

Supporting Information

Exploring dual electrophiles in peptide-based proteasome inhibitors: carbonyls and epoxides

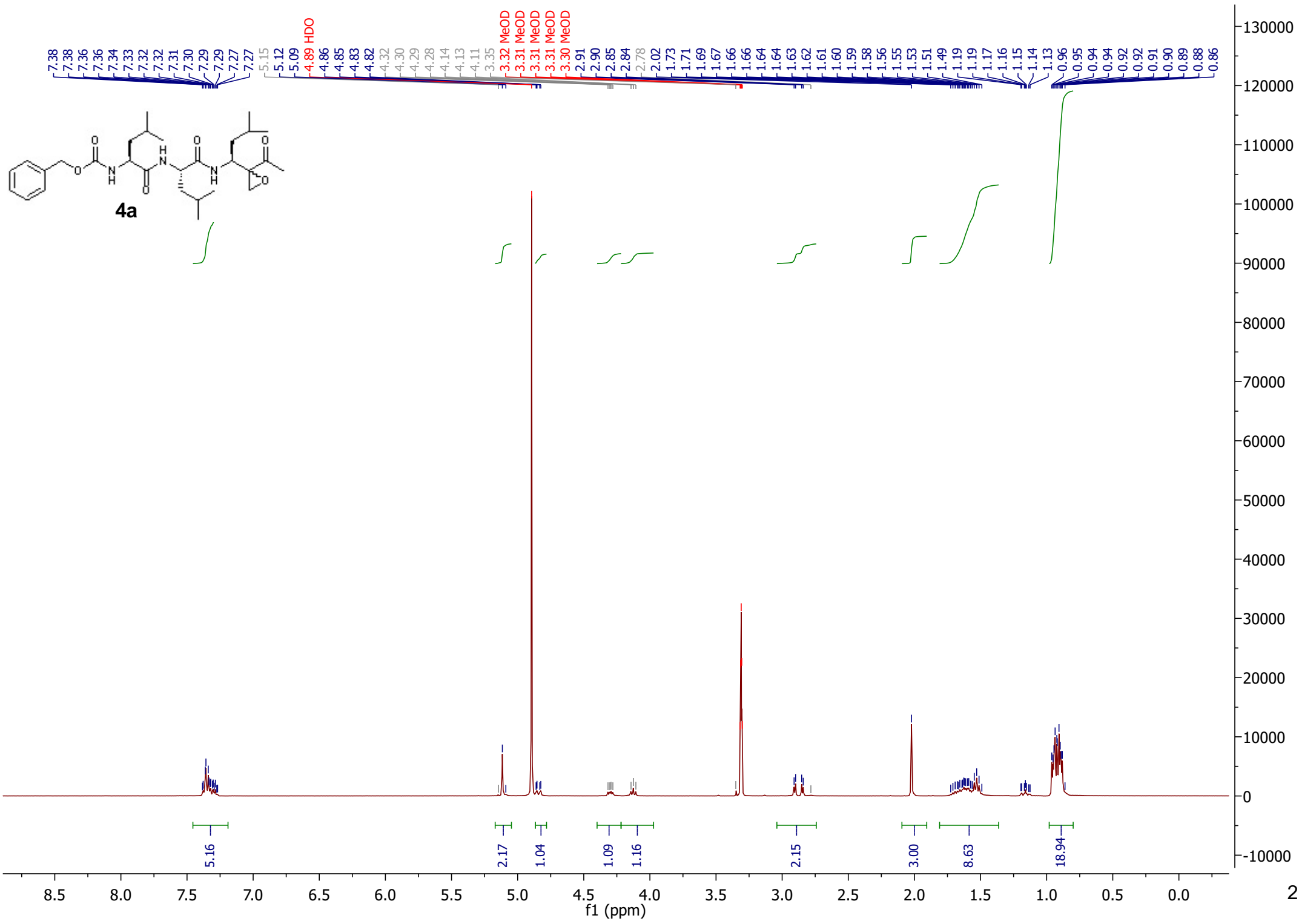
Bo-Tao Xin^a, Gerjan de Bruin^a, Martijn Verdoes^b, Dmitri V. Filippov, Gijs A. van der Marel^a
and Herman S. Overkleeft^{a*}

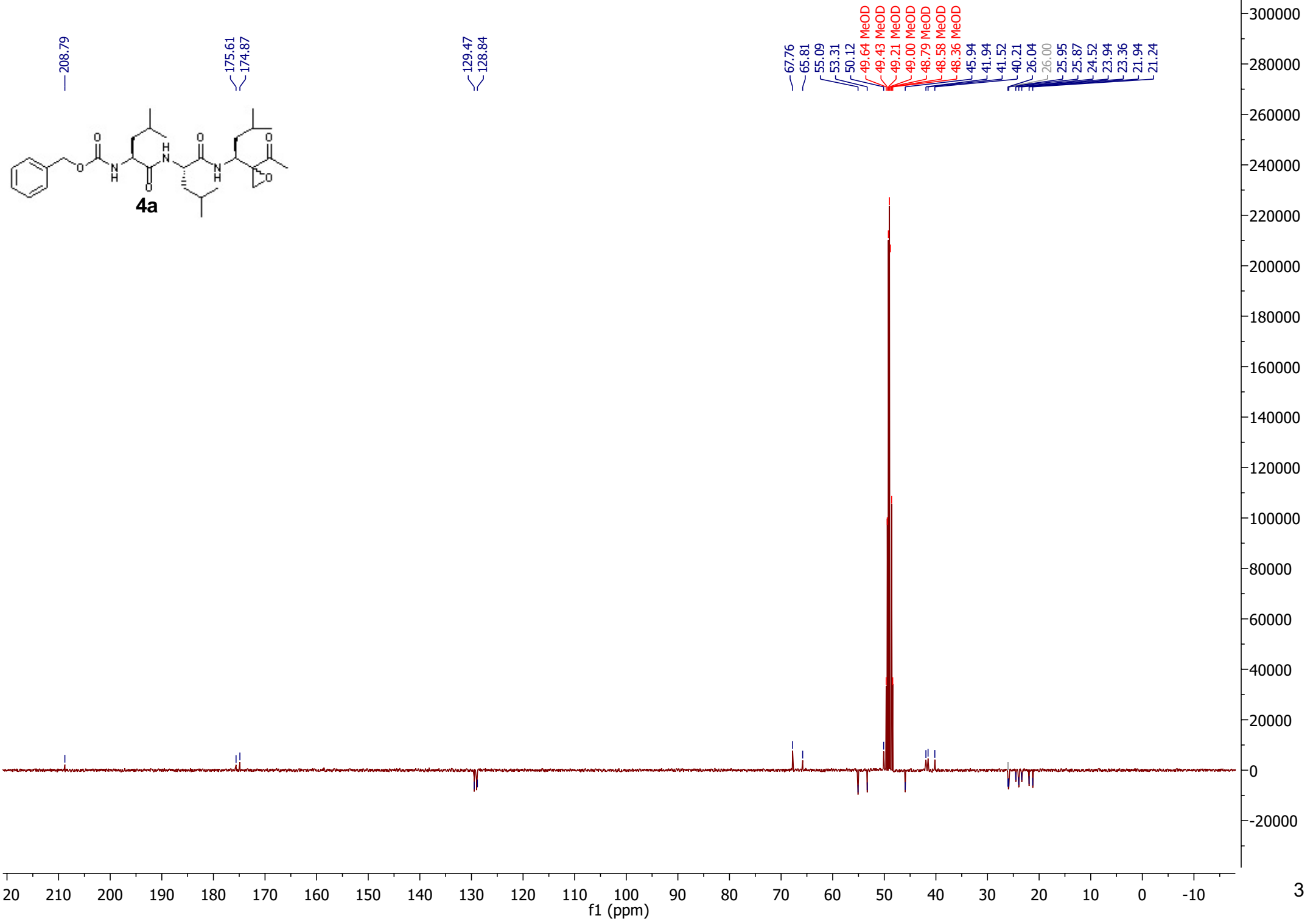
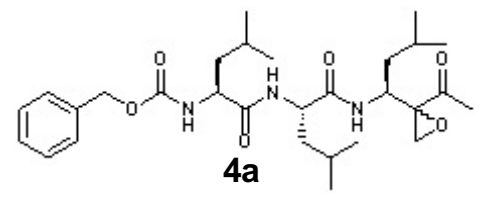
^aLeiden Institute of Chemistry, Leiden University, Einsteinweg 55, 2300 RA Leiden, the Netherlands. ^bDepartment of Tumor Immunology, Nijmegen Centre for Molecular Life Sciences, Radboud University Nijmegen Medical Centre, Nijmegen, The Netherlands.

*h.s.overkleeft@chem.leidenuniv.nl

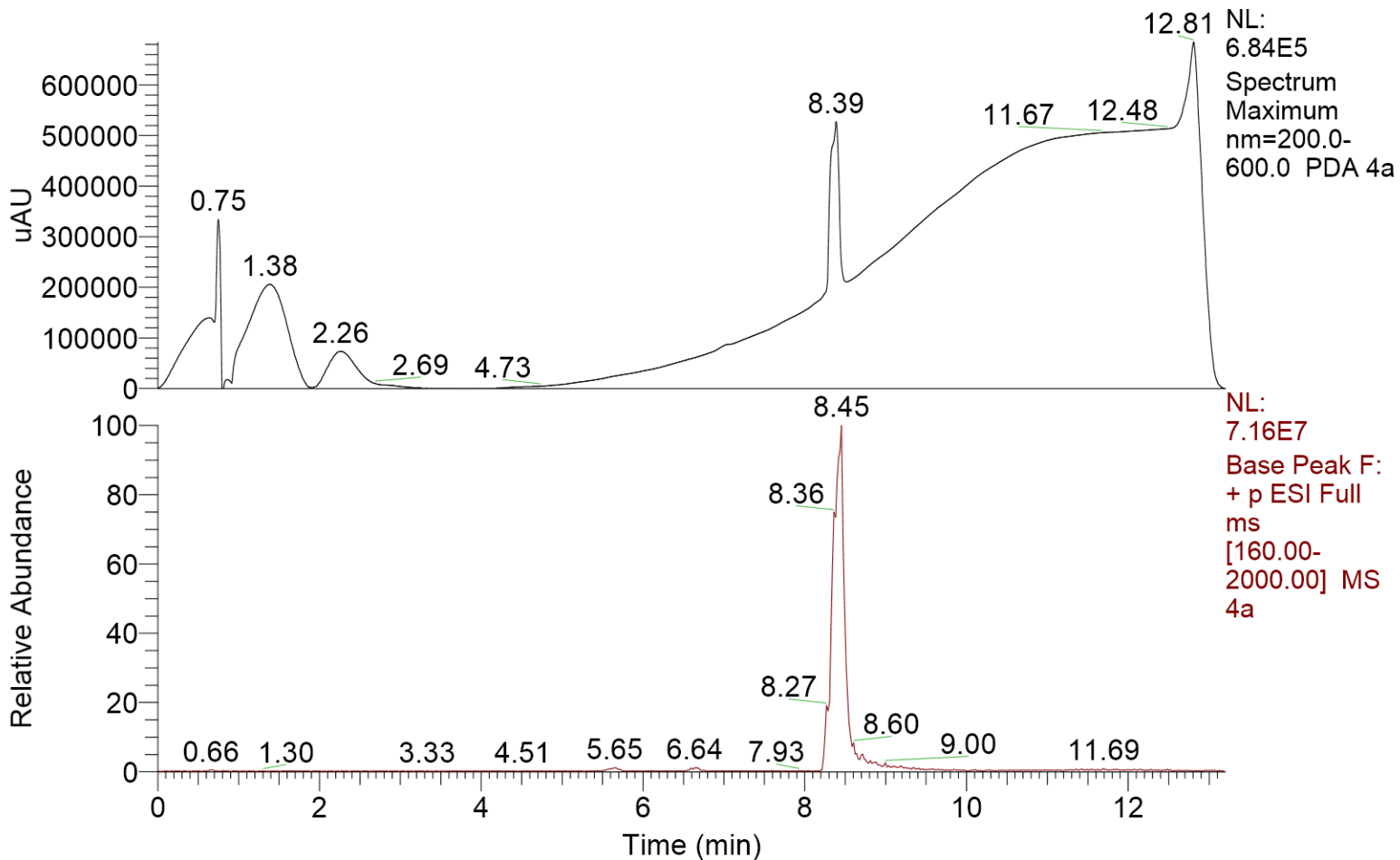
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RT: 0.00 - 13.20



4a

Type: Unknown ID: 1 Row: 1

Instrument Method: C:\Xcalibur\methods\General(TFA)\1090%B10_C=TFA_20ul_+pf_12,5min.meth

Processing Method:

Vial: B:37

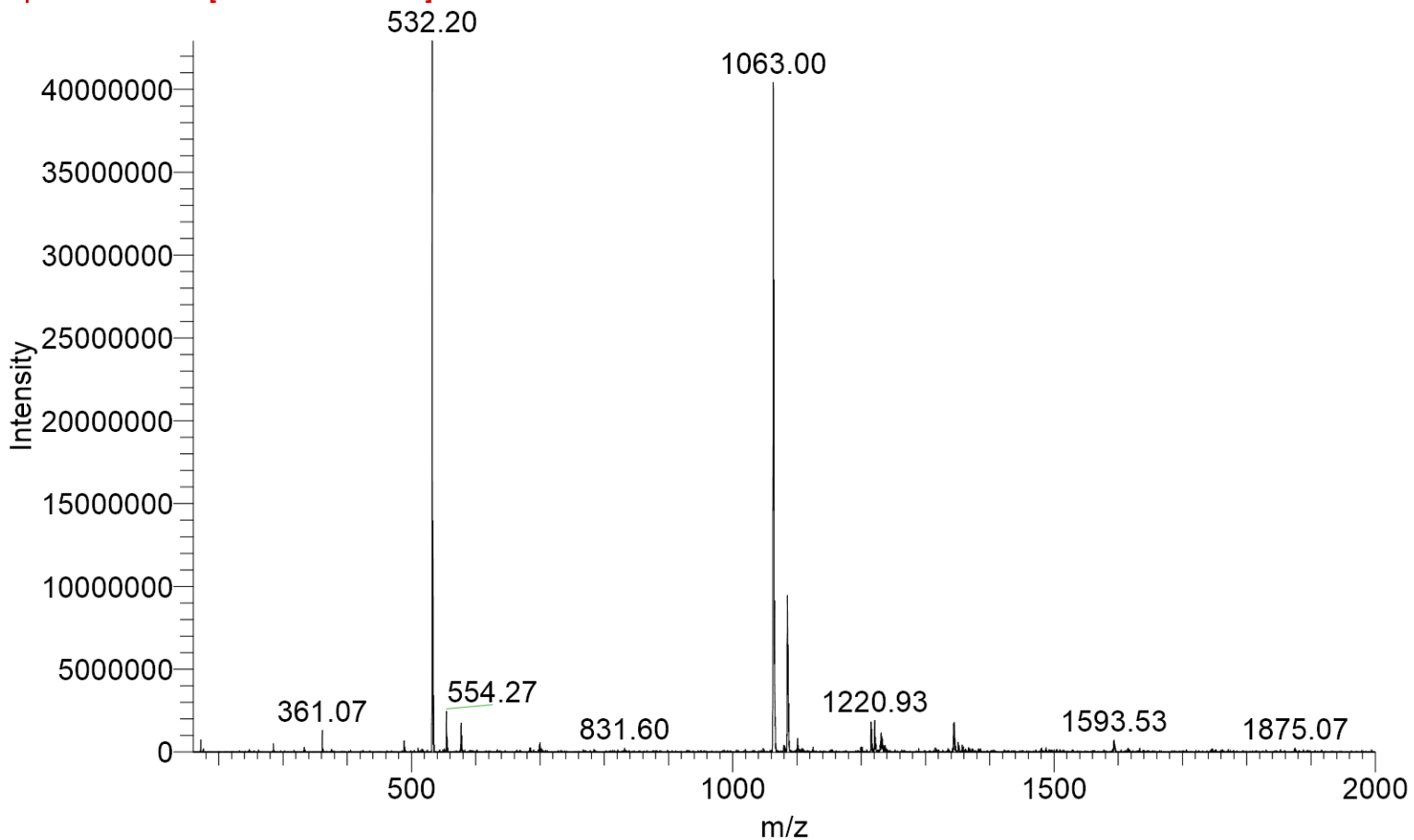
Injection Volume (µl): 20.00

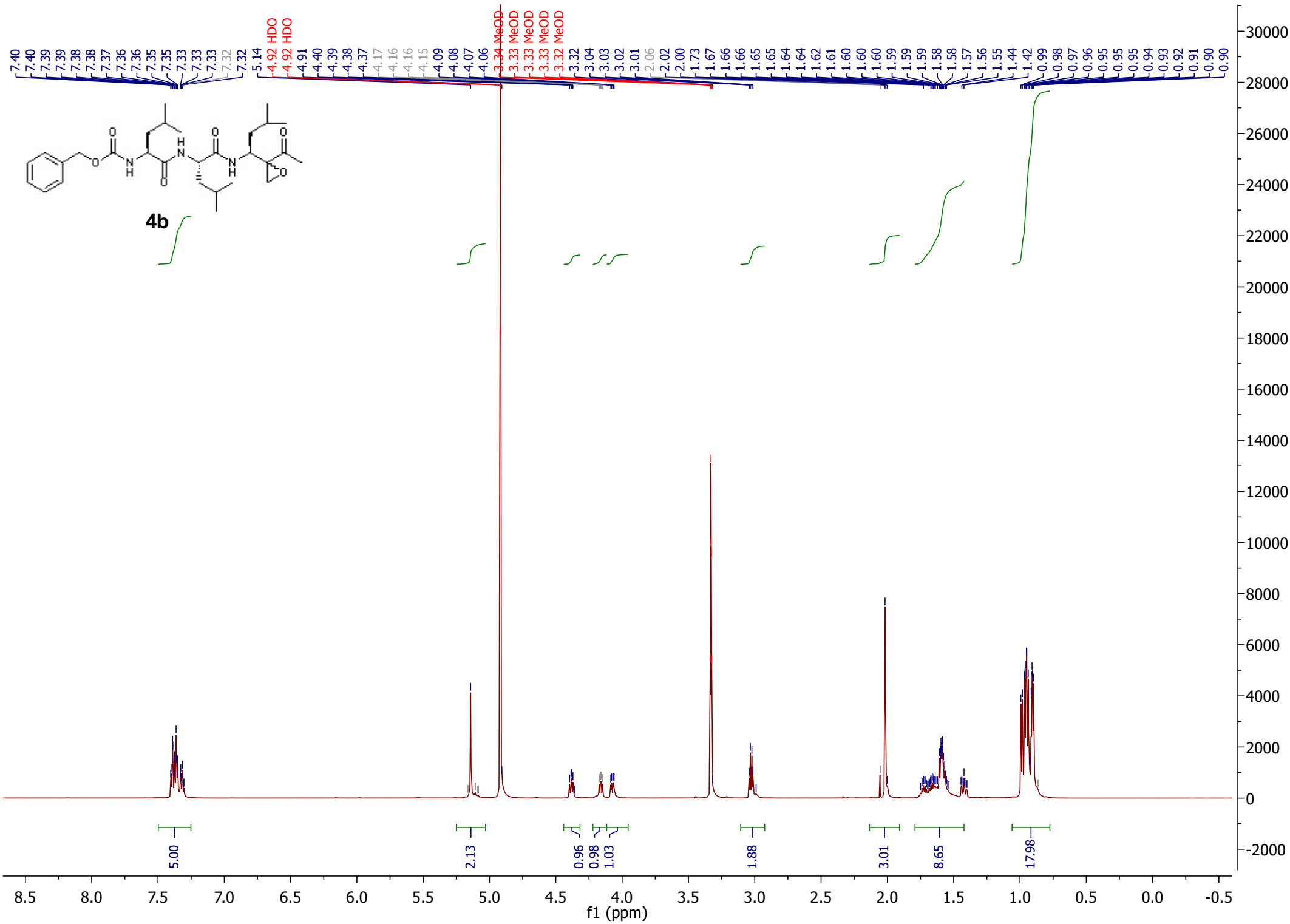
Sample Weight: 0.00

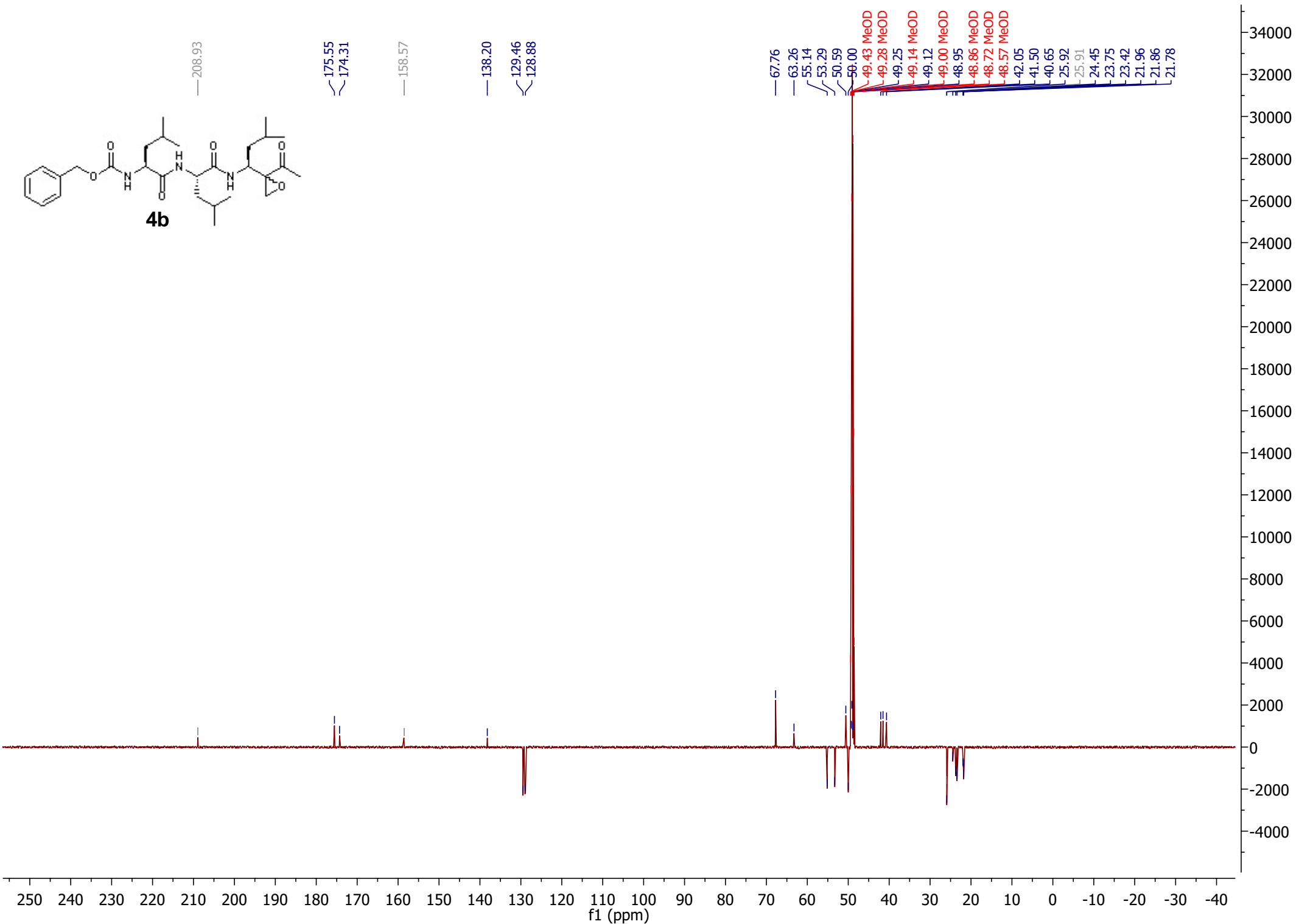
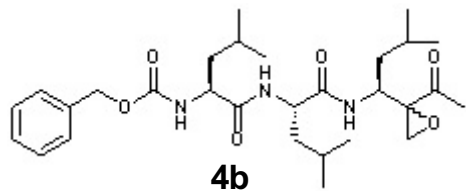
Sample Volume (µl): 0.00

4a #436-446 RT: 8.29-8.47 AV: 11 NL: 4.29E7

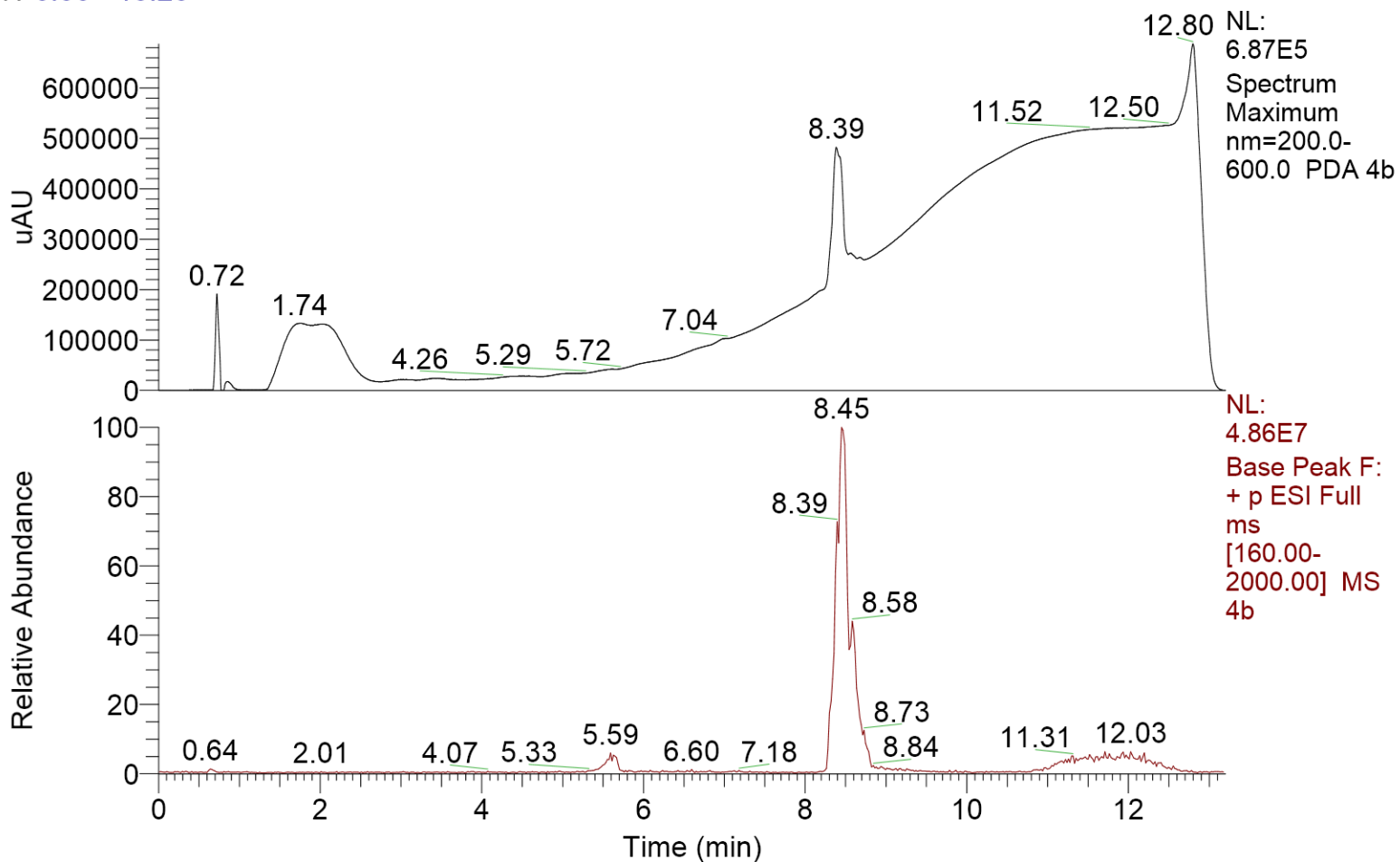
F: + p ESI Full ms [160.00-2000.00]







RT: 0.00 - 13.20



4b

Type: Unknown ID: 1 Row: 1

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Processing Method:

Vial: B:39

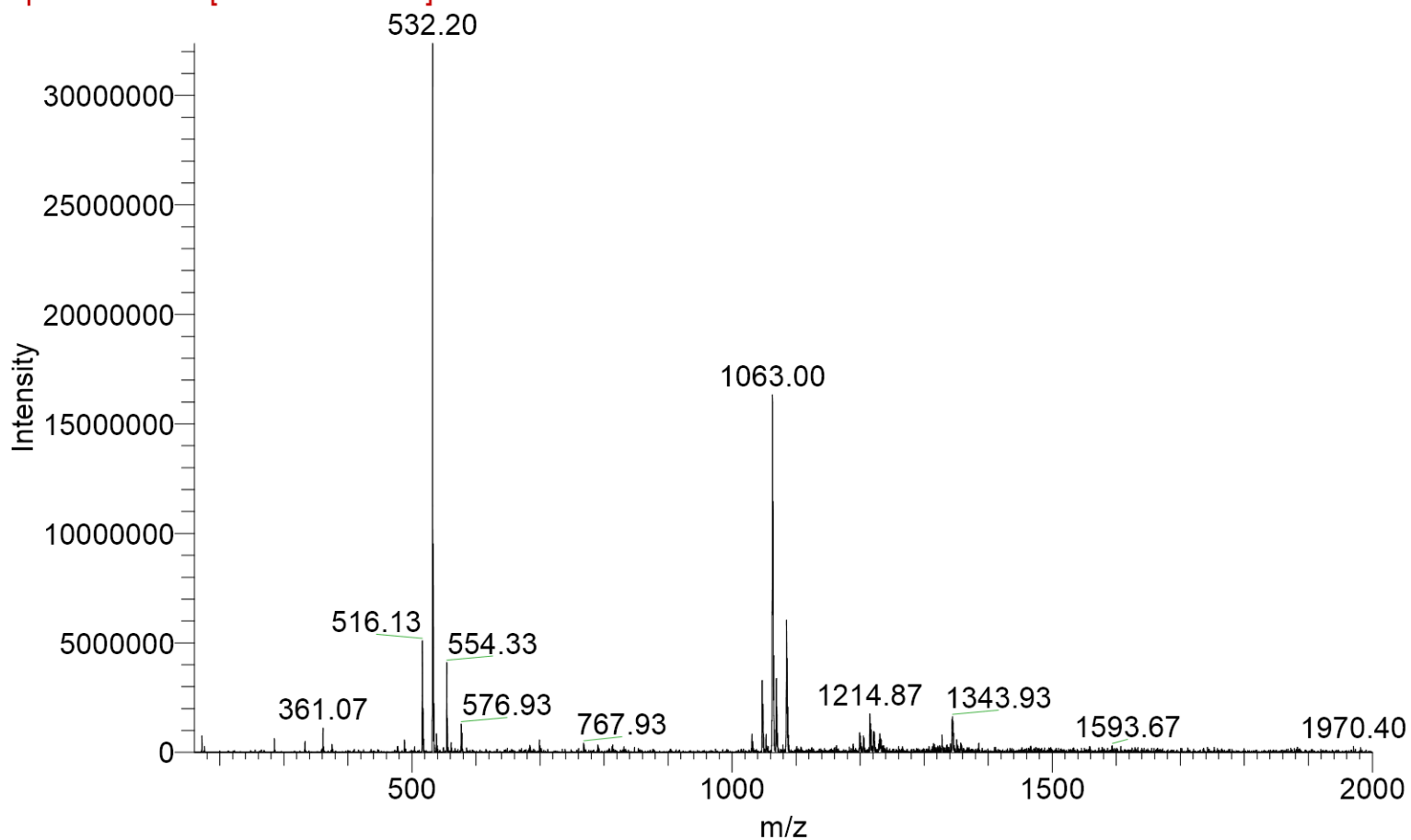
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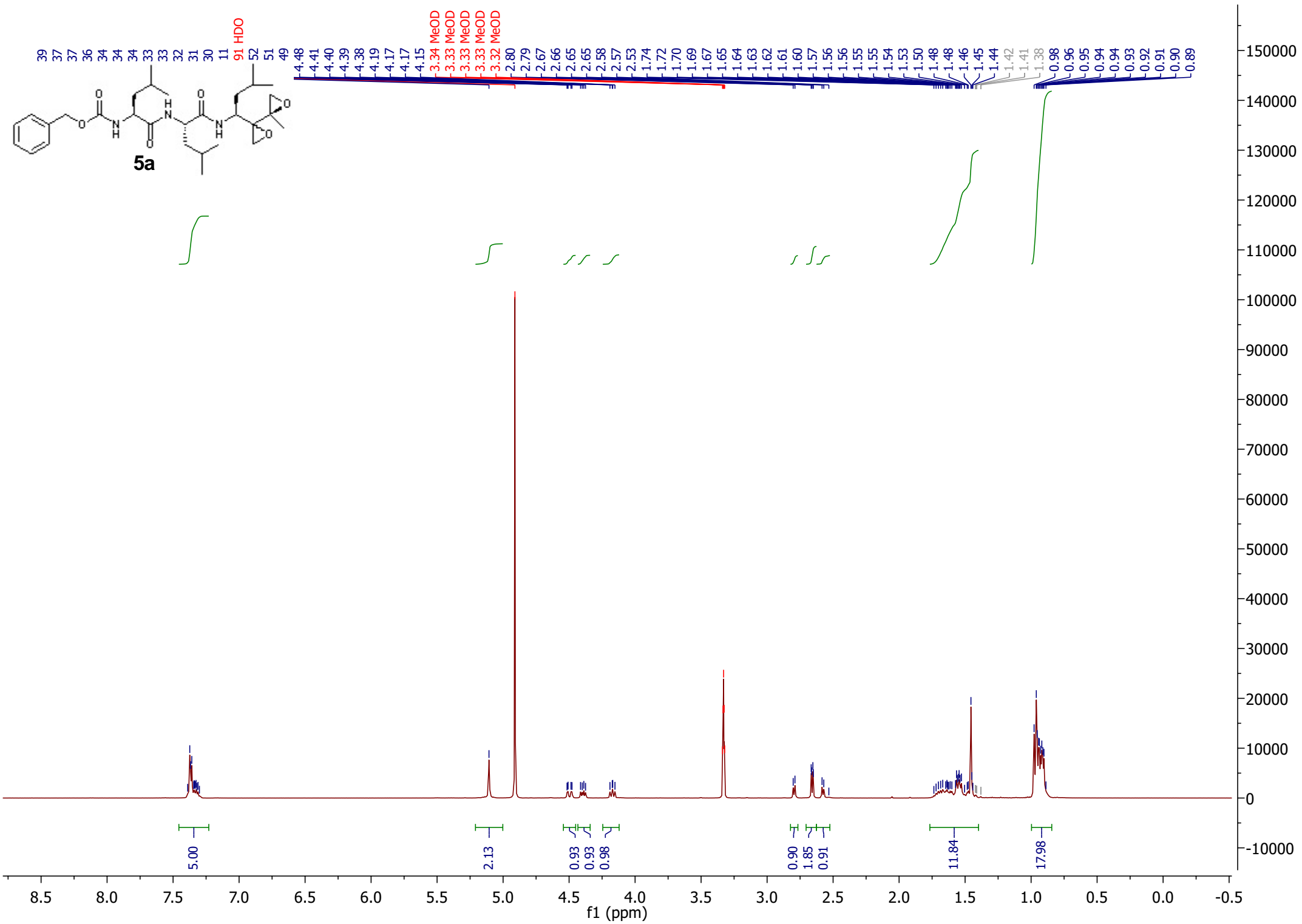
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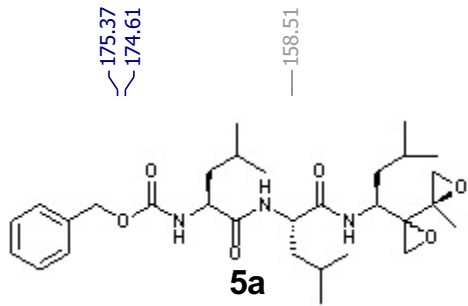
Sample Volume (µl): 0.00

4b #439-446 RT: 8.34-8.47 AV: 8 NL: 3.24E7

F: + p ESI Full ms [160.00-2000.00]

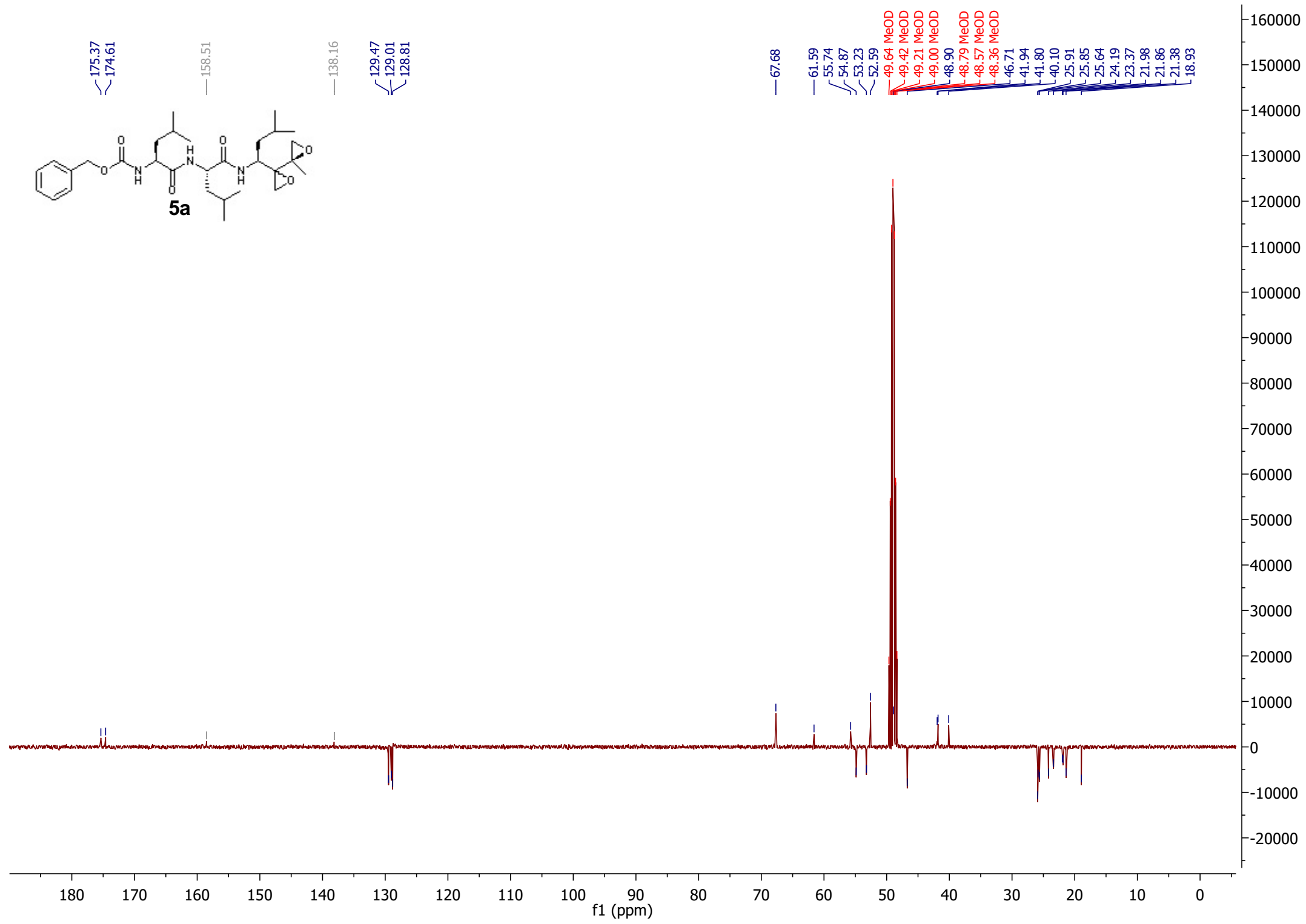




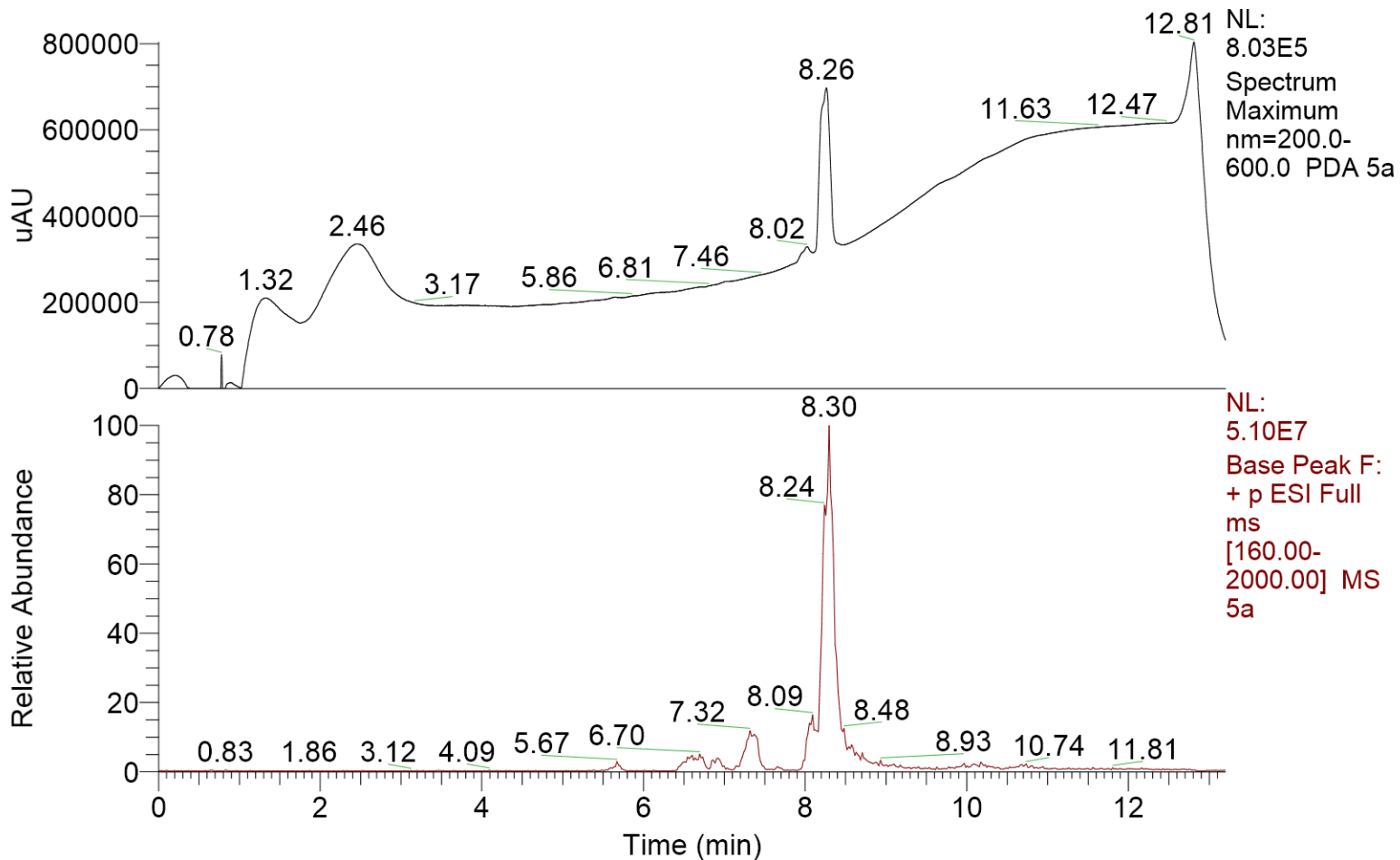


175.37
174.61
158.51
138.16
129.47
129.01
128.81

67.68
61.59
55.74
54.87
53.23
52.59
49.64 MeOD
49.42 MeOD
49.21 MeOD
49.00 MeOD
48.90
48.79 MeOD
48.57 MeOD
48.36 MeOD
46.71
41.94
41.80
40.10
25.91
25.85
25.64
24.19
23.37
21.98
21.86
21.38
18.93



RT: 0.00 - 13.20



5a

Type: Unknown ID: 1 Row: 1

Instrument Method: C:\Xcalibur\methods\General(TFA)\1090%B10_C=TFA_20ul_+pf_12,5min.meth

Processing Method:

Vial: C:20

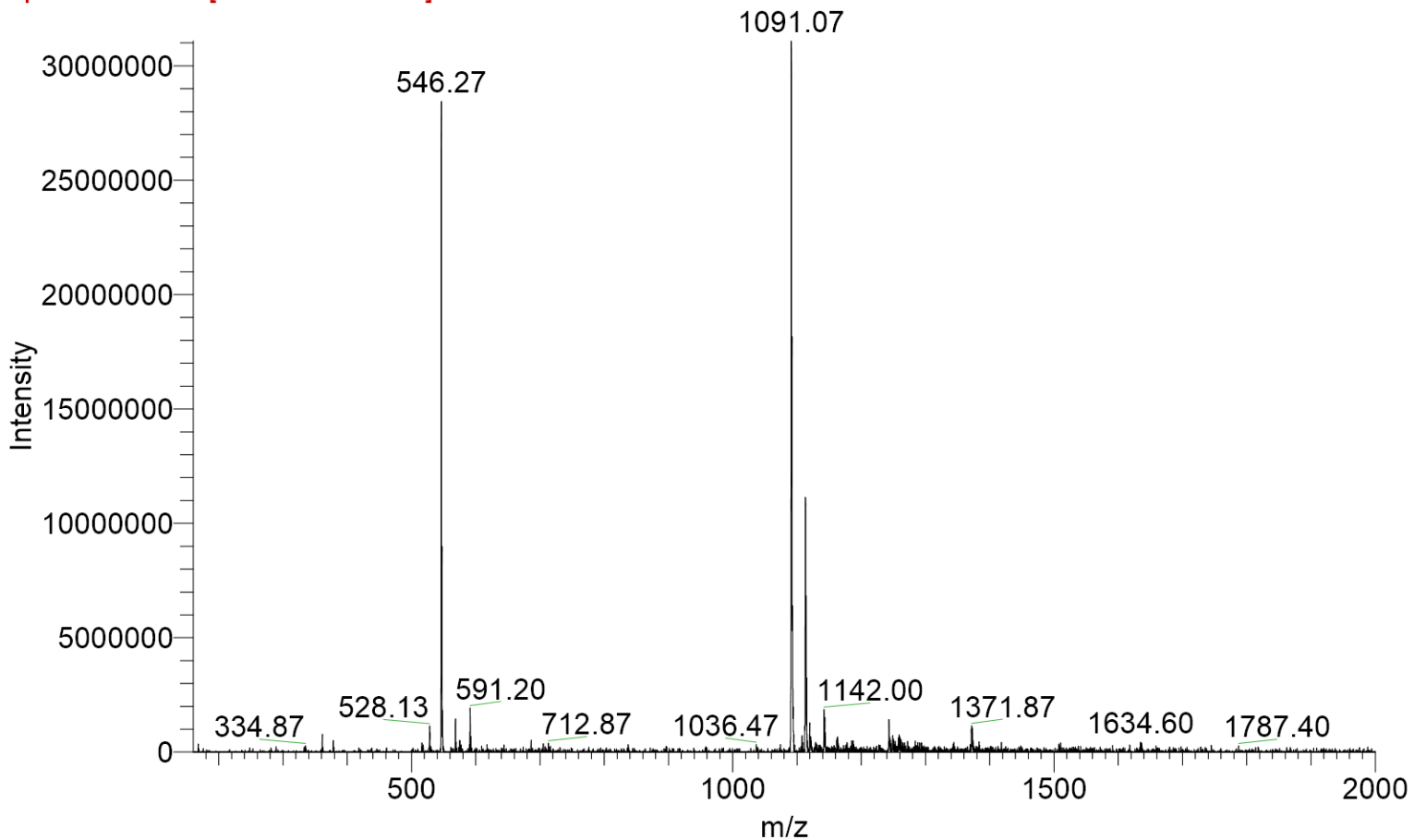
Injection Volume (µl): 20.00

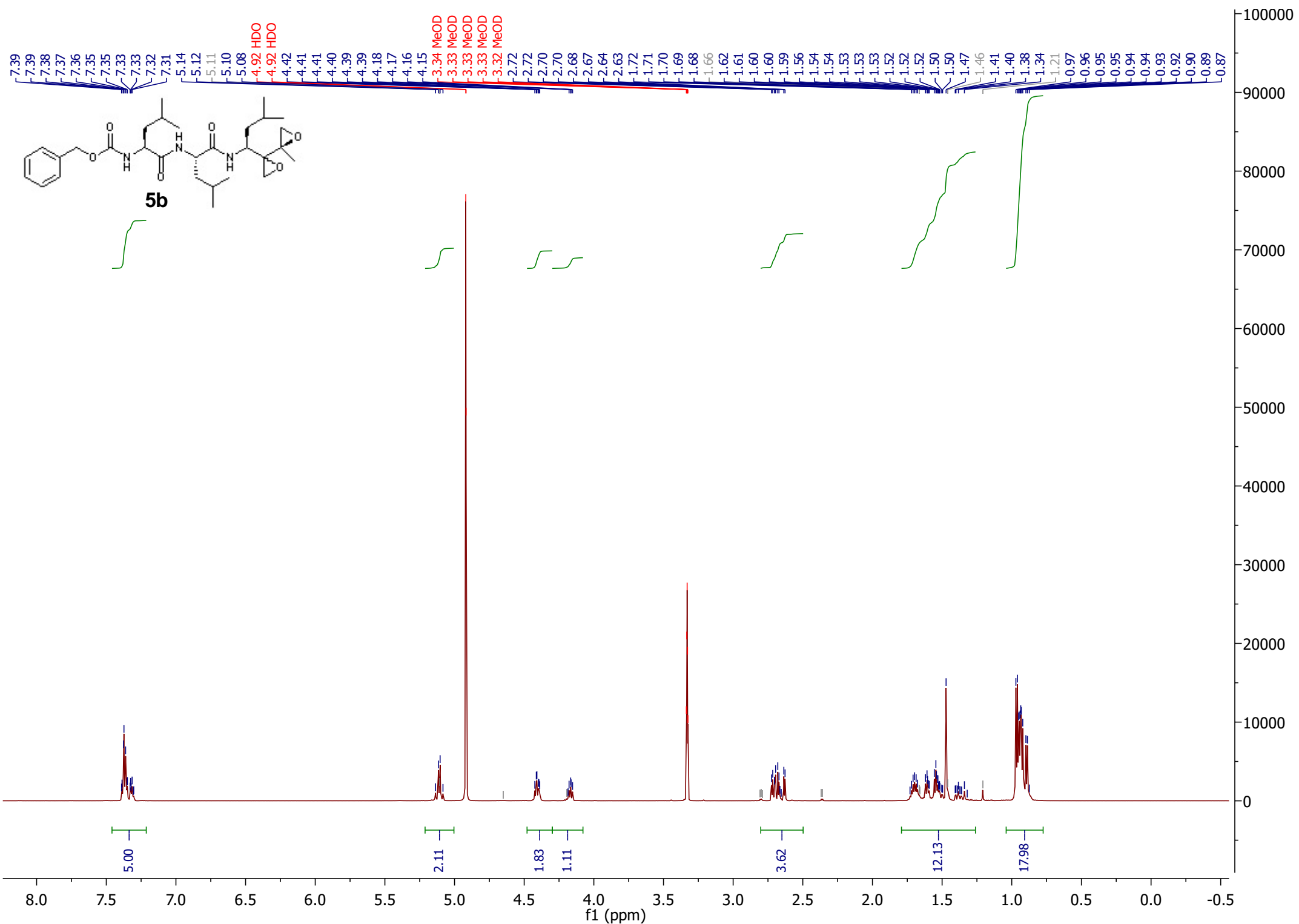
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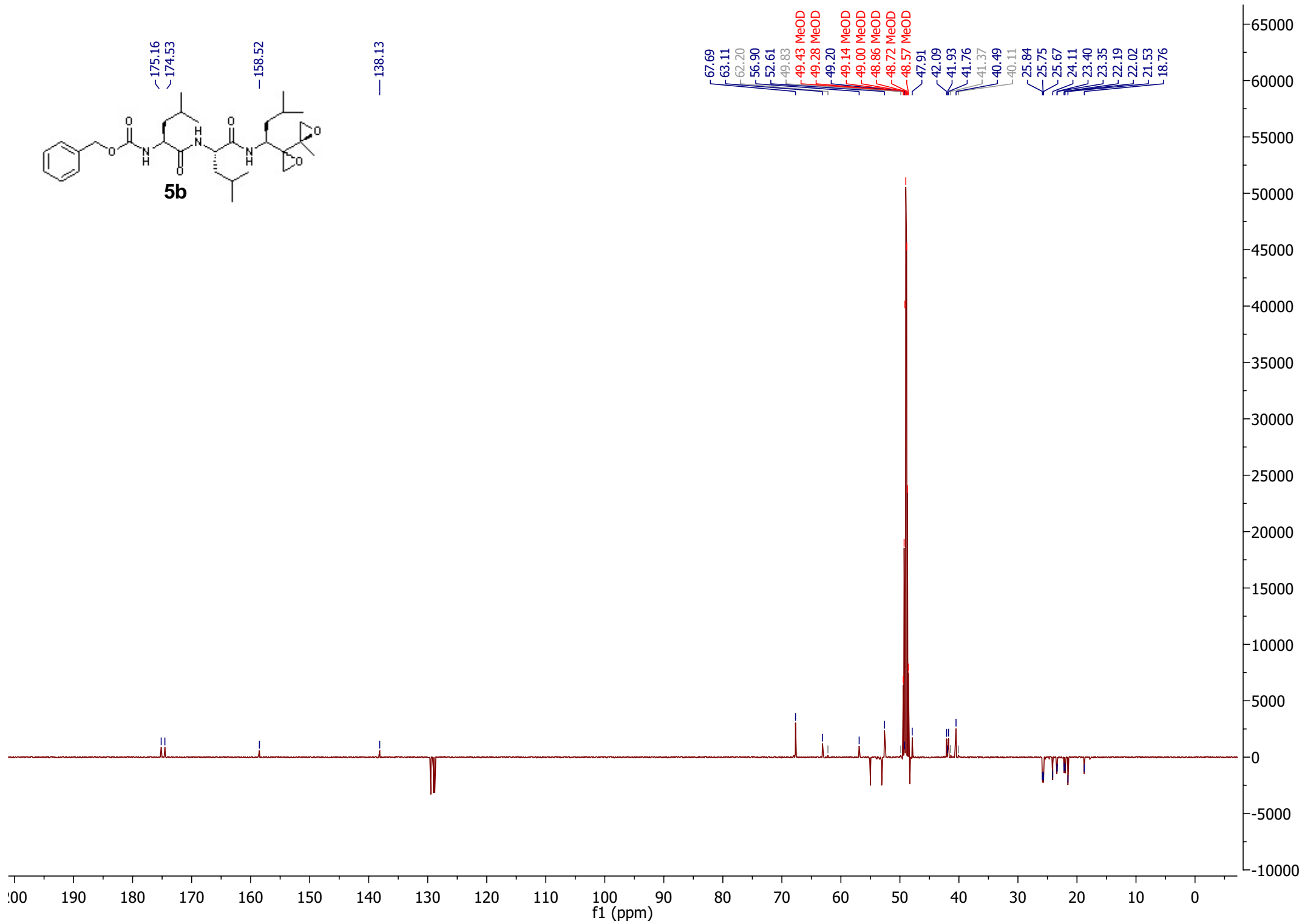
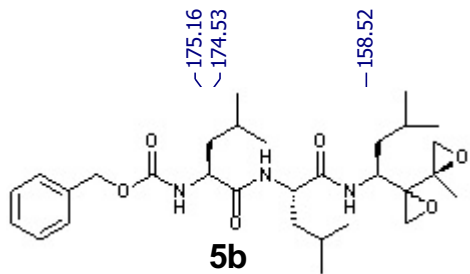
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5a #437-442 RT: 8.30-8.39 AV: 6 NL: 3.11E7

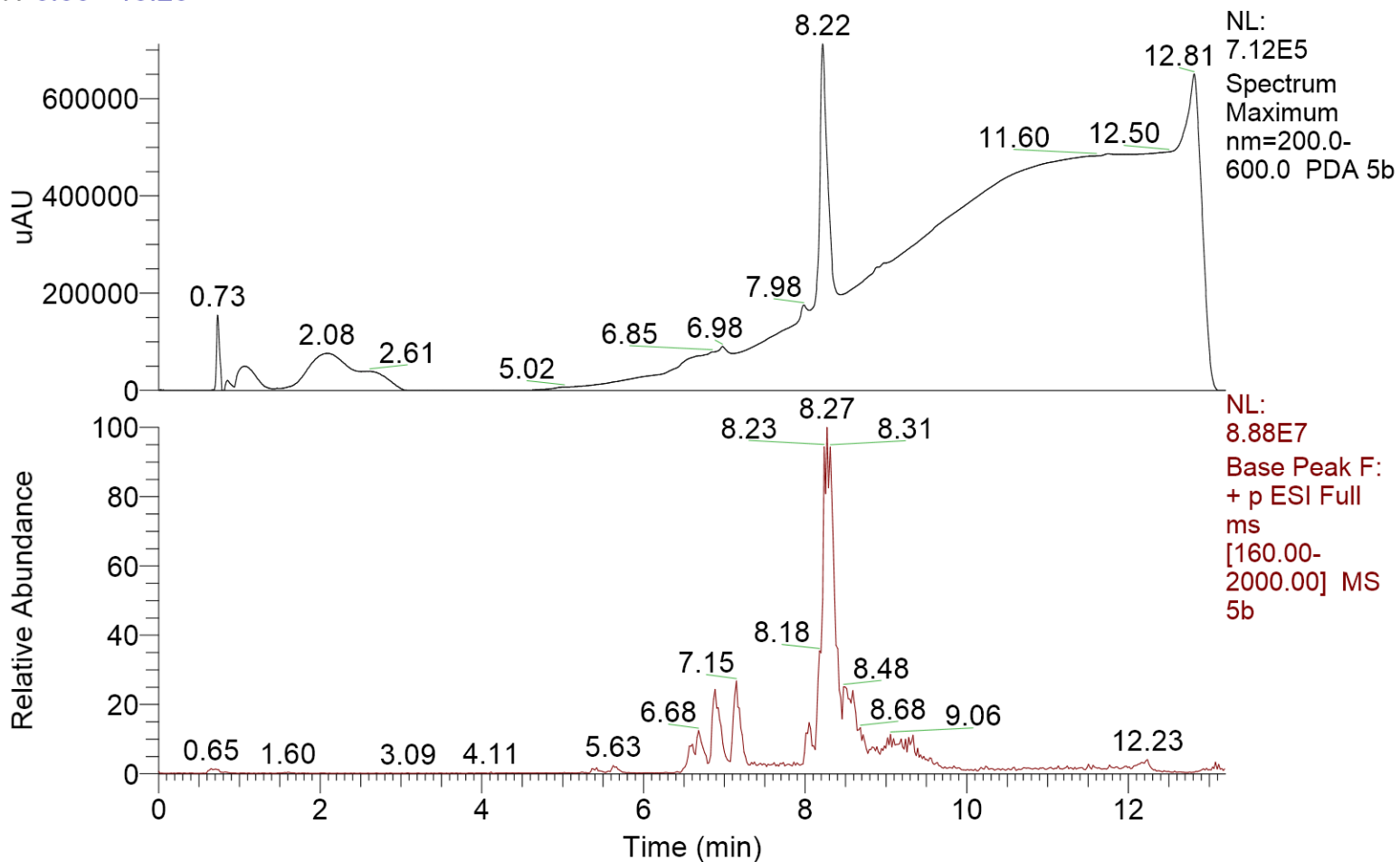
F: + p ESI Full ms [160.00-2000.00]







RT: 0.00 - 13.20



5b

Type: Unknown ID: 1 Row: 1

Instrument Method: C:\Xcalibur\methods\General(TFA)\1090%B10_C=TFA_20ul_+pf_12,5min.meth

Processing Method:

Vial: C:38

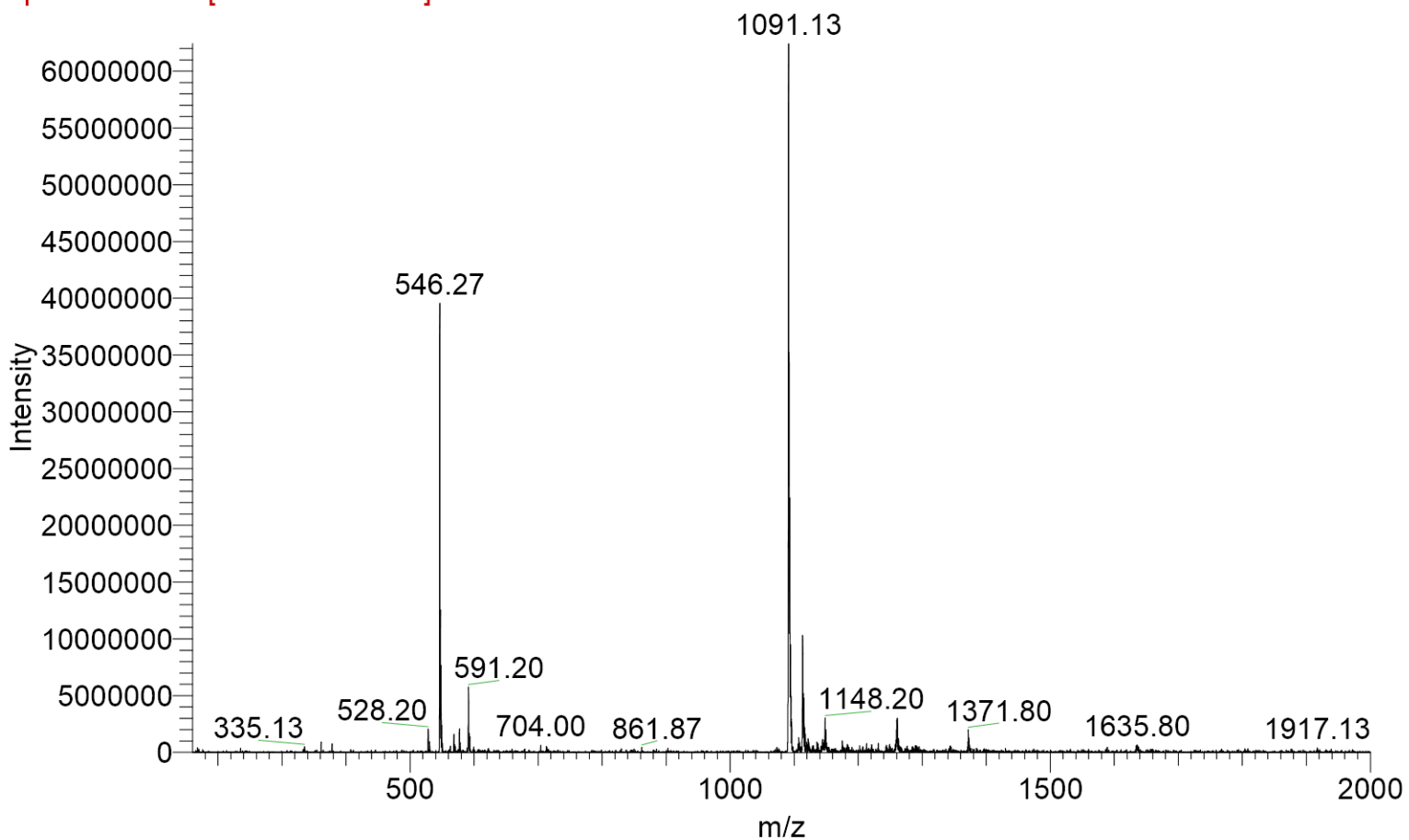
Injection Volume (µl): 20.00

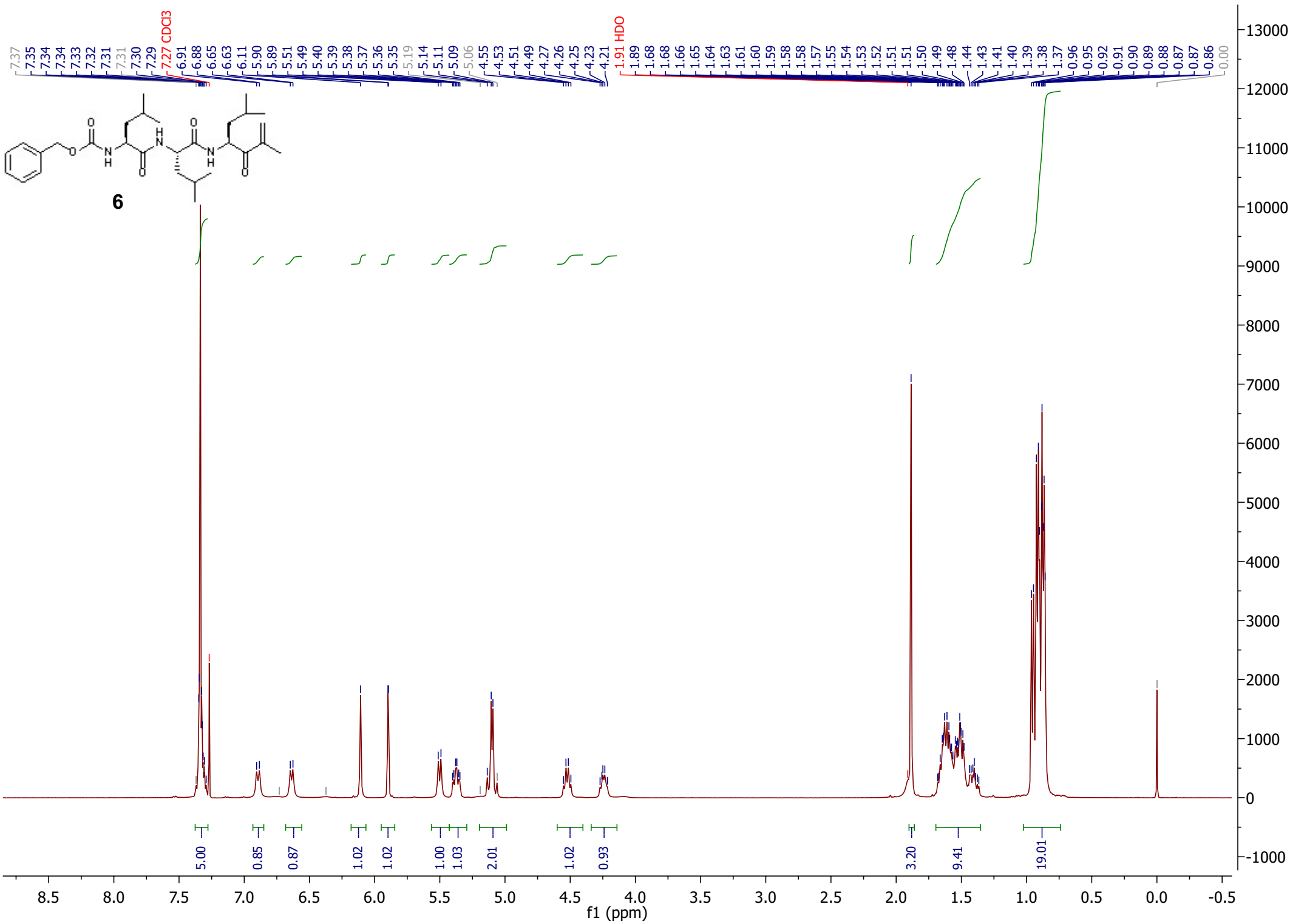
Sample Weight: 0.00

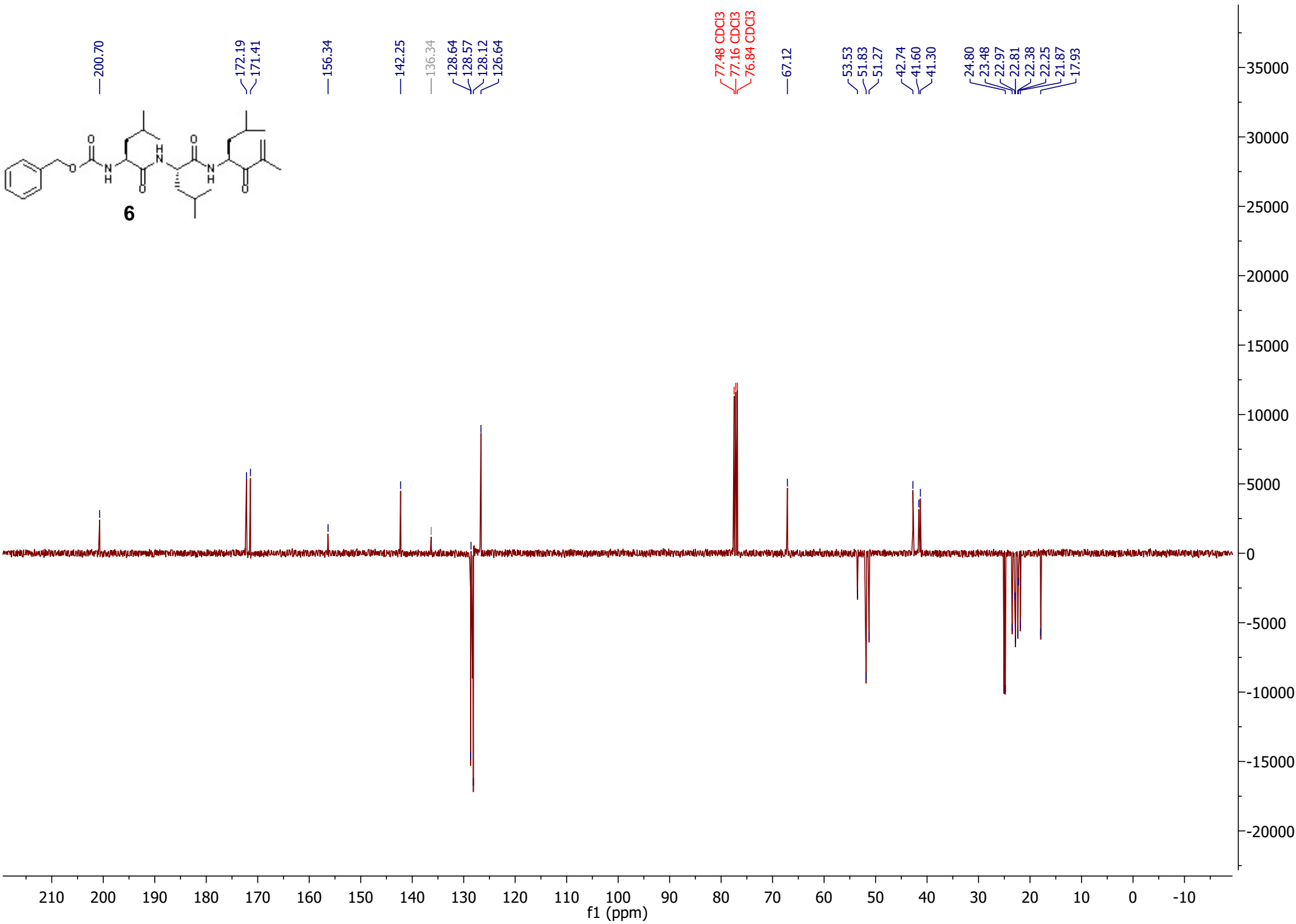
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5b #434-442 RT: 8.20-8.35 AV: 9 NL: 6.24E7

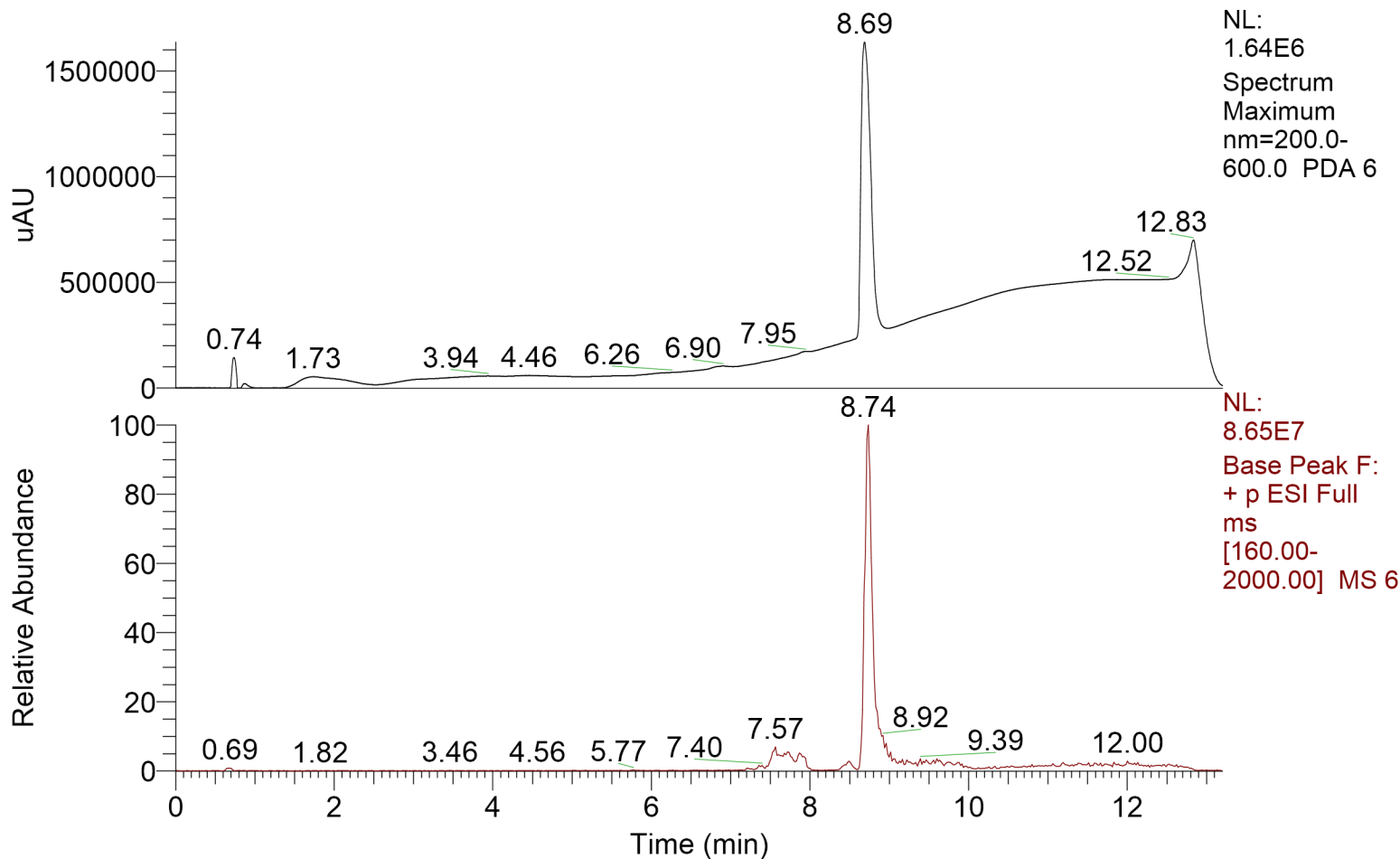
F: + p ESI Full ms [160.00-2000.00]







RT: 0.00 - 13.20



6

Type: Unknown ID: 1 Row: 1

Instrument Method: C:\Xcalibur\methods\General(TFA)\1090%B10_C=TFA_20ul_+pf_12,5min.meth

Processing Method:

Vial: C:18

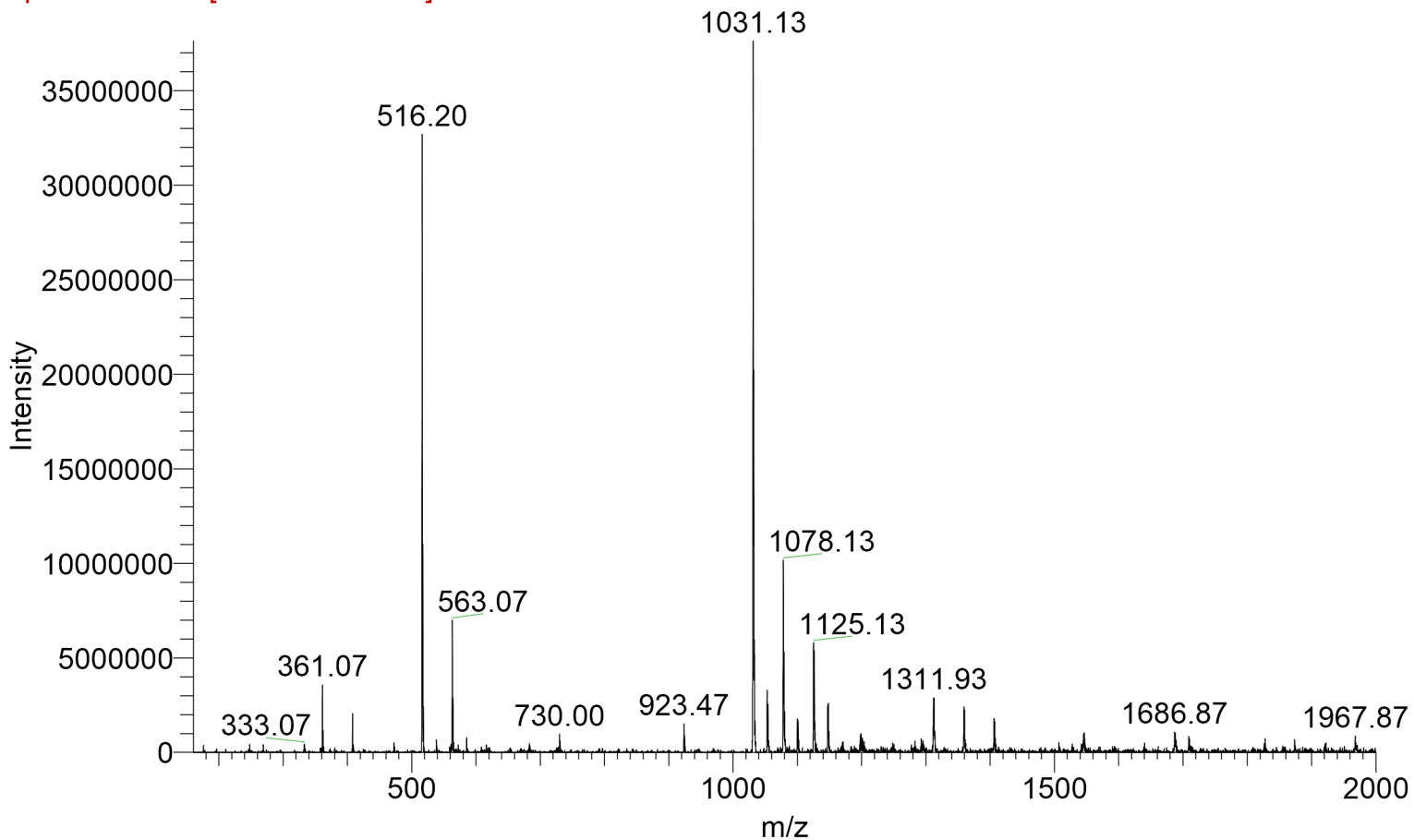
Injection Volume (µl): 20.00

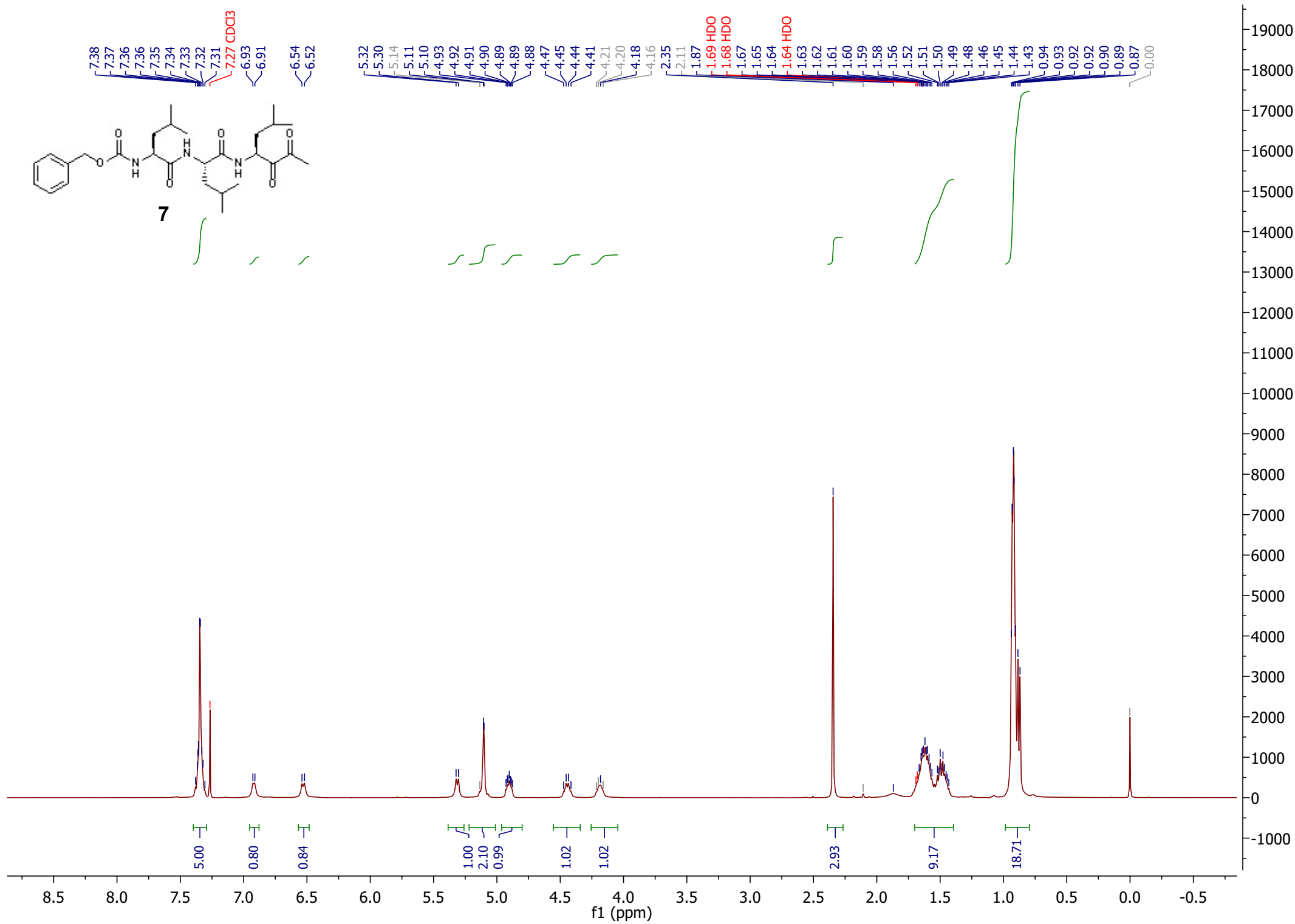
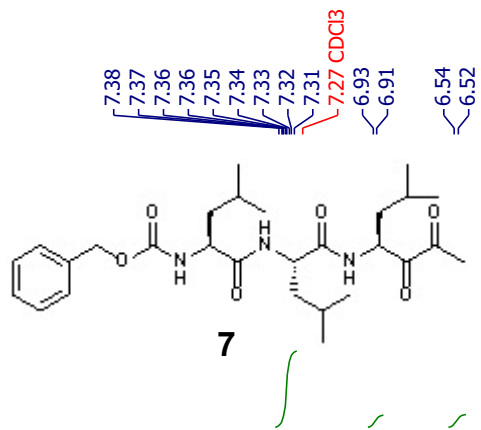
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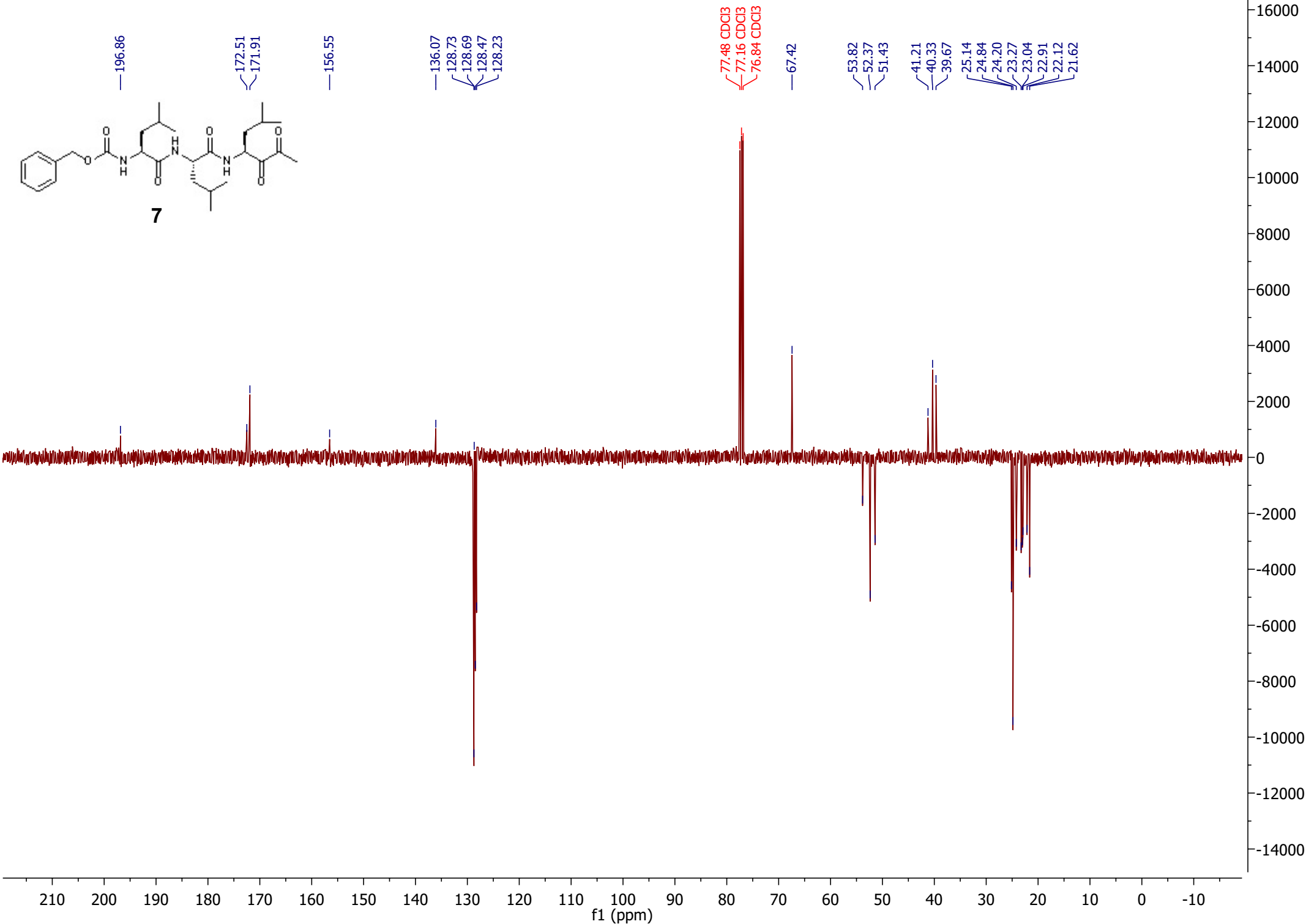
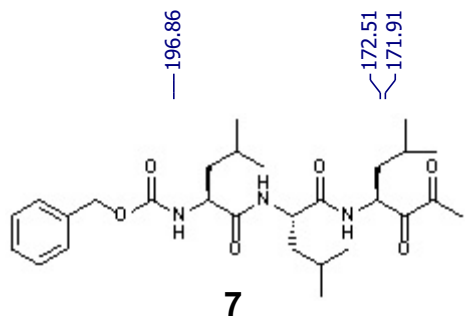
Sample Volume (µl): 0.00

6 #454-461 RT: 8.74-8.87 AV: 8 NL: 3.76E7

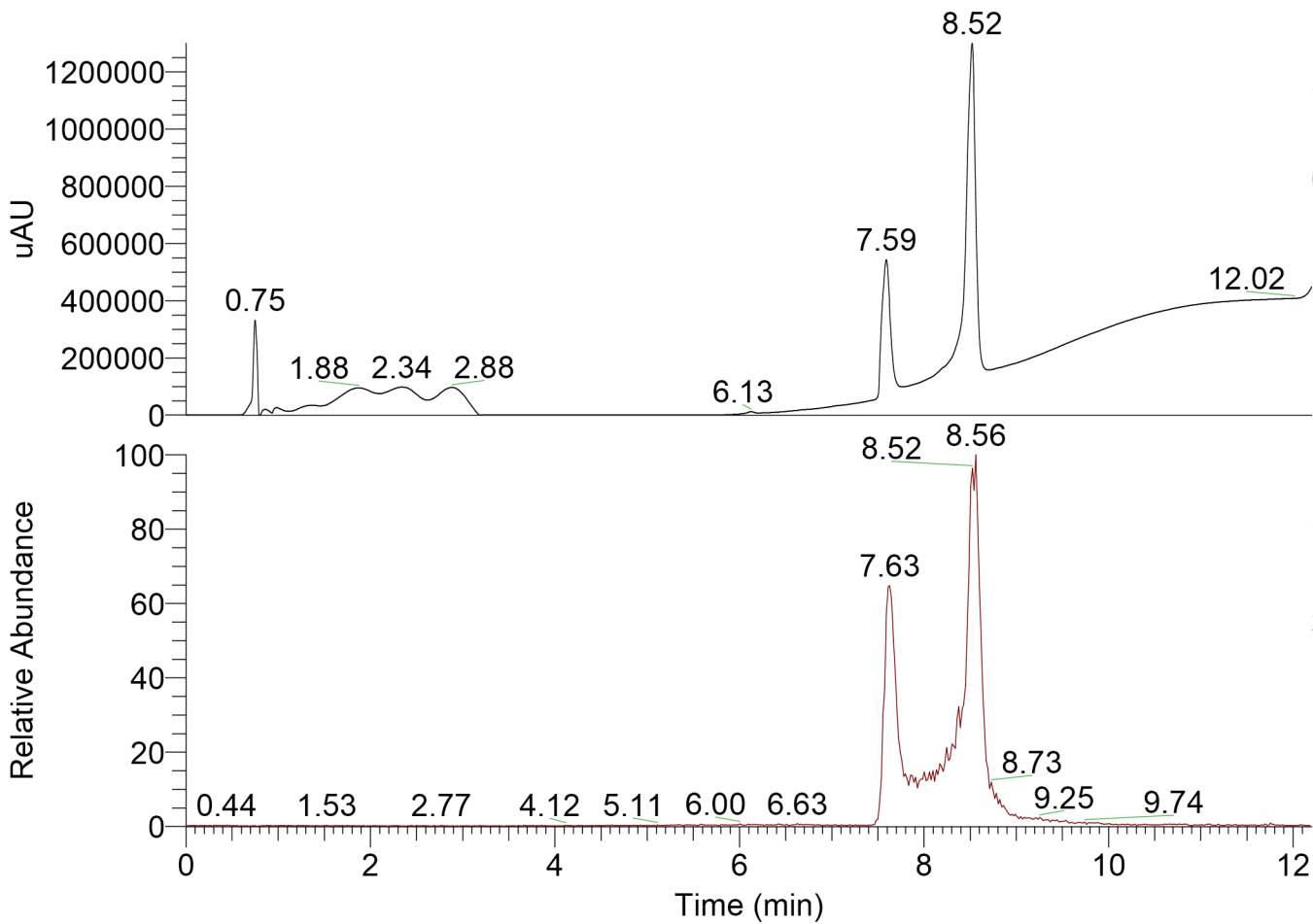
F: + p ESI Full ms [160.00-2000.00]



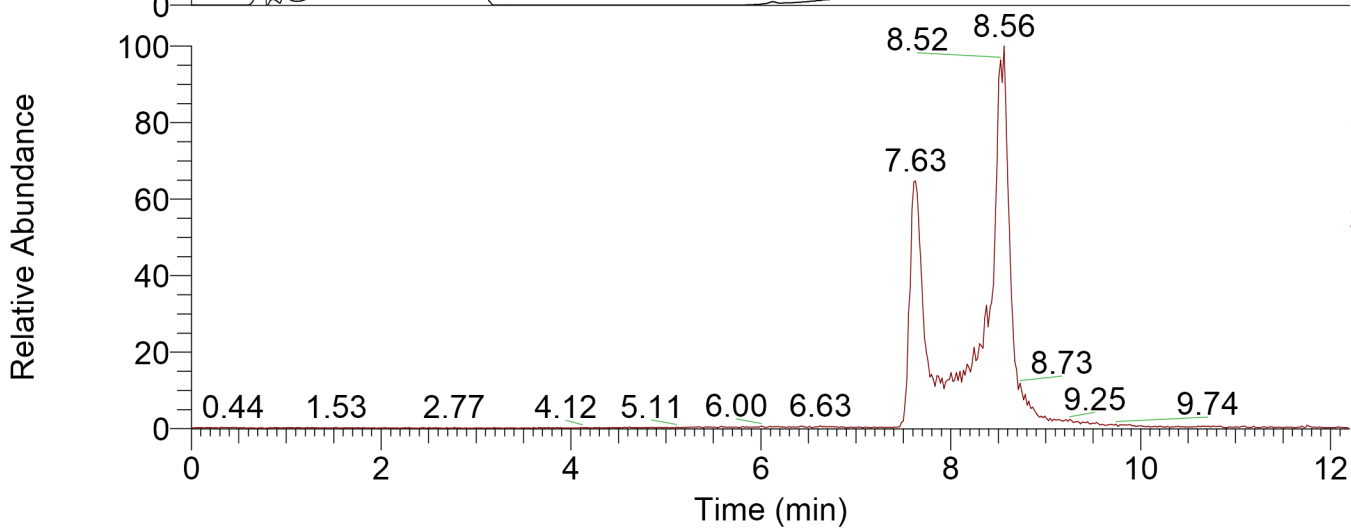




RT: 0.00 - 12.20



NL: 1.30E6
 Spectrum Maximum
 nm=200.0-600.0 PDA 7



NL: 1.24E8
 Base Peak F:
 + p ESI Full
 ms
 [160.00-2000.00] MS 7

7

Type: Unknown ID: 1 Row: 1

Instrument Method: C:\Xcalibur\methods\General(TFA)\1090%B00_C=TFA_20ul_+pf_12,5min.meth

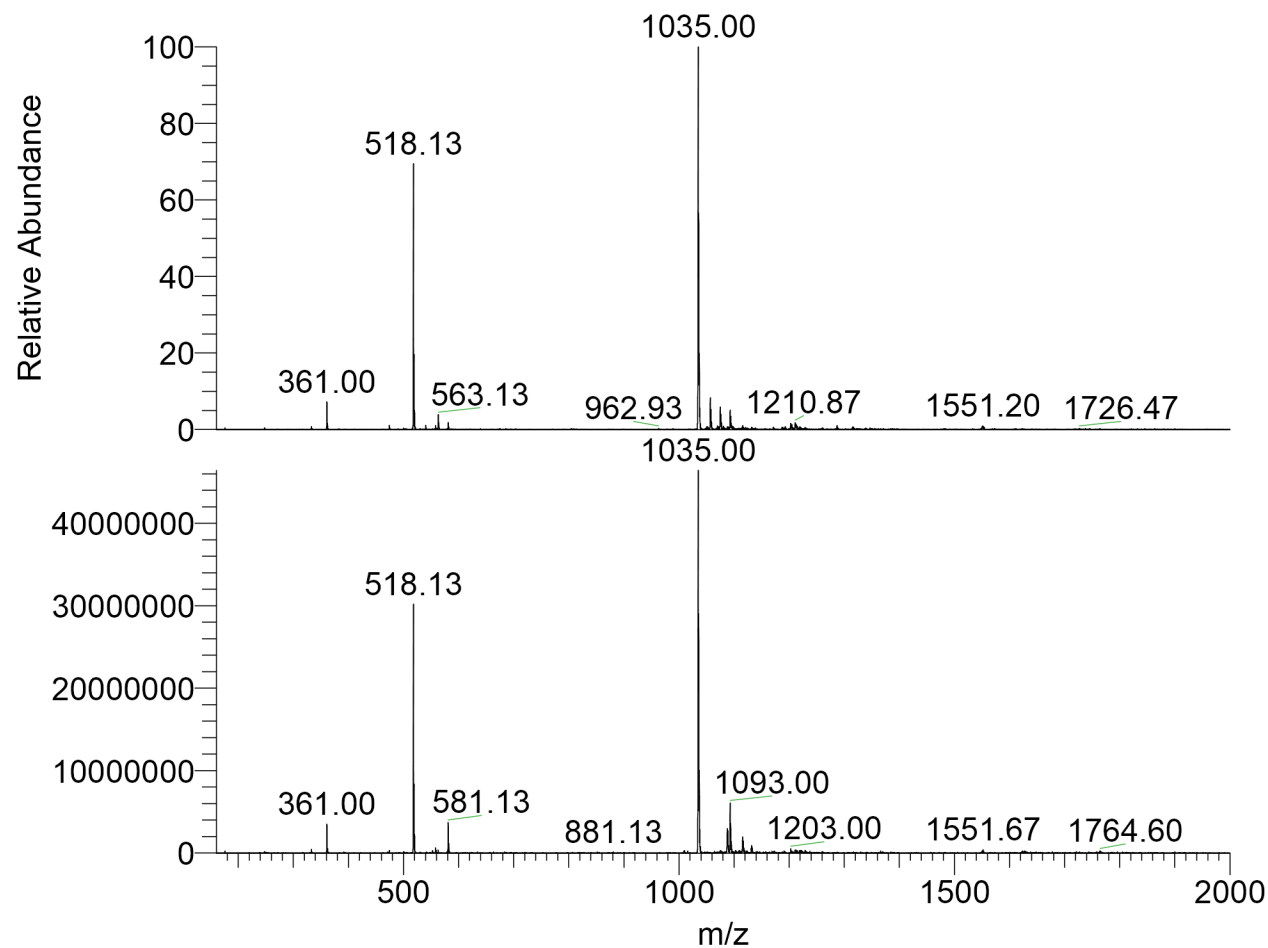
Processing Method:

Vial: B:39

Injection Volume (µl): 20.00

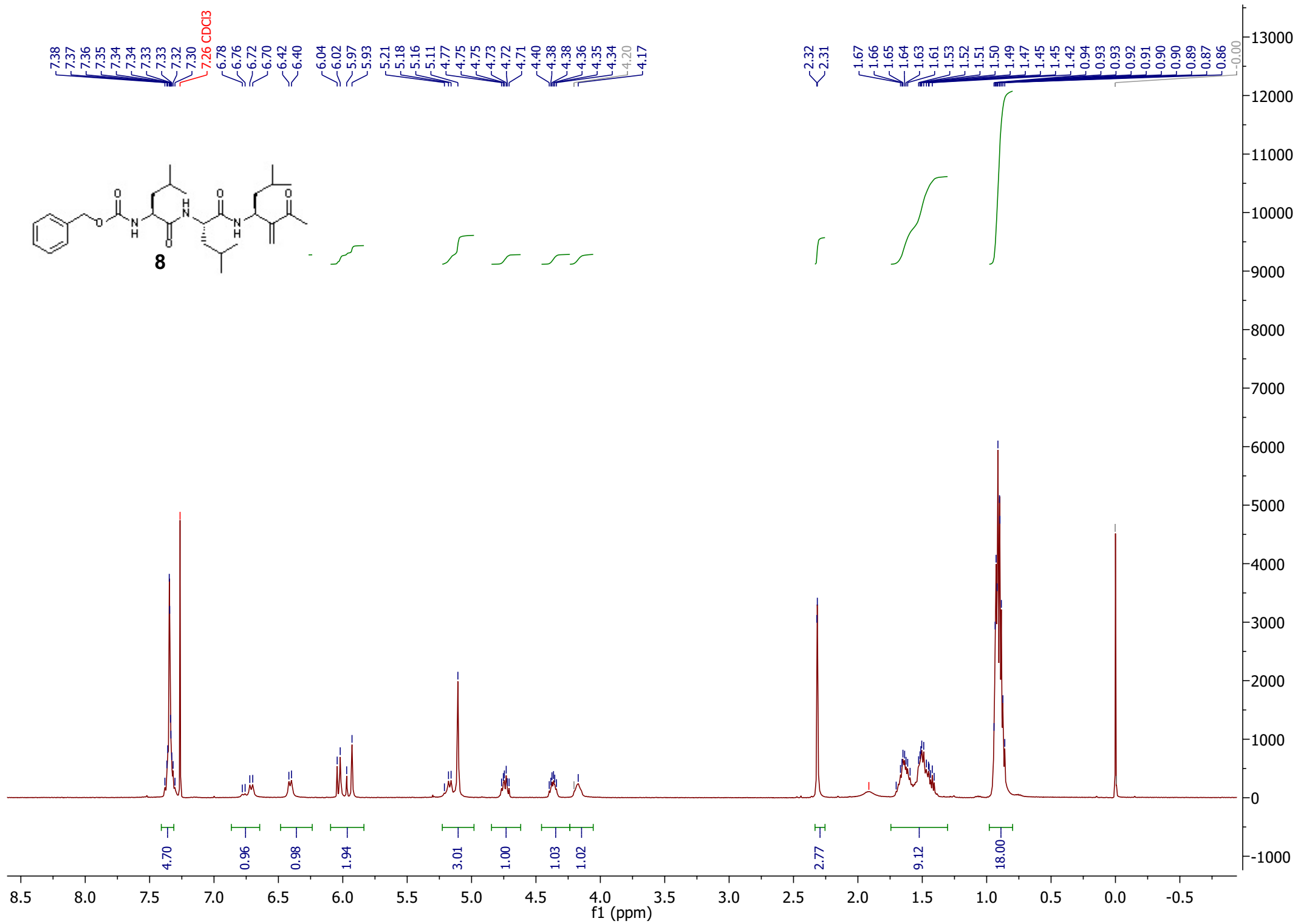
Sample Weight: 0.00

Sample Volume (µl): 0.00

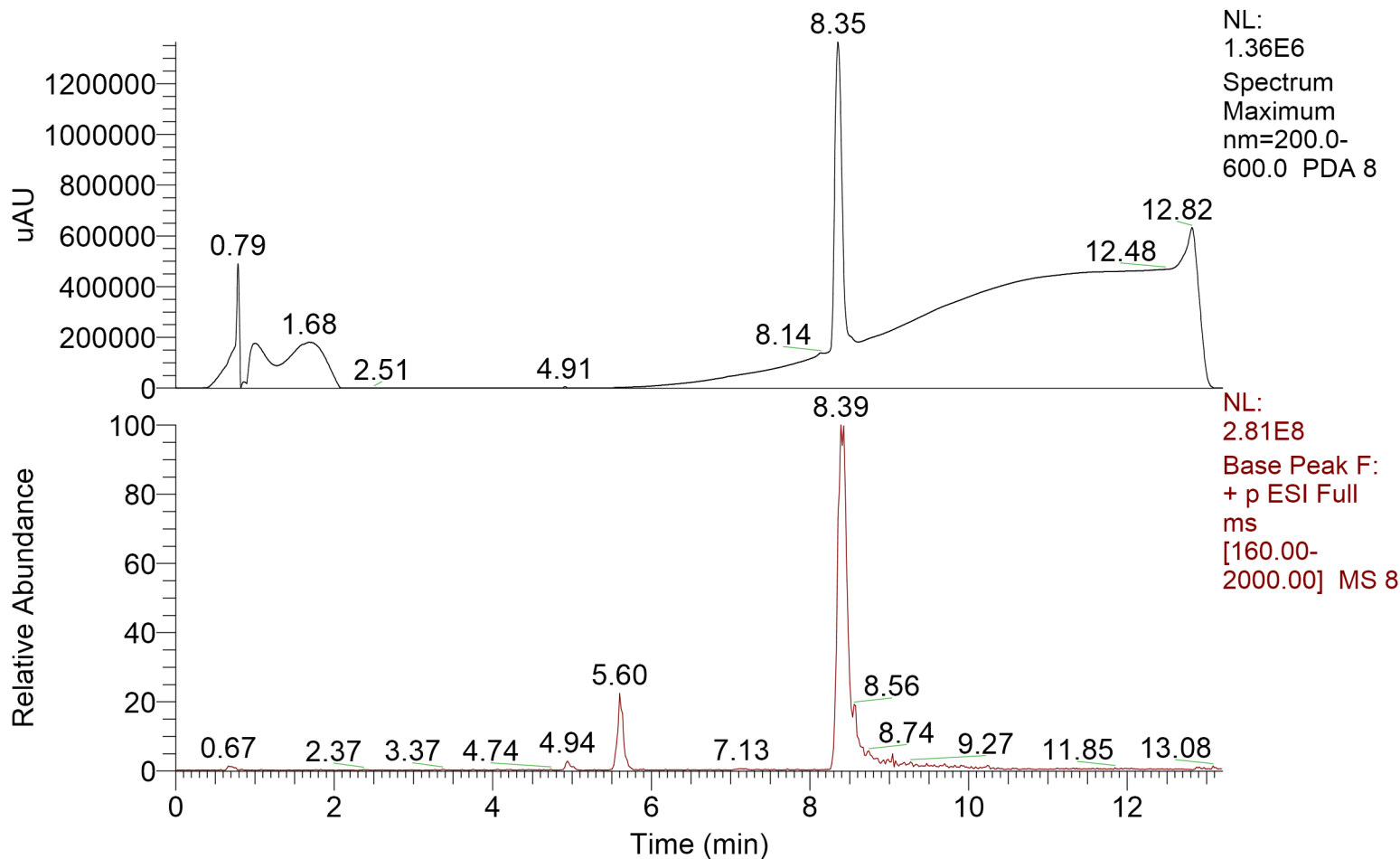


NL: 4.90E7
 7#440-464 RT:
 8.34-8.79 AV: 25 F:
 + p ESI Full ms
 [160.00-2000.00]

NL: 4.64E7
 7#395-404 RT:
 7.50-7.67 AV: 10 F:
 + p ESI Full ms
 [160.00-2000.00]



RT: 0.00 - 13.20



8

Type: Unknown ID: 1 Row: 1

Instrument Method: C:\Xcalibur\methods\General(TFA)\1090%B10_C=TFA_20ul_+pf_12,5min.meth

Processing Method:

Vial: C:40

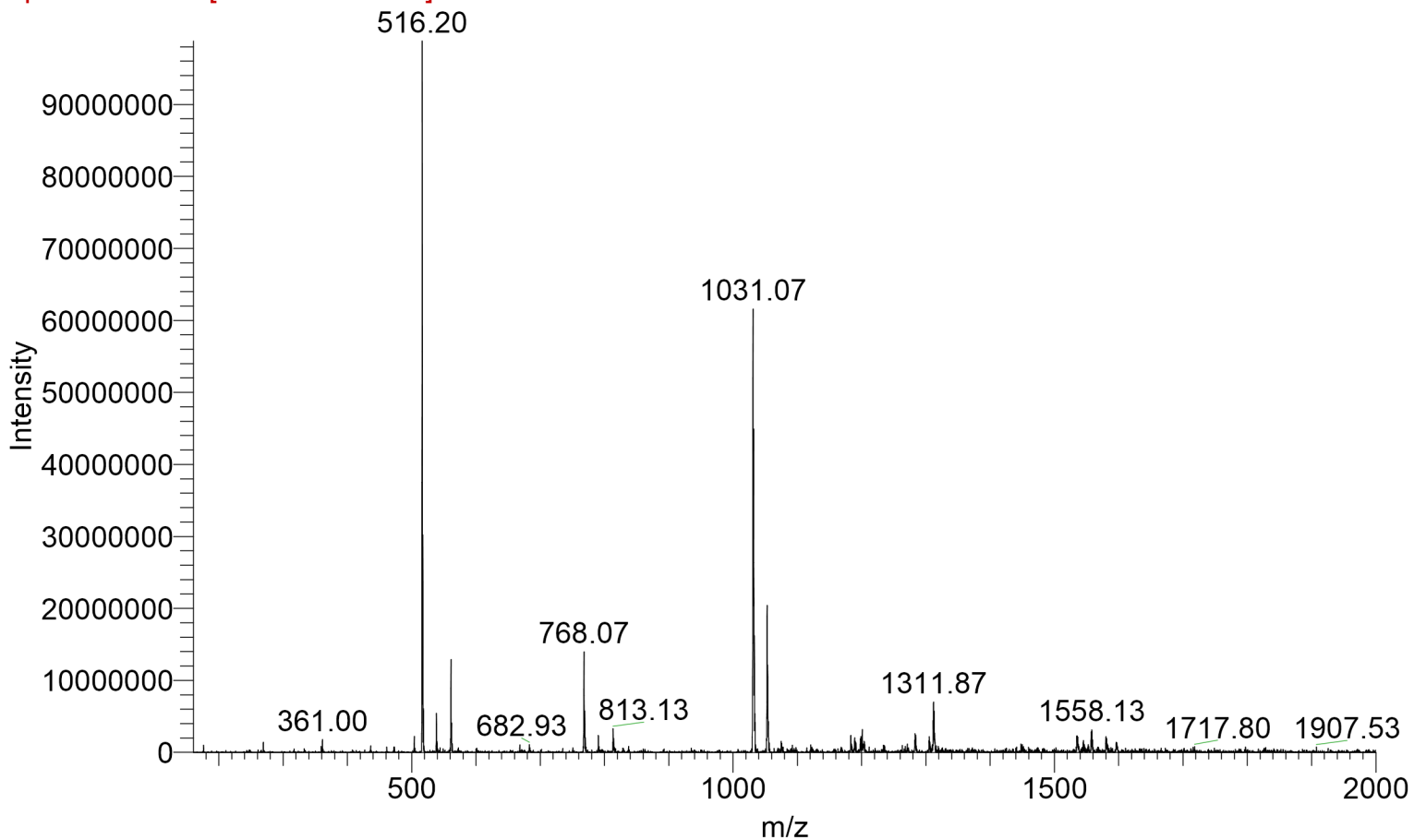
Injection Volume (µl): 20.00

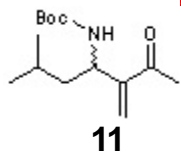
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Sample Volume (µl): 0.00

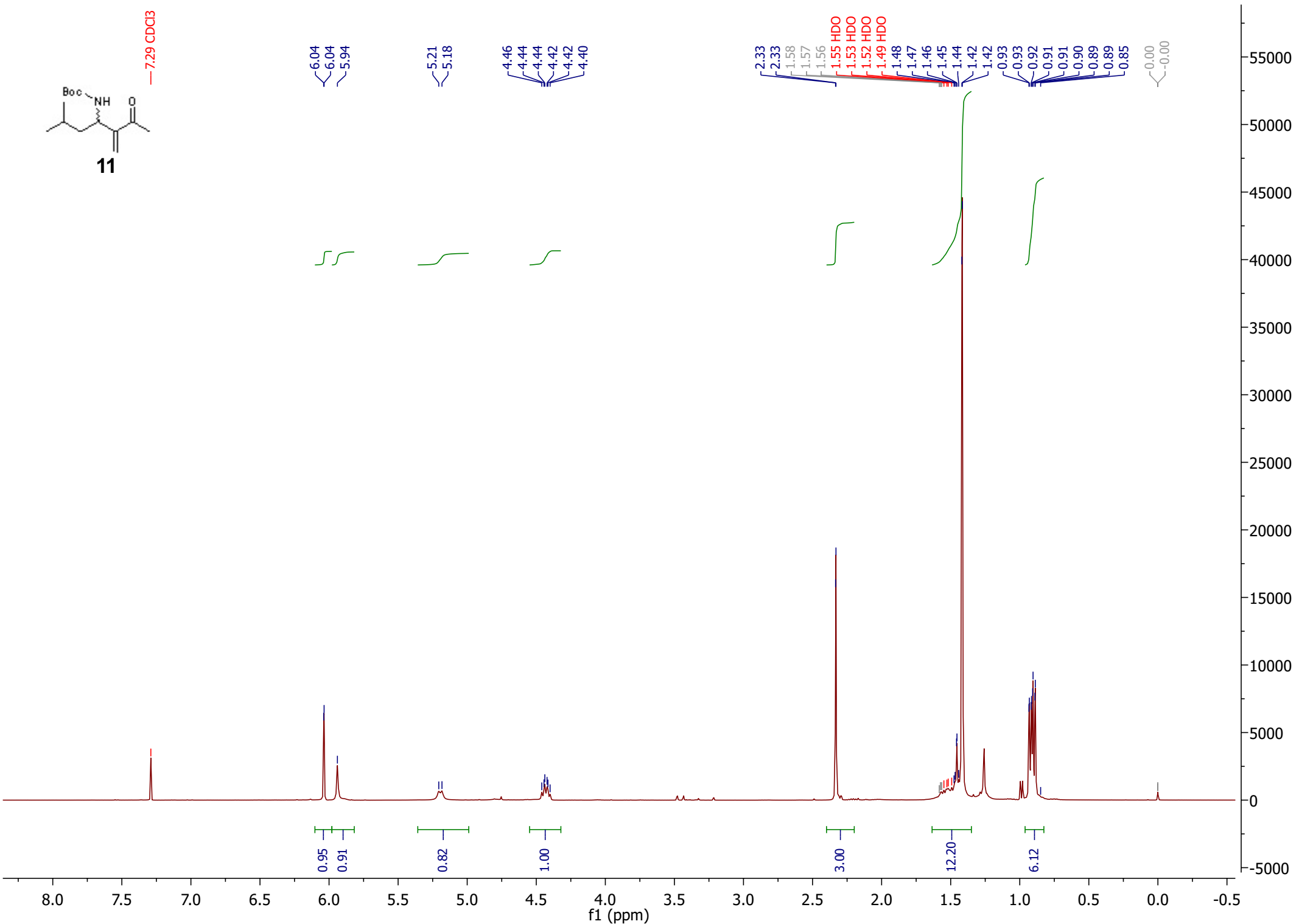
8 #441-461 RT: 8.26-8.63 AV: 21 NL: 9.88E7

F: + p ESI Full ms [160.00-2000.00]

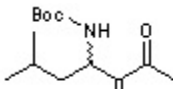




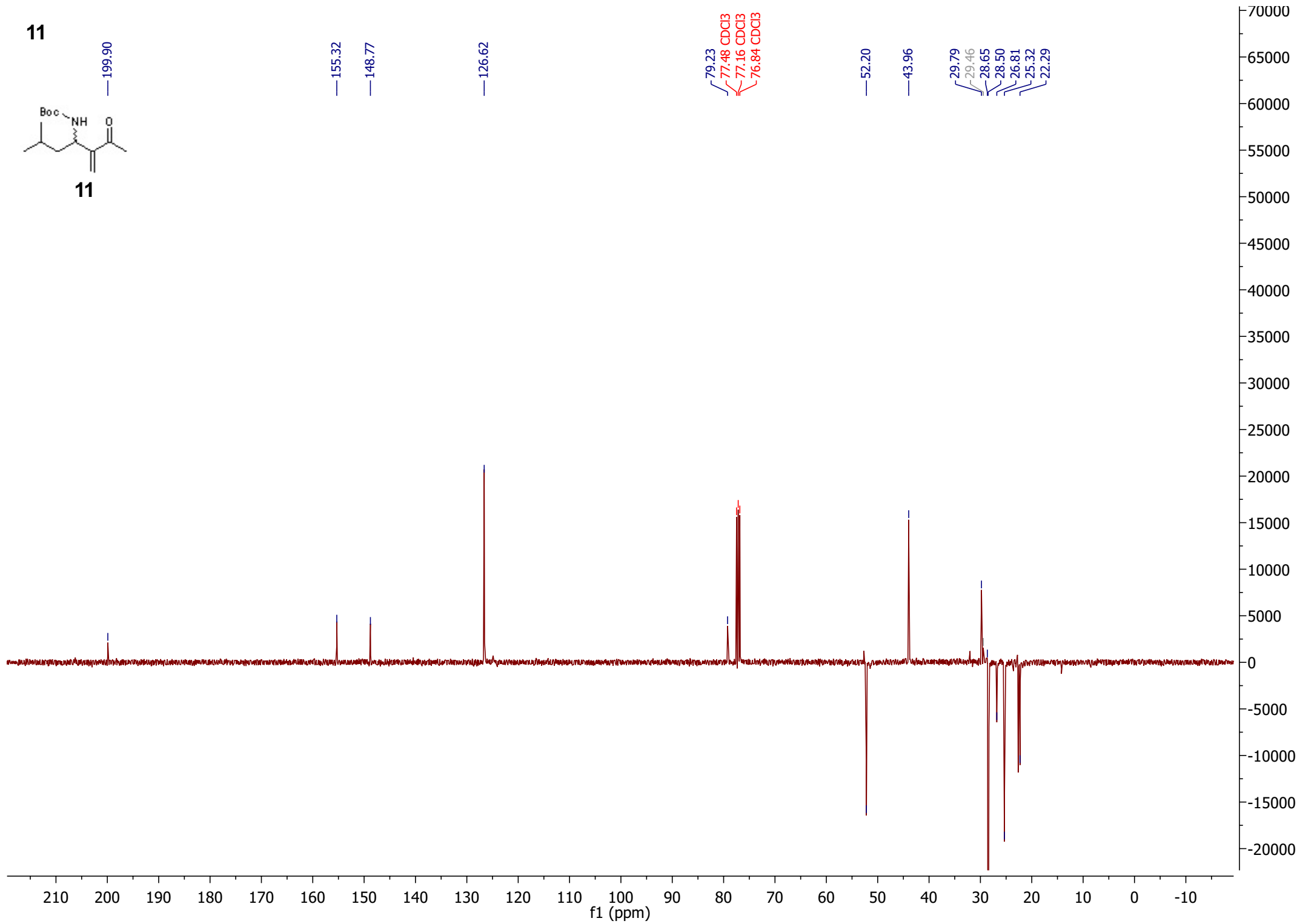
— 7.29 CDCl₃

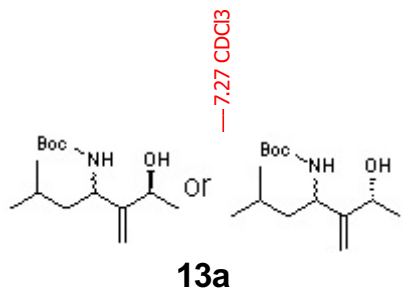


11

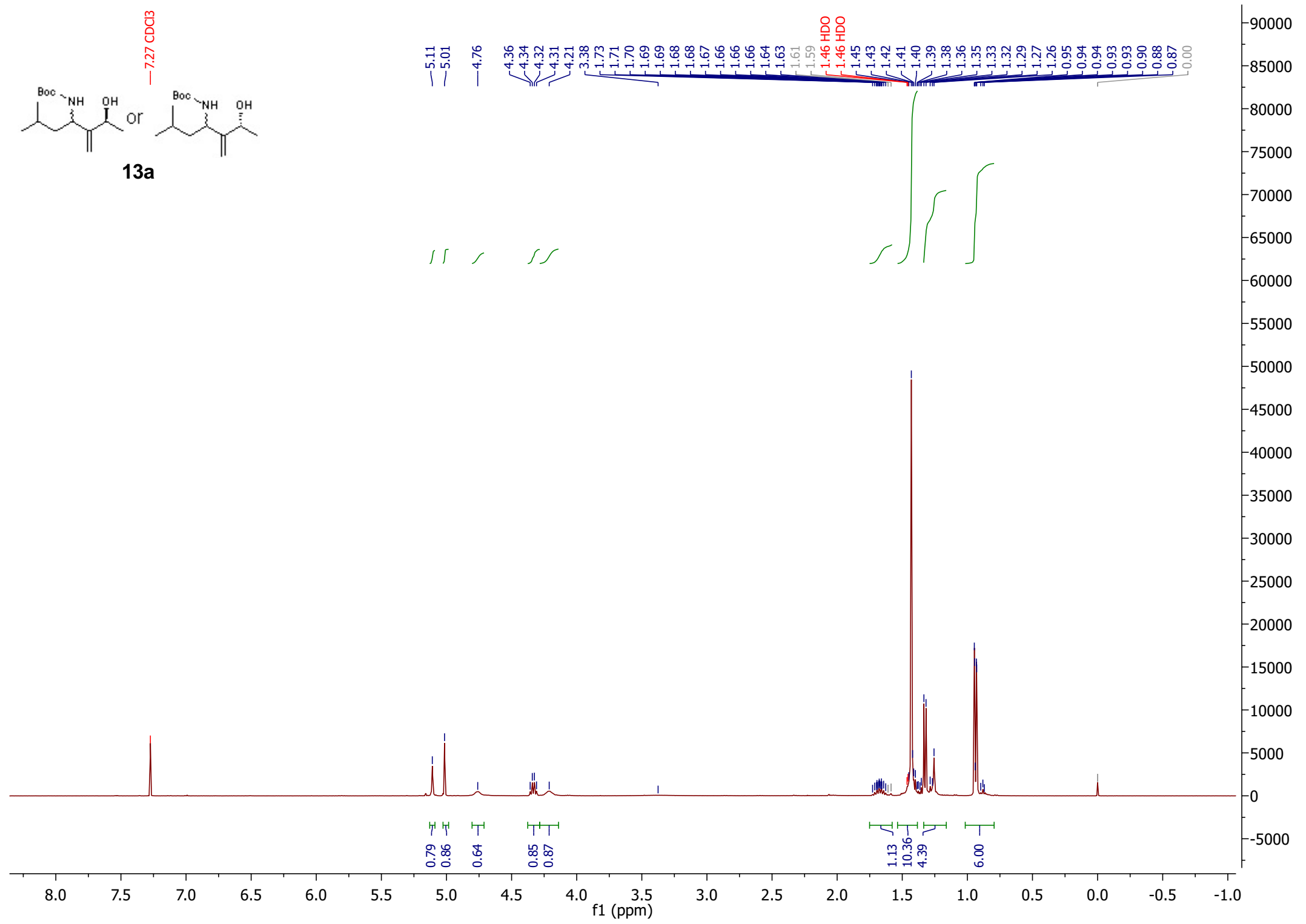


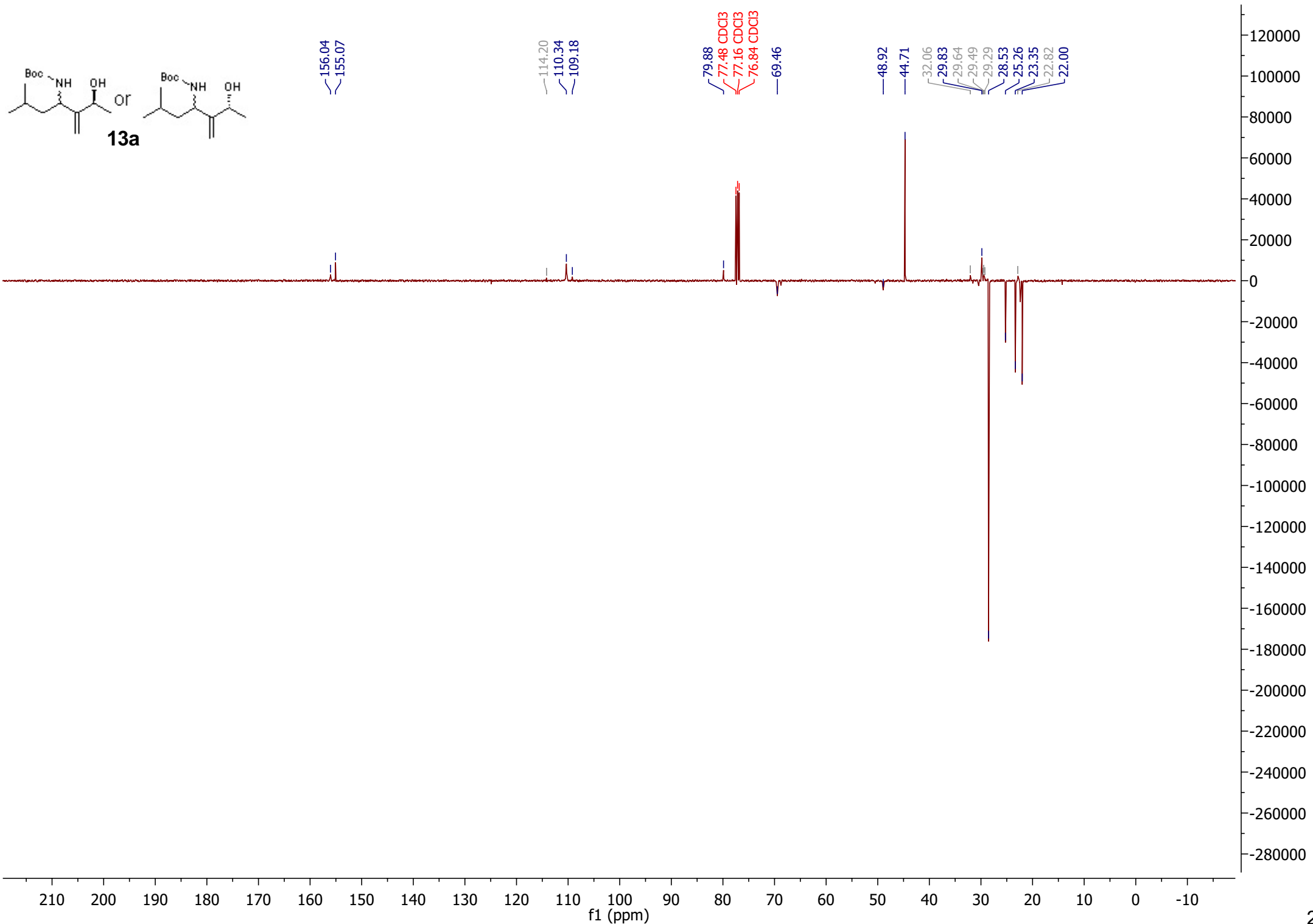
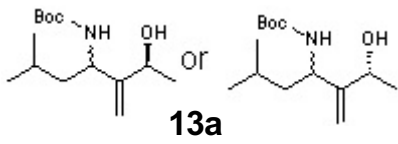
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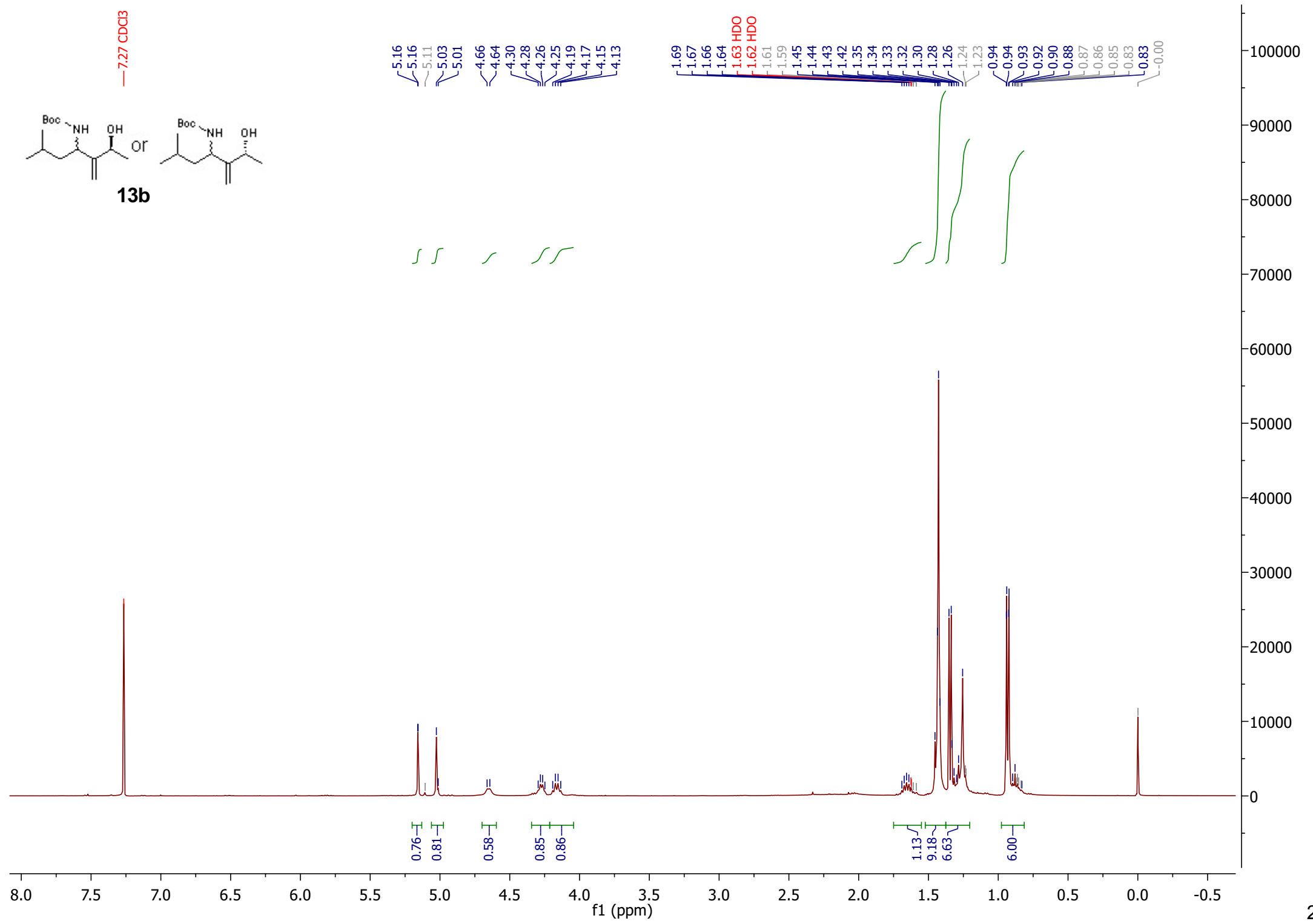
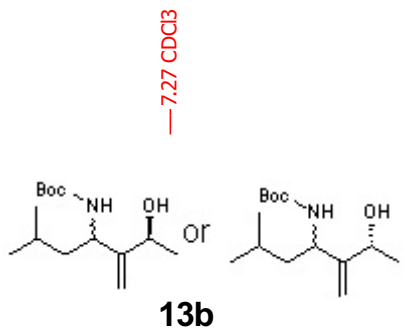


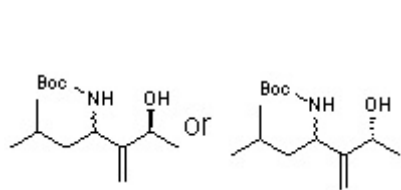


7.27 CDCl3









13b

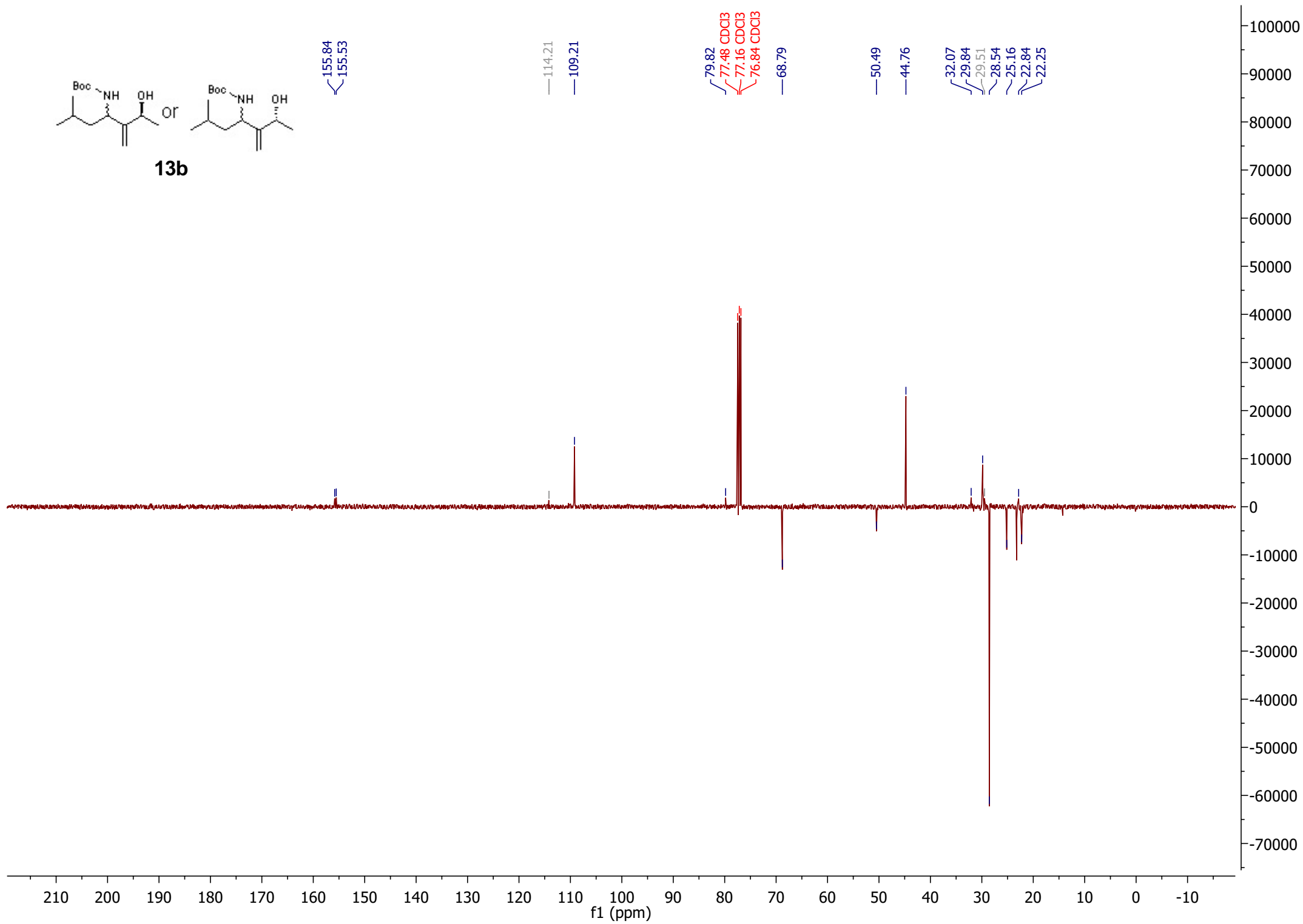
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155.53

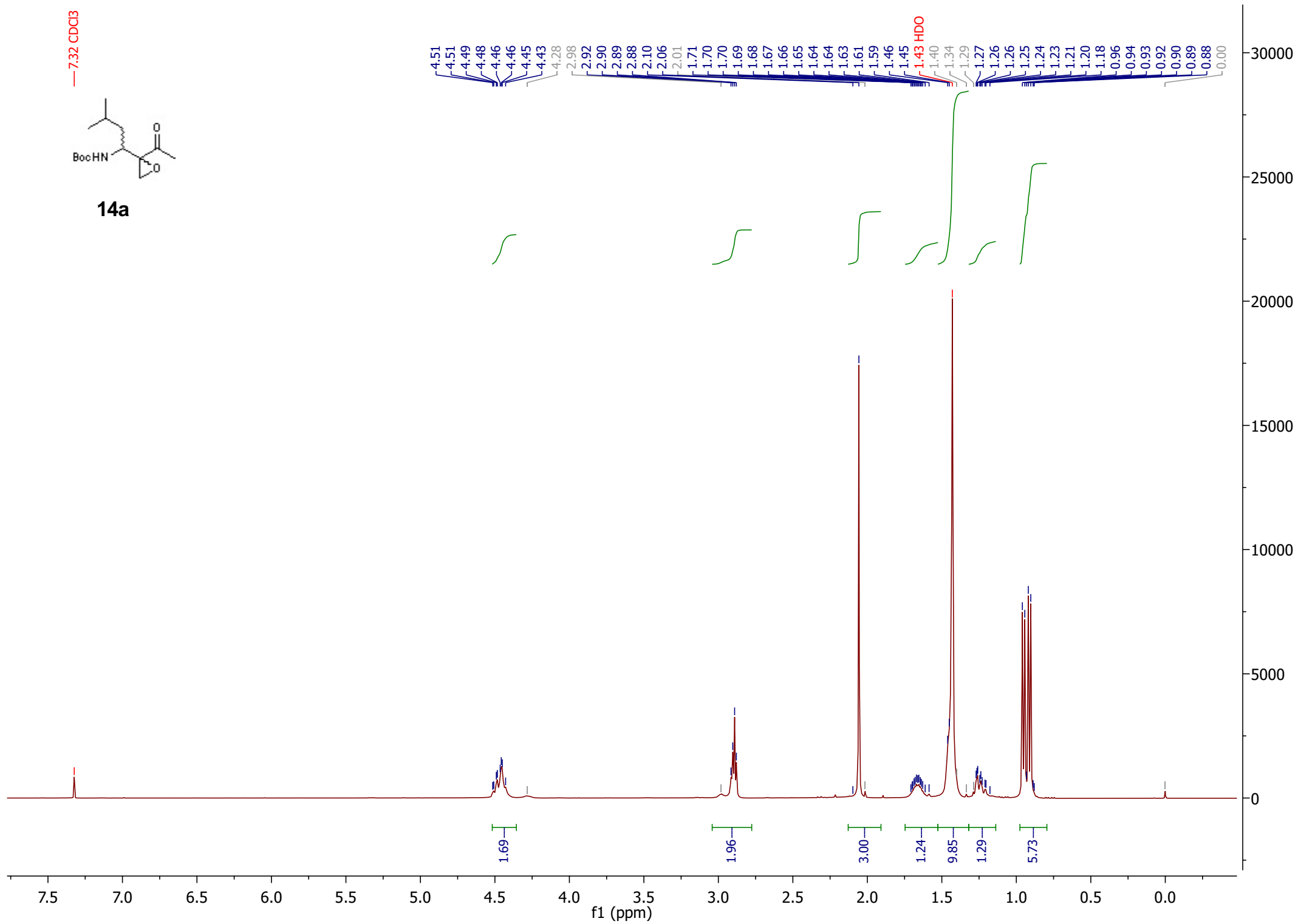
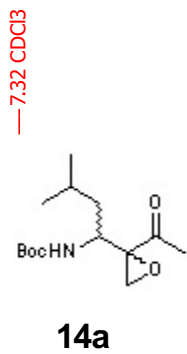
114.21
109.21

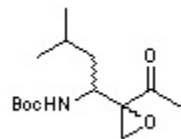
79.82
77.48 CDCl3
77.16 CDCl3
76.84 CDCl3
68.79

50.49
44.76

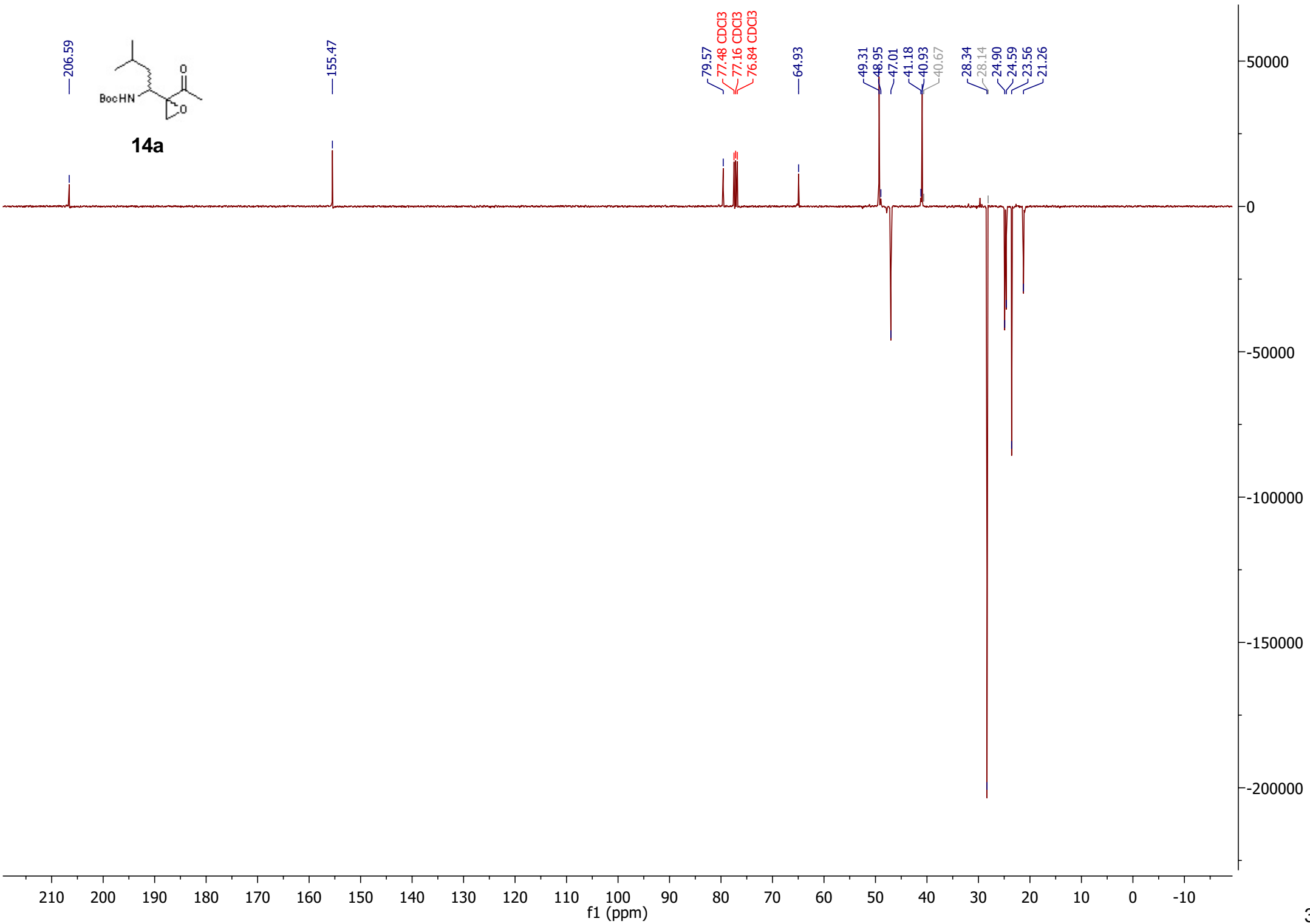
32.07
29.84
29.51
28.54
25.16
22.84
22.25

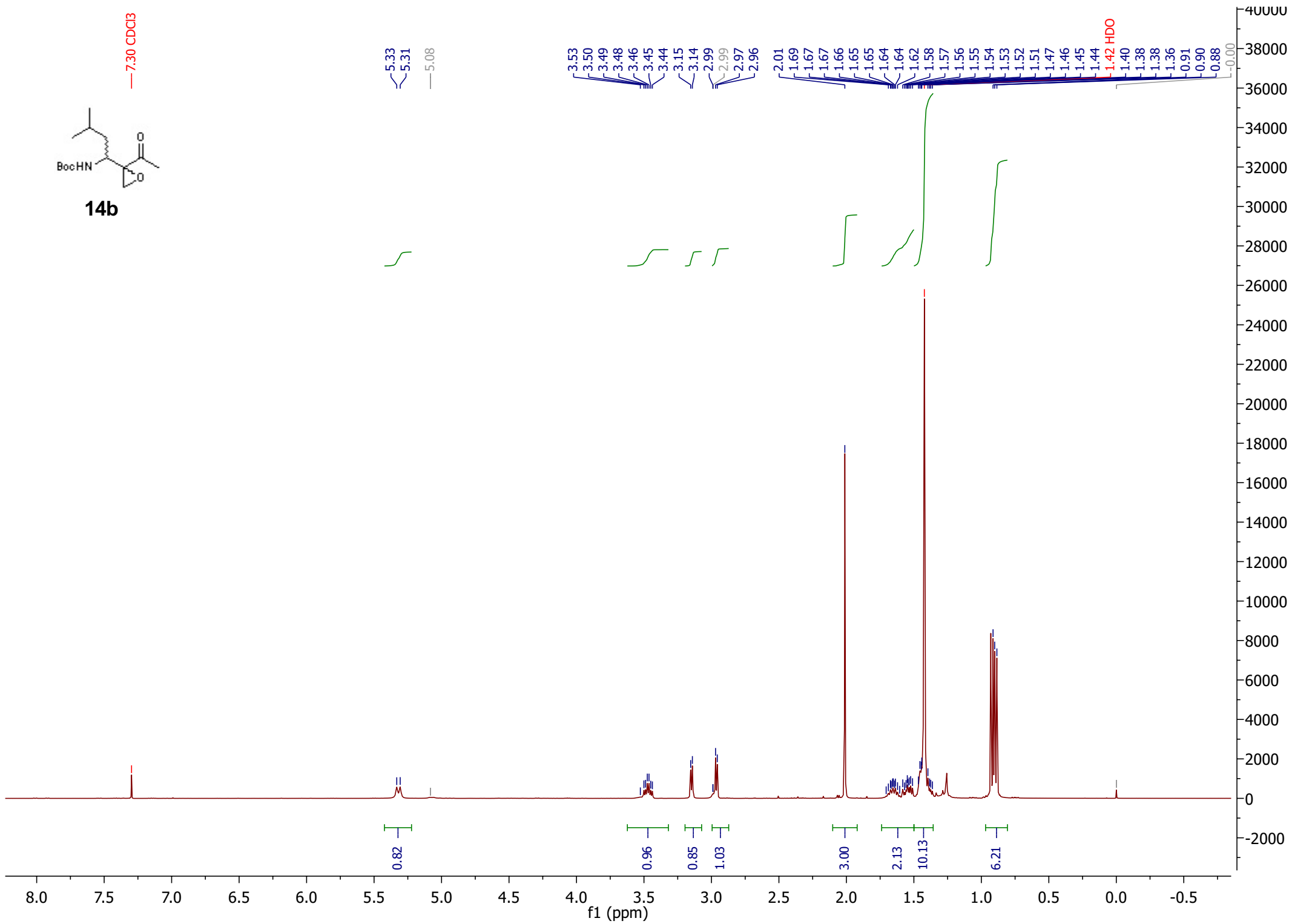
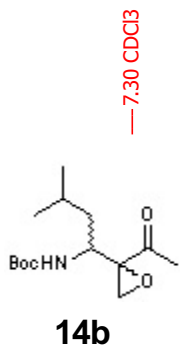




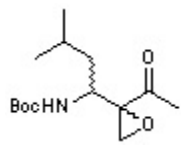


14a





208.62



14b

155.47

79.41
77.48 CDCl3
77.16 CDCl3
76.84 CDCl3

62.60

52.60

51.26

50.81

40.73

29.77

29.44

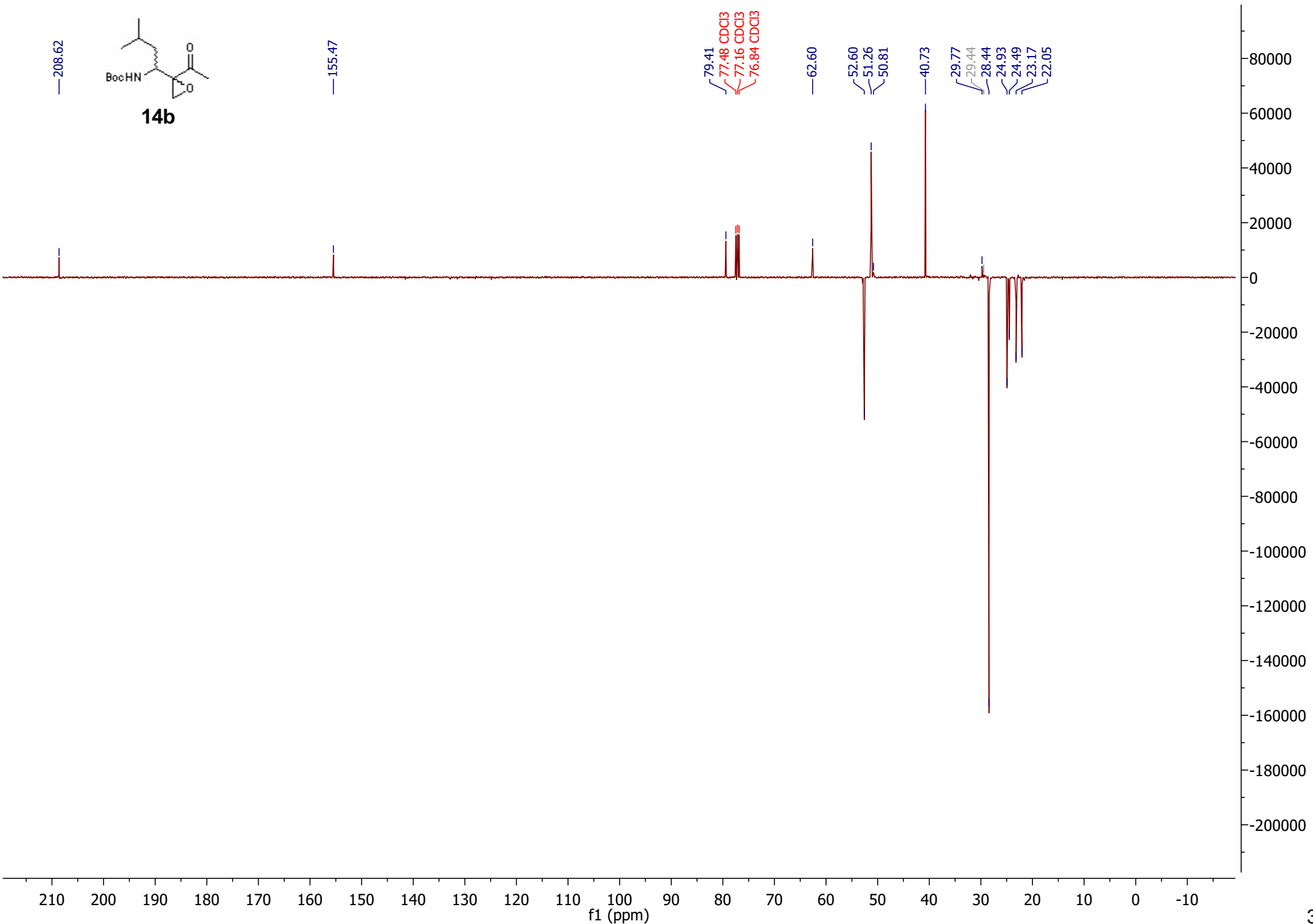
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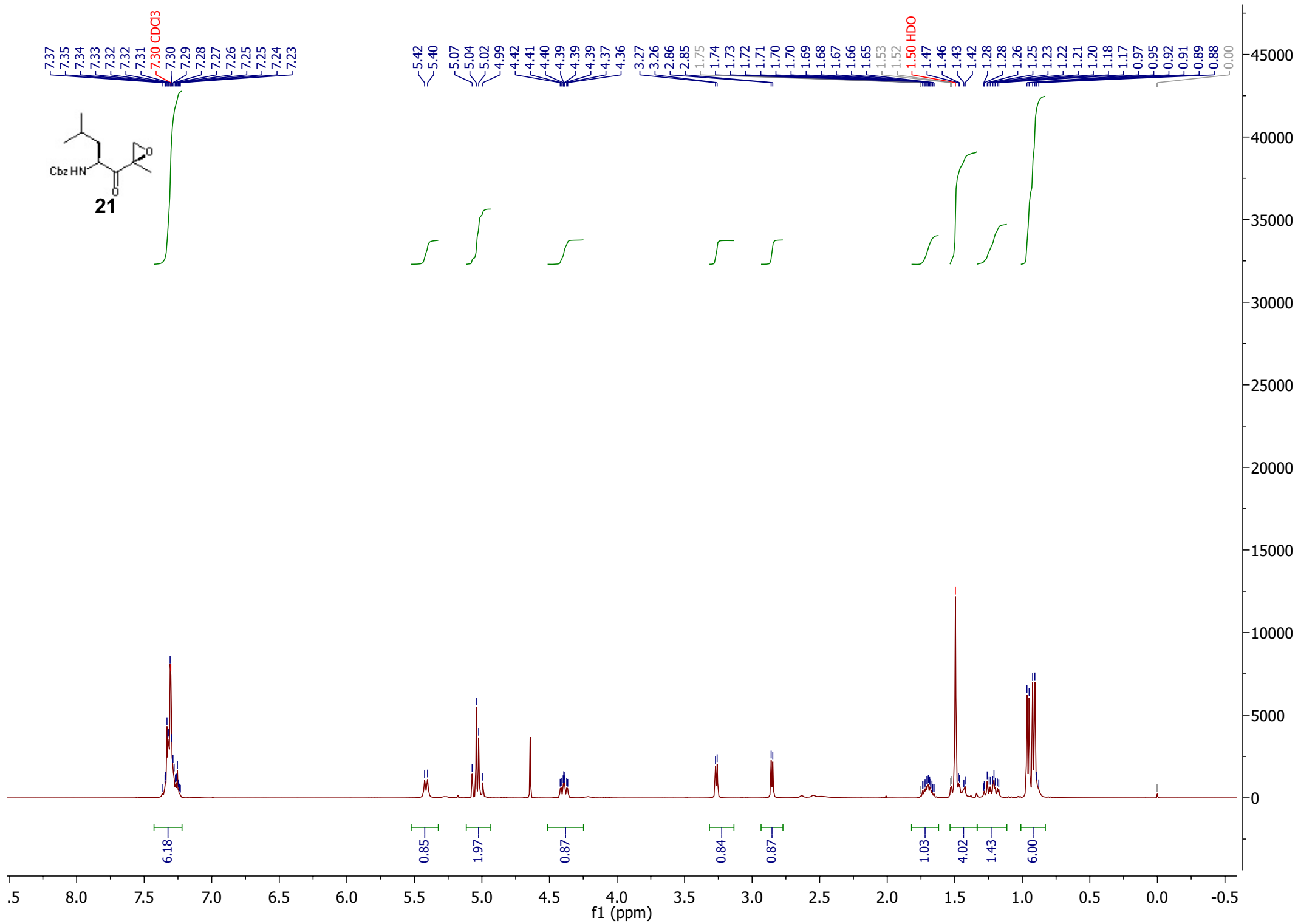
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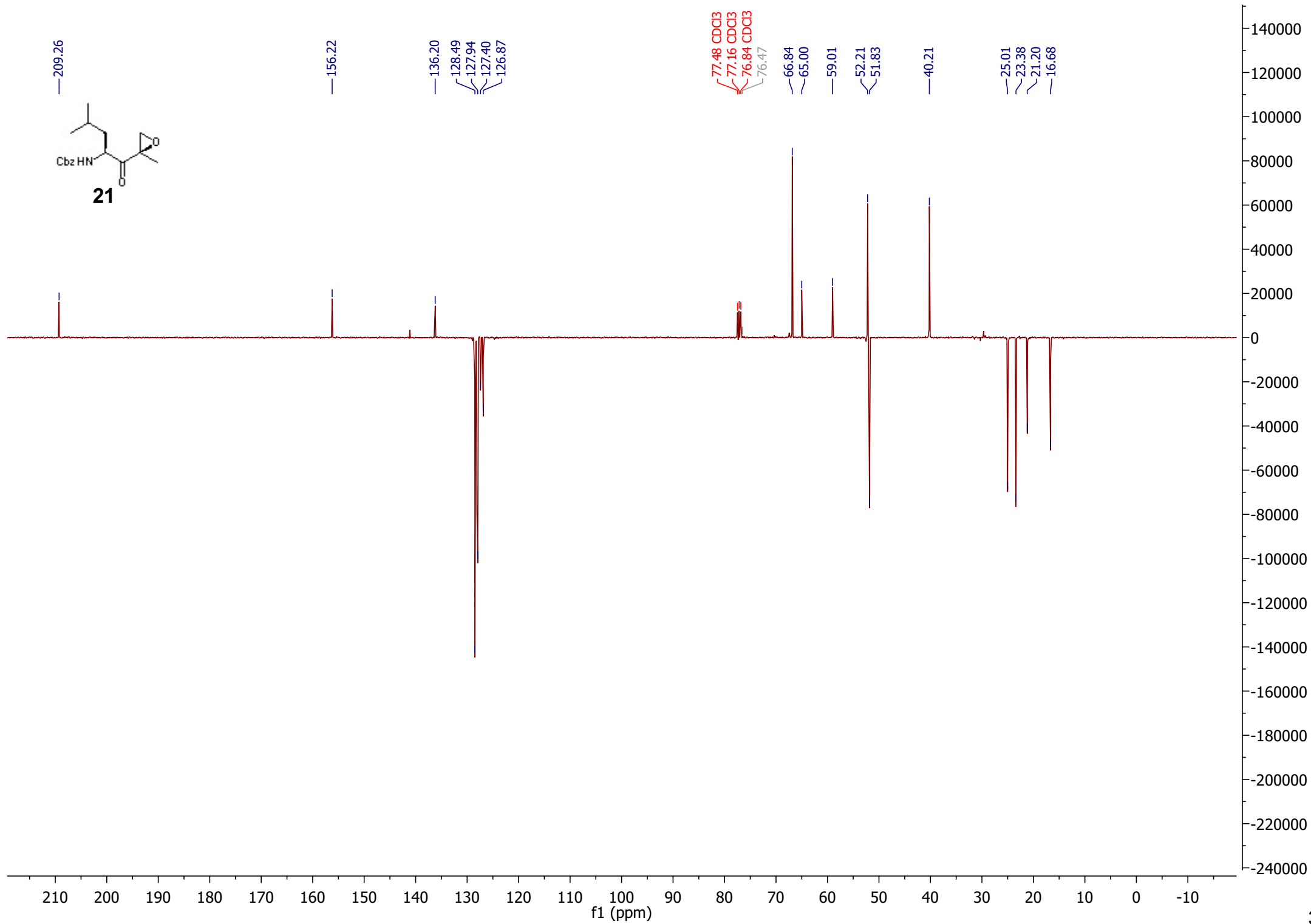
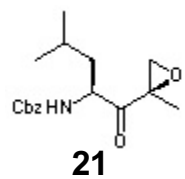
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23.17

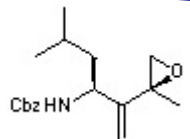
22.05



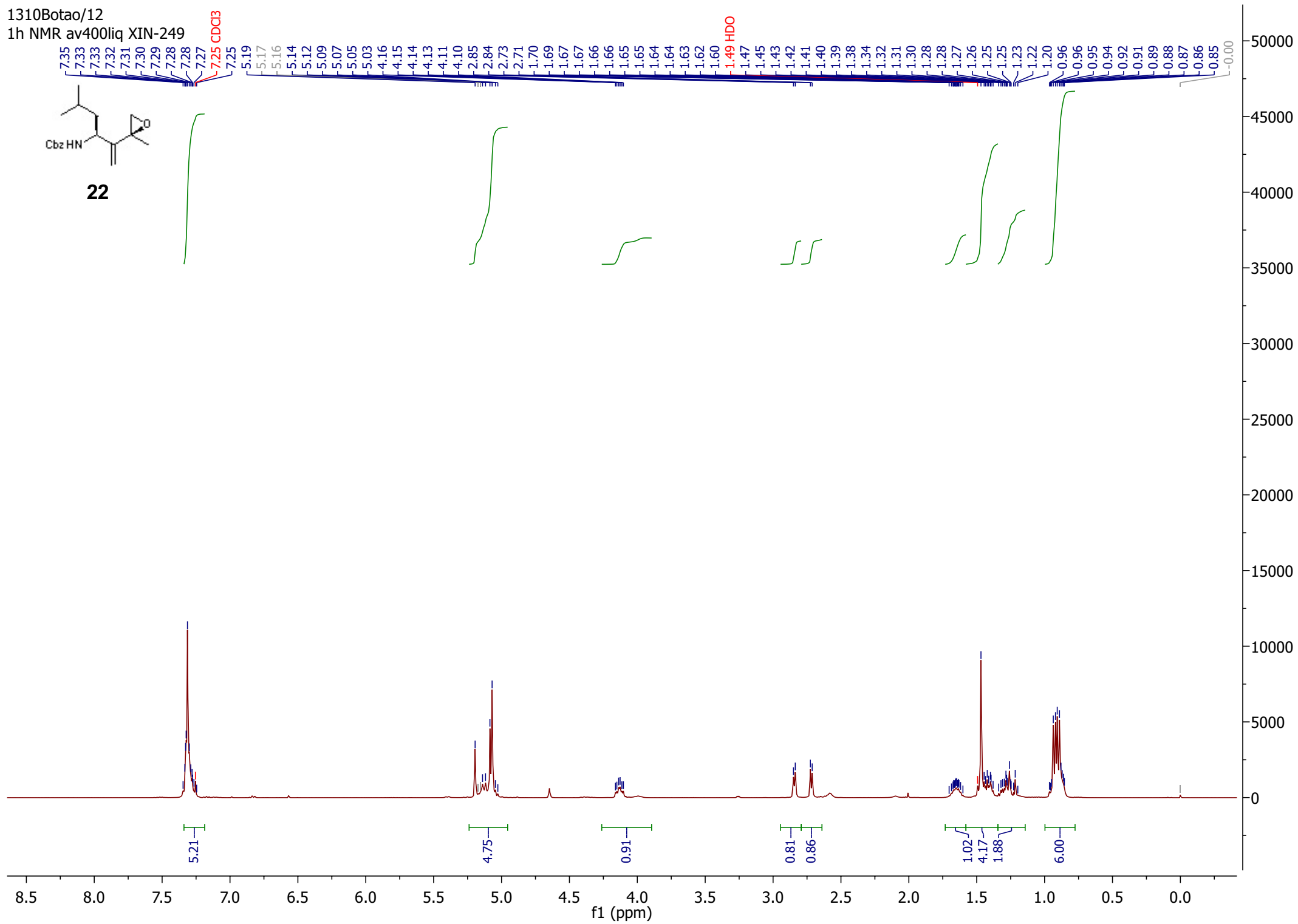


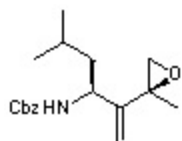


1310Botao/12
1h NMR av400liq XIN-249

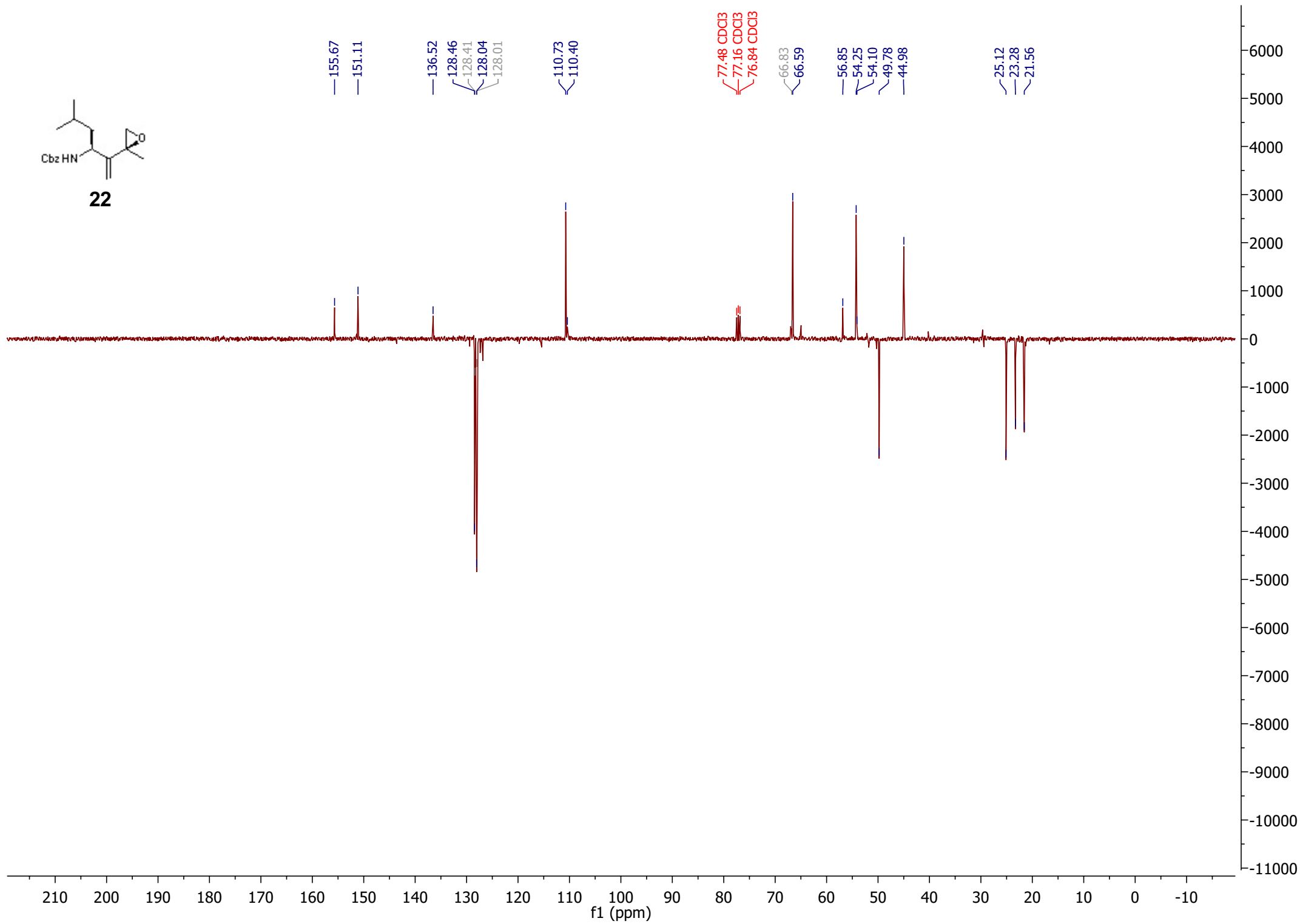


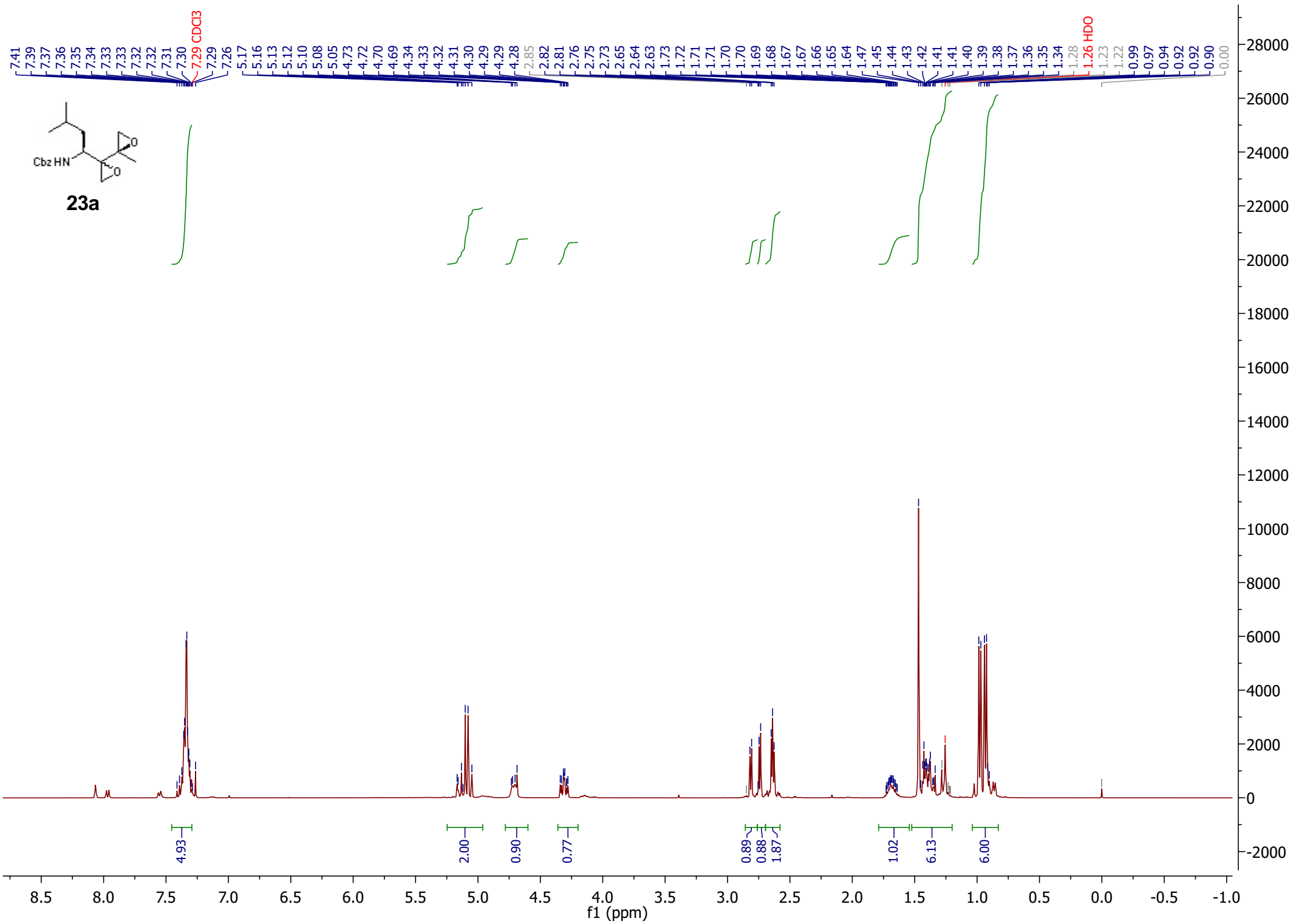
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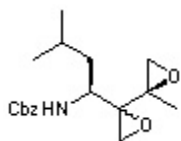




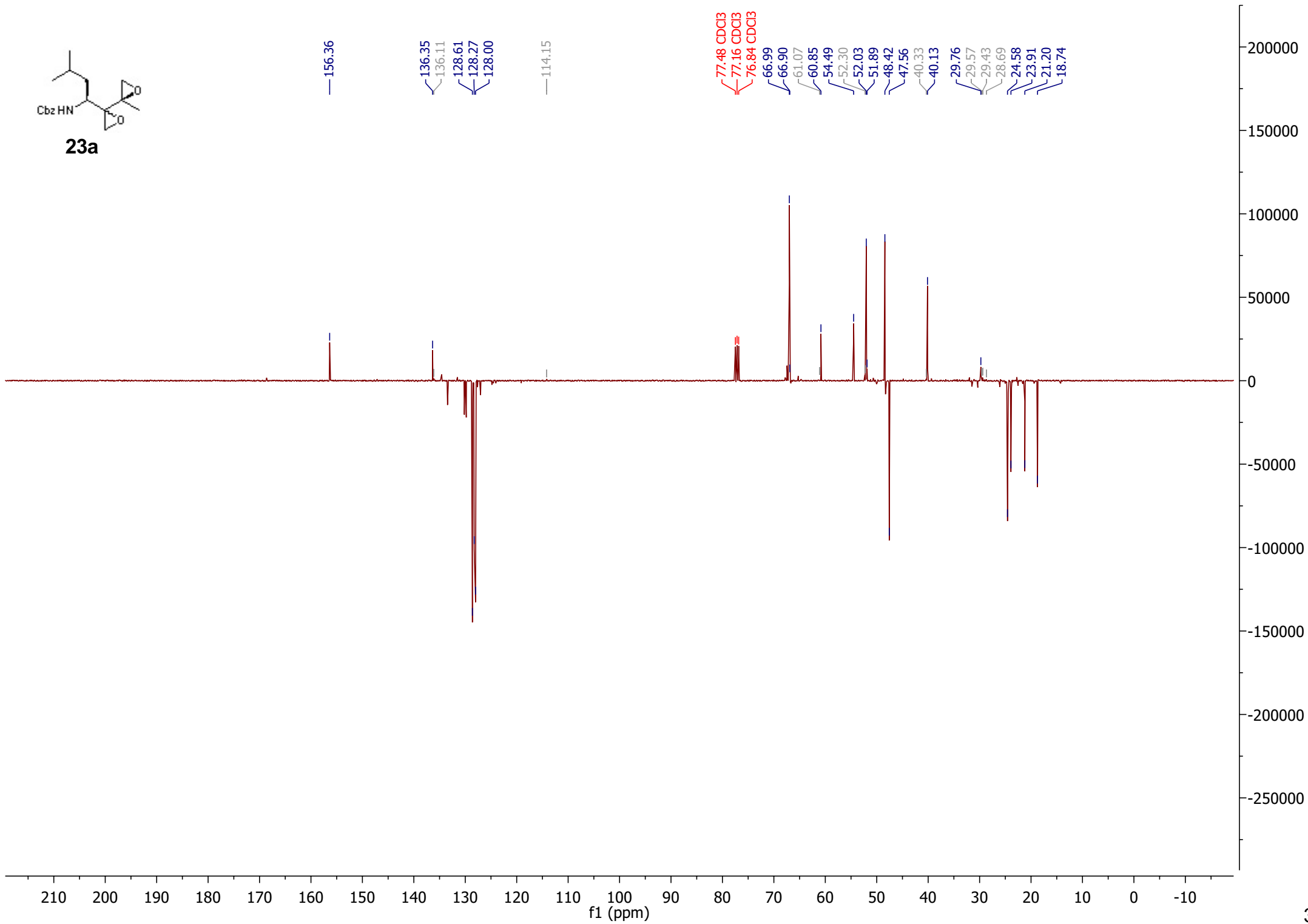
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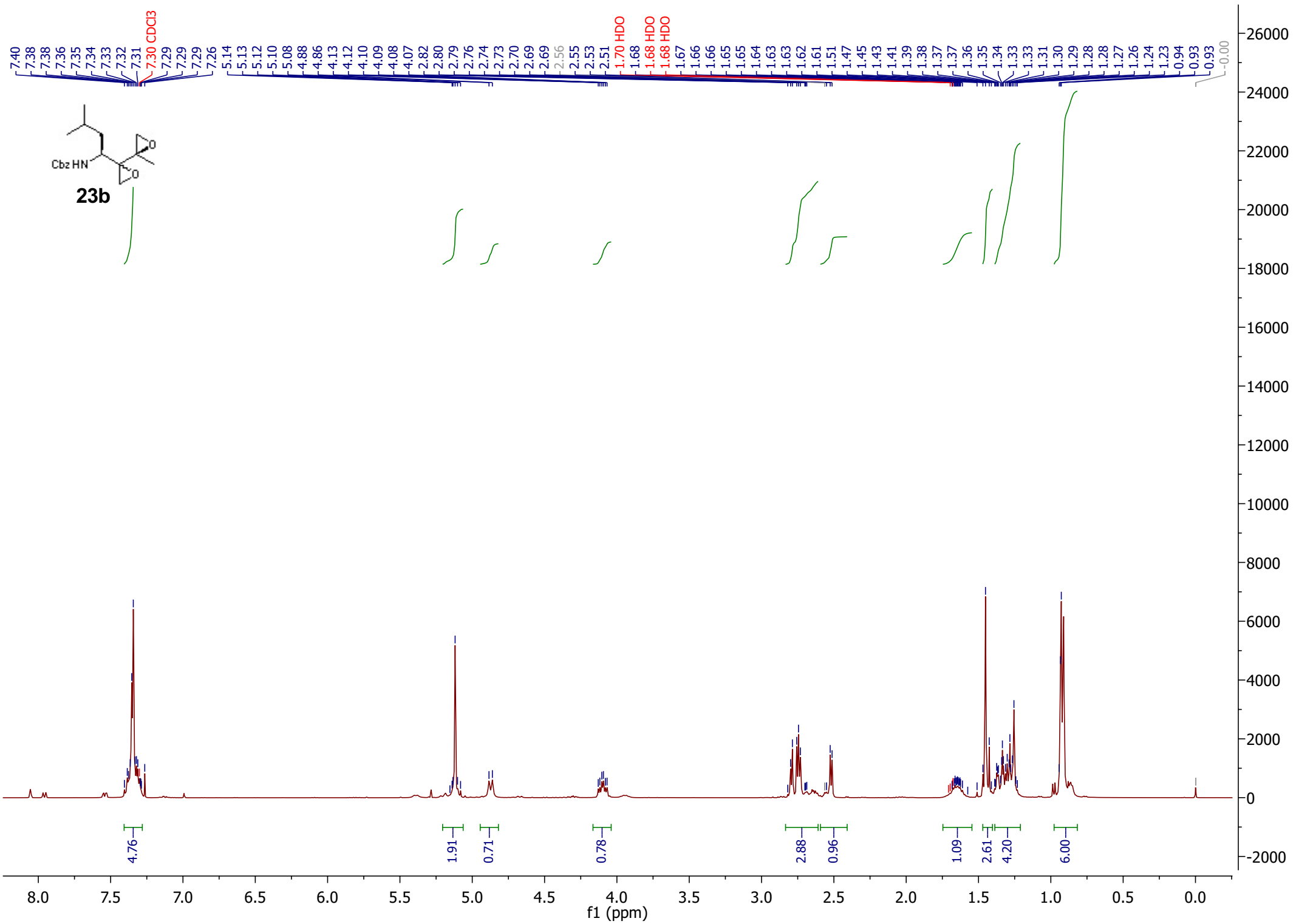


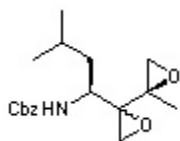




23a







23b

