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Total Synthesis of (+) Herboxidiene/GEX 1A

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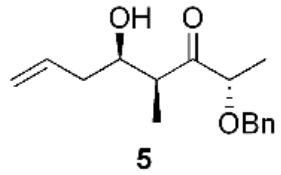
1. ^{1}H and ^{13}C NMR Spectra of Compounds

^{1}H NMR (400 MHz, $CDCl_3$)



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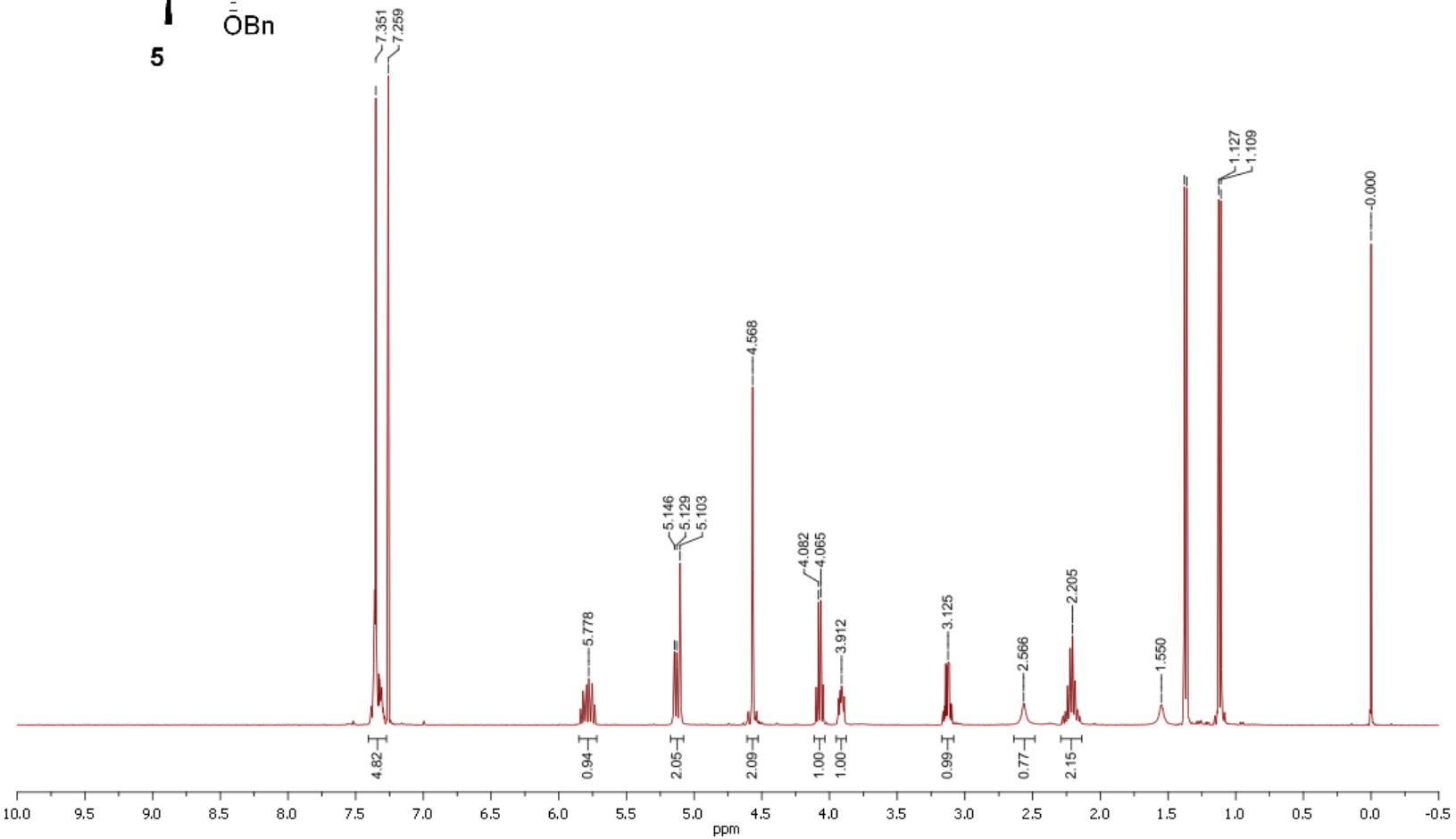
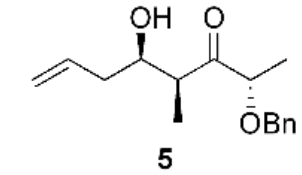
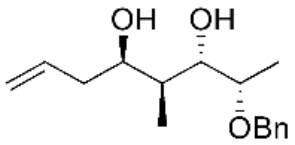


^{13}C NMR (100.6 MHz, $CDCl_3$)



5

^{1}H NMR (400 MHz, $CDCl_3$)



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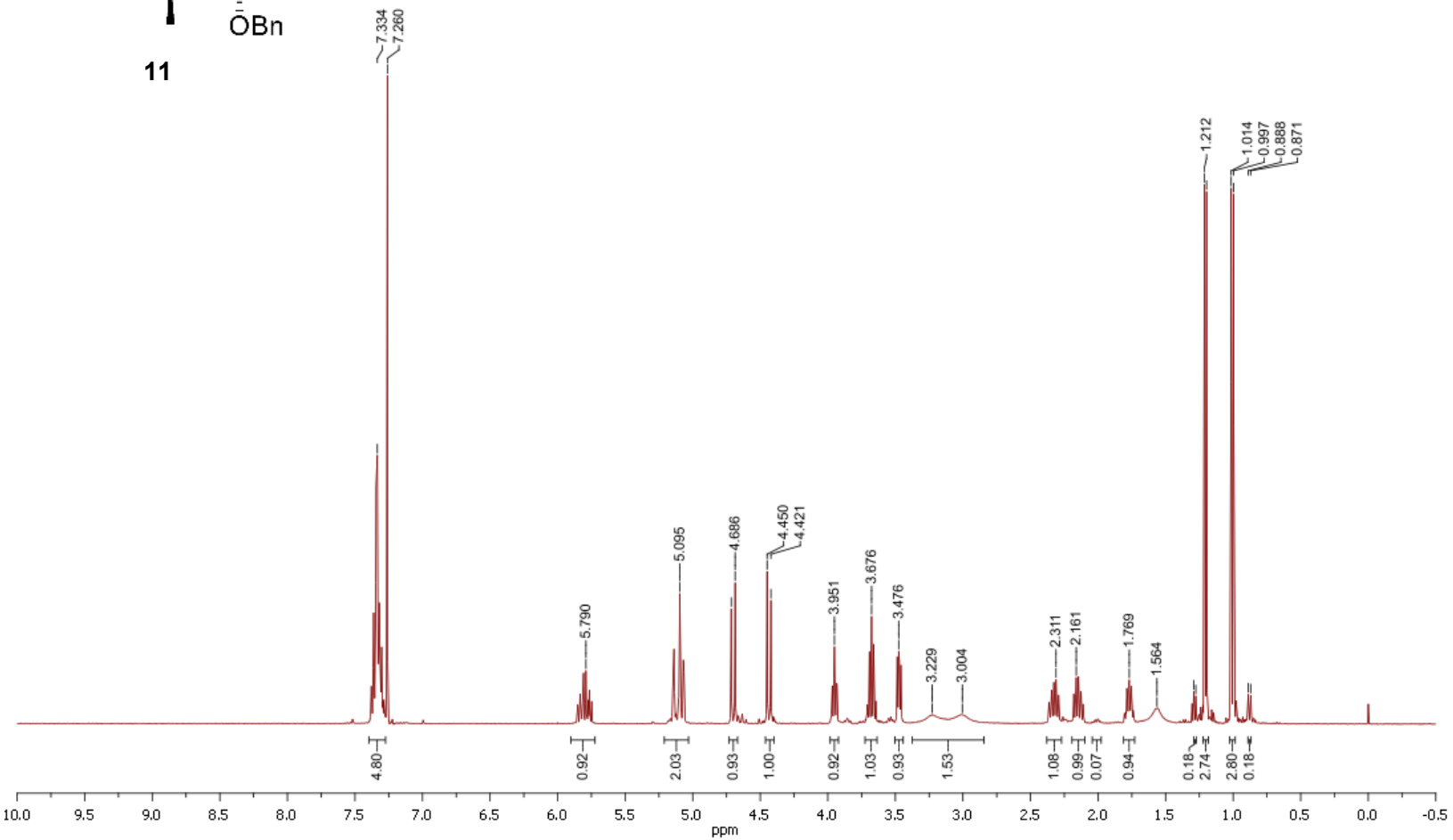
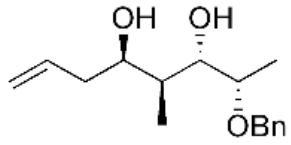
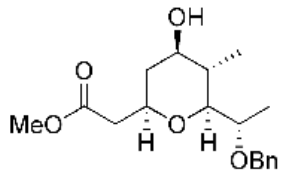


^{13}C NMR (100.6 MHz, $CDCl_3$)



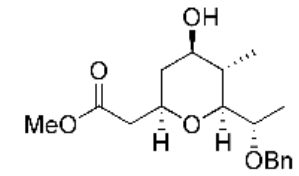
11

^{1}H NMR (400 MHz, $CDCl_3$)



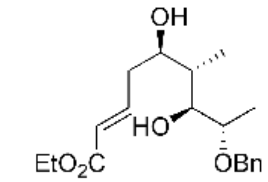
12

^{13}C NMR (100.6 MHz, $CDCl_3$)



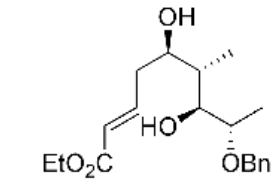
12

^{1}H NMR (400 MHz, $CDCl_3$)



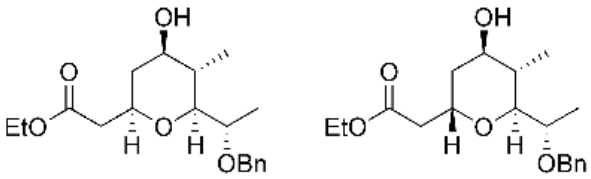
13

^{13}C NMR (100.6 MHz, $CDCl_3$)



13

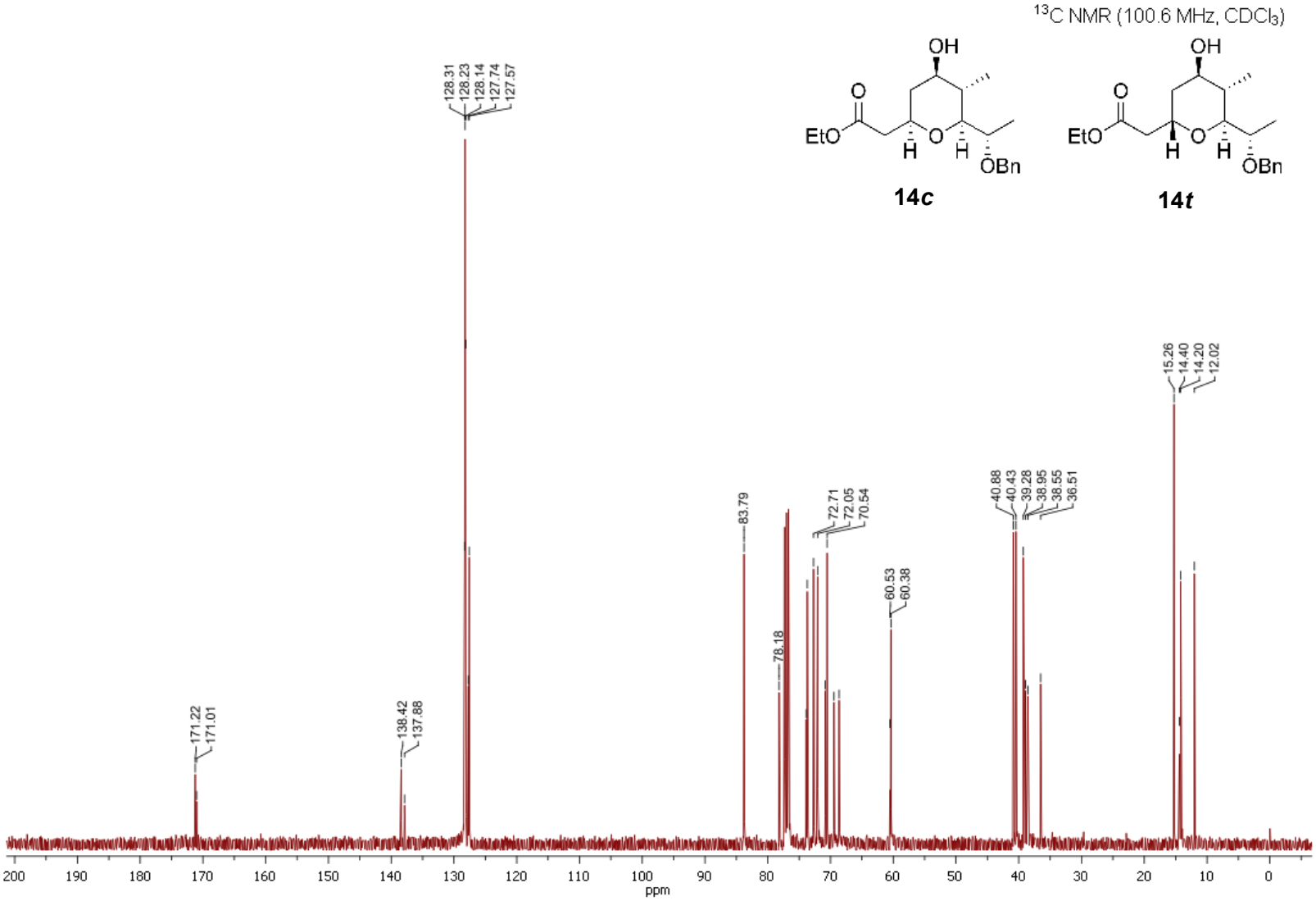
^{1}H NMR (400 MHz, $CDCl_3$)



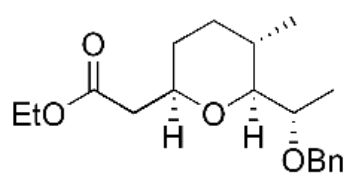
14*c*

14*t*

rd 69:31

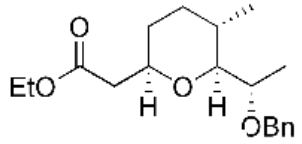

^{13}C NMR (100.6 MHz, CDCl$_3$)
OH
O
EtO
H
O
H
OBn
14c
14t
128.31
128.23
128.14
127.74
127.57
171.22
171.01
138.42
137.88
83.79
78.18
72.71
72.05
70.54
60.53
60.38
40.88
40.43
39.28
38.95
38.55
36.51
15.26
14.40
14.20
12.02
ppm

^{1}H NMR (400 MHz, $CDCl_3$)



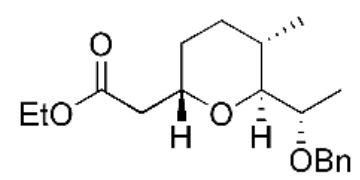
15c

^{13}C NMR (100.6 MHz, $CDCl_3$)

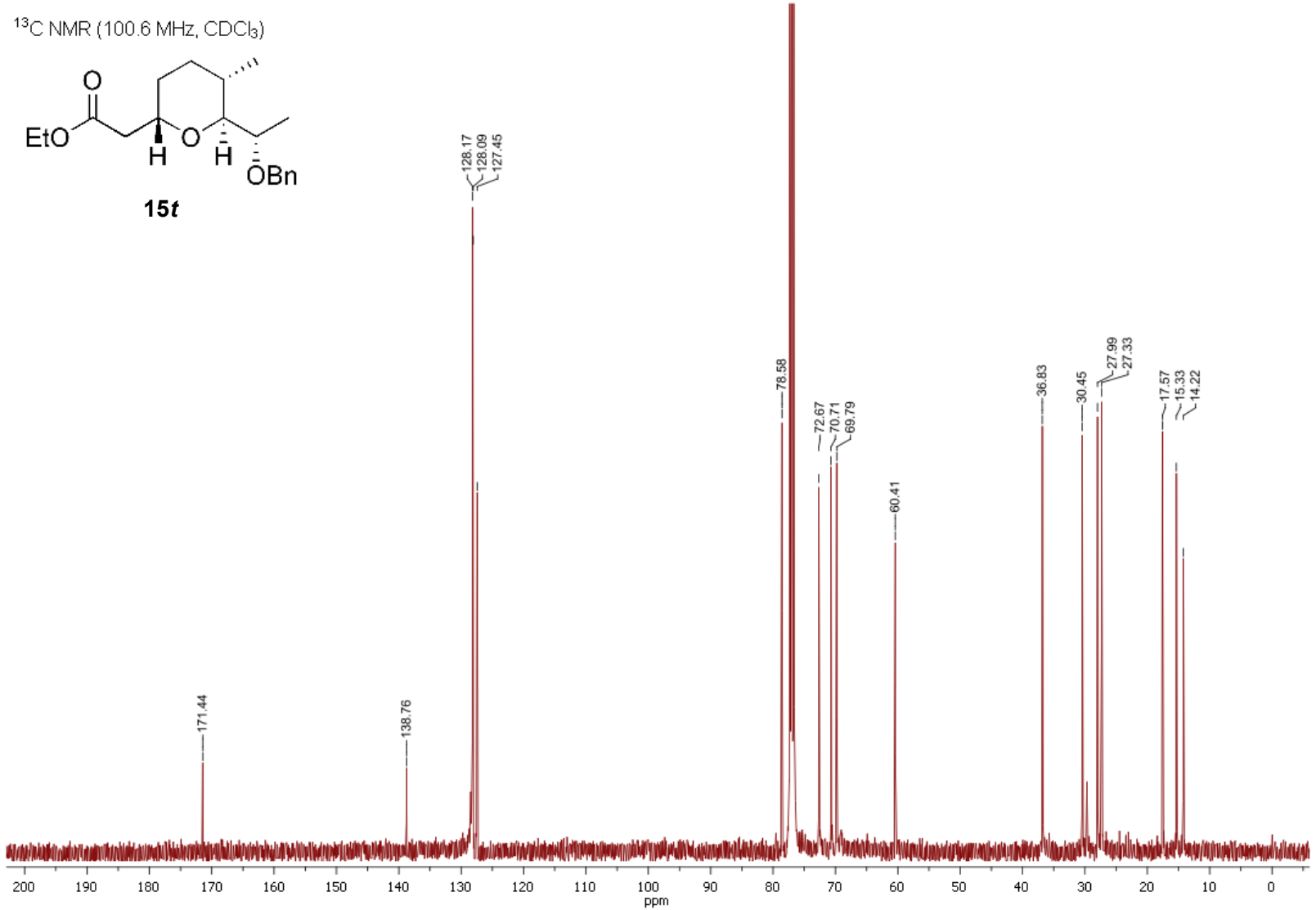


15*c*

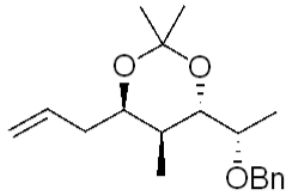
^{1}H NMR (400 MHz, $CDCl_3$)



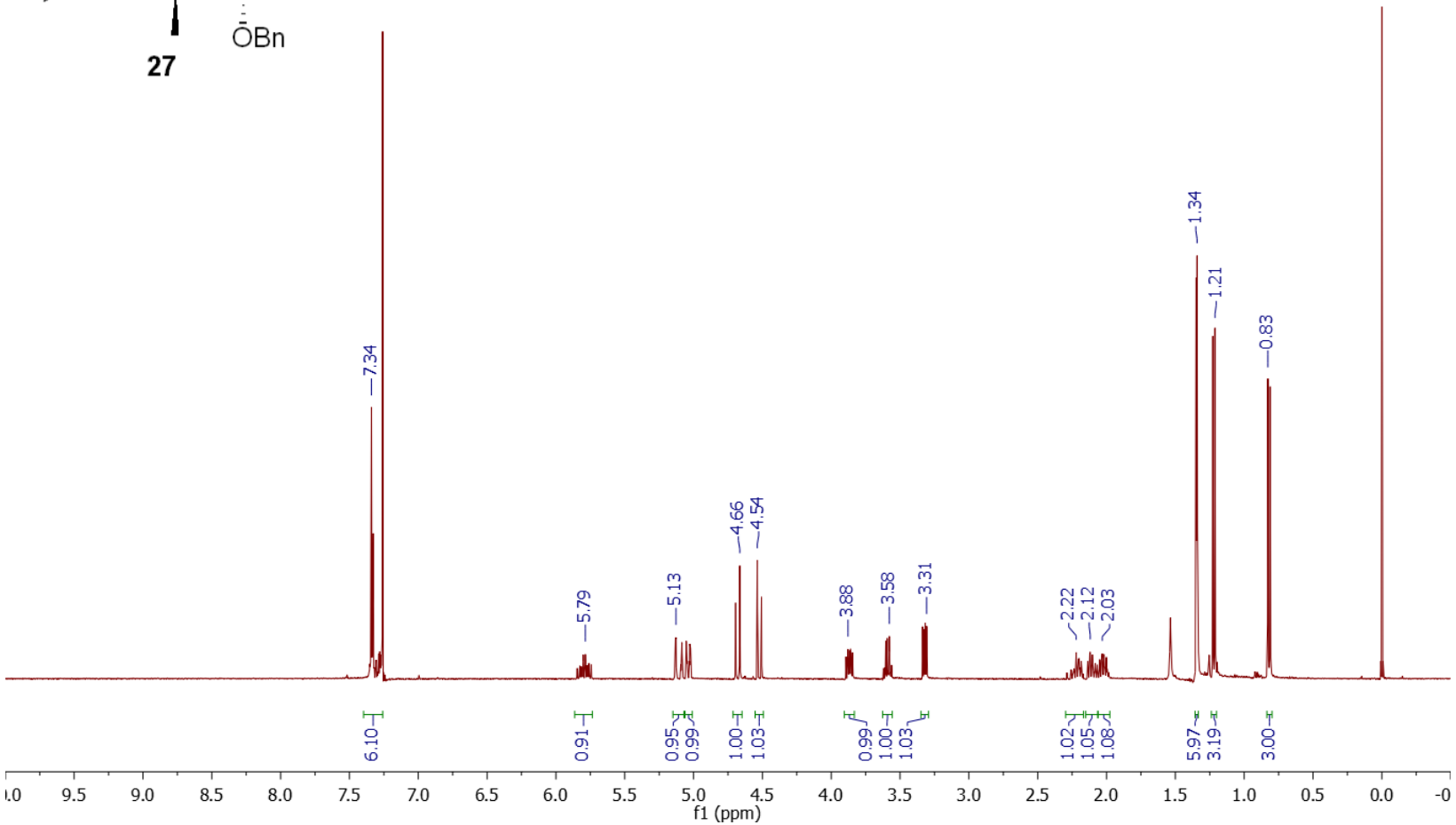
15*t*


^{13}C NMR (100.6 MHz, CDCl$_3$)
EtO
O
H
O
H
OBn
15*t*
128.17
128.09
127.45
78.58
72.67
70.71
69.79
60.41
36.83
30.45
27.99
27.33
17.57
15.33
14.22
171.44
138.76
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
ppm

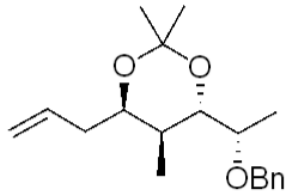
^{1}H NMR (400 MHz, $CDCl_3$)



27

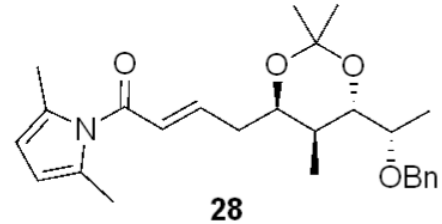


^{13}C NMR (100.6 MHz, $CDCl_3$)



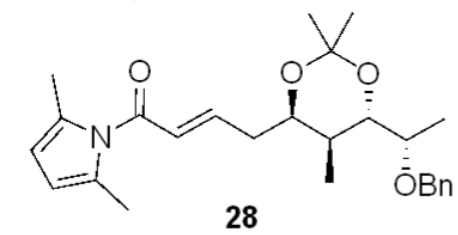
27

^{1}H NMR (400 MHz, $CDCl_3$)



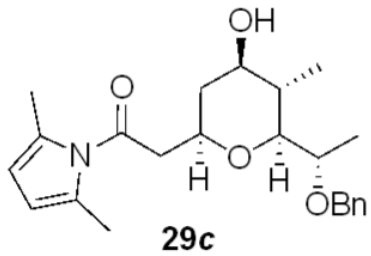
28

^{13}C NMR (100.6 MHz, $CDCl_3$)



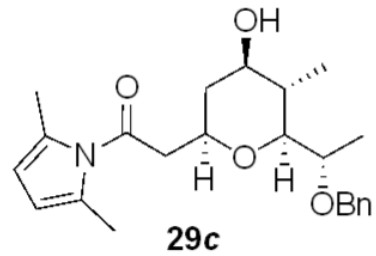
28

^{1}H NMR (400 MHz, $CDCl_3$)



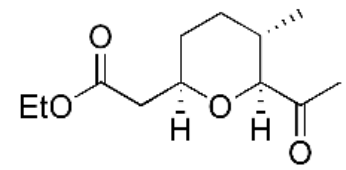
29c

^{13}C NMR (100.6 MHz, $CDCl_3$)



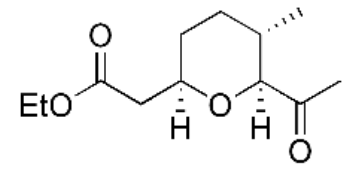
29c

^{1}H NMR (400 MHz, $CDCl_3$)

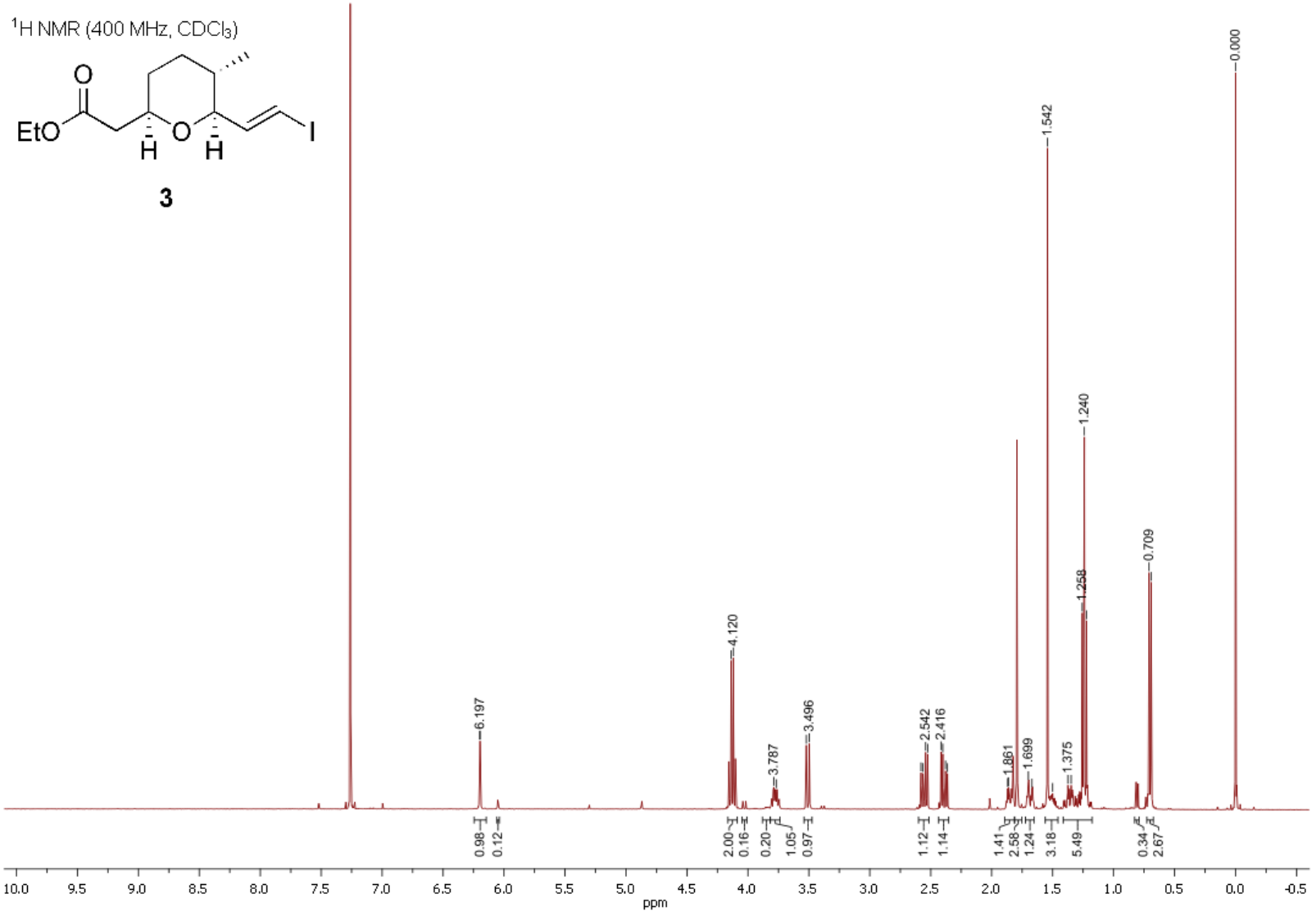


30

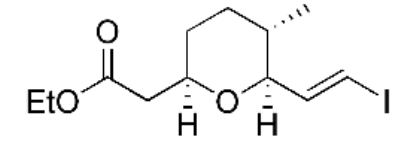
^{13}C NMR (100.6 MHz, $CDCl_3$)



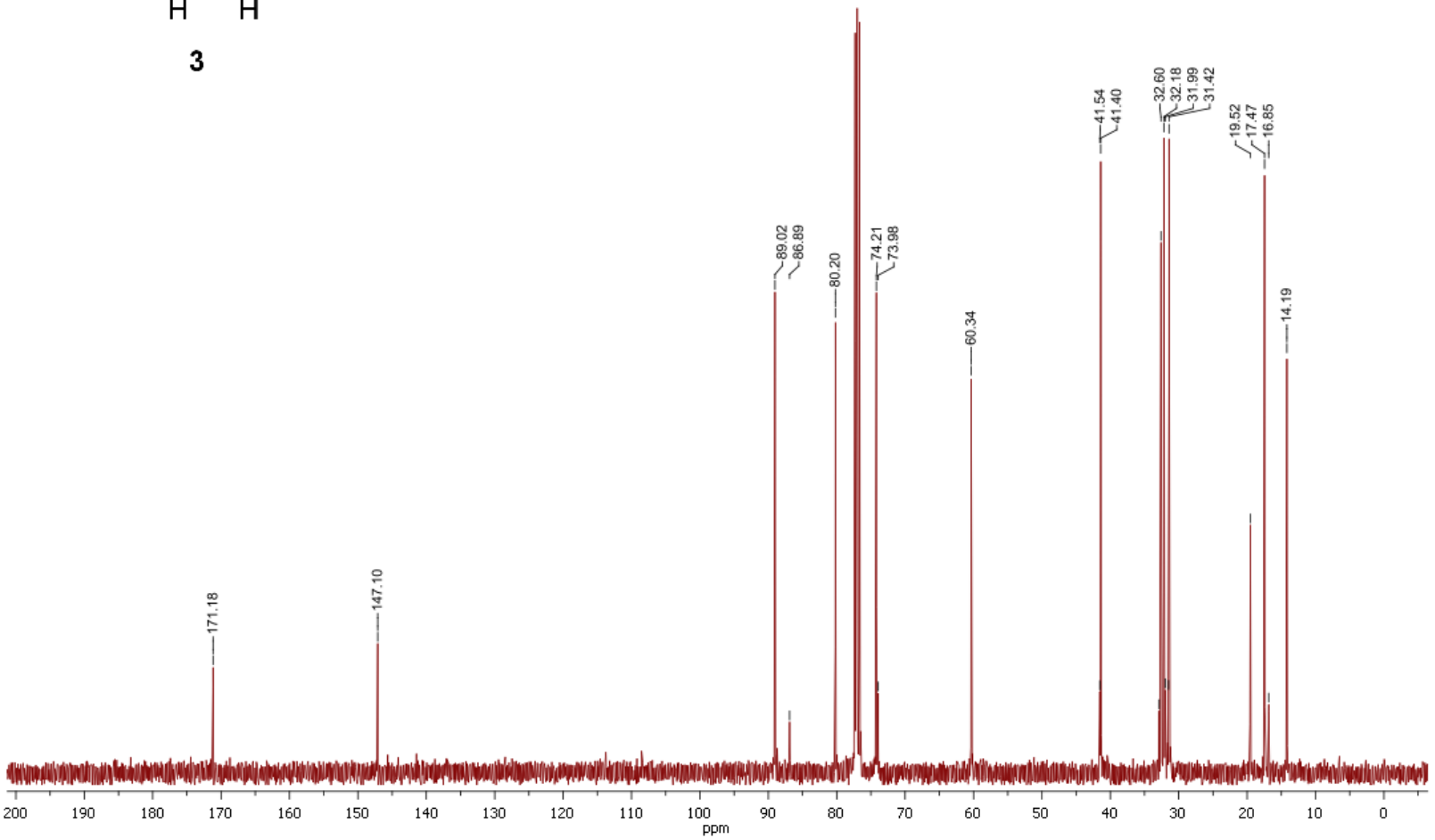
30


^{1}H NMR (400 MHz, $CDCl_3$)
EtO
O
H
O
H
I
3
0.000
1.542
1.240
1.258
0.709
4.120
6.197
3.496
3.787
2.542
2.416
1.861
1.699
1.375
0.98
0.12
2.00
0.16
0.20
1.05
0.97
1.12
1.14
1.41
2.58
1.24
3.18
5.49
0.34
2.67
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
ppm

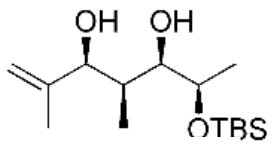
^{13}C NMR (100.6 MHz, $CDCl_3$)



3

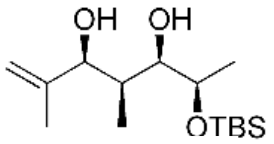


^{1}H NMR (400 MHz, $CDCl_3$)



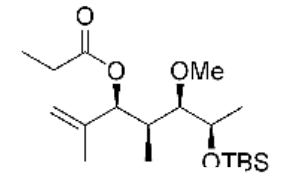
32

^{13}C NMR (100.6 MHz, $CDCl_3$)



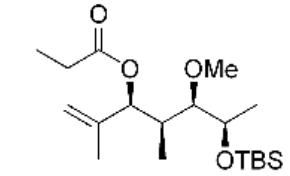
32

^{1}H NMR (400 MHz, $CDCl_3$)



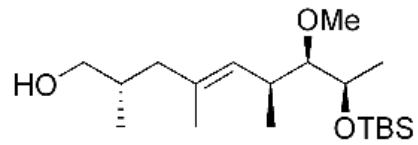
35

^{13}C NMR (100.6 MHz, $CDCl_3$)



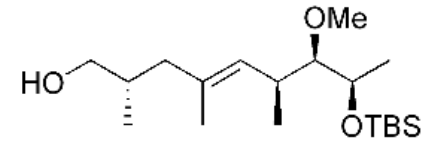
35

^{1}H NMR (400 MHz, $CDCl_3$)



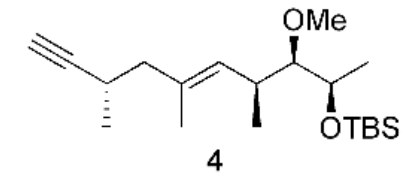
38

^{13}C NMR (100.6 MHz, $CDCl_3$)



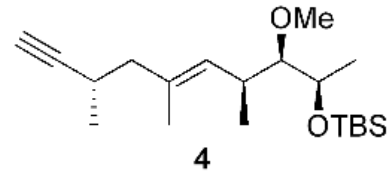
38

^{1}H NMR (400 MHz, $CDCl_3$)



4

^{13}C NMR (100.6 MHz, $CDCl_3$)



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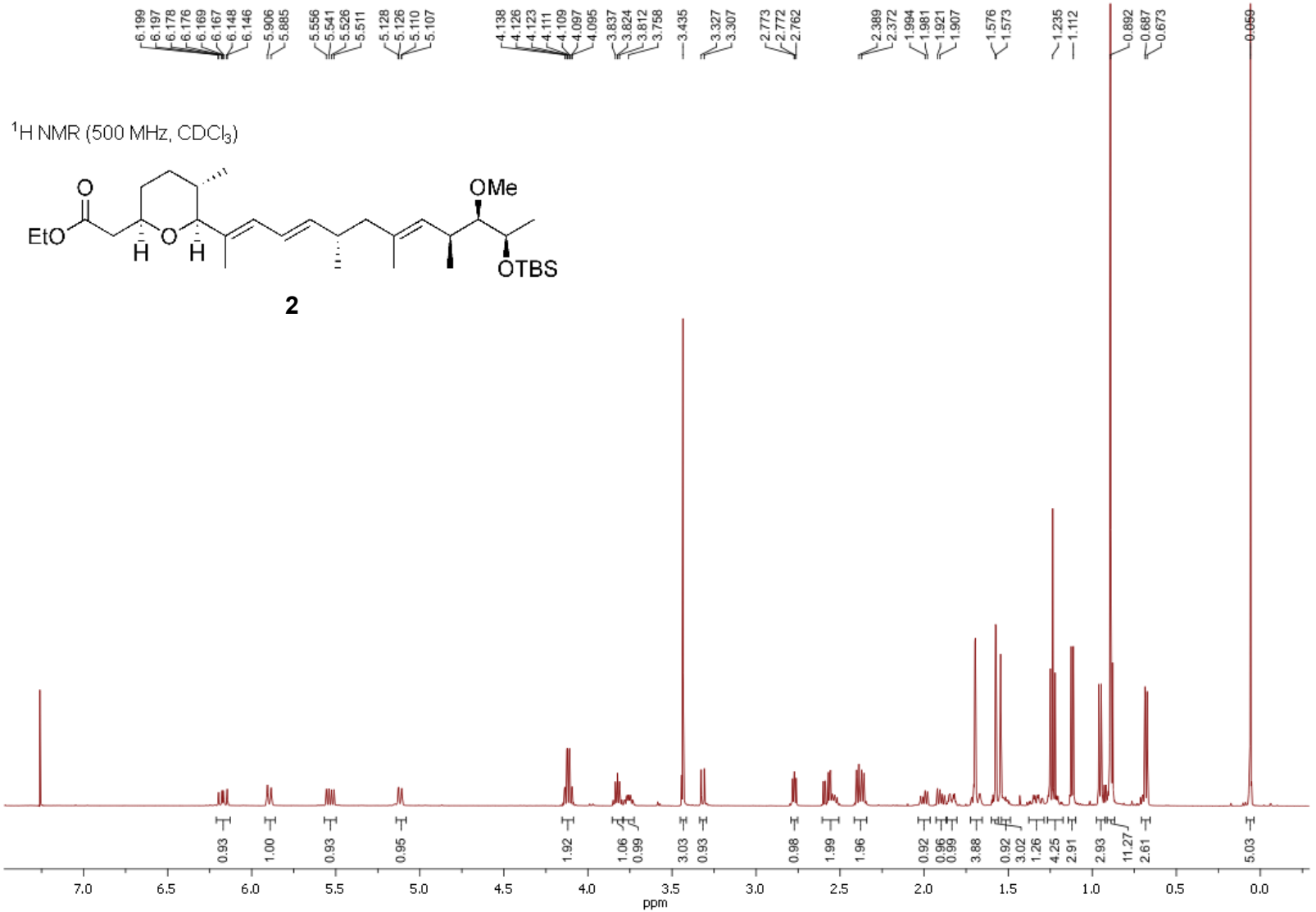
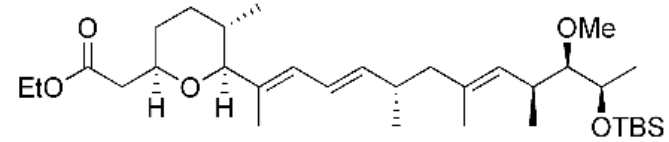
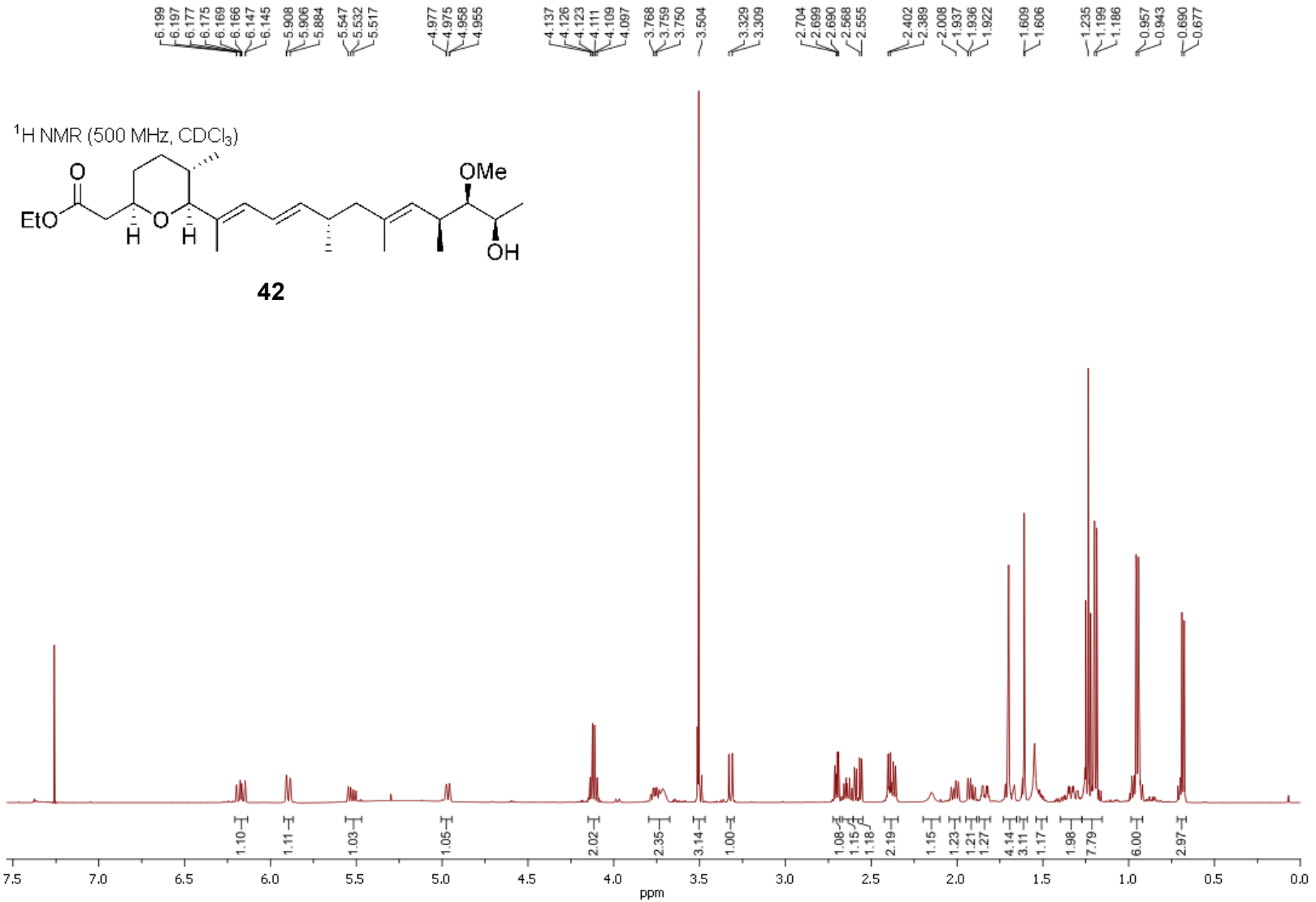

6.199
6.197
6.178
6.176
6.169
6.167
6.148
6.146
5.906
5.885
5.556
5.541
5.526
5.511
5.128
5.126
5.110
5.107
4.138
4.126
4.123
4.111
4.109
4.097
4.095
3.837
3.824
3.812
3.758
3.435
3.327
3.307
2.773
2.772
2.762
2.389
2.372
1.994
1.981
1.921
1.907
1.576
1.573
1.235
1.112
0.892
0.687
0.673
0.050
^{1}H NMR (500 MHz, $CDCl_3$)
O
EtO
H
O
H
OMe
OTBS
2
0.93
1.00
0.93
0.95
1.92
1.06
0.99
3.03
0.93
0.98
1.99
1.96
0.92
0.96
0.99
3.88
0.92
3.02
1.26
4.25
2.91
2.93
11.27
2.61
5.03
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
ppm

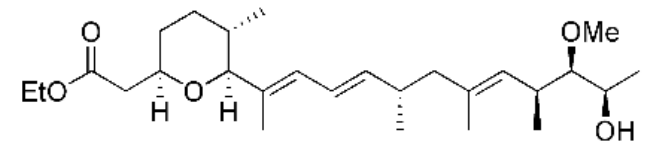
^{13}C NMR (100.6 MHz, $CDCl_3$)



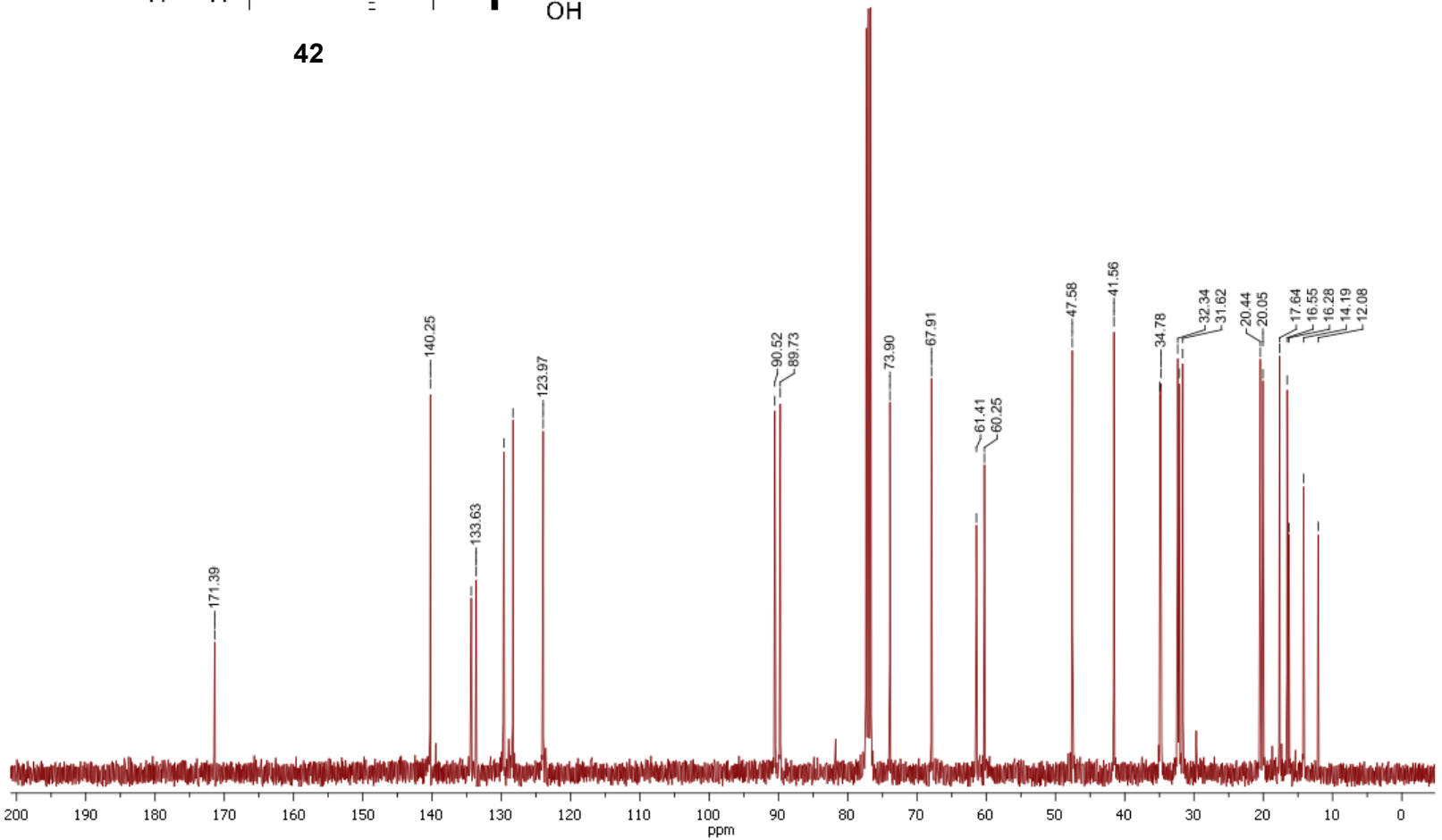
2

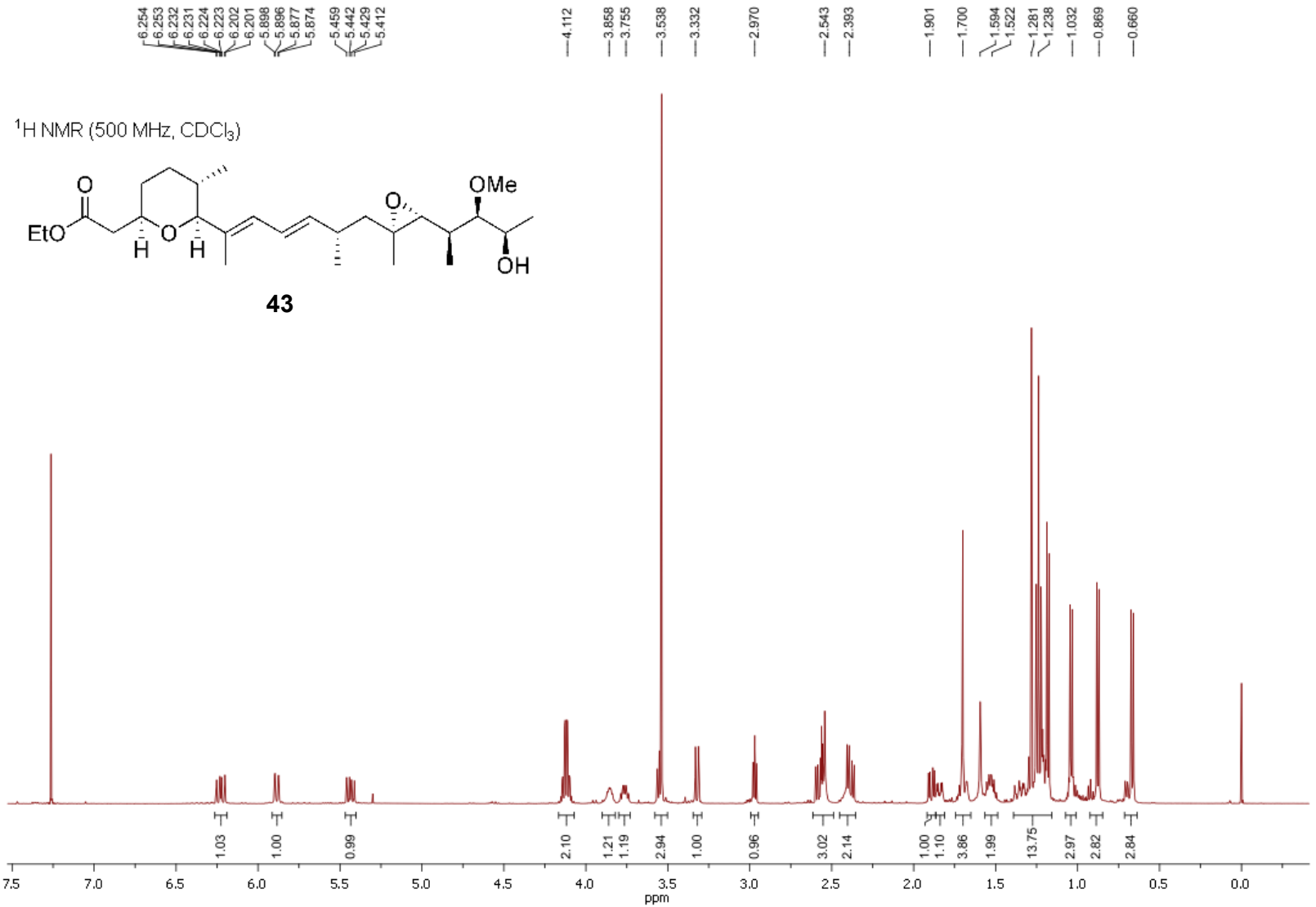

6.199
6.197
6.177
6.175
6.169
6.166
6.147
6.145
5.908
5.906
5.884
5.547
5.532
5.517
4.977
4.975
4.958
4.955
4.137
4.126
4.123
4.111
4.109
4.097
3.768
3.759
3.750
3.504
3.329
3.309
2.704
2.699
2.690
2.568
2.555
2.402
2.389
2.008
1.937
1.936
1.922
1.609
1.606
1.235
1.199
1.186
0.957
0.943
0.690
0.677
1H NMR (500 MHz, CDCl3)
O
EtO
H
O
H
OMe
OH
42
1.10
1.11
1.03
1.05
2.02
2.35
3.14
1.00
1.08
1.15
1.18
2.19
1.15
1.23
1.21
1.27
4.14
3.11
1.17
1.98
7.79
6.00
2.97
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
ppm

^{13}C NMR (100.6 MHz, $CDCl_3$)

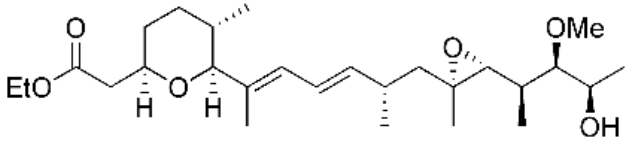


42

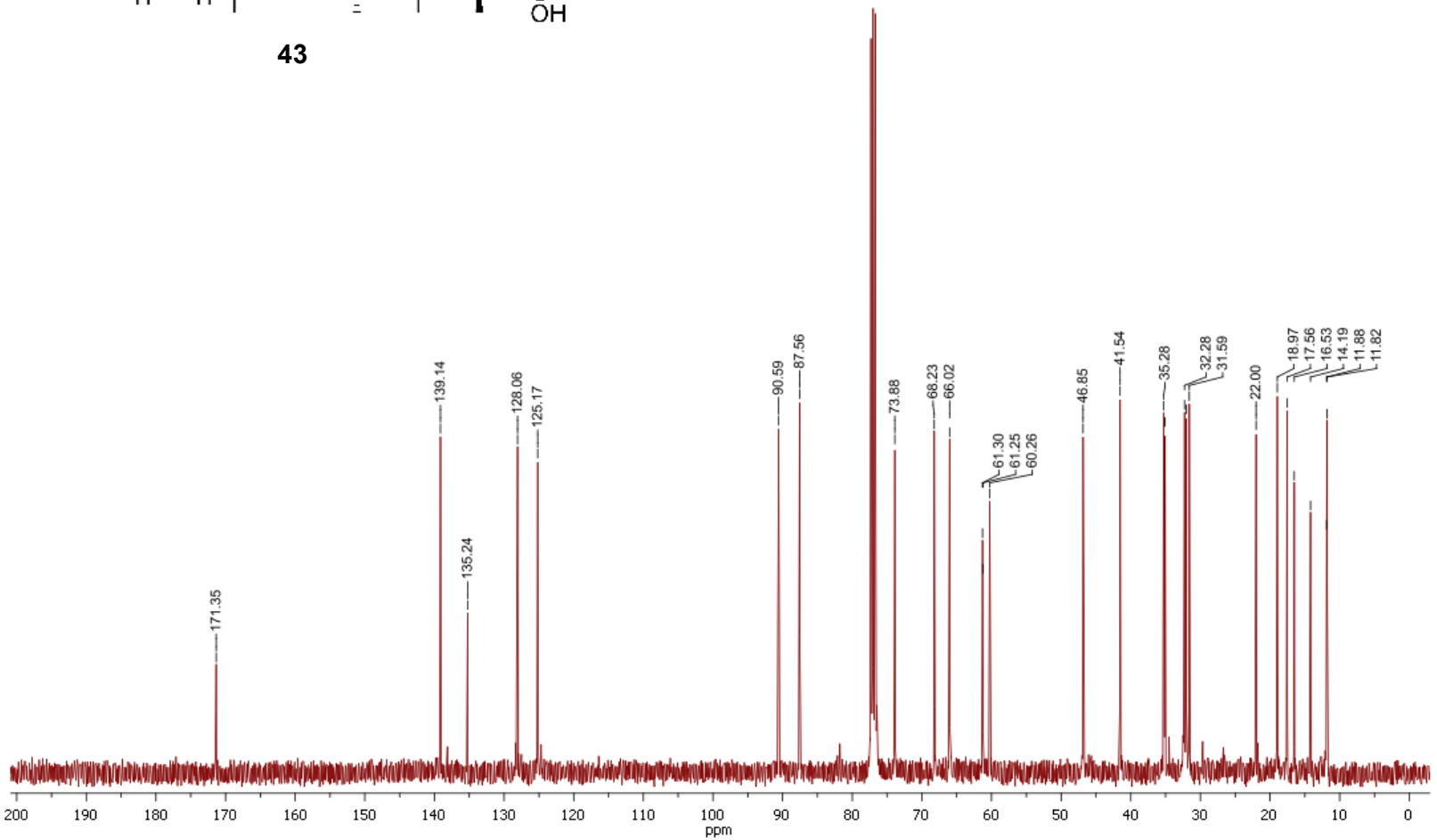


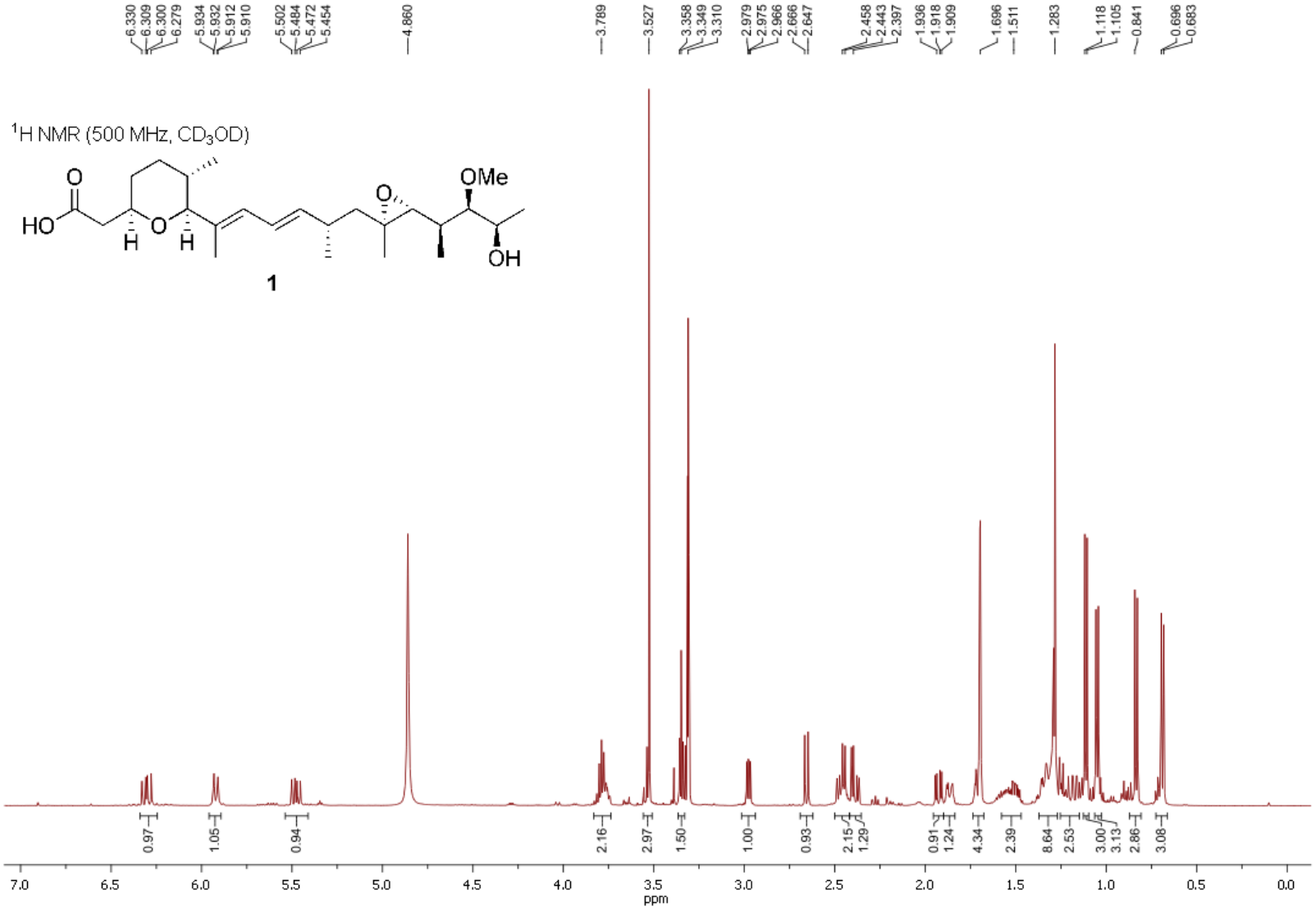

6.254
6.253
6.232
6.231
6.224
6.223
6.202
6.201
5.898
5.896
5.877
5.874
5.459
5.442
5.429
5.412
4.112
3.858
3.755
3.538
3.332
2.970
2.543
2.393
1.901
1.700
1.594
1.522
1.281
1.238
1.032
0.869
0.660
1H NMR (500 MHz, CDCl3)
O
EtO
H
O
H
O
OMe
OH
43
1.03
1.00
0.99
2.10
1.21
1.19
2.94
1.00
0.96
3.02
2.14
1.00
1.10
3.86
1.99
13.75
2.97
2.82
2.84
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
ppm

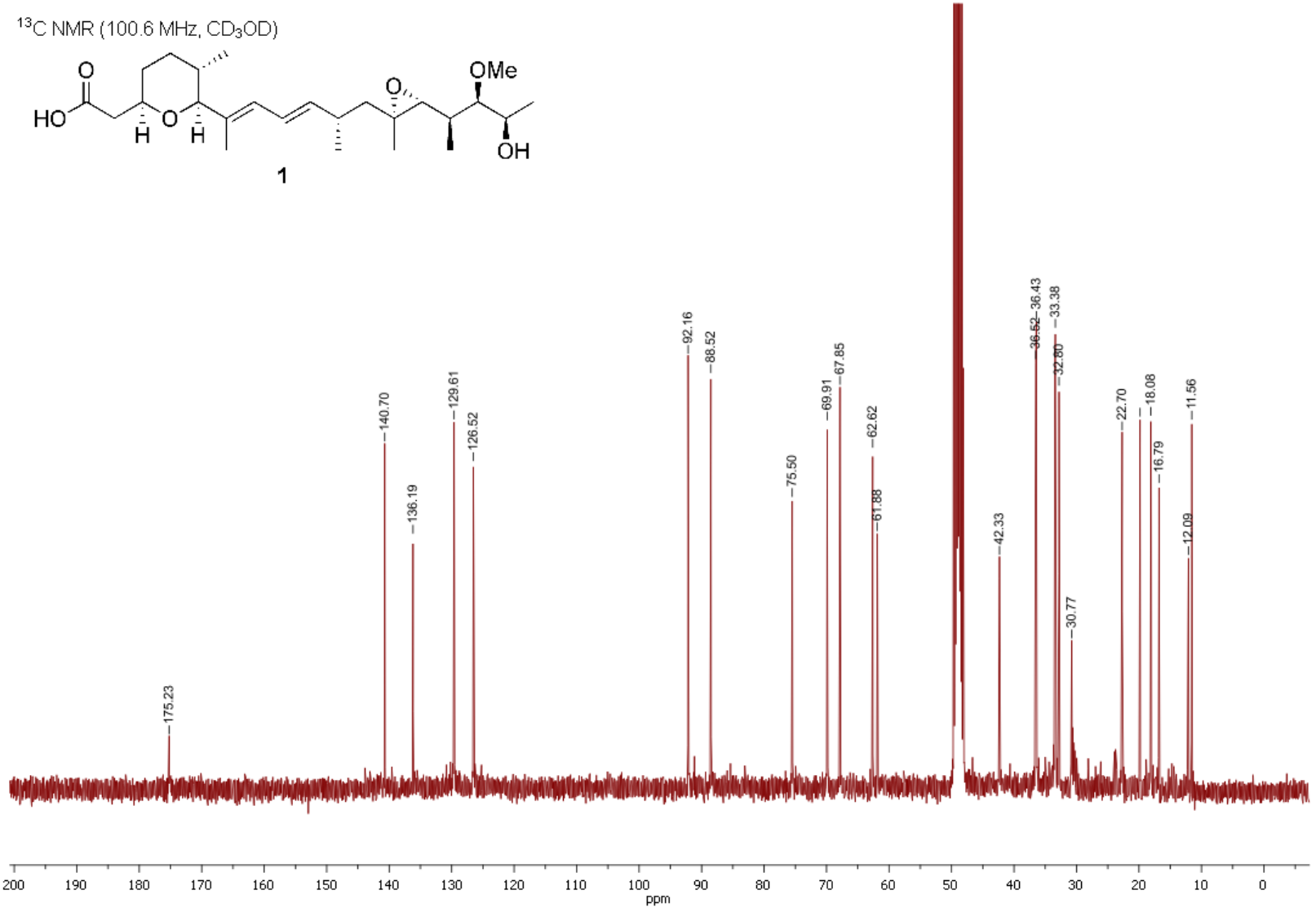
^{13}C NMR (100.6 MHz, $CDCl_3$)



43




6.330
6.309
6.300
6.279
5.934
5.932
5.912
5.910
5.502
5.484
5.472
5.454
4.860
3.789
3.527
3.358
3.349
3.310
2.979
2.975
2.966
2.666
2.647
2.458
2.443
2.397
1.936
1.918
1.909
1.696
1.511
1.283
1.118
1.105
0.841
0.696
0.683
^{1}H NMR (500 MHz, CD$_3$OD)
HO
O
H
O
H
O
OMe
OH
1
0.97
1.05
0.94
2.16
2.97
1.50
1.00
0.93
2.15
1.29
0.91
1.24
4.34
2.39
8.64
2.53
3.00
3.13
2.86
3.08
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
ppm


^{13}C NMR (100.6 MHz, CD_3OD)
HO
O
H
O
H
O
OMe
OH
1
175.23
140.70
136.19
129.61
126.52
92.16
88.52
75.50
69.91
67.85
62.62
61.88
42.33
36.52
36.43
33.38
32.80
30.77
22.70
18.08
16.79
12.09
11.56
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
ppm

2. Theoretical Calculations: Tables of Atom Coordinates and Absolute Energies

Table S1. Electronic energies (in Hartrees) for optimized minima (in Hartrees), and relative energies (in kcal/mol) for compouns **I** and **II**. The energy of conformer ***cis*-I** *chair* is taken as zero for each one.

Compounds	E_{el}/Ha	E_{rel}/kcal mol^{-1}
***cis*-I** *chair*	-731.7543468	0.00
***cis*-I** *boat*	-731.7577363	-2.13
***trans*-I** *chair*	-731.7567384	-1.50
***trans*-I** *boat*	-731.7557879	-0.90
***cis*-II** *chair*	-656.5100739	0.00
***cis*-II** *boat*	-656.5007855	+5.83
***trans*-II** *chair*	-656.5088965	+0.74
***trans*-II** *boat*	-656.5028187	+4.55

Table S2. Cartesian coordinates (in Å) for optimized minima shown in Table S1.

a) ***cis*-I** *chair*

O	-0.113571	1.956978	1.405351
C	0.082854	1.521453	2.733270
H	-0.691783	0.773118	2.991665
C	-0.106874	2.741592	3.631704
H	0.677000	3.481012	3.437782
H	-1.070131	3.204214	3.406178
H	-0.086162	2.477571	4.693207
C	1.463910	0.842330	2.900746
H	2.219659	1.599002	2.642877
C	1.725101	0.336100	4.324951
H	1.815944	1.157983	5.040360
H	0.907360	-0.311963	4.663160
H	2.647993	-0.247686	4.356903
C	1.586617	-0.298705	1.878158
H	0.929939	-1.117849	2.196185
O	2.910751	-0.884574	1.896372
H	3.466573	-0.330751	1.337695
C	1.192543	0.140371	0.470603
H	1.947384	0.842934	0.086168
H	1.184038	-0.728846	-0.192947
C	-0.175815	0.841003	0.408138
H	-0.959588	0.163928	0.775356
C	-0.546971	1.315877	-0.926621
H	0.191397	1.813827	-1.544551
C	-1.852269	1.200626	-1.388712
O	-2.859608	0.693948	-0.860935
O	-2.001543	1.755448	-2.705173
C	-3.291455	1.639514	-3.271749
H	-3.582271	0.584580	-3.363260
H	-4.042356	2.112892	-2.626952
C	-3.258261	2.306724	-4.640677
H	-2.522058	1.823308	-5.289957
H	-2.984927	3.362237	-4.549611
H	-4.240518	2.243604	-5.123786

b) ***cis*-I** *boat*

O	-1.018336	0.608136	0.707255
C	-2.223005	1.106344	0.149442
H	-1.977443	1.594425	-0.809581
C	-2.783194	2.164151	1.094644
H	-3.697935	2.607121	0.683373
H	-3.023861	1.720069	2.065246
H	-2.047668	2.957415	1.249027
C	-3.238126	-0.051538	-0.136722
H	-4.095982	0.056746	0.537753
C	-3.759432	-0.026853	-1.579437
H	-4.489792	-0.825118	-1.753823
H	-4.251835	0.926199	-1.801546
H	-2.946182	-0.149405	-2.301260
C	-2.576770	-1.395286	0.232343
H	-3.236142	-2.217317	-0.068682
O	-2.472709	-1.509176	1.660897
H	-1.808374	-0.842368	1.901892
C	-1.197058	-1.565972	-0.423496
H	-0.708873	-2.419697	0.054266
H	-1.313663	-1.822124	-1.483311
C	-0.300395	-0.309221	-0.294609
H	-0.323431	0.284132	-1.216398
C	1.081348	-0.579002	0.073919
H	1.312869	-1.394122	0.749172
C	2.118334	0.224192	-0.398800
O	2.096491	1.196938	-1.171512
O	3.390580	-0.203671	0.098850
C	4.506720	0.527784	-0.370862
H	4.589433	0.448984	-1.462929
H	4.391838	1.594690	-0.144151
C	5.749090	-0.038694	0.303515
H	5.870602	-1.099458	0.064620
H	5.675217	0.055198	1.390959
H	6.645785	0.496399	-0.030456

c) ***trans*-I** *chair*

O	0.064516	1.783129	1.095430
C	0.020090	1.380874	2.446021
H	-0.732609	0.582054	2.556686
C	-0.429413	2.594071	3.256400
H	0.314964	3.395619	3.194021
H	-1.367810	2.970928	2.843422
H	-0.588822	2.345347	4.309944
C	1.391892	0.816622	2.898795
H	2.117220	1.641277	2.812160
C	1.384338	0.305945	4.345722
H	1.242784	1.117477	5.064902
H	0.573969	-0.417459	4.494324
H	2.326935	-0.195035	4.578791
C	1.849203	-0.288527	1.928688
H	1.246484	-1.185056	2.101108
O	3.201661	-0.715233	2.224961
H	3.789237	-0.038845	1.870281
C	1.715251	0.143970	0.471297
H	2.425440	0.966718	0.293096
H	1.985798	-0.688016	-0.184566
C	0.290583	0.634949	0.146296
H	0.278950	1.152989	-0.813546
C	-0.739431	-0.417247	0.138749
H	-0.687582	-1.260490	0.816303
C	-1.773613	-0.393306	-0.793123
O	-2.031275	0.417022	-1.699138
O	-2.645399	-1.525307	-0.645297
C	-3.695846	-1.612227	-1.588036
H	-4.309562	-0.703334	-1.568504
H	-3.296163	-1.695016	-2.607590
C	-4.531502	-2.836982	-1.239513
H	-4.946470	-2.747431	-0.231149
H	-3.921787	-3.744875	-1.273199
H	-5.361431	-2.950804	-1.946838

d) ***trans*-I** *boat*

O	-1.039992	-0.099459	1.064462
C	-1.735499	0.709840	0.137280
H	-1.154868	0.738675	-0.799284
C	-1.815044	2.126330	0.695003
H	-2.371432	2.786547	0.019229
H	-2.319924	2.122661	1.666612
H	-0.810198	2.532567	0.832461
C	-3.134193	0.092719	-0.160401
H	-3.868029	0.532131	0.527416
C	-3.596487	0.367190	-1.596632
H	-4.608171	-0.016220	-1.769650
H	-3.608920	1.441506	-1.809467
H	-2.929214	-0.101672	-2.327076
C	-3.087097	-1.417573	0.175726
H	-3.928092	-1.925153	-0.310226
O	-3.291538	-1.625202	1.581421
H	-2.547615	-1.158965	1.996333
C	-1.761348	-2.033960	-0.290462
H	-1.772785	-3.112932	-0.110162
H	-1.671396	-1.898000	-1.374717
C	-0.530309	-1.411405	0.410287
H	-0.271553	-1.958040	1.317835
C	0.636924	-1.272146	-0.452524
H	0.514268	-1.105712	-1.516548
C	1.933840	-1.357318	0.057712
O	2.335194	-1.576038	1.210163
O	2.916975	-1.176594	-0.969342
C	4.263161	-1.312694	-0.554697
H	4.478307	-0.638020	0.282248
H	4.454508	-2.331083	-0.190495
C	5.151667	-0.995853	-1.750152
H	4.975891	0.025072	-2.101890
H	4.944826	-1.678415	-2.579859
H	6.209544	-1.091386	-1.478905

e) ***cis*-II** *chair*

O	-0.085885	1.946077	1.398232
C	0.117354	1.504429	2.724492
H	-0.655662	0.753481	2.982966
C	-0.068407	2.722487	3.627341
H	0.716812	3.460914	3.434287
H	-1.031087	3.188565	3.405966
H	-0.045884	2.454556	4.688320
C	1.495804	0.820986	2.875946
H	2.249200	1.584844	2.635537
C	1.761253	0.294579	4.292248
H	1.812119	1.098245	5.032591
H	0.971461	-0.399064	4.604760
H	2.710458	-0.251753	4.331143
C	1.608838	-0.309052	1.839841
H	0.939291	-1.126910	2.145087
H	2.626680	-0.723399	1.854046
C	1.223328	0.147137	0.426648
H	1.972611	0.849117	0.038523
H	1.202996	-0.709983	-0.253982
C	-0.147132	0.838513	0.385710
H	-0.921567	0.151366	0.755298
C	-0.542098	1.333370	-0.936562
H	0.184249	1.848006	-1.555283
C	-1.846386	1.201307	-1.393295
O	-2.846326	0.675351	-0.868572
O	-2.009453	1.763745	-2.708754
C	-3.308394	1.664903	-3.254961
H	-3.633958	0.617631	-3.298344
H	-4.037385	2.189332	-2.622950
C	-3.272596	2.274853	-4.650613
H	-2.562132	1.740013	-5.288236
H	-2.962238	3.323208	-4.607257
H	-4.263163	2.225846	-5.118470

f) ***cis*-II** *boat*

O	-1.068515	0.593007	0.813149
C	-2.258465	1.120390	0.265586
H	-1.997106	1.747340	-0.606324
C	-2.887887	2.016105	1.329064
H	-3.779209	2.521146	0.938576
H	-3.179189	1.422542	2.202000
H	-2.169007	2.771763	1.655191
C	-3.240959	-0.002913	-0.223242
H	-4.207174	0.148894	0.276980
C	-3.498678	0.065511	-1.735542
H	-4.217146	-0.700645	-2.050055
H	-3.906487	1.041860	-2.020903
H	-2.577342	-0.081706	-2.305871
C	-2.691067	-1.369307	0.220778
H	-3.346788	-2.172762	-0.141338
H	-2.723425	-1.407016	1.313976
C	-1.235658	-1.602111	-0.233727
H	-0.783700	-2.373620	0.398155
H	-1.201977	-1.987250	-1.259416
C	-0.372140	-0.320017	-0.160140
H	-0.411420	0.221732	-1.114426
C	1.031632	-0.557033	0.181145
H	1.284896	-1.294950	0.933716
C	2.049618	0.189719	-0.400477
O	2.010688	1.078306	-1.271225
O	3.341372	-0.183249	0.110603
C	4.447838	0.421934	-0.526451
H	4.543906	0.062514	-1.561939
H	4.312186	1.507436	-0.586020
C	5.696266	0.070051	0.272574
H	5.833212	-1.014435	0.323483
H	5.616004	0.447503	1.296308
H	6.587420	0.509958	-0.190886

g) ***trans*-II** *chair*

O	0.059539	1.789098	1.142516
C	0.027690	1.381169	2.493901
H	-0.715921	0.573180	2.606512
C	-0.432523	2.589084	3.306650
H	0.304516	3.397540	3.243525
H	-1.375174	2.958501	2.896245
H	-0.587586	2.337963	4.360741
C	1.407748	0.830296	2.929423
H	2.118301	1.666232	2.844021
C	1.423756	0.316977	4.375114
H	1.242924	1.113995	5.102327
H	0.655910	-0.451429	4.523126
H	2.392292	-0.136262	4.616320
C	1.854473	-0.272498	1.951877
H	1.237235	-1.164883	2.115292
H	2.888892	-0.565248	2.179403
C	1.727635	0.172688	0.489474
H	2.431290	0.996067	0.306147
H	1.991535	-0.648699	-0.184305
C	0.299234	0.654015	0.175617
H	0.277201	1.185996	-0.776408
C	-0.727496	-0.403324	0.155137
H	-0.691761	-1.234271	0.848918
C	-1.742931	-0.394843	-0.794856
O	-1.986953	0.396537	-1.722250
O	-2.622721	-1.525496	-0.638581
C	-3.605163	-1.675965	-1.642968
H	-4.158880	-0.741117	-1.784770
H	-3.138267	-1.910815	-2.610990
C	-4.537735	-2.803289	-1.218562
H	-5.023844	-2.563060	-0.268258
H	-3.984040	-3.737885	-1.086517
H	-5.315176	-2.965655	-1.974622

h) ***trans*-II** *boat*

O	-1.033889	-0.057631	0.976684
C	-1.822934	0.706214	0.098815
H	-1.325639	0.759101	-0.885801
C	-1.915880	2.122992	0.657968
H	-2.553427	2.759657	0.033314
H	-2.333535	2.097908	1.669914
H	-0.920370	2.569736	0.711727
C	-3.218652	0.041407	-0.092200
H	-3.885199	0.427219	0.691500
C	-3.835185	0.394636	-1.452952
H	-4.855179	0.003677	-1.541024
H	-3.880797	1.478515	-1.605355
H	-3.244392	-0.027017	-2.273212
C	-3.069595	-1.486458	0.104542
H	-3.895961	-2.010949	-0.394062
H	-3.141806	-1.721010	1.171163
C	-1.713613	-1.978010	-0.418136
H	-1.638751	-3.067633	-0.343673
H	-1.622759	-1.742096	-1.485539
C	-0.524710	-1.348162	0.344604
H	-0.304044	-1.920470	1.248078
C	0.684166	-1.214542	-0.474717
H	0.600754	-0.980650	-1.530492
C	1.956443	-1.376500	0.066665
O	2.320031	-1.675250	1.216387
O	2.981749	-1.175142	-0.923157
C	4.304478	-1.413400	-0.486335
H	4.524949	-0.829816	0.415210
H	4.439376	-2.469578	-0.213014
C	5.245092	-1.033630	-1.622795
H	5.127991	0.022639	-1.882939
H	5.032459	-1.626114	-2.517875
H	6.288627	-1.205842	-1.333494

Table S3. Electronic energies (in Hartrees) for stationary points (in Hartrees) involved in the cyclation of compound **I**. Rlative energies (in kcal/mol) are also shown, as Table S1.

Compounds	E_{el}/Ha	E_{rel}/kcal mol^{-1}
*alkoxyde **A***	-731.7526749	+1.05
TS$_A$	-731.7489385	+3.39
***cis*-I** *boat*	-731.7577363	-2.13
*alkoxyde **B***	-731.7589304	-2.88
TS$_B$	-731.7512865	+1.91
***trans*-I** *boat*	-731.7557879	-0.90

Table S4. Cartesian coordinates (in Å) for stationary points (reactant alkoxydes and transition states) shown in Table S3.

a) *alkoxyde **A***

O	-0.156527	2.131528	2.122250
C	0.217663	1.053426	2.873320
H	-0.397938	0.141737	2.635598
C	-0.007398	1.302126	4.385017
H	0.220638	0.425786	5.008662
H	0.612921	2.144627	4.712903
H	-1.054887	1.575935	4.542073
C	1.704798	0.637754	2.599745
H	2.337706	1.350759	3.147567
C	2.053549	-0.775856	3.082340
H	3.078373	-1.055493	2.804158
H	1.977043	-0.853835	4.171123
H	1.377540	-1.527179	2.658190
C	2.086144	0.874342	1.115275
H	3.148879	0.599641	1.005830
O	1.955523	2.235504	0.794114
H	1.048375	2.444801	1.250909
C	1.345916	-0.022884	0.069482
H	1.911298	0.050983	-0.865899
H	1.410879	-1.068979	0.402365
C	-0.089781	0.291673	-0.216457
H	-0.812037	0.194266	0.585583
C	-0.525048	0.664393	-1.431662
H	0.168528	0.838652	-2.247175
C	-1.939462	0.900393	-1.722646
O	-2.901328	0.655107	-1.026326
O	-2.086355	1.453254	-2.977423
C	-3.430297	1.753004	-3.375584
H	-4.025169	0.834288	-3.368510
H	-3.878942	2.434952	-2.647690
C	-3.372797	2.371931	-4.760656
H	-2.924125	1.680491	-5.478740
H	-2.778031	3.288639	-4.751379
H	-4.382548	2.618633	-5.103554

b) ***TS$_A$:*** *alkoxyde* ***A*** → ***cis*-I** *boat*

O	-1.076062	0.745955	0.763369
C	-2.240311	1.128889	0.118587
H	-2.003187	1.489458	-0.908890
C	-2.911482	2.304029	0.846100
H	-3.832375	2.623962	0.339287
H	-3.161775	2.012339	1.871549
H	-2.224111	3.153316	0.890660
C	-3.226508	-0.082896	-0.047363
H	-3.986226	-0.024974	0.743371
C	-3.947973	-0.080127	-1.400234
H	-4.662607	-0.908196	-1.481239
H	-4.505384	0.852127	-1.543510
H	-3.240597	-0.164313	-2.232226
C	-2.459309	-1.391113	0.232065
H	-3.117314	-2.244459	0.020032
O	-2.142086	-1.472372	1.620418
H	-1.592767	-0.659669	1.735747
C	-1.178238	-1.568038	-0.612288
H	-0.716453	-2.504184	-0.284042
H	-1.458856	-1.709077	-1.665825
C	-0.144920	-0.453837	-0.540014
H	-0.248923	0.346707	-1.265175
C	1.150063	-0.738982	-0.144969
H	1.364770	-1.613011	0.458578
C	2.235607	0.140380	-0.438532
O	2.249110	1.168599	-1.106142
O	3.433387	-0.326103	0.128809
C	4.585360	0.471504	-0.120953
H	4.765866	0.543820	-1.199637
H	4.419373	1.491748	0.241435
C	5.761613	-0.179630	0.589365
H	5.928543	-1.193825	0.215829
H	5.578437	-0.240669	1.665565
H	6.674402	0.403642	0.426201

c) *alkoxyde* ***B***

O	-2.291565	0.569950	2.251861
C	-2.055672	0.859259	0.887200
H	-1.029191	0.555681	0.608998
C	-2.144219	2.377304	0.709801
H	-1.823414	2.698523	-0.286549
H	-3.171465	2.719417	0.879806
H	-1.501930	2.860232	1.452333
C	-3.044634	0.072630	-0.004232
H	-4.046324	0.375120	0.334190
C	-2.923105	0.410404	-1.496625
H	-3.539954	-0.271031	-2.094706
H	-3.257319	1.429577	-1.716755
H	-1.890750	0.318386	-1.852864
C	-2.997749	-1.476166	0.283119
H	-3.898371	-1.872794	-0.260270
O	-2.996224	-1.771673	1.599394
H	-2.575601	-0.411916	2.234223
C	-1.814259	-2.238884	-0.469604
H	-2.048786	-3.286047	-0.238264
H	-1.853225	-2.121286	-1.560036
C	-0.450031	-1.975357	0.044669
H	-0.353170	-1.945121	1.127691
C	0.646883	-1.799416	-0.717707
H	0.588542	-1.820474	-1.801120
C	1.975484	-1.576738	-0.151205
O	2.301431	-1.542143	1.017121
O	2.905269	-1.408532	-1.157474
C	4.255707	-1.184175	-0.731337
H	4.295002	-0.284871	-0.109575
H	4.583981	-2.022016	-0.108957
C	5.113758	-1.041576	-1.975490
H	4.776782	-0.200474	-2.586604
H	5.068726	-1.947312	-2.585754
H	6.156795	-0.867085	-1.693574

d) ***TS*$_B$:** *alkoxyde* ***B*** **→** ***trans*-I** *boat*

O	-1.090173	0.010263	1.206054
C	-1.729596	0.749604	0.226971
H	-1.121675	0.745465	-0.705900
C	-1.870747	2.219310	0.652460
H	-2.369786	2.825929	-0.115625
H	-2.450672	2.284182	1.579736
H	-0.880698	2.643516	0.841173
C	-3.113504	0.111710	-0.126981
H	-3.873490	0.534378	0.544467
C	-3.551068	0.379760	-1.572197
H	-4.542050	-0.042329	-1.779077
H	-3.602118	1.454867	-1.774665
H	-2.846913	-0.050739	-2.292269
C	-3.058136	-1.394239	0.220162
H	-3.939897	-1.893624	-0.202614
O	-3.140862	-1.570817	1.633501
H	-2.387546	-1.008821	1.935225
C	-1.797440	-2.082472	-0.342111
H	-1.921265	-3.165884	-0.214234
H	-1.737521	-1.903184	-1.422513
C	-0.480989	-1.697401	0.306412
H	-0.311831	-2.070731	1.308207
C	0.636530	-1.512185	-0.487255
H	0.535105	-1.286526	-1.542766
C	1.963186	-1.537856	0.043474
O	2.346586	-1.790430	1.178486
O	2.909236	-1.250253	-0.955198
C	4.271029	-1.277178	-0.541148
H	4.426098	-0.569344	0.280144
H	4.526688	-2.270834	-0.155760
C	5.127564	-0.918891	-1.745259
H	4.874086	0.077161	-2.118327
H	4.974767	-1.634482	-2.558023
H	6.188501	-0.926524	-1.472847