New Journal of Chemistry

Supporting Information

C2/C3 Alkynylation of L-Ascorbic Acid by Sonogashira Coupling and Efficient Access to Some Potent and Highly Selective Novel Anticancer Agents

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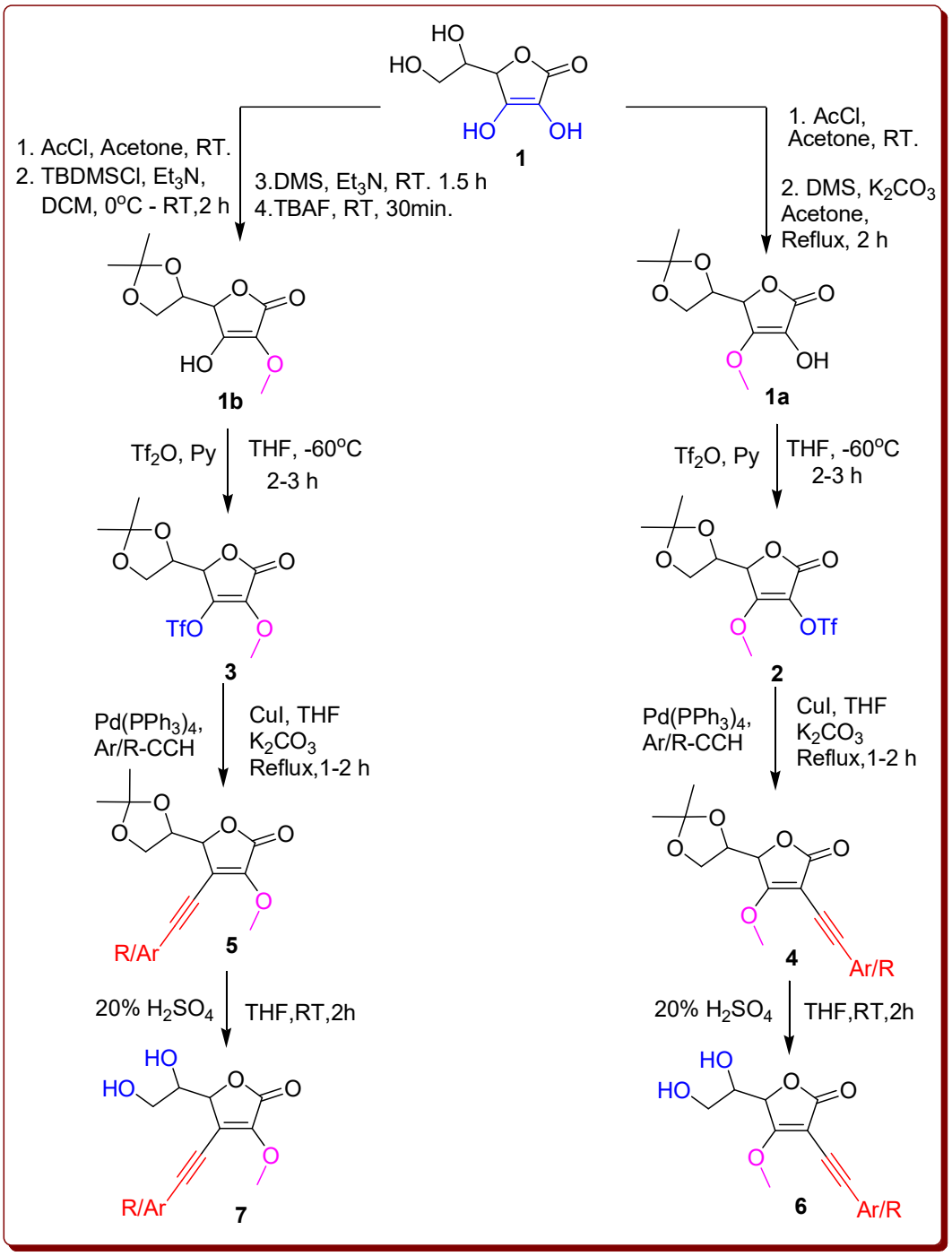
A. Scheme 1.



Scheme 1.

1awas synthesized following a published procedure.[1]

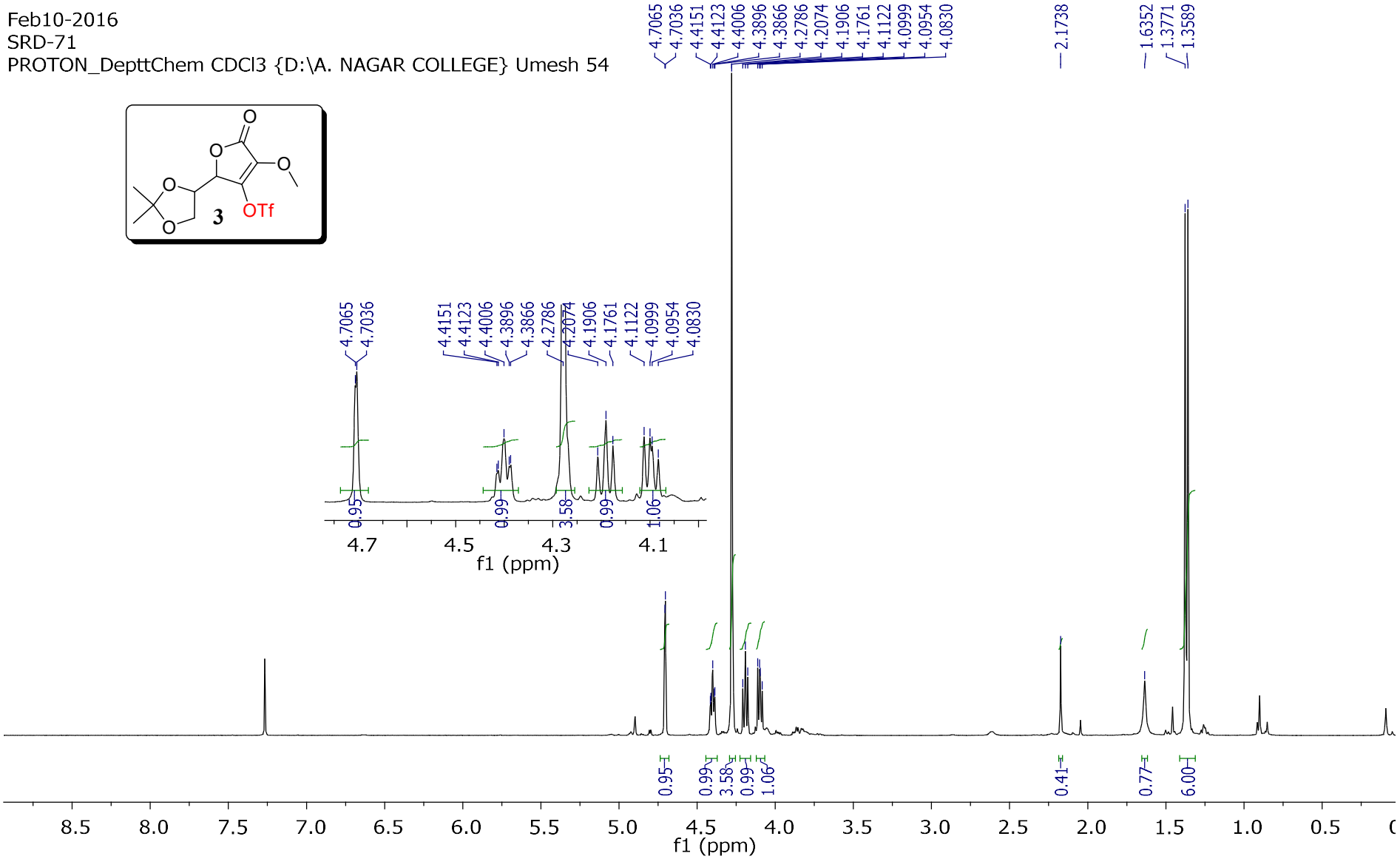
1bwas synthesized following a published procedure.[2]

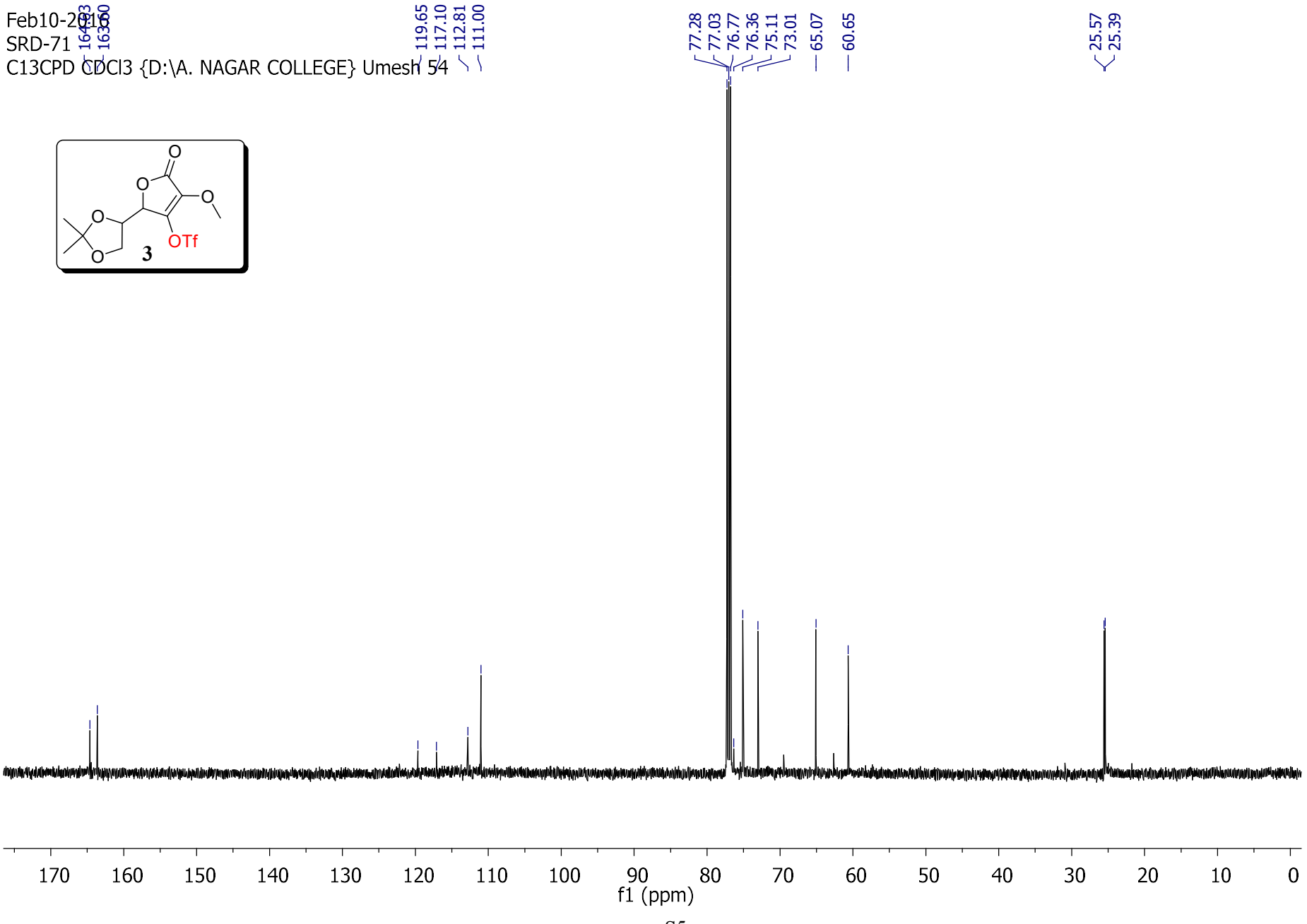
2was synthesized following a published procedure.[3]

B. References

1. M. G. Kulkarni, S. R. Thopate, *Tetrahedron*, **1996**, *52*, 1293.
2. S. R. Thopate, R. A. Dengale, M. G. Kulkarni, *Synlett***2013**, *24*, 1555
3. S. R. Kote, G. R. Dhage, S. R. Thopate R. Mishra, A. A. Khan, *Synthesis*, **2015,***47*, 2603.

C. Copies of ^{1}H and ^{13}C NMR spectra

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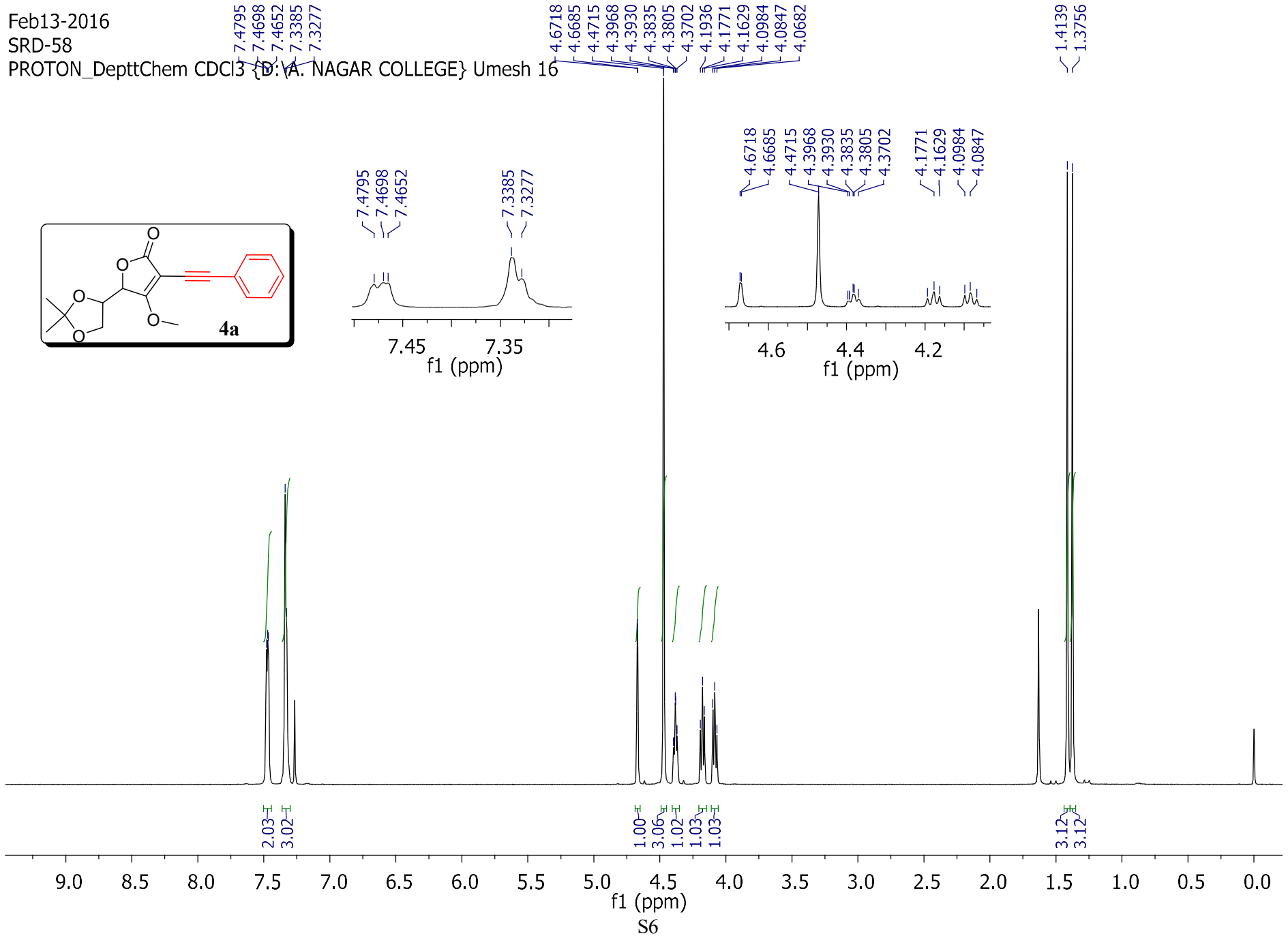
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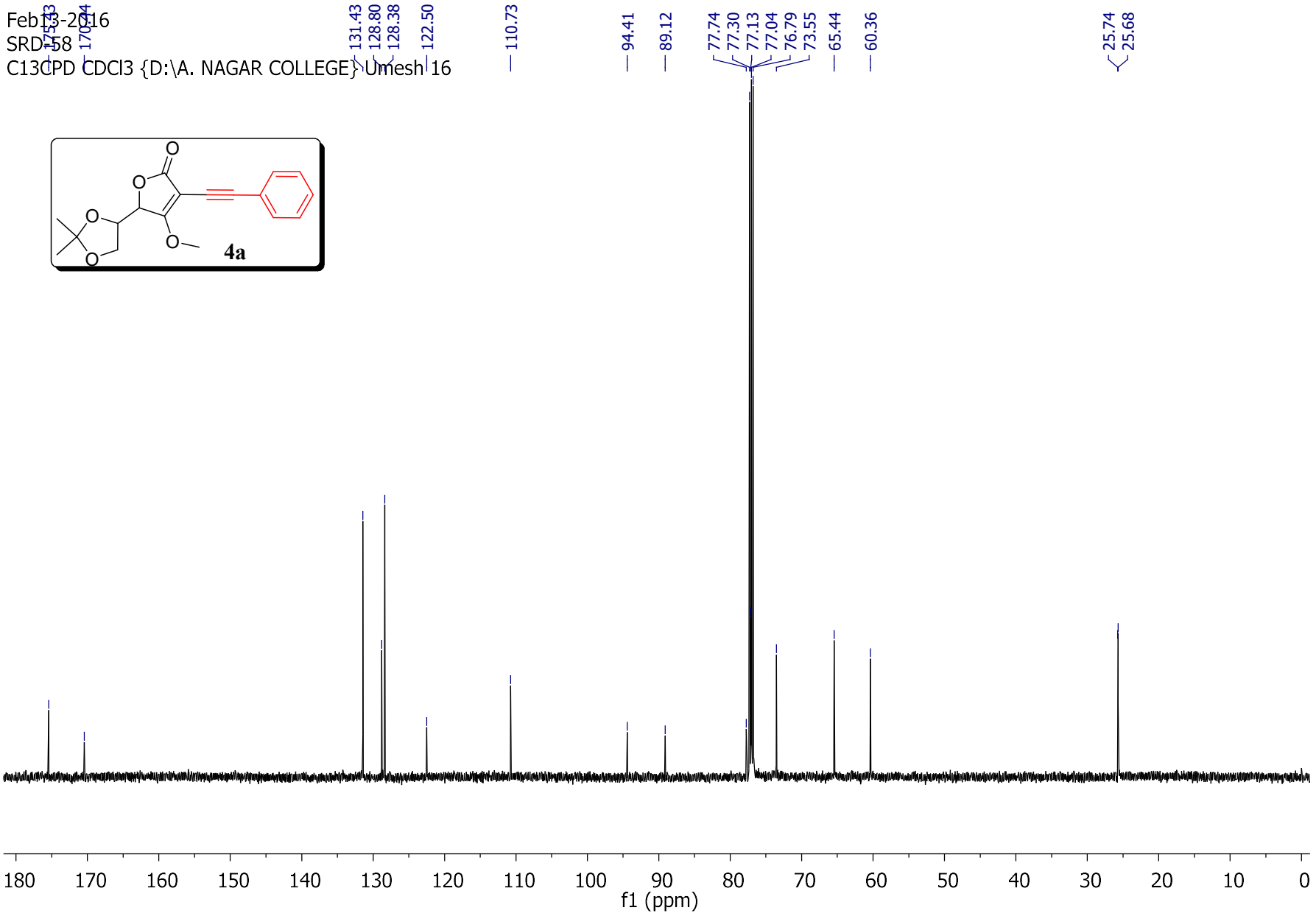
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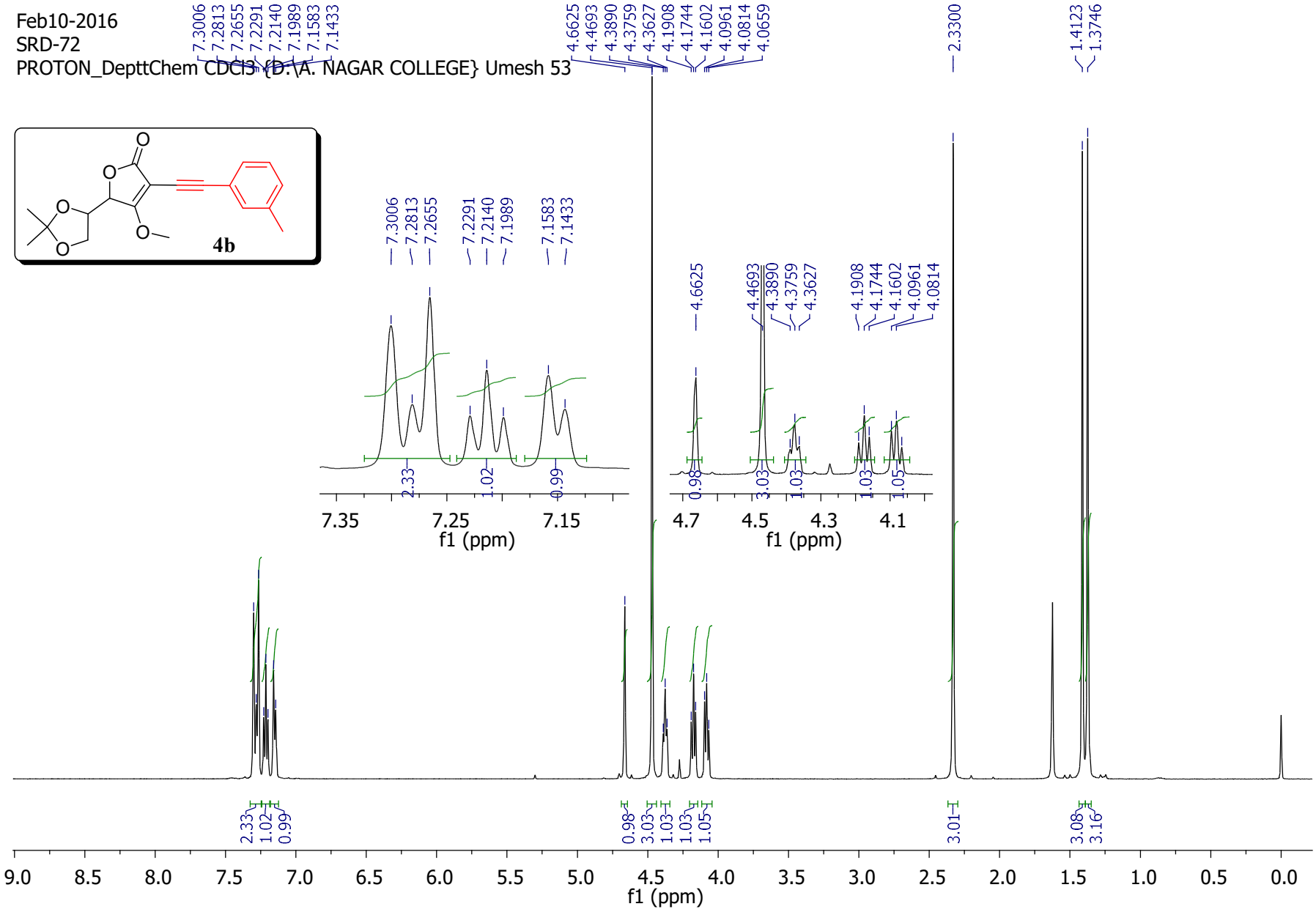
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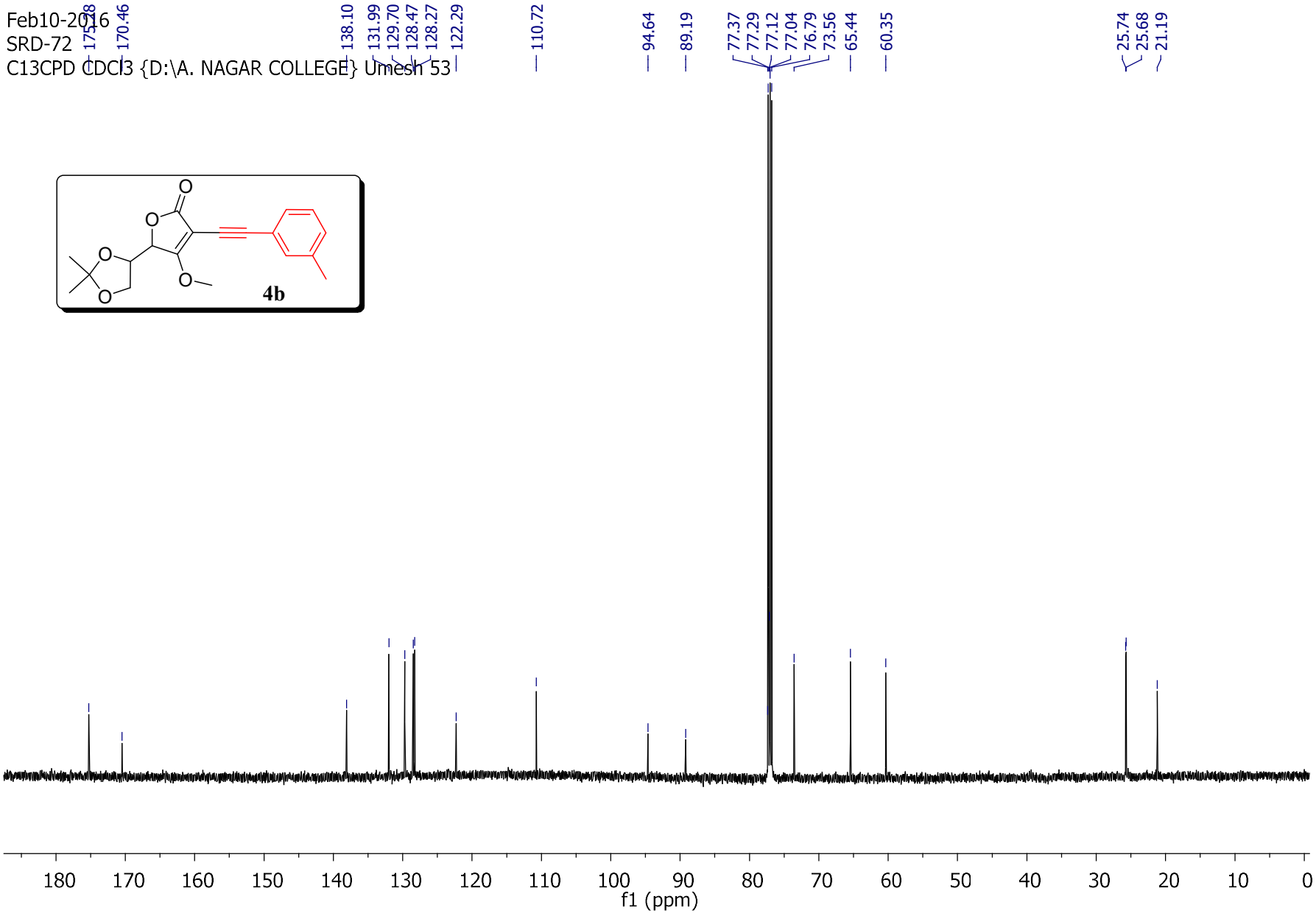
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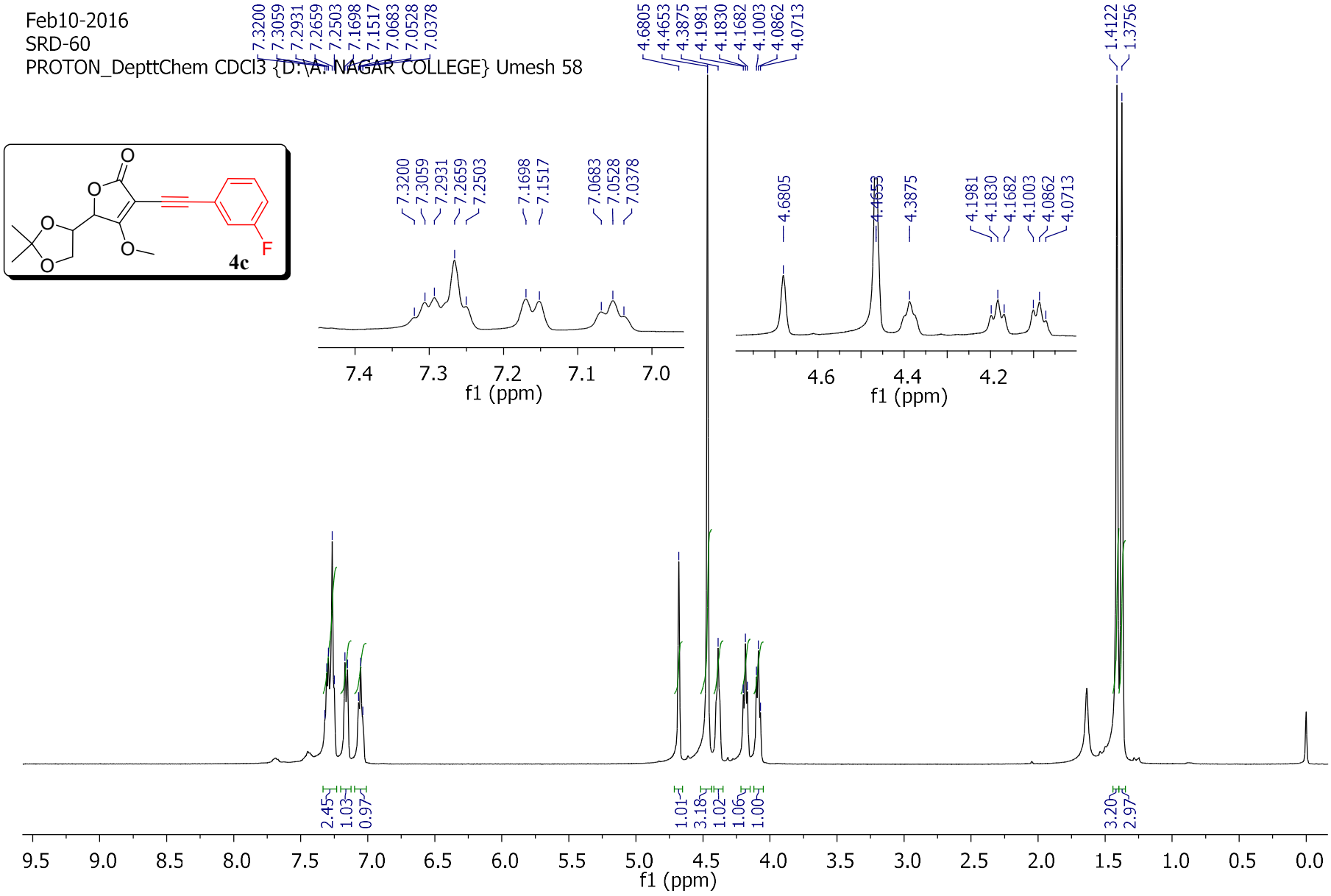
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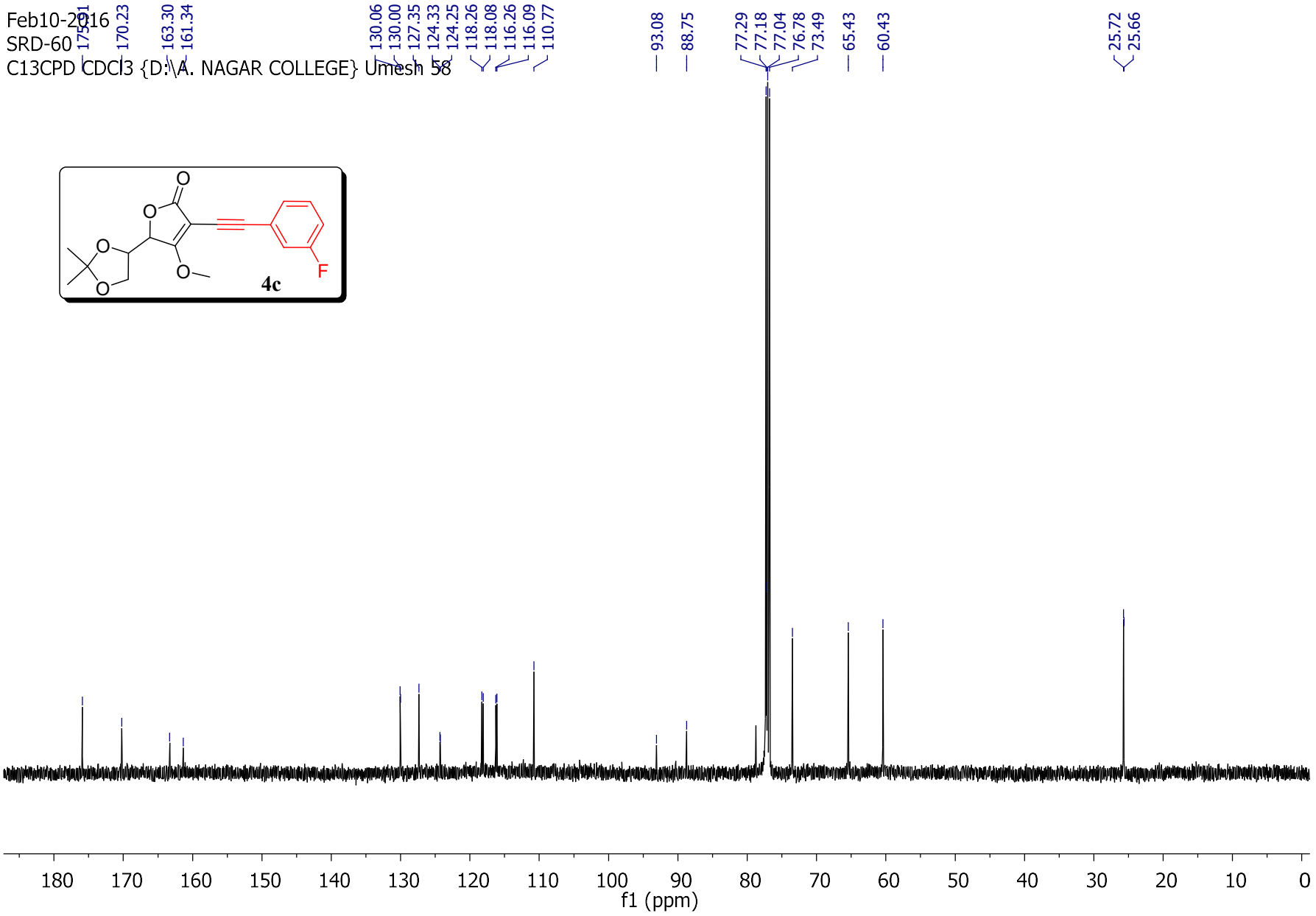
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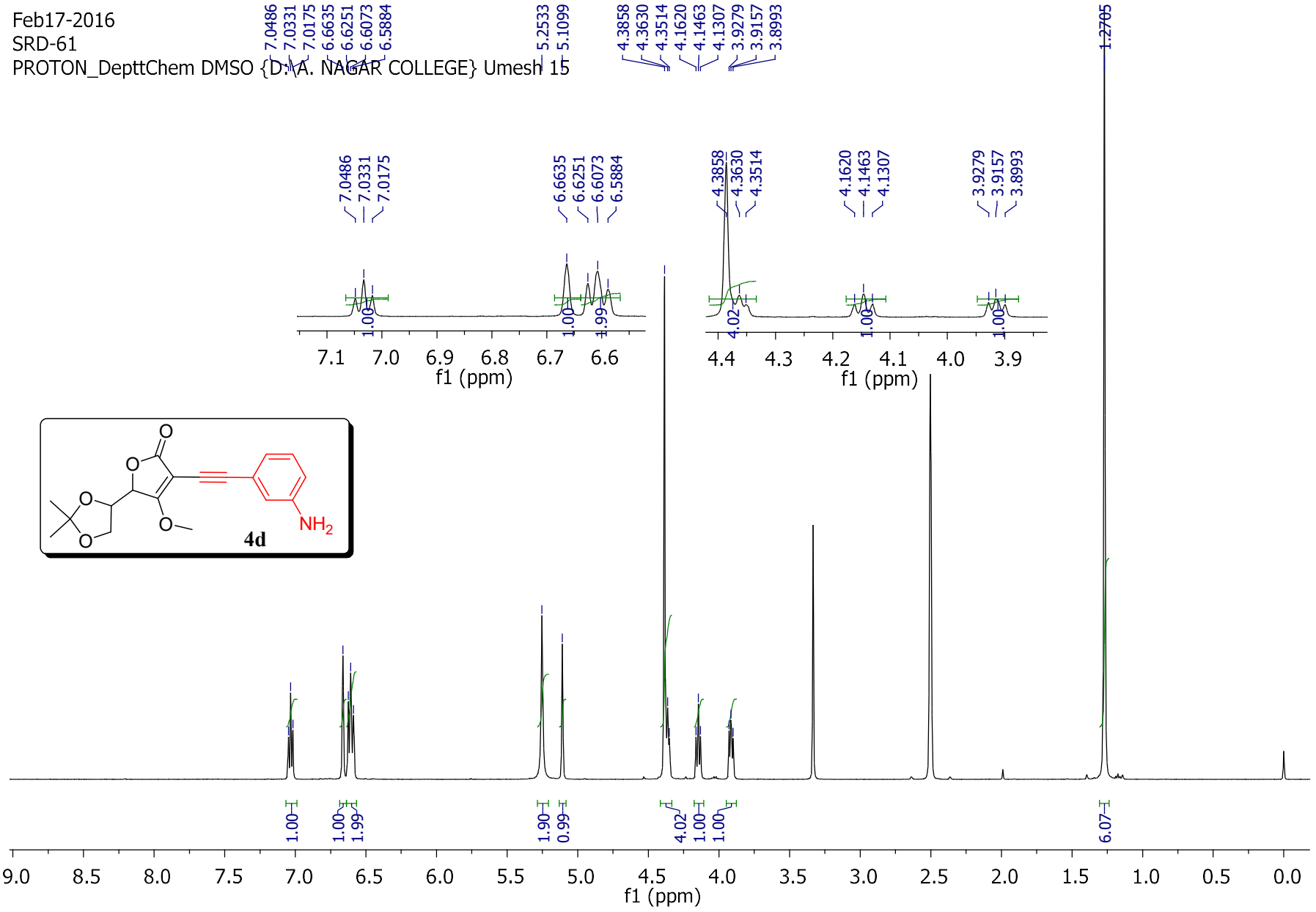
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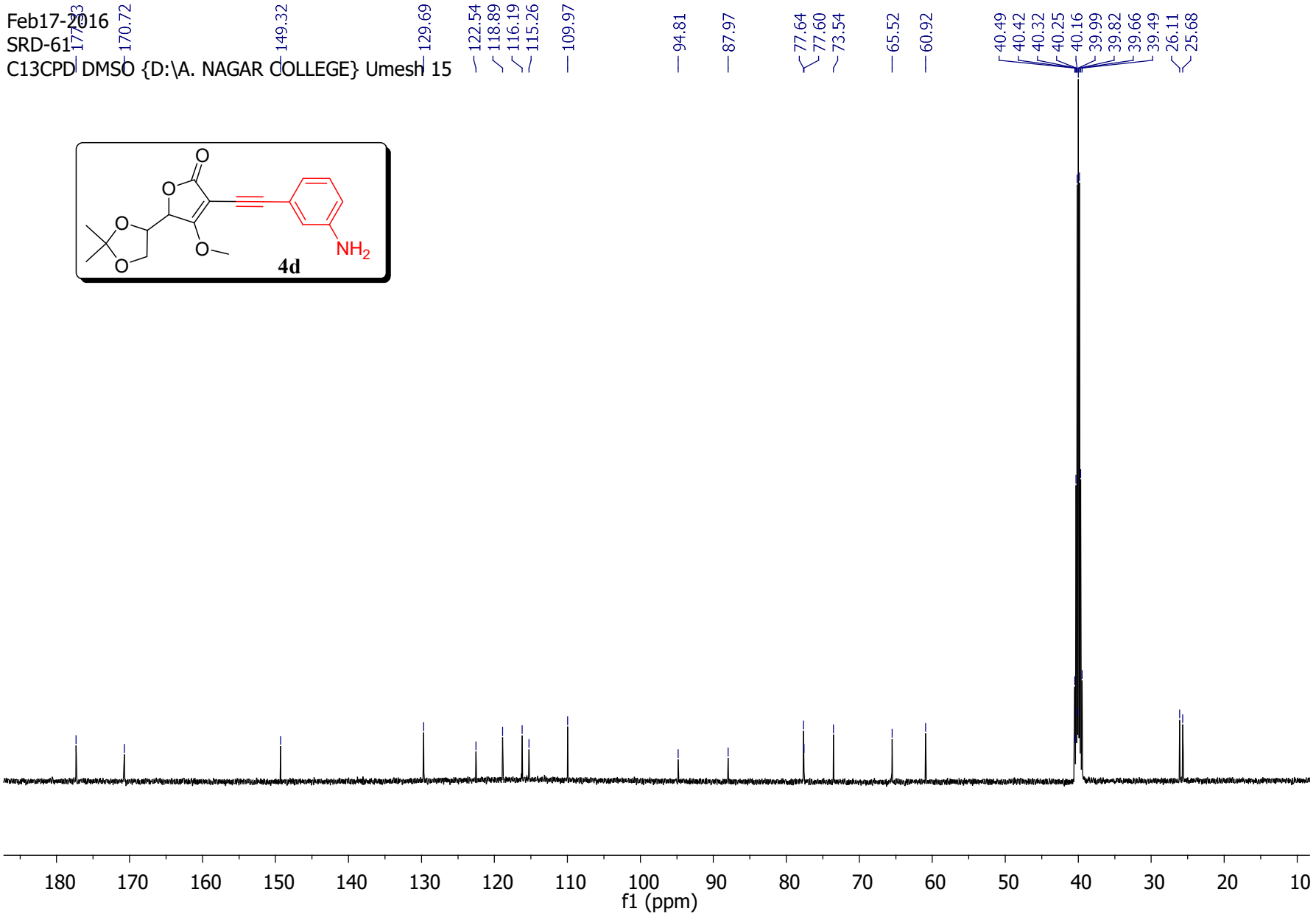
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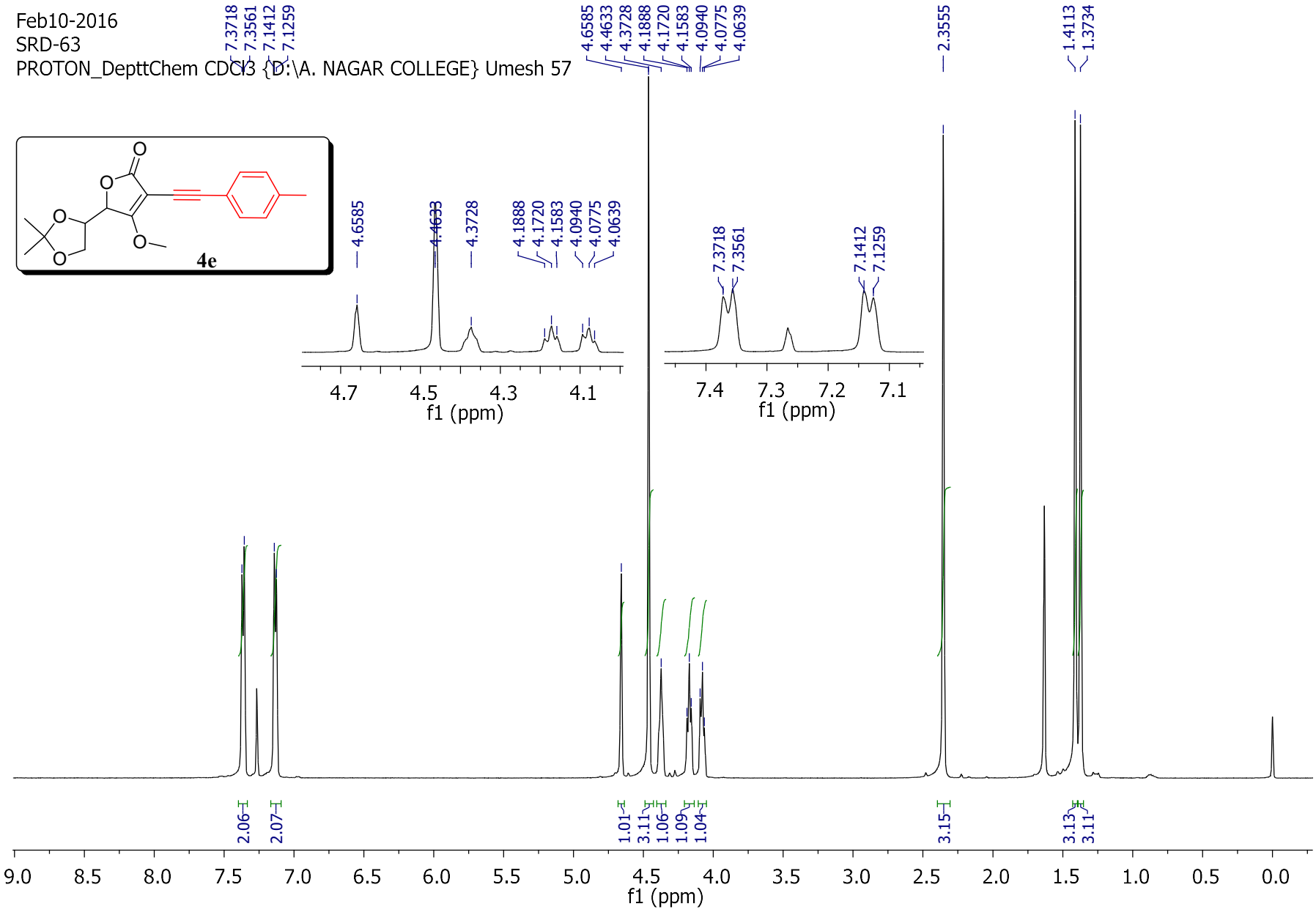
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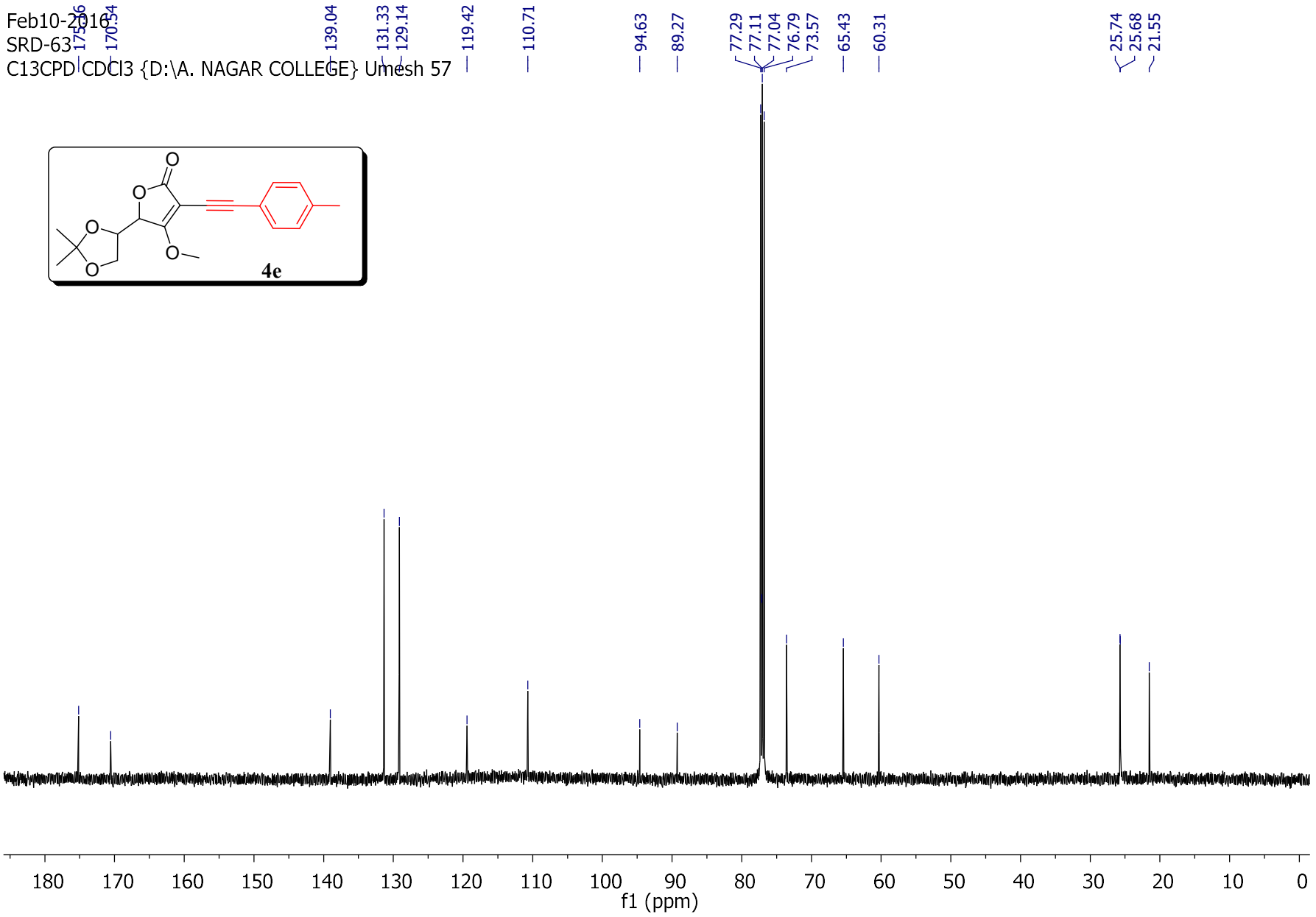
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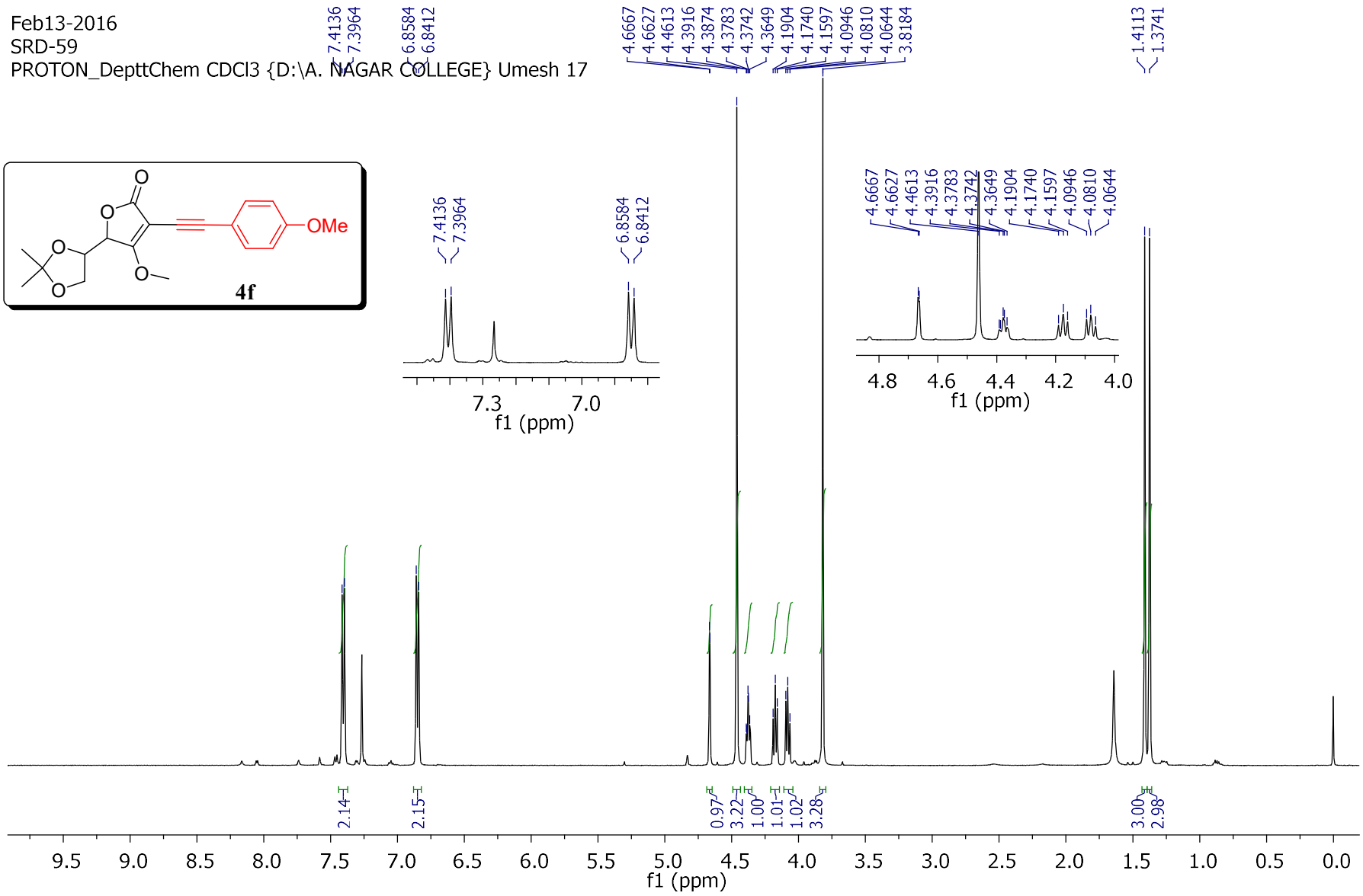
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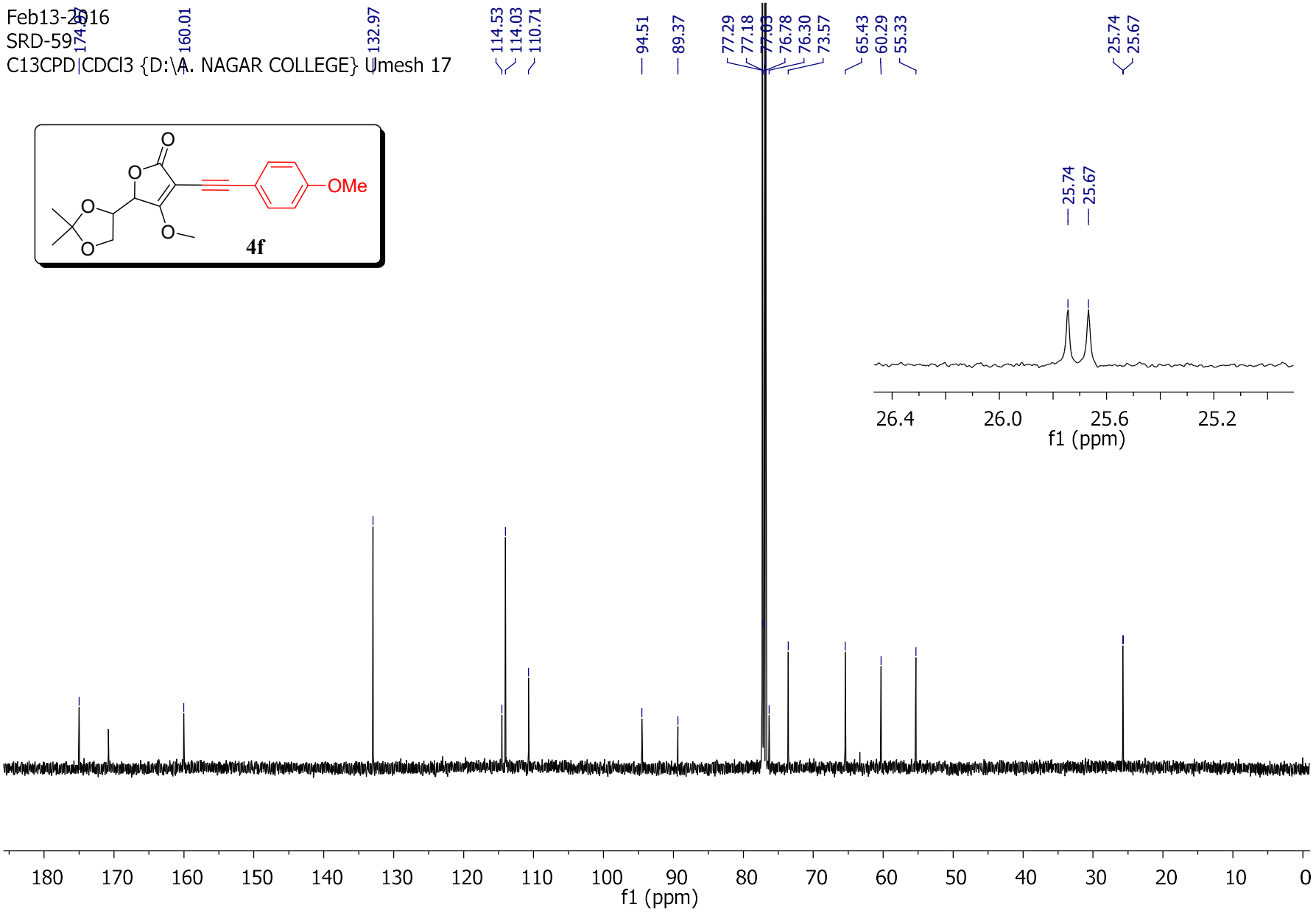
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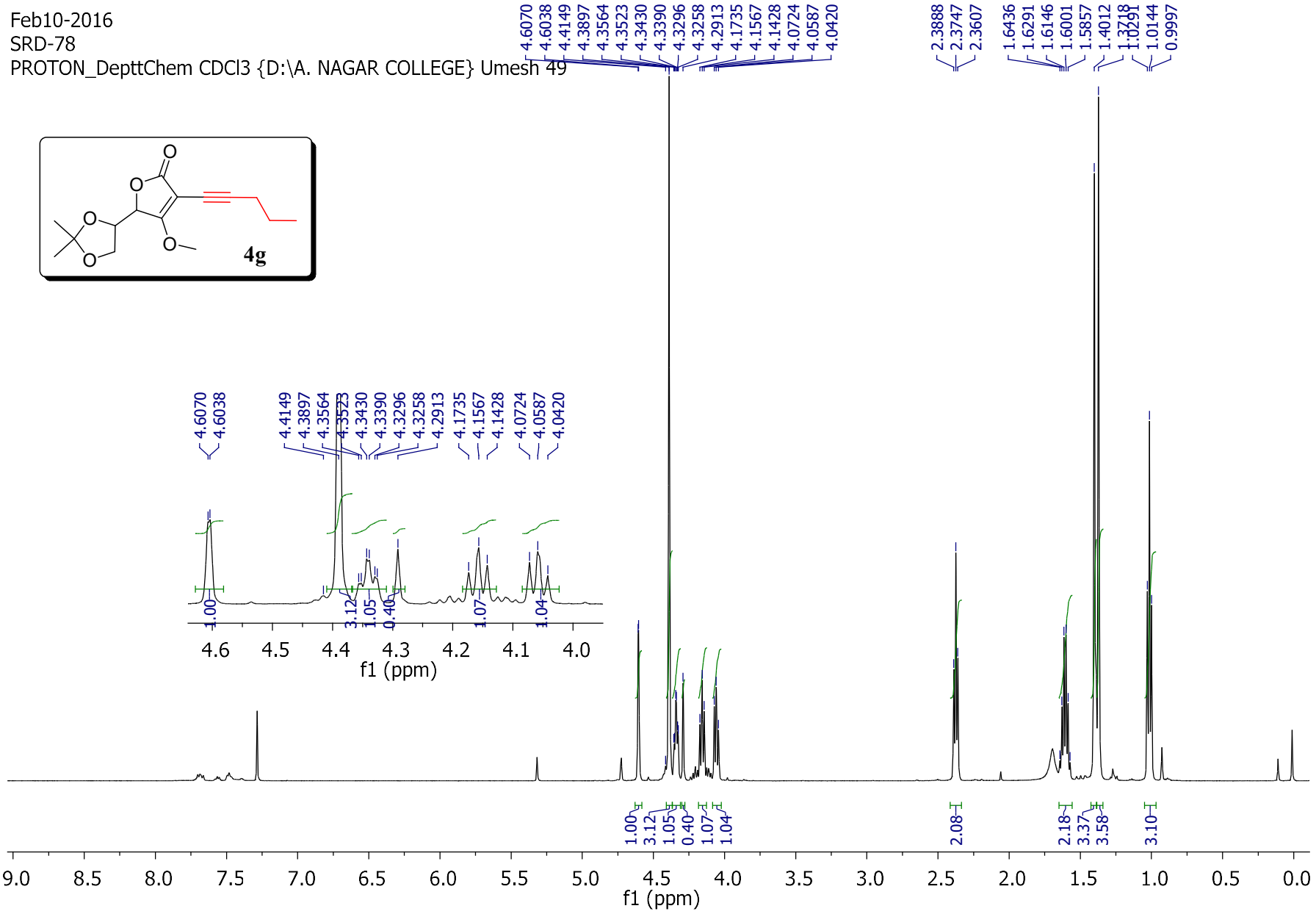
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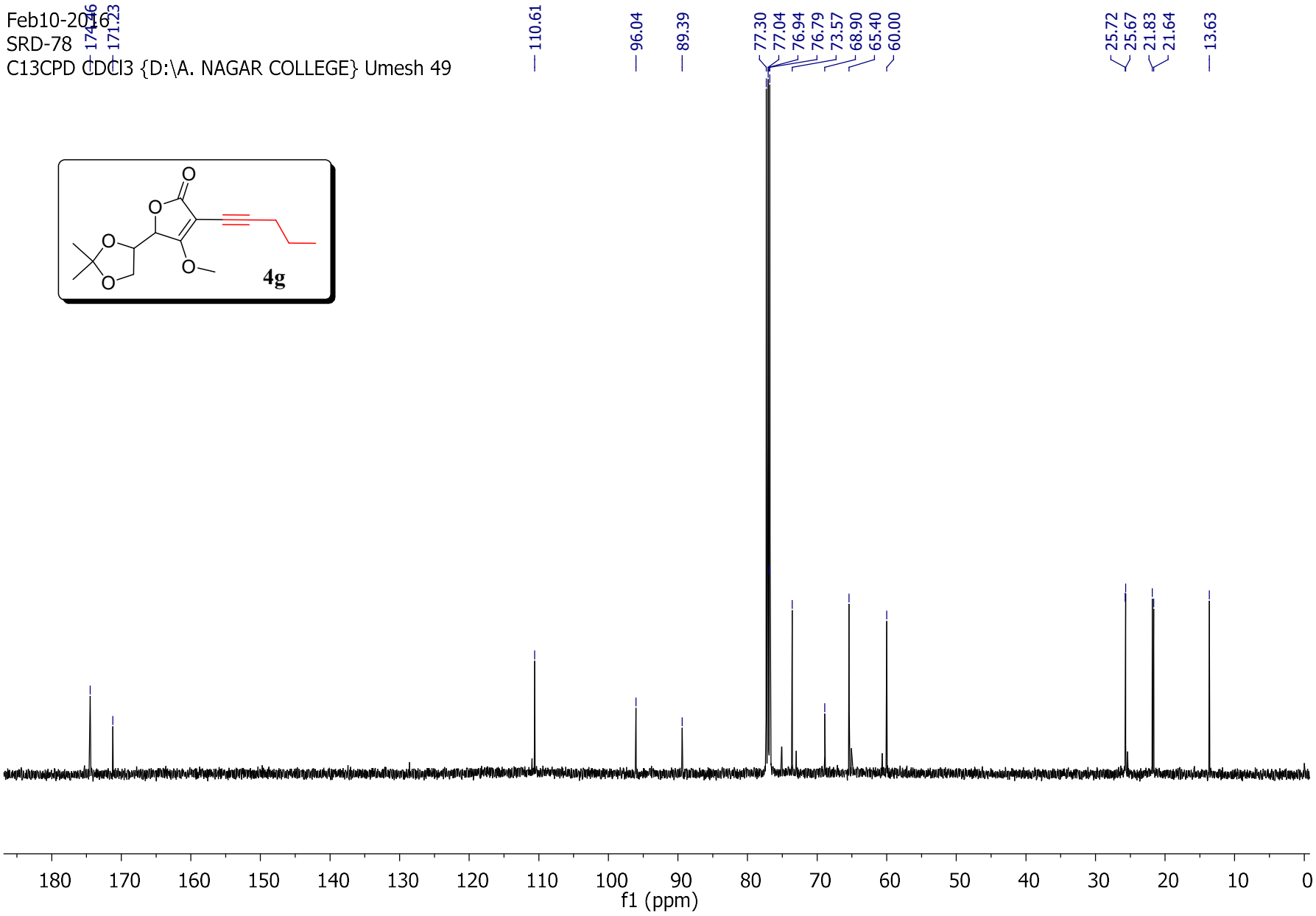
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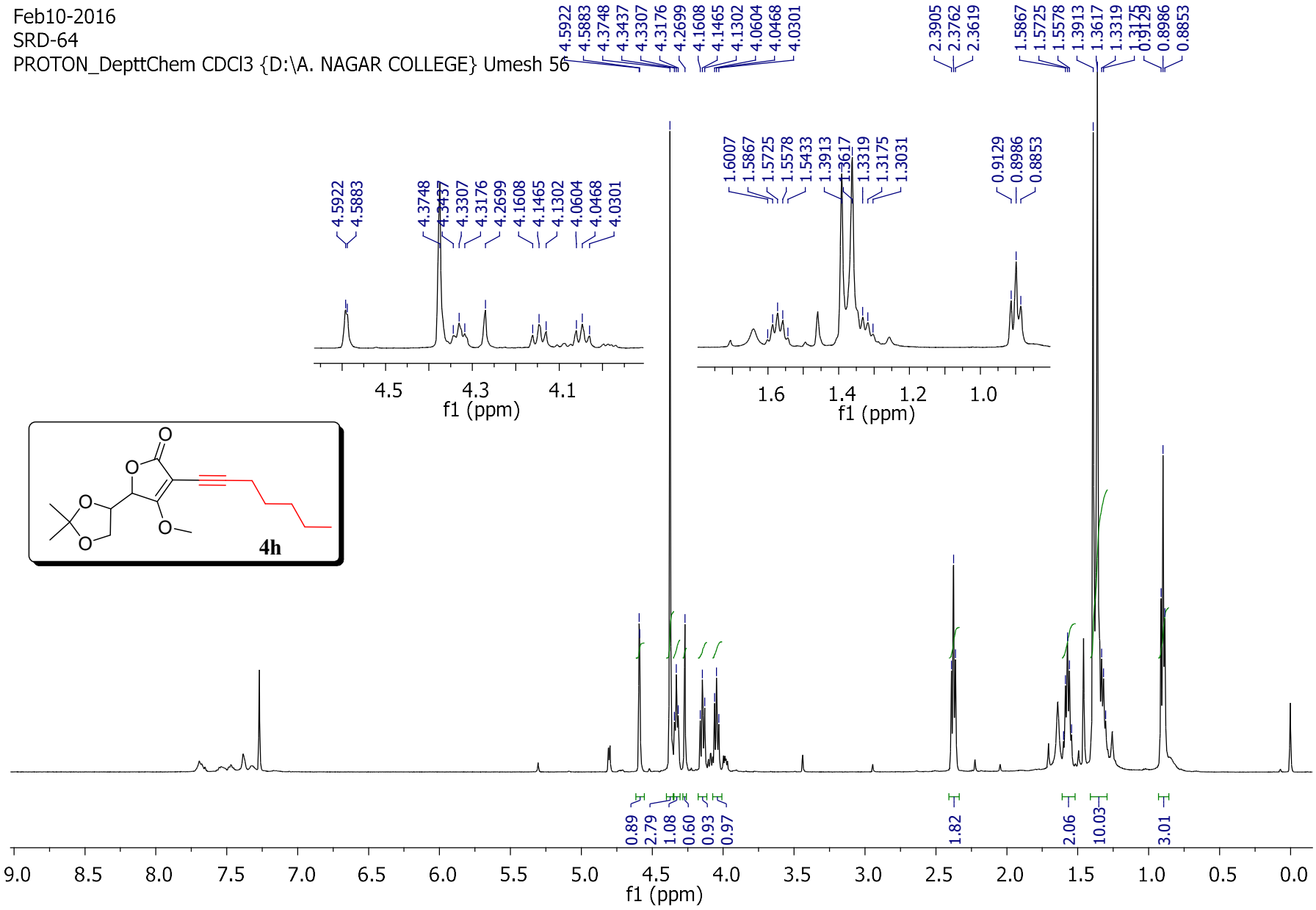
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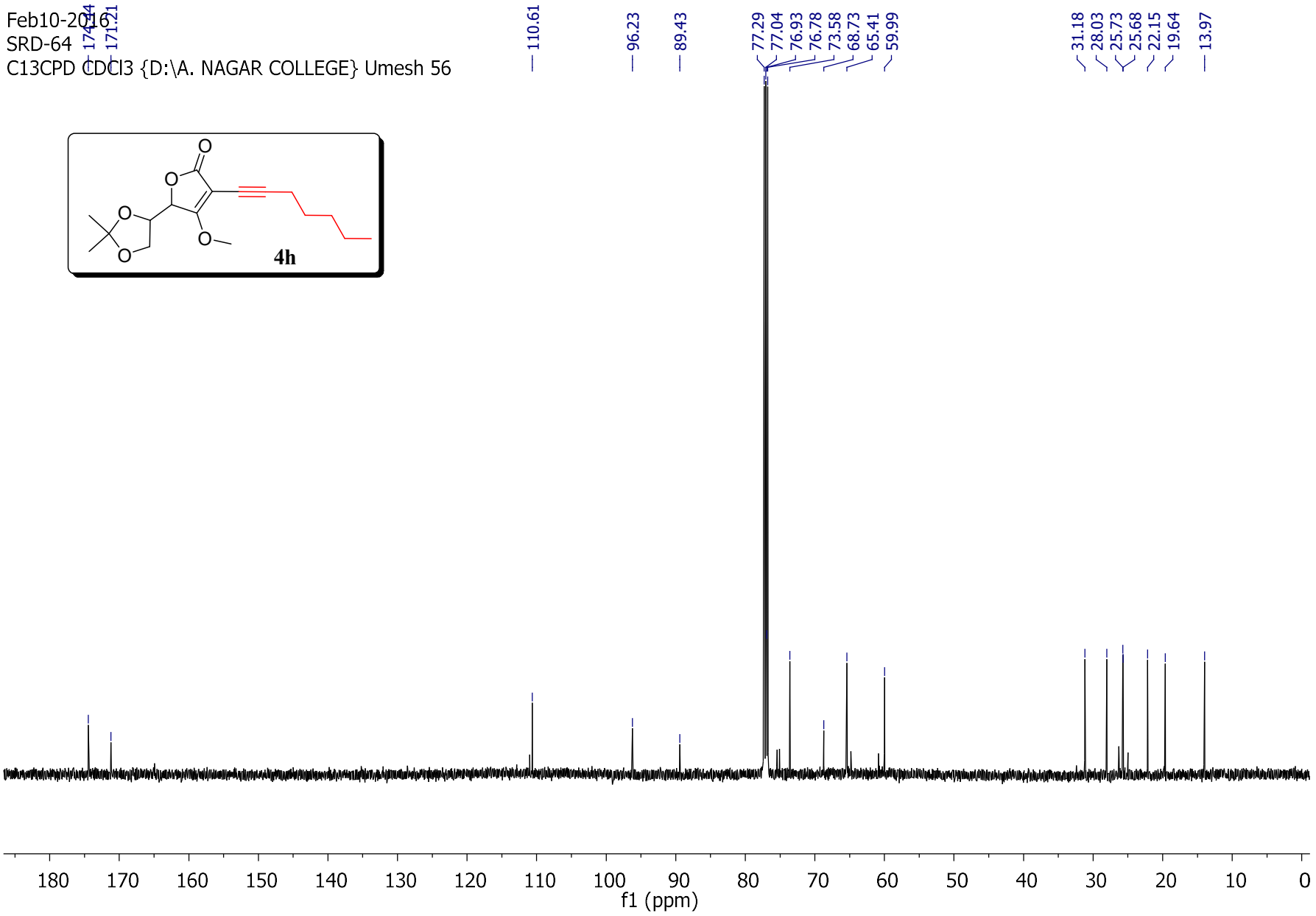
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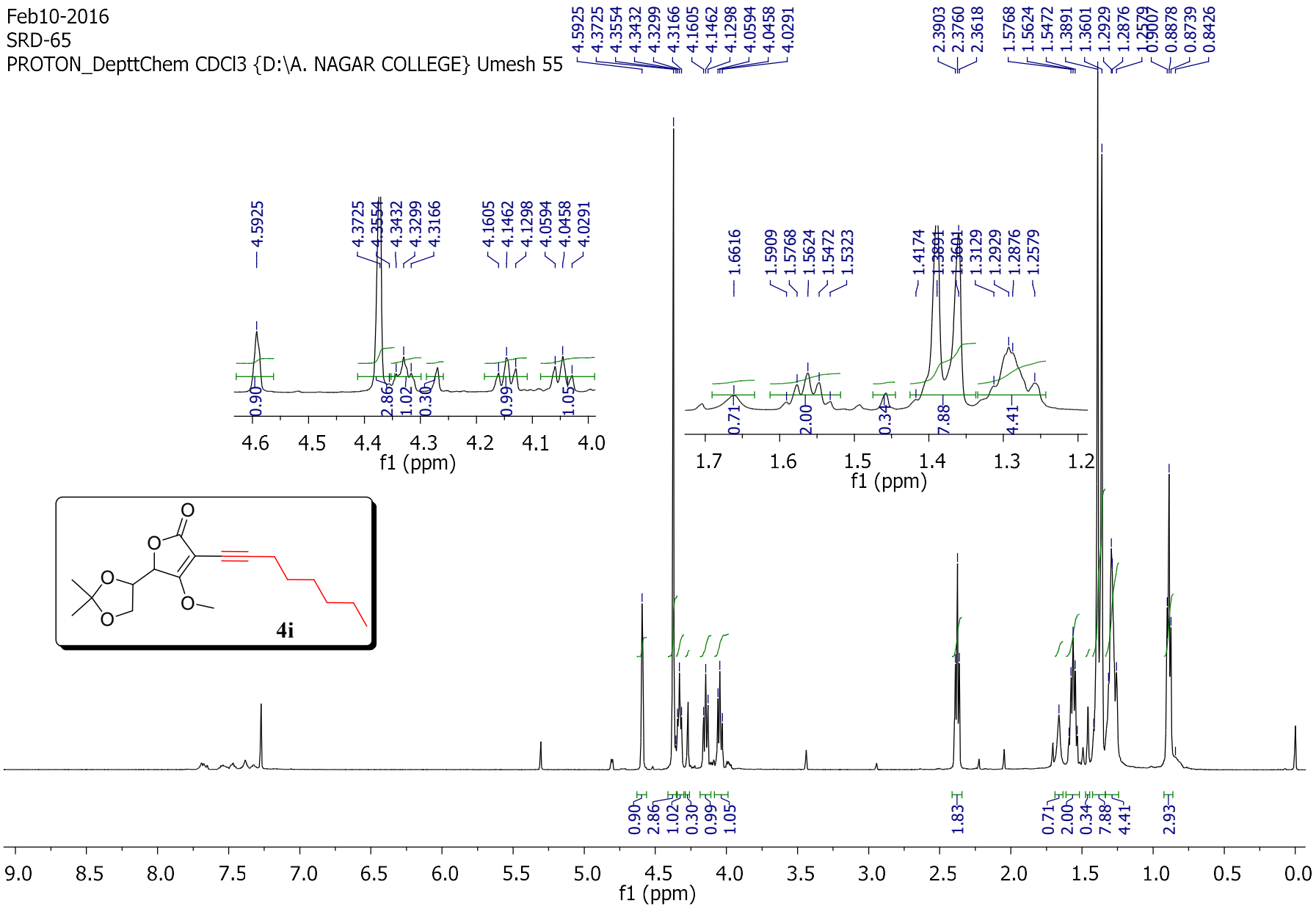
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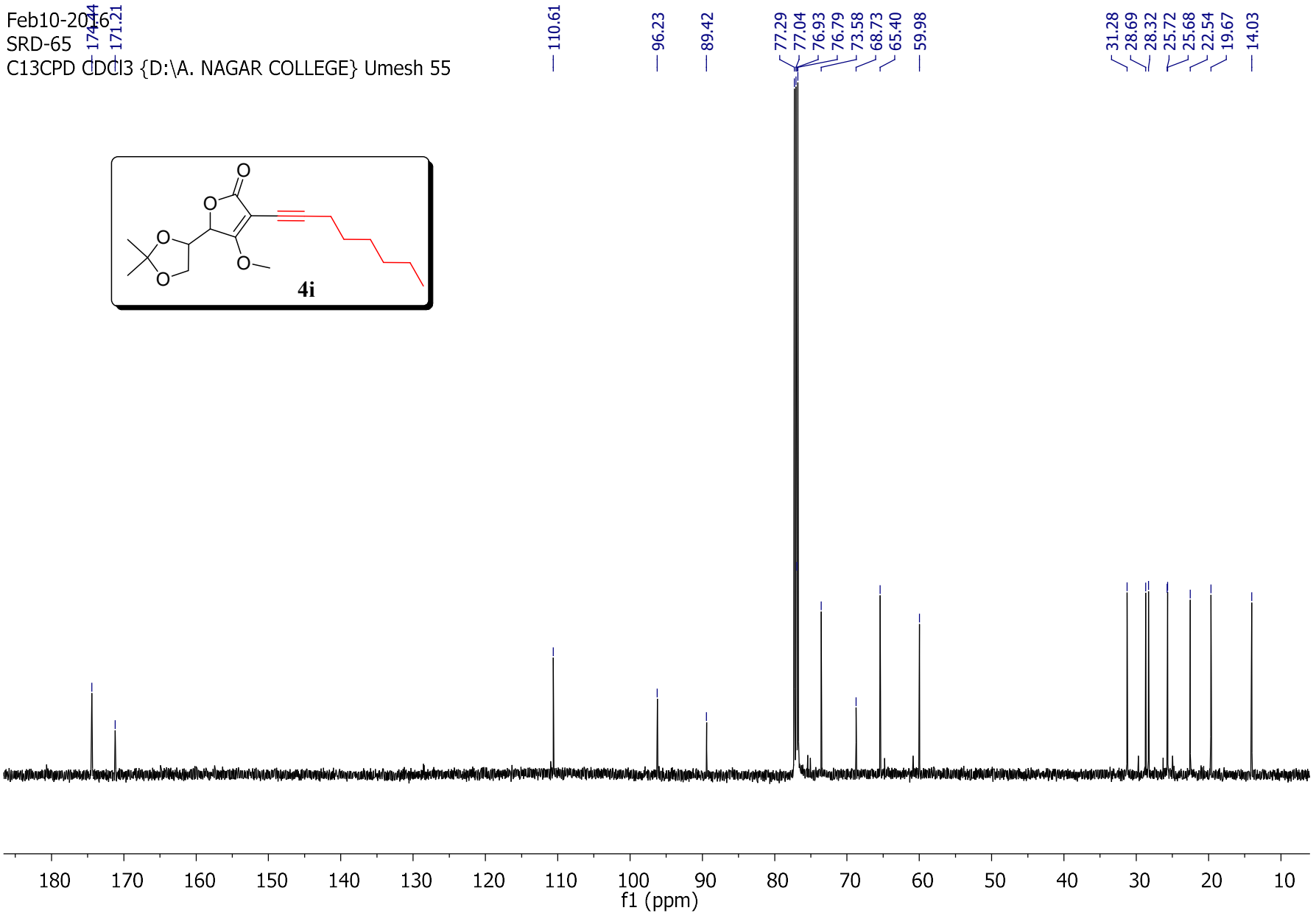
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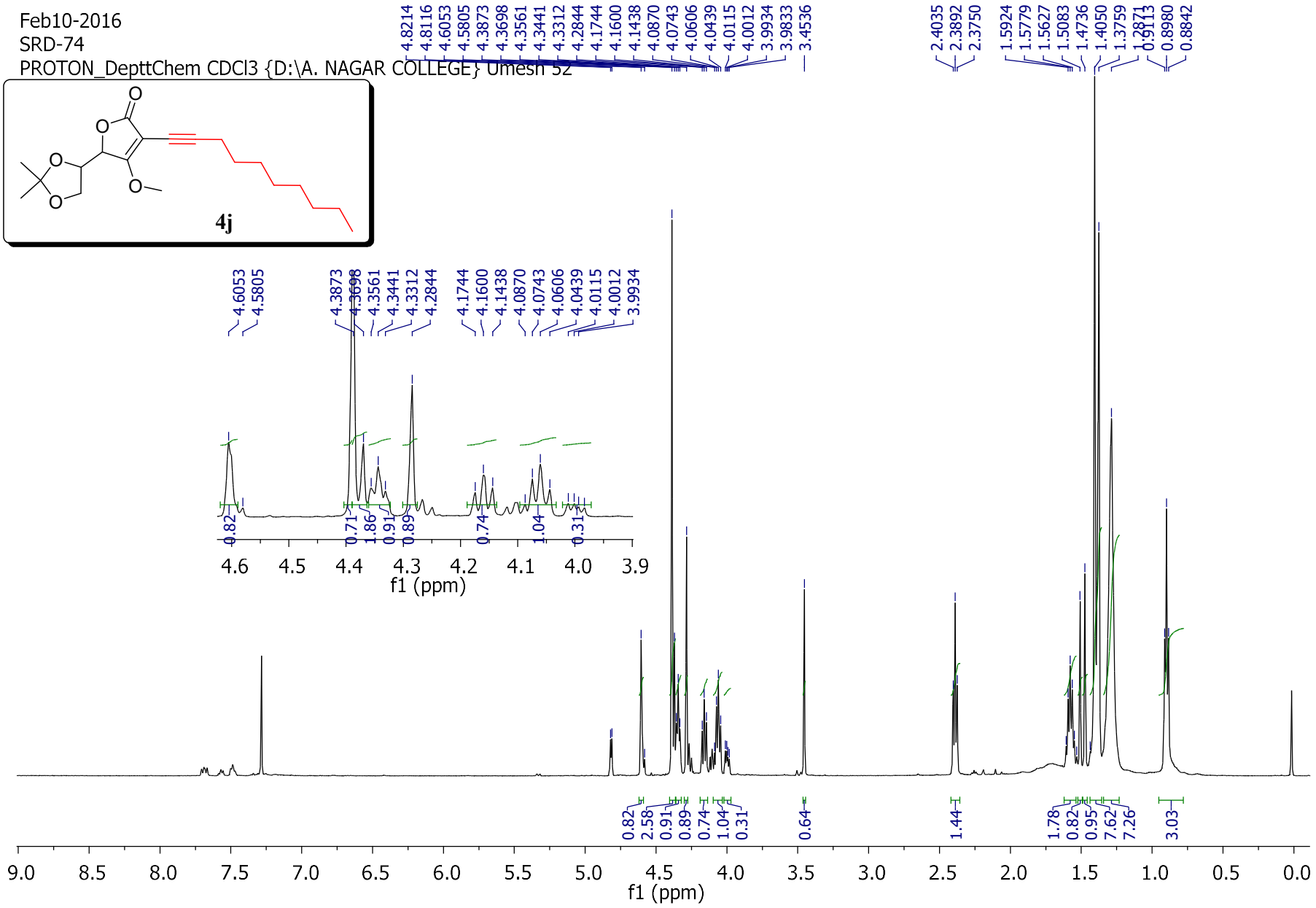
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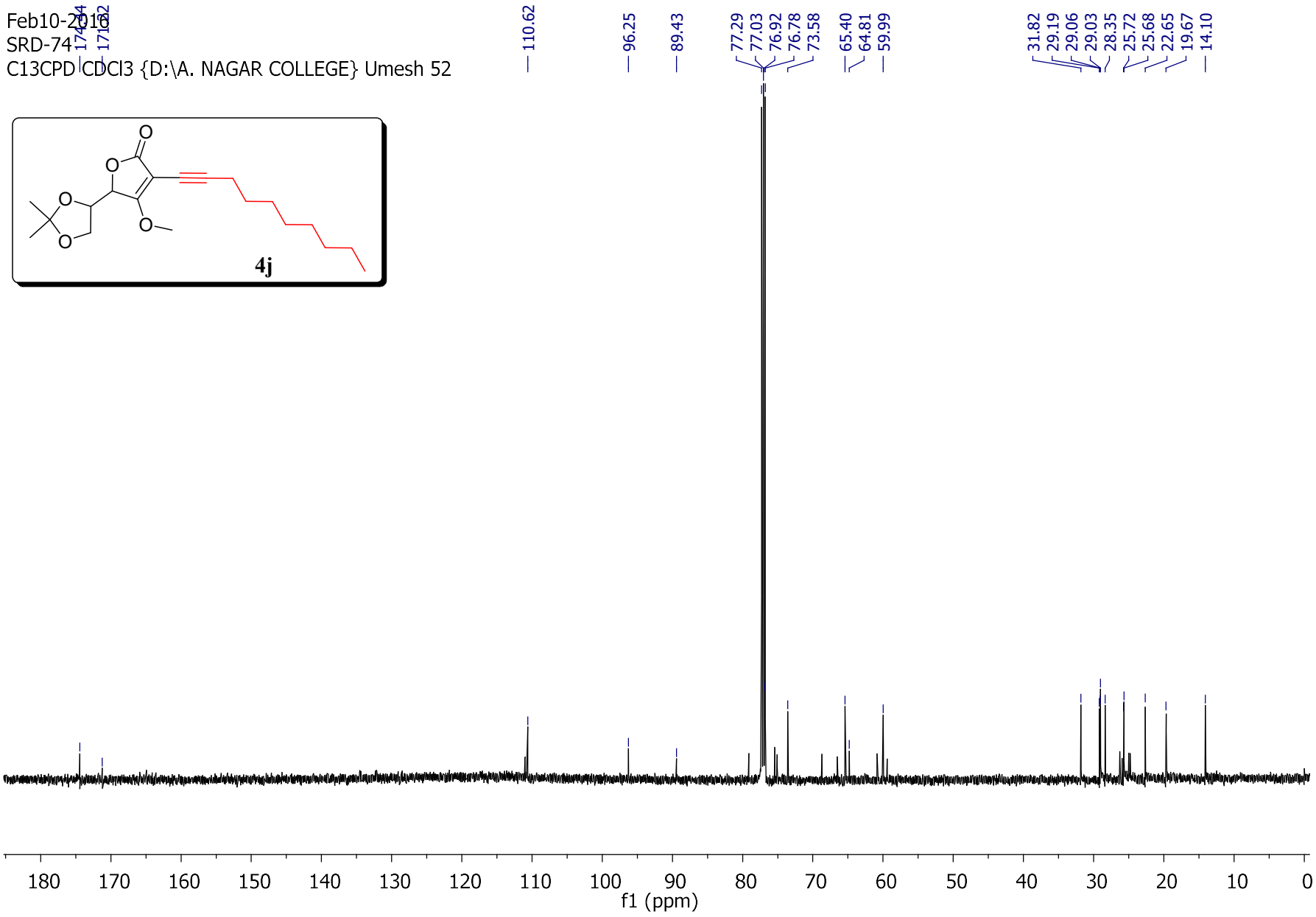
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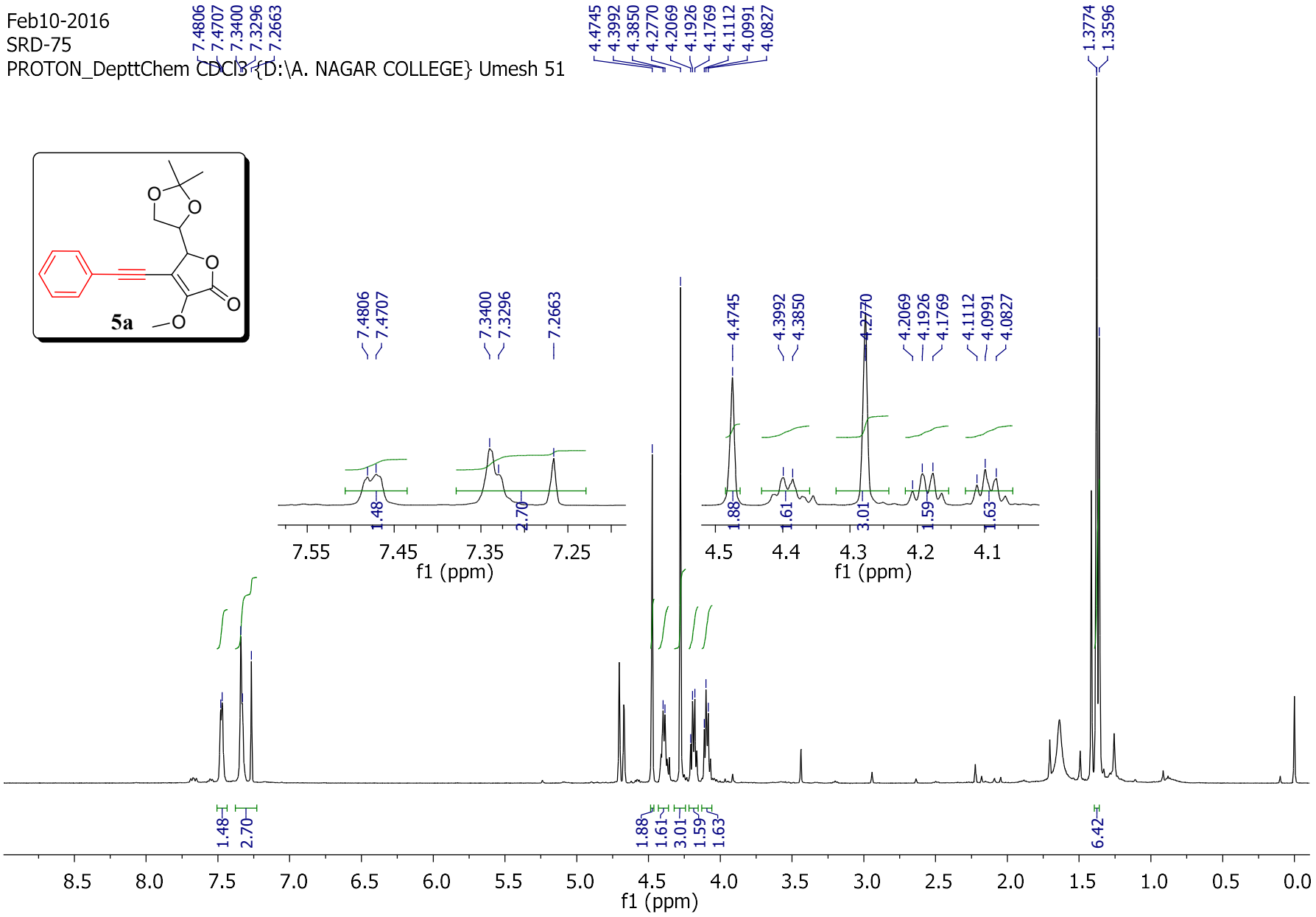
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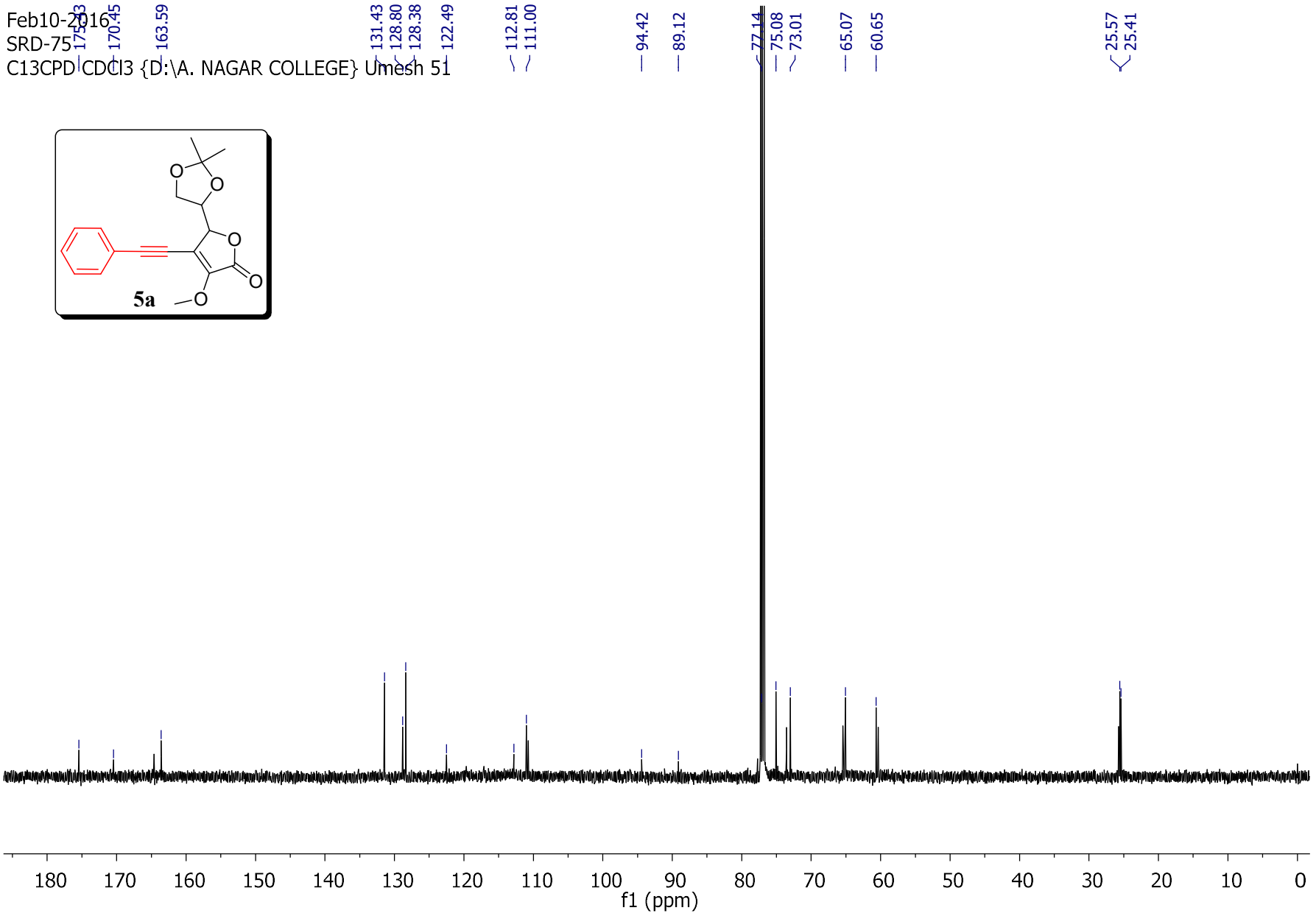
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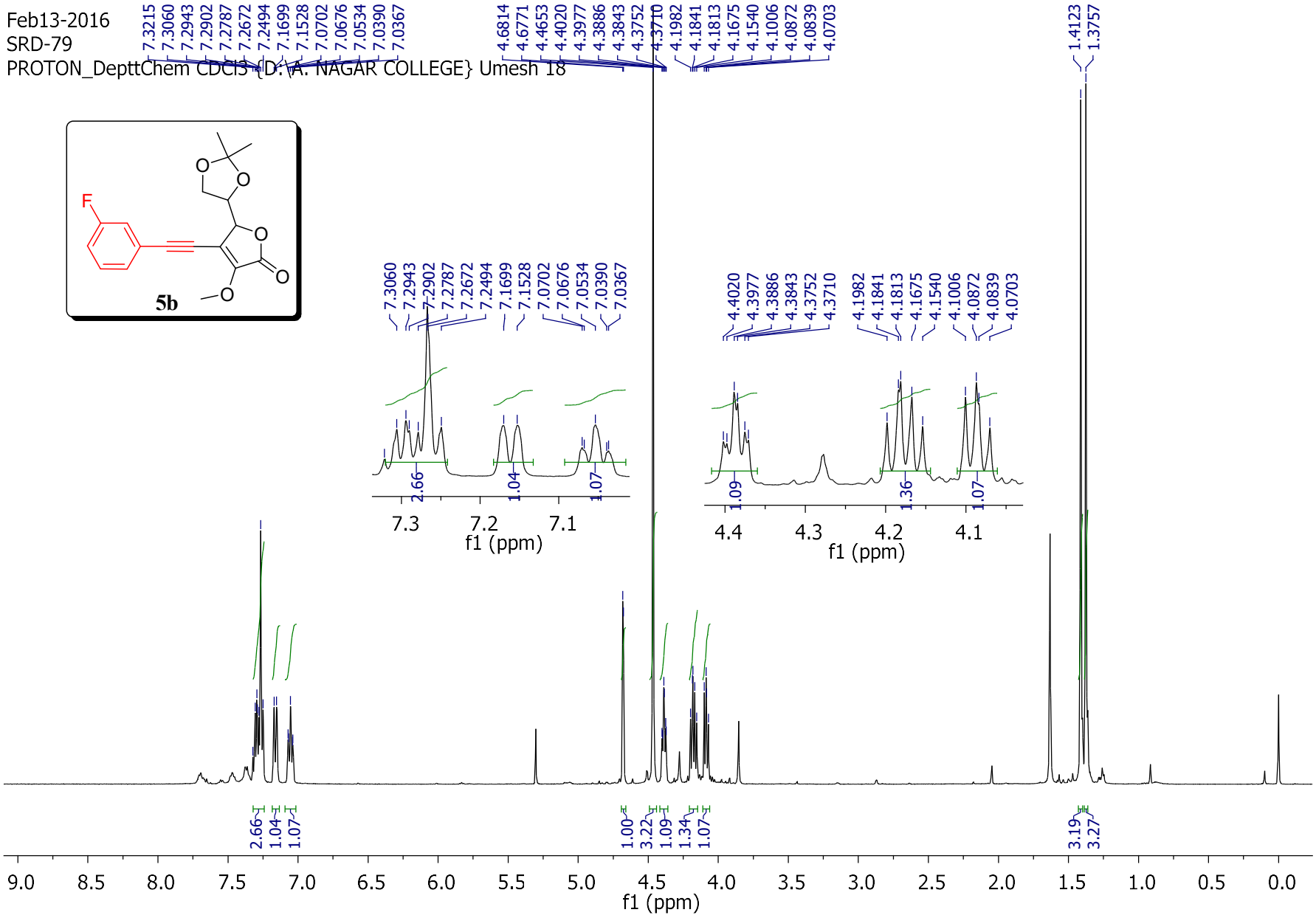
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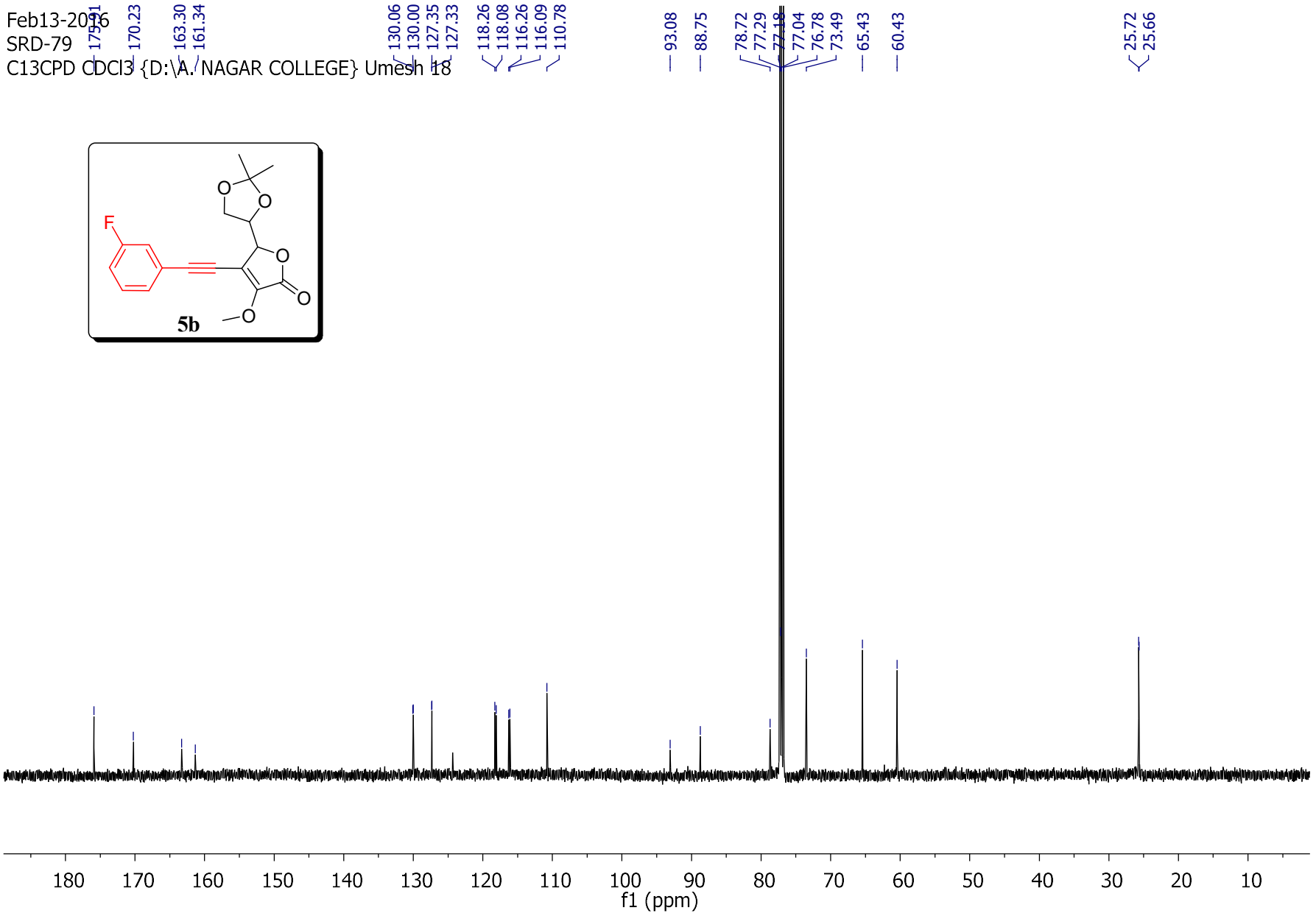
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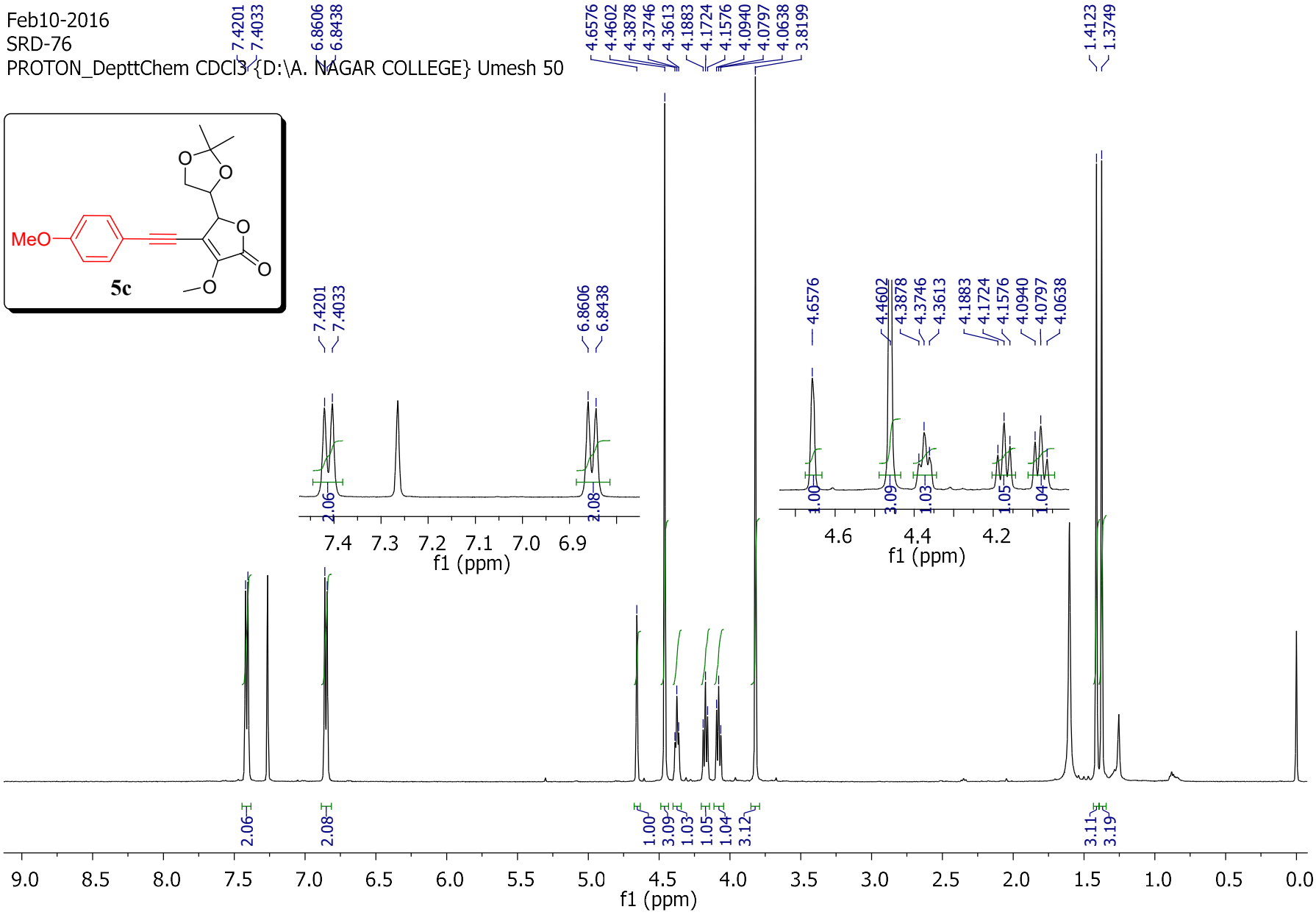
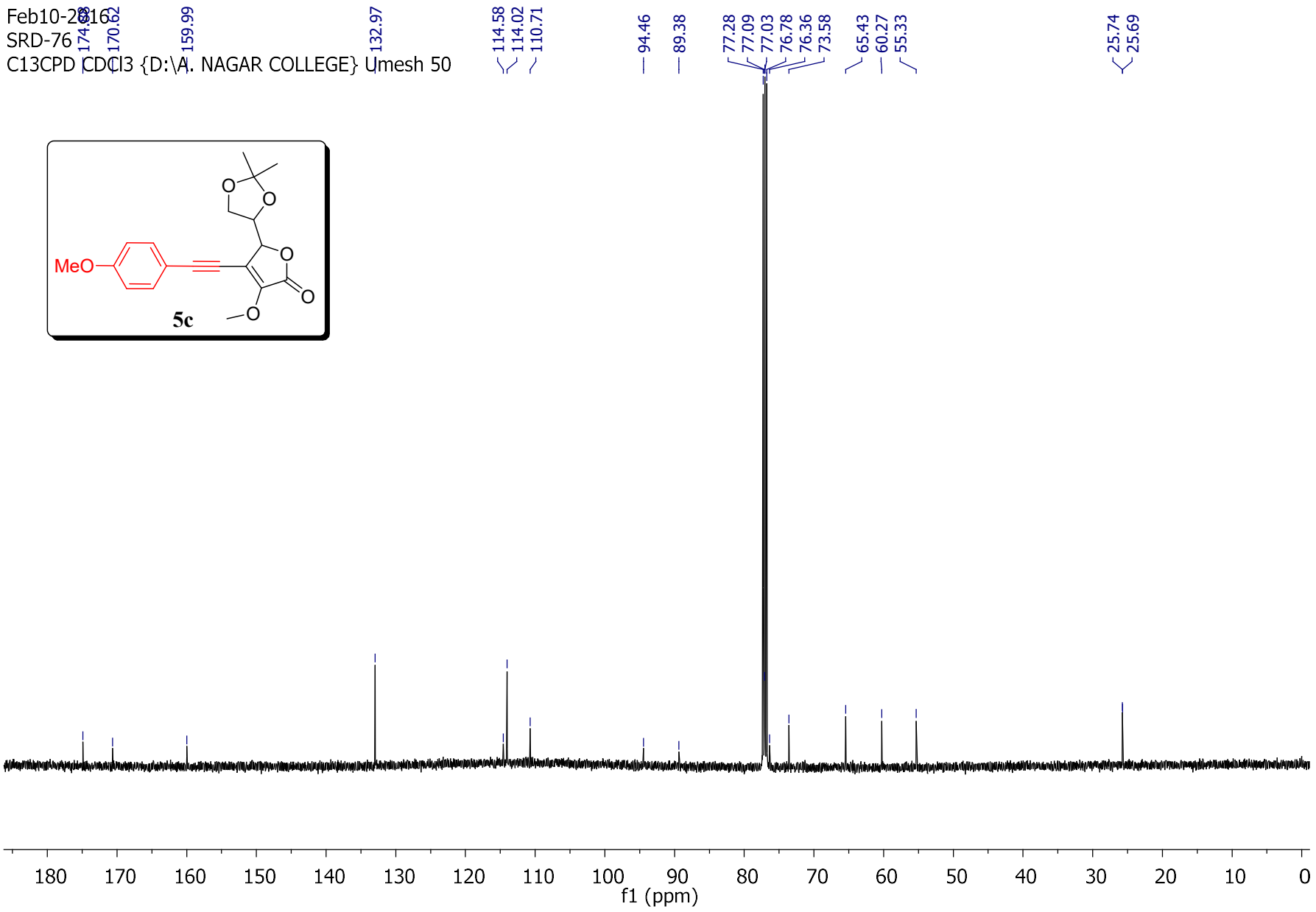
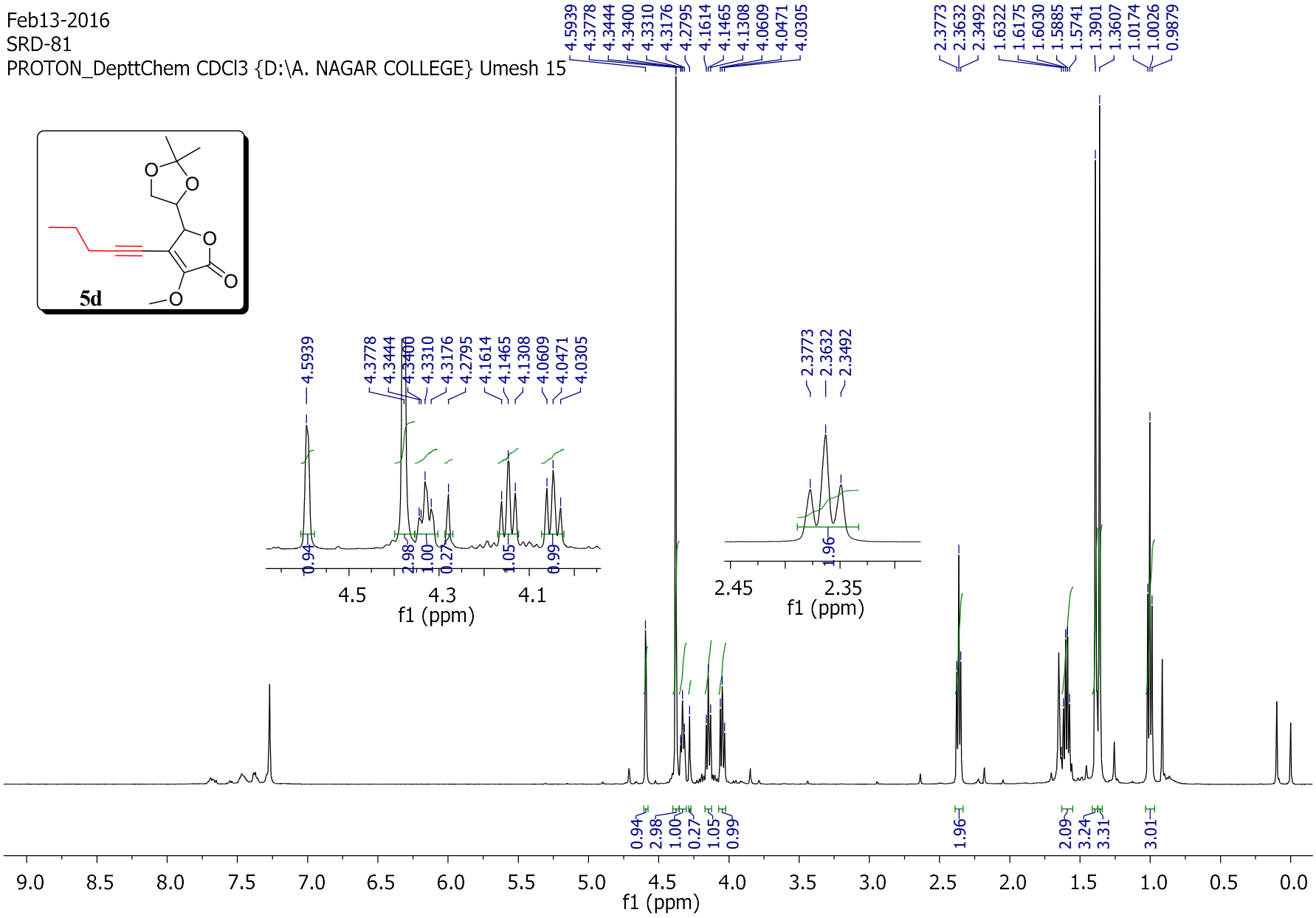
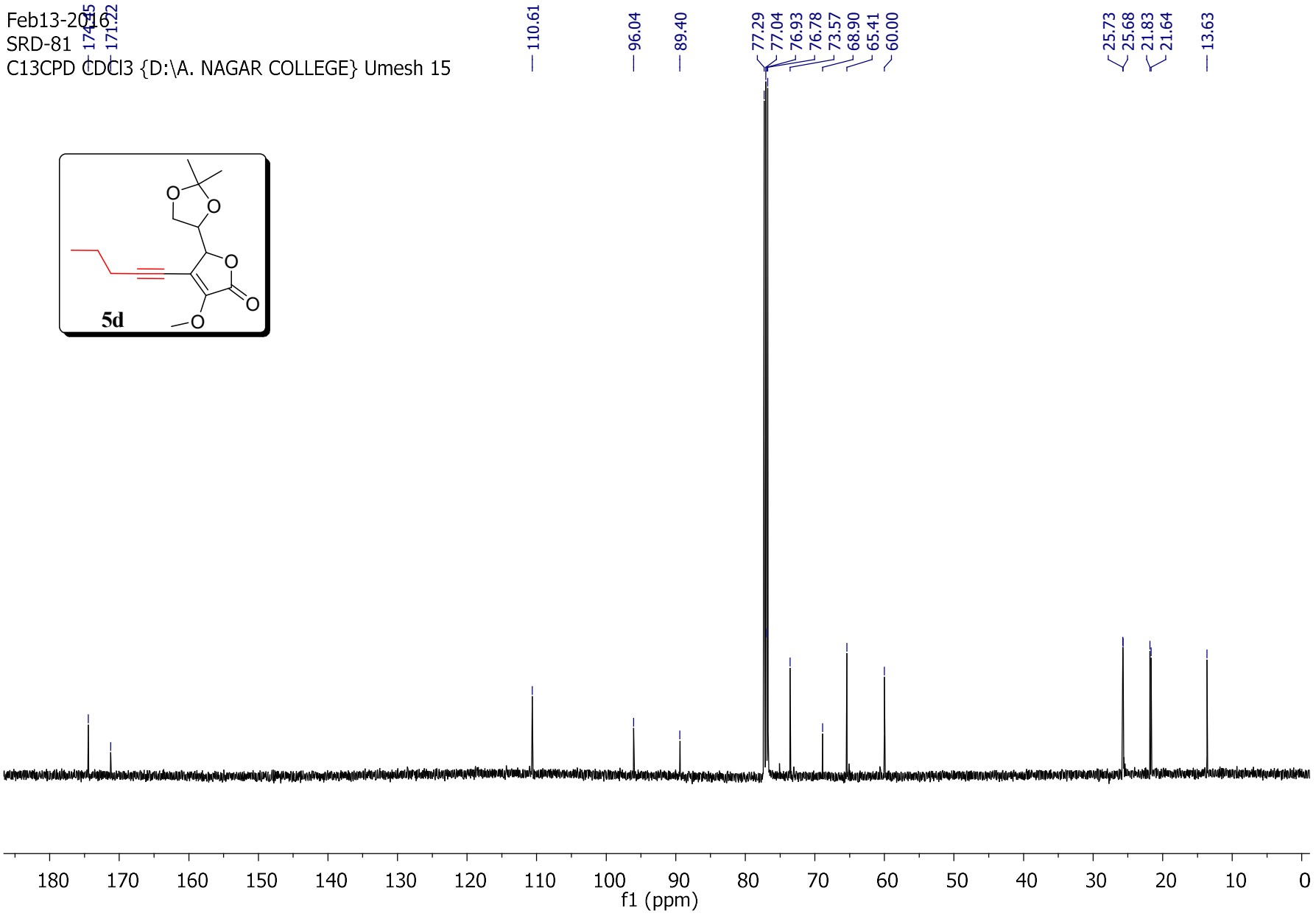
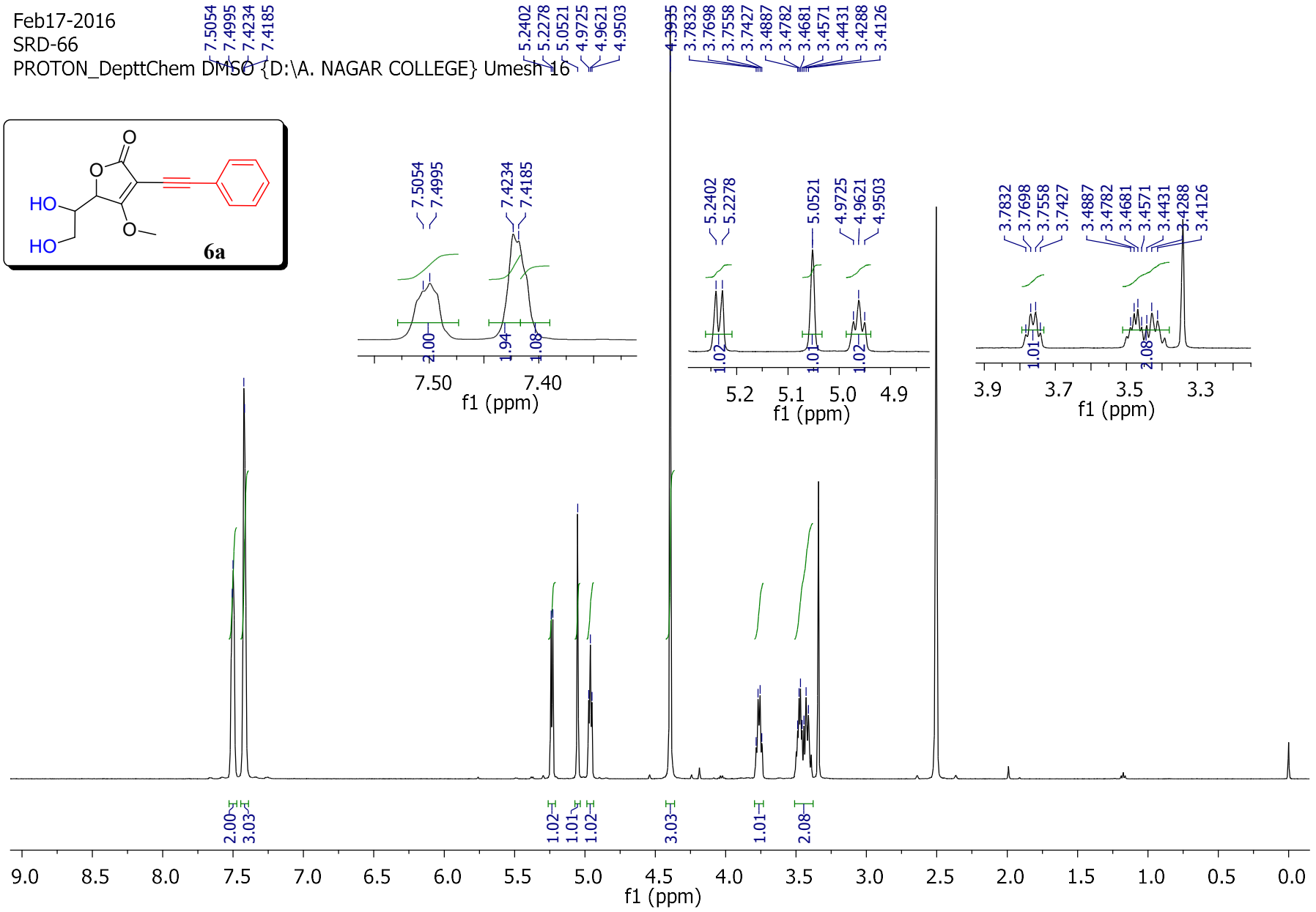
25.66
F
O
O
O
O
O
5b
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)

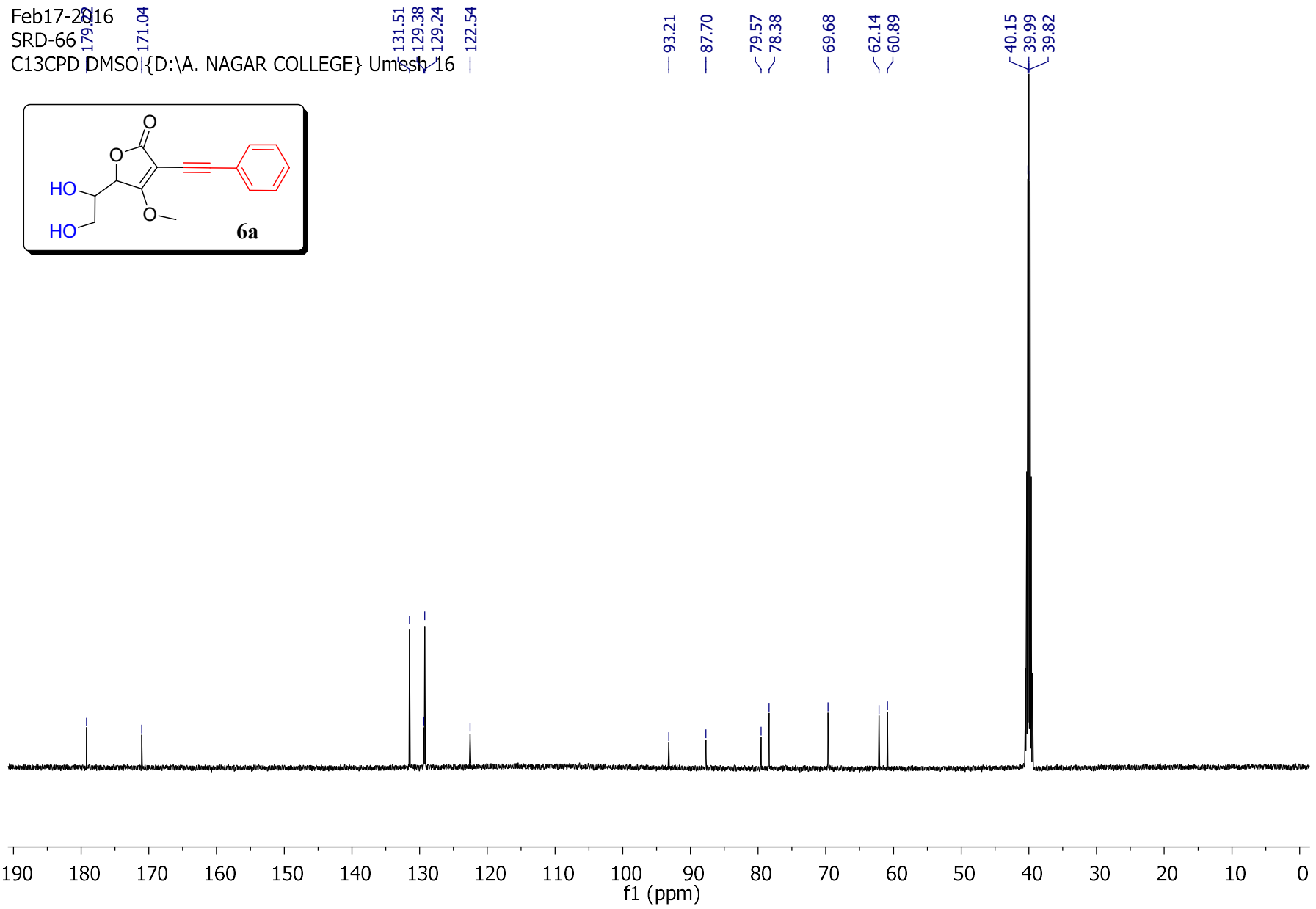

Feb10-2016
SRD-76
PROTON_DepttChem CDCl3 {D:\A. NAGAR COLLEGE} Umesh 50
MeO
5c
f1 (ppm)

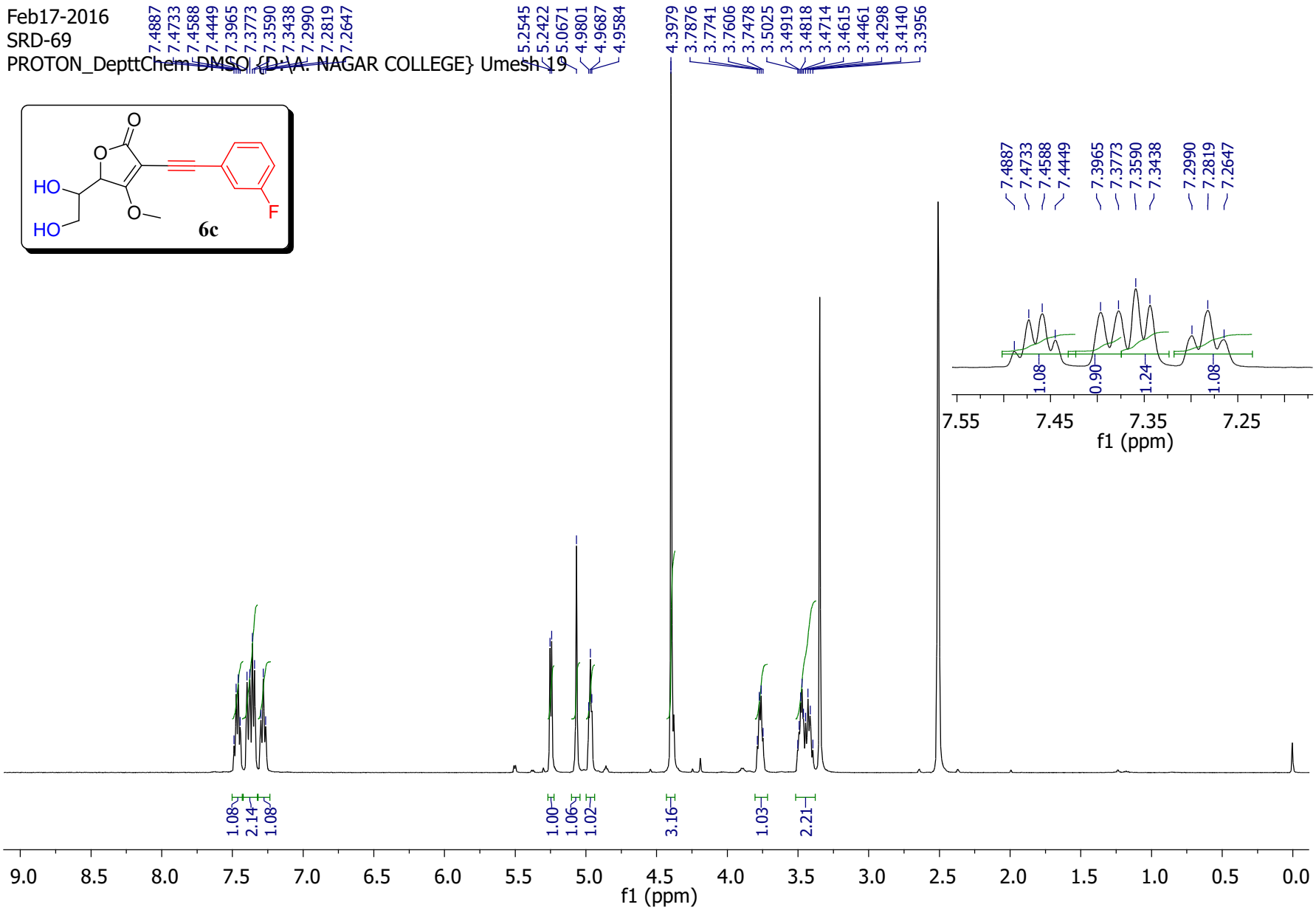

Feb10-2016
SRD-76
C13CPD CDCl3 {D:\A. NAGAR COLLEGE} Umesh 50
174.88
170.62
159.99
132.97
114.58
114.02
110.71
94.46
89.38
77.28
77.09
77.03
76.78
76.36
73.58
65.43
60.27
55.33
25.74
25.69
MeO
O
O
O
O
O
5c
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

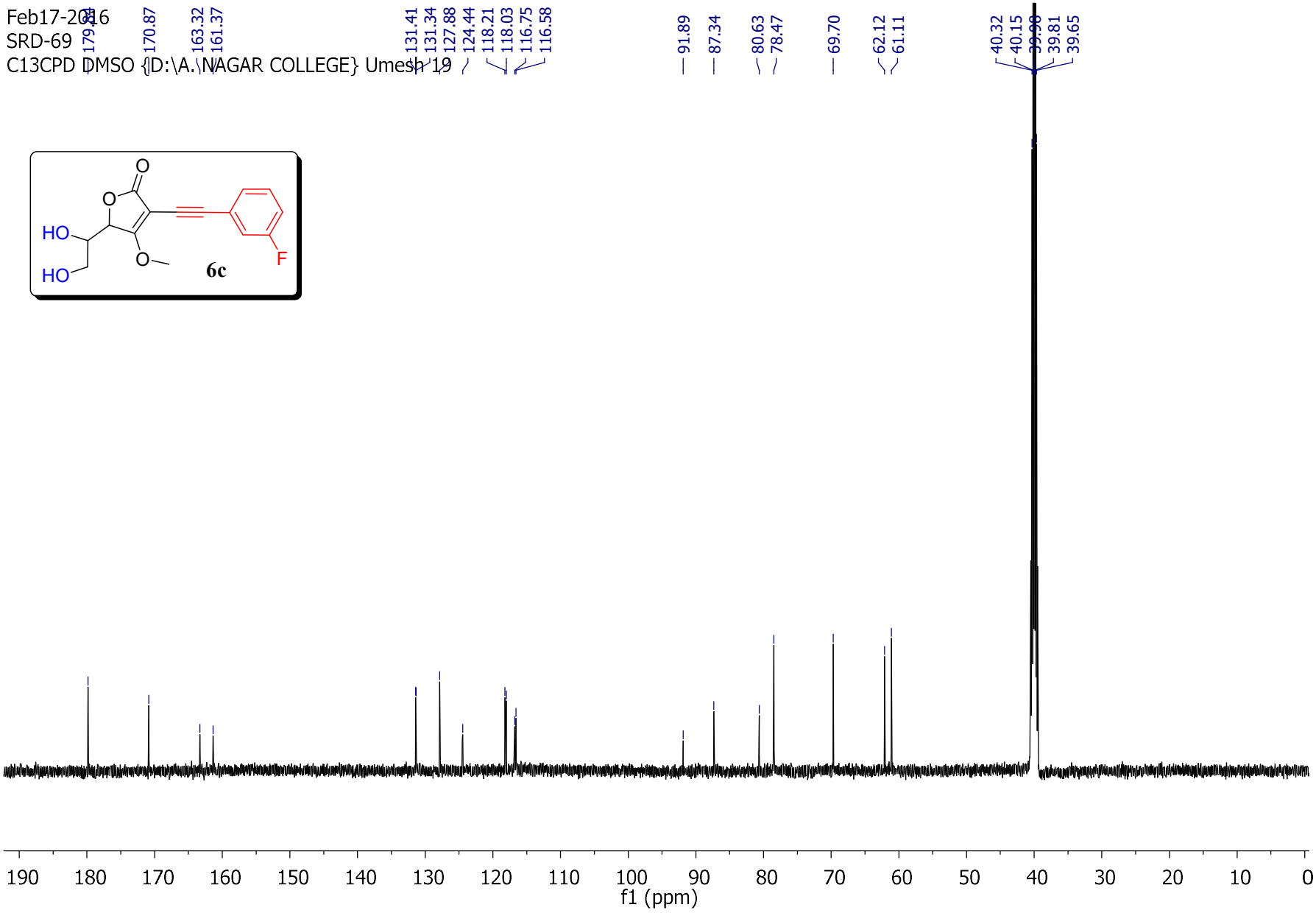

Feb13-2016
SRD-81
PROTON_DepttChem CDCl3 {D:\A. NAGAR COLLEGE} Umesh 15
5d
4.5939
4.3778
4.3444
4.3400
4.3310
4.3176
4.2795
4.1614
4.1465
4.1308
4.0609
4.0471
4.0305
2.3773
2.3632
2.3492
1.6322
1.6175
1.6030
1.5885
1.5741
1.3901
1.3607
1.0174
1.0026
0.9879
0.94
2.98
1.00
0.27
1.05
0.99
1.96
2.09
3.24
3.31
3.01
f1 (ppm)

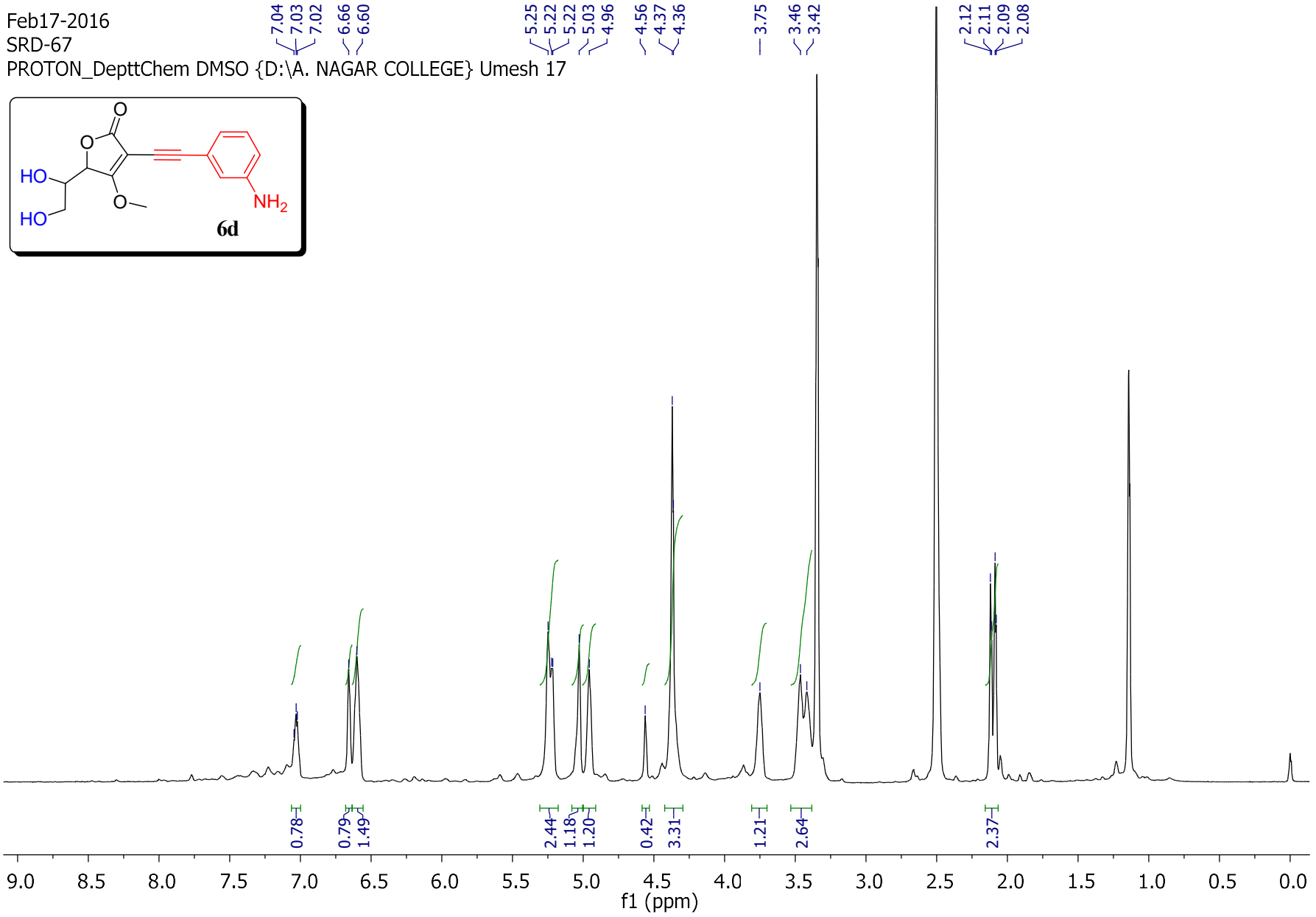

Feb13-2016
SRD-81
C13CPD CDCl3 {D:\A. NAGAR COLLEGE} Umesh 15
174.45
171.22
110.61
96.04
89.40
77.29
77.04
76.93
76.78
73.57
68.90
65.41
60.00
25.73
25.68
21.83
21.64
13.63
5d
O
O
O
O
O
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

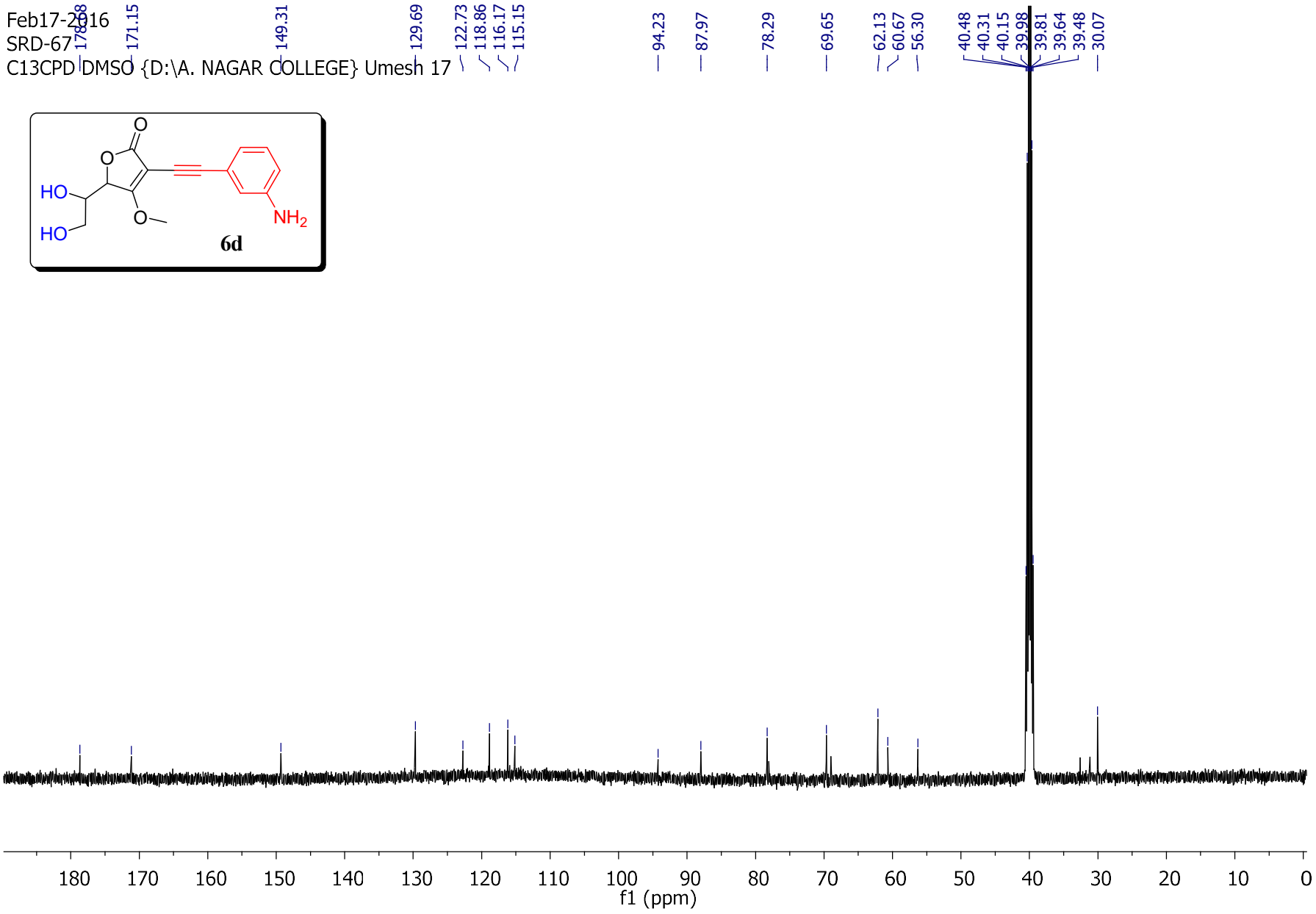

Feb17-2016
SRD-66
PROTON_DepttChem DMSO {D:\A. NAGAR COLLEGE} Umesh 16
7.5054
7.4995
7.4234
7.4185
5.2402
5.2278
5.0521
4.9725
4.9621
4.9503
4.3935
3.7832
3.7698
3.7558
3.7427
3.4887
3.4782
3.4681
3.4571
3.4431
3.4288
3.4126
HO
HO
O
O
O
6a
2.00
1.94
1.08
1.02
1.01
1.02
1.01
1.02
3.03
1.01
2.08
f1 (ppm)

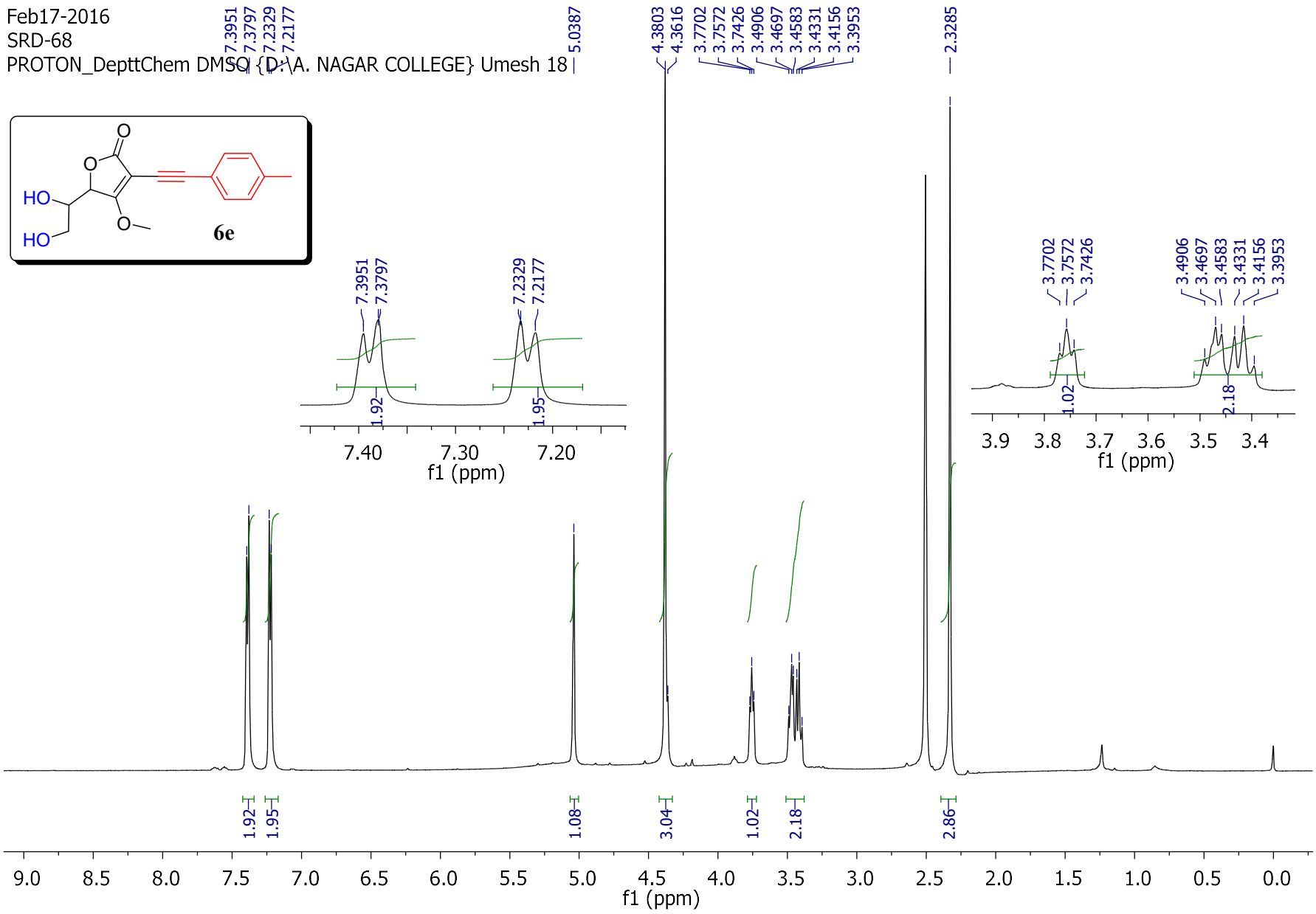

Feb17-2016
SRD-66
C13CPD DMSO {D:\A. NAGAR COLLEGE} Umesh 16
179.51
171.04
131.51
129.38
129.24
122.54
93.21
87.70
79.57
78.38
69.68
62.14
60.89
40.15
39.99
39.82
HO
HO
O
O
O
6a
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

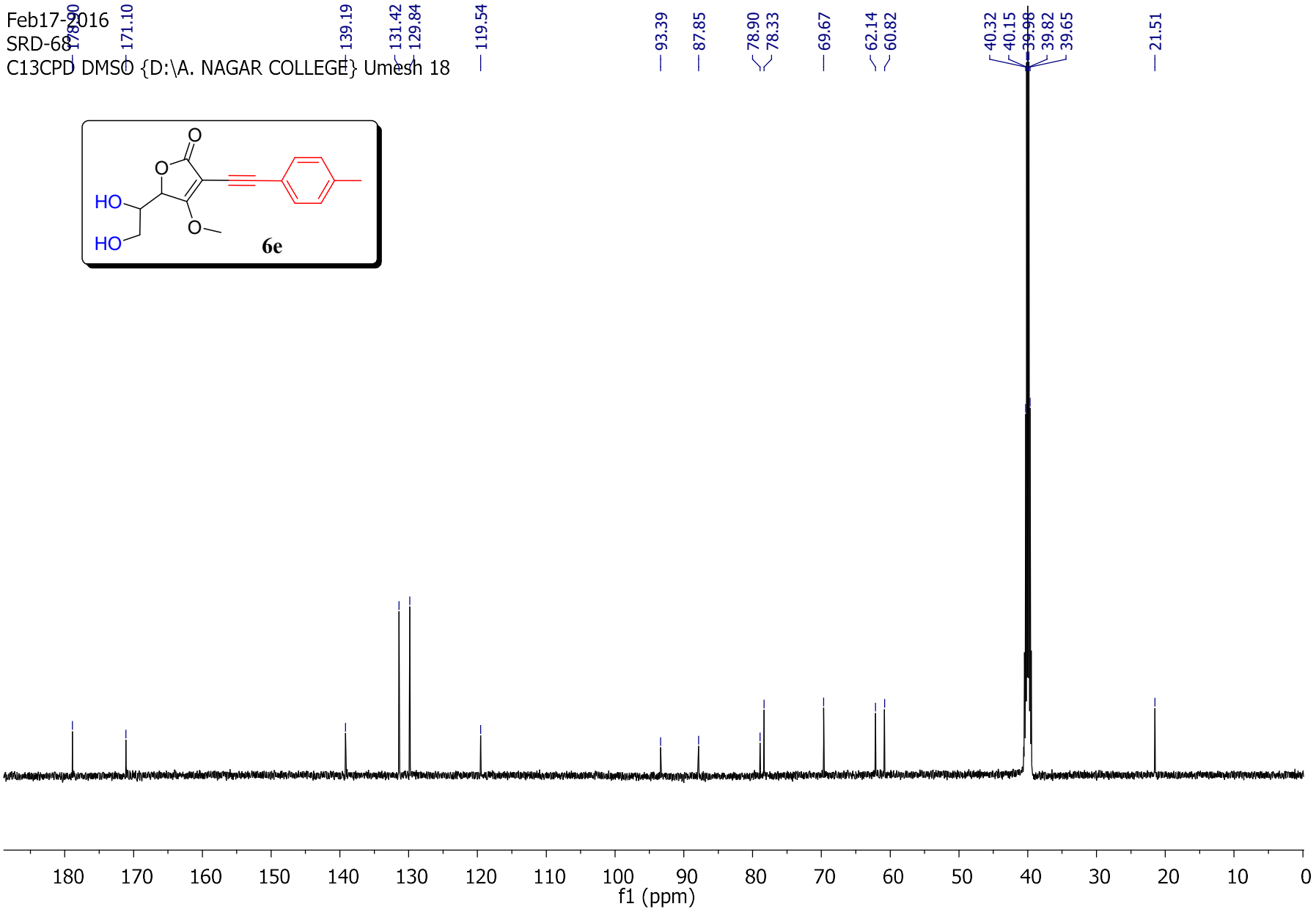

Feb17-2016
SRD-69
PROTON_DepttChem DMSO {D:\A. NAGAR COLLEGE} Umesh 19
7.4887
7.4733
7.4588
7.4449
7.3965
7.3773
7.3590
7.3438
7.2990
7.2819
7.2647
5.2545
5.2422
5.0671
4.9801
4.9687
4.9584
4.3979
3.7876
3.7741
3.7606
3.7478
3.5025
3.4919
3.4818
3.4714
3.4615
3.4461
3.4298
3.4140
3.3956
HO
HO
O
O
O
F
6c
1.08
2.14
1.08
1.00
1.06
1.02
3.16
1.03
2.21
1.08
0.90
1.24
1.08
7.55
7.45
7.35
7.25
f1 (ppm)
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
f1 (ppm)

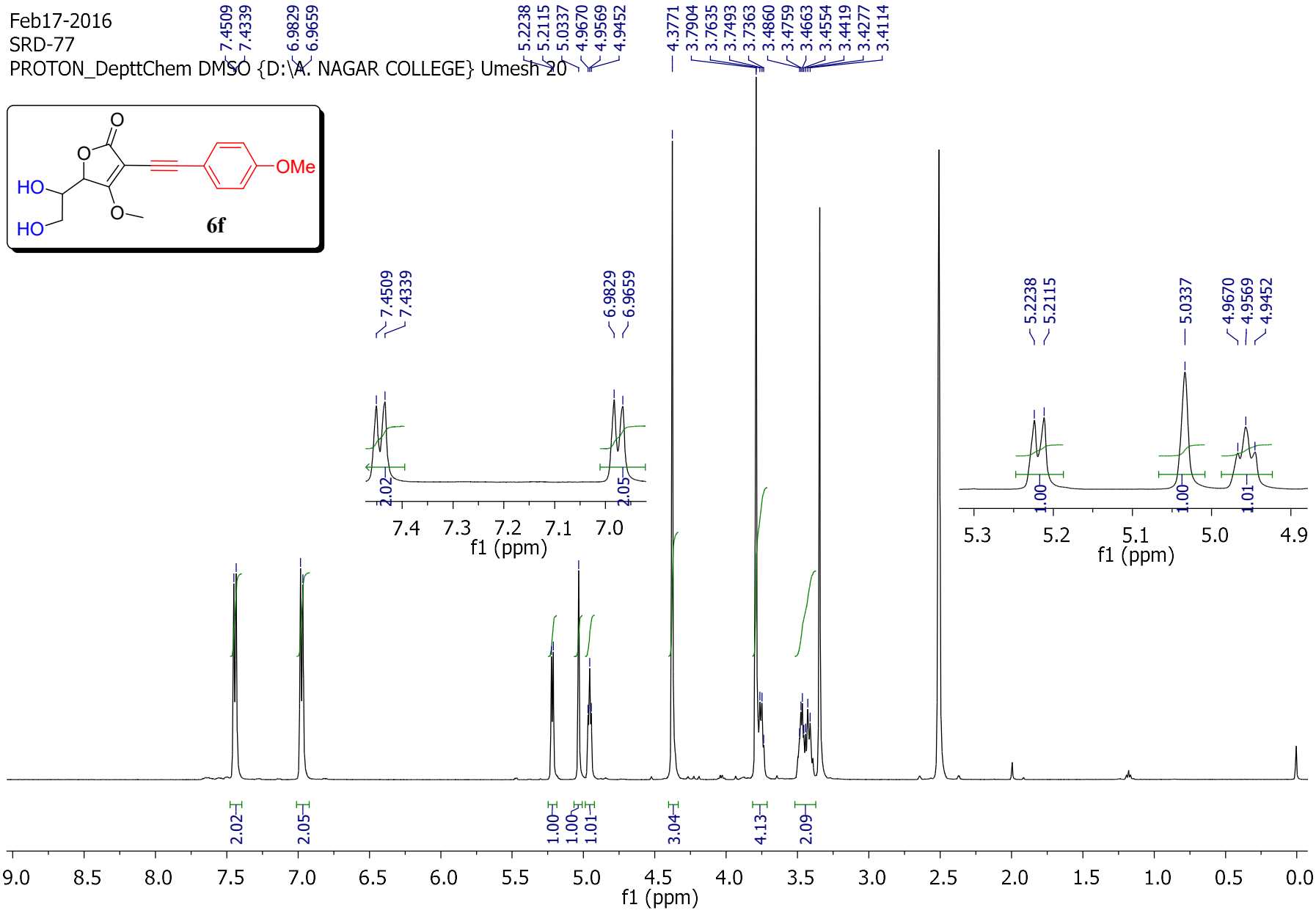

Feb17-2016
SRD-69
C13CPD DMSO {D:\A.\NAGAR COLLEGE} Umesh 19
179.41
170.87
163.32
161.37
131.41
131.34
127.88
124.44
118.21
118.03
116.75
116.58
91.89
87.34
80.63
78.47
69.70
62.12
61.11
40.32
40.15
39.98
39.81
39.65
HO
HO
O
O
O
F
6c
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

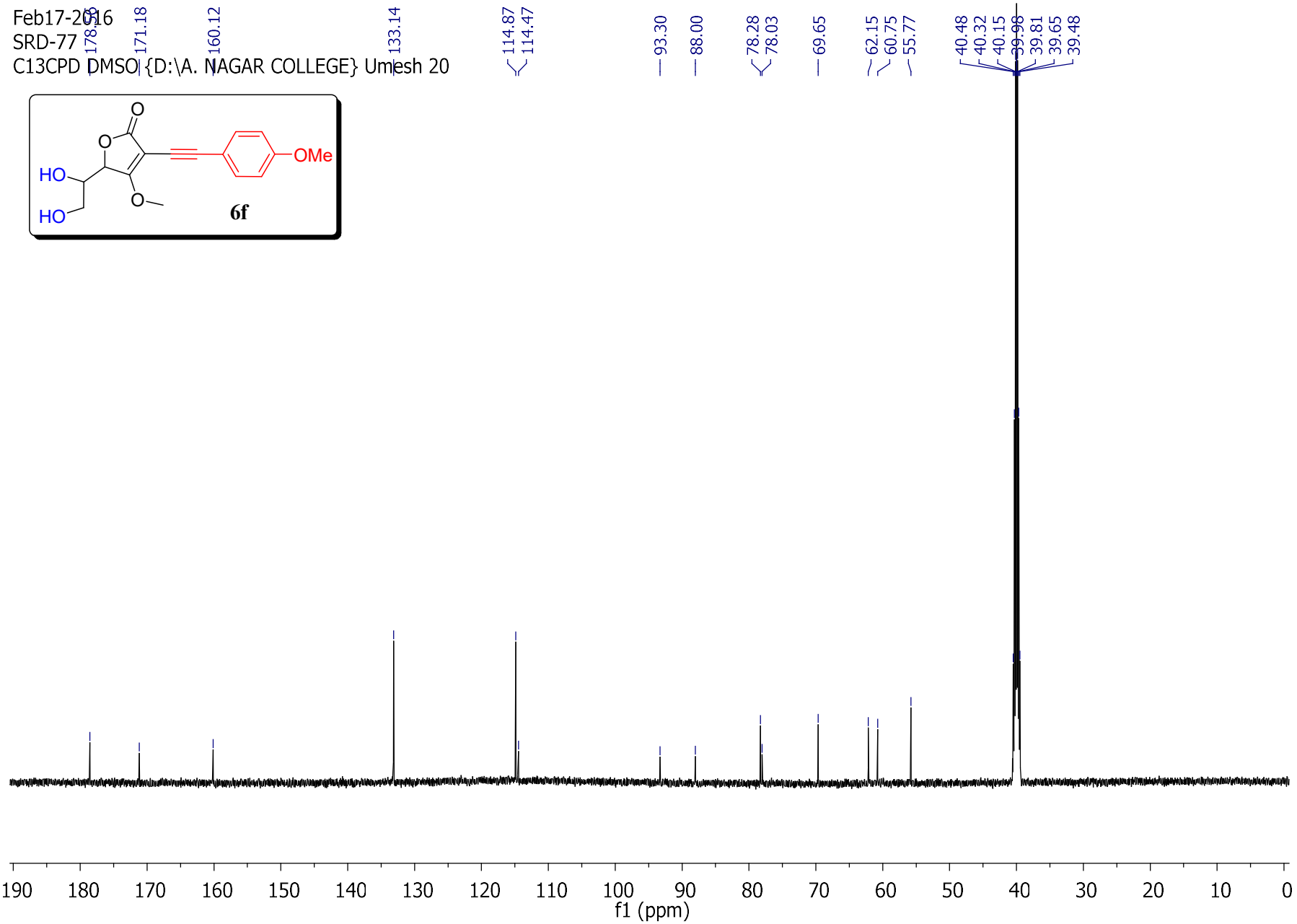

Feb17-2016
SRD-67
PROTON_DepttChem DMSO {D:\A. NAGAR COLLEGE} Umesh 17
7.04
7.03
7.02
6.66
6.60
5.25
5.22
5.22
5.03
4.96
4.56
4.37
4.36
3.75
3.46
3.42
2.12
2.11
2.09
2.08
HO
HO
O
O
O
NH2
6d
0.78
0.79
1.49
2.44
1.18
1.20
0.42
3.31
1.21
2.64
2.37
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

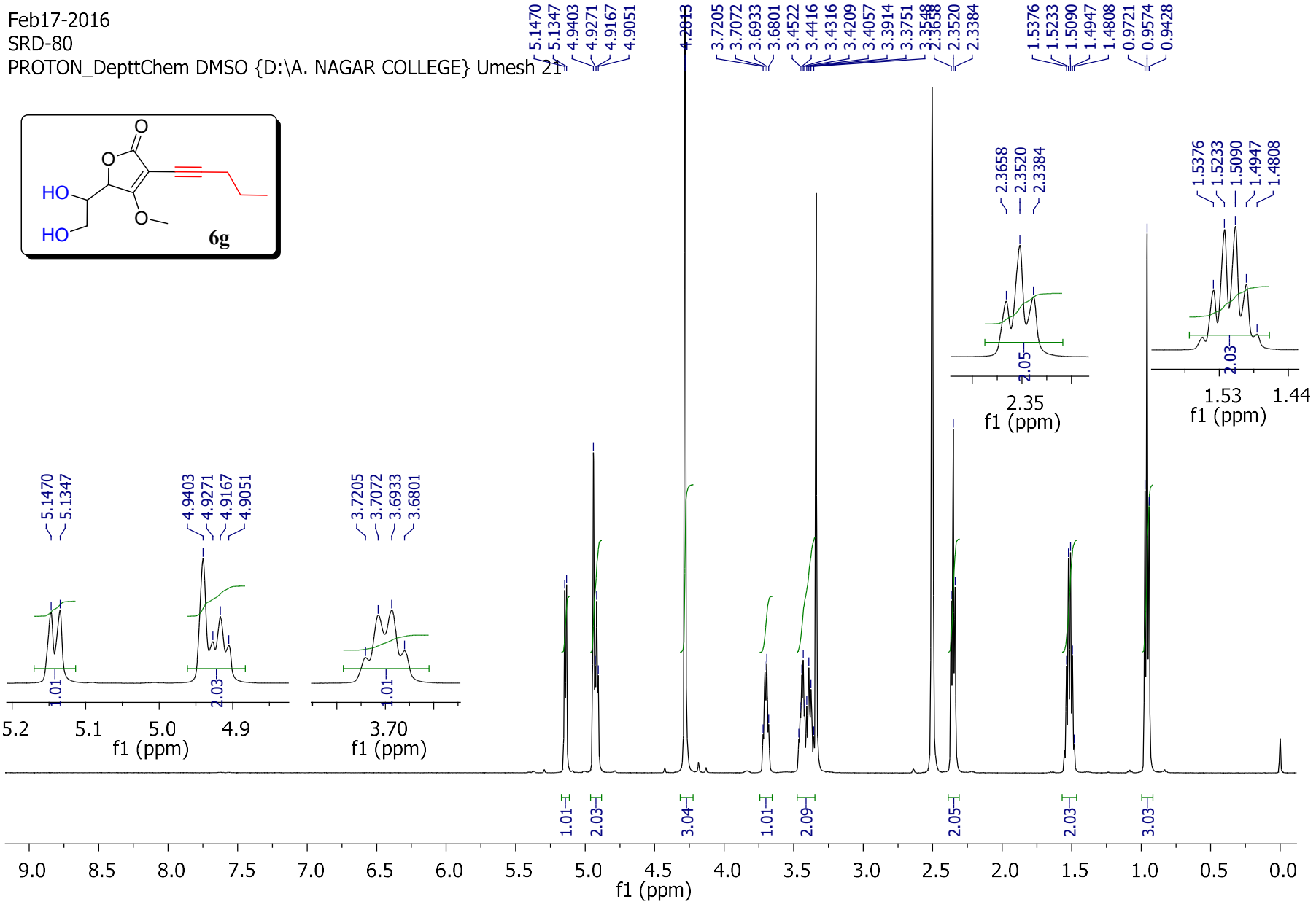

Feb17-2016
SRD-67
C13CPD DMSO {D:\A. NAGAR COLLEGE} Umesh 17
178.88
171.15
149.31
129.69
122.73
118.86
116.17
115.15
94.23
87.97
78.29
69.65
62.13
60.67
56.30
40.48
40.31
40.15
39.98
39.81
39.64
39.48
30.07
HO
HO
O
O
O
NH2
6d
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

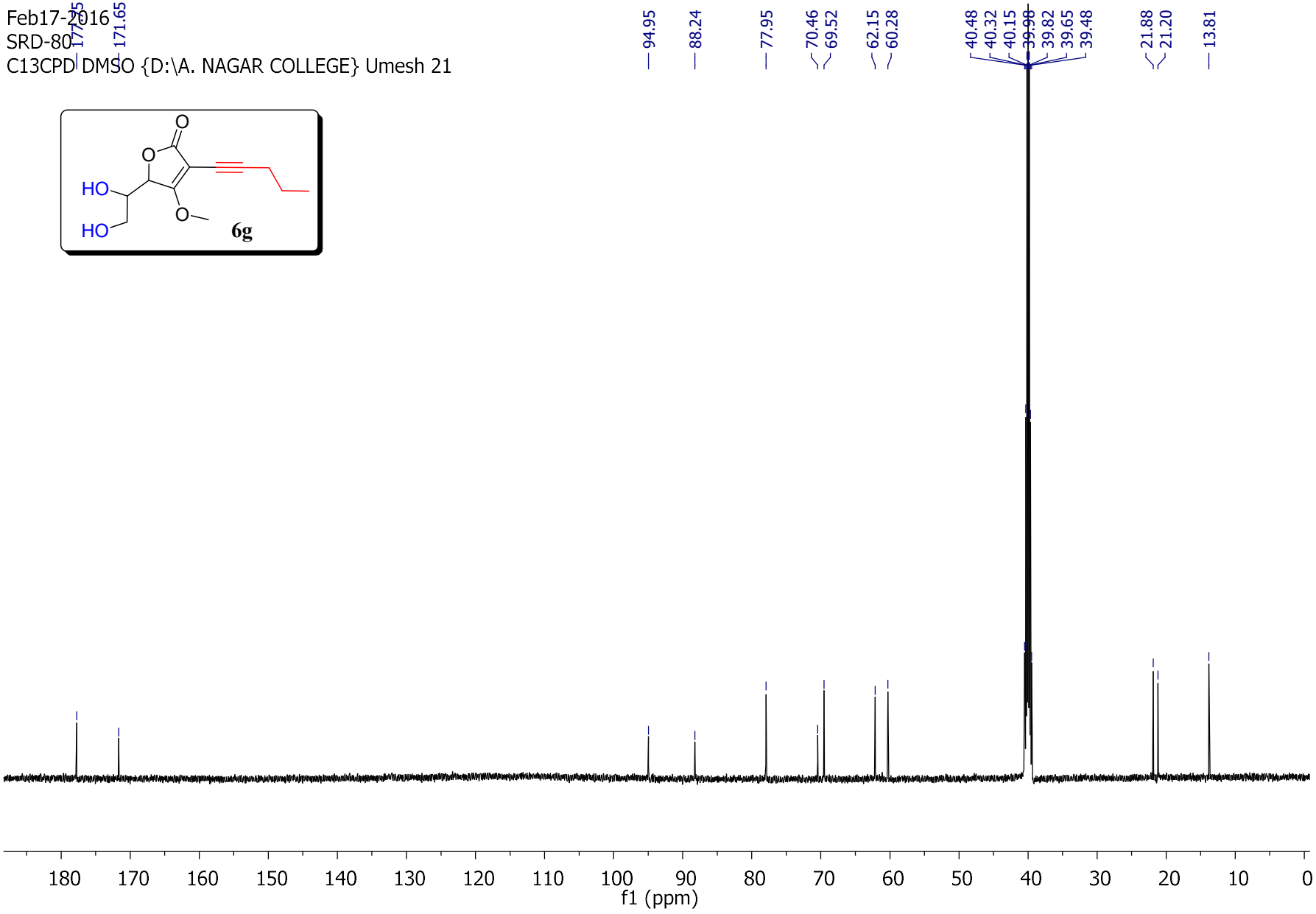

Feb17-2016
SRD-68
PROTON_DepttChem DMSO {D:\A. NAGAR COLLEGE} Umesh 18
7.3951
7.3797
7.2329
7.2177
5.0387
4.3803
4.3616
3.7702
3.7572
3.7426
3.4906
3.4697
3.4583
3.4331
3.4156
3.3953
2.3285
HO
HO
O
O
O
6e
1.92
1.95
1.08
3.04
1.02
2.18
2.86
f1 (ppm)

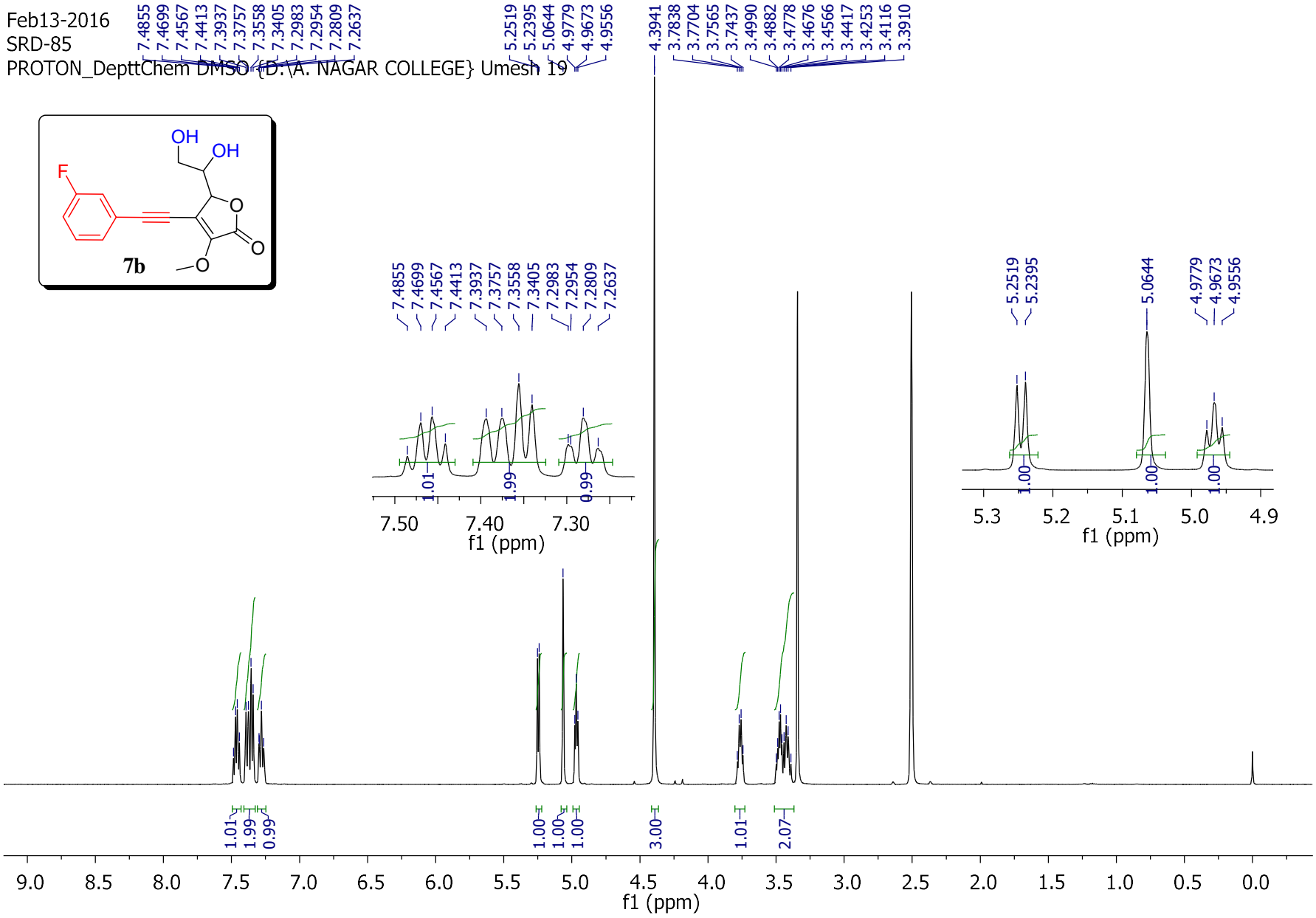

Feb17-2016
SRD-68
C13CPD DMSO {D:\A. NAGAR COLLEGE} Umesh 18
178.90
171.10
139.19
131.42
129.84
119.54
93.39
87.85
78.90
78.33
69.67
62.14
60.82
40.32
40.15
39.98
39.82
39.65
21.51
HO
HO
O
O
O
6e
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

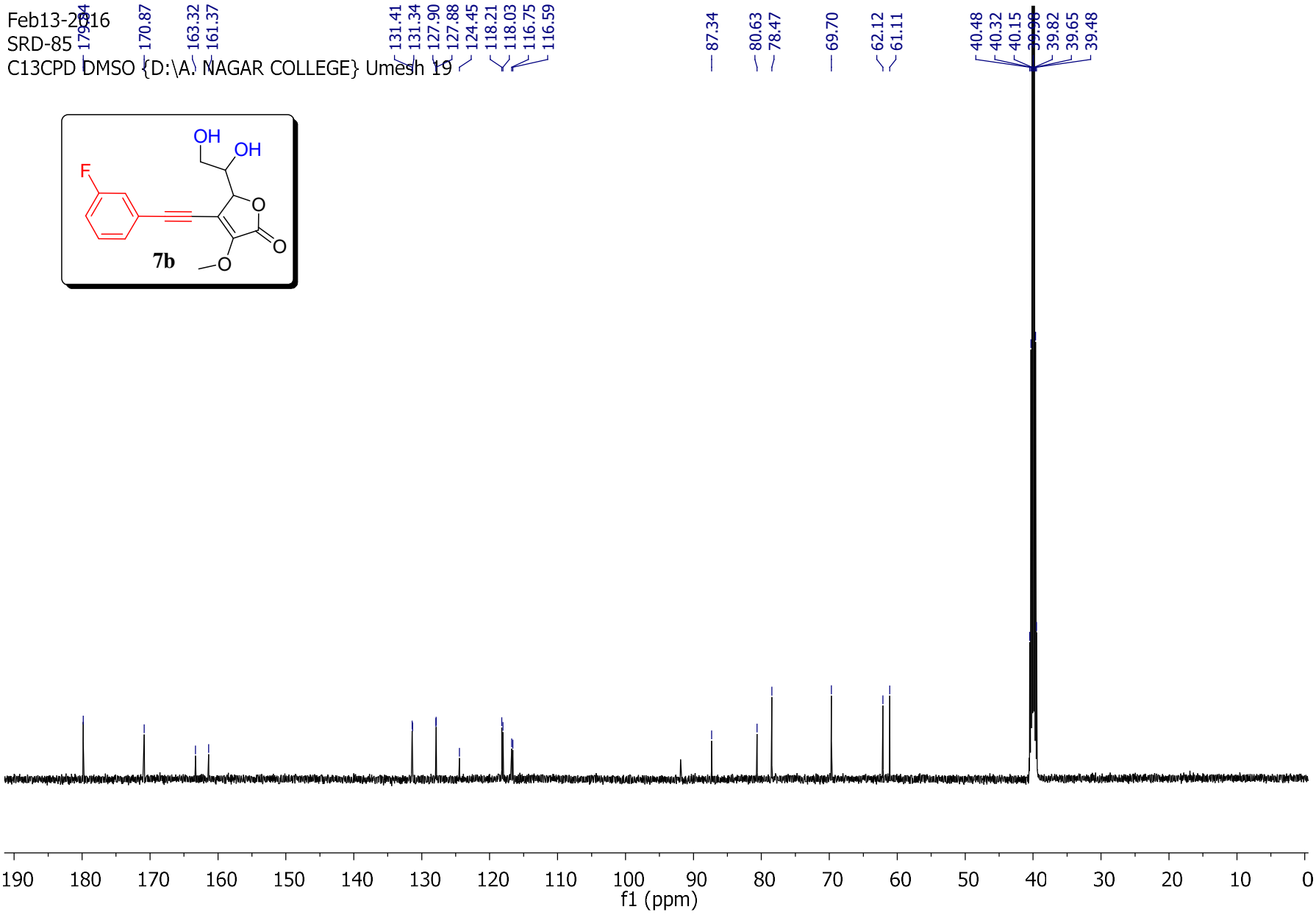

Feb17-2016
SRD-77
PROTON_DepttChem DMSO {D:\A. NAGAR COLLEGE} Umesh 20
7.4509
7.4339
6.9829
6.9659
5.2238
5.2115
5.0337
4.9670
4.9569
4.9452
4.3771
3.7904
3.7635
3.7493
3.7363
3.4860
3.4759
3.4663
3.4554
3.4419
3.4277
3.4114
HO
HO
O
O
O
OMe
6f
f1 (ppm)
2.02
2.05
1.00
1.00
1.01
3.04
4.13
2.09

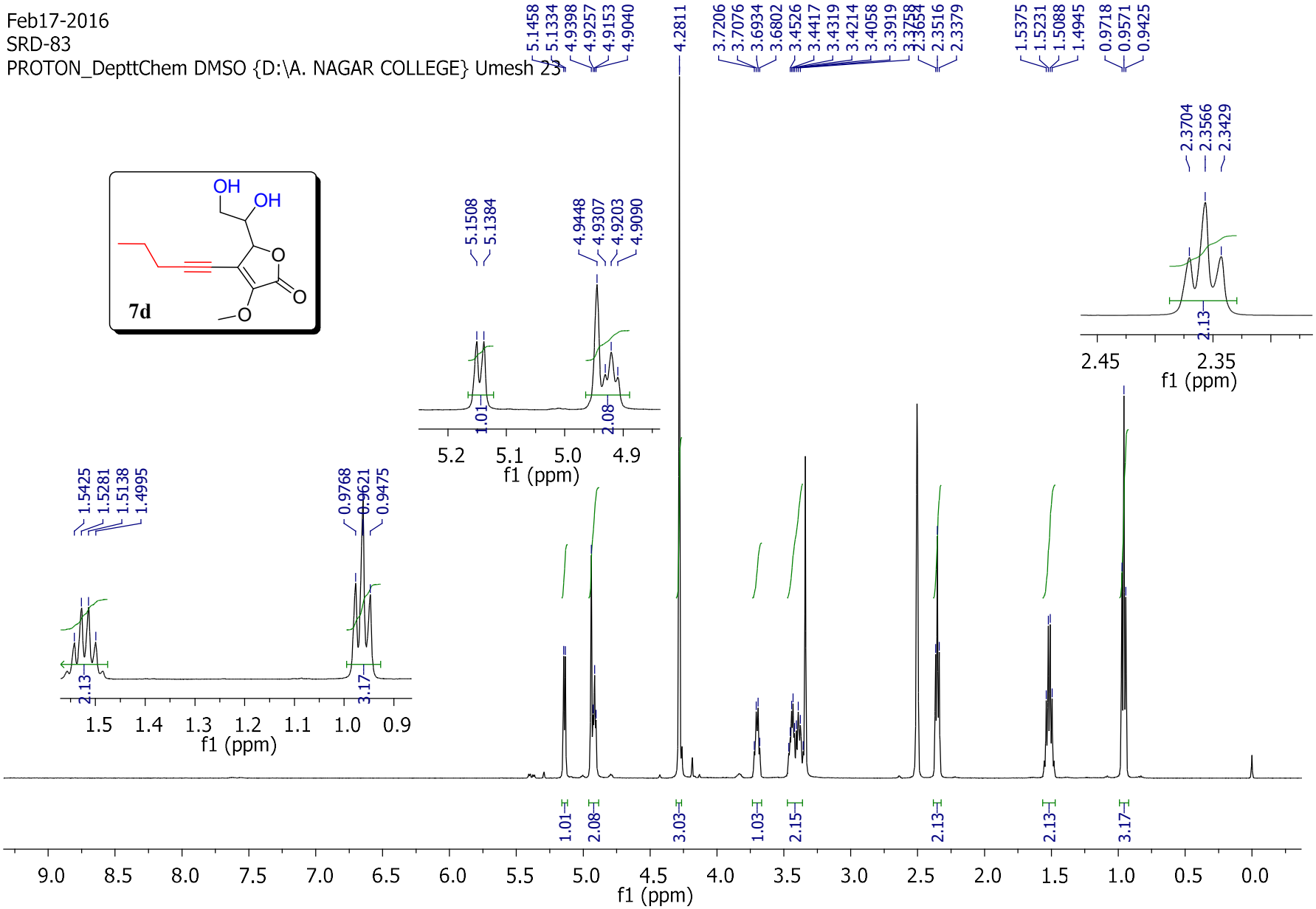

Feb17-2016
SRD-77
C13CPD DMSO {D:\A. NAGAR COLLEGE} Umesh 20
178.1
171.18
160.12
133.14
114.87
114.47
93.30
88.00
78.28
78.03
69.65
62.15
60.75
55.77
40.48
40.32
40.15
39.98
39.81
39.65
39.48
HO
HO
O
O
O
OMe
6f
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

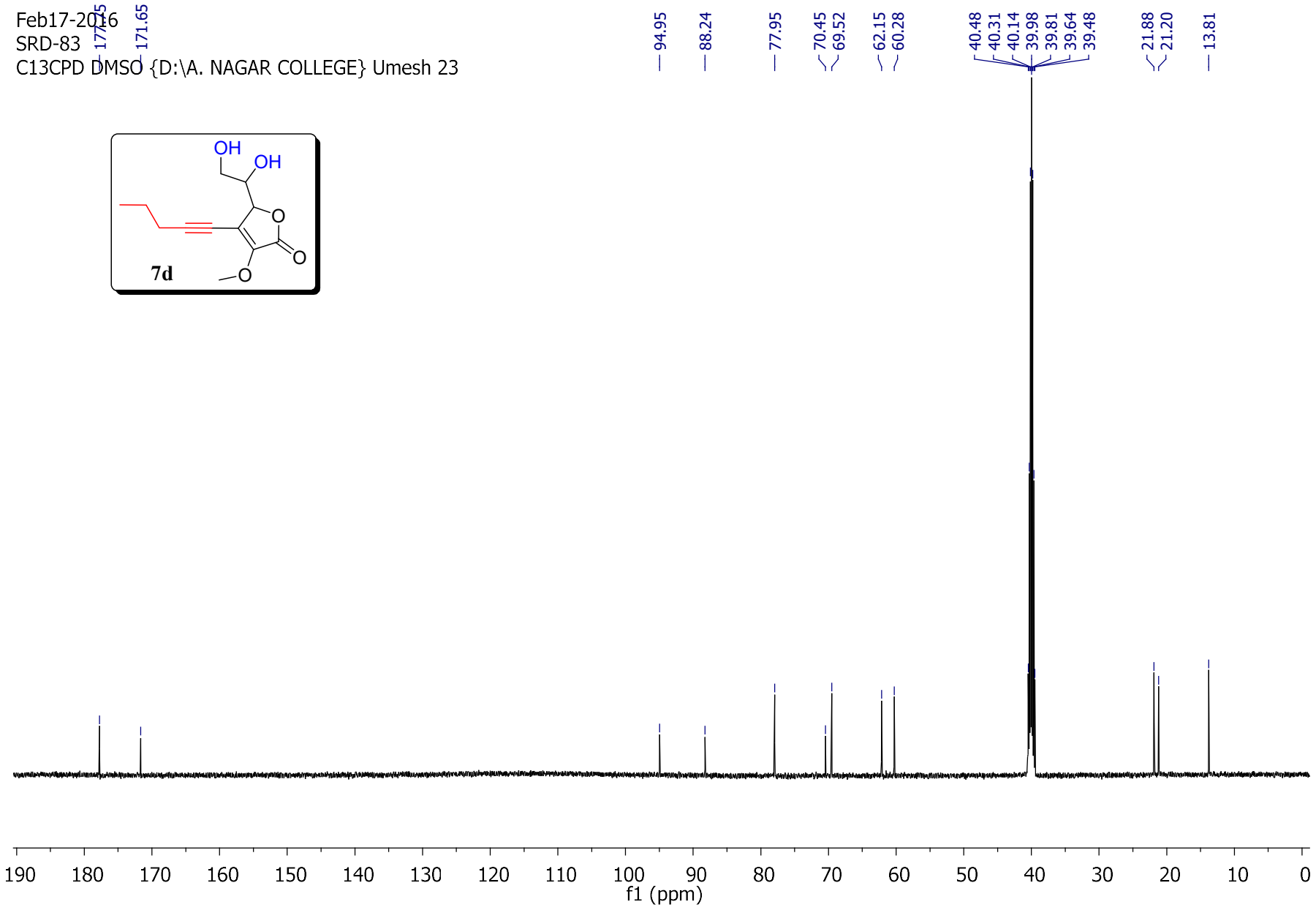

Feb17-2016
SRD-80
PROTON_DepttChem DMSO {D:\A. NAGAR COLLEGE} Umesh 21
HO
HO
O
O
O
6g
5.1470
5.1347
4.9403
4.9271
4.9167
4.9051
4.2813
3.7205
3.7072
3.6933
3.6801
3.4522
3.4416
3.4316
3.4209
3.4057
3.3914
3.3751
3.3548
3.3658
2.3520
2.3384
1.5376
1.5233
1.5090
1.4947
1.4808
0.9721
0.9574
0.9428
1.01
2.03
3.04
1.01
2.09
2.05
2.03
3.03
f1 (ppm)

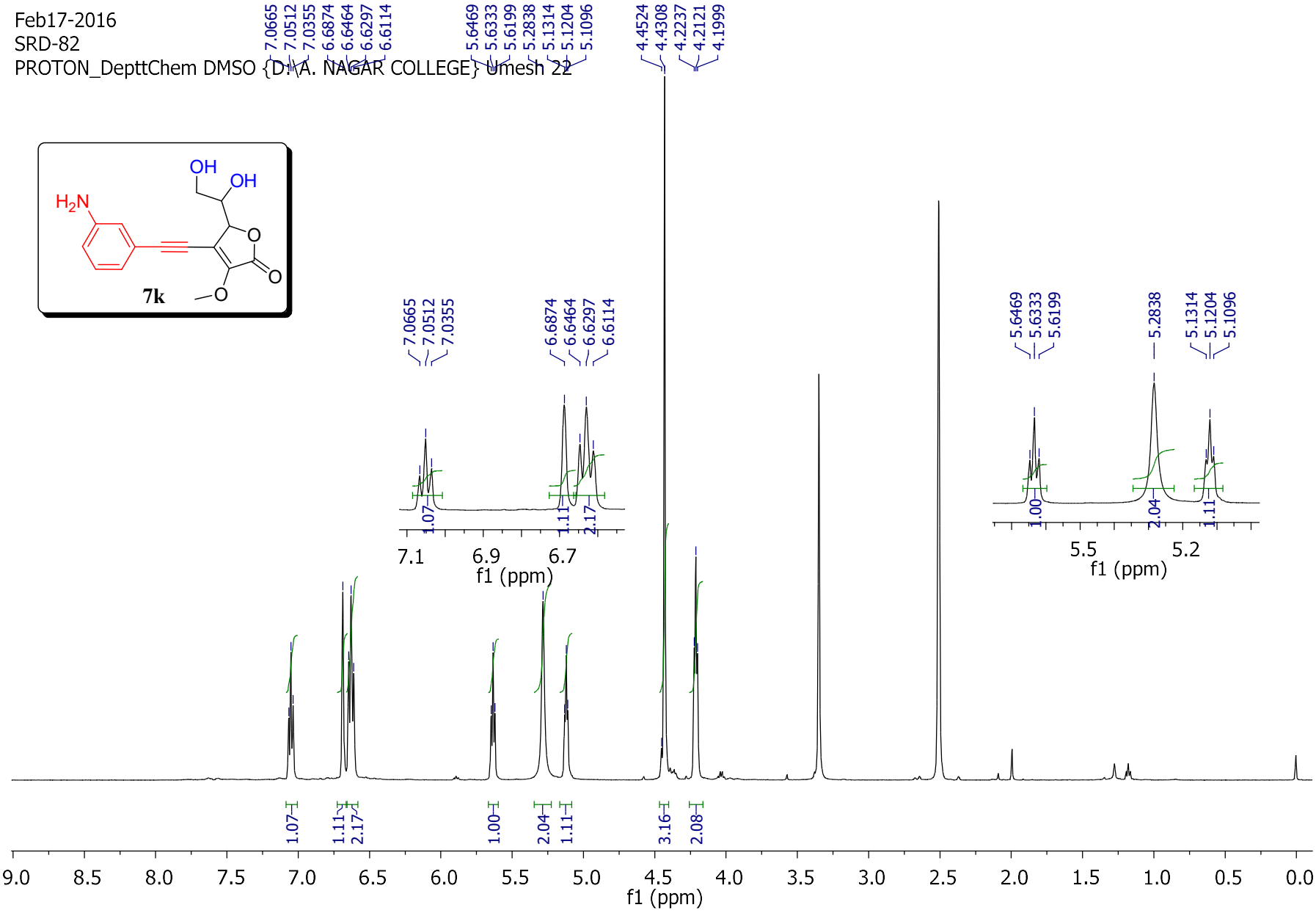

Feb17-2016
SRD-80
C13CPD DMSO {D:\A. NAGAR COLLEGE} Umesh 21
177.55
171.65
94.95
88.24
77.95
70.46
69.52
62.15
60.28
40.48
40.32
40.15
39.98
39.82
39.65
39.48
21.88
21.20
13.81
HO
HO
O
O
O
6g
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

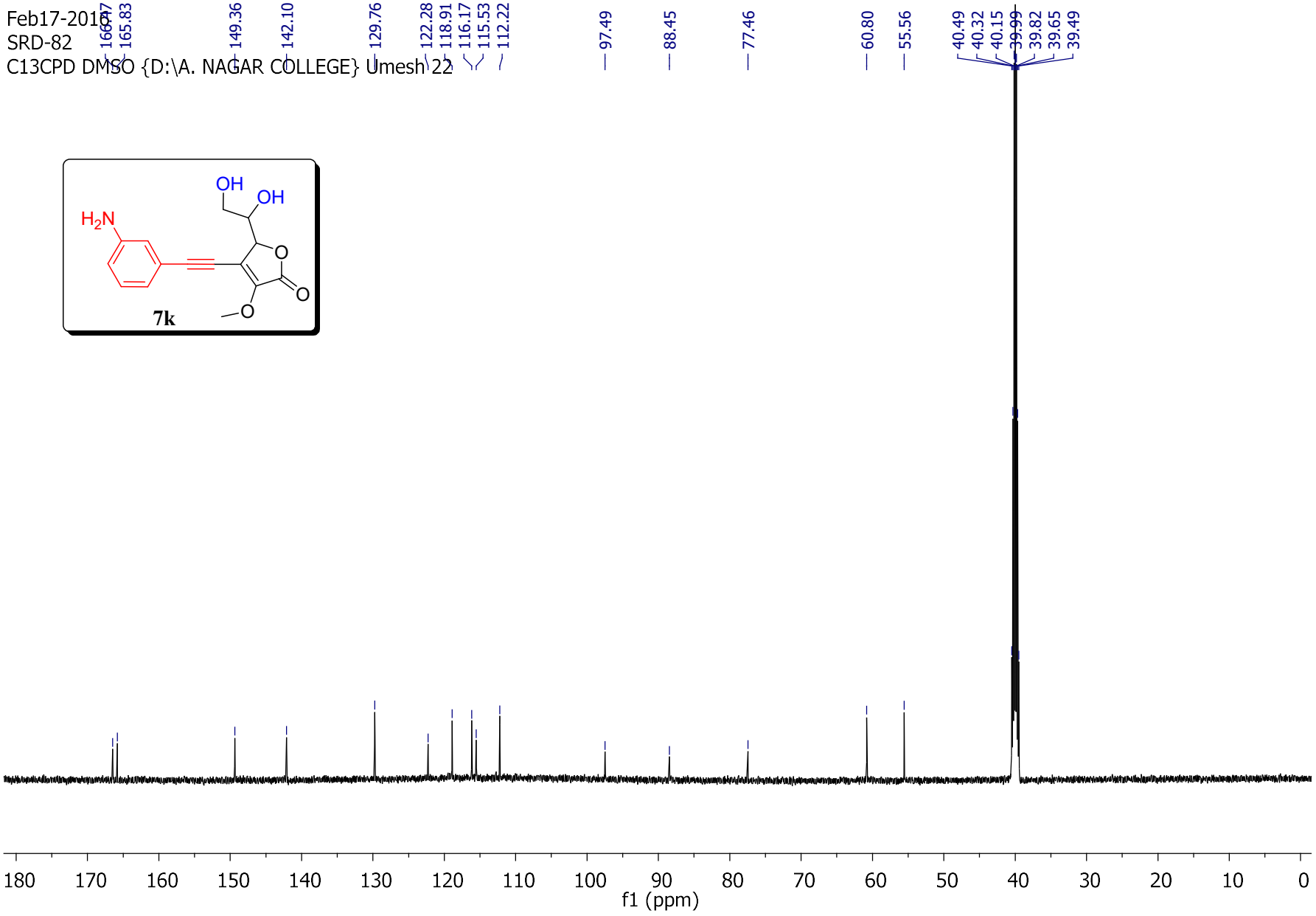

Feb13-2016
SRD-85
PROTON_DepttChem DMSO {D:\A. NAGAR COLLEGE} Umesh 19
7.4855
7.4699
7.4567
7.4413
7.3937
7.3757
7.3558
7.3405
7.2983
7.2954
7.2809
7.2637
5.2519
5.2395
5.0644
4.9779
4.9673
4.9556
4.3941
3.7838
3.7704
3.7565
3.7437
3.4990
3.4882
3.4778
3.4676
3.4566
3.4417
3.4253
3.4116
3.3910
OH
OH
F
O
O
O
7b
1.01
1.99
0.99
1.00
1.00
1.00
3.00
1.01
2.07
7.50
7.40
7.30
f1 (ppm)
5.3
5.2
5.1
5.0
4.9
f1 (ppm)
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
f1 (ppm)


Feb13-2016
SRD-85
C13CPD DMSO {D:\A. NAGAR COLLEGE} Umesh 19
179.04
170.87
163.32
161.37
131.41
131.34
127.90
127.88
124.45
118.21
118.03
116.75
116.59
87.34
80.63
78.47
69.70
62.12
61.11
40.48
40.32
40.15
39.98
39.82
39.65
39.48
OH
OH
F
O
O
O
7b
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


Feb17-2016
SRD-83
PROTON_DepttChem DMSO {D:\A. NAGAR COLLEGE} Umesh 23
OH
OH
O
O
O
O
7d
5.1458
5.1334
4.9398
4.9257
4.9153
4.9040
4.2811
3.7206
3.7076
3.6934
3.6802
3.4526
3.4417
3.4319
3.4214
3.4058
3.3919
3.3758
3.3654
2.3516
2.3379
1.5375
1.5231
1.5088
1.4945
0.9718
0.9571
0.9425
2.3704
2.3566
2.3429
2.13
2.45
2.35
f1 (ppm)
5.1508
5.1384
4.9448
4.9307
4.9203
4.9090
1.01
2.08
5.2
5.1
5.0
4.9
f1 (ppm)
1.5425
1.5281
1.5138
1.4995
0.9768
0.9621
0.9475
2.13
3.17
1.5
1.4
1.3
1.2
1.1
1.0
0.9
f1 (ppm)
1.01
2.08
3.03
1.03
2.15
2.13
2.13
3.17
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
f1 (ppm)


Feb17-2016
SRD-83
C13CPD DMSO {D:\A. NAGAR COLLEGE} Umesh 23
177.05
171.65
94.95
88.24
77.95
70.45
69.52
62.15
60.28
40.48
40.31
40.14
39.98
39.81
39.64
39.48
21.88
21.20
13.81
OH
OH
O
O
O
7d
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


Feb17-2016
SRD-82
PROTON_DepttChem DMSO {D:\A. NAGAR COLLEGE} Umesh 22
7.0665
7.0512
7.0355
6.6874
6.6464
6.6297
6.6114
5.6469
5.6333
5.6199
5.2838
5.1314
5.1204
5.1096
4.4524
4.4308
4.2237
4.2121
4.1999
OH
OH
H2N
O
O
O
O
7k
1.07
1.11
2.17
1.00
2.04
1.11
3.16
2.08
f1 (ppm)


Feb17-2016
SRD-82
C13CPD DMSO {D:\A. NAGAR COLLEGE} Umesh 22
166.47
165.83
149.36
142.10
129.76
122.28
118.91
116.17
115.53
112.22
97.49
88.45
77.46
60.80
55.56
40.49
40.32
40.15
39.99
39.82
39.65
39.49
OH
OH
H2N
O
O
O
7k
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

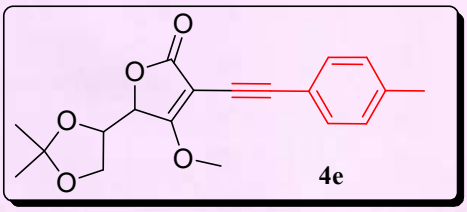
F: HPLC Data

7/24/2017 15:20:56 1

==== Shimadzu LCsolution Analysis Report ====

C:\Chandu\2017\July2017\24072017\Data\03.lcd

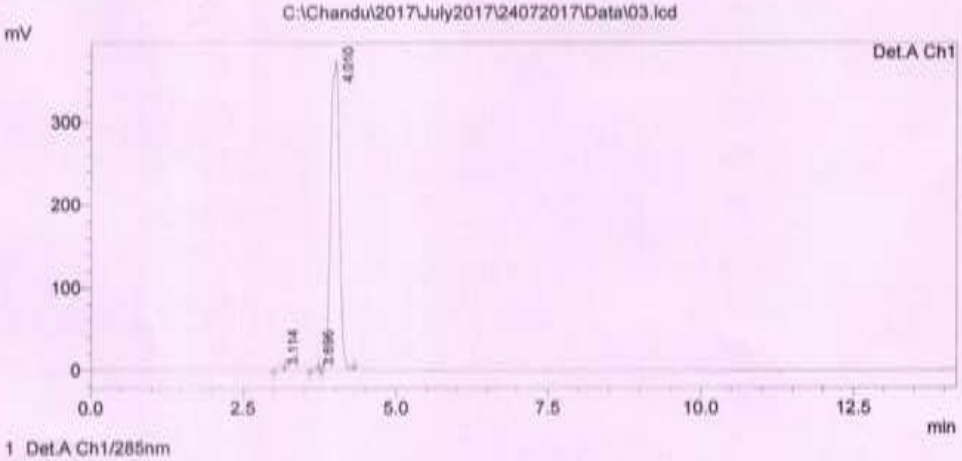
Acquired by	: Admin
Sample Name	: SRD-63
Sample ID	: Mthanol
Tray#	: 1
Vail #	: 3
Injection Volume	: 2 uL
Data File Name	: 03.lcd
Method File Name	: wat-8.lcm
Batch File Name	: 01.lcb
Report File Name	: Default.lcr
Data Acquired	: 7/24/2017 2:17:55 PM
Data Processed	: 7/24/2017 2:32:12 PM



4e

<Chromatogram>

C:\Chandu\2017\July2017\24072017\Data\03.lcd



1 Det.A Ch1/285nm

PeakTable

Detector A Ch1 285nm

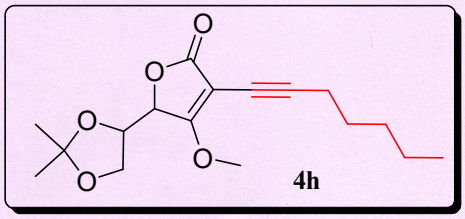
Peak#	Ret. Time	Area	Height	Area %
1	3.114	7021	1024	0.187
2	3.696	1223	208	0.033
3	4.010	3739140	373322	99.780
Total		3747384	374554	100.000

C:\Chandu\2017\July2017\24072017\Data\03

==== Shimadzu LCsolution Analysis Report ====

C:\Chandu\2017\July2017\24072017\Data\04.lcd

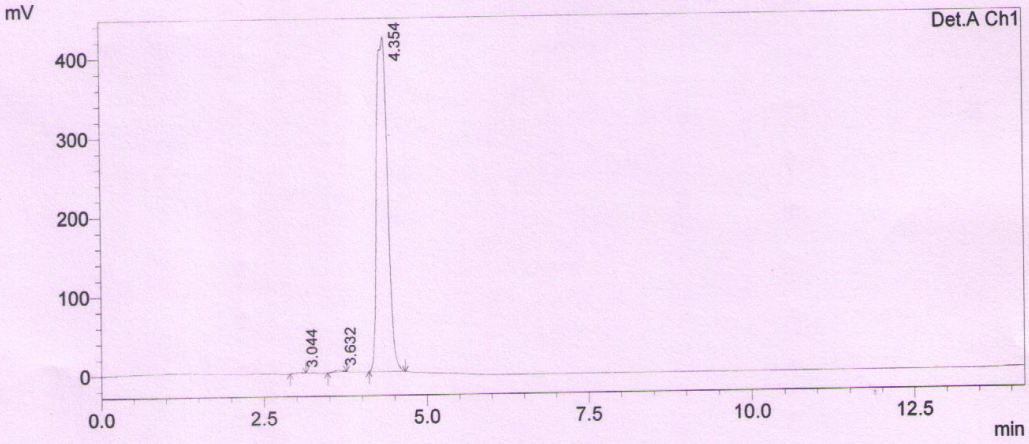
Acquired by	: Admin
Sample Name	: SRD-64
Sample ID	: Mthanol
Tray#	: 1
Vail #	: 4
Injection Volume	: 5 uL
Data File Name	: 04.lcd
Method File Name	: wat-8.lcm
Batch File Name	: 01.lcb
Report File Name	: Default.lcr
Data Acquired	: 7/24/2017 2:50:07 PM
Data Processed	: 7/24/2017 3:04:21 PM



4h

<Chromatogram>

C:\Chandu\2017\July2017\24072017\Data\04.lcd



1 Det.A Ch1/257nm

PeakTable

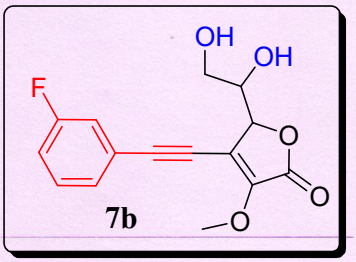
Detector A Ch1 257nm

Peak#	Ret. Time	Area	Height	Area %
1	3.044	10954	1563	0.222
2	3.632	20369	2252	0.413
3	4.354	4904070	421598	99.365
Total		4935393	425412	100.000

==== Shimadzu LCsolution Analysis Report ====

C:\Chandu\2017\July2017\24072017\Data\02.lcd

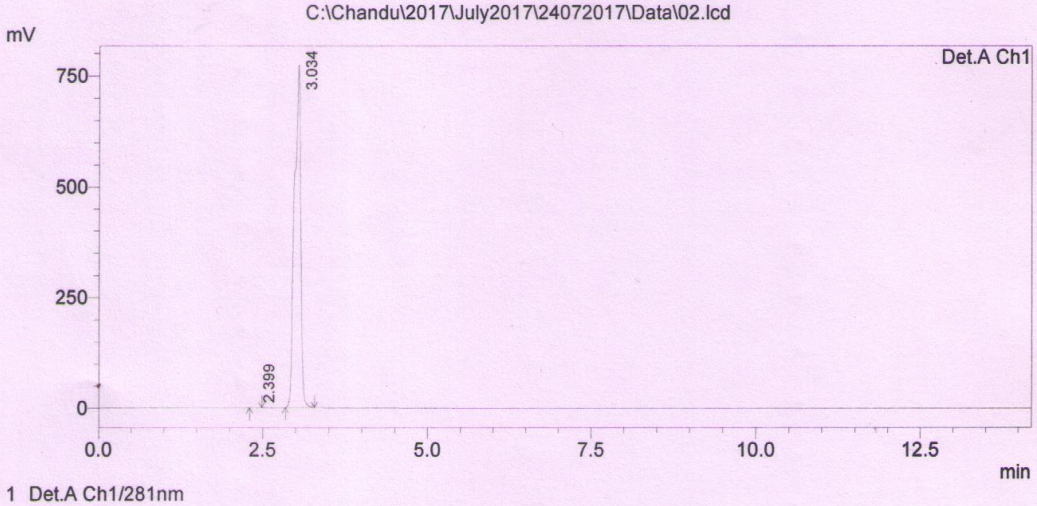
Acquired by	: Admin
Sample Name	: SRD-85
Sample ID	: Mthanol
Tray#	: 1
Vail #	: 2
Injection Volume	: 5 uL
Data File Name	: 02.lcd
Method File Name	: wat-8.lcm
Batch File Name	: 01.lcb
Report File Name	: Default.lcr
Data Acquired	: 7/24/2017 12:21:44 PM
Data Processed	: 7/24/2017 12:35:59 PM



7b

<Chromatogram>

C:\Chandu\2017\July2017\24072017\Data\02.lcd



1 Det.A Ch1/281nm

PeakTable

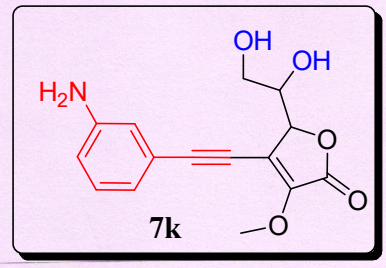
Detector A Ch1 281nm

Peak#	Ret. Time	Area	Height	Area %
1	2.399	3285	727	0.063
2	3.034	5177838	770581	99.937
Total		5181124	771309	100.000

==== Shimadzu LCsolution Analysis Report ====

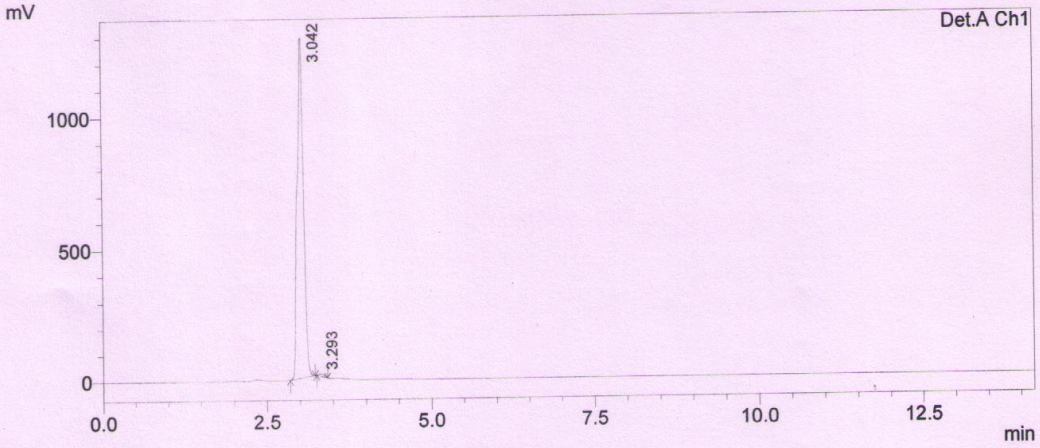
C:\Chandu\2017\July2017\24072017\Data\01.lcd

Acquired by	: Admin
Sample Name	: SRD-82
Sample ID	: Mthanol
Tray#	: 1
Vail #	: 1
Injection Volume	: 5 uL
Data File Name	: 01.lcd
Method File Name	: wat-8.lcm
Batch File Name	: 01.lcb
Report File Name	: Default.lcr
Data Acquired	: 4/28/2002 9:11:30 PM
Data Processed	: 7/24/2017 11:54:19 AM



<Chromatogram>

C:\Chandu\2017\July2017\24072017\Data\01.lcd



1 Det.A Ch1/325nm

PeakTable

Detector A Ch1 325nm

Peak#	Ret. Time	Area	Height	Area %
1	3.042	8434658	1282467	99.388
2	3.293	51954	6606	0.612
Total		8486612	1289073	100.000