Supporting Information

Janus-Faced Oxidant and Antioxidant Profiles of Organo Diselenides

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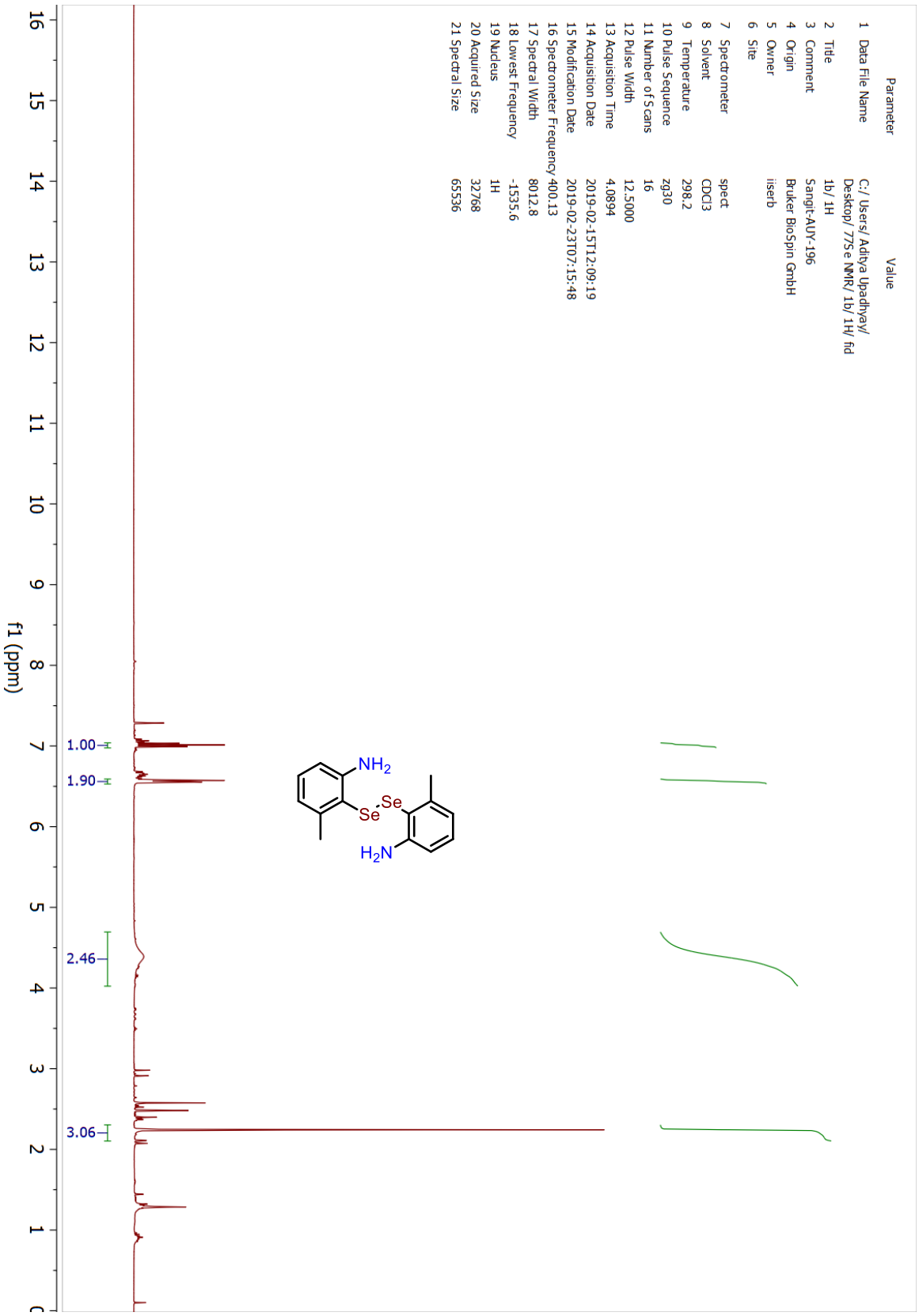
1. General experimental details:

All reactions were carried out in oven-dried glassware with magnetic stirring. NMR experiments were carried out on Bruker 400/500MHz spectrometer in $CDCl_3$/DMSO-*d6* solvents and chemical shifts are reported in ppm. The following abbreviations were used to indicate multiplicity: s (singlet), d (doublet), t (triplet), q (quartet), dd (doublet of doublet), td (triplet of doublet) and m (multiplet). Electron paramagnetic resonance was carried out on Bruker EMX micro-X CW-EPR (34 GHz) series spectrophotometer. High-resolution mass spectroscopic (HRMS) analysis is performed on quadrupole-time-of-flight Bruker MicroTOF-Q II mass spectrometer equipped with an ESI and APCI source; GC-MS analysis is performed on Agilent 7200/Agilent Technologies MS-S975C inert XLEI/CIMSD with triple-axis detector. TLC plates (Merck silica gel (60F254) plates) used for monitoring the reactions were purchased from Merck. Single crystal X-ray data for compound 4 were collected on a Bruker D8 VENTURE diffractometer equipped with CMOS Photon 100 detector and Mo-Kα (λ = 0.71073 Å) radiation was used.

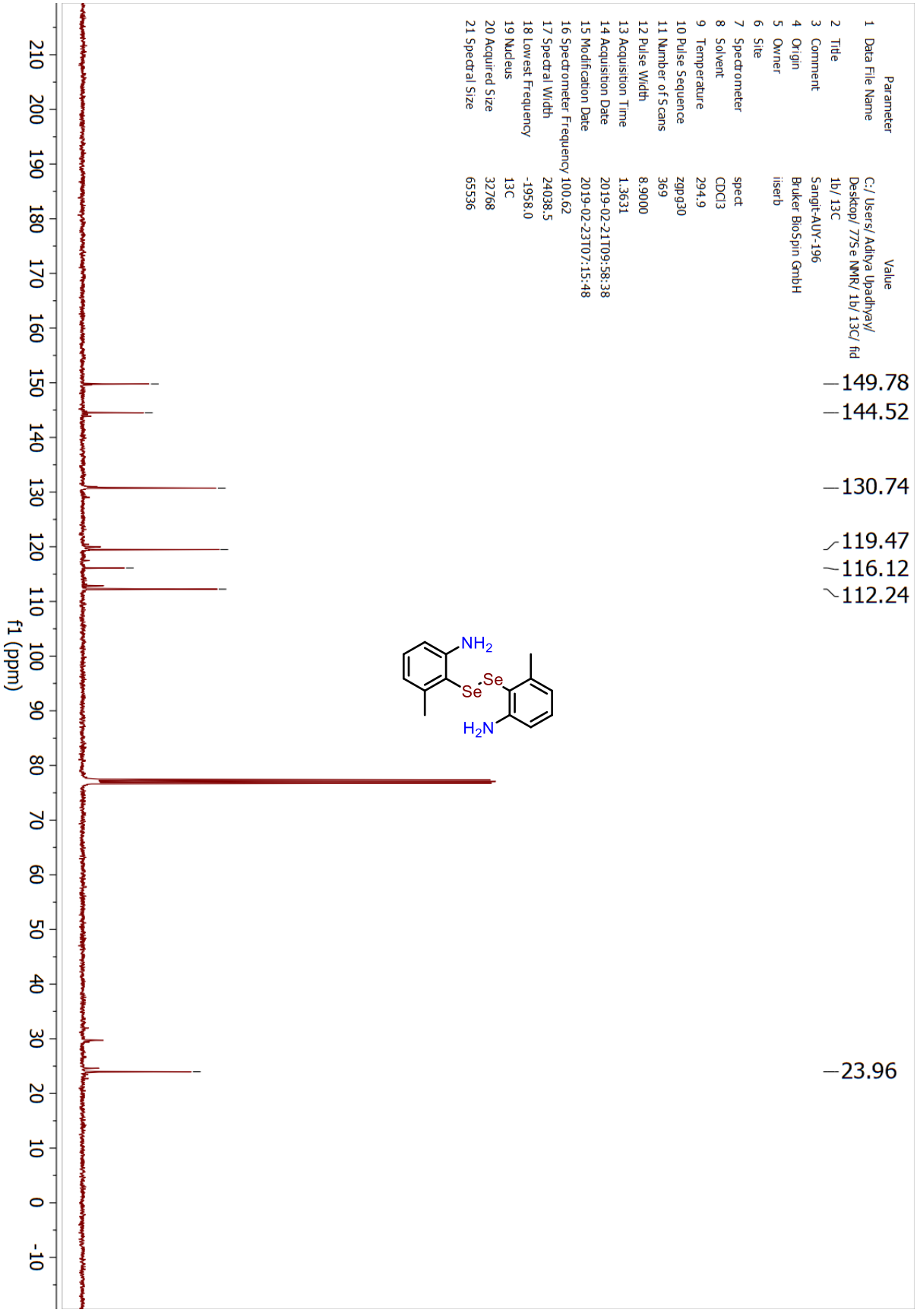
2. NMR spectra

^{1}H NMR of **1b**



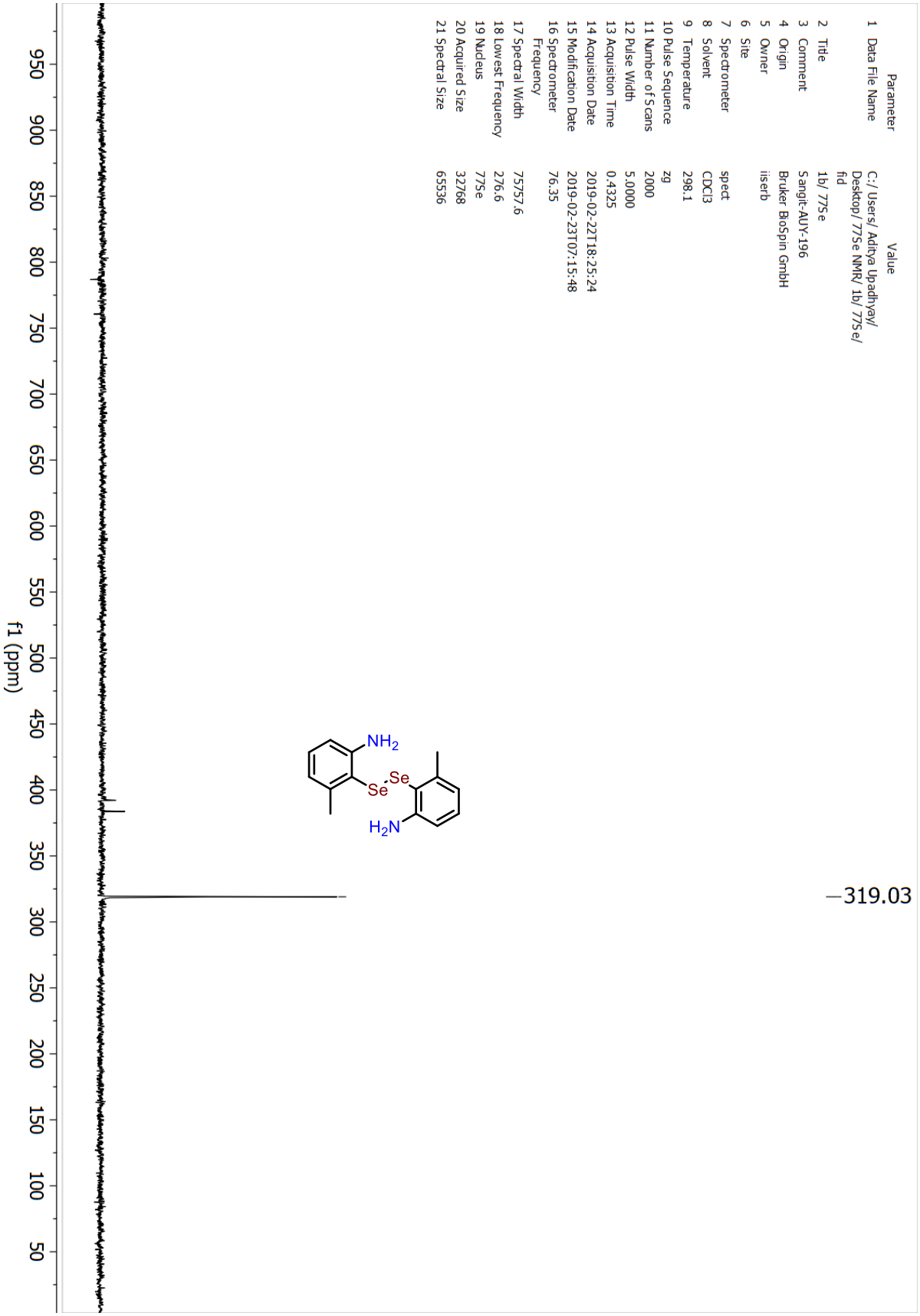
This compound is light and air sensitive

^{13}C NMR of **1b**



This compound is light and air sensitive

^{77}Se NMR of **1b**



This compound is light and air sensitive

HRMS of **1b**

Display Report

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Comment			

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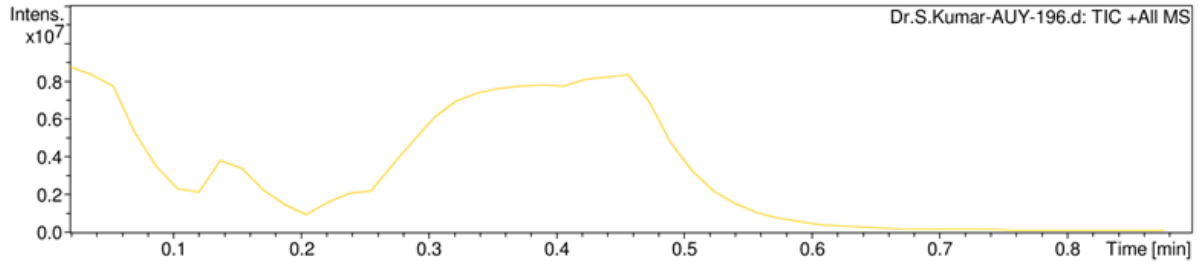

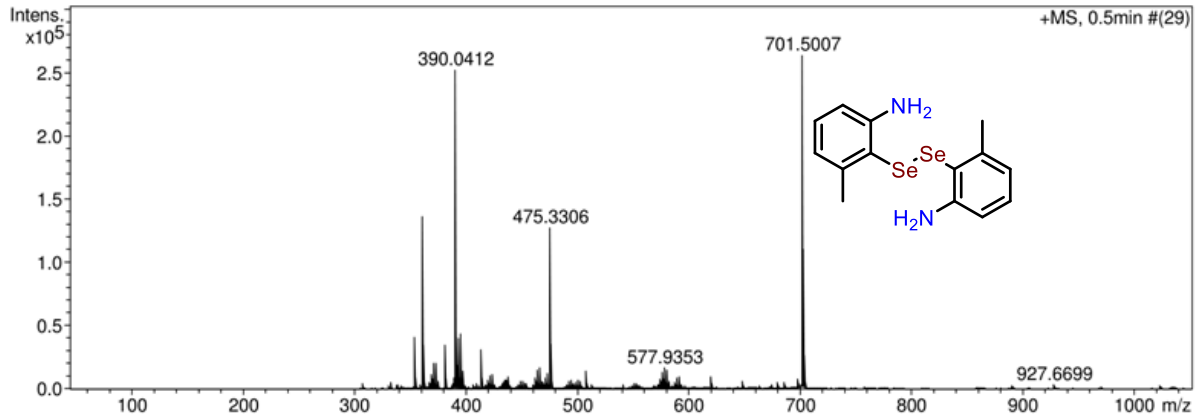

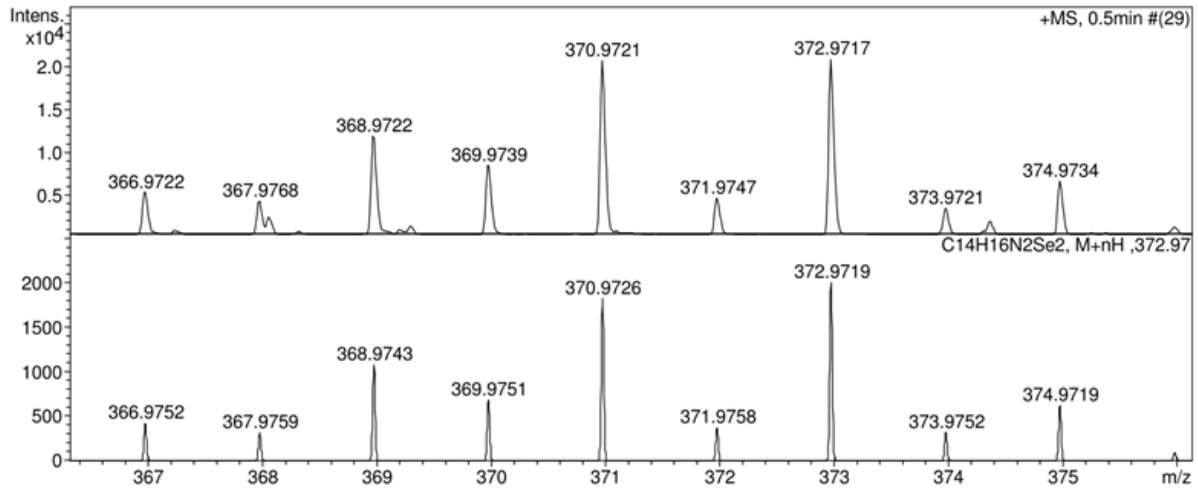

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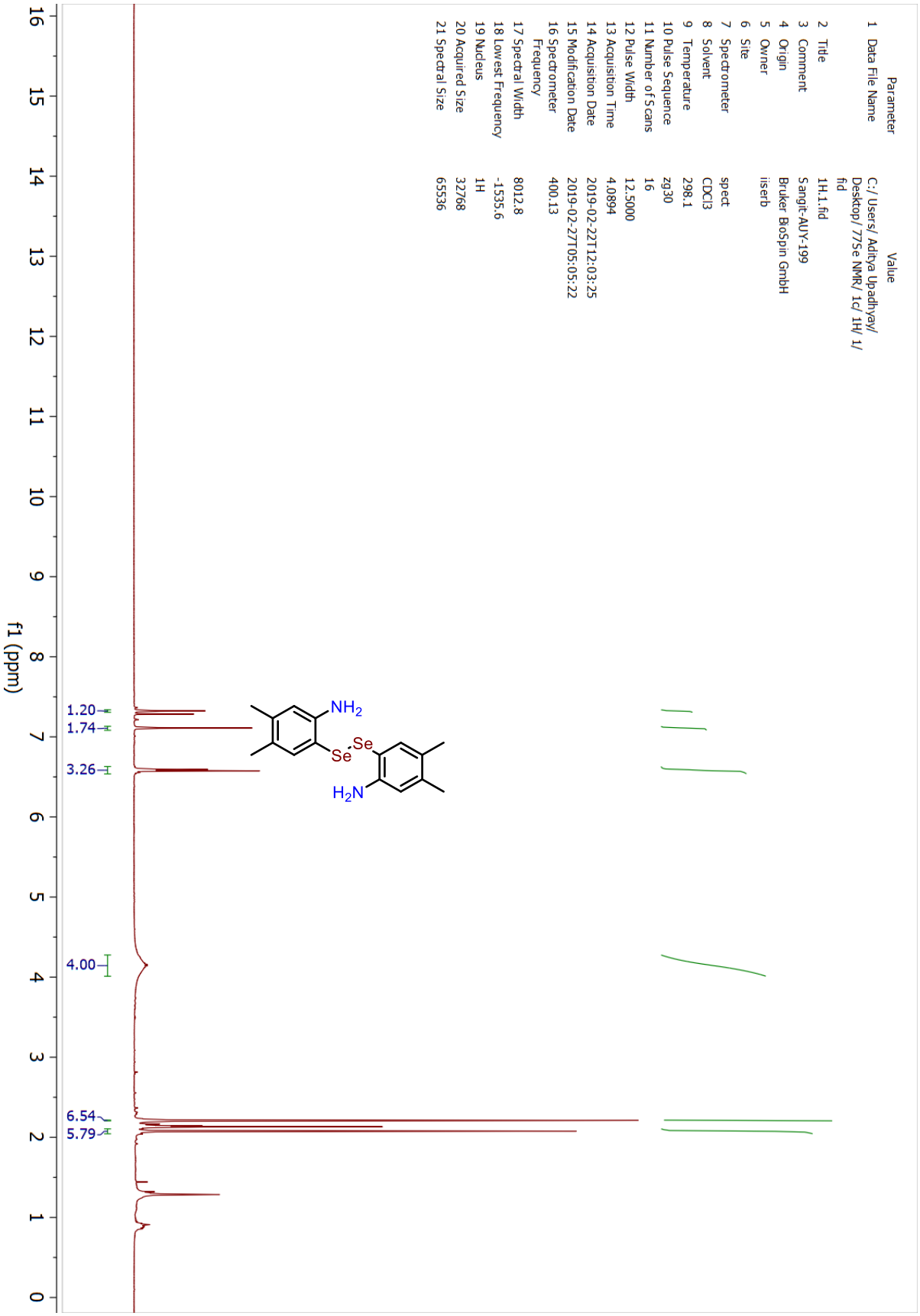

This compound is light and air sensitive

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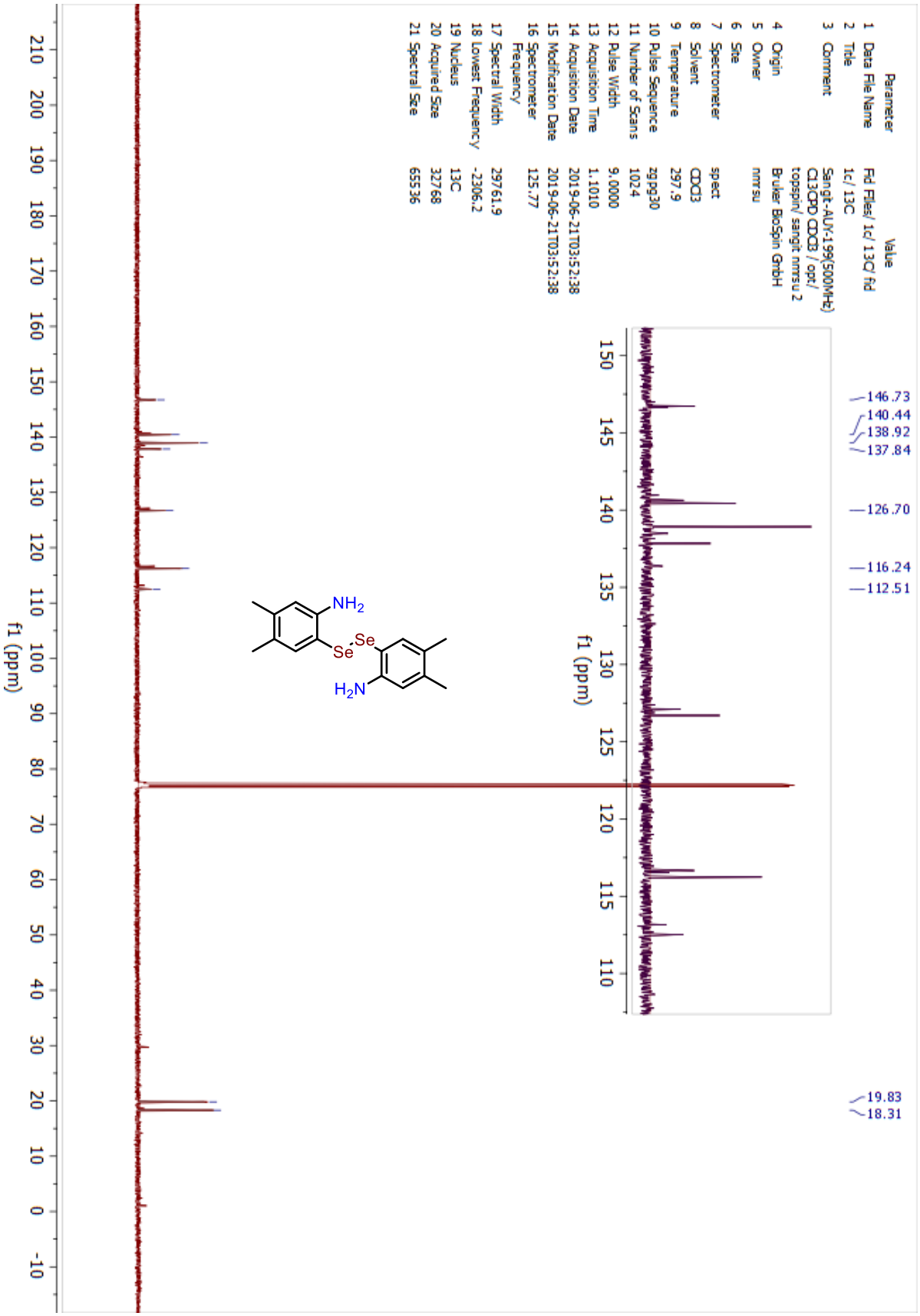

This compound is light and air sensitive

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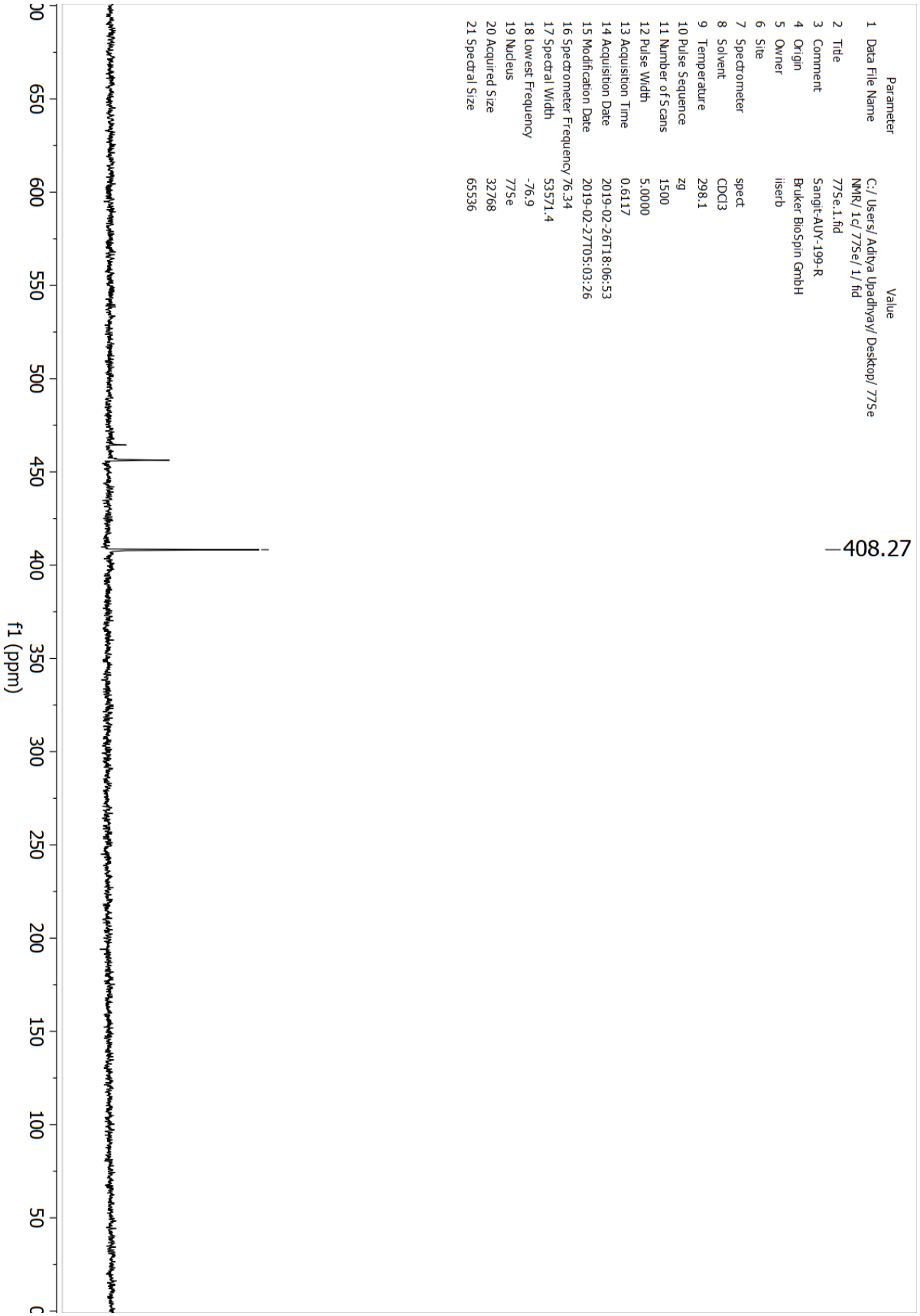

This compound is light and air sensitive

HRMS of **1c**

Display Report

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Sample Name	AUY-199	Instrument	micrOTOF-Q II 10330
Comment			

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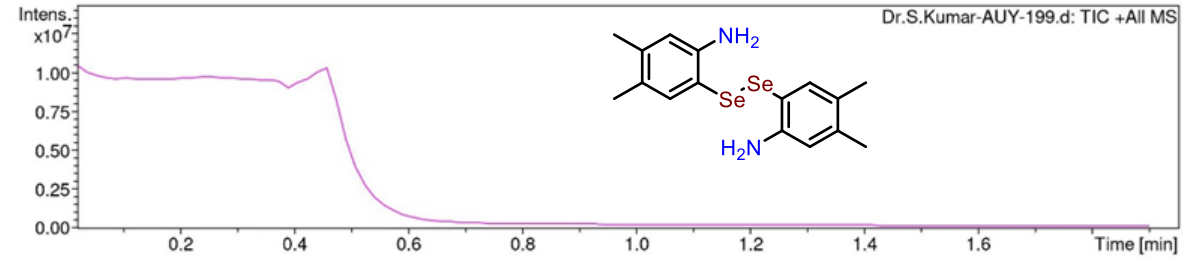

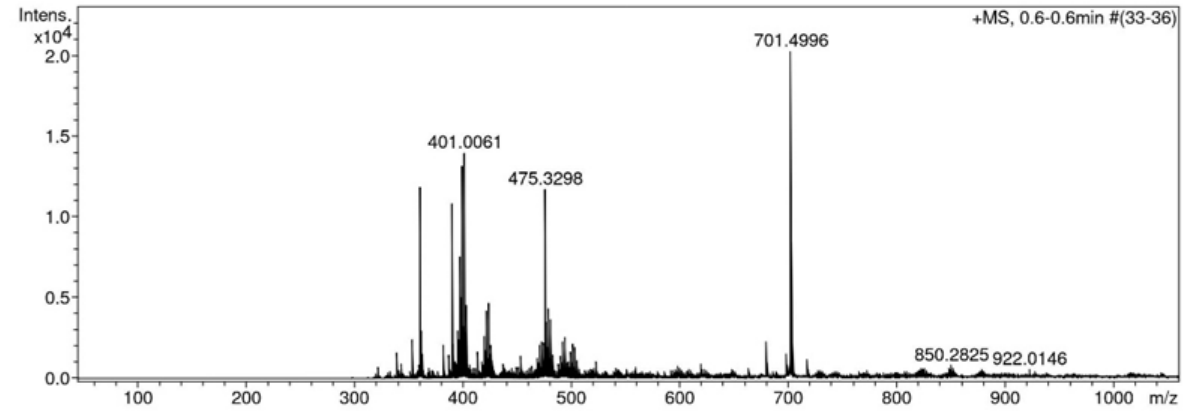

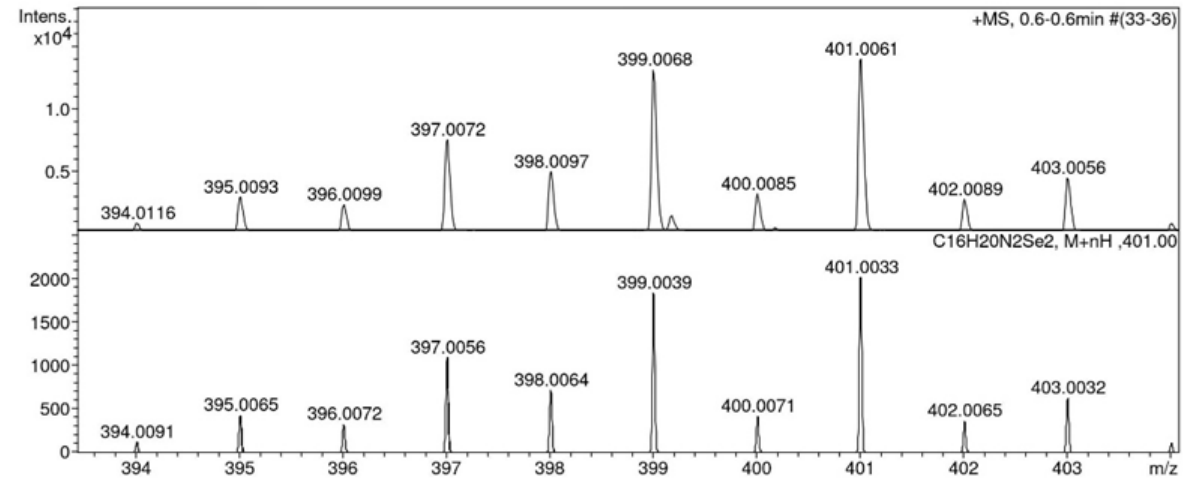

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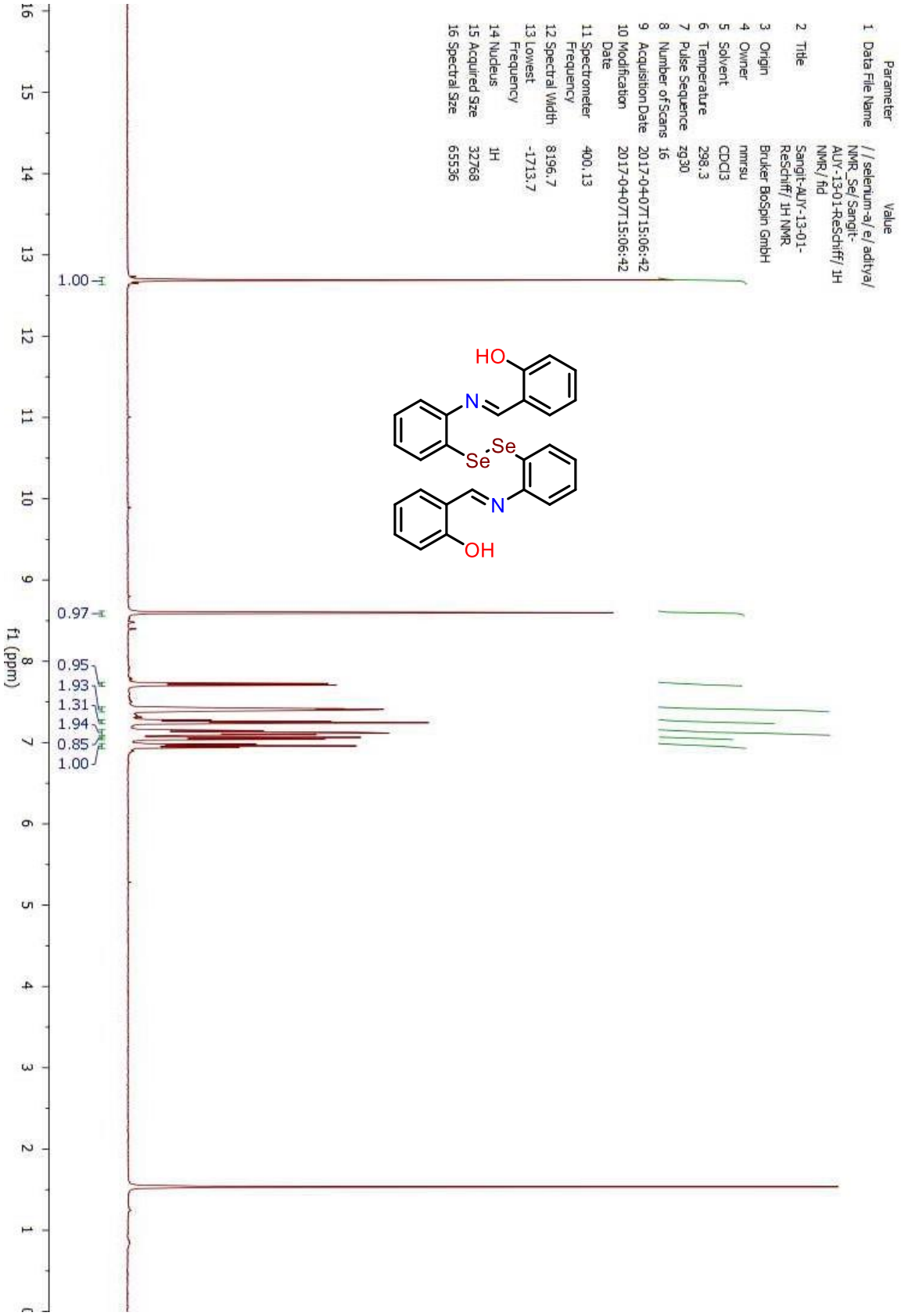
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16 Spectral Size 65536
HO
N
Se
Se
N
OH
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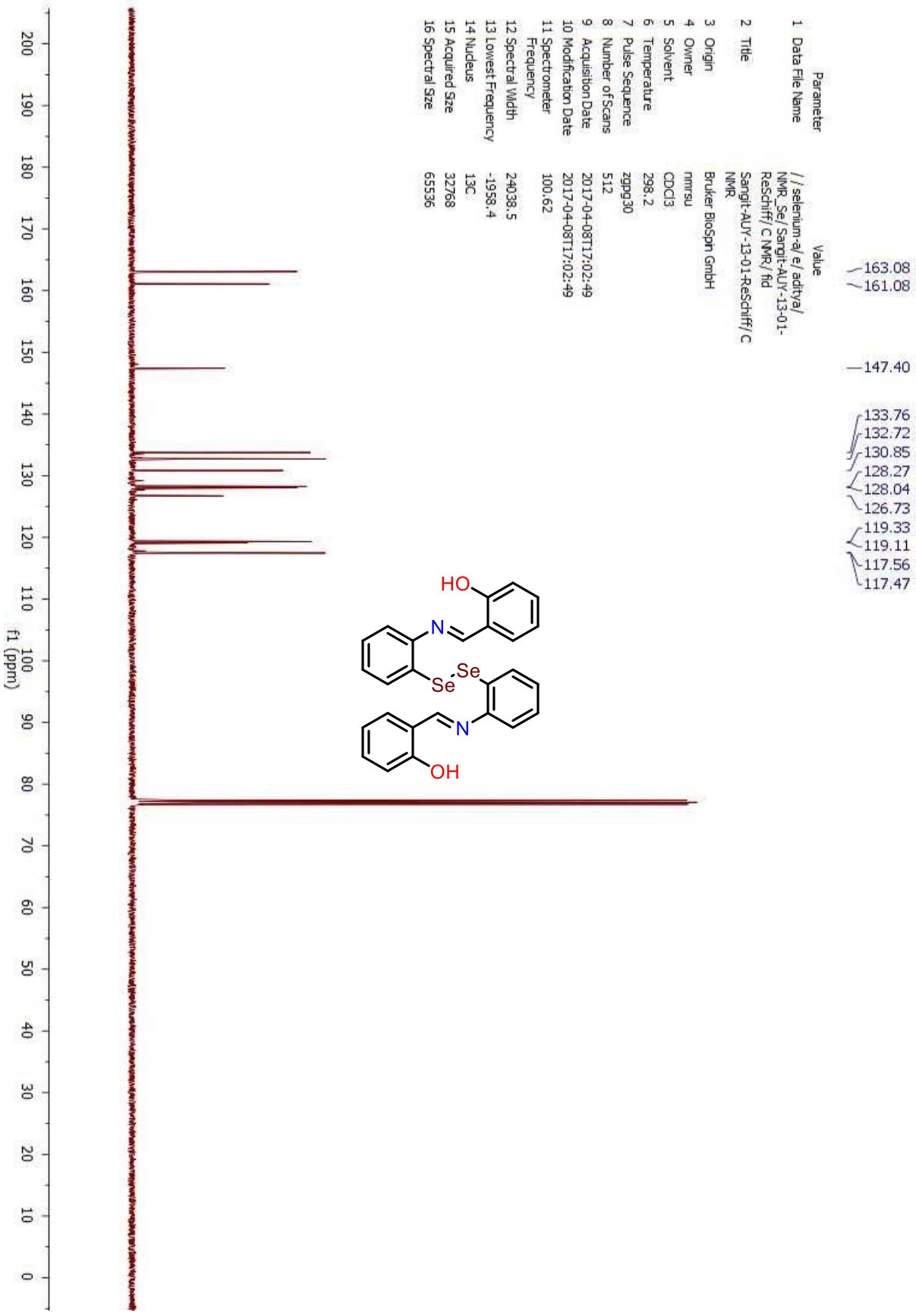
0.95
1.93
1.31
1.94
0.85
1.00
f1 (ppm)

^{13}C NMR of **2a**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Bruker BioSpin GmbH
4 Owner
nmrsu
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CDCl3
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298.2
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2017-04-08T17:02:49
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100.62
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13C
15 Acquired Size
32768
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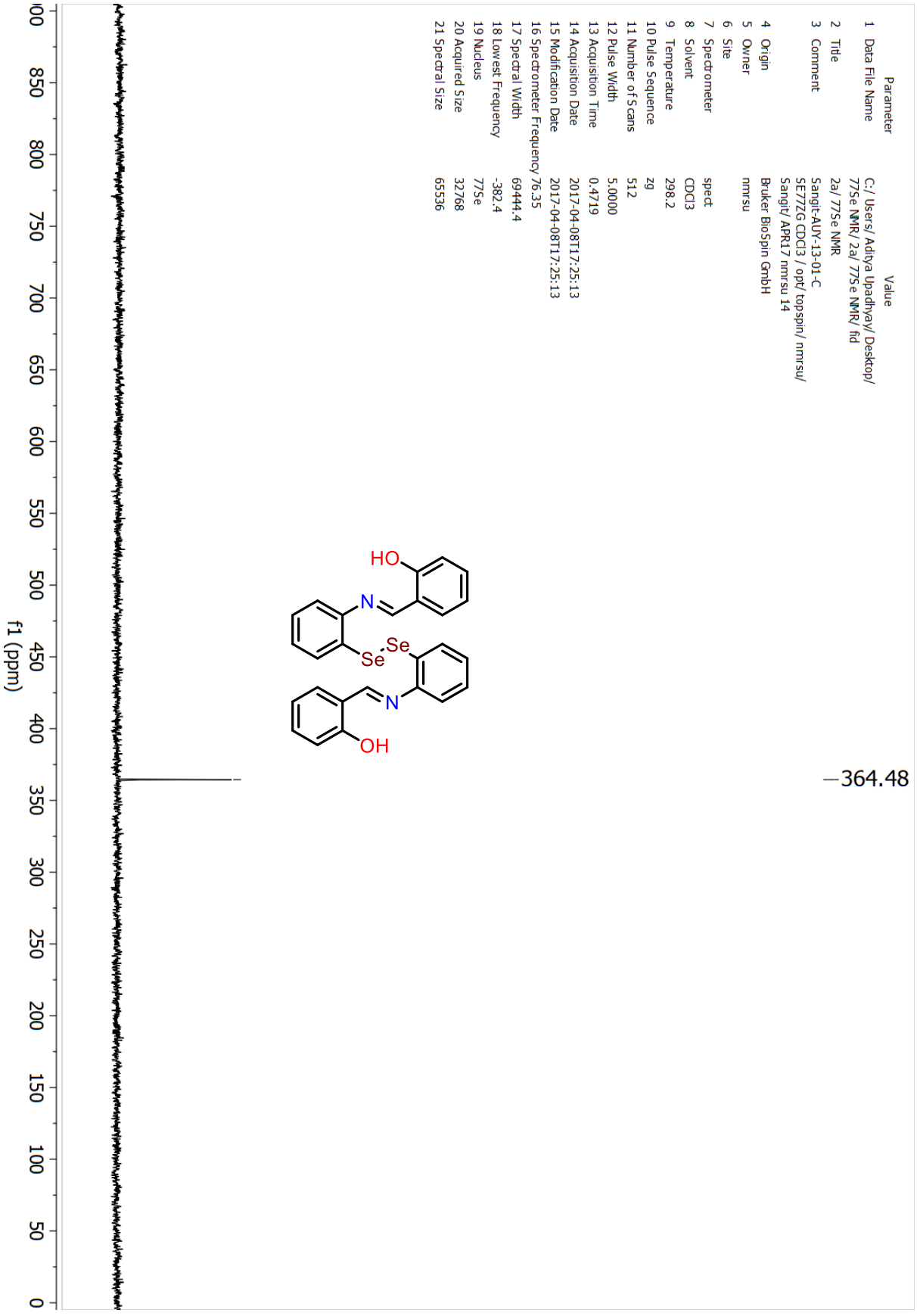
65536
163.08
161.08
147.40
133.76
132.72
130.85
128.27
128.04
126.73
119.33
119.11
117.56
117.47
HO
N
Se
Se
N
OH
f1 (ppm)
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0

^{77}Se NMR of **2a**



HRMS of **2a**

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Comment			

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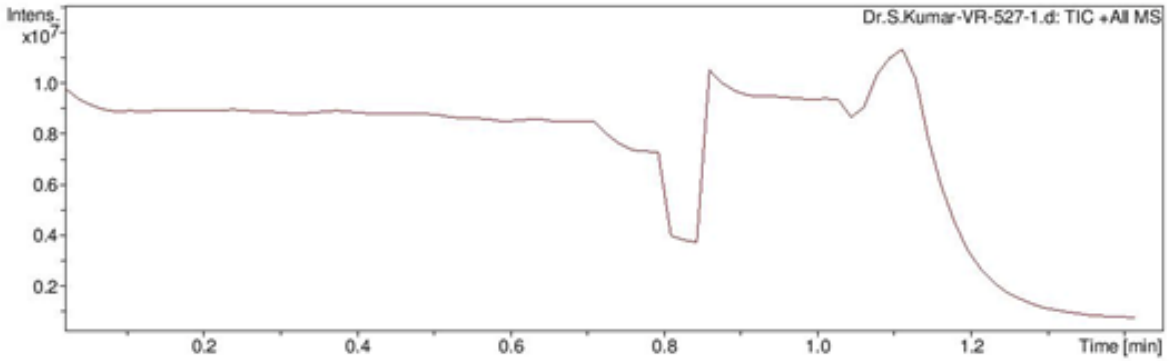
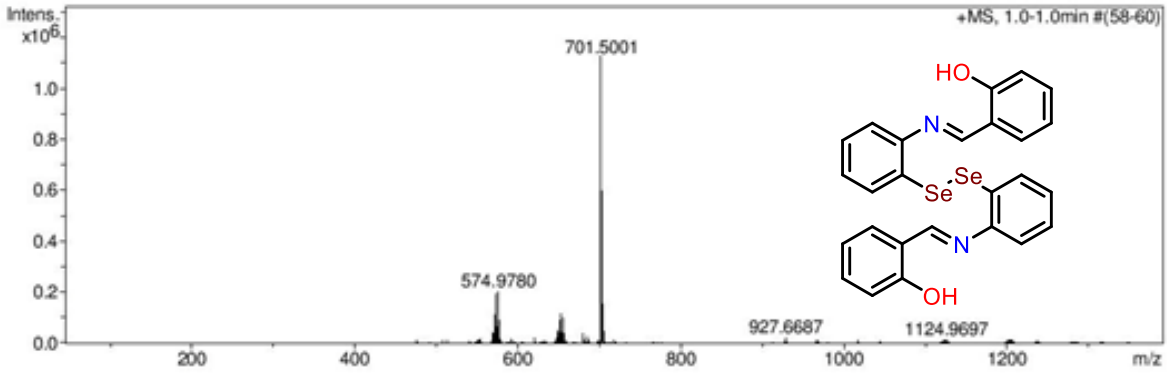
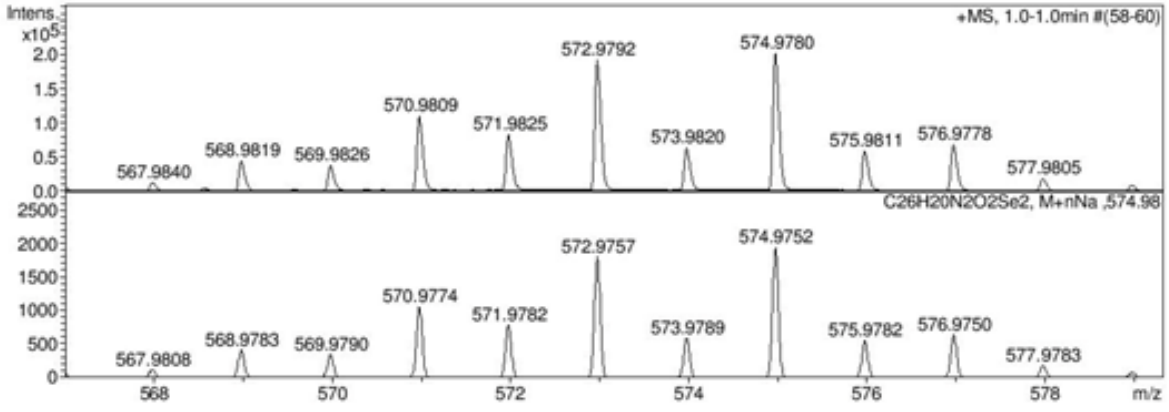
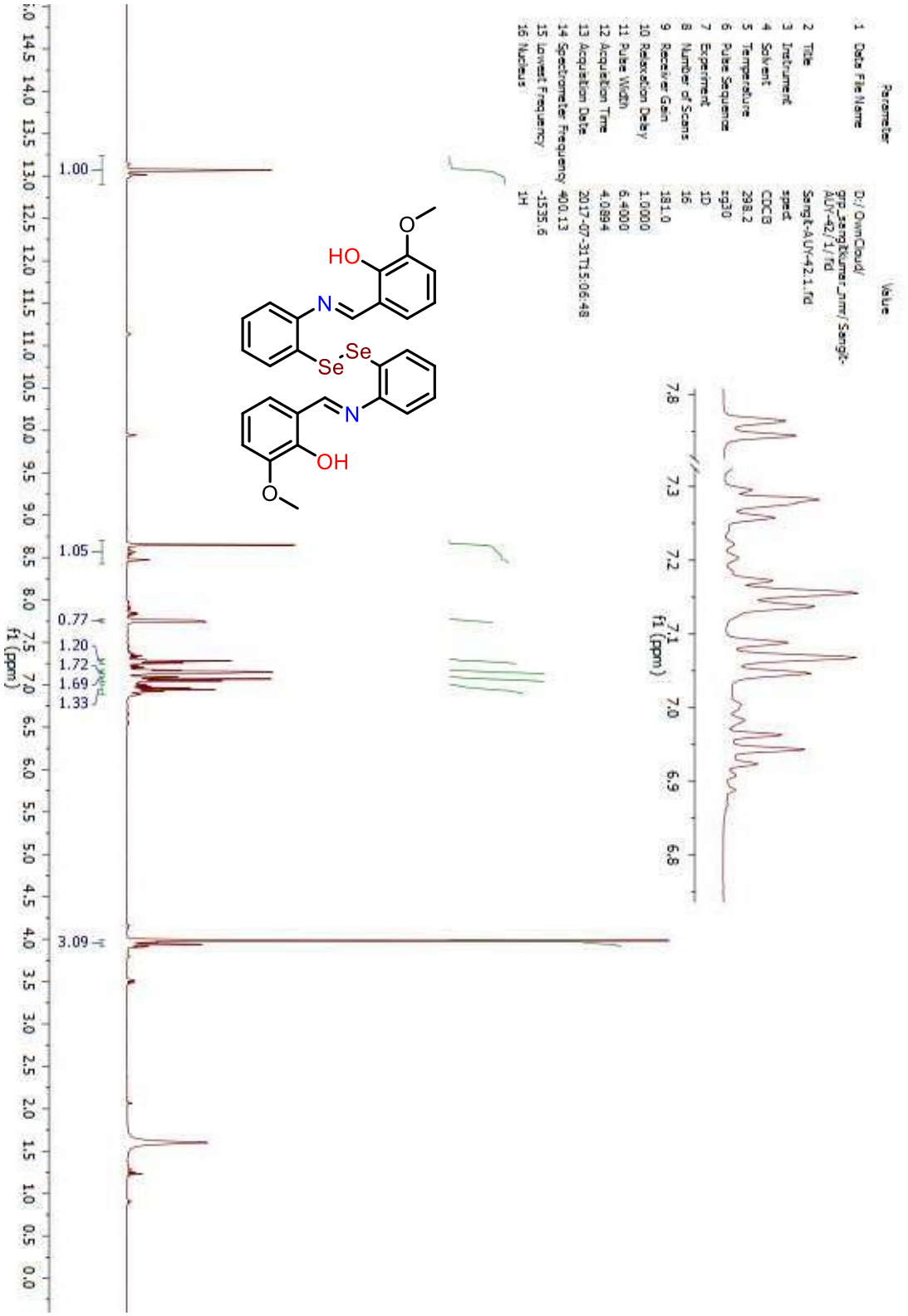




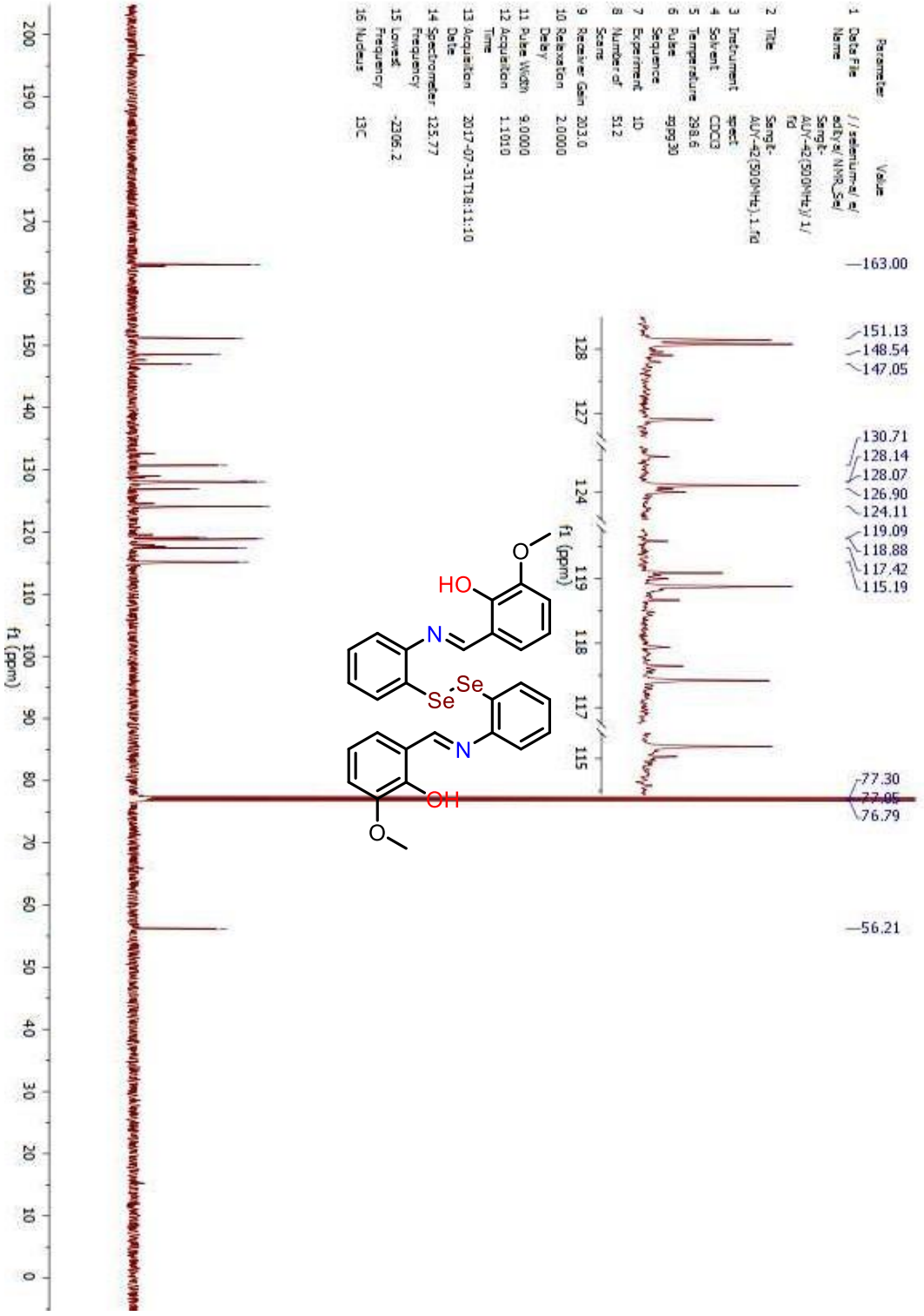


^{1}H NMR of **2b**



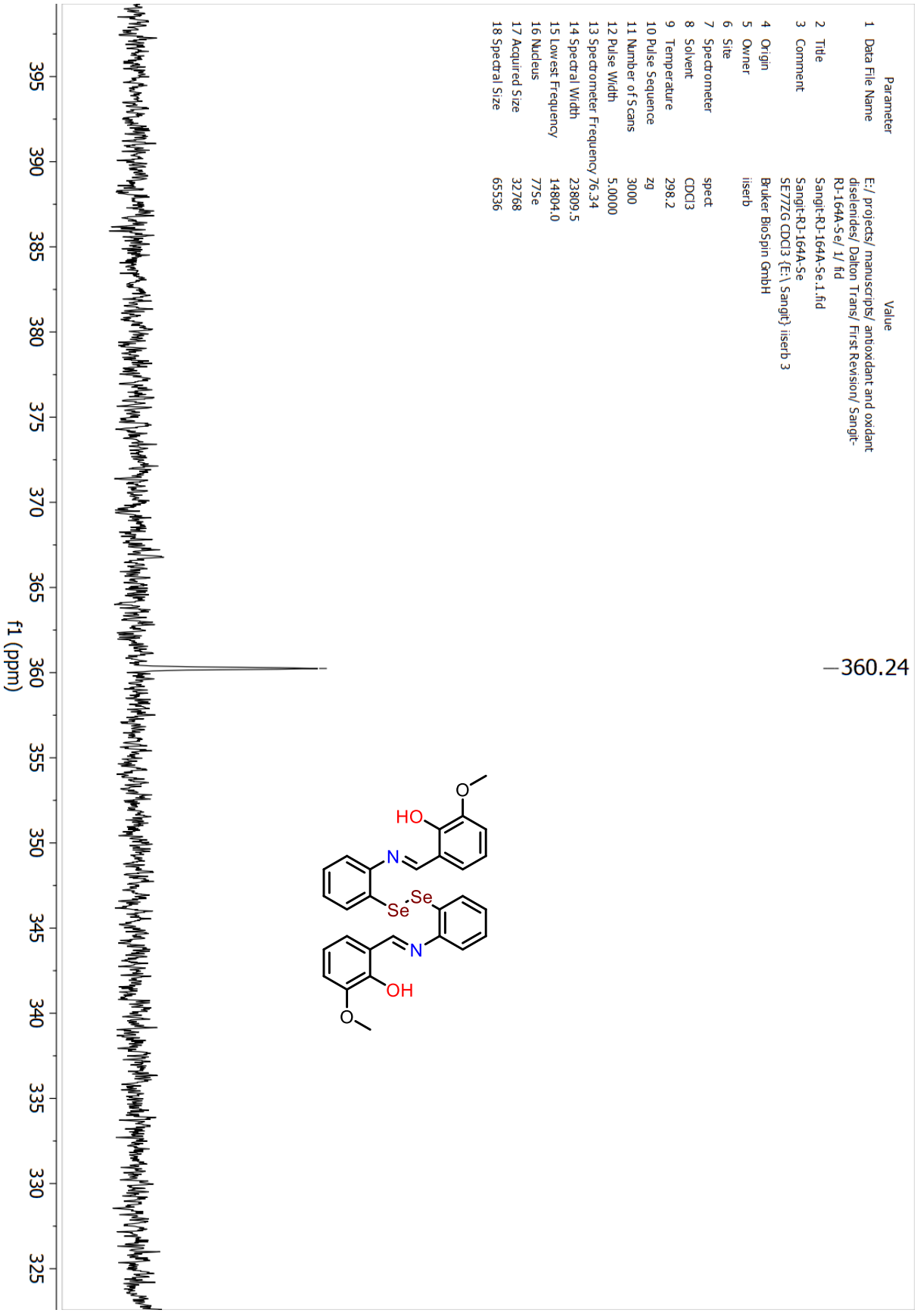
Two regioisomers were observed due to the *E*:*Z* formation around C=N.

^{13}C NMR of **2b**



Two regioisomers were observed due to the *E*:*Z* formation around C=N.

^{77}Se NMR of **2b**



HRMS of **2b**

Display Report

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Comment			

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.3 Bar
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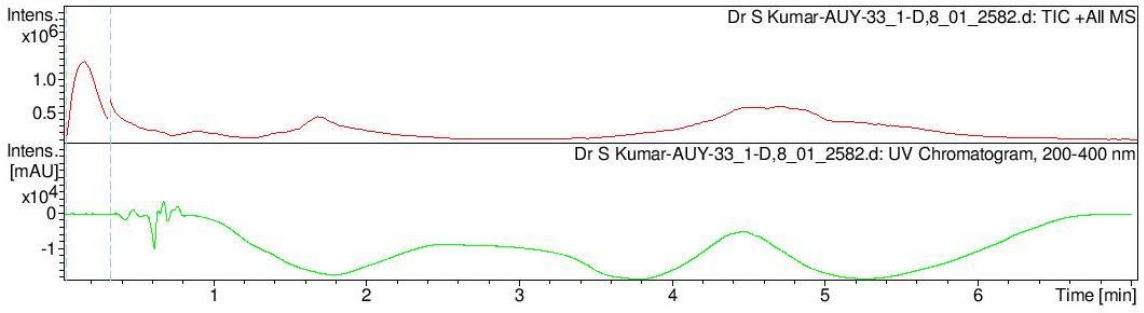

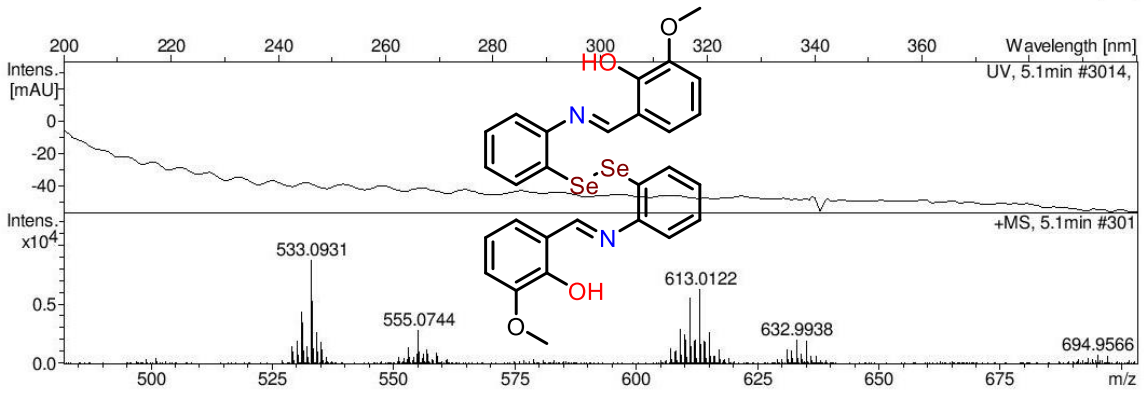

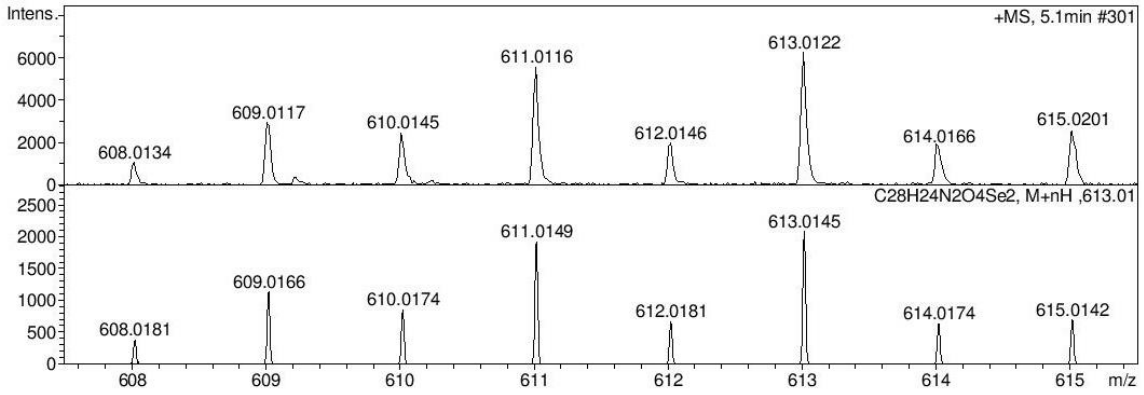

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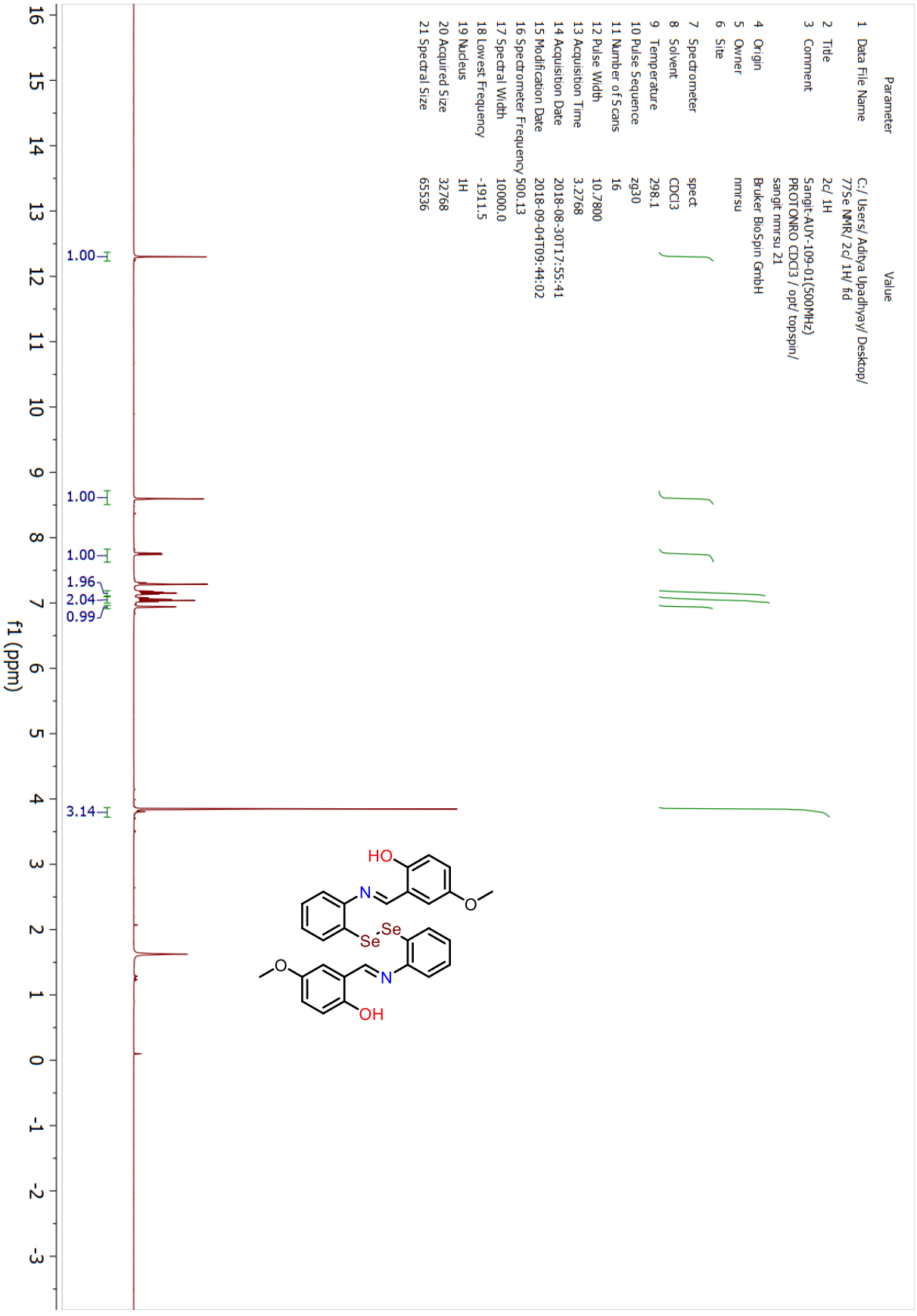
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1H
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1.00
1.00
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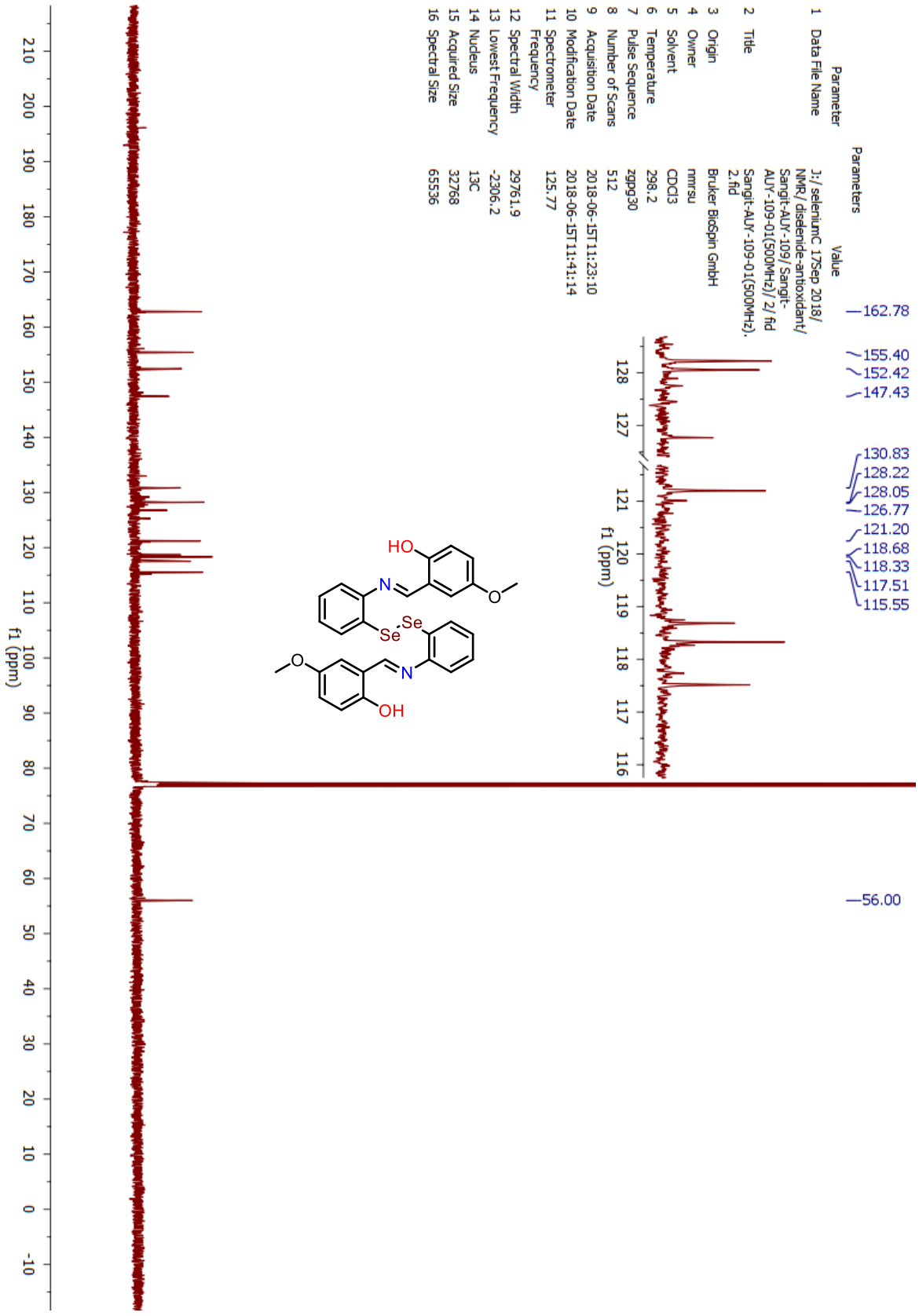
2.04
0.99
3.14
HO
N
O
Se
Se
N
O
OH
f1 (ppm)

^{13}C NMR of **2c**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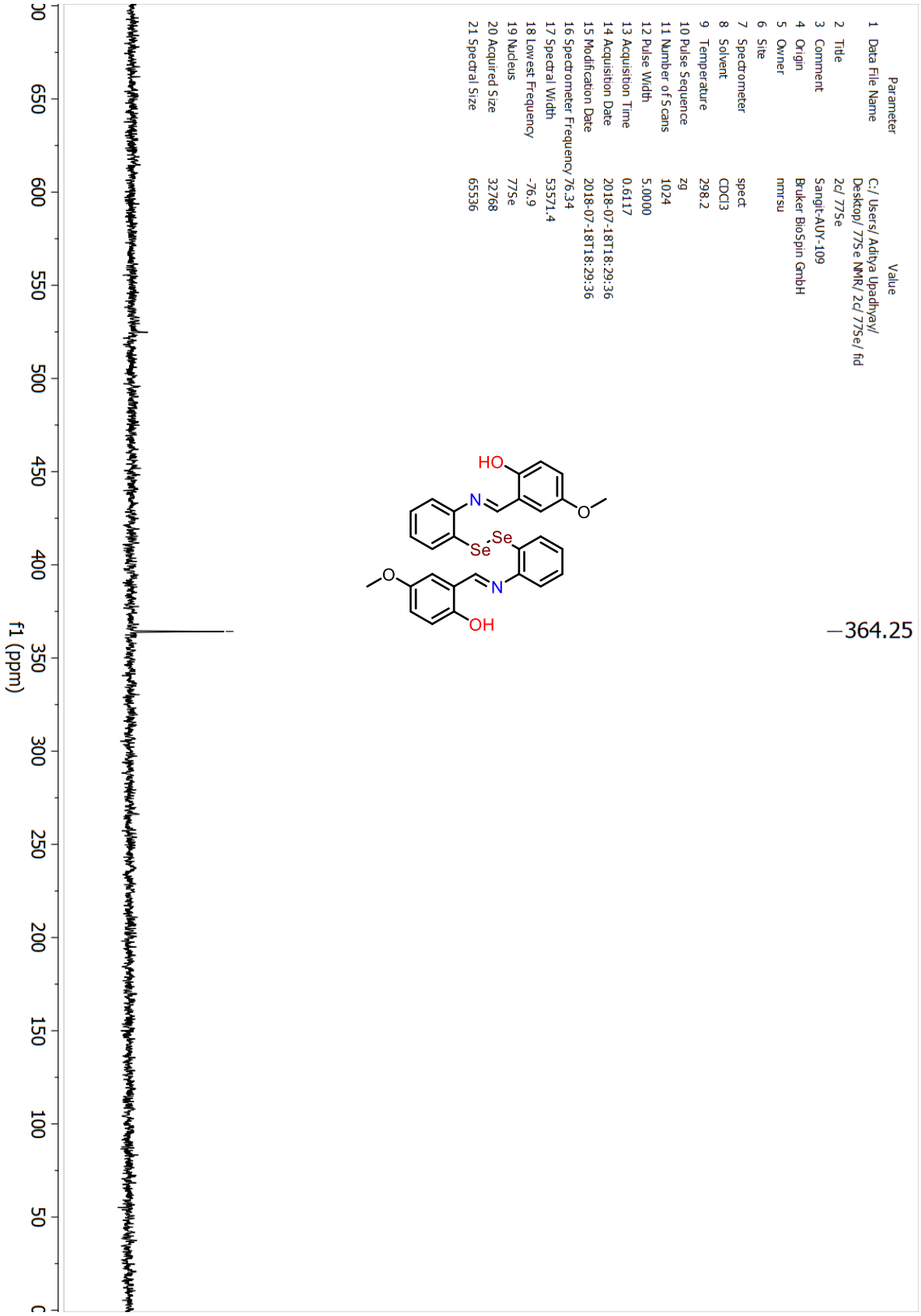
147.43
130.83
128.22
128.05
126.77
121.20
118.68
118.33
117.51
115.55
56.00
HO
N
O
Se
Se
N
O
OH
f1 (ppm)

^{77}Se NMR of **2c**



HRMS of **2c**

Display Report

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Sample Name	AUY-109	Instrument	micrOTOF-Q II 10330
Comment			

Acquisition Parameter

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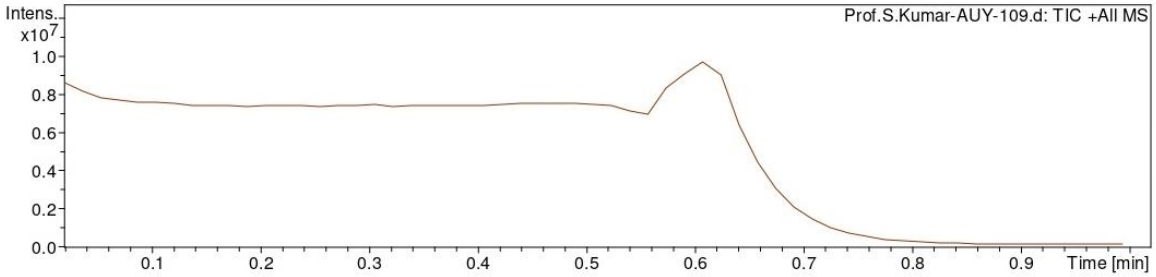
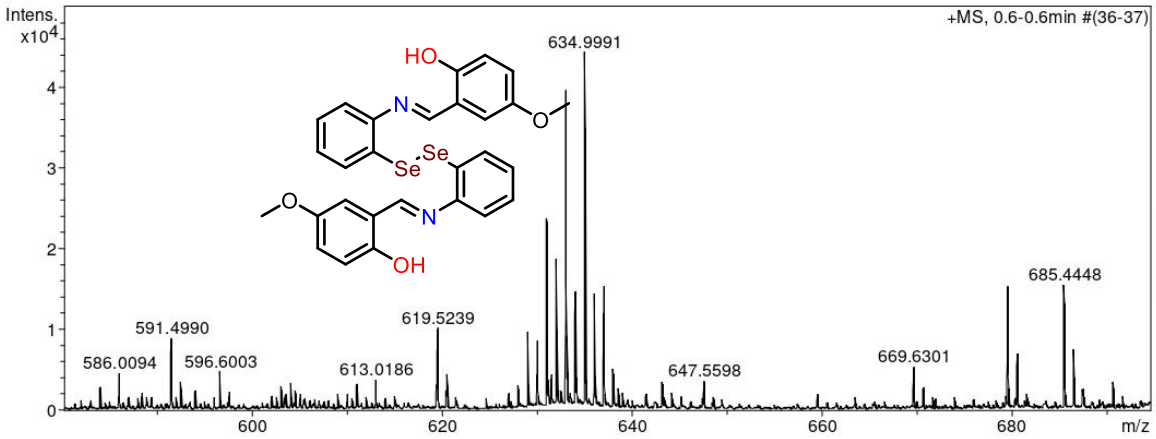
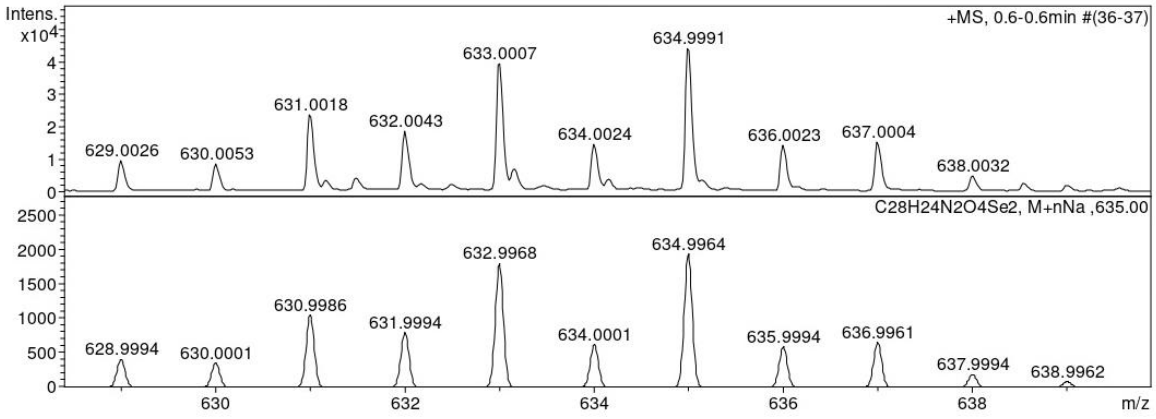
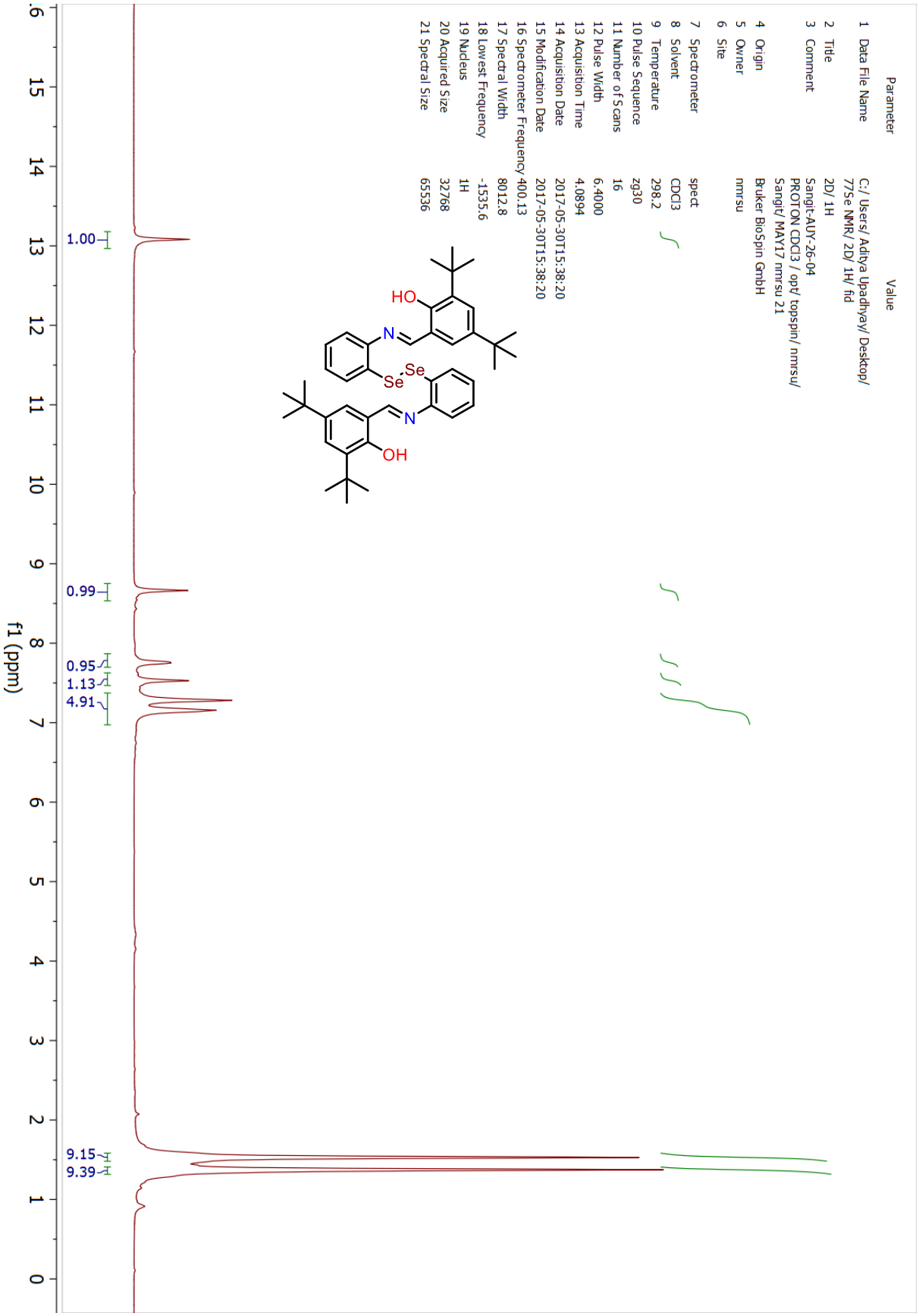






Bruker Compass DataAnalysis 4.0 printed: 6/15/2018 4:22:59 PM Page 1 of 1

^{1}H NMR of **2d**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2D/ 1H
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4 Origin
Bruker BioSpin GmbH
5 Owner
nmrsu
6 Site
7 Spectrometer
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CDCl3
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18 Lowest Frequency
-1535.6
19 Nucleus
1H
20 Acquired Size
32768
21 Spectral Size
65536
HO
N
Se
Se
N
OH
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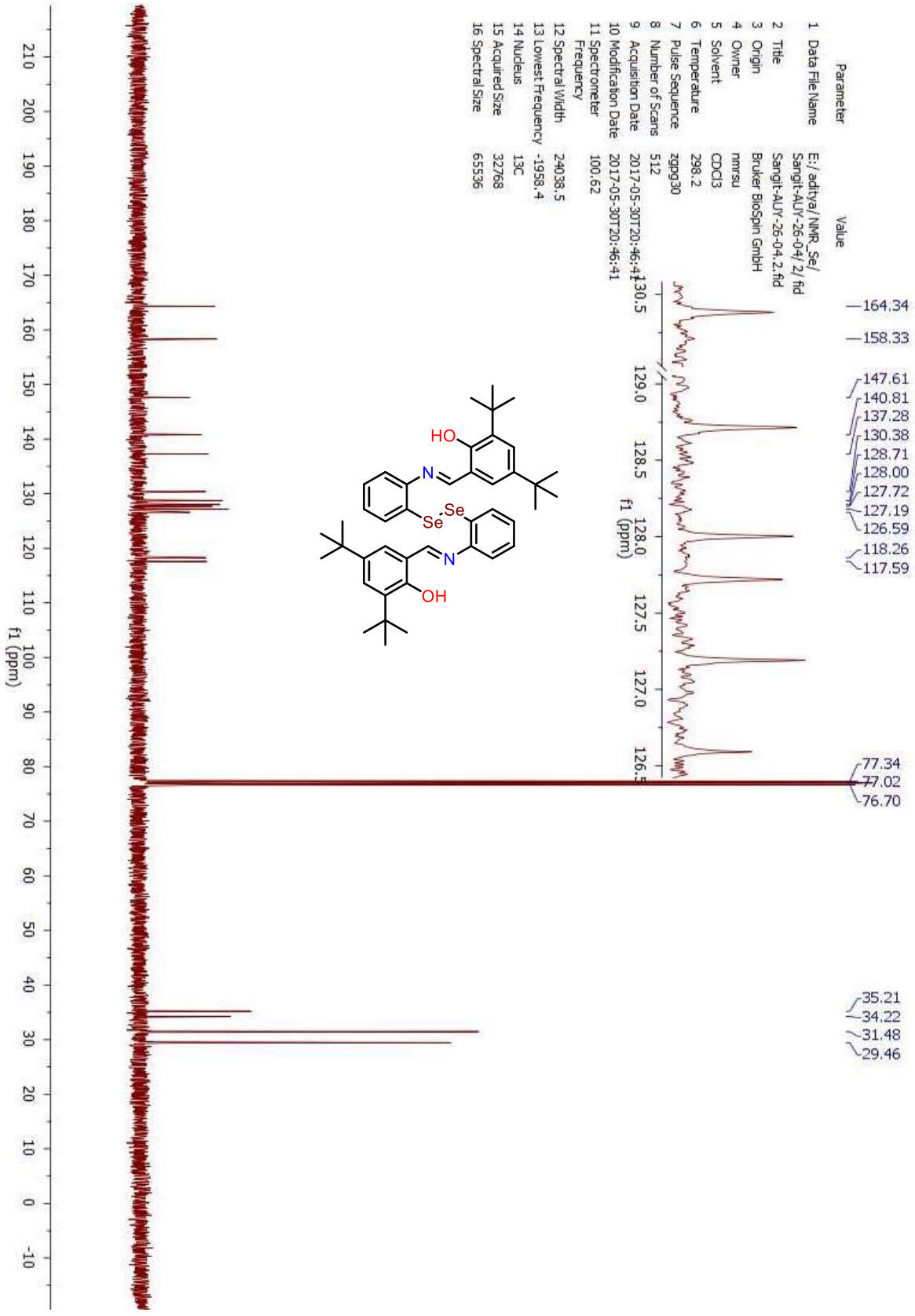
0.99
0.95
1.13
4.91
9.15
9.39
f1 (ppm)

^{13}C NMR of **2d**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10 Modification Date 2017-05-30T20:46:41
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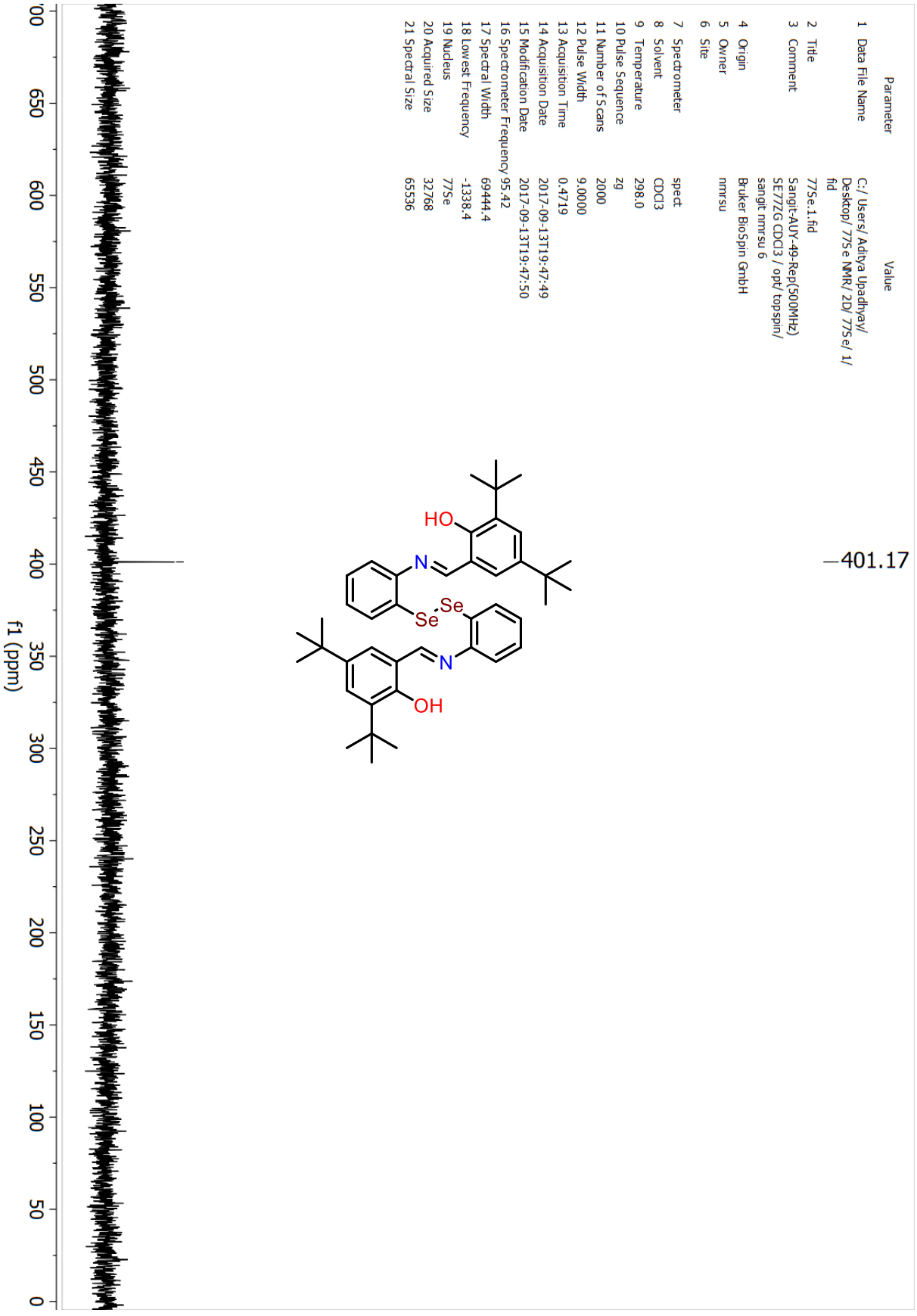
12 Spectral Width 24038.5
13 Lowest Frequency -1958.4
14 Nucleus 13C
15 Acquired Size 32768
16 Spectral Size 65536
HO
N
Se
Se
N
OH
164.34
158.33
147.61
140.81
137.28
130.38
128.71
128.00
127.72
127.19
126.59
118.26
117.59
77.34
77.02
76.70
35.21
34.22
31.48
29.46
f1 (ppm)

^{77}Se NMR of **2d**



HRMS of **2d**

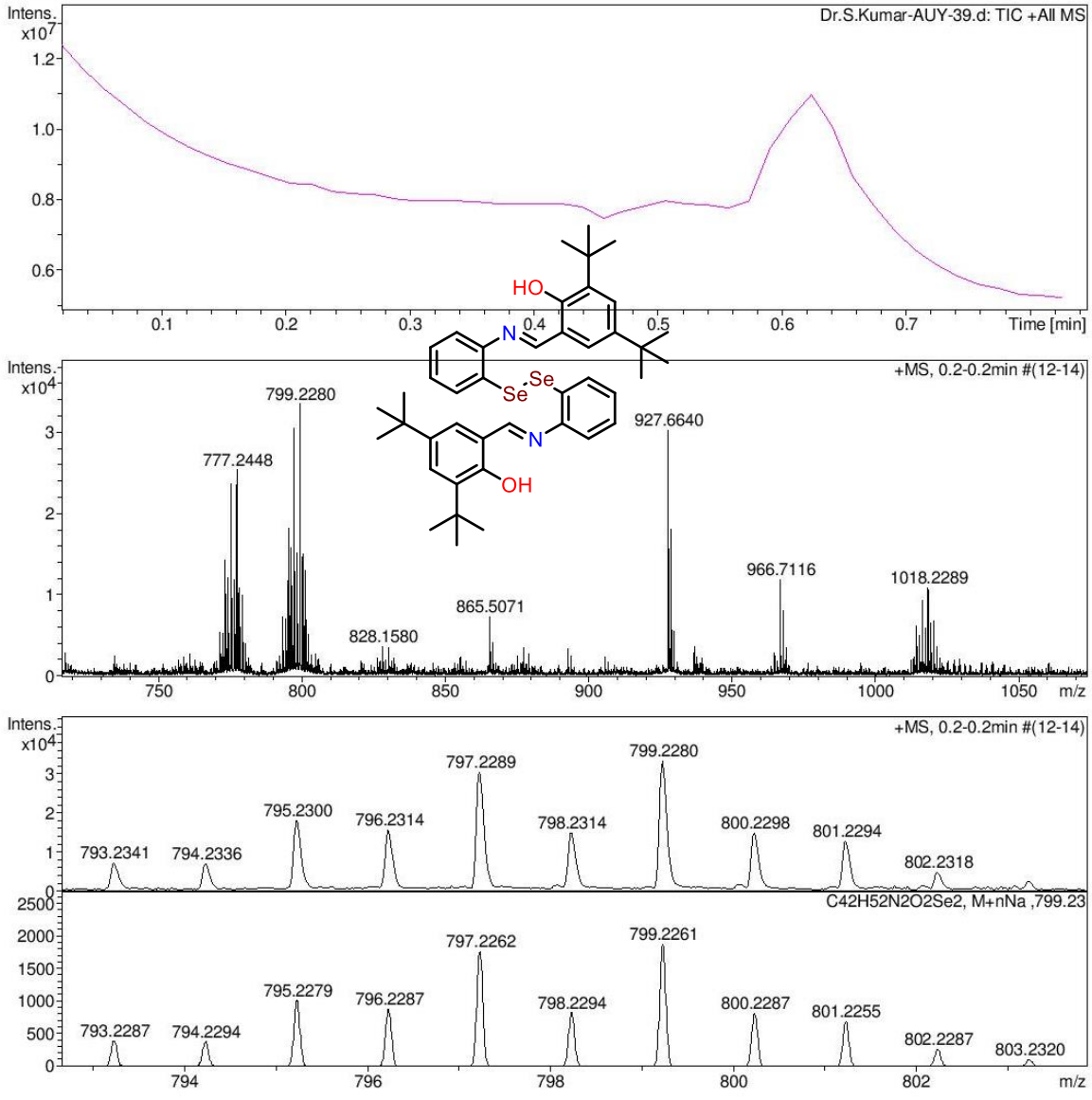
Display Report

Analysis Info

Analysis Name	D:\Data\NEW USER DATA 2017\NOV\28 NOV\Dr.S.Kumar-AUY-39.d	Acquisition Date	11/28/2017 4:46:08 PM
Method	tune_wide.m	Operator	RUCHI
Sample Name	AUY-39	Instrument	micrOTOF-Q II 10330
Comment			

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	5.8 psi
Focus	Not active	Set Capillary	4500 V	Set Dry Heater	180 °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



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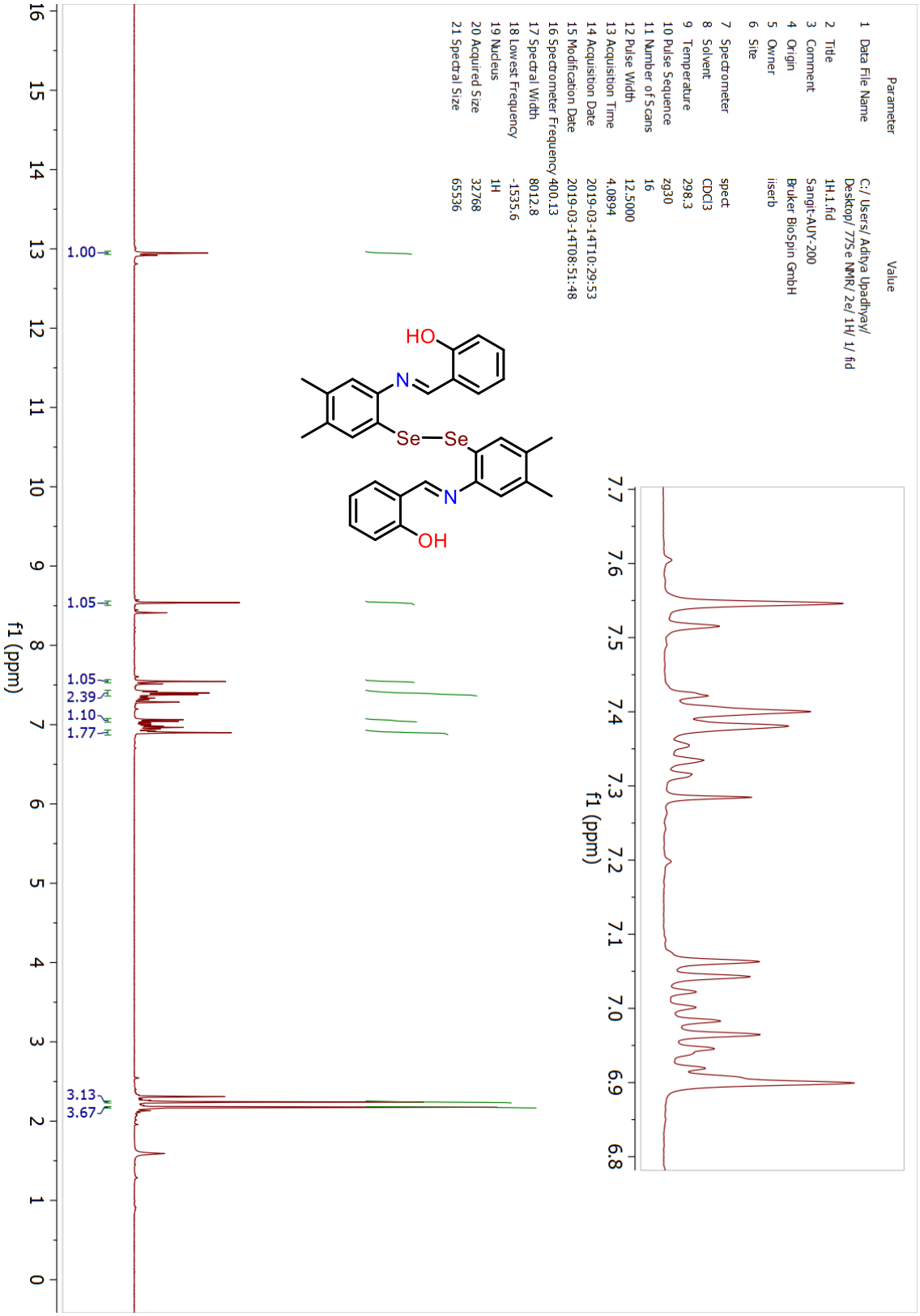
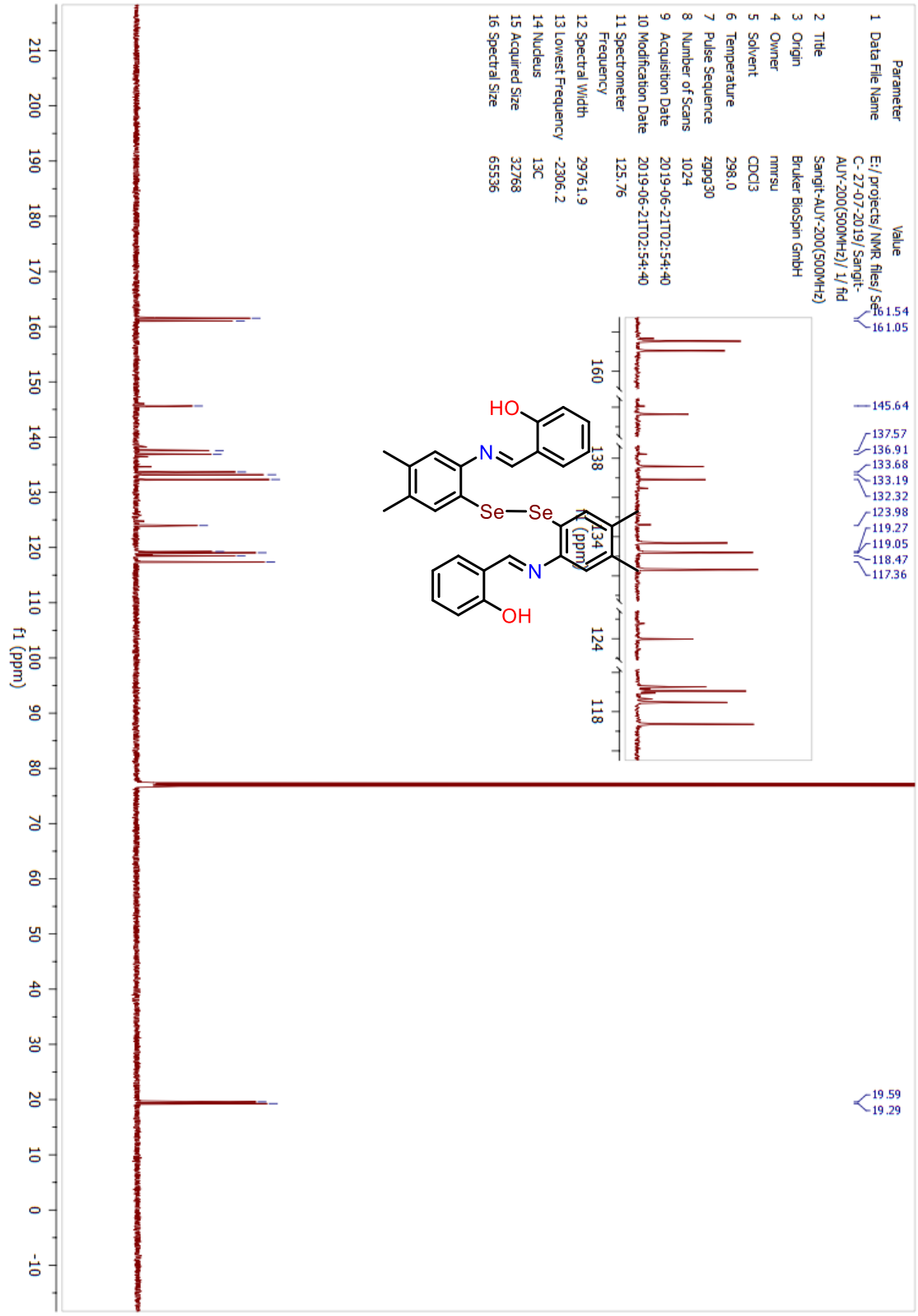
^{1}H NMR of **2e**



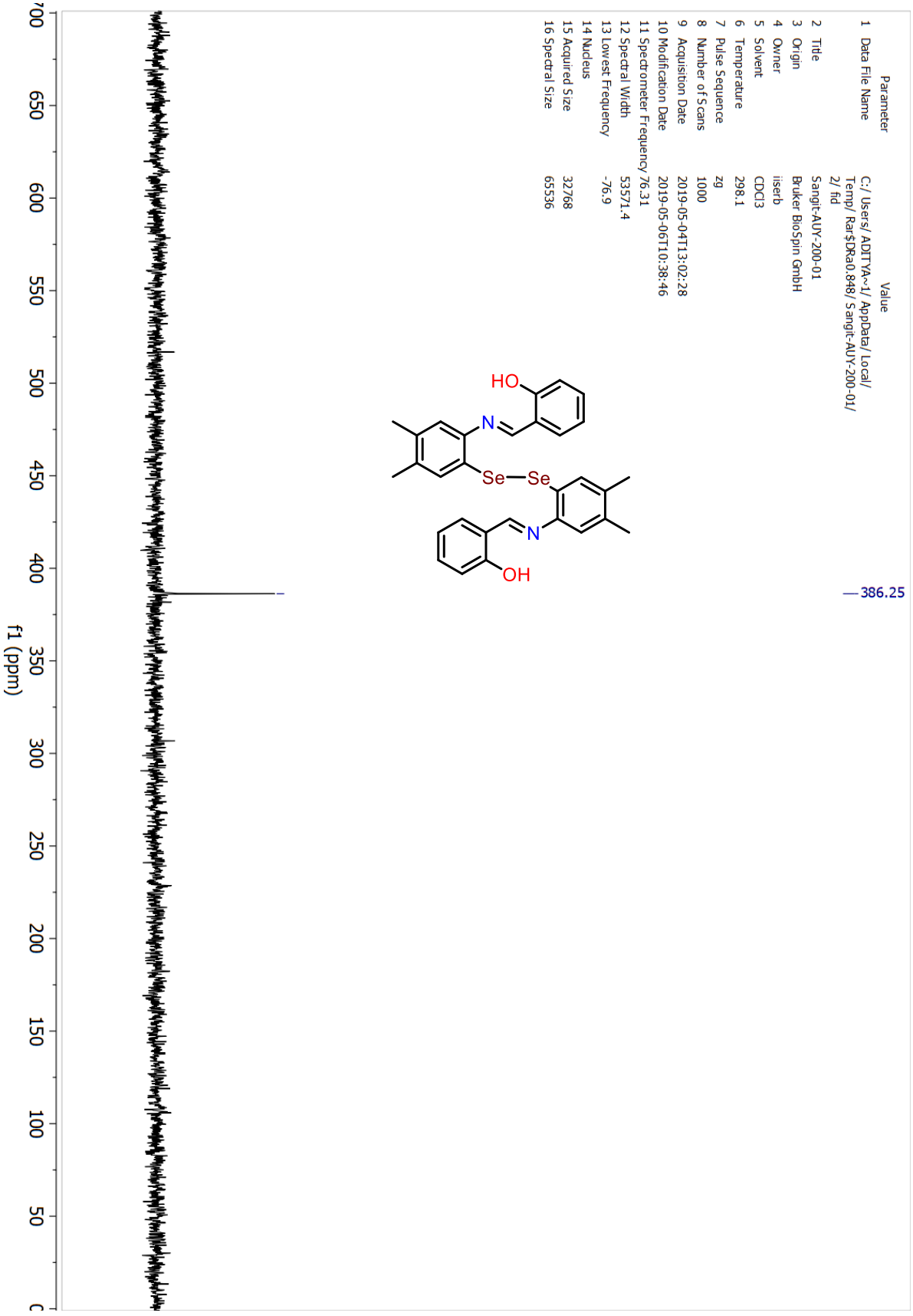
Two regioisomers were observed due to the *E*:*Z* formation around C=N.

^{13}C NMR of **2e**



Two regioisomers were observed due to the *E*:*Z* formation around C=N.

^{77}Se NMR of **2e**



HRMS of **2e**

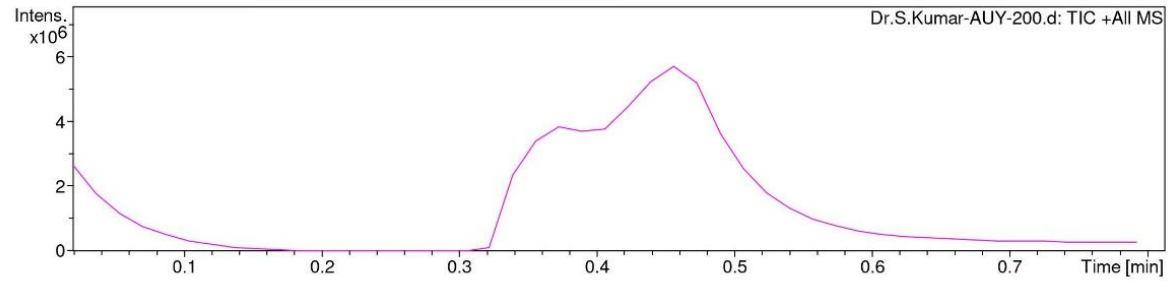
Display Report

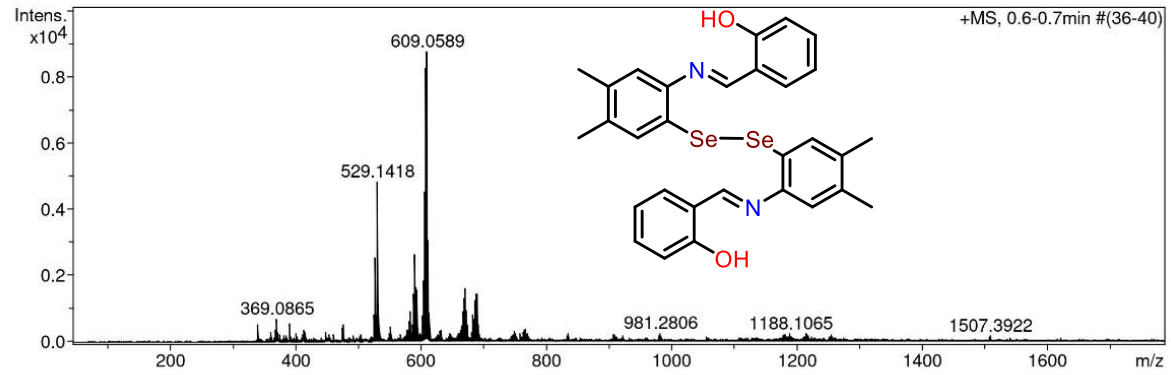
Analysis Info

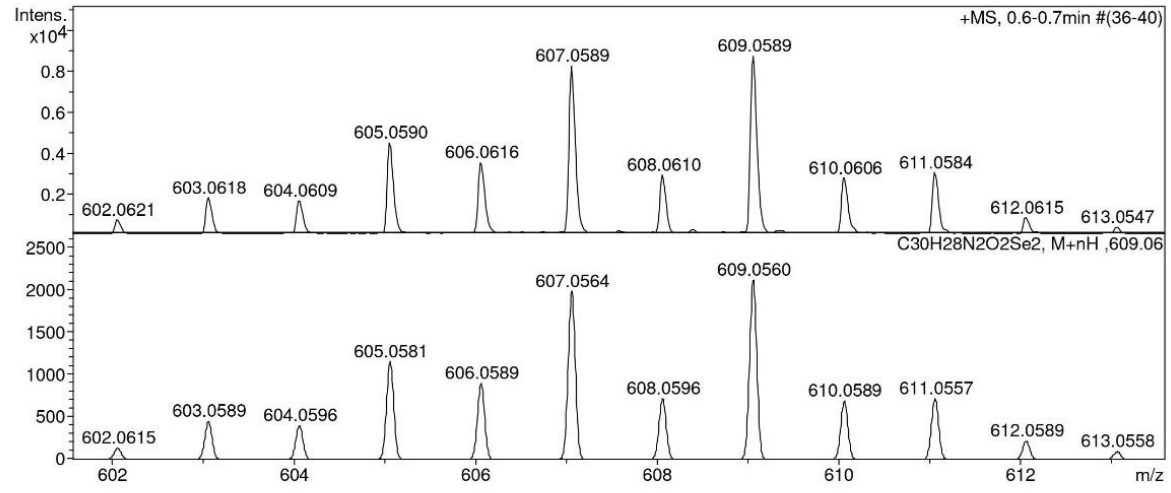
Analysis Name	D:\Data\NEW USER DATA 2017\2019\APR\30 APR\Dr.S.Kumar-AUY-200.d	Acquisition Date	4/30/2019 3:48:49 PM
Method	tune_wide.m	Operator	RUCHI
Sample Name	AUY-200	Instrument	micrOTOF-Q II 10330
Comment			

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Not active	Set Capillary	4500 V	Set Dry Heater	180 °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







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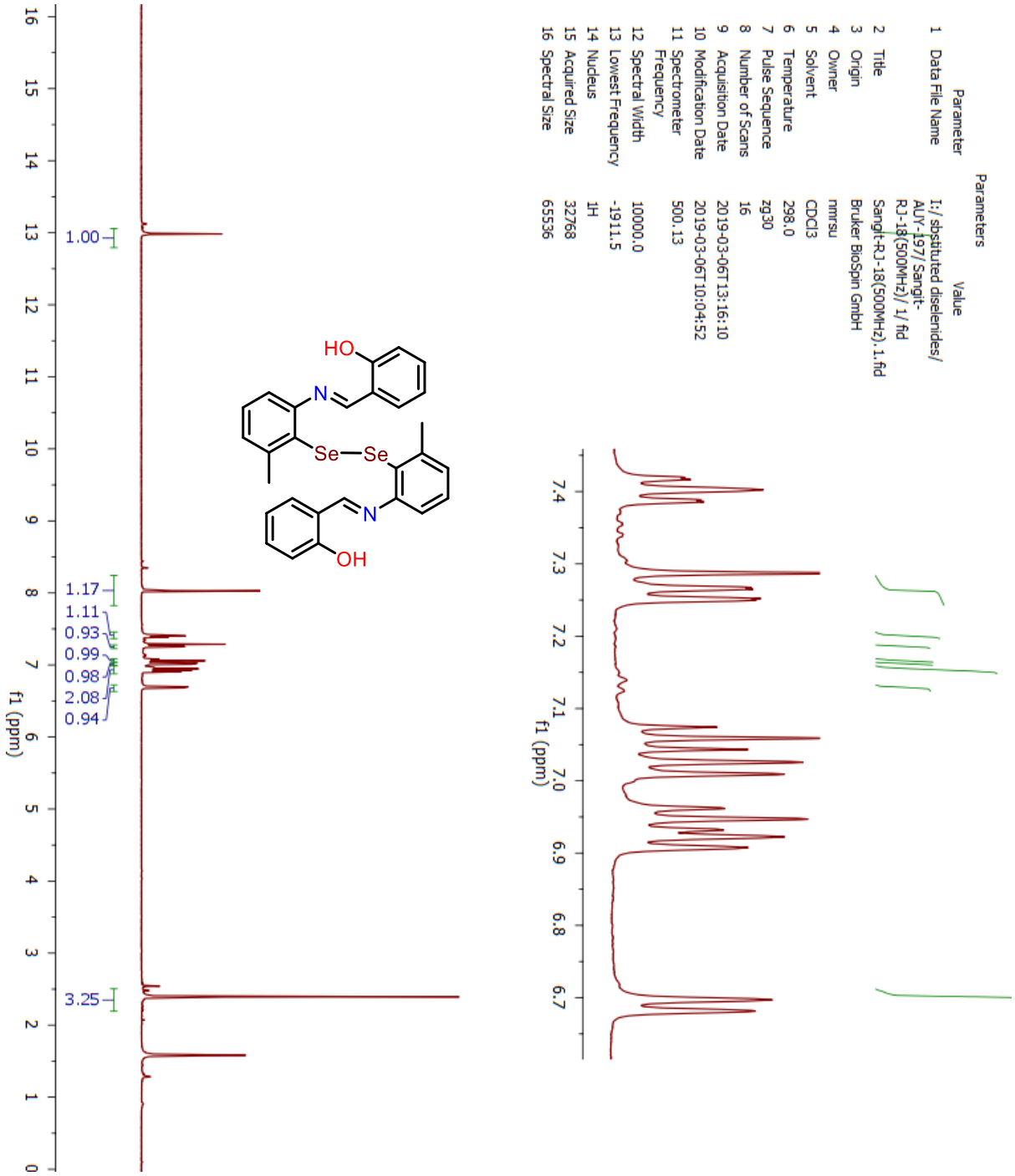
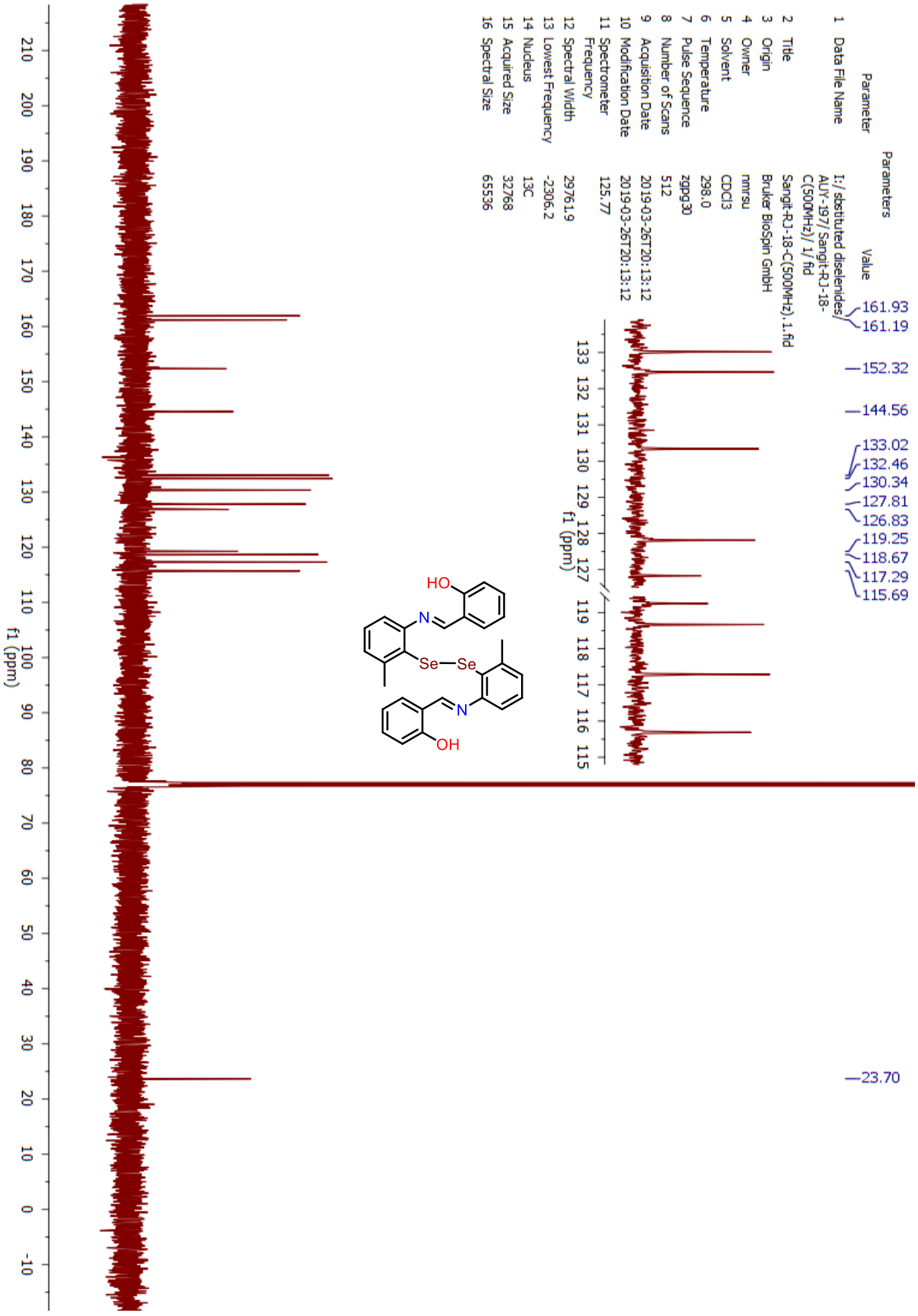
^{1}H NMR of **2f**


HO
N
Se
Se
N
OH
1.00
1.17
1.11
0.93
0.99
0.98
2.08
0.94
3.25
f1 (ppm)
Parameters
Parameter
Value
1 Data File Name I:/ sbstituted diselenides/ AUY-197/ Sangit-RJ-18(500MHz)/ 1/ fid
2 Title Sangit-RJ-18(500MHz),1.fid
3 Origin Bruker BioSpin GmbH
4 Owner nmrsu
5 Solvent CDCl3
6 Temperature 298.0
7 Pulse Sequence zg30
8 Number of Scans 16
9 Acquisition Date 2019-03-06T13:16:10
10 Modification Date 2019-03-06T10:04:52
11 Spectrometer Frequency 500.13
12 Spectral Width 10000.0
13 Lowest Frequency -1911.5
14 Nucleus 1H
15 Acquired Size 32768
16 Spectral Size 65536
7.4
7.3
7.2
7.1
7.0
6.9
6.8
6.7
f1 (ppm)

^{13}C NMR of **2f**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Parameter Value
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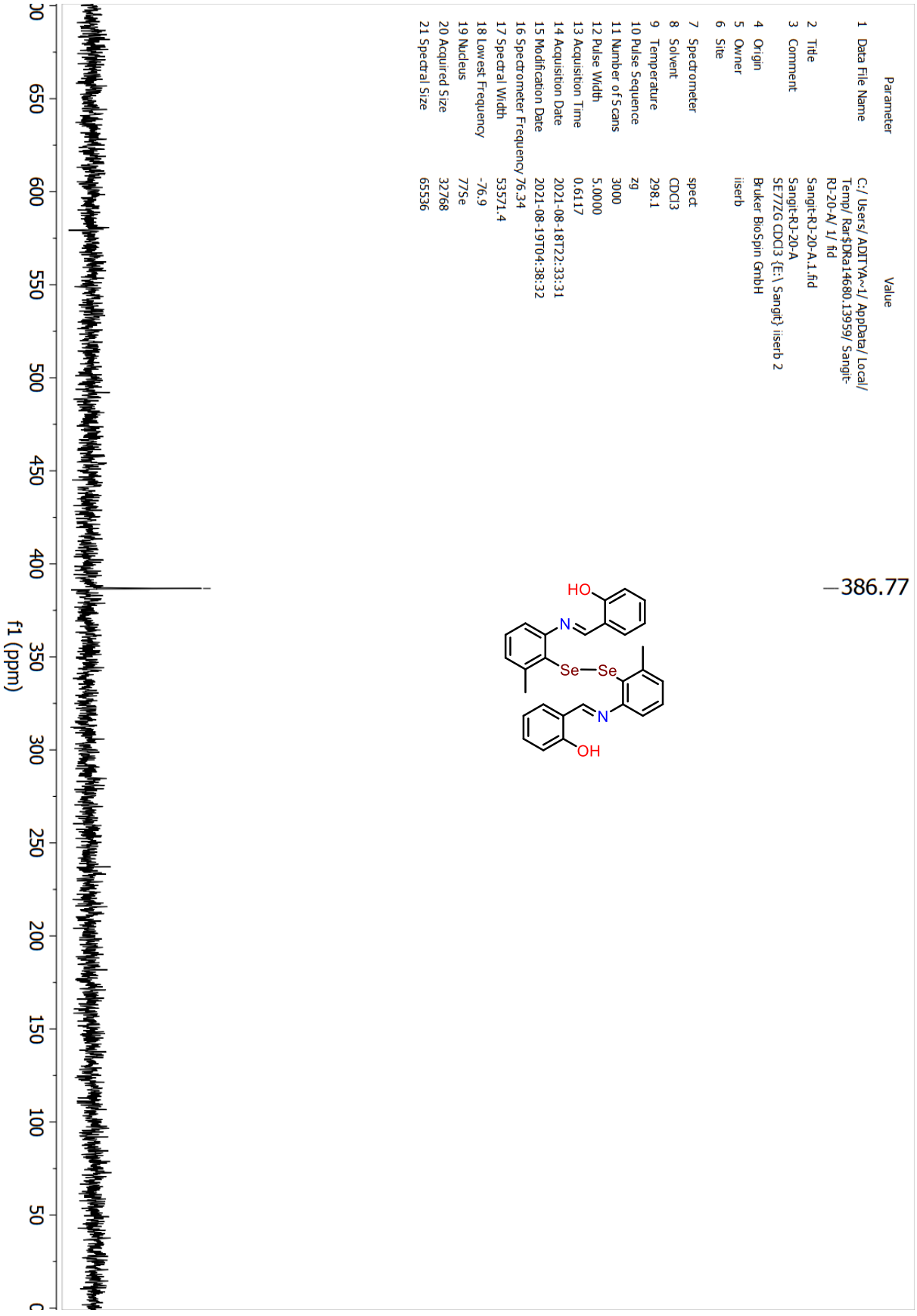
2 Title Sangit-RJ-18-C(500MHz).1.fid
3 Origin Bruker BioSpin GmbH
4 Owner nmrsu
5 Solvent CDCl3
6 Temperature 298.0
7 Pulse Sequence zgpg30
8 Number of Scans 512
9 Acquisition Date 2019-03-26T20:13:12
10 Modification Date 2019-03-26T20:13:12
11 Spectrometer Frequency 125.77
12 Spectral Width 29761.9
13 Lowest Frequency -2306.2
14 Nucleus 13C
15 Acquired Size 32768
16 Spectral Size 65536
161.93
161.19
152.32
144.56
133.02
132.46
130.34
127.81
126.83
119.25
118.67
117.29
115.69
23.70
f1 (ppm)
HO
N
Se
Se
N
OH

^{77}Se NMR of **2f**



HRMS of **2f**

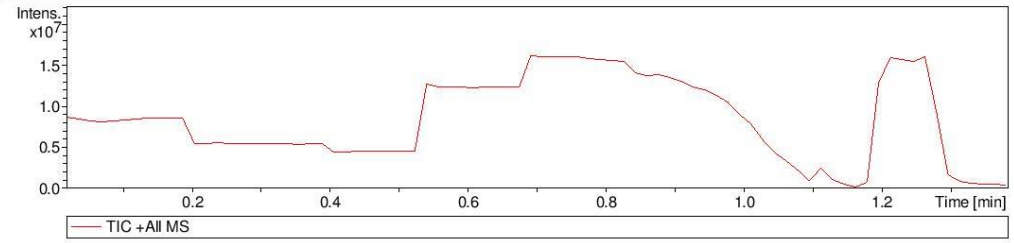
Display Report

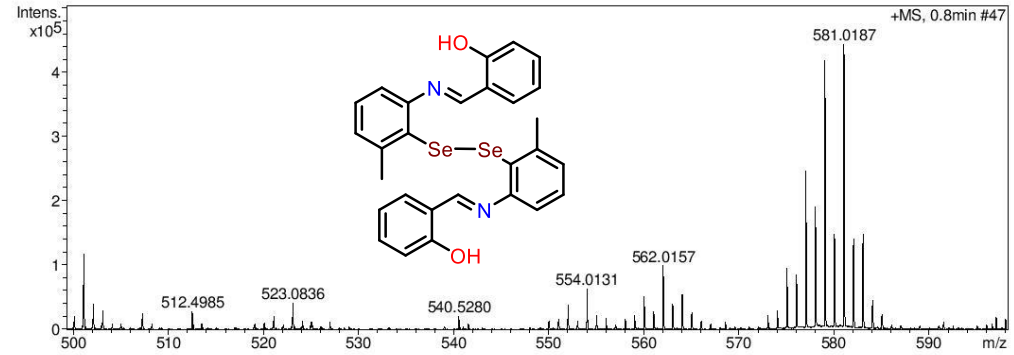
Analysis Info

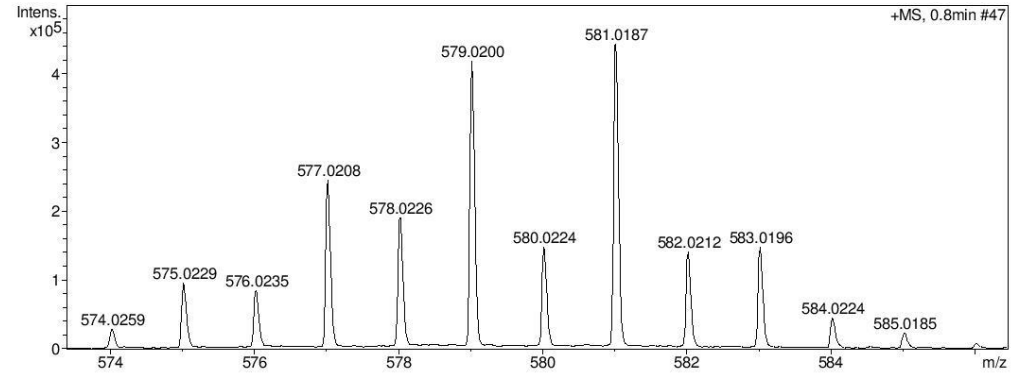
Analysis Name	D:\Data\NEW USER DATA 2017\2019\FEB\18 feb\Dr S Kimar-AUY-197-R.d	Acquisition Date	2/19/2019 11:25:33 AM
Method	tune mix_low.New.021117.m	Operator	RUCHI
Sample Name	AUY-197-R	Instrument	micrOTOF-Q II 10330
Comment			

Acquisition Parameter

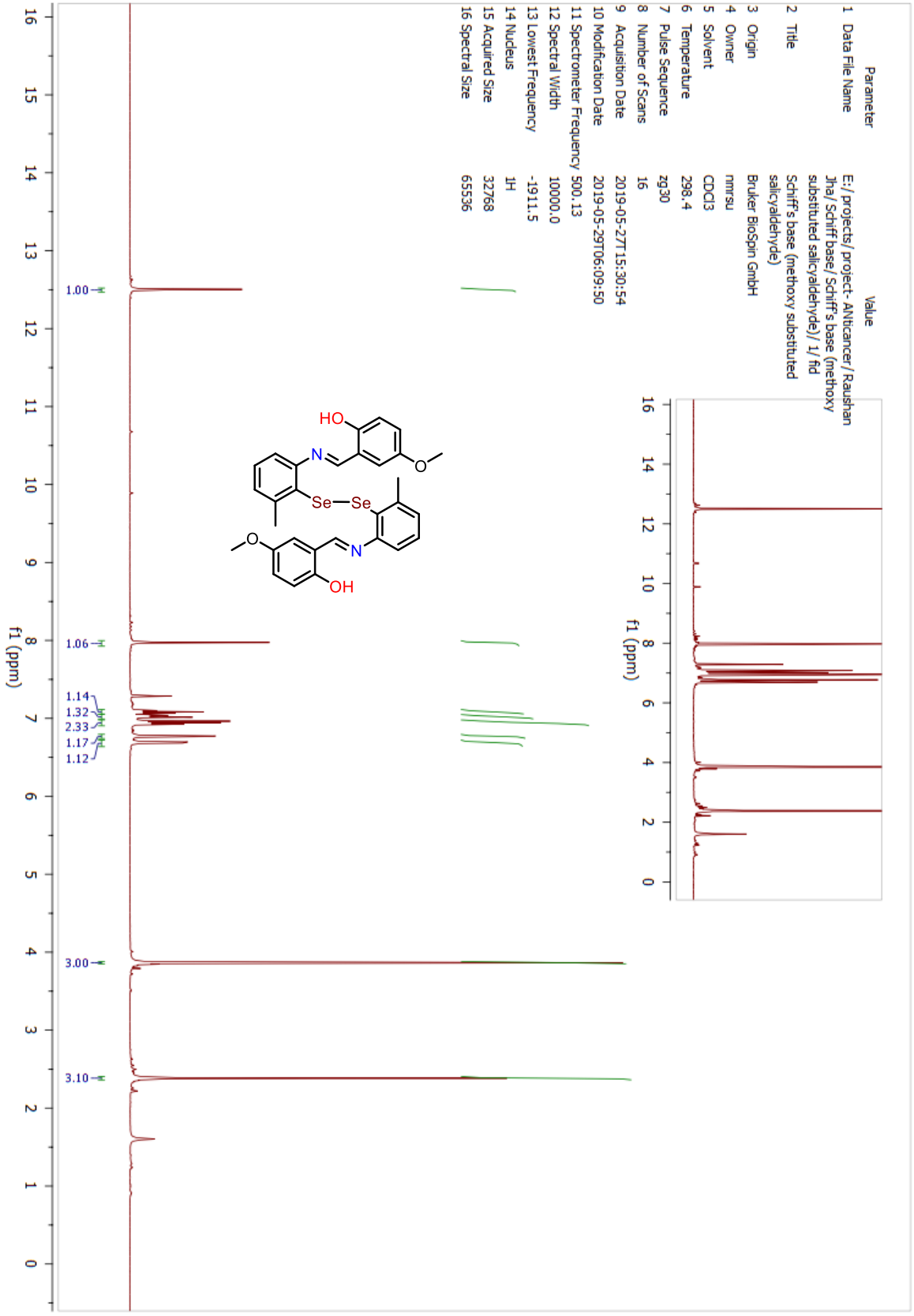
Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Not active	Set Capillary	4600 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	3000 m/z	Set Collision Cell RF	100.0 Vpp	Set Divert Valve	Waste







^{1}H NMR of **2g**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Value
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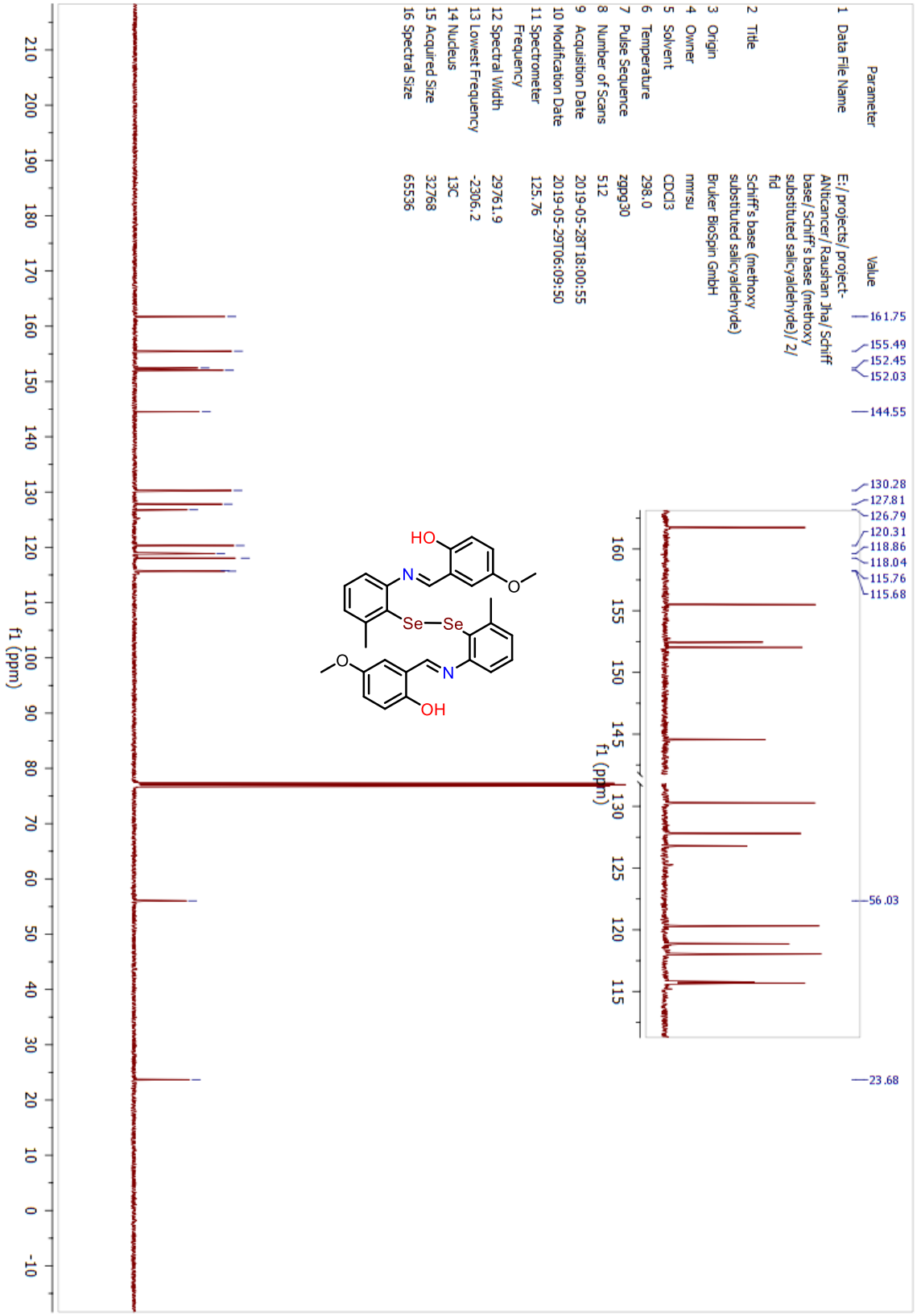
2 Title
Schiff's base (methoxy substituted salicyaldehyde)
3 Origin
Bruker BioSpin GmbH
4 Owner
nmrsu
5 Solvent
CDCl3
6 Temperature
298.4
7 Pulse Sequence
zg30
8 Number of Scans
16
9 Acquisition Date
2019-05-27T15:30:54
10 Modification Date
2019-05-29T06:09:50
11 Spectrometer Frequency
500.13
12 Spectral Width
10000.0
13 Lowest Frequency
-1911.5
14 Nucleus
1H
15 Acquired Size
32768
16 Spectral Size
65536
HO
N
O
Se
Se
O
N
OH
1.00
1.06
1.14
1.32
2.33
1.17
1.12
3.00
3.10
f1 (ppm)

^{13}C NMR of **2g**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Value
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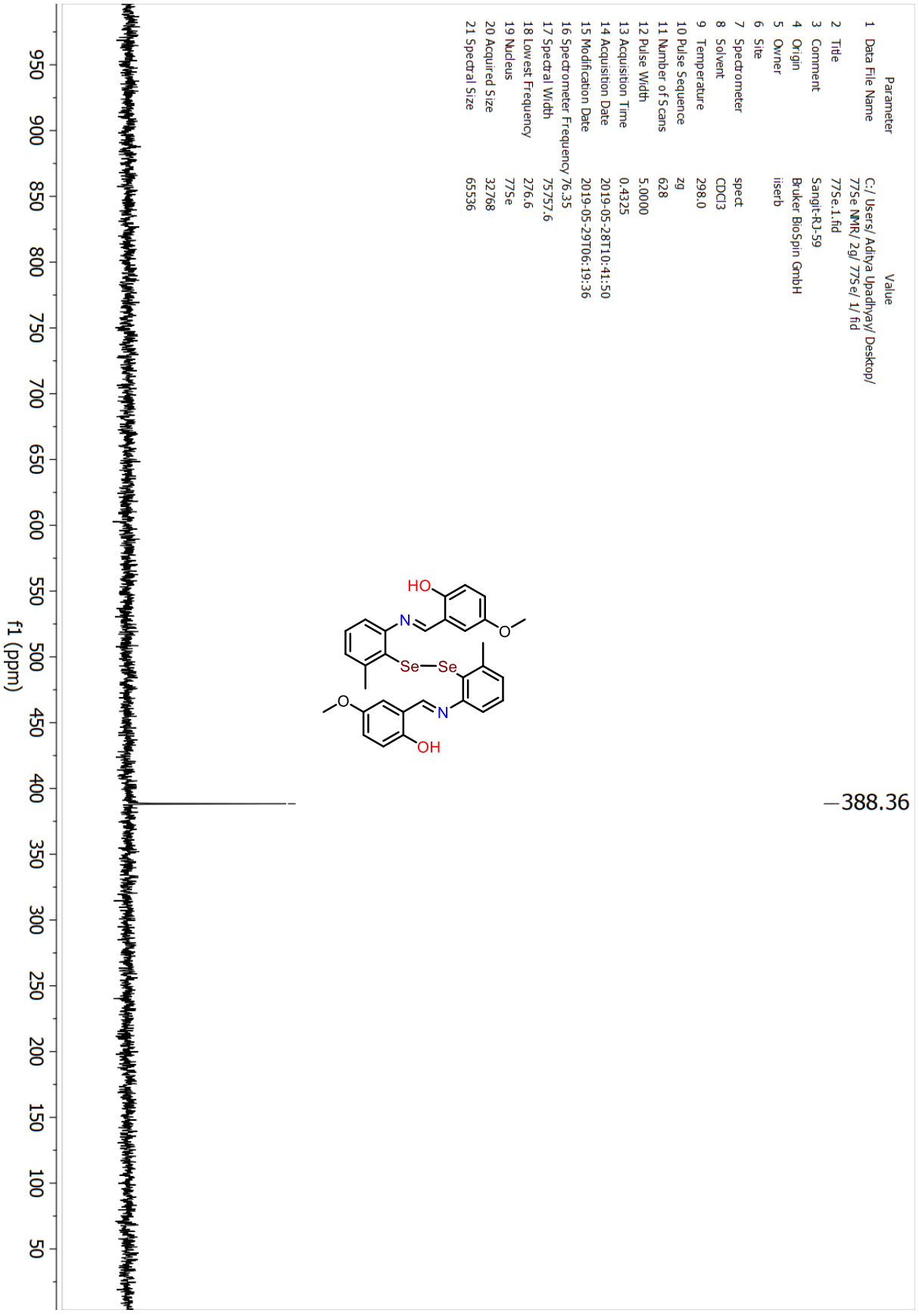
E:/projects/project-ANticancer/Raushan Jha/ Schiff base/ Schiff's base (methoxy substituted salicyaldehyde)/ 2/ fid
2 Title
Schiff's base (methoxy substituted salicyaldehyde)
3 Origin
Bruker BioSpin GmbH
4 Owner
nmrsu
5 Solvent
CDCl3
6 Temperature
298.0
7 Pulse Sequence
zgpg30
8 Number of Scans
512
9 Acquisition Date
2019-05-28T18:00:55
10 Modification Date
2019-05-29T06:09:50
11 Spectrometer Frequency
125.76
12 Spectral Width
29761.9
13 Lowest Frequency
-2306.2
14 Nucleus
13C
15 Acquired Size
32768
16 Spectral Size
65536
161.75
155.49
152.45
152.03
144.55
130.28
127.81
126.79
120.31
118.86
118.04
115.76
115.68
56.03
23.68
HO
N
O
Se
Se
O
N
OH
f1 (ppm)
f1 (ppm)

^{77}Se NMR of **2g**



HRMS of **2g**

Display Report

Analysis Info

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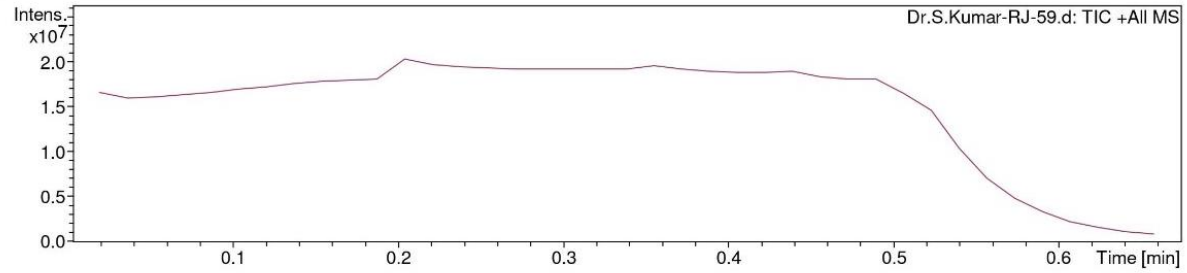
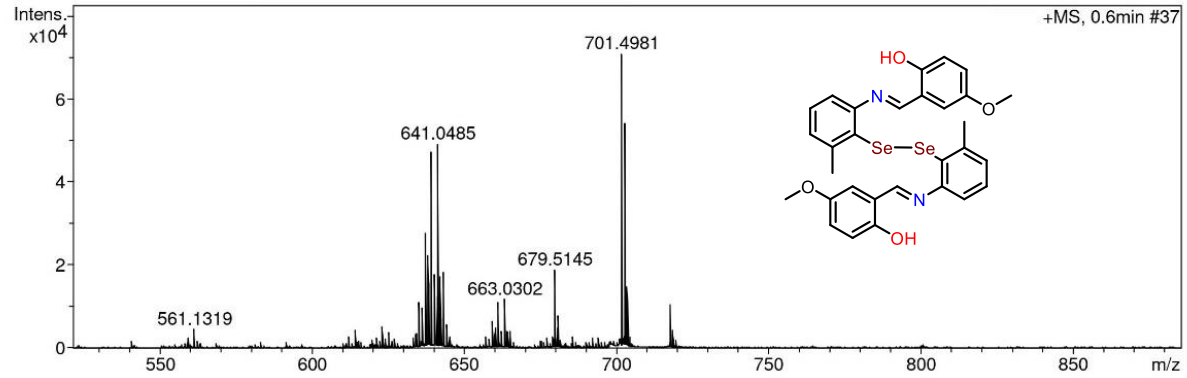
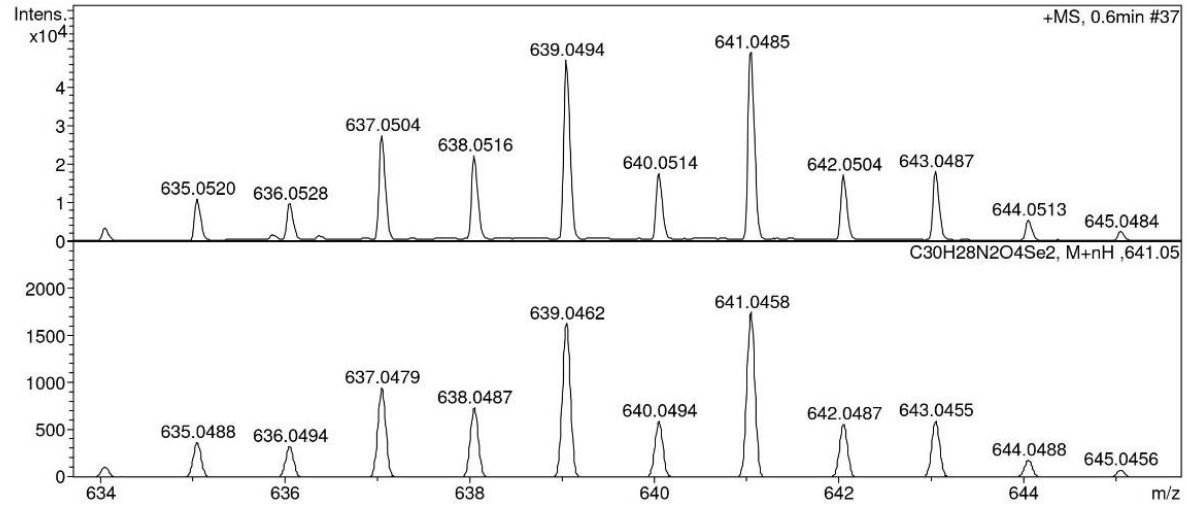
Method	tune_wide.m	Operator	RUCHI
Sample Name	-RJ-59	Instrument	micrOTOF-Q II 10330
Comment			

Acquisition Parameter

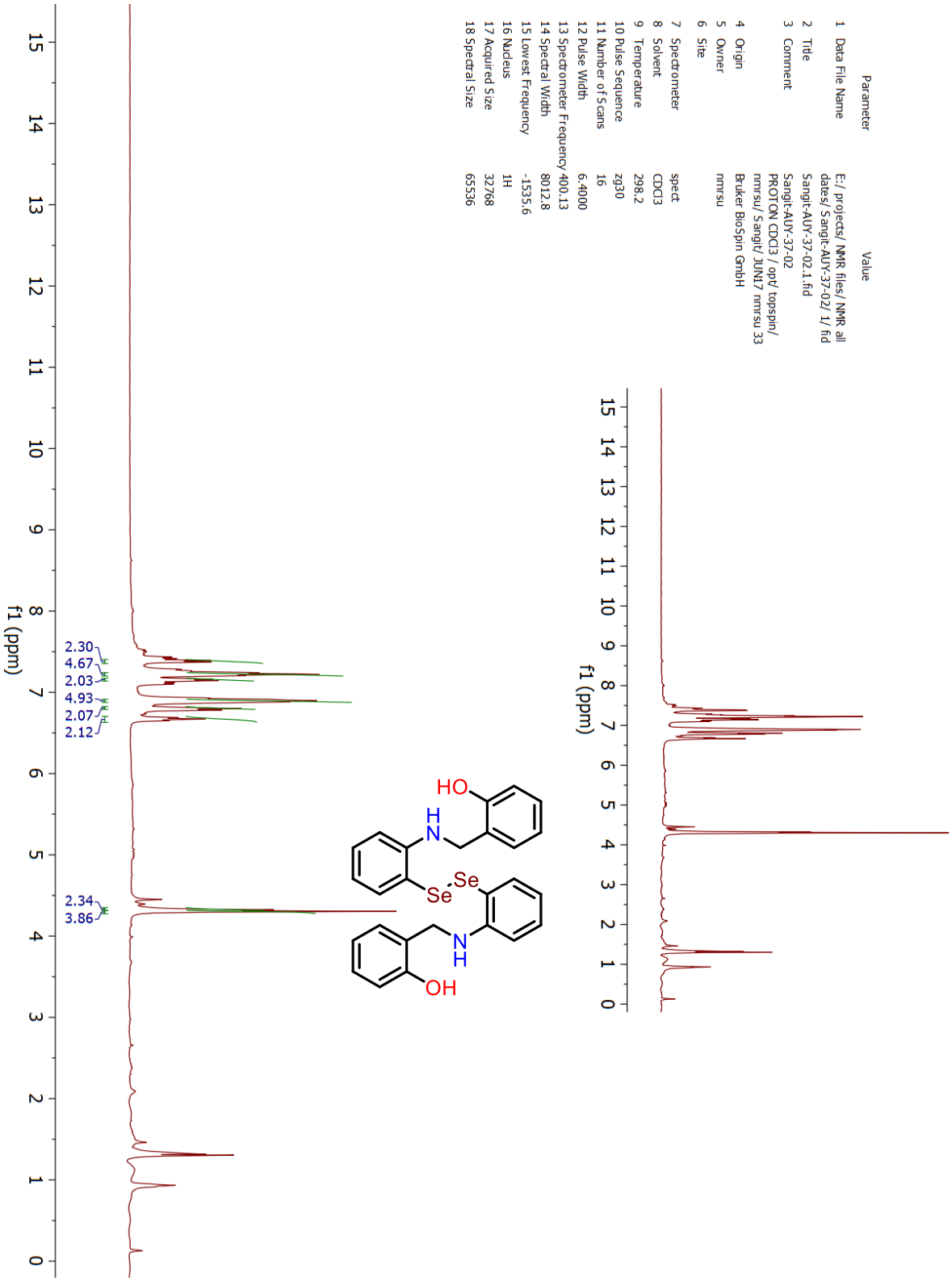
Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Not active	Set Capillary	4500 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	3000 m/z	Set Collision Cell RF	600.0 Vpp	Set Divert Valve	Waste







^{1}H NMR of **3a**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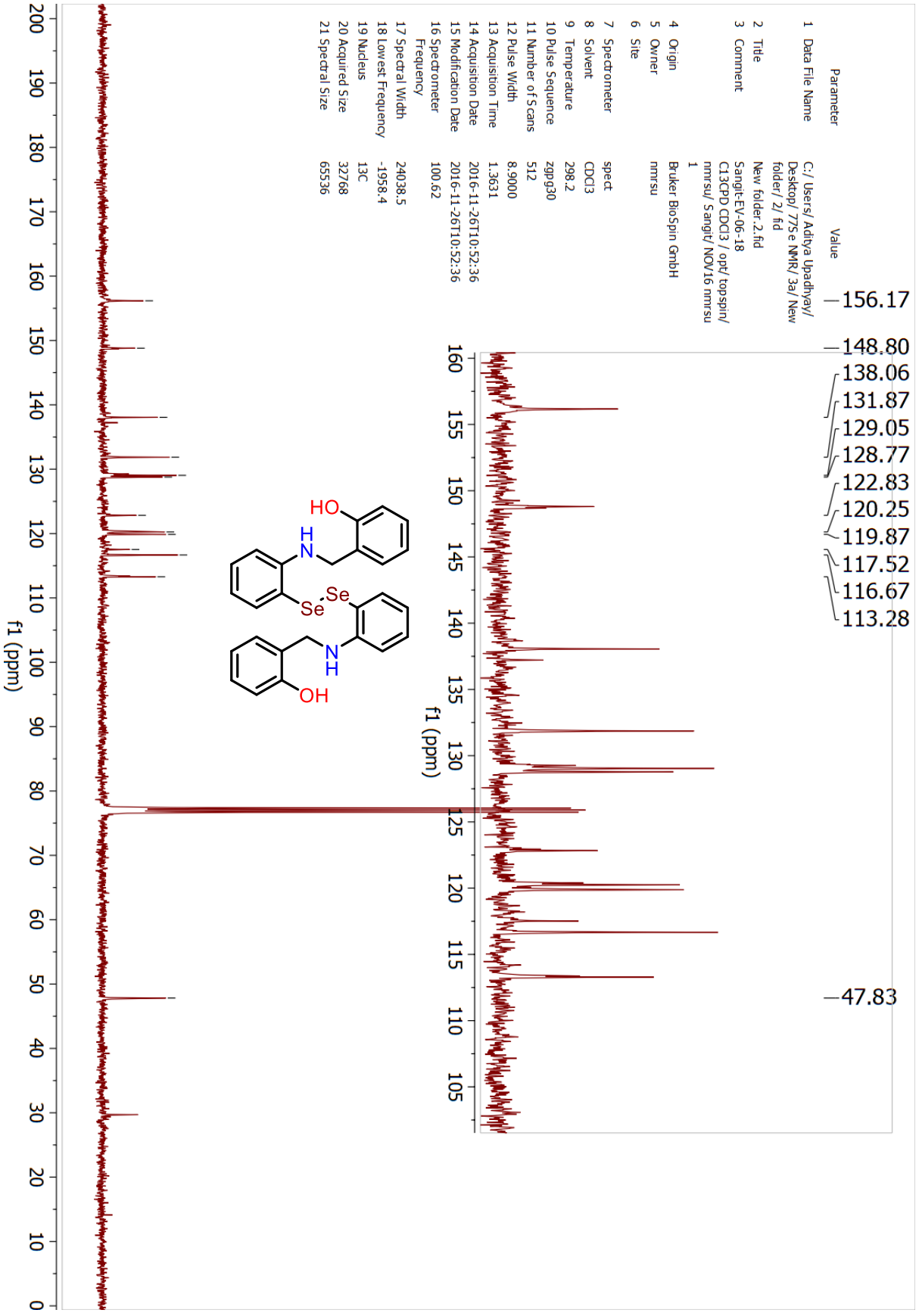
2 Title
Sangit-AUY-37-02.1.fid
3 Comment
Sangit-AUY-37-02
PROTON CDCl3 / opt/ topspin/ nmrsu/ Sangit/ JUN17 nmrsu 33
4 Origin
Bruker BioSpin GmbH
5 Owner
nmrsu
6 Site
7 Spectrometer
spect
8 Solvent
CDCl3
9 Temperature
298.2
10 Pulse Sequence
zg30
11 Number of Scans
16
12 Pulse Width
6.4000
13 Spectrometer Frequency
400.13
14 Spectral Width
8012.8
15 Lowest Frequency
-1535.6
16 Nucleus
1H
17 Acquired Size
32768
18 Spectral Size
65536
f1 (ppm)
2.30
4.67
2.03
4.93
2.07
2.12
2.34
3.86
HO
H
N
Se
Se
N
H
OH

^{13}C NMR of **3a**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2 Title
New folder.2.fid
3 Comment
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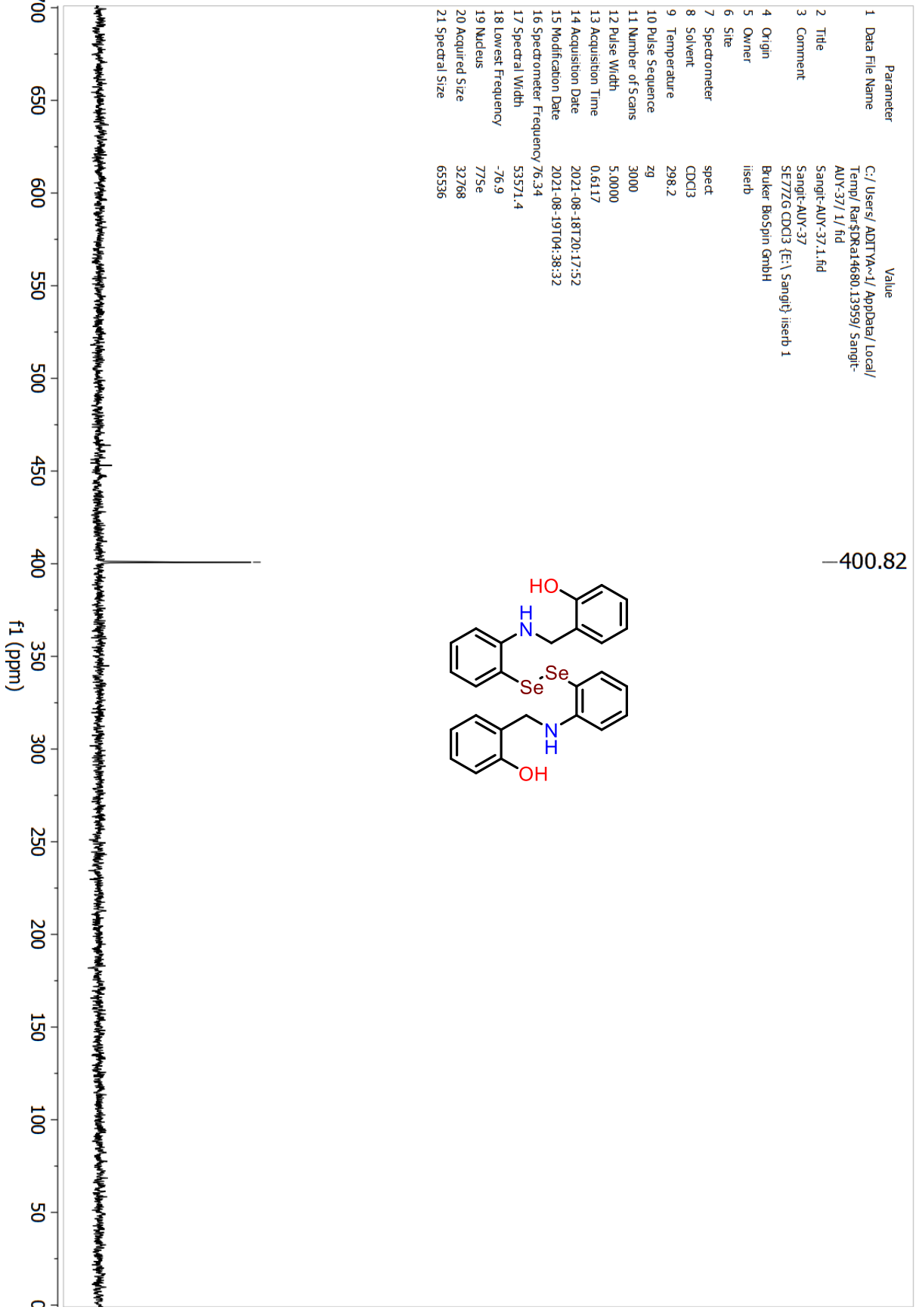
4 Origin
Bruker BioSpin GmbH
5 Owner
nmrsu
6 Site
7 Spectrometer
spect
8 Solvent
CDCl3
9 Temperature
298.2
10 Pulse Sequence
zgpg30
11 Number of Scans
512
12 Pulse Width
8.9000
13 Acquisition Time
1.3631
14 Acquisition Date
2016-11-26T10:52:36
15 Modification Date
2016-11-26T10:52:36
16 Spectrometer Frequency
100.62
17 Spectral Width
24038.5
18 Lowest Frequency
-1958.4
19 Nucleus
13C
20 Acquired Size
32768
21 Spectral Size
65536
156.17
148.80
138.06
131.87
129.05
128.77
122.83
120.25
119.87
117.52
116.67
113.28
47.83
HO
H
N
Se
Se
N
H
OH
f1 (ppm)
f1 (ppm)

^{77}Se NMR of **3a**



HRMS of **3a**

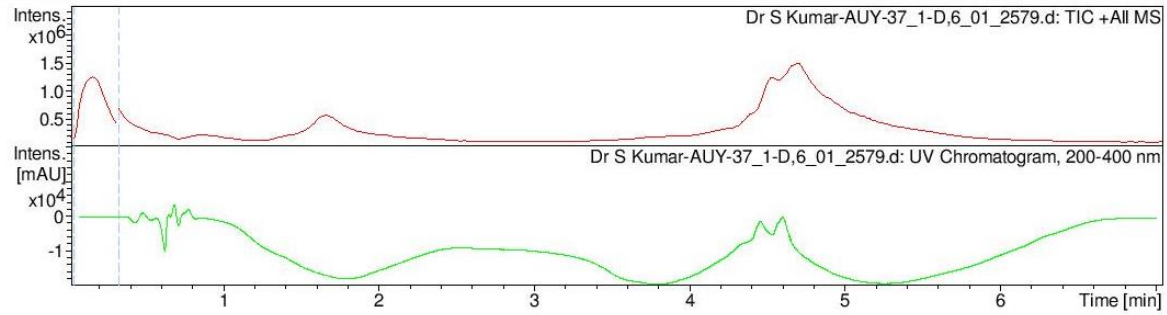
Display Report

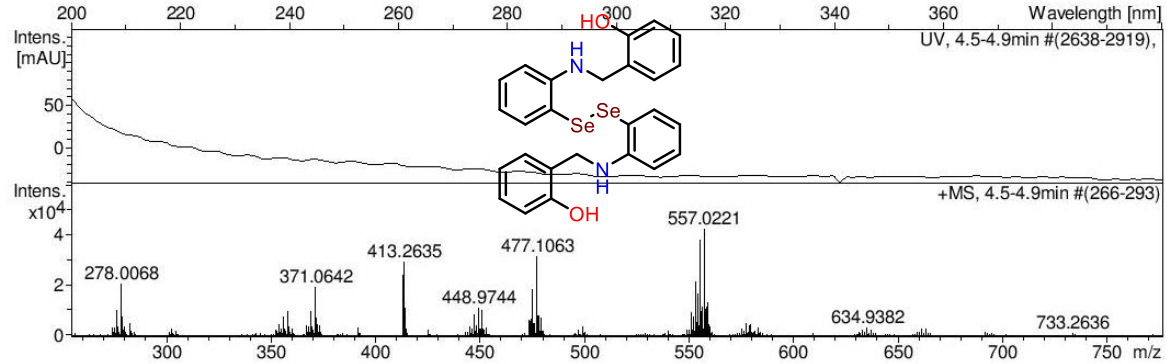
Analysis Info

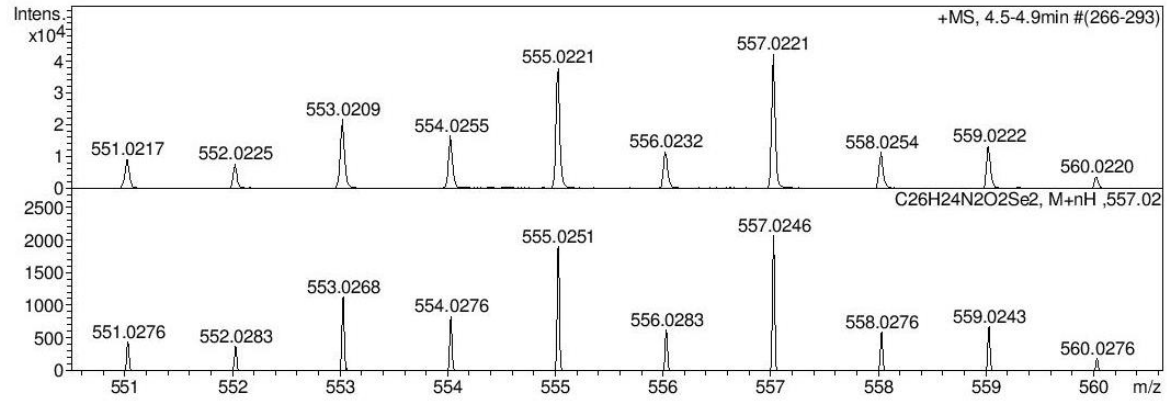
Analysis Name	D:\Data\user data\2017\JULY 2017\26 july\Dr S Kumar-AUY-37_1-D,6_01_2579.d	Acquisition Date	7/26/2017 12:18:57 PM
Method	hrlcms_pos_mid_tunemix.m	Operator	RUCHI SHRIVASTAVA
Sample Name	Dr S Kumar-AUY-37	Instrument	micrOTOF-Q II 10330
Comment			

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	450.0 Vpp	Set Divert Valve	Waste







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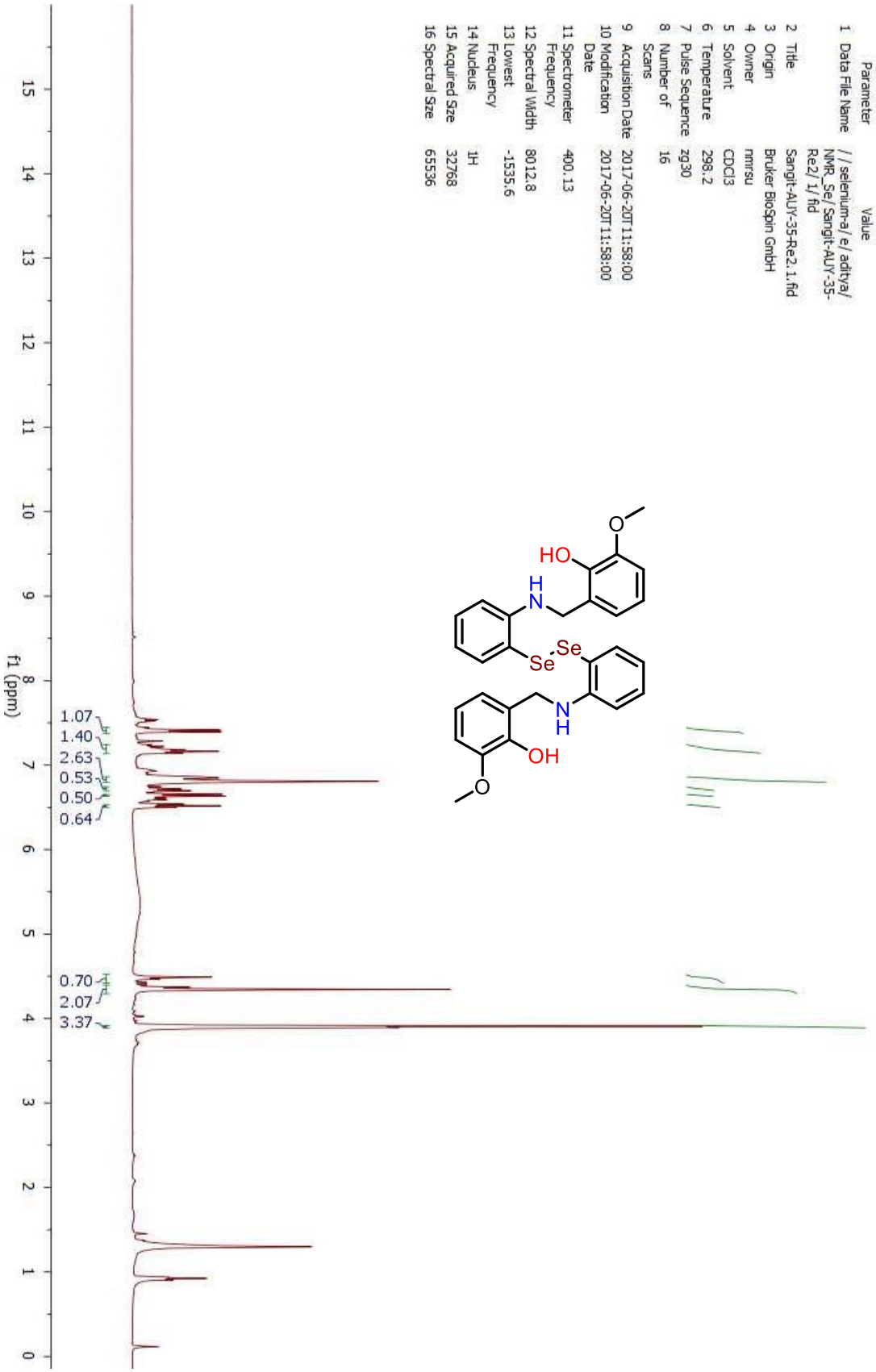
^{1}H NMR of **3b**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Value
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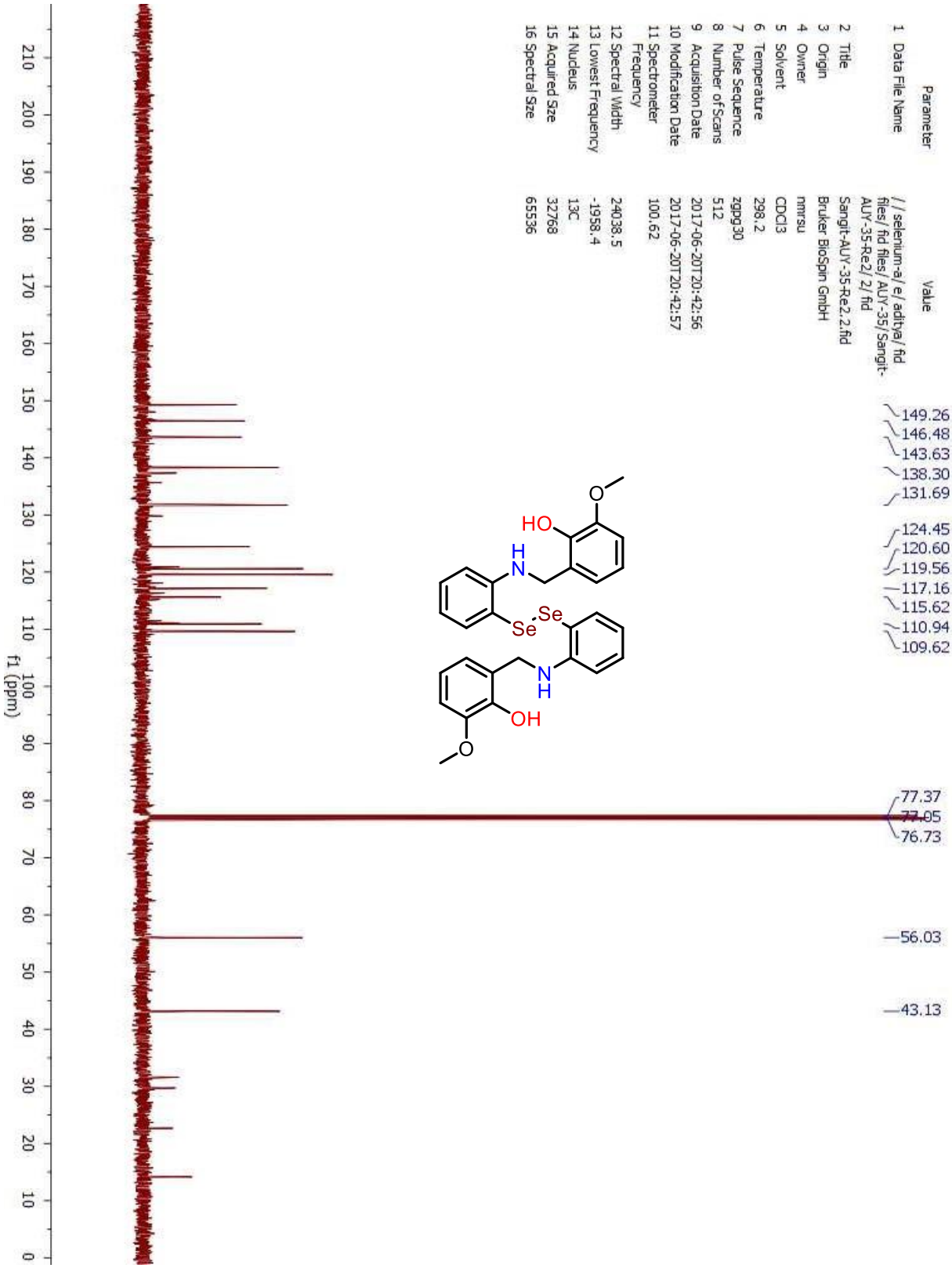
2 Title Sangit-AUY-35-Re2. 1. fid
3 Origin Bruker BioSpin GmbH
4 Owner nmrsu
5 Solvent CDCl3
6 Temperature 298. 2
7 Pulse Sequence zg30
8 Number of Scans 16
9 Acquisition Date 2017-06-20T11:58:00
10 Modification Date 2017-06-20T11:58:00
11 Spectrometer Frequency 400. 13
12 Spectral Width 8012. 8
13 Lowest Frequency -1535. 6
14 Nucleus 1H
15 Acquired Size 32768
16 Spectral Size 65536
HO
H
N
Se
Se
N
H
OH
O
O
f1 (ppm)
1.07
1.40
2.63
0.53
0.50
0.64
0.70
2.07
3.37

^{13}C NMR of **3b**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Value
1 Data File Name
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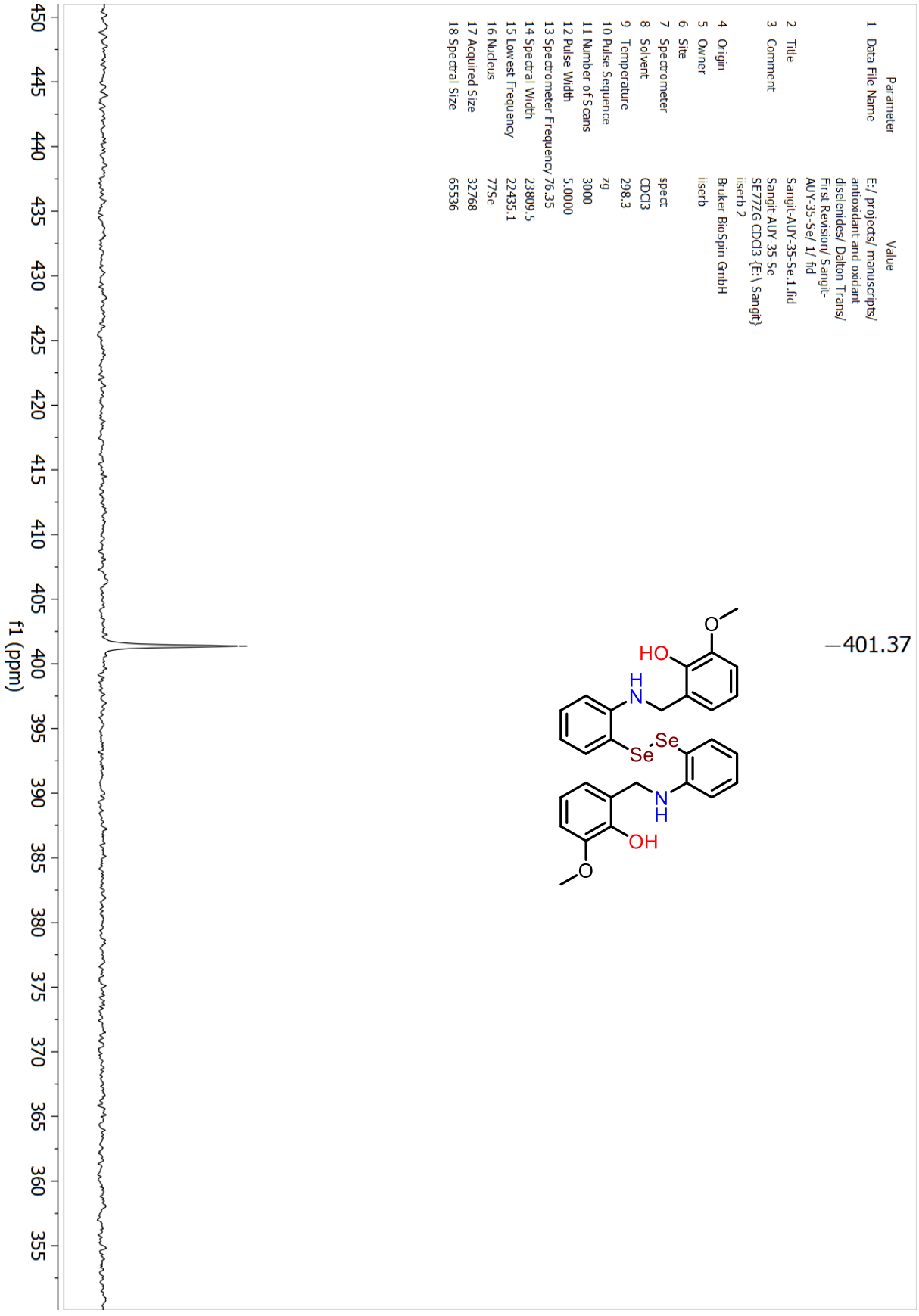
2 Title
Sangit-AUY-35-Re2.2.fid
3 Origin
Bruker BioSpin GmbH
4 Owner
nmrsu
5 Solvent
CDCl3
6 Temperature
298.2
7 Pulse Sequence
zgpg30
8 Number of Scans
512
9 Acquisition Date
2017-06-20T20:42:56
10 Modification Date
2017-06-20T20:42:57
11 Spectrometer Frequency
100.62
12 Spectral Width
24038.5
13 Lowest Frequency
-1958.4
14 Nucleus
13C
15 Acquired Size
32768
16 Spectral Size
65536
149.26
146.48
143.63
138.30
131.69
124.45
120.60
119.56
117.16
115.62
110.94
109.62
77.37
77.05
76.73
56.03
43.13
HO
O
H
N
Se
Se
N
H
OH
O
f1 (ppm)

^{77}Se NMR of **3b**



HRMS of **3b**

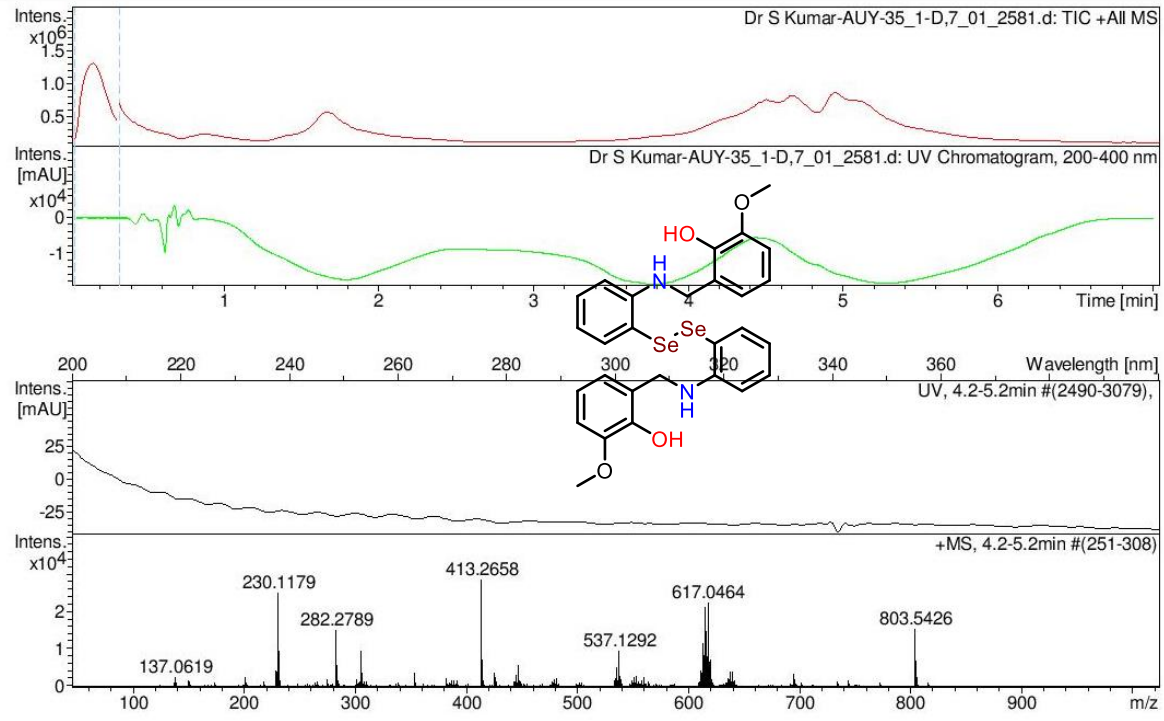
Display Report

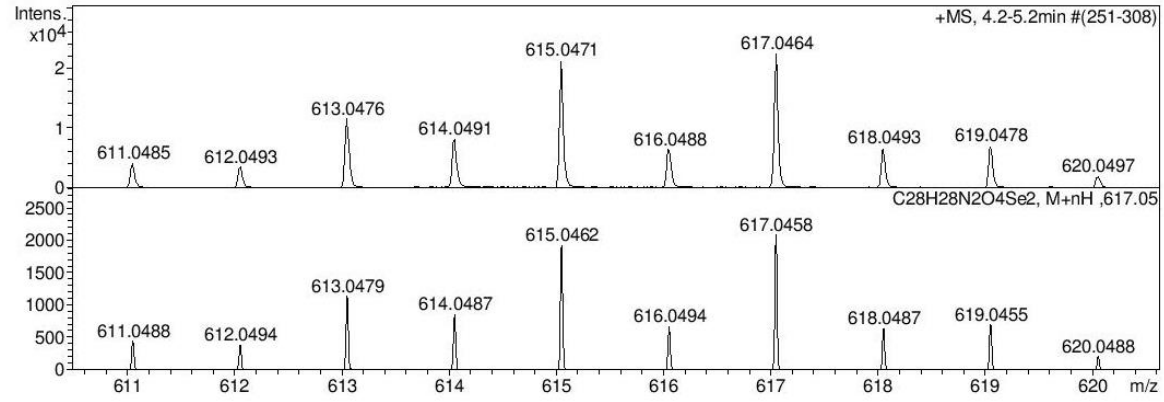
Analysis Info

Analysis Name	D:\Data\user data\2017\JULY 2017\26 july\Dr S Kumar-AUY-35_1-D,7_01_2581.d	Acquisition Date	7/26/2017 12:35:24 PM
Method	hrlcms_pos_mid_tunemix.m	Operator	RUCHI SHRIVASTAVA
Sample Name	Dr S Kumar-AUY-35	Instrument	micrOTOF-Q II 10330
Comment			

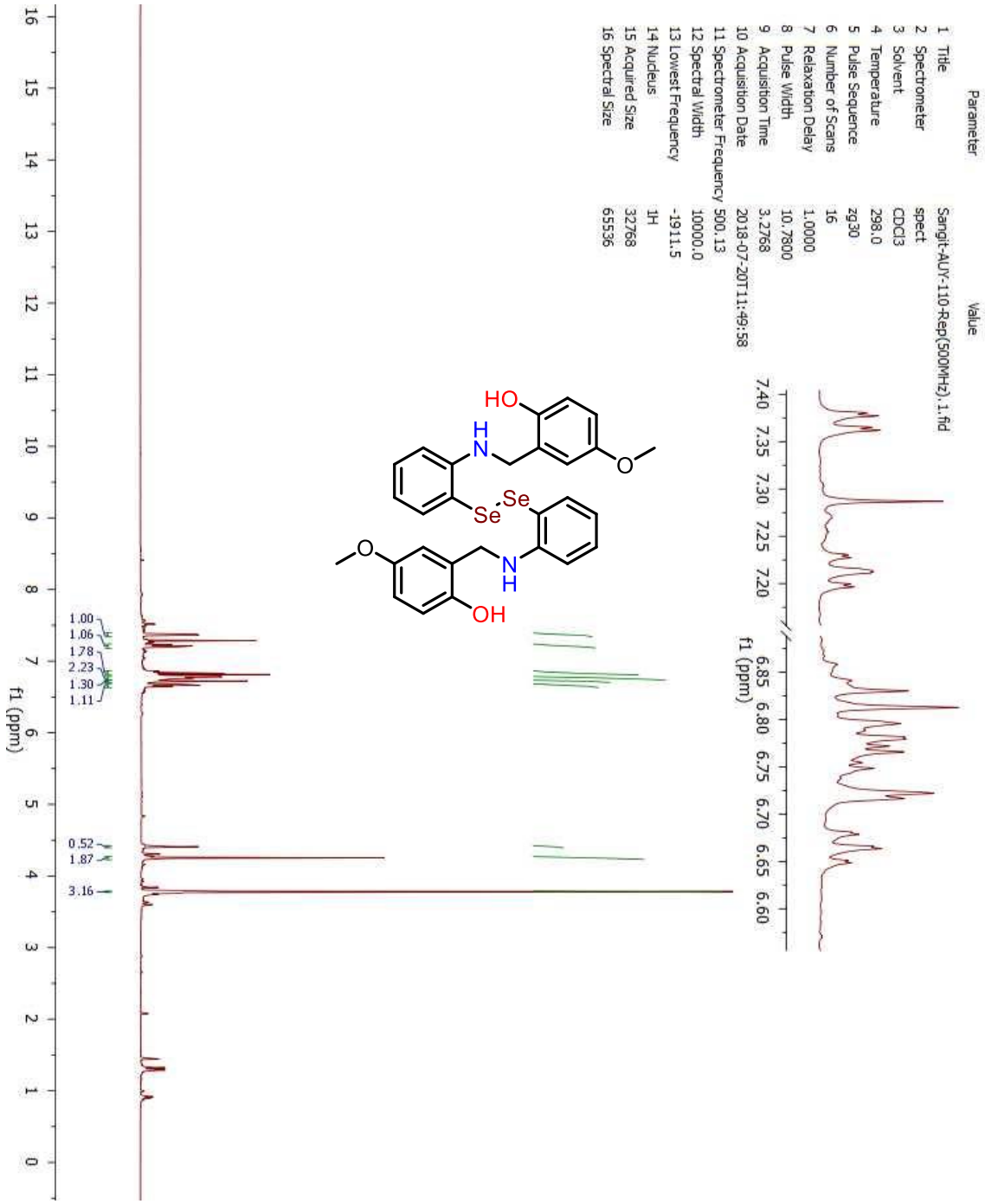
Acquisition Parameter

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	450.0 Vpp	Set Divert Valve	Waste

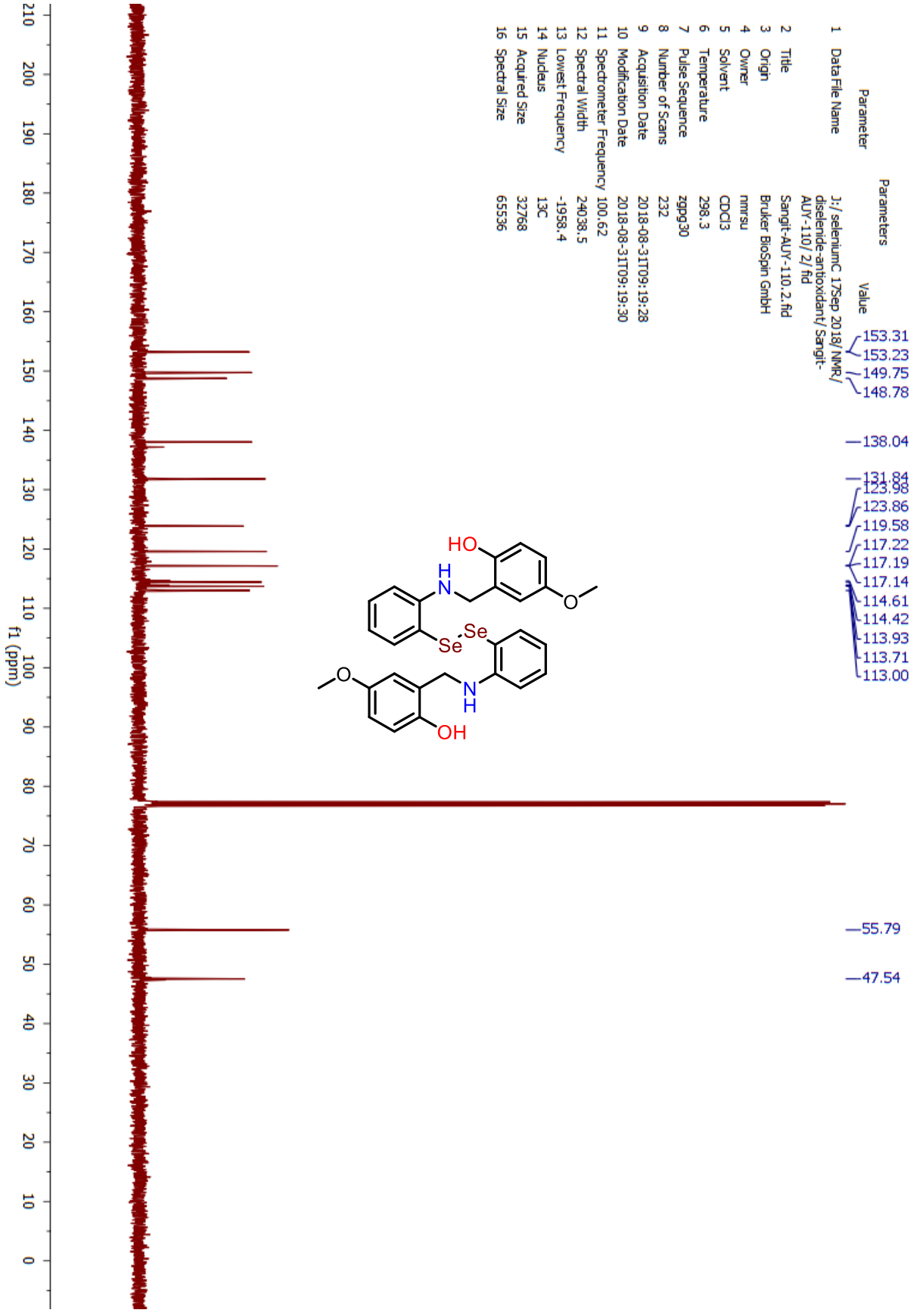




^{1}H NMR of **3c**


Parameter
Value
1 Title
Sangit-AUY-110-Rep(500MHz).1.fid
2 Spectrometer
spect
3 Solvent
CDCl3
4 Temperature
298.0
5 Pulse Sequence
zg30
6 Number of Scans
16
7 Relaxation Delay
1.0000
8 Pulse Width
10.7800
9 Acquisition Time
3.2768
10 Acquisition Date
2018-07-20T11:49:58
11 Spectrometer Frequency
500.13
12 Spectral Width
10000.0
13 Lowest Frequency
-1911.5
14 Nucleus
1H
15 Acquired Size
32768
16 Spectral Size
65536
HO
H
N
Se
Se
O
N
H
O
OH
1.00
1.06
1.78
2.23
1.30
1.11
0.52
1.87
3.16
f1 (ppm)

^{13}C NMR of **3c**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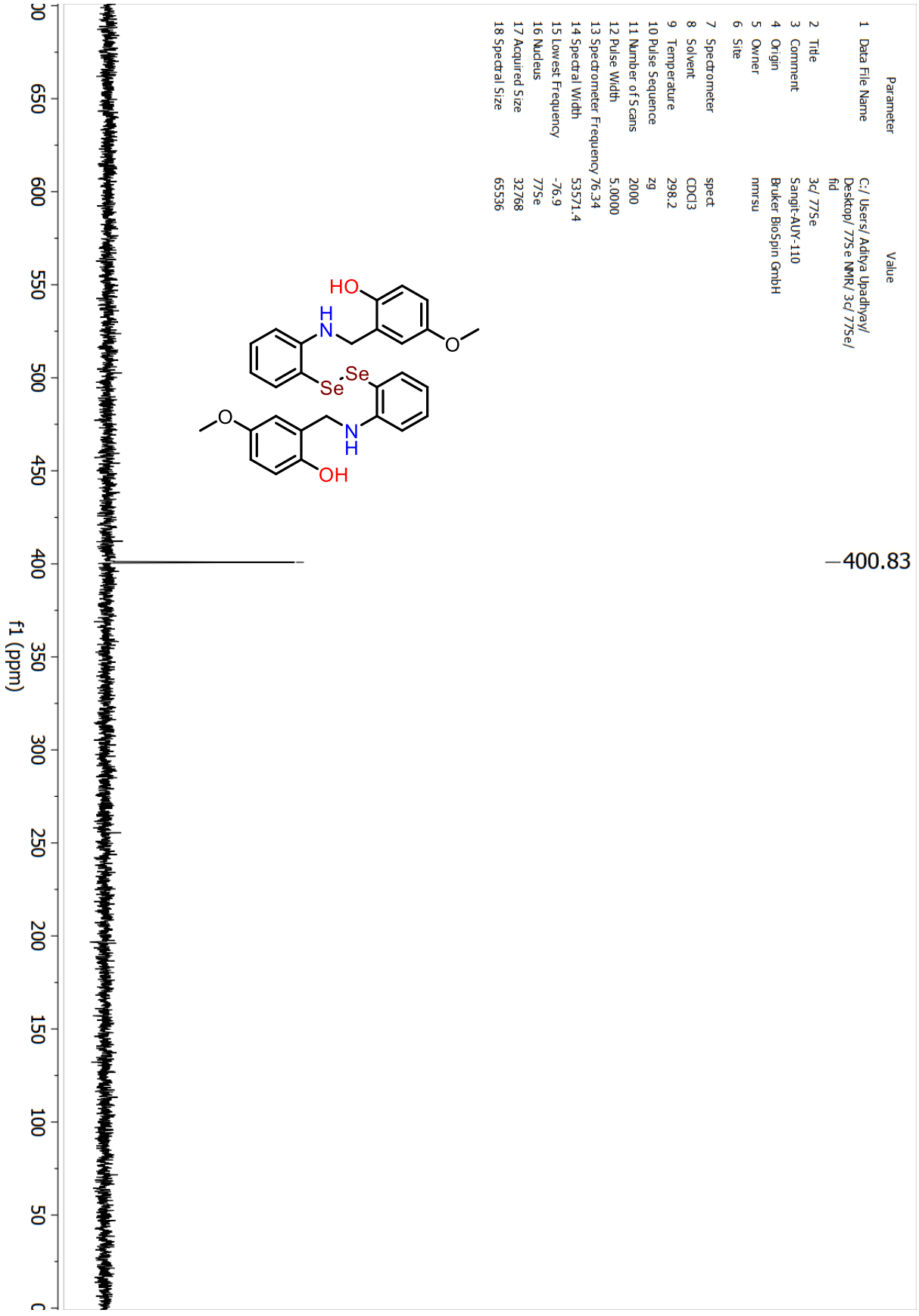
Value
1 Data File Name J:/ seleniumC 17Sep 2018/ NMR/ diselenide-antioxidant/ Sangit-AUY-110/ 2/ fid
2 Title Sangit-AUY-110.2.fid
3 Origin Bruker BioSpin GmbH
4 Owner nmrsu
5 Solvent CDCl3
6 Temperature 298.3
7 Pulse Sequence zgpg30
8 Number of Scans 232
9 Acquisition Date 2018-08-31T09:19:28
10 Modification Date 2018-08-31T09:19:30
11 Spectrometer Frequency 100.62
12 Spectral Width 24038.5
13 Lowest Frequency -1958.4
14 Nucleus 13C
15 Acquired Size 32768
16 Spectral Size 65536
153.31
153.23
149.75
148.78
138.04
131.84
123.98
123.86
119.58
117.22
117.19
117.14
114.61
114.42
113.93
113.71
113.00
55.79
47.54
HO
H
N
Se
Se
O
O
N
H
OH
f1 (ppm)

^{77}Se NMR of **3c**



HRMS of **3c**

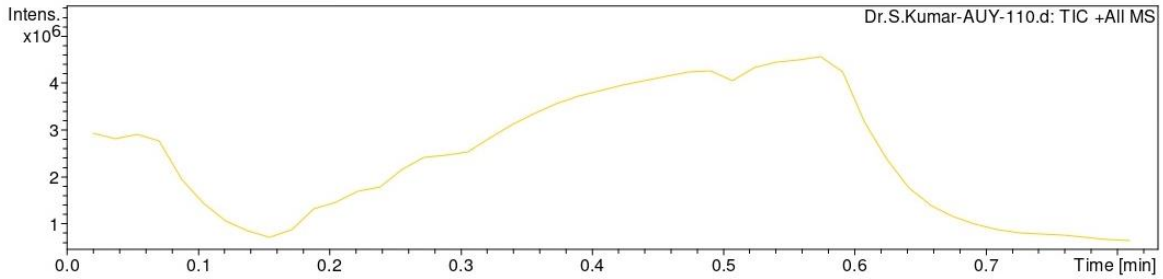
Display Report

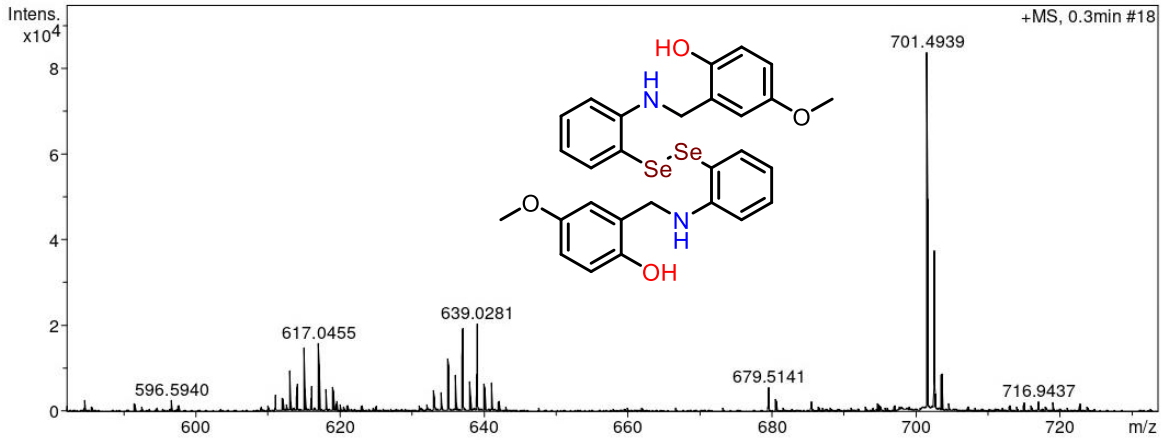
Analysis Info

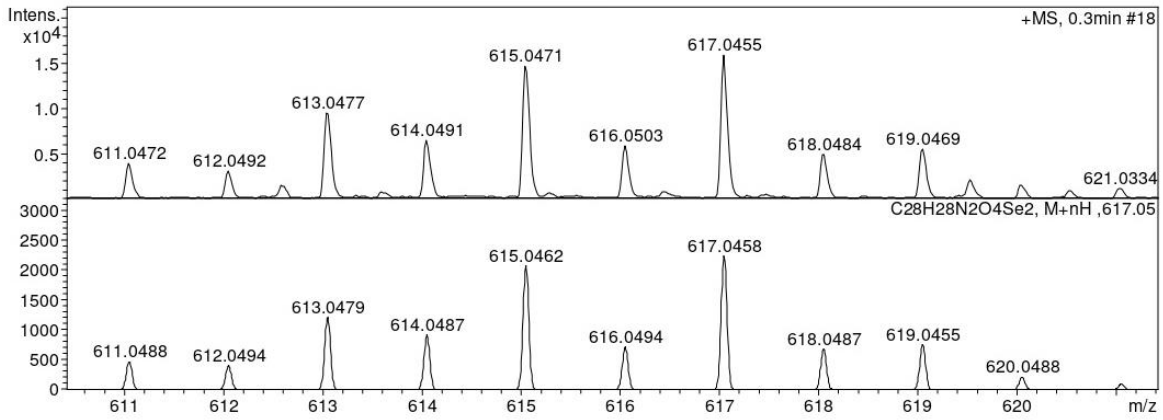
Analysis Name	D:\Data\NEW USER DATA 2017\2018\AUGUST 2018\29 AUG\Dr.S.Kumar-AUY-110.d	Acquisition Date	8/29/2018 4:29:14 PM
Method	tune_wide.m	Operator	RUCHI
Sample Name	AUY-110	Instrument	micrOTOF-Q II 10330
Comment			

Acquisition Parameter

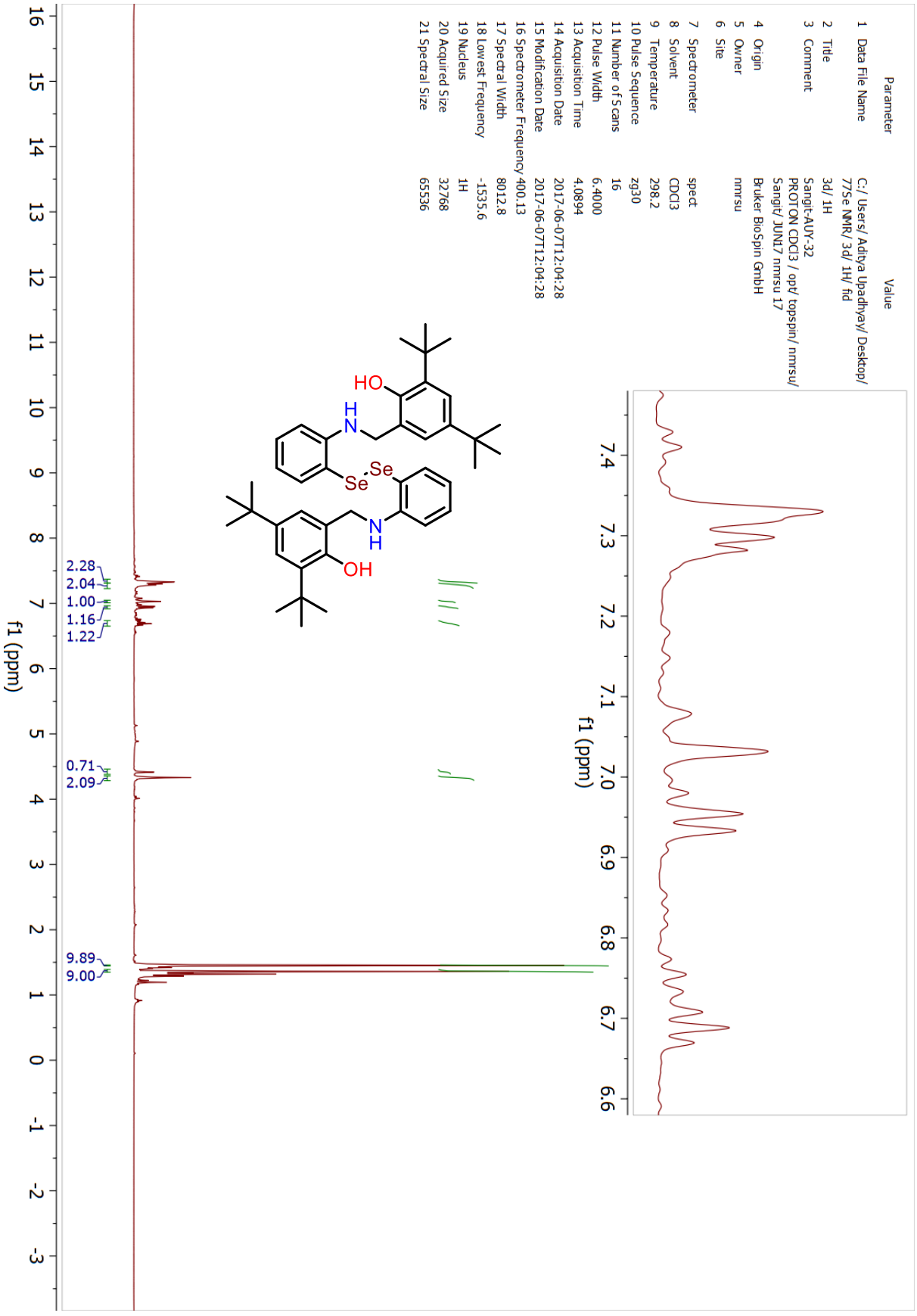
Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Not active	Set Capillary	4500 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	3000 m/z	Set Collision Cell RF	600.0 Vpp	Set Divert Valve	Waste







^{1}H NMR of **3d**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Value
1 Data File Name
C:/ Users/ Aditya Upadhyay/ Desktop/ 77Se NMR/ 3d/ 1H/ fid
2 Title
3d/ 1H
3 Comment
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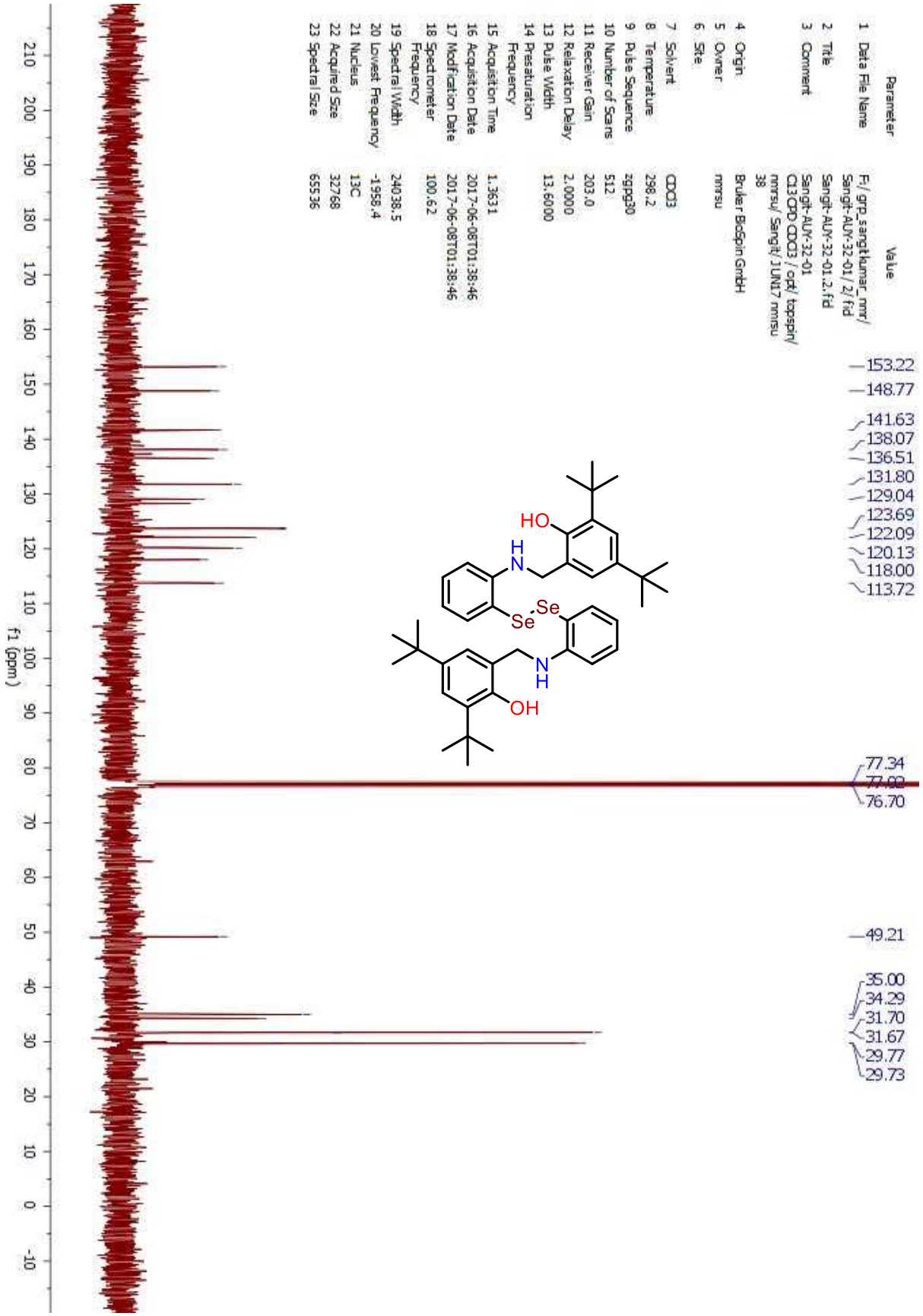
4 Origin
Bruker BioSpin GmbH
5 Owner
nmrsu
6 Site
7 Spectrometer
spect
8 Solvent
CDCl3
9 Temperature
298.2
10 Pulse Sequence
zg30
11 Number of Scans
16
12 Pulse Width
6.4000
13 Acquisition Time
4.0894
14 Acquisition Date
2017-06-07T12:04:28
15 Modification Date
2017-06-07T12:04:28
16 Spectrometer Frequency
400.13
17 Spectral Width
8012.8
18 Lowest Frequency
-1535.6
19 Nucleus
1H
20 Acquired Size
32768
21 Spectral Size
65536
HO
H
N
Se
Se
N
H
OH
2.28
2.04
1.00
1.16
1.22
0.71
2.09
9.89
9.00
f1 (ppm)
f1 (ppm)

^{13}C NMR of **3d**


Parameter
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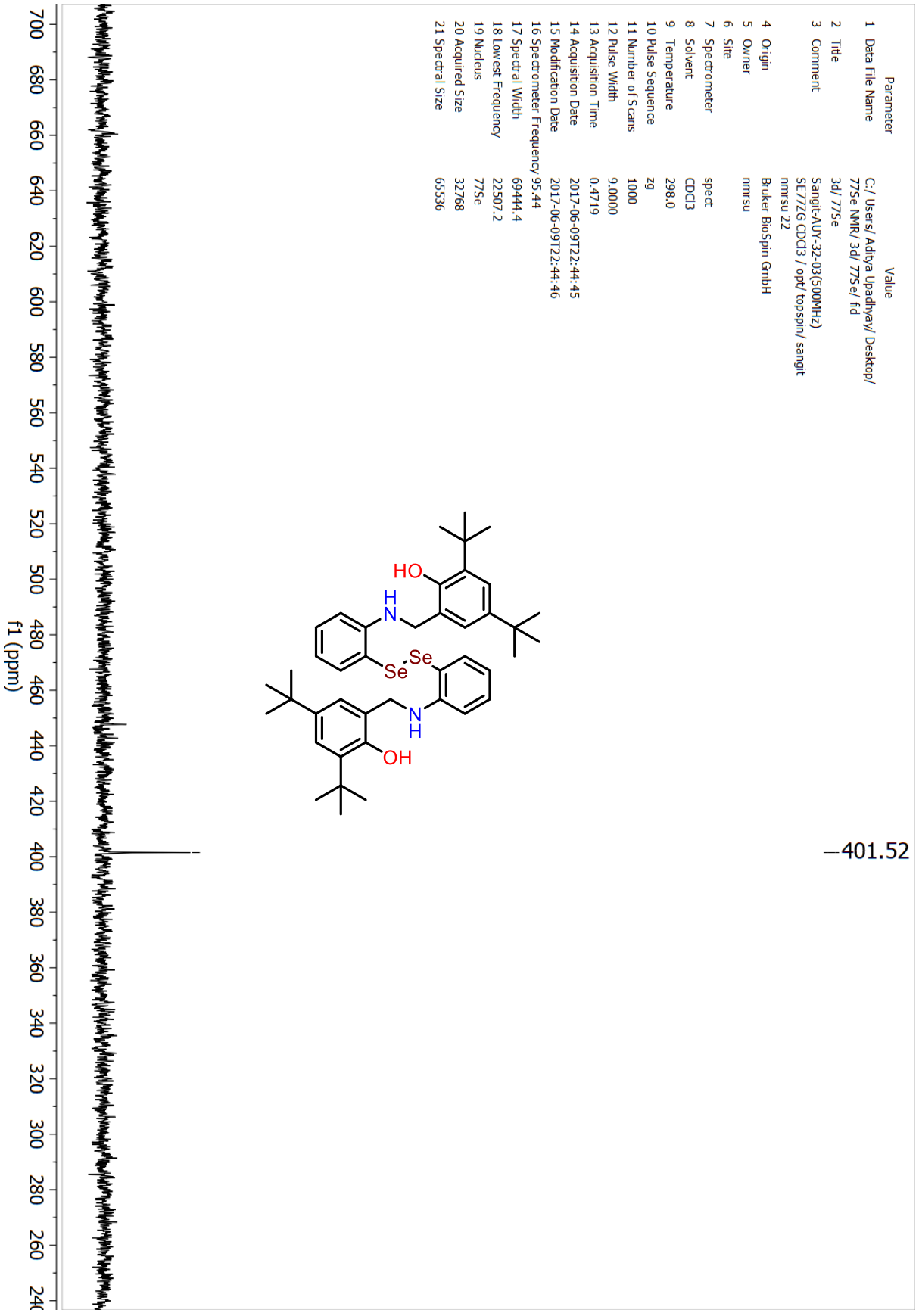
1 Data File Name
F:/ grp sangtkumar nmr/ Sangit-AUY-32-01/ 2/ fid
2 Title
Sangit-AUY-32-01.2.fid
3 Comment
Sangit-AUY-32-01 CL3 CPD CDCl3 / opt/ topspin/ nmrsu/ Sangit/ JUN17 nmrsu 38
4 Origin
Bruker BioSpin GmbH
5 Owner
nmrsu
6 Site
7 Solvent
CDCl3
8 Temperature
298.2
9 Pulse Sequence
zgpg30
10 Number of Scans
512
11 Receiver Gain
203.0
12 Relaxation Delay
2.0000
13 Pulse Width
13.6000
14 Presaturation Frequency
15 Acquisition Time
1.3631
16 Acquisition Date
2017-06-08T01:38:46
17 Modification Date
2017-06-08T01:38:46
18 Spectrometer Frequency
100.62
19 Spectral Width
24038.5
20 Lowest Frequency
-1958.4
21 Nucleus
13C
22 Acquired Size
32768
23 Spectral Size
65536
153.22
148.77
141.63
138.07
136.51
131.80
129.04
123.69
122.09
120.13
118.00
113.72
77.34
77.02
76.70
49.21
35.00
34.29
31.70
31.67
29.77
29.73
HO
HN
Se
Se
N
H
OH
f1 (ppm)

^{77}Se NMR of **3d**



HRMS of **3d**

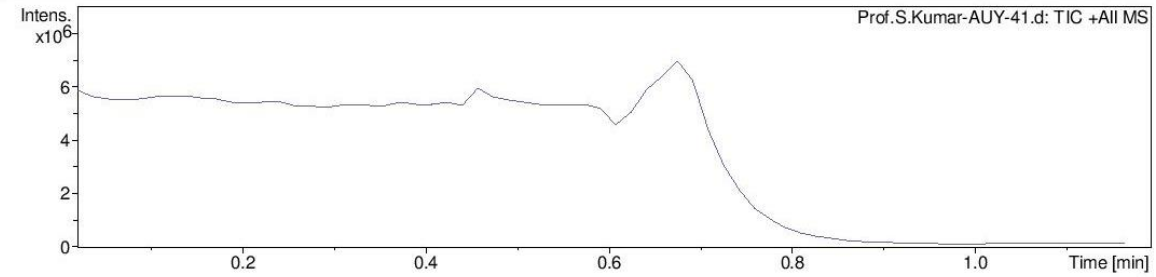
Display Report

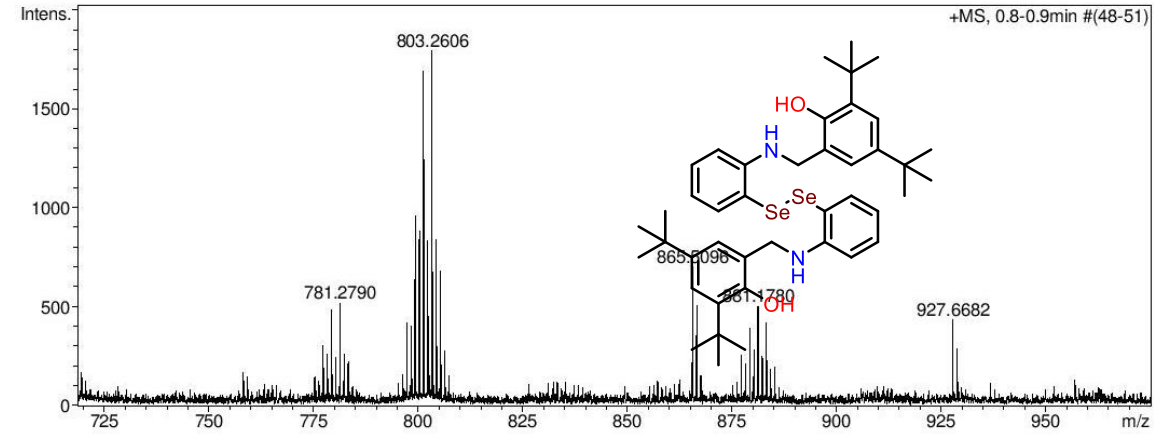
Analysis Info

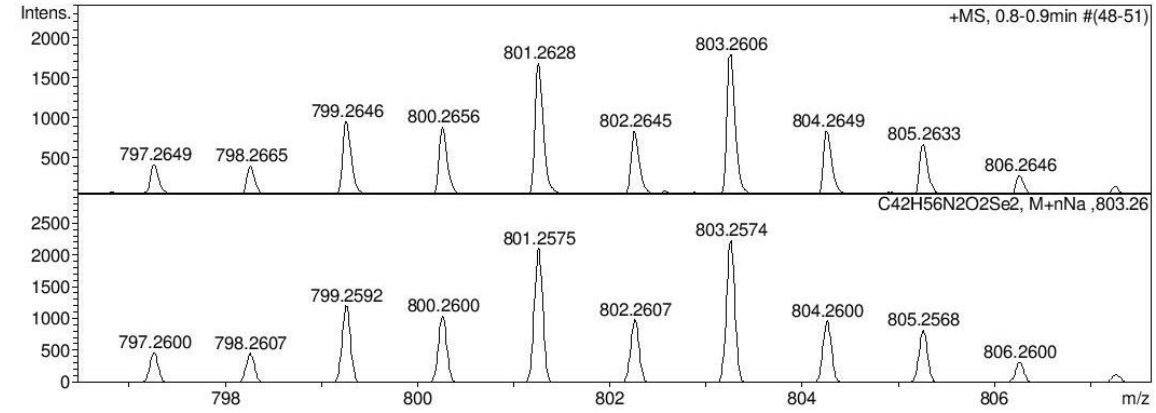
Analysis Name	D:\Data\NEW USER DATA 2017\2018\JUNE 2018\15 june\Prof.S.Kumar-AUY-41.d	Acquisition Date	6/15/2018 4:24:33 PM
Method	tune_wide.m	Operator	RUCHI
Sample Name	AUY-41	Instrument	micrOTOF-Q II 10330
Comment			

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Not active	Set Capillary	4500 V	Set Dry Heater	180 °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	700.0 Vpp	Set Divert Valve	Waste

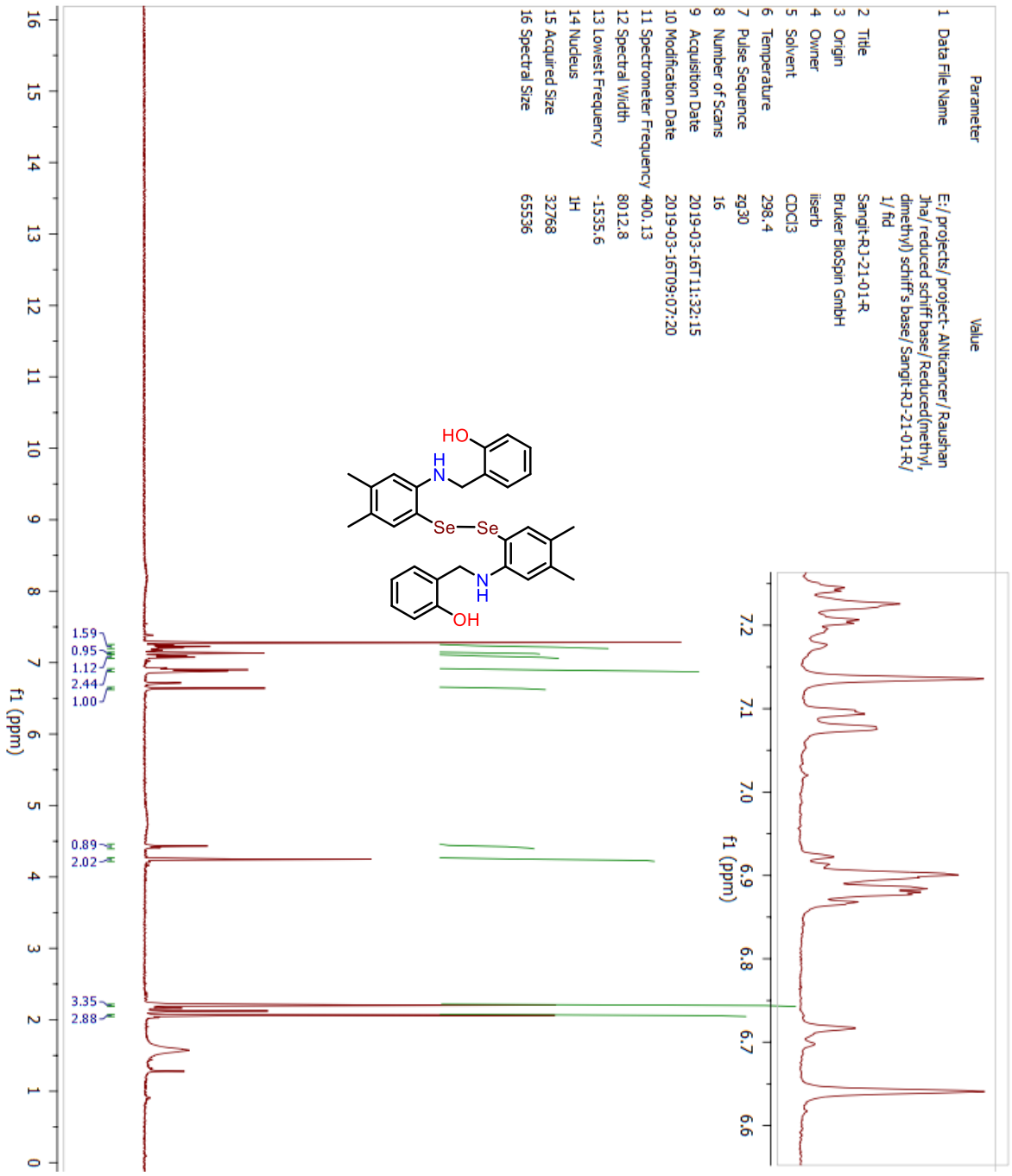




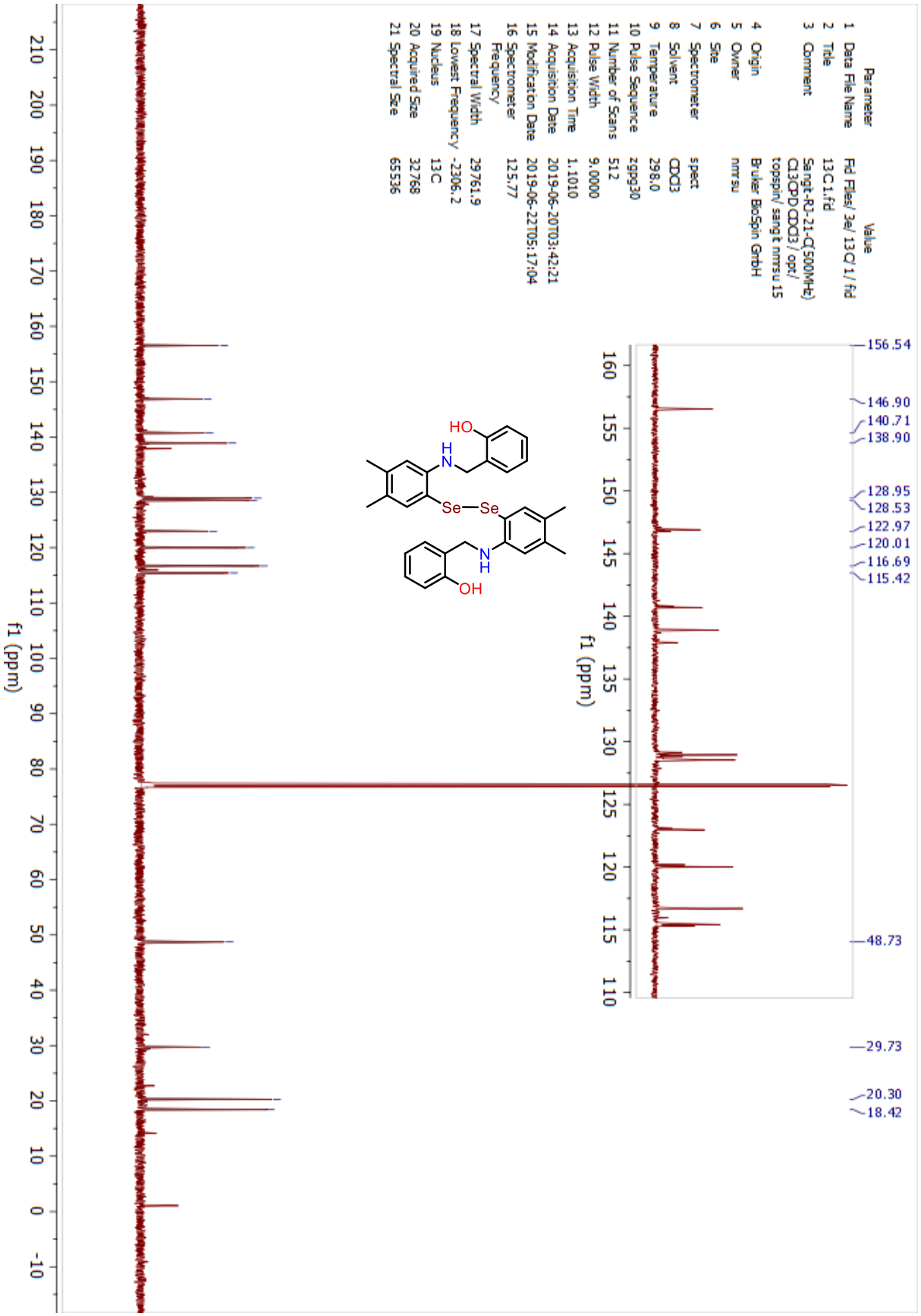


Bruker Compass DataAnalysis 4.0 printed: 6/15/2018 4:26:33 PM Page 1 of 1

^{1}H NMR of **3e**


Parameter
Value
1 Data File Name
E:/ projects/ project- ANticancer/ Raushan Jha/ reduced schiff base/ Reduced(methyl, dimethyl) schiff's base/ Sangit-RJ-21-01-R/ 1/ fid
2 Title
Sangit-RJ-21-01-R
3 Origin
Bruker BioSpin GmbH
4 Owner
iiserb
5 Solvent
CDCl3
6 Temperature
298.4
7 Pulse Sequence
zg30
8 Number of Scans
16
9 Acquisition Date
2019-03-16T11:32:15
10 Modification Date
2019-03-16T09:07:20
11 Spectrometer Frequency
400.13
12 Spectral Width
8012.8
13 Lowest Frequency
-1535.6
14 Nucleus
1H
15 Acquired Size
32768
16 Spectral Size
65536
HO
HN
Se
Se
NH
OH
1.59
0.95
1.12
2.44
1.00
0.89
2.02
3.35
2.88
f1 (ppm)
f1 (ppm)

^{13}C NMR of **3e**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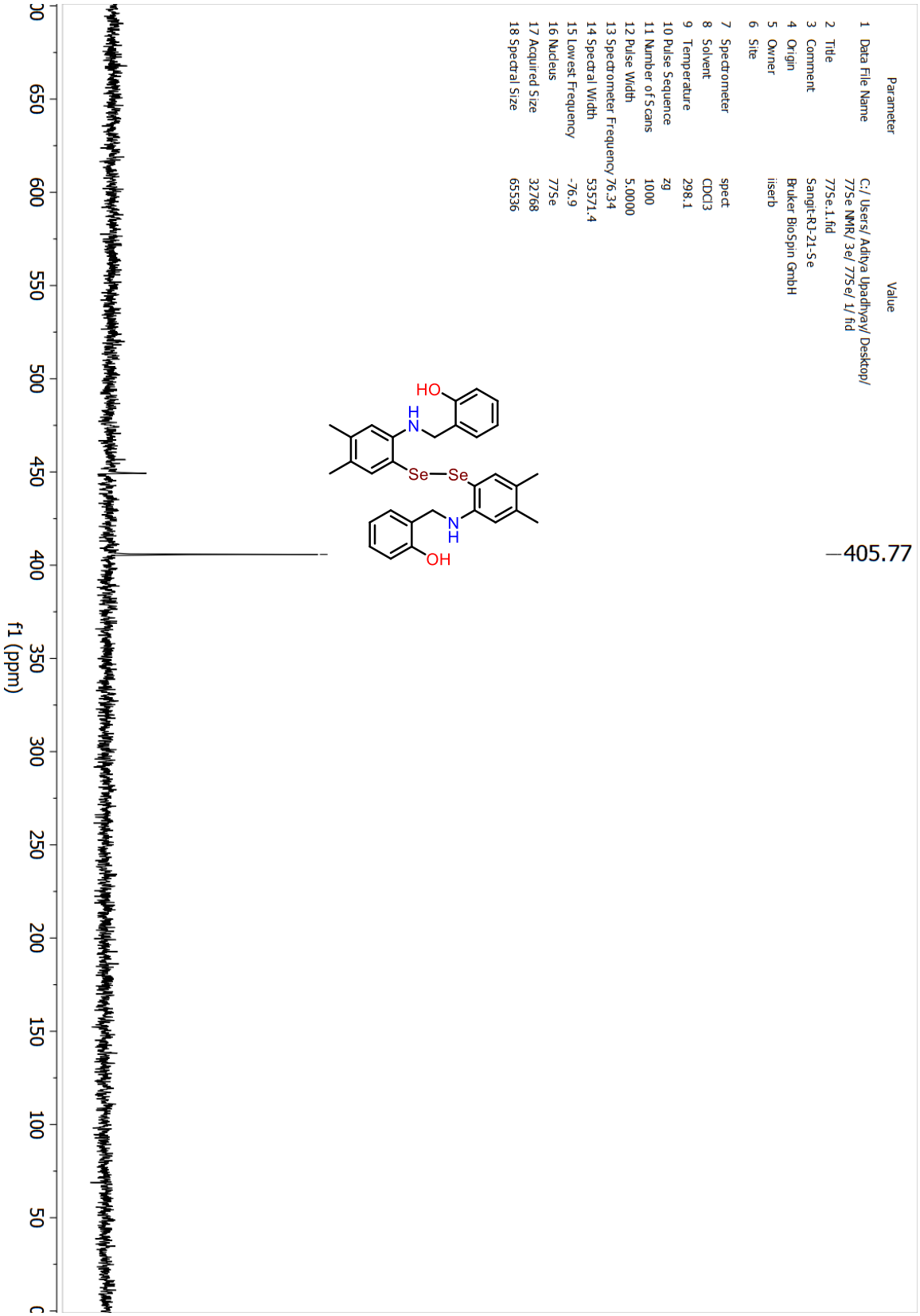
2 Title 13C1.fid
3 Comment Sangit-RJ-21-C[500MHz] CL3OPD CDCl3 / opt/ topspin/ sangit nmrsu 15
4 Origin Bruker BioSpin GmbH
5 Owner nmrsu
6 Site
7 Spectrometer spect
8 Solvent CDCl3
9 Temperature 298.0
10 Pulse Sequence zgpg30
11 Number of Scans 512
12 Pulse Width 9.0000
13 Acquisition Time 1.1010
14 Acquisition Date 2019-06-20T03:42:21
15 Modification Date 2019-06-22T05:17:04
16 Spectrometer Frequency 125.77
17 Spectral Width 29761.9
18 Lowest Frequency -2306.2
19 Nucleus 13C
20 Acquired Size 32768
21 Spectral Size 65536
HO
H
N
Se—Se
N
H
OH
156.54
146.90
140.71
138.90
128.95
128.53
122.97
120.01
116.69
115.42
48.73
29.73
20.30
18.42
f1 (ppm)
f1 (ppm)

^{77}Se NMR of **3e**



An additional peak at 451ppm was observed due to the impurity and could not be removed because of the greasy nature

HRMS of **3e**

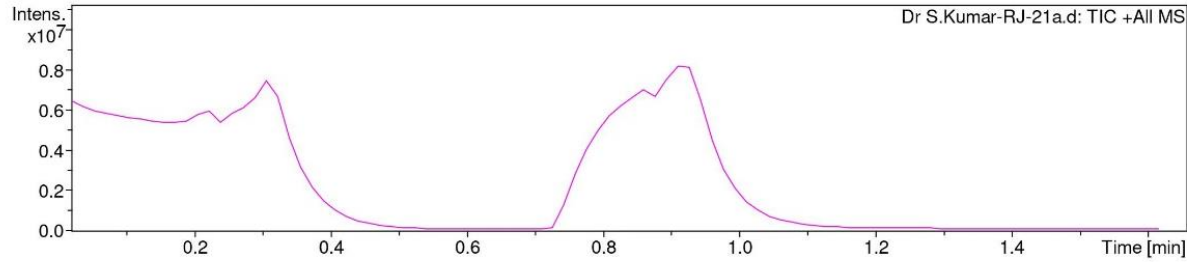
Display Report

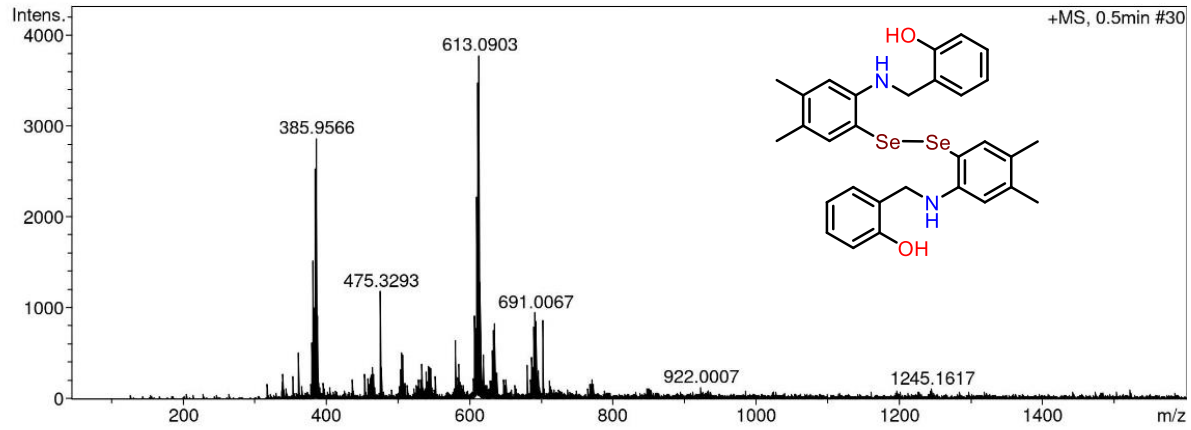
Analysis Info

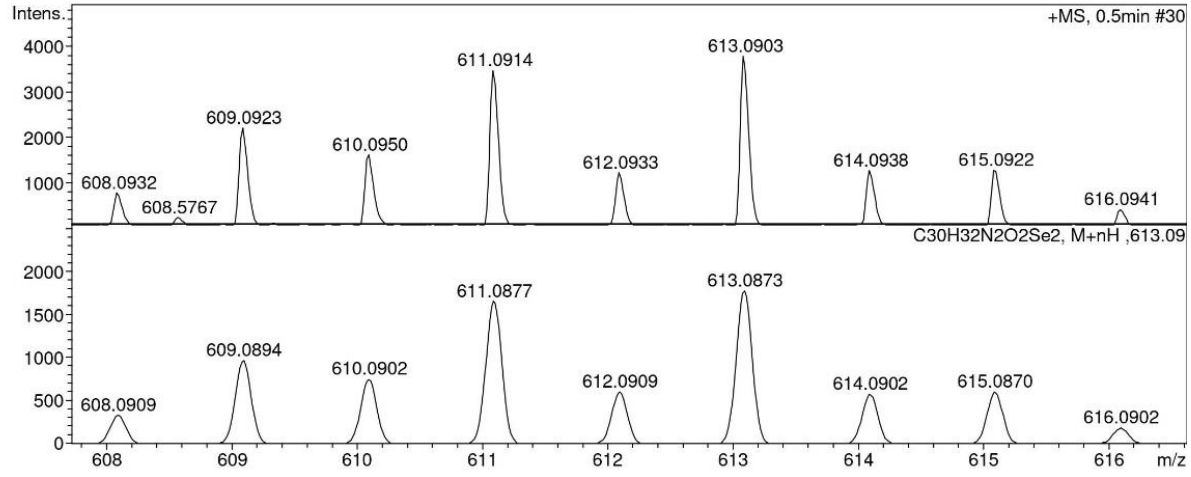
Analysis Name	D:\Data\NEW USER DATA 2017\2019\MAR\15 MAR\Dr S.Kumar-RJ-21a.d	Acquisition Date	3/15/2019 3:45:16 PM
Method	tune_wide.m	Operator	RUCHI
Sample Name	RJ-21a	Instrument	micrOTOF-Q II 10330
Comment			

Acquisition Parameter

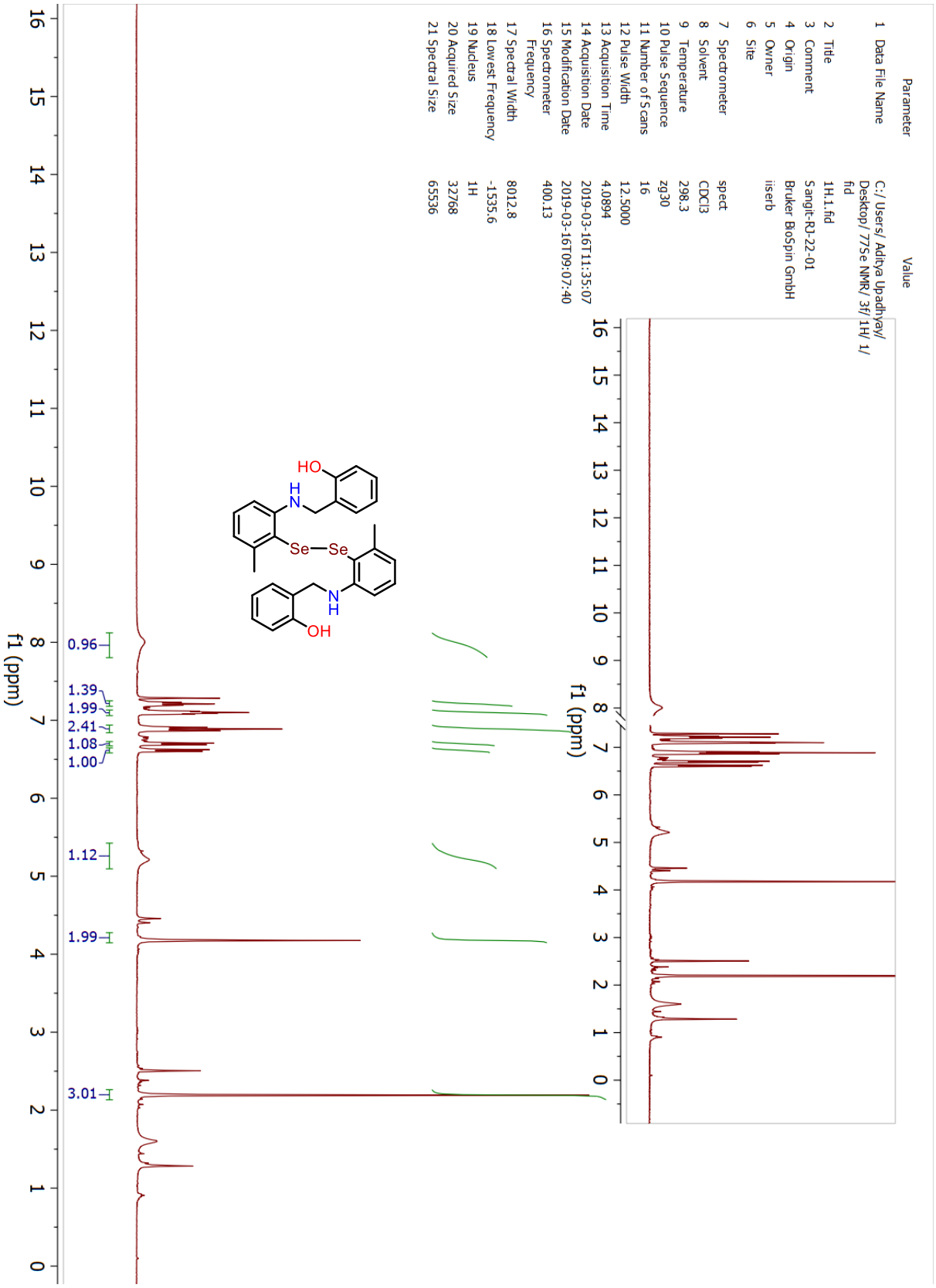
Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Not active	Set Capillary	4500 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	3000 m/z	Set Collision Cell RF	600.0 Vpp	Set Divert Valve	Waste



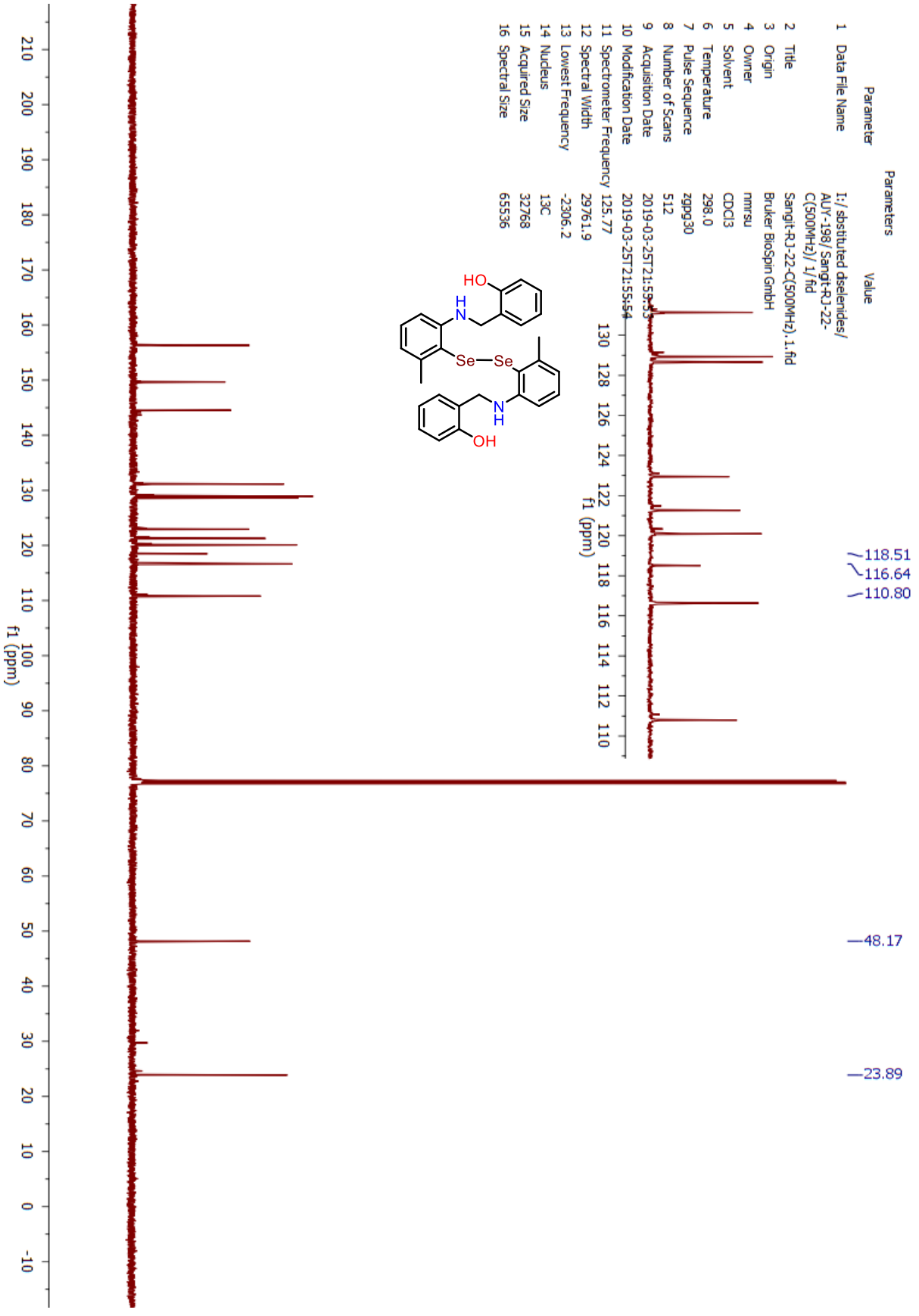




^{1}H NMR of **3f**


Parameter
Value
1 Data File Name
C:/ Users/ Aditya Upadhyay/ Desktop/ 77Se NMR/ 3f/ 1H/ 1/ fid
2 Title
1H.1.fid
3 Comment
Sangit-RJ-22-01
4 Origin
Bruker BioSpin GmbH
5 Owner
iiserb
6 Site
7 Spectrometer
spect
8 Solvent
CDCl3
9 Temperature
298.3
10 Pulse Sequence
zg30
11 Number of Scans
16
12 Pulse Width
12.5000
13 Acquisition Time
4.0894
14 Acquisition Date
2019-03-16T11:35:07
15 Modification Date
2019-03-16T09:07:40
16 Spectrometer Frequency
400.13
17 Spectral Width
8012.8
18 Lowest Frequency
-1535.6
19 Nucleus
1H
20 Acquired Size
32768
21 Spectral Size
65536
HO
H
N
Se
Se
N
H
OH
0.96
1.39
1.99
2.41
1.08
1.00
1.12
1.99
3.01
f1 (ppm)

^{13}C NMR of **3f**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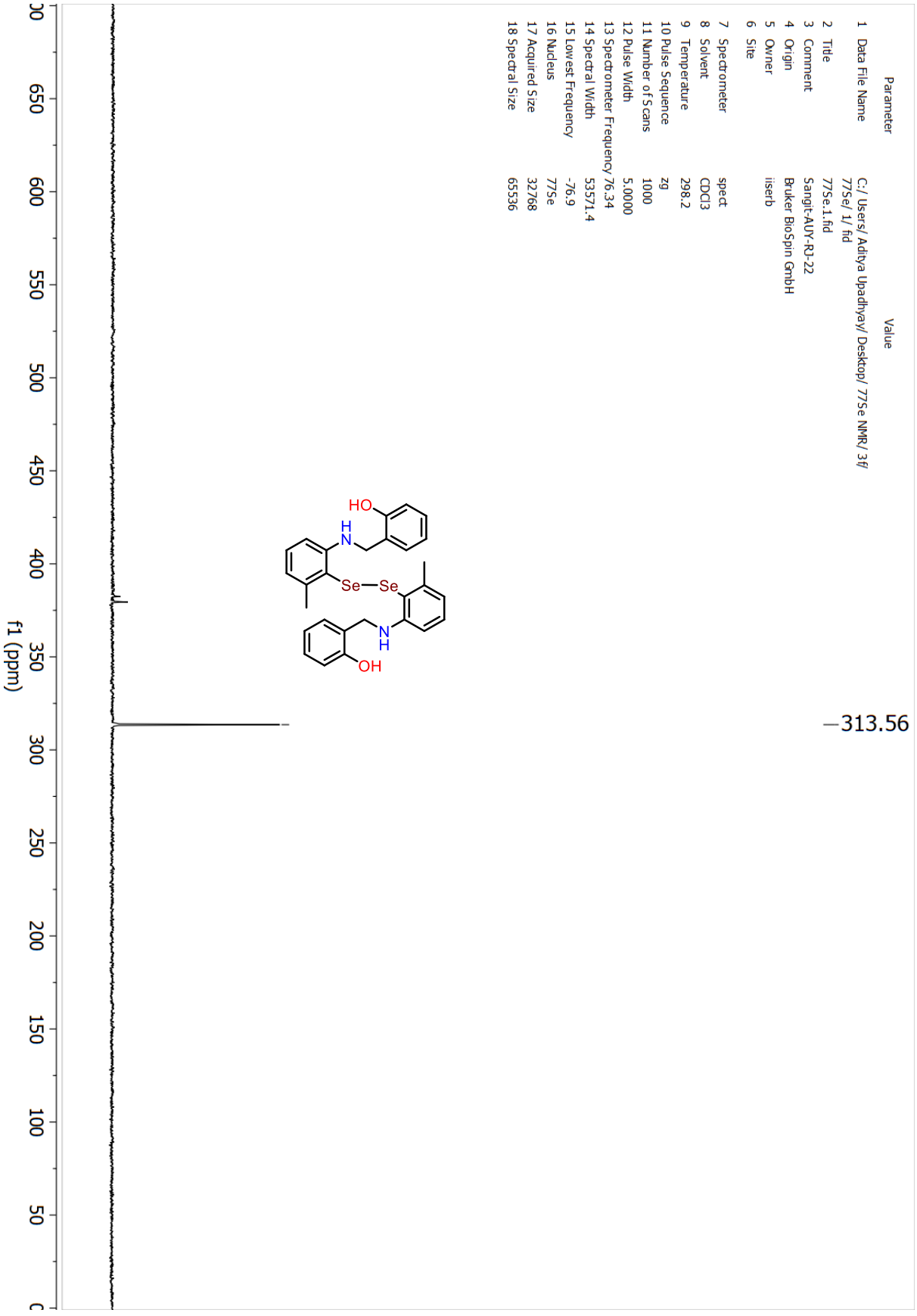
Parameter
Value
1 Data File Name I:/.sbstituted dselenides/AUY-198/Sangit-RJ-22-C(500MHz)/ 1/ fid
2 Title Sangit-RJ-22-C(500MHz).1.fid
3 Origin Bruker BioSpin GmbH
4 Owner nmrsu
5 Solvent CDCl3
6 Temperature 298.0
7 Pulse Sequence zgpg30
8 Number of Scans 512
9 Acquisition Date 2019-03-25T21:55:33
10 Modification Date 2019-03-25T21:55:54
11 Spectrometer Frequency 125.77
12 Spectral Width 29761.9
13 Lowest Frequency -2306.2
14 Nucleus 13C
15 Acquired Size 32768
16 Spectral Size 65536
HO
H
N
Se
Se
N
H
OH
118.51
116.64
110.80
48.17
23.89
f1 (ppm)

^{77}Se NMR of **3f**



HRMS of **3f**

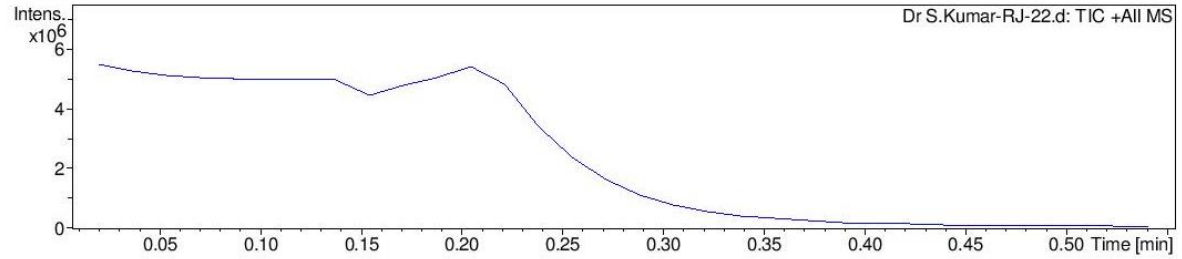
Display Report

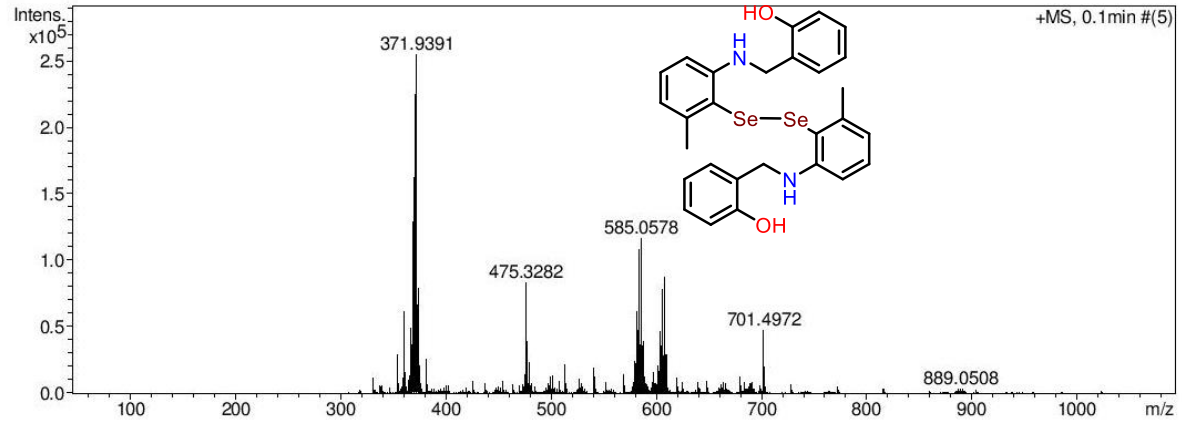
Analysis Info

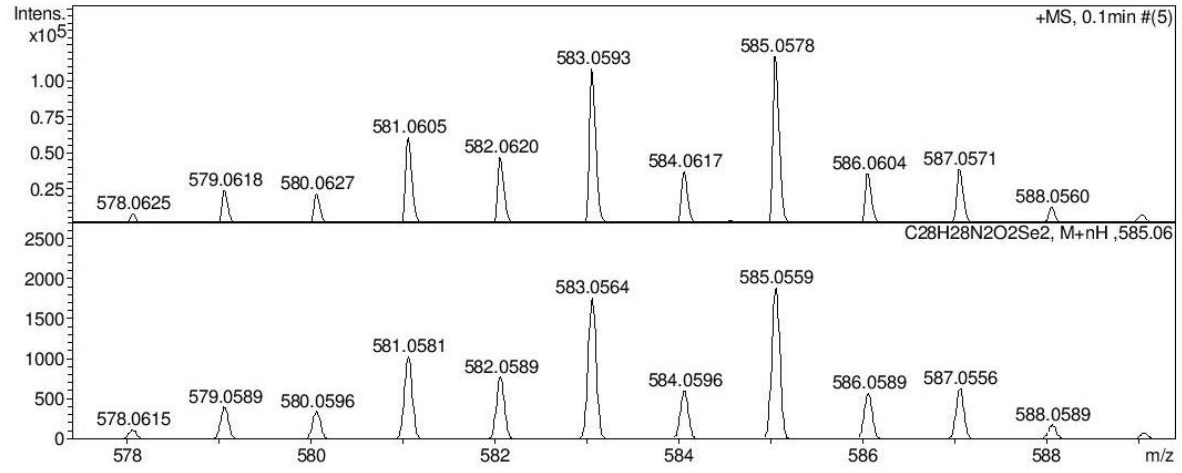
Analysis Name	D:\Data\NEW USER DATA 2017\2019\MAR\15 MAR\Dr S.Kumar-RJ-22.d	Acquisition Date	3/15/2019 3:50:08 PM
Method	tune_wide.m	Operator	RUCHI
Sample Name	RJ-22	Instrument	micrOTOF-Q II 10330
Comment			

Acquisition Parameter

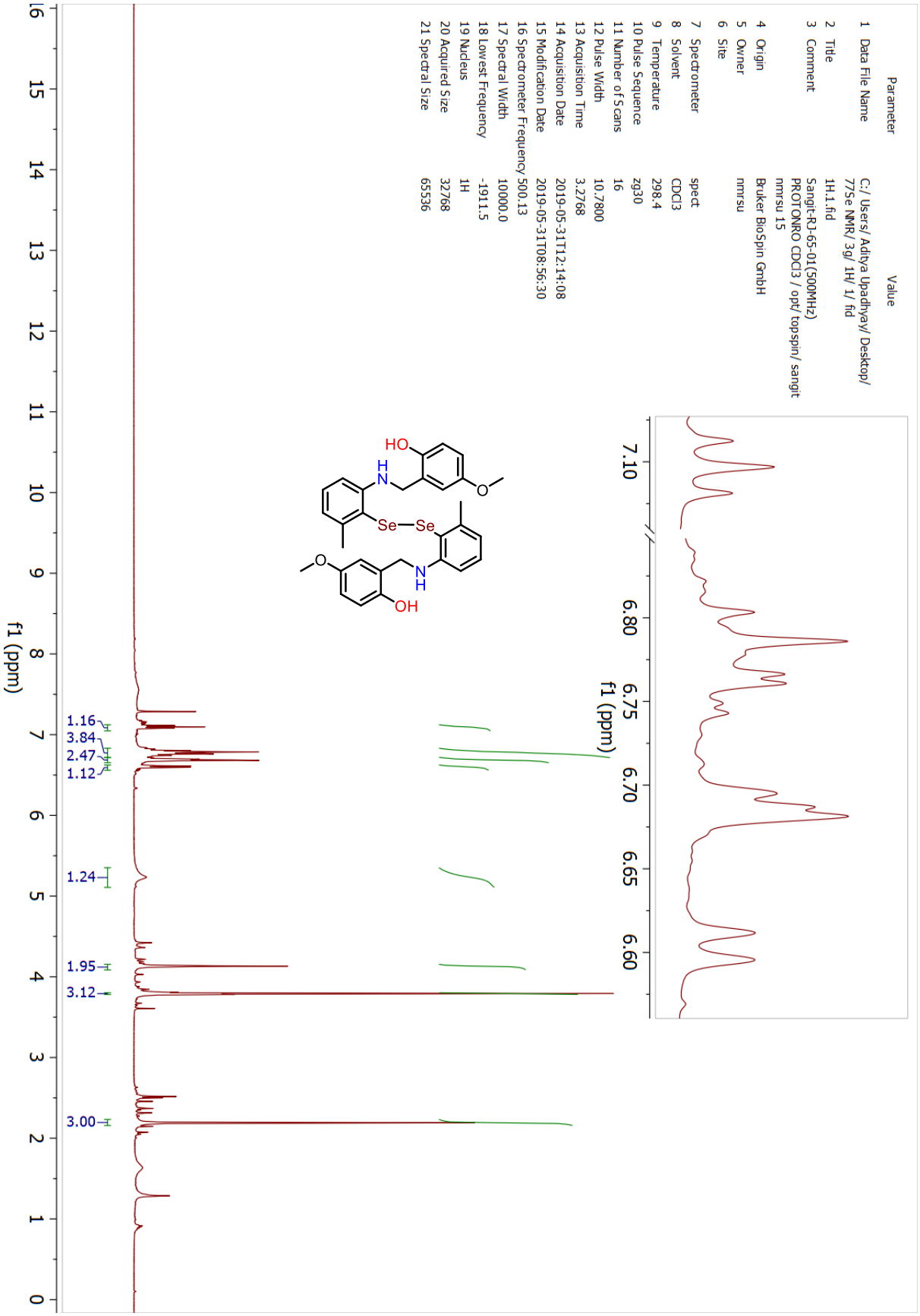
Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Not active	Set Capillary	4500 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	3000 m/z	Set Collision Cell RF	600.0 Vpp	Set Divert Valve	Waste







^{1}H NMR of **3g**


Parameter
Value
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2 Title
1H.1.fid
3 Comment
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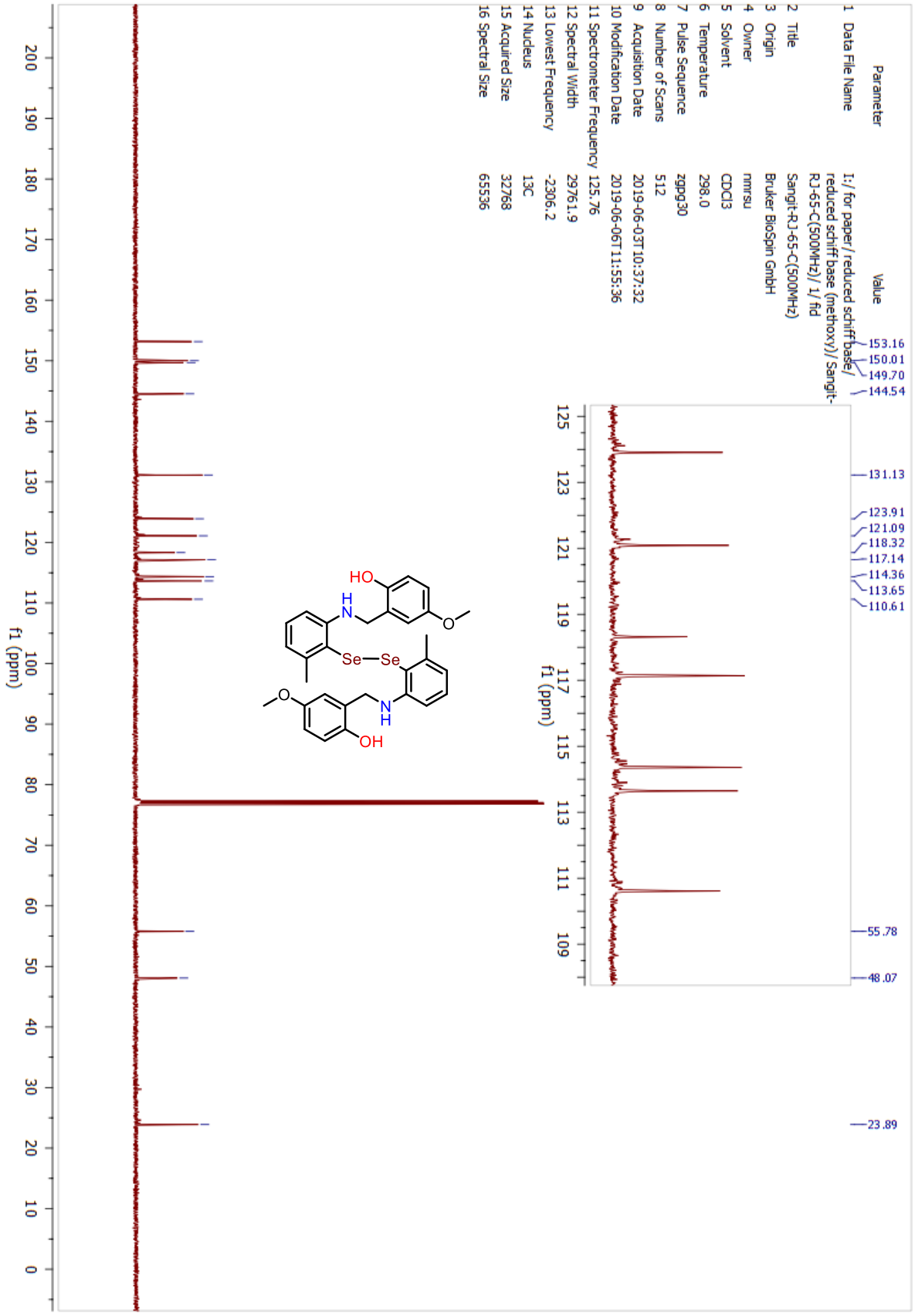
4 Origin
Bruker BioSpin GmbH
5 Owner
nmrsu
6 Site
7 Spectrometer
spect
8 Solvent
CDCl3
9 Temperature
298.4
10 Pulse Sequence
zg30
11 Number of Scans
16
12 Pulse Width
10.7800
13 Acquisition Time
3.2768
14 Acquisition Date
2019-05-31T12:14:08
15 Modification Date
2019-05-31T08:56:30
16 Spectrometer Frequency 500.13
17 Spectral Width
10000.0
18 Lowest Frequency
-1911.5
19 Nucleus
1H
20 Acquired Size
32768
21 Spectral Size
65536
HO
H
N
O
Se
Se
O
N
H
OH
7.10
6.80
6.75
6.70
6.65
6.60
f1 (ppm)
1.16
3.84
2.47
1.12
1.24
1.95
3.12
3.00
f1 (ppm)

^{13}C NMR of **3g**


Parameter
Value
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2 Title
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3 Origin
Bruker BioSpin GmbH
4 Owner
nmrsu
5 Solvent
CDCl3
6 Temperature
298.0
7 Pulse Sequence
zgpg30
8 Number of Scans
512
9 Acquisition Date
2019-06-03T10:37:32
10 Modification Date
2019-06-06T11:55:36
11 Spectrometer Frequency
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113.65
110.61
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H
N
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Se
Se
O
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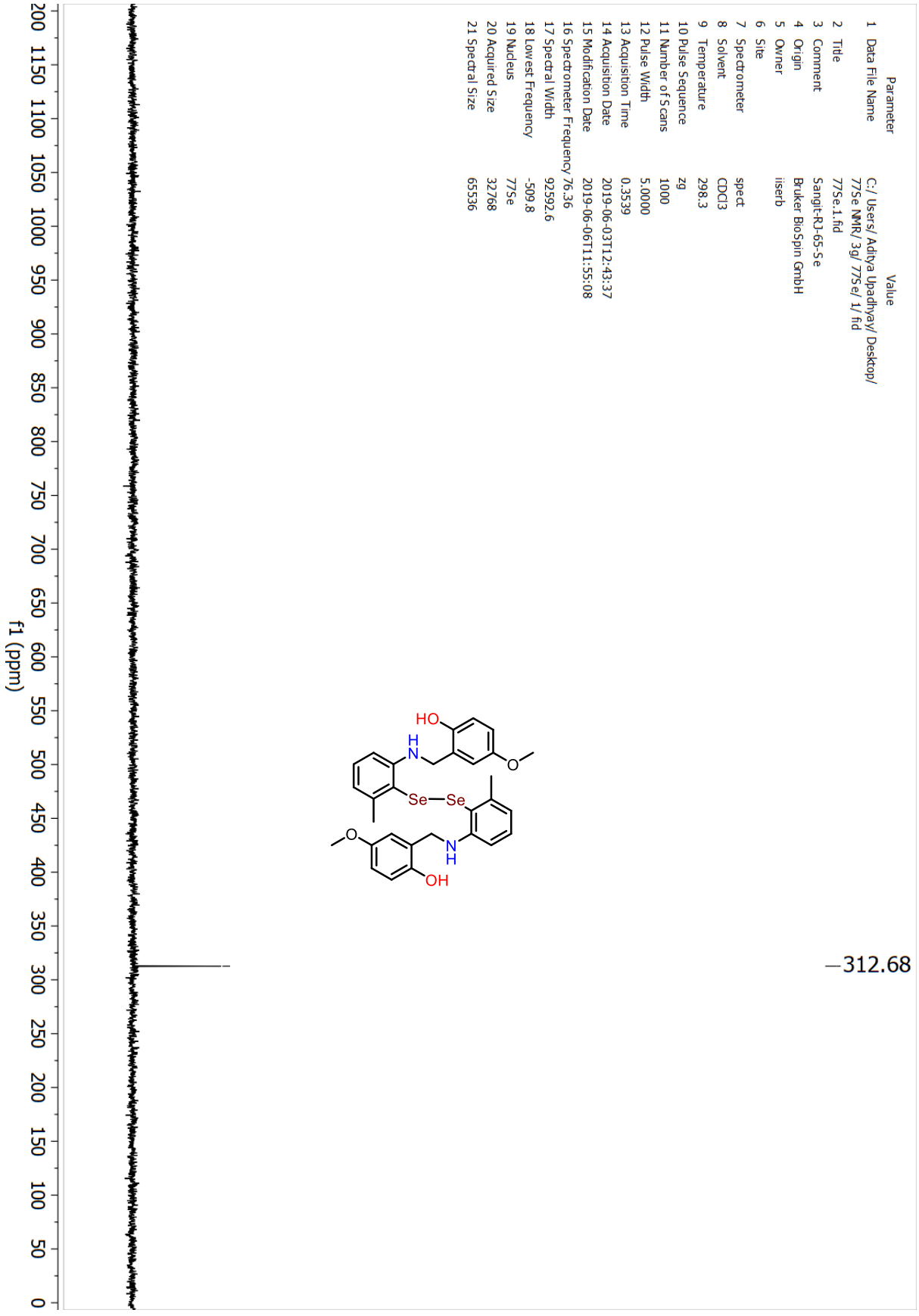
H
OH
f1 (ppm)

77Se NMR of **3g**



HRMS of **3g**

Display Report

Analysis Info

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Sample Name	RJ-65	Instrument	micrOTOF-Q II 10330
Comment			

Acquisition Parameter

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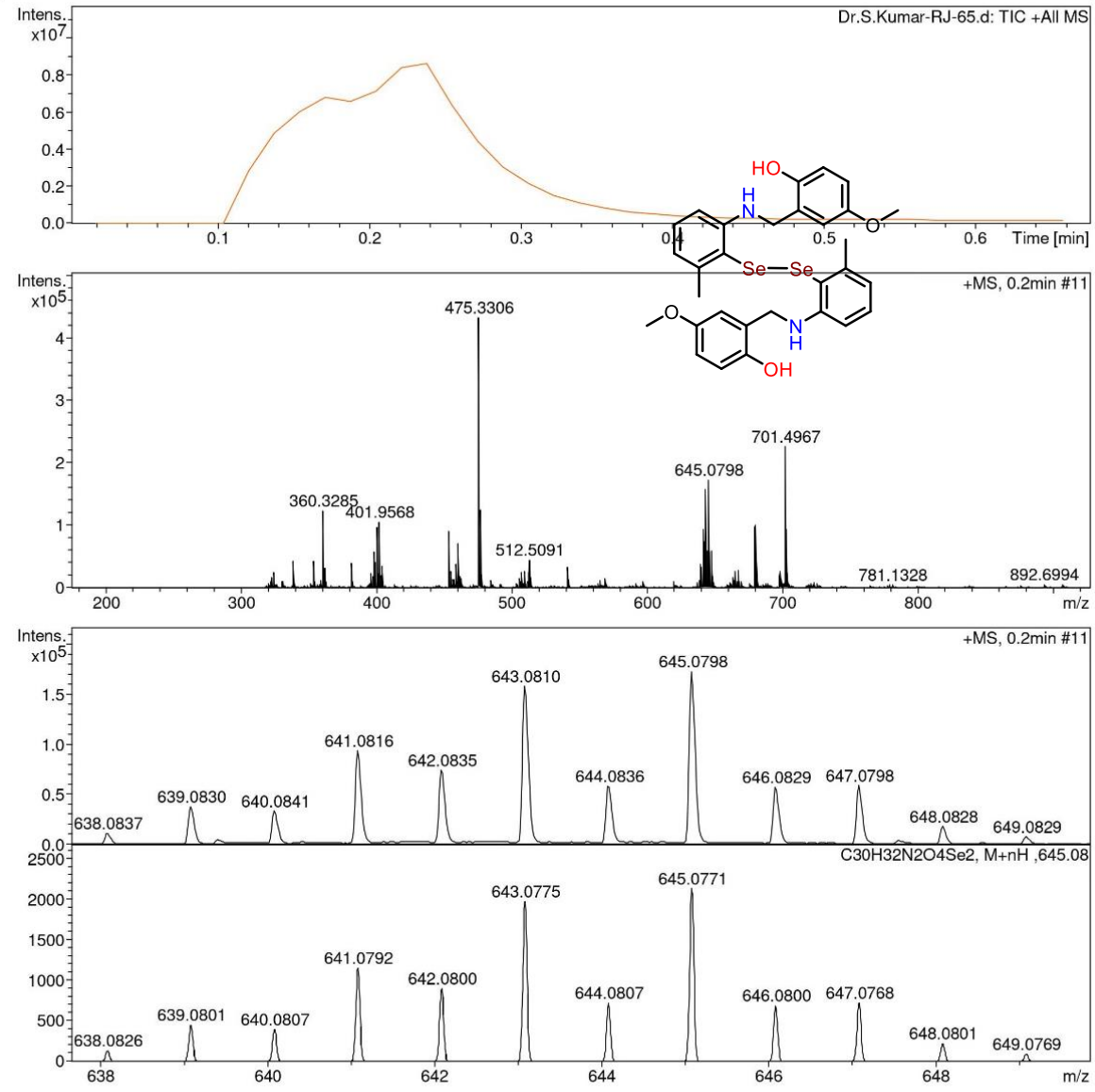
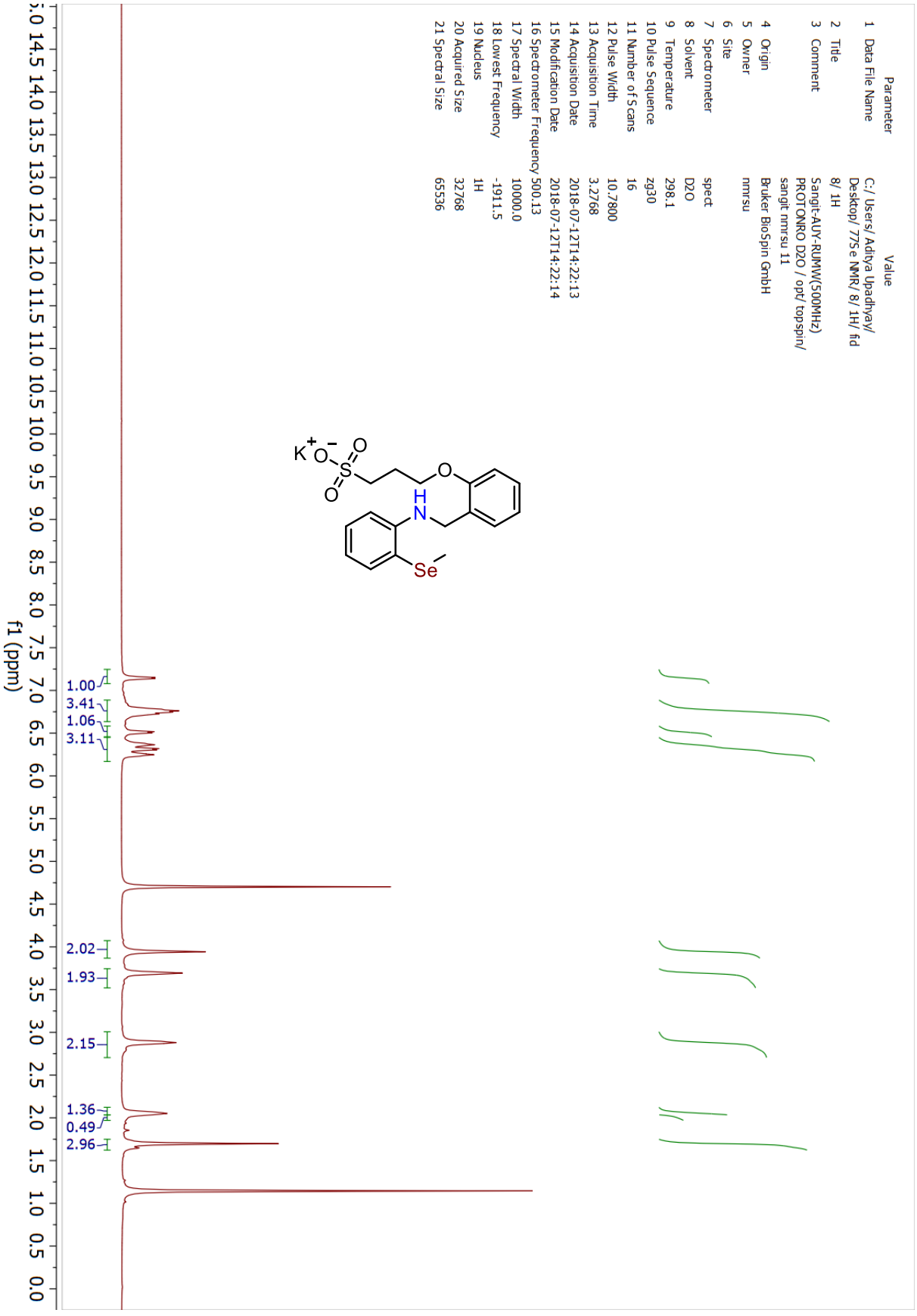


^{1}H NMR of **8**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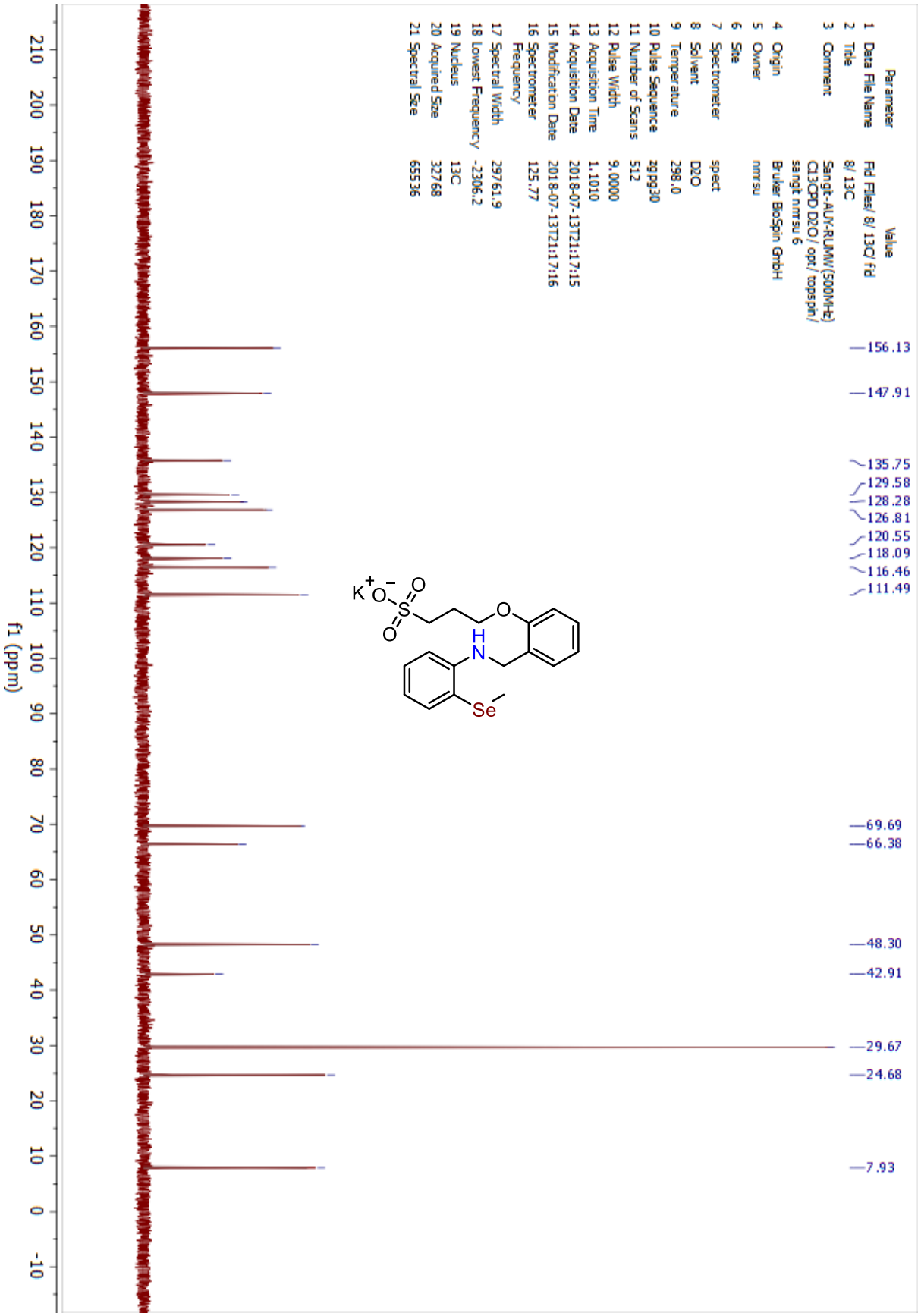
2.02
1.93
2.15
1.36
0.49
2.96
f1 (ppm)
5.0 14.5 14.0 13.5 13.0 12.5 12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0

^{13}C NMR of **8**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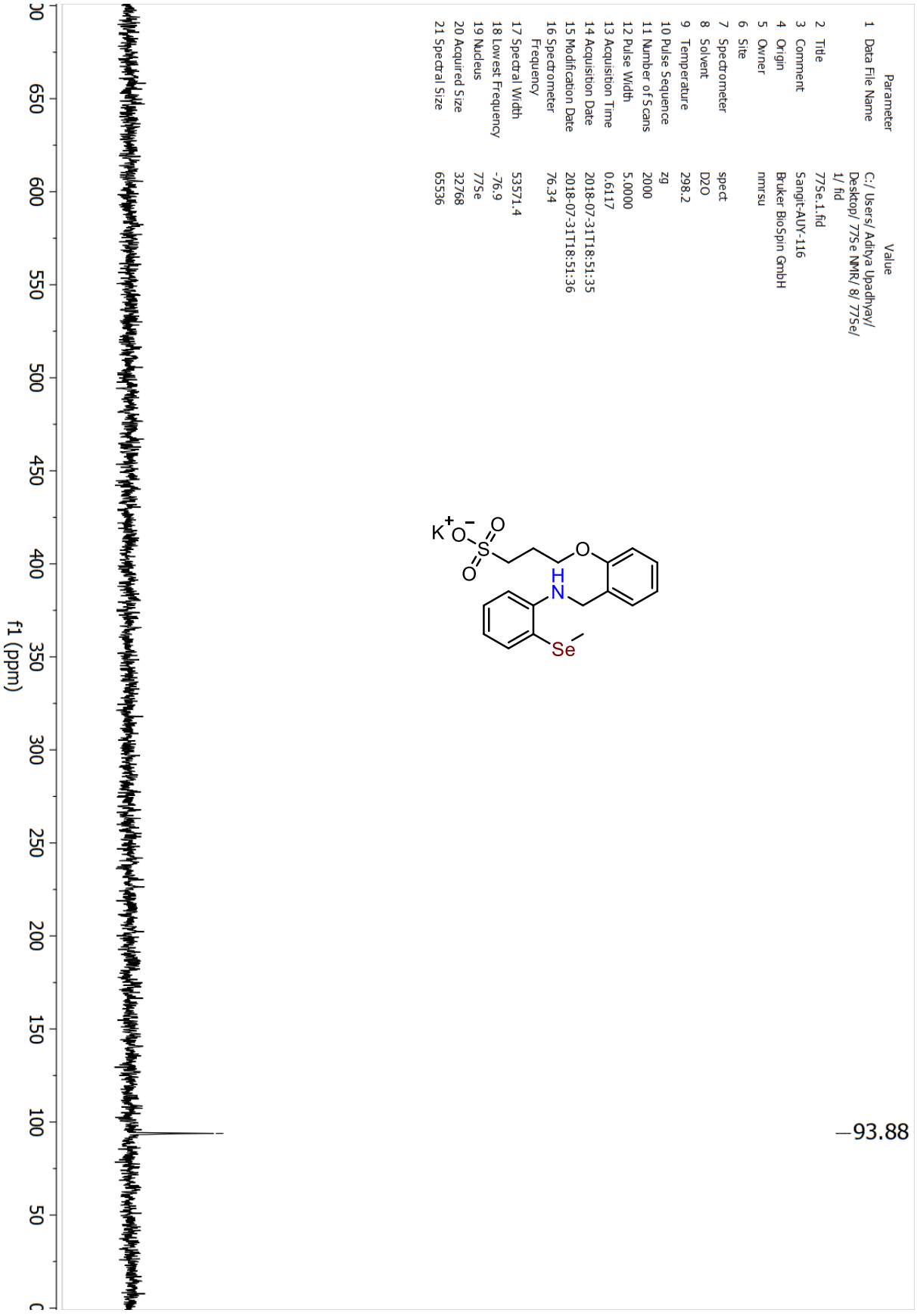
-10

^{77}Se NMR of **8**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200
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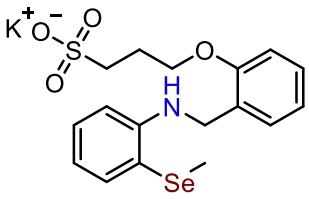
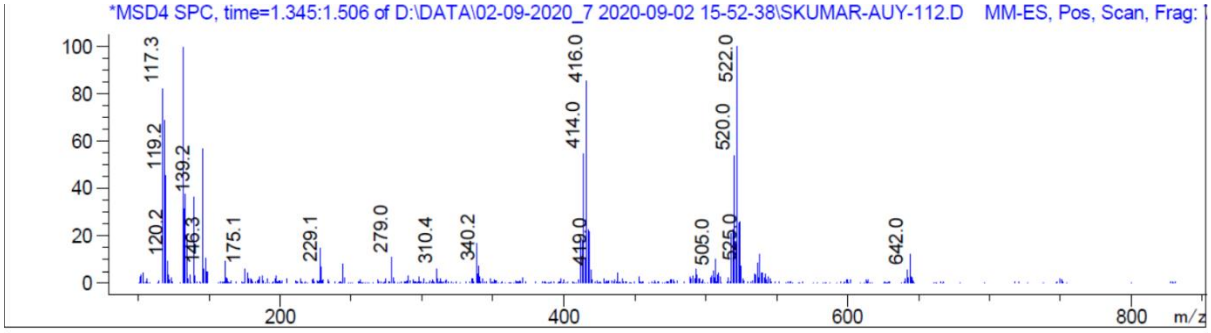
100
50

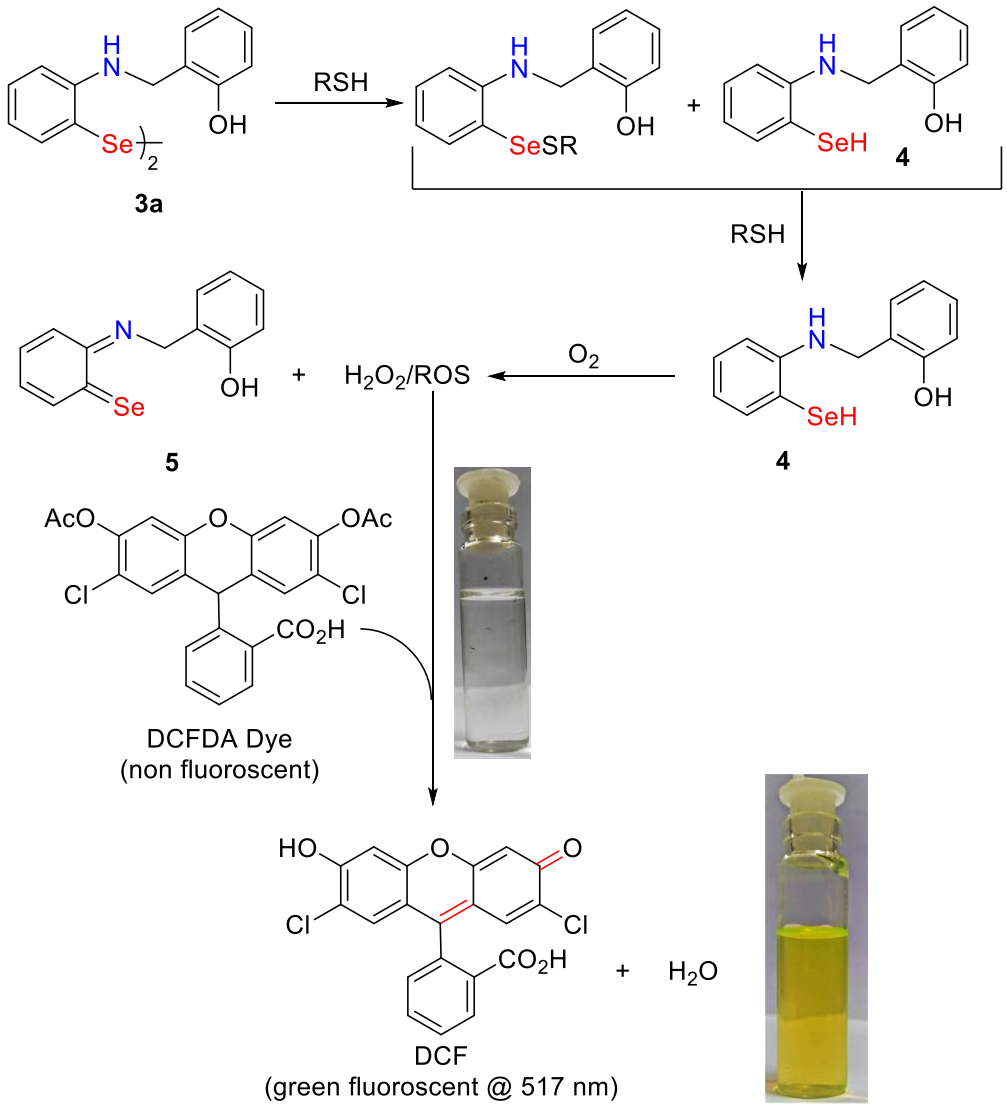
LRGCMS of **8**

Exact Mass: 414.02





3. Reactive oxygen generation assay



Scheme S1. Schematic representation of ROS generation by catalyst **3a**.

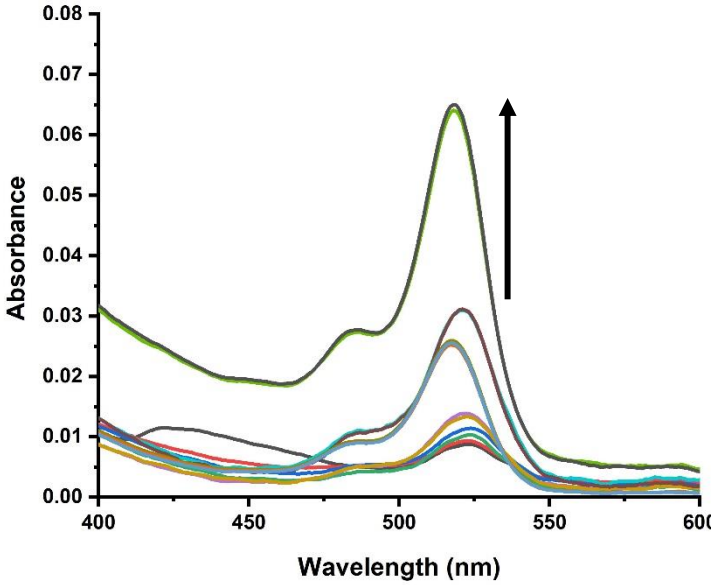


Figure S1. ROS generation by diselenide catalysts **3a.**

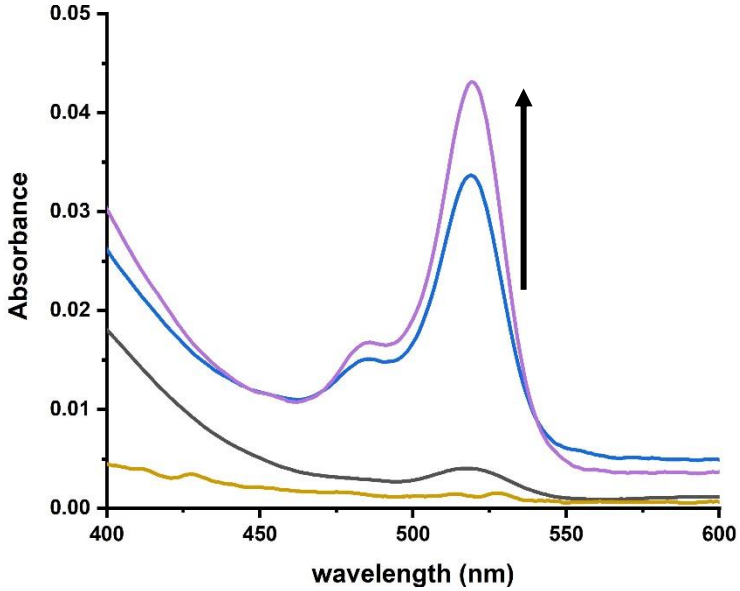


Figure S2. ROS generation by diselenide catalysts **3b.**

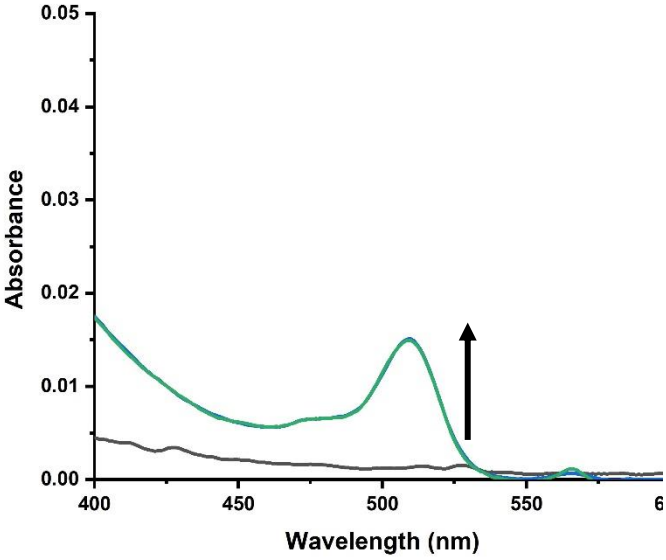


Figure S3. ROS generation by diselenide catalysts **3c.**

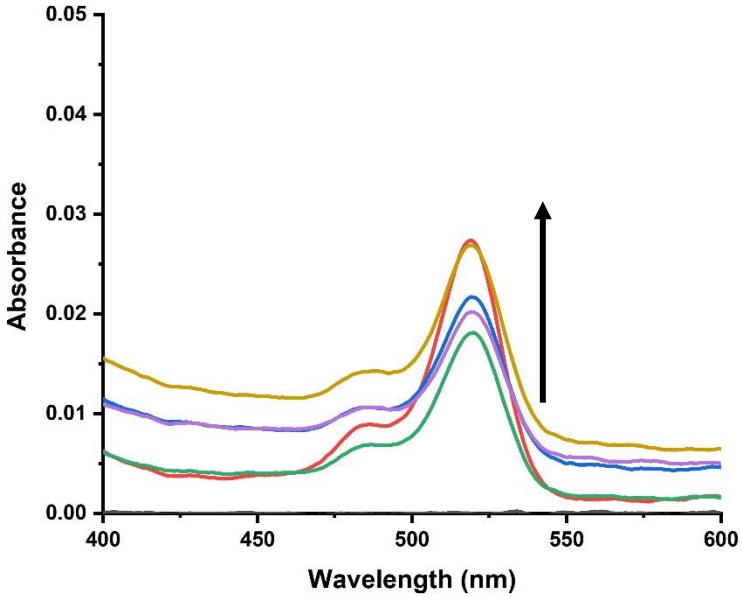


Figure S4. ROS generation by diselenide catalysts **3d.**

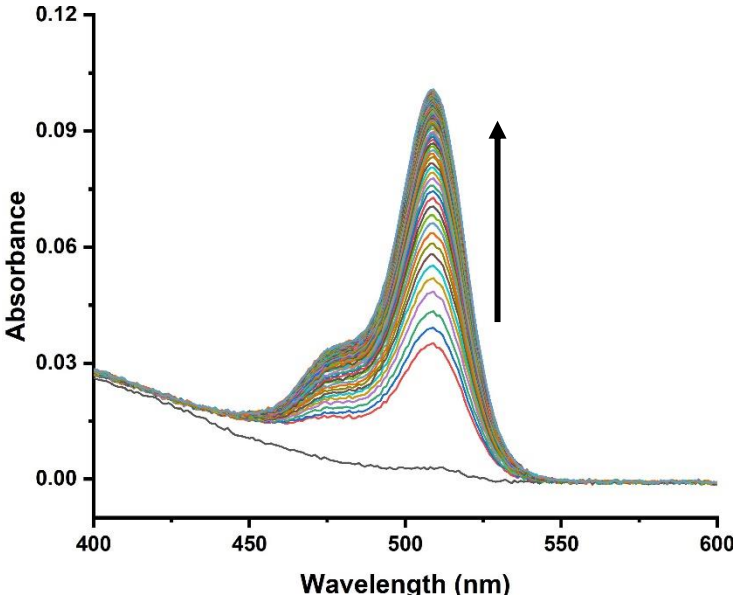


Figure S5. ROS generation by diselenide catalysts **3e**

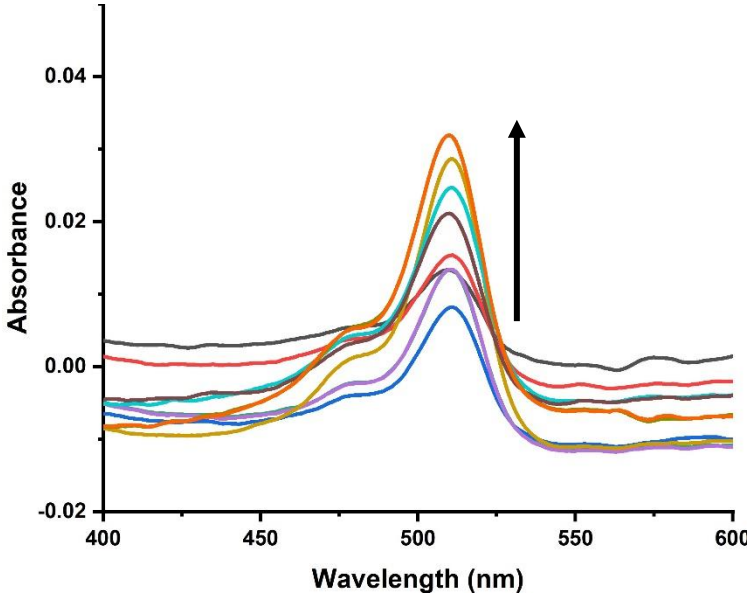


Figure S6. ROS generation by diselenide catalysts **3f.**

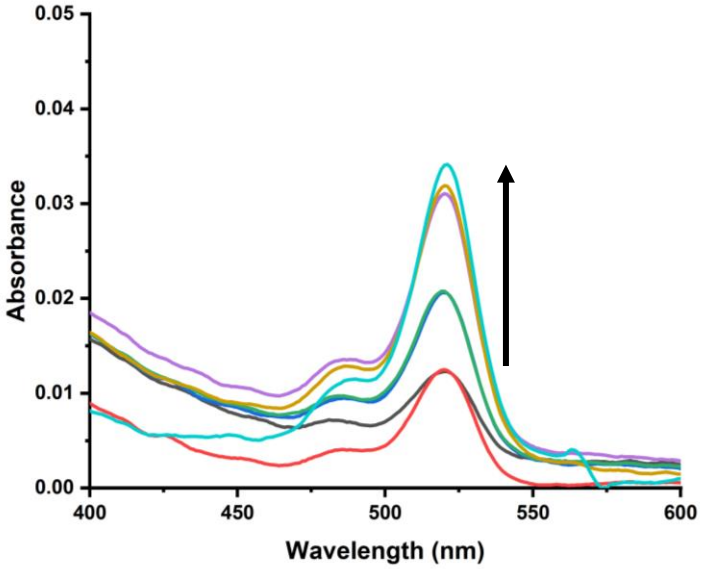


Figure S7. ROS generation by diselenide catalysts **3g.**

4. Control experiment for ROS generation assay

1. Reaction mixture of benzenethiol (40 µM) and DCFDA (10 µM) dye in acetonitrile solvent under oxygen atmosphere

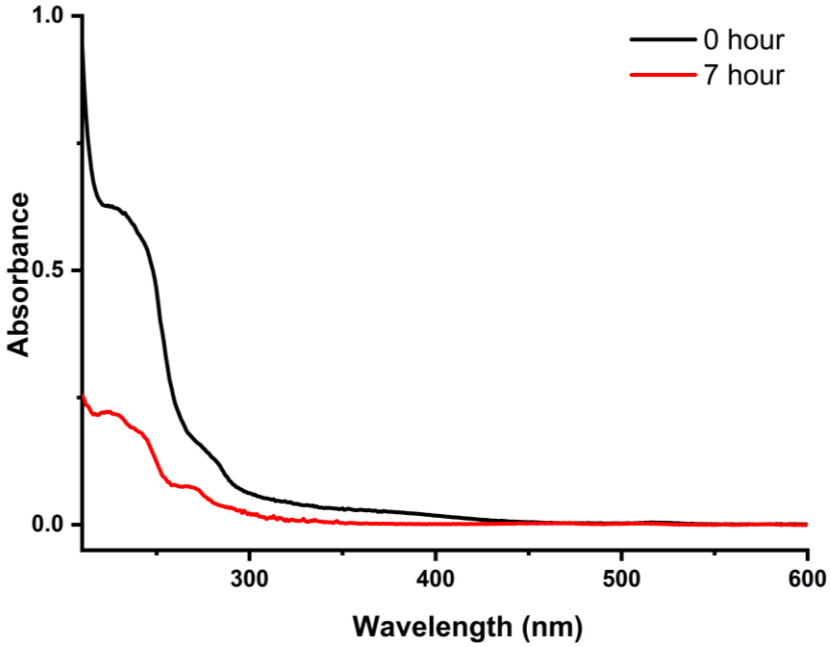


Figure S8. Reaction mixture of benzenethiol (40 µM) and DCFDA dye (10 µM) in acetonitrile solvent under oxygen atmosphere at room temperature.

2. Reaction mixture of DCFDA in acetonitrile solvent under oxygen atmosphere

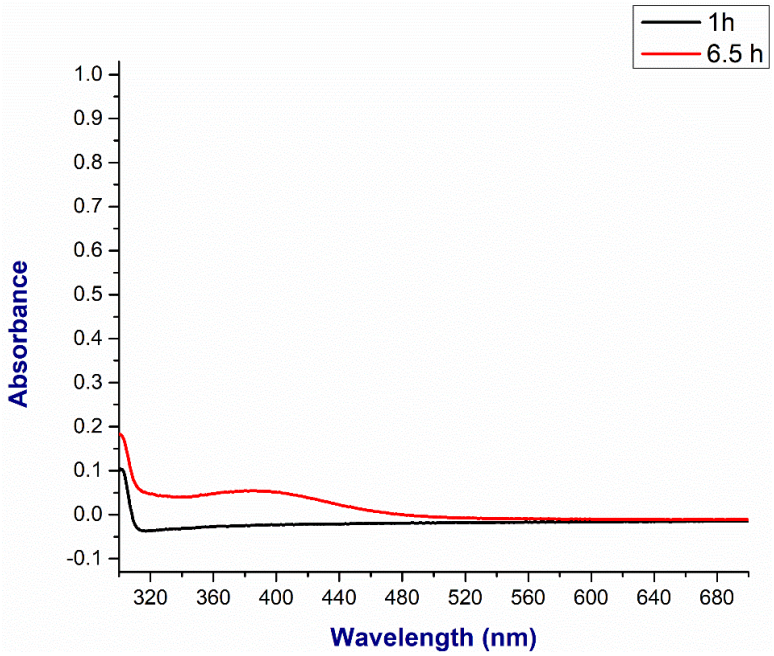


Figure S9. UV-Visible spectra of DCFDA dye in acetonitrile solvent under oxygen atmosphere at room temperature.

3. Reaction mixture of catalyst **3a** (10 µM) and DCFDA dye (10 µM) in acetonitrile solvent under oxygen atmosphere

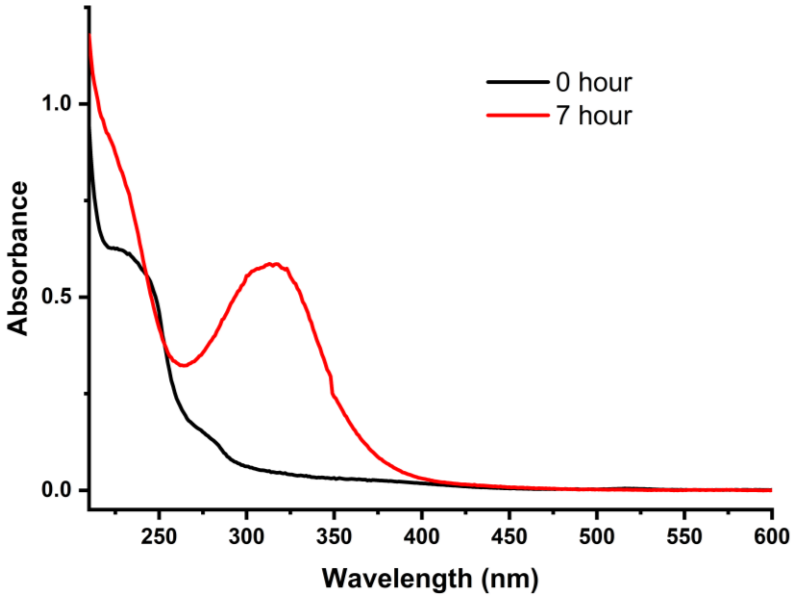
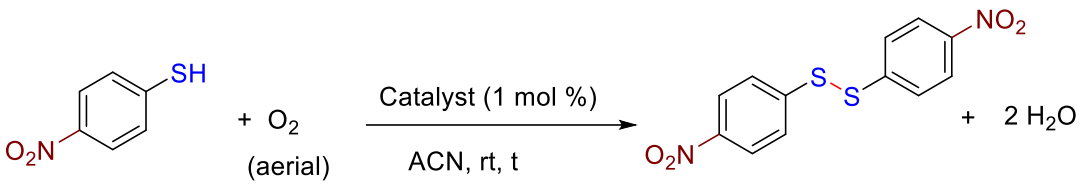


Figure S10. UV-Visible spectra of catalyst **3a** (10 µM), and DCFDA dye (10 µM) in acetonitrile solvent under oxygen atmosphere at room temperature.

5. Aerial Oxidation of *para*-nitrothiophenol



Scheme S2. Aerial oxidation of *para* nitrothiophenol in the presence of 1 mol% catalyst at room temperature.

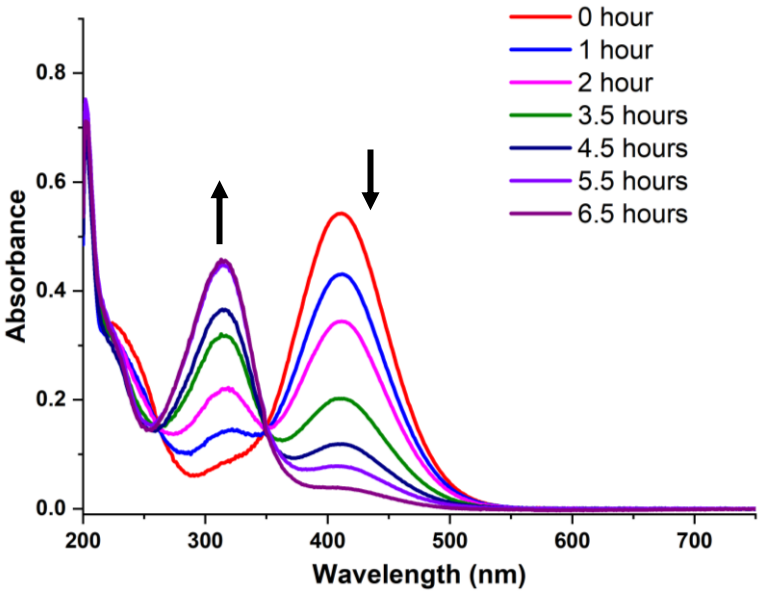


Figure S11. ROS generation by diselenide catalysts **3a.**

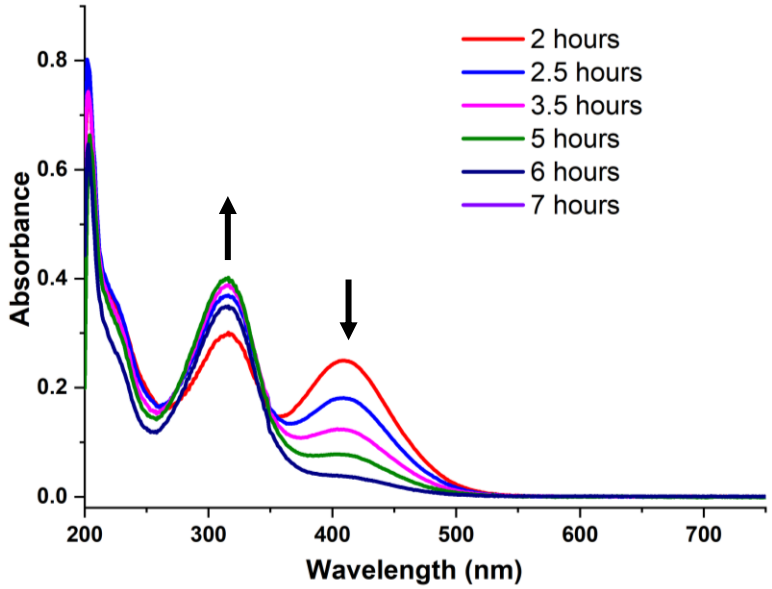


Figure S12. ROS generation by diselenide catalysts **3b.**

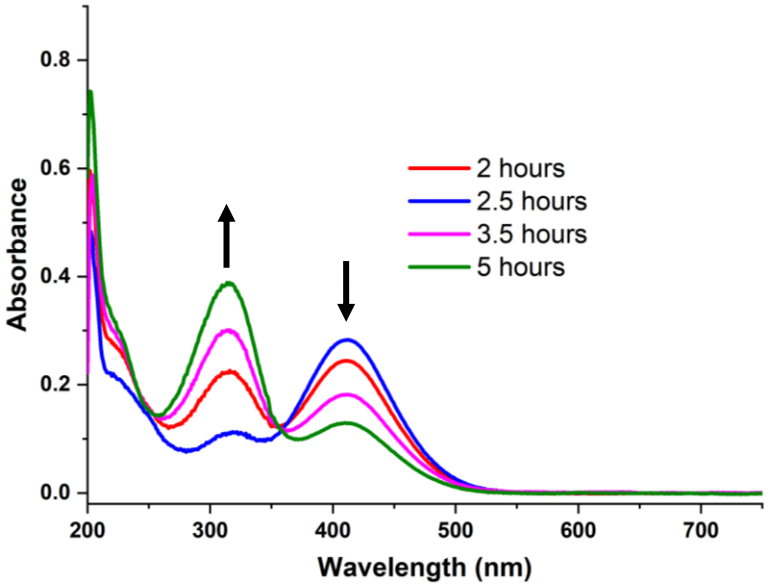


Figure S13. ROS generation by diselenide catalysts **3c.**

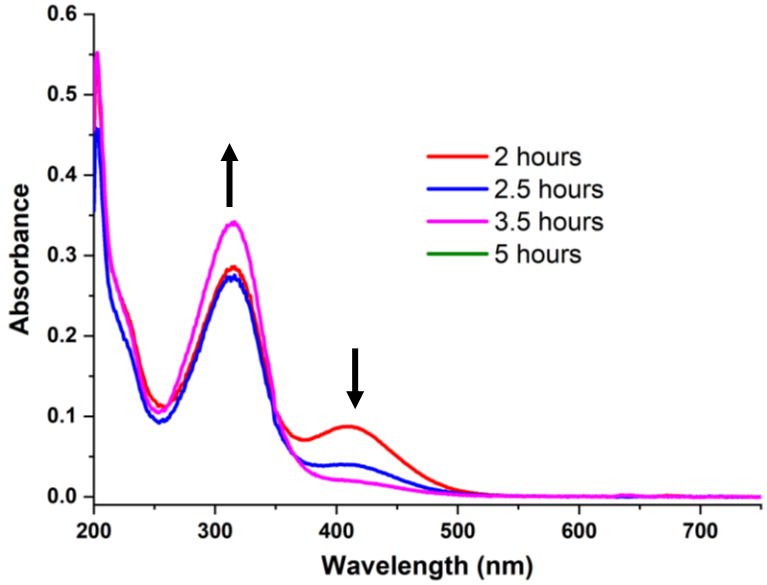


Figure S14. ROS generation by diselenide catalysts **3d.**

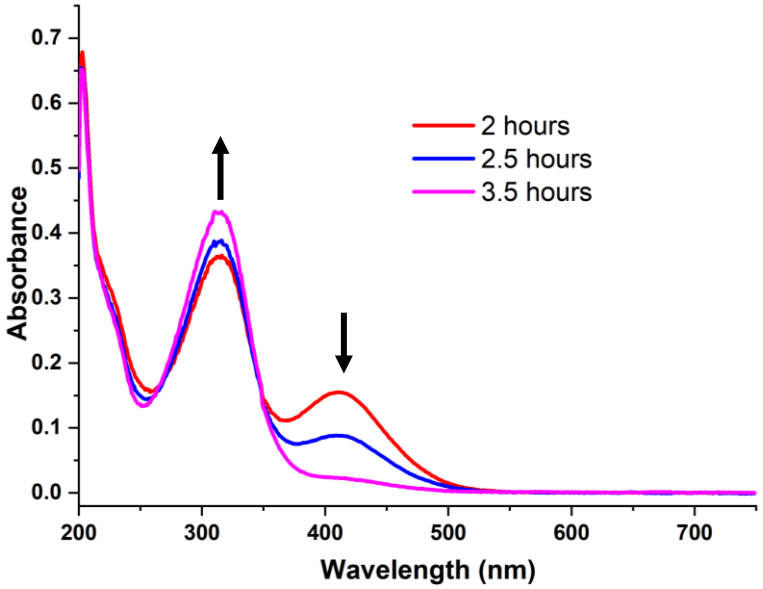


Figure S15. ROS generation by diselenide catalysts **3e.**

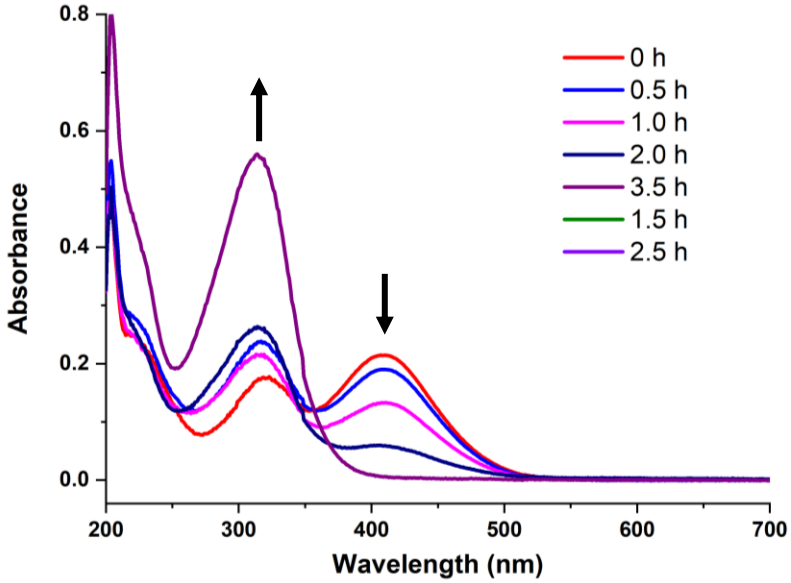


Figure S16. ROS generation by diselenide catalysts **3f.**

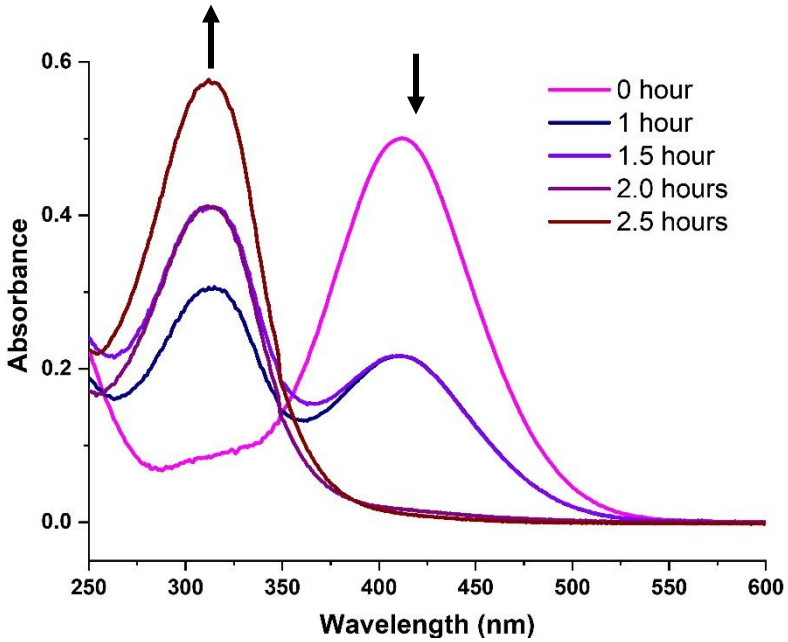
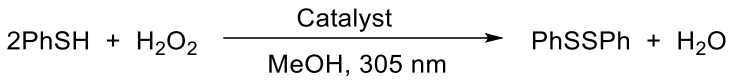


Figure S17. ROS generation by diselenide catalysts **3g.**

6. Initial reduction rate of hydrogen peroxide



Peroxide decomposing antioxidant activity of catalyst 1a was evaluated by thiol peroxidase assay. The test mixture contained benzenethiol (1 mM), organoselenium catalyst (0.1 mM) and hydrogen peroxide (3.75 mM). The Reaction of the model compound with PhSH and H_2O_2 was studied in methanol by following the appearance of diphenyl disulfide absorption at 305 nm at 25 ^oC. Each initial reduction rate was measured at least three times by using 1.24 $mM^{-1}cm^{-1}$ as the molar extinction coefficient for PhSSPh.

Initial reduction rate for hydrogen peroxide by catalyst **3b**

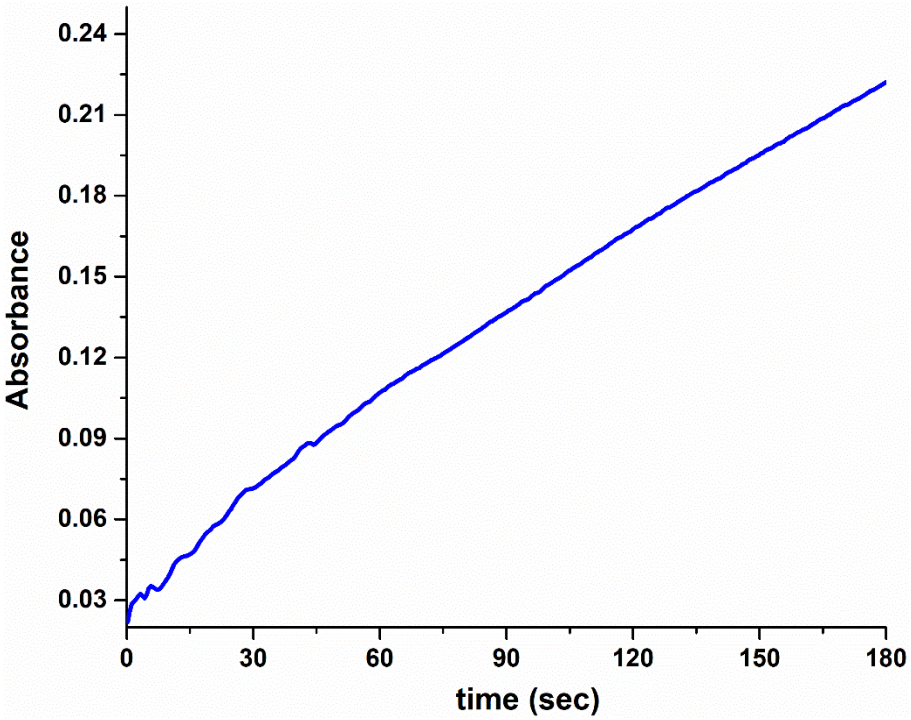


Figure S18: A model plot of absorbance vs time (sec). The initial concentration of benzenethiol, catalyst **3b** and H_2O_2 were fixed to 1 mM, 0.1 mM, 3.75 mM respectively.

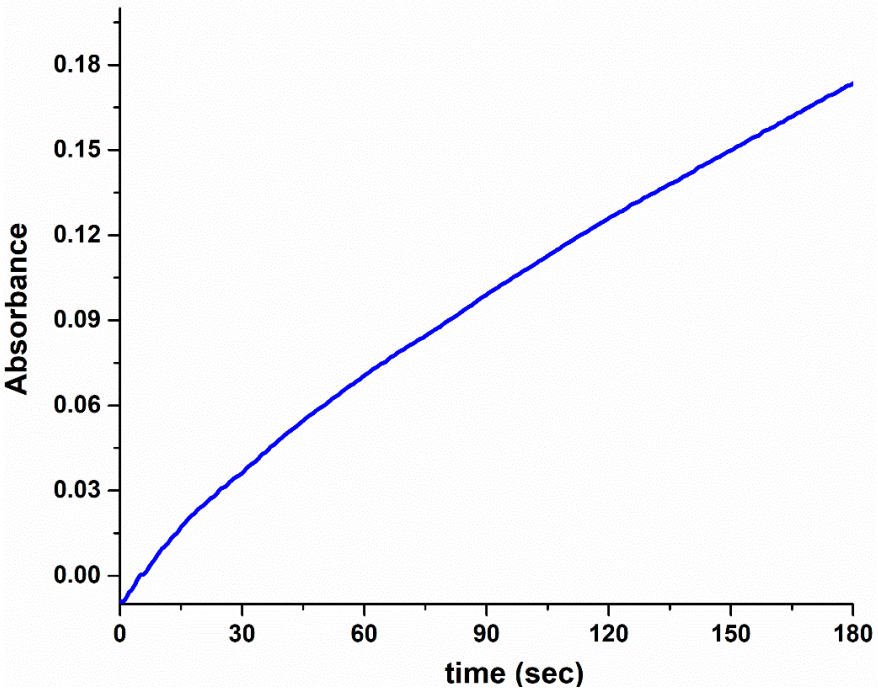


Figure S19: A model plot of absorbance vs time (sec). The initial concentration of benzenethiol, catalyst **3b** and H_2O_2 were fixed to 1 mM, 0.1 mM, 3.75 mM respectively.

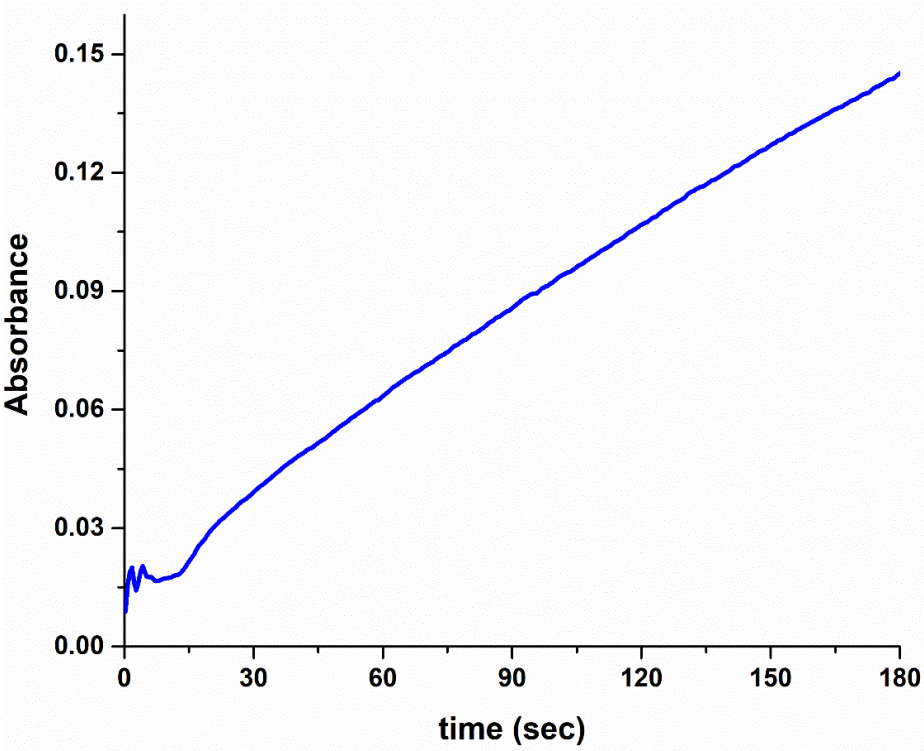


Figure S20: A model plot of absorbance vs time (sec). The initial concentration of benzenethiol, catalyst **3b** and H_2O_2 were fixed to 1 mM, 0.1 mM, 3.75 mM respectively.

Initial reduction rate of 3c

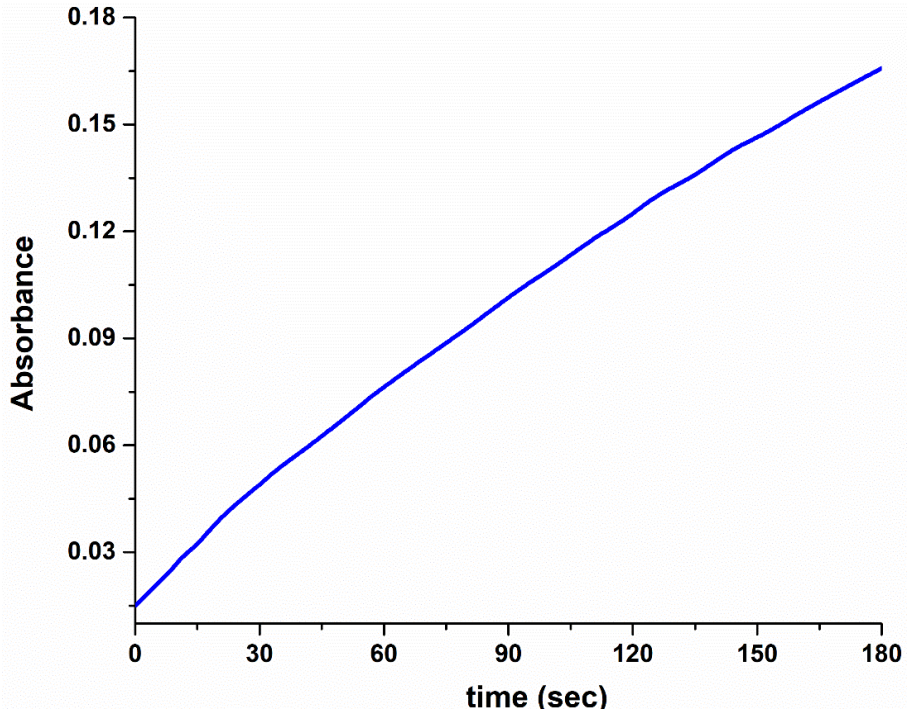


Figure S21: A model plot of absorbance vs time (sec). The initial concentration of benzenethiol, catalyst **3c** and H_2O_2 were fixed to 1 mM, 0.1 mM, 3.75 mM respectively

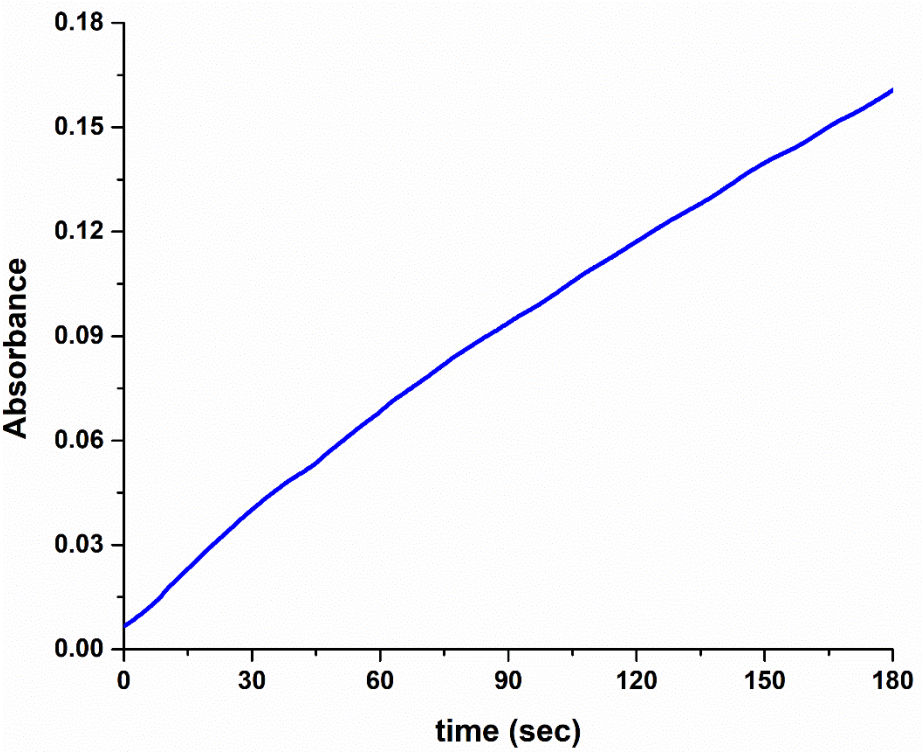


Figure S22: A model plot of absorbance vs time (sec). The initial concentration of benzenethiol, catalyst **3c** and H_2O_2 were fixed to 1 mM, 0.1 mM, 3.75 mM respectively

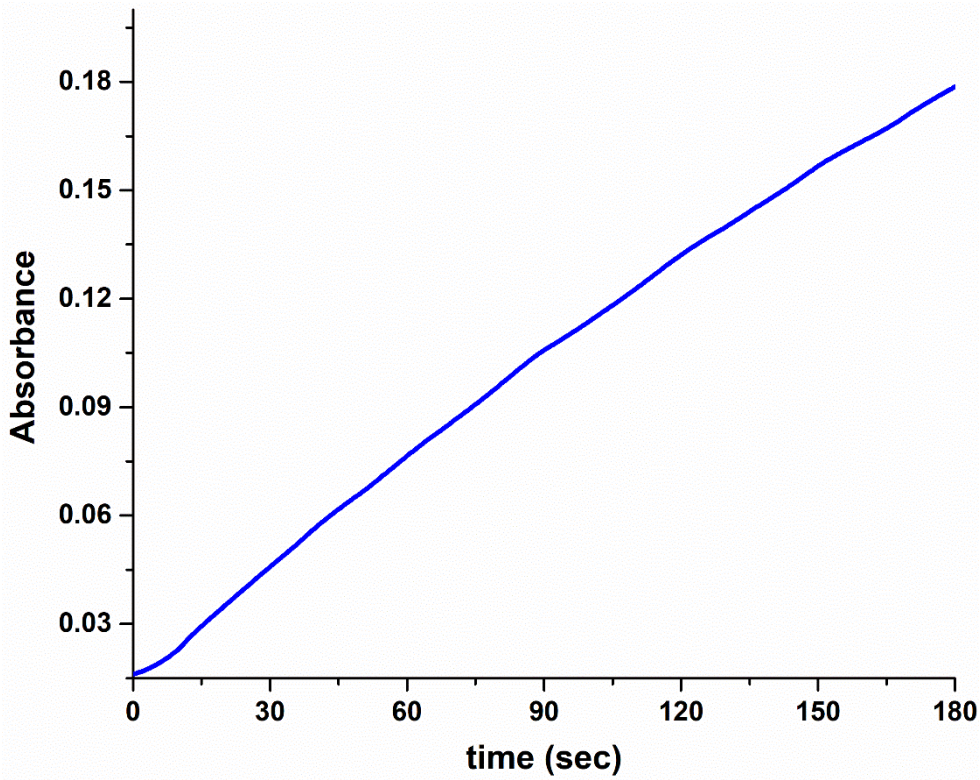


Figure S23: A model plot of absorbance vs time (sec). The initial concentration of benzenethiol, catalyst **3c** and H_2O_2 were fixed to 1 mM, 0.1 mM, 3.75 mM respectively.

Initial reduction rate of 3d

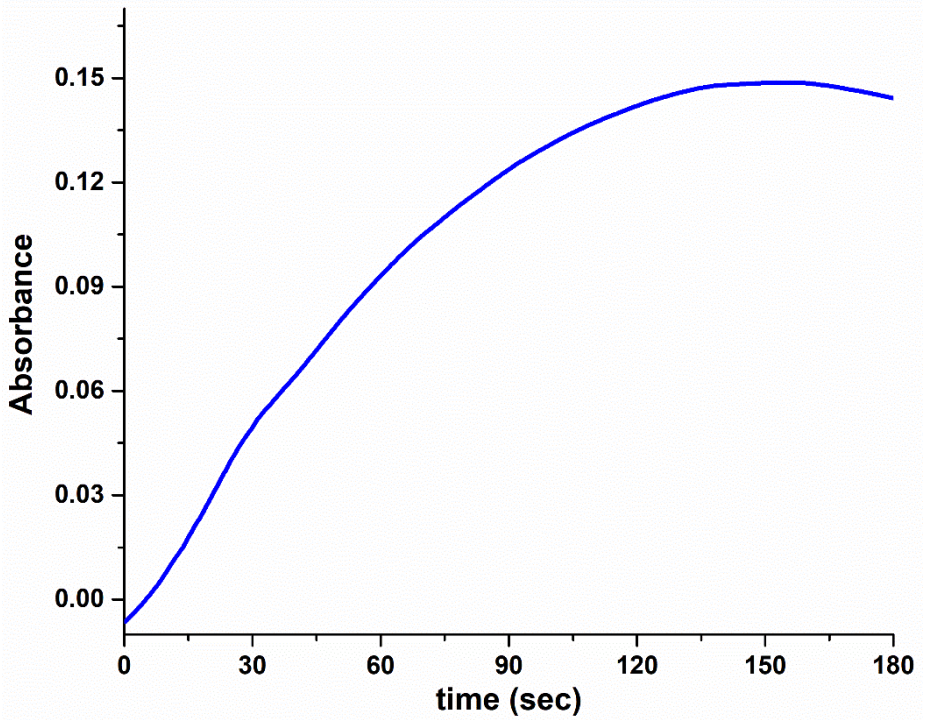


Figure S24: A model plot of absorbance vs time (sec). The initial concentration of benzenethiol, catalyst **3d** and H_2O_2 were fixed to 1 mM, 0.1 mM, 3.75 mM respectively.

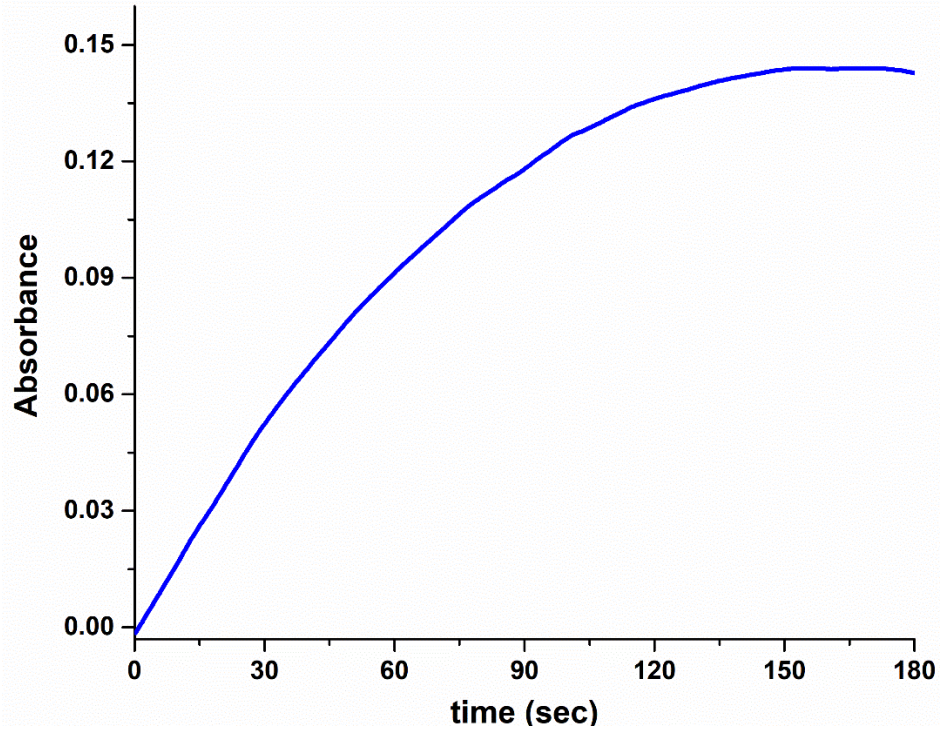


Figure S25: A model plot of absorbance vs time (sec). The initial concentration of benzenethiol, catalyst **3d** and H_2O_2 were fixed to 1 mM, 0.1 mM, 3.75 mM respectively**.**

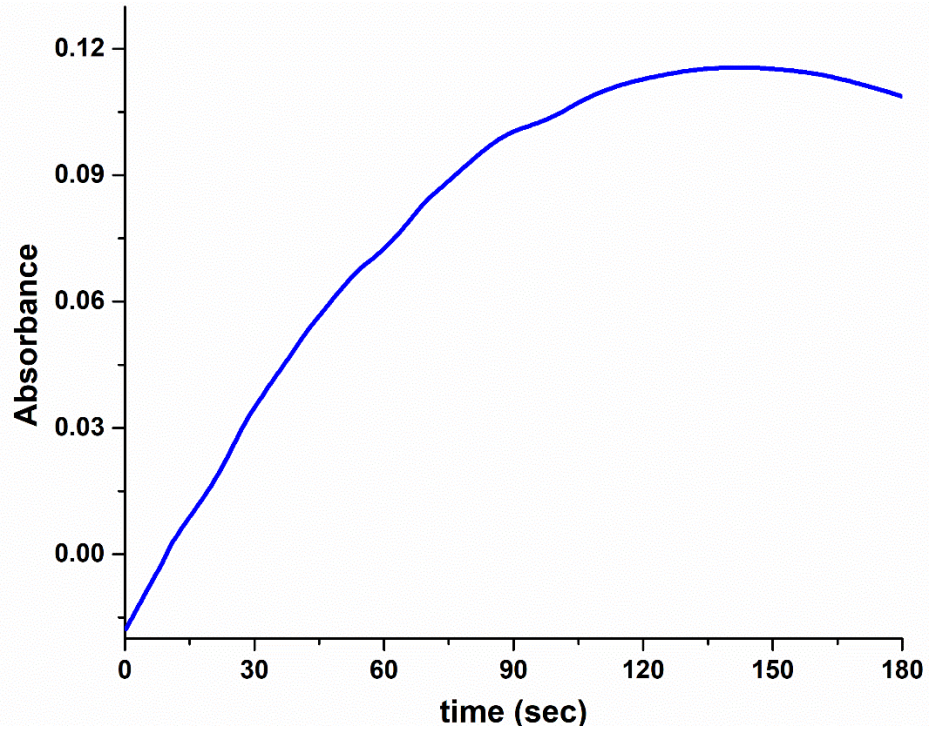


Figure S26: A model plot of absorbance vs time (sec). The initial concentration of benzenethiol, catalyst **3d** and H_2O_2 were fixed to 1 mM, 0.1 mM, 3.75 mM respectively.

Initial reduction rate of 3e:

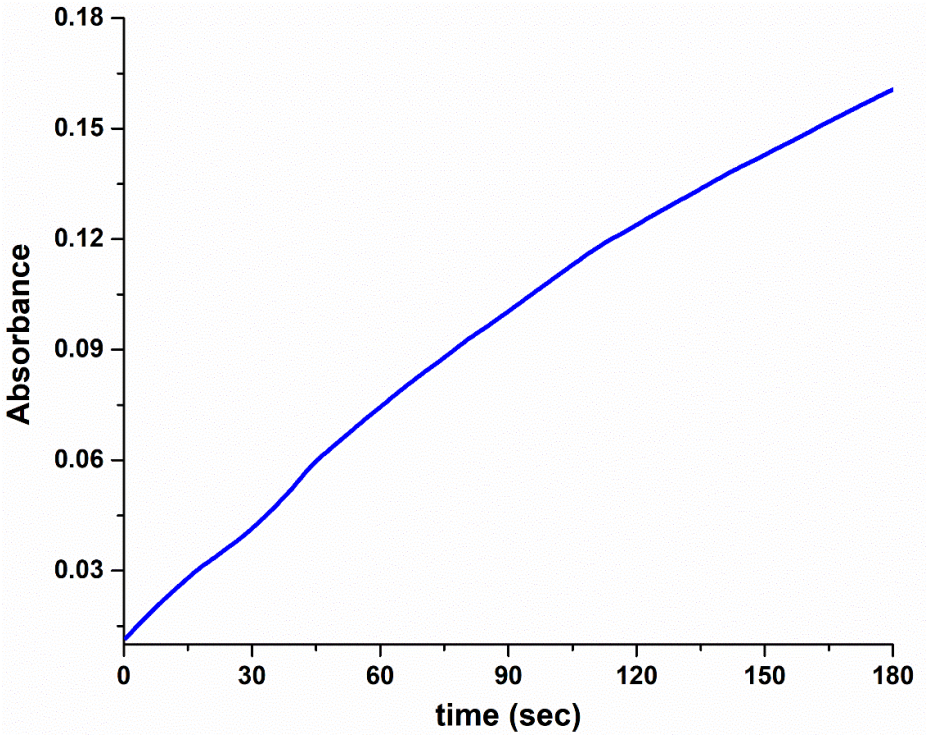


Figure S27: A model plot of absorbance vs time (sec). The initial concentration of benzenethiol, catalyst **3e** and H_2O_2 were fixed to 1 mM, 0.1 mM, 3.75 mM respectively.

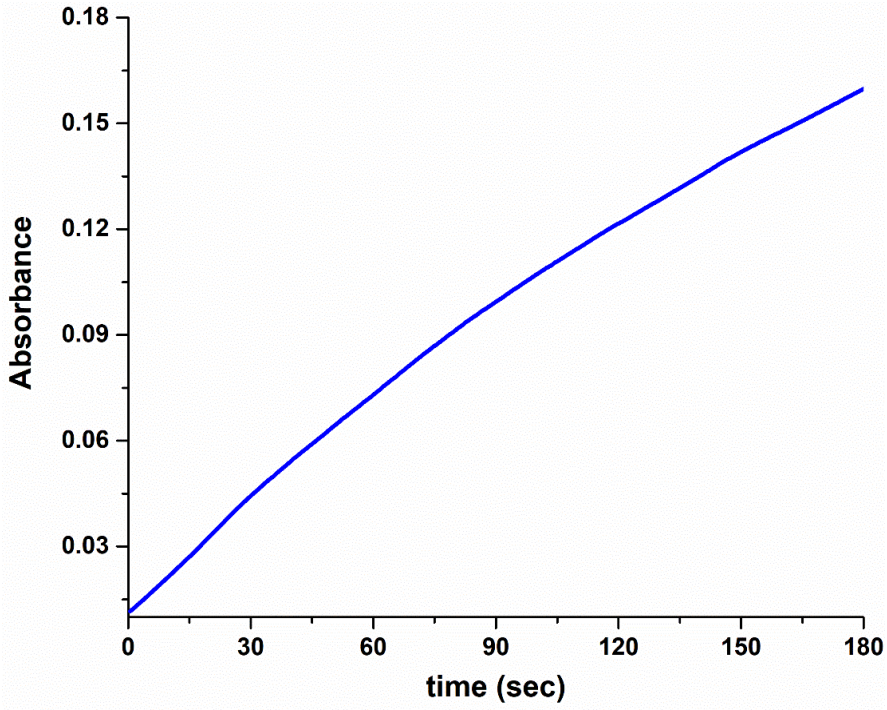


Figure S28: A model plot of absorbance vs time (sec). The initial concentration of benzenethiol, catalyst **3e** and H_2O_2 were fixed to 1 mM, 0.1 mM, 3.75 mM respectively.

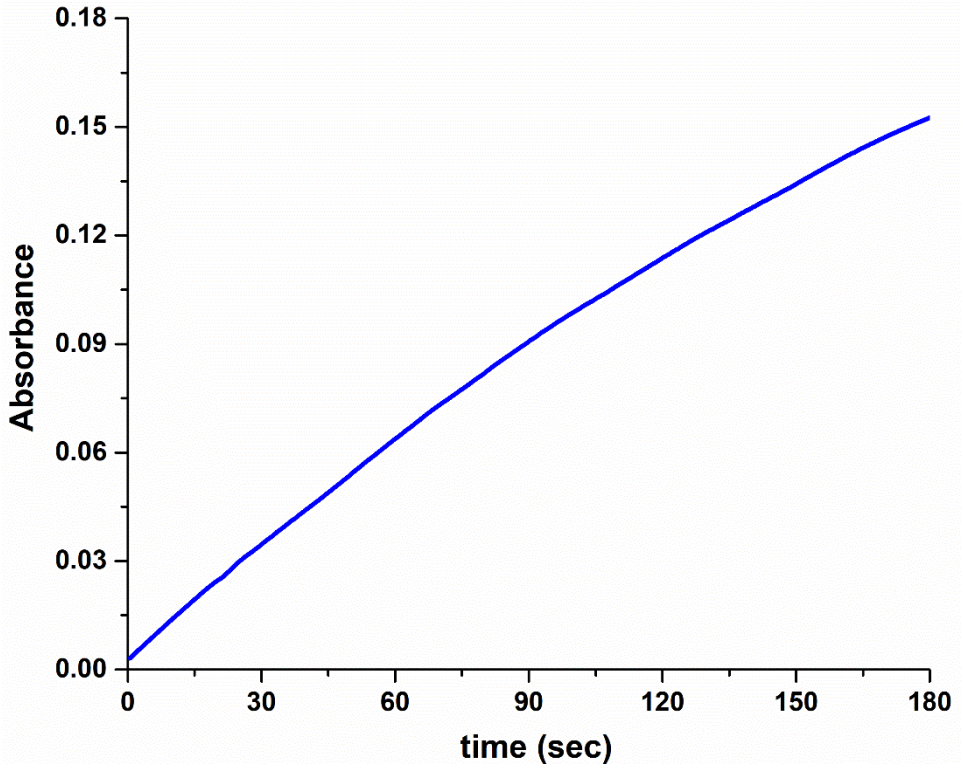


Figure S29: A model plot of absorbance vs time (sec). The initial concentration of benzenethiol, catalyst **3e** and H_2O_2 were fixed to 1 mM, 0.1 mM, 3.75 mM respectively.

Initial reduction rate of 3f

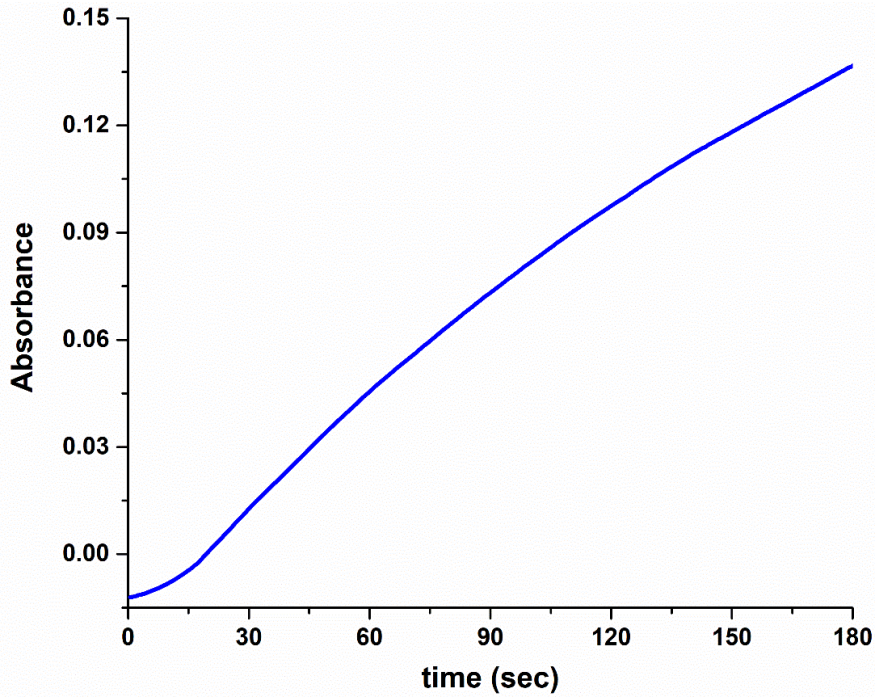


Figure S30: A model plot of absorbance vs time (sec). The initial concentration of benzenethiol, catalyst **3f** and H_2O_2 were fixed to 1 mM, 0.1 mM, 3.75 mM respectively.

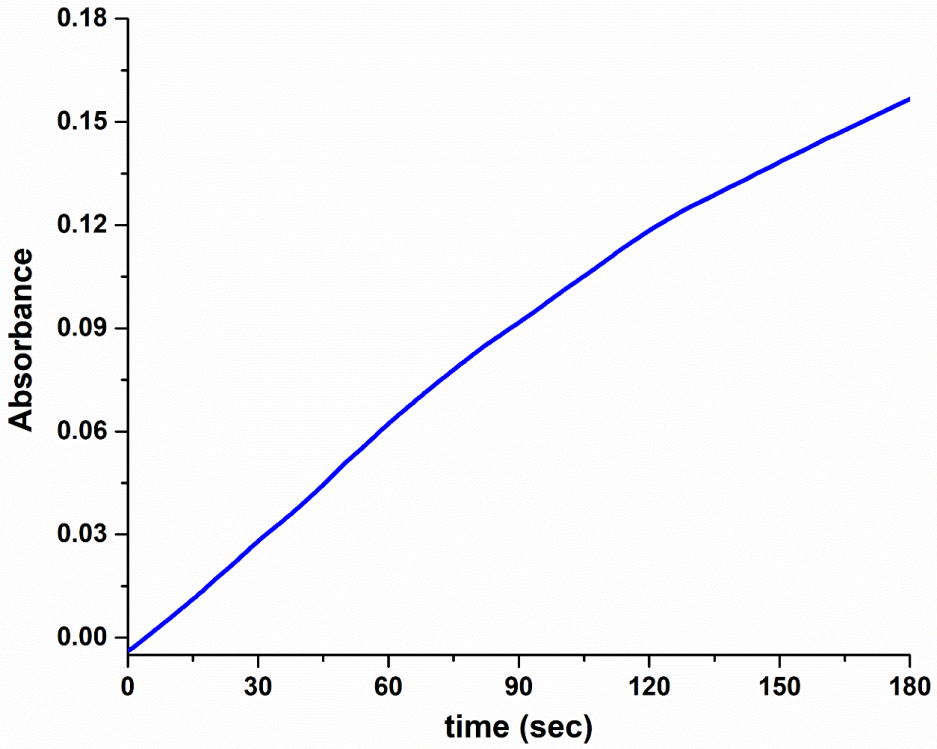


Figure S31: A model plot of absorbance vs time (sec). The initial concentration of benzenethiol, catalyst **3f** and H_2O_2 were fixed to 1 mM, 0.1 mM, 3.75 mM respectively.

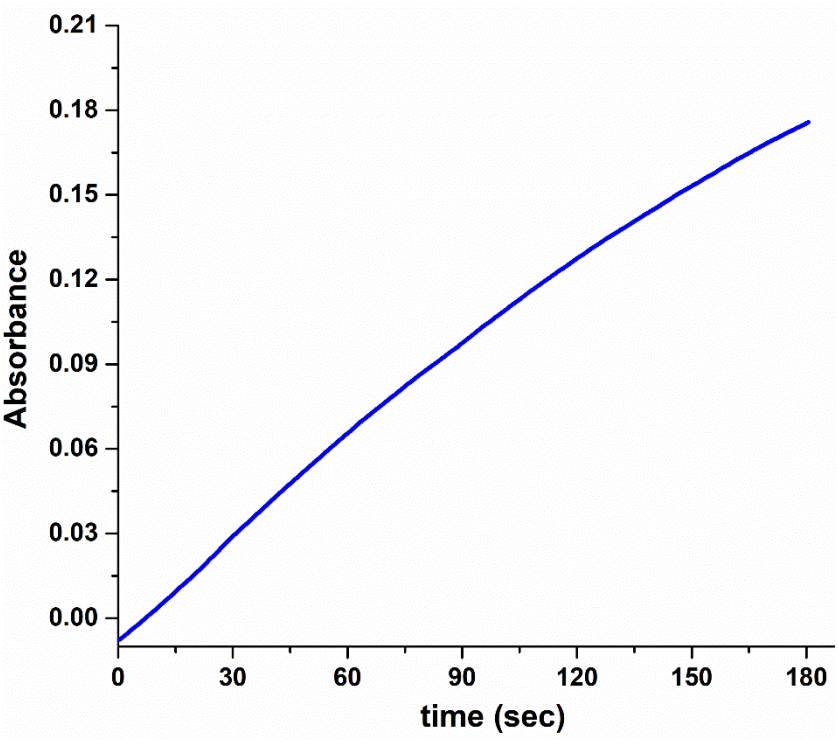


Figure S32: A model plot of absorbance vs time (sec). The initial concentration of benzenethiol, catalyst **3f** and H_2O_2 were fixed to 1 mM, 0.1 mM, 3.75 mM respectively.

Initial reduction rate 3g

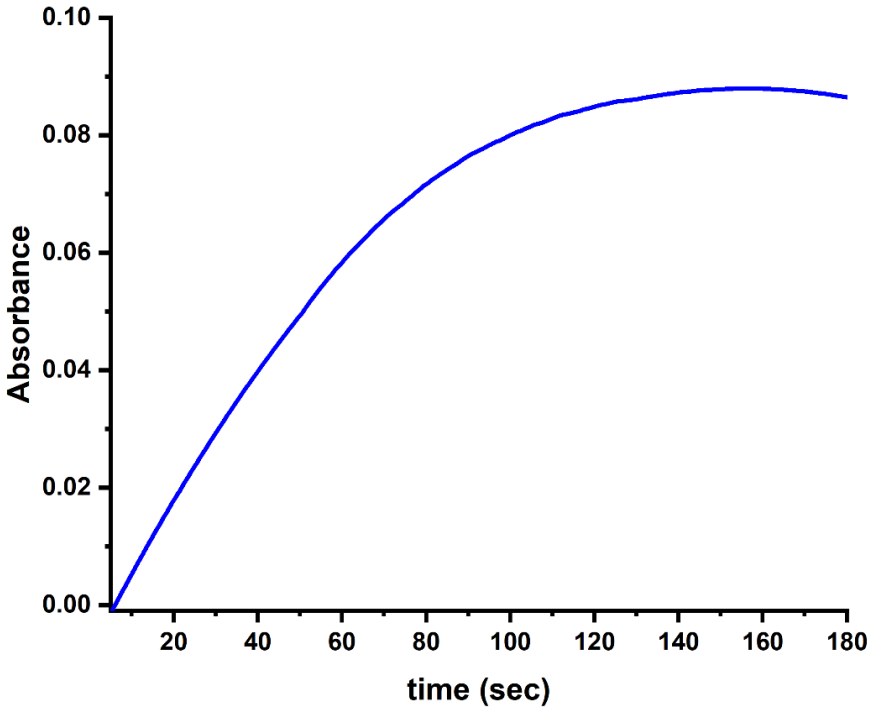


Figure S33: A model plot of absorbance vs time (sec). The initial concentration of benzenethiol, catalyst **3g** and H_2O_2 were fixed to 1 mM, 0.1 mM, 3.75 mM respectively.

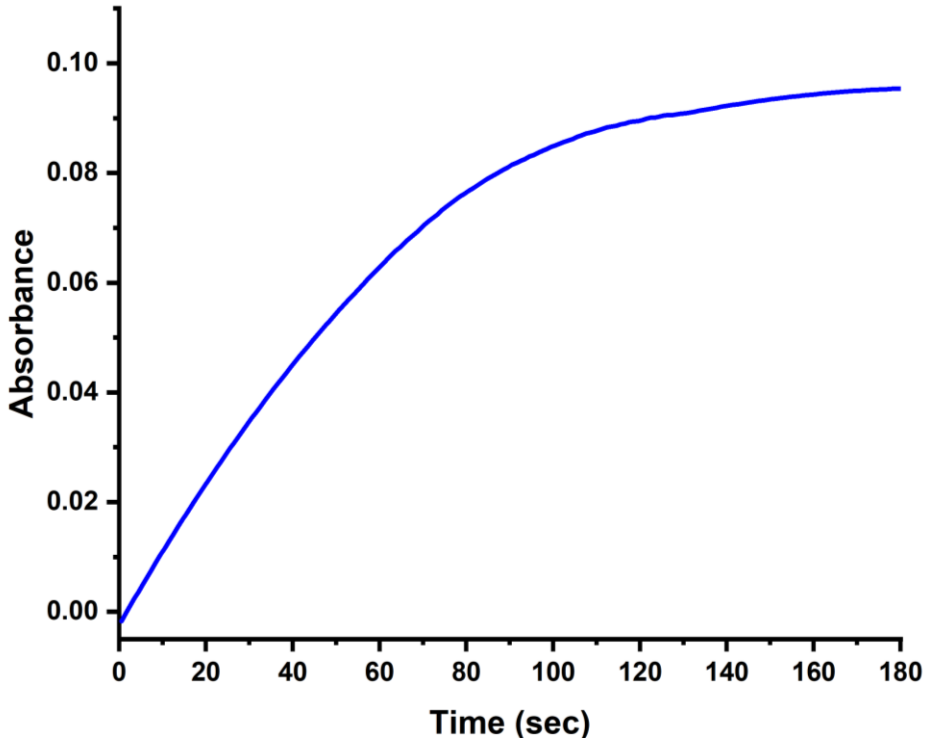


Figure S34: A model plot of absorbance vs time (sec). The initial concentration of benzenethiol, catalyst **3g** and H_2O_2 were fixed to 1 mM, 0.1 mM, 3.75 mM respectively.

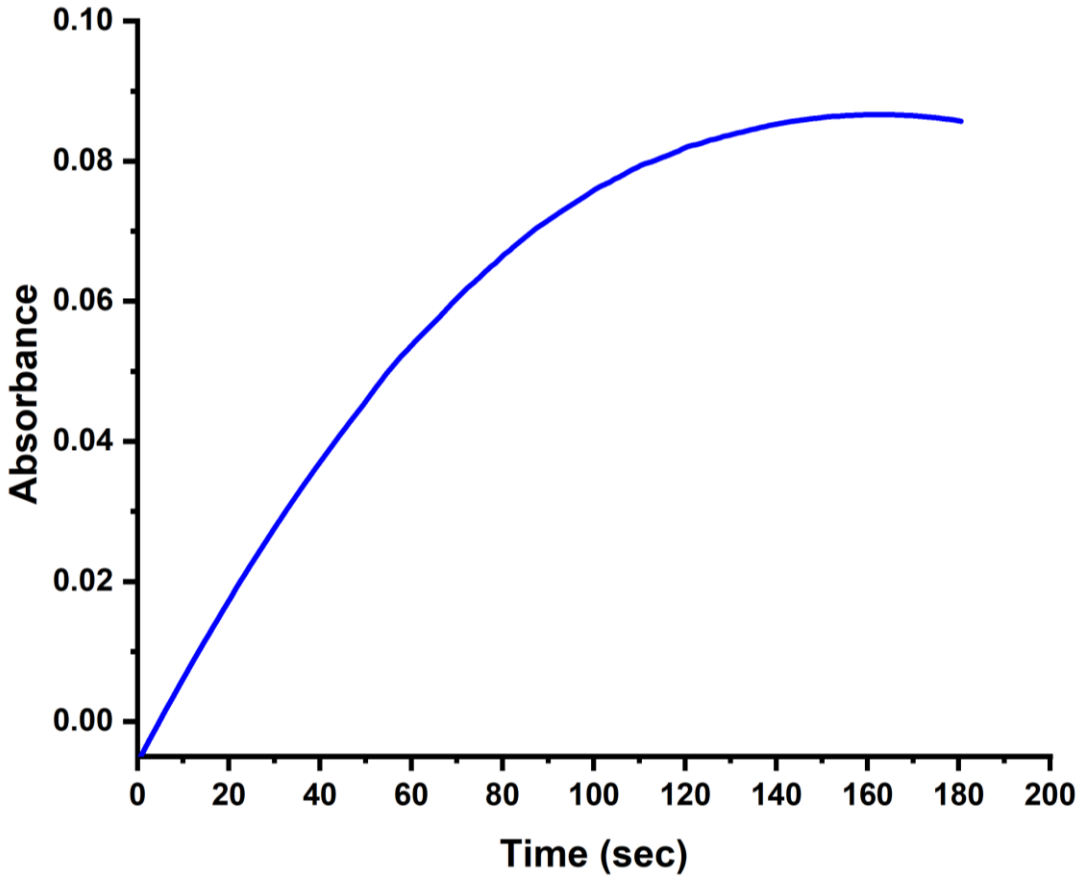


Figure S35: A model plot of absorbance vs time (sec). The initial concentration of benzenethiol, catalyst **3g** and H_2O_2 were fixed to 1 mM, 0.1 mM, 3.75 mM respectively.

7. MTT Assay

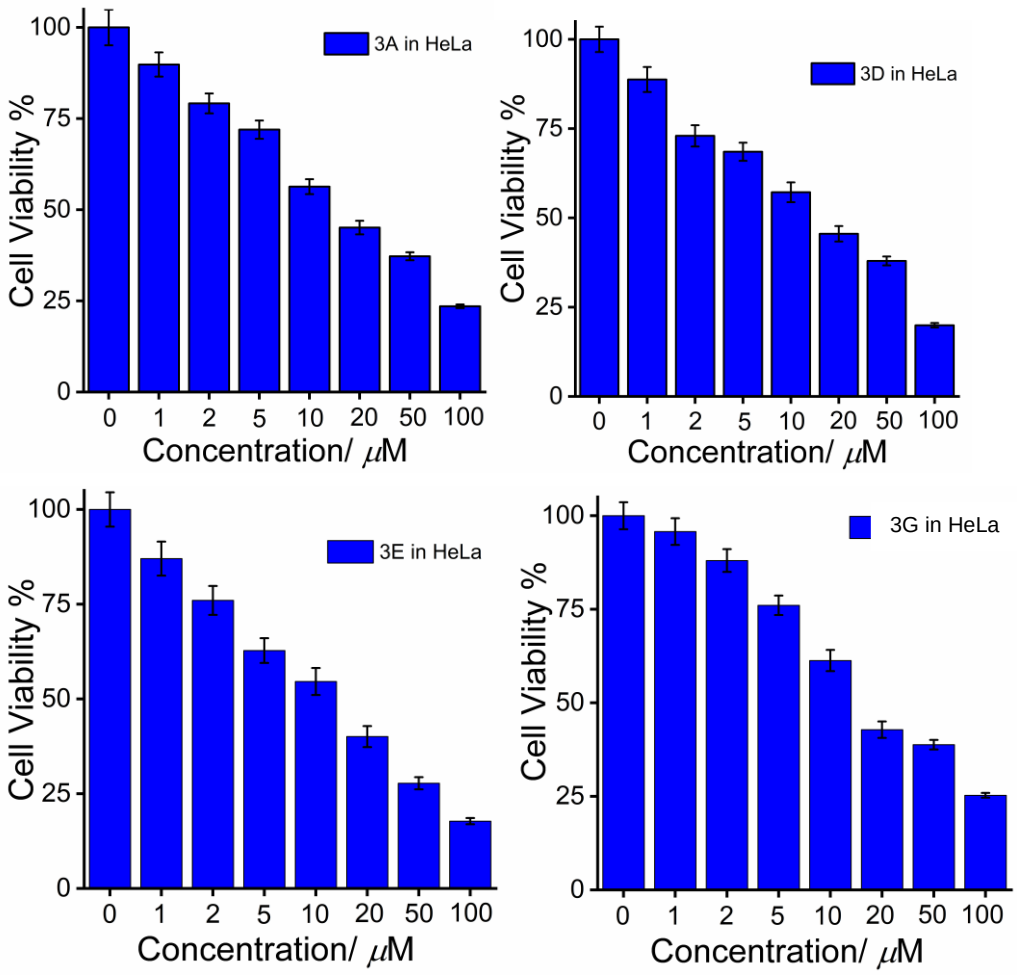


Figure S36. MTT assay of selected diselenides on Hela cancer cells.

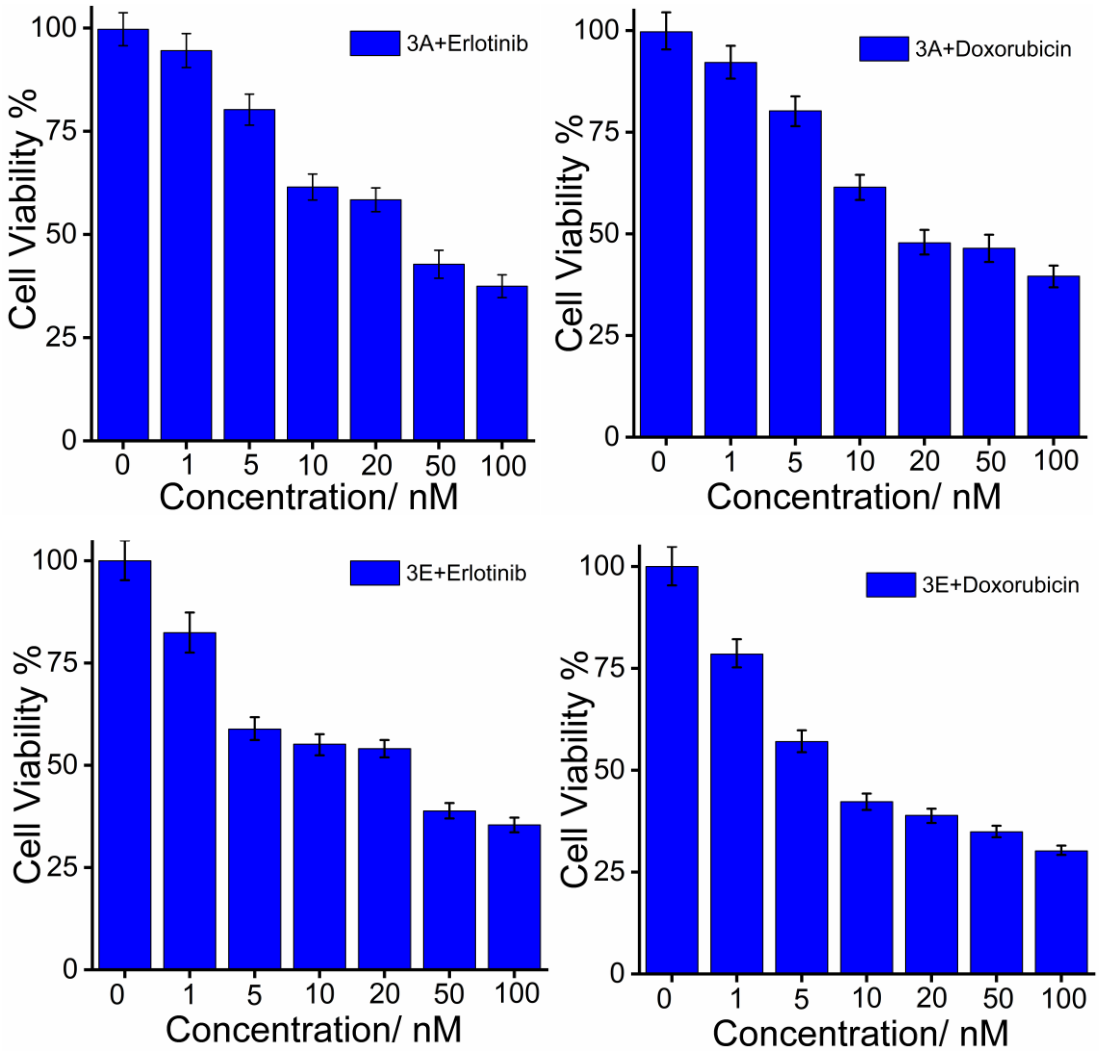


Figure S37. MTT of diselenides **3a** and **3e** in the combination with Erlotinib and Dox drugs on HeLa cancer cells.

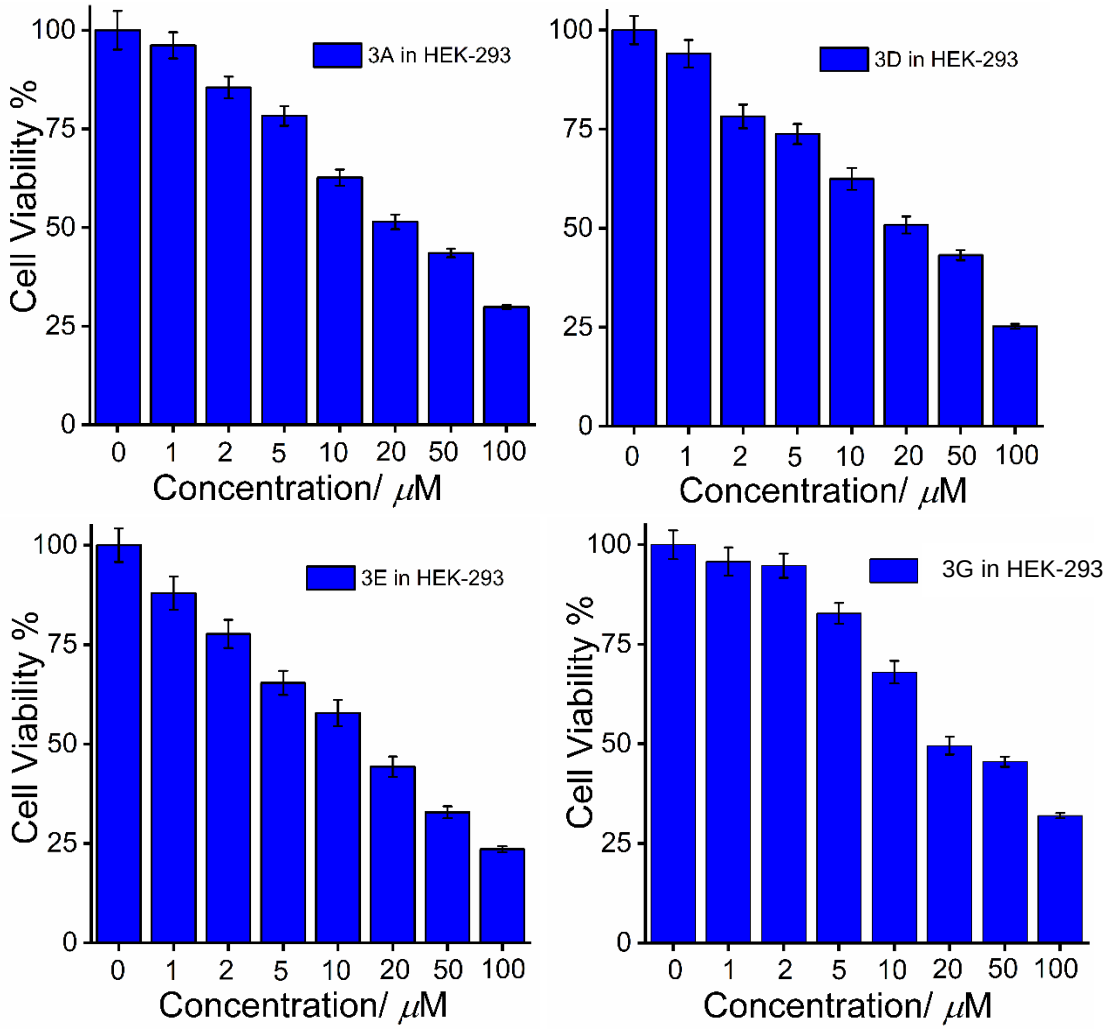
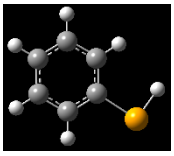


Figure S38. MTT assay of selected diselenides on HEK-293 cells.

8. Computational details

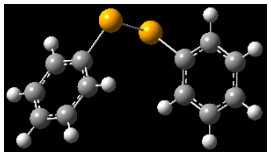
6



Gibb's free energy: -2633.779785

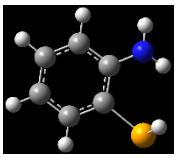
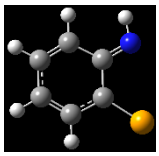
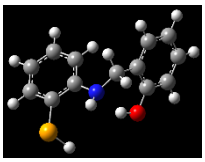
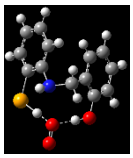
Symbol	X	Y	Z
Se	-1.828825	-0.043833	-0.001668
C	0.107008	0.017673	0.001618
C	0.795343	-1.199538	0.002622
C	0.819659	1.220007	-0.000525
C	2.188996	-1.209895	0.00078
H	0.252743	-2.139543	0.005578
C	2.213961	1.198306	-0.001194
H	0.299162	2.171293	-0.002017
C	2.904331	-0.012948	-0.00093
H	2.713857	-2.159661	0.001603
H	2.759008	2.136728	-0.002521
H	3.988882	-0.024078	-0.001832
H	-2.009373	1.423928	0.041685

6a



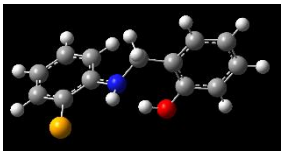
Gibb's free energy: -5266.377278

Symbol	X	Y	Z
C	0.03021	2.893248	2.334099
C	0.540042	2.055333	1.342387
C	-0.03021	2.063388	0.065329
C	-1.106742	2.910778	-0.216814
C	-1.614222	3.741206	0.780448
C	-1.046488	3.734022	2.055245
H	0.474636	2.886107	3.323833
H	1.376028	1.400699	1.560619
H	-1.544889	2.920673	-1.20837
H	-2.45	4.396947	0.559828
H	-1.441972	4.38388	2.82866
Se	0.72888	0.947118	-1.330257
Se	-0.72888	-0.947118	-1.330257
C	0.03021	-2.063388	0.065329
C	-0.540042	-2.055333	1.342387
C	1.106742	-2.910778	-0.216814
C	-0.03021	-2.893248	2.334099
H	-1.376028	-1.400699	1.560619
C	1.614222	-3.741206	0.780448
H	1.544889	-2.920673	-1.20837
C	1.046488	-3.734022	2.055245
H	-0.474636	-2.886107	3.323833

				H	2.45	-4.396947	0.559828
				H	1.441972	-4.38388	2.82866
7				**7a**			
							
Gibb's free energy: -2689.137379				Gibb's free energy: -2687.885087			
Symbol	X	Y	Z	Symbol	X	Y	Z
C	-2.16811	-1.499345	0.002967	C	-2.000797	-1.537209	0.000013
C	-0.776647	-1.451754	0.025744	C	0.045699	-0.191397	-0.000046
C	-0.099776	-0.230622	0.027156	C	-0.801894	1.053336	-0.000008
C	-0.816863	0.986442	0.003396	C	-2.260373	0.871582	-0.000004
C	-2.22334	0.91842	-0.005251	C	-2.82536	-0.351599	0.000005
C	-2.885364	-0.301976	-0.007976	H	-2.482672	-2.509679	0.000037
H	-2.681273	-2.454558	0.002002	H	-2.871122	1.770419	-0.000005
H	-0.204621	-2.373045	0.047831	H	-3.905157	-0.461105	0.000011
H	-2.791582	1.844132	-0.017101	N	-0.240067	2.209814	0.000008
H	-3.970554	-0.316857	-0.020835	H	-0.951998	2.945261	0.000027
Se	1.841252	-0.249416	-0.039643	Se	1.848633	-0.153029	0.000005
H	2.049865	0.522155	1.213102	C	-0.644779	-1.454545	-0.000008
N	-0.174261	2.21474	0.060734	H	-0.037087	-2.351606	0.000001
H	0.761325	2.227469	-0.324481				
H	-0.725301	3.000668	-0.253996				
4				**TS-I**			
							
Gibb's free energy: -3034.703127				Gibb's free energy: -3185.019577			
Correction to Gibbs Free Energy= 0.185689				Correction to Gibbs Free Energy= 0.180766			
Zero-point correction= 0.228780				Zero-point correction= 0.227879			
Symbol	X	Y	Z	Imaginary vibration frequency: 1 (-823.97)			
C	-0.847202	2.912069	-0.274032	Symbol	X	Y	Z

C	-2.187949	2.823574	-0.638031	C	1.850934	2.920706	0.72712
C	-2.830856	1.58964	-0.556304	C	2.639308	1.827196	0.399454
C	-2.150413	0.45701	-0.111758	C	2.063981	0.636757	-0.057893
C	-0.791685	0.541511	0.270374	C	0.651454	0.545814	-0.209669
C	-0.156267	1.789651	0.173738	C	-0.131273	1.674844	0.122749
N	-0.105936	-0.607315	0.694278	C	0.461443	2.838159	0.576643
C	1.13633	-0.502076	1.482018	H	2.311743	3.834853	1.083824
C	2.390624	-0.283464	0.654476	H	3.717186	1.890176	0.487646
C	3.425446	0.51321	1.152401	H	-1.20671	1.625211	0019796
C	4.630082	0.660988	0.468325	H	-0.162467	3.691324	0.819674
C	4.807902	0.002241	-0.74854	N	0.069662	-0.650249	-0.586282
C	3.788133	-0.785178	-1.272764	H	0.764036	-1.328925	-0.881114
C	2.582537	-0.933129	-0.580636	C	-1.172942	-0.77374	-1.386683
O	1.6240s01	-1.726385	-1.137284	H	-1.041736	-0.232279	-2.328862
H	-0.326432	3.862017	-0.335844	H	-1.226378	-1.836275	-1.639035
H	-2.727965	3.696362	-0.987687	C	-2.491262	-0.352226	-0.761686
H	-3.872398	1.501924	-0.84438	C	-2.854089	-0.683814	0.557787
H	0.887695	1.883075	0.444083	C	-3.435841	0.291825	-1.567972
H	1.055649	0.281165	2.244129	C	-4.138471	-0.392753	1.027069
H	1.22447	-1.452189	2.017249	C	-4.715847	0.584066	-1.104464
H	3.281565	1.023573	2.100905	H	-3.159177	0.562012	-2.583194
H	5.41754	1.28356	0.878817	C	-5.065389	0.230583	0.199304
H	5.738577	0.107318	-1.296778	H	-4.385587	-0.658986	2.049381
H	3.903916	-1.297038	-2.222411	H	-5.429605	1.081189	-1.751979
H	0.782604	-1.552925	-0.663924	H	-6.058205	0.450617	0.578204
H	-0.745418	-1.294607	1.078982	O	-1.98416	-1.269446	1.414744
Se	-3.155198	-1.197634	0.07726	H	-1.074148	-1.255847	1.055008
H	-2.373618	-1.976662	-0.917249	Se	3.249417	-0.761193	-0.727056
				H	3.412057	-1.438347	0.580458
				O	1.371334	-0.915046	2.062092
				O	0.687718	-1.820125	1.548603

TS-II



Gibb's free energy: -3034.092858

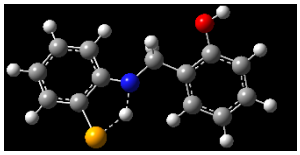
Correction to Gibbs Free Energy= 0.178712

Zero-point correction= 0.220711

Imaginary vibration frequency: 1 (-33.37)

Symbol	X	Y	Z
C	-2.508854	2.274739	-1.228029
C	-2.609759	0.900061	-1.087763
C	-1.833281	0.212749	-0.142019
C	-0.955383	0.942606	0.715639
C	-0.835226	2.3354	0.520555
C	-1.60064	2.987296	-0.429117
H	-3.112671	2.791608	-1.965782
H	-3.276582	0.337656	-1.732248
H	-0.160746	2.902167	1.151996
H	-1.502879	4.061209	-0.54704
N	-0.250975	0.305555	1.714457
H	-0.506623	-0.664094	1.828114
C	1.169699	0.557794	1.930654
H	1.328167	1.586442	2.259744
H	1.471695	-0.082544	2.764529
C	2.047973	0.270476	0.72097
C	1.915064	-0.977775	0.019693
C	3.012231	1.176182	0.309629
C	2.750461	-1.212628	-1.110335
C	3.836984	0.914029	-0.793875
H	3.119978	2.117314	0.841069
C	3.700808	-0.28688	-1.501083

TS-III



Gibb's free energy: -3034.055355

Correction to Gibbs Free Energy= 0.167895

Zero-point correction= 0.212204

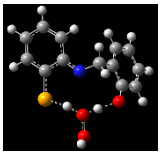
Imaginary vibration frequency: 1 (-1037.47)

Symbol	X	Y	Z
C	3.802272	0.234879	0.089258
C	2.471312	-0.190332	0.086909
C	1.429325	0.772961	0.413106
C	1.856842	2.120596	0.713714
C	3.172249	2.500453	0.689625
C	4.15518	1.547737	0.374961
H	4.589904	-0.471493	-0.143173
H	1.083673	2.824578	0.99524
H	3.452877	3.520187	0.92476
H	5.202282	1.827751	0.359843
N	0.102774	0.612141	0.484372
H	-0.498953	1.810262	-0.15906
C	-0.57488	-0.653353	0.251239
H	-0.328482	-1.045236	-0.745533
H	-0.212651	-1.388646	0.980882
C	-2.078936	-0.550488	0.359635
C	-2.858191	-0.176322	-0.749299
C	-2.728831	-0.895866	1.547814
C	-4.252132	-0.188027	-0.663119
C	-4.118817	-0.893529	1.640919
H	-2.133448	-1.185444	2.40873
C	-4.880757	-0.547434	0.52509

H	2.633296	-2.15687	-1.631278
H	4.566185	1.652372	-1.108475
H	4.337186	-0.488072	-2.356382
O	1.091866	-1.903114	0.422408
H	-0.28357	-1.808155	0.198398
Se	-1.886235	-1.697862	-0.07743

H	-4.824623	0.097891	-1.538618
H	-4.601922	-1.168711	2.572129
H	-5.964386	-0.549907	0.580703
O	-2.289482	0.139319	-1.959257
H	-1.644634	0.863096	-1.843613
Se	2.107353	-2.016646	-0.350278
H	3.534692	-2.341603	-0.574747
O	-2.083692	2.874248	-0.472242
O	-0.925771	2.361506	-0.940729

TS-IV



Gibb's free energy: -3185.019577

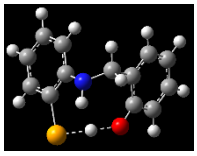
Correction to Gibbs Free Energy= 0.180766

Zero-point correction= 0.227879

Imaginary vibration frequency: 1 (-823.97)

Symbol	X	Y	Z
C	1.375222	2.972659	0.106098
C	2.22303	2.483588	1.16463
C	2.302899	1.162061	1.412788
C	1.599743	0.166398	0.568825
C	0.646284	0.744072	-0.456445
C	0.608596	2.154426	-0.668261
N	-0.140273	-0.116623	-1.057155
C	-1.408253	0.121682	-1.760244
C	-2.569565	0.094119	-0.783136
C	-3.437771	1.185419	-0.691303
C	-4.523856	1.171275	0.182715
C	-4.746441	0.053649	0.985229

TS-V



Gibb's free energy: -3034.063479

Correction to Gibbs Free Energy= 0.170489

Zero-point correction= 0.212700

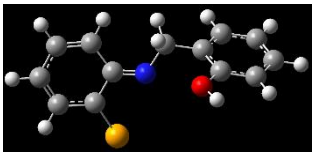
Imaginary vibration frequency: 1 (-1802.91)

Symbol	X	Y	Z
C	-2.508854	2.274739	-1.228029
C	-2.609759	0.900061	-1.087763
C	-1.833281	0.212749	-0.142019
C	-0.955383	0.942606	0.715639
C	-0.835226	2.3354	0.520555
C	-1.60064	2.987296	-0.429117
H	-3.112671	2.791608	-1.965782
H	-3.276582	0.337656	-1.732248
H	-0.160746	2.902167	1.151996
H	-1.502879	4.061209	-0.54704
N	-0.250975	0.305555	1.714457
H	-0.506623	-0.664094	1.828114

C	-3.884959	-1.039601	0.91241
C	-2.797368	-1.025856	0.039139
O	-2.008668	-2.153963	-0.061118
H	1.331901	4.042983	-0.064397
H	2.785888	3.193662	1.758201
H	2.910359	0.756822	2.212369
H	-0.042598	2.571558	-1.424605
H	-1.372536	1.068854	-2.293125
H	-1.499568	-0.672571	-2.503158
H	-3.264875	2.054248	-1.318914
H	-5.188763	2.026554	0.234556
H	-5.588126	0.030263	1.669524
H	-4.045274	-1.918534	1.52753
H	0.02235	-1.086056	-0.77075
Se	3.088819	-0.861768	-0.430428
H	1.9935	-1.964597	-0.043534
H	-1.140404	-2.084872	0.406457
O	0.648089	-2.000647	0.712119
O	0.952434	-0.766039	1.420224

C	1.169699	0.557794	1.930654
H	1.328167	1.586442	2.259744
H	1.471695	-0.082544	2.764529
C	2.047973	0.270476	0.72097
C	1.915064	-0.977775	0.019693
C	3.012231	1.176182	0.309629
C	2.750461	-1.212628	-1.110335
C	3.836984	0.914029	-0.793875
H	3.119978	2.117314	0.841069
C	3.700808	-0.28688	-1.501083
H	2.633296	-2.15687	-1.631278
H	4.566185	1.652372	-1.108475
H	4.337186	-0.488072	-2.356382
O	1.091866	-1.903114	0.422408
H	-0.28357	-1.808155	0.198398
Se	-1.886235	-1.697862	-0.07743

Selone 5



Gibb’s free energy: -3033.466578

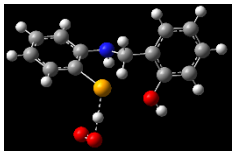
Correction to Gibbs Free Energy= 0.161201

Zero-point correction= 0.207209

Imaginary vibration frequency: 0

Symbol	X	Y	Z
C	-3.158826	0.986385	-0.628718
C	-1.972599	0.264032	-0.337514

TS-VI



Gibb’s free energy: -3185.010556

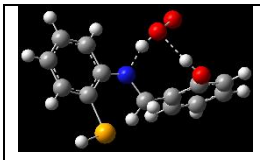
Correction to Gibbs Free Energy= 0.184479

Zero-point correction= 0.231822

Imaginary vibration frequency: 1 (-25.86)

Symbol	X	Y	Z
C	-3.158826	0.986385	-0.628718
C	-1.972599	0.264032	-0.337514

C	-0.900202	0.929660.34998		C	-0.900202	0.929660.34998	
C	-1.167904	2.243064	0.844381	C	-1.167904	2.243064	0.844381
C	-2.346356	2.892712	0.581673	C	-2.346356	2.892712	0.581673
C	-3.355976	2.273203	-0.187938	C	-3.355976	2.273203	-0.187938
H	-3.936231	0.480419	-1.188995	H	-3.936231	0.480419	-1.188995
H	-0.387358	2.746267	1.406925	H	-0.387358	2.746267	1.406925
H	-2.491752	3.900849	0.955352	H	-2.491752	3.900849	0.955352
H	-4.279601	2.795583	-0.408447	H	-4.279601	2.795583	-0.408447
N	0.341678	0.440473	0.594907	N	0.341678	0.440473	0.594907
H	0.914297	1.039841	1.172104	H	0.914297	1.039841	1.172104
C	1.102958	-0.617968	-0.088523	C	1.102958	-0.617968	-0.088523
H	0.828796	-0.625386	-1.142994	H	0.828796	-0.625386	-1.142994
H	0.84667	-1.596874	0.320721	H	0.84667	-1.596874	0.320721
C	2.584229	-0.375076	0.06892	C	2.584229	-0.375076	0.06892
C	3.239124	0.588072	-0.716943	C	3.239124	0.588072	-0.716943
C	3.340514	-1.105615	0.988912	C	3.340514	-1.105615	0.988912
C	4.611369	0.805389	-0.578701	C	4.611369	0.805389	-0.578701
C	4.711187	-0.895736	1.136425	C	4.711187	-0.895736	1.136425
H	2.842059	-1.855657	1.595658	H	2.842059	-1.855657	1.595658
C	5.342816	0.064384	0.34749	C	5.342816	0.064384	0.34749
H	5.103734	1.551302	-1.196105	H	5.103734	1.551302	-1.196105
H	5.277756	-1.475898	1.856212	H	5.277756	-1.475898	1.856212
H	6.408721	0.240601	0.447133	H	6.408721	0.240601	0.447133
O	2.478186	1.289077	-1.612543	O	2.478186	1.289077	-1.612543
H	3.02551	1.909918	-2.110593	H	3.02551	1.909918	-2.110593
Se	-1.905793	-1.520017	-1.039695	Se	-1.905793	-1.520017	-1.039695
H	-1.849056	-2.150109	0.3322	H	-1.849056	-2.150109	0.3322
O	-2.665658	-1.690634	1.924322	O	-2.665658	-1.690634	1.924322
O	-2.572569	-0.433271	1.996901	O	-2.572569	-0.433271	1.996901
TS-VII				**TS-VIII**			



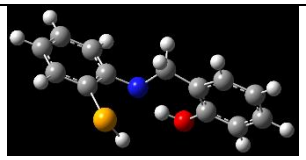
Gibb’s free energy: -3184.983718

Correction to Gibbs Free Energy= 0.180010

Zero-point correction= 0.228767

Imaginary vibration frequency: 1 (-101.40)

Symbol	X	Y	Z
C	3.802272	0.234879	0.089258
C	2.471312	-0.190332	0.086909
C	1.429325	0.772961	0.413106
C	1.856842	2.120596	0.713714
C	3.172249	2.500453	0.689625
C	4.15518	1.547737	0.374961
H	4.589904	-0.471493	-0.143173
H	1.083673	2.824578	0.99524
H	3.452877	3.520187	0.92476
H	5.202282	1.827751	0.359843
N	0.102774	0.612141	0.484372
H	-0.498953	1.810262	-0.15906
C	-0.57488	-0.653353	0.251239
H	-0.328482	-1.045236	-0.745533
H	-0.212651	-1.388646	0.980882
C	-2.078936	-0.550488	0.359635
C	-2.858191	-0.176322	-0.749299
C	-2.728831	-0.895866	1.547814
C	-4.252132	-0.188027	-0.663119
C	-4.118817	-0.893529	1.640919
H	-2.133448	-1.185444	2.40873
C	-4.880757	-0.547434	0.52509
H	-4.824623	0.097891	-1.538618



Gibb’s free energy: -3034.055288

Correction to Gibbs Free Energy= 0.169424

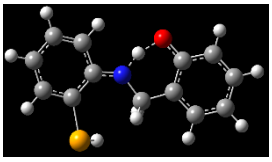
Zero-point correction= 0.213133

Imaginary vibration frequency: 1 (-59.48)

Symbol	X	Y	Z
C	3.565304	0.474696	-0.212611
C	2.275637	-0.011154	0.005144
C	1.188577	0.926358	0.13508
C	1.523458	2.322709	0.1006
C	2.806275	2.76687	-0.108006
C	3.841916	1.837731	-0.281345
H	4.381986	-0.231863	-0.30835
H	0.712427	3.030972	0.225791
H	3.012443	3.830515	-0.139464
H	4.86	2.170916	-0.445803
N	-0.126889	0.685593	0.264388
C	-0.865298	-0.559949	0.276916
H	-0.701804	-1.06138	1.242787
H	-0.477829	-1.250745	-0.480954
C	-2.351522	-0.32457	0.084647
C	-3.193908	-1.428794	-0.053991
C	-2.900164	0.993561	0.061377
C	-4.568119	-1.282483	-0.222775
H	-2.760695	-2.426515	-0.033109
C	-4.299303	1.120689	-0.11526
C	-5.113527	0.006715	-0.252485
H	-5.203077	-2.154848	-0.333587
H	-4.713478	2.124278	-0.136546

H	-4.601922	-1.168711	2.572129
H	-5.964386	-0.549907	0.580703
O	-2.289482	0.139319	-1.959257
H	-1.644634	0.863096	-1.843613
Se	2.107353	-2.016646	-0.350278
H	3.534692	-2.341603	-0.574747
O	-2.083692	2.874248	-0.472242
O	-0.925771	2.361506	-0.940729
H	-6.183548	0.139206	-0.38485
O	-2.134086	2.058917	0.199653
H	-0.954589	1.550009	0.269513
Se	2.154838	-1.939959	-0.017204
H	1.268624	-2.086703	1.157815

TS-IX



Gibb's free energy: -3034.056848

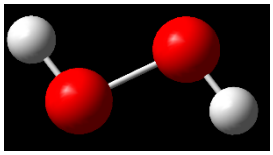
Correction to Gibbs Free Energy= 0.165416

Zero-point correction= 0.209658

Imaginary vibration frequency: 1 (-1278.85s)

Symbol	X	Y	Z
C	3.565304	0.474696	-0.212611
C	2.275637	-0.011154	0.005144
C	1.188577	0.926358	0.13508
C	1.523458	2.322709	0.1006
C	2.806275	2.76687	-0.108006
C	3.841916	1.837731	-0.281345
H	4.381986	-0.231863	-0.30835
H	0.712427	3.030972	0.225791
H	3.012443	3.830515	-0.139464
H	4.860000	2.170916	-0.445803
N	-0.126889	0.685593	0.264388
C	-0.865298	-0.559949	0.276916
H	-0.701804	-1.06138	1.242787

H_2O_2



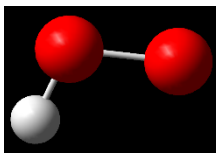
Gibb's free energy: -151.592371

Correction to Gibbs Free Energy= 0.003530

Zero-point correction= 0.025674

Symbol	X	Y	Z
O	0.717192	0.141625	-0.000024
H	1.066568	-0.761861	0.000134
O	-0.717192	-0.141625	-0.000032
H	-1.066568	0.761861	0.000309

HOO radical



Gibb's free energy: -150.967003

Correction to Gibbs Free Energy= -0.007981

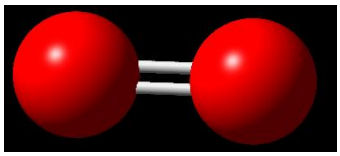
Zero-point correction= 0.014186

Symbol	X	Y	Z
O	0.055061	-0.606043	0

H	-0.477829	-1.250745	-0.480954
C	-2.351522	-0.32457	0.084647
C	-3.193908	-1.428794	-0.053991
C	-2.900164	0.993561	0.061377
C	-4.568119	-1.282483	-0.222775
H	-2.760695	-2.426515	-0.033109
C	-4.299303	1.120689	-0.11526
C	-5.113527	0.006715	-0.252485
H	-5.203077	-2.154848	-0.333587
H	-4.713478	2.124278	-0.136546
H	-6.183548	0.139206	-0.38485
O	-2.134086	2.058917	0.199653
H	-0.954589	1.550009	0.269513
Se	2.154838	-1.939959	-0.017204
H	1.268624	-2.086703	1.157815

H	0.880972	-0.892572	0
O	0.055061	0.717614	0

O_2



Gibb's free energy: -150.325240

Symbol	X	Y	Z
O	0	0	0.603038
O	0	0	0.603038

References

1. M. J. Frisch, G. W. Frisch, H. B. Schlegel et al. Gaussian 09, Revision A.02, Gaussian, Inc., Wallingford CT, 2009.