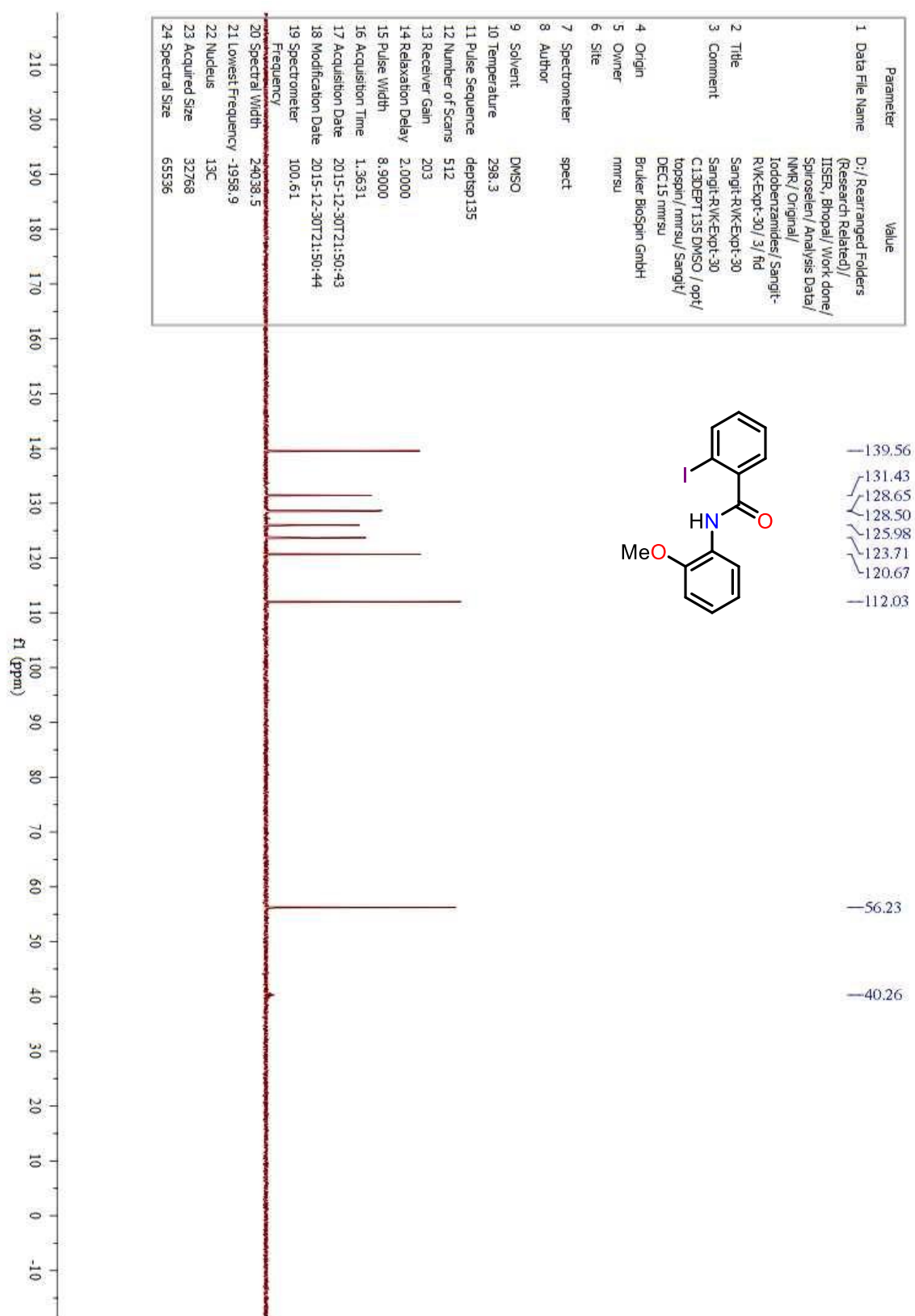
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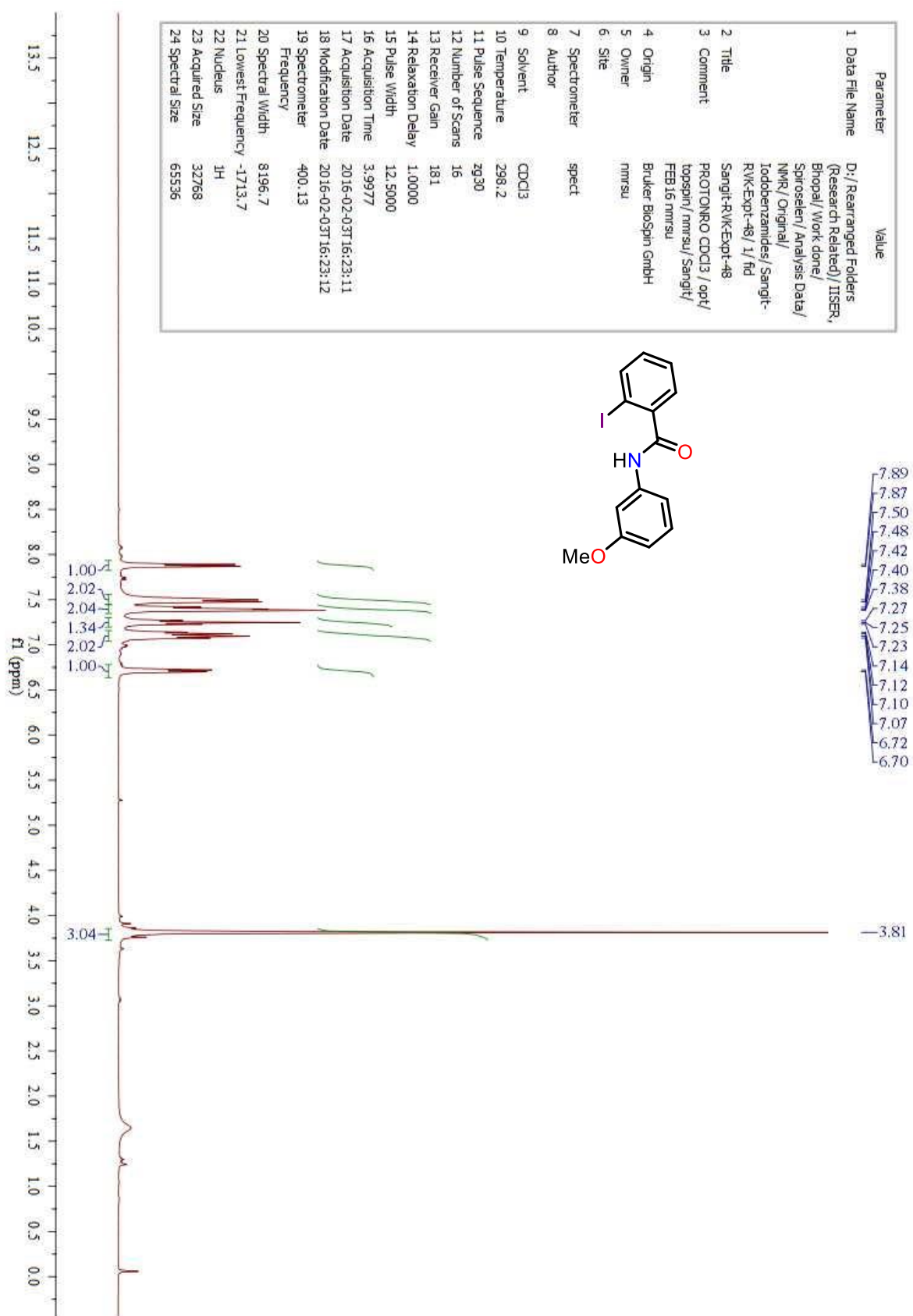
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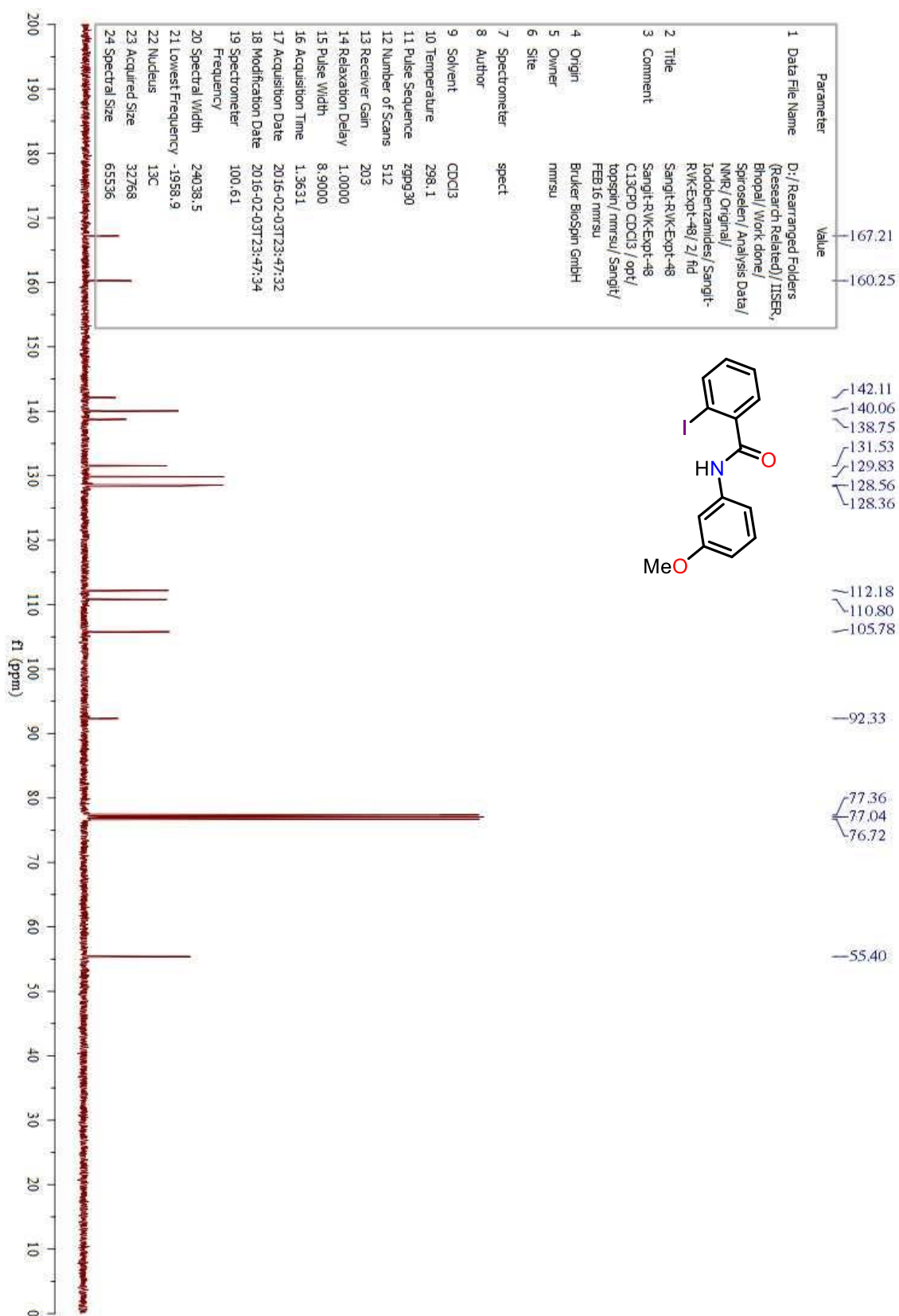
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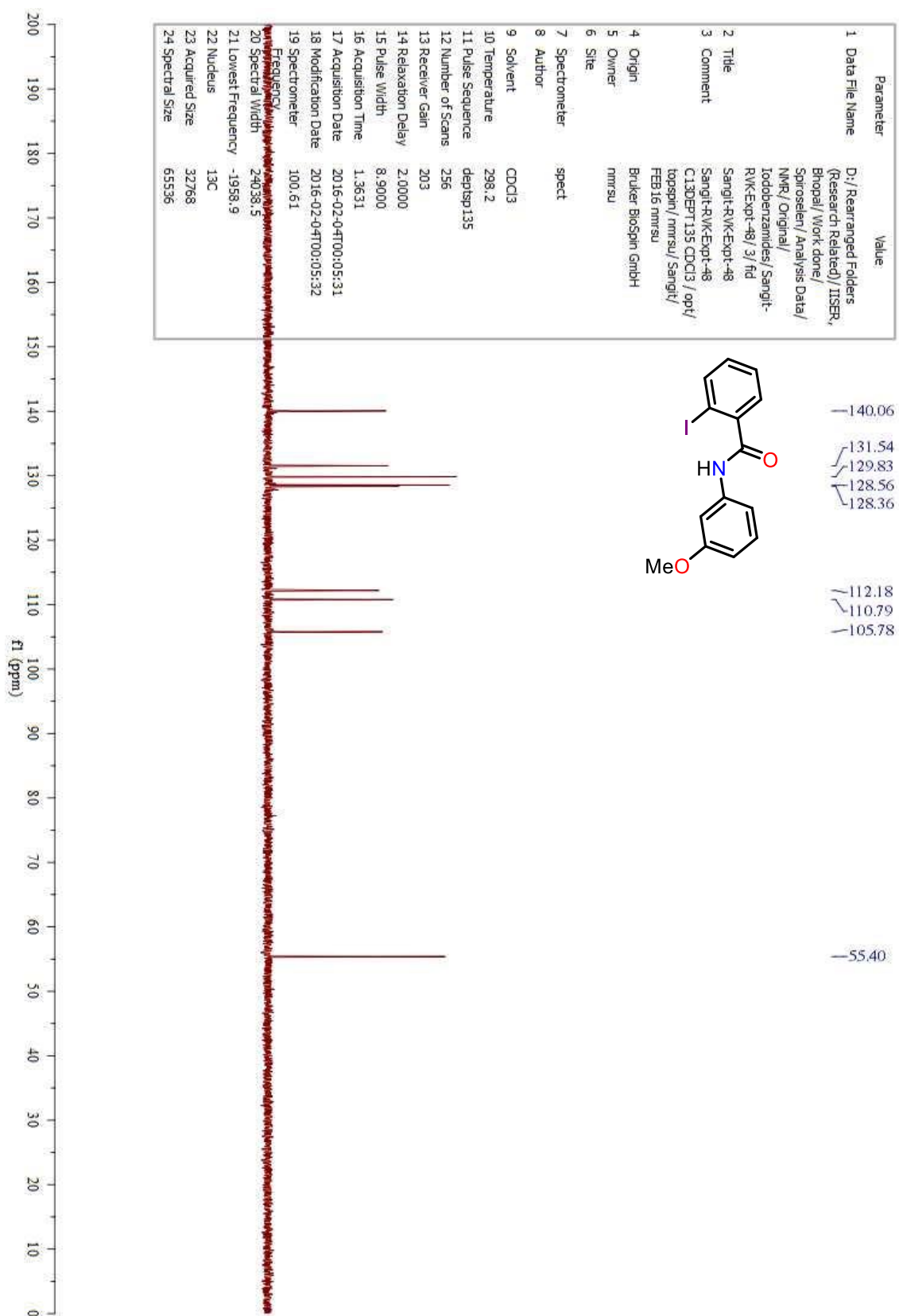
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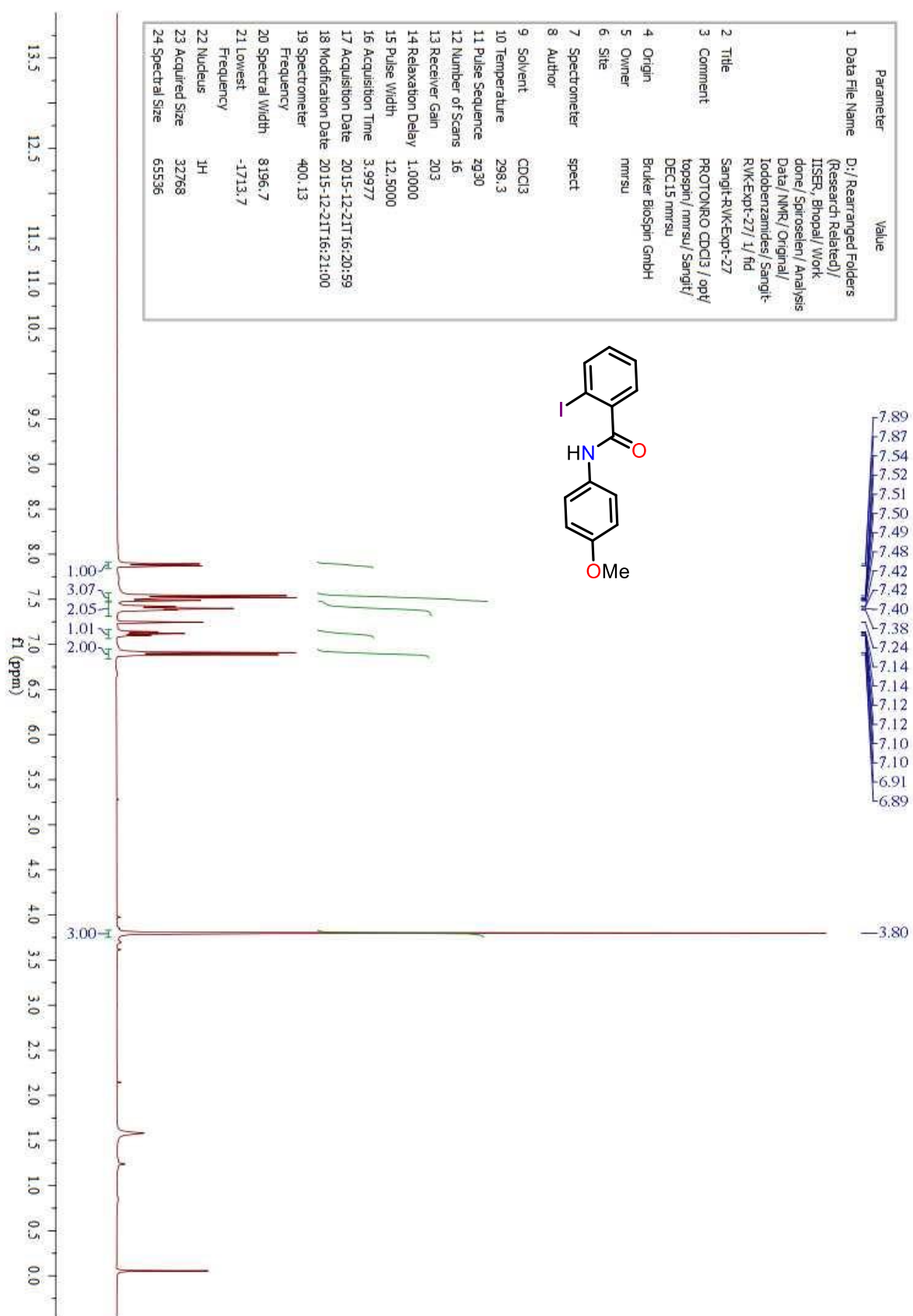
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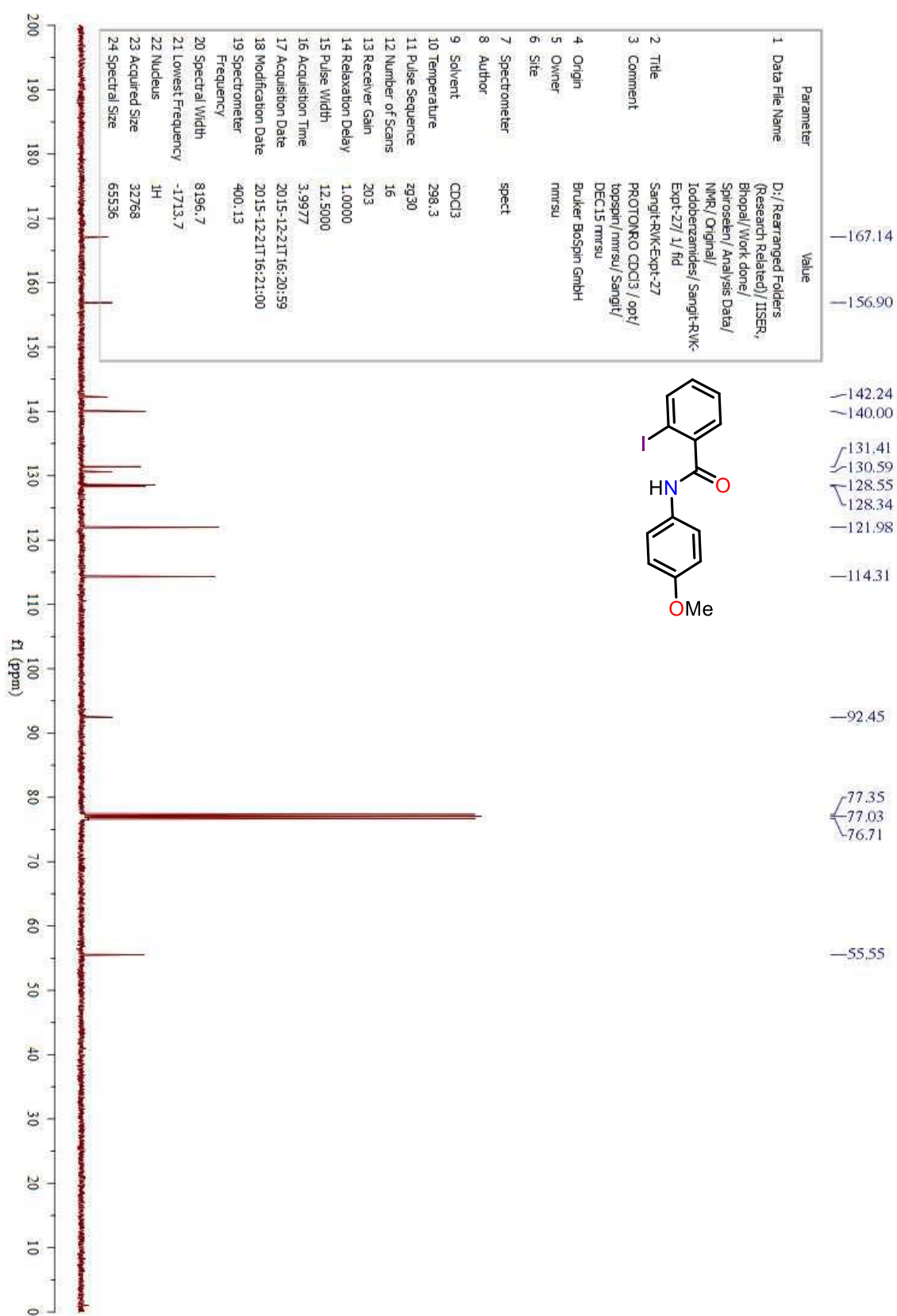
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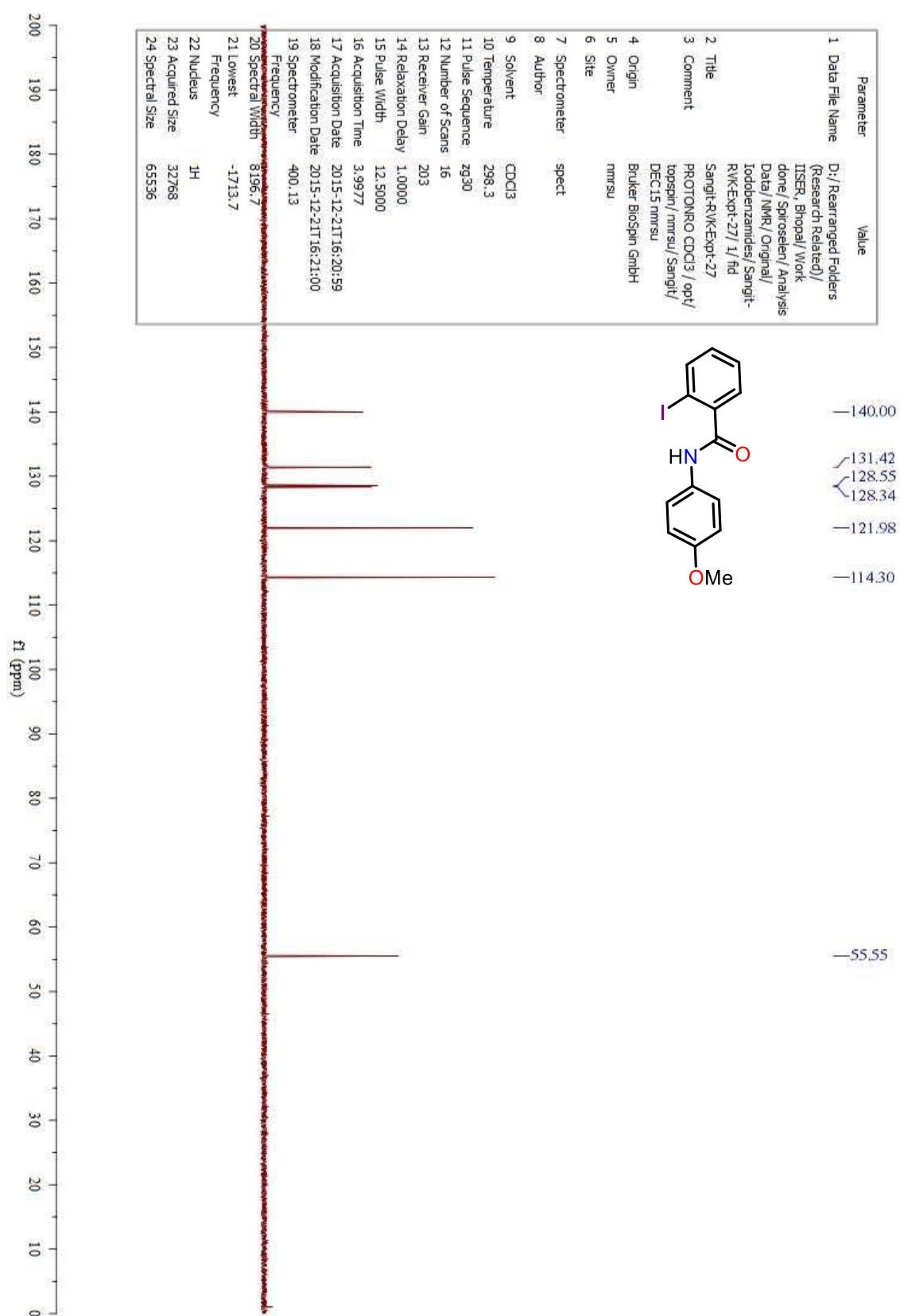


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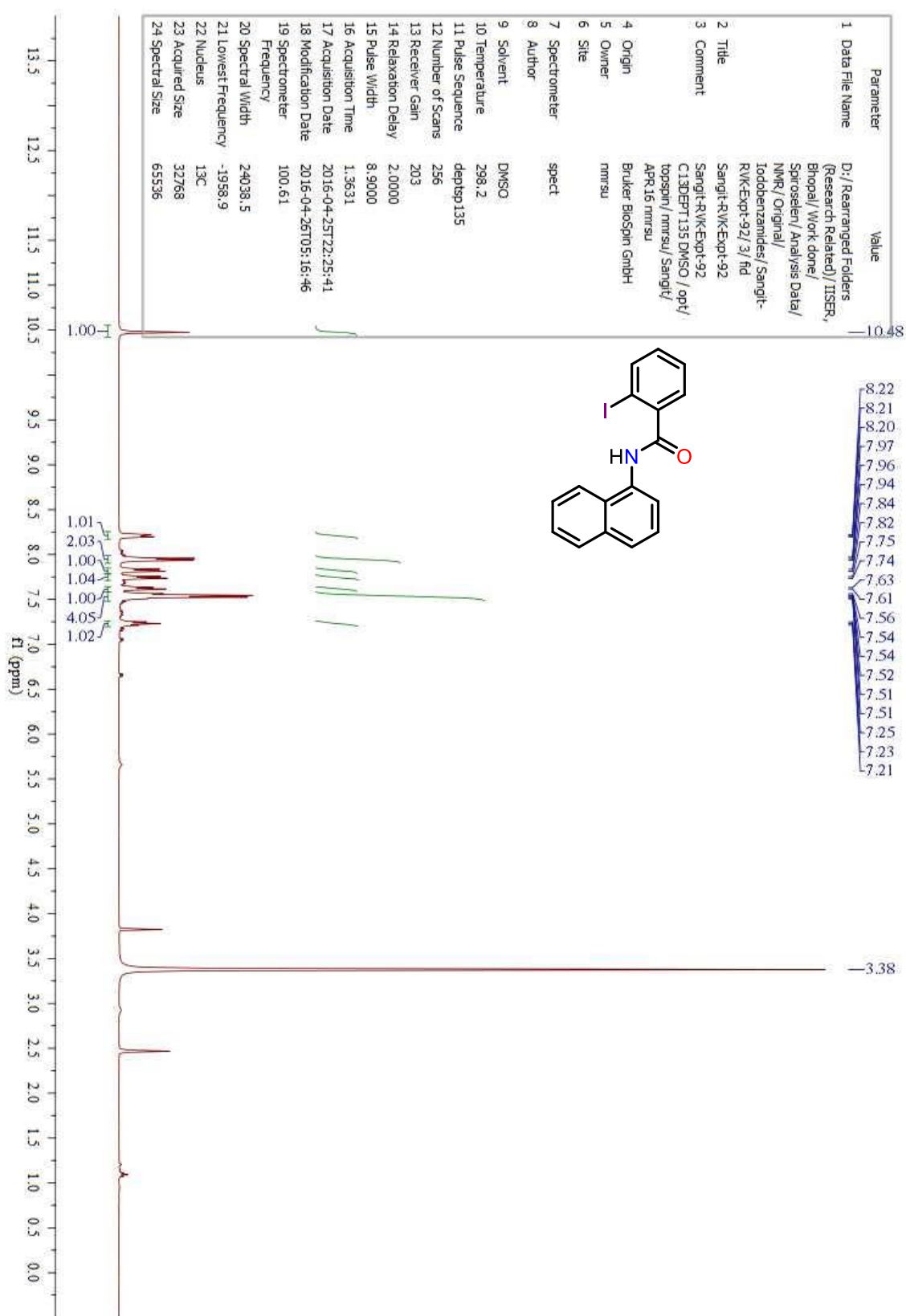


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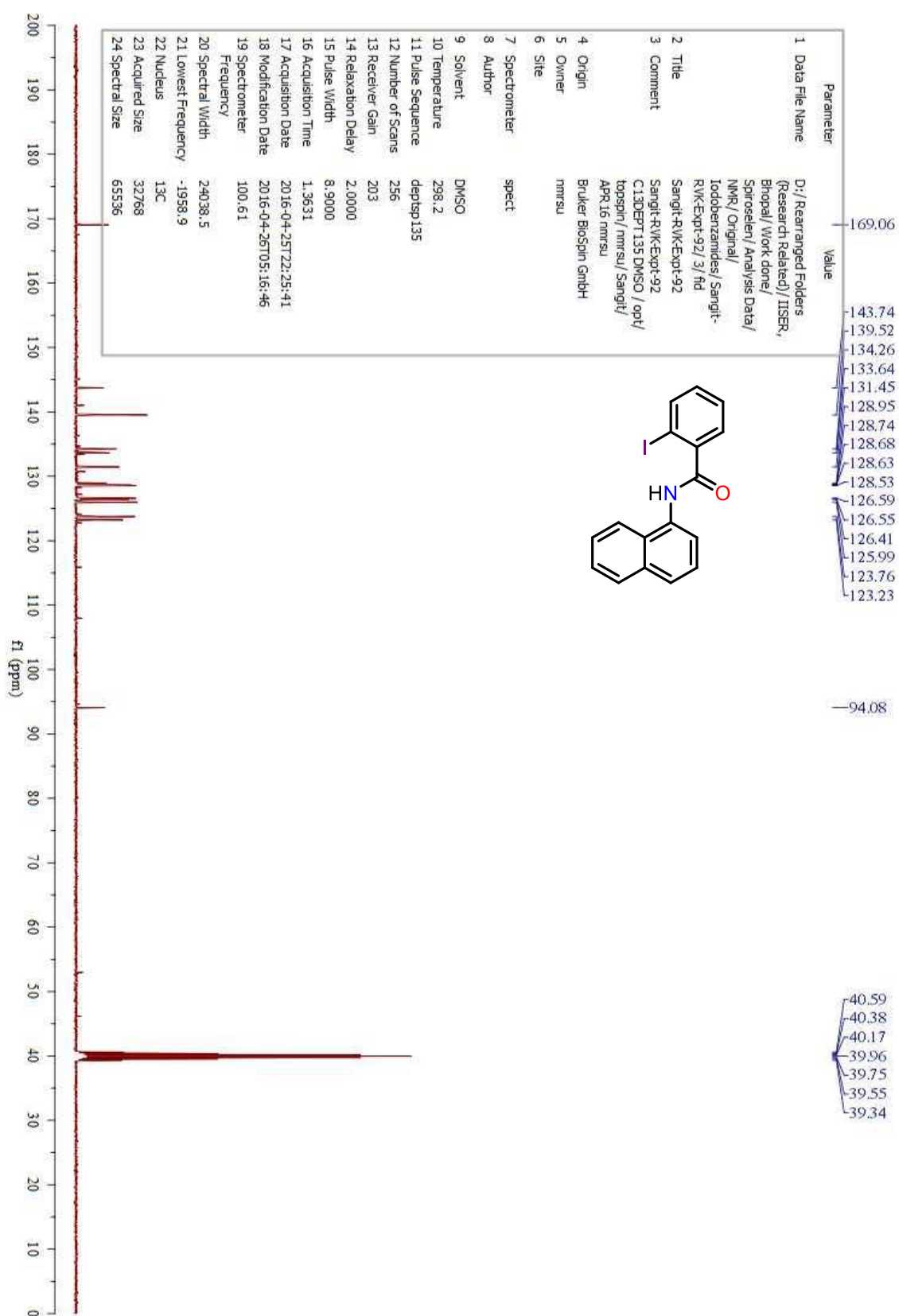




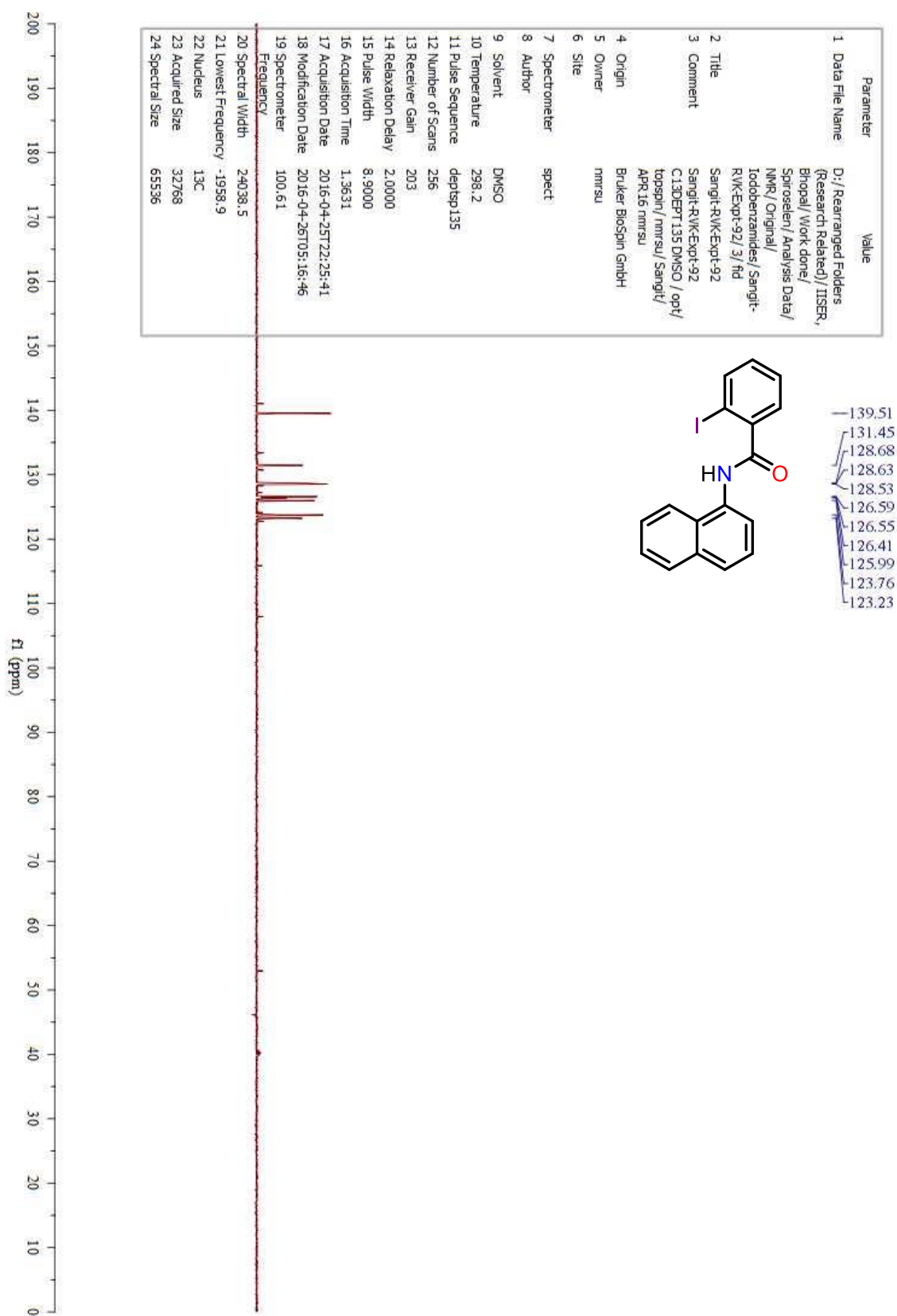
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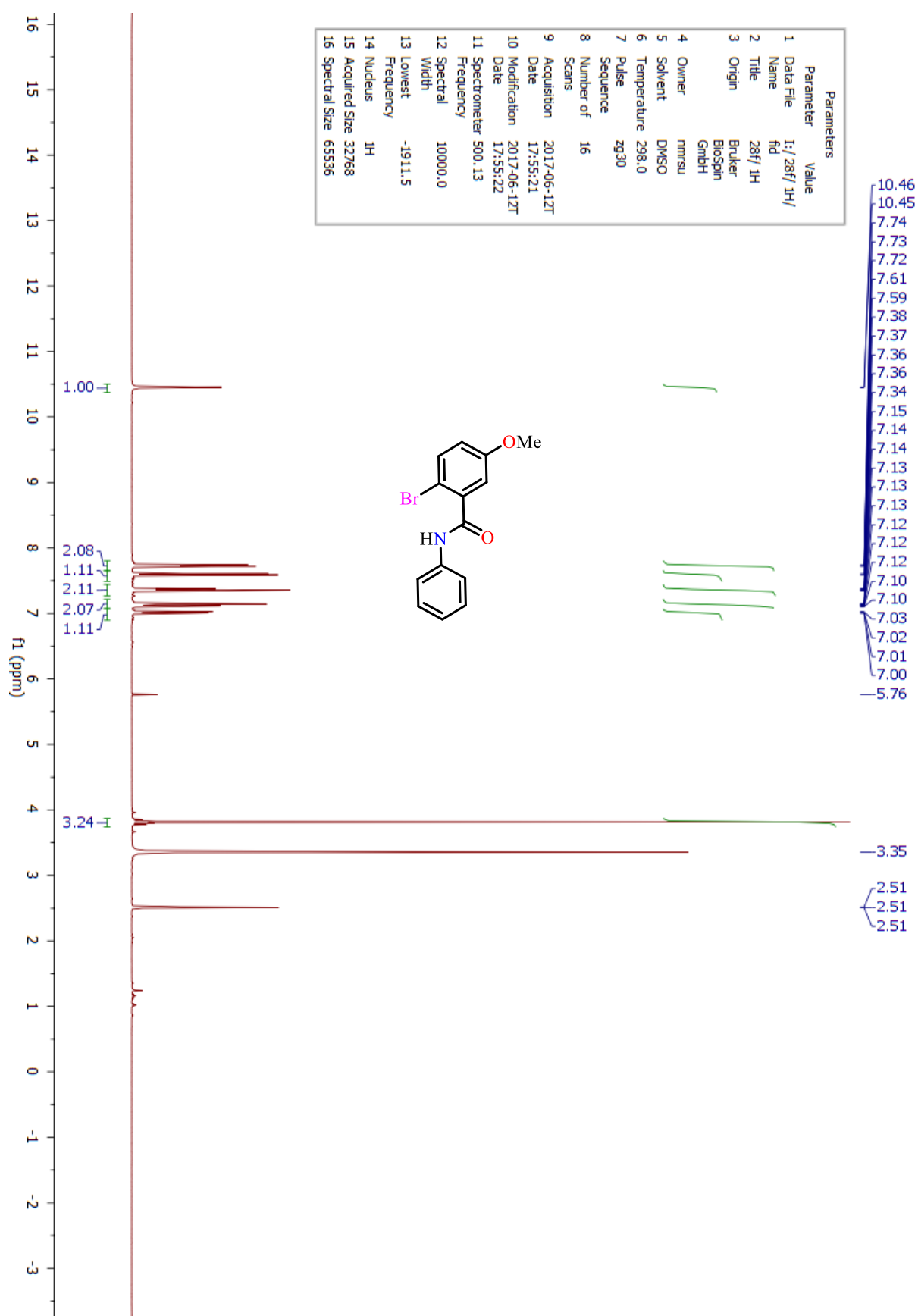
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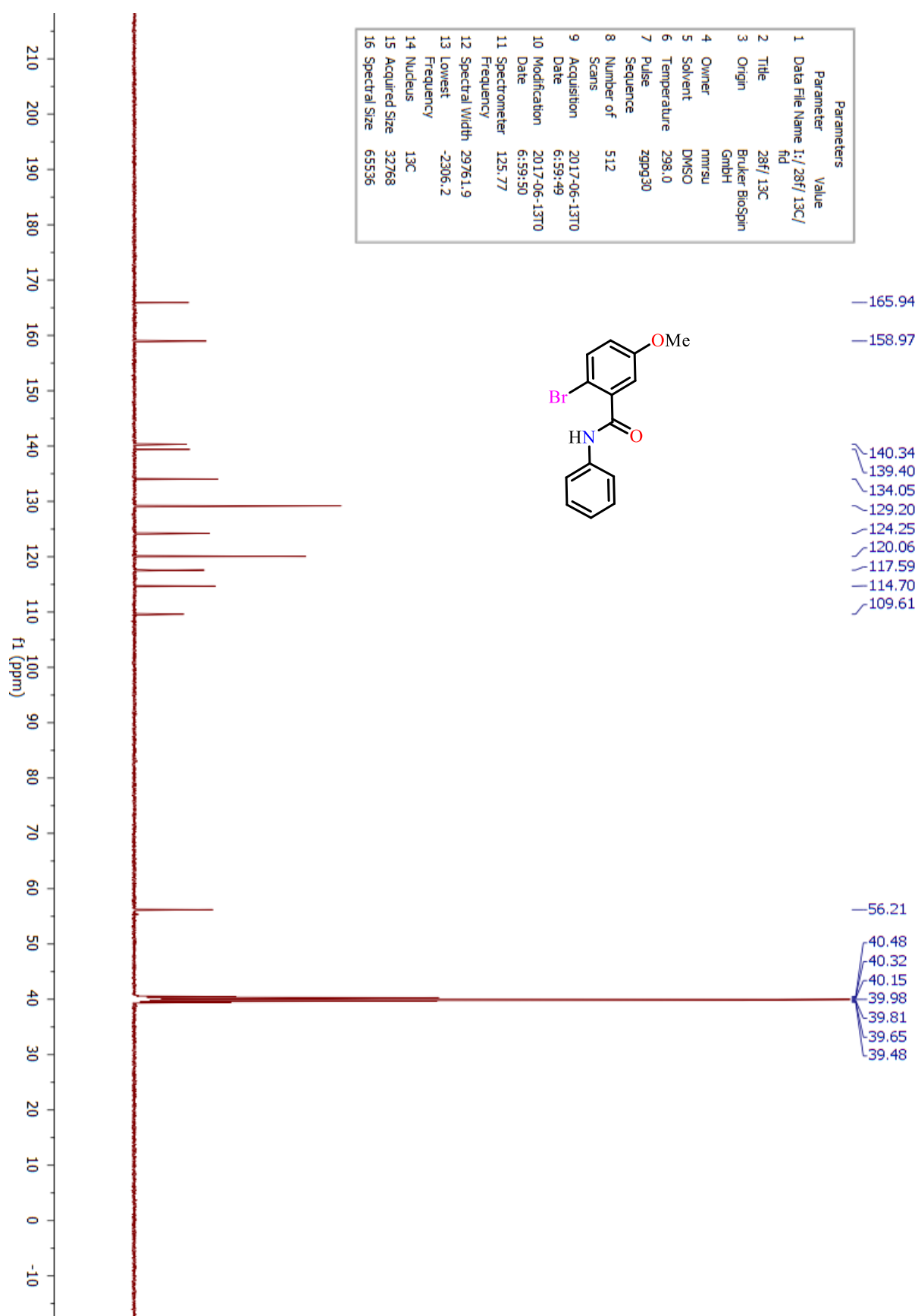
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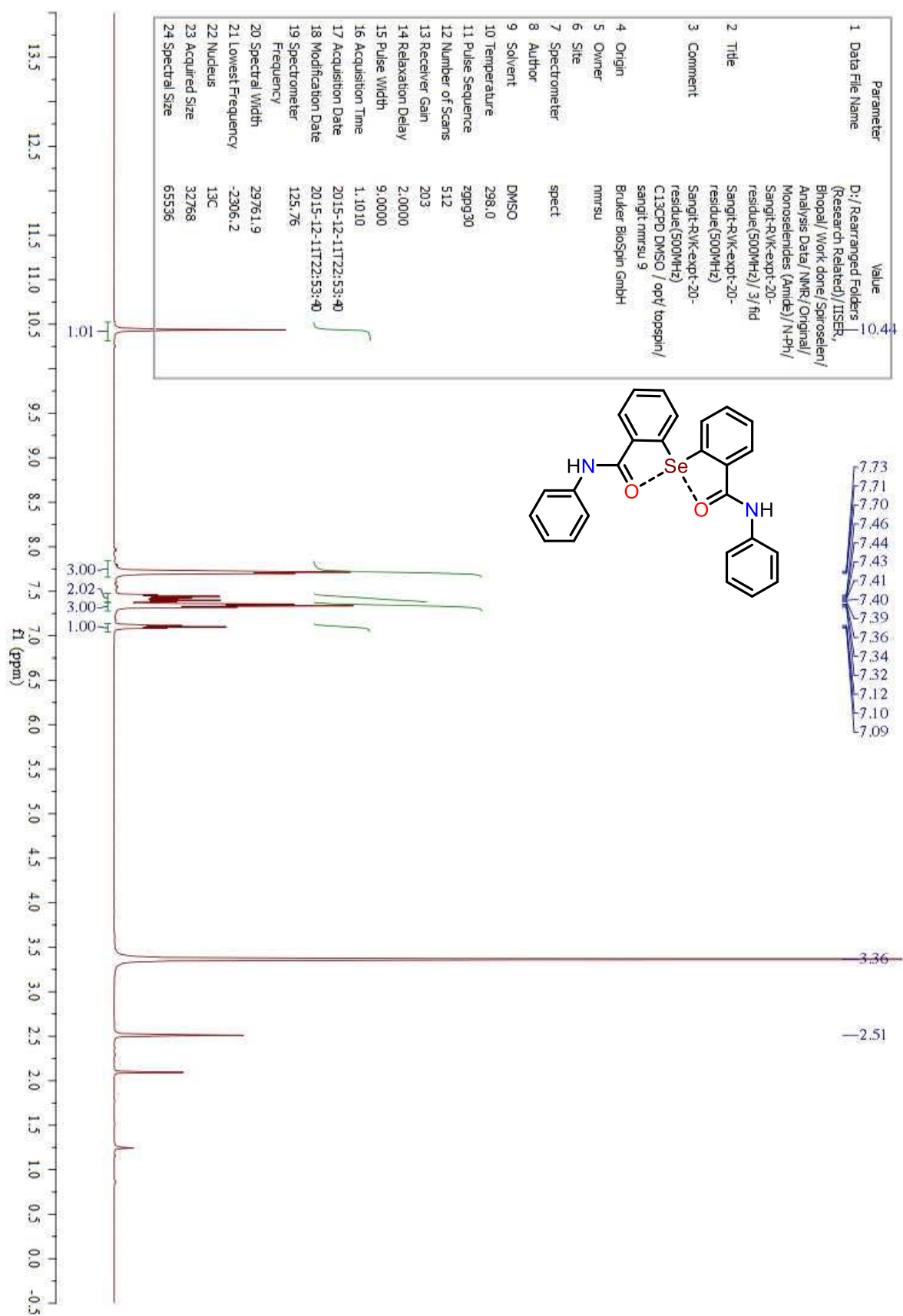
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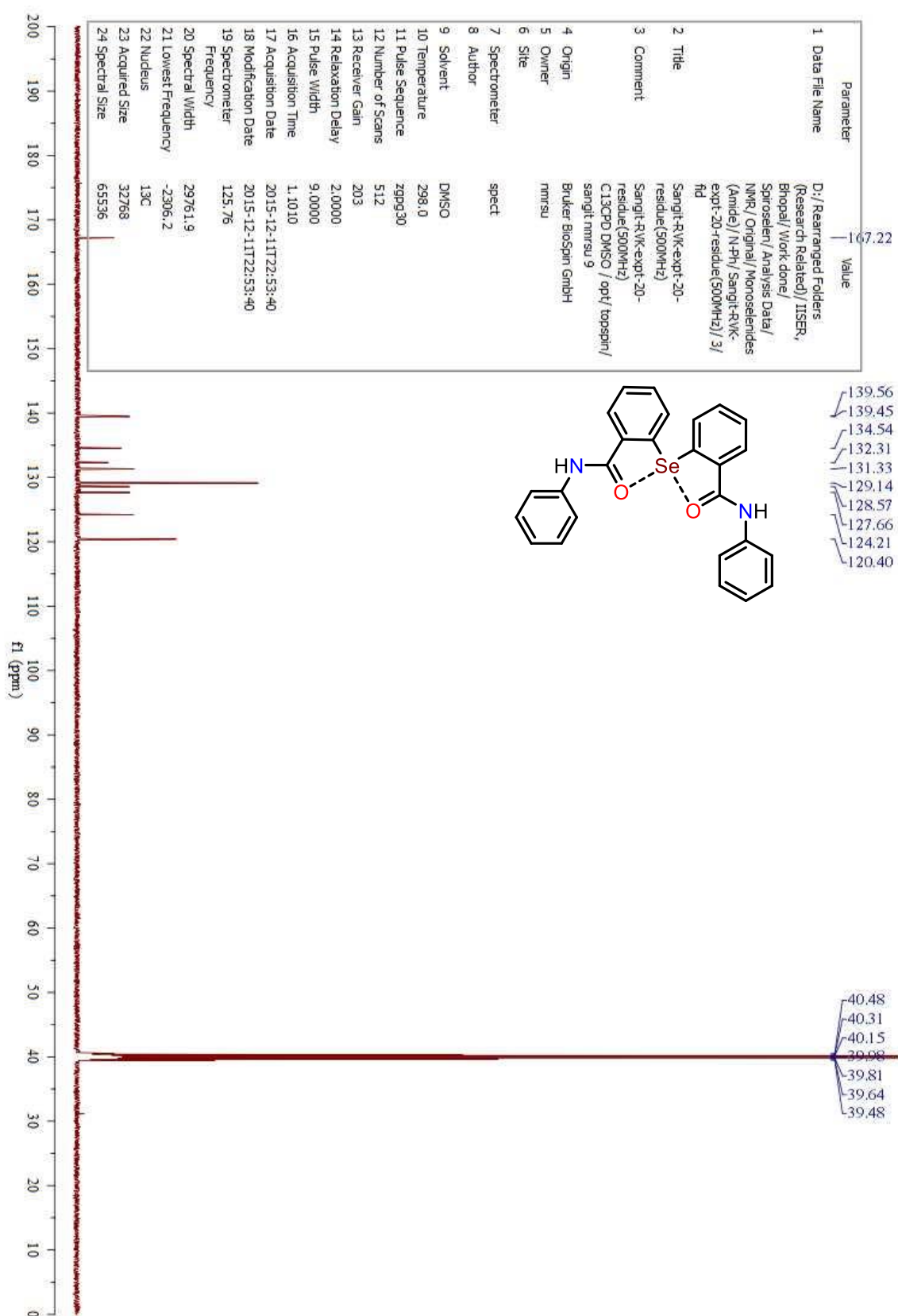
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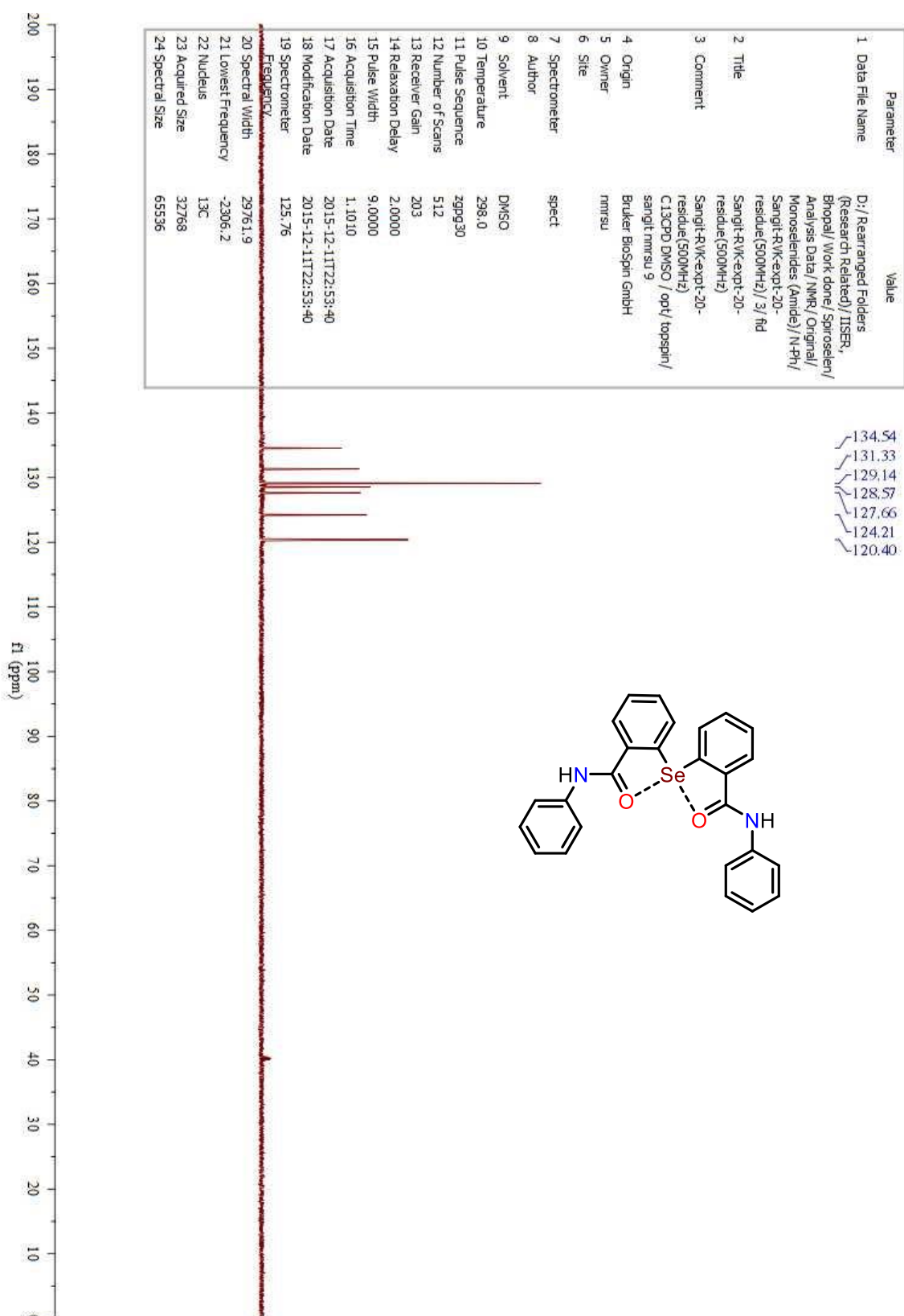


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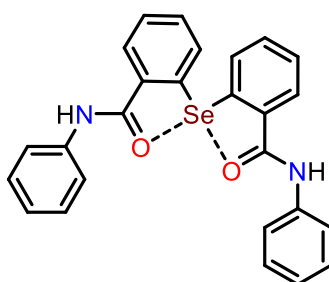
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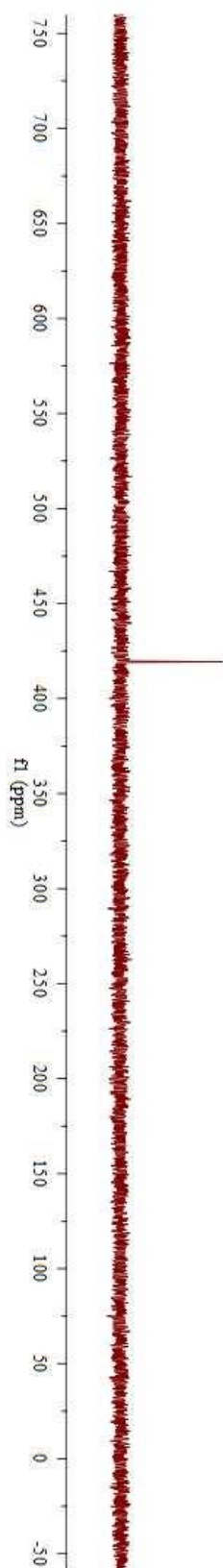


⁷⁷Se NMR of 24

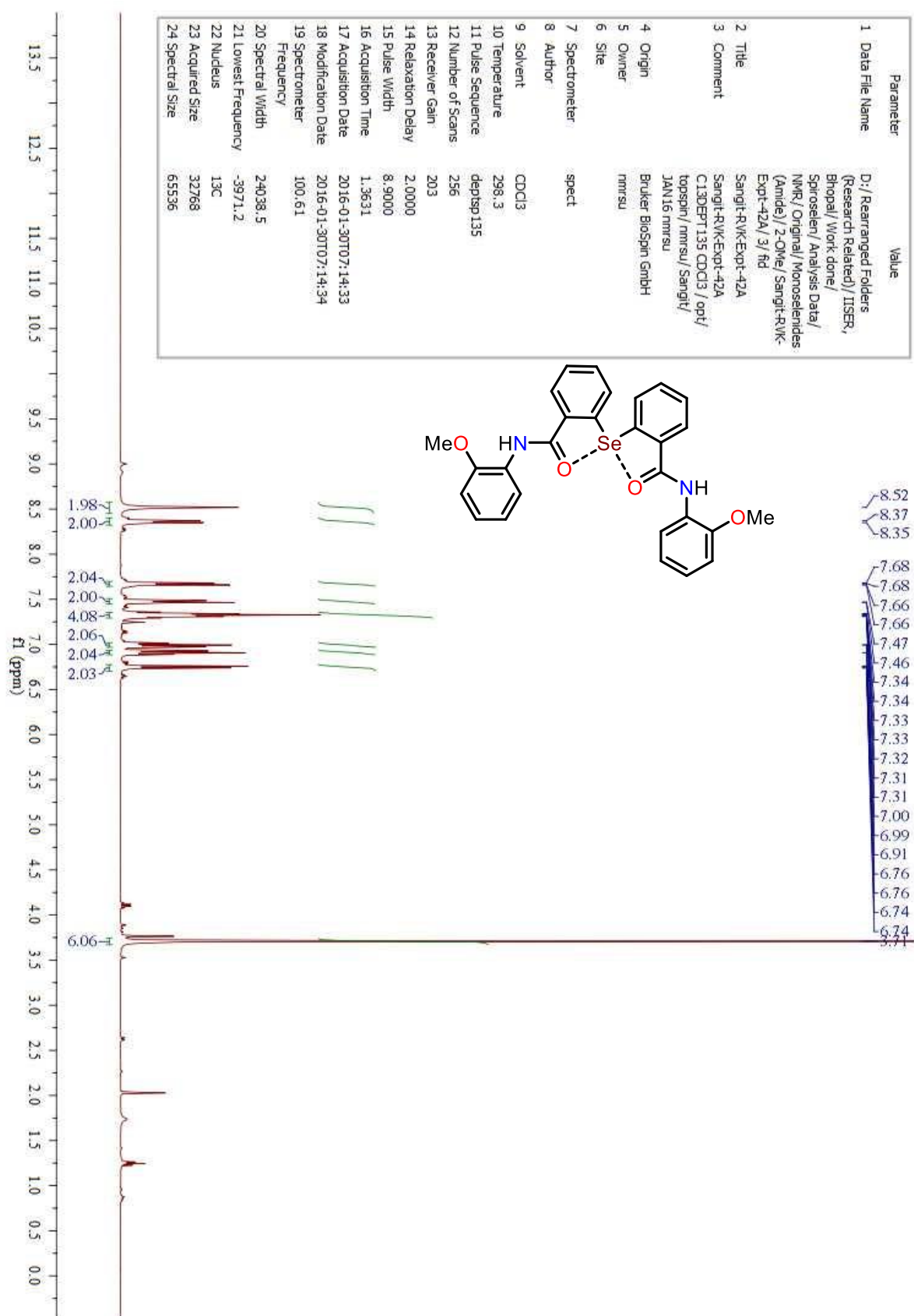
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4 Owner	nmrsu
5 Site	
6 Spectrometer	spect
7 Author	
8 Solvent	DMSO
9 Temperature	298.2
10 Pulse Sequence	zg
11 Number of Scans	512
12 Receiver Gain	203
13 Relaxation Delay	4.0000
14 Pulse Width	5.0000
15 Acquisition Time	0.5243
16 Acquisition Date	2015-10-26T18:12:31
17 Modification Date	2015-10-26T18:12:32
18 Spectrometer	76.31
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Frequency	
21 Nucleus	
22 Acquired Size	32768
23 Spectral Size	65536



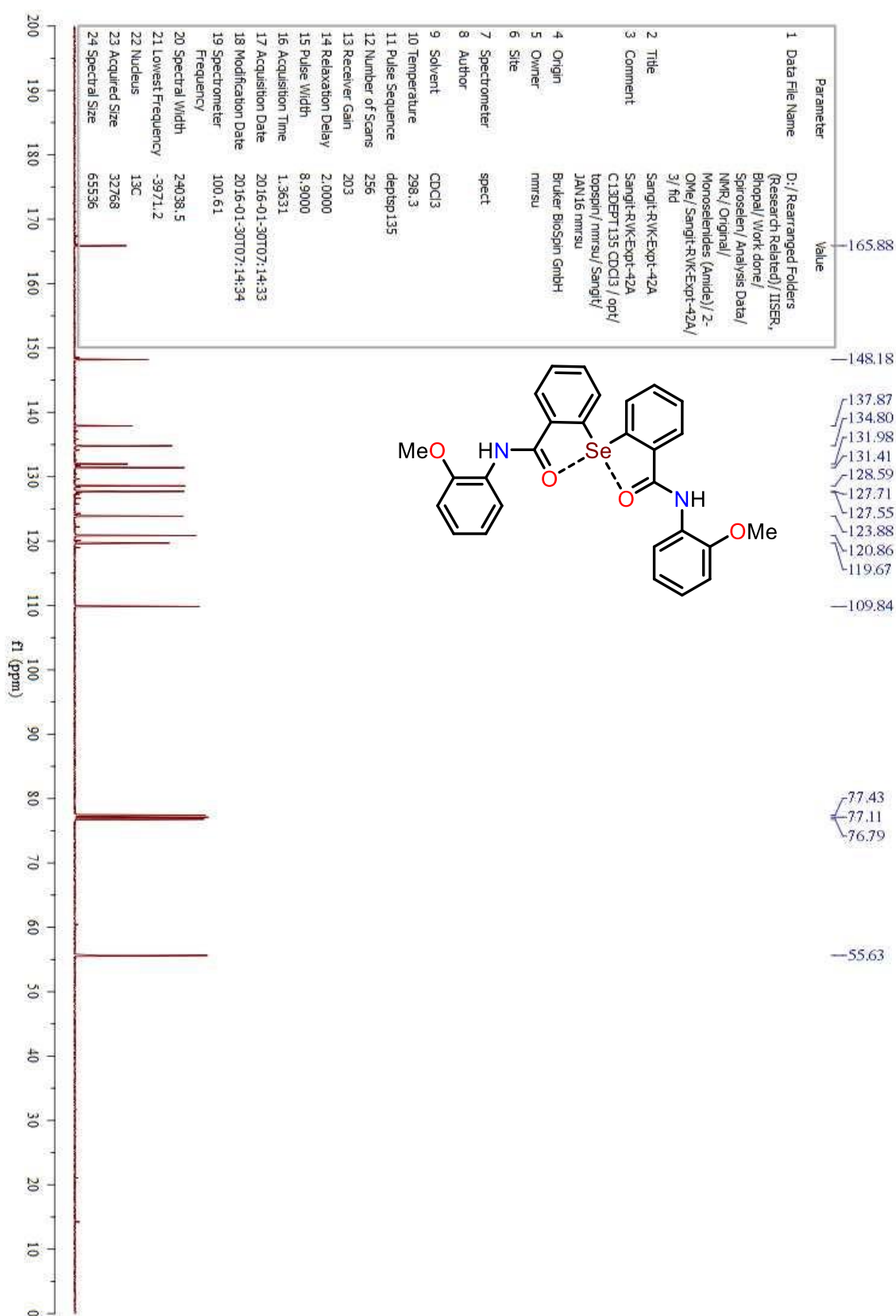
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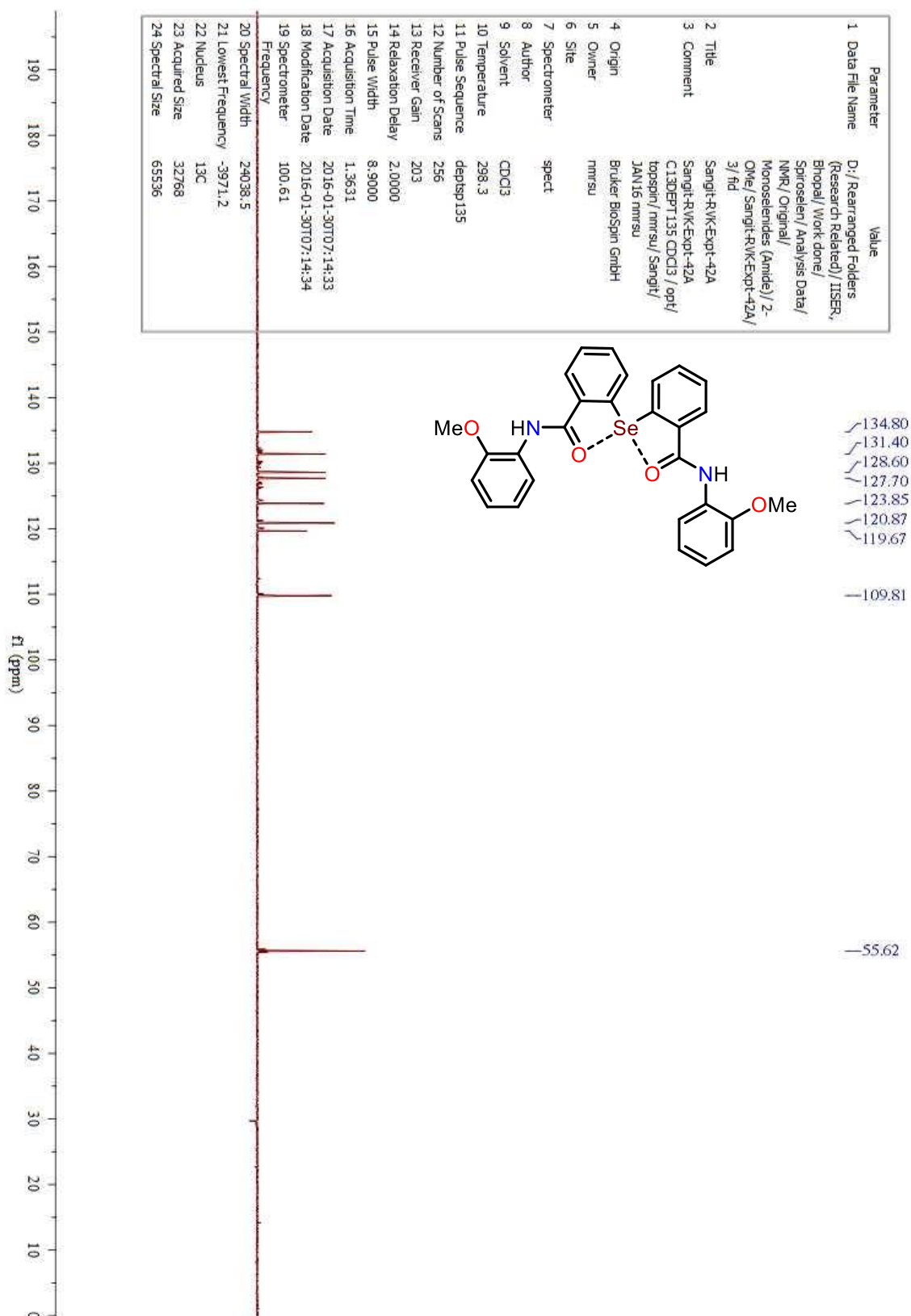
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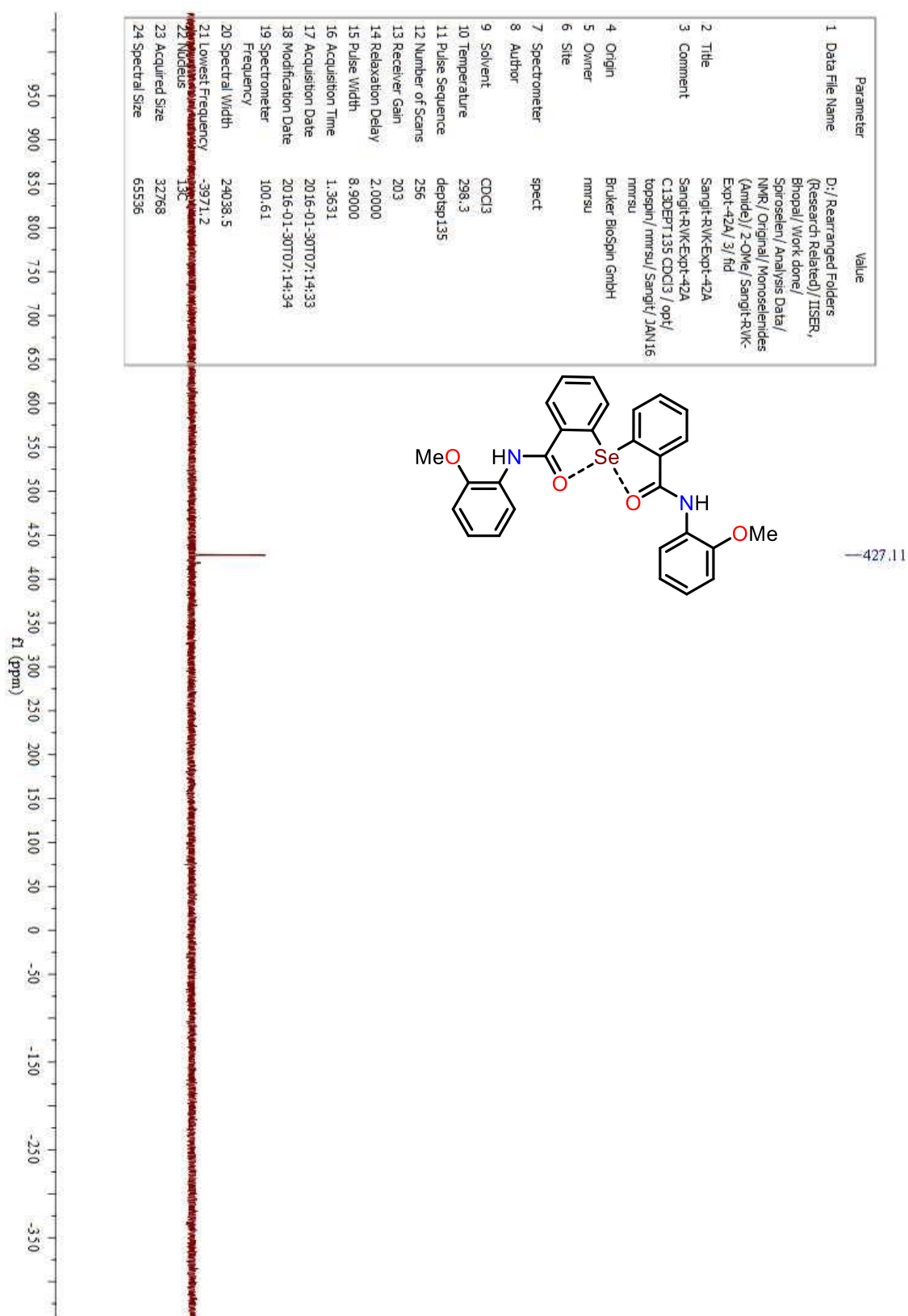
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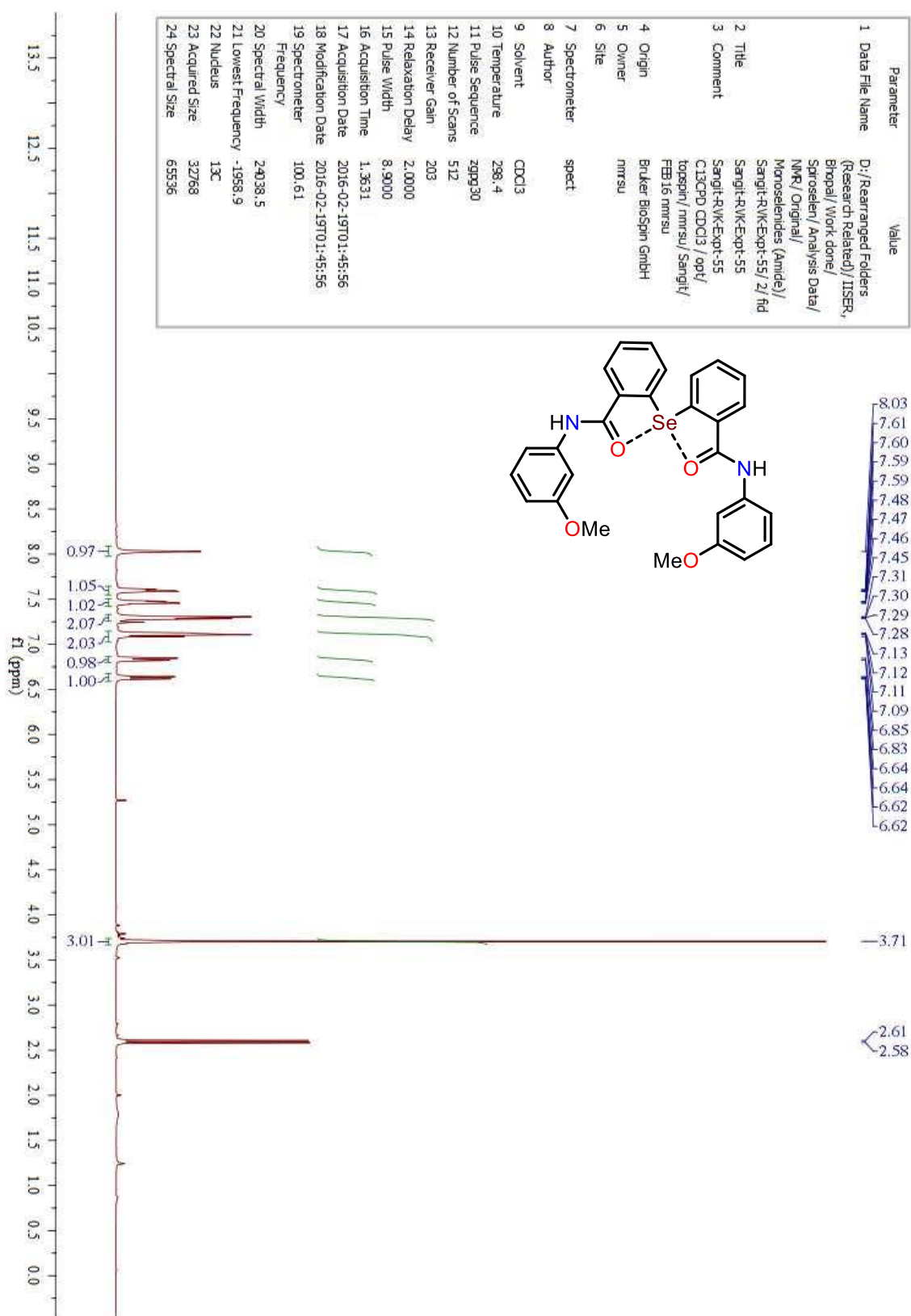
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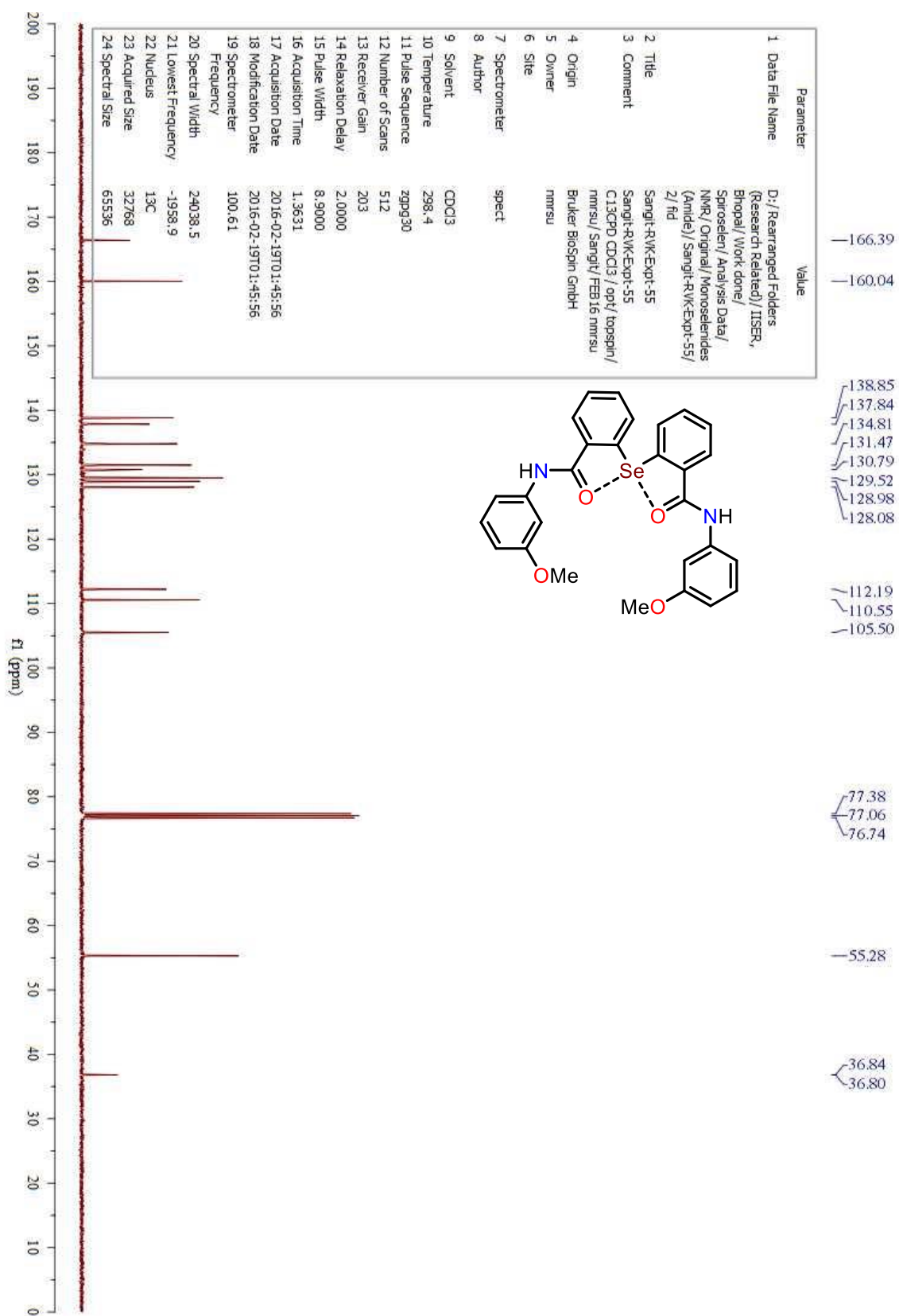
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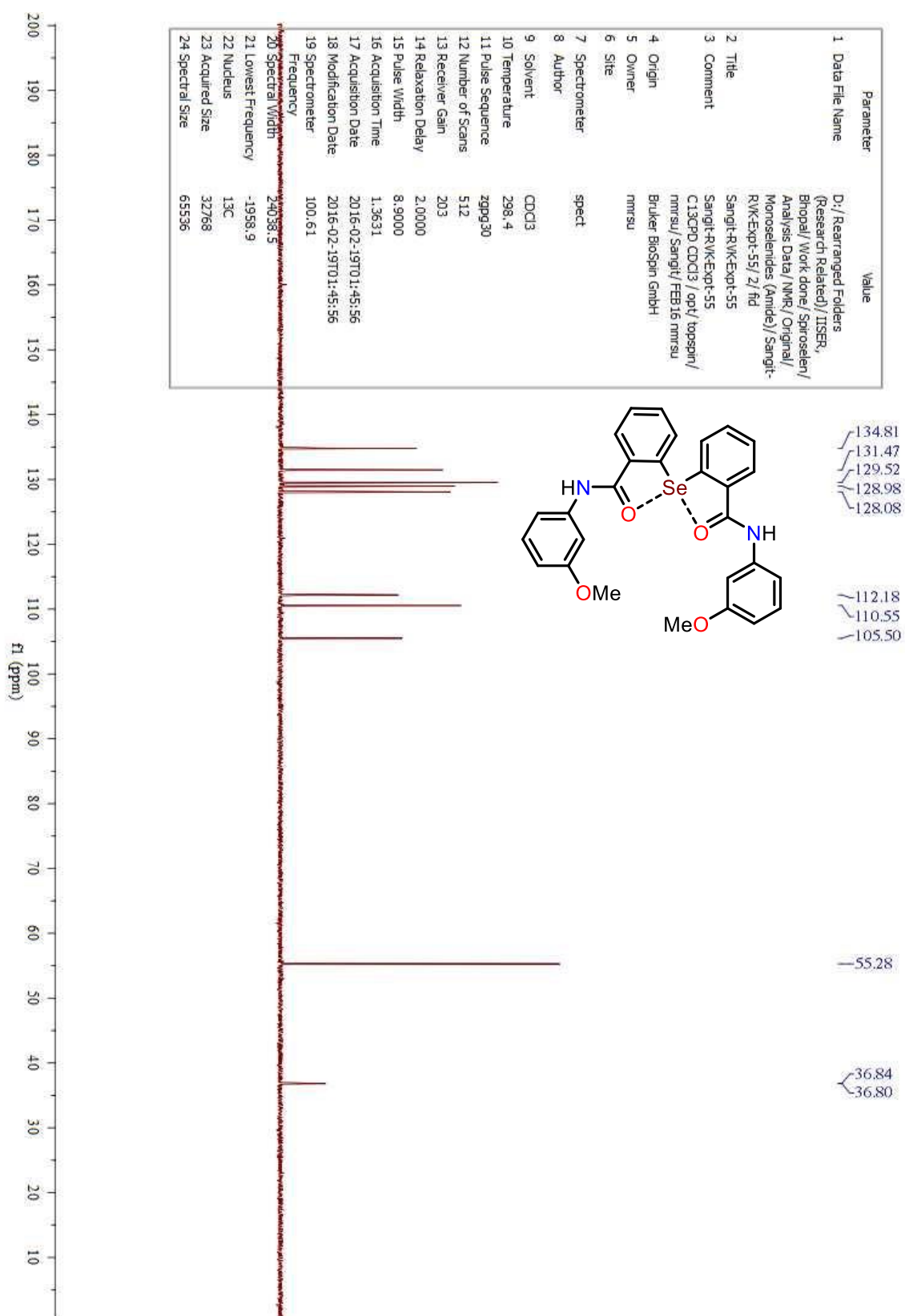


¹H NMR of 38

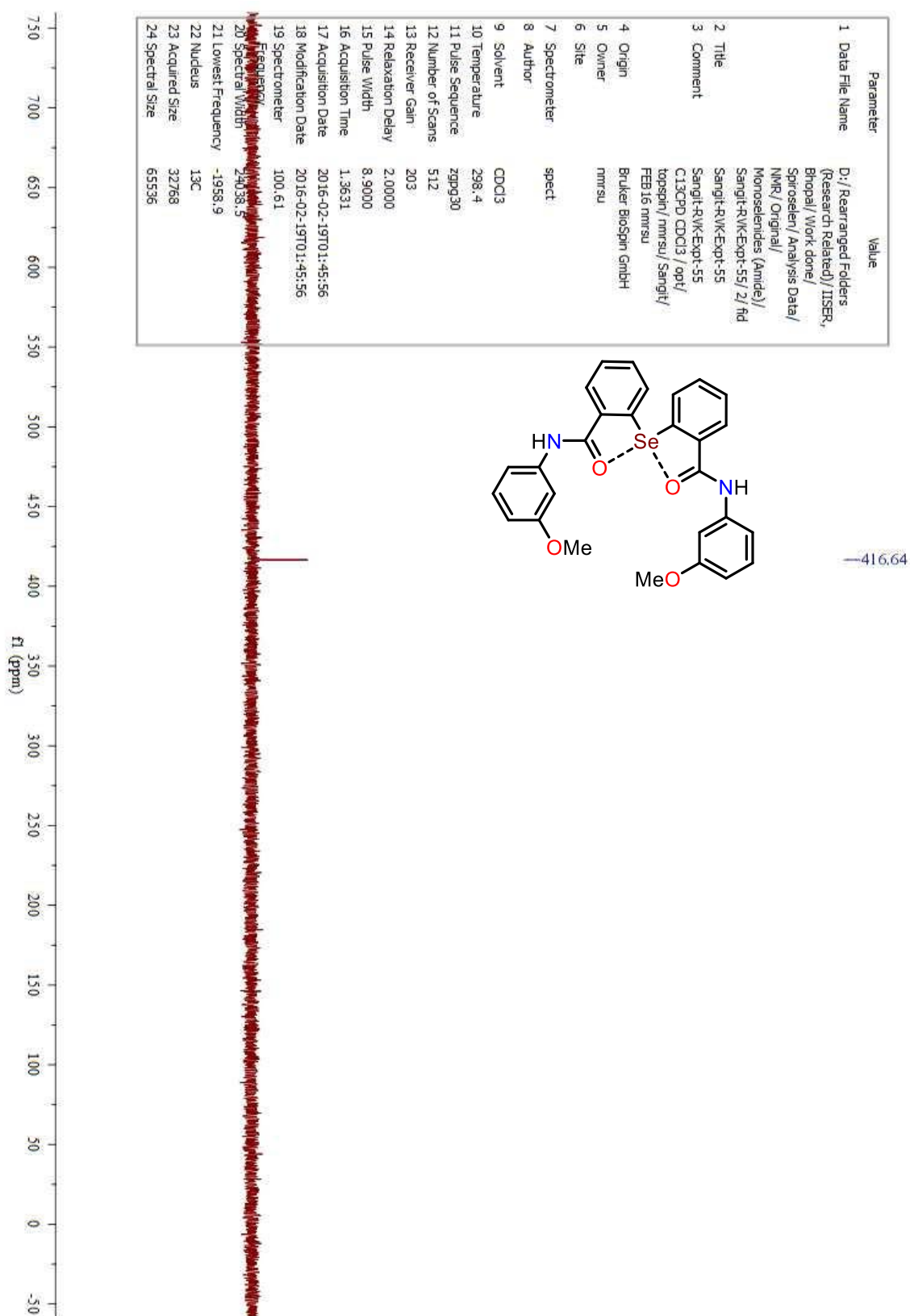


¹³C NMR of **38**

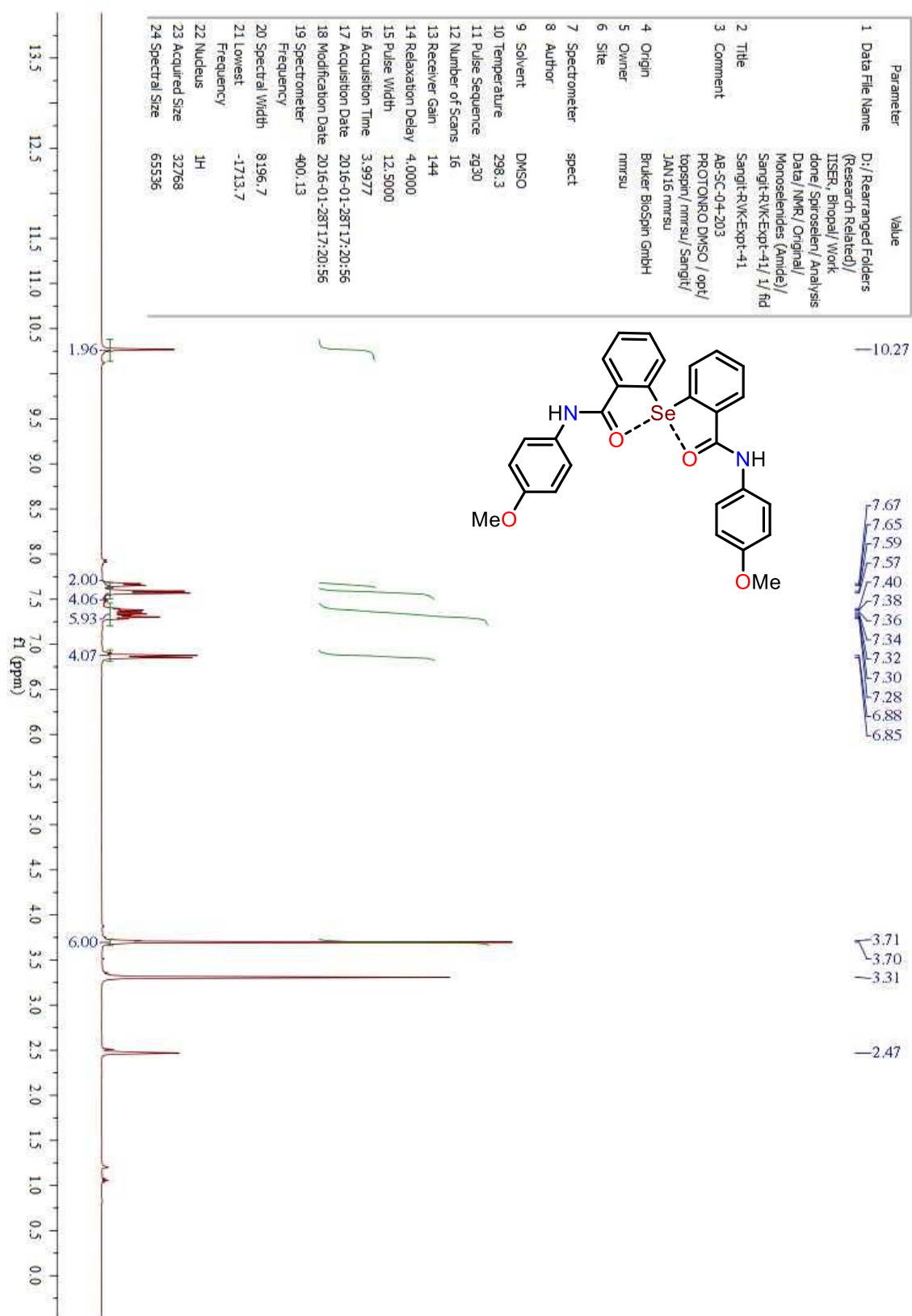


DEPT-135 of **38**


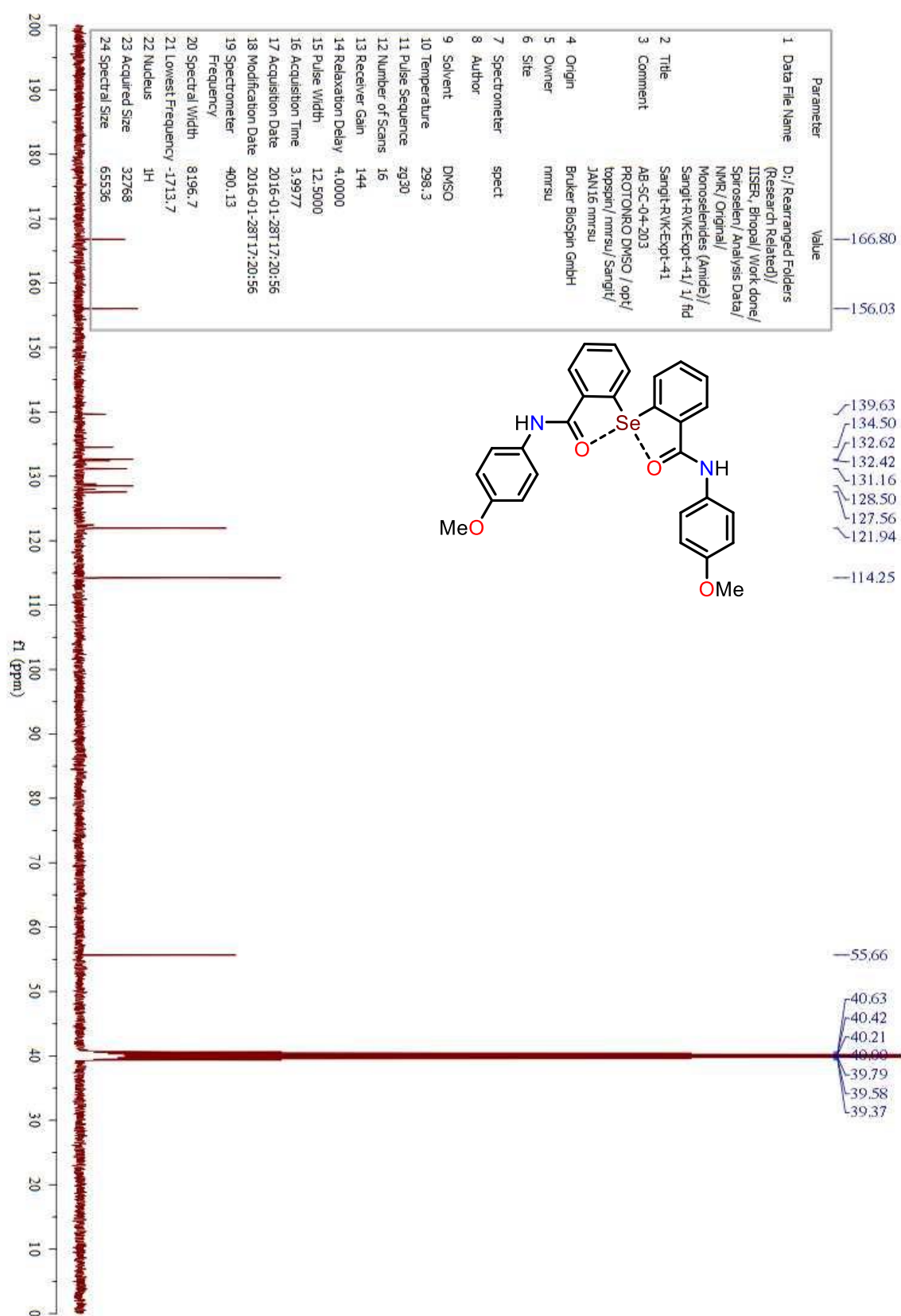
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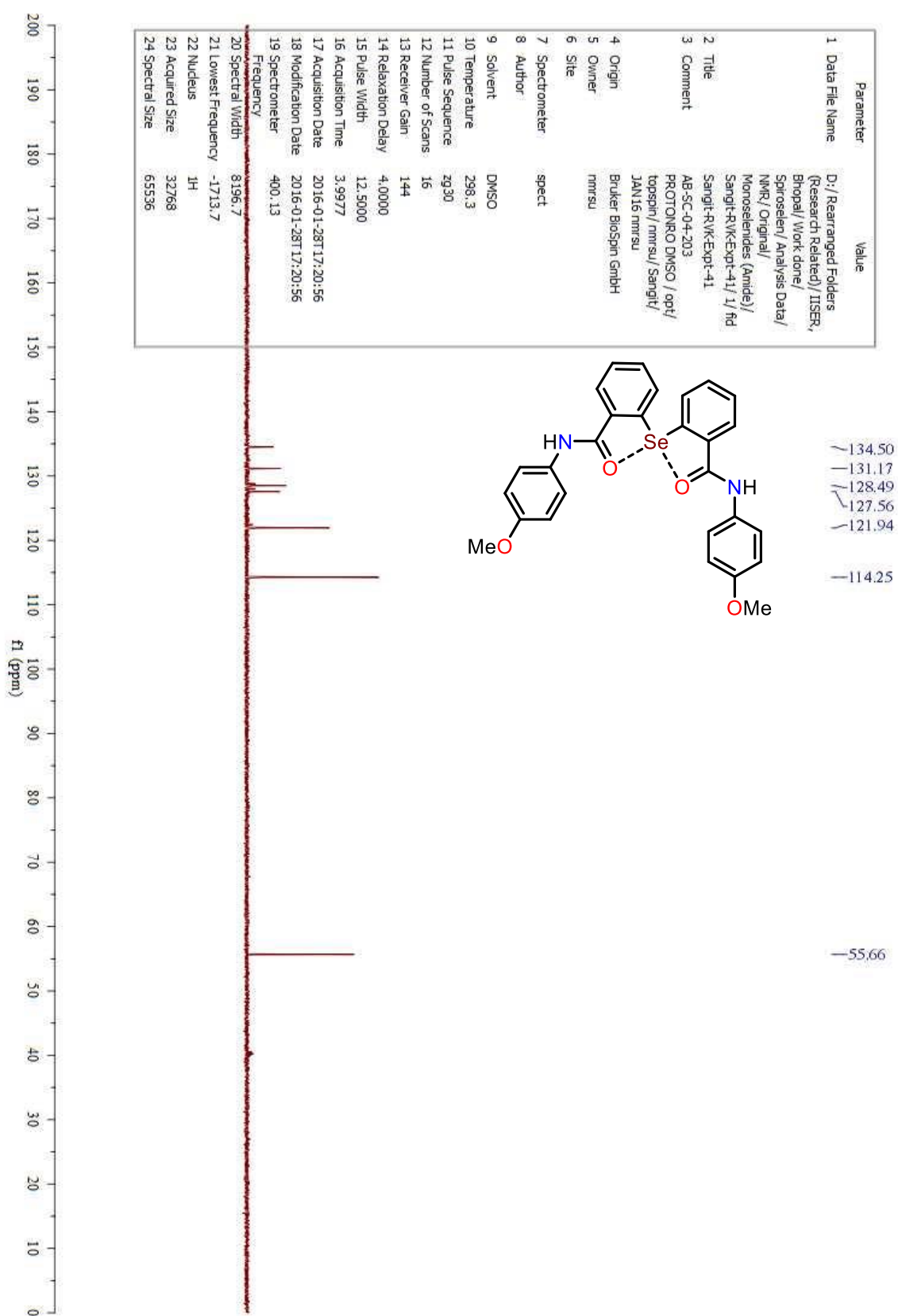


¹H NMR of 39

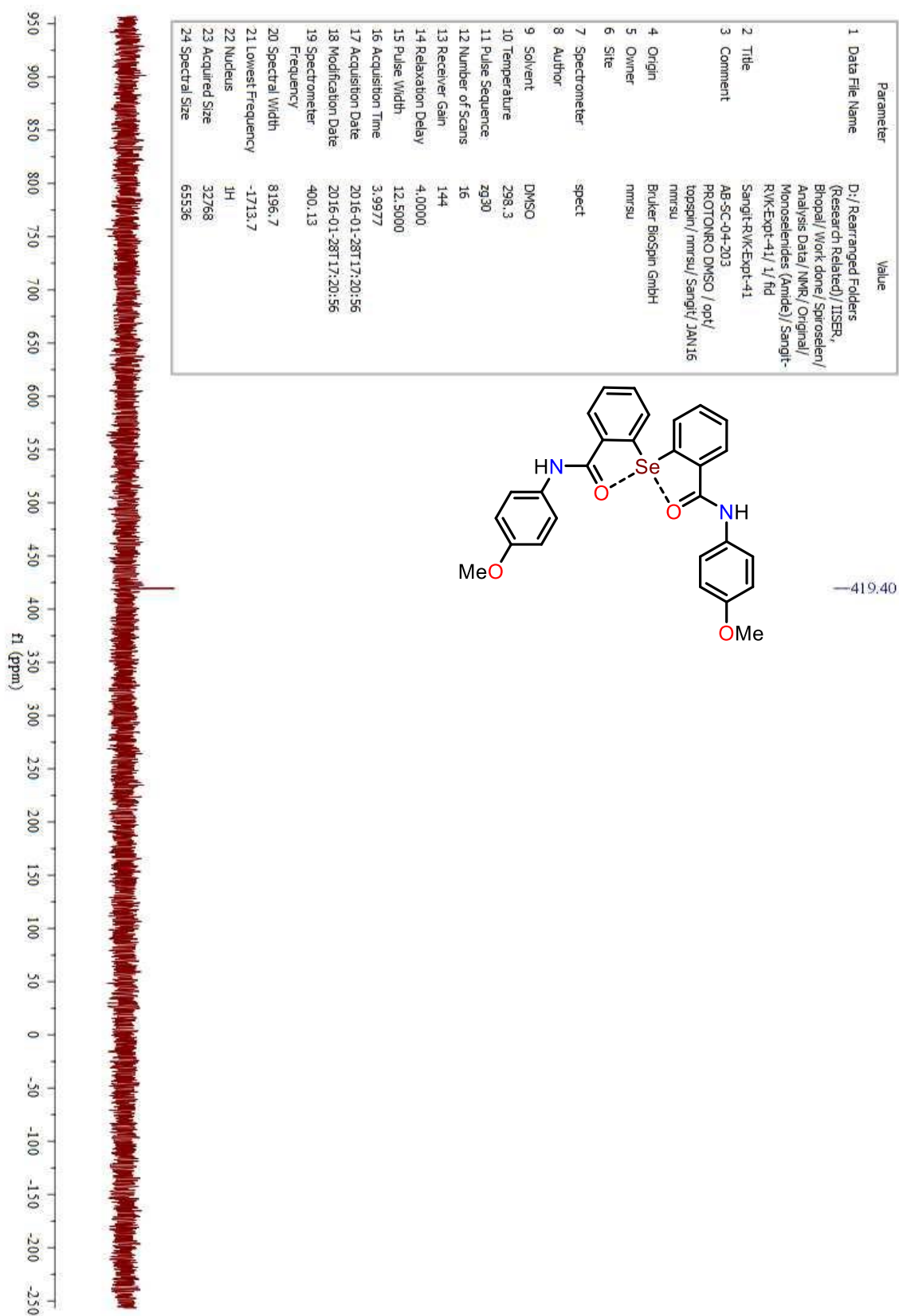


¹³C NMR of **39**

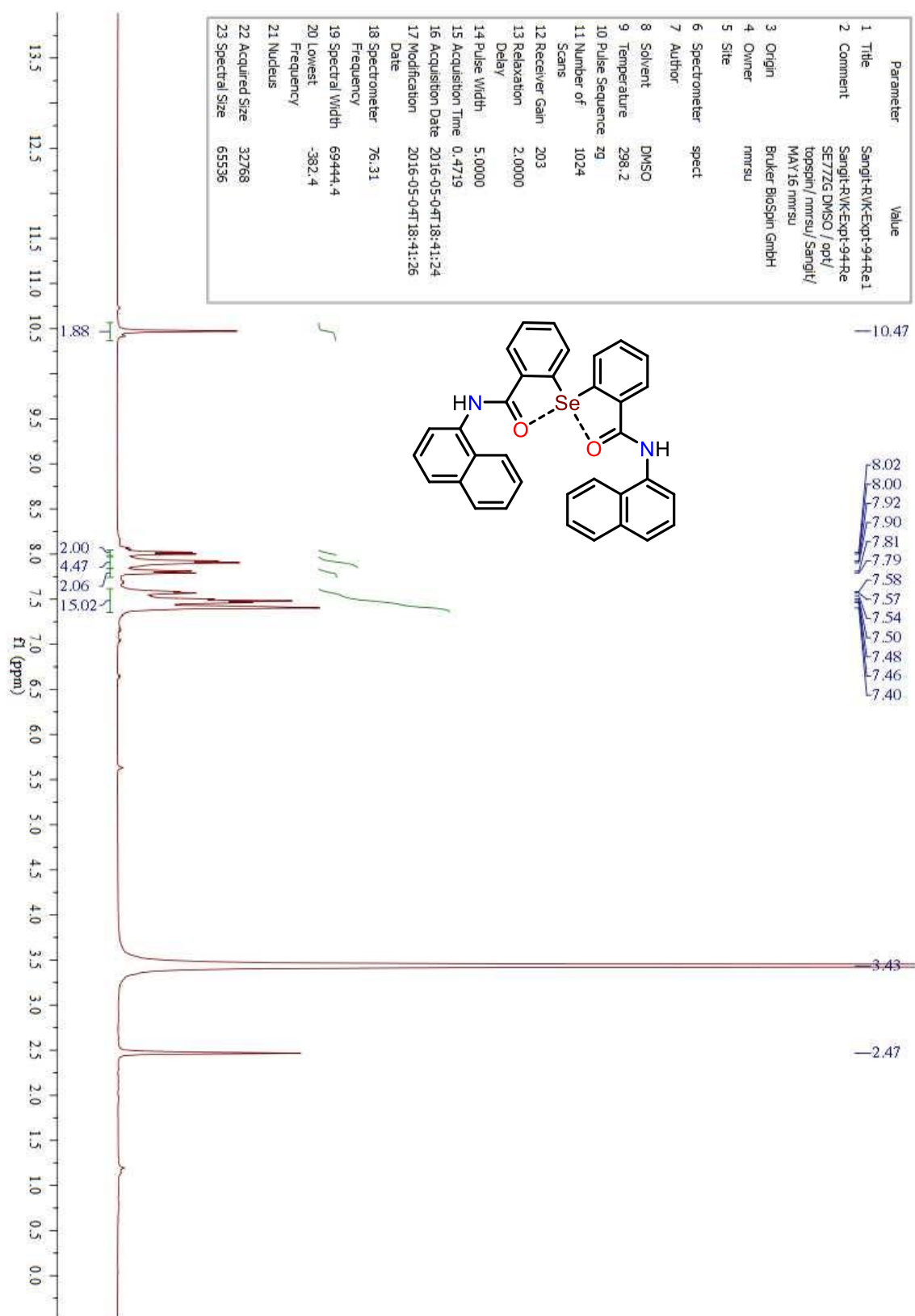




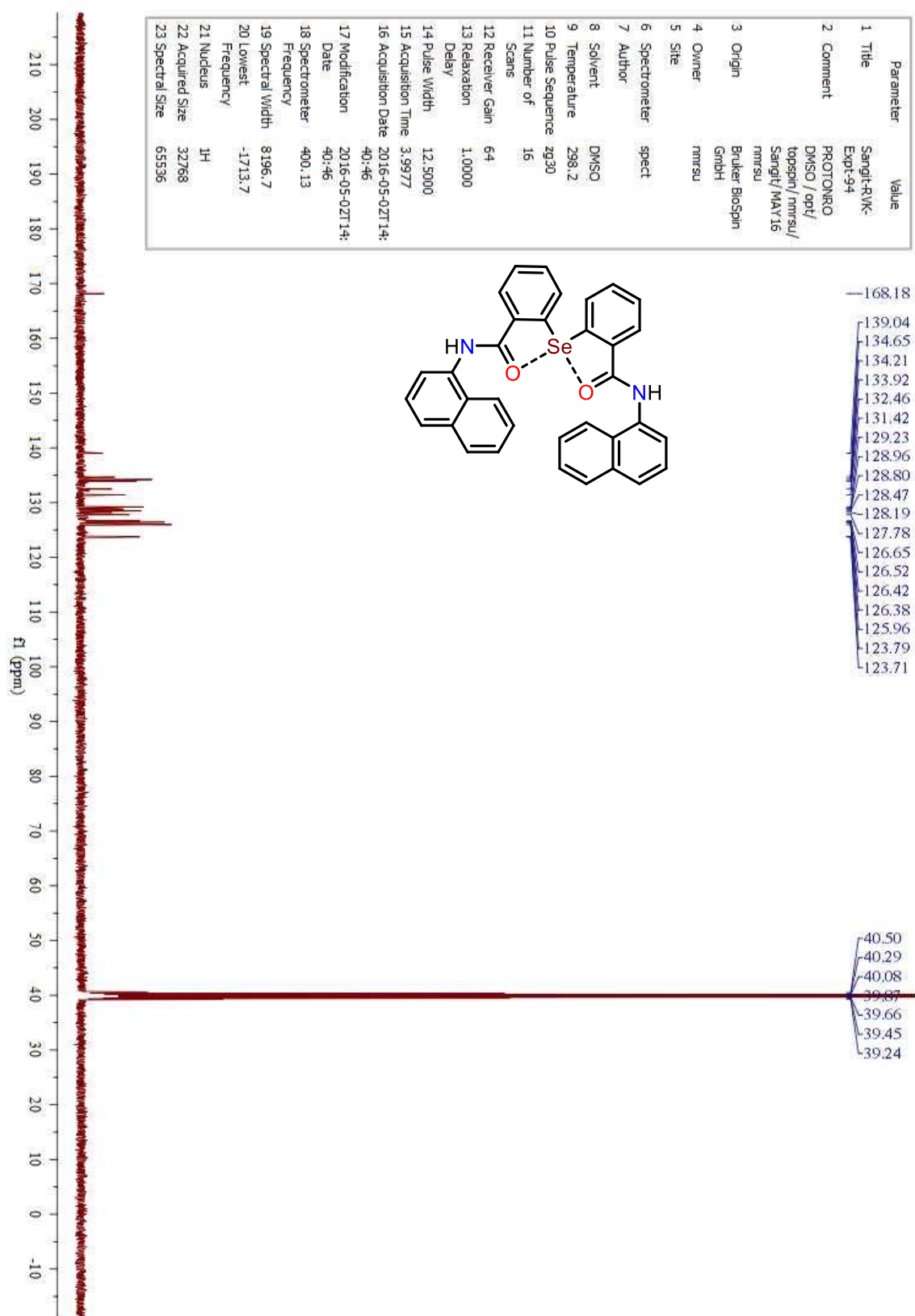
⁷⁷Se NMR of 39



¹H NMR of 40

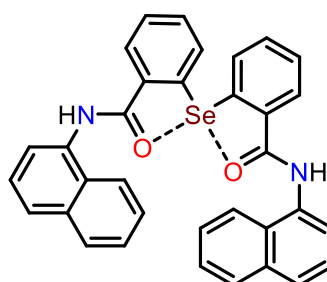


¹³C NMR of 40



DEPT-135 of 40

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4 Owner	nmrsu
5 Site	
6 Spectrometer	spect
7 Author	
8 Solvent	DMSO
9 Temperature	298.2
10 Pulse Sequence	zg30
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12 Receiver Gain	64
13 Relaxation Delay	1.0000
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21 Nucleus	¹ H
22 Acquired Size	32768
23 Spectral Size	65536

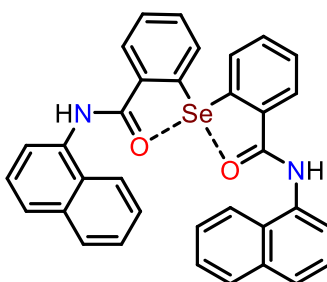


134.65
131.42
128.80
128.47
127.78
126.65
126.52
126.38
125.96
123.79
123.71

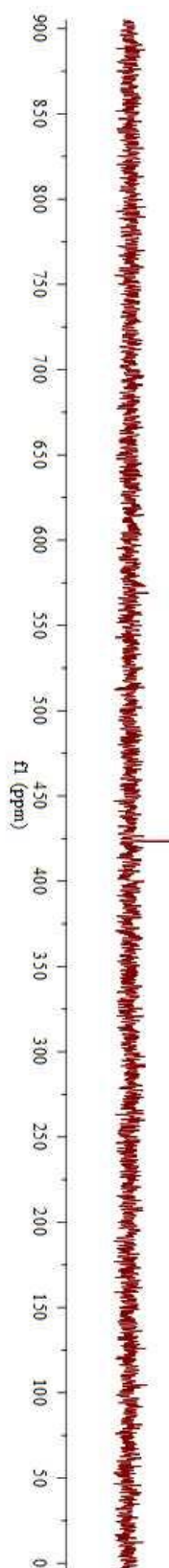


⁷⁷Se NMR of 40

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5 Site	
6 Spectrometer	spect
7 Author	
8 Solvent	DMSO
9 Temperature	298.2
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11 Number of Scans	256
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21 Nucleus	13C
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—423.46



HR-MS of 40

Display Report

Analysis Info

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 Sample Name Dr.S.kumar-RVK-EXPT-94
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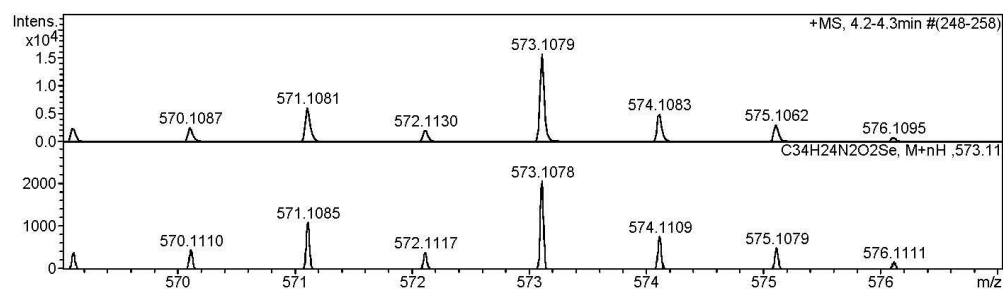
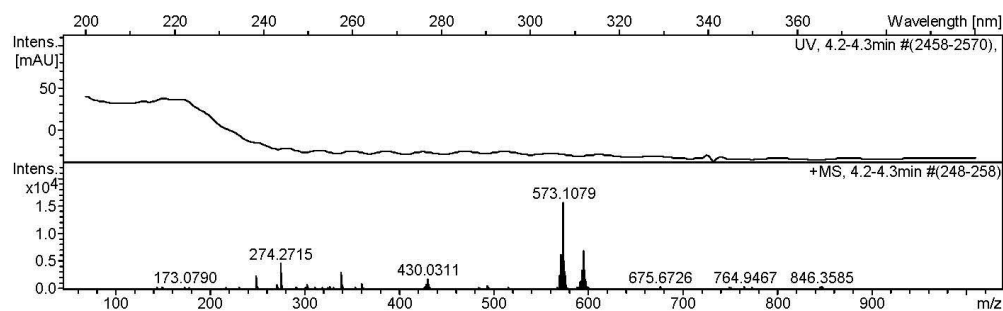
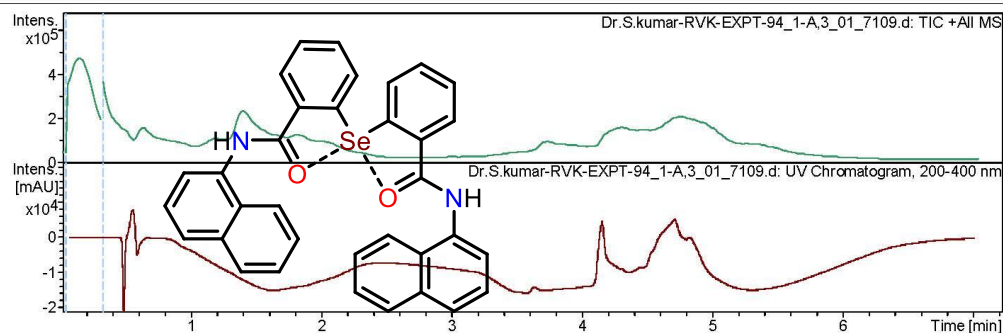
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Operator DIMPLE

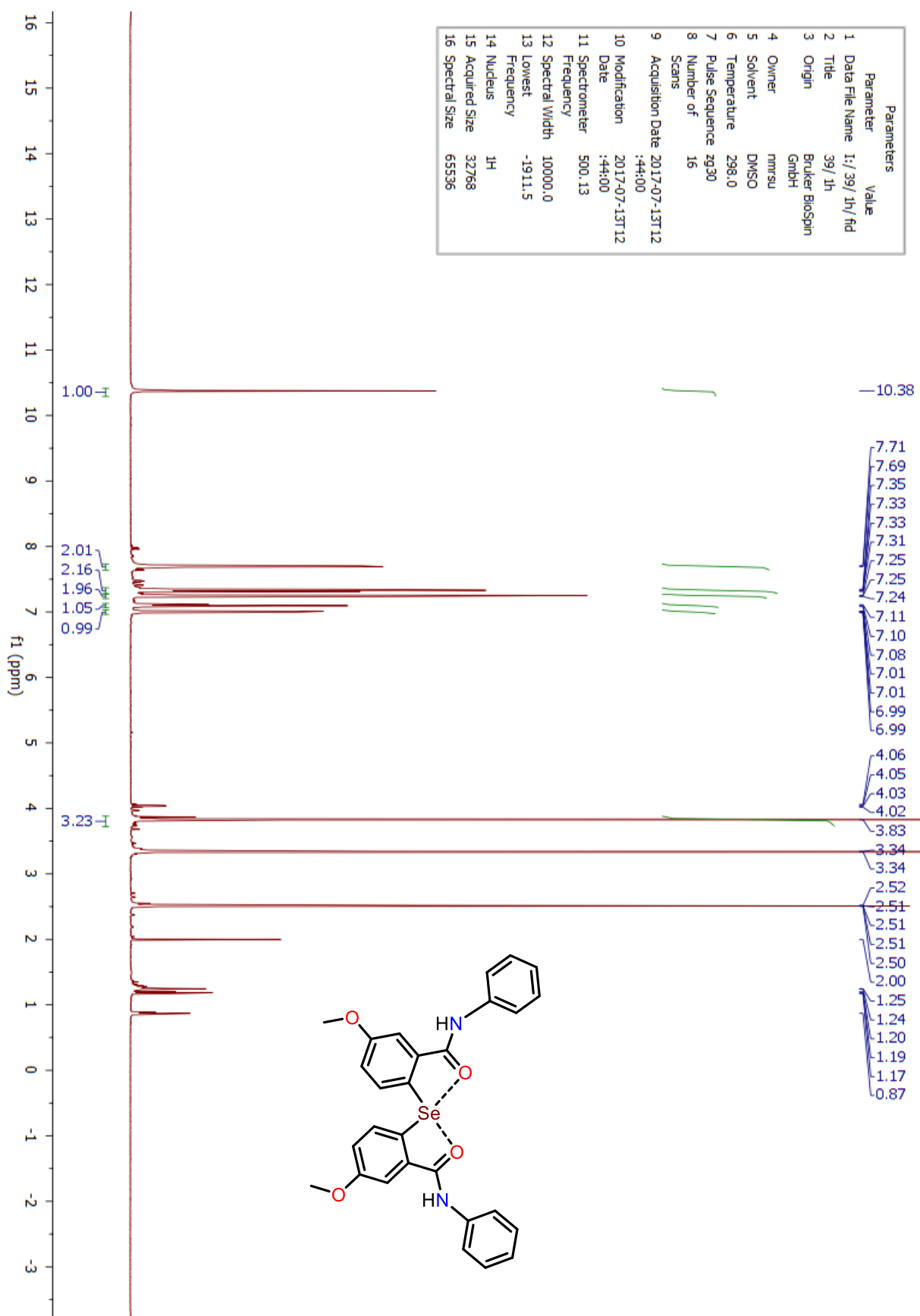
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Acquisition Parameter

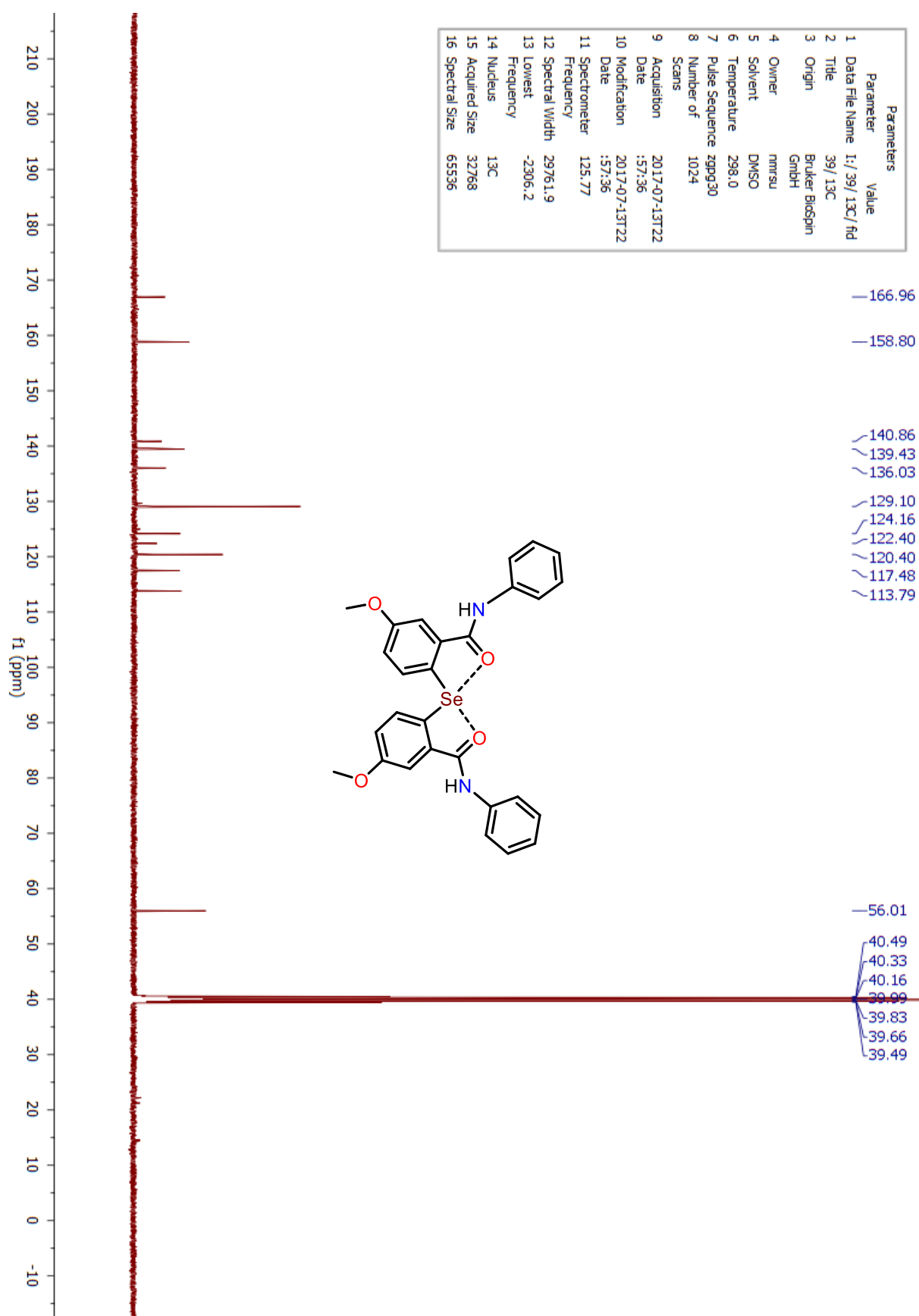
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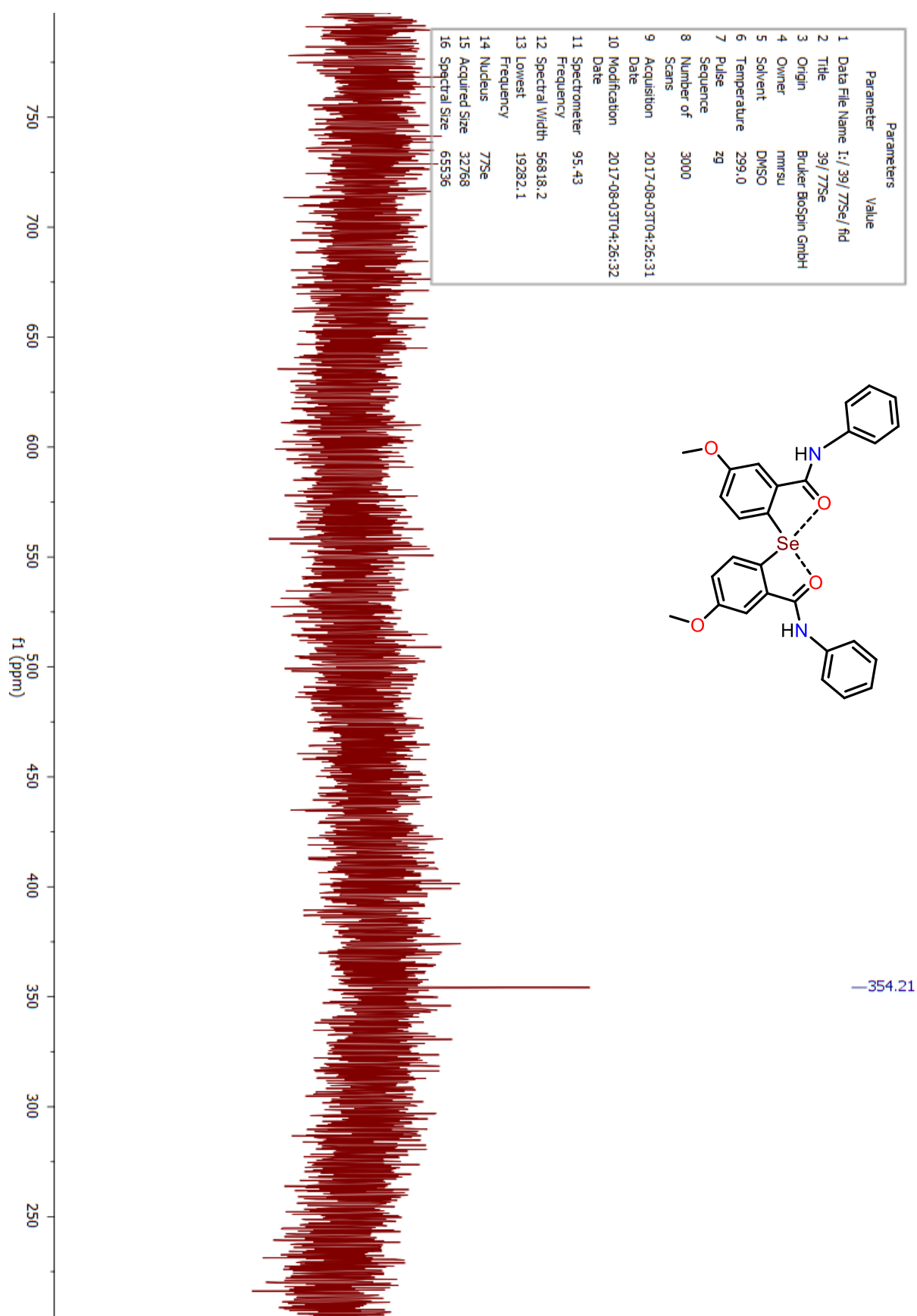
¹H NMR of 41



¹³C NMR of **41**



⁷⁷Se NMR of **41**



Display Report

Analysis Info

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 Sample Name RVK-EXP-52
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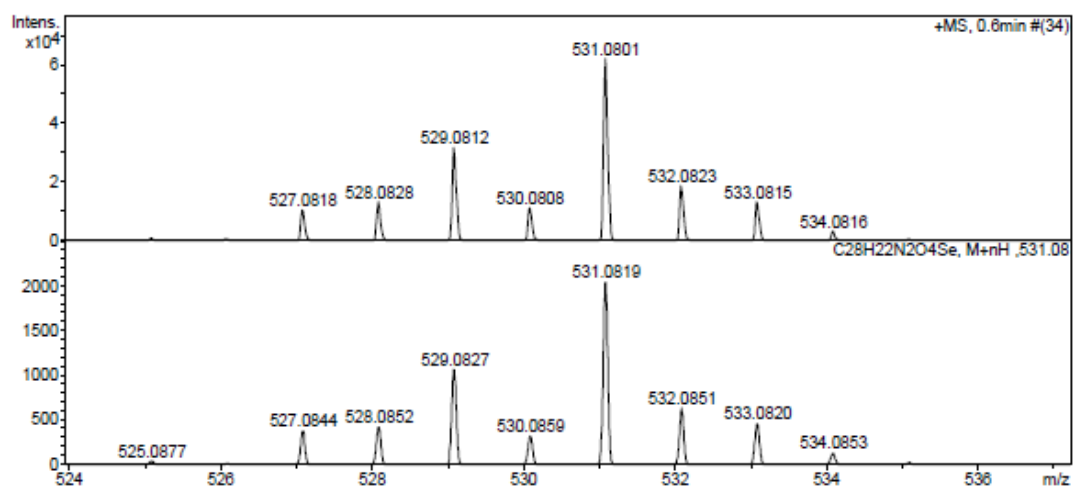
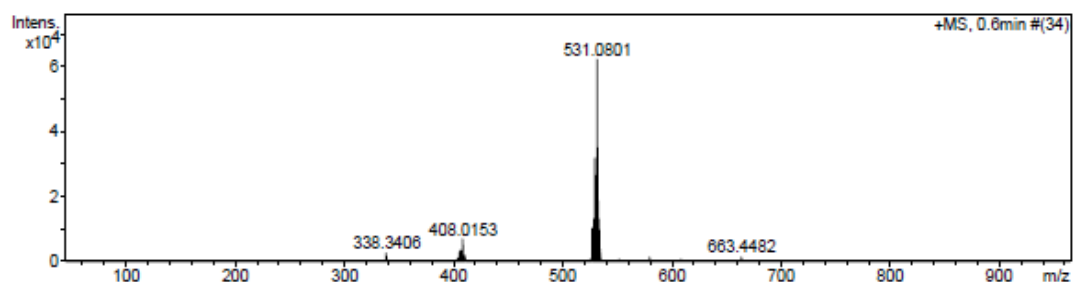
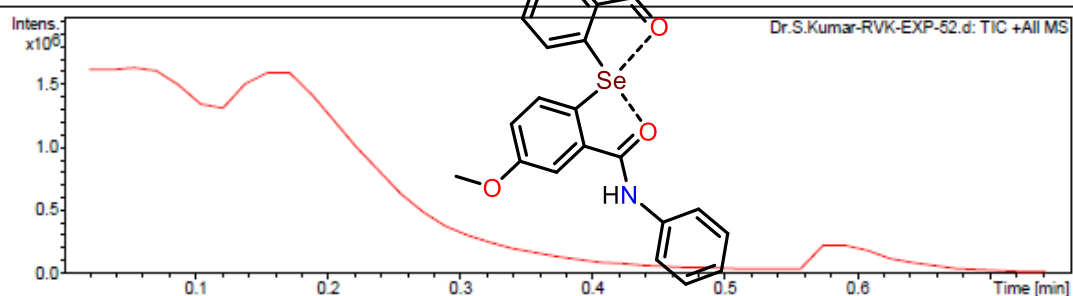
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Set Nebulizer
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2.5 Bar
 200 °C
 4.0 l/min
 Waste



Parameters

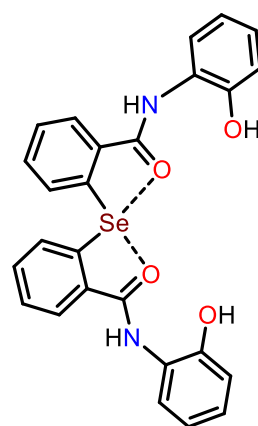
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10 Acquisition Date	2017-04-13T12:53:51
11 Modification Date	2018-11-22T06:13:32
12 Spectrometer	500.13
13 Spectral Width	10000.0
14 Lowest Frequency	-1911.5
15 Nucleus	¹ H
16 Acquired Size	32768
17 Spectral Size	65536

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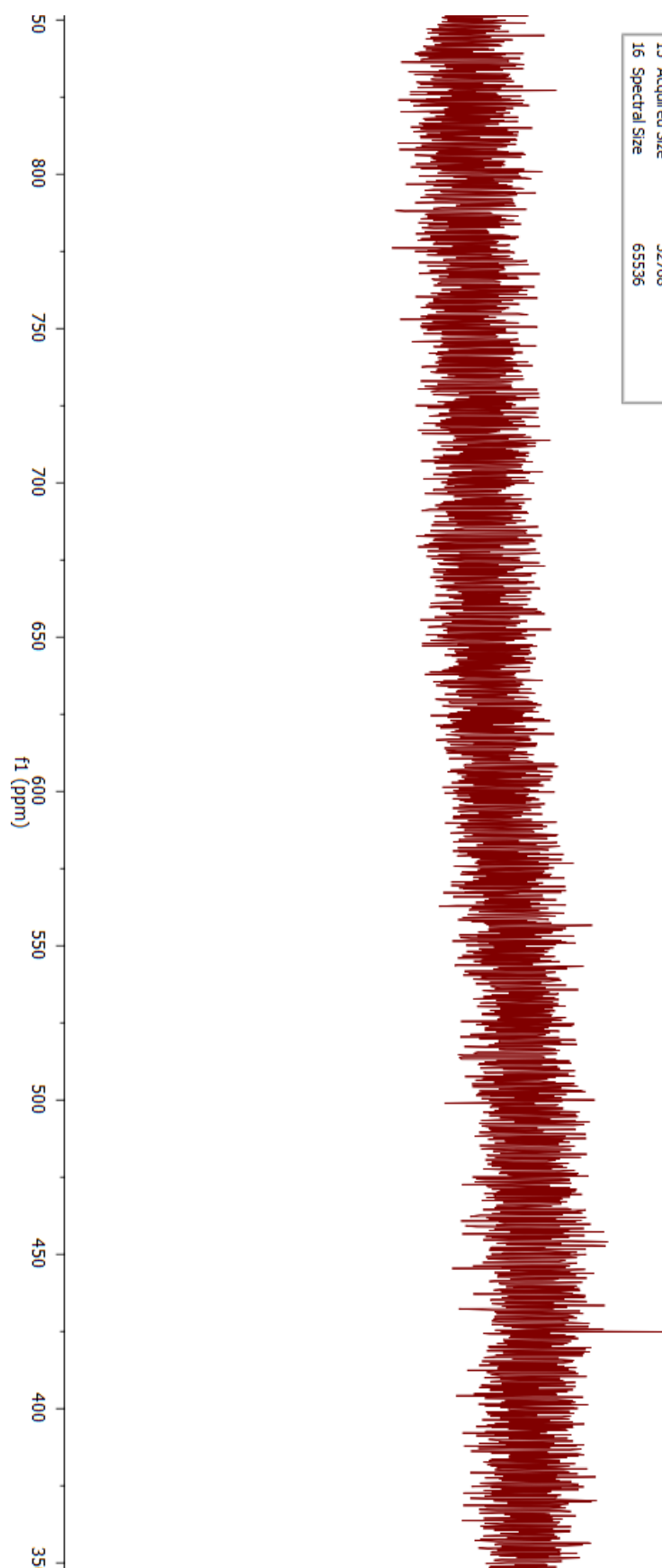
¹H NMR spectrum (DMSO-d₆) showing peaks from 5.77 to 9.71 ppm. Integration values are provided for each peak.

Chemical Shift (ppm)	Integration
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7.80	2.12
7.78	3.28
7.72	0.99
7.70	0.93
7.40	0.95
7.38	
7.37	
7.05	
7.04	
7.03	
7.02	
7.01	
6.93	
6.92	
6.91	
6.83	
6.82	
6.80	
5.77	
2.51	
2.51	
2.51	
2.00	
1.25	
1.24	

Parameters	
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4 Owner	nmrsu
5 Solvent	DMSO
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15 Acquired Size	32768
16 Spectral Size	65536



—424.91

⁷⁷Se NMR of 45

Display Report

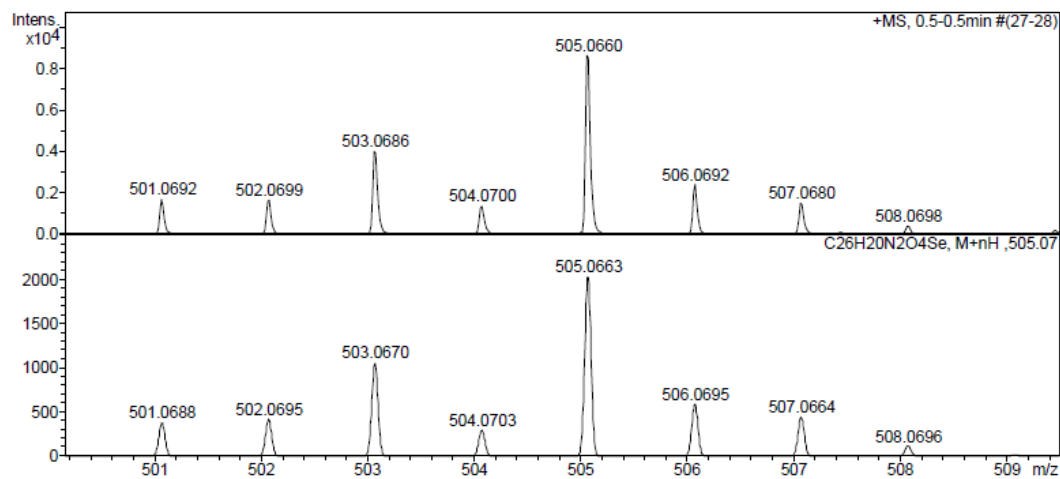
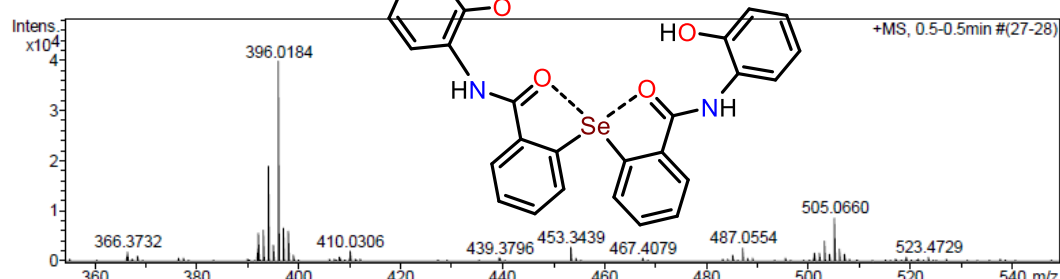
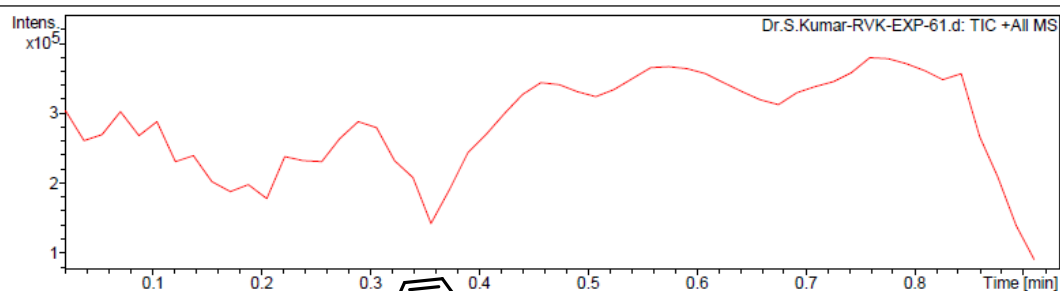
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Sample Name RVK-EXP-61
Comment

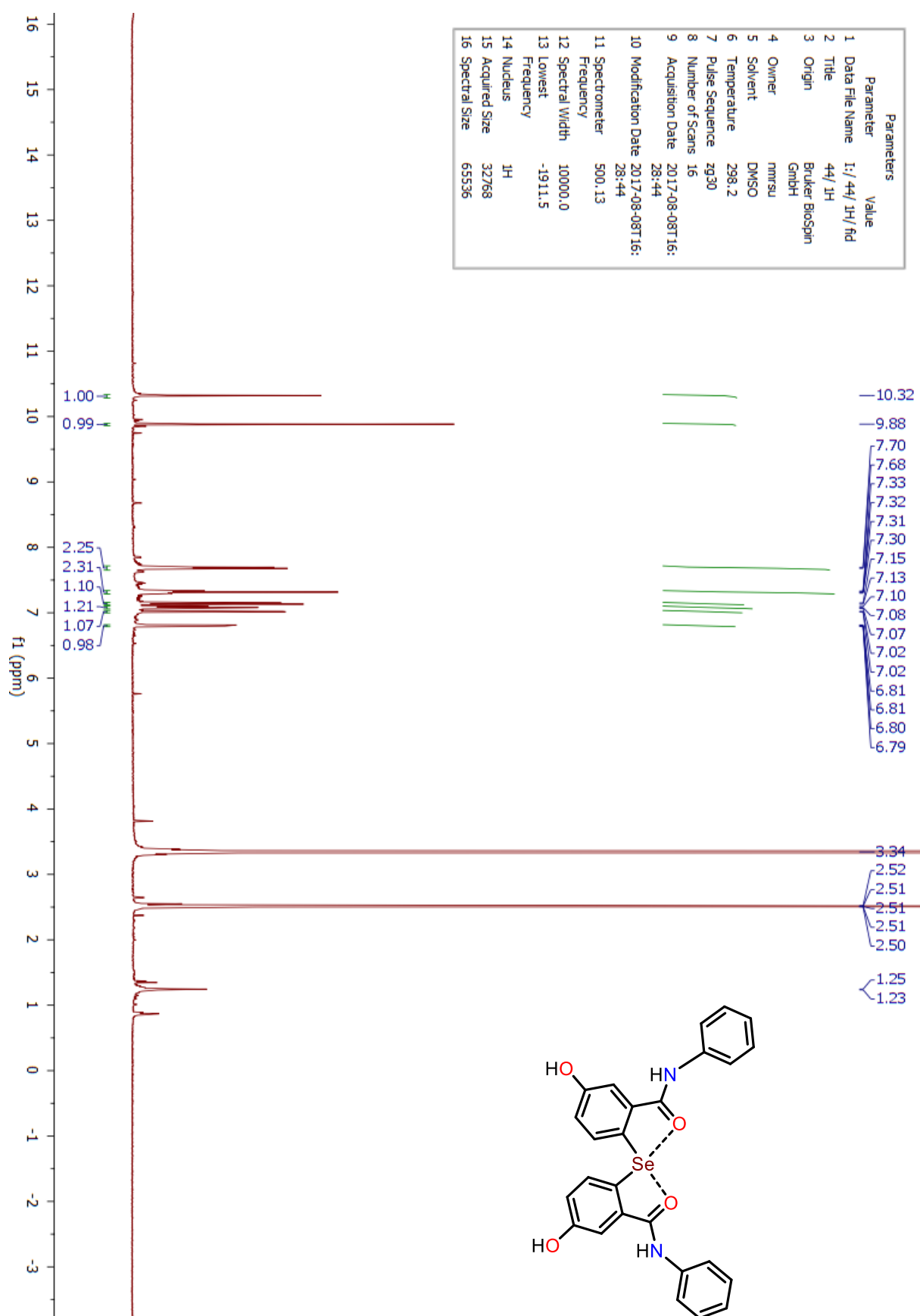
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Operator DIMPLE
Instrument microTOF-Q II 10330

Acquisition Parameter

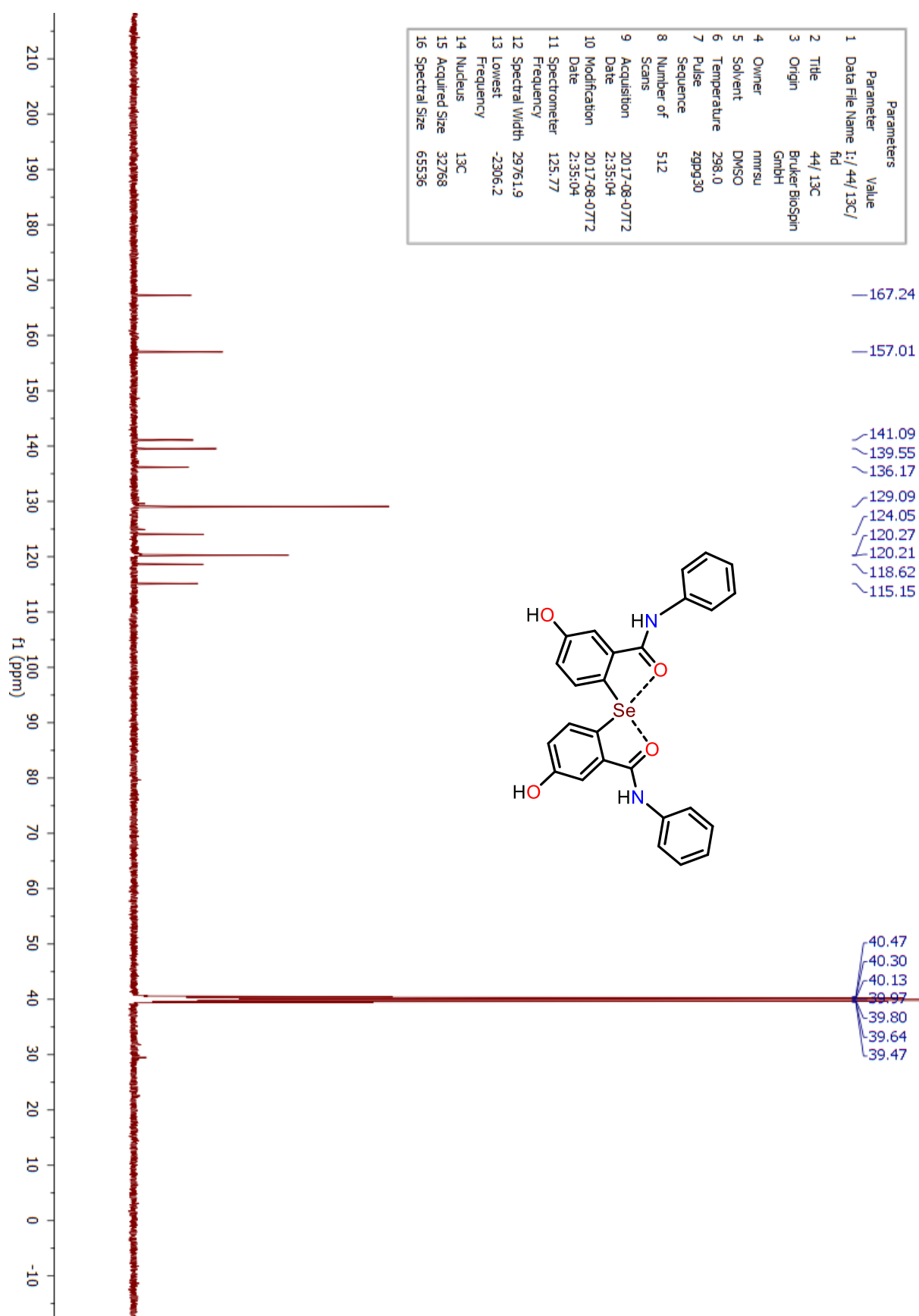
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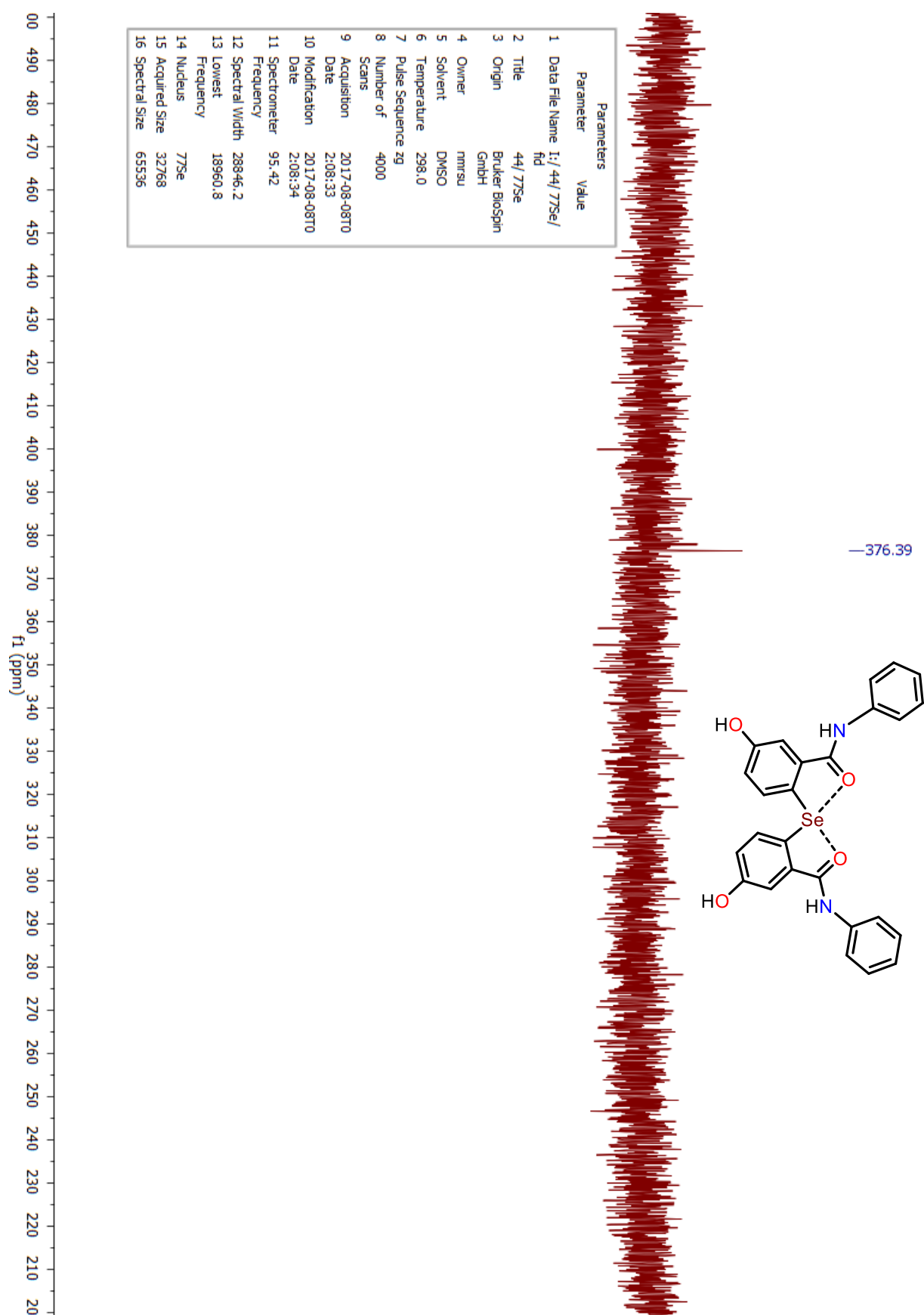


¹H NMR of **46**



¹³C NMR of 46



⁷⁷Se NMR of **46**

Display Report

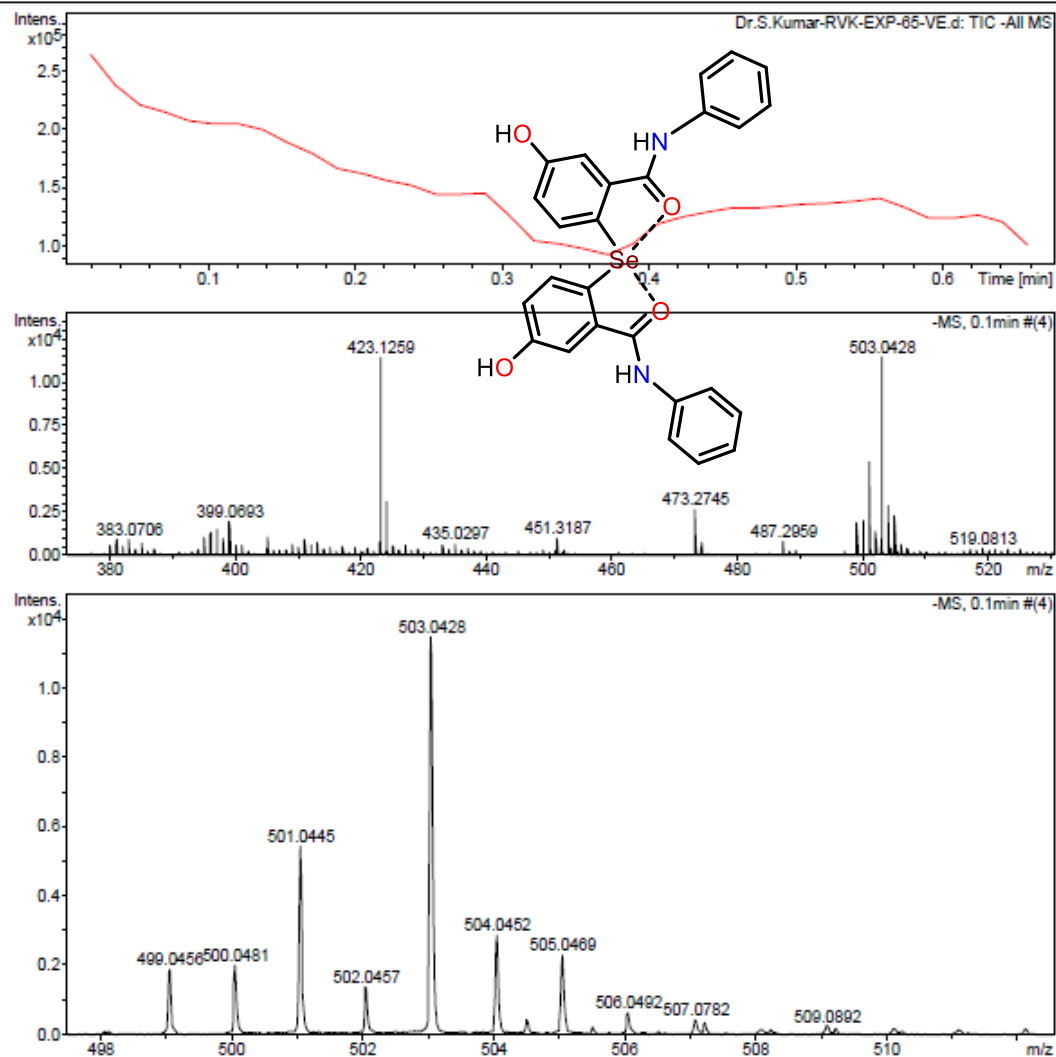
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Method tune_wide_APCI_23.06.m
Sample Name RVK-EXP-65-VE
Comment

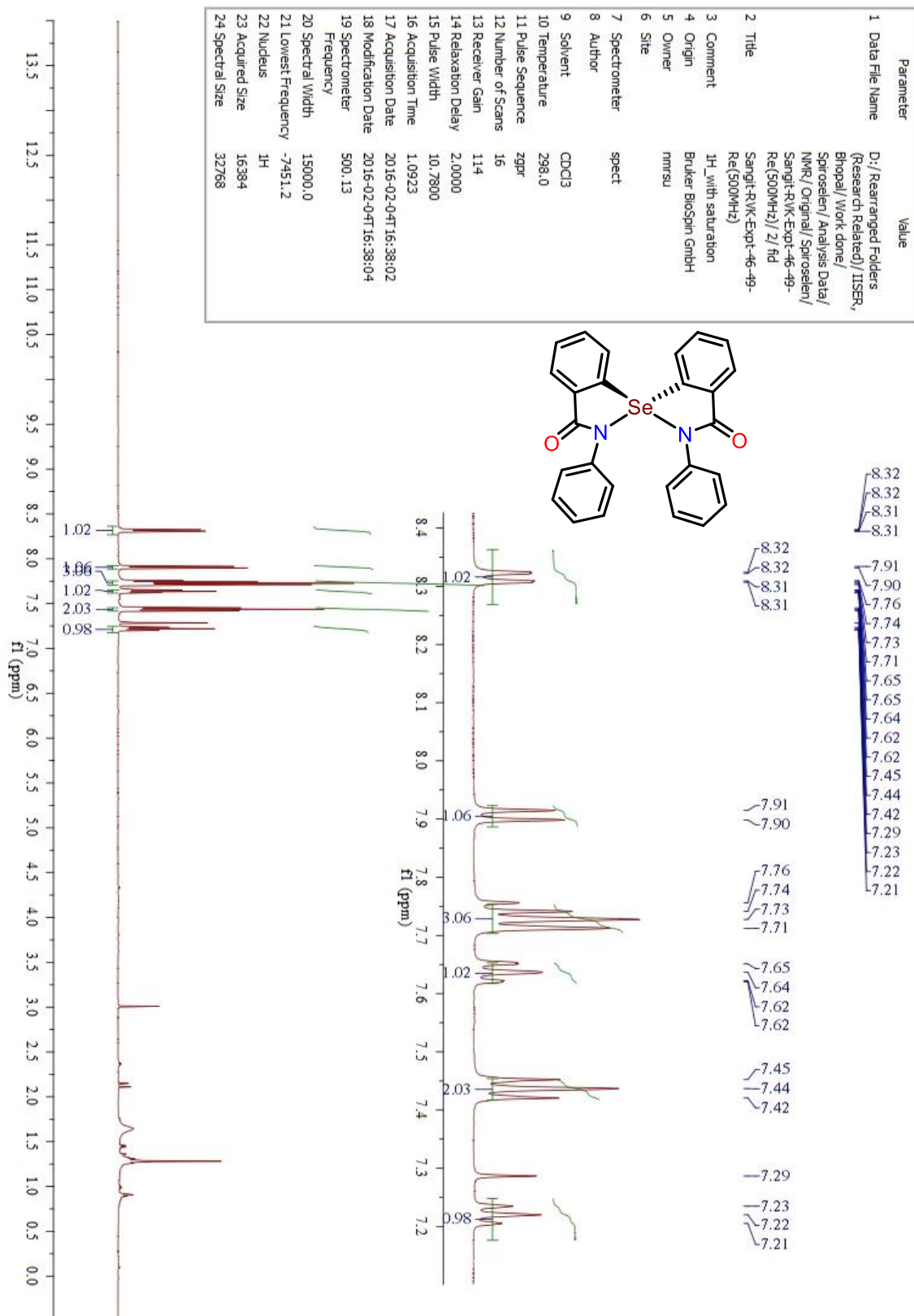
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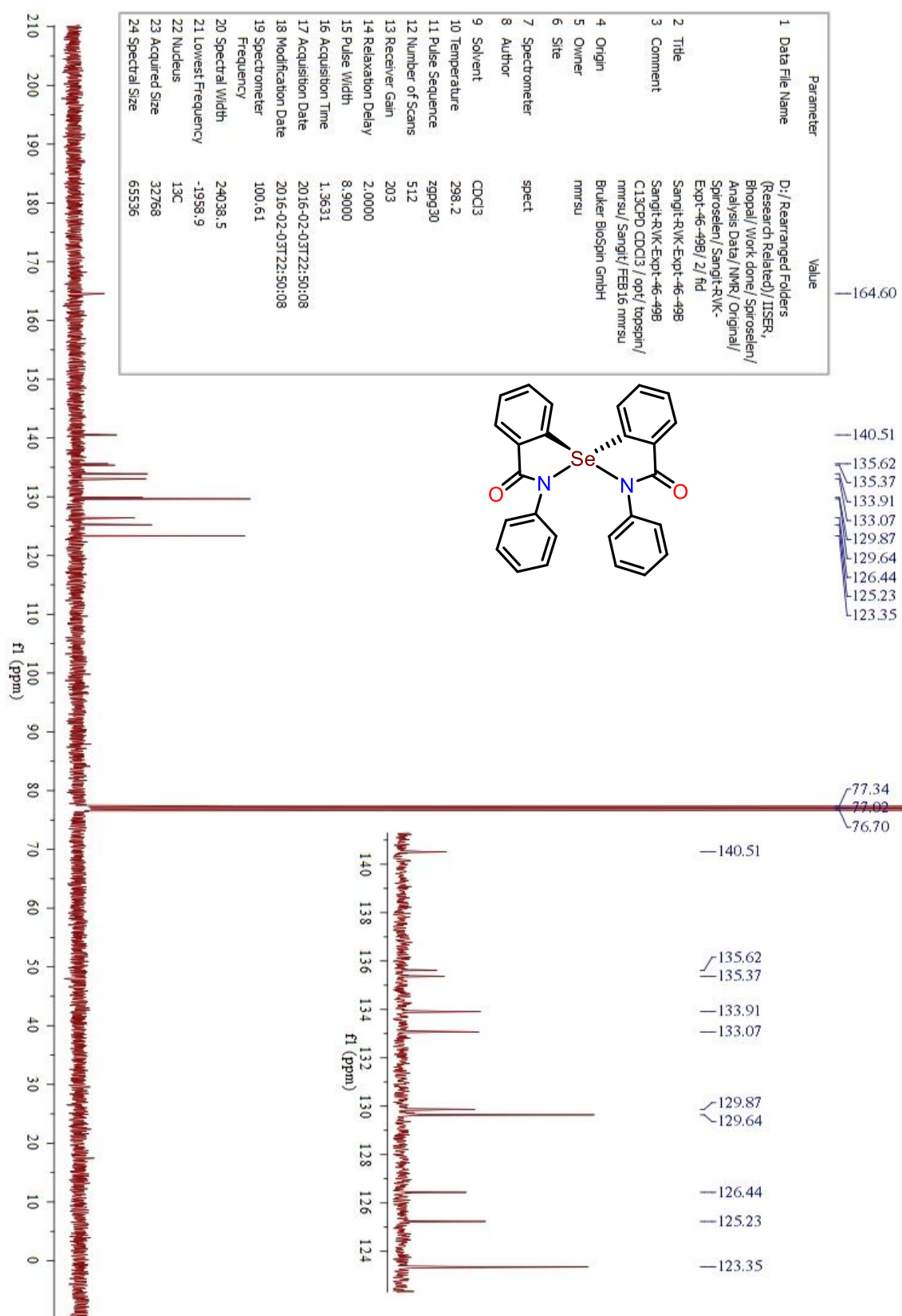
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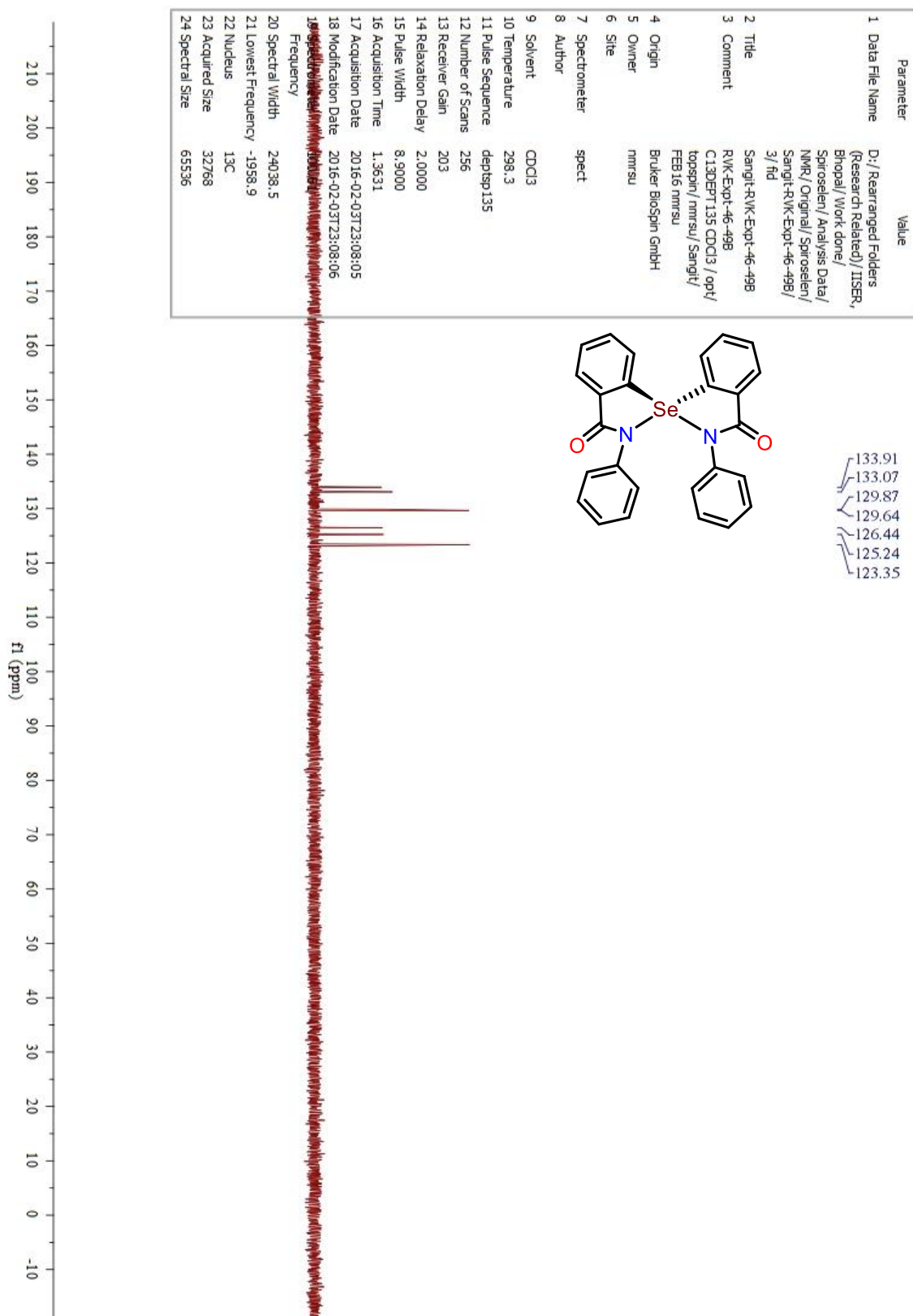
¹H NMR of 14



¹³C NMR of **14**

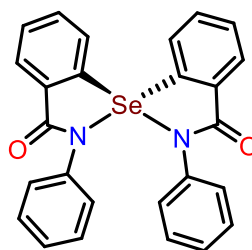


DEPT-135 of 14



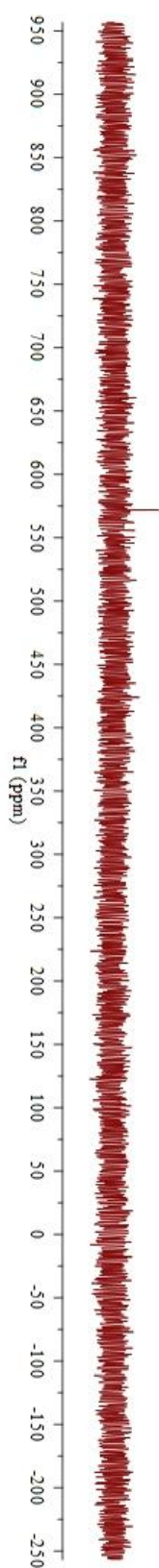
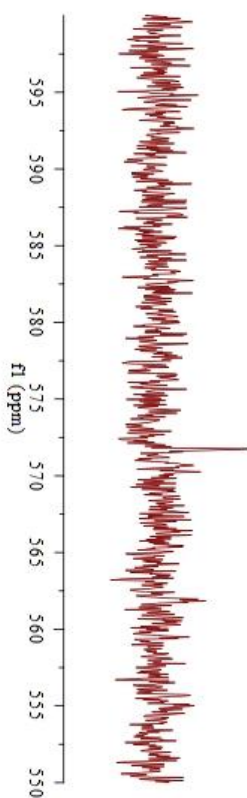
⁷⁷Se NMR of 14

Parameter	Value
1 Data File Name	D:/Rearranged Folders (Research Related)/IISER, Bhopal/Work done/ Spiroselen/ Analysis Data/ NMR/ Original/ Spiroselen/ Sangit-RVK-Expt -46/ 3/ ftd
2 Title	Sangit-RVK-Expt -46
3 Comment	Sangit-RVK-Expt -46 SE77Z6 CDCl3 / opt/ topspin/ nmrsu/ Sangit/ JAN16 nmrsu
4 Origin	Bruker Biospin GmbH
5 Owner	nmrsu
6 Site	
7 Spectrometer	spect
8 Author	
9 Solvent	CDCl3
10 Temperature	298.2
11 Pulse Sequence	zg
12 Number of Scans	512
13 Receiver Gain	203
14 Relaxation Delay	1.0000
15 Pulse Width	5.0000
16 Acquisition Time	0.3539
17 Acquisition Date	2016-01-29T06:26:54
18 Modification Date	2016-01-29T06:26:56
19 Spectrometer Frequency	76.31
20 Spectral Width	92592.6
21 Lowest Frequency	-19587.5
22 Nucleus	
23 Acquired Size	32768
24 Spectral Size	65536

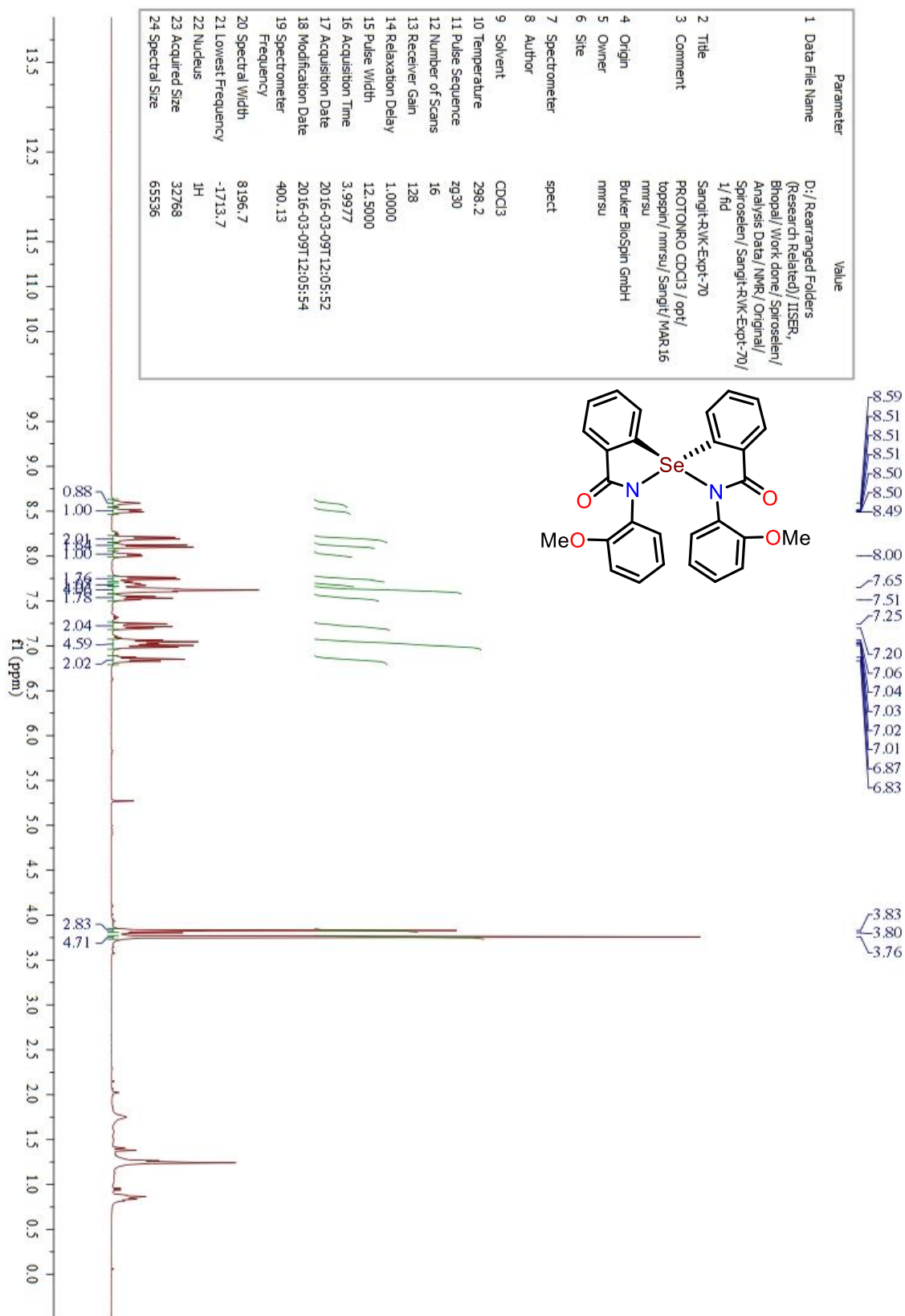


—571.79

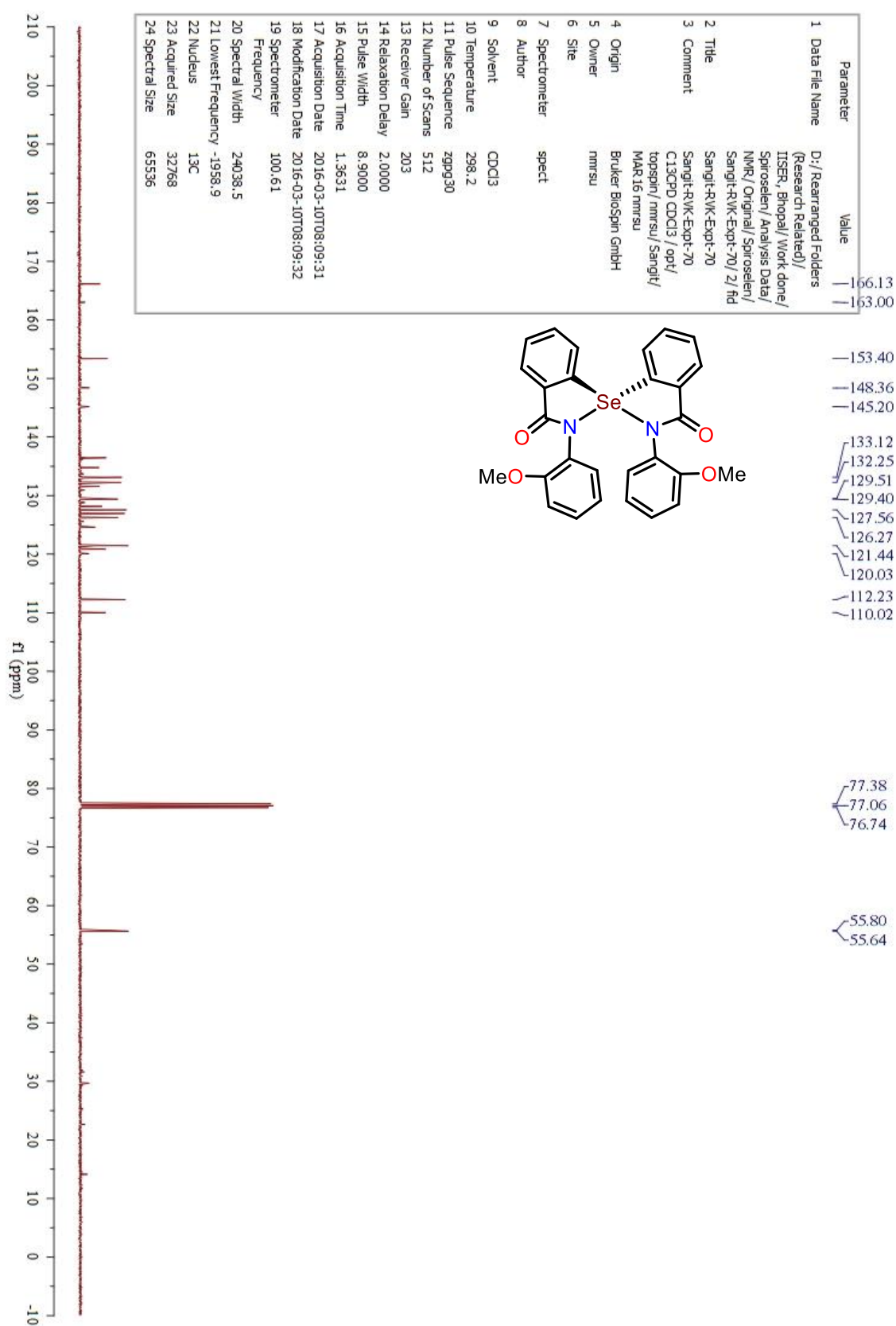
—571.79



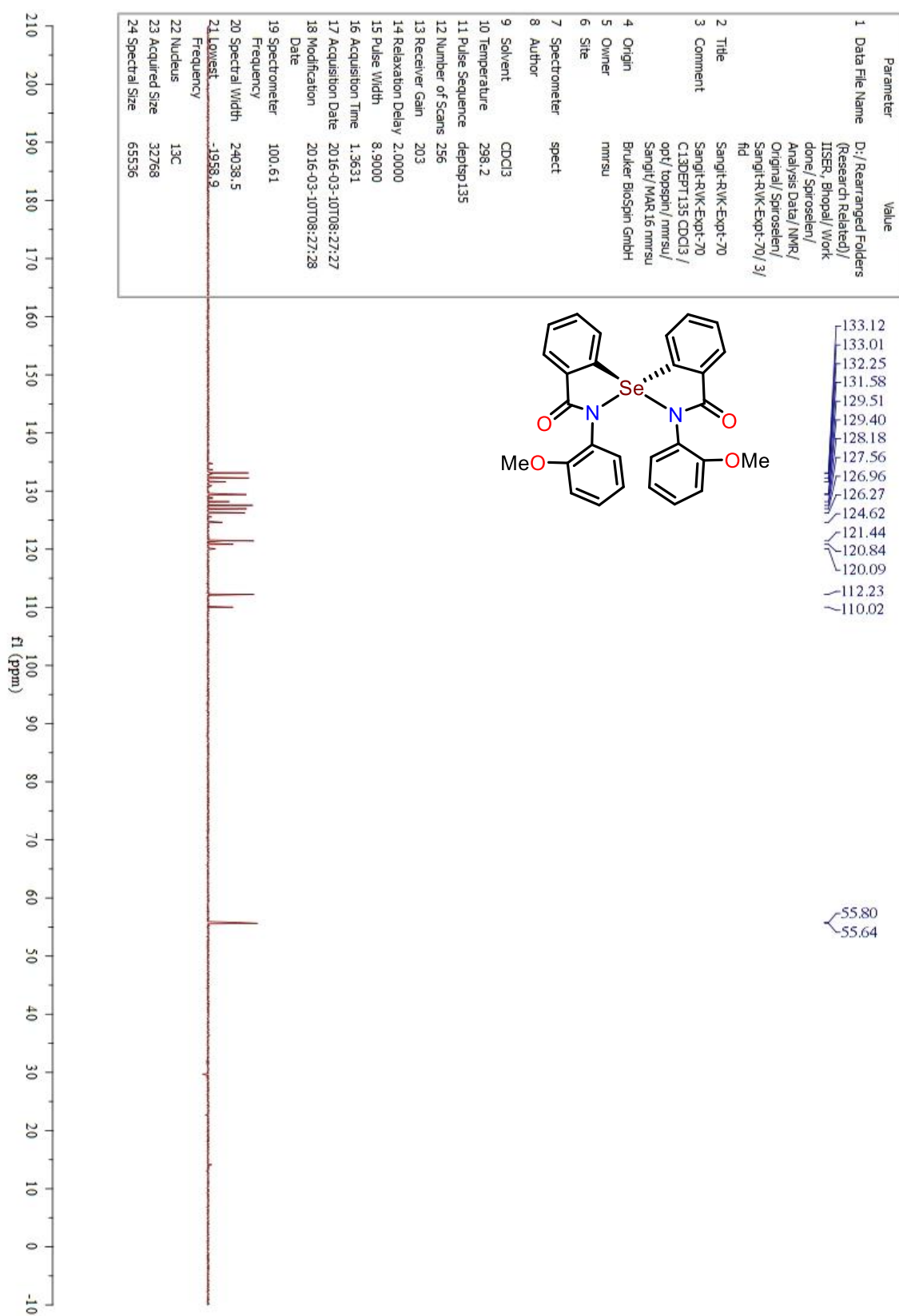
¹H NMR of 15



¹³C NMR of 15

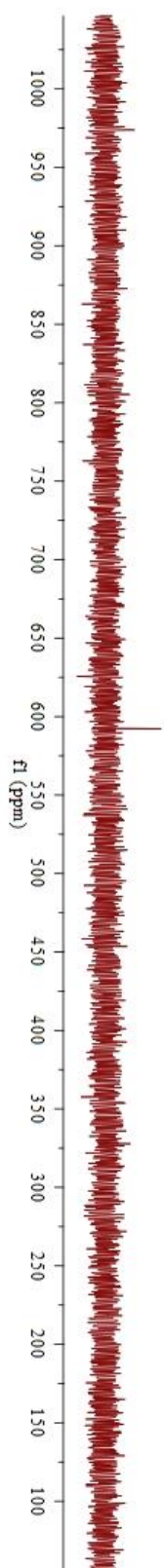
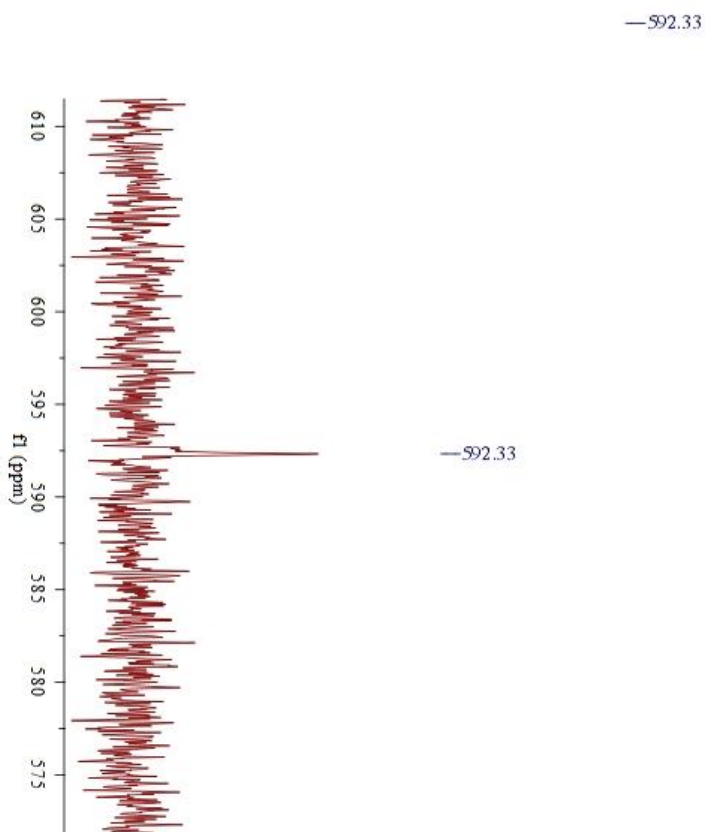
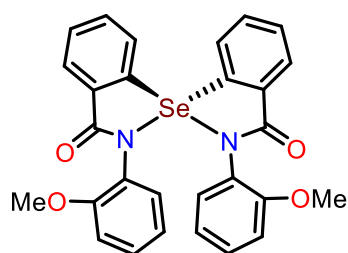


DEPT-135 of 15

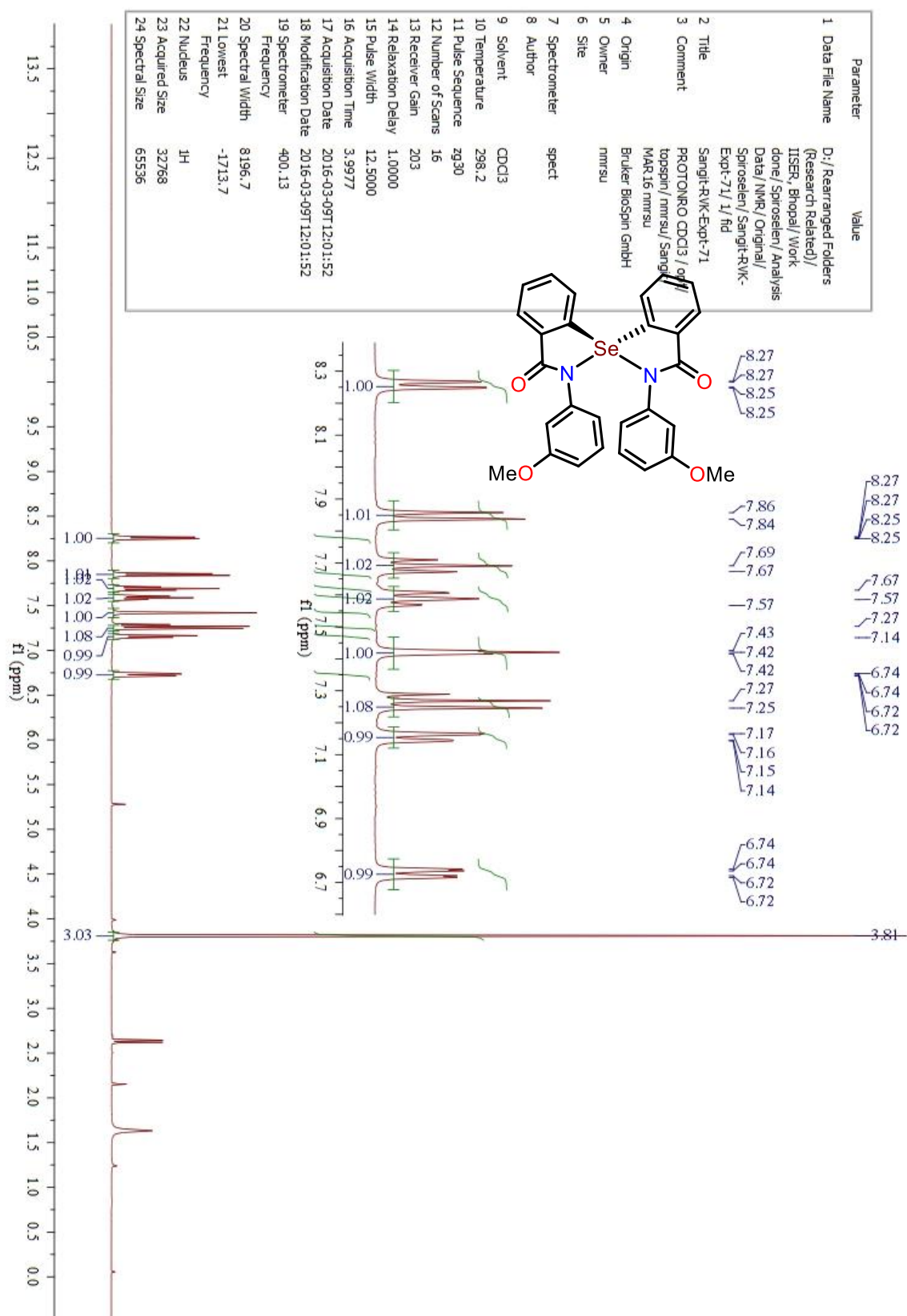


⁷⁷Se NMR of 15

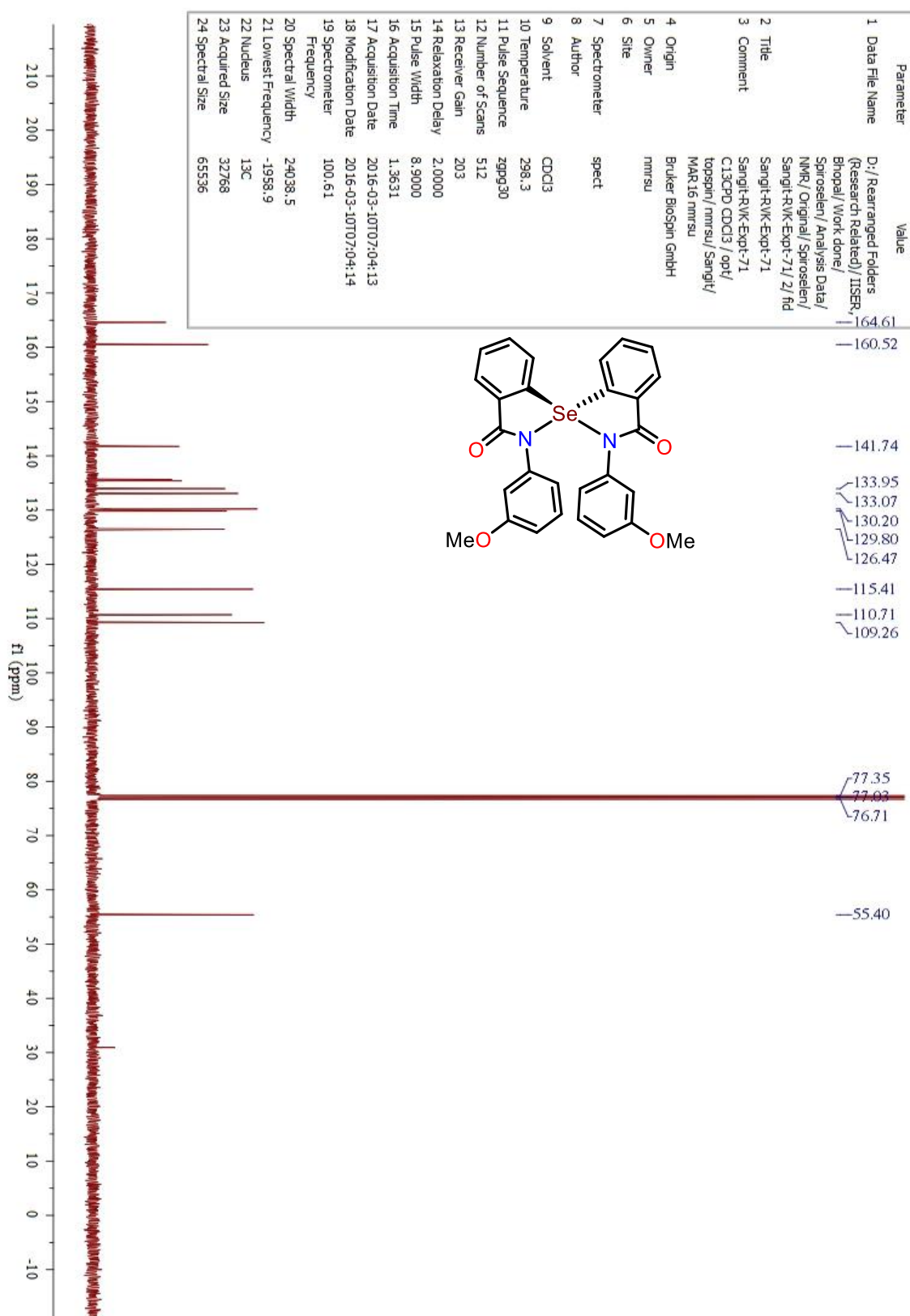
Parameter	Value
1 Data File Name	D:/Rearranged Folders (Research Related)/ITSER, Bhopal/ Work done/ Spiroselen/ Analysis Data/ NMR/ Original/ Spiroselen/ Sangit-RVK-Expt-70/ 4/ f1d
2 Title	Sangit-RVK-Expt-70
3 Comment	Sangit-RVK-Expt-70 SE77ZG CDCl3 / opt/ topspin/ nmrsu/ Sangit/ MAR 16 nmrsu
4 Origin	nmrsu
5 Owner	nmrsu
6 Site	nmrsu
7 Spectrometer	spect
8 Author	
9 Solvent	CDCl3
10 Temperature	298.3
11 Pulse Sequence	zg
12 Number of Scans	512
13 Receiver Gain	203
14 Relaxation Delay	1.0000
15 Pulse Width	5.0000
16 Acquisition Time	0.4325
17 Acquisition Date	2016-03-10T08:42:09
18 Modification Date	2016-03-10T08:42:10
19 Spectrometer	76.31
Frequency	
20 Spectral Width	75757.6
21 Lowest Frequency	4092.2
22 Nucleus	
23 Acquired Size	32768
24 Spectral Size	65536



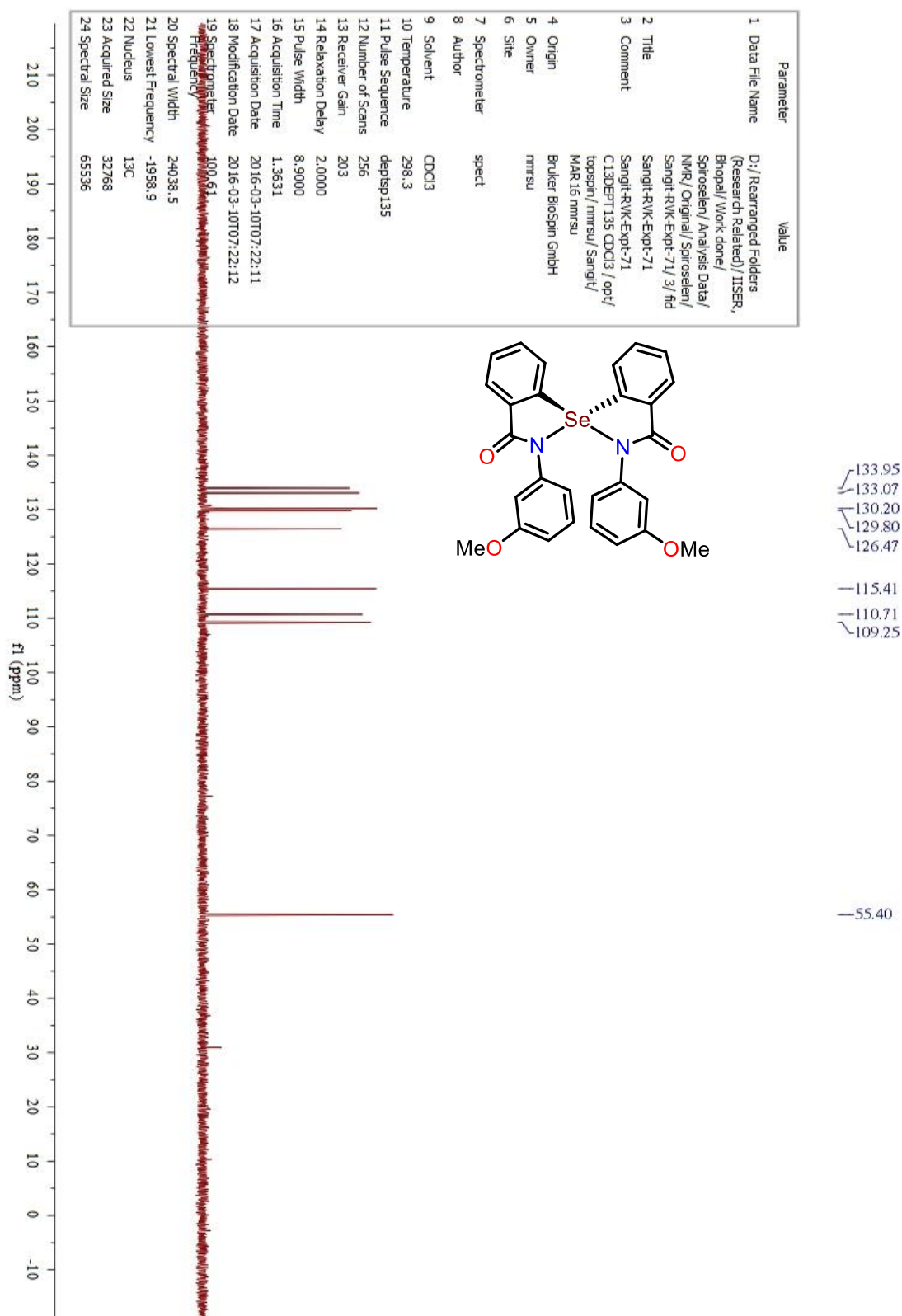
¹H NMR of 17



¹³C NMR of **17**

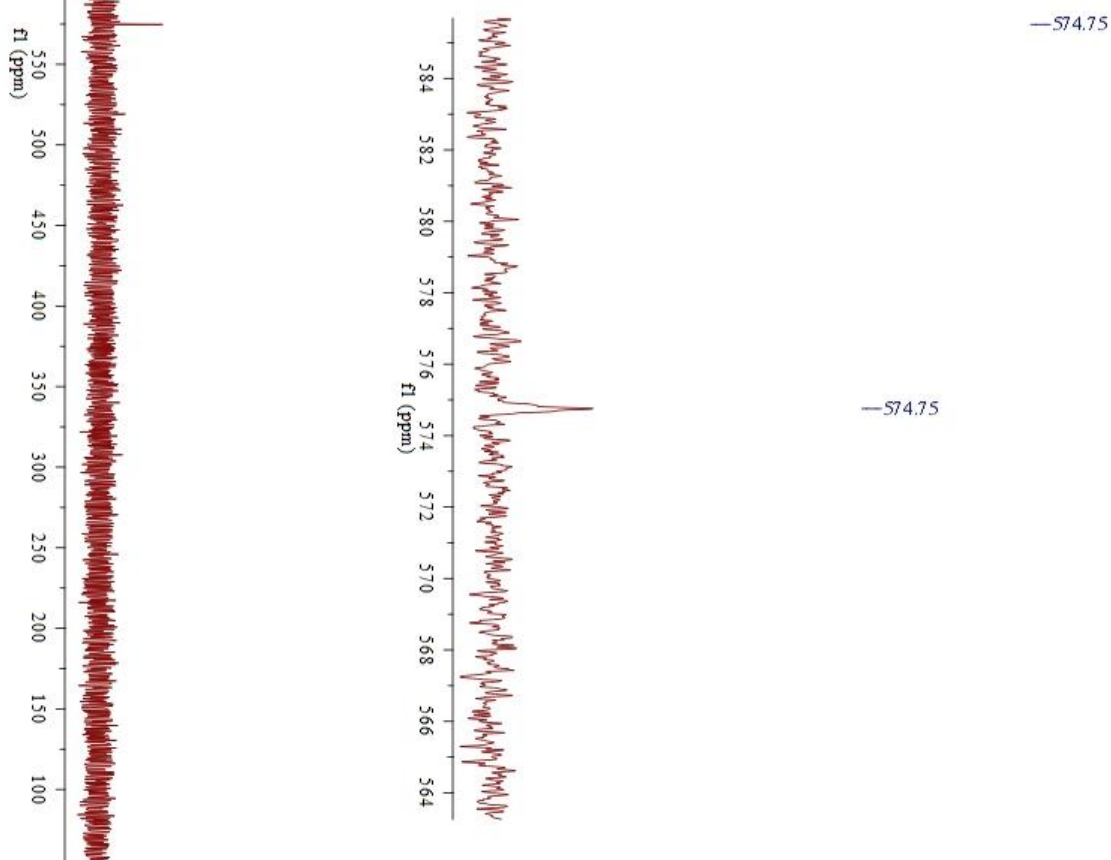
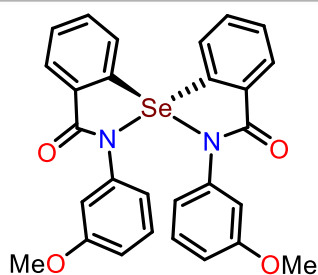


DEPT-135 of 17

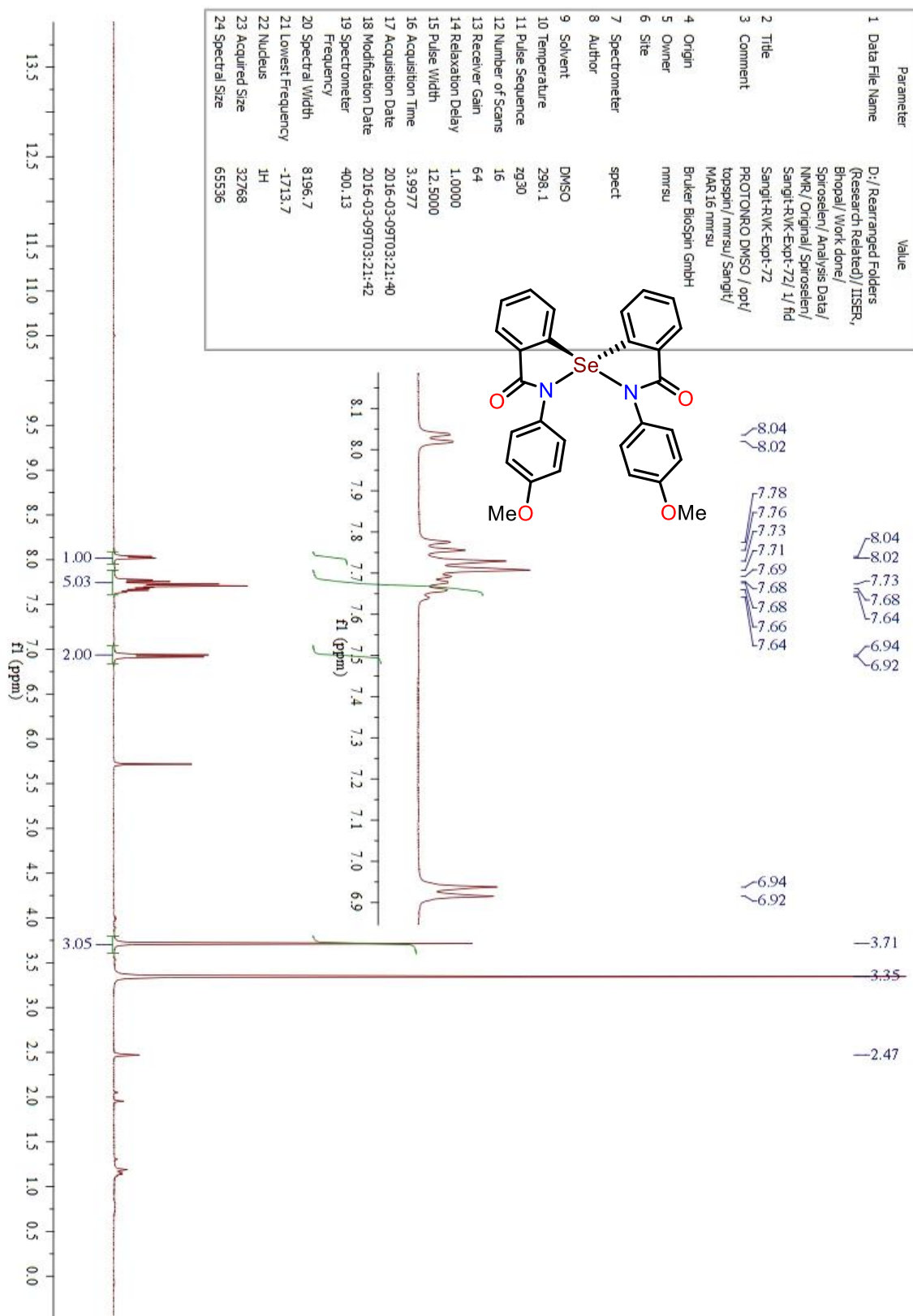


⁷⁷Se NMR of 17

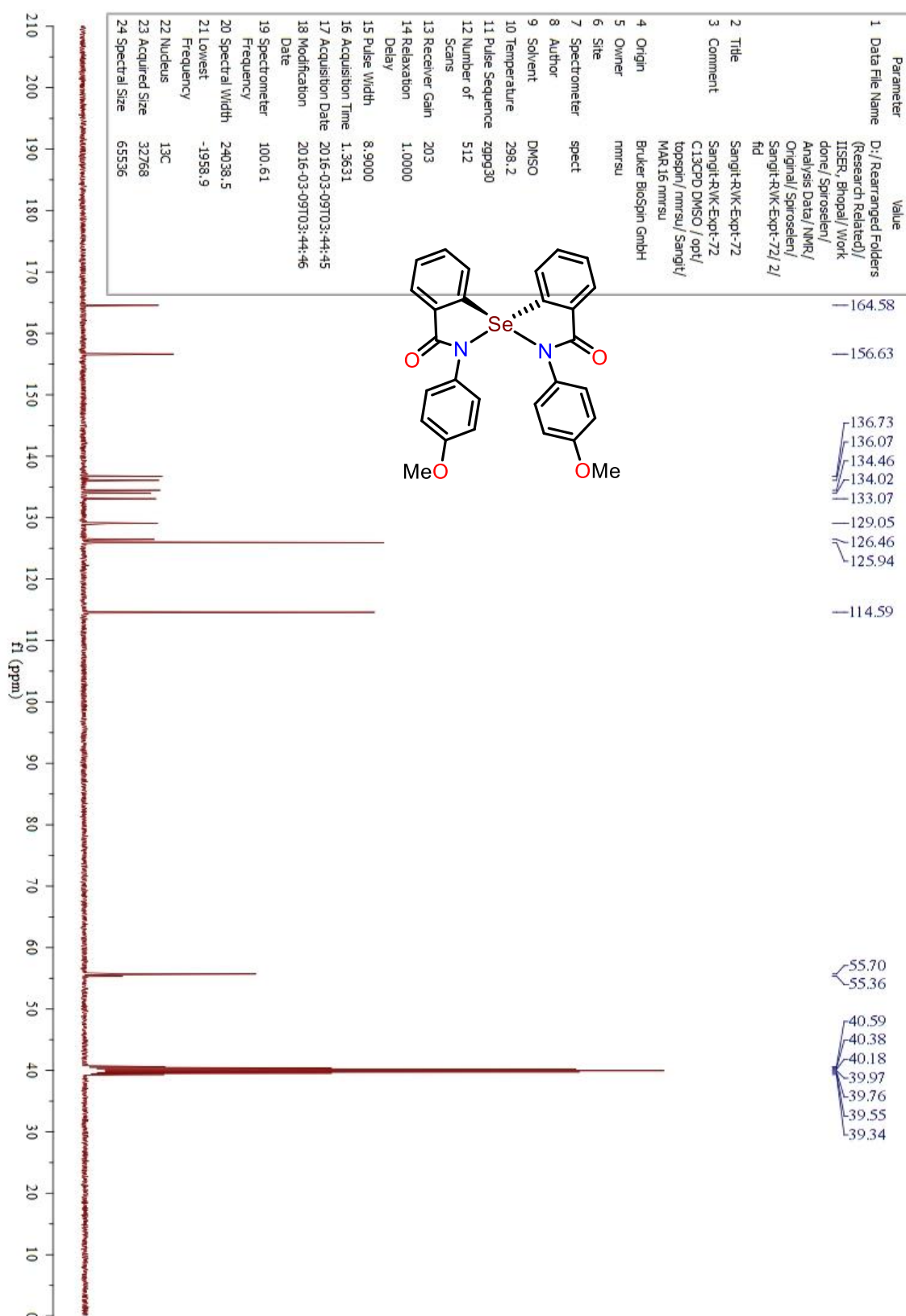
Parameter	Value
1 Data File Name	D:\Rearranged Folders (Research Related)/IISER, Bhopal/Work done/ Spiroselen/Analysis Data/ NMR/Original/Spiroselen/ Sangit-RVK-Expt-71/ Sangit- RVK-Expt-71-Re/ 1 (Double Scan)/ fid
2 Title	Sangit-RVK-Expt-71-Re
3 Comment	Sangit-RVK-Expt-71-Re SE77ZG CDCl3 / opt/ topspin/ nmr/su/ Sangit/ MAR 16 nmr/su Bruker Biospin GmbH nmr/su
4 Origin	
5 Owner	
6 Site	
7 Spectrometer	spect
8 Author	
9 Solvent	CDCl3
10 Temperature	298.2
11 Pulse Sequence	zg
12 Number of Scans	1024
13 Receiver Gain	203
14 Relaxation Delay	1.0000
15 Pulse Width	5.0000
16 Acquisition Time	0.4325
17 Acquisition Date	2016-03-10T19:19:56
18 Modification Date	2016-03-10T19:19:56
19 Spectrometer Frequency	76.31
20 Spectral Width	75757.6
21 Lowest Frequency	4092.2
22 Nucleus	
23 Acquired Size	32768
24 Spectral Size	65536



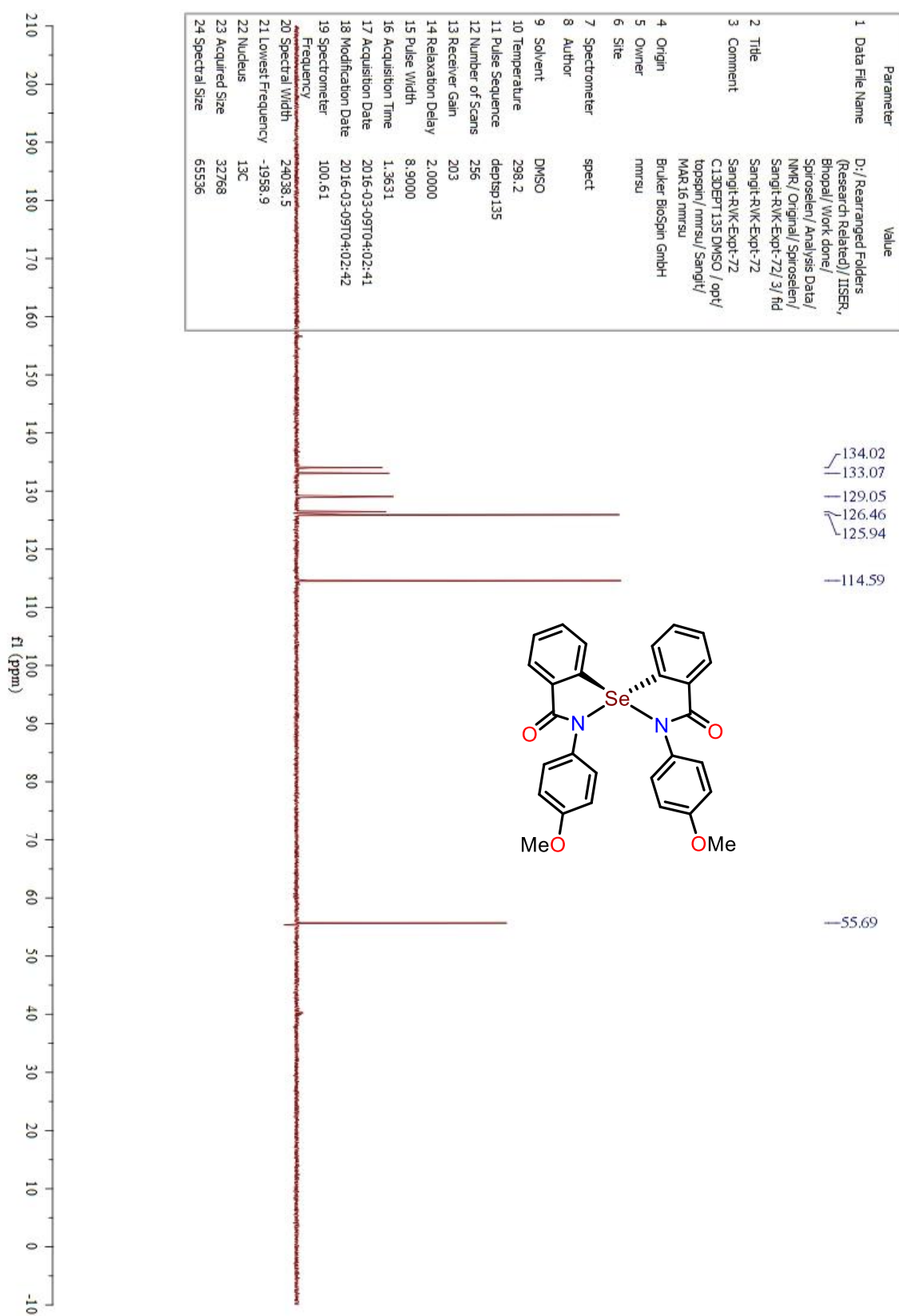
¹H NMR of 42



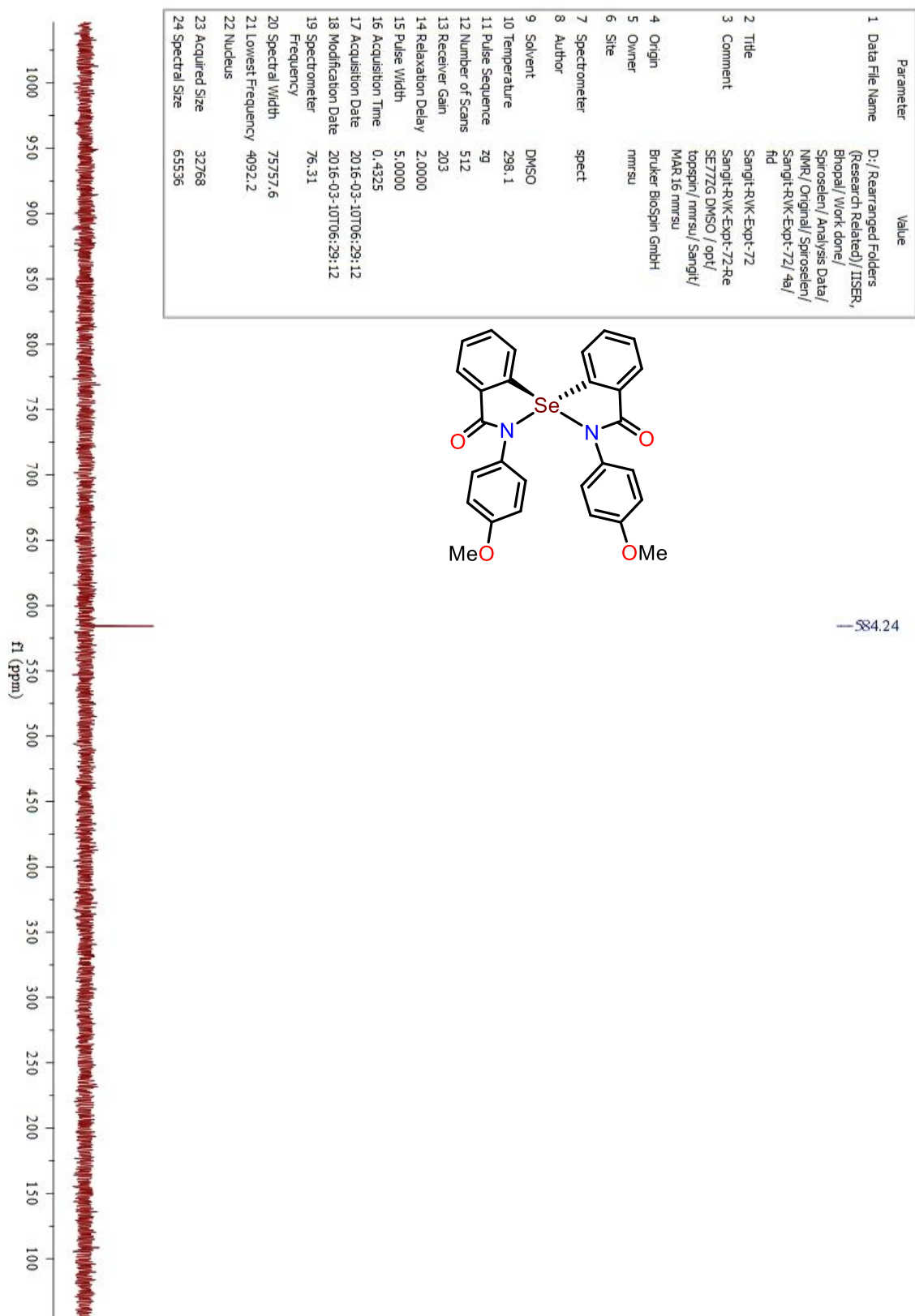
¹³C NMR of 42



DEPT-135 of 42



⁷⁷Se NMR of 42



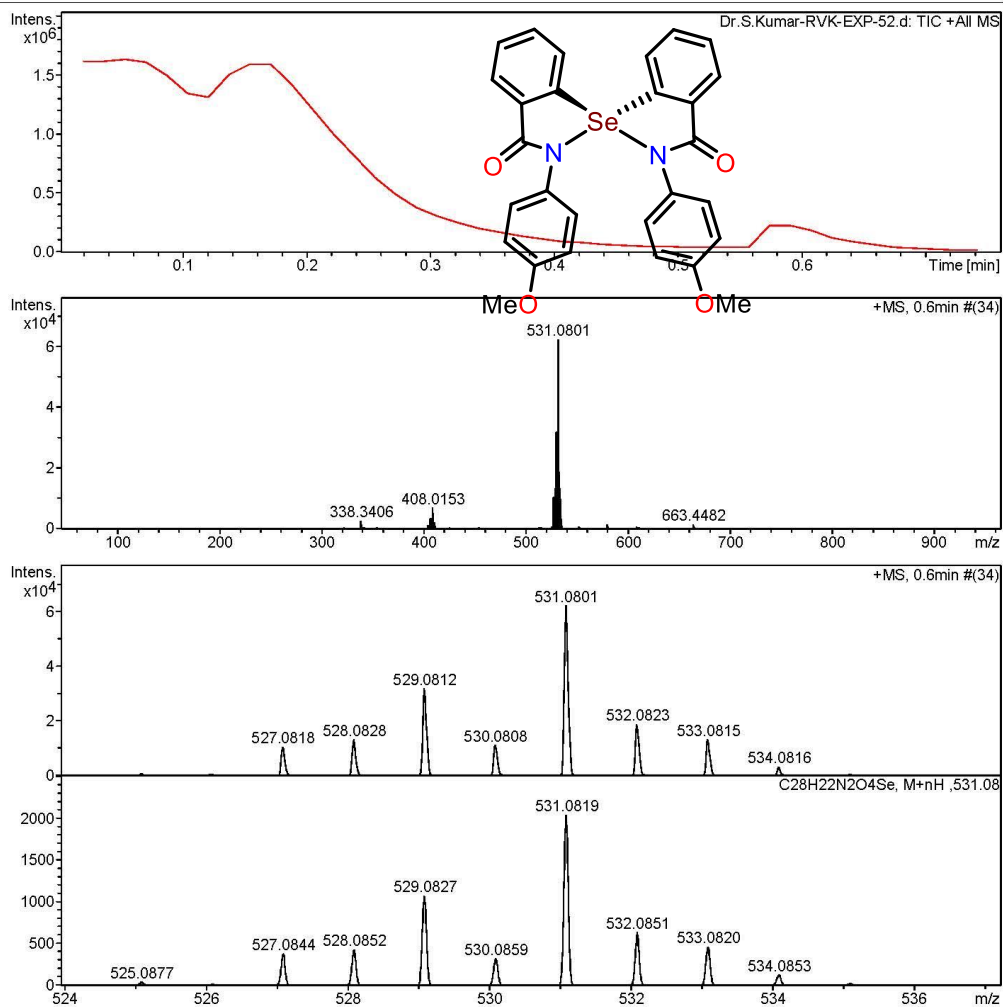
Display Report

Analysis Info

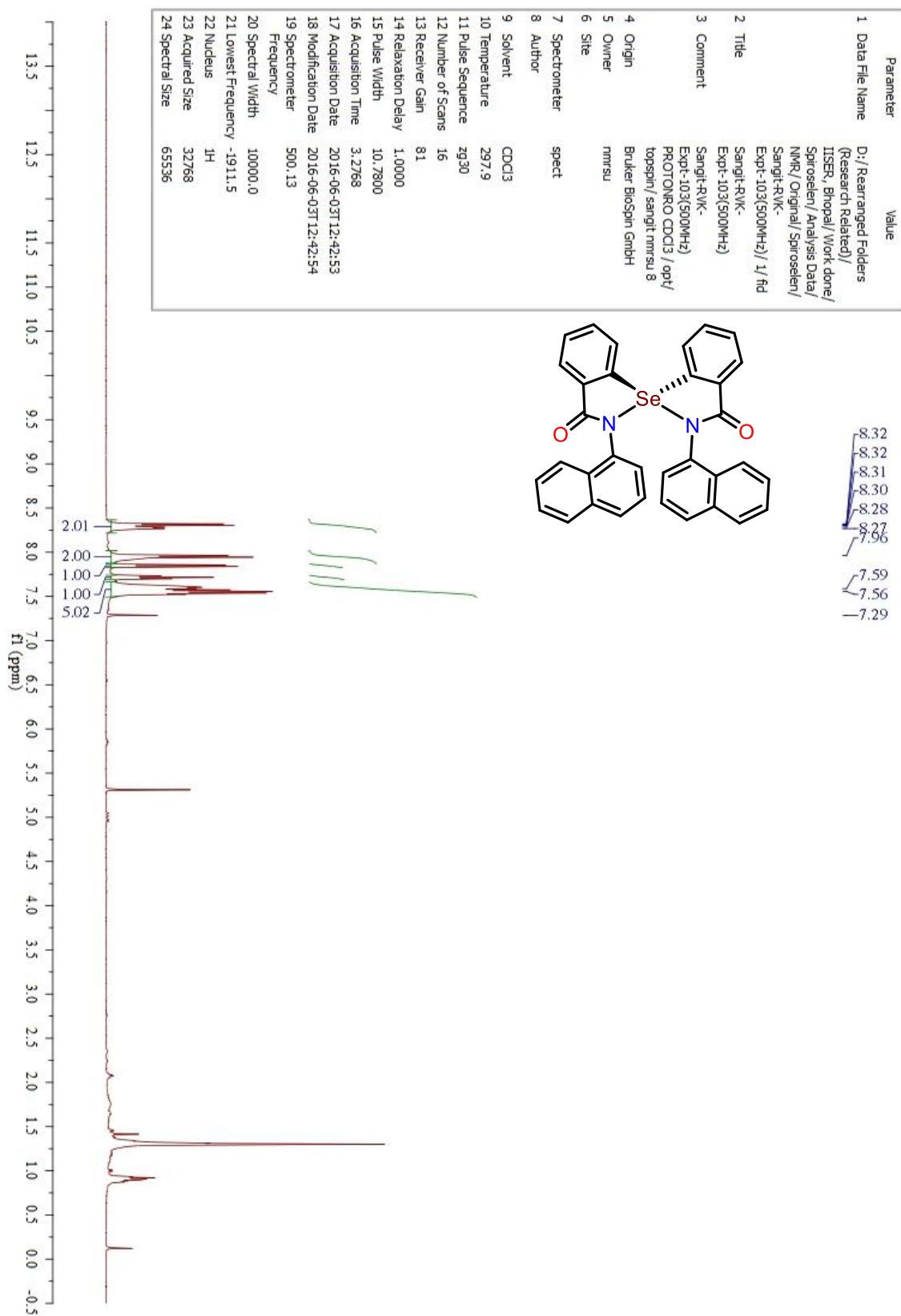
Analysis Name	D:\Data\user data\2016\MARCH 2016\03-03-2016\Dr.S.Kumar-RVK-EXP-52.d	Acquisition Date	3/3/2016 4:08:05 PM
Method	tune_wide_APCI_23.06.m	Operator	DIMPLE
Sample Name	RVK-EXP-52	Instrument	micrOTOF-Q II 10330
Comment			

Acquisition Parameter

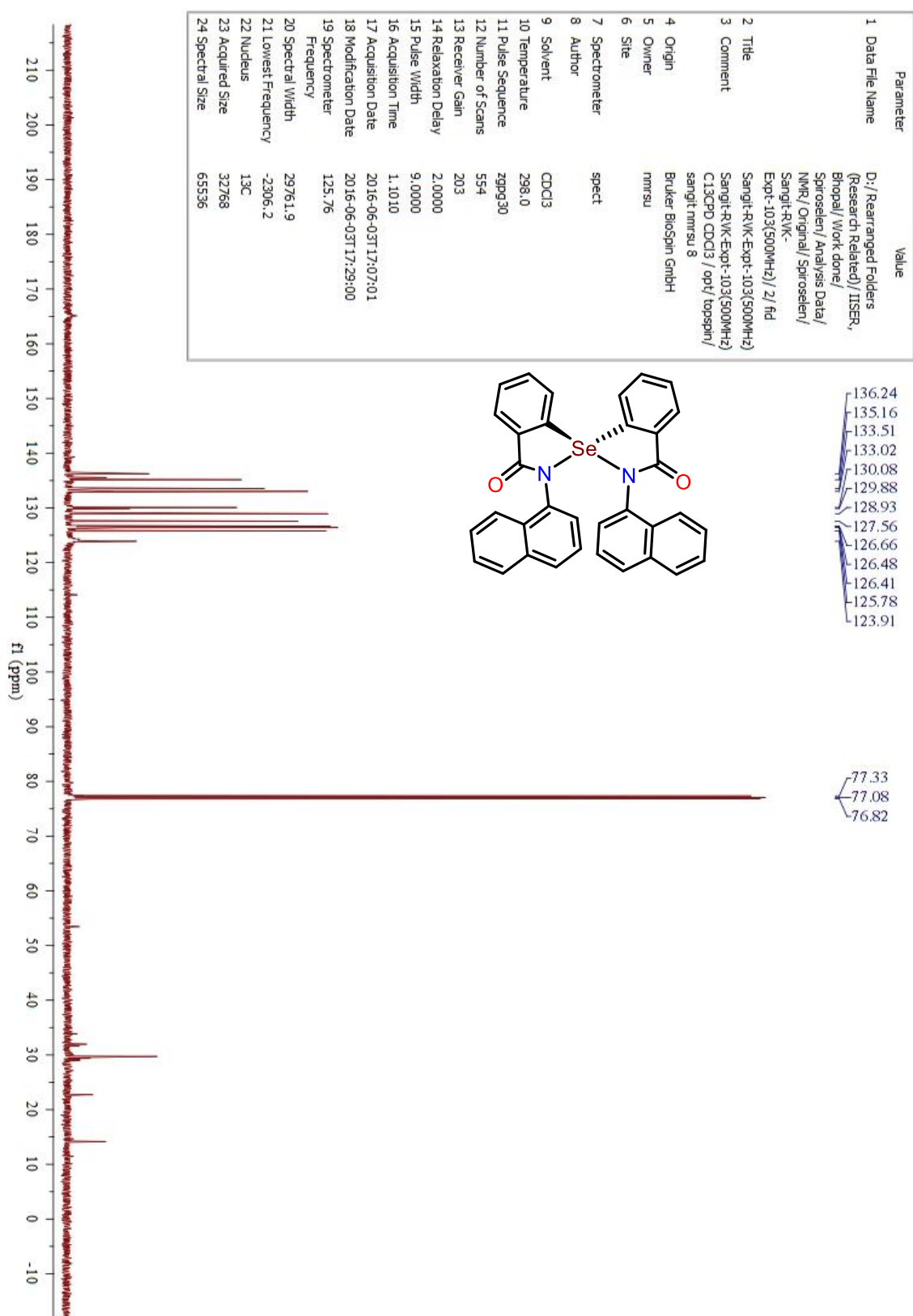
Source Type	APCI	Ion Polarity	Positive	Set Nebulizer	2.5 Bar
Focus	Not active	Set Capillary	4000 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	3000 m/z	Set Collision Cell RF	600.0 Vpp	Set Divert Valve	Waste



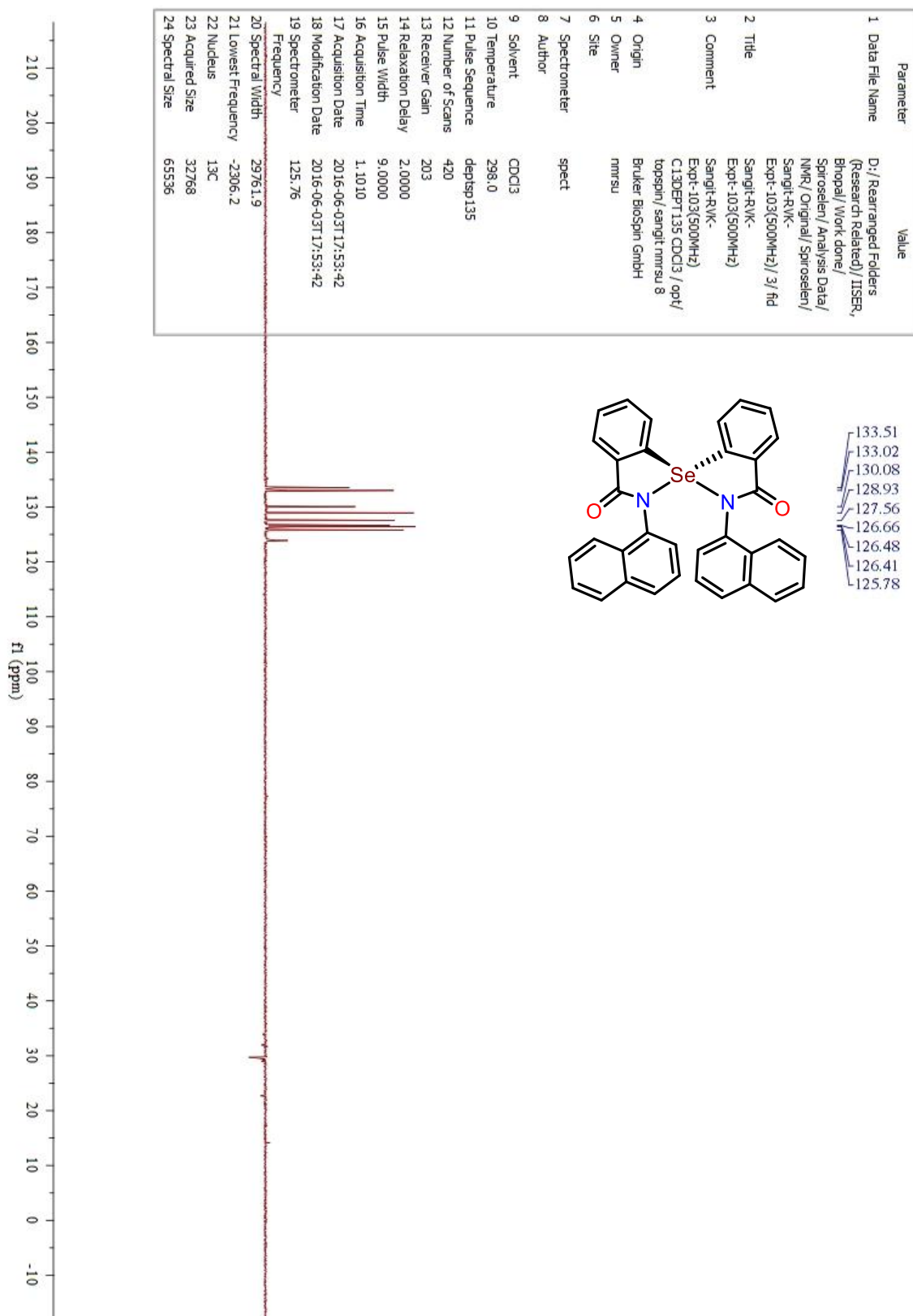
¹H NMR of 43



¹³C NMR of 43

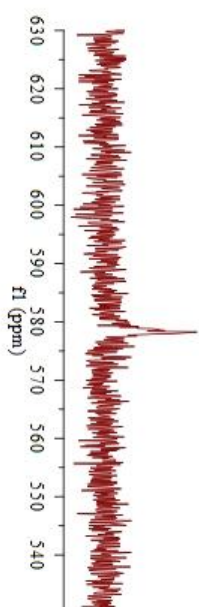
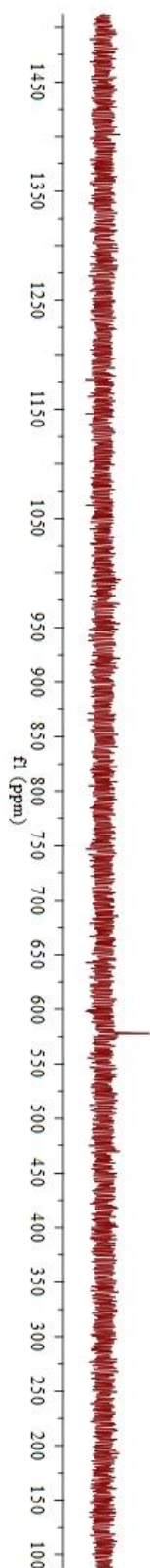
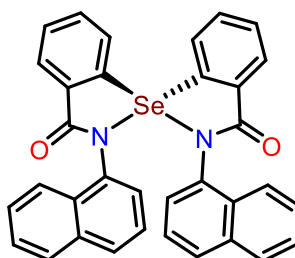


DEPT-135 of 43



⁷⁷Se NMR of 43

Parameter	Value
1 Data File Name	D:/Rearranged Folders (Research Related)/IISER, Bhopal/Work done/ Spiroselen/Analysis Data/ NMR/Original/Spiroselen/ Sangit-RVK-Expt-103/2/ftd
2 Title	Sangit-RVK-Expt-103
3 Comment	Sangit-RVK-Expt-103 SE77ZG CDCl3 / opt/ topspin / nmrsu / Sangit/ JUN16 nmrsu
4 Origin	Brucker Biospin GmbH
5 Owner	nmrsu
6 Site	
7 Spectrometer	spect
8 Author	
9 Solvent	CDCl3
10 Temperature	298.1
11 Pulse Sequence	zg
12 Number of Scans	5000
13 Receiver Gain	203
14 Relaxation Delay	2.0000
15 Pulse Width	5.0000
16 Acquisition Time	0.3015
17 Acquisition Date	2016-06-06T23:21:36
18 Modification Date	2016-06-06T23:21:38
19 Spectrometer Frequency	76.31
20 Spectral Width	108695.6
21 Lowest Frequency	6700.8
22 Nucleus	
23 Acquired Size	32768
24 Spectral Size	65536



—578.27

—578.27

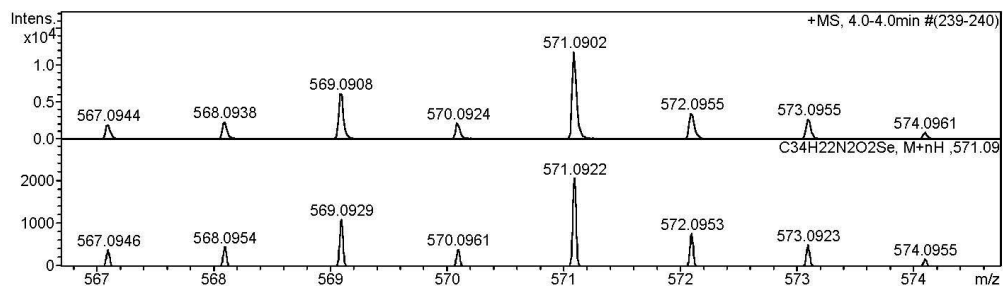
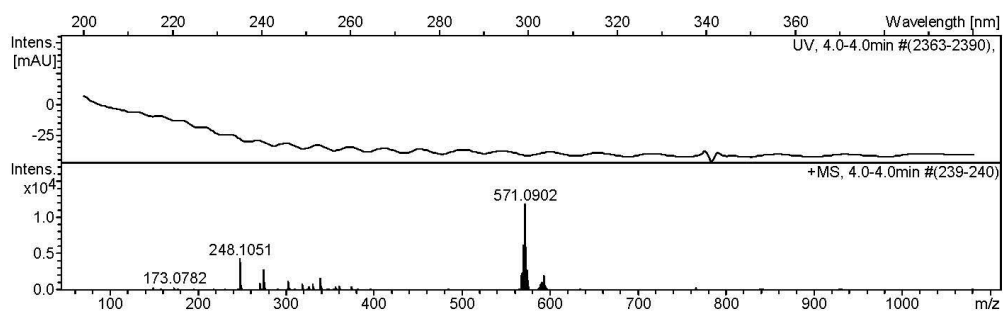
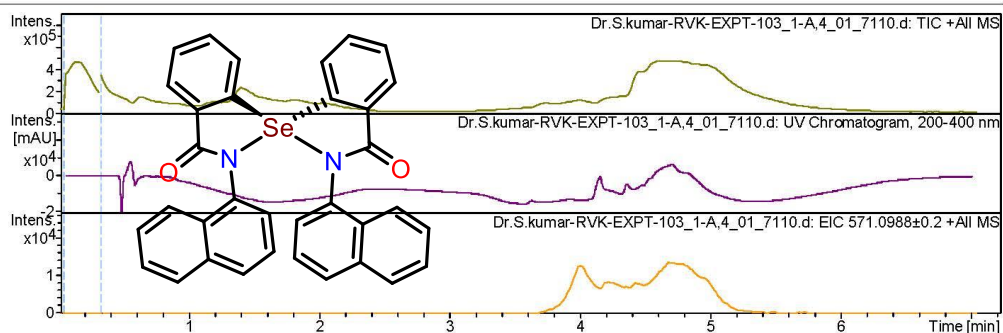
Display Report

Analysis Info

Analysis Name D:\Data\user data\2016\August 2016\08-08-2016\Dr.S.kumar-RVK-EXPT-103_1-A_4_01_7110.d Acquisition Date 8/8/2016 2:08:58 PM
Method hrlcms_pos_low_tunemix.m Operator DIMPLE
Sample Name Dr.S.kumar-RVK-EXPT-103 Instrument micrOTOF-Q II 10330
Comment

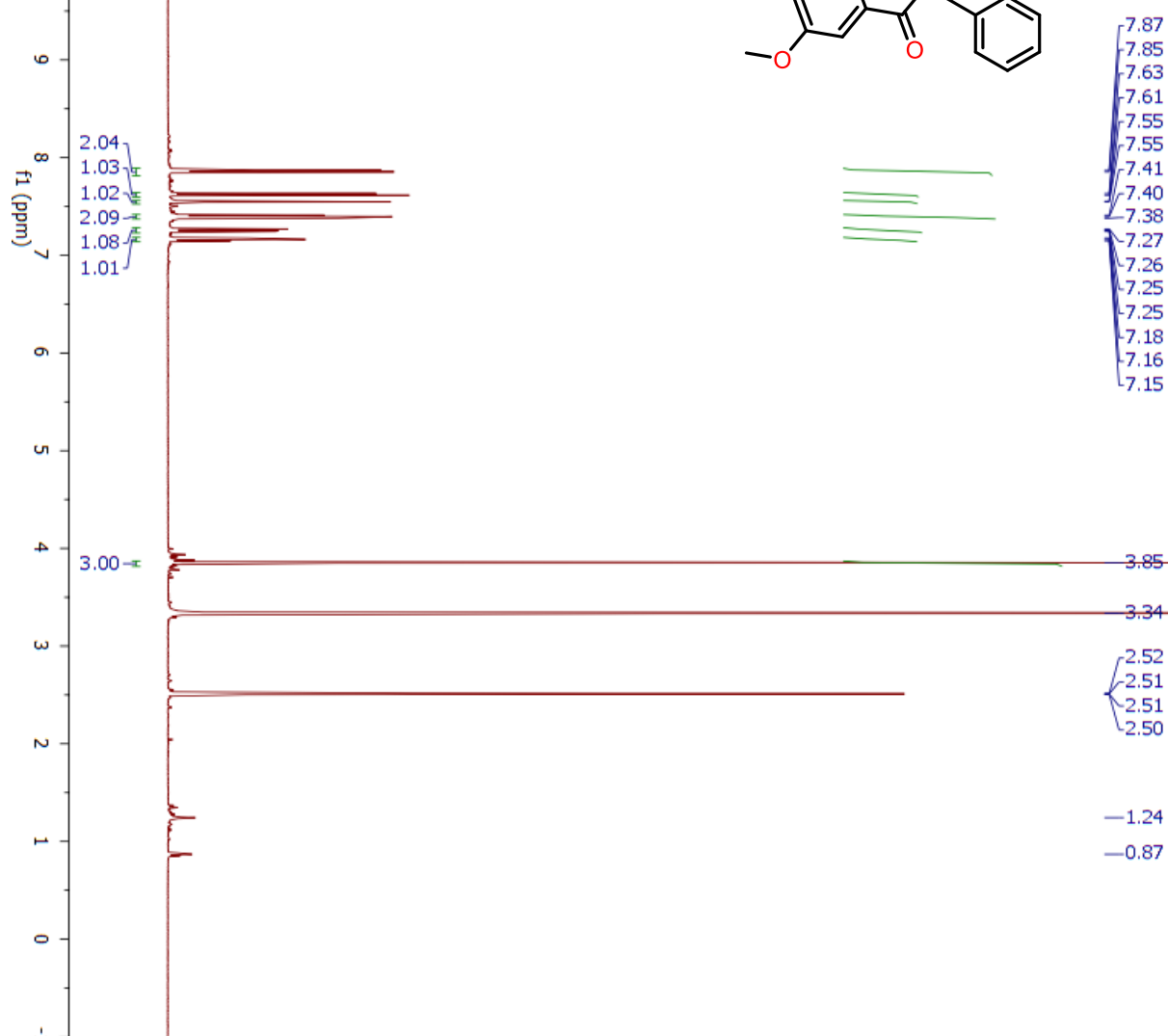
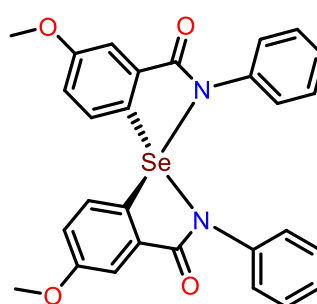
Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	1.0 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	250 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	7.0 l/min
Scan End	3000 m/z	Set Collision Cell RF	130.0 Vpp	Set Divert Valve	Waste

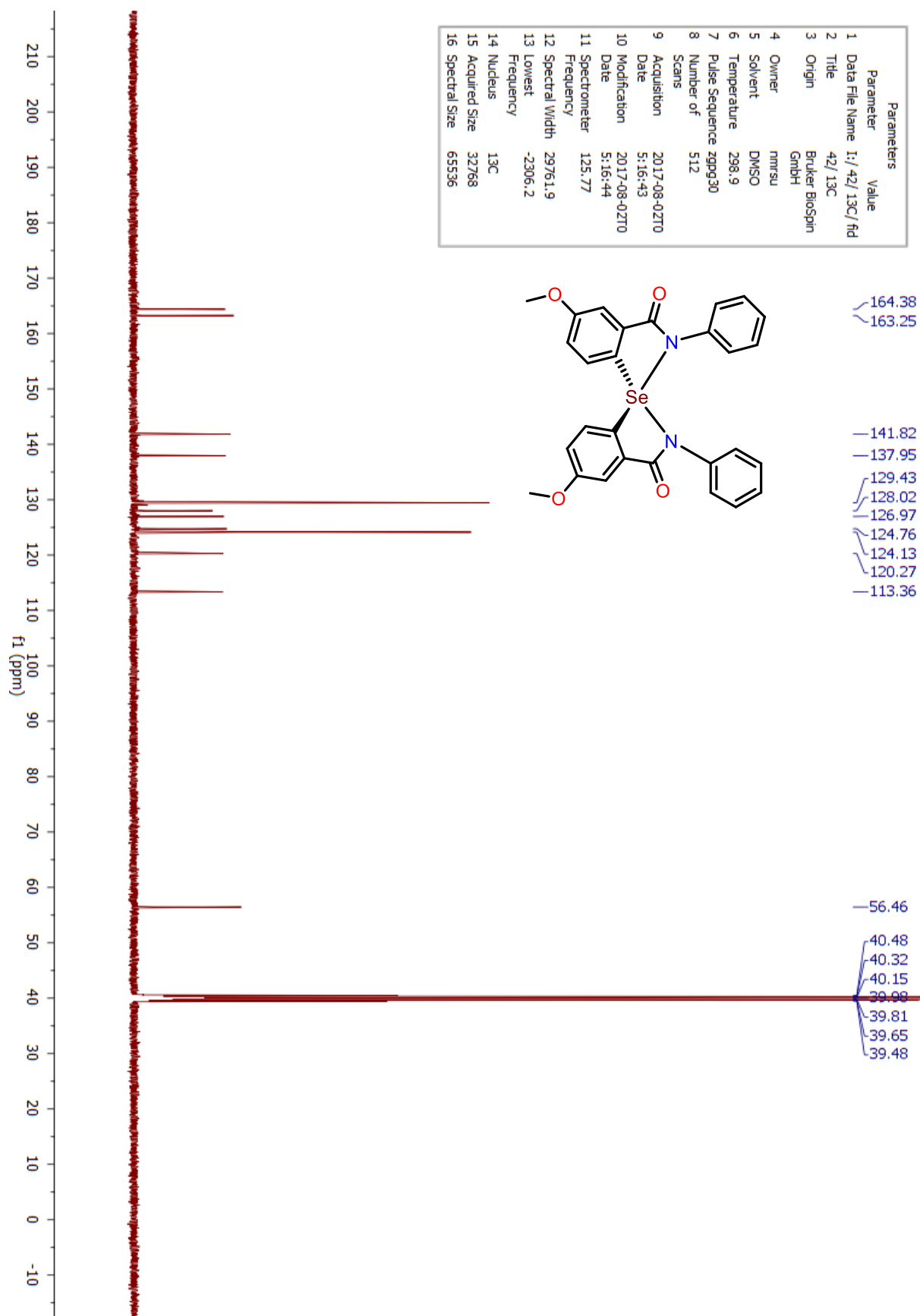


¹H NMR of 44

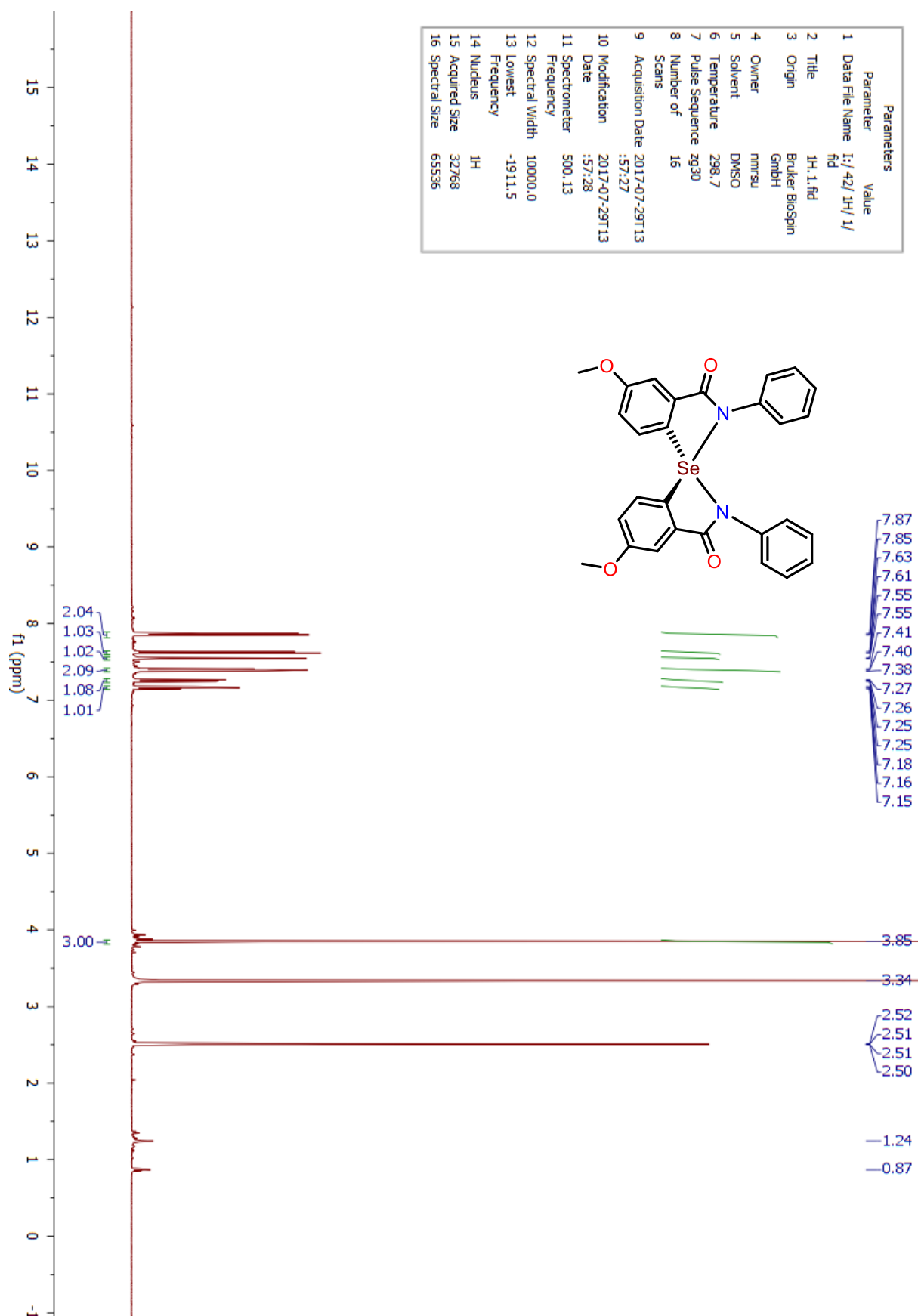
Parameter	Value
1 Data File Name	1:/42/ 1H/ 1/ f1d
2 Title	1H, 1.f1d
3 Origin	Brüker Biospin GmbH
4 Owner	nmrsu
5 Solvent	DMSO
6 Temperature	298.7
7 Pulse Sequence	zg30
8 Number of Scans	16
9 Acquisition Date	2017-07-29T13:57:27
10 Modification Date	2017-07-29T13:57:28
11 Spectrometer	500.13
12 Spectral Width	10000.0
13 Lowest Frequency	-1911.5
14 Nucleus	¹ H
15 Acquired Size	32768
16 Spectral Size	65536



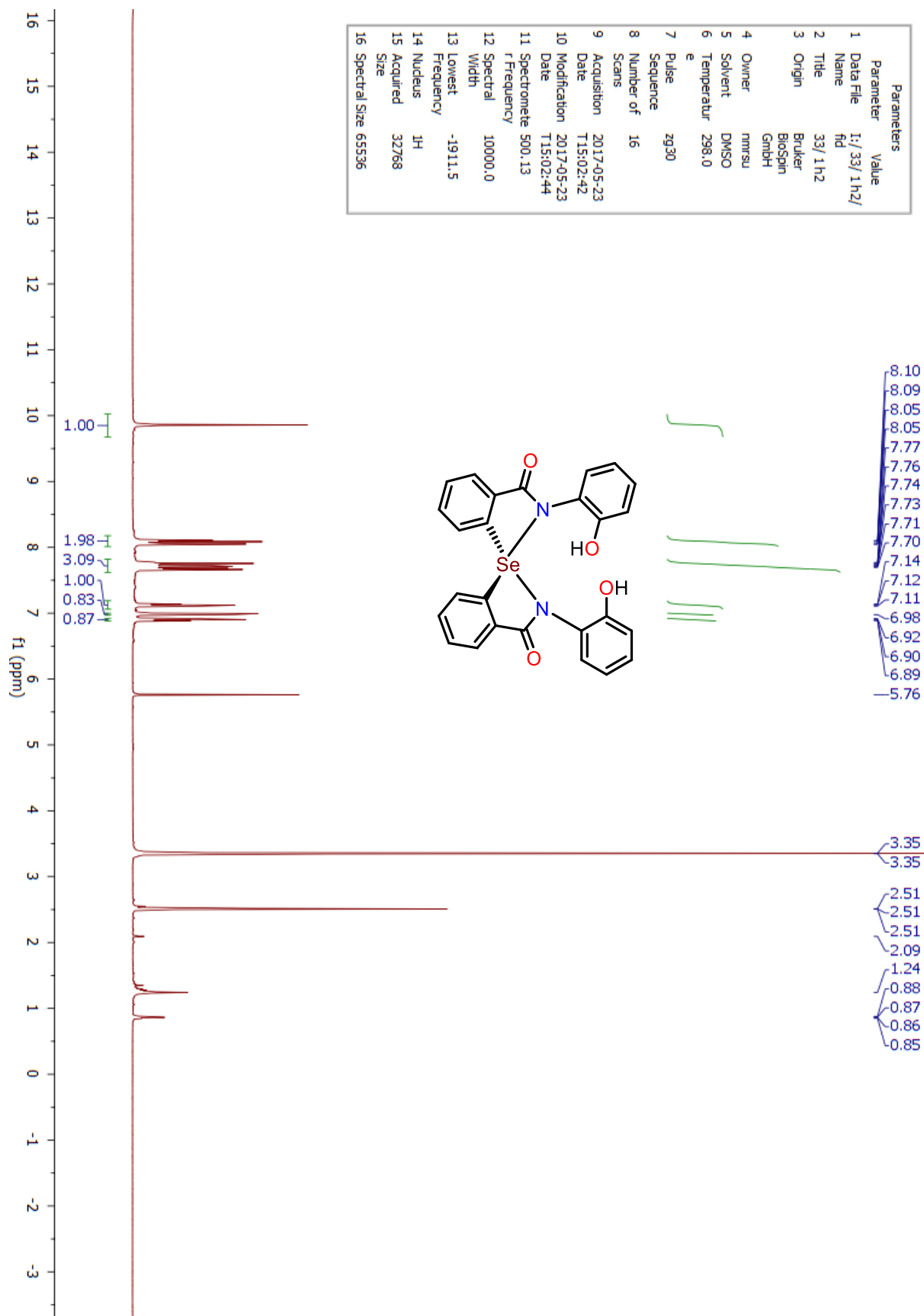
¹³C NMR of 44



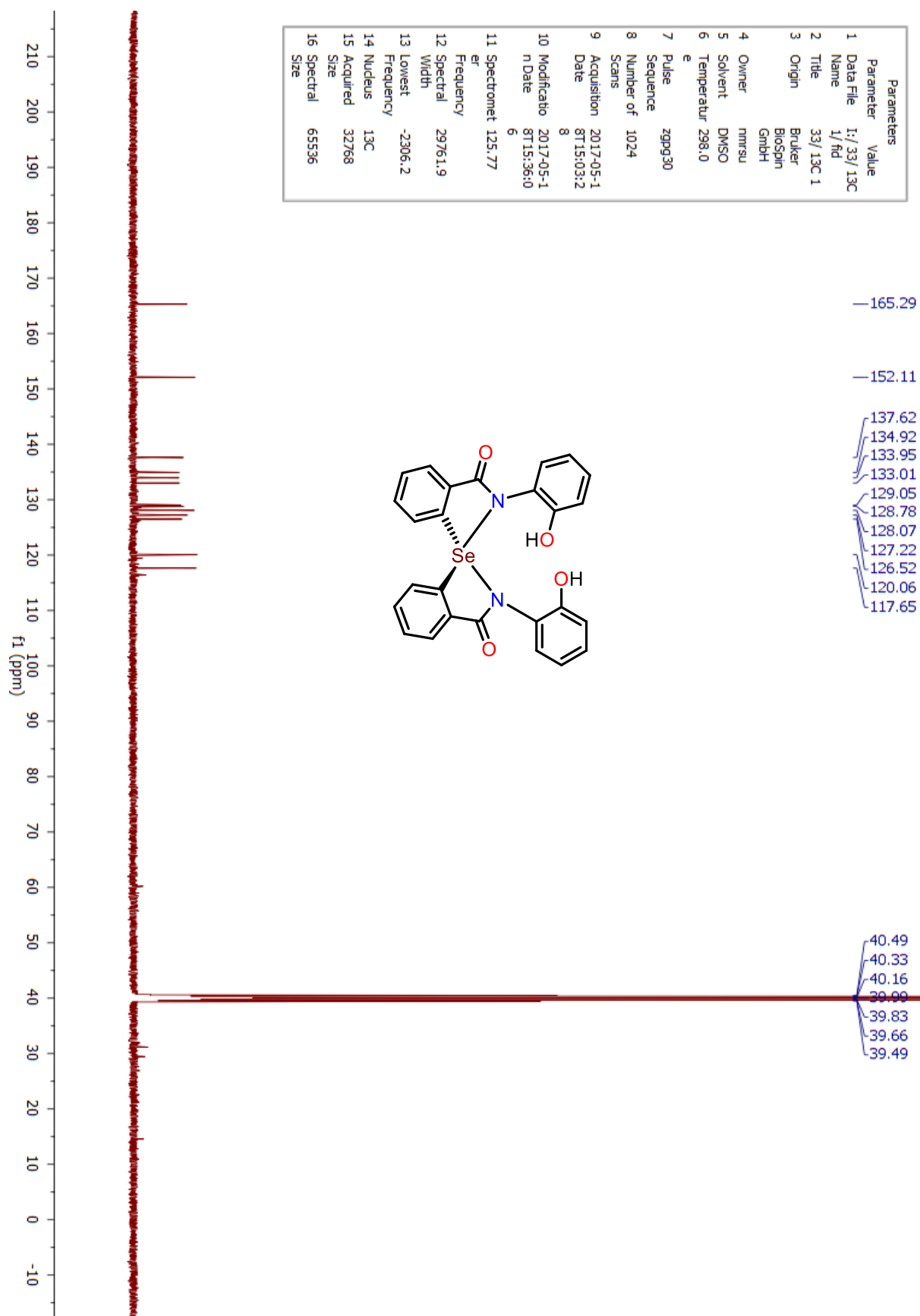
⁷⁷Se NMR of 44



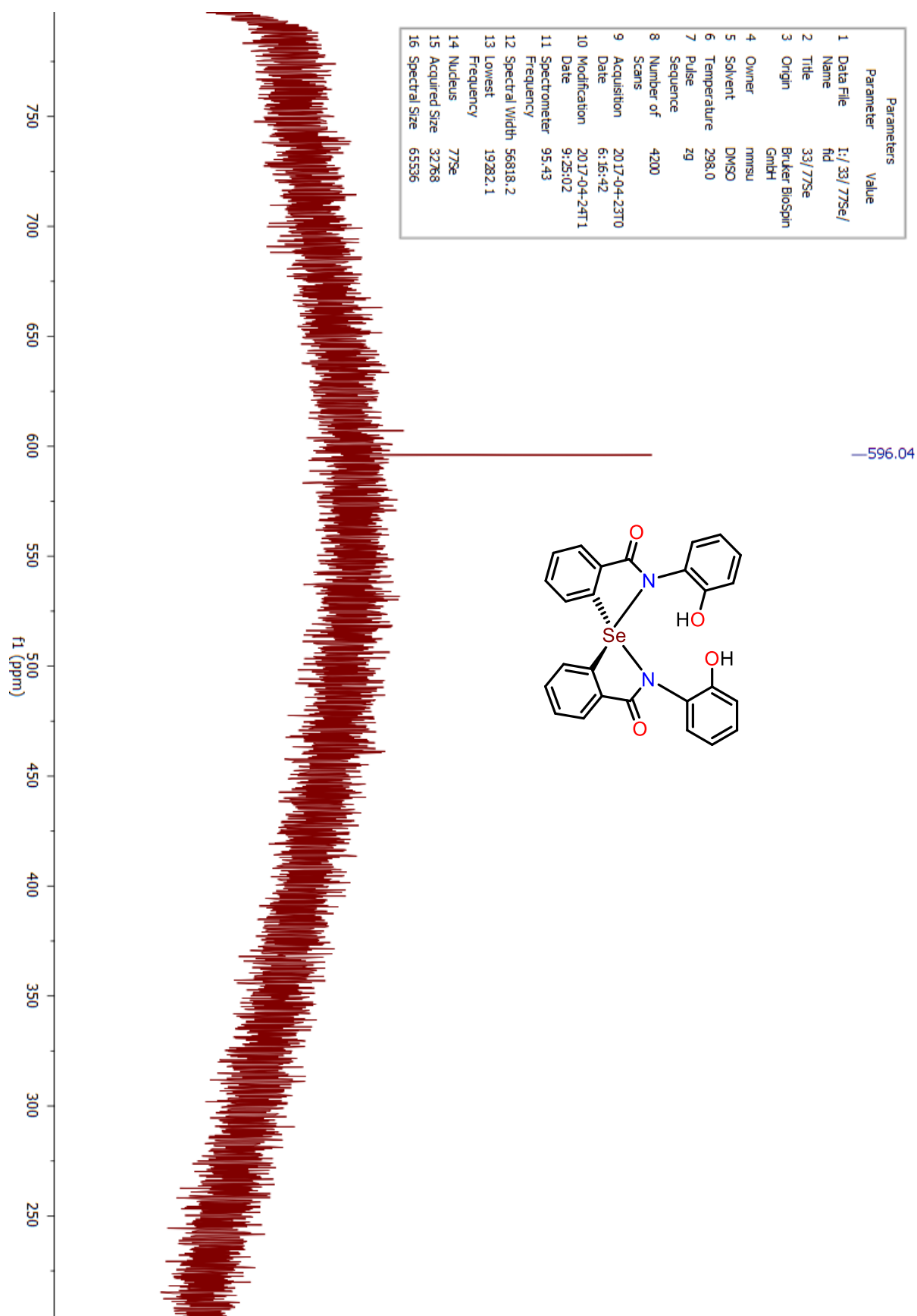
¹H NMR of 29



¹³C NMR of 29



⁷⁷Se NMR of 29



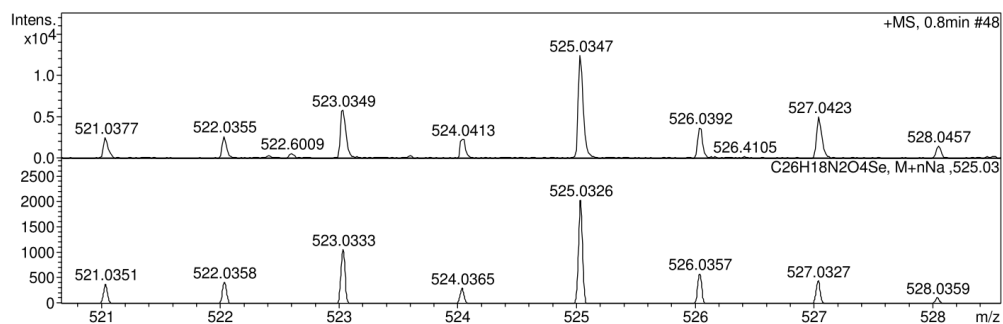
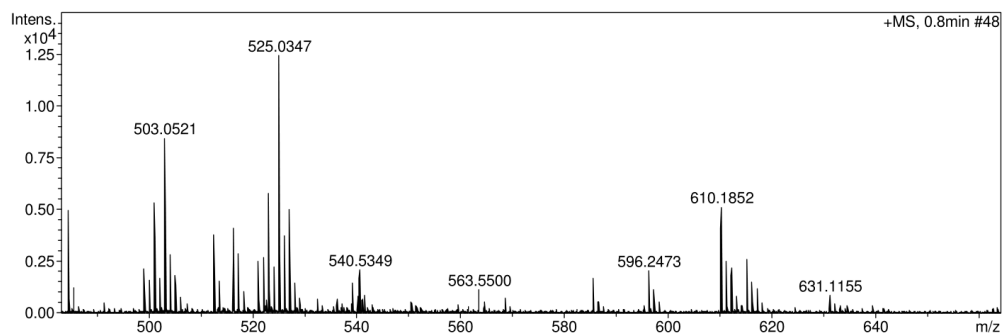
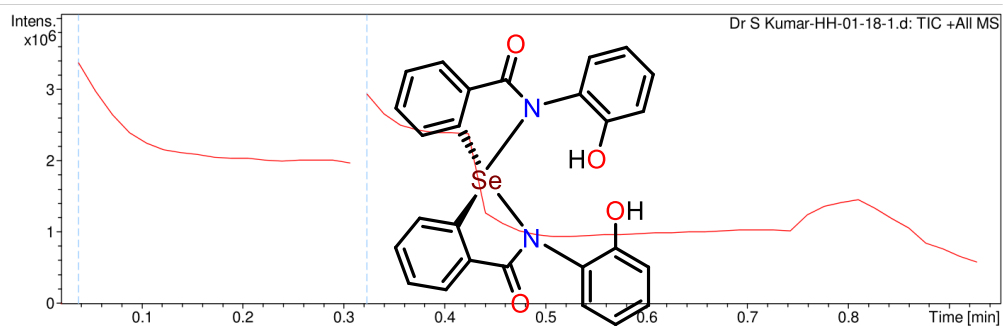
Display Report

Analysis Info

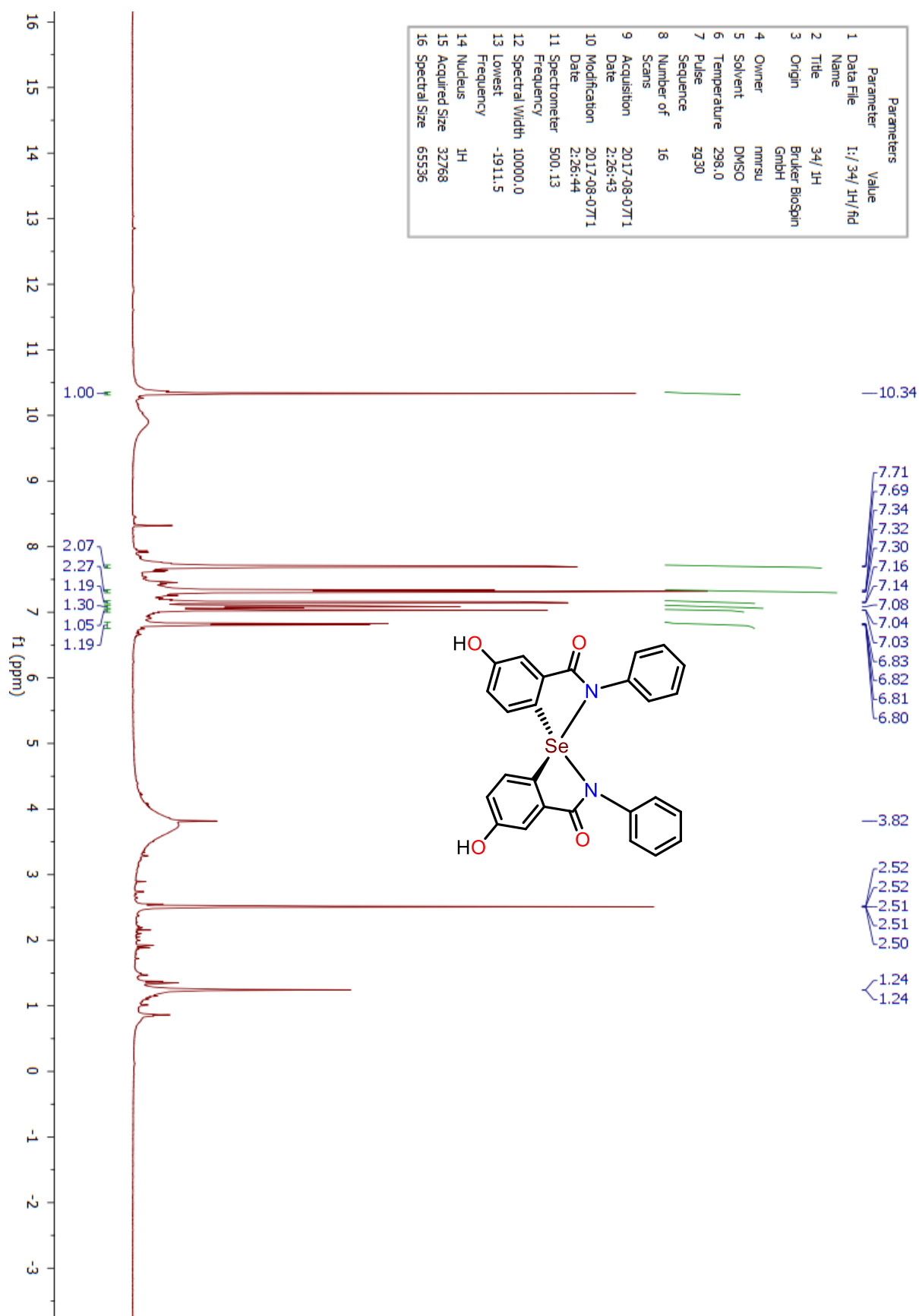
Analysis Name	D:\Data\user data\2017\APRIL 2017\19 april\Dr S Kumar-HH-01-18-1.d	Acquisition Date	4/19/2017 10:30:47 AM
Method	Pos_HIGH_tunemix.m	Operator	RUCHI SHRIVASTAVA
Sample Name	HH-01-18-1	Instrument	micrOTOF-Q II 10330
Comment			

Acquisition Parameter

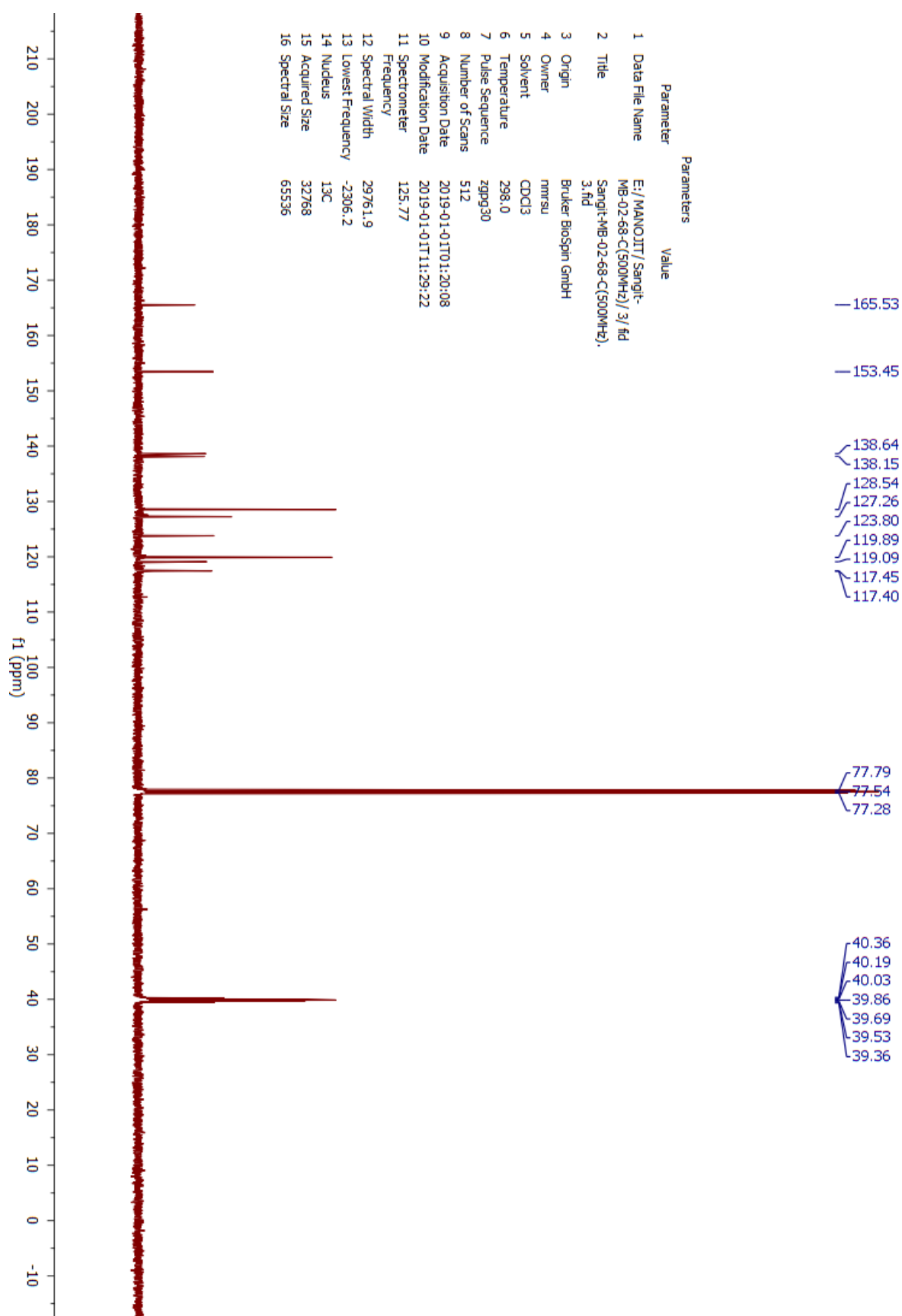
Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.3 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	3000 m/z	Set Collision Cell RF	1000.0 Vpp	Set Divert Valve	Waste



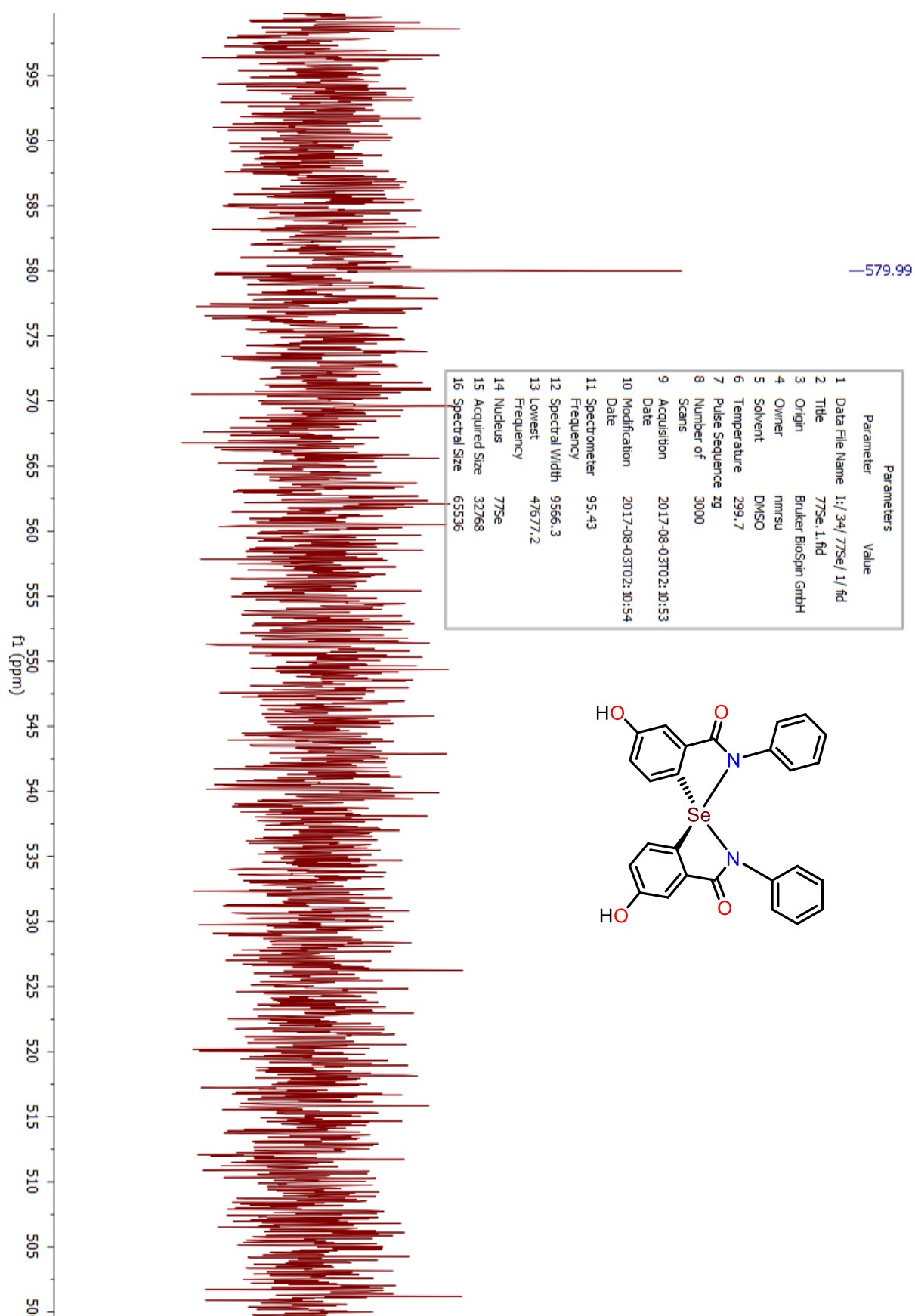
¹H NMR of 30



¹³C NMR of 30



⁷⁷Se NMR of **30**



Display Report

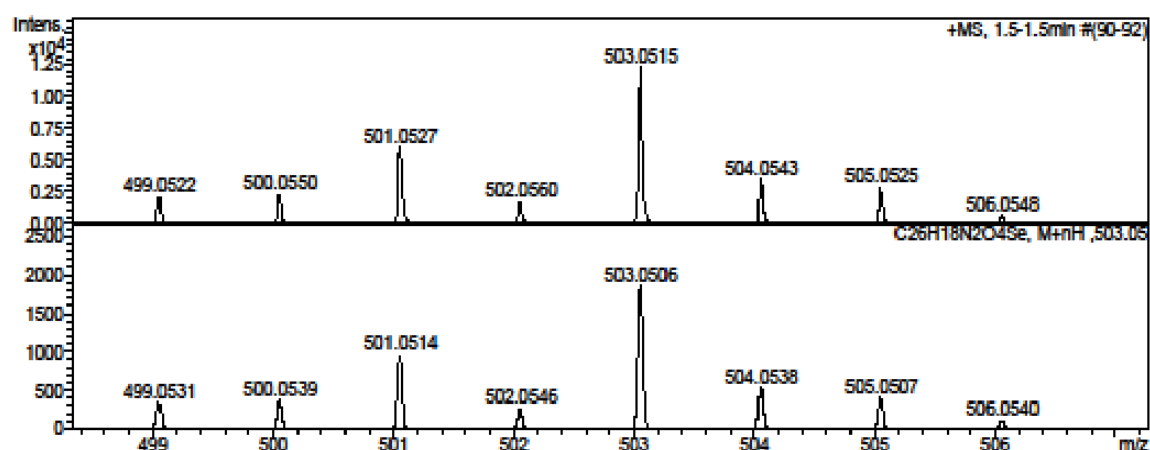
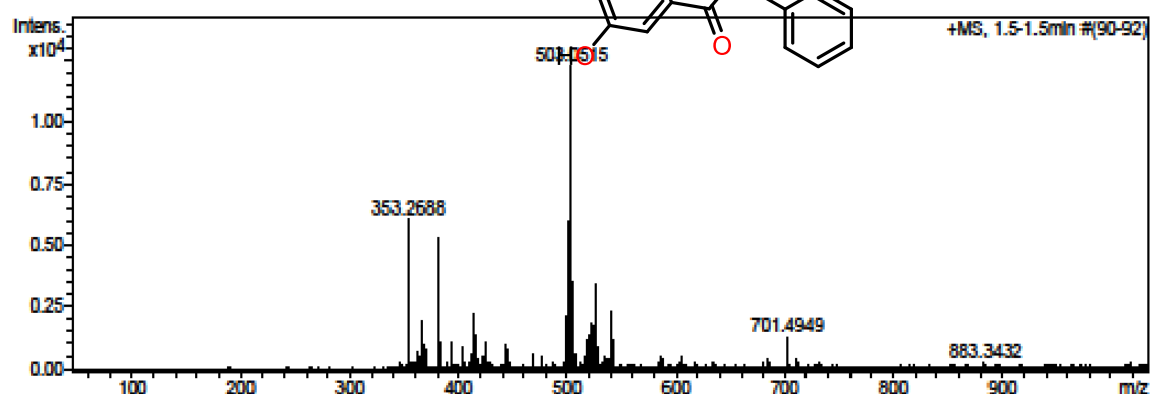
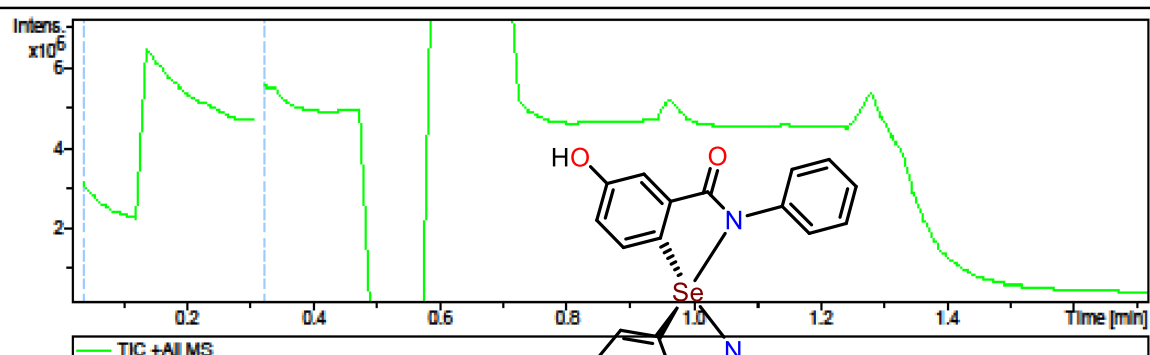
Analysis Info

Analysis Name D:\Data\user data\2017\AUGUST 2017\24 Aug 17\Dr. S.Kumar-HH-01-43-1.d
Method Pos_Mid_tunemix.m
Sample Name HH-01-43-1
Comment

Acquisition Date 8/24/2017 3:38:42 PM
Operator RUCHI SHRIVASTAVA
Instrument microTOF-Q II 10330

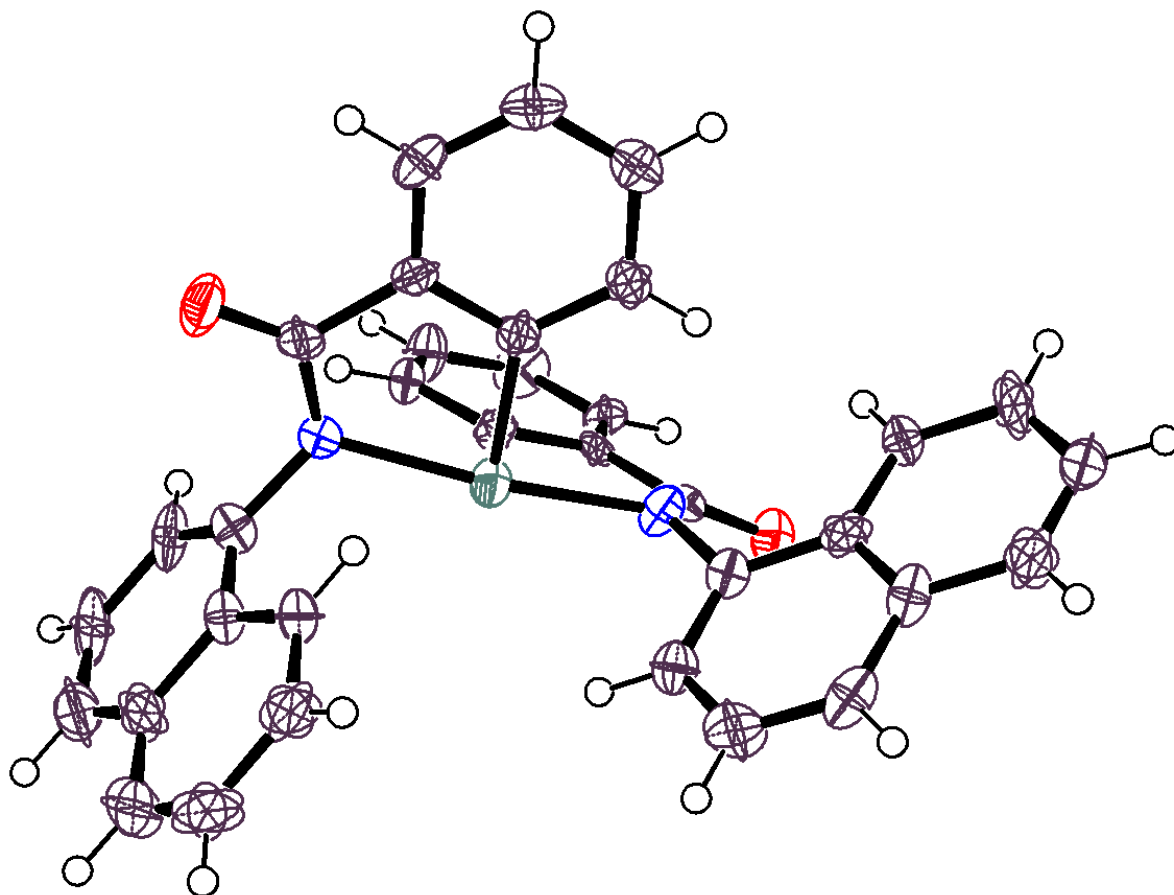
Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.3 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	3000 m/z	Set Collision Cell RF	450.0 Vpp	Set Divert Valve	Waste

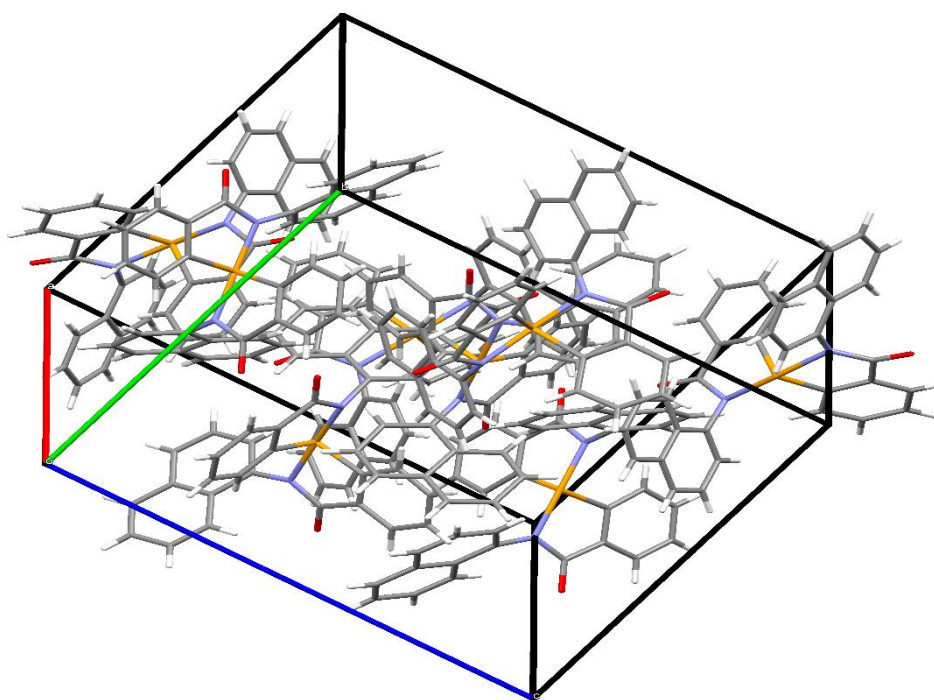


Crystal Structure of 43

ORTEP view of 43 with 50% thermal ellipsoid probability



Packing diagram of 43



Crystal data

Identification code	RVK-43
Empirical formula	C ₂₆ H ₂₀ N ₂ O ₂ Se ₂
Formula weight	569.49
Temperature/K	293
Crystal System	Orthorhombic
Space group	Pca2 ₁
a/Å	21.073 (3)
b/Å	14.264 (2)
c/Å	16.949(3)
α /°	90
β /°	90
γ /°	90
Volume/ Å ³	5094.7 (19)
Z	8
$\rho_{\text{calc}}/\text{cm}^3$	1.485
μ/mm^{-1}	1.51
F(000)	2320
Radiation	Mo K α (λ =0.71073 Å)
2 θ range for data collection/°	2.4-22.09°
Index ranges	-14 $\leq$ h $\leq$ 17, -14 $\leq$ k $\leq$ 17, -15 $\leq$ l $\leq$ 20
Reflections collected	18263
Independent reflections	7747
Data/restraints/parameters	7747/1/703
Goodness-of-fit on F ²	0.96
Final R indexes [$I \geq 2\sigma(I)$]	R ₁ =0.052, wR ₂ = 0.0898
Final R indexes [all data]	R ₁ =0.0518, wR ₂ =0.1067
Largest diff. peak/hole/e Å ⁻³	0.4 and -0.64
Computing publication material:	Olex2 (Dolomanov et al., 2009)

Atomic coordinates (x 104) and equivalent isotropic displacement parameters (Å² x 103) for AV-567. U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
Se1	0.32674 (4)	0.60881 (6)	0.51946 (6)	0.0295 (2)
Se2	0.55180 (4)	0.13265 (7)	0.47217 (6)	0.0303 (2)
N1	0.3600 (3)	0.4821 (5)	0.5546 (5)	0.029 (2)
O4	0.5896 (3)	-0.0923 (5)	0.6115 (4)	0.0361 (17)
O3	0.4508 (3)	0.3317 (5)	0.3548 (4)	0.0414 (18)
O2	0.2998 (3)	0.8277 (5)	0.3676 (4)	0.0438 (18)

O1	0.4263 (3)	0.4172 (5)	0.6482 (4)	0.047 (2)
N4	0.5772 (3)	−0.0008 (6)	0.5003 (5)	0.033 (2)
N2	0.3025 (3)	0.7408 (5)	0.4831 (5)	0.034 (2)
N3	0.5171 (3)	0.2621 (5)	0.4463 (5)	0.031 (2)
C40	0.4480 (4)	0.1663 (7)	0.3745 (6)	0.030 (3)
C58	0.5672 (4)	−0.0244 (7)	0.5763 (6)	0.027 (2)
C59	0.6209 (4)	−0.0450 (7)	0.4483 (6)	0.038 (3)
C25	0.2591 (4)	0.7930 (6)	0.5293 (7)	0.031 (2)
C12	0.2267 (5)	0.3134 (7)	0.5884 (6)	0.038 (3)
C32	0.3381 (4)	1.0252 (8)	0.5506 (6)	0.041 (3)
H32	0.3735	1.0569	0.5316	0.049*
C18	0.3734 (4)	0.6098 (7)	0.4215 (6)	0.030 (2)
C56	0.4988 (4)	0.0340 (7)	0.6883 (6)	0.033 (2)
H56	0.5082	−0.0194	0.7175	0.039*
C67	0.5622 (4)	−0.1980 (7)	0.4528 (6)	0.036 (3)
H67	0.5351	−0.1745	0.4914	0.043*
C26	0.2063 (4)	0.7475 (7)	0.5573 (6)	0.037 (3)
H26	0.1970	0.6873	0.5397	0.044*
C44	0.5947 (5)	0.4760 (7)	0.5272 (8)	0.054 (3)
H44	0.5892	0.5175	0.5690	0.064*
C57	0.5246 (4)	0.0450 (6)	0.6143 (6)	0.023 (2)
C42	0.5592 (5)	0.3413 (7)	0.4546 (7)	0.042 (3)
C33	0.3252 (4)	0.9375 (6)	0.5254 (8)	0.034 (2)
H33	0.3522	0.9105	0.4884	0.041*

C50	0.6215 (5)	0.2861 (8)	0.3382 (6)	0.042 (3)
H50	0.5929	0.2376	0.3291	0.050*
C20	0.4467 (5)	0.5524 (8)	0.3286 (6)	0.041 (3)
H20	0.4753	0.5067	0.3123	0.049*
C34	0.2731 (4)	0.8849 (8)	0.5522 (6)	0.038 (3)
C11	0.2343 (5)	0.2559 (7)	0.5234 (8)	0.046 (3)
H11	0.2060	0.2069	0.5147	0.055*
C2	0.4112 (4)	0.7469 (7)	0.5943 (6)	0.037 (3)
H2	0.3883	0.7940	0.5691	0.044*
C8	0.3185 (4)	0.4048 (7)	0.5458 (6)	0.033 (3)
C27	0.1664 (5)	0.7912 (8)	0.6124 (7)	0.047 (3)
H27	0.1320	0.7587	0.6332	0.056*
C43	0.5523 (5)	0.4019 (7)	0.5159 (8)	0.048 (3)
H43	0.5188	0.3940	0.5509	0.058*
C19	0.4152 (4)	0.5396 (7)	0.3991 (6)	0.032 (3)
H19	0.4217	0.4866	0.4300	0.039*
C53	0.4717 (4)	0.1972 (7)	0.6041 (7)	0.034 (3)
H53	0.4631	0.2517	0.5759	0.040*
C41	0.4711 (4)	0.2628 (7)	0.3912 (6)	0.031 (2)
C51	0.6108 (5)	0.3503 (7)	0.4020 (7)	0.038 (3)
C14	0.1668 (5)	0.3572 (8)	0.7041 (7)	0.051 (3)
H14	0.1336	0.3459	0.7390	0.062*
C52	0.5107 (4)	0.1266 (7)	0.5738 (6)	0.029 (2)
C17	0.2690 (5)	0.3897 (7)	0.6011 (6)	0.033 (2)

C60	0.6692 (4)	0.0073 (7)	0.4162 (6)	0.038 (3)
H60	0.6753	0.0688	0.4329	0.046*
C68	0.6106 (4)	−0.1399 (7)	0.4227 (6)	0.033 (3)
C5	0.4793 (4)	0.6054 (8)	0.6696 (6)	0.041 (3)
H5	0.5017	0.5583	0.6953	0.049*
C28	0.1778 (5)	0.8805 (8)	0.6353 (6)	0.041 (3)
H28	0.1499	0.9101	0.6698	0.049*
C7	0.4051 (5)	0.4851 (7)	0.6116 (6)	0.036 (3)
C1	0.3941 (4)	0.6529 (7)	0.5861 (6)	0.032 (3)
C49	0.6728 (5)	0.2961 (8)	0.2914 (7)	0.048 (3)
H49	0.6795	0.2538	0.2505	0.057*
C4	0.4973 (5)	0.6974 (8)	0.6781 (6)	0.043 (3)
H4	0.5324	0.7123	0.7089	0.052*
C24	0.3187 (5)	0.7606 (7)	0.4065 (6)	0.034 (3)
C29	0.2315 (4)	0.9288 (7)	0.6075 (6)	0.033 (3)
C36	0.4643 (4)	0.0016 (7)	0.3950 (6)	0.035 (3)
H36	0.4875	−0.0475	0.4167	0.041*
C15	0.2075 (5)	0.4326 (8)	0.7160 (7)	0.055 (3)
H15	0.1999	0.4737	0.7576	0.066*
C63	0.6520 (5)	−0.1769 (7)	0.3650 (6)	0.036 (3)
C64	0.6435 (5)	−0.2695 (8)	0.3383 (7)	0.048 (3)
H64	0.6702	−0.2937	0.2997	0.058*
C35	0.4820 (4)	0.0930 (7)	0.4074 (6)	0.030 (2)
C31	0.2979 (5)	1.0684 (8)	0.6056 (7)	0.051 (3)

H31	0.3073	1.1278	0.6250	0.061*
C16	0.2587 (5)	0.4472 (7)	0.6674 (6)	0.044 (3)
H16	0.2868	0.4957	0.6784	0.053*
C55	0.4589 (5)	0.1018 (8)	0.7199 (6)	0.041 (3)
H55	0.4406	0.0930	0.7692	0.050*
C21	0.4380 (5)	0.6287 (8)	0.2817 (7)	0.049 (3)
H21	0.4601	0.6347	0.2345	0.059*
C39	0.3962 (4)	0.1479 (8)	0.3276 (6)	0.038 (3)
H39	0.3737	0.1968	0.3045	0.045*
C37	0.4108 (4)	−0.0160 (8)	0.3490 (6)	0.038 (3)
H37	0.3972	−0.0774	0.3413	0.046*
C6	0.4272 (4)	0.5827 (7)	0.6223 (6)	0.032 (3)
C61	0.7090 (5)	−0.0305 (8)	0.3595 (7)	0.045 (3)
H61	0.7416	0.0061	0.3392	0.054*
C30	0.2448 (5)	1.0218 (7)	0.6305 (7)	0.046 (3)
H30	0.2164	1.0525	0.6636	0.055*
C13	0.1762 (5)	0.3000 (8)	0.6405 (8)	0.049 (3)
H13	0.1482	0.2507	0.6317	0.059*
C22	0.3954 (5)	0.6976 (7)	0.3057 (6)	0.041 (3)
H22	0.3889	0.7503	0.2744	0.050*
C66	0.5542 (5)	−0.2862 (7)	0.4272 (7)	0.047 (3)
H66	0.5214	−0.3229	0.4472	0.056*
C23	0.3629 (5)	0.6879 (7)	0.3755 (6)	0.035 (3)
C3	0.4634 (5)	0.7680 (8)	0.6411 (7)	0.045 (3)

H3	0.4757	0.8301	0.6476	0.054*
C46	0.6544 (5)	0.4243 (8)	0.4127 (7)	0.045 (3)
C38	0.3781 (4)	0.0565 (8)	0.3151 (6)	0.040 (3)
H38	0.3432	0.0438	0.2833	0.048*
C65	0.5964 (5)	−0.3238 (8)	0.3689 (7)	0.048 (3)
H65	0.5916	−0.3854	0.3519	0.057*
C62	0.7018 (5)	−0.1188 (8)	0.3330 (6)	0.042 (3)
H62	0.7287	−0.1422	0.2943	0.050*
C54	0.4470 (5)	0.1816 (8)	0.6778 (6)	0.043 (3)
H54	0.4209	0.2271	0.7001	0.052*
C45	0.6449 (5)	0.4869 (8)	0.4757 (9)	0.062 (3)
H45	0.6730	0.5364	0.4829	0.074*
C48	0.7160 (5)	0.3682 (10)	0.3032 (8)	0.056 (3)
H48	0.7517	0.3729	0.2712	0.067*
C47	0.7062 (5)	0.4319 (9)	0.3614 (8)	0.056 (4)
H47	0.7344	0.4815	0.3672	0.067*
C9	0.3246 (4)	0.3462 (8)	0.4816 (7)	0.044 (3)
H9	0.3564	0.3565	0.4445	0.052*
C10	0.2825 (5)	0.2707 (7)	0.4727 (8)	0.051 (3)
H10	0.2880	0.2297	0.4305	0.061*

Bond length (Å) and Bond Angle

Se1—N1	2.028 (7)	C43—H43	0.9300
Se1—N2	2.046 (8)	C19—H19	0.9300

Se1—C18	1.930 (10)	C53—H53	0.9300
Se1—C1	1.921 (9)	C53—C52	1.396 (12)
Se2—N4	2.034 (8)	C53—C54	1.372 (14)
Se2—N3	2.034 (8)	C51—C46	1.411 (13)
Se2—C52	1.931 (9)	C14—H14	0.9300
Se2—C35	1.921 (9)	C14—C15	1.389 (14)
N1—C8	1.414 (11)	C14—C13	1.366 (15)
N1—C7	1.356 (12)	C17—C16	1.408 (13)
O4—C58	1.231 (10)	C60—H60	0.9300
O3—C41	1.237 (11)	C60—C61	1.384 (13)
O2—C24	1.229 (11)	C68—C63	1.413 (13)
O1—C7	1.234 (11)	C5—H5	0.9300
N4—C58	1.348 (12)	C5—C4	1.374 (14)
N4—C59	1.423 (11)	C5—C6	1.396 (13)
N2—C25	1.416 (12)	C28—H28	0.9300
N2—C24	1.372 (12)	C28—C29	1.407 (13)
N3—C42	1.443 (12)	C7—C6	1.479 (13)
N3—C41	1.346 (11)	C1—C6	1.366 (13)
C40—C41	1.487 (13)	C49—H49	0.9300
C40—C35	1.384 (12)	C49—C48	1.388 (15)
C40—C39	1.376 (13)	C4—H4	0.9300
C58—C57	1.483 (12)	C4—C3	1.385 (14)
C59—C60	1.374 (12)	C24—C23	1.490 (13)
C59—C68	1.438 (13)	C29—C30	1.409 (13)

C25—C26	1.373 (12)	C36—H36	0.9300
C25—C34	1.398 (13)	C36—C35	1.373 (12)
C12—C11	1.383 (15)	C36—C37	1.393 (13)
C12—C17	1.424 (13)	C15—H15	0.9300
C12—C13	1.396 (14)	C15—C16	1.373 (13)
C32—H32	0.9300	C63—C64	1.406 (14)
C32—C33	1.349 (12)	C63—C62	1.443 (14)
C32—C31	1.401 (14)	C64—H64	0.9300
C18—C19	1.386 (12)	C64—C65	1.361 (14)
C18—C23	1.378 (13)	C31—H31	0.9300
C56—H56	0.9300	C31—C30	1.369 (14)
C56—C57	1.375 (13)	C16—H16	0.9300
C56—C55	1.389 (13)	C55—H55	0.9300
C67—H67	0.9300	C55—C54	1.365 (14)
C67—C68	1.410 (12)	C21—H21	0.9300
C67—C66	1.342 (13)	C21—C22	1.391 (14)
C26—H26	0.9300	C39—H39	0.9300
C26—C27	1.404 (14)	C39—C38	1.375 (14)
C44—H44	0.9300	C37—H37	0.9300
C44—C43	1.397 (13)	C37—C38	1.369 (13)
C44—C45	1.381 (16)	C61—H61	0.9300
C57—C52	1.383 (12)	C61—C62	1.346 (14)
C42—C43	1.359 (14)	C30—H30	0.9300
C42—C51	1.413 (14)	C13—H13	0.9300

C33—H33	0.9300	C22—H22	0.9300
C33—C34	1.406 (12)	C22—C23	1.374 (14)
C50—H50	0.9300	C66—H66	0.9300
C50—C51	1.434 (14)	C66—C65	1.434 (14)
C50—C49	1.350 (13)	C3—H3	0.9300
C20—H20	0.9300	C46—C45	1.407 (16)
C20—C19	1.379 (13)	C46—C47	1.399 (15)
C20—C21	1.359 (15)	C38—H38	0.9300
C34—C29	1.428 (13)	C65—H65	0.9300
C11—H11	0.9300	C62—H62	0.9300
C11—C10	1.348 (14)	C54—H54	0.9300
C2—H2	0.9300	C45—H45	0.9300
C2—C1	1.395 (13)	C48—H48	0.9300
C2—C3	1.390 (13)	C48—C47	1.356 (17)
C8—C17	1.419 (12)	C47—H47	0.9300
C8—C9	1.379 (13)	C9—H9	0.9300
C27—H27	0.9300	C9—C10	1.404 (13)
C27—C28	1.352 (14)	C10—H10	0.9300
N1—Se1—N2	174.2 (3)	C67—C68—C59	123.6 (9)
C18—Se1—N1	94.7 (4)	C67—C68—C63	118.6 (10)
C18—Se1—N2	82.1 (4)	C63—C68—C59	117.8 (9)
C1—Se1—N1	82.2 (4)	C4—C5—H5	120.0
C1—Se1—N2	93.5 (4)	C4—C5—C6	120.0 (10)
C1—Se1—C18	97.3 (4)	C6—C5—H5	120.0

N3—Se2—N4	174.1 (3)	C27—C28—H28	119.7
C52—Se2—N4	82.4 (4)	C27—C28—C29	120.6 (10)
C52—Se2—N3	94.1 (4)	C29—C28—H28	119.7
C35—Se2—N4	93.4 (4)	N1—C7—C6	109.8 (9)
C35—Se2—N3	82.4 (4)	O1—C7—N1	126.0 (10)
C35—Se2—C52	98.8 (4)	O1—C7—C6	124.2 (10)
C8—N1—Se1	116.8 (6)	C2—C1—Se1	124.3 (7)
C7—N1—Se1	115.0 (6)	C6—C1—Se1	113.7 (8)
C7—N1—C8	122.2 (8)	C6—C1—C2	121.9 (9)
C58—N4—Se2	114.6 (6)	C50—C49—H49	119.4
C58—N4—C59	125.6 (8)	C50—C49—C48	121.3 (12)
C59—N4—Se2	116.1 (6)	C48—C49—H49	119.4
C25—N2—Se1	118.6 (7)	C5—C4—H4	119.9
C24—N2—Se1	114.3 (6)	C5—C4—C3	120.3 (10)
C24—N2—C25	125.2 (8)	C3—C4—H4	119.9
C42—N3—Se2	117.9 (6)	O2—C24—N2	126.0 (9)
C41—N3—Se2	114.6 (6)	O2—C24—C23	123.7 (10)
C41—N3—C42	120.3 (8)	N2—C24—C23	110.2 (9)
C35—C40—C41	117.0 (9)	C28—C29—C34	119.9 (10)
C39—C40—C41	123.1 (9)	C28—C29—C30	121.9 (10)
C39—C40—C35	119.9 (10)	C30—C29—C34	118.2 (9)
O4—C58—N4	126.8 (9)	C35—C36—H36	120.8
O4—C58—C57	123.1 (9)	C35—C36—C37	118.5 (10)
N4—C58—C57	110.1 (9)	C37—C36—H36	120.8

N4—C59—C68	120.4 (9)	C14—C15—H15	119.5
C60—C59—N4	119.0 (9)	C16—C15—C14	121.0 (11)
C60—C59—C68	120.3 (10)	C16—C15—H15	119.5
C26—C25—N2	117.8 (8)	C68—C63—C62	119.6 (9)
C26—C25—C34	121.2 (10)	C64—C63—C68	119.6 (10)
C34—C25—N2	120.7 (8)	C64—C63—C62	120.8 (10)
C11—C12—C17	120.1 (10)	C63—C64—H64	119.8
C11—C12—C13	120.7 (10)	C65—C64—C63	120.3 (11)
C13—C12—C17	119.1 (10)	C65—C64—H64	119.8
C33—C32—H32	120.1	C40—C35—Se2	113.8 (7)
C33—C32—C31	119.8 (10)	C36—C35—Se2	125.1 (8)
C31—C32—H32	120.1	C36—C35—C40	121.1 (9)
C19—C18—Se1	123.7 (8)	C32—C31—H31	120.5
C23—C18—Se1	114.2 (7)	C30—C31—C32	119.0 (10)
C23—C18—C19	122.1 (10)	C30—C31—H31	120.5
C57—C56—H56	119.6	C17—C16—H16	119.6
C57—C56—C55	120.8 (9)	C15—C16—C17	120.7 (10)
C55—C56—H56	119.6	C15—C16—H16	119.6
C68—C67—H67	119.2	C56—C55—H55	120.3
C66—C67—H67	119.2	C54—C55—C56	119.4 (10)
C66—C67—C68	121.6 (10)	C54—C55—H55	120.3
C25—C26—H26	119.8	C20—C21—H21	120.6
C25—C26—C27	120.4 (10)	C20—C21—C22	118.8 (11)
C27—C26—H26	119.8	C22—C21—H21	120.6

C43—C44—H44	120.4	C40—C39—H39	120.3
C45—C44—H44	120.4	C38—C39—C40	119.3 (10)
C45—C44—C43	119.2 (12)	C38—C39—H39	120.3
C56—C57—C58	124.0 (9)	C36—C37—H37	119.8
C56—C57—C52	117.6 (9)	C38—C37—C36	120.4 (10)
C52—C57—C58	118.4 (9)	C38—C37—H37	119.8
C43—C42—N3	120.5 (9)	C5—C6—C7	122.5 (10)
C43—C42—C51	120.4 (10)	C1—C6—C5	119.2 (10)
C51—C42—N3	118.9 (10)	C1—C6—C7	118.3 (9)
C32—C33—H33	118.3	C60—C61—H61	119.0
C32—C33—C34	123.3 (10)	C62—C61—C60	121.9 (11)
C34—C33—H33	118.3	C62—C61—H61	119.0
C51—C50—H50	120.0	C29—C30—H30	118.9
C49—C50—H50	120.0	C31—C30—C29	122.3 (10)
C49—C50—C51	120.0 (11)	C31—C30—H30	118.9
C19—C20—H20	118.4	C12—C13—H13	119.1
C21—C20—H20	118.4	C14—C13—C12	121.8 (11)
C21—C20—C19	123.2 (10)	C14—C13—H13	119.1
C25—C34—C33	125.1 (9)	C21—C22—H22	119.9
C25—C34—C29	117.7 (9)	C23—C22—C21	120.1 (11)
C33—C34—C29	117.2 (10)	C23—C22—H22	119.9
C12—C11—H11	119.9	C67—C66—H66	120.1
C10—C11—C12	120.2 (10)	C67—C66—C65	119.7 (10)
C10—C11—H11	119.9	C65—C66—H66	120.1

C1—C2—H2	121.0	C18—C23—C24	117.7 (10)
C3—C2—H2	121.0	C22—C23—C18	119.2 (10)
C3—C2—C1	118.0 (10)	C22—C23—C24	123.0 (10)
N1—C8—C17	120.2 (9)	C2—C3—H3	119.7
C9—C8—N1	119.9 (9)	C4—C3—C2	120.6 (10)
C9—C8—C17	119.9 (9)	C4—C3—H3	119.7
C26—C27—H27	119.9	C45—C46—C51	118.6 (11)
C28—C27—C26	120.2 (10)	C47—C46—C51	119.0 (12)
C28—C27—H27	119.9	C47—C46—C45	122.3 (11)
C44—C43—H43	119.4	C39—C38—H38	119.6
C42—C43—C44	121.2 (11)	C37—C38—C39	120.8 (10)
C42—C43—H43	119.4	C37—C38—H38	119.6
C18—C19—H19	121.7	C64—C65—C66	120.1 (11)
C20—C19—C18	116.6 (10)	C64—C65—H65	119.9
C20—C19—H19	121.7	C66—C65—H65	119.9
C52—C53—H53	121.9	C63—C62—H62	120.2
C54—C53—H53	121.9	C61—C62—C63	119.6 (10)
C54—C53—C52	116.2 (10)	C61—C62—H62	120.2
O3—C41—N3	127.0 (9)	C53—C54—H54	118.7
O3—C41—C40	121.8 (9)	C55—C54—C53	122.7 (10)
N3—C41—C40	111.1 (9)	C55—C54—H54	118.7
C42—C51—C50	122.5 (10)	C44—C45—C46	121.2 (11)
C46—C51—C42	119.3 (11)	C44—C45—H45	119.4
C46—C51—C50	118.2 (10)	C46—C45—H45	119.4

C15—C14—H14	120.4	C49—C48—H48	119.9
C13—C14—H14	120.4	C47—C48—C49	120.1 (11)
C13—C14—C15	119.2 (10)	C47—C48—H48	119.9
C57—C52—Se2	112.6 (7)	C46—C47—H47	119.4
C57—C52—C53	123.3 (9)	C48—C47—C46	121.3 (12)
C53—C52—Se2	124.1 (8)	C48—C47—H47	119.4
C8—C17—C12	118.5 (9)	C8—C9—H9	120.3
C16—C17—C12	118.0 (9)	C8—C9—C10	119.5 (10)
C16—C17—C8	123.5 (9)	C10—C9—H9	120.3
C59—C60—H60	119.6	C11—C10—C9	121.9 (11)
C59—C60—C61	120.7 (10)	C11—C10—H10	119.1
C61—C60—H60	119.6	C9—C10—H10	119.1
Se1—N1—C8—C17	−78.7 (10)	C11—C12—C17—C8	0.0 (15)
Se1—N1—C8—C9	98.7 (9)	C11—C12—C17—C16	178.9 (10)
Se1—N1—C7—O1	170.8 (9)	C11—C12—C13—C14	−178.4 (11)
Se1—N1—C7—C6	−11.1 (10)	C2—C1—C6—C5	0.8 (15)
Se1—N2—C25—C26	−43.8 (11)	C2—C1—C6—C7	178.9 (9)
Se1—N2—C25—C34	129.8 (8)	C8—N1—C7—O1	19.0 (15)
Se1—N2—C24—O2	166.7 (8)	C8—N1—C7—C6	−162.8 (8)
Se1—N2—C24—C23	−13.0 (10)	C8—C17—C16—C15	175.8 (10)
Se1—C18—C19—C20	−177.6 (7)	C8—C9—C10—C11	2.8 (17)
Se1—C18—C23—C24	0.6 (12)	C27—C28—C29—C34	2.5 (15)
Se1—C18—C23—C22	177.7 (7)	C27—C28—C29—C30	−179.8 (11)
Se1—C1—C6—C5	177.2 (8)	C43—C44—C45—C46	−0.6 (18)

Se1—C1—C6—C7	−4.8 (12)	C43—C42—C51—C50	177.7 (10)
Se2—N4—C58—O4	−164.3 (8)	C43—C42—C51—C46	−1.4 (15)
Se2—N4—C58—C57	15.1 (9)	C19—C18—C23—C24	−178.0 (9)
Se2—N4—C59—C60	38.0 (11)	C19—C18—C23—C22	−0.9 (15)
Se2—N4—C59—C68	−135.0 (8)	C19—C20—C21—C22	0.2 (17)
Se2—N3—C42—C43	−106.3 (9)	C41—N3—C42—C43	105.0 (11)
Se2—N3—C42—C51	68.4 (11)	C41—N3—C42—C51	−80.2 (12)
Se2—N3—C41—O3	−165.5 (8)	C41—C40—C35—Se2	2.0 (11)
Se2—N3—C41—C40	11.5 (9)	C41—C40—C35—C36	−179.8 (9)
N1—C8—C17—C12	177.5 (8)	C41—C40—C39—C38	179.9 (9)
N1—C8—C17—C16	−1.4 (15)	C51—C42—C43—C44	1.8 (16)
N1—C8—C9—C10	−178.8 (9)	C51—C50—C49—C48	−0.5 (15)
N1—C7—C6—C5	−171.4 (9)	C51—C46—C45—C44	0.9 (17)
N1—C7—C6—C1	10.6 (13)	C51—C46—C47—C48	−1.8 (17)
O4—C58—C57—C56	−9.4 (14)	C14—C15—C16—C17	4.1 (18)
O4—C58—C57—C52	169.3 (9)	C52—C53—C54—C55	−0.3 (16)
O2—C24—C23—C18	−171.2 (10)	C17—C12—C11—C10	1.4 (17)
O2—C24—C23—C22	11.8 (16)	C17—C12—C13—C14	−1.0 (17)
O1—C7—C6—C5	6.7 (16)	C17—C8—C9—C10	−1.4 (15)
O1—C7—C6—C1	−171.3 (10)	C60—C59—C68—C67	179.9 (9)
N4—C58—C57—C56	171.1 (8)	C60—C59—C68—C63	0.8 (14)
N4—C58—C57—C52	−10.2 (11)	C60—C61—C62—C63	−1.0 (17)
N4—C59—C60—C61	−173.6 (9)	C68—C59—C60—C61	−0.6 (15)
N4—C59—C68—C67	−7.2 (14)	C68—C67—C66—C65	1.3 (16)

N4—C59—C68—C63	173.7 (8)	C68—C63—C64—C65	−1.2 (15)
N2—C25—C26—C27	170.9 (9)	C68—C63—C62—C61	1.2 (15)
N2—C25—C34—C33	7.9 (15)	C5—C4—C3—C2	−0.6 (16)
N2—C25—C34—C29	−171.5 (9)	C28—C29—C30—C31	177.9 (10)
N2—C24—C23—C18	8.4 (13)	C7—N1—C8—C17	72.6 (12)
N2—C24—C23—C22	−168.6 (9)	C7—N1—C8—C9	−110.0 (11)
N3—C42—C43—C44	176.5 (10)	C1—C2—C3—C4	0.2 (15)
N3—C42—C51—C50	2.9 (15)	C49—C50—C51—C42	−177.6 (10)
N3—C42—C51—C46	−176.2 (9)	C49—C50—C51—C46	1.5 (15)
C40—C39—C38—C37	0.3 (15)	C49—C48—C47—C46	2.8 (18)
C58—N4—C59—C60	−119.1 (11)	C4—C5—C6—C7	−179.2 (10)
C58—N4—C59—C68	67.8 (12)	C4—C5—C6—C1	−1.2 (16)
C58—C57—C52—Se2	−0.1 (10)	C24—N2—C25—C26	119.6 (10)
C58—C57—C52—C53	−179.3 (8)	C24—N2—C25—C34	−66.8 (13)
C59—N4—C58—O4	−6.9 (15)	C36—C37—C38—C39	−1.9 (15)
C59—N4—C58—C57	172.6 (8)	C15—C14—C13—C12	1.9 (18)
C59—C60—C61—C62	0.7 (17)	C63—C64—C65—C66	1.4 (16)
C59—C68—C63—C64	180.0 (9)	C64—C63—C62—C61	−179.9 (10)
C59—C68—C63—C62	−1.1 (14)	C35—C40—C41—O3	168.1 (9)
C25—N2—C24—O2	2.6 (16)	C35—C40—C41—N3	−9.1 (12)
C25—N2—C24—C23	−177.0 (8)	C35—C40—C39—C38	1.2 (15)
C25—C26—C27—C28	3.4 (16)	C35—C36—C37—C38	2.1 (15)
C25—C34—C29—C28	−1.7 (14)	C31—C32—C33—C34	−0.7 (17)
C25—C34—C29—C30	−179.4 (9)	C55—C56—C57—C58	−179.7 (8)

C12—C11—C10—C9	−2.8 (18)	C55—C56—C57—C52	1.7 (14)
C12—C17—C16—C15	−3.1 (16)	C21—C20—C19—C18	−0.5 (16)
C32—C33—C34—C25	−178.0 (10)	C21—C22—C23—C18	0.5 (15)
C32—C33—C34—C29	1.4 (15)	C21—C22—C23—C24	177.4 (9)
C32—C31—C30—C29	5.2 (17)	C39—C40—C41—O3	−10.7 (15)
C56—C57—C52—Se2	178.7 (6)	C39—C40—C41—N3	172.1 (9)
C56—C57—C52—C53	−0.5 (14)	C39—C40—C35—Se2	−179.1 (7)
C56—C55—C54—C53	1.4 (17)	C39—C40—C35—C36	−1.0 (15)
C67—C68—C63—C64	0.9 (14)	C37—C36—C35—Se2	177.3 (7)
C67—C68—C63—C62	179.8 (9)	C37—C36—C35—C40	−0.7 (14)
C67—C66—C65—C64	−1.5 (16)	C6—C5—C4—C3	1.1 (16)
C26—C25—C34—C33	−178.7 (10)	C13—C12—C11—C10	178.7 (10)
C26—C25—C34—C29	1.8 (14)	C13—C12—C17—C8	−177.4 (9)
C26—C27—C28—C29	−3.3 (16)	C13—C12—C17—C16	1.5 (15)
C57—C56—C55—C54	−2.1 (15)	C13—C14—C15—C16	−3.4 (18)
C42—N3—C41—O3	−15.9 (14)	C66—C67—C68—C59	180.0 (10)
C42—N3—C41—C40	161.1 (9)	C66—C67—C68—C63	−1.0 (15)
C42—C51—C46—C45	0.0 (15)	C23—C18—C19—C20	0.9 (15)
C42—C51—C46—C47	178.7 (10)	C3—C2—C1—Se1	−176.3 (7)
C33—C32—C31—C30	−2.6 (17)	C3—C2—C1—C6	−0.3 (15)
C33—C34—C29—C28	178.8 (9)	C62—C63—C64—C65	179.9 (10)
C33—C34—C29—C30	1.0 (14)	C54—C53—C52—Se2	−179.3 (8)
C50—C51—C46—C45	−179.1 (10)	C54—C53—C52—C57	−0.2 (14)
C50—C51—C46—C47	−0.4 (15)	C45—C44—C43—C42	−0.8 (16)

C50—C49—C48—C47	−1.7 (17)	C45—C46—C47—C48	176.9 (11)
C20—C21—C22—C23	−0.1 (16)	C47—C46—C45—C44	−177.7 (10)
C34—C25—C26—C27	−2.6 (15)	C9—C8—C17—C12	0.1 (14)
C34—C29—C30—C31	−4.4 (16)	C9—C8—C17—C16	−178.8 (10)