

Electronic Supplementary Information

A straightforward TBHP-mediated synthesis of 2-amidobenzoic acids from 2 arylindoles and their antimicrobial activity

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‡Equal contribution to this work

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1. Procedure for the synthesis of **3a**:

To a solution of 2-phenylindole **1a** (0.518 mmol) and 2-aminopyridine (0.62 mmol) and Cu(OAc)₂.H₂O (20 mol %) in chlorobenzene (5 mL) was added TBHP (1.55 mmol, 70% aqueous solution) at room temperature and the reaction mixture was stirred at 120 °C with a reflux condenser for 2 h. After completion of the reaction, observed by TLC, the mixture was allowed to attain room temperature. The reaction mixture was poured into water (20 mL) and extracted with ethyl acetate (3 × 15 mL). The combined organic layer was dried over Na₂SO₄ and evaporated under vacuum. The resulting crude solid was purified by column chromatography (silica gel 100-200 mesh) using *n*-hexane (100%) as an eluent to afford as the red color amorphous solid product in 70% yield.

***Note:** The ¹H NMR analysis of isolated product showed the mixture of two compounds *i.e.* 2-phenyl-3H-indol-3-one (**3a**) and 2-phenyl-4*H*-benzo[d][1,3]oxazin-4-one (**4a**) in 10: 3.5 NMR ratio. We have tried multiple column chromatographies to separate out the mixture of **3a** and **4a**. However due to inseparable spots on TLC and highly non-polar in nature, we could not isolate them in a pure form. The mixture was directly used for the control reaction as described in the manuscript.

2. Copies of the NMR and ESI-HRMS data for all the compounds

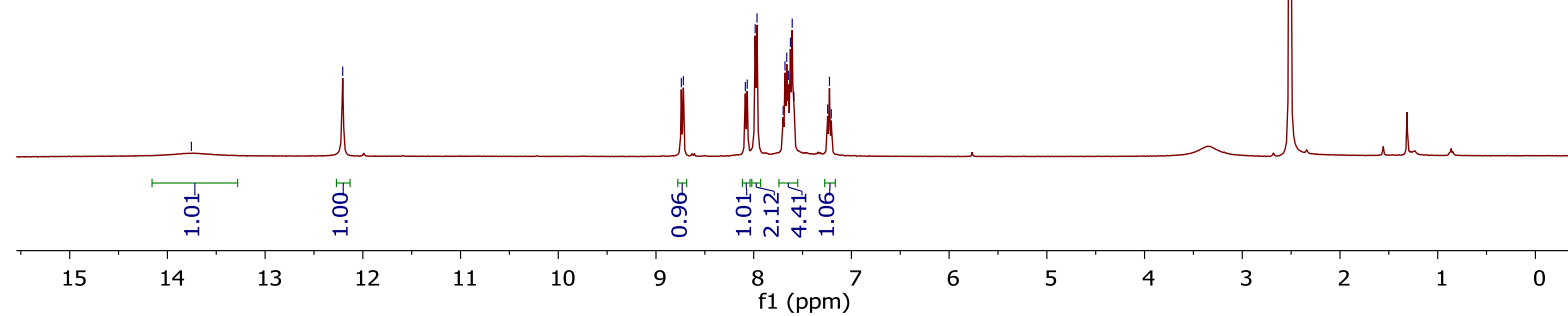
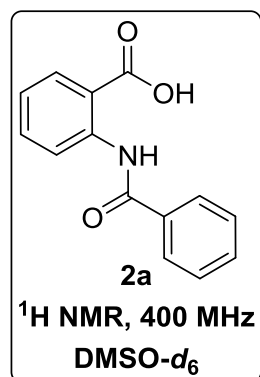
Apr02-2018
MS/SD-1013

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— 12.2060

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— 2.5124

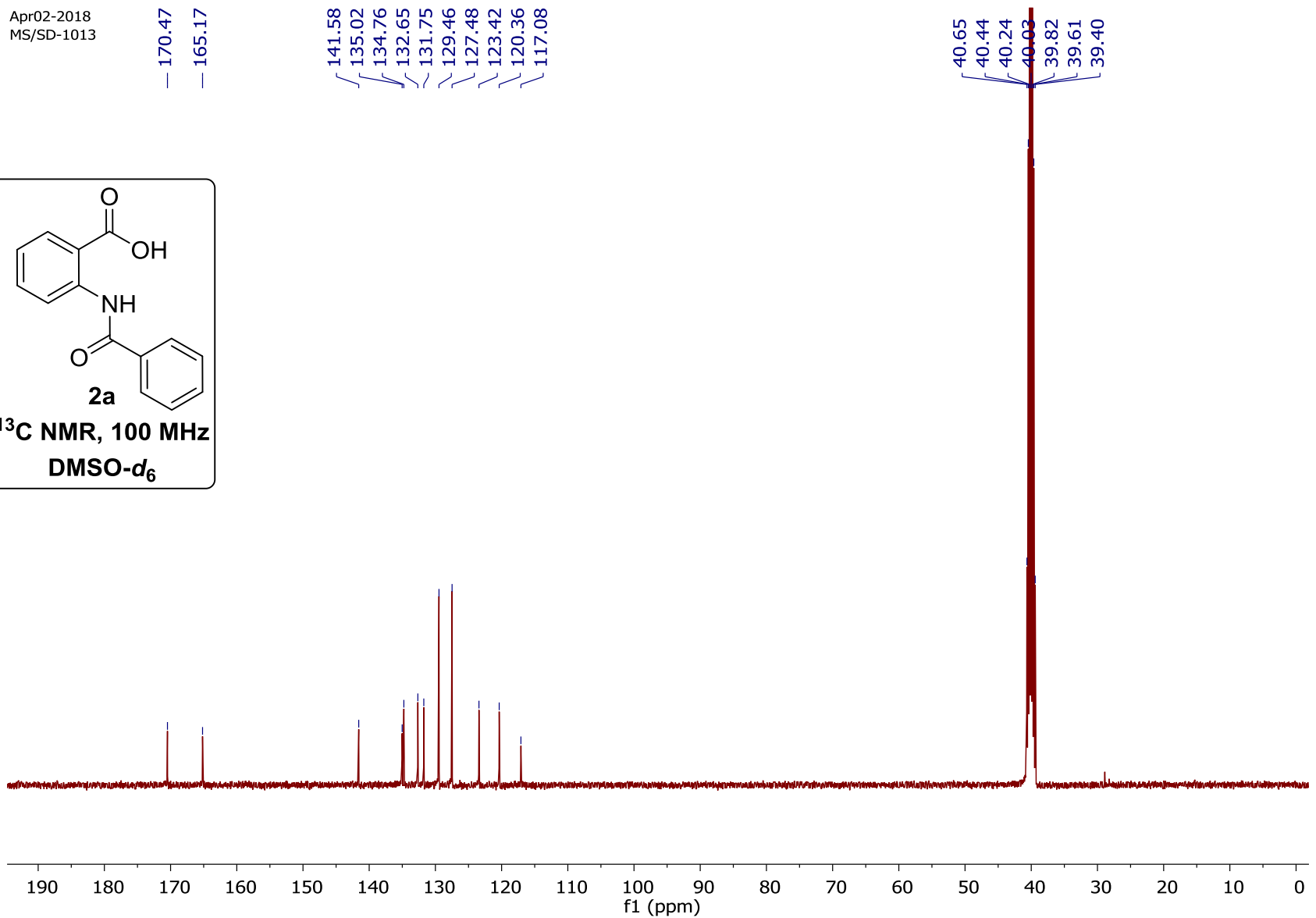
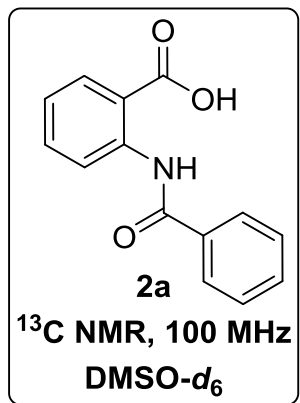


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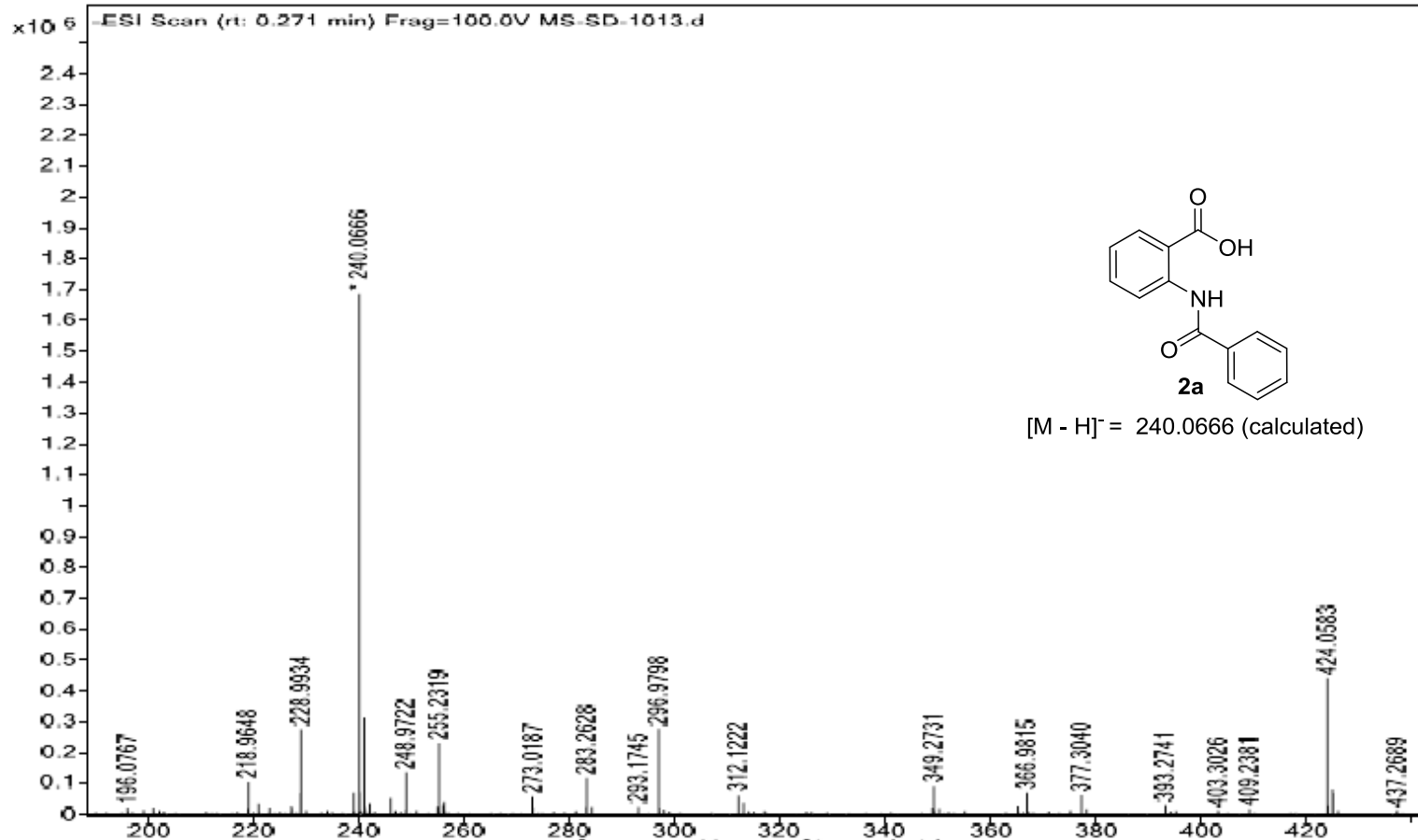
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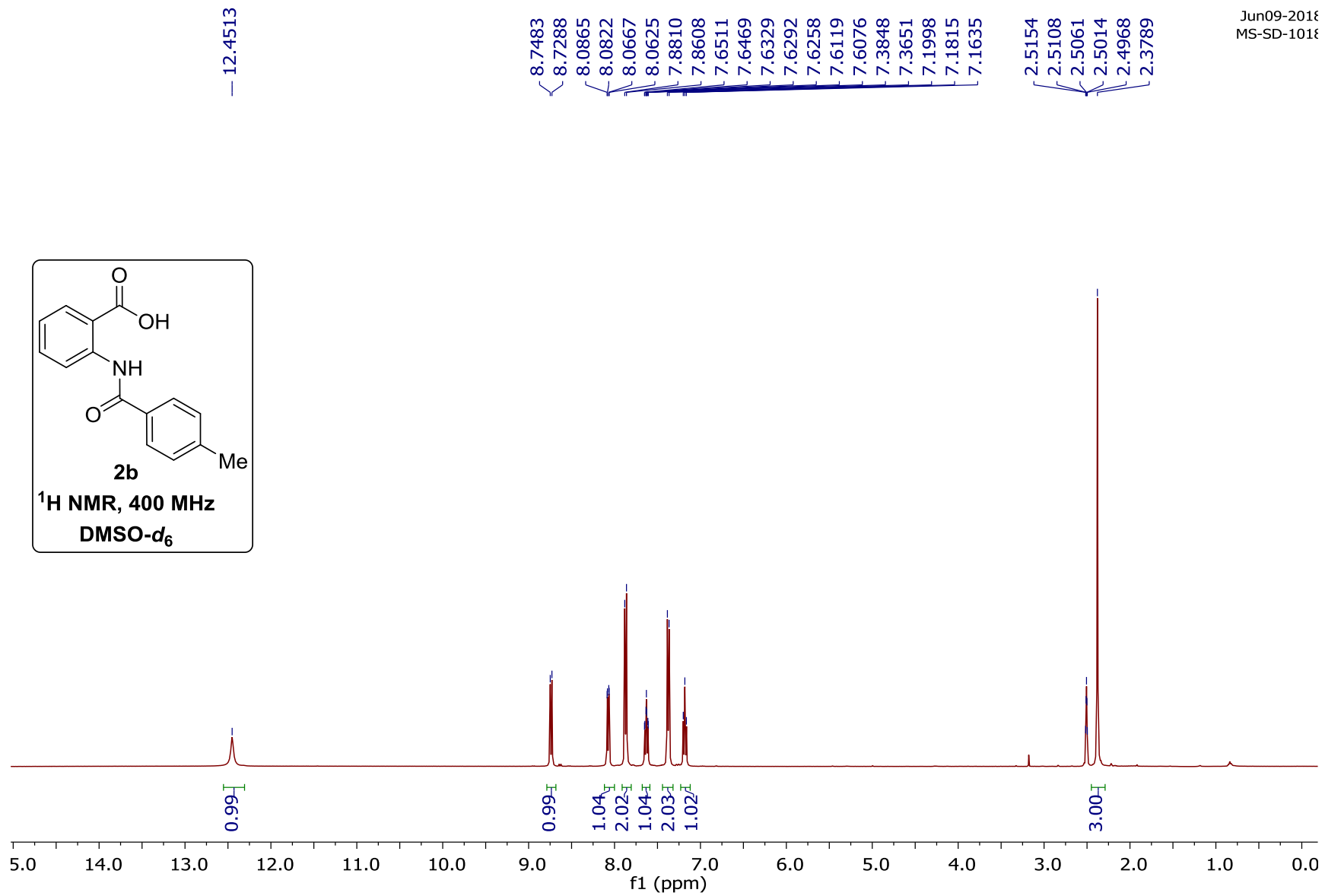
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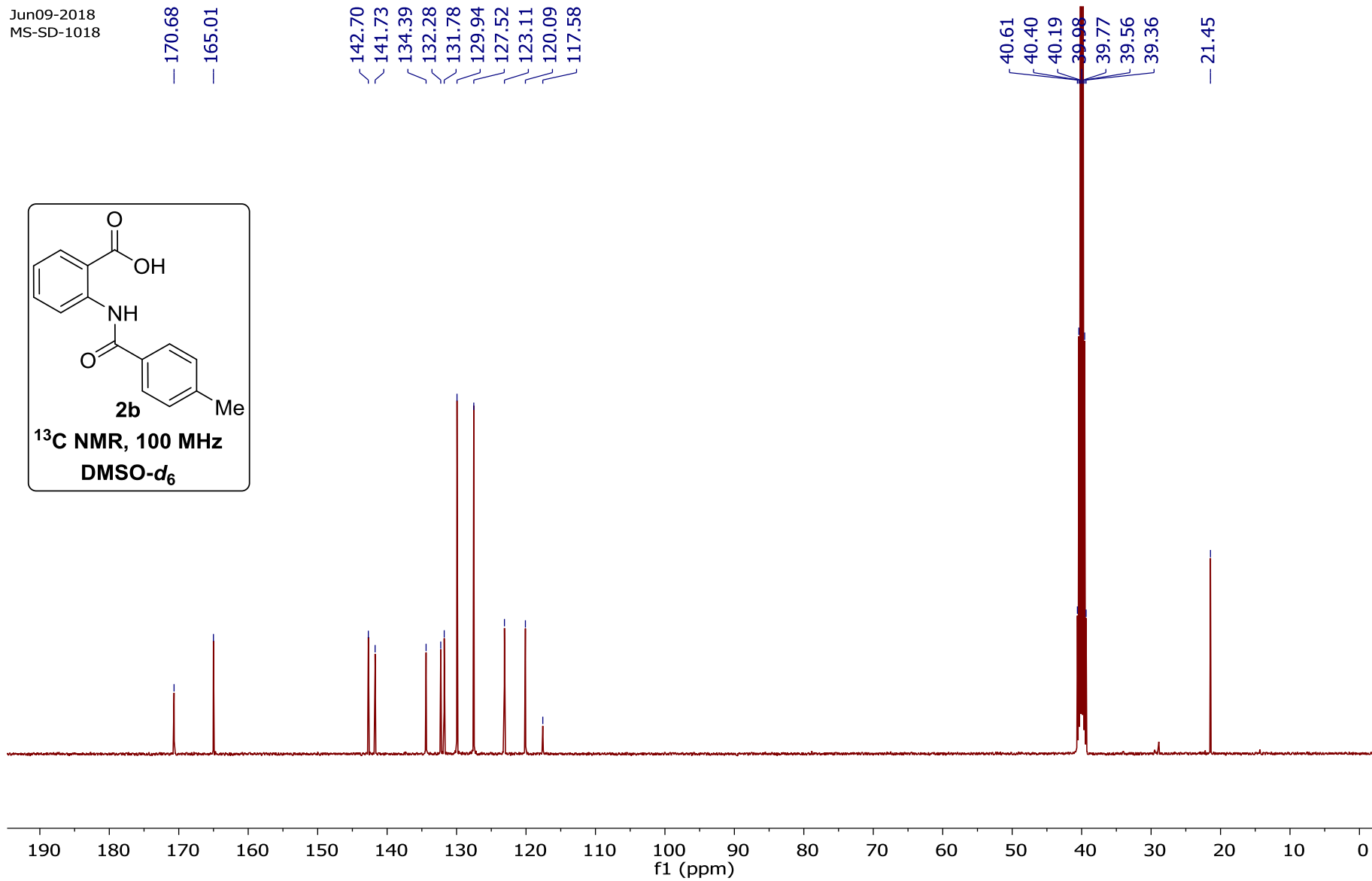
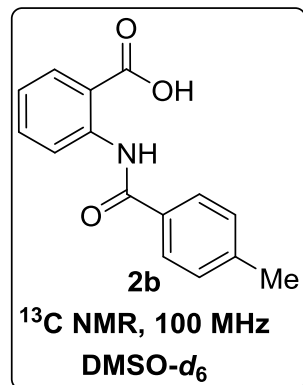
Jun09-2018
MS-SD-1018

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— 165.01

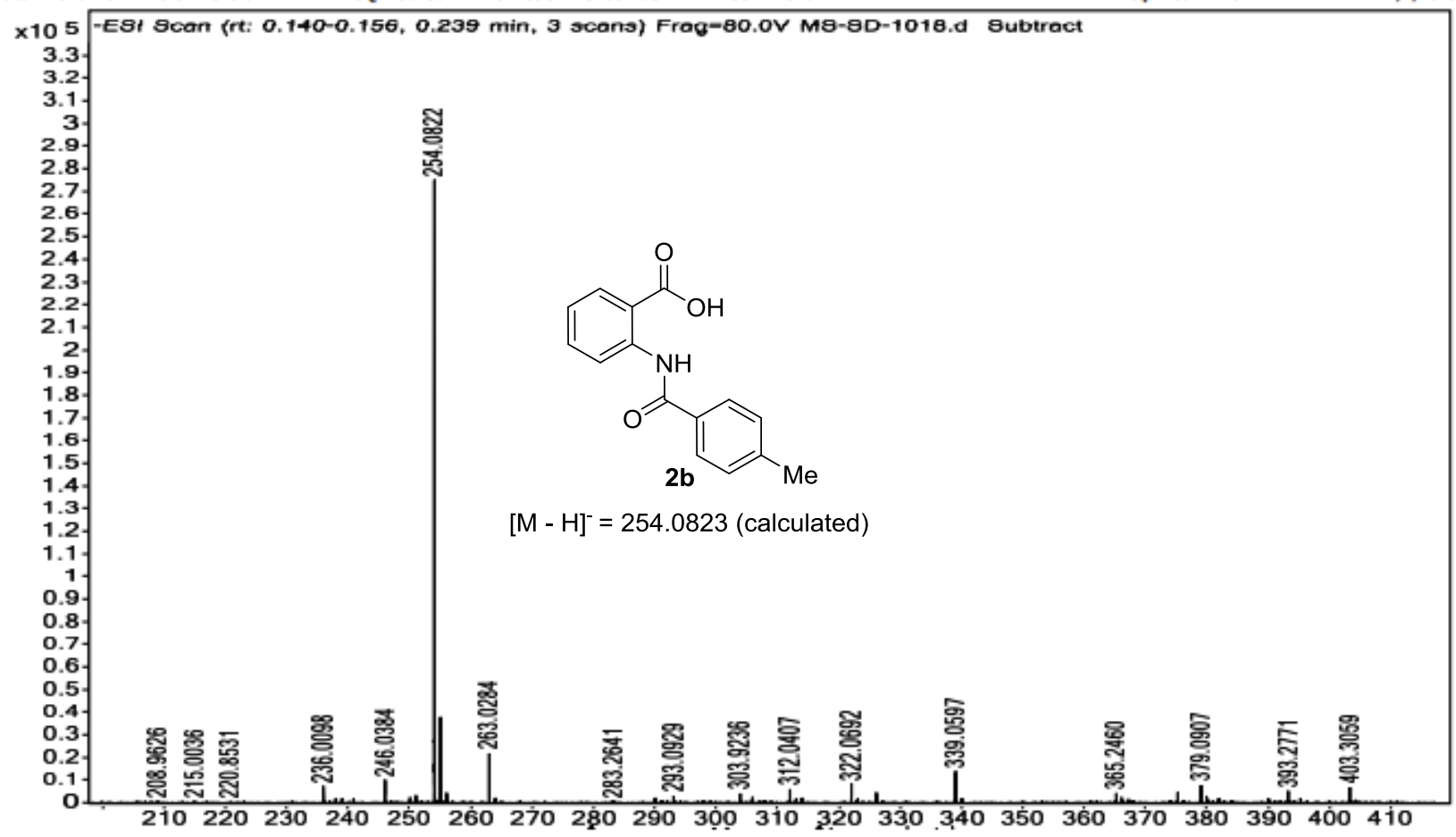
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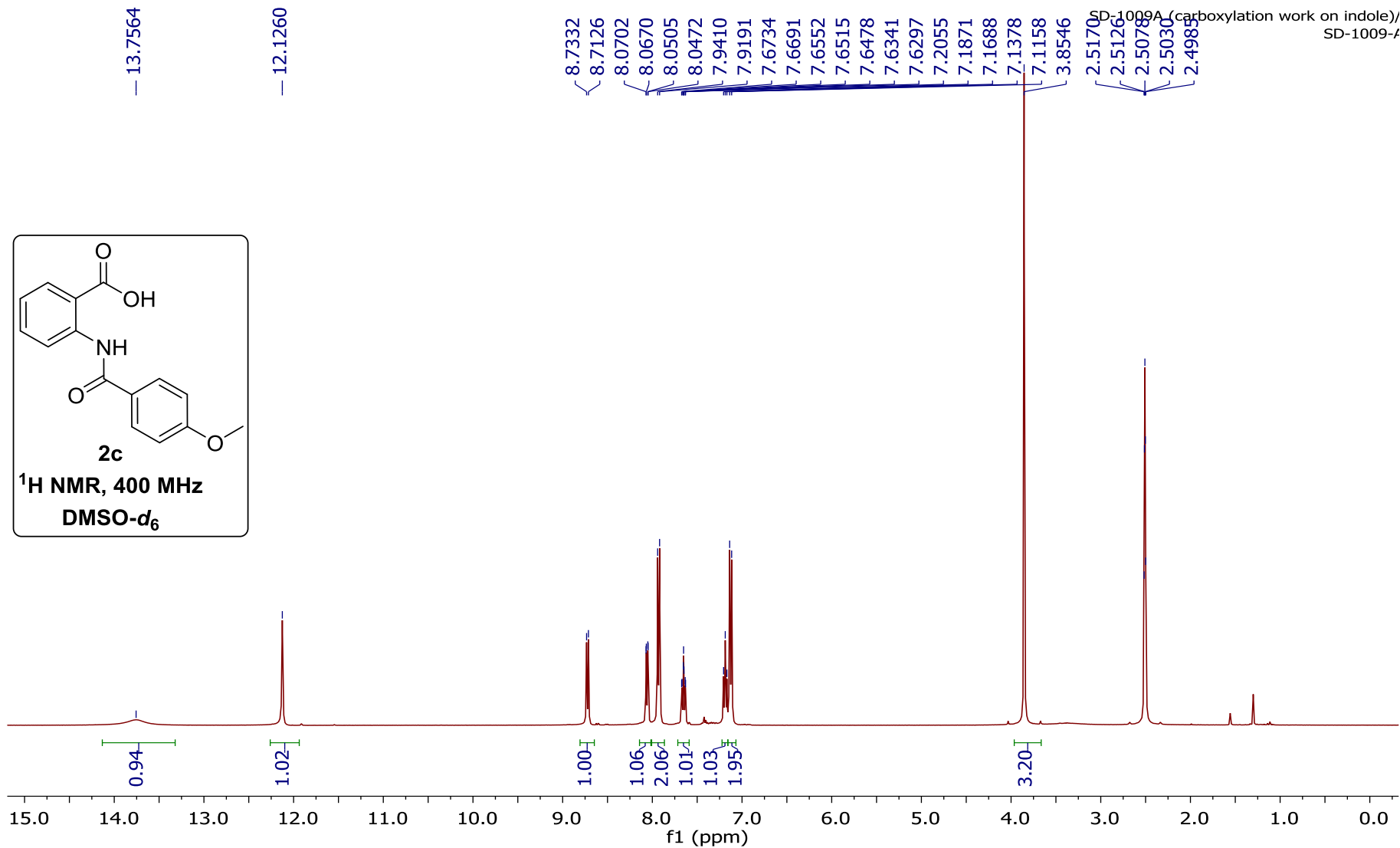
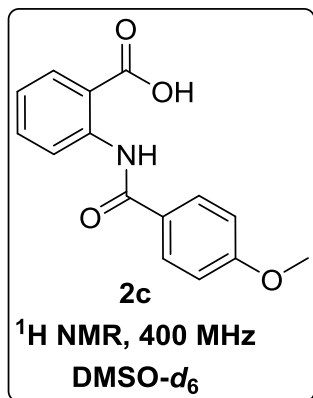
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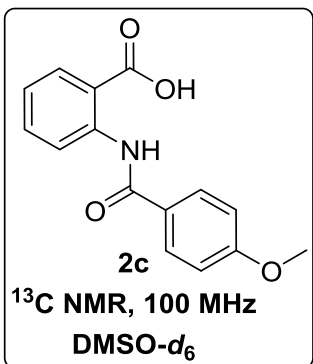
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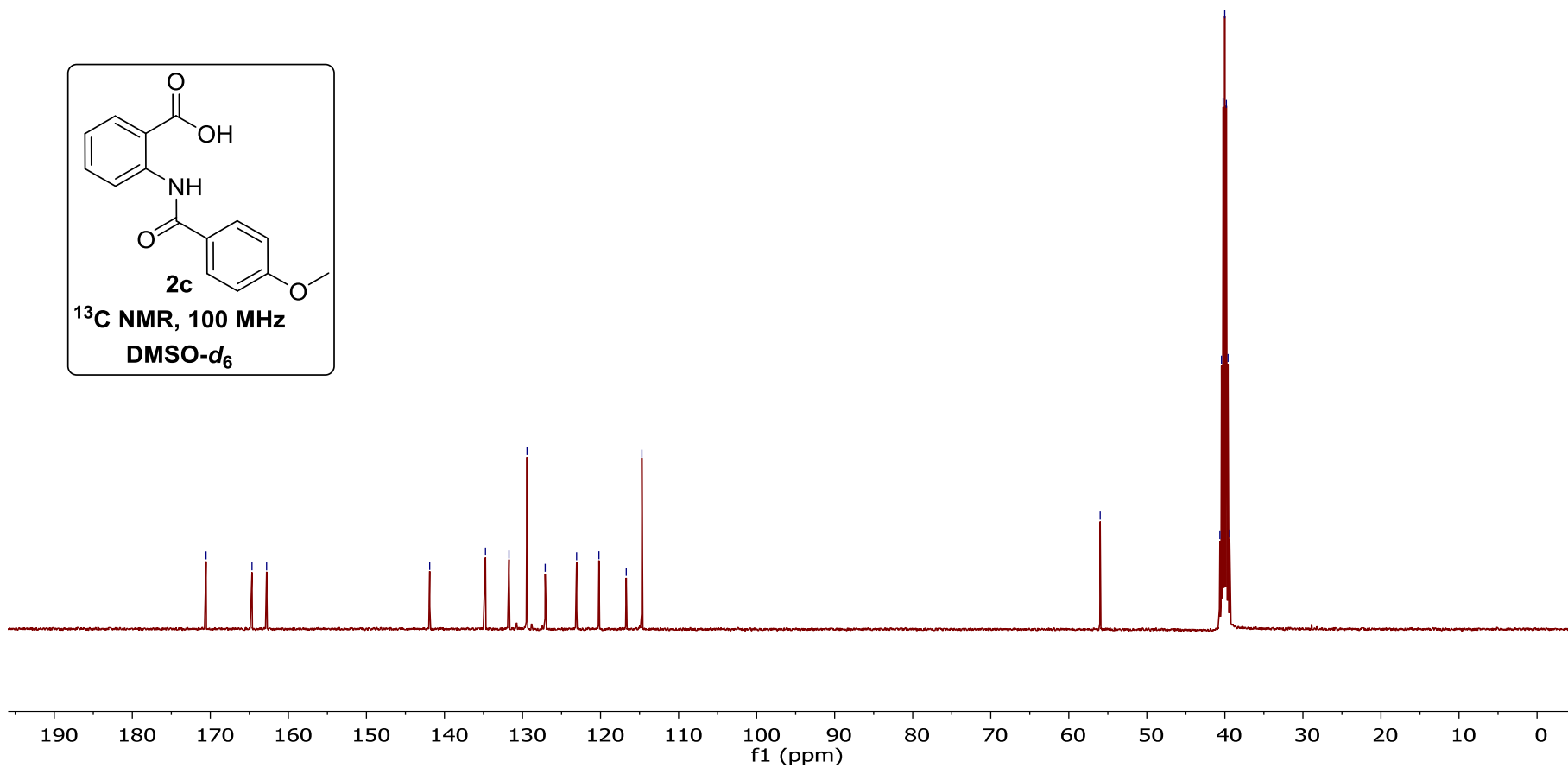




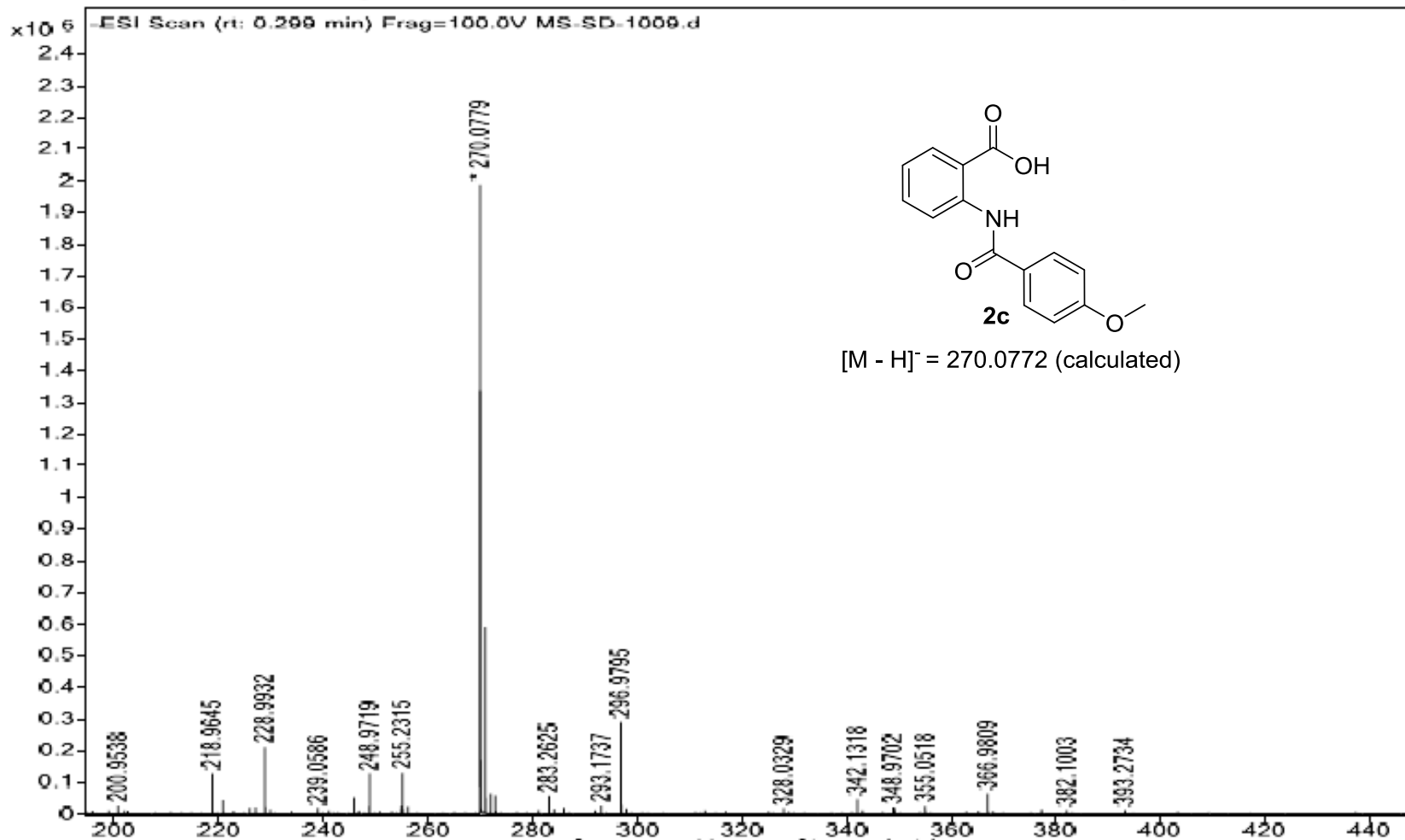
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 / 162.79

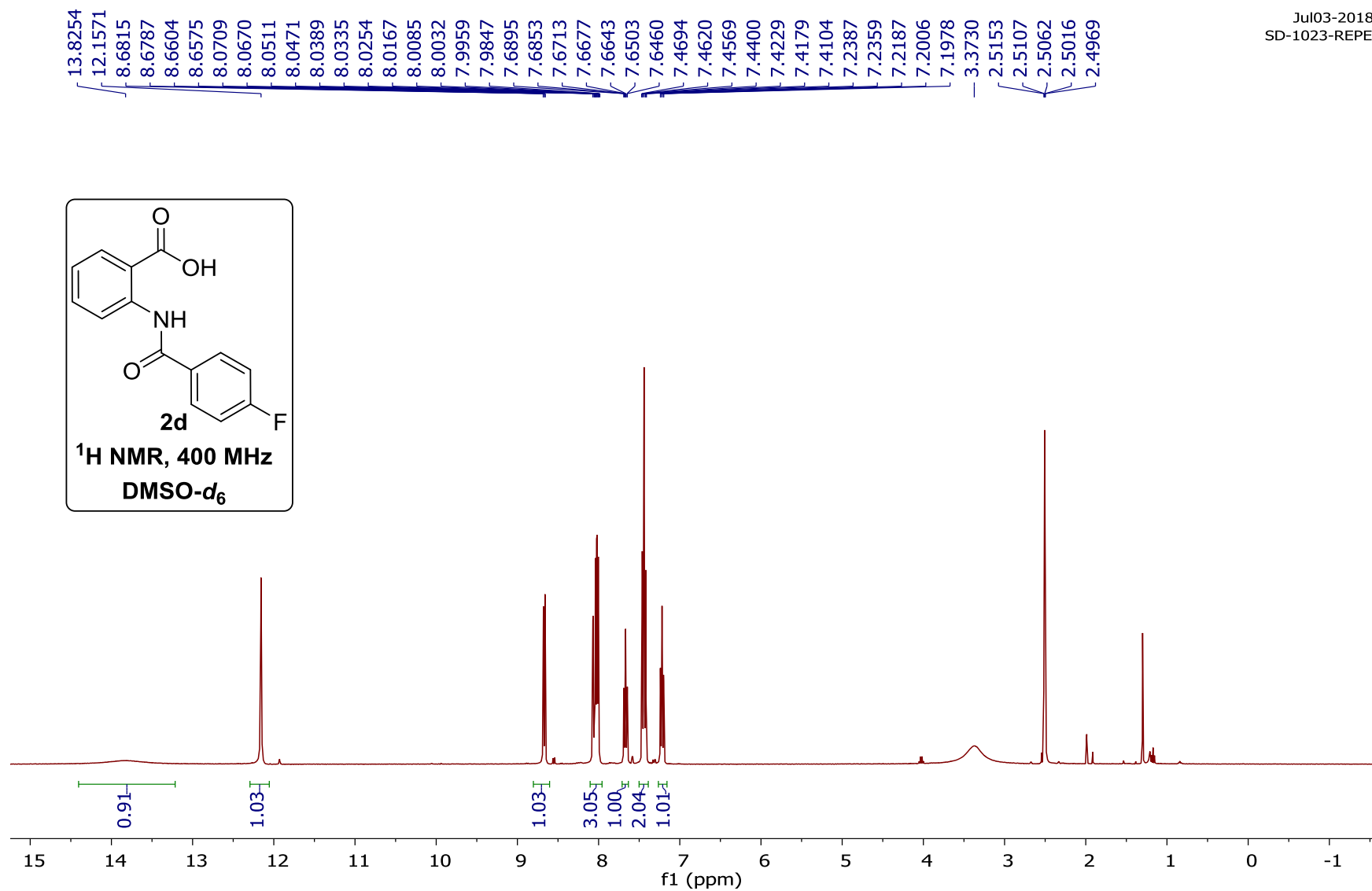
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 / 116.71
 / 114.70

— 55.98
 { 40.64
 { 40.43
 { 40.22
 { 40.01
 { 39.81
 { 39.60
 { 39.39
 SD-1009A (carboxylation work on indole)/
 SD-1009-7



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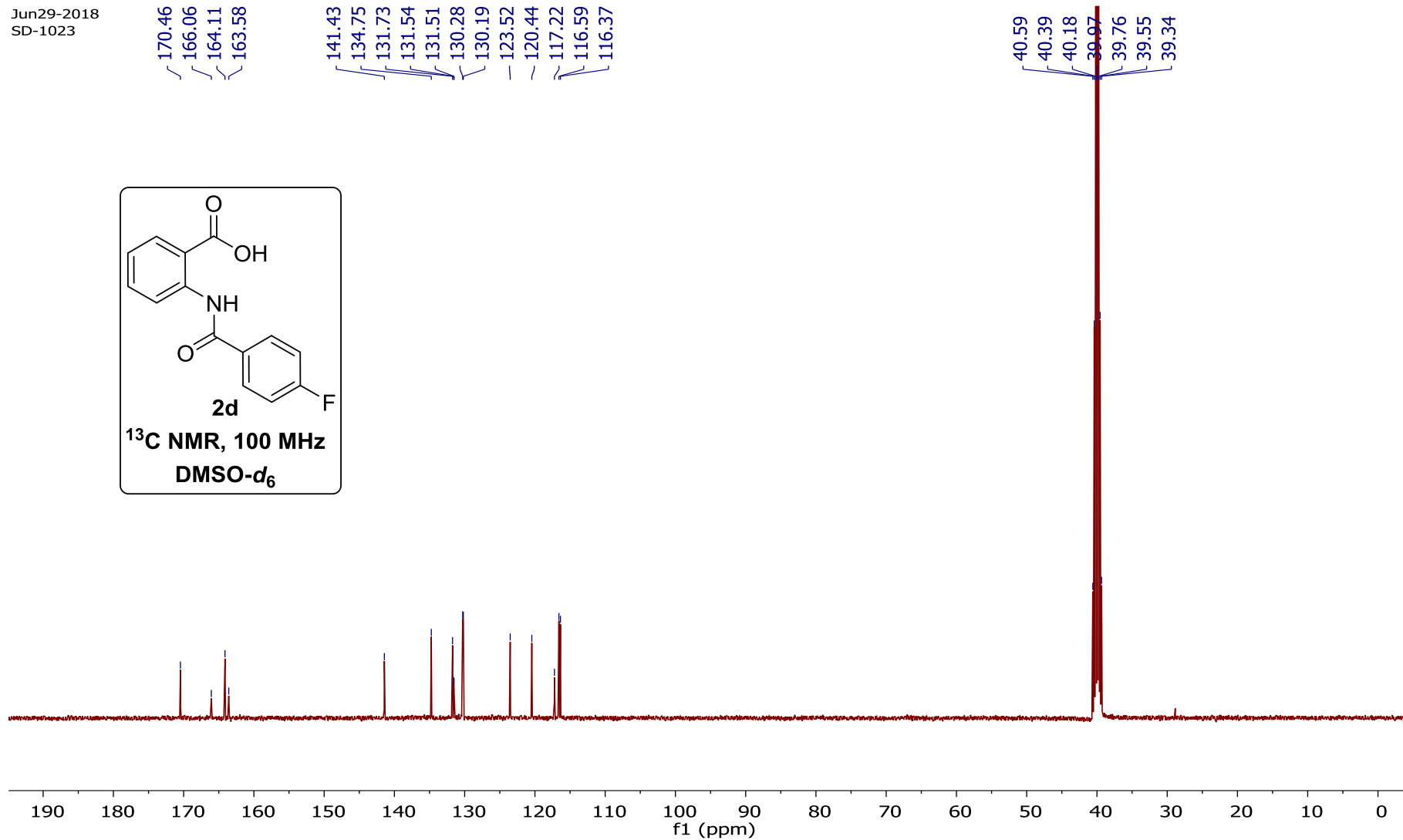
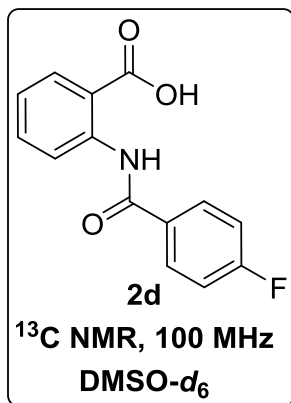


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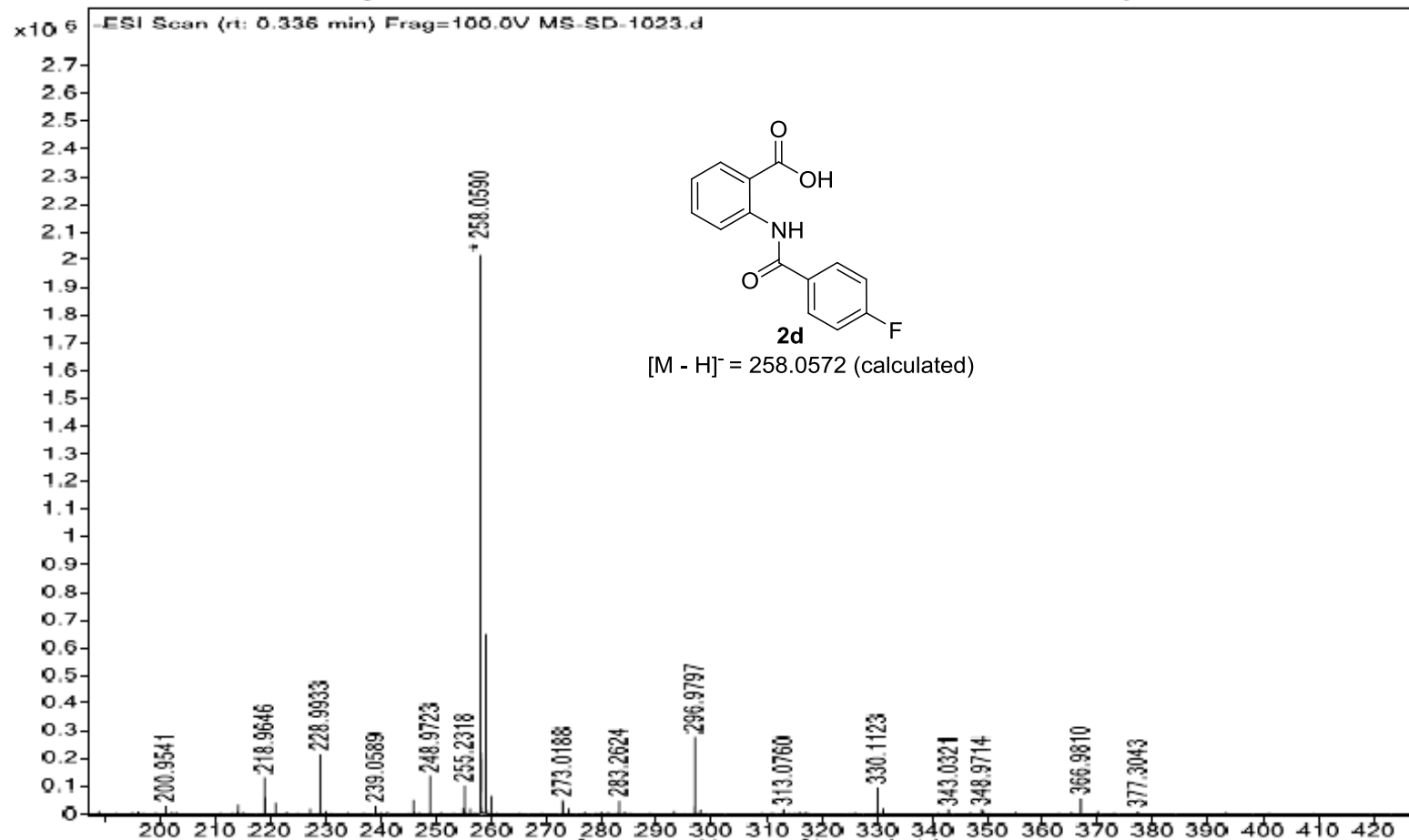
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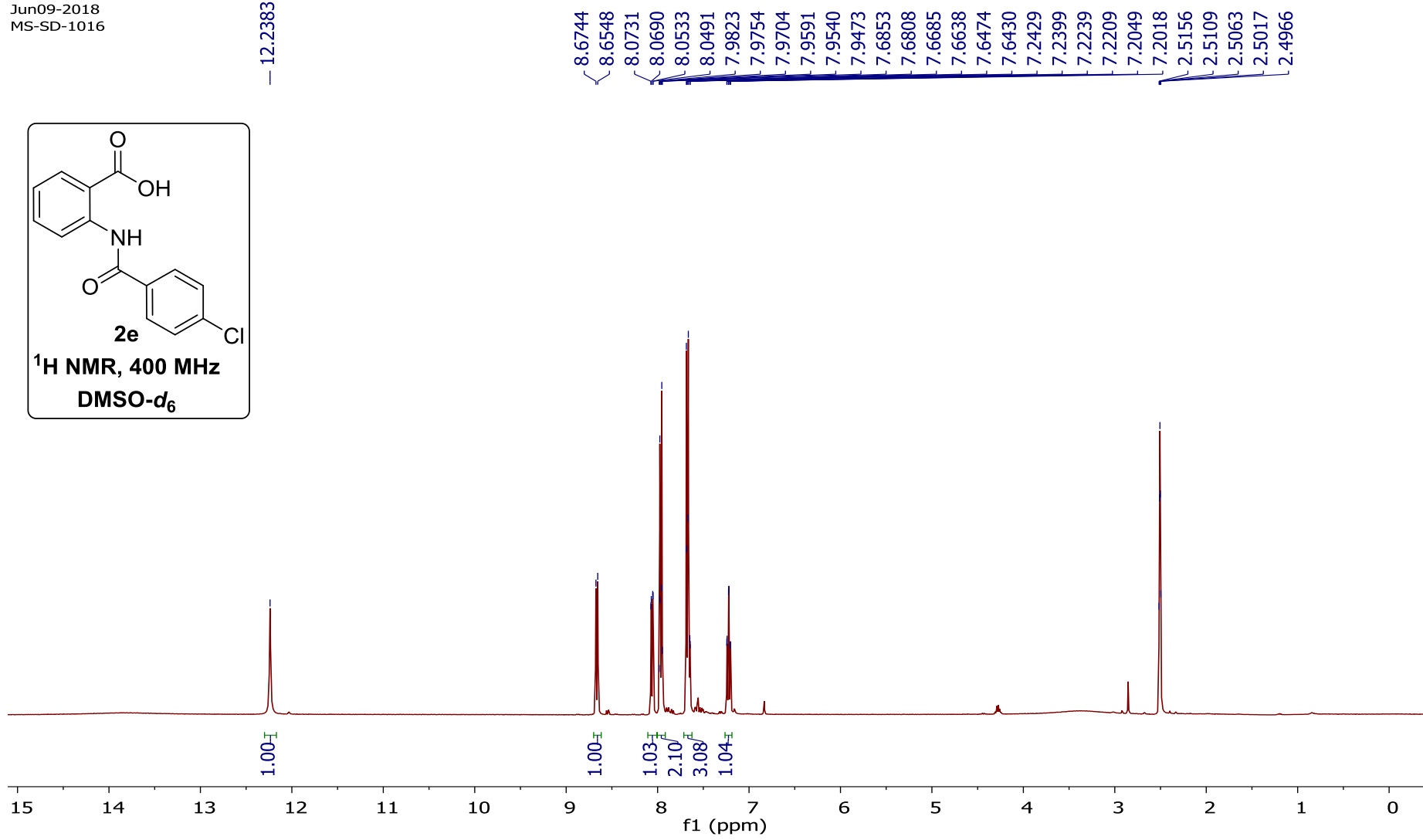
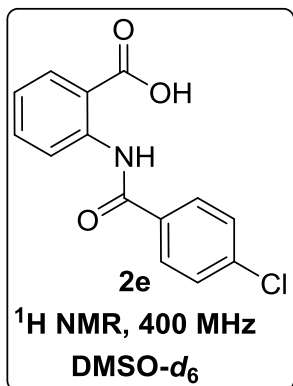


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Jun09-2018
MS-SD-1016

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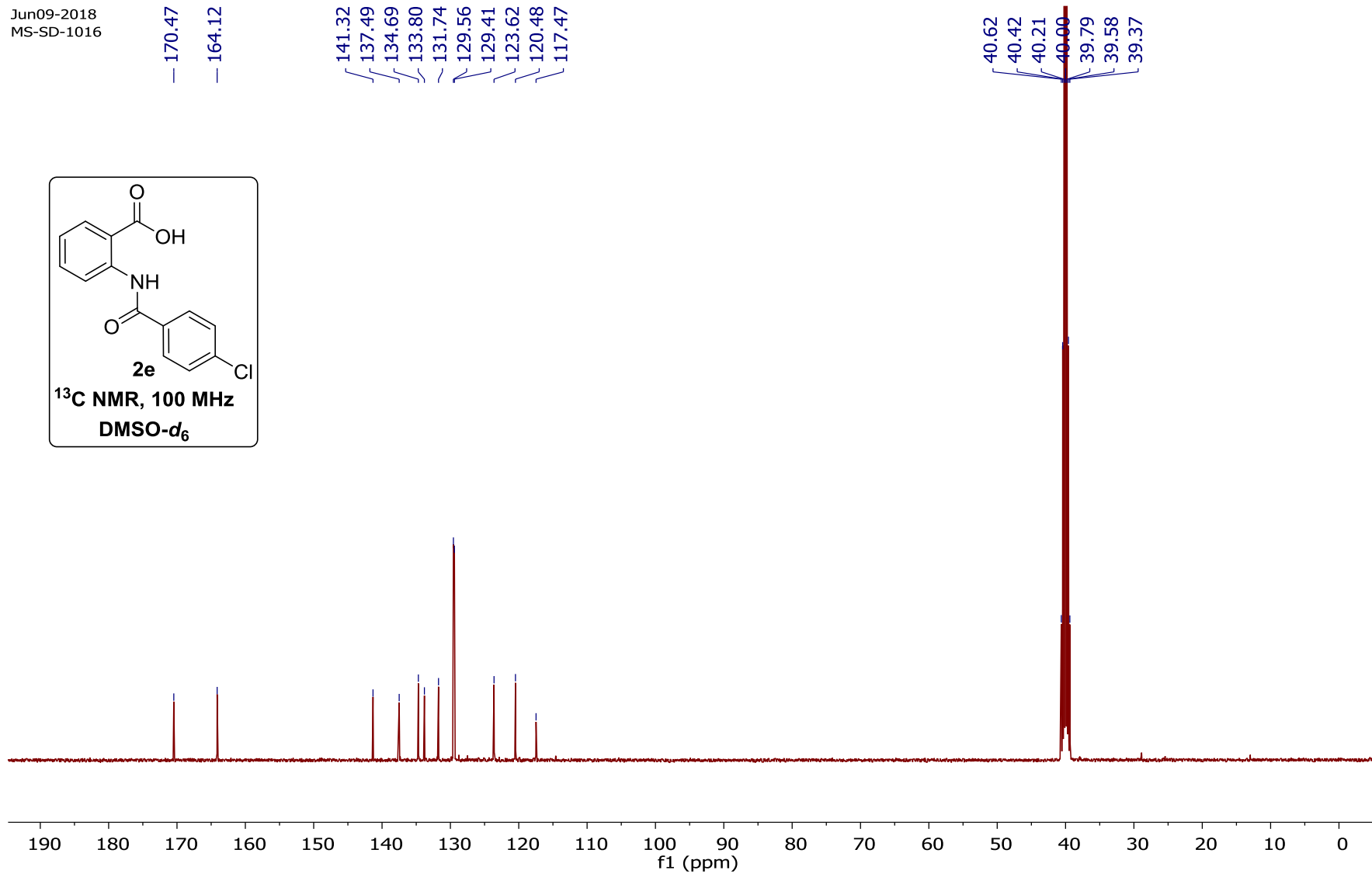
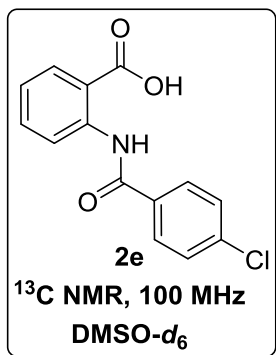


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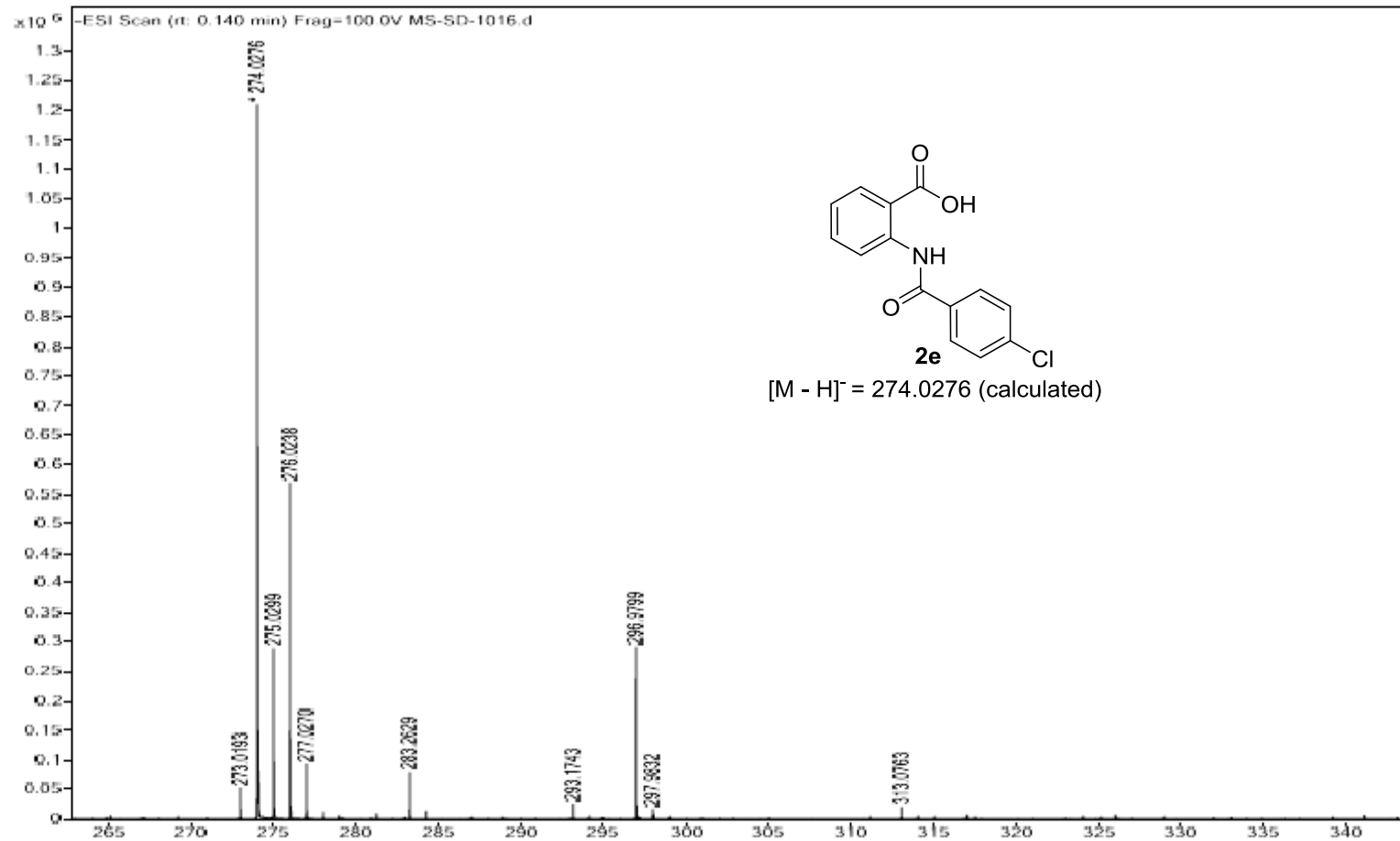
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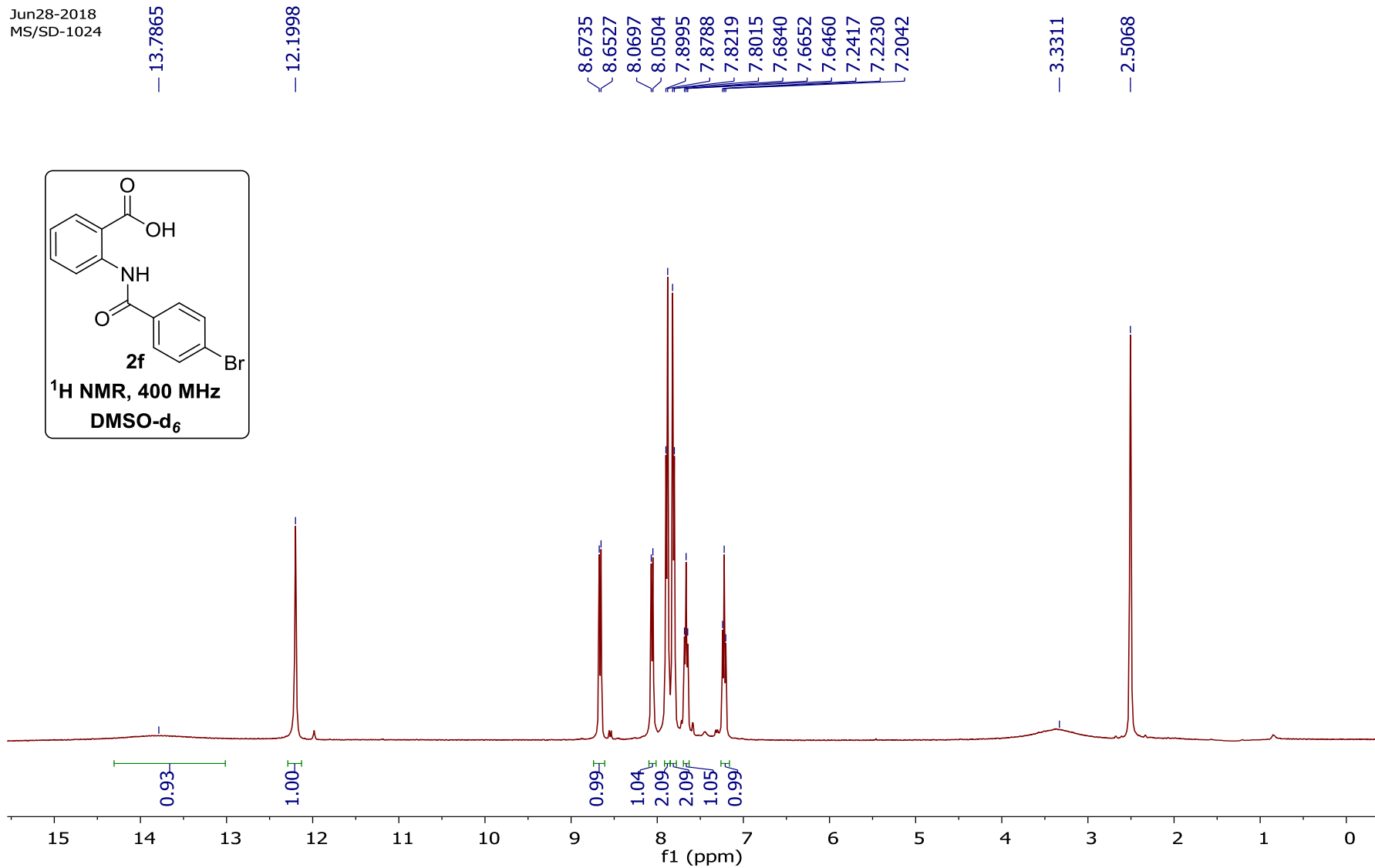
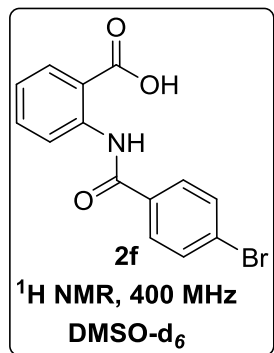
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Jun28-2018
MS/SD-1024

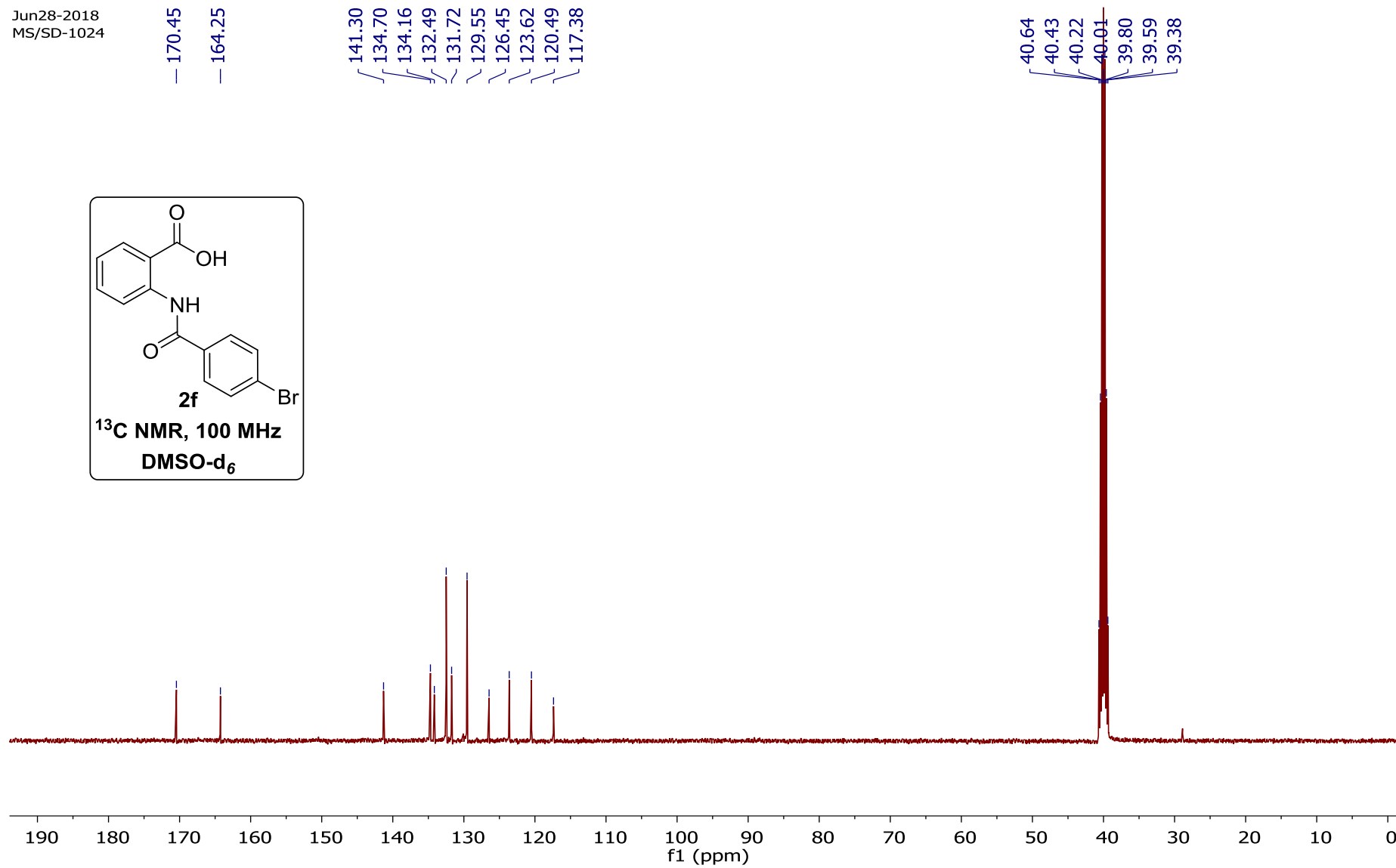
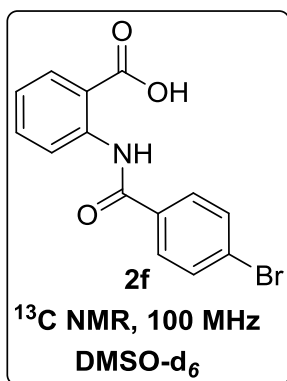


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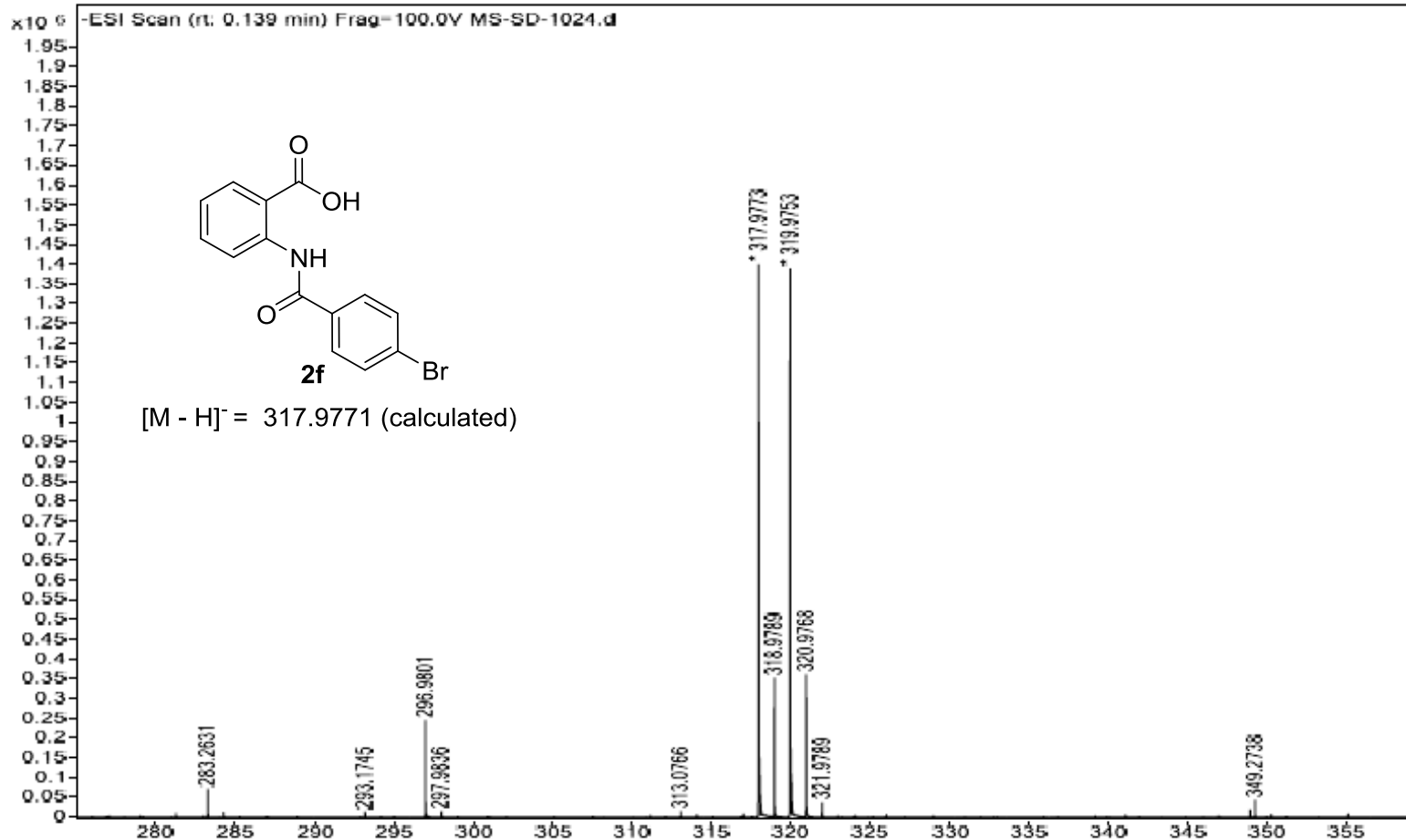
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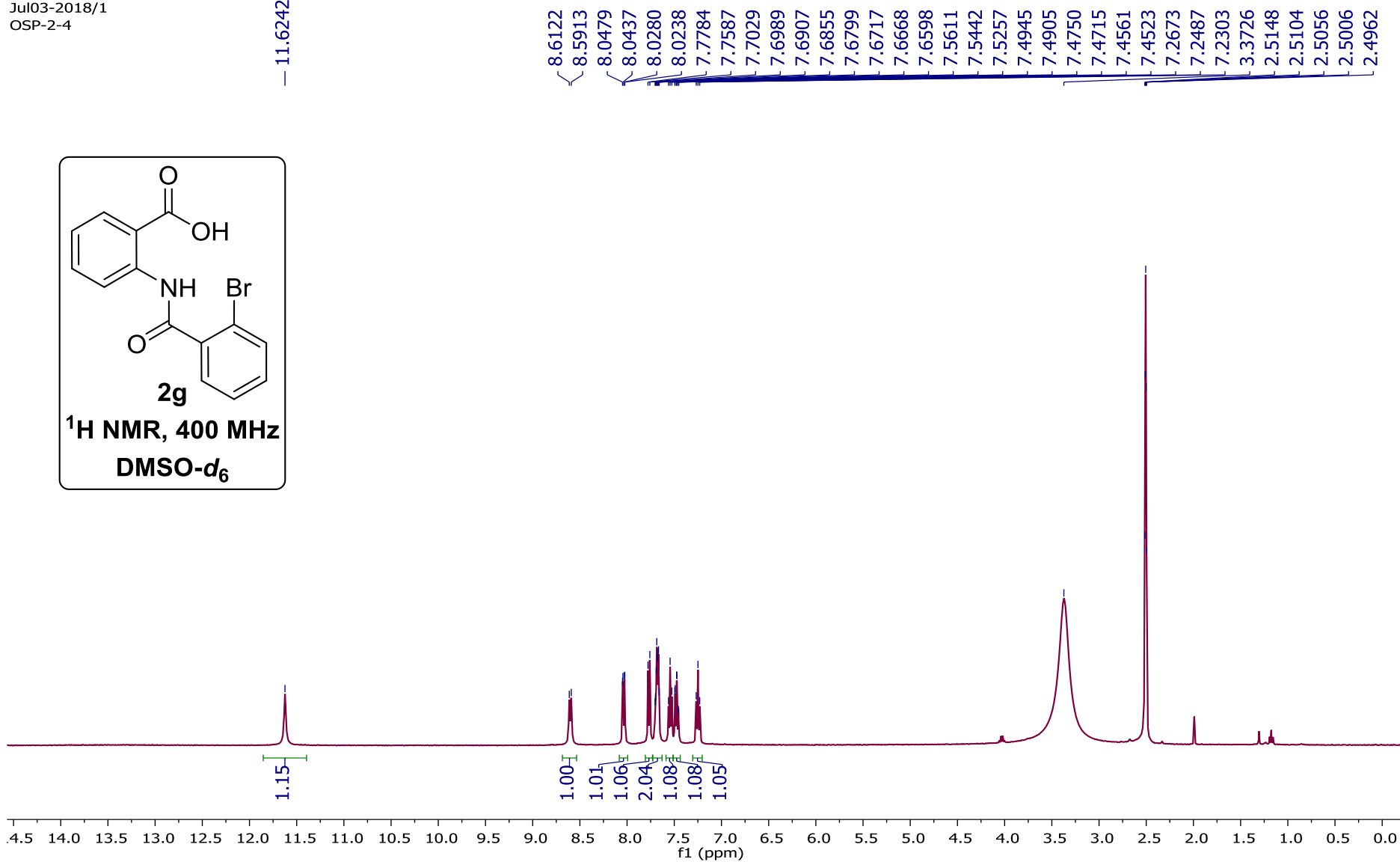
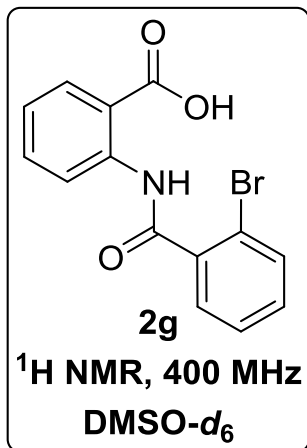
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— 11.6242

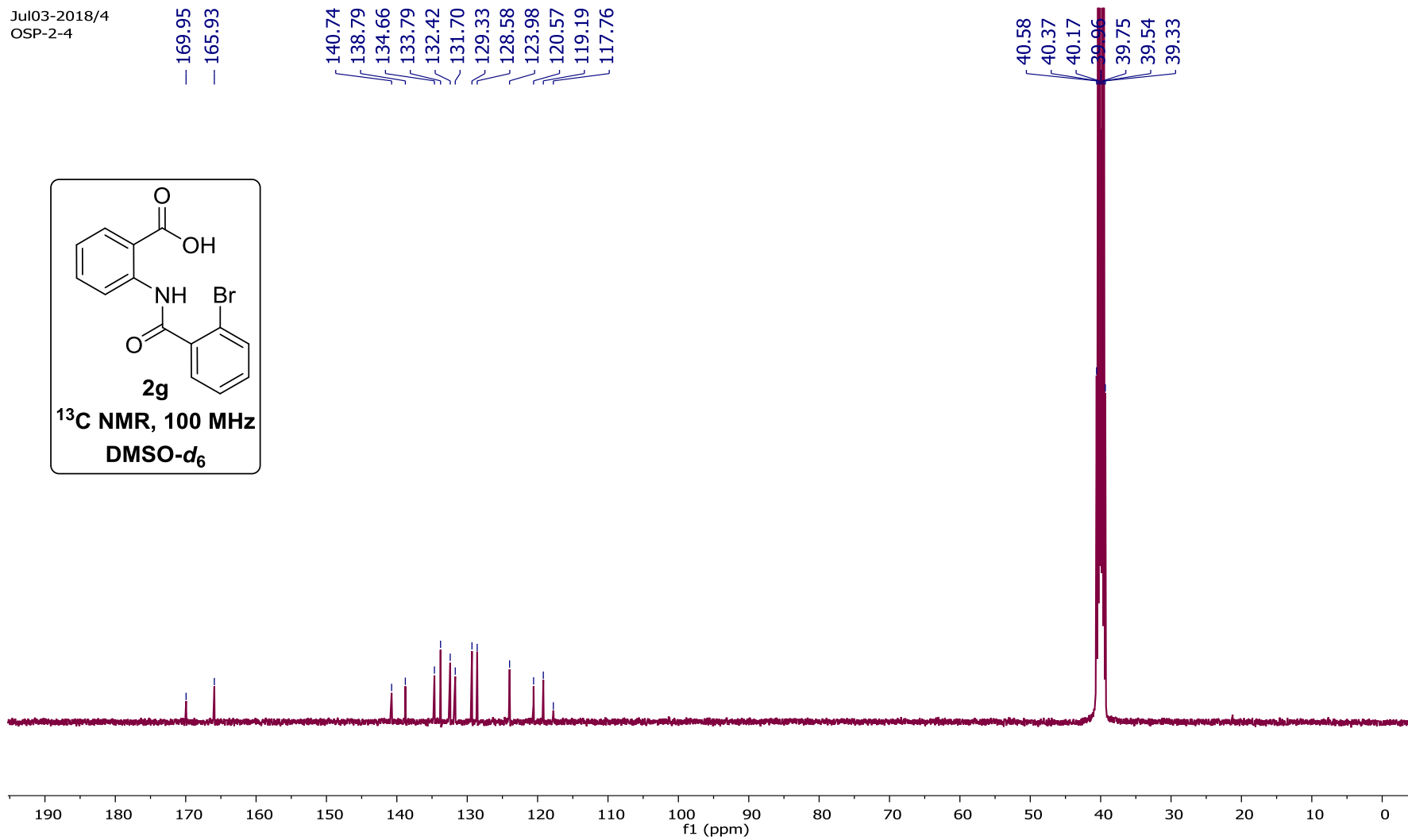
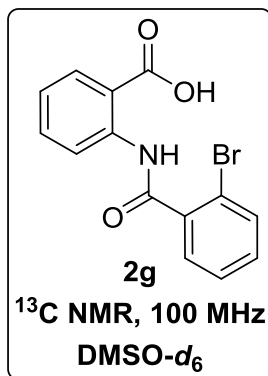


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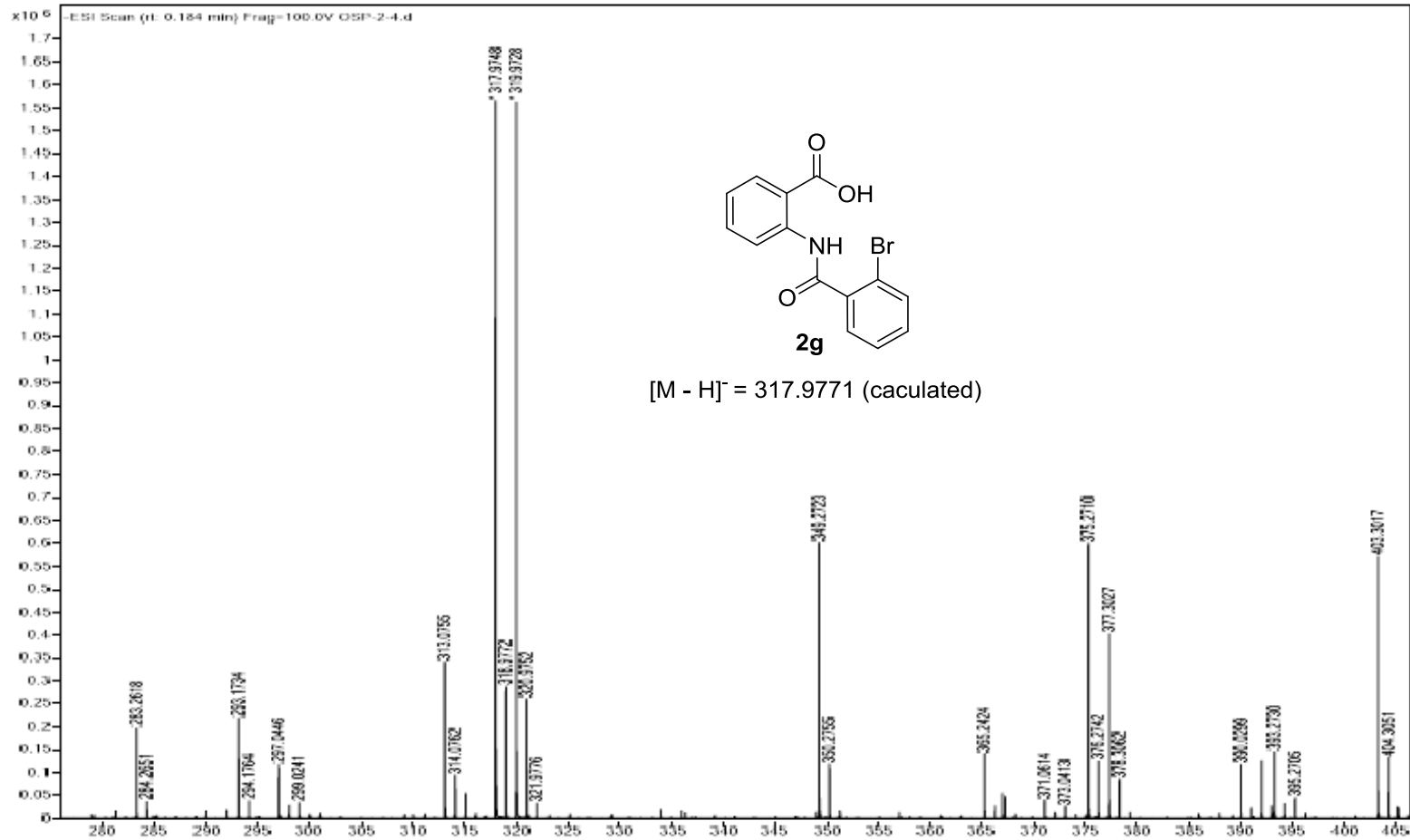
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— 165.93

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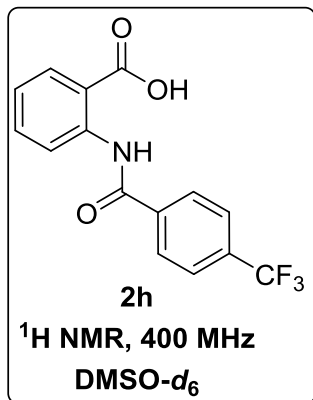
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MS/SD-1017

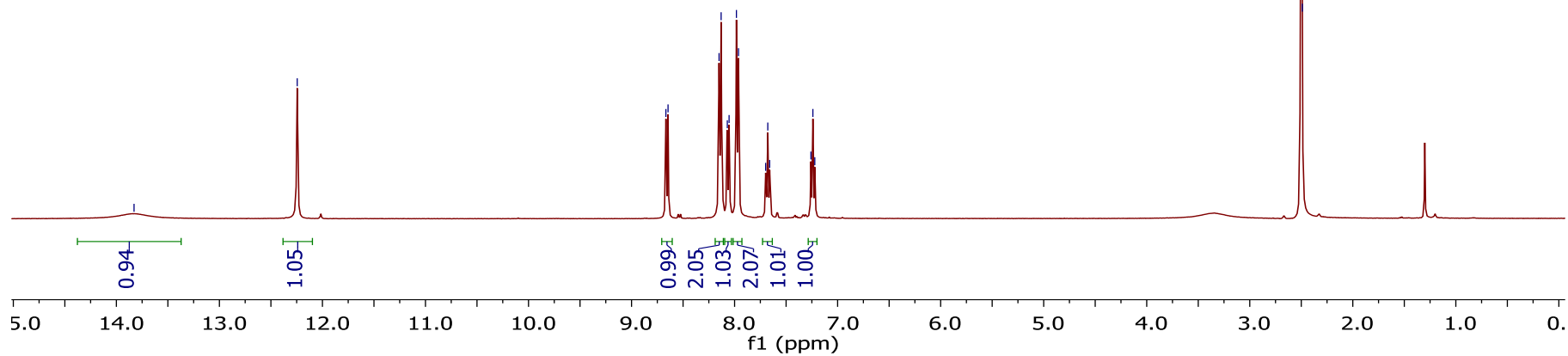
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— 12.2447



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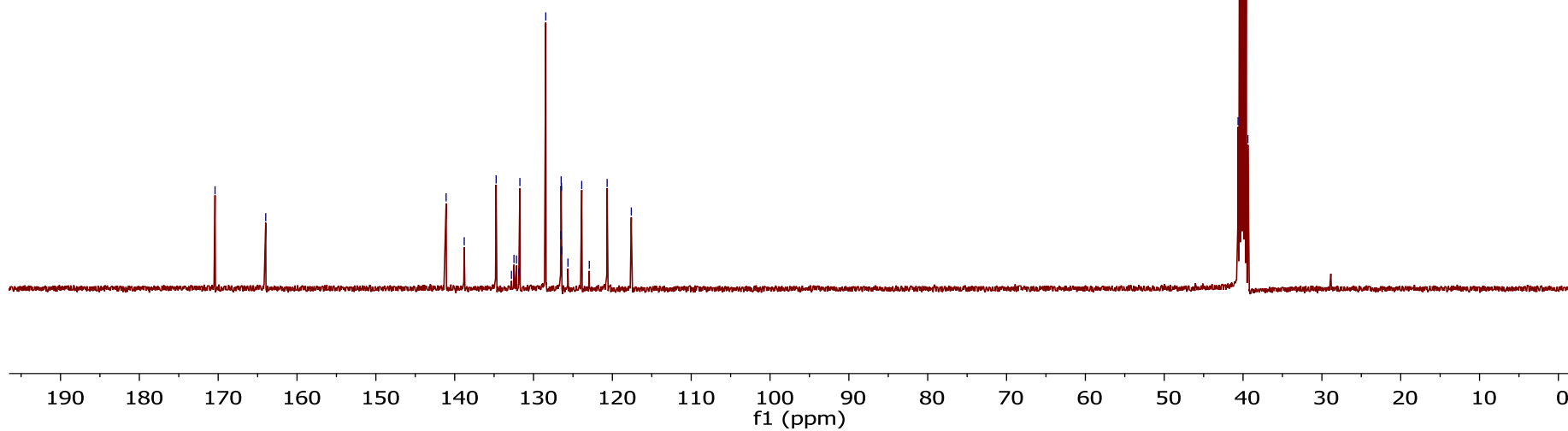
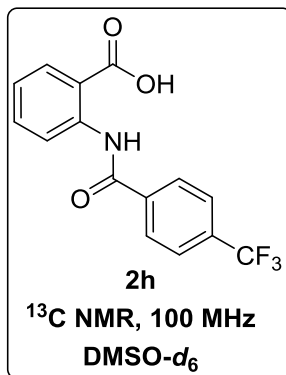
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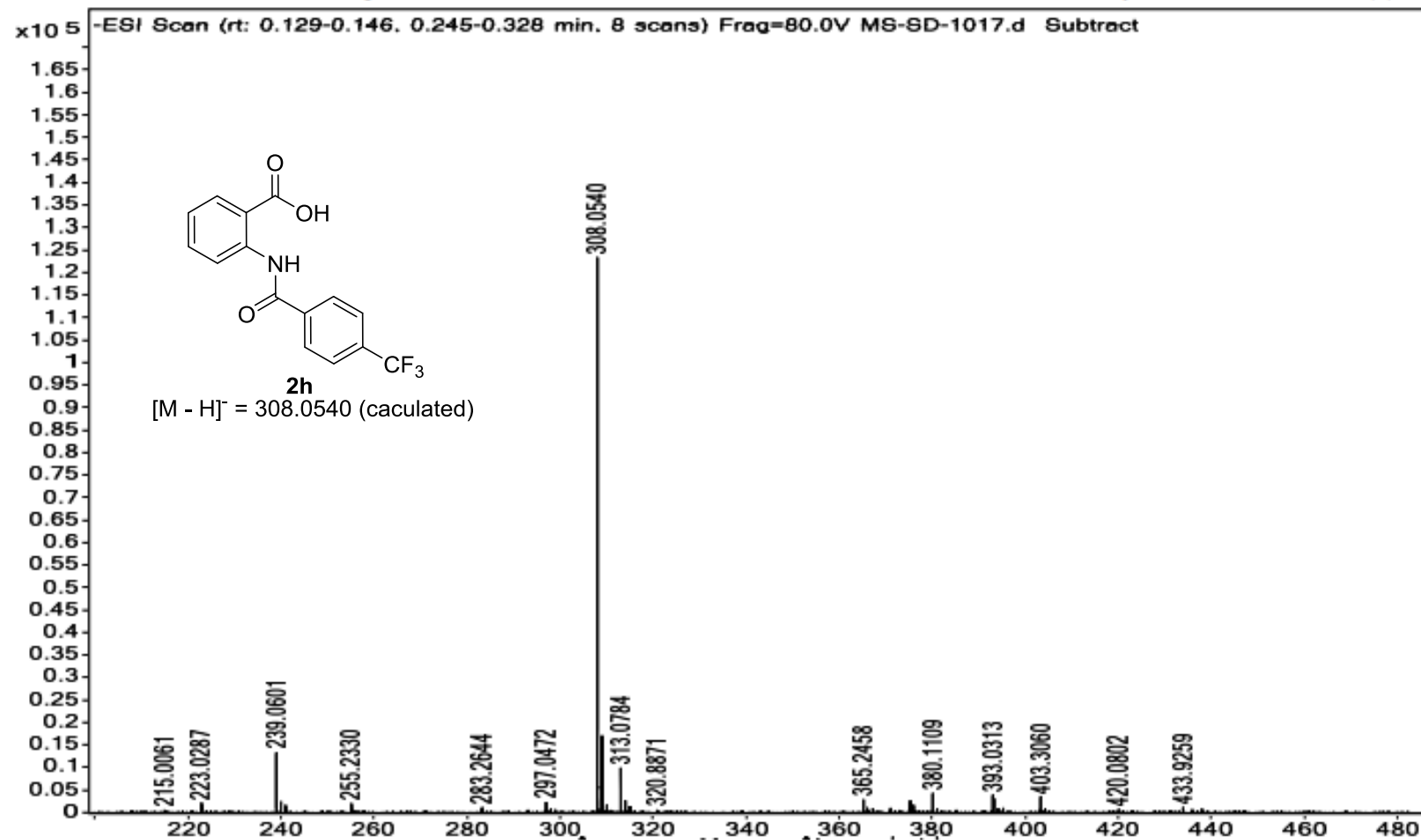
Apr02-2018
MS/SD-1017

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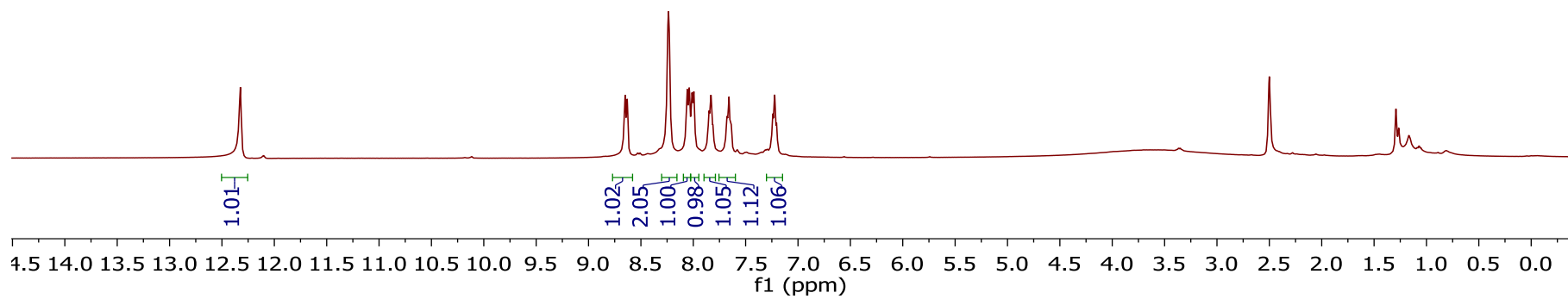
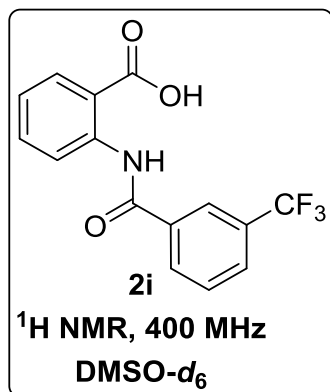


Nov28-2018/5
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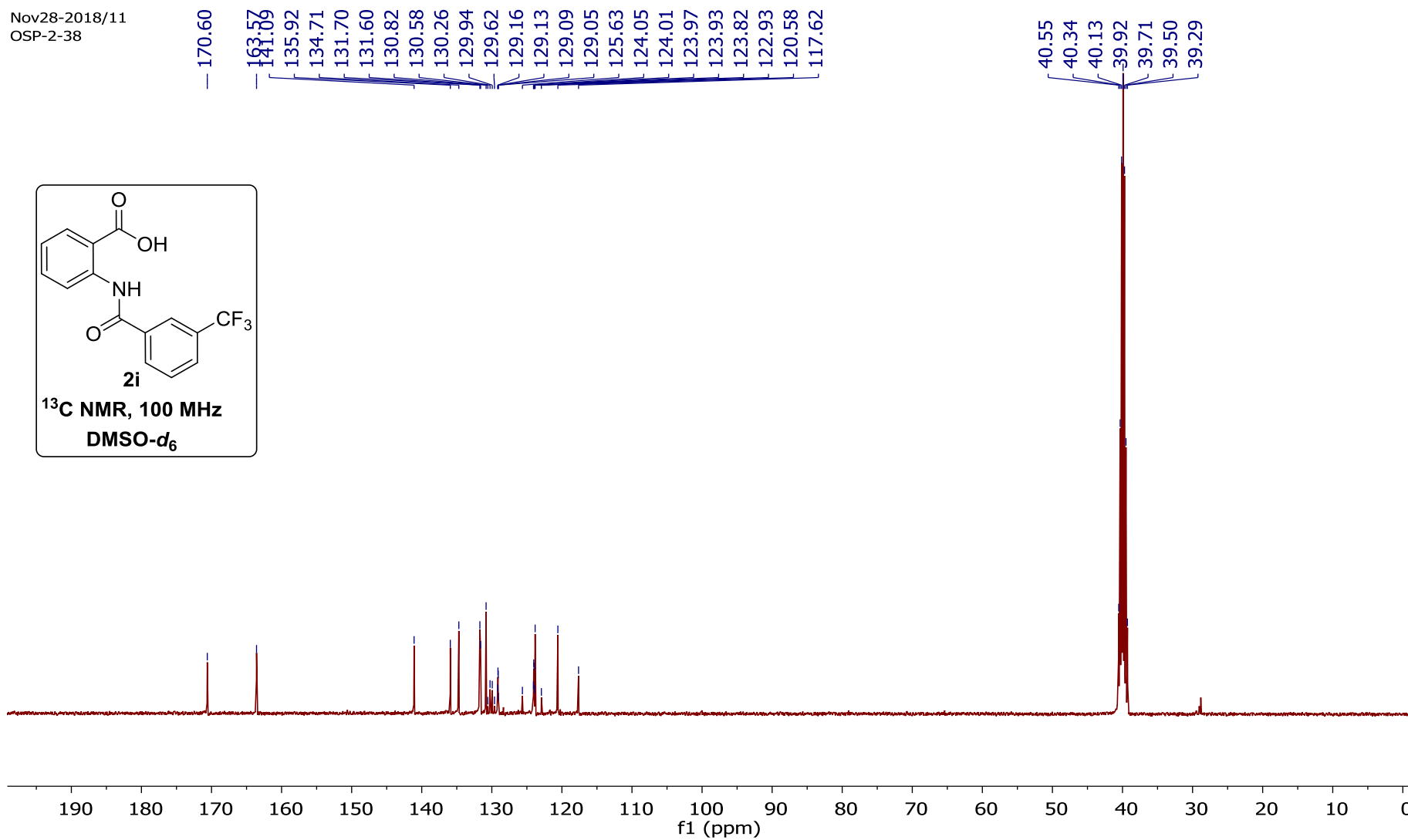
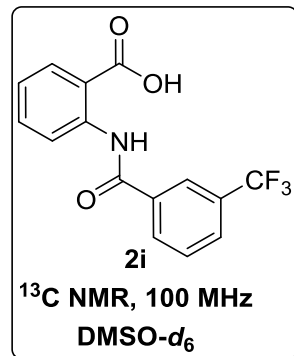
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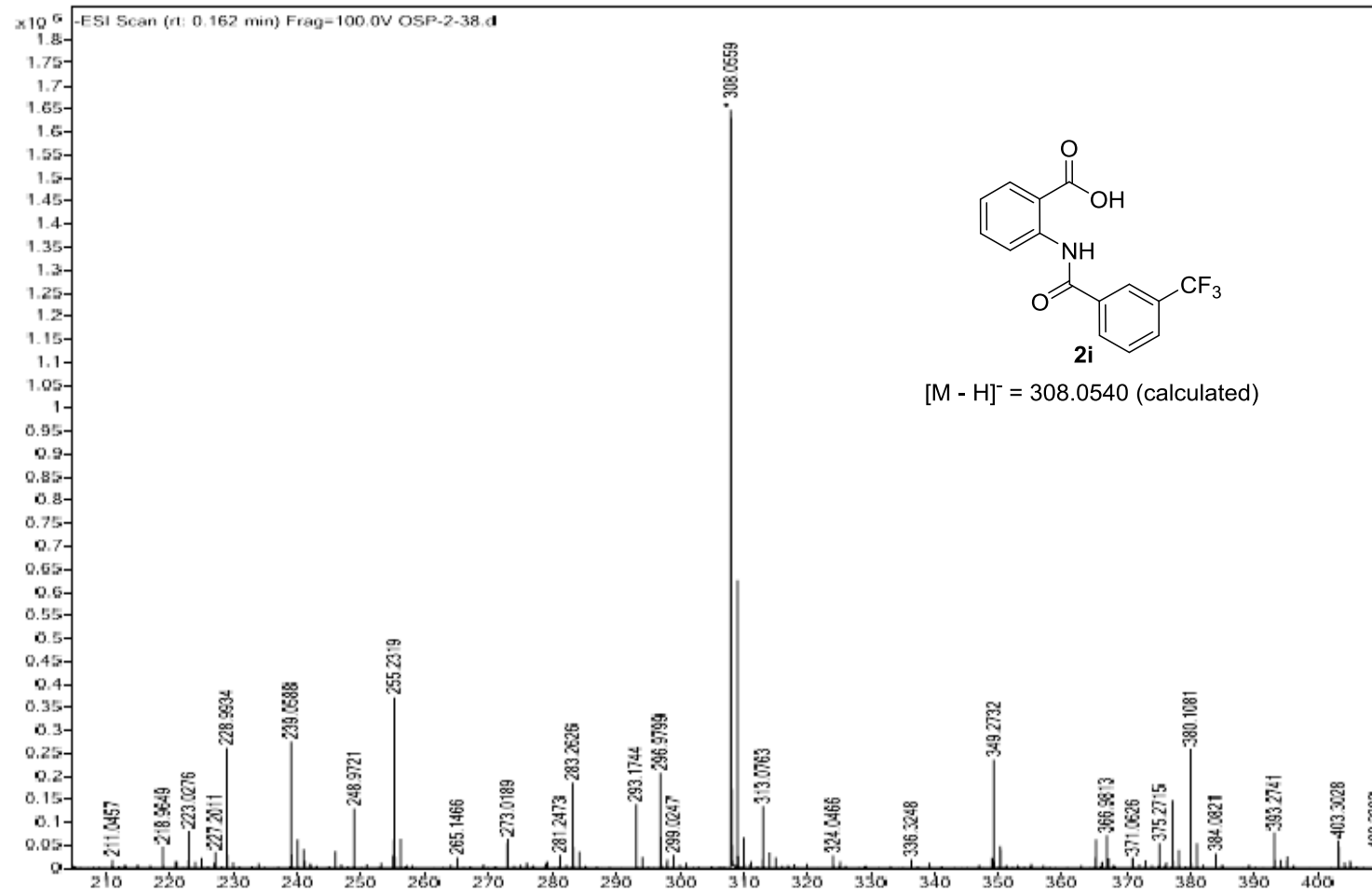
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Nov28-2018/11
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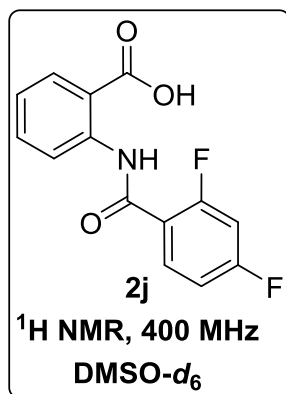


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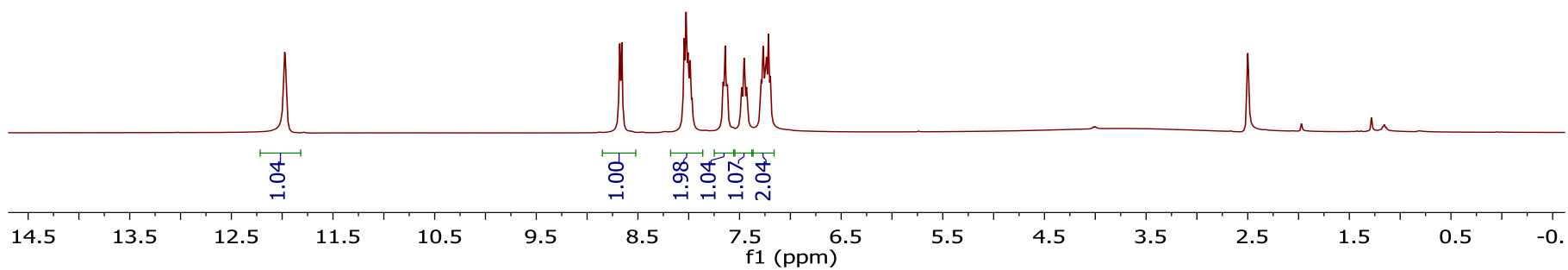
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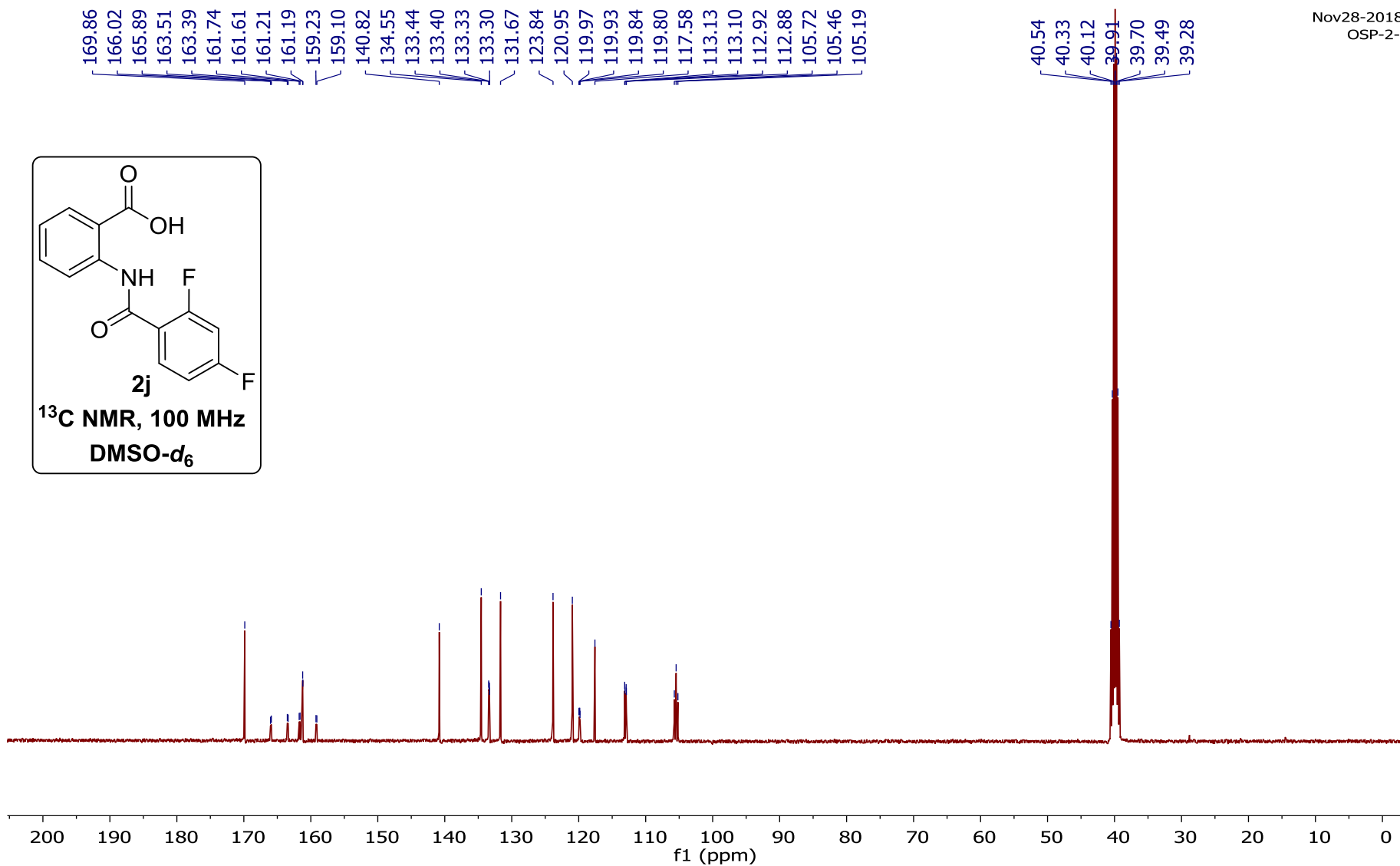
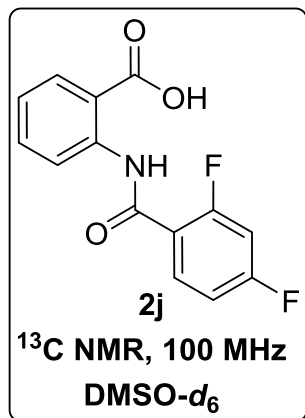
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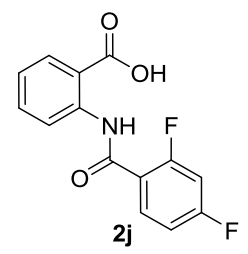
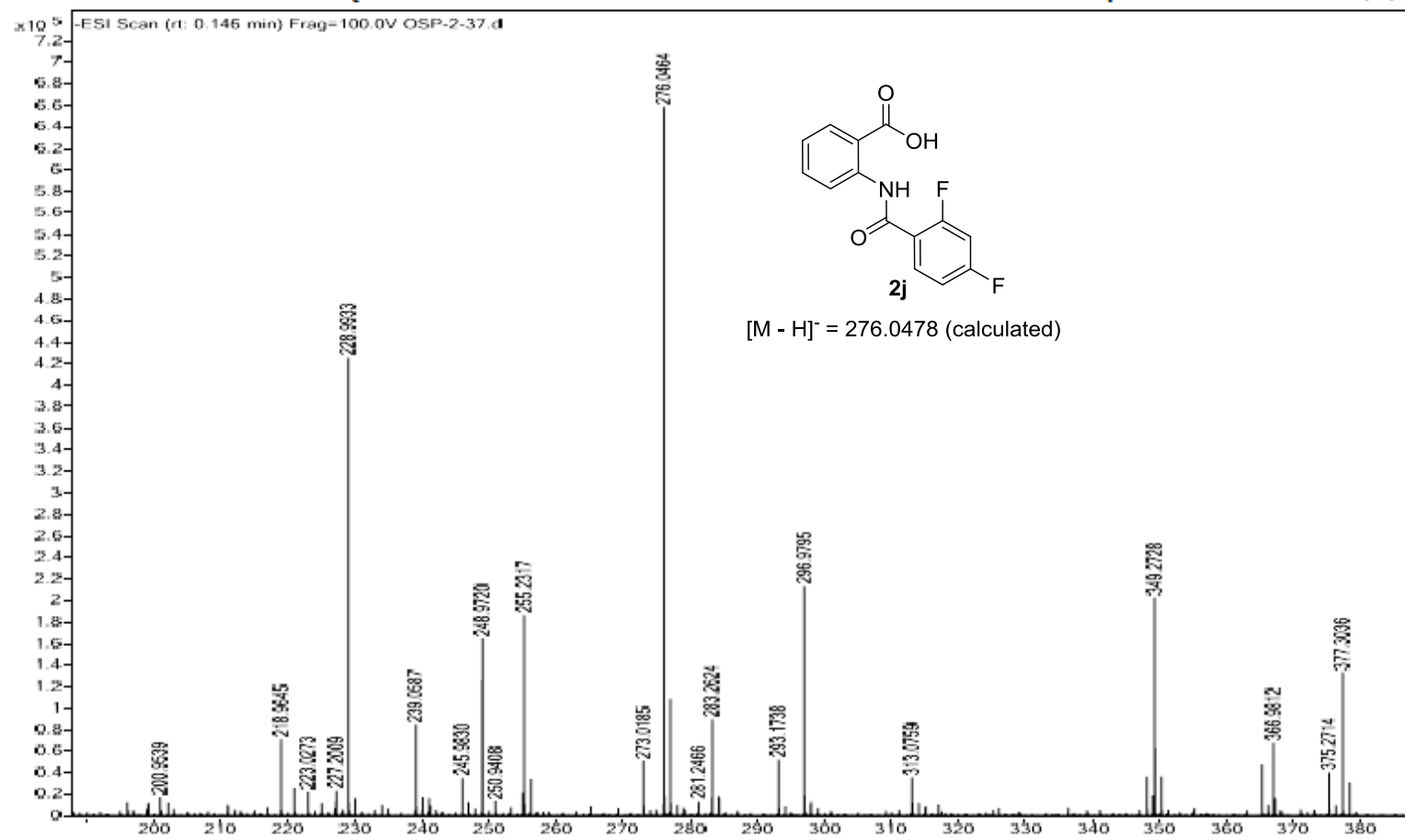
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7.1964

— 2.4995



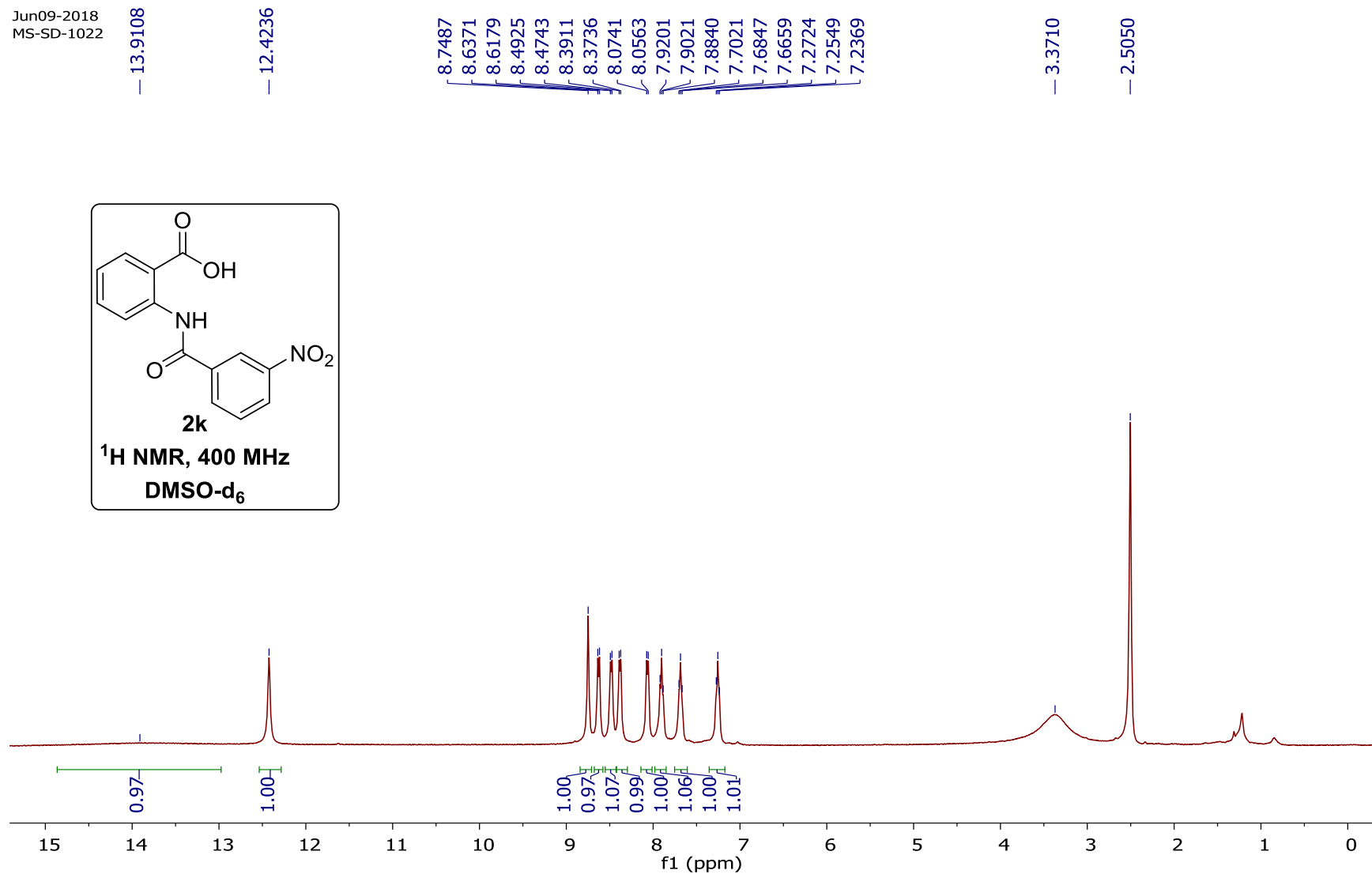
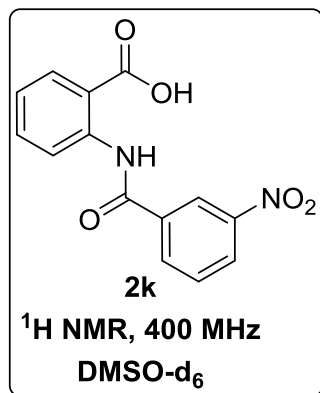


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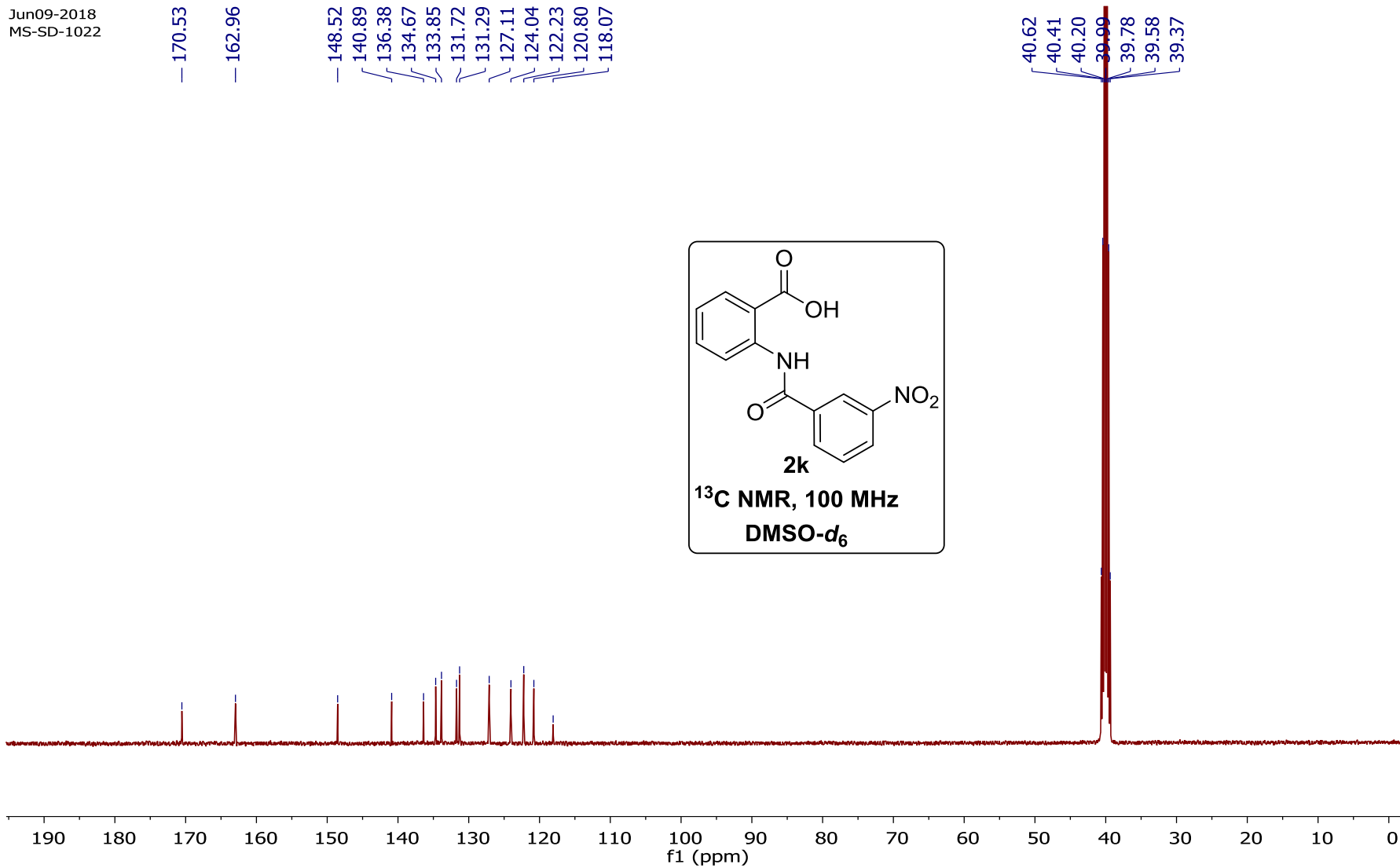


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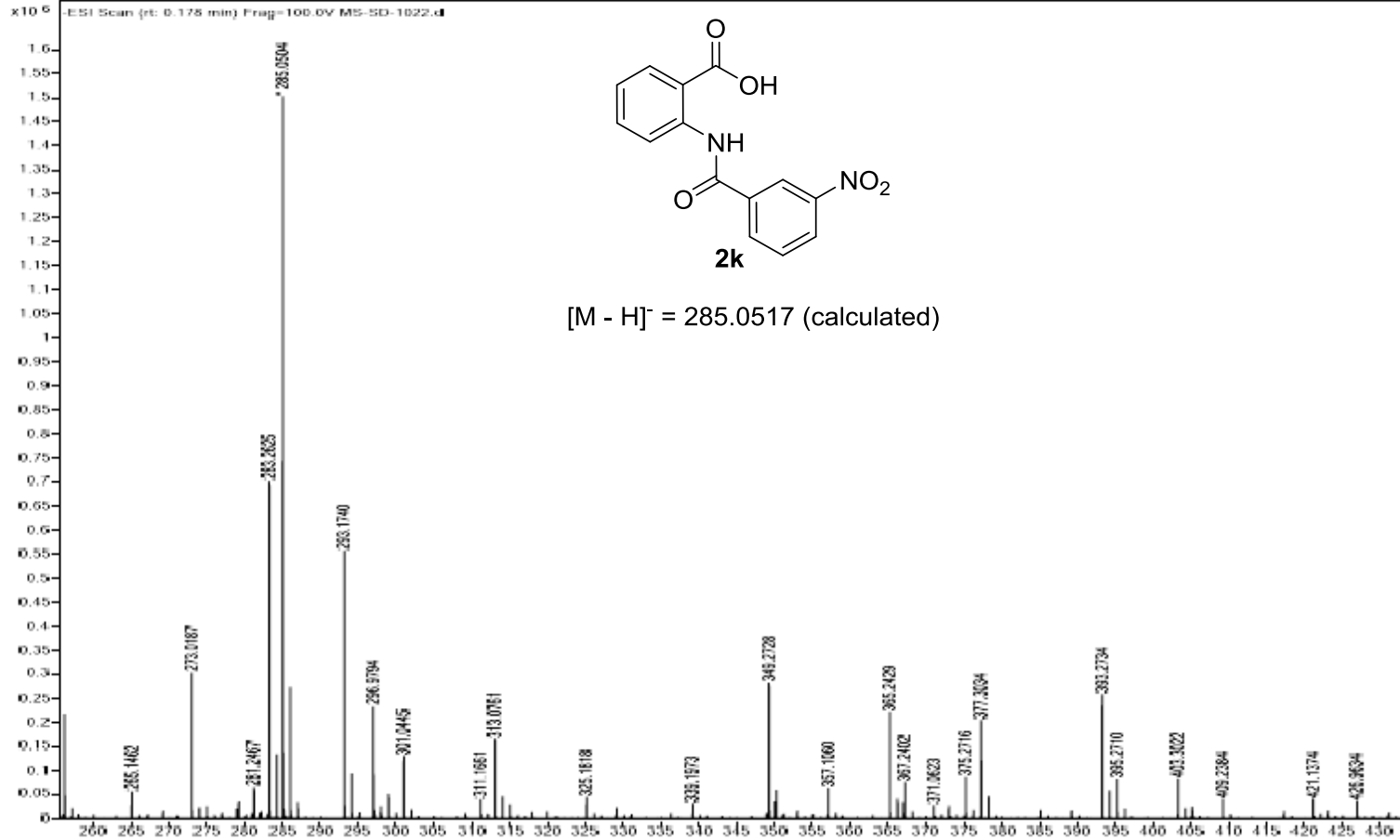
Jun09-2018
MS-SD-1022



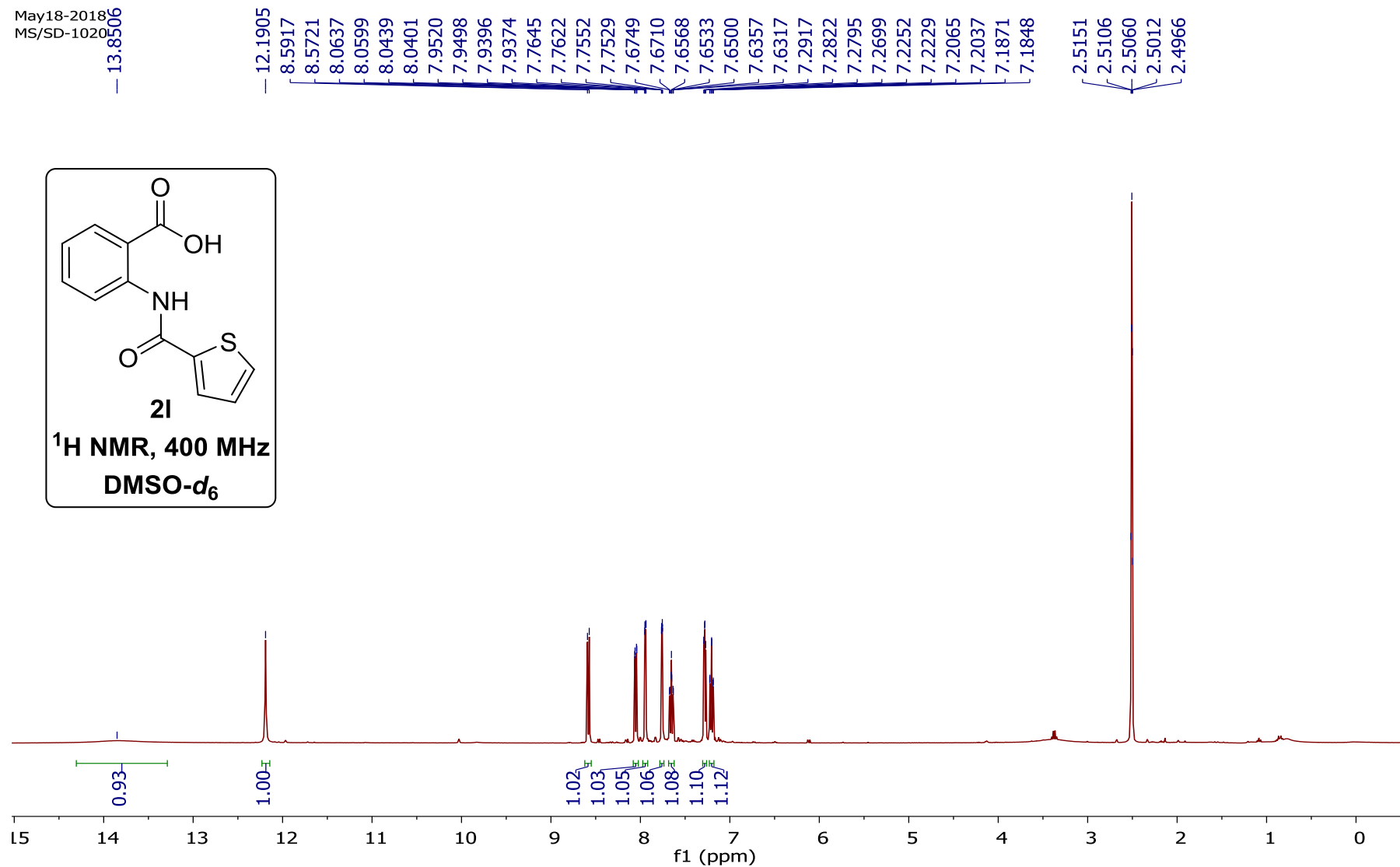
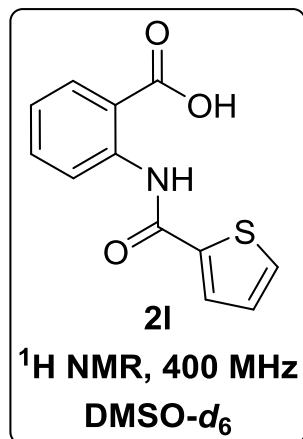
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MS-SD-1022



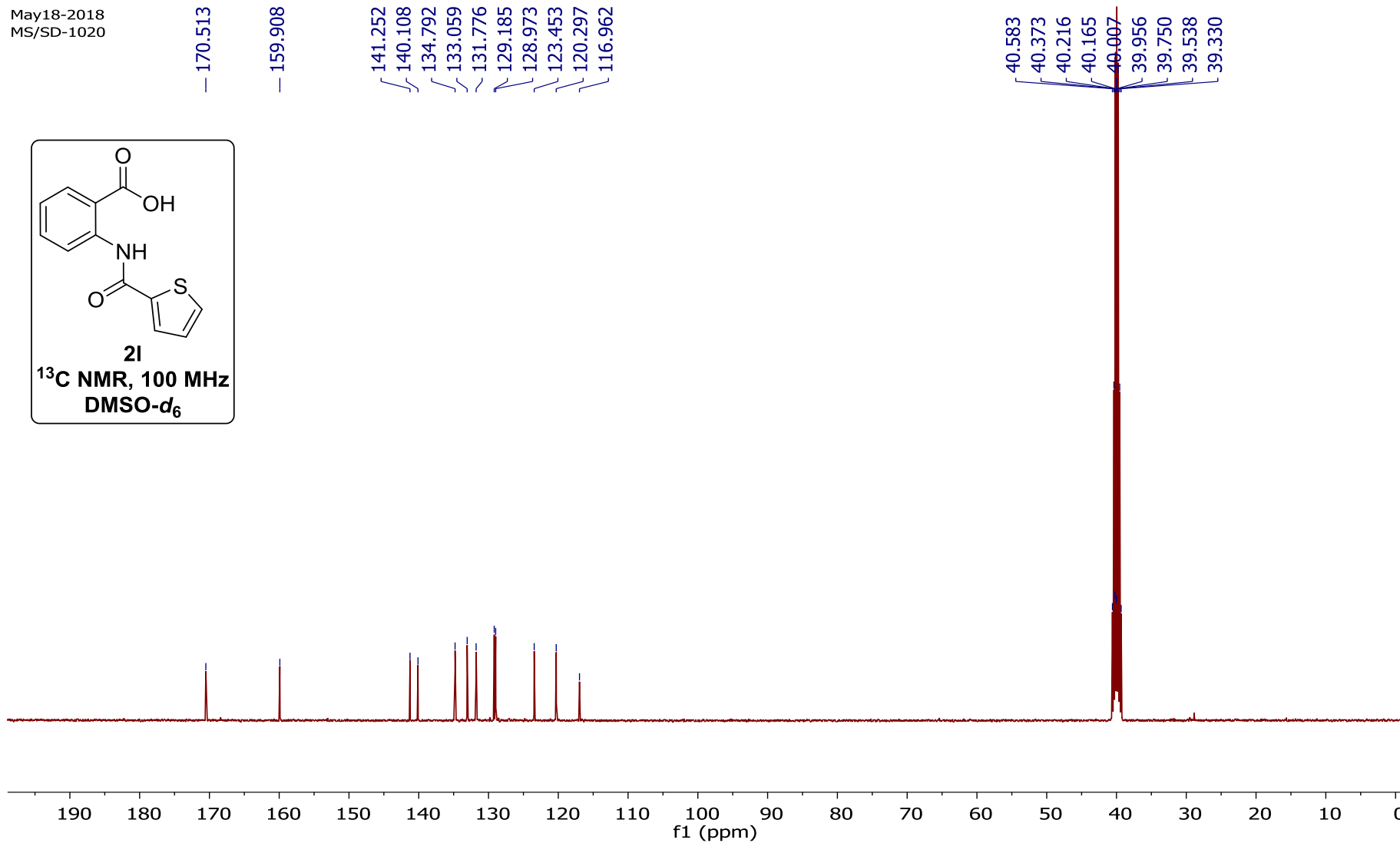
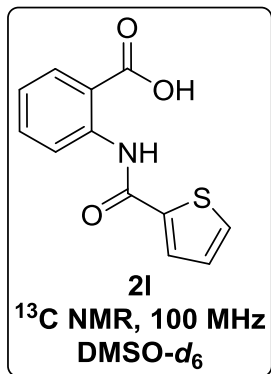
Sample Name	MS-SD-1022	Position	P2-F2	Instrument Name	Instrument 1	User Name	
Inj Vol	0.25	InjPosition		SampleType	Sample	IRM Calibration Status	Success
Data Filename	MS-SD-1022.d	ACQ Method	ChB60ChA40Dual AJS E	Comment		Acquired Time	10/29/2018 12:46:39 PM



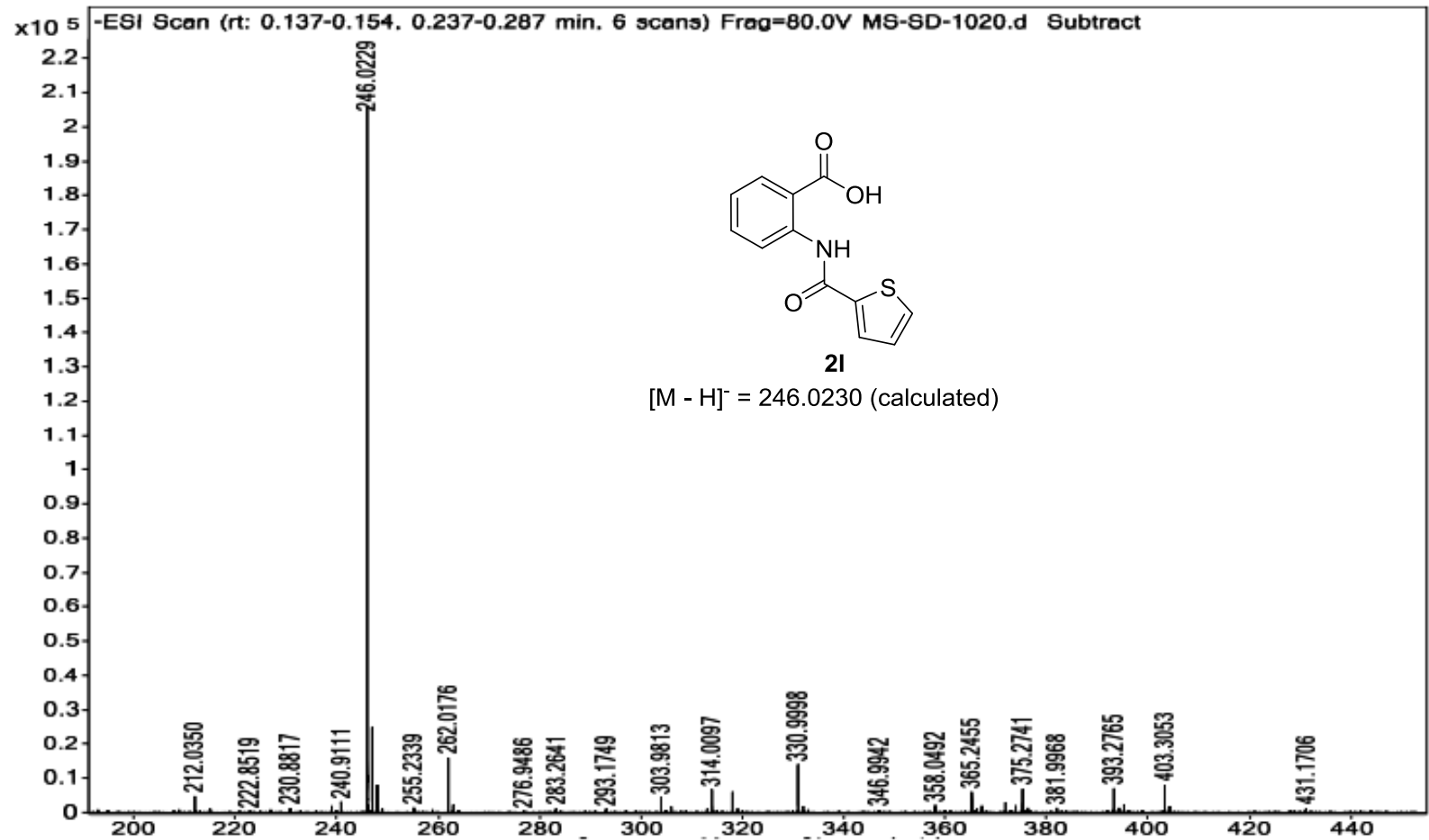
May18-2018
MS/SD-1020



May18-2018
MS/SD-1020



Sample Name	MS-SD-1020	Position	P1-B3	Instrument Name	Instrument 1	User Name	
Inj Vol	0.25	InjPosition		SampleType	Sample	IRM Calibration Status	Success
Data Filename	MS-SD-1020.d	ACQ Method	Ch860ChD40Dual AJS E	Comment		Acquired Time	1/2/2019 5:30:09 PM



Jun28-2018
MS/SD-1021

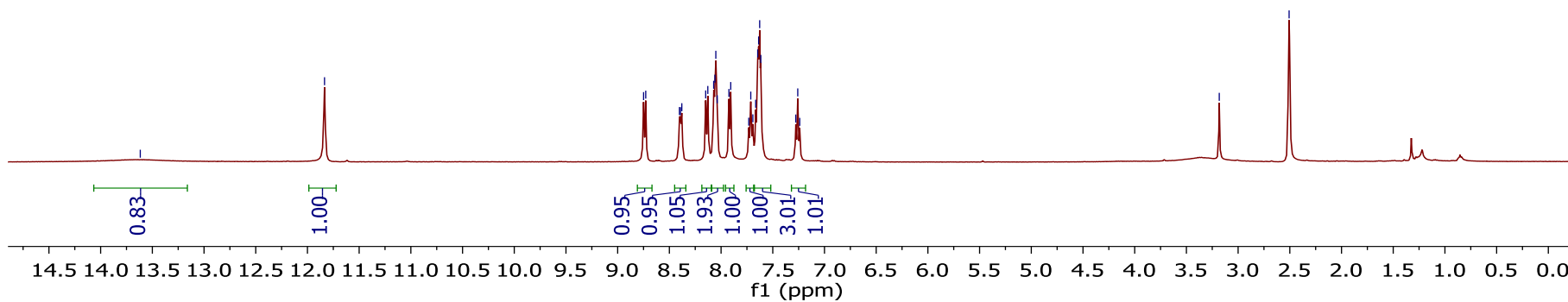
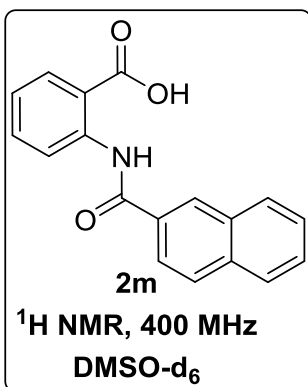
— 13.6167

— 11.8348

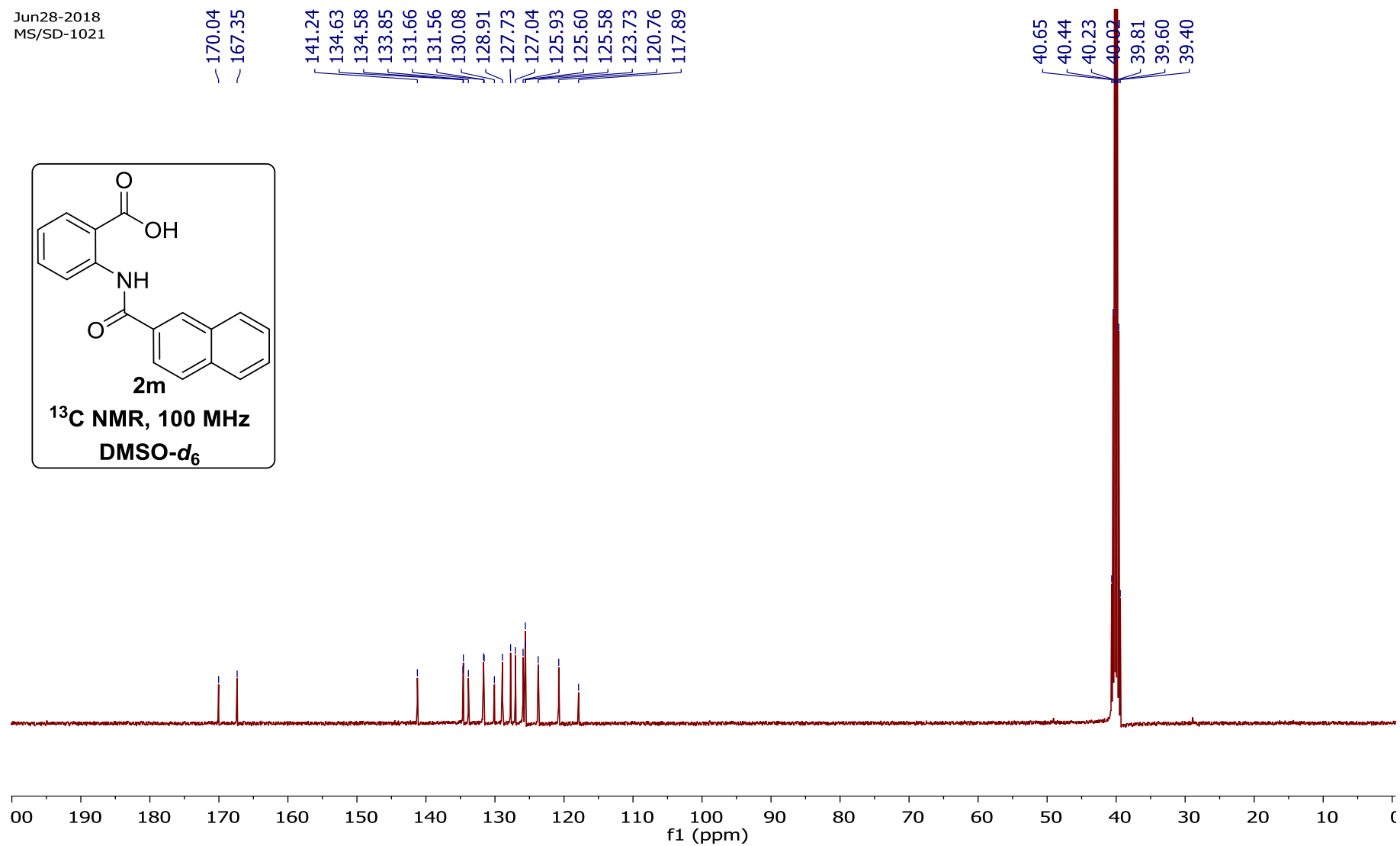
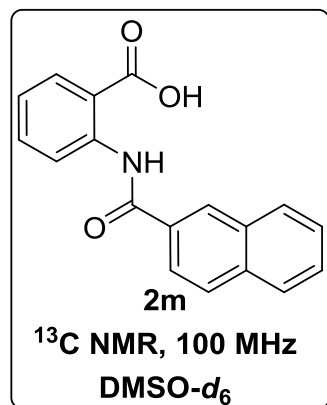
8.7494
8.7286
8.4026
8.3930
8.3796
8.1488
8.1282
8.0715
8.0598
8.0508
8.0375
7.9243
7.9066
7.7323
7.7127
7.6928
7.6654
7.6457
7.6368
7.6267
7.6158
7.2774
7.2584
7.2394

— 3.1823

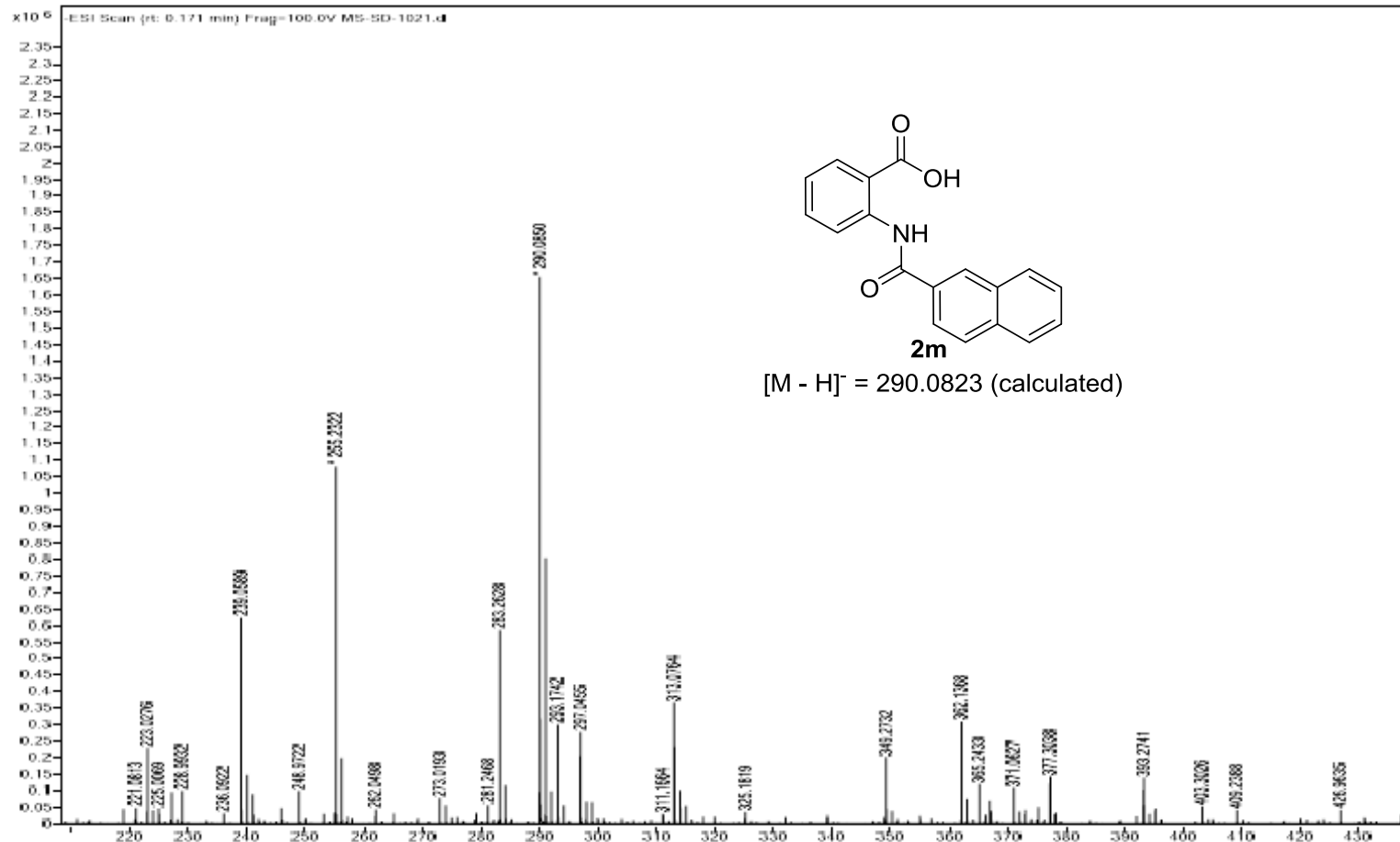
— 2.5067



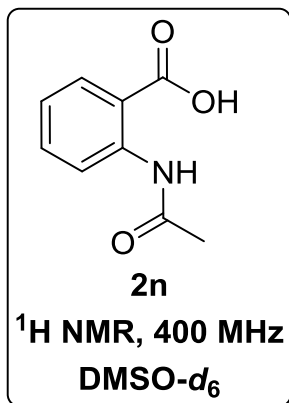
Jun28-2018
MS/SD-1021



Sample Name	M5-SD-1021	Position	P2-F1	Instrument Name	Instrument 1	User Name	
Inj Vol	0.25	InjPosition		SampleType	Sample	IRM Calibration Status	Success
Data Filename	M5-SD-1021.d	ACQ Method	ChB60ChA40Dual AJS E	Comment		Acquired Time	10/29/2018 12:38:14 PM



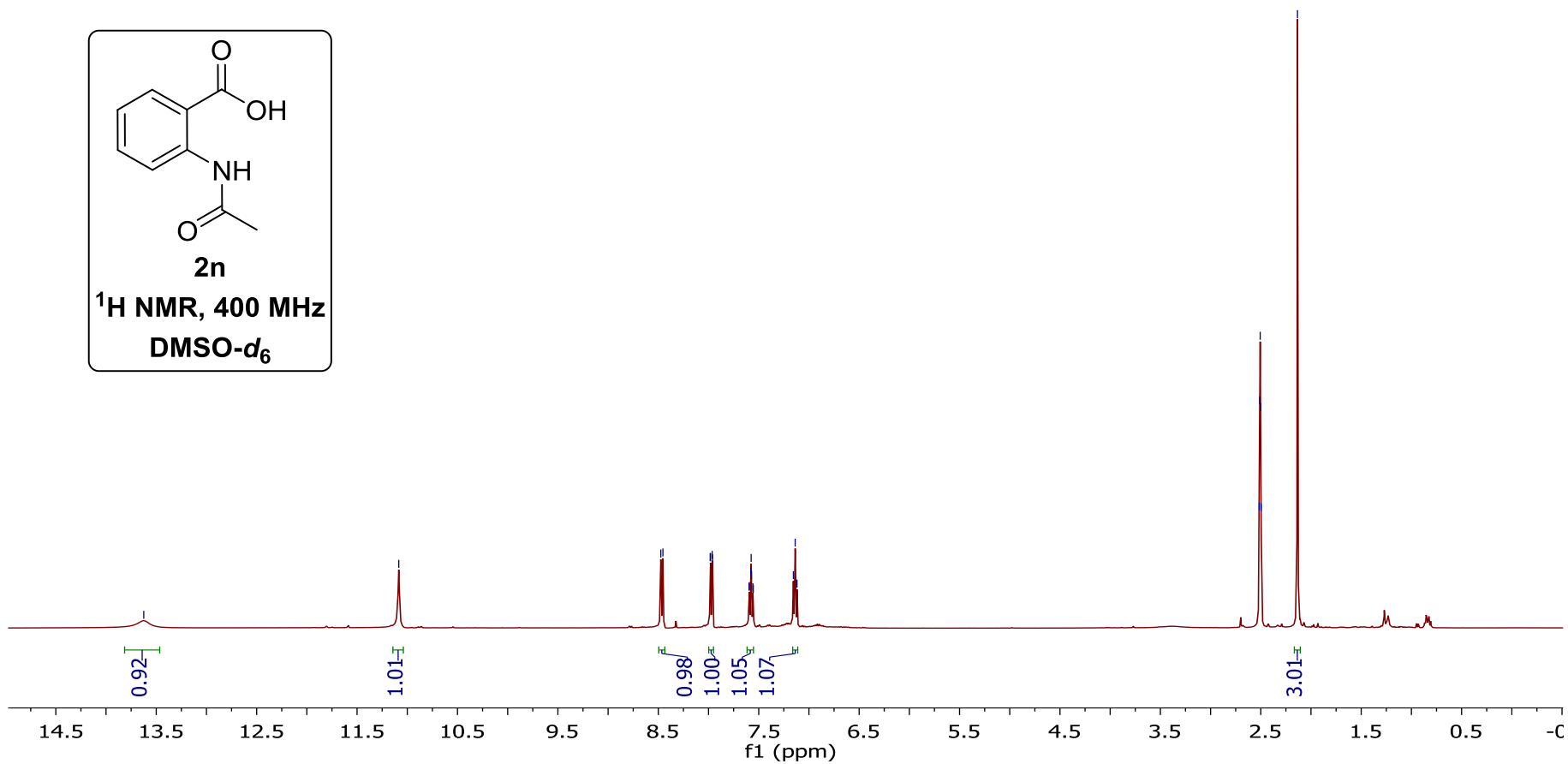
May18-2018
MS/SD-1030
— 13.6242



— 11.0847

8.4750
8.4542
7.9832
7.9797
7.9634
7.9600
7.5967
7.5932
7.5789
7.5754
7.5720
7.5576
7.5540
7.1549
7.1368
7.1187

2.5151
2.5105
2.5057
2.5011
2.4968
2.1345



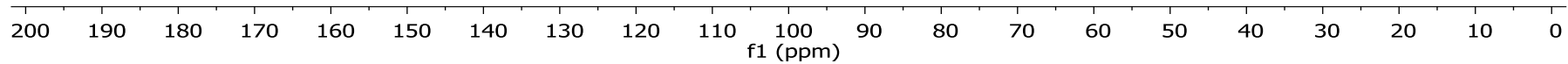
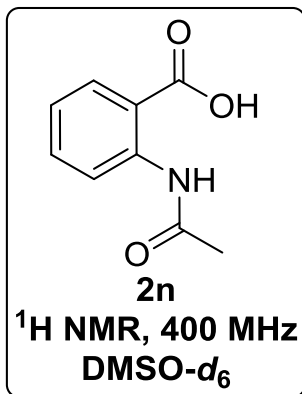
May18-2018
MS/SD-1030

169.950
168.929

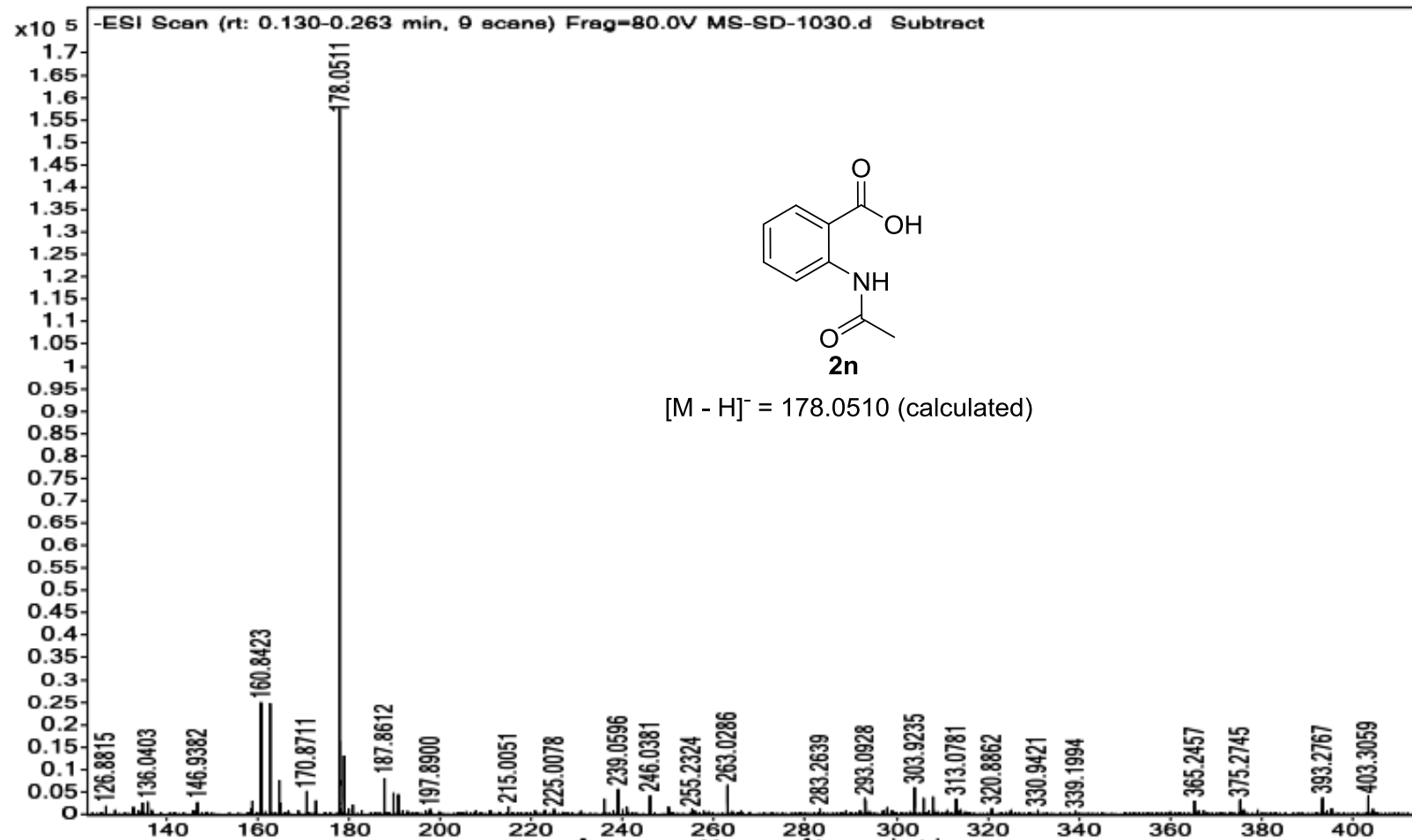
141.313
134.455
131.516

123.011
120.381
116.941

40.578
40.369
40.160
39.954
39.742
39.534
39.325
25.464

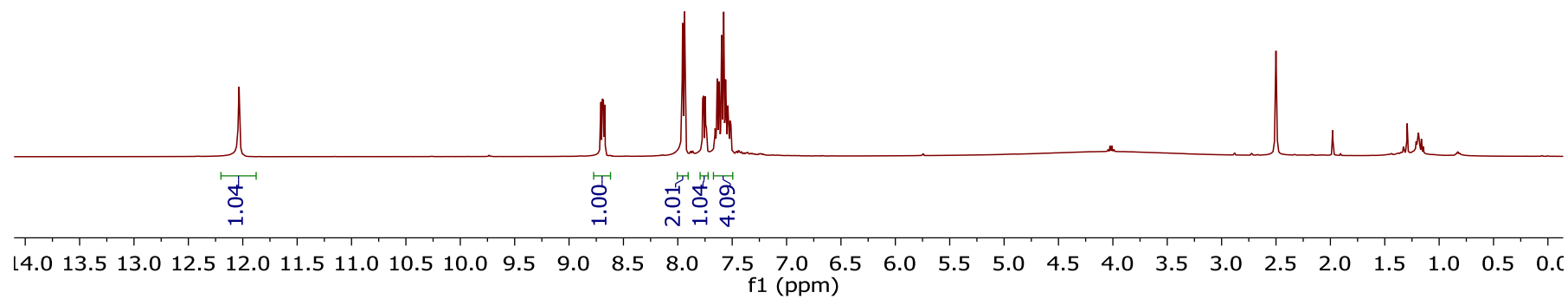
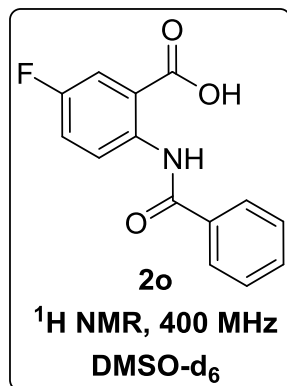


Sample Name	MS-SD-1030	Position	P1-810	Instrument Name	Instrument 1	User Name	
Inj Vol	0.25	InjPosition		SampleType	Sample	IRM Calibration Status	Success
Data Filename	MS-SD-1030.d	ACQ Method	ChB60ChD40Dual AJS E	Comment		Acquired Time	1/2/2019 6:02:45 PM



Nov28-2018/4
OSP-2-36

— 12.0346

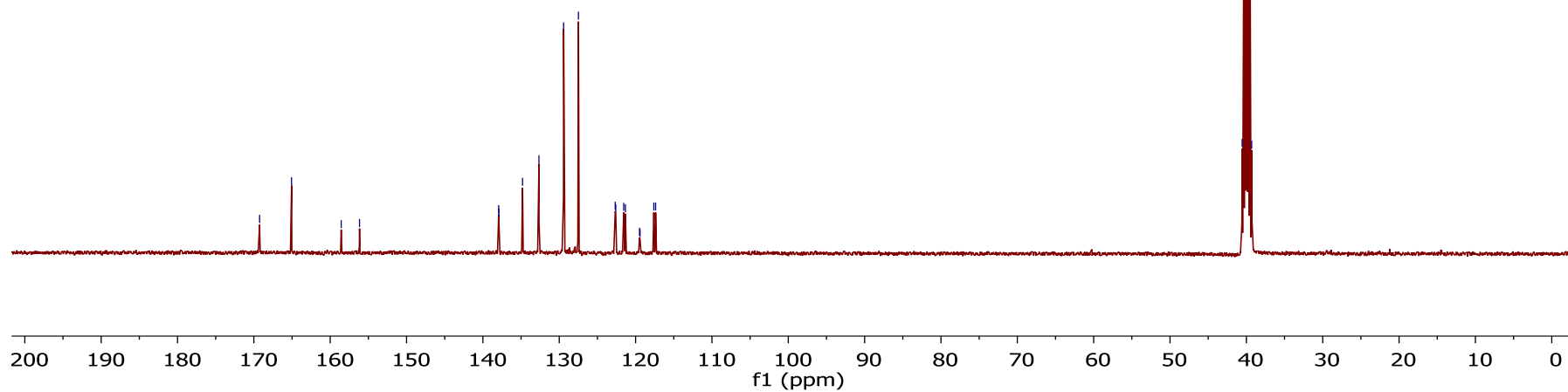
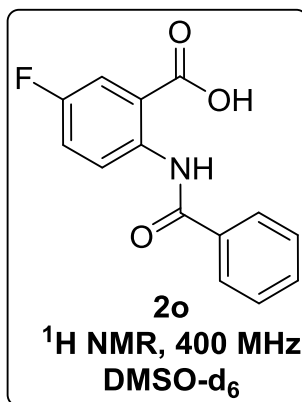


8.7072
8.6942
8.6841
8.6712
7.9584
7.9553
7.9511
7.9436
7.9382
7.9339
7.7711
7.7631
7.7476
7.7397
7.6561
7.6379
7.6200
7.5969
7.5779
7.5610
7.5565
7.5422
7.5398
7.5344
7.5196
7.5117
2.5097
2.5050
2.5004
2.4958
2.4912

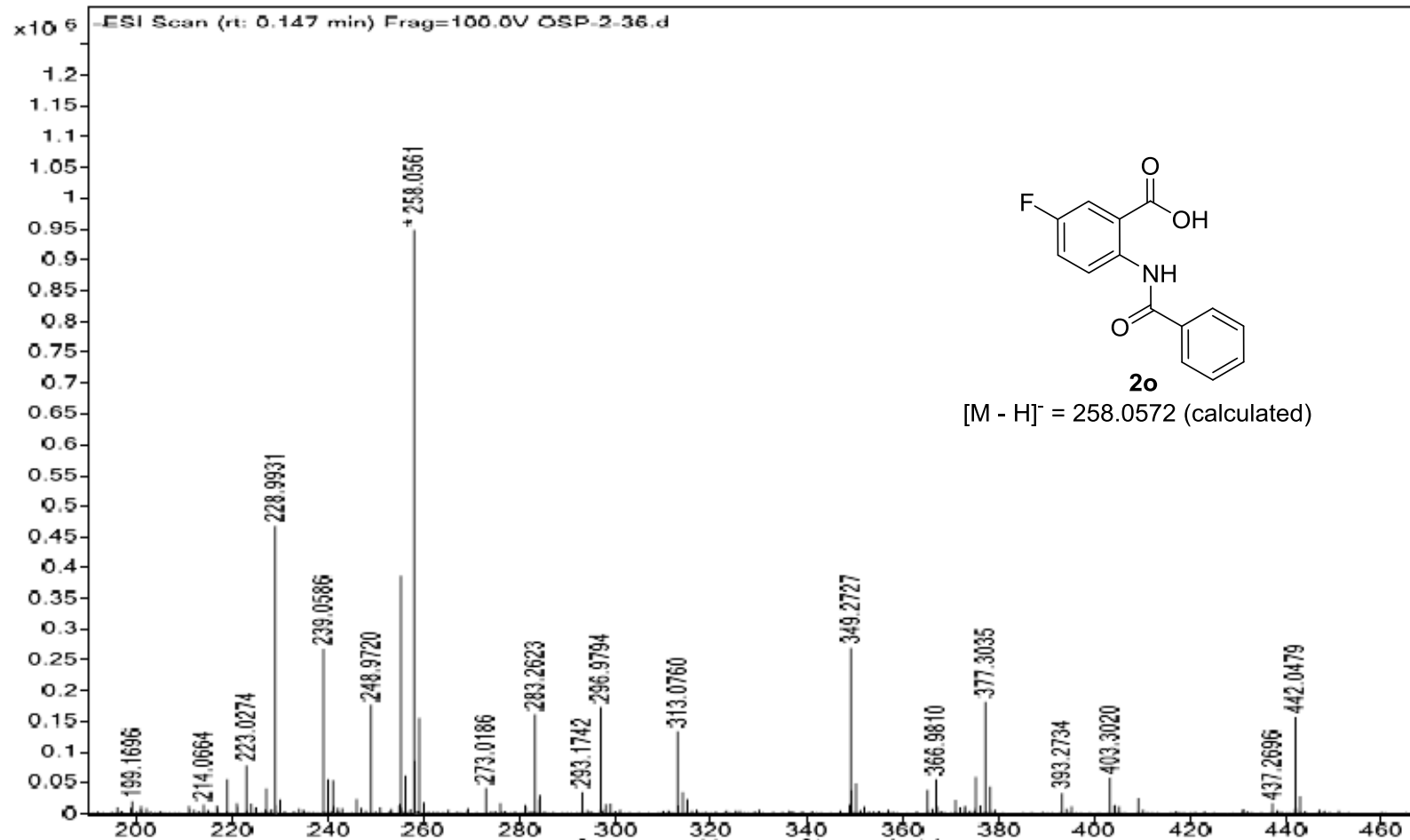
Nov28-2018/10
OSP-2-36

169.25
165.06
158.56
156.16
137.94
137.91
134.81
132.66
129.43
127.49
122.67
122.60
121.56
121.34
119.49
119.42
117.61
117.38

40.55
40.34
40.14
39.93
39.72
39.51
39.30

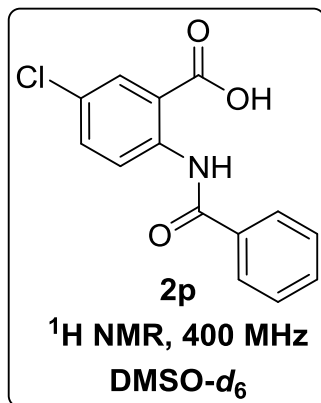


Sample Name	OSP-2-36	Position	P2-E5	Instrument Name	Instrument 1	User Name	
Inj Vol	0.25	InjPosition		SampleType	Sample	IRM Calibration Status	Success
Data Filename	OSP-2-36.d	ACQ Method	ChB60ChA40Dual AJS E	Comment		Acquired Time	10/29/2018 11:40:27 AM



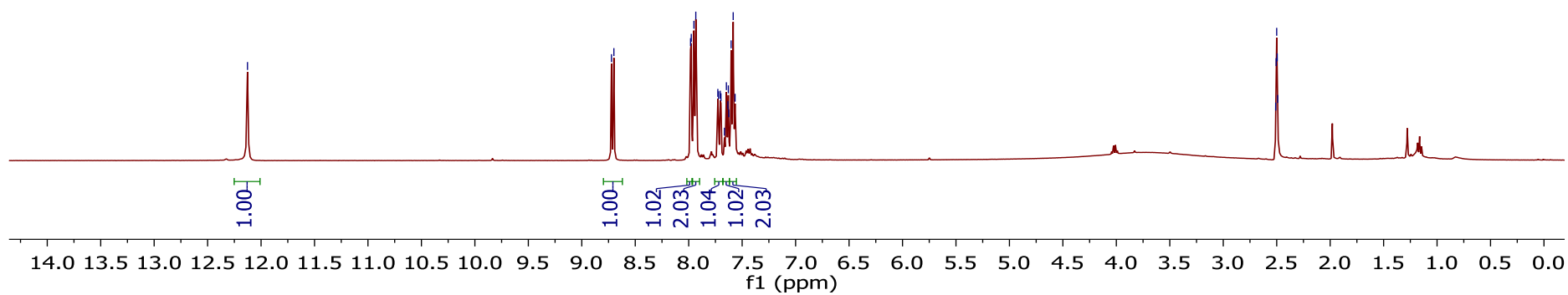
Dec21-2018/1
OSP-2-41

— 12.1269



8.7223
8.6997
7.9826
7.9759
7.9512
7.9336
7.7275
7.7211
7.7050
7.6986
7.6655
7.6474
7.6329
7.6293
7.6254
7.6030
7.5839
7.5662

2.5093
2.5050
2.5001
2.4954
2.4909

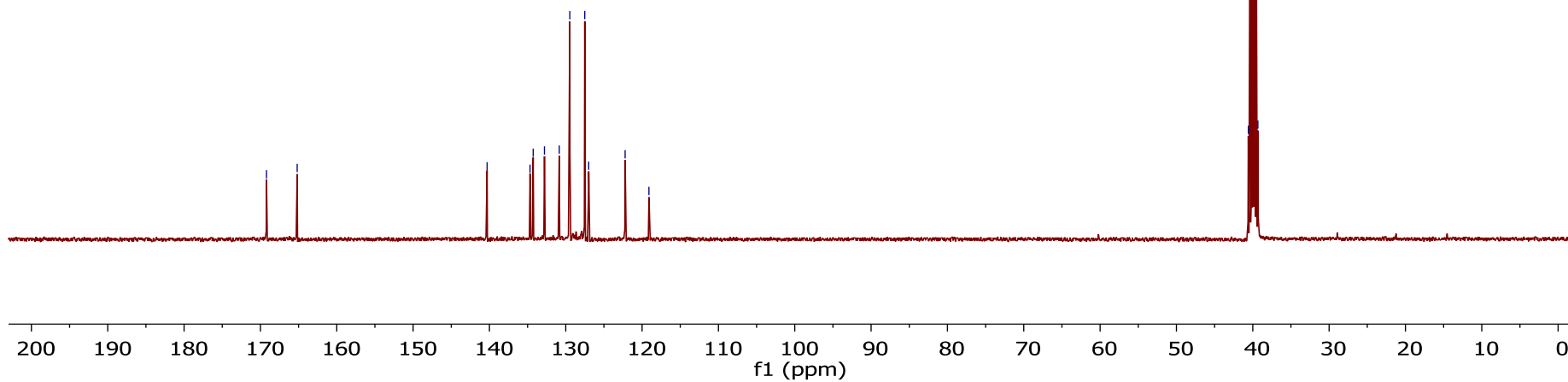
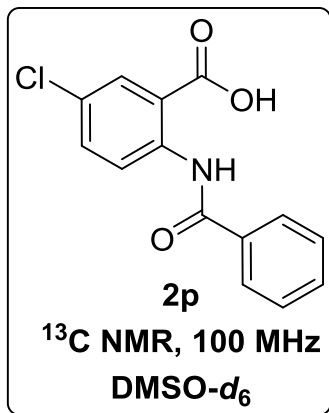


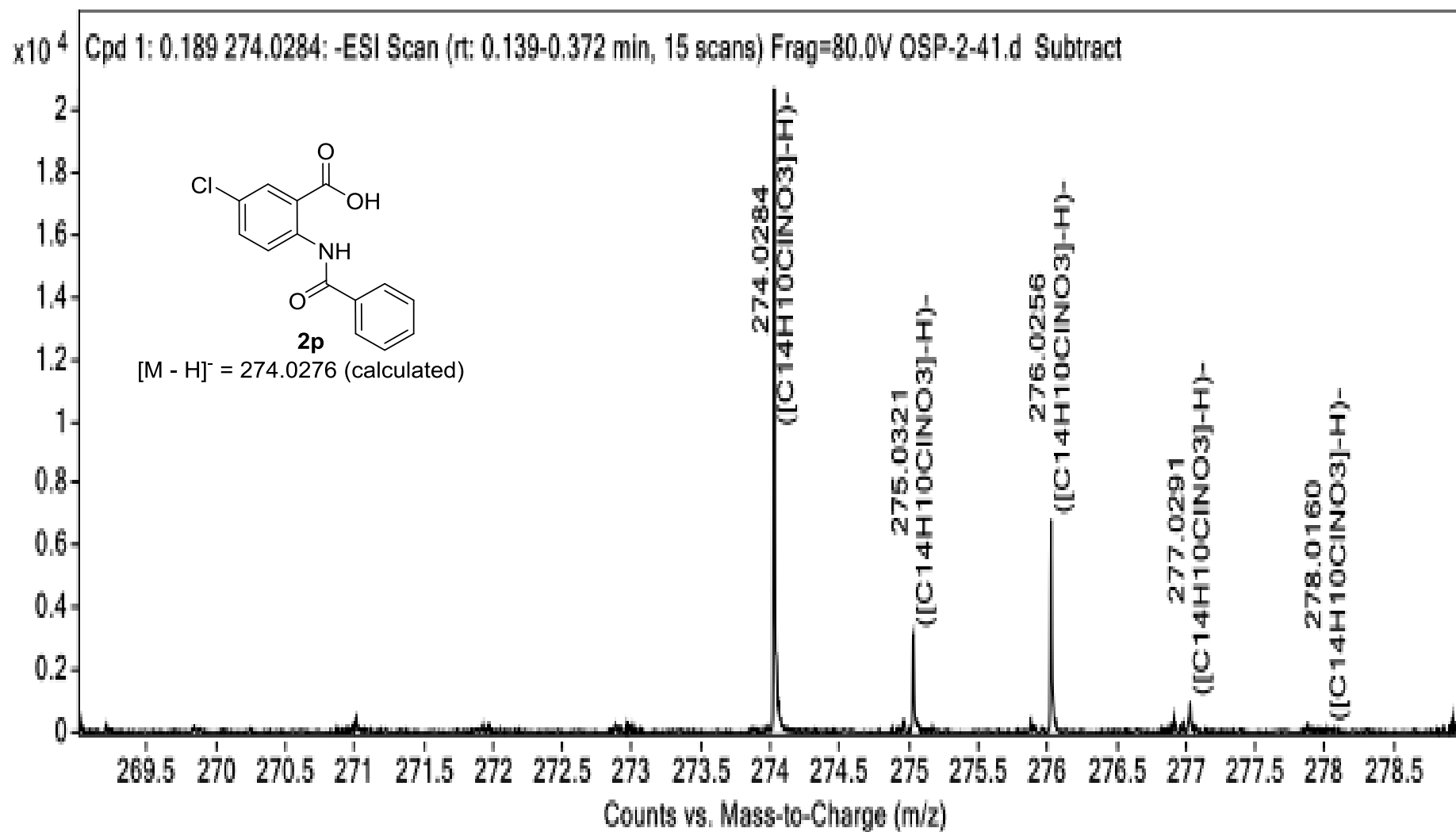
Dec21-2018/2
OSP-2-41

— 169.20
— 165.18

140.31
134.68
134.27
132.79
130.85
129.47
127.51
126.99
122.22
119.10

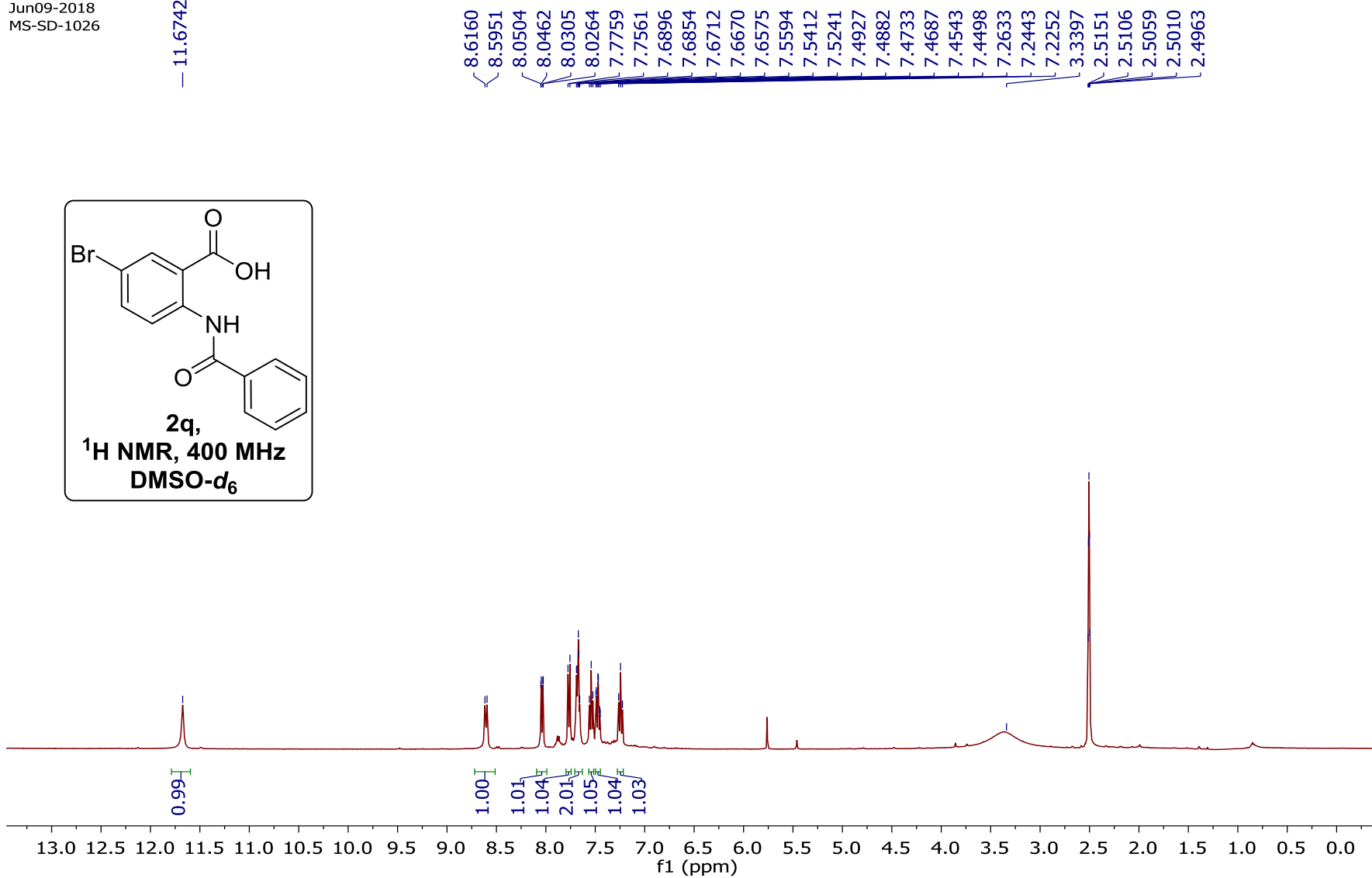
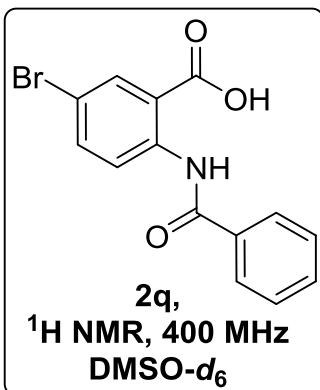
40.58
40.37
40.17
39.96
39.75
39.54
39.33





Jun09-2018
MS-SD-1026

— 11.6742

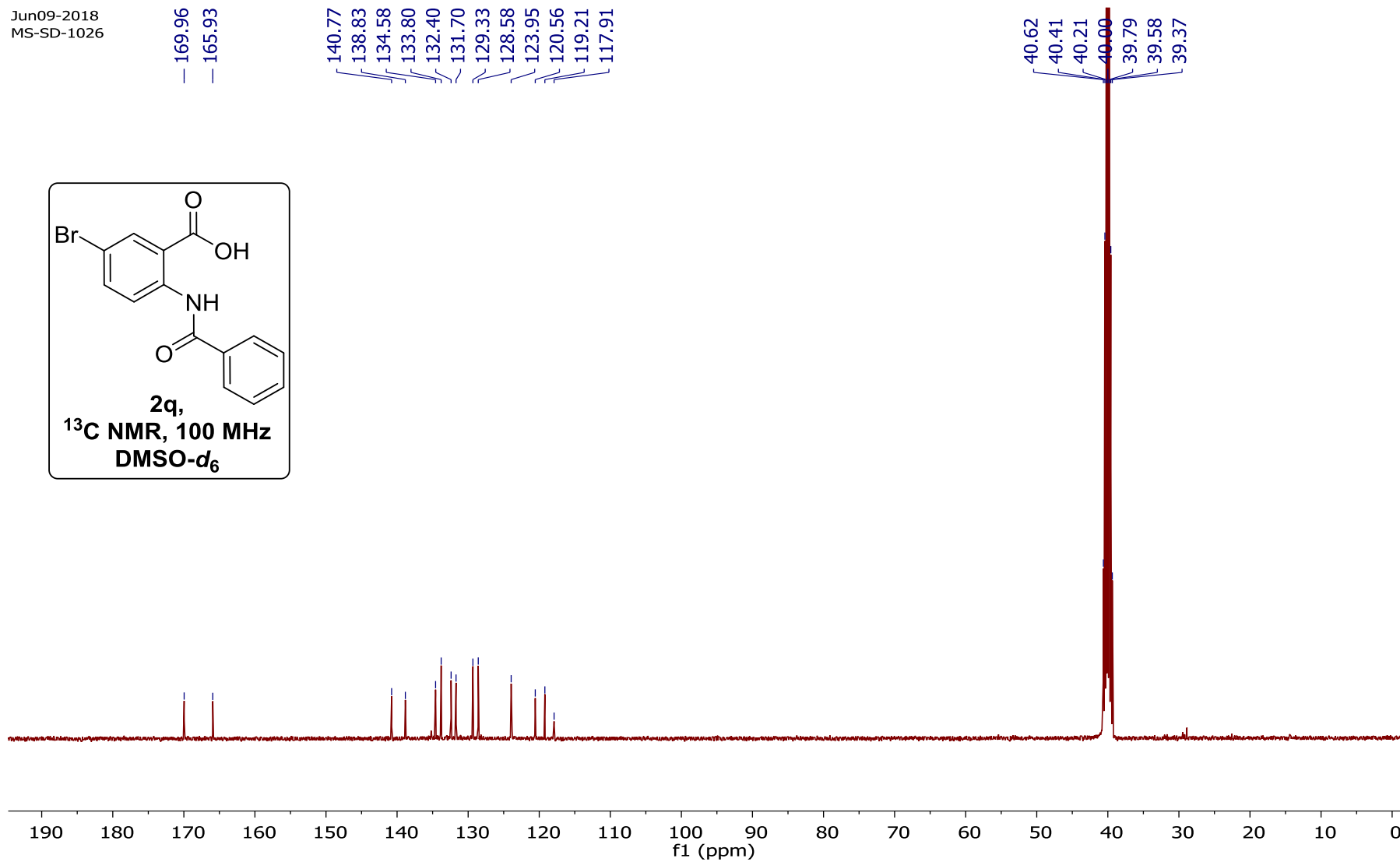
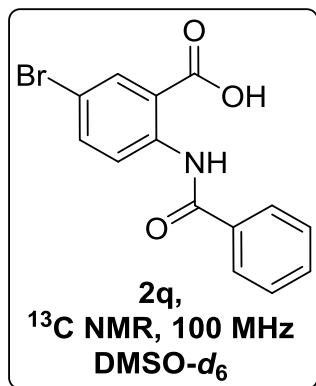


Jun09-2018
MS-SD-1026

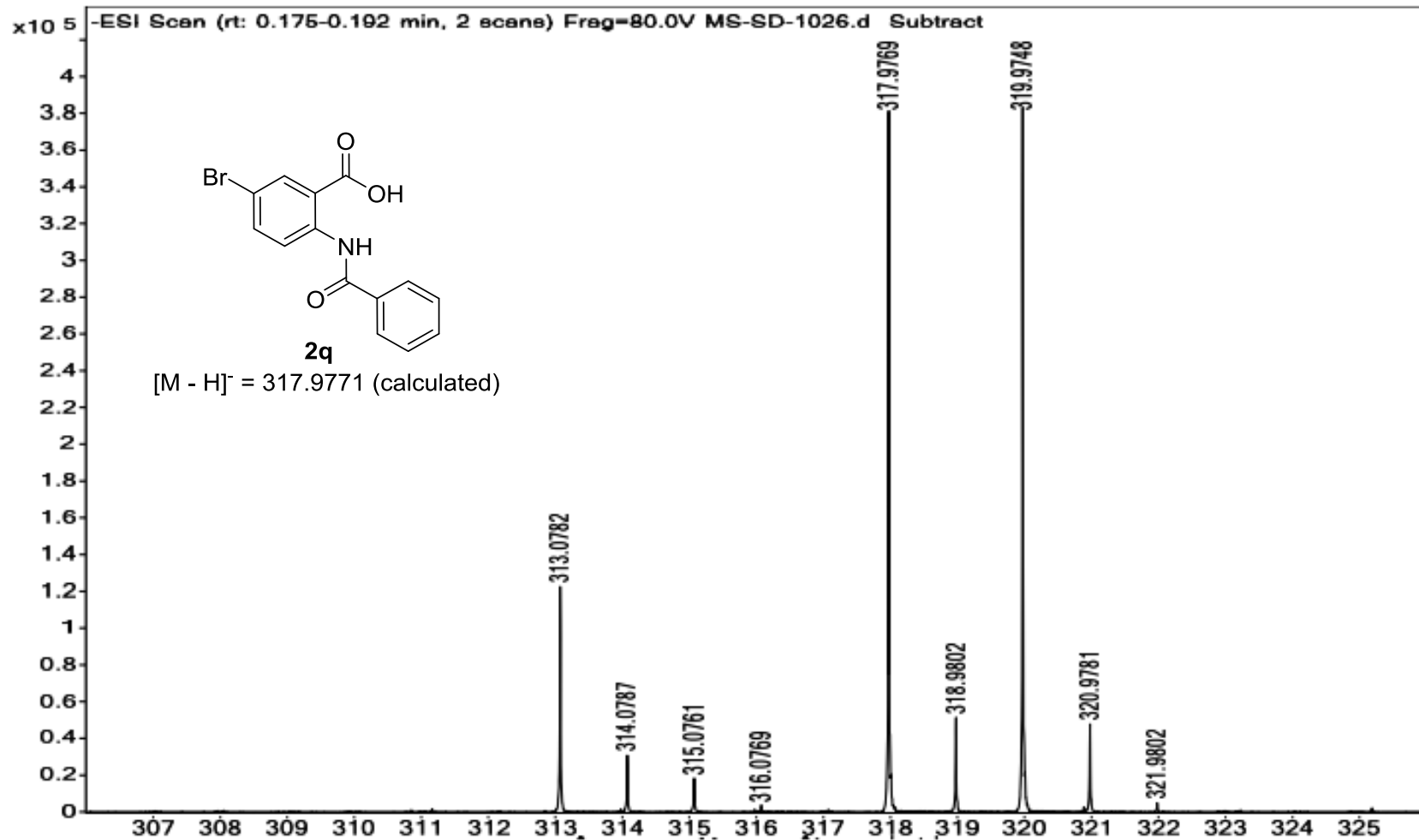
— 169.96
— 165.93

140.77
138.83
134.58
133.80
132.40
131.70
129.33
128.58
123.95
120.56
119.21
117.91

40.62
40.41
40.21
40.00
39.79
39.58
39.37



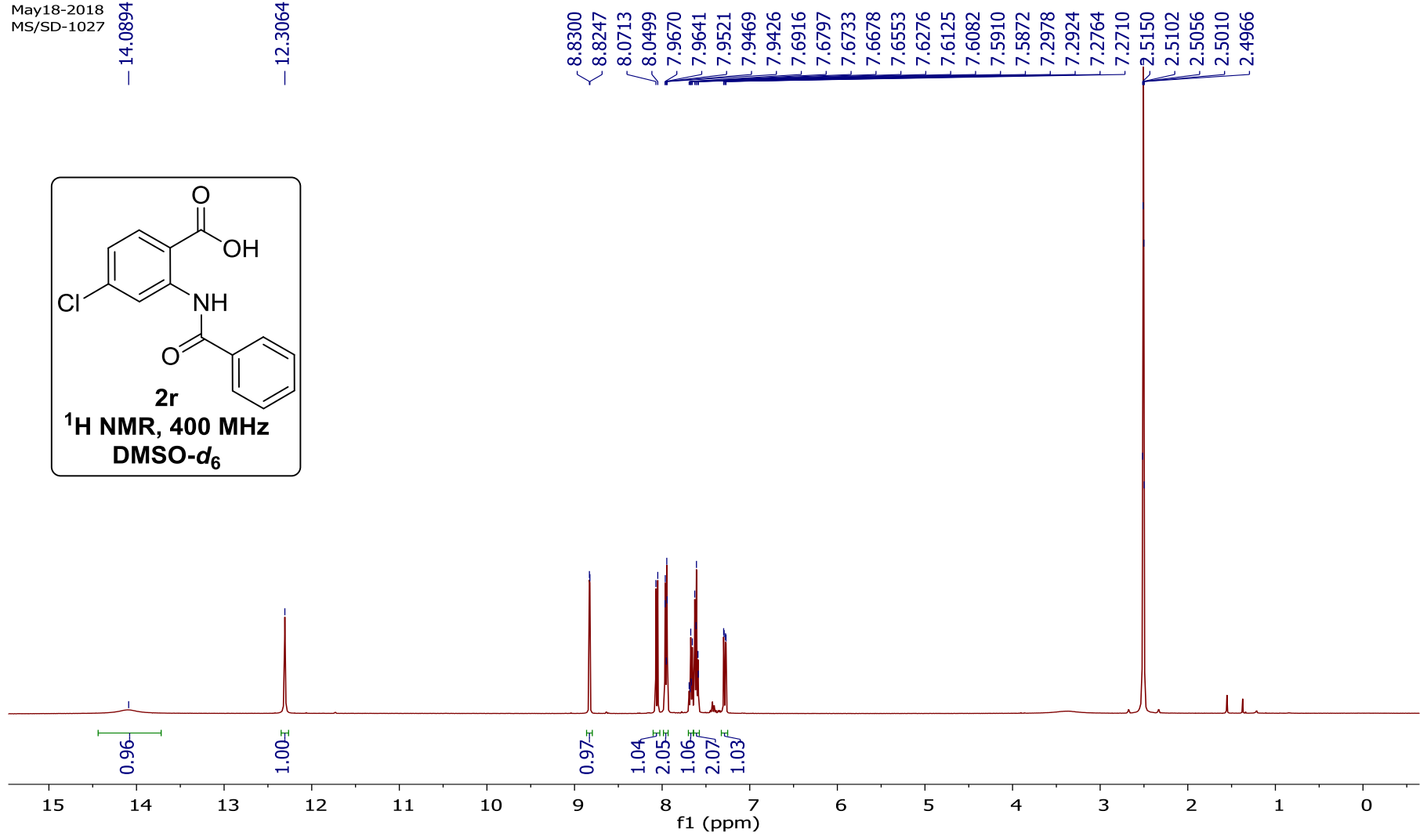
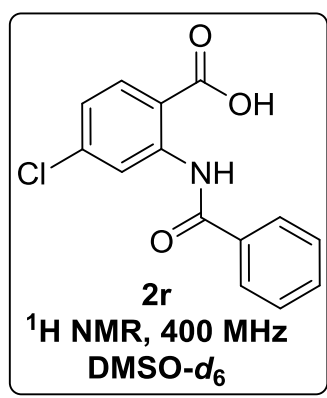
Sample Name	MS-SD-1026	Position	P1-B11	Instrument Name	Instrument 1	User Name	
Inj Vol	0.25	InjPosition		SampleType	Sample	IRM Calibration Status	Success
Data Filename	MS-SD-1026.d	ACQ Method	ChB60ChD40Dual AJS E	Comment		Acquired Time	1/2/2019 6:10:57 PM



May18-2018
MS/SD-1027

— 14.0894

— 12.3064

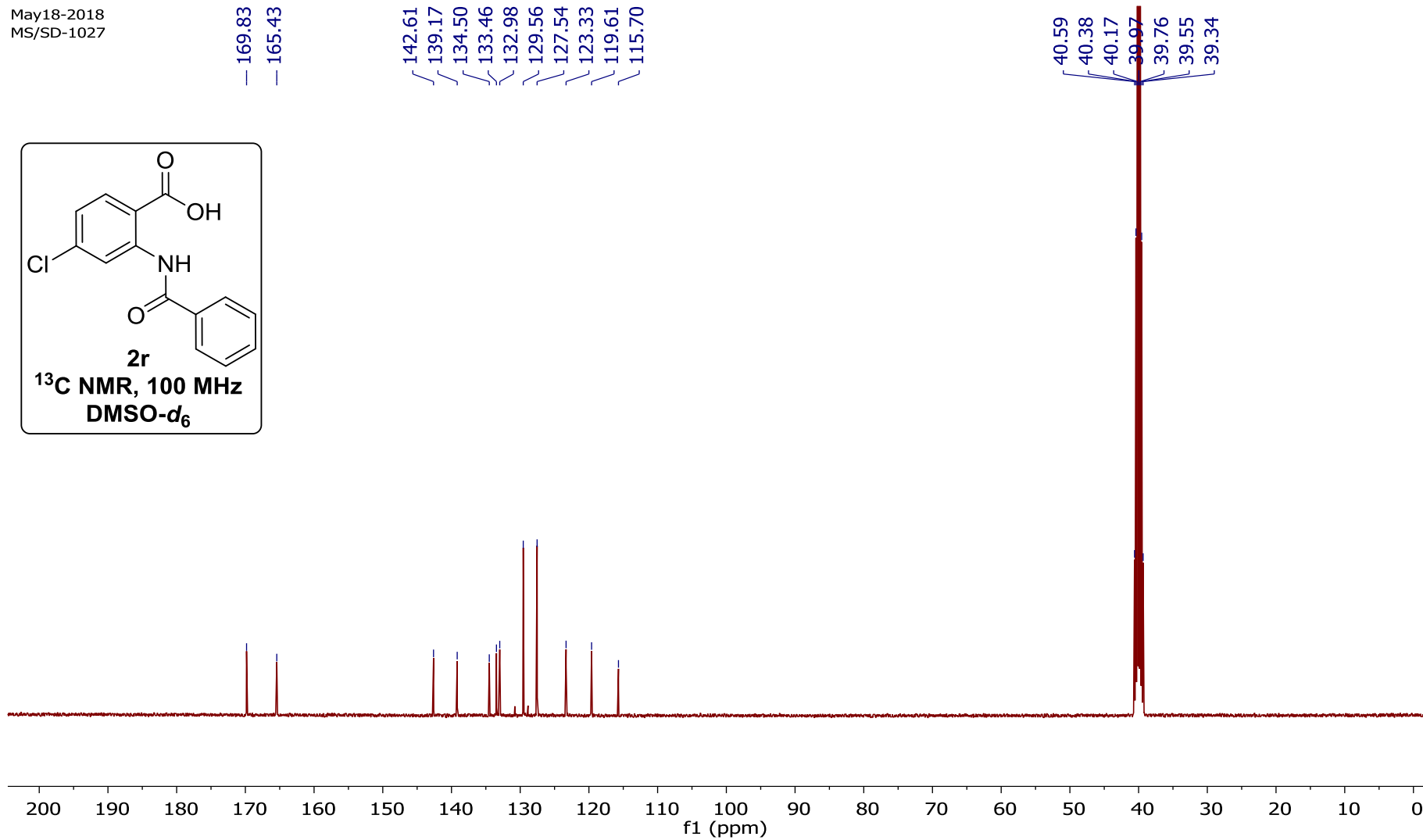
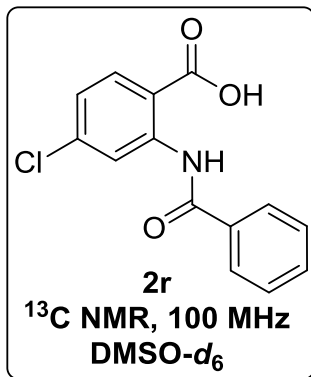


May18-2018
MS/SD-1027

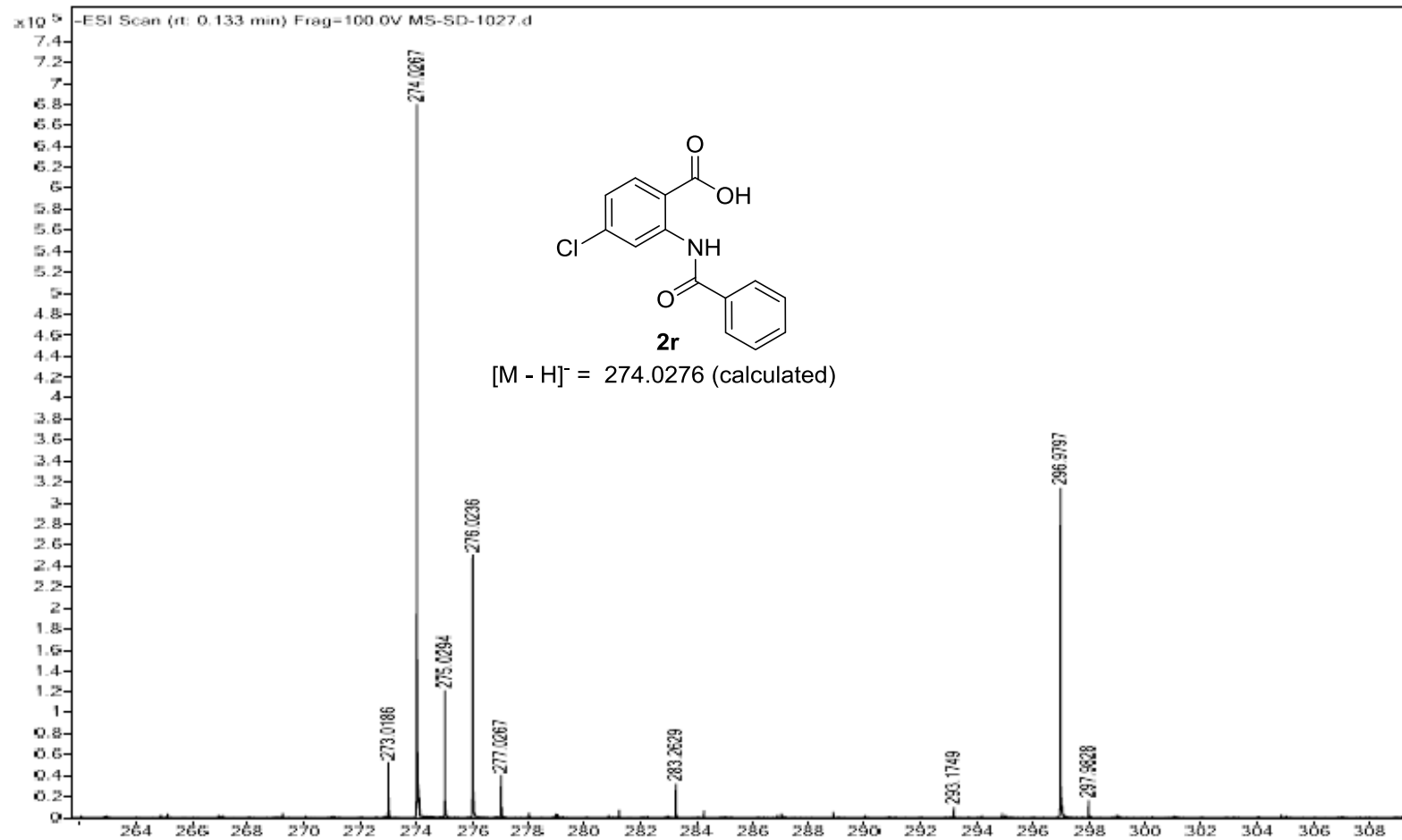
— 169.83
— 165.43

142.61
139.17
134.50
133.46
132.98
129.56
127.54
123.33
119.61
115.70

40.59
40.38
40.17
39.97
39.76
39.55
39.34

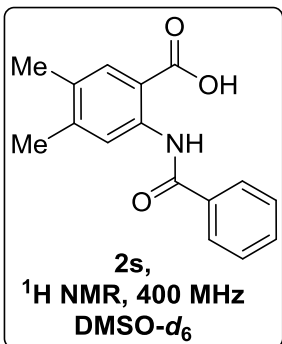


Sample Name	MS-SD-1027	Position	P2-F8	Instrument Name	Instrument 1	User Name	
Inj Vol	0.25	InjPosition		SampleType	Sample	IRM Calibration Status	Success
Data Filename	MS-SD-1027.d	ACQ Method	ChB60ChA40Dual AJS E	Comment		Acquired Time	10/29/2018 1:36:16 PM



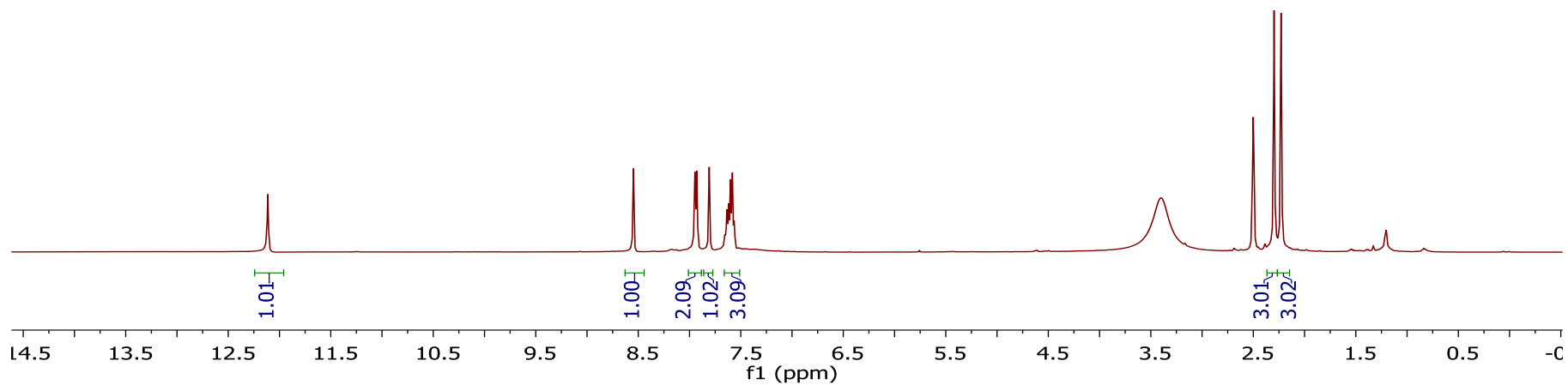
Nov29-2018/1
OSP-ACID-56 Me

-12.1140



-8.5474
7.9467
7.9281
7.8075
7.6542
7.6364
7.6191
7.6004
7.5821
7.5637

-3.4012
2.5055
2.5002
2.4950
2.2974
2.2293



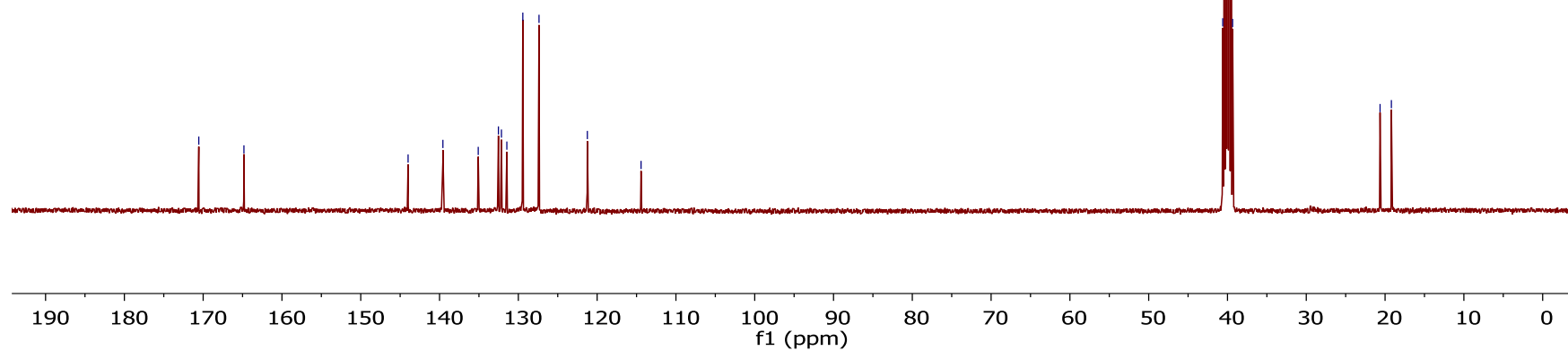
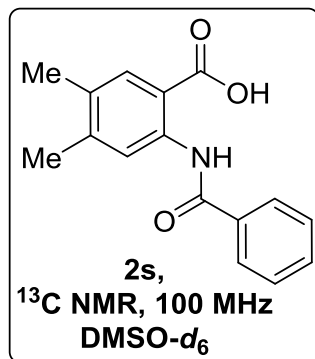
Nov29-2018/2
OSP-ACID-56 Me

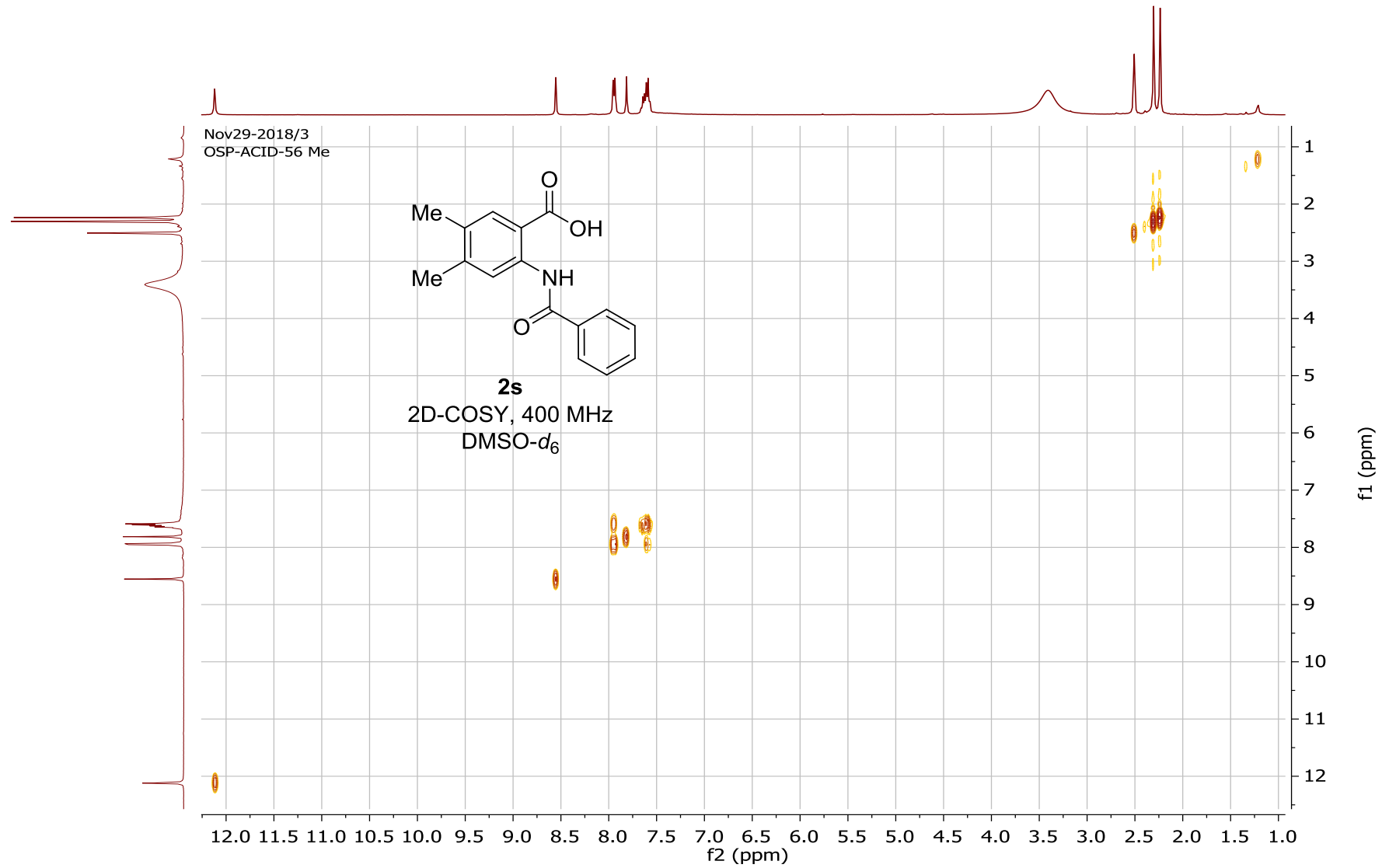
— 170.55
— 164.83

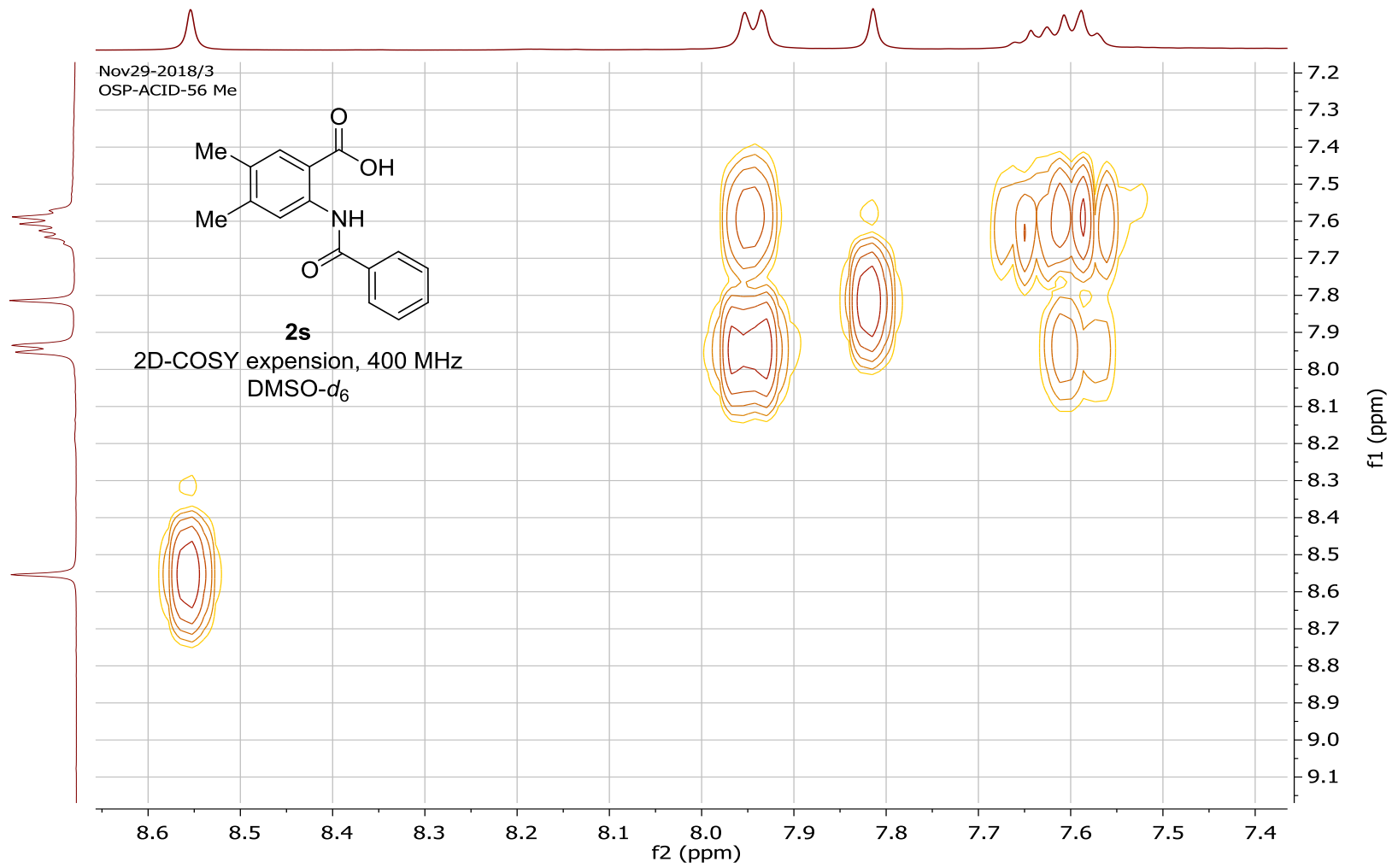
~ 143.99
~ 139.57
~ 135.09
~ 132.53
~ 132.14
~ 131.46
~ 129.43
~ 127.38
~ 121.24
~ 114.42

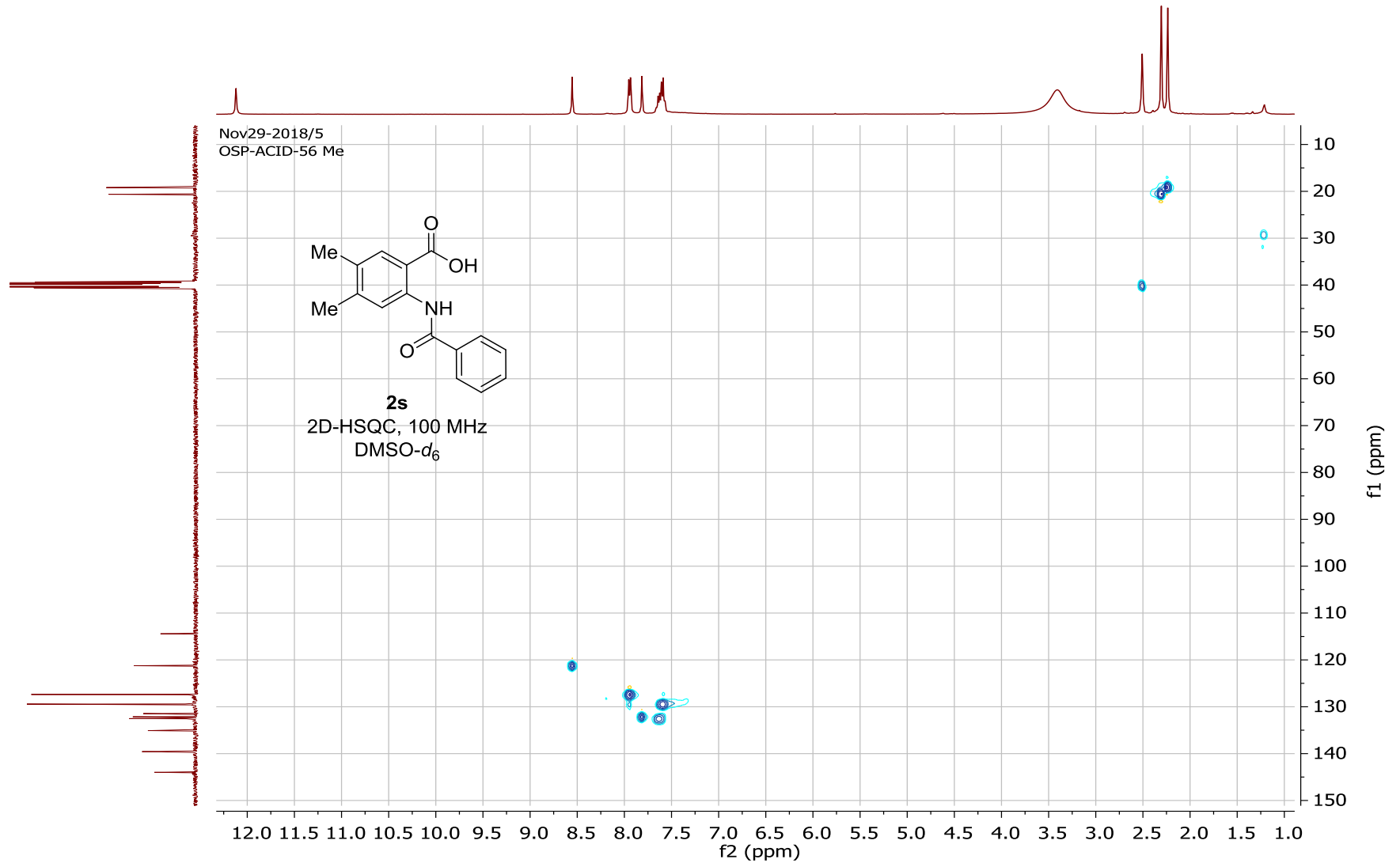
40.60
40.39
40.18
39.98
39.77
39.56
39.35

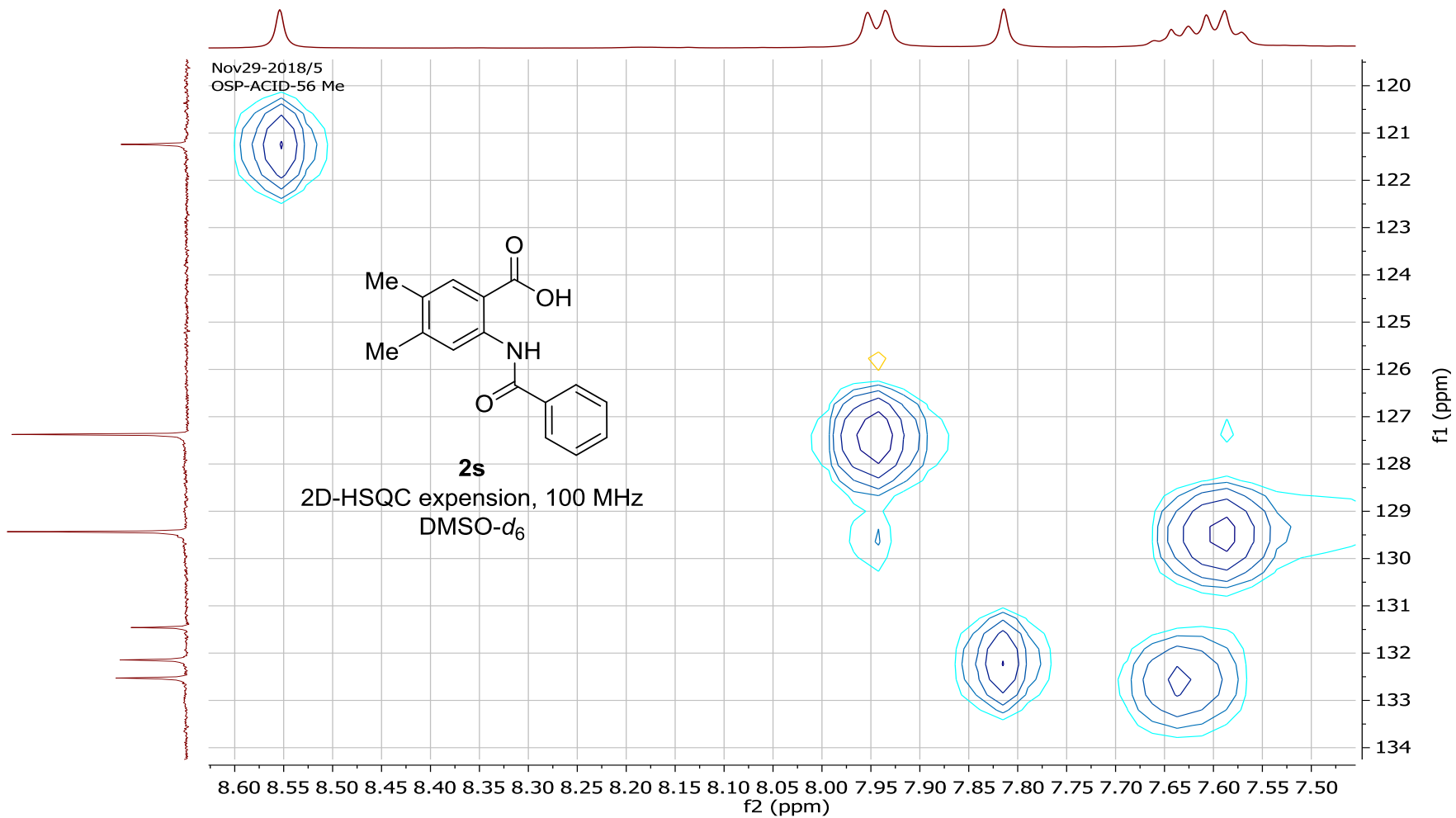
~ 20.64
~ 19.20

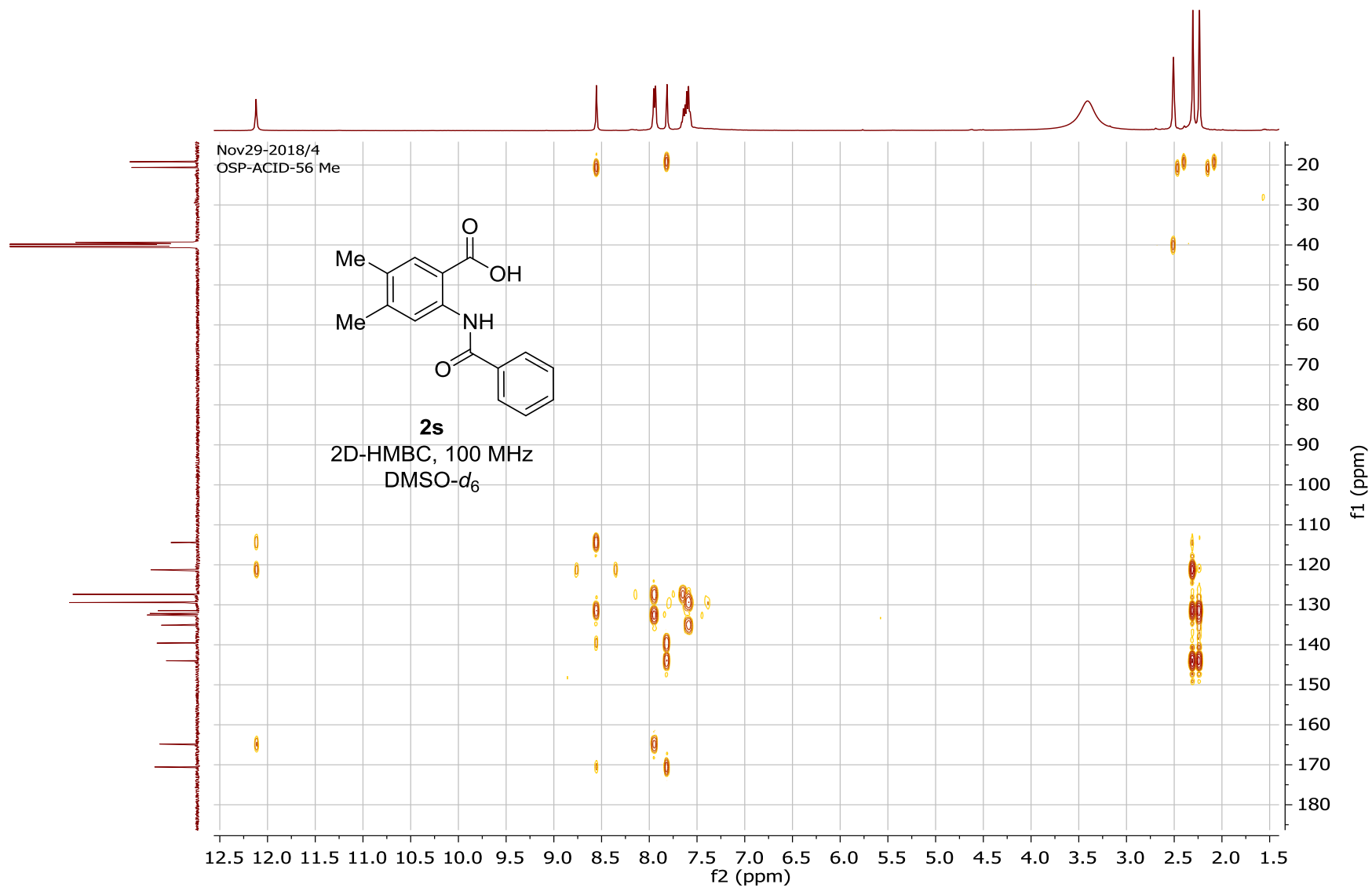


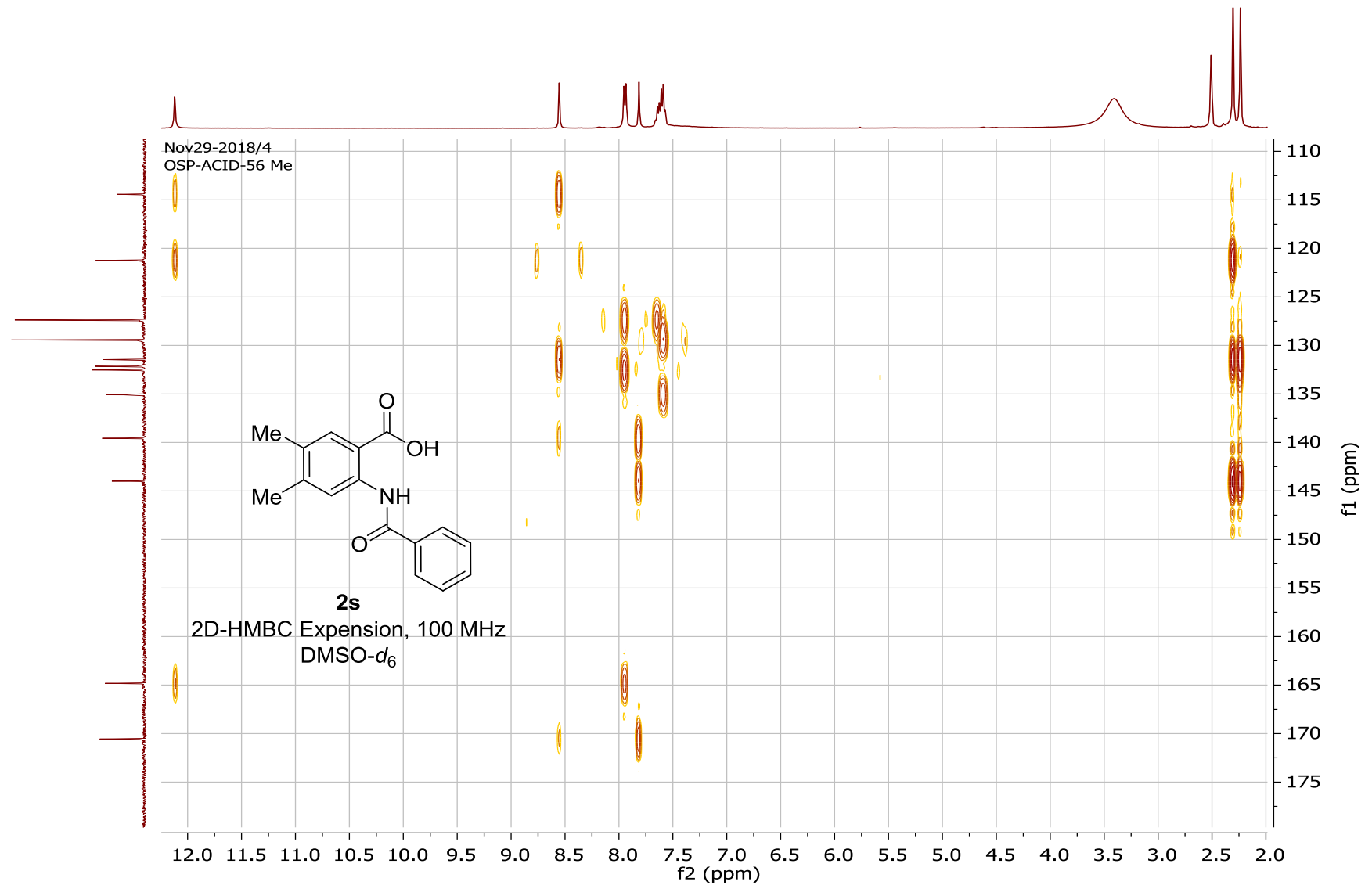




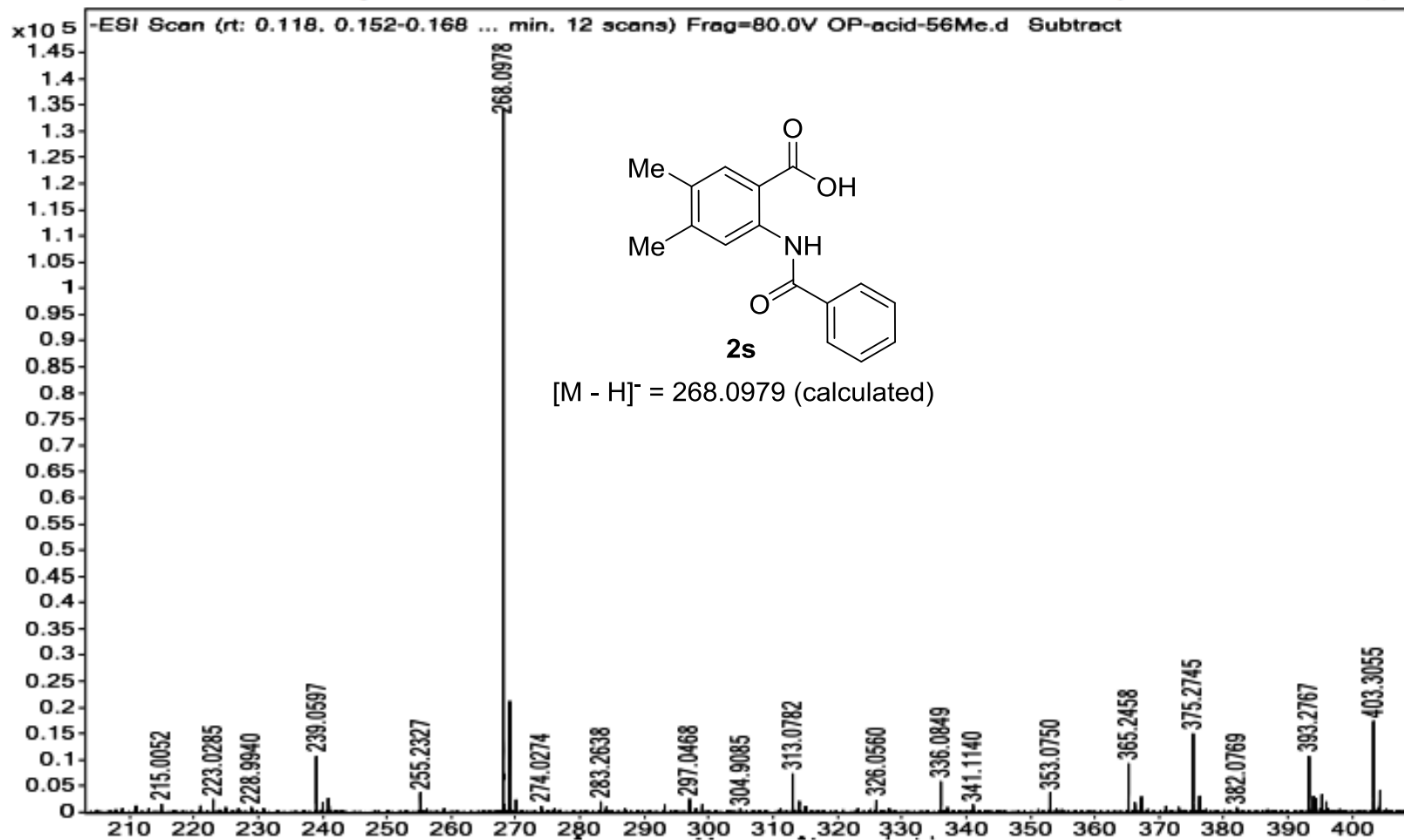


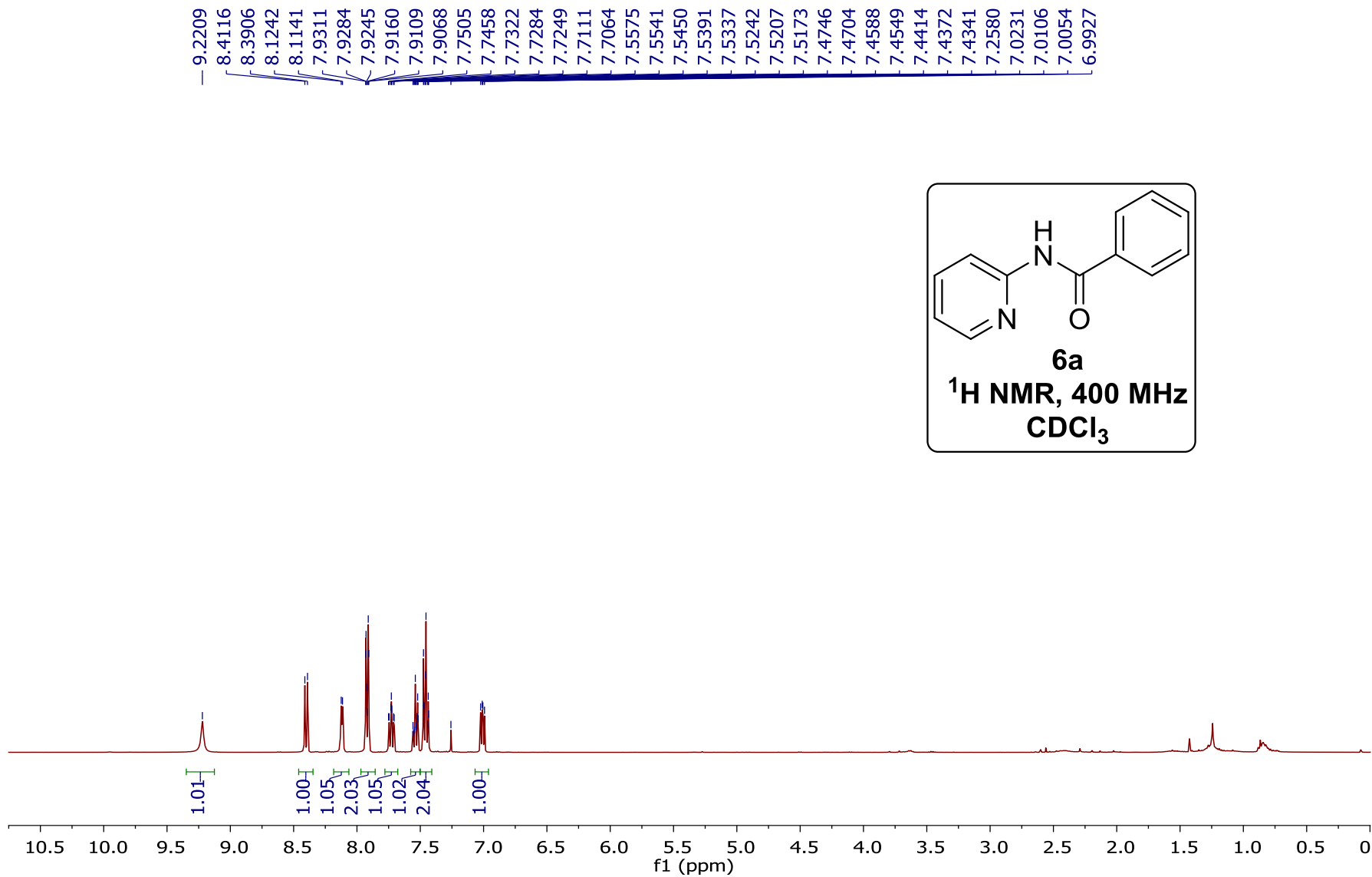


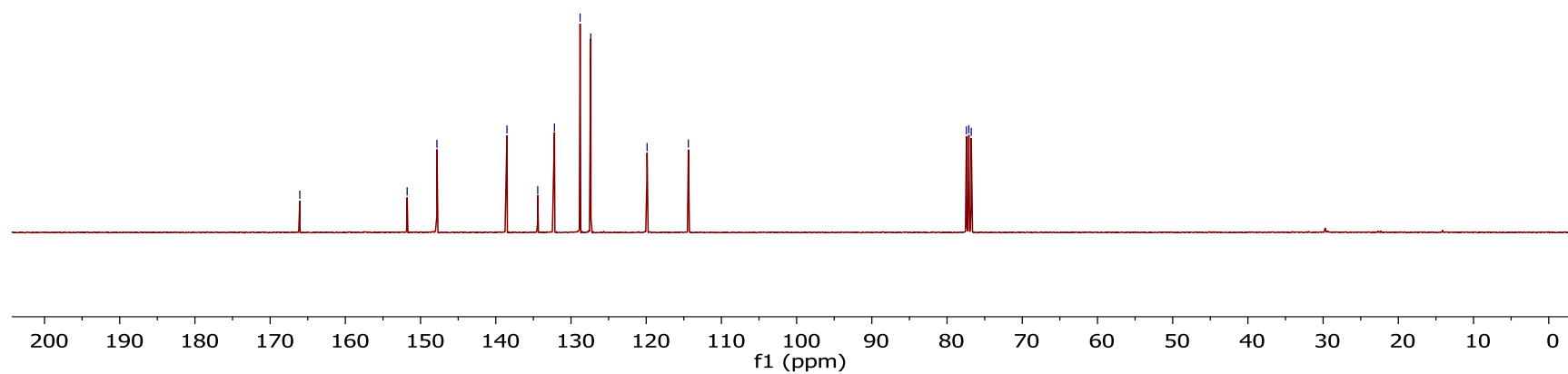
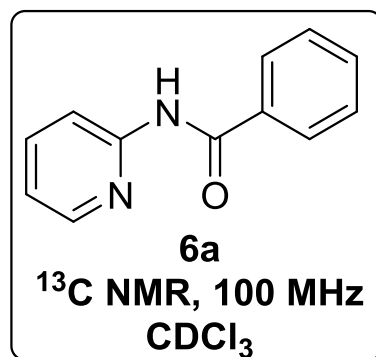


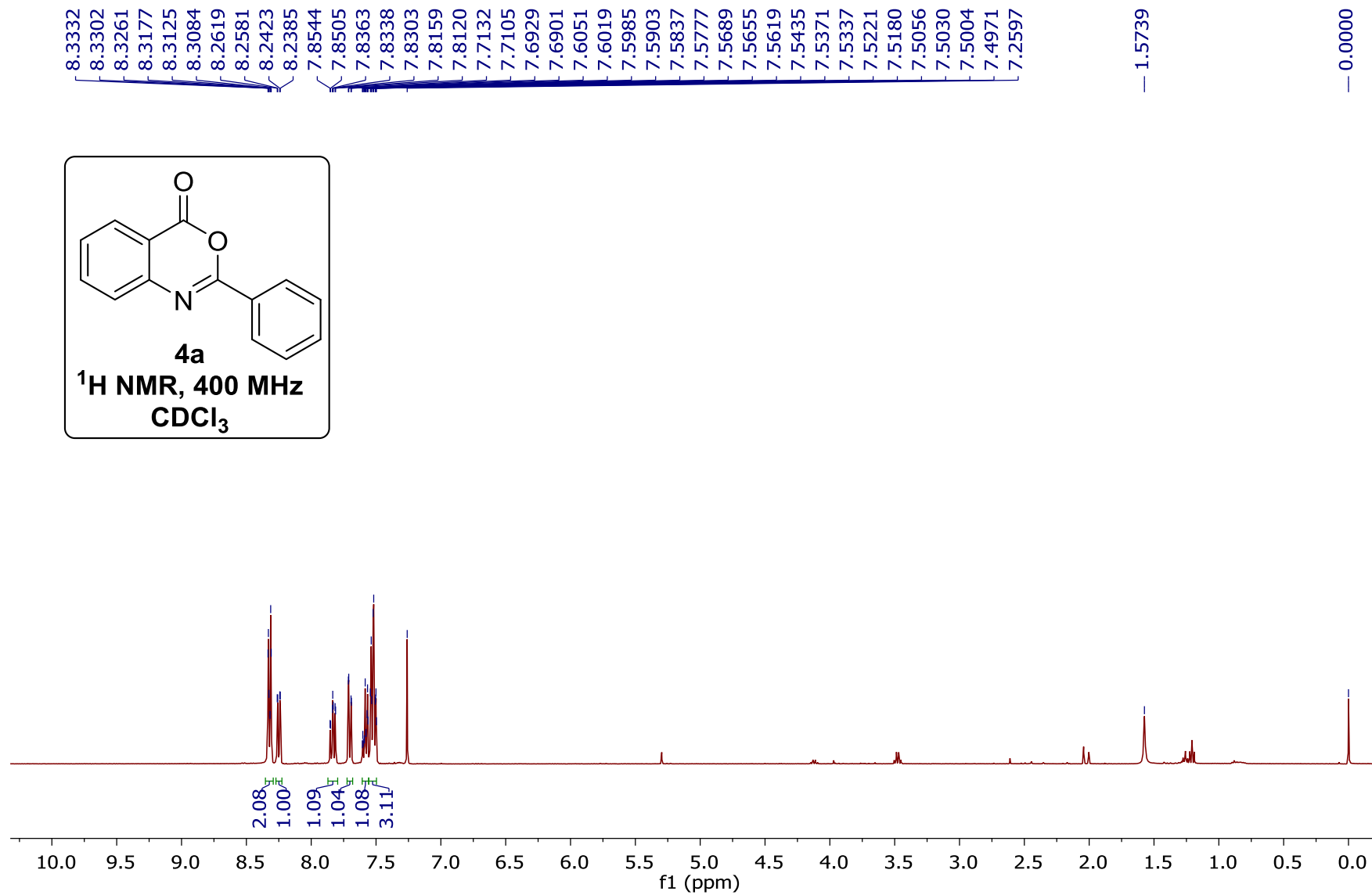


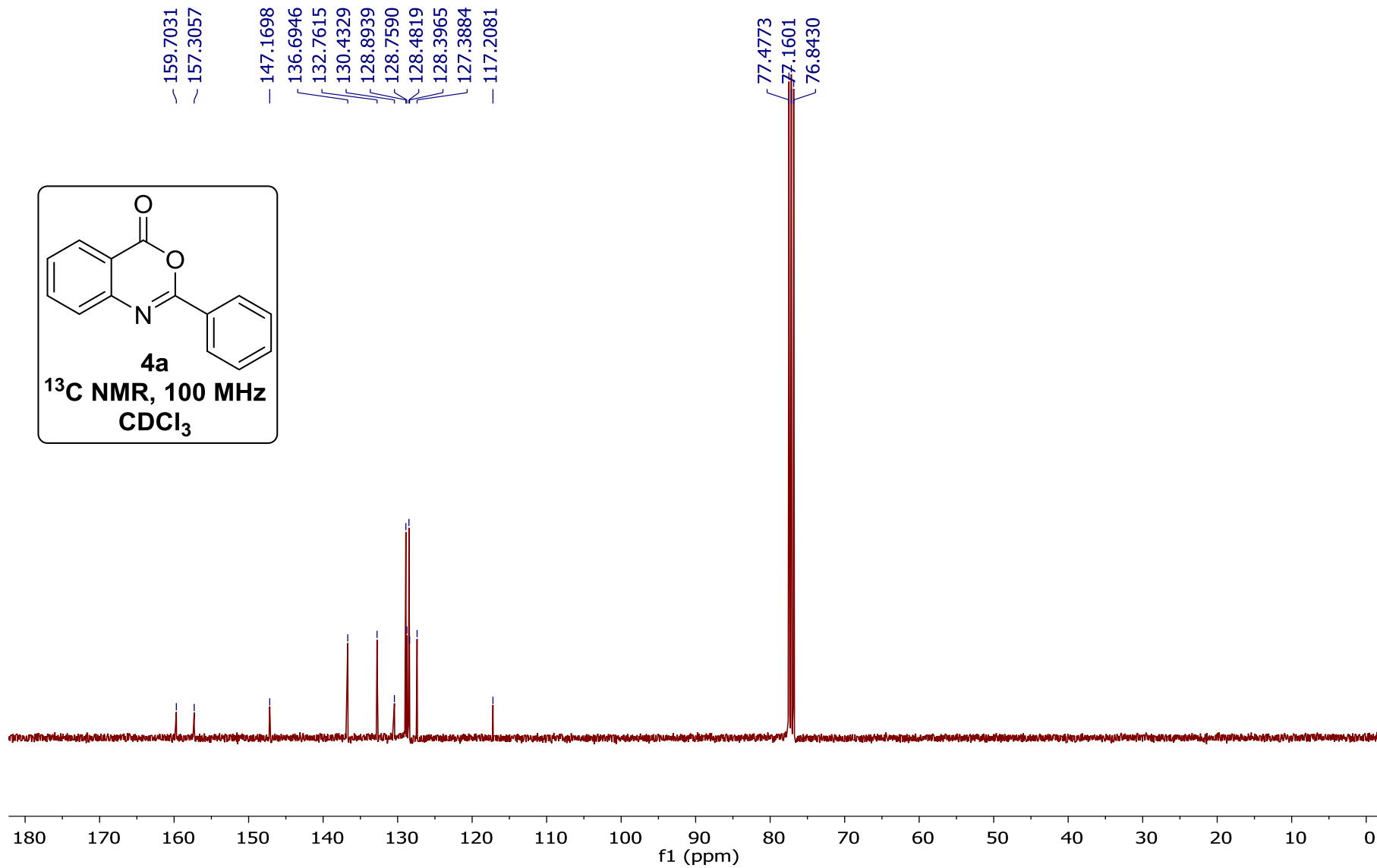
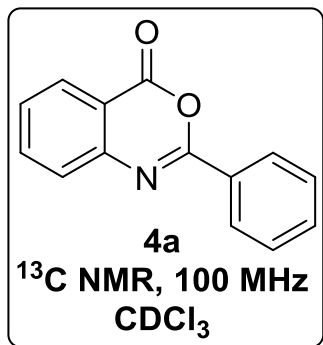
Sample Name	OP-add-56Me	Position	P1-B2	Instrument Name	Instrument 1	User Name	
Inj Vol	0.25	InjPosition		SampleType	Sample	IRM Calibration Status	Success
Data Filename	OP-add-56Me.d	ACQ Method	ChB60ChD40Dual AJS E	Comment		Acquired Time	1/2/2019 5:22:02 PM



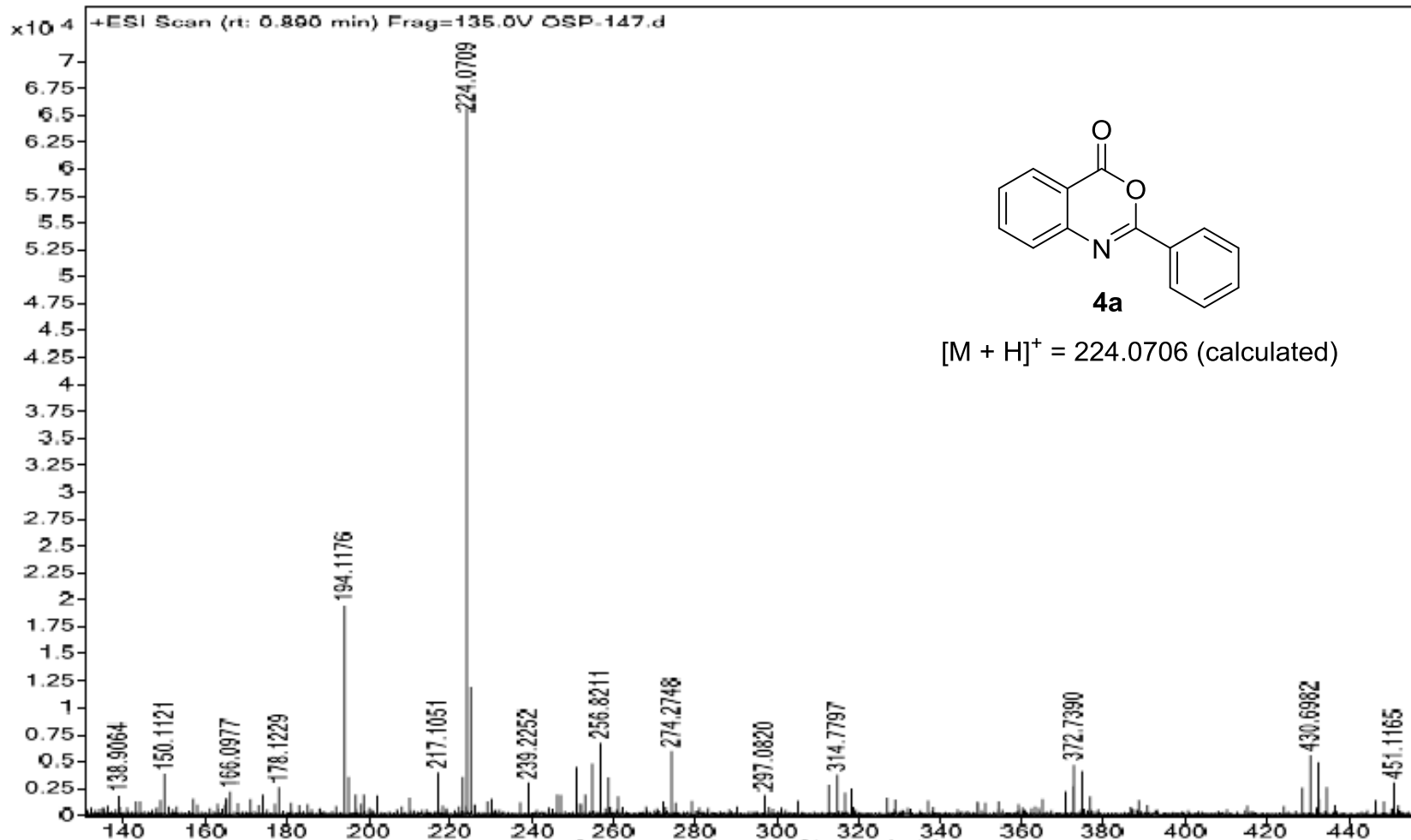


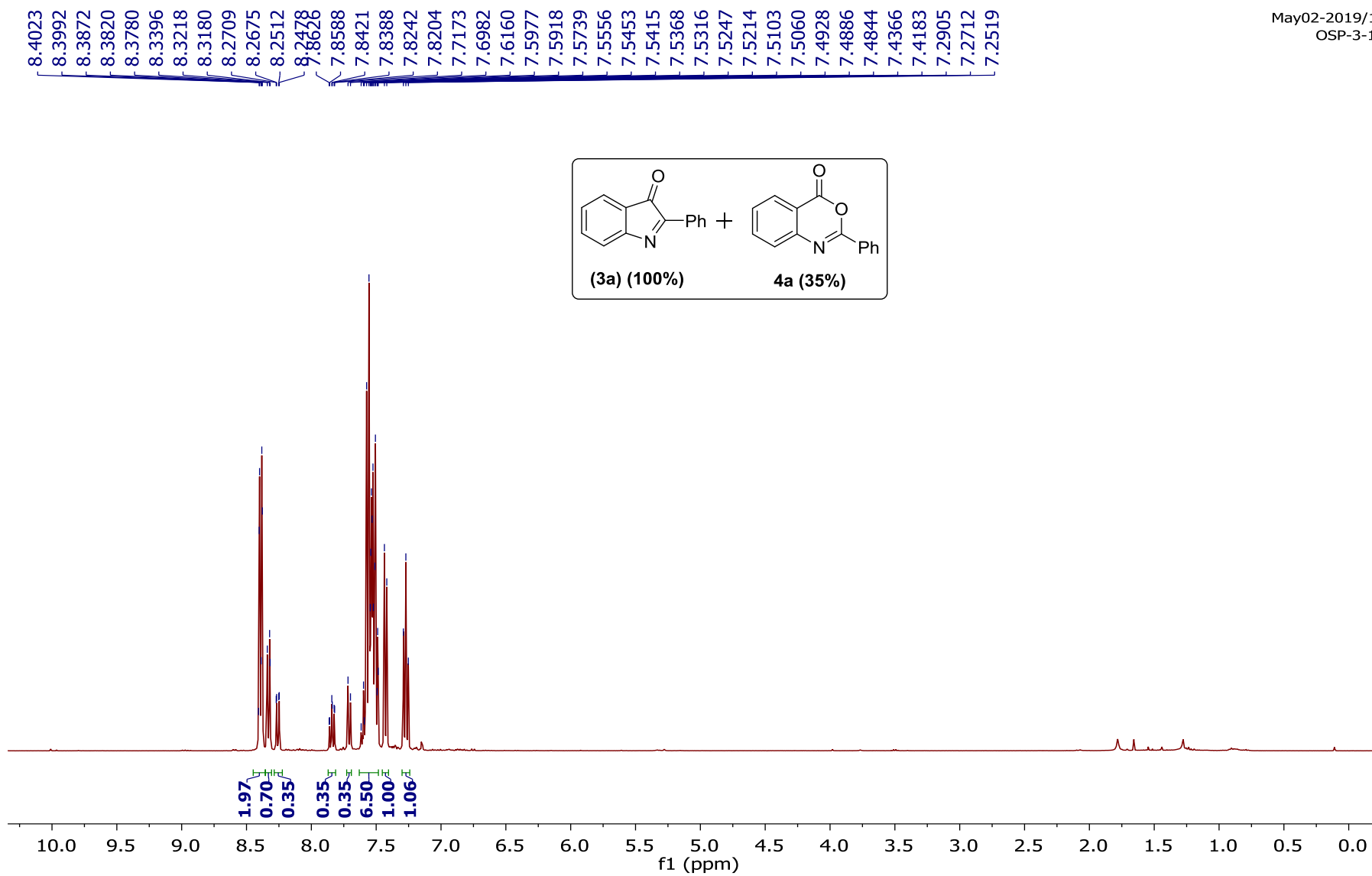


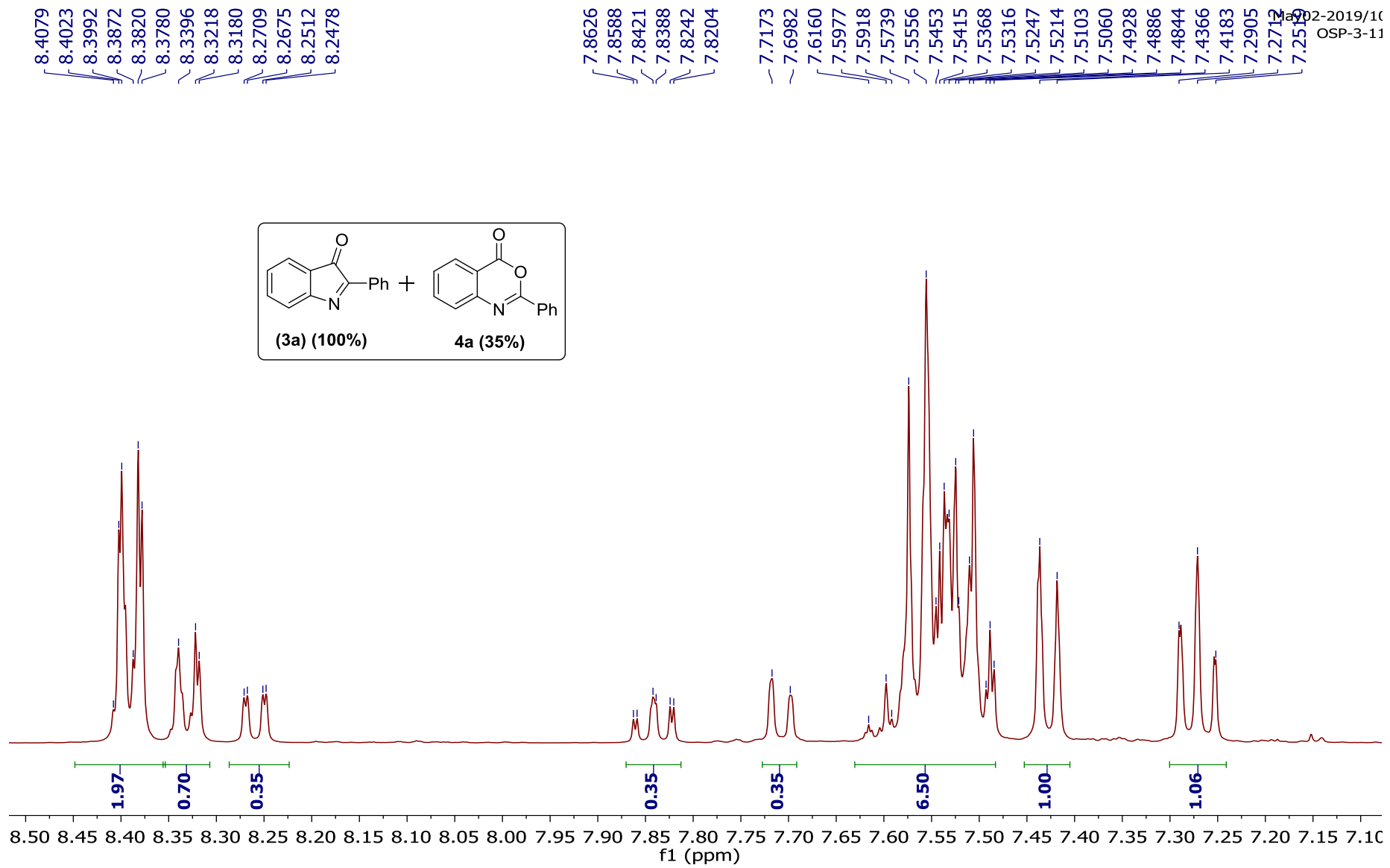




Sample Name	OSP-147	Position	P1-B7	Instrument Name	Instrument 1	User Name	
Inj Vol	0.25	InjPosition		SampleType	Sample	IRM Calibration Status	Success
Data Filename	OSP-147.d	ACQ Method	water_acn_grad_6min_	Comment		Acquired Time	4/3/2018 12:51:51 PM

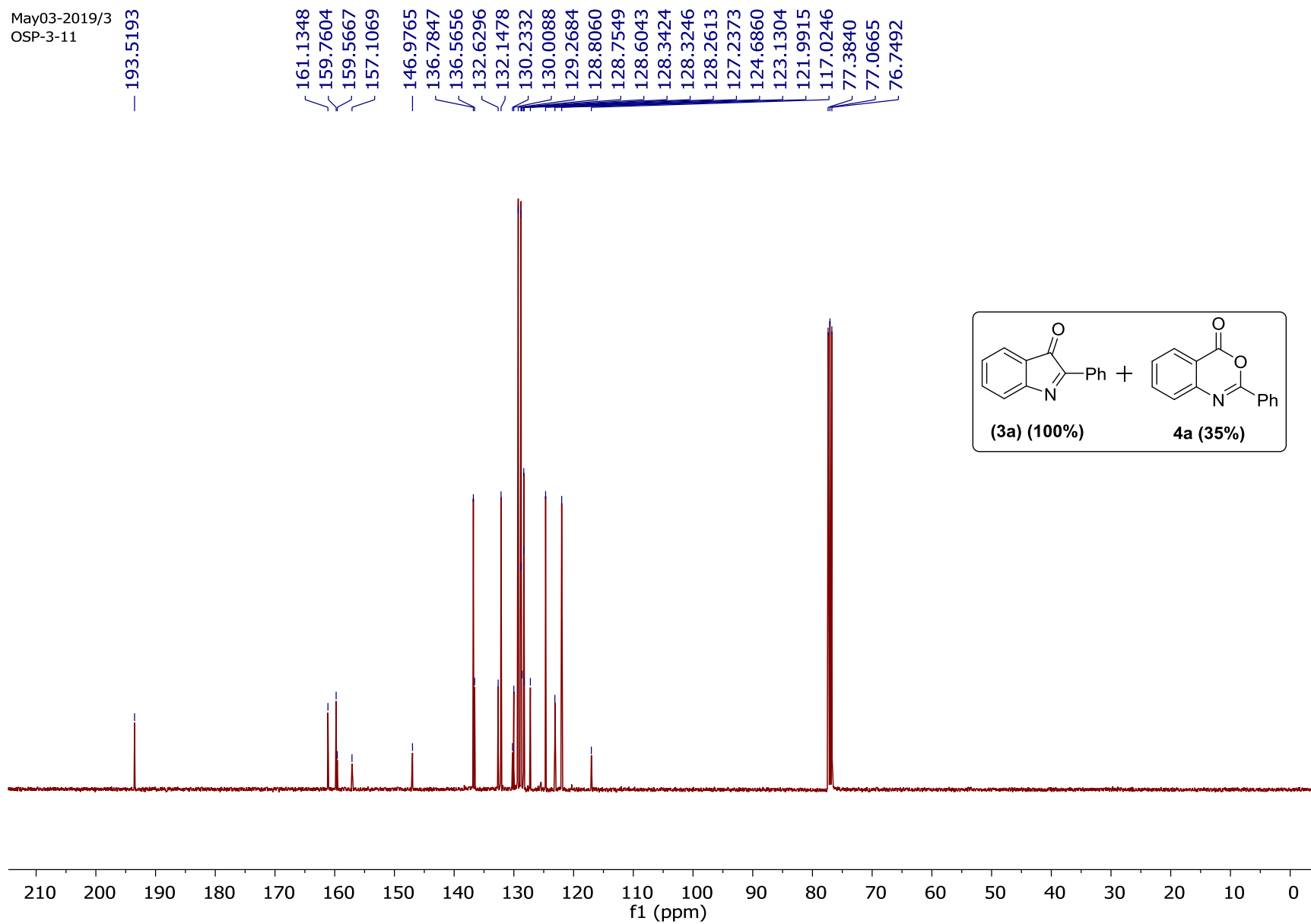




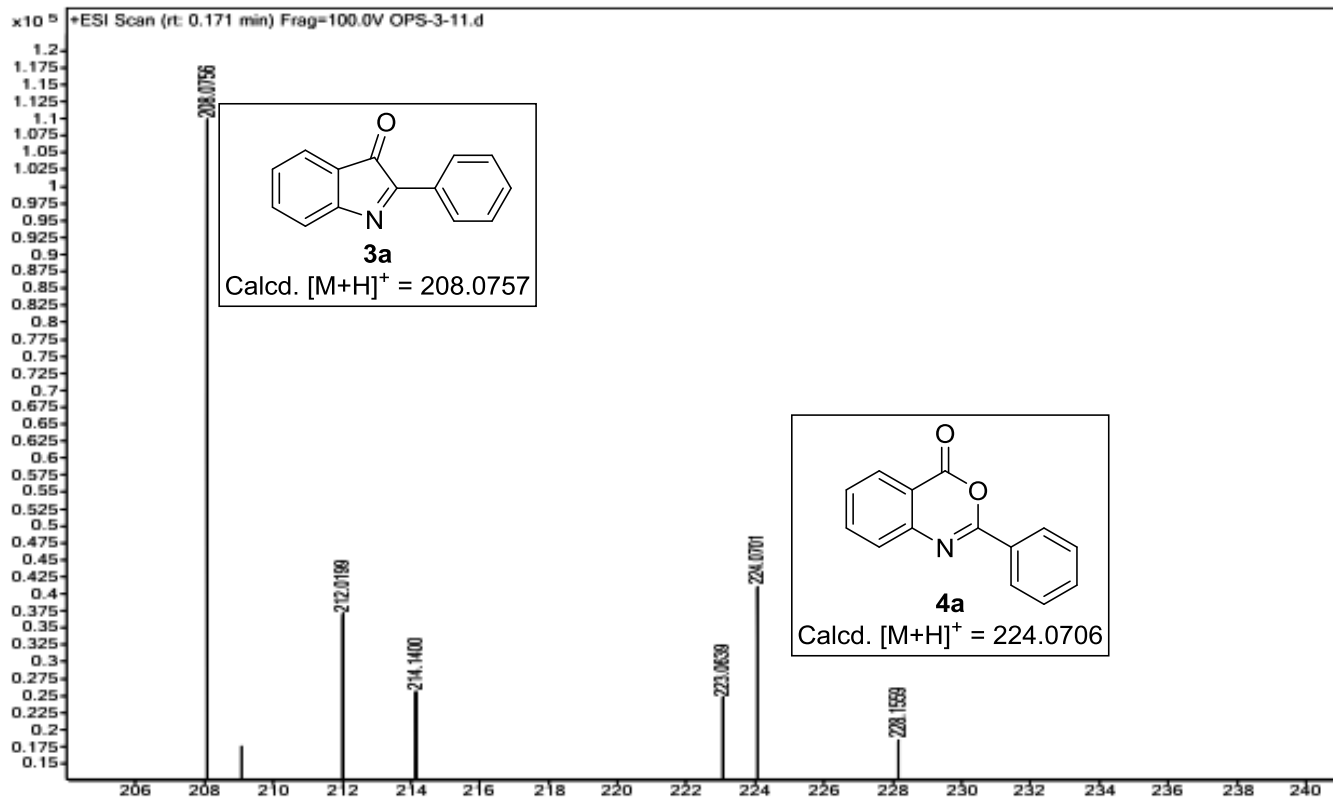


02-2019/10
OSP-3-11

May03-2019/3
OSP-3-11

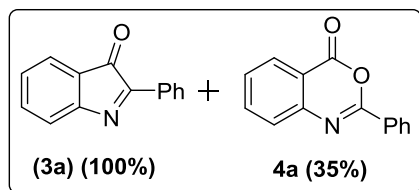


Sample Name	Position	Instrument Name	Instrument 1	User Name
OPS-3-11	P1-F1			
Inj Vol	InjPosition	SampleType	Sample	IRM Calibration Status
0.25				Success
Data Filename	ACQ Method	Comment	Acquired Time	
OPS-3-11.d	ChB60ChD40_Isocratic			5/4/2019 11:31:16 AM

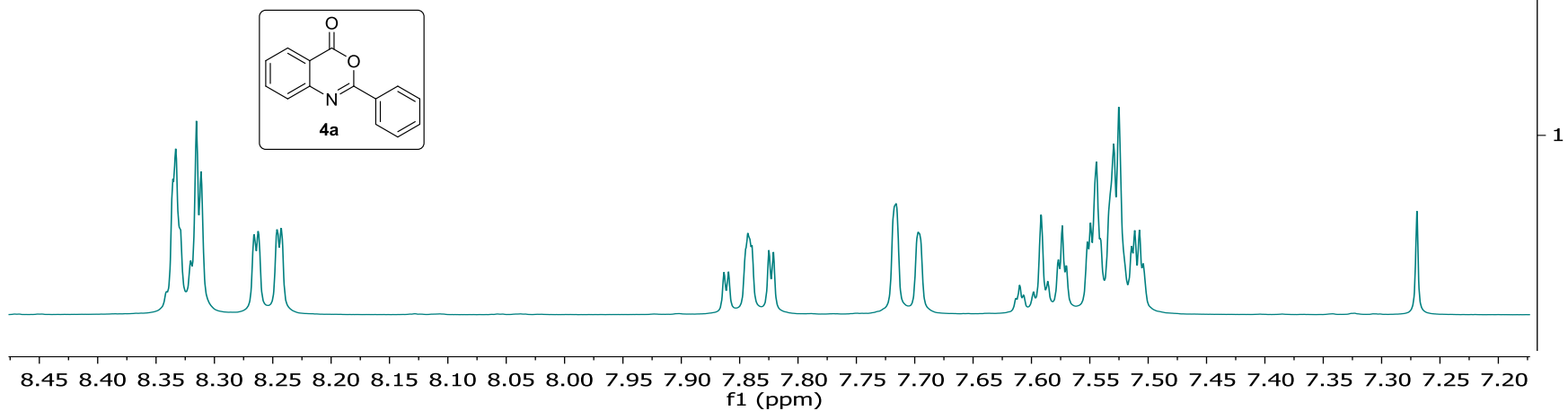


ESI-HRMS analysis of mixture of 3a and 4a

May02-2019/10
OSP-3-11

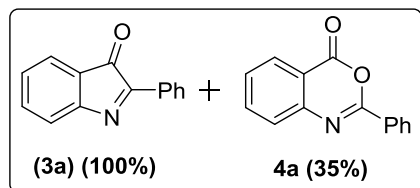


Dec31-2018/1
OSP-2-109

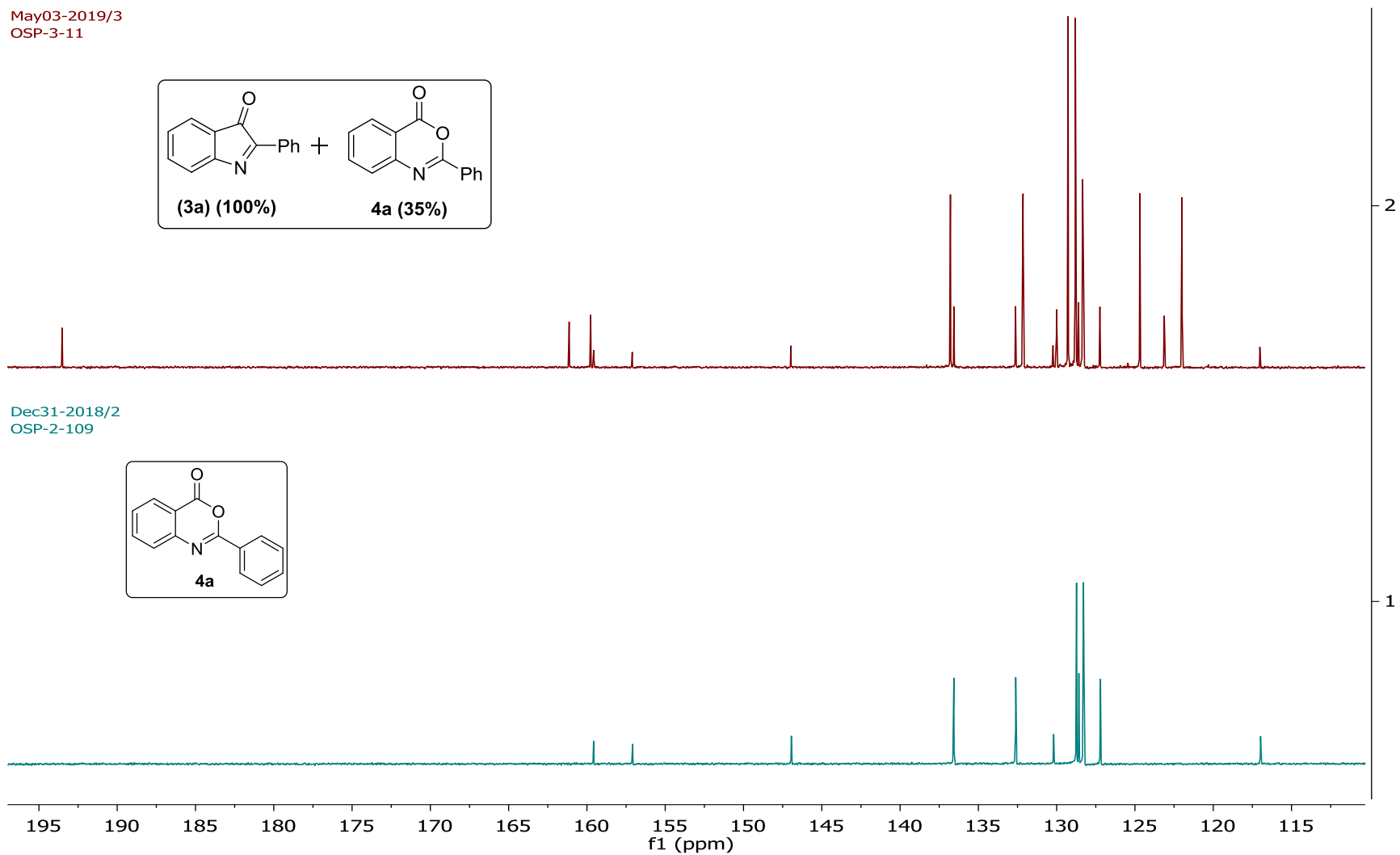
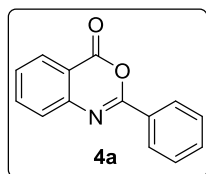


Comparative ¹H NMR of a mixture of 3a and 4a with pure intermediate 4a

May03-2019/3
OSP-3-11



Dec31-2018/2
OSP-2-109



Comparative ^{13}C NMR of a mixture of 3a and 4a with pure intermediate 4a

3. Unambiguous molecular structure determination of **3s**

