

Supporting Information

For

**Pyrolysis of azetidinone derivatives: A versatile route toward electron-rich alkenes, C-1
allylation and/or homologation of aldehydes**

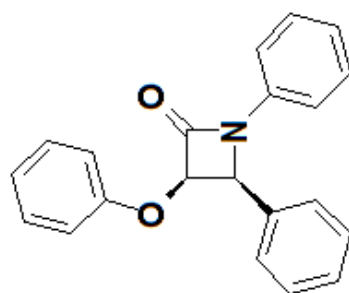
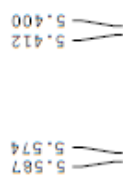
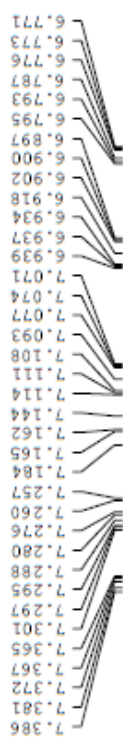
Nouf Al-Hamdan, Osama M. Habib, Yehia A. Ibrahim, Nouria A. Al-Awadi.*

Chemistry Department, Faculty of science, Kuwait University, P.O. Box 5969, Safat
13060, Kuwait.

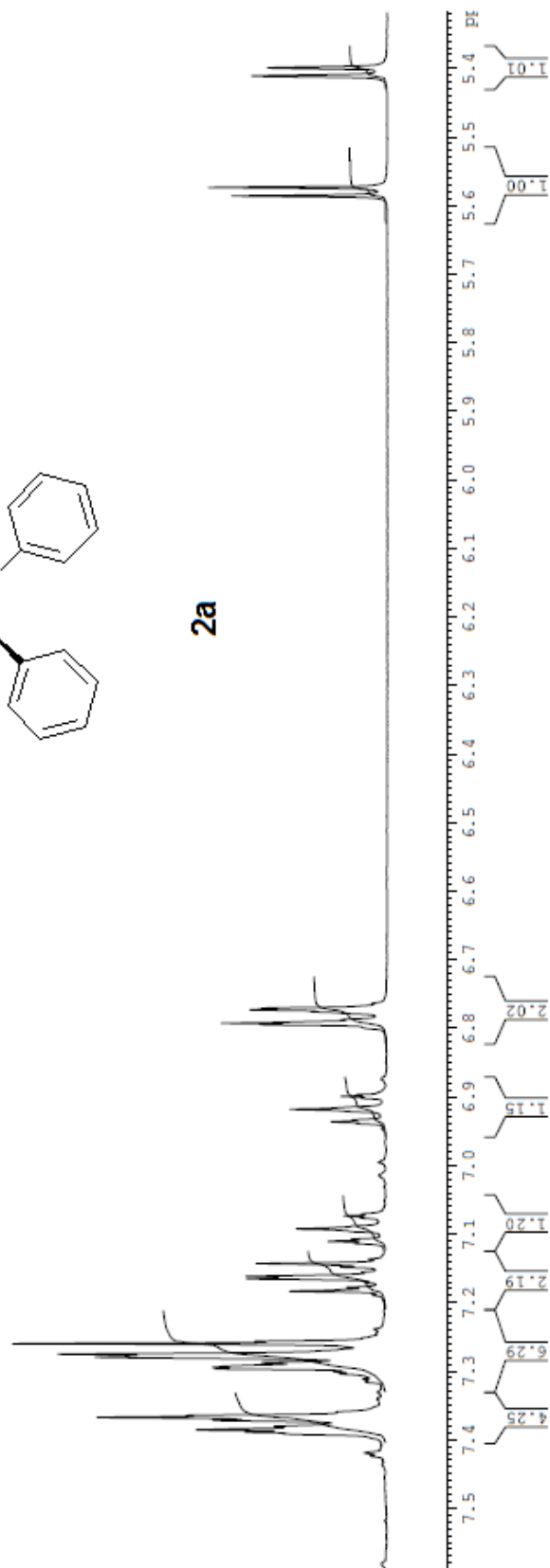
Correspondence author: *E*-mail address: n.alawadi@ku.edu.kw

Tel: (+) 96524985537; Fax: (+) 96524816482

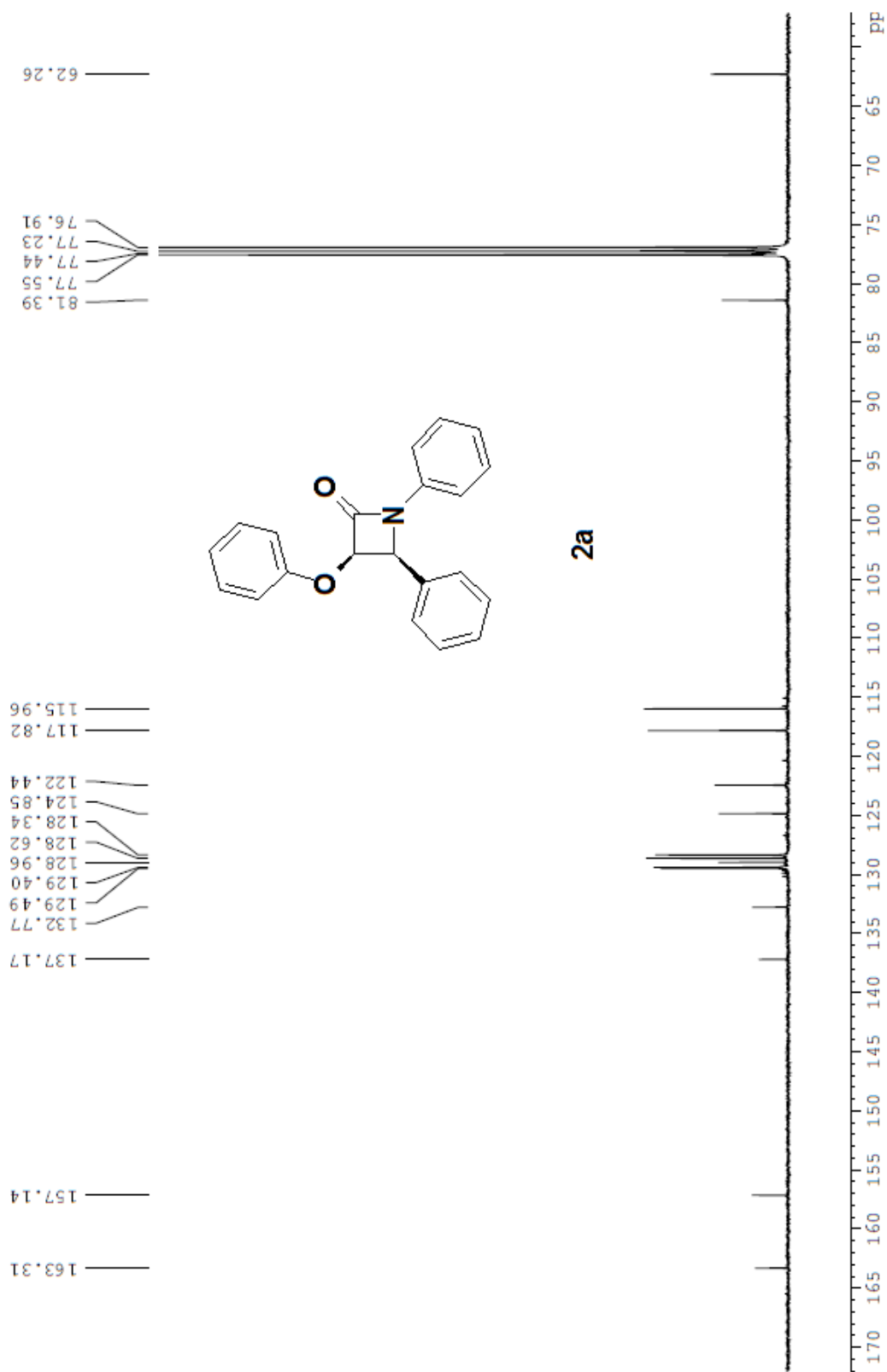
¹H spectrum Nouf 2a in CDCl₃



2a



¹³C decoupled spectra Nouf 2a in CDCl₃

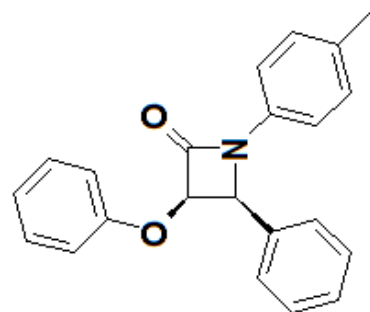


¹H spectra Osama 2B in CDCL₃

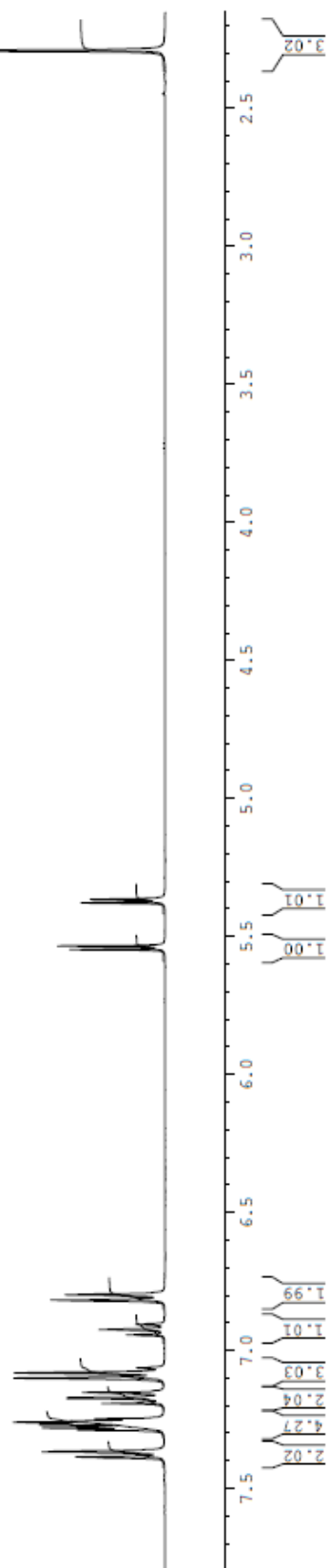
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7.365
7.288
7.261
7.248
7.192
7.171
7.152
7.101
7.082
7.066
6.943
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6.906
6.817
6.796

5.547
5.535
5.378
5.365

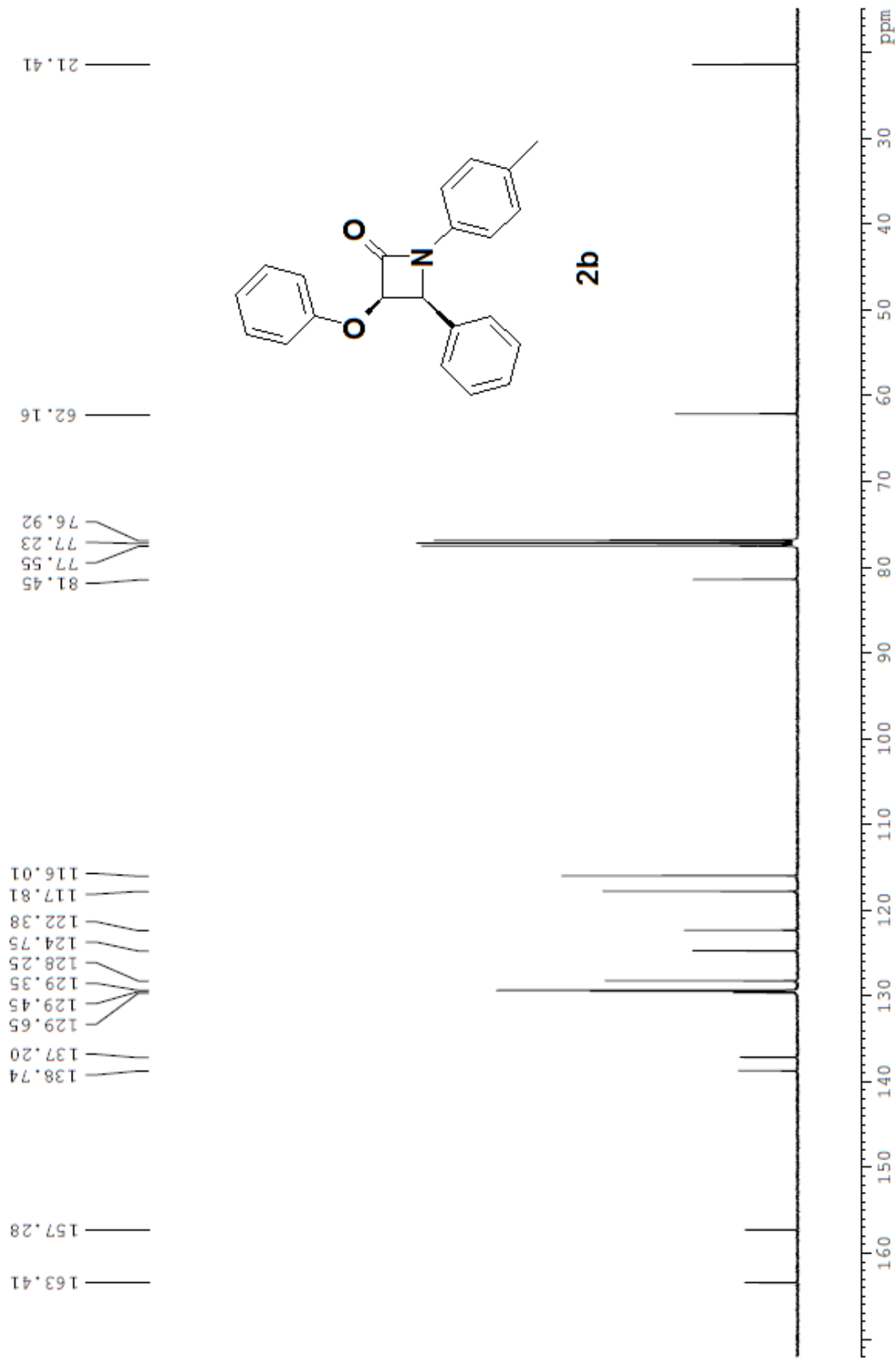
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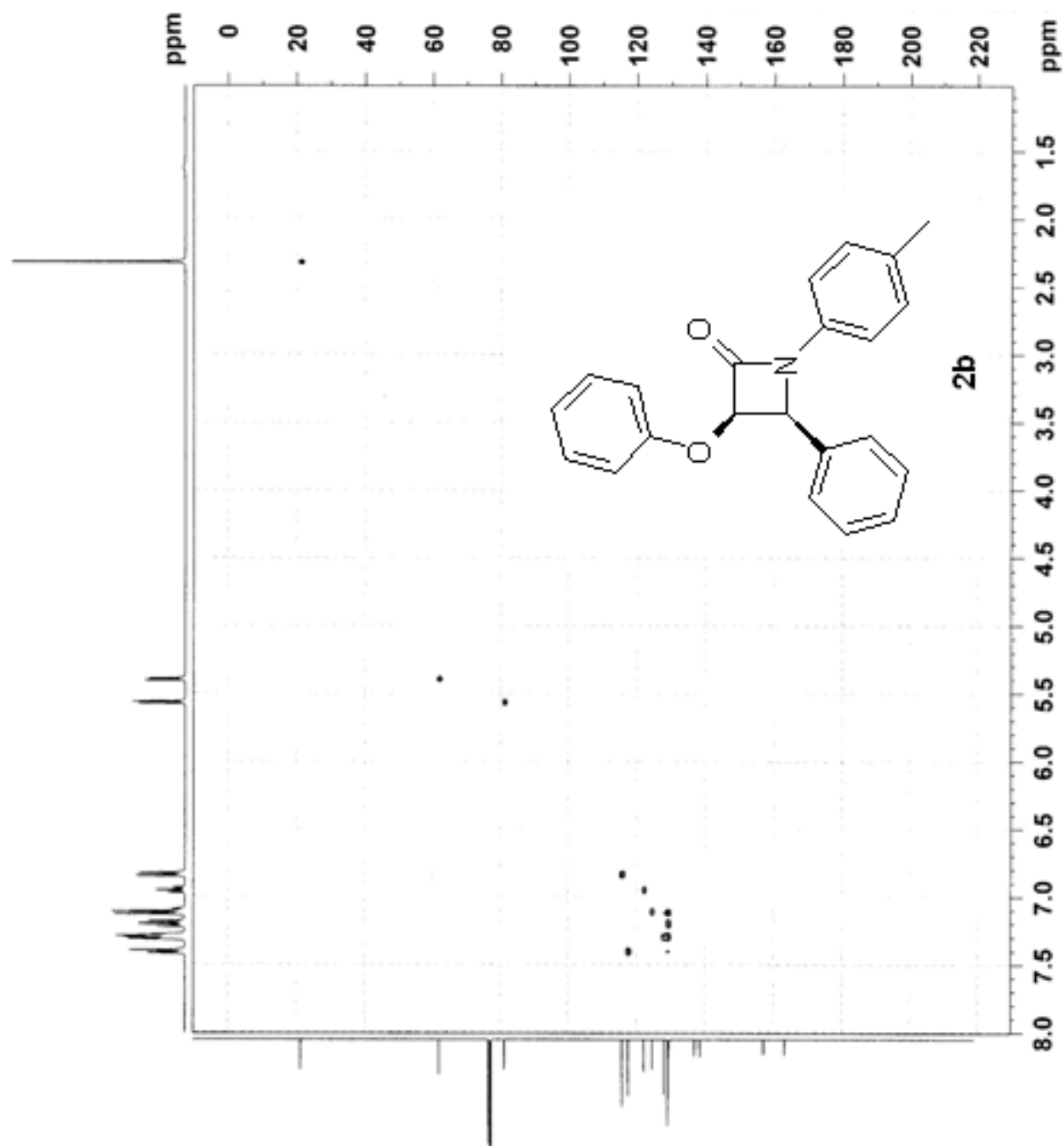


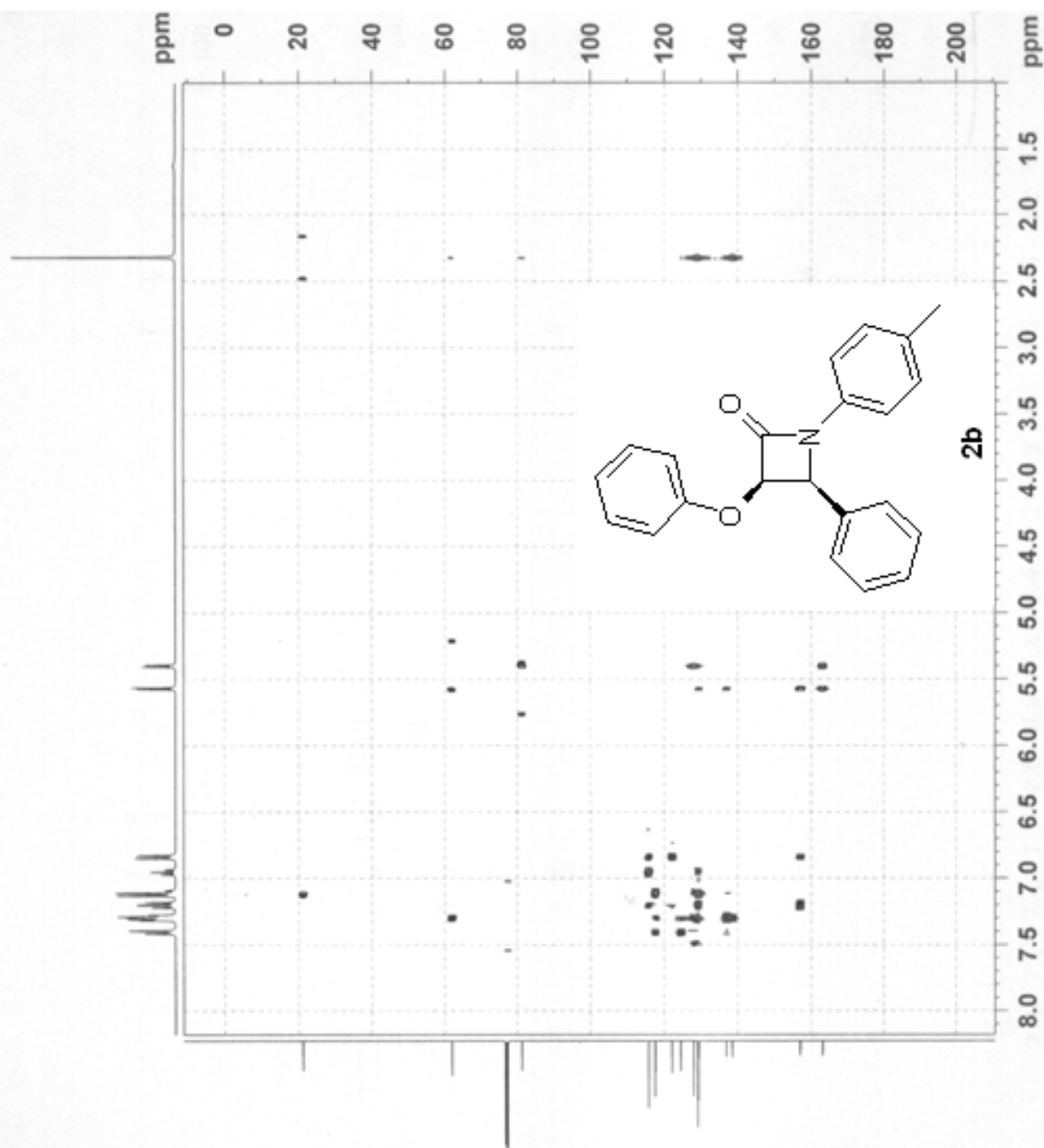
2b



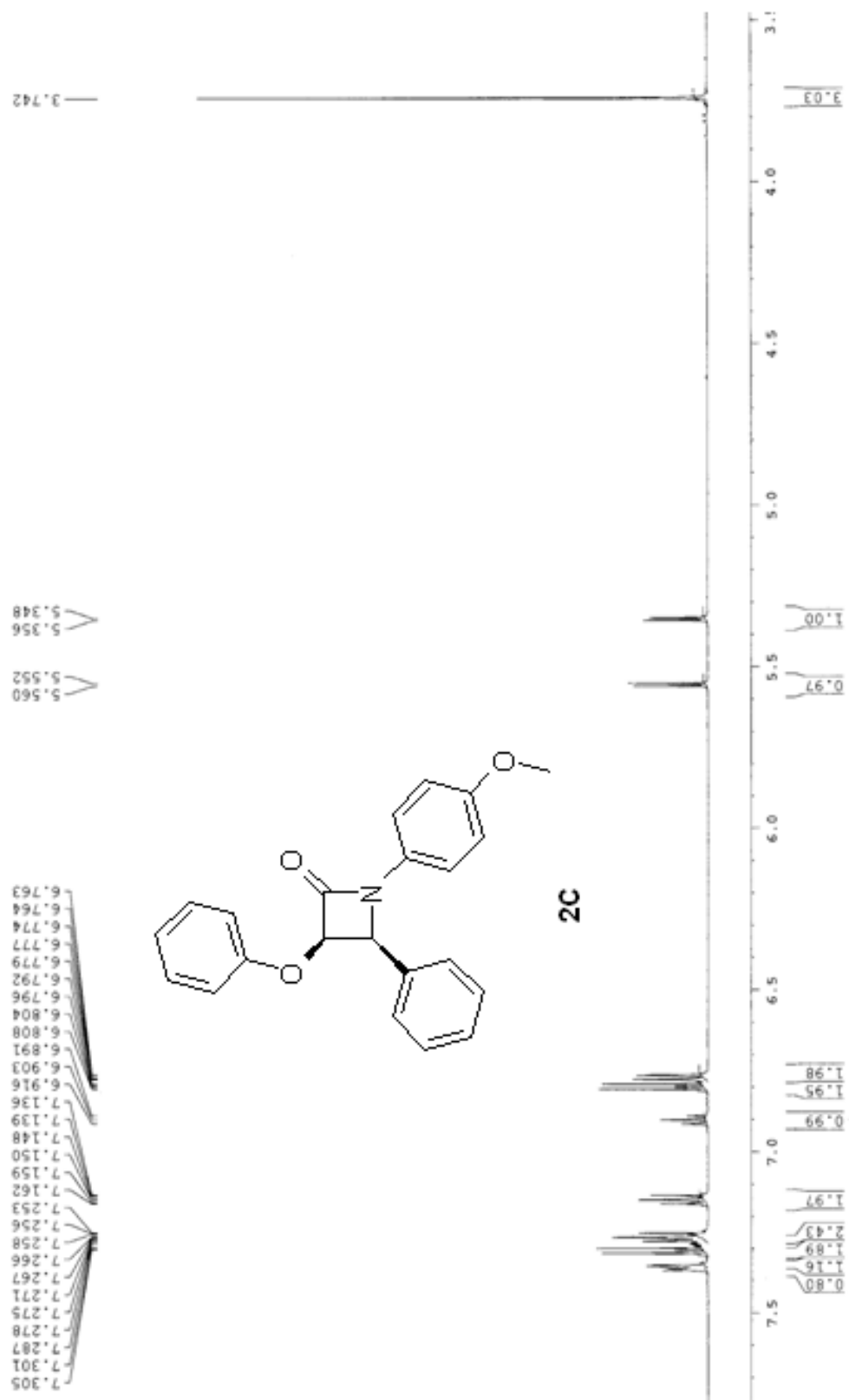
¹³C decoupled spectra Osama 2B in CDCL₃



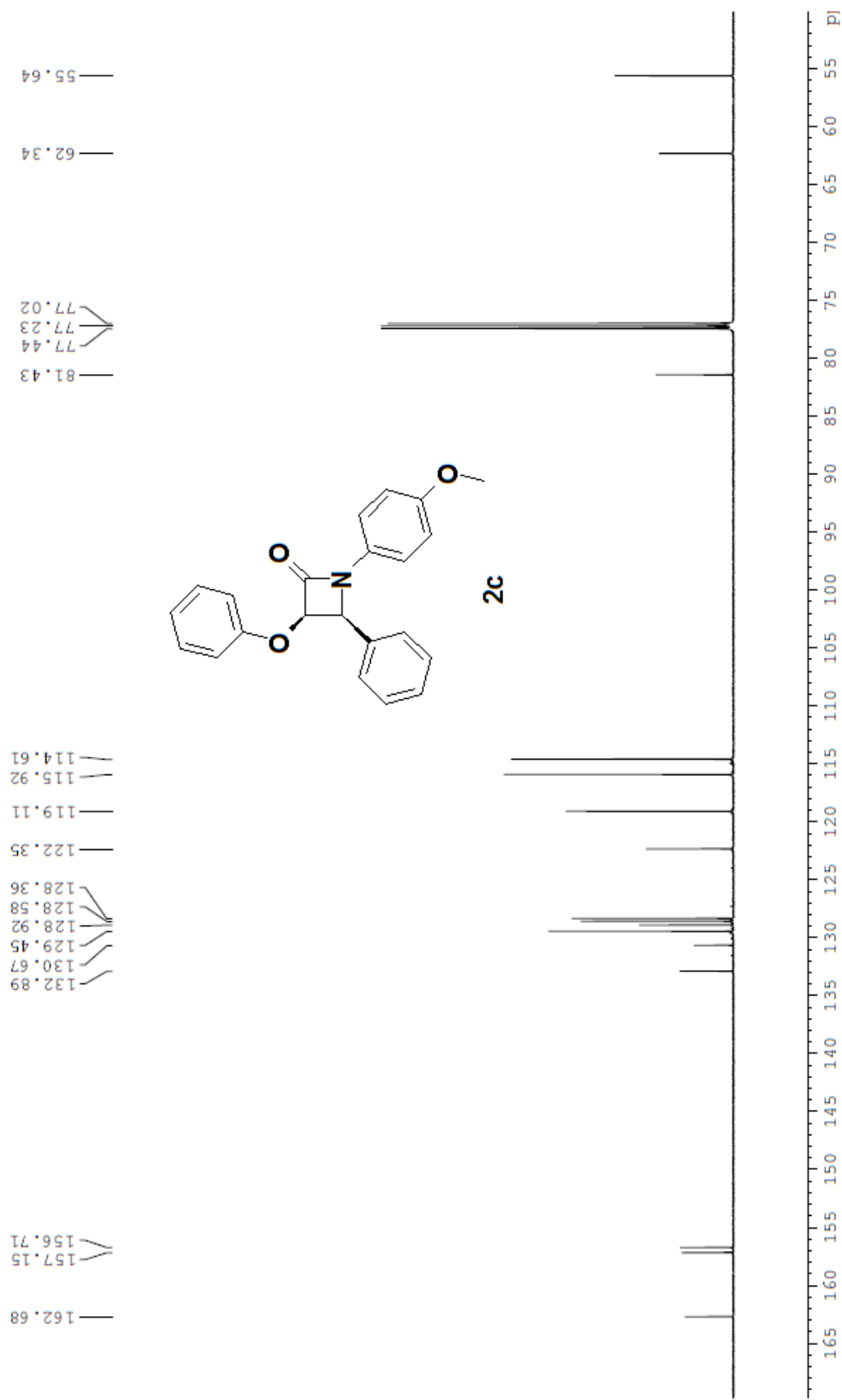




¹H spectrum Osama 2C in CDCl₃



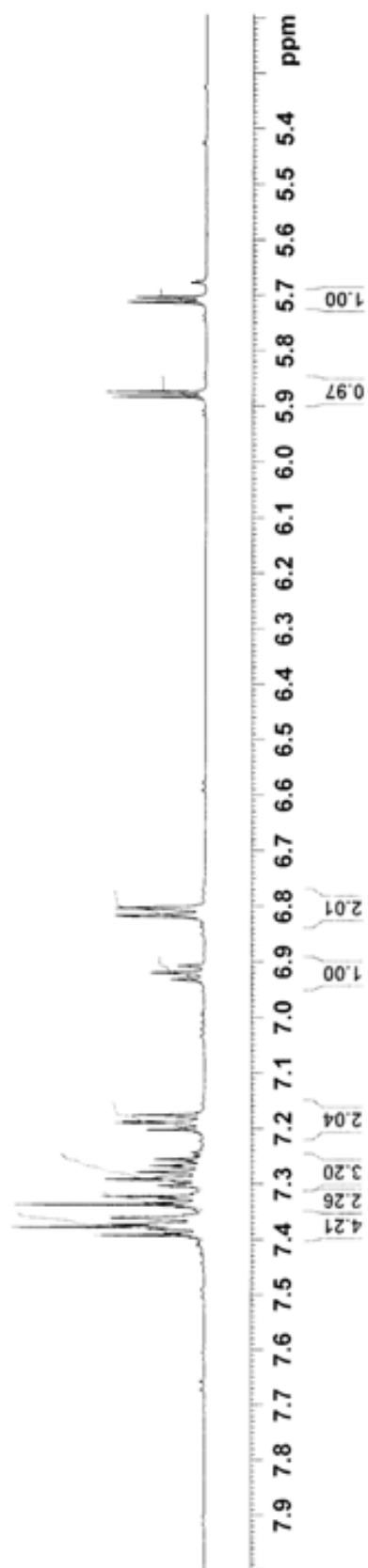
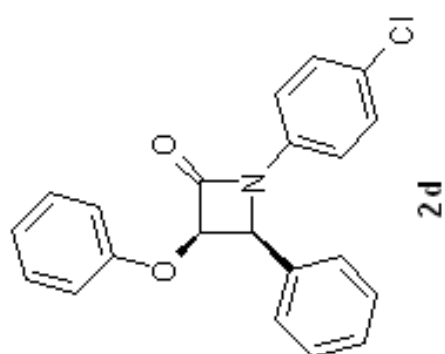
¹³C decoupled spectrum Osama 2c in CDCl₃



¹H Spectra Dr.OSAMA Cis ClA in DMSO (at 90c)

7.392
7.377
7.377
7.337
7.337
7.322
7.372
7.359
7.304
7.290
7.278
7.268
7.254
7.204
7.189
7.176
6.933
6.918
6.908
6.816
6.804

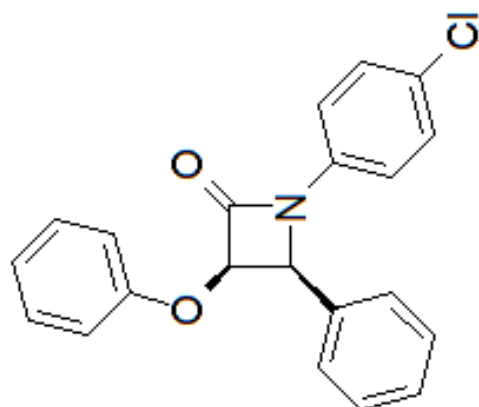
5.885
5.875
5.713
5.703
5.679



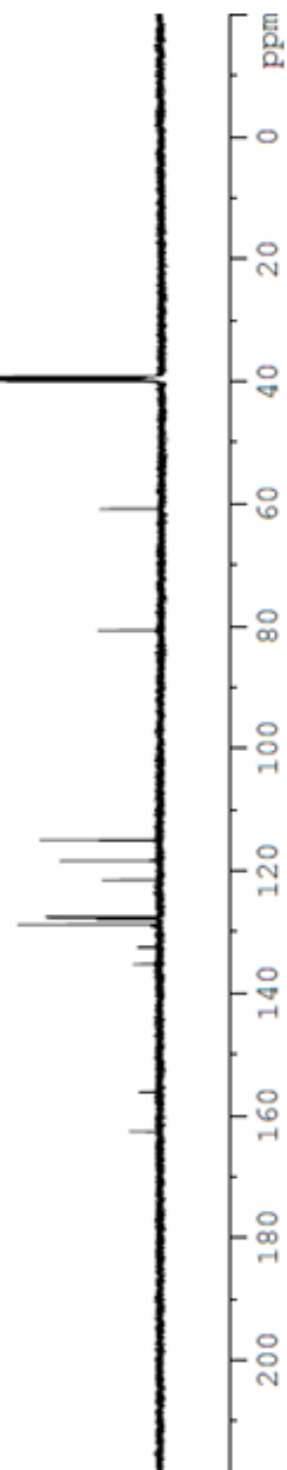
¹³C decoupled spectra Dr.OSAMA Cis ClA in DMSO (at90c)

162.65
156.21
135.27
132.53
129.18
128.83
128.78
127.94
127.86
127.73
127.63
121.53
118.46
115.00

60.86
40.06
39.94
39.80
39.66
39.52
39.38
39.24
39.10



2d

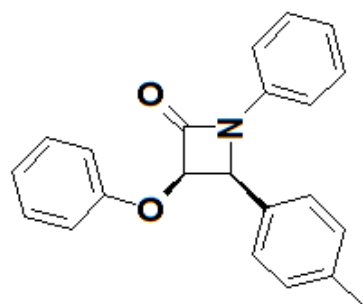


¹H spectrum Osama 2e in CDCl₃

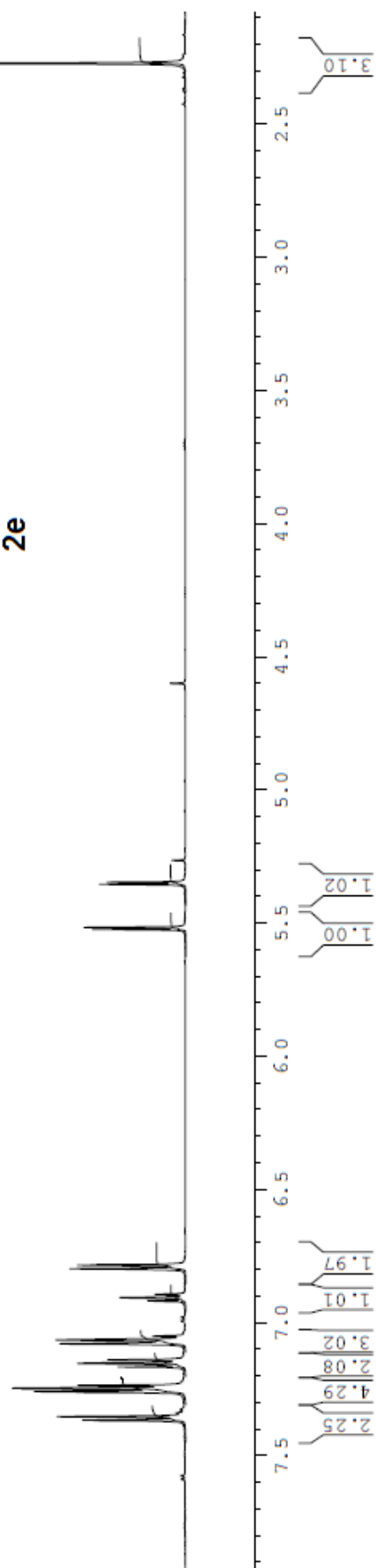
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7.354
7.263
7.260
7.249
7.247
7.237
7.167
7.164
7.155
7.153
7.141
7.080
7.067
7.052
6.920
6.907
6.895
6.798
6.785

5.525
5.517
5.355
5.347

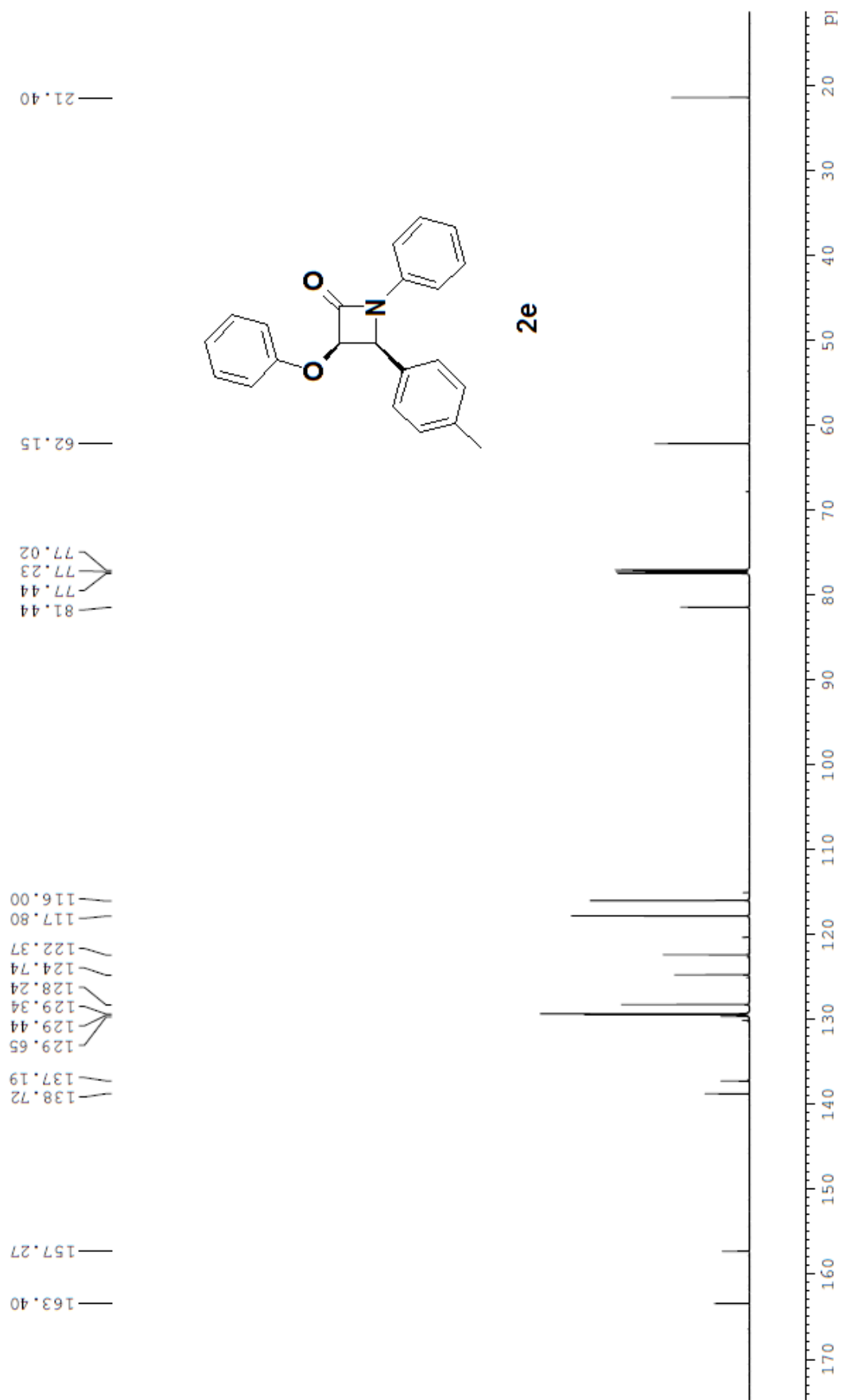
2.272



2e



¹³C decoupled spectrum Osama 2e in CDCl₃

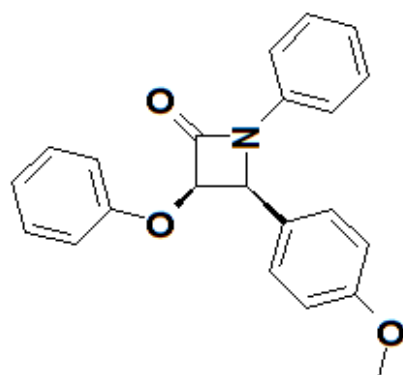


¹H spectra Osama methoxy B in CDCL₃

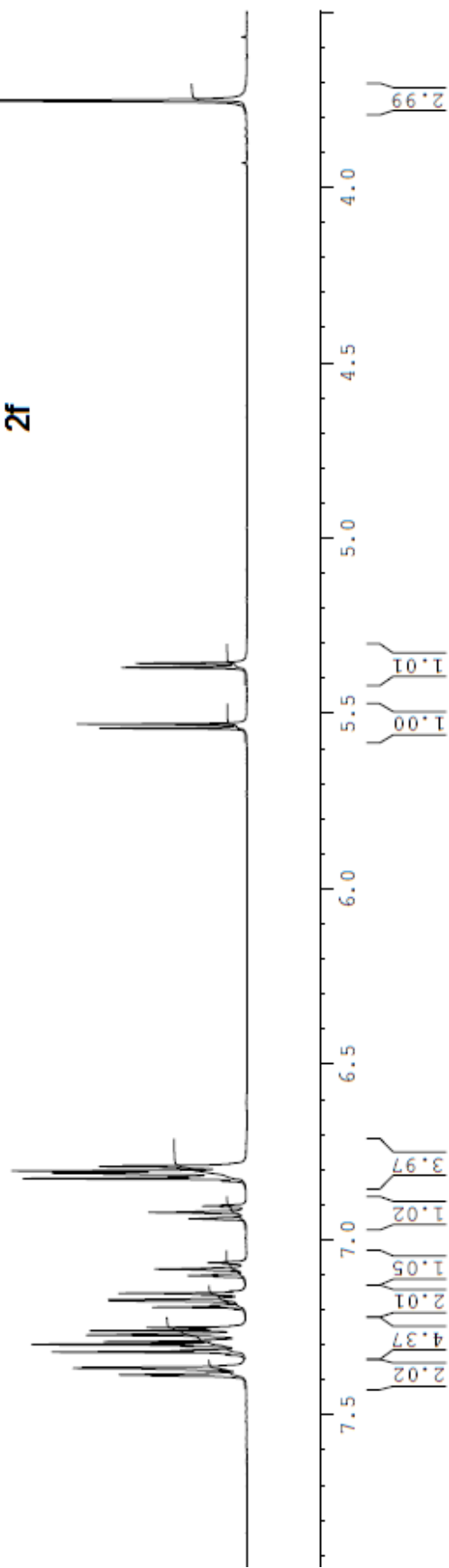
7.390
7.368
7.365
7.322
7.300
7.292
7.273
7.260
7.252
7.194
7.176
7.172
7.154
7.104
7.086
7.067
6.942
6.923
6.905
6.827
6.815
6.812
6.805
6.793
6.790

5.543
5.531
5.370
5.358

3.754



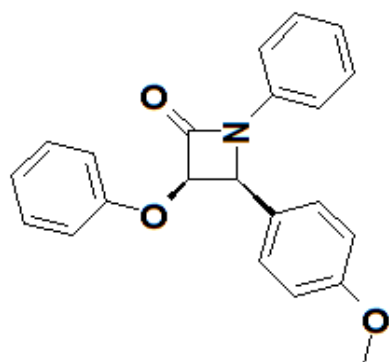
2f



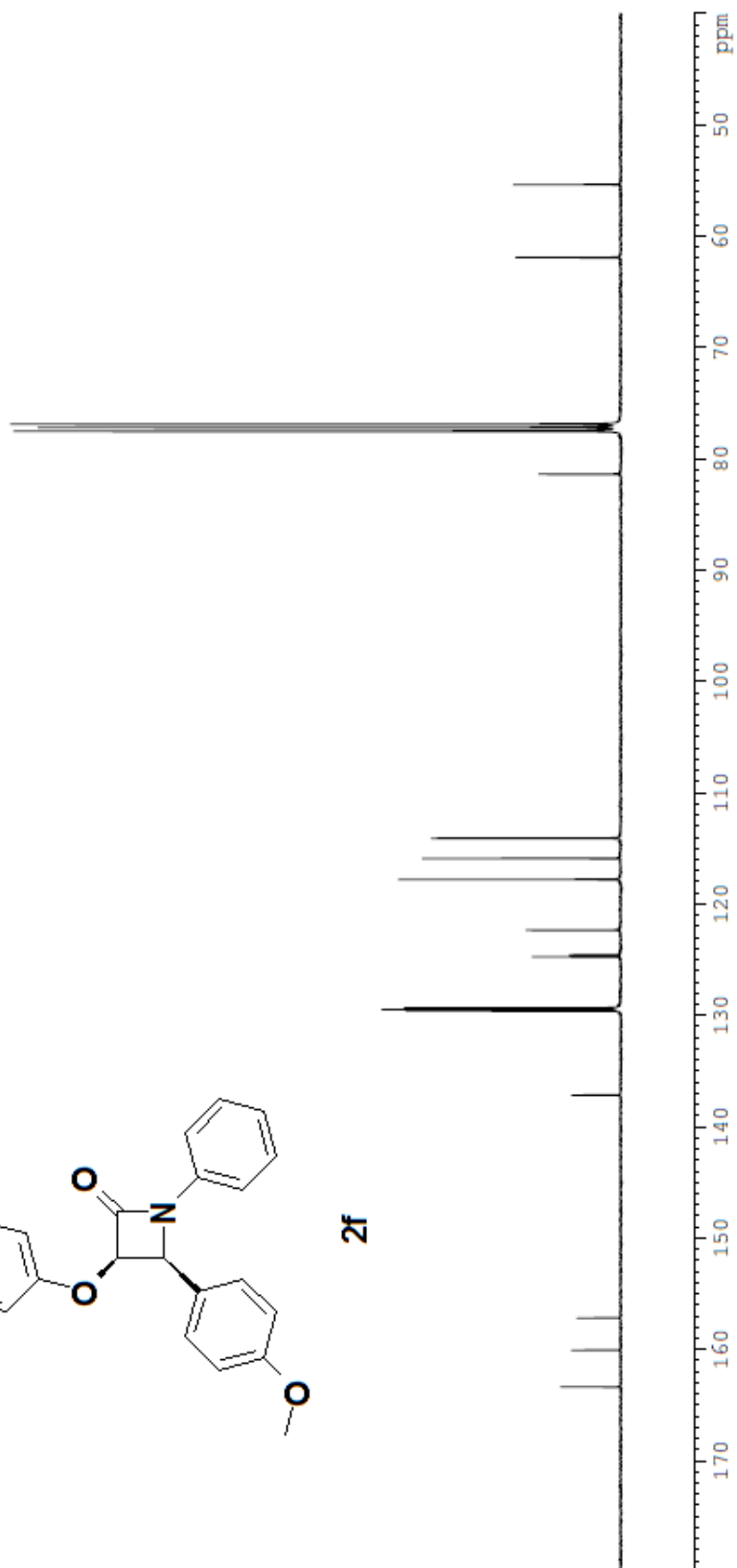
¹³C decoupled spectra Osama methoxyB in CDCl₃

163.39
160.09
157.22
137.19
129.62
129.49
129.35
124.77
124.58
122.38
117.83
115.93
114.10

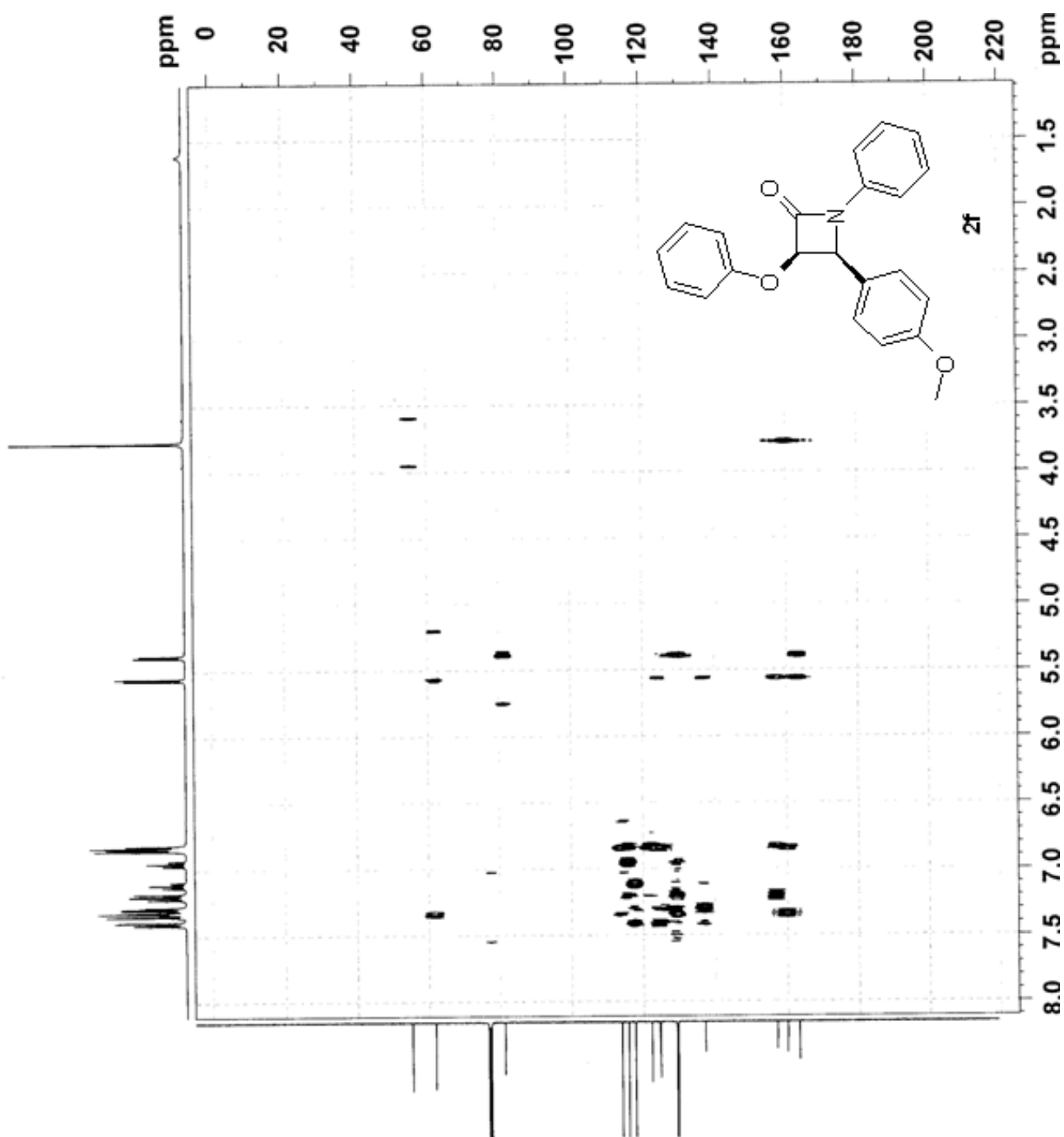
81.41
77.55
77.23
76.92
61.93
55.40



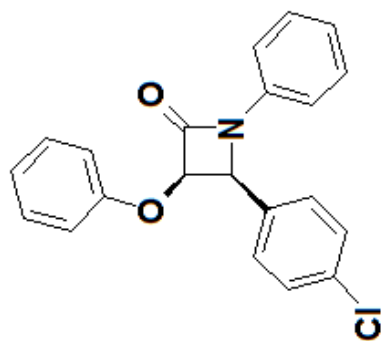
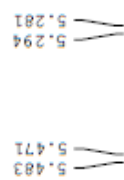
2f



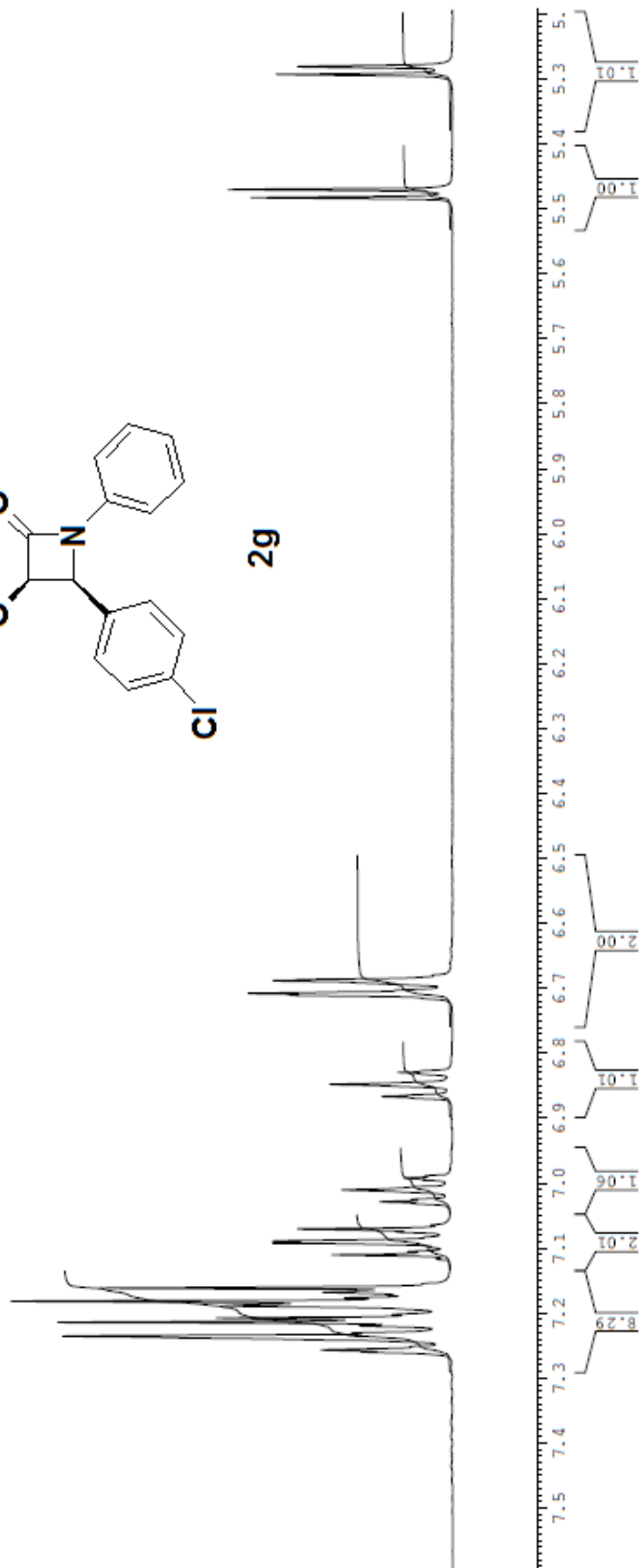
¹³C HMBC spectra Methoxy B in CDCl₃



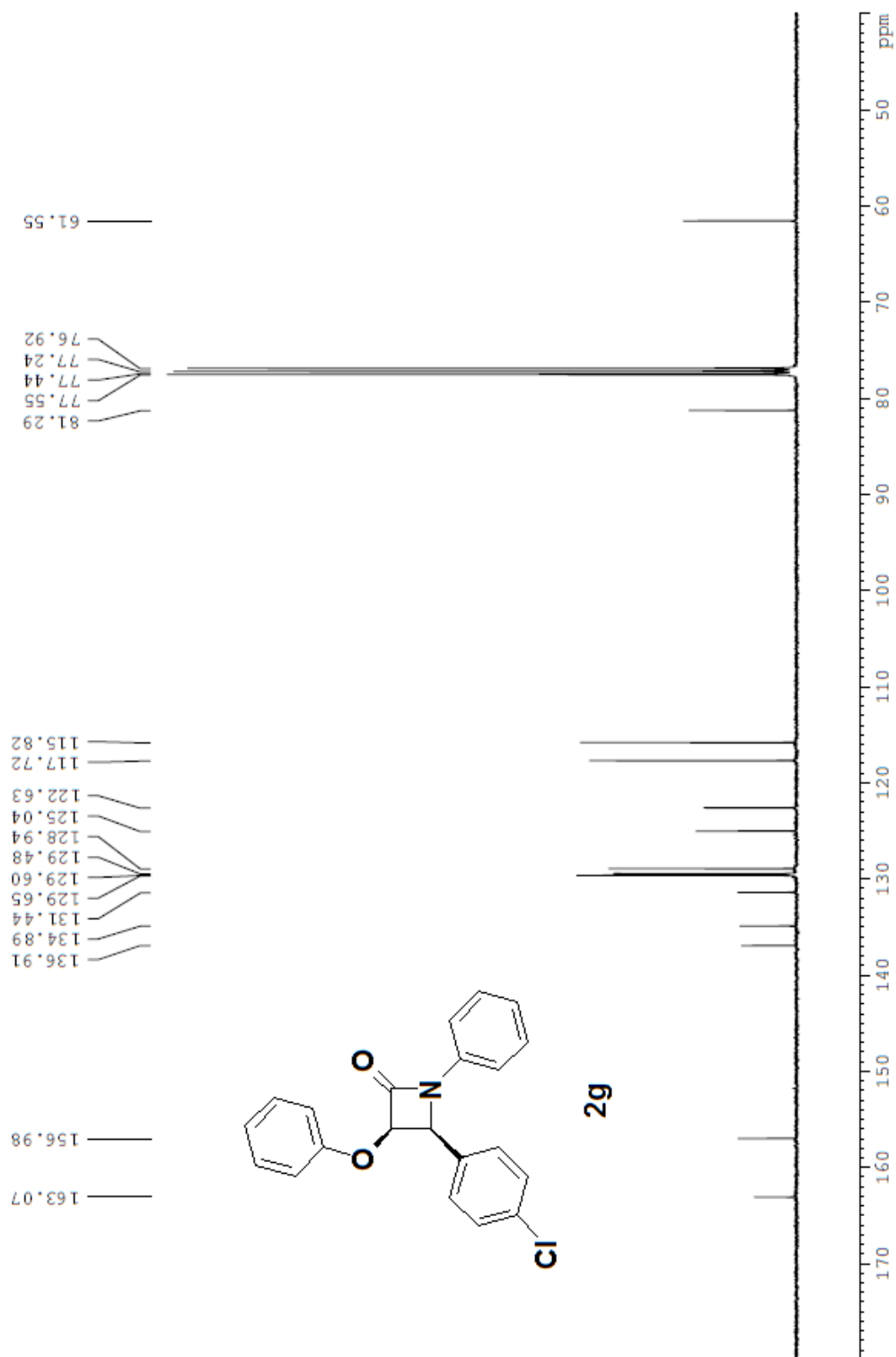
¹H spectra Osama ClB in CDCL₃

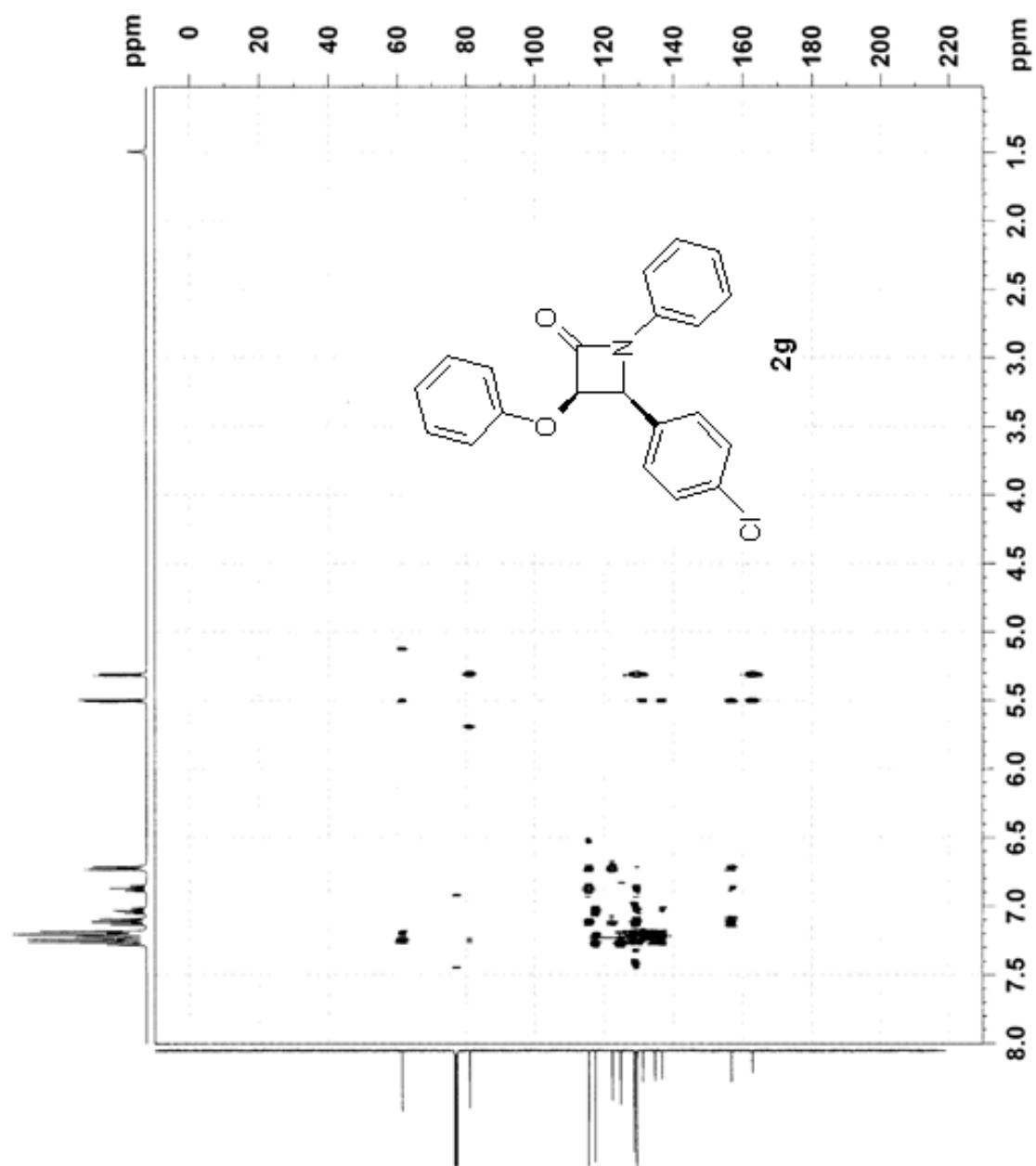


2g

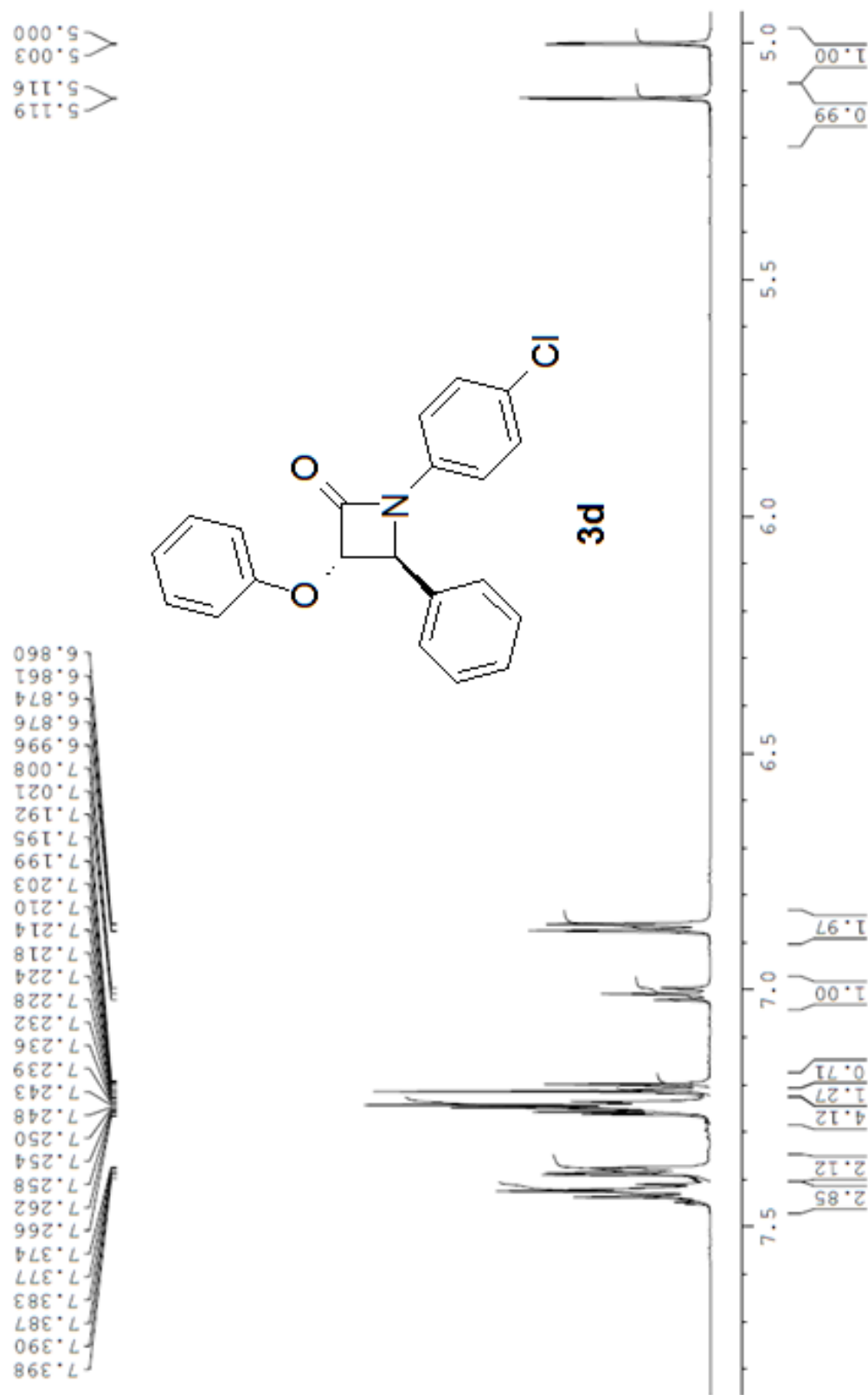


¹³C decoupled spectra Osama C1B in CDCl₃

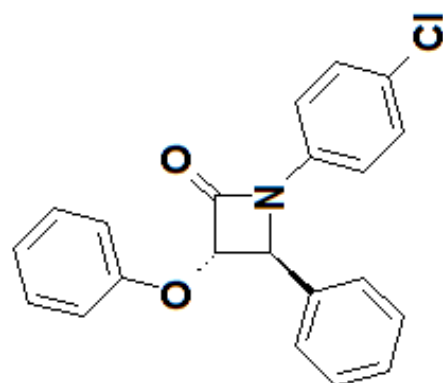




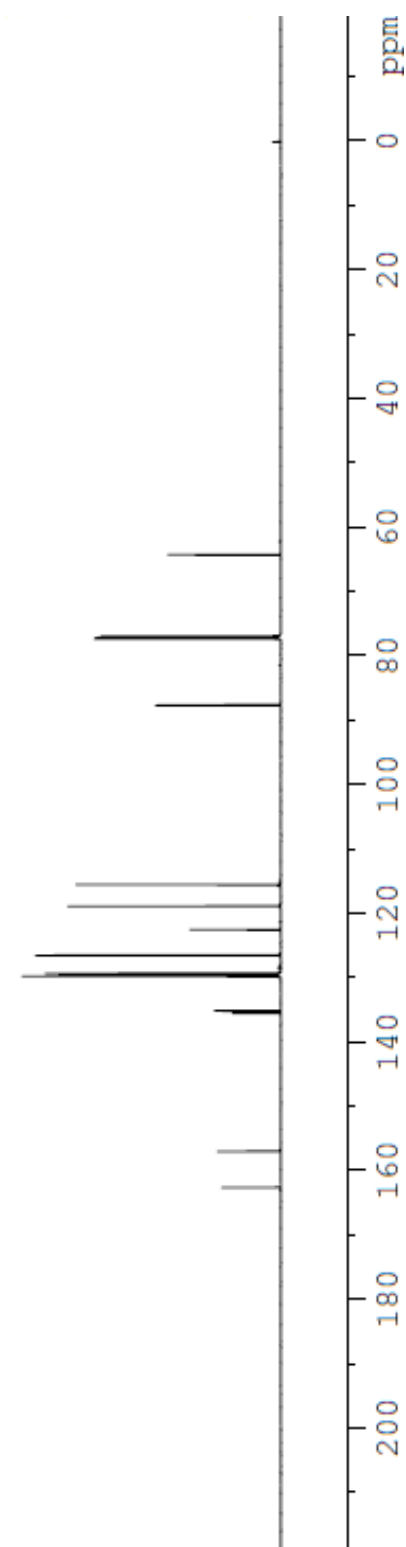
¹H spectrum Osama 3D in CDCl₃



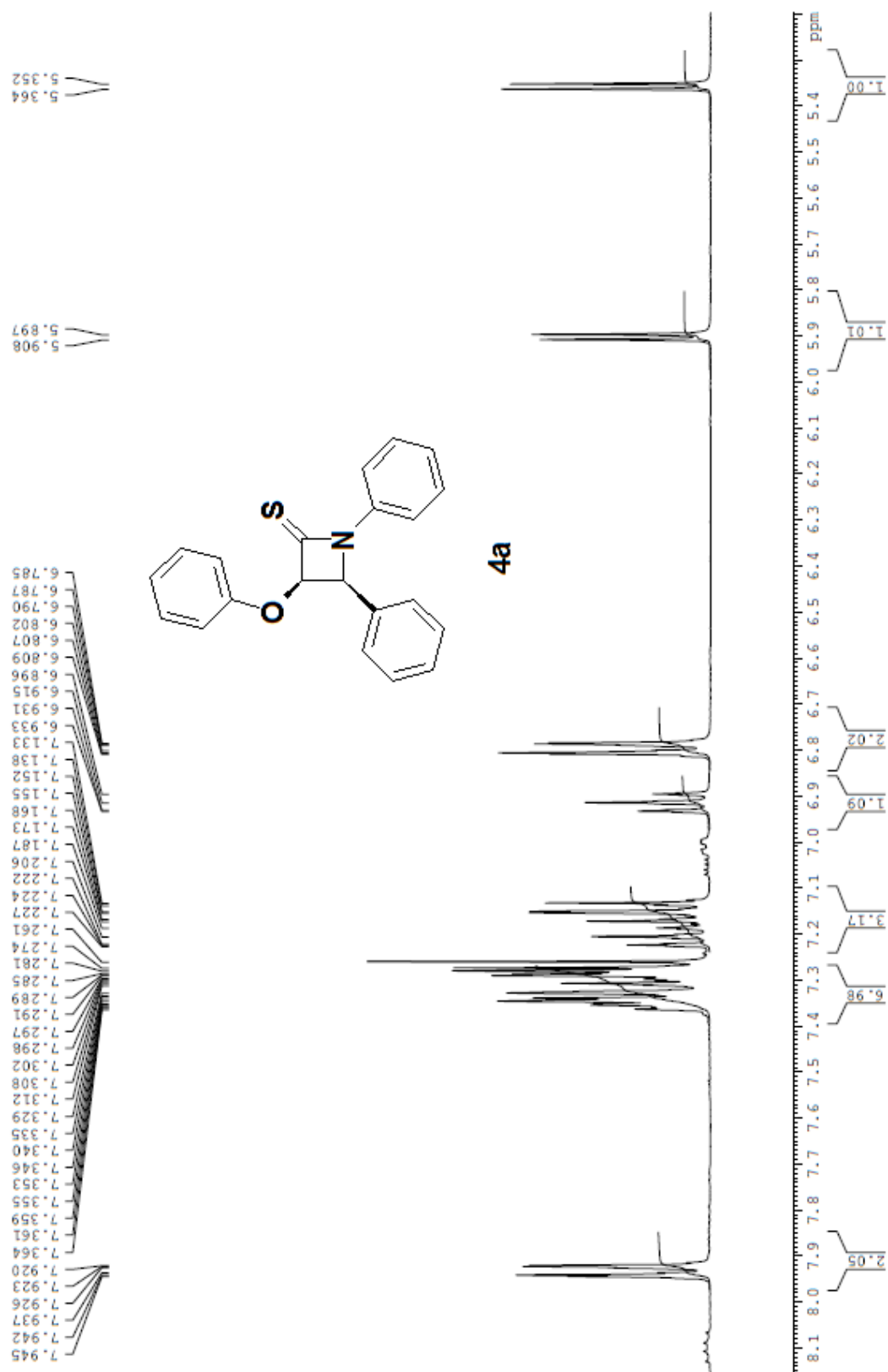
¹³C decoupled spectrum Osama 3D in CDCl₃



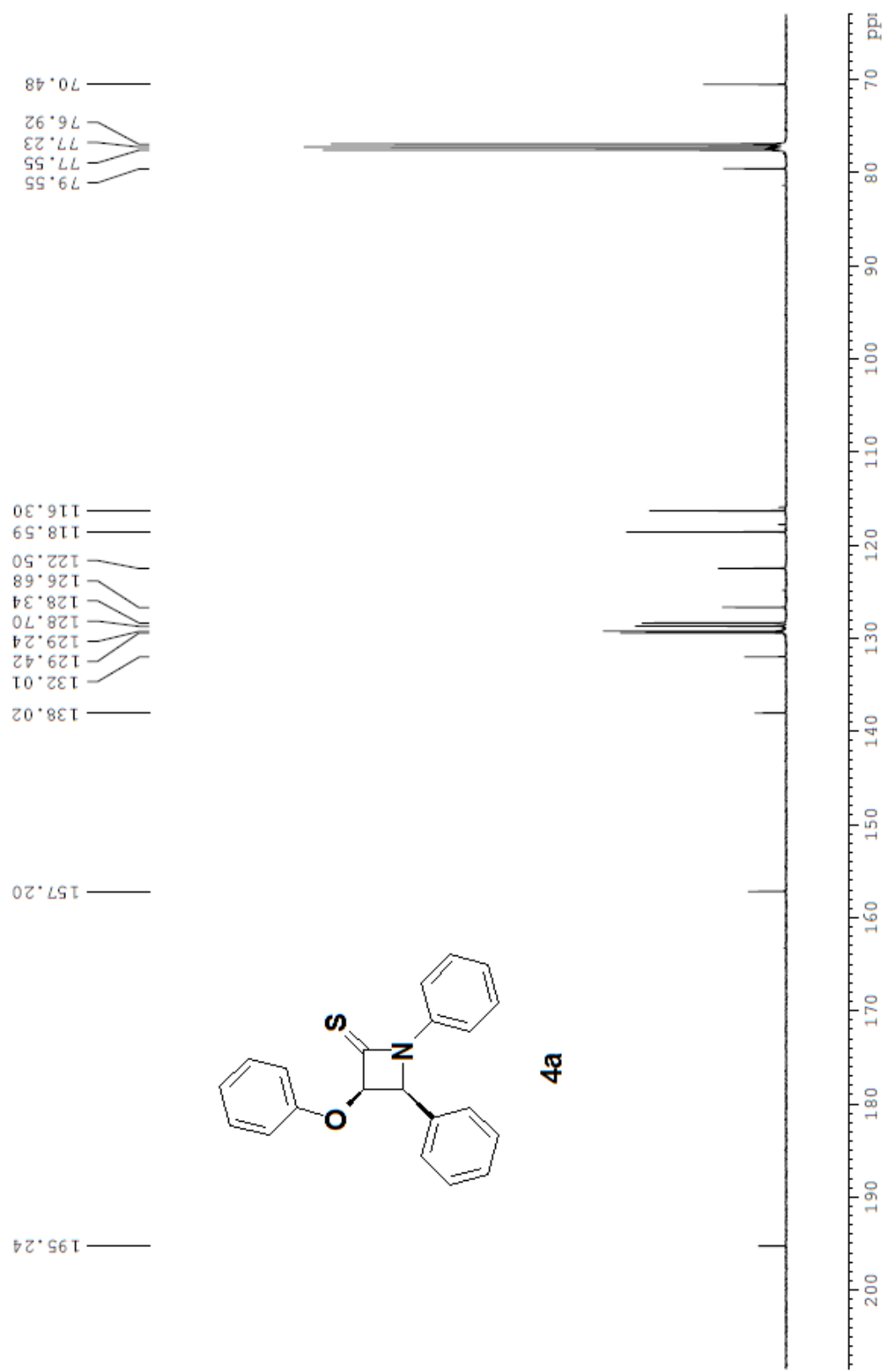
3d



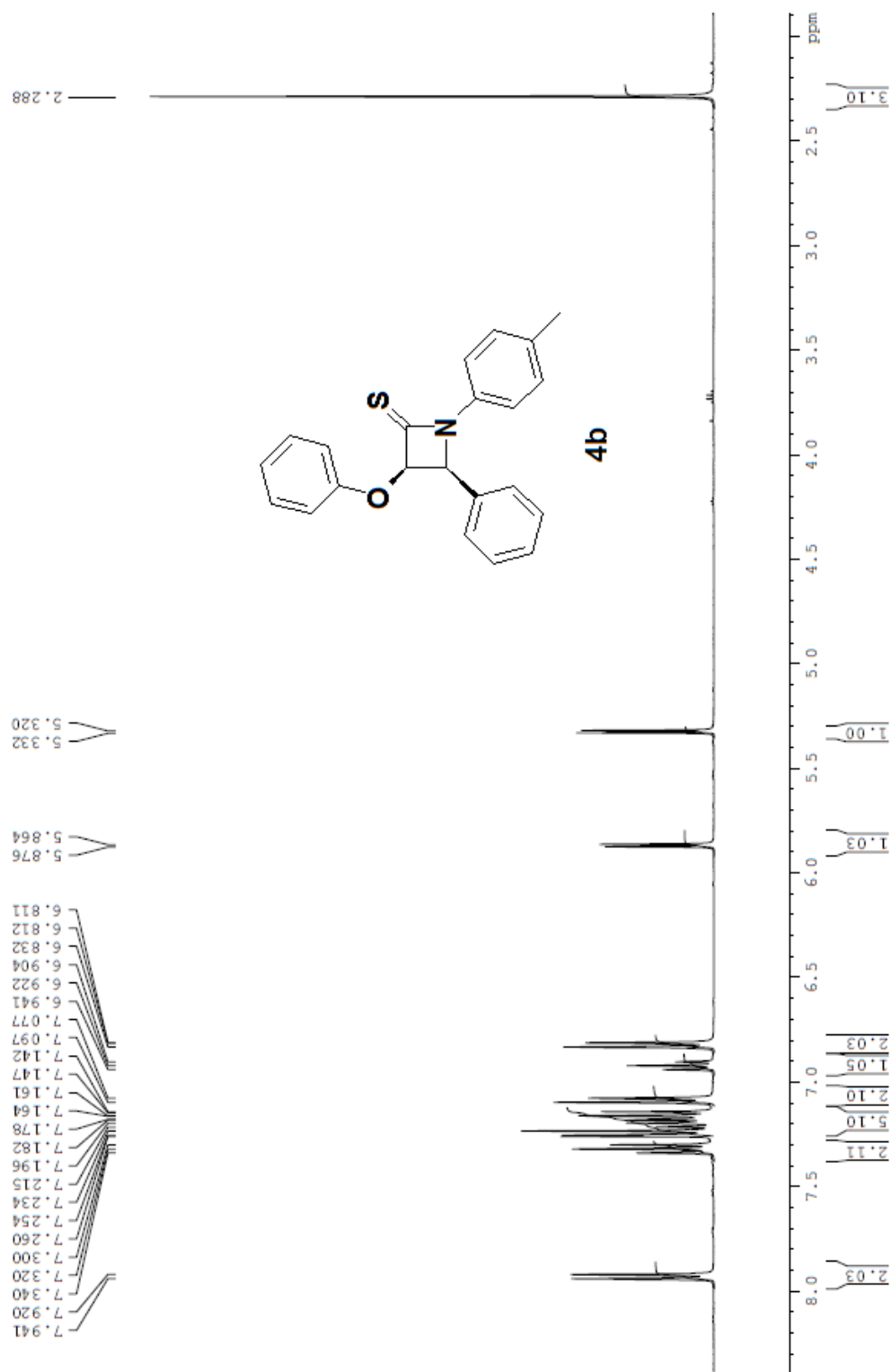
¹H spectra Nouf thio in CDCl₃



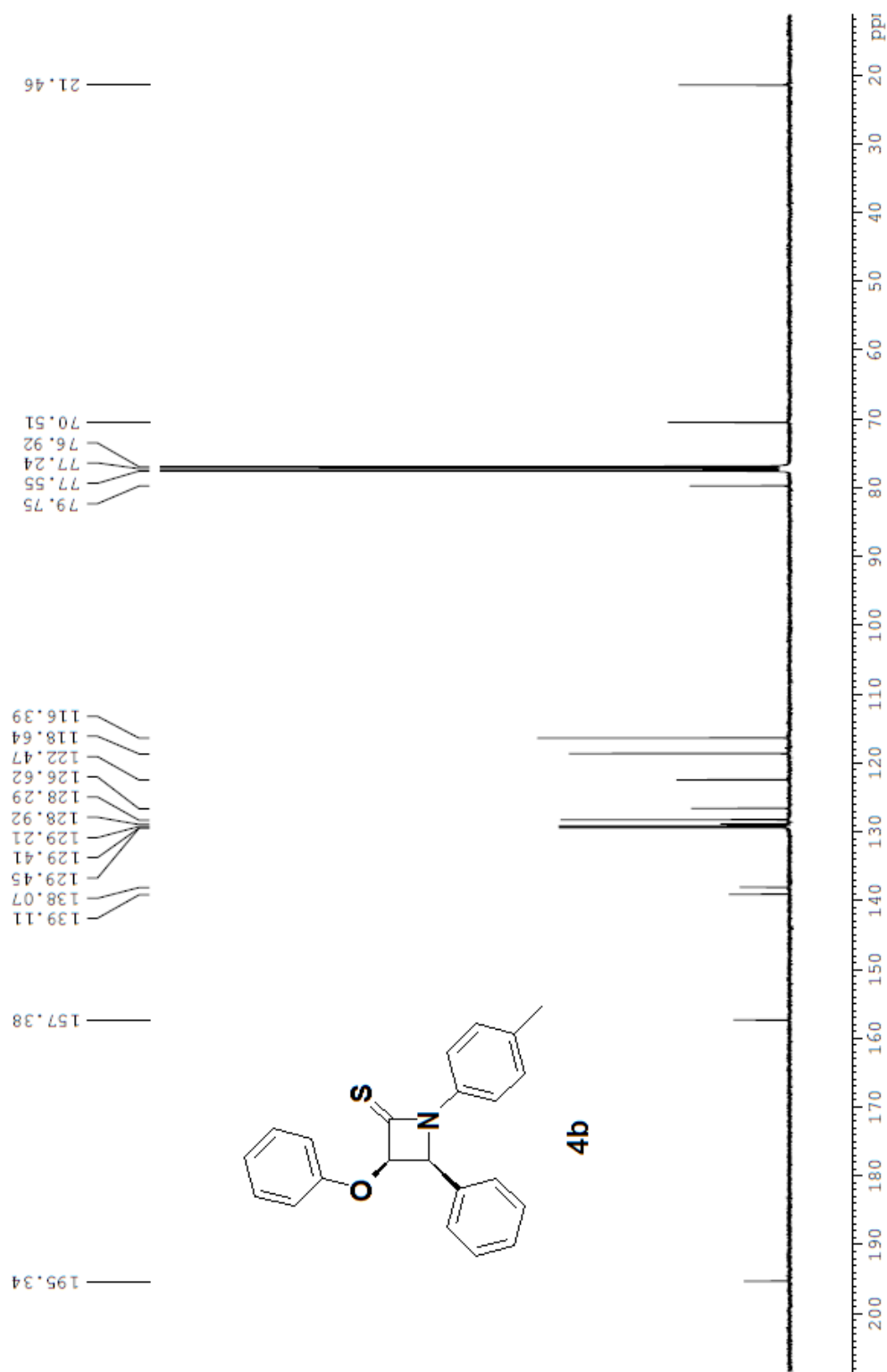
¹³C decoupled spectra Nouf T phenyl in CDCl₃



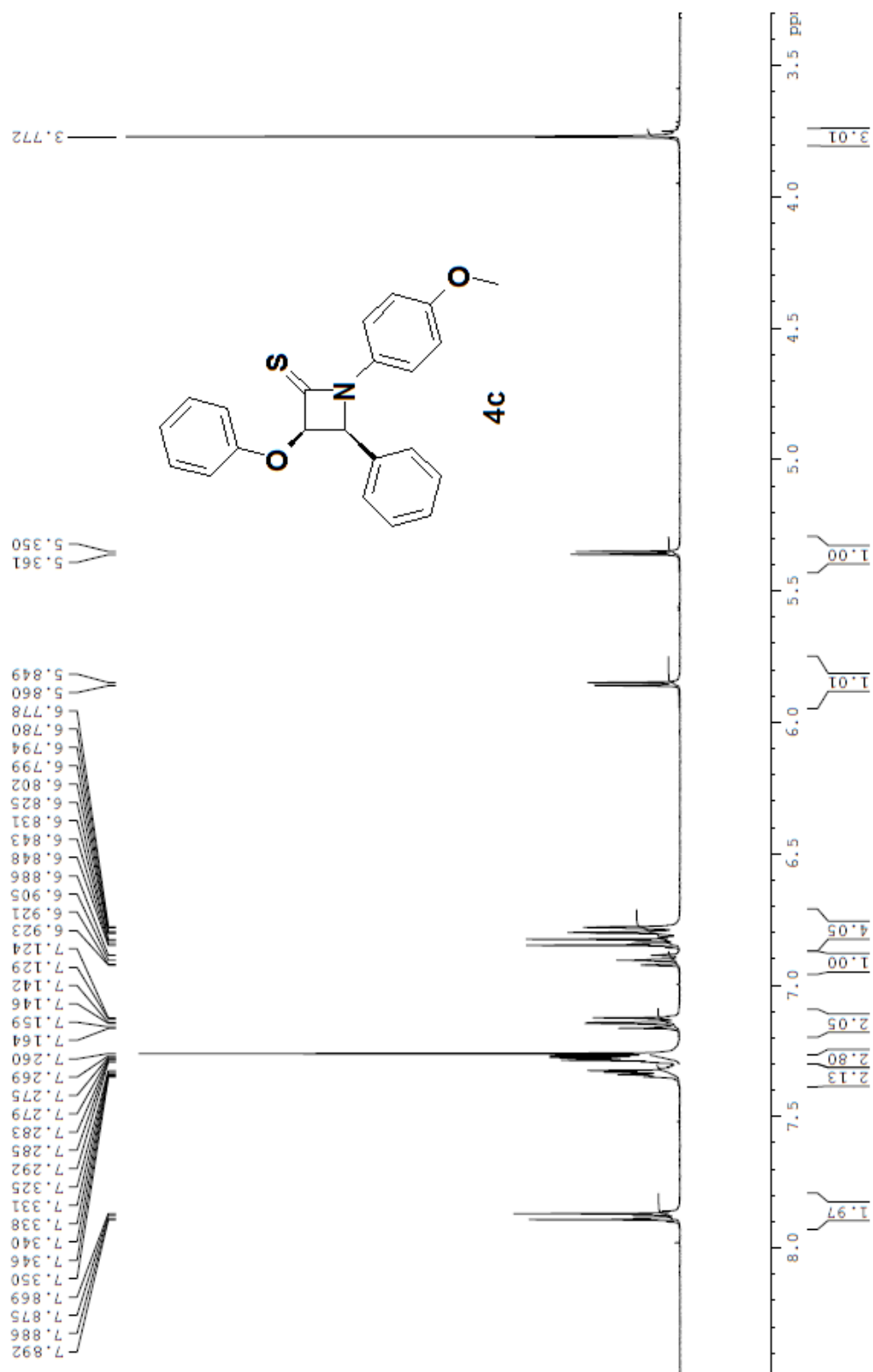
¹H spectra Osama 4B in CDCl₃



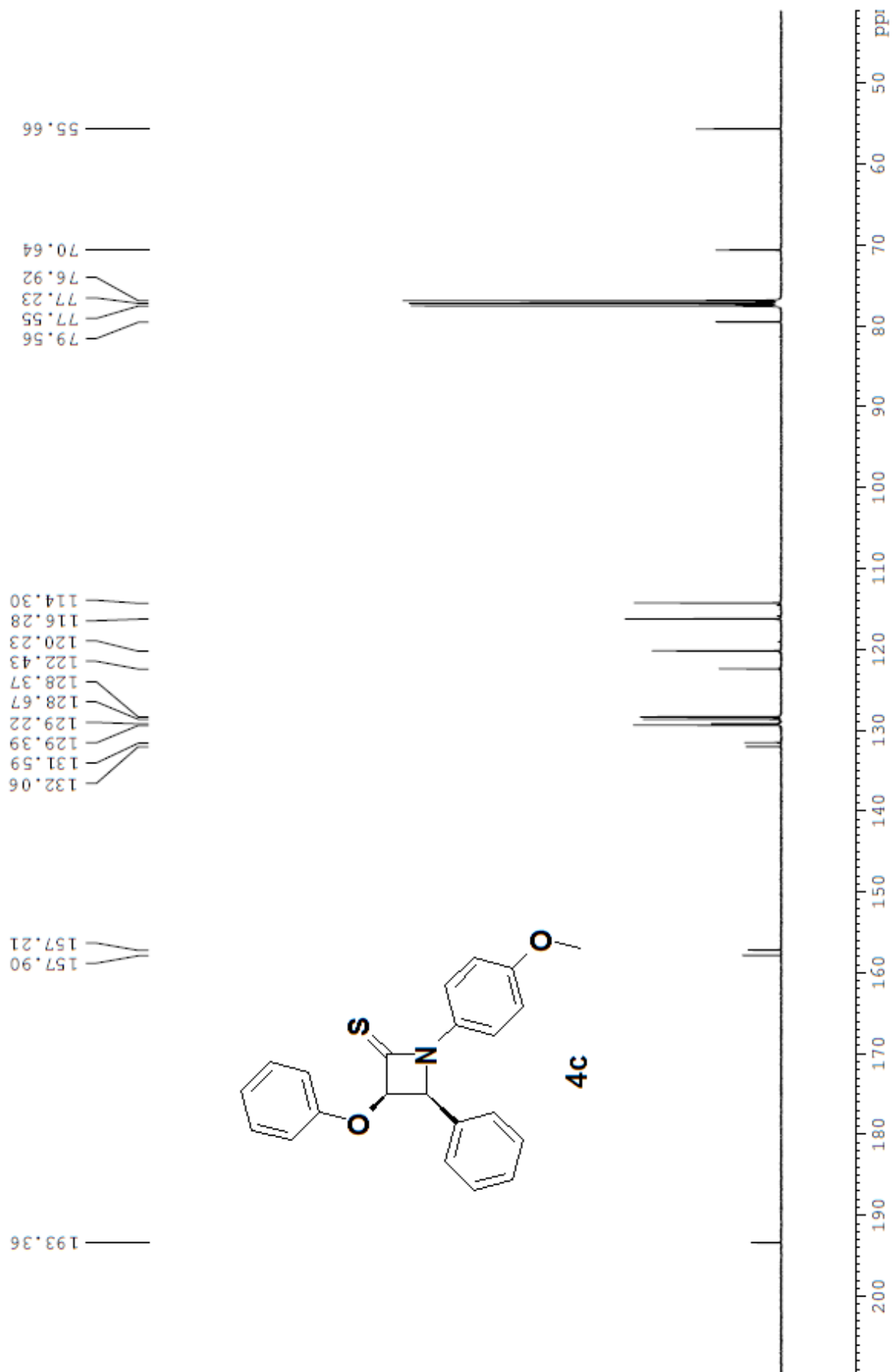
¹³C decoupled spectra Osama 4B in CDCL₃



¹H spectra Nouf Thio CH3A in CDCL₃



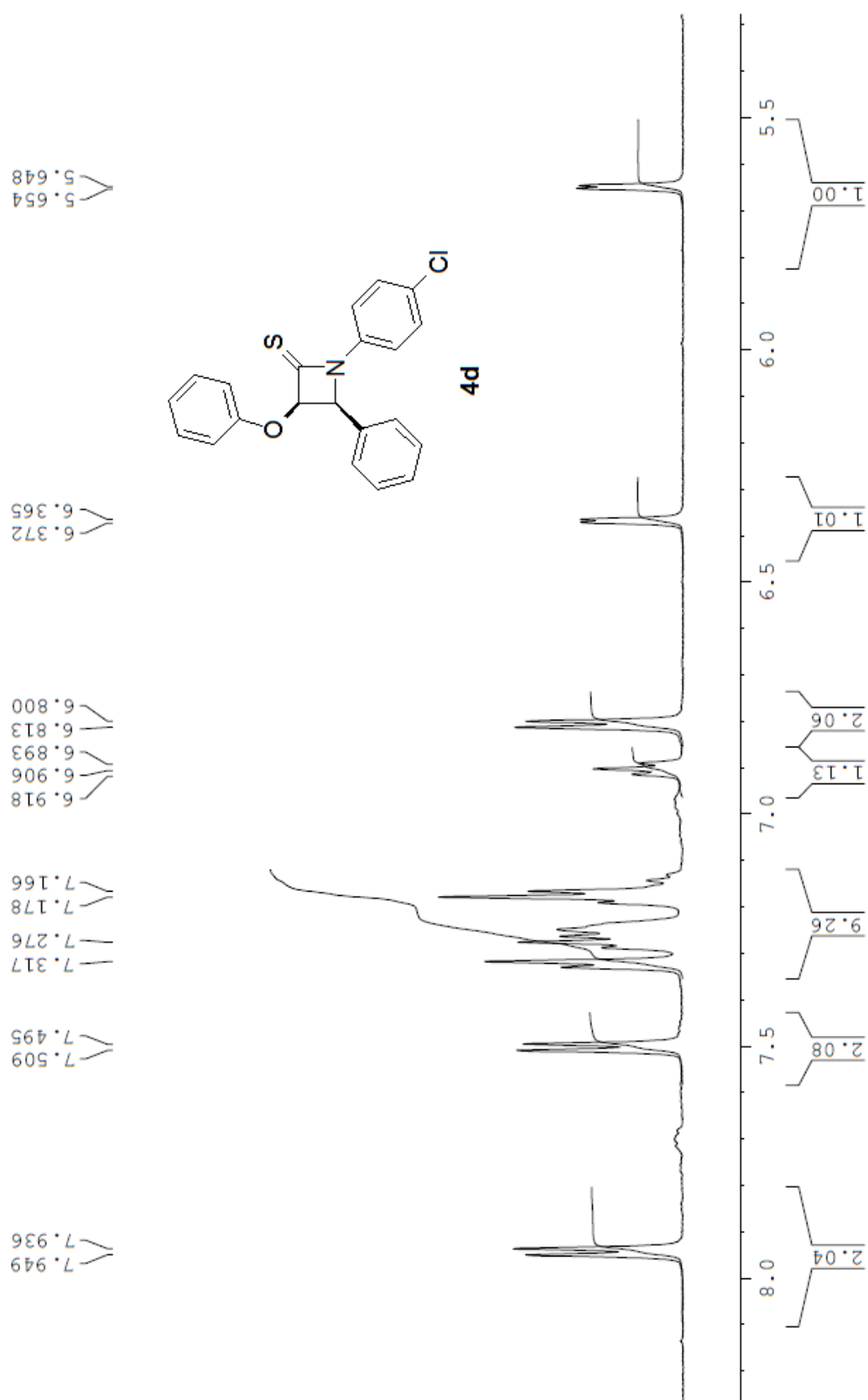
¹³C decoupled spectra Nouf T-OCH3A in CDCL3



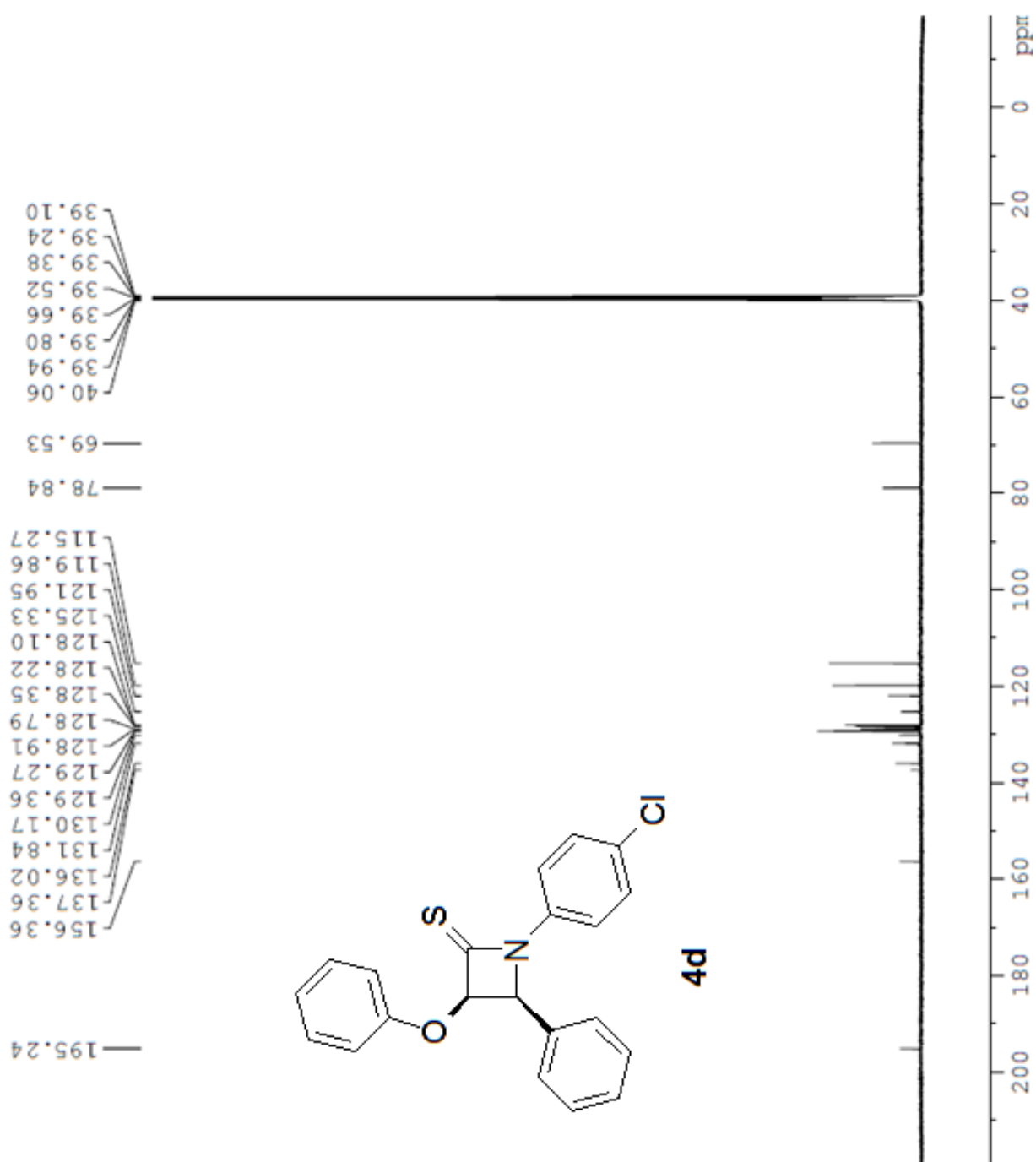
¹H spectrum Dr.Osama 4 in DMSO



¹H spectrum Dr.Osama 4 in DMSO



¹³C decoupled spectrum Dr.Osama 4 in DMSO

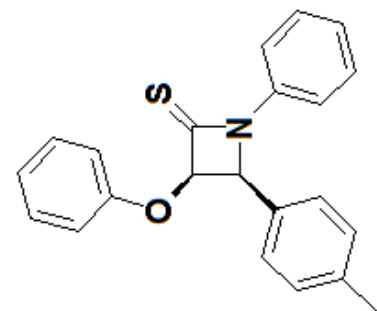


¹H spectrum Dr.Osama 3 in CDCl₃

7.909
7.896
7.287
7.284
7.274
7.260
7.215
7.212
7.201
7.165
7.152
7.140
7.138
7.134
7.131
7.121
7.120
7.110
7.107
7.051
7.037
6.894
6.882
6.869
6.795
6.794
6.781

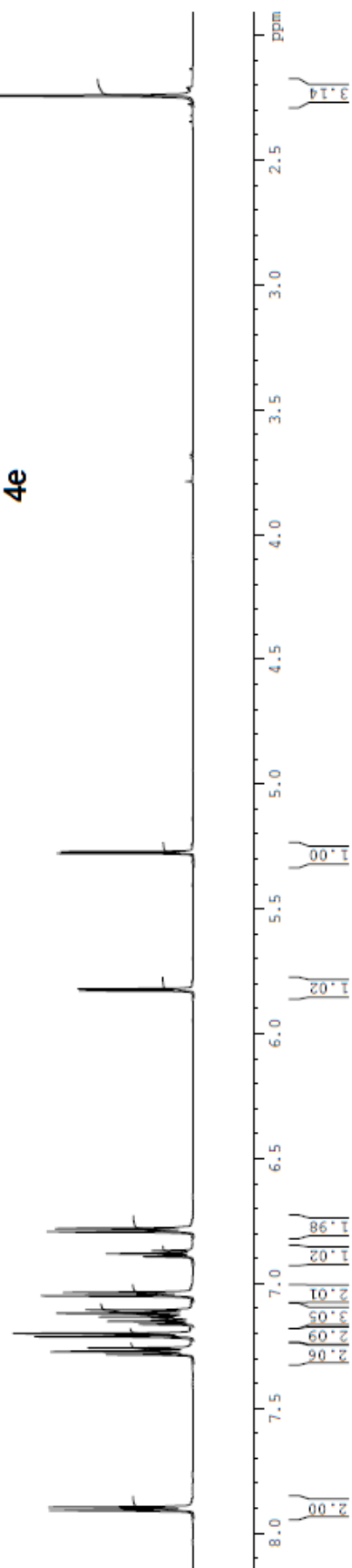
5.828
5.821
5.278
5.271

2.242

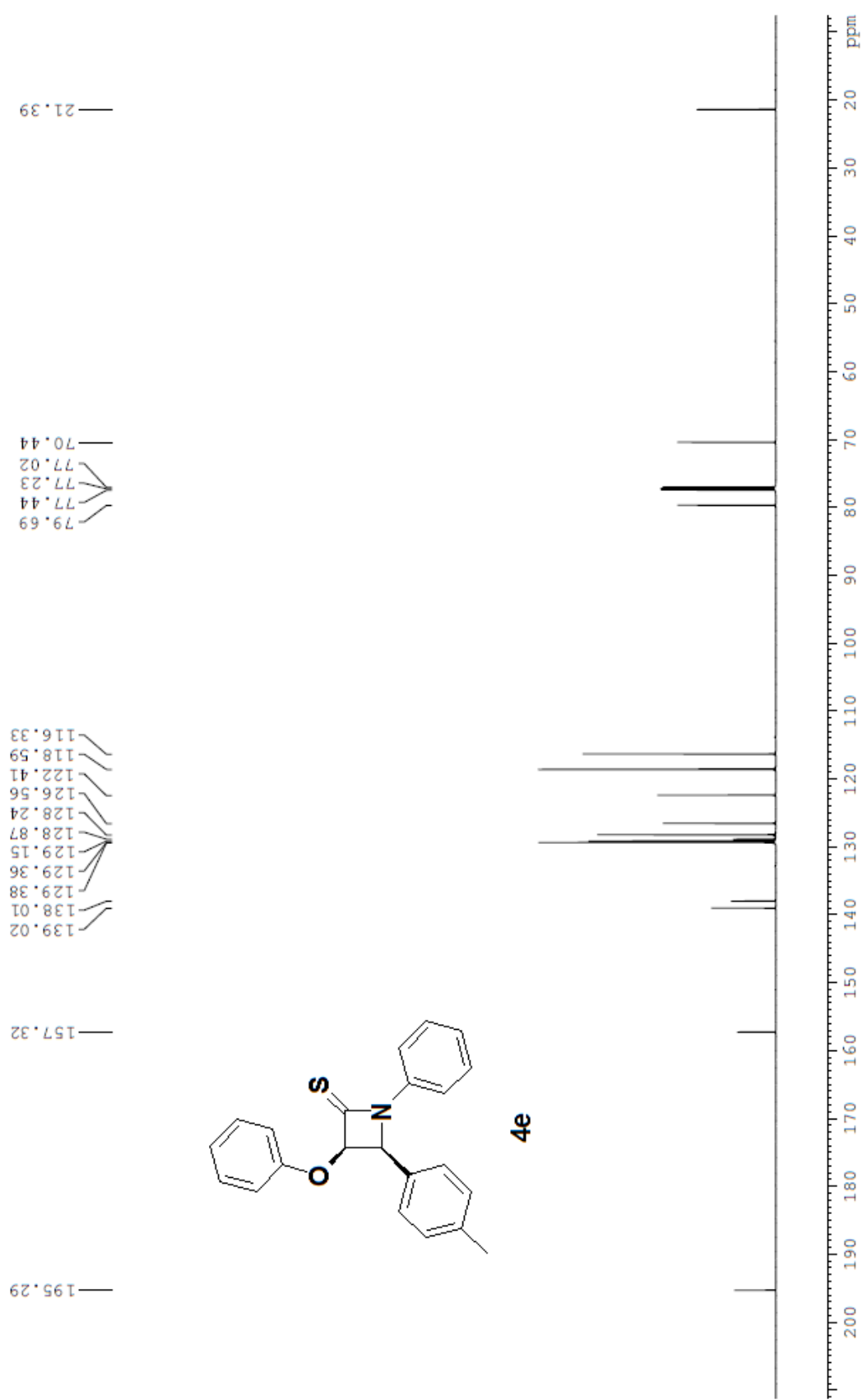


4e

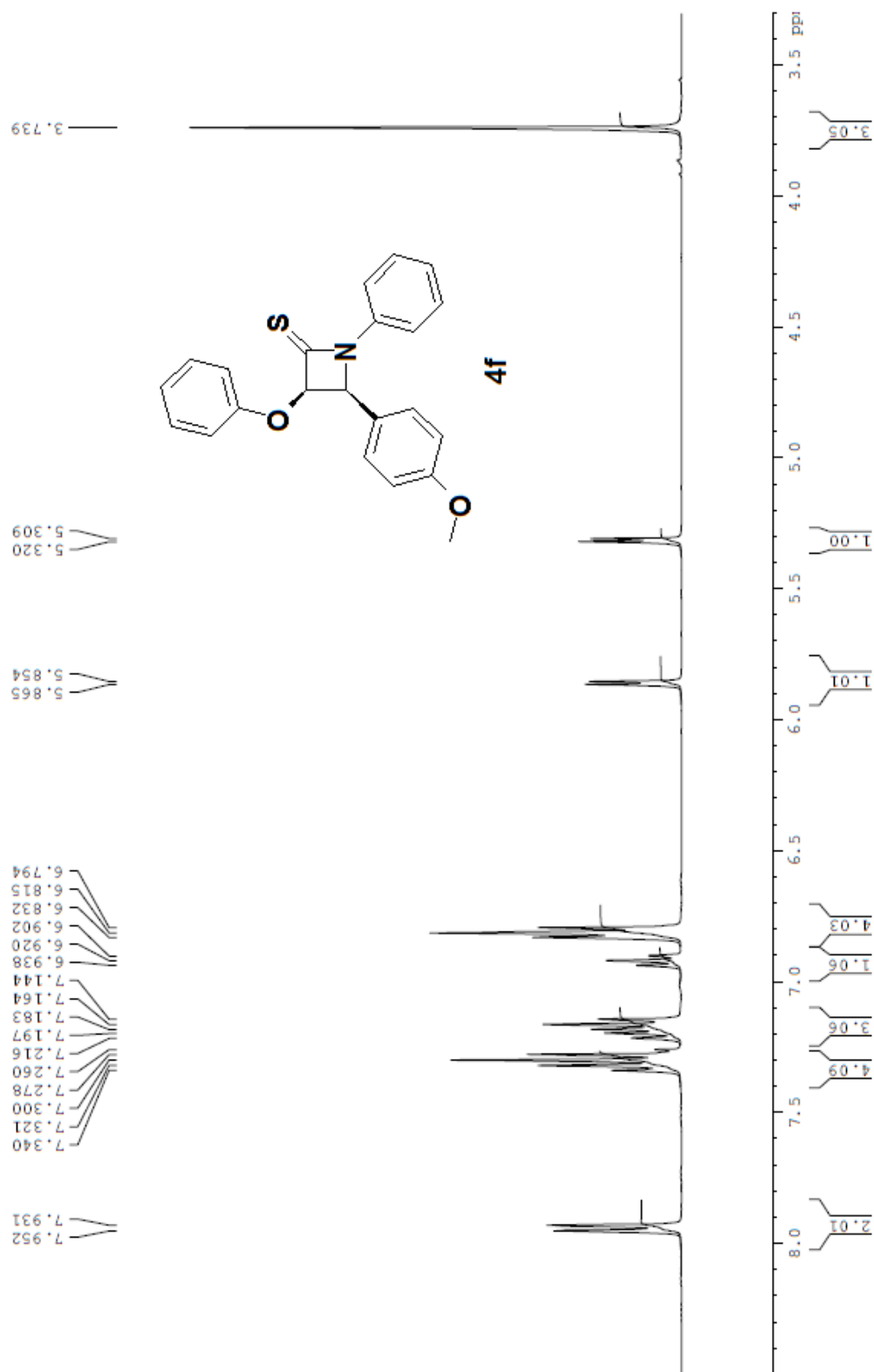
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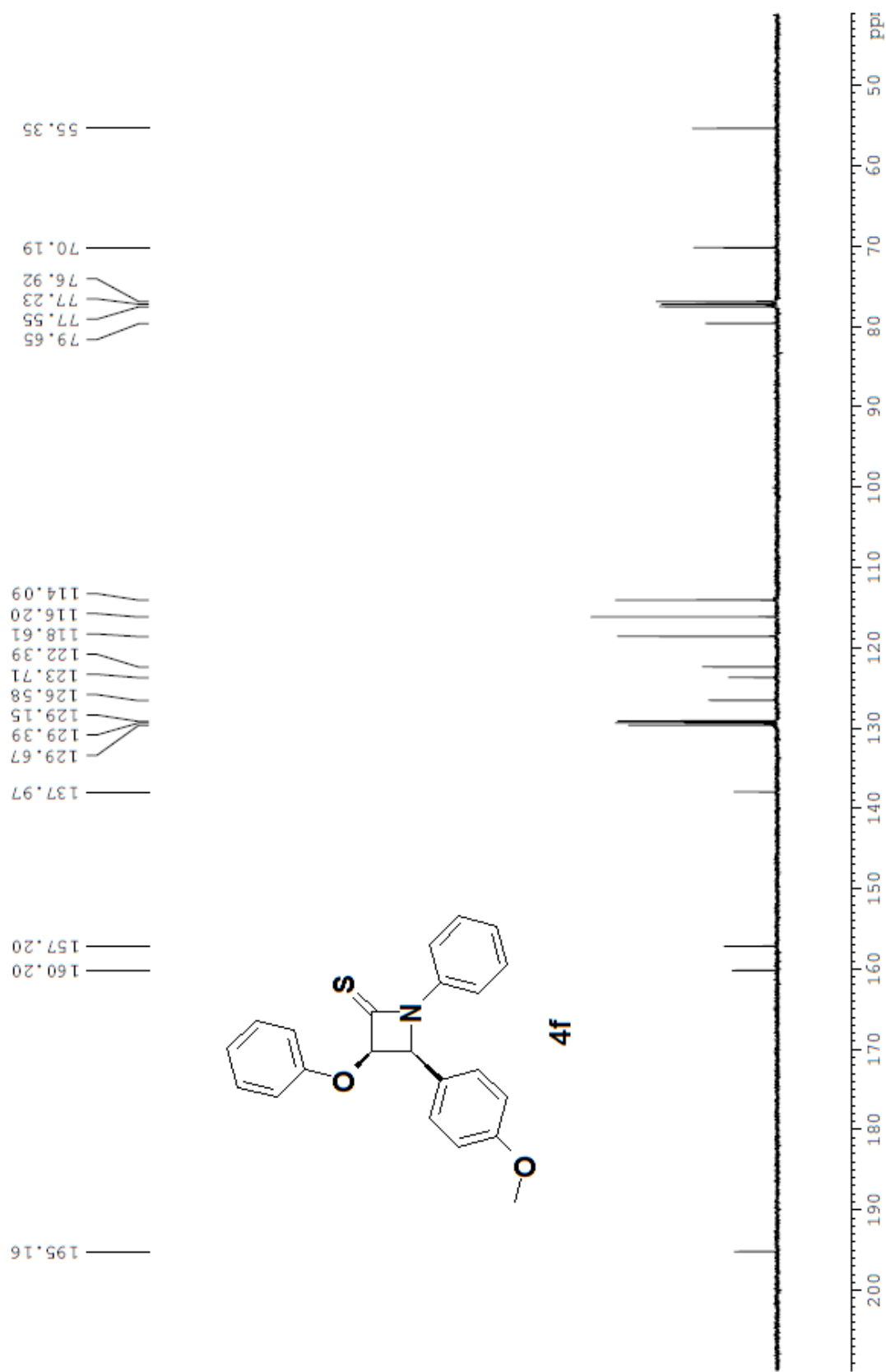
¹³C decoupled spectrum Dr.Osama 3 in CDCl₃



¹H spectra Osama 4f in CDCl₃



¹³C decoupled spectra Osama 4f in CDCL₃



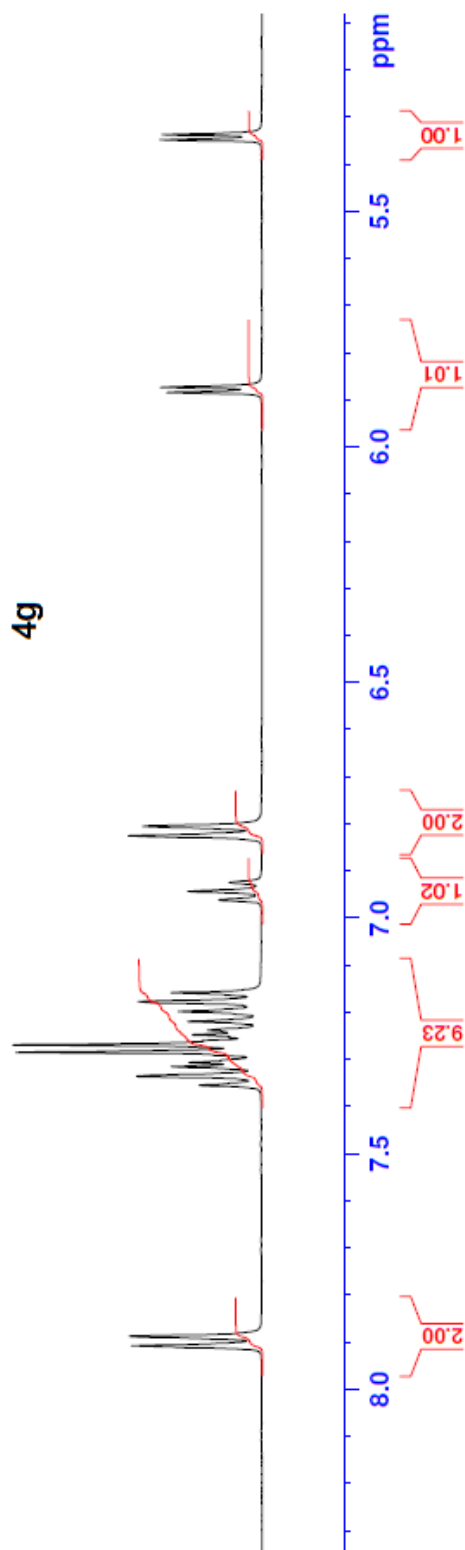
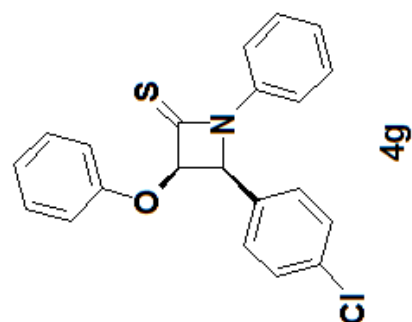
¹H spectra Osama 4g in CDCl₃

7.908
7.888

7.355
7.336
7.316
7.307
7.285
7.269
7.261
7.253
7.248
7.238
7.220
7.199
7.177
7.159
6.962
6.943
6.925
6.825
6.806

5.885
5.874

5.349
5.338



¹³C decoupled spectra Osama 4G in CDCL₃

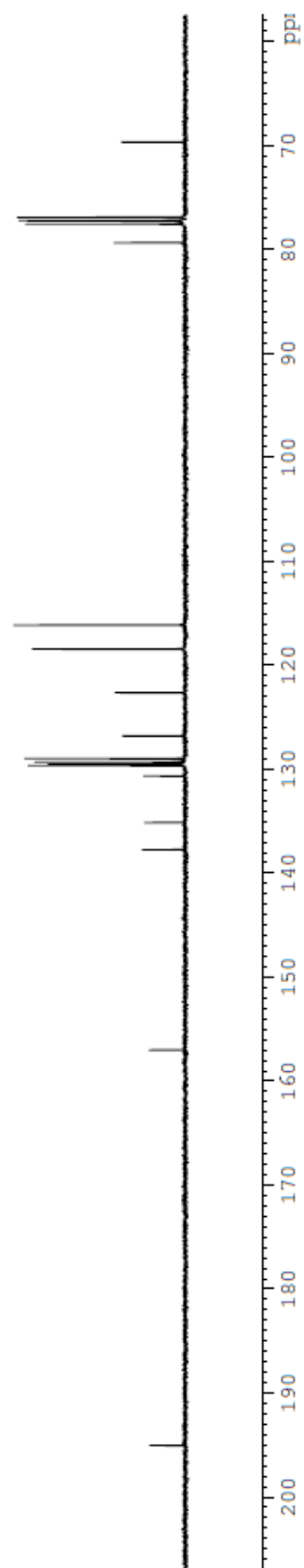
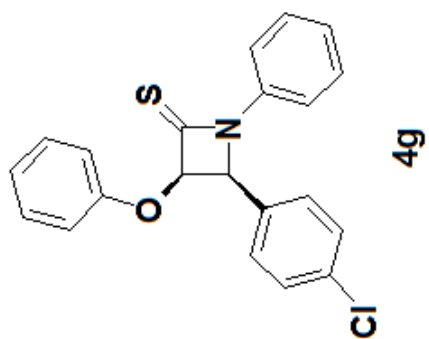
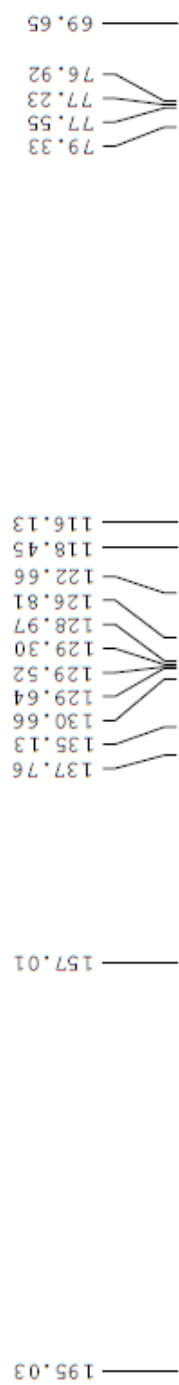


Table 1. Yield, ^1H -NMR and ^{13}C -NMR of azetidinones **2a-g**, **3d** and **4a-g** (H-3/C-3 and H-4/C-4)

Comp.	%yield	H3/C3	H4/C4
2a	67%,	5.60 (d, <i>J</i> 4.8)/81.1	5.43 (d, <i>J</i> 4.8)/62.1
2b	60%,	5.60 (d, <i>J</i> 4.8)/81.0	5.40 (d, <i>J</i> 4.8)/61.9
2c	60%,	5.67 (d, <i>J</i> 4.8)/81.2	5.40 (d, <i>J</i> 4.8)/62.2
2d	30%	5.58 (d, <i>J</i> 4.8)/81.4	5.38 (d, <i>J</i> 4.8)/62.2
2e	74%	5.57 (d, <i>J</i> 4.8)/81.2	5.40 (d, <i>J</i> 4.8)/61.9
2f	61%	5.56 (d, <i>J</i> 4.8)/81.2	5.40 (d, <i>J</i> 4.8)/61.7
2g	58%	5.60 (d, <i>J</i> 4.8)/81.0	5.40 (d, <i>J</i> 4.8)/61.1
3d	45%	5.11(d, <i>J</i> 1.8)/87.5	5.00 (d, <i>J</i> 1.8)/64.1
4a	67%	5.93 (d, <i>J</i> 4.8)/79.3	5.38 (d, <i>J</i> 4.8)/70.3
4b	69%	5.89 (d, <i>J</i> 4.4)/79.5	5.35 (d, <i>J</i> 4.4)/70.2
4c	71%	5.87 (d, <i>J</i> 4.4)/79.3	5.35 (d, <i>J</i> 4.4)/70.4
4d	77%	5.90 (d, <i>J</i> 4.8)/79.3	5.38 (d, <i>J</i> 4.8)/70.2
4e	65%	5.89 (d, <i>J</i> 4.4)/79.5	5.35 (d, <i>J</i> 4.4)/70.2
4f	73%	5.87 (d, <i>J</i> 4.4)/79.4	5.34 (d, <i>J</i> 4.4)/69.9
4g	72%	5.88 (d, <i>J</i> 4.8)/79.1	5.35 (d, <i>J</i> 4.8)/69.4

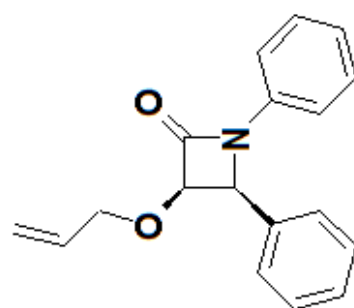
Assignment of H3, H4 proton signals is based on their cross correlations with their respective carbon signals in the 2D-HSQC NMR spectra.

¹H spectra Osama ADP1 in CDCl₃

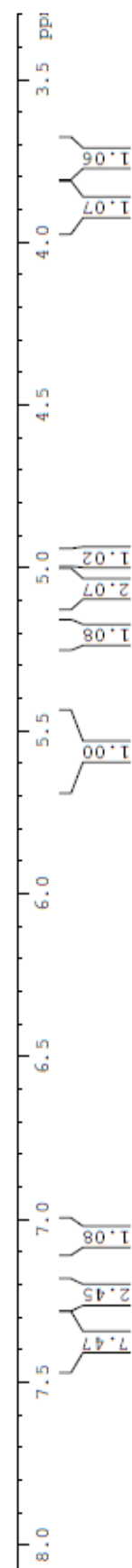
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7.416
7.406
7.397
7.393
7.379
7.367
7.361
7.345
7.343
7.324
7.265
7.260
7.246
7.225
7.077
7.059
7.040

5.621
5.607
5.594
5.580
5.572
5.565
5.552
5.538
5.524
5.210
5.198
5.083
5.059
5.080
5.057
5.038
5.034
4.978
4.966

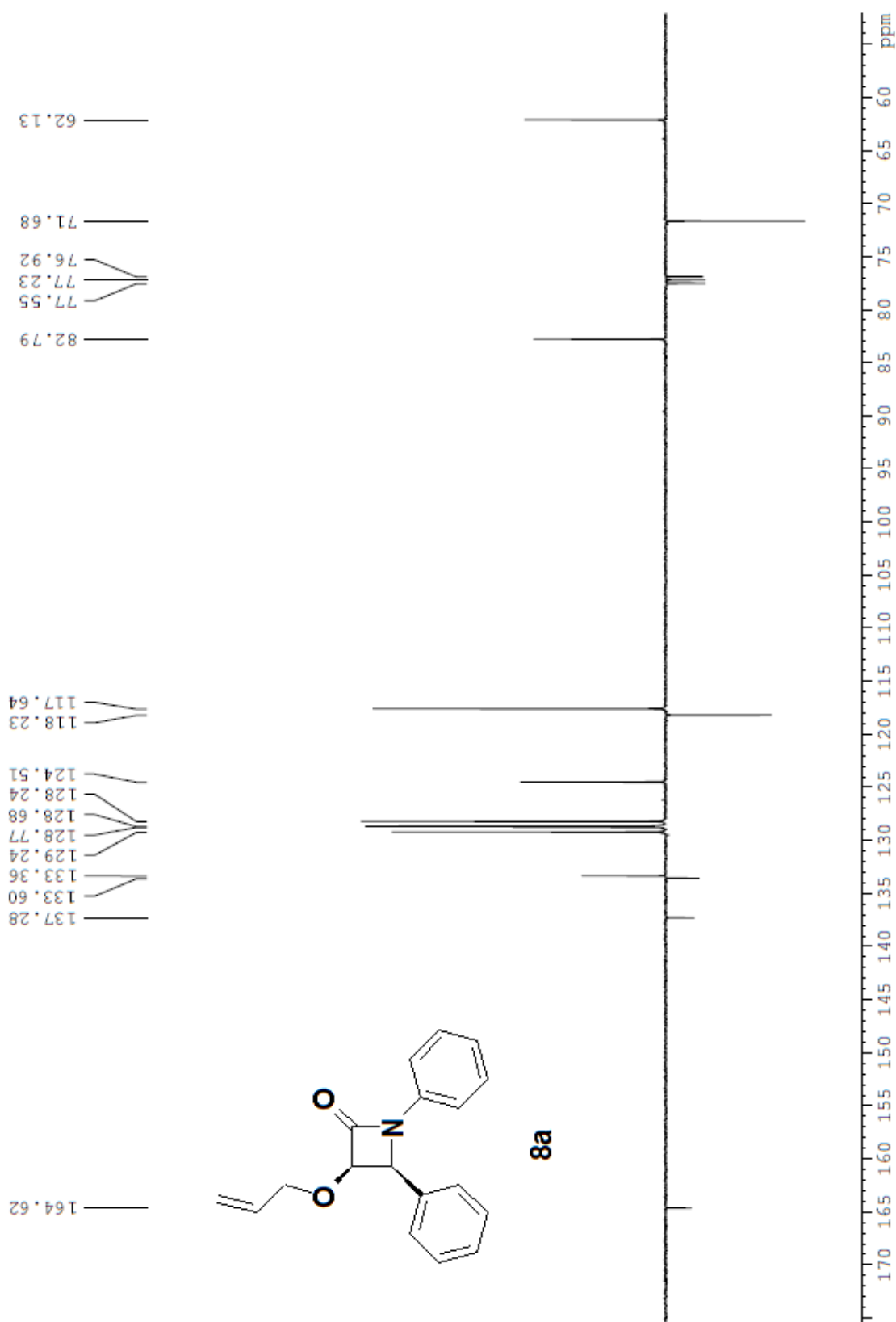
3.925
3.910
3.894
3.879
3.780
3.765
3.749
3.734

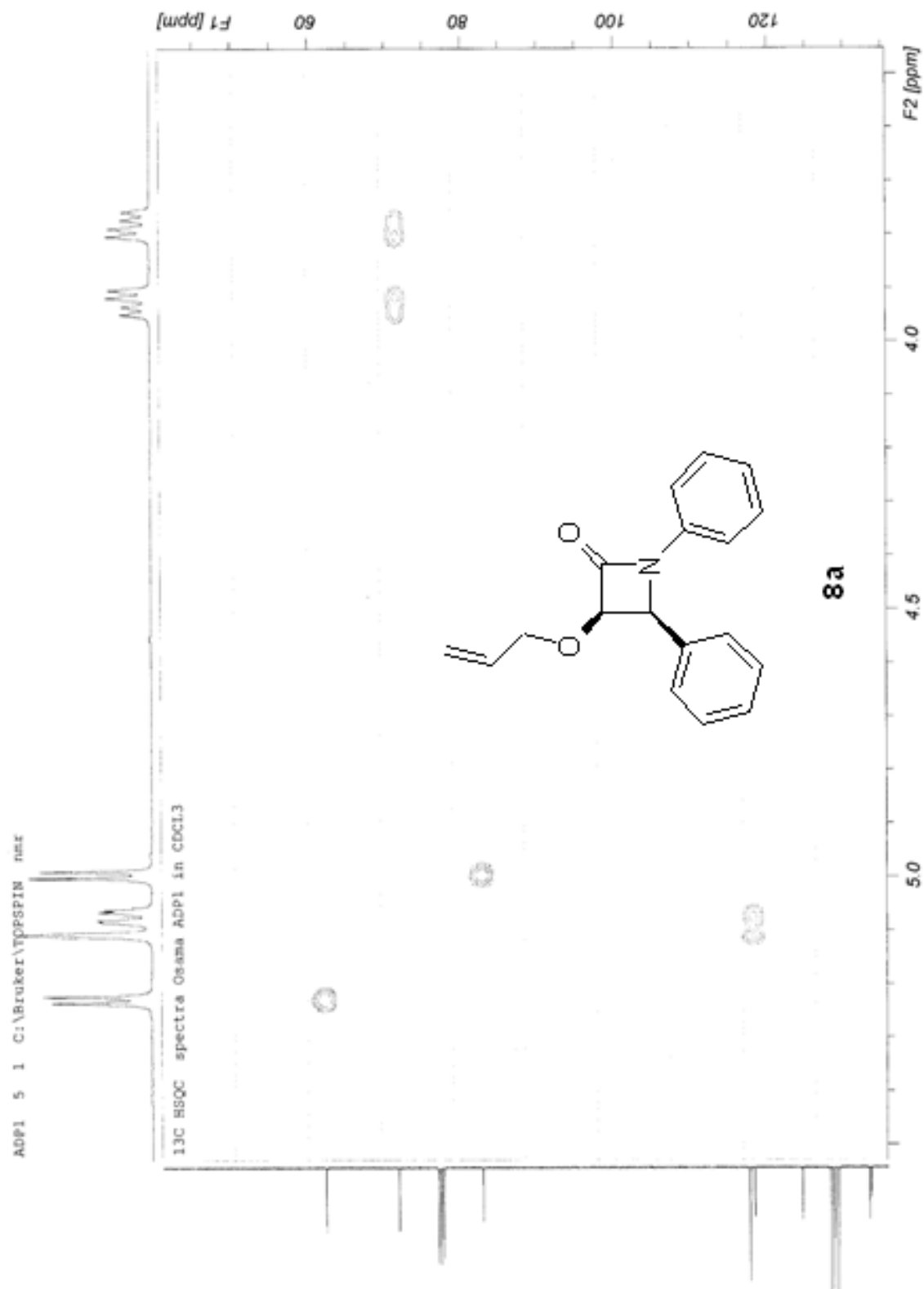


8a



¹³C APT spectra Osama ADP1 in CDCL₃





C:\Xcalibur\Data\nouria\ADP1

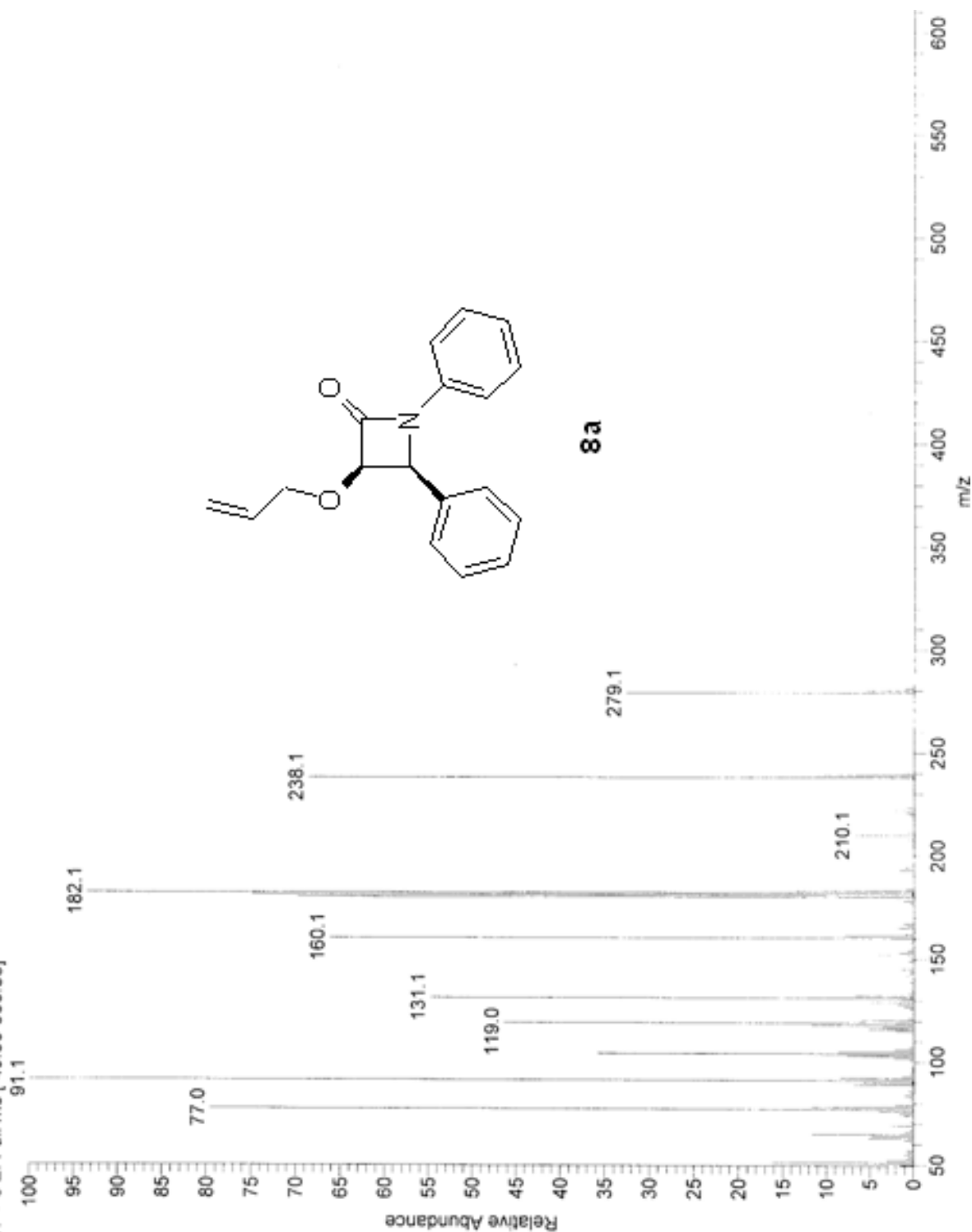
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ADP1#50 RT: 2.17 AV: 1 NL: 7.73E6

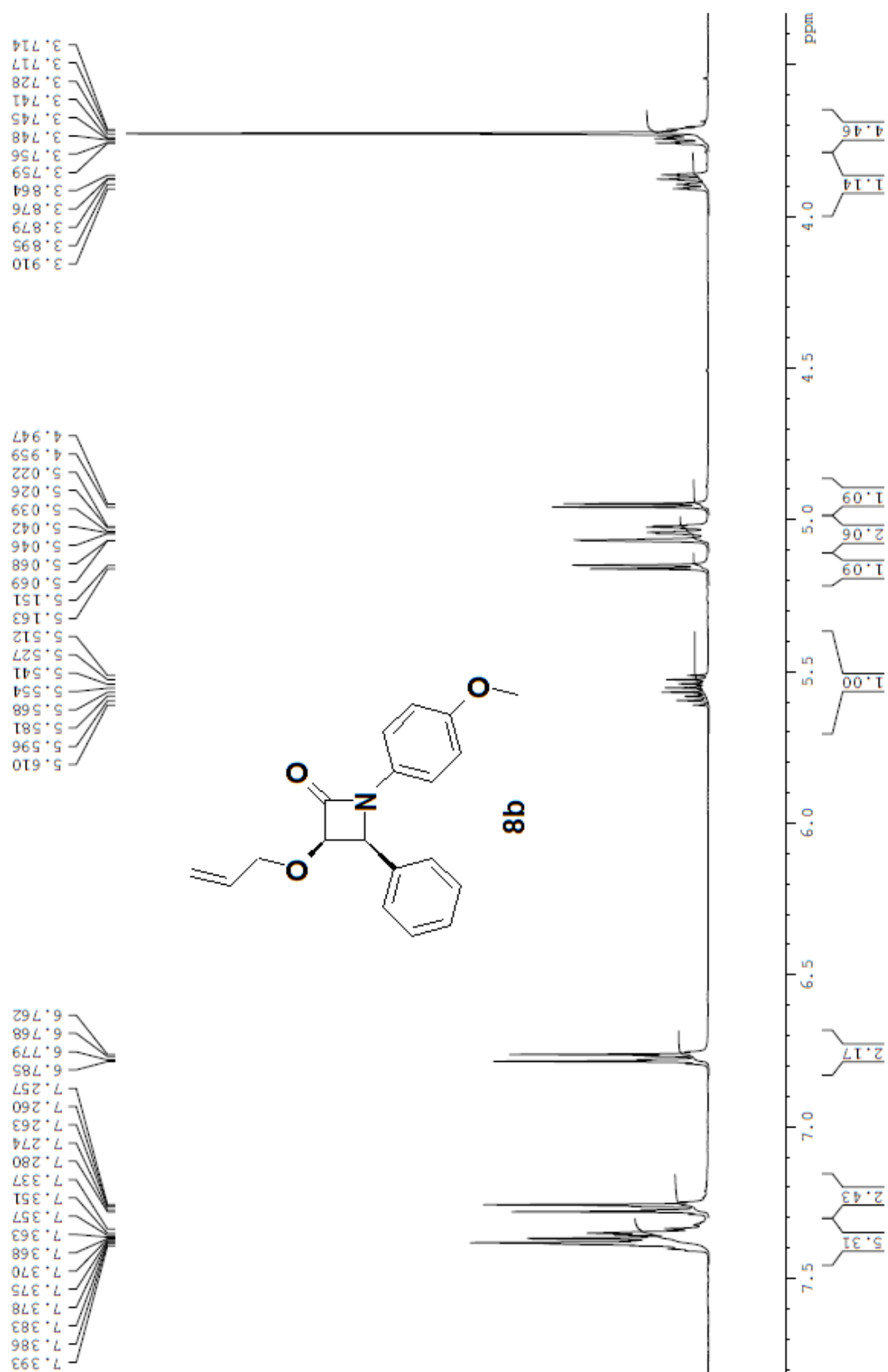
T: + c EI Full ms [49.50-900.50]

GC MS DFS- Thermo
Project No. GS01/03

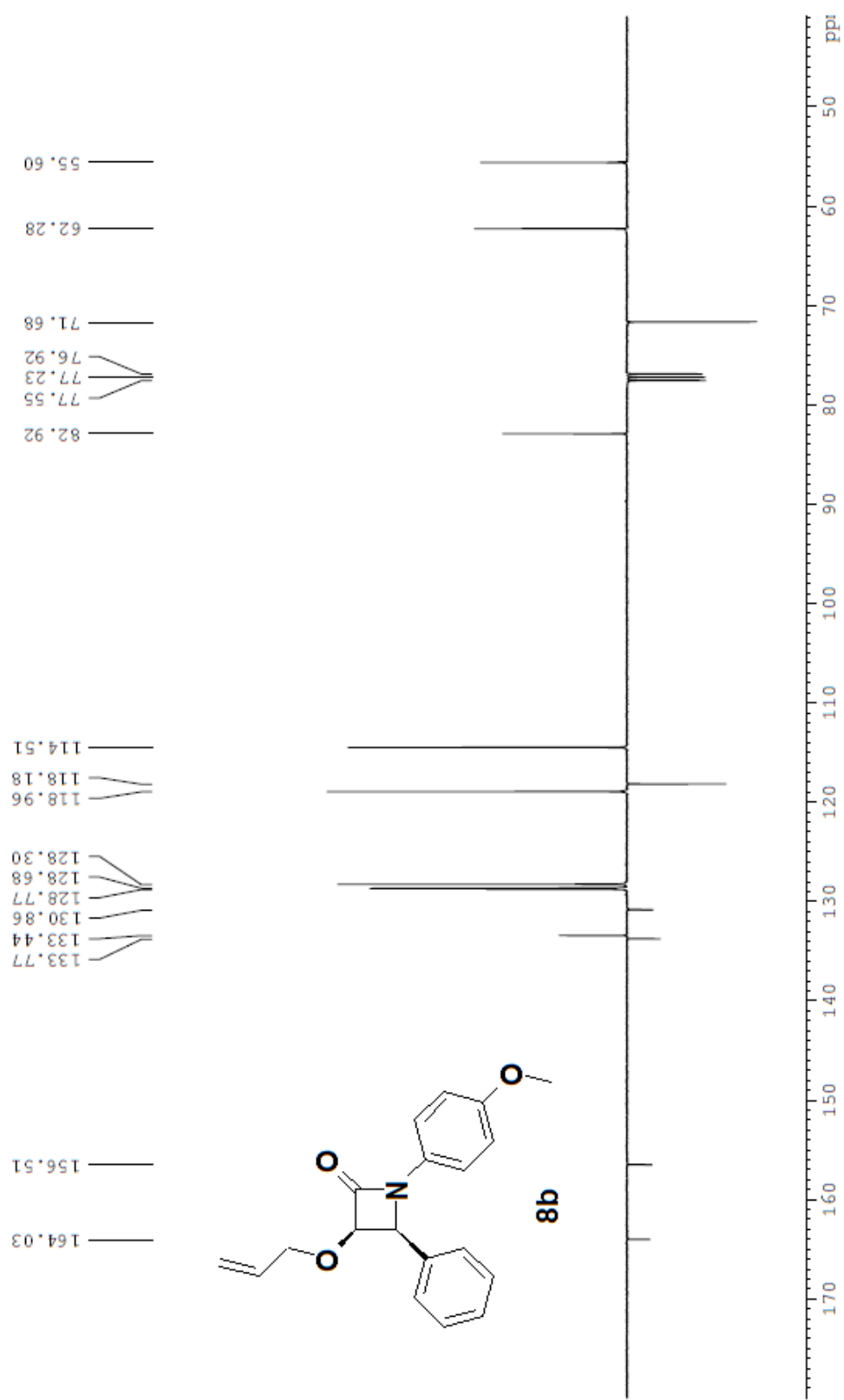
ADP1



¹H spectra Osama APM4 in CDCL₃



¹³C APT spectra Osama APM4 in CDCL₃



C:\Xcalibur\Data\Inouria\APM4

11/14/2011 11:43:05 AM

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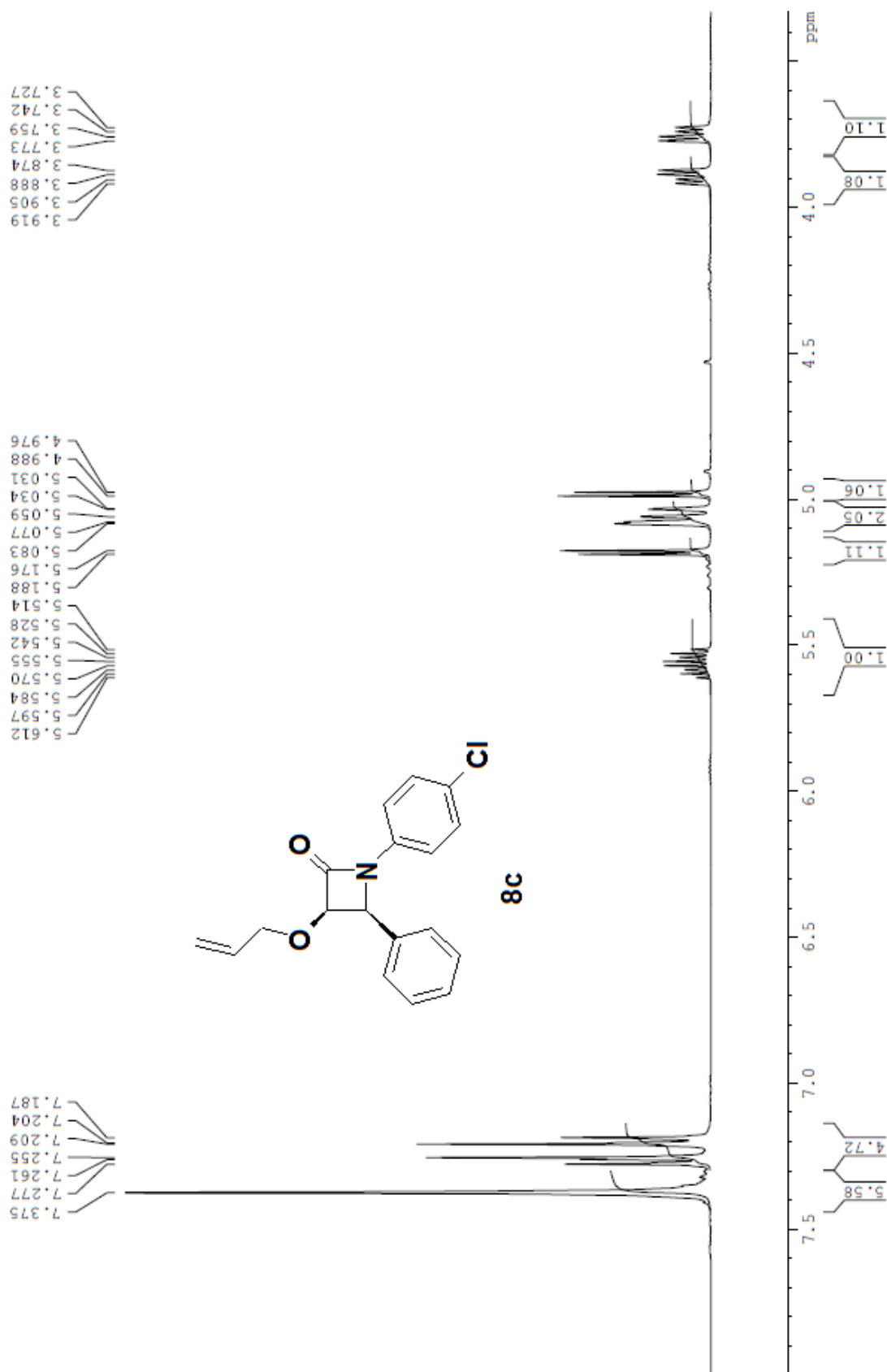
T: + c EI Full ms [49.50-900.50]

GC MS DFS- Thermo
Project No: GS01/03

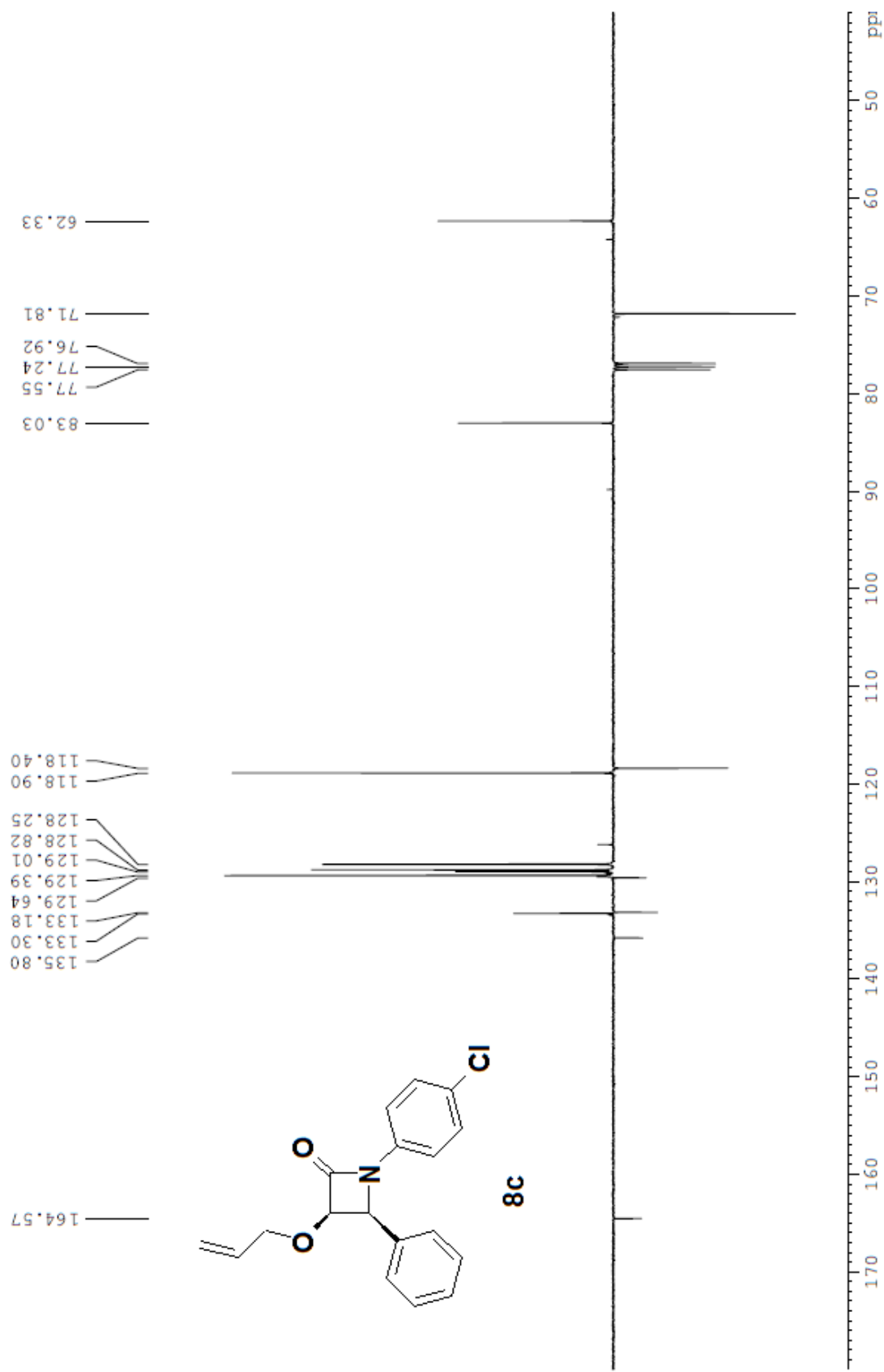
APM4

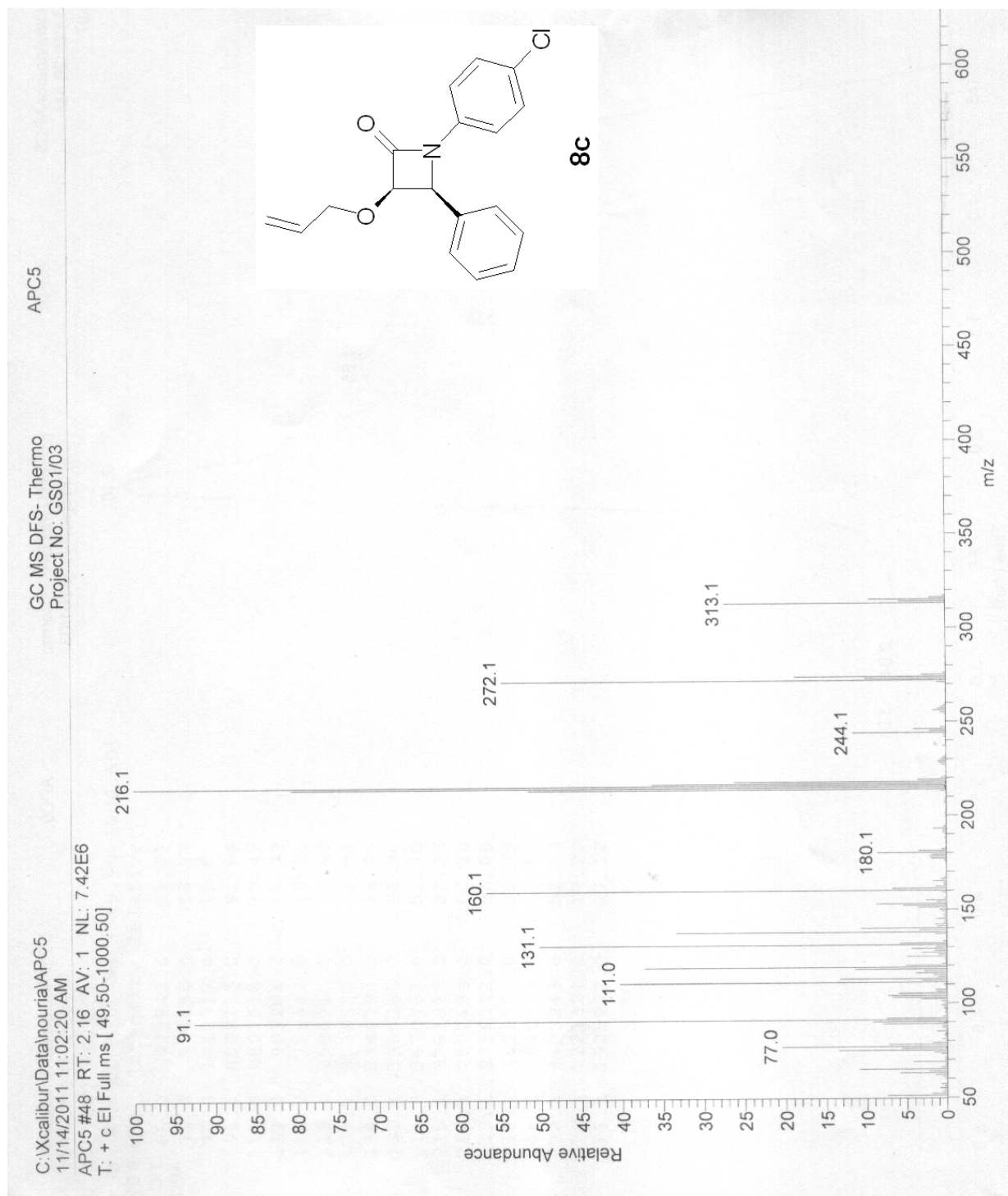


¹H spectra Osama APC5 in CDCl₃

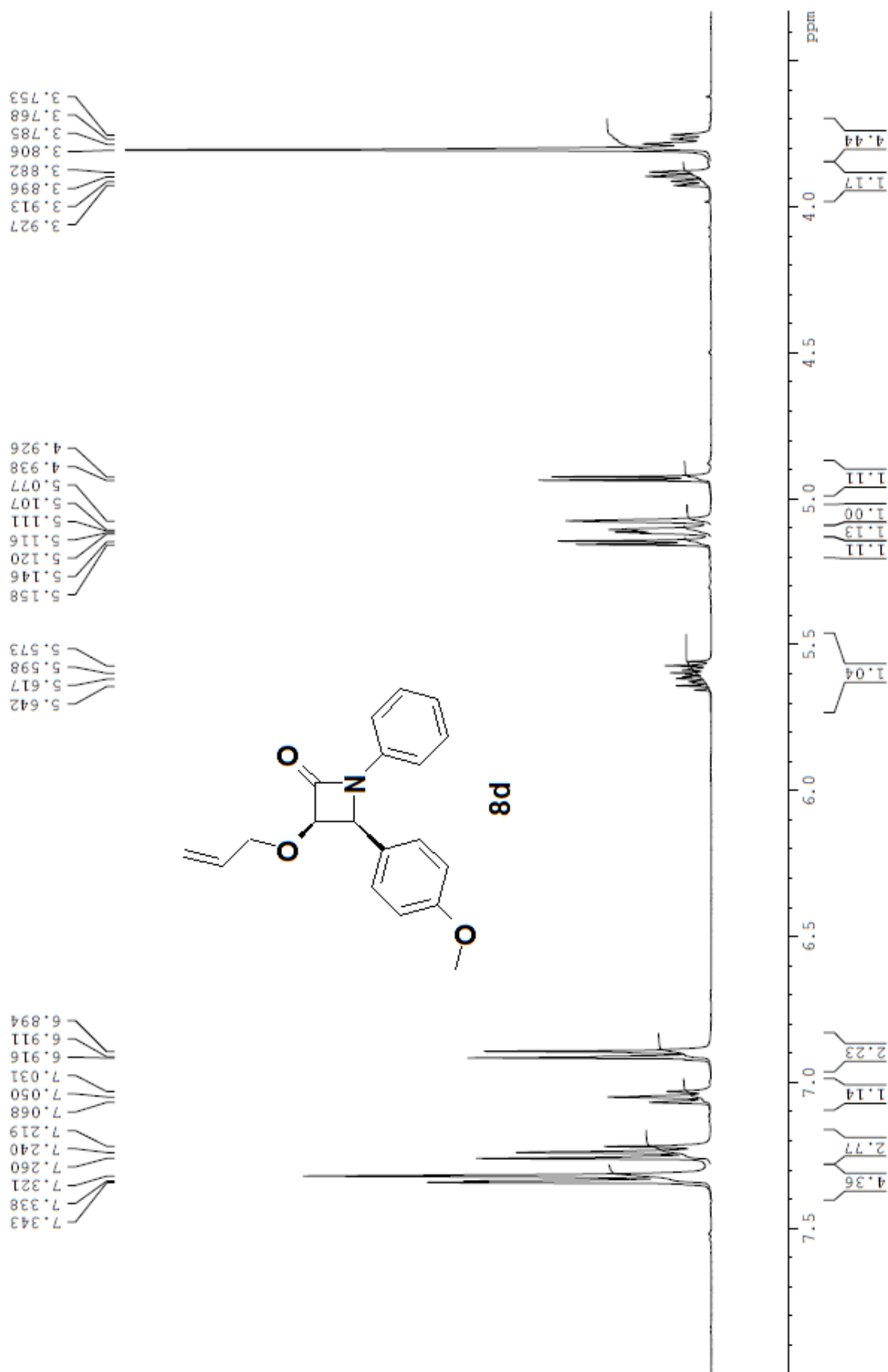


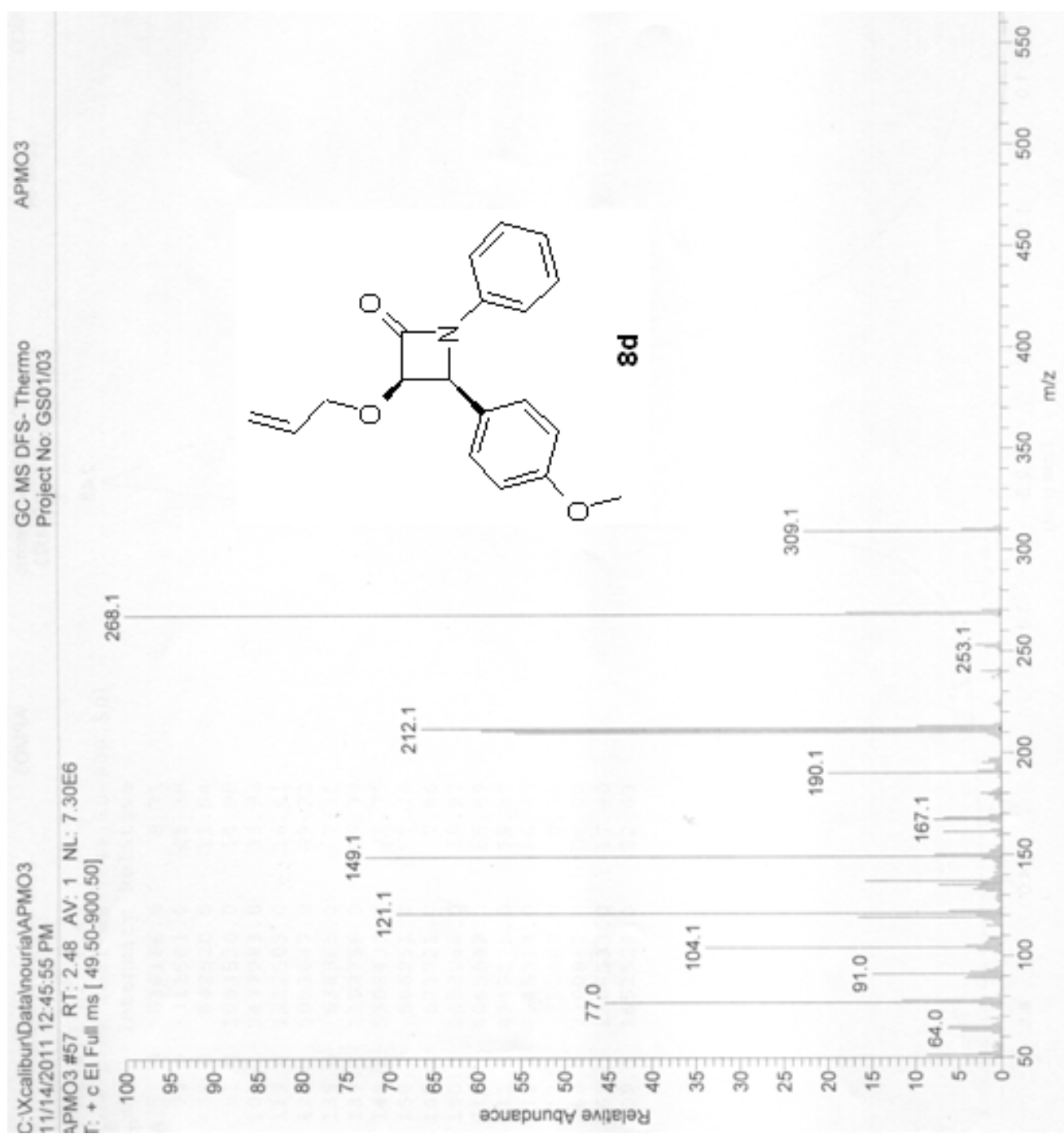
¹³C APT spectra Osama APC5 in CDCl₃





¹H spectra Osama APNO3 in CDCl₃



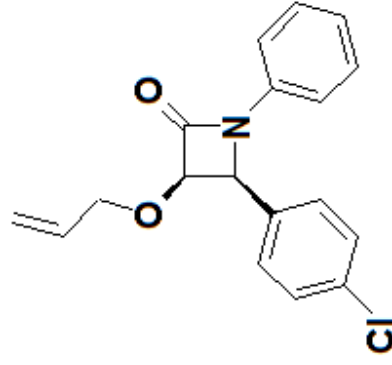


¹H spectra Osama ACP6 in CDCl₃

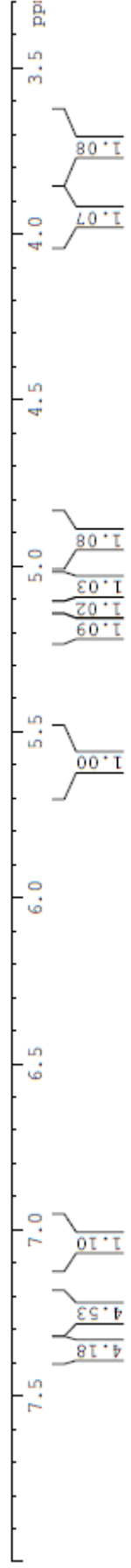
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7.363
7.349
7.328
7.326
7.312
7.308
7.304
7.290
7.287
7.270
7.264
7.261
7.251
7.235
7.230
7.092
7.088
7.085
7.070
7.056
7.053
7.049

5.652
5.638
5.624
5.617
5.611
5.603
5.596
5.591
5.583
5.577
5.569
5.555
5.186
5.174
5.120
5.118
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5.097
5.094
5.091
5.080
5.077
5.073
5.069
4.968
4.956

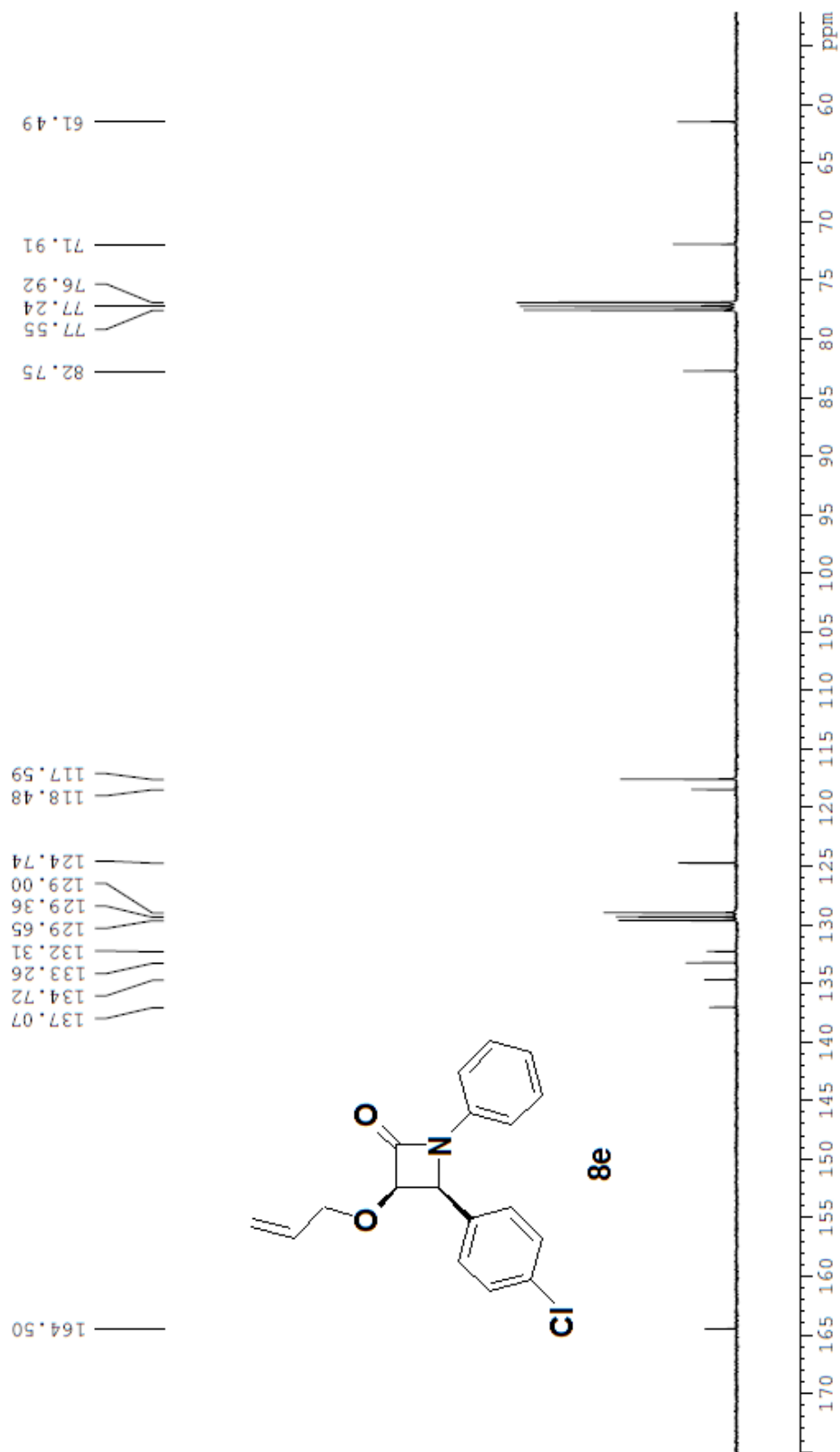
3.964
3.950
3.933
3.919
3.820
3.805
3.788
3.773

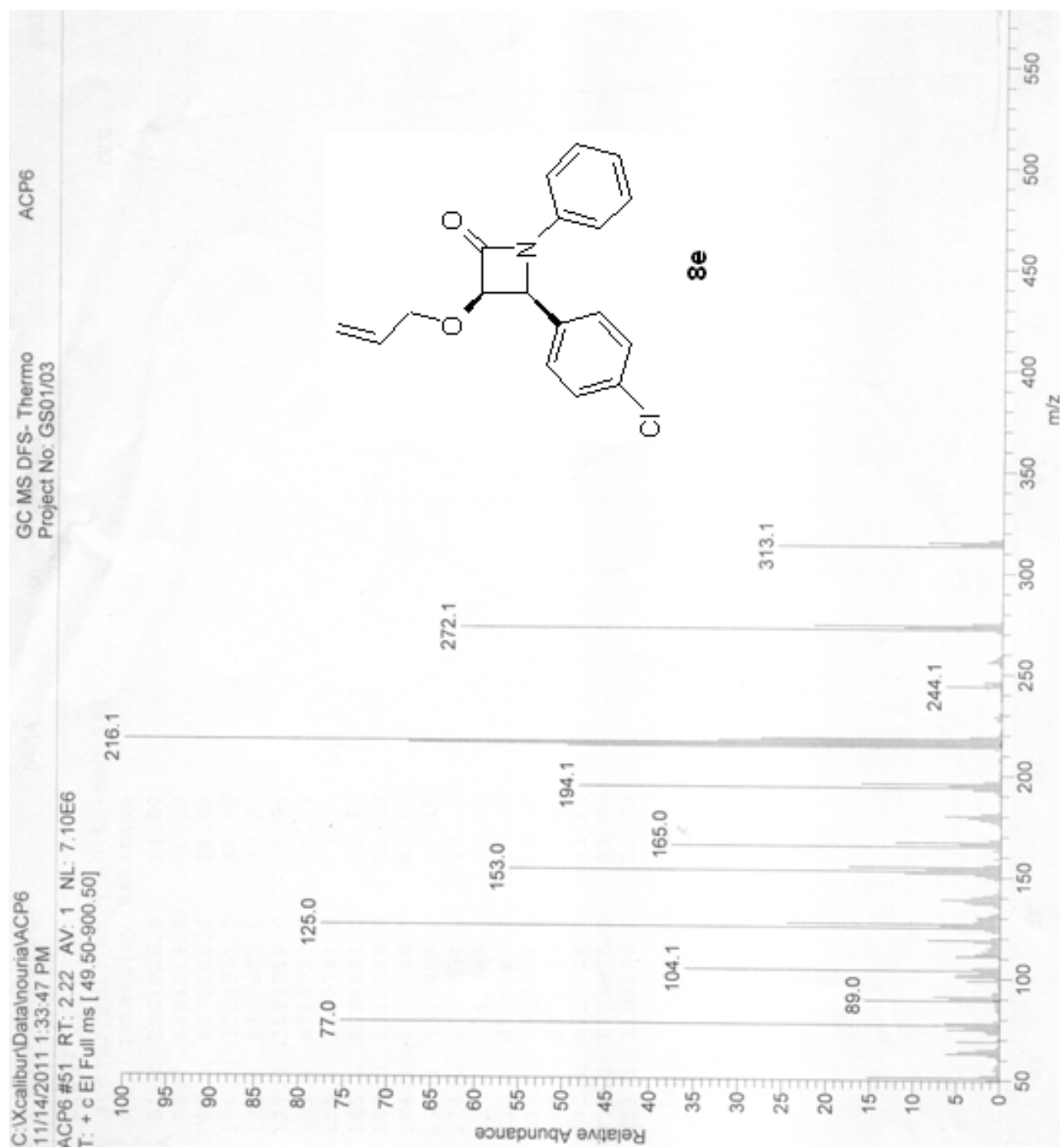


8e

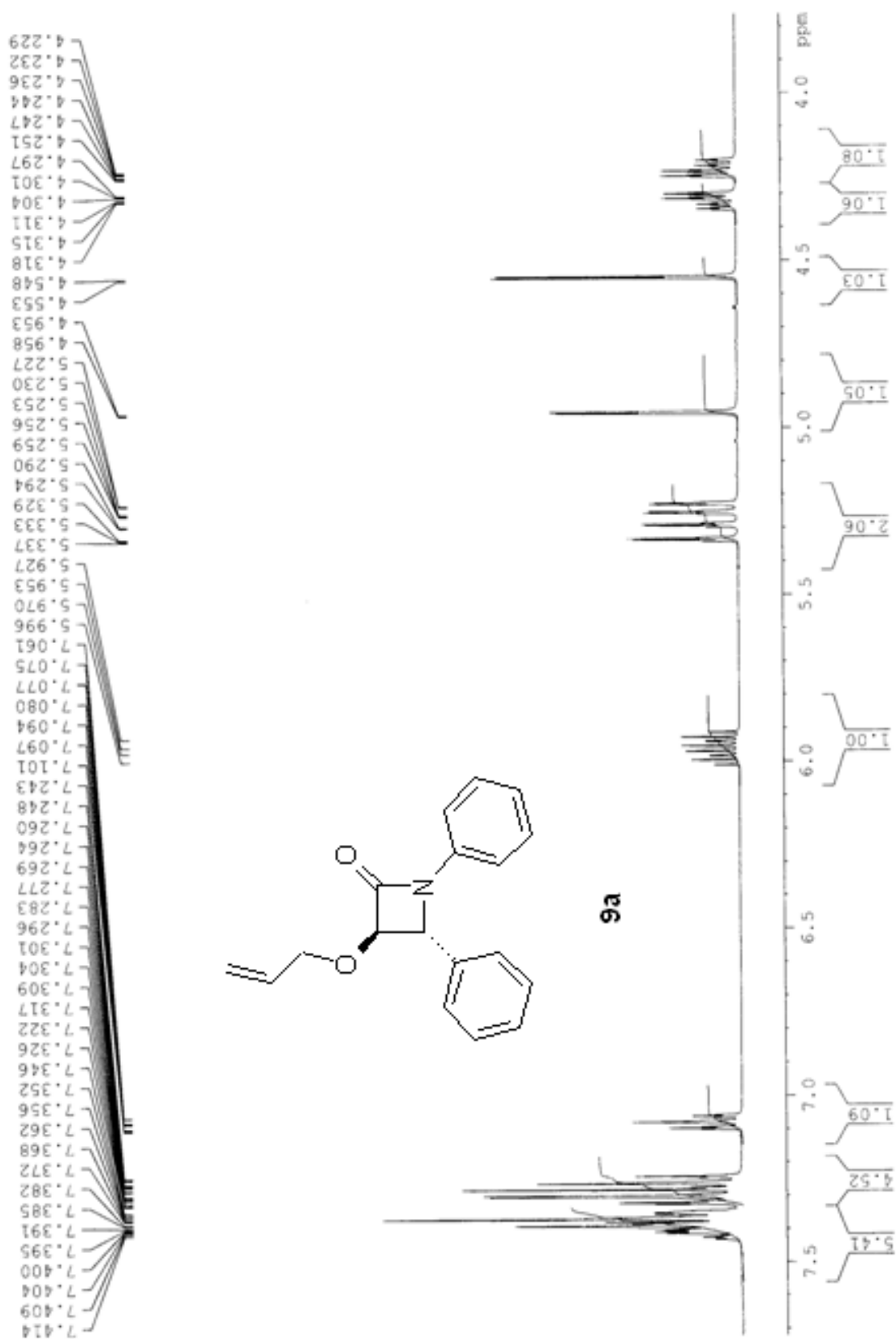


¹³C decoupled spectra Osama ACP6 in CDCL₃

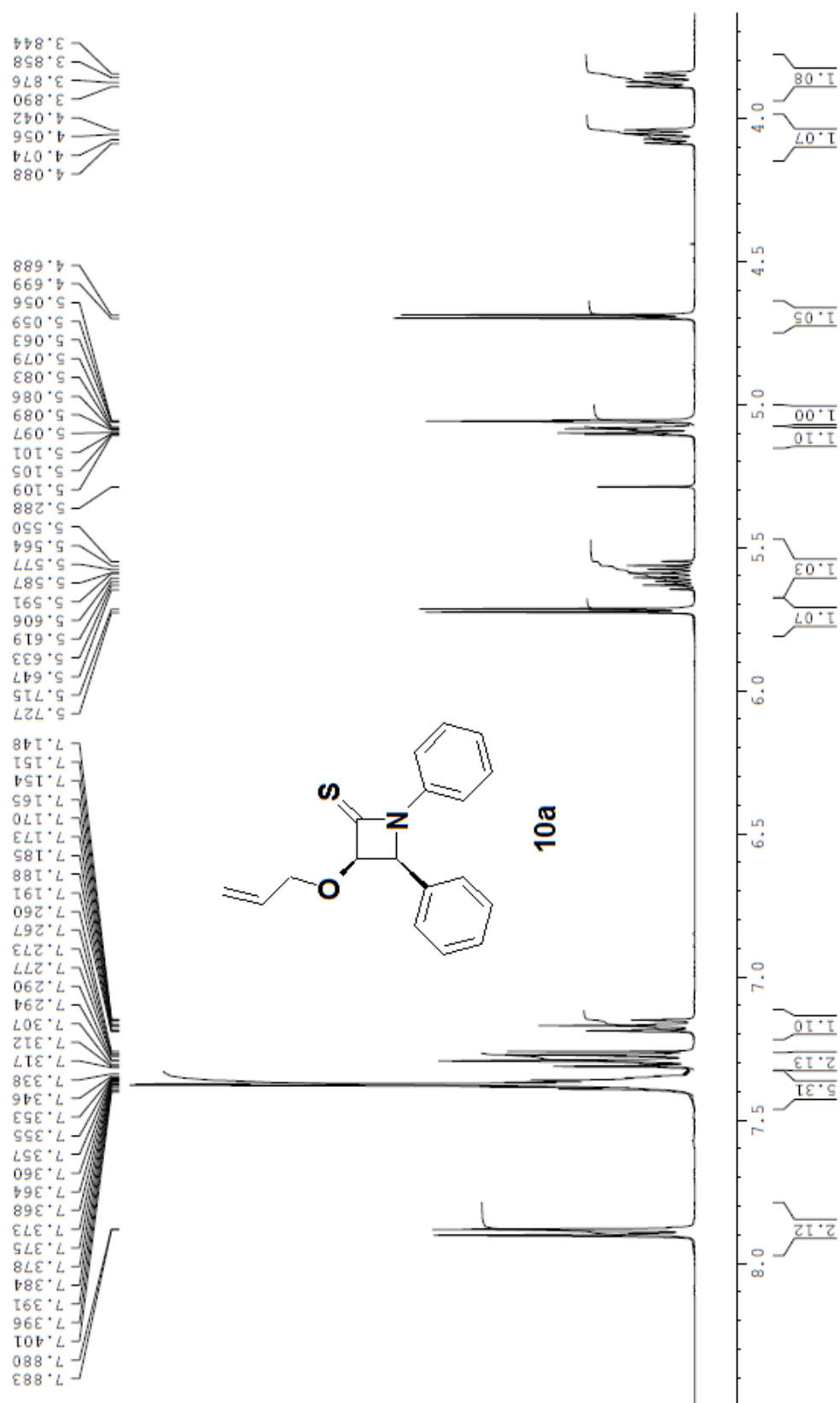




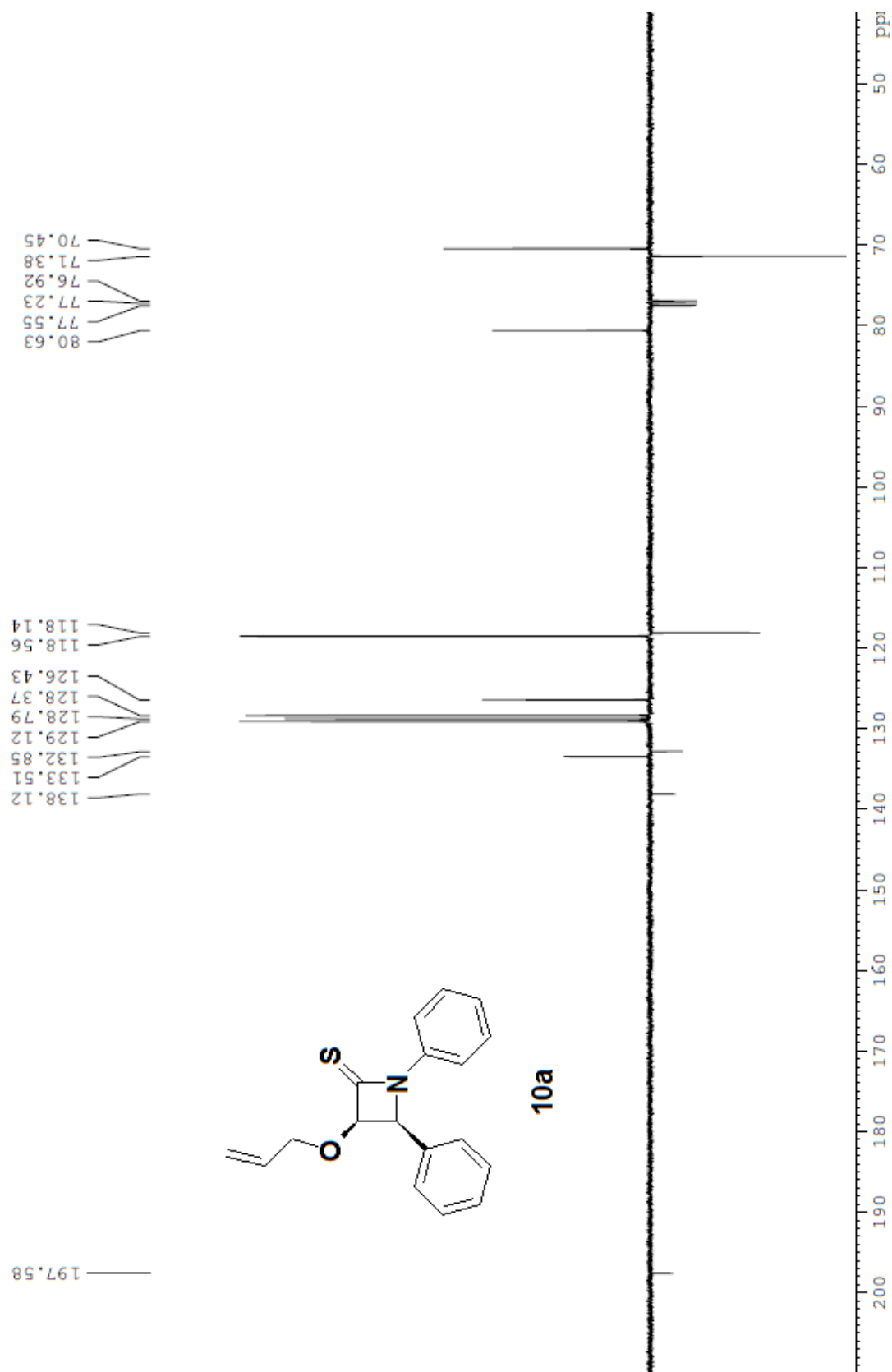
¹H spectra Osama F2 in CDCl₃

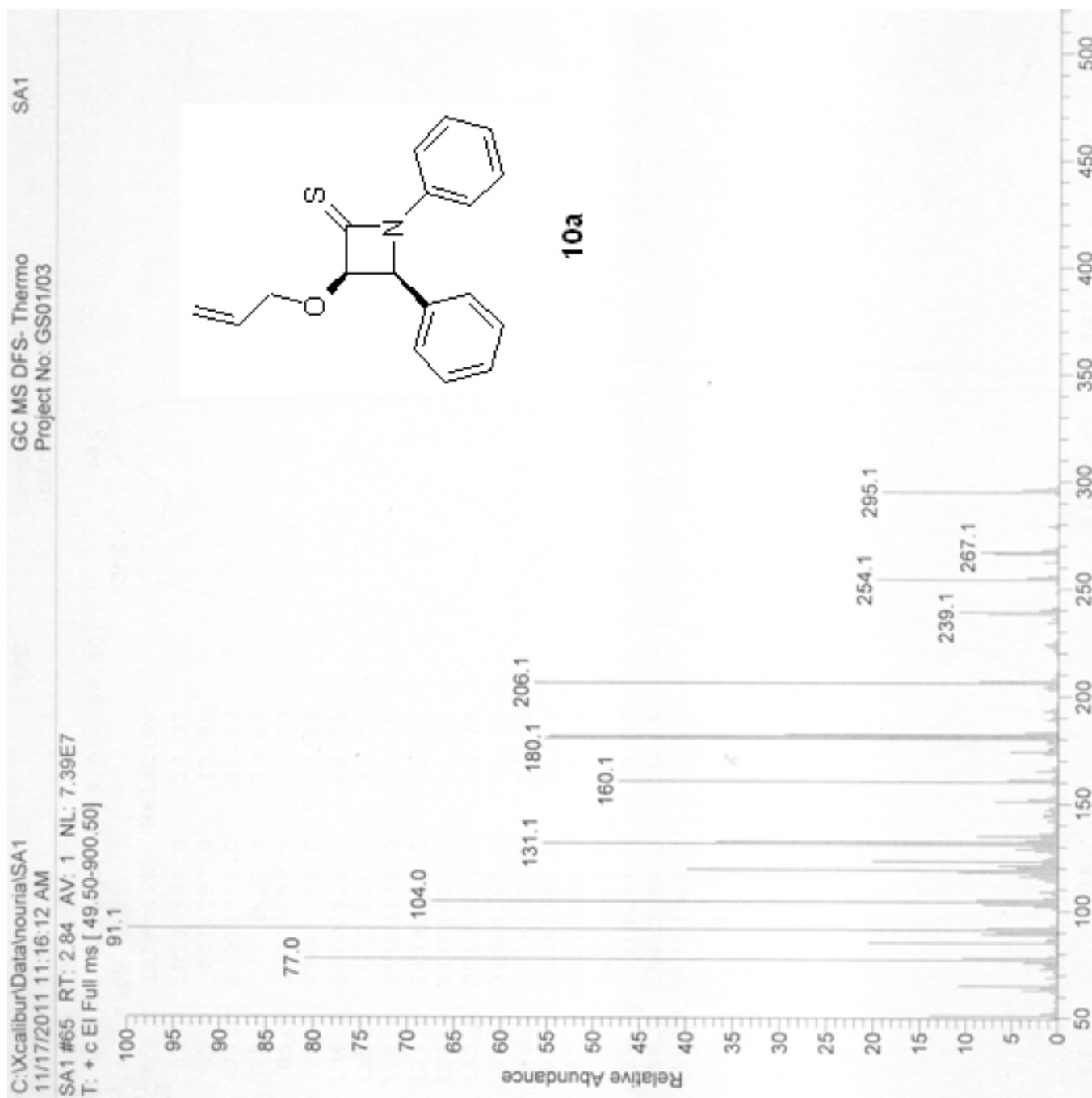


¹H spectra Osama SA1 in CDCl₃

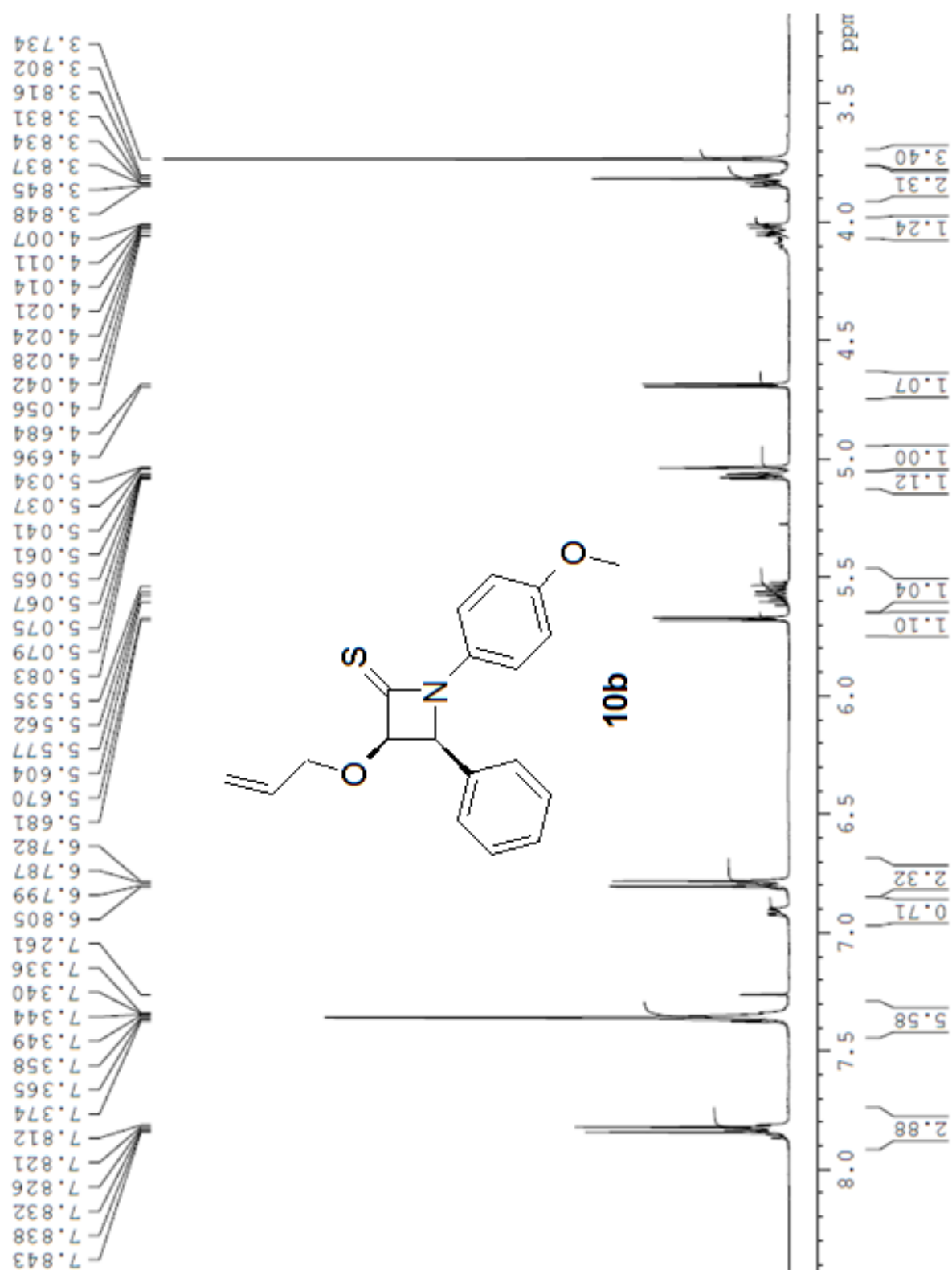


¹³C APT spectra Osama SA1 in CDCl₃

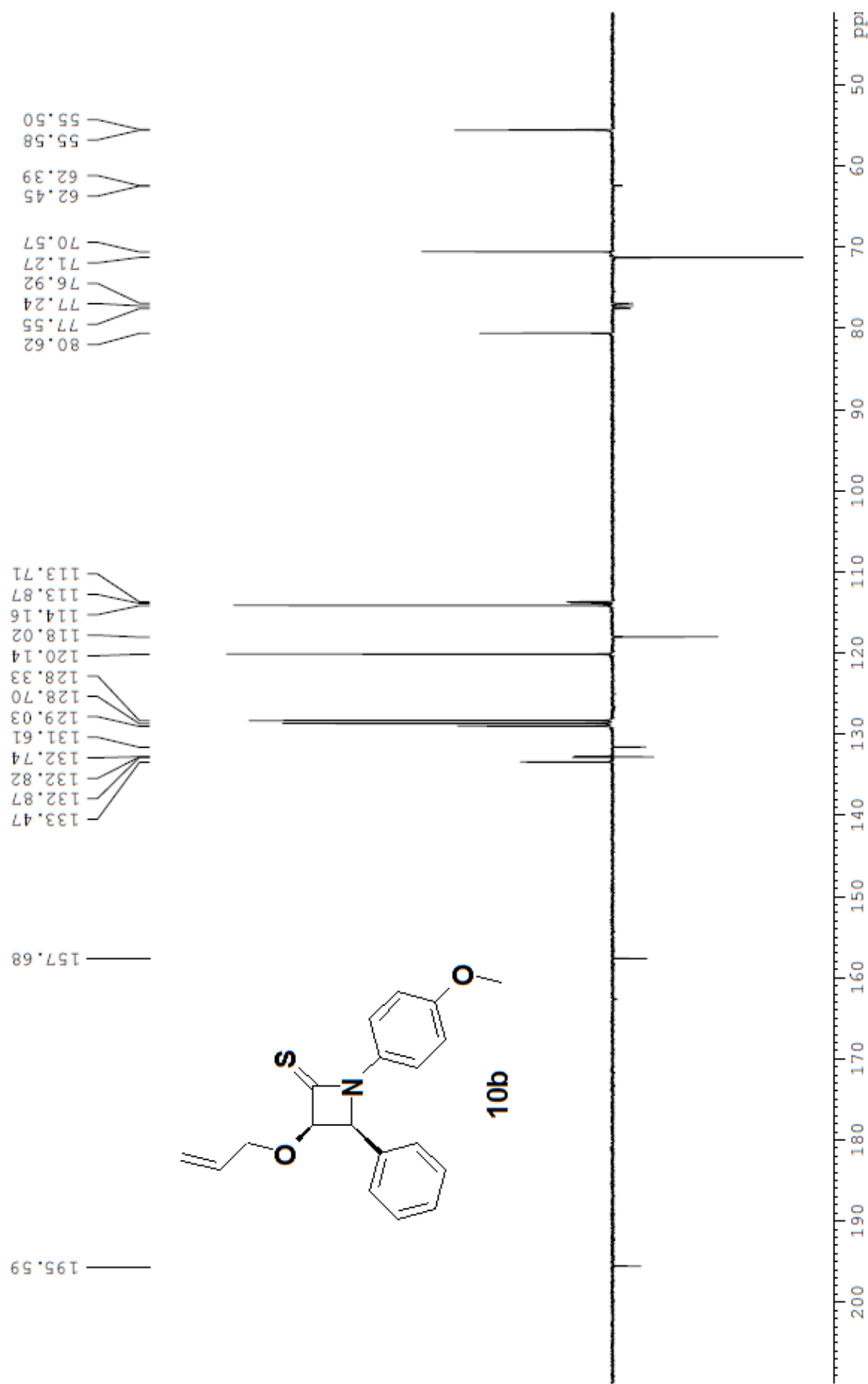




¹H spectra Osama SA2 in CDCL3



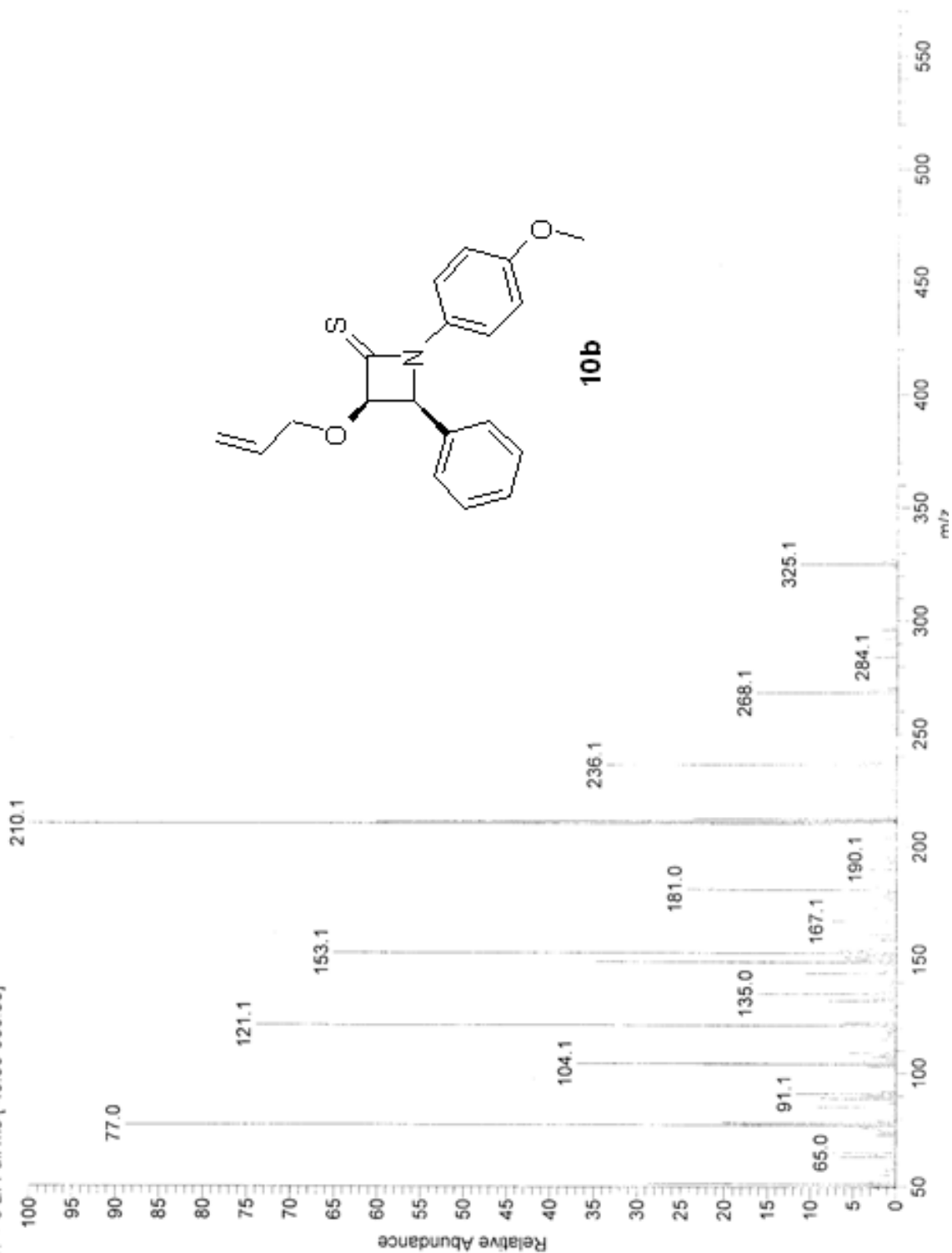
¹³C APT spectra Osama SA2 in CDCL₃



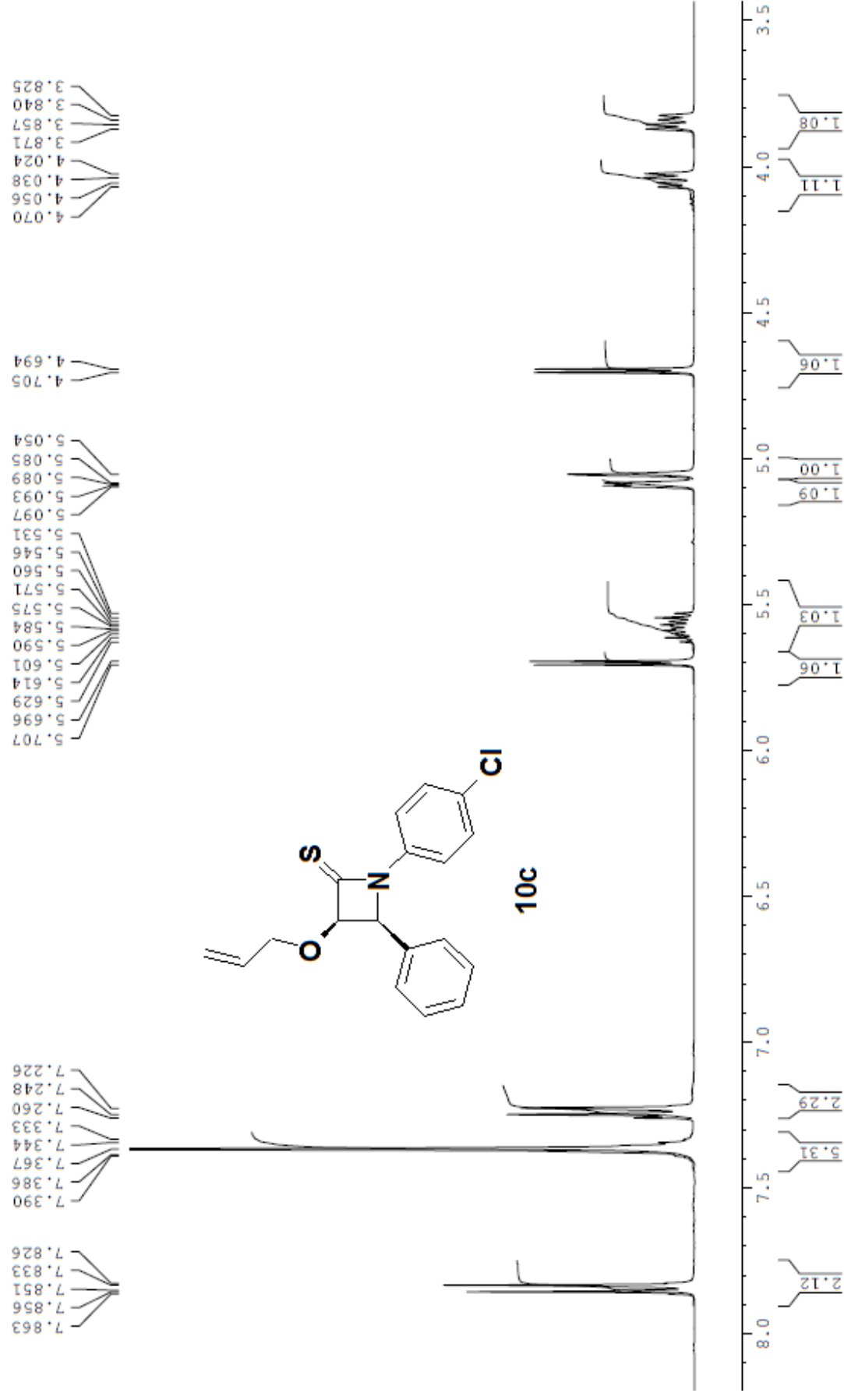
C:\Xcalibur\Data\nouria\SA2
5/27/2012 12:46:00 PM
SA2 #97 RT: 4.26 AV: 1 NL: 1.03E6
T: + c EI Full ms [49.50-900.50]

GC MS DFS- Thermo
Project No: GS01/03

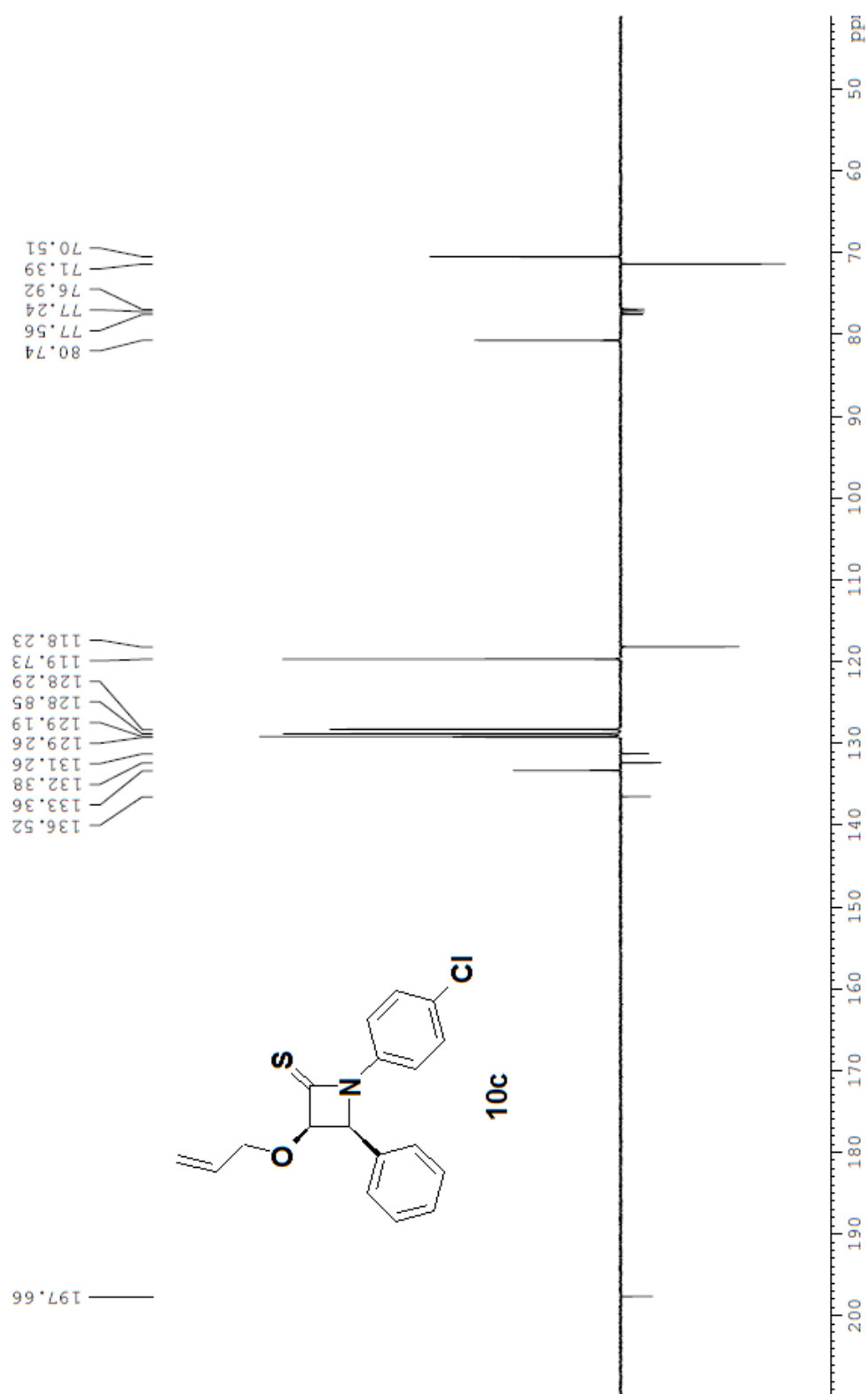
SA2



¹H spectra Osama SA3 in CDCL₃



¹³C APT spectra Osama SA3 in CDCl₃



C:\Xcalibur\Data\ncouria\SA3

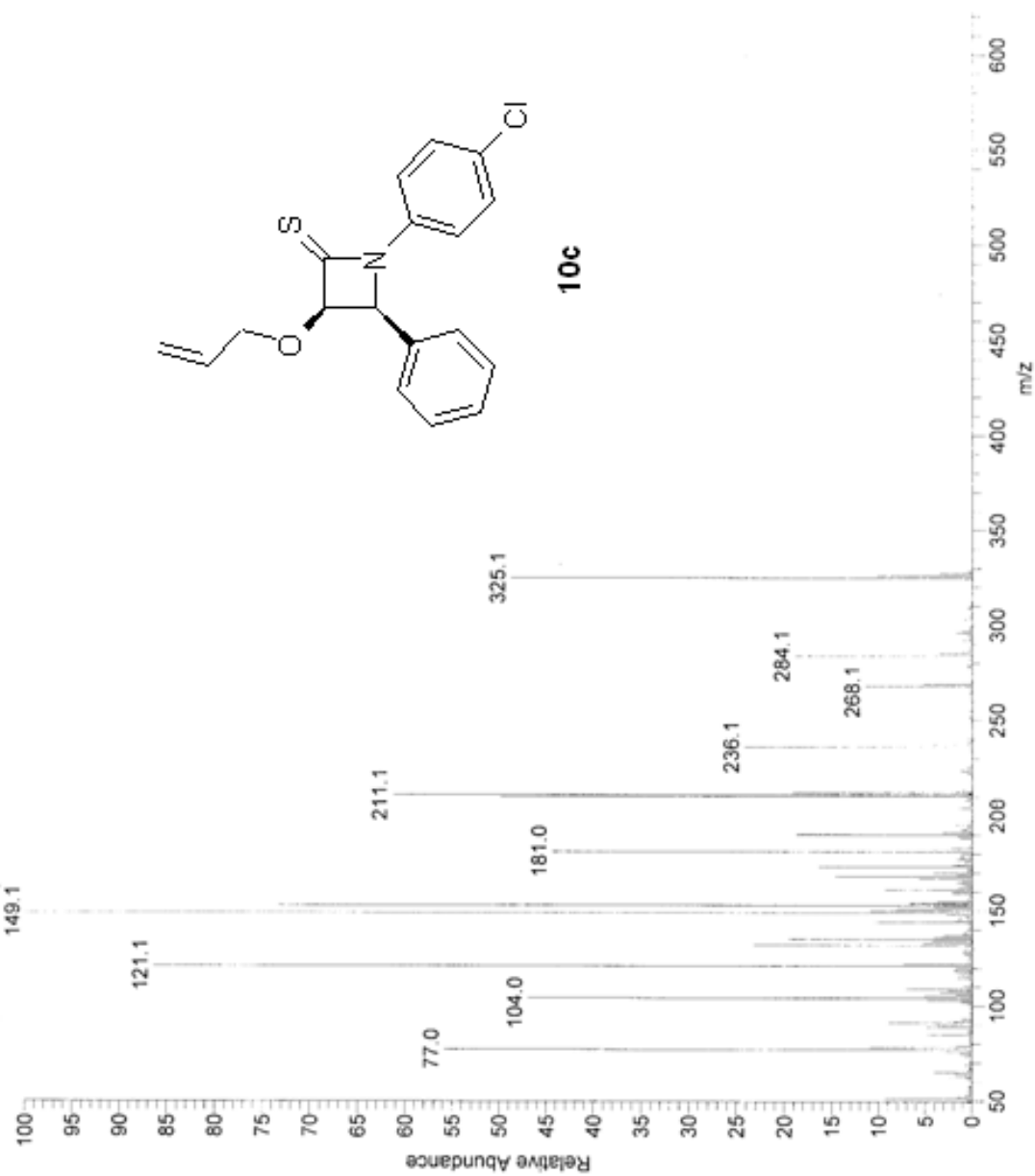
11/17/2011 11:36:02 AM

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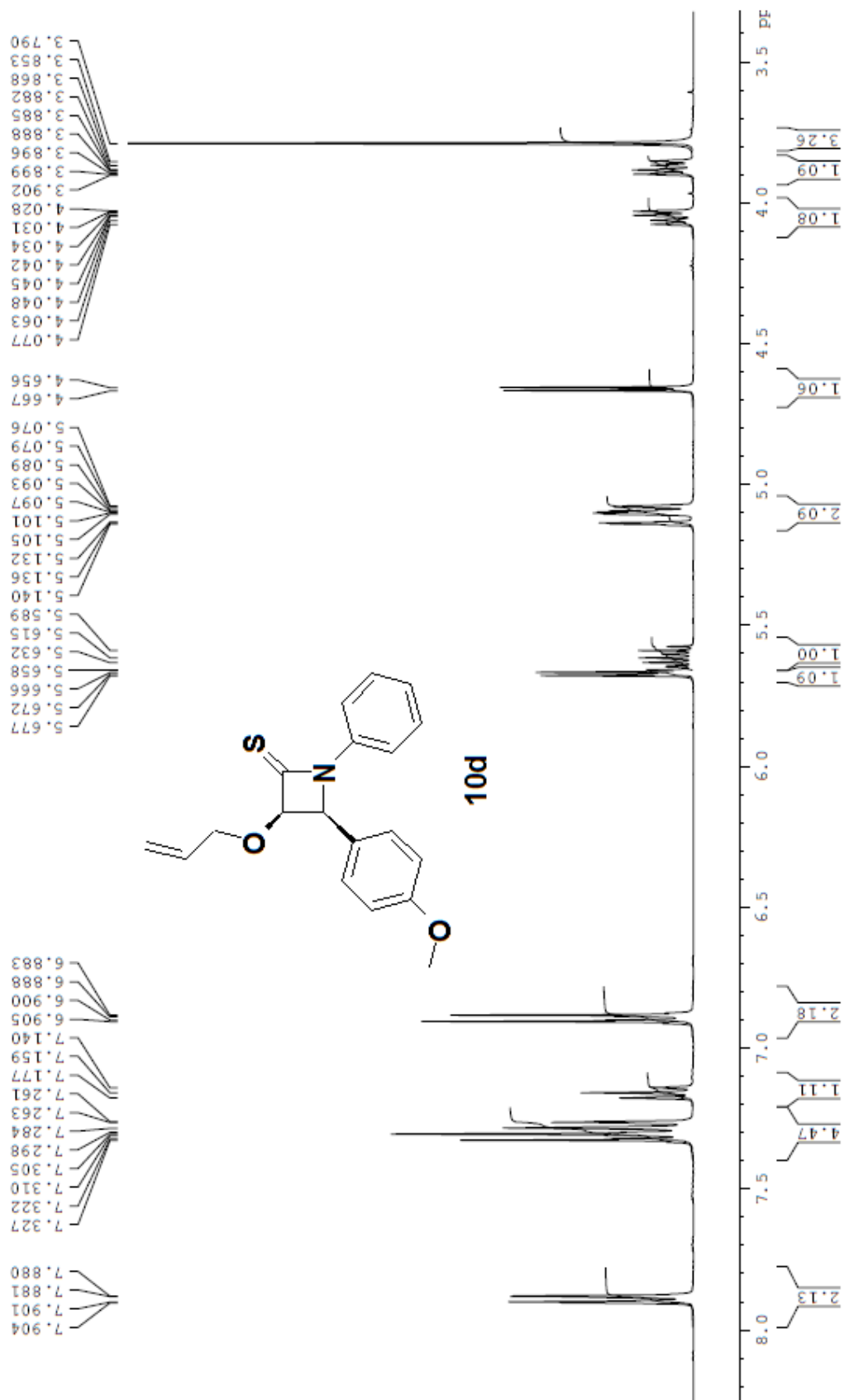
T: + c EI Full ms [49.50-900.50]

GC MS DFS- Thermo
Project No: GS01/03

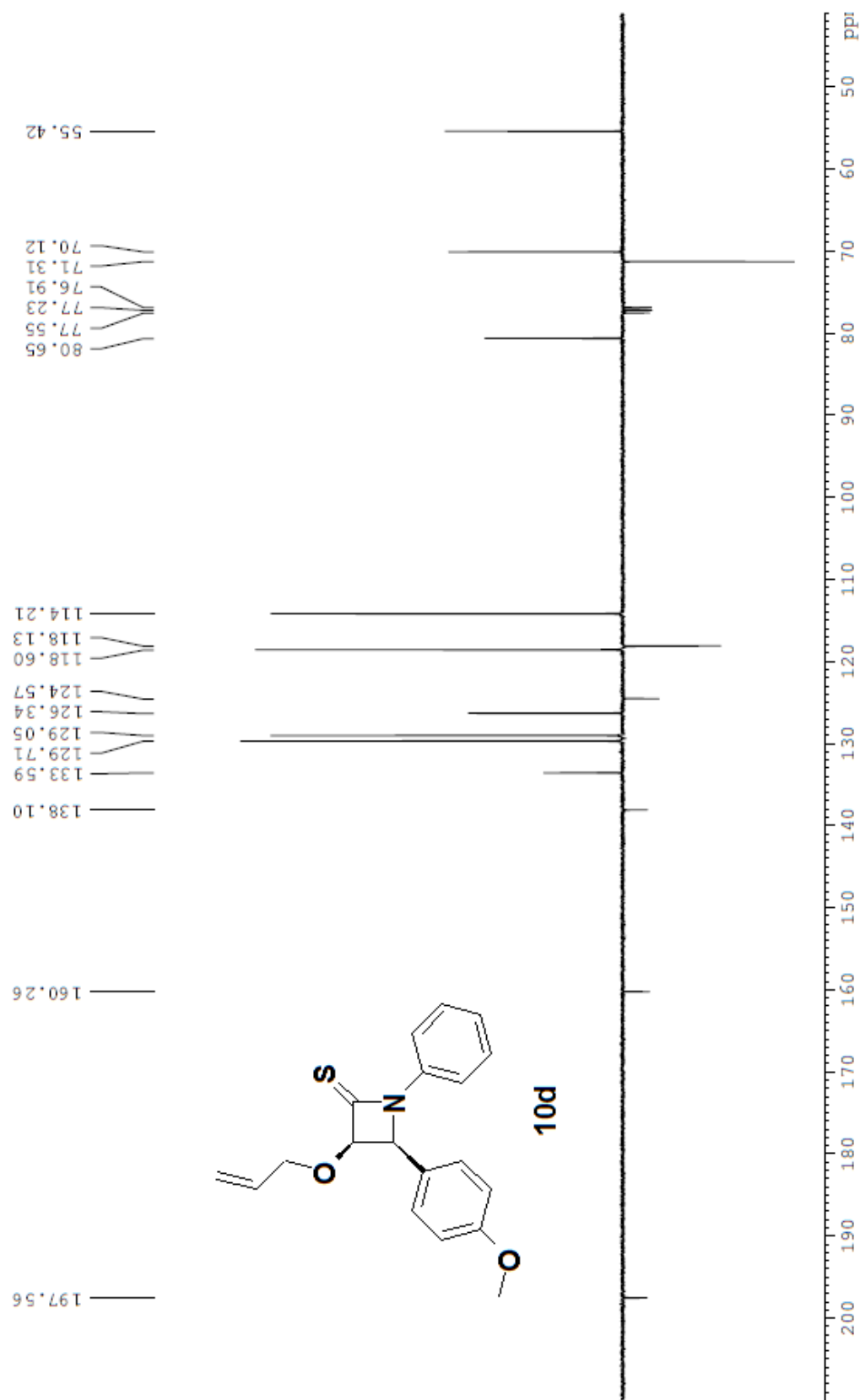
SA3

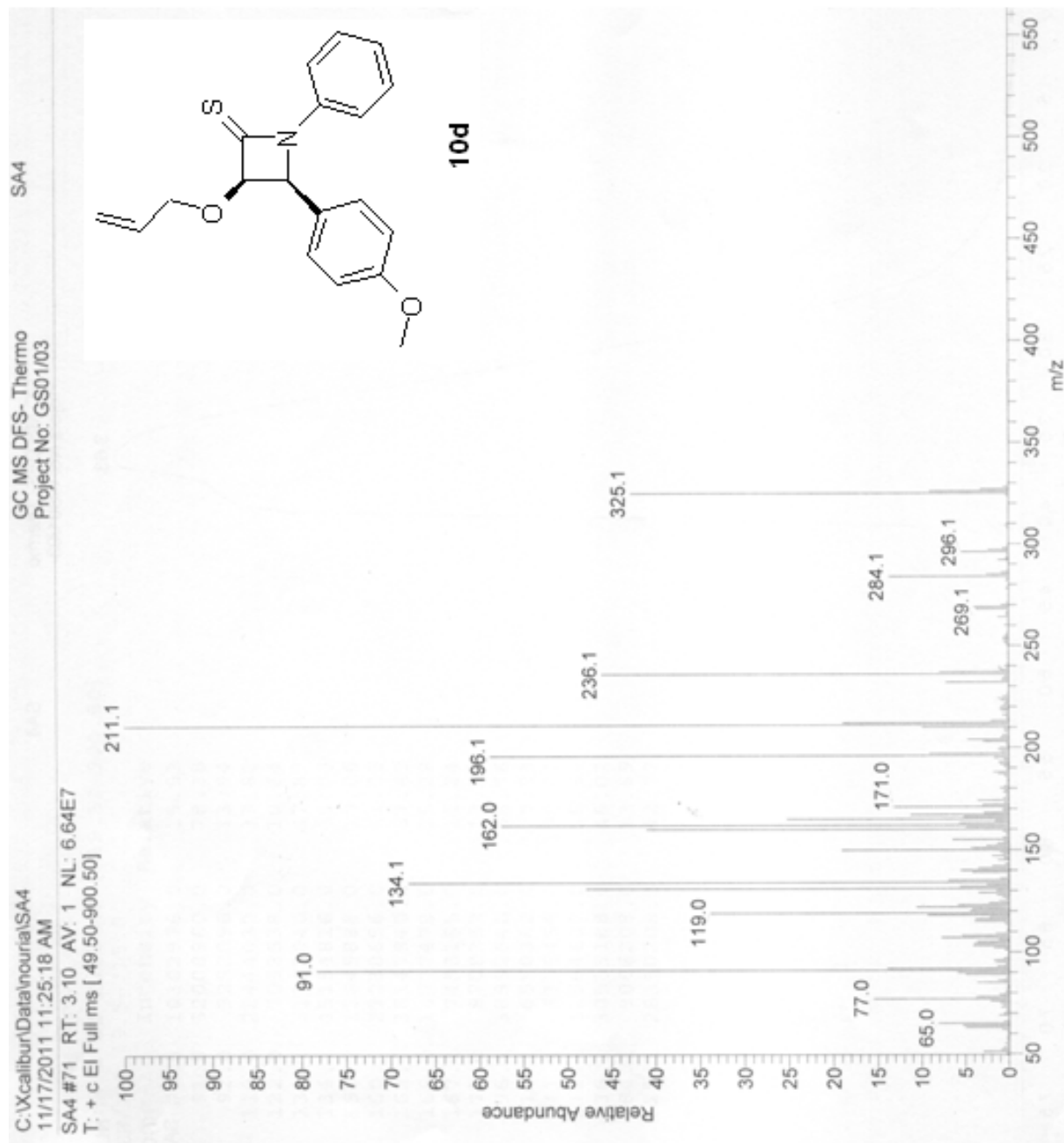


¹H spectra Osama SA4 in CDCl₃

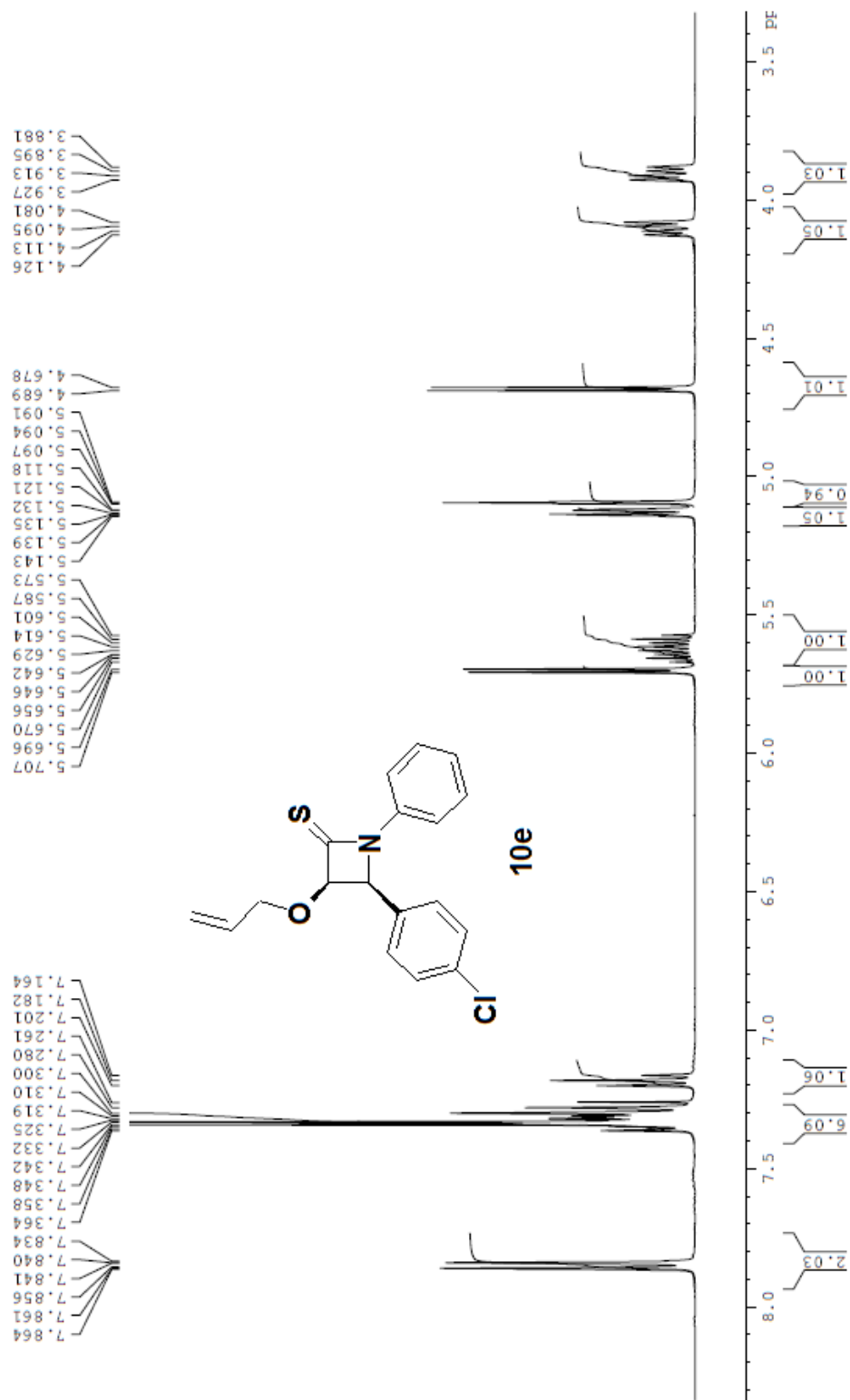


¹³C APT spectra Osama SA4 in CDCl₃

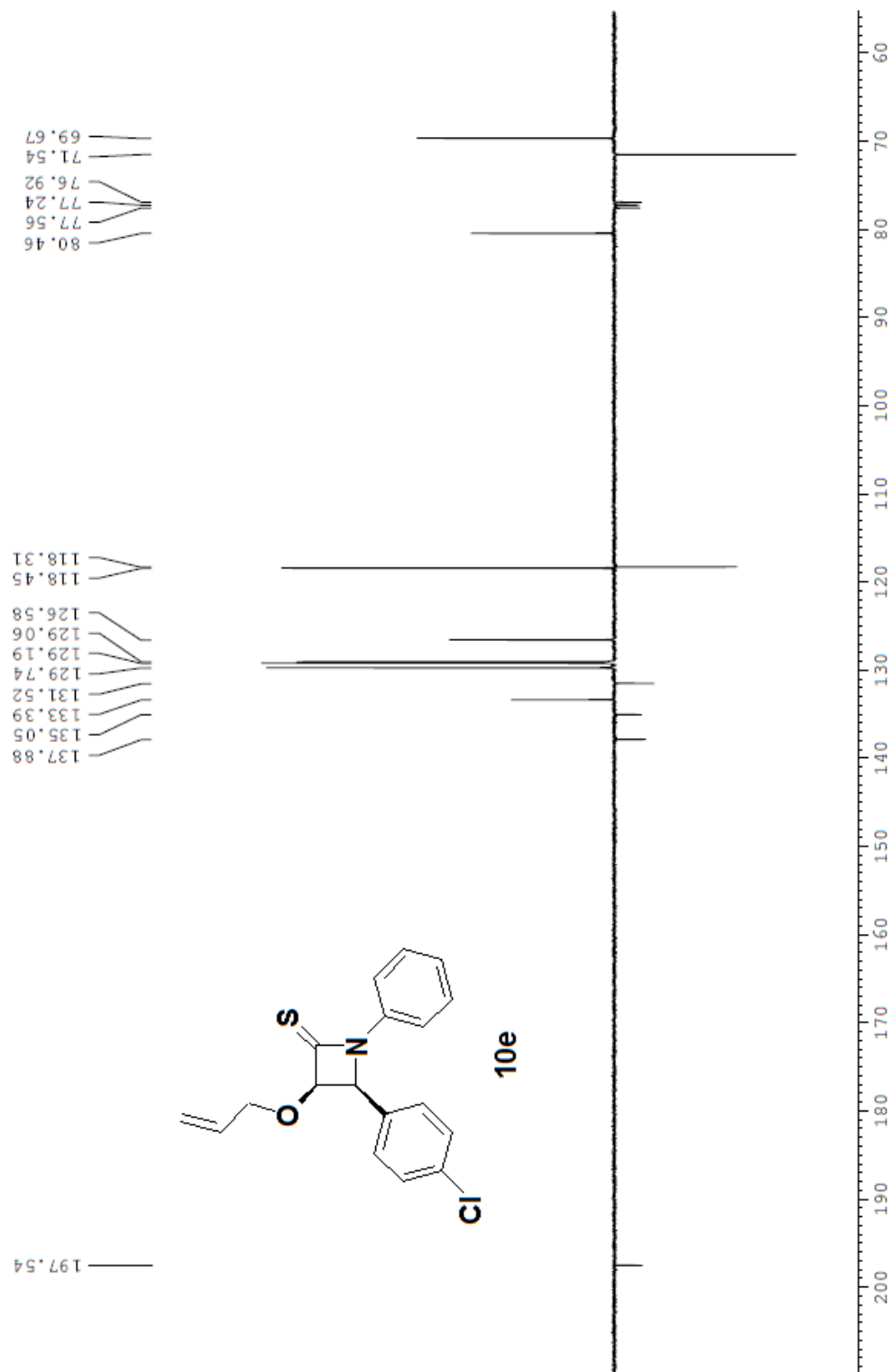




¹H spectra Osama SA5 in CDCl₃



¹³C APT spectra Osama SA5 in CDCl₃



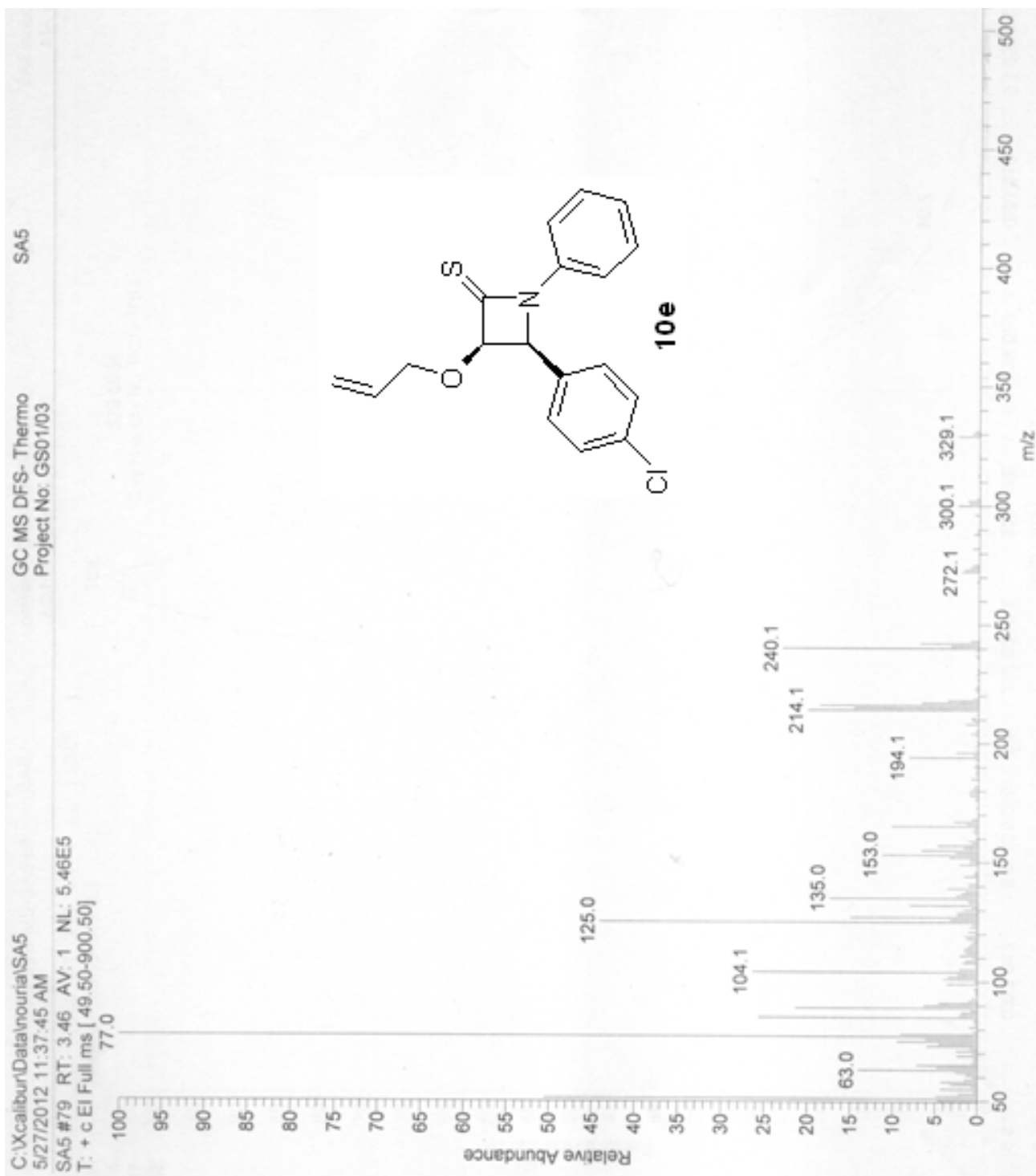
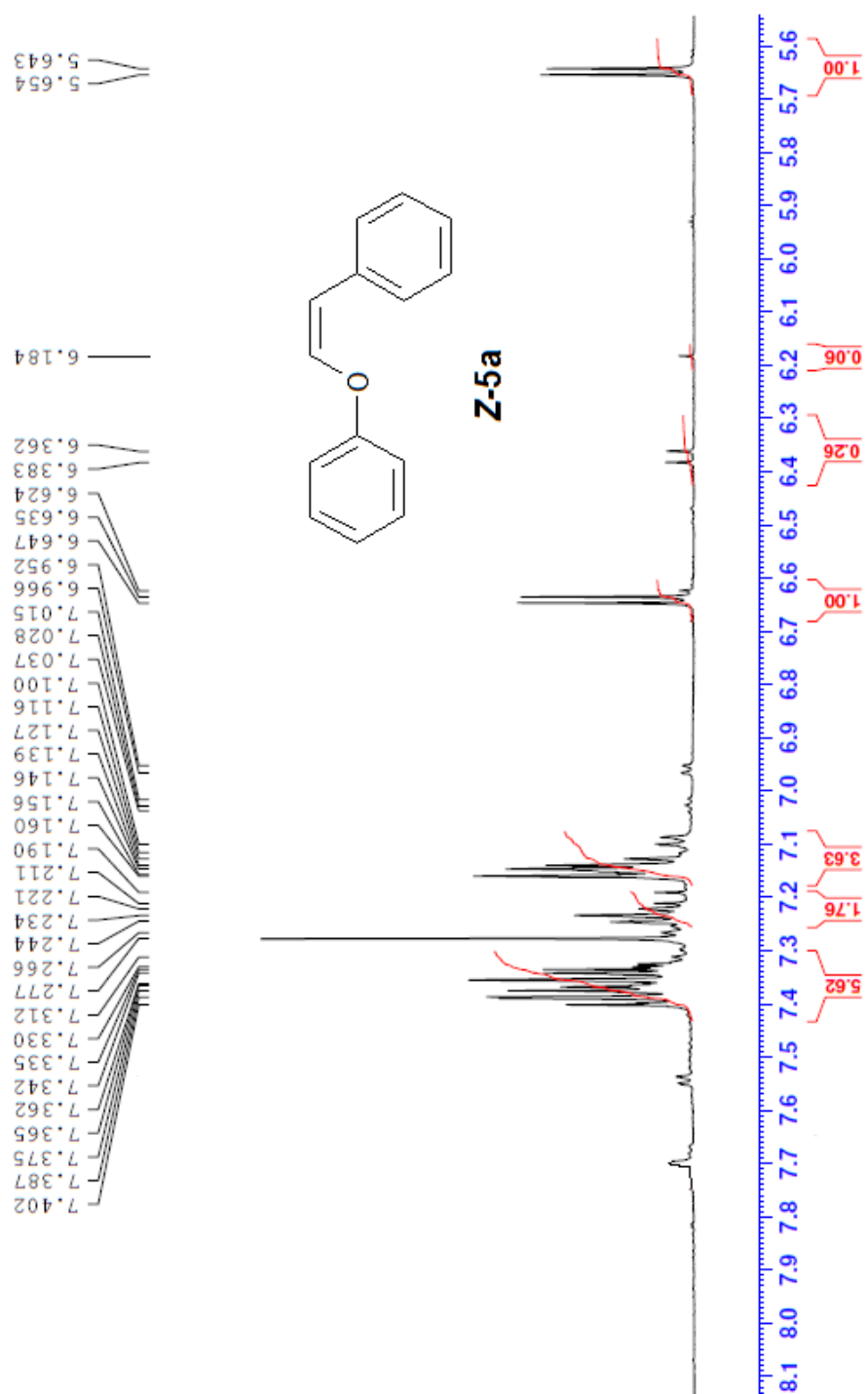


Table 2. H-3/C-3 and H-4/C-4 of azetidinone rings of 8a-e, 9a and 10a-e.

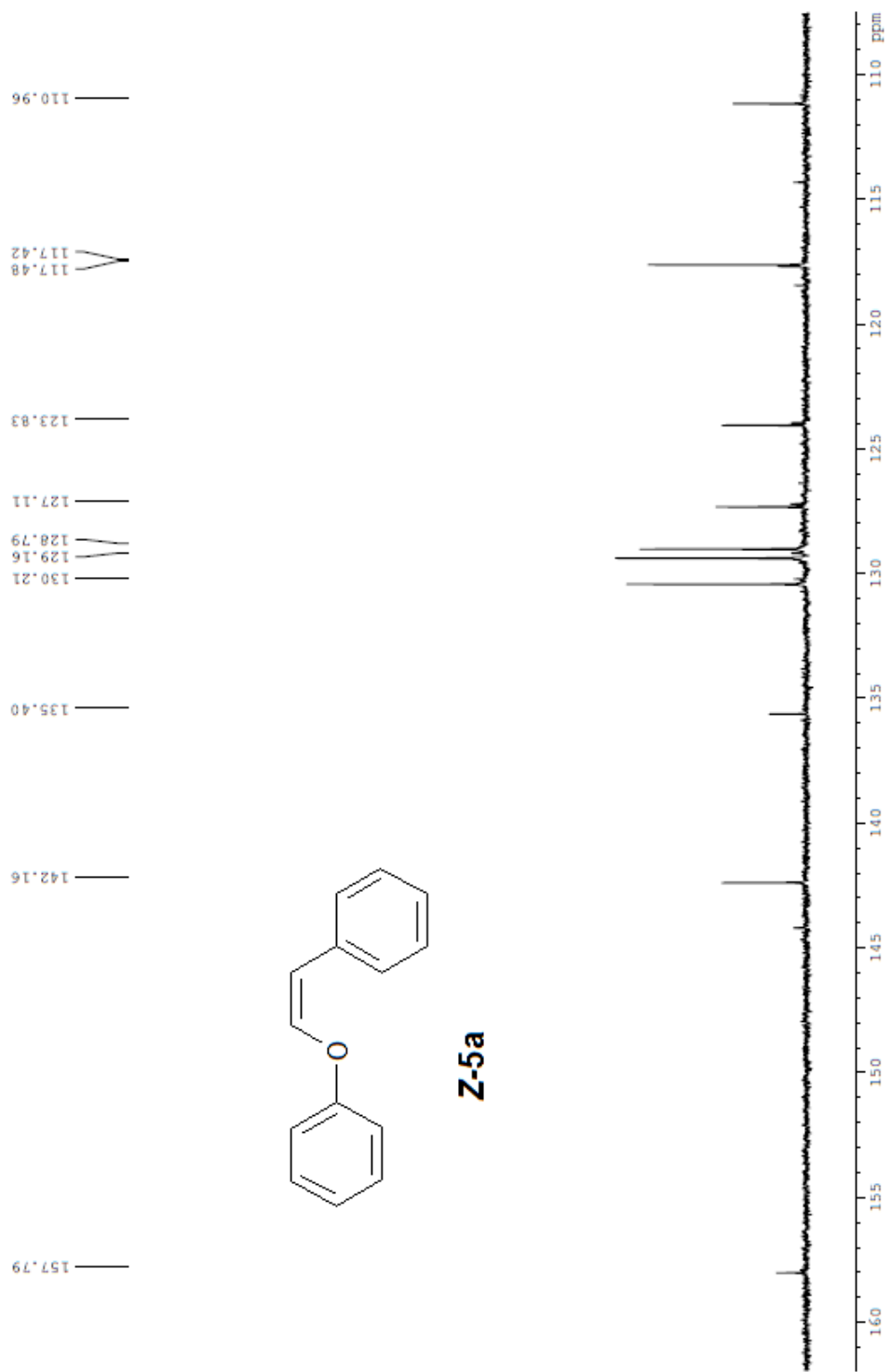
8a	75%	4.99 (d, J 4.8)/82.5	5.22 (d, J 4.8)/61.0
8b	84%	4.97 (d, J 4.8)/82.7	5.17 (d, J 4.8)/62.1
8c	69%	4.92 (d, J 4.8)/82.8	5.19 (d, J 4.8)/62.1
8d	82%	4.94 (d, J 4.8)/82.4	5.16 (d, J 4.8)/61.5
8e	70%	4.98 (d, J 4.8)/82.5	5.19 (d, J 4.8)/61.3
9a	4%	4.55 (d, J 2.4)	4.95 (d, J 2.4)
10a	70%	4.72 (d, J 4.4)/80.4	5.75(d, J 4.4)/70.2
10b	75%	4.71 (d, J 4.4)/80.3	5.70(d, J 4.4)/70.3
10c	65%	4.72 (d, J 4.4)/80.6	5.73(d, J 4.4)/70.3
10d	72%	4.68 (d, J 4.4)/80.5	5.70(d, J 4.4)/69.9
10e	68%	4.70 (d, J 4.4)/80.3	5.73(d, J 4.4)/69.5

Assignment of H3, H4 proton signals is based on their cross correlations with their respective carbon signals in the 2D-HSQC NMR spectra.

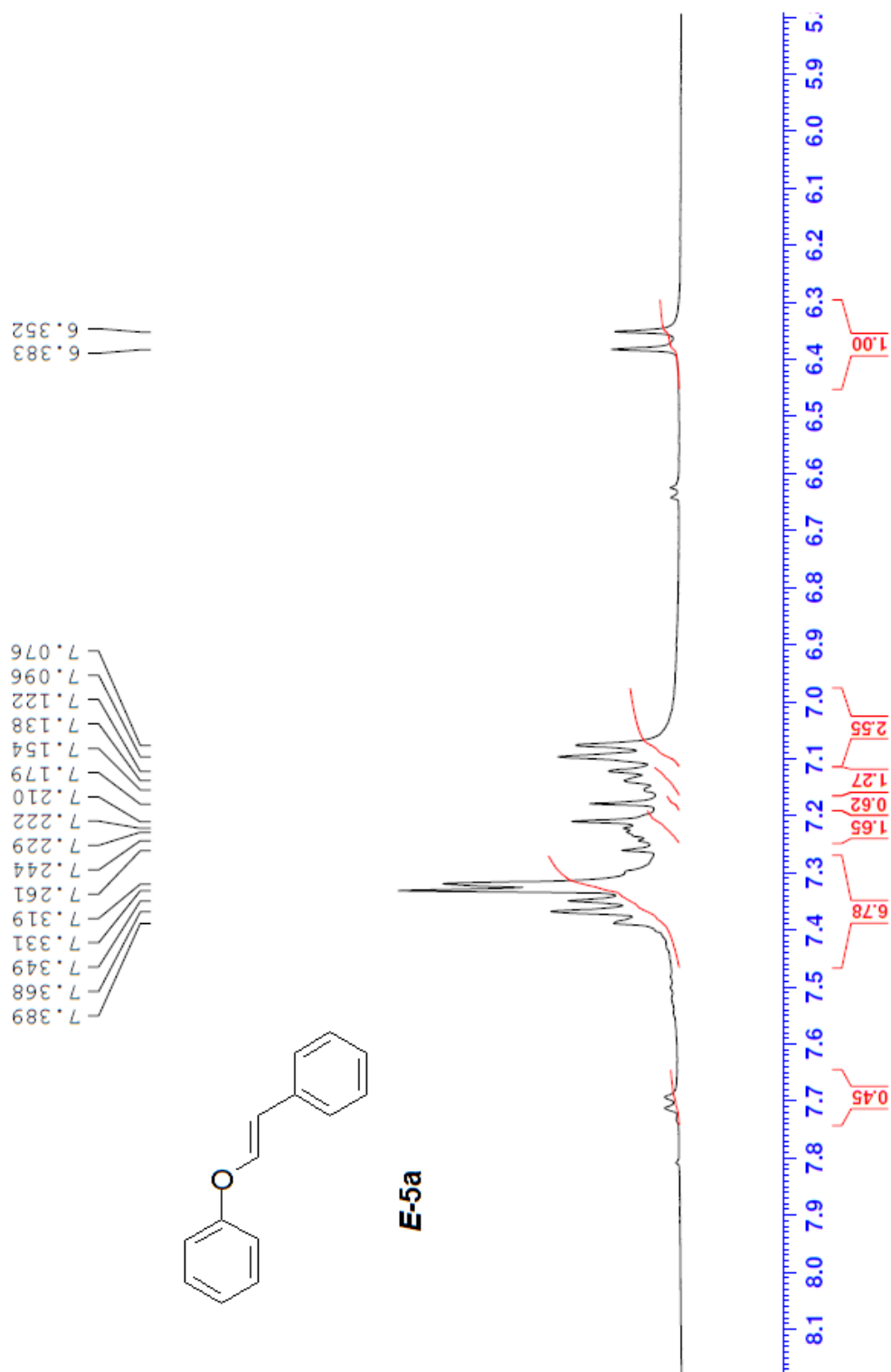
Spectra of some selected product after preparative TLC separation



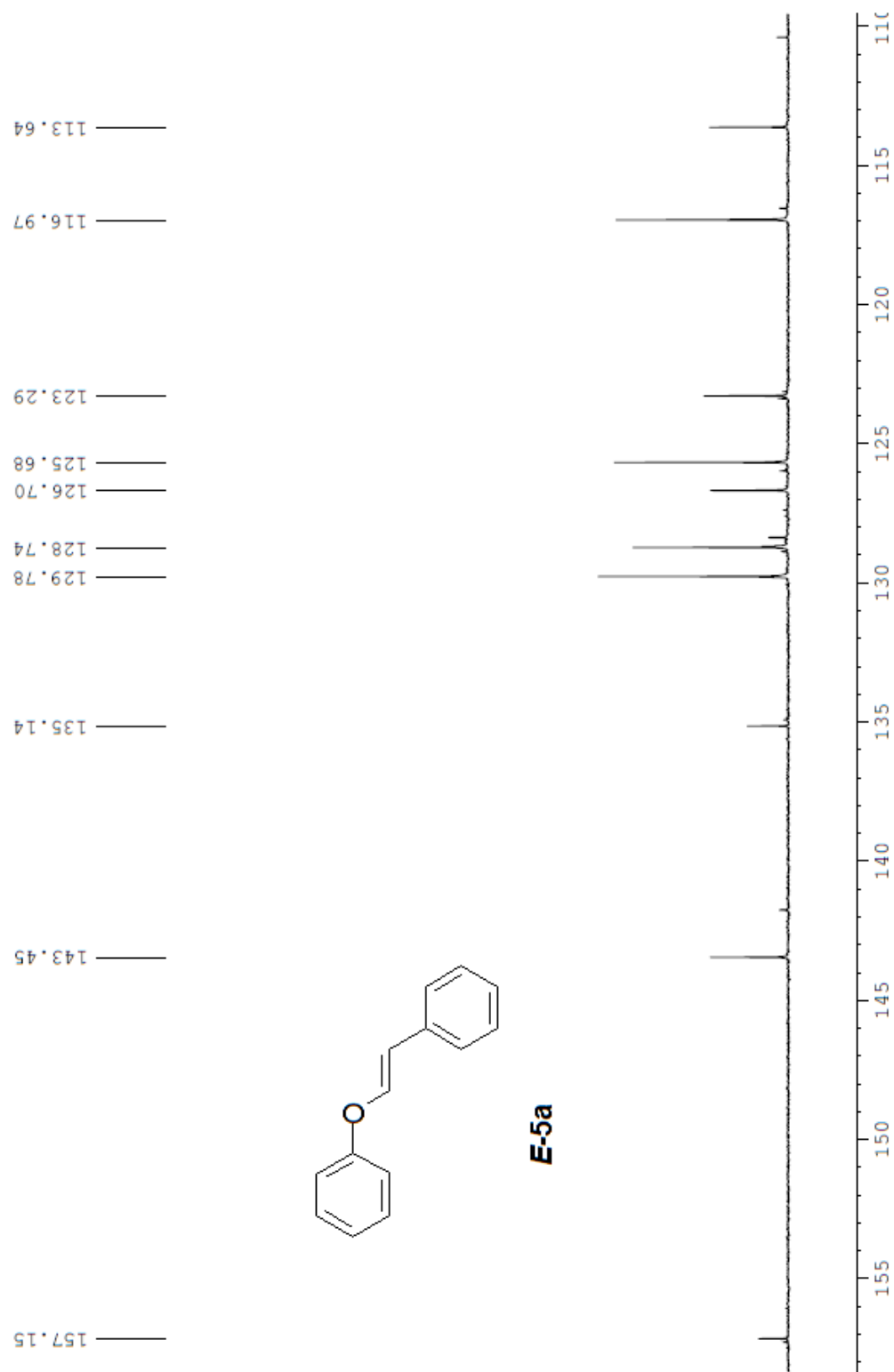
¹³C Spectra Dr.YEHIA C3 in CDCL3



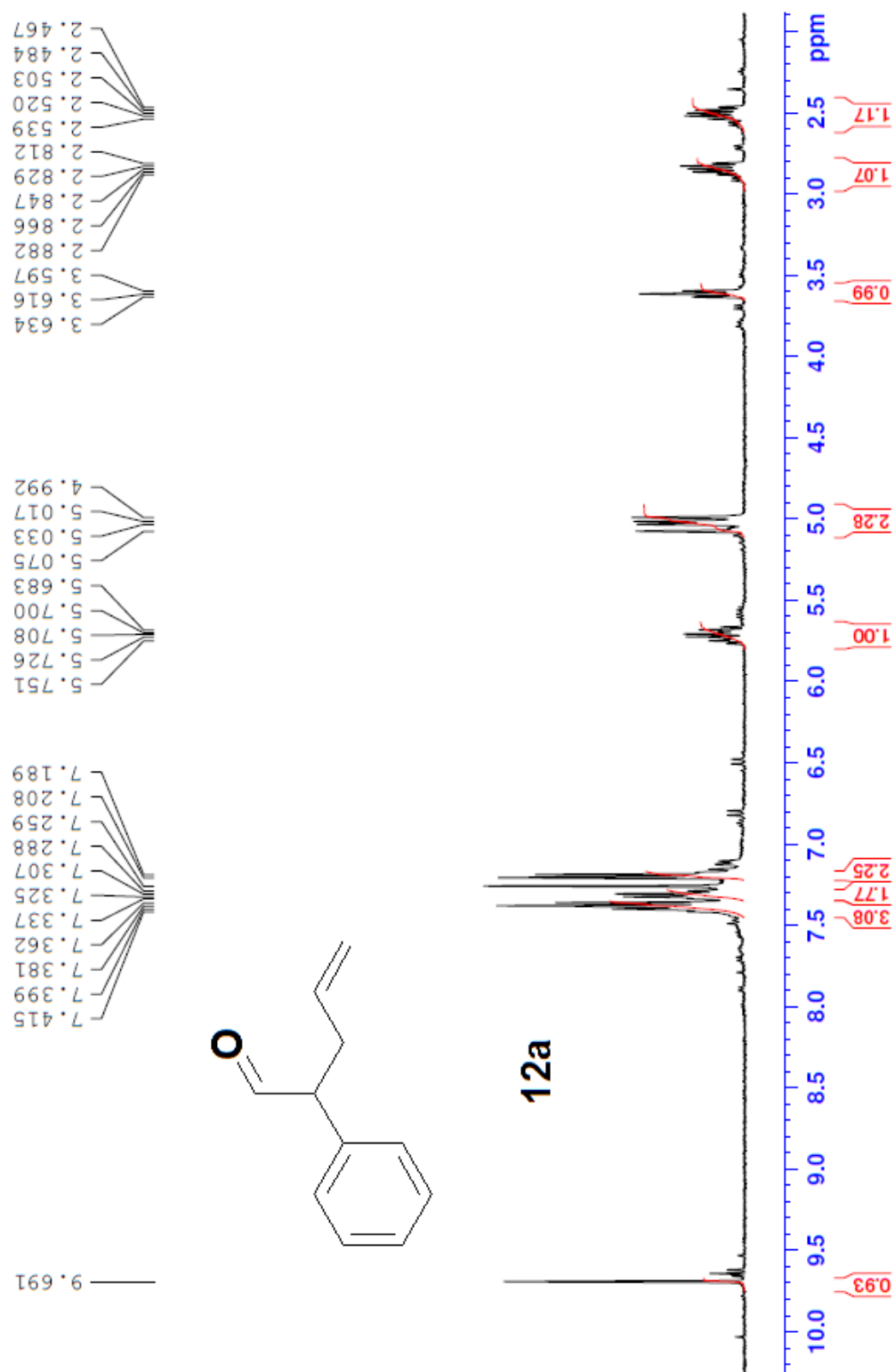
¹H spectra Dr.Yehia C1 in CDCL3



¹³C decoupled spectra Dr.Yehia C1 in CDCL3



¹H spectrum Osama AL in CDCl₃



¹³C decoupled Spectra Osama AL in CDCl₃

