BEILSTEIN JOURNAL OF ORGANIC CHEMISTRY

Supporting Information

for

Influence of per-O-sulfation upon the conformational behaviour of common furanosides

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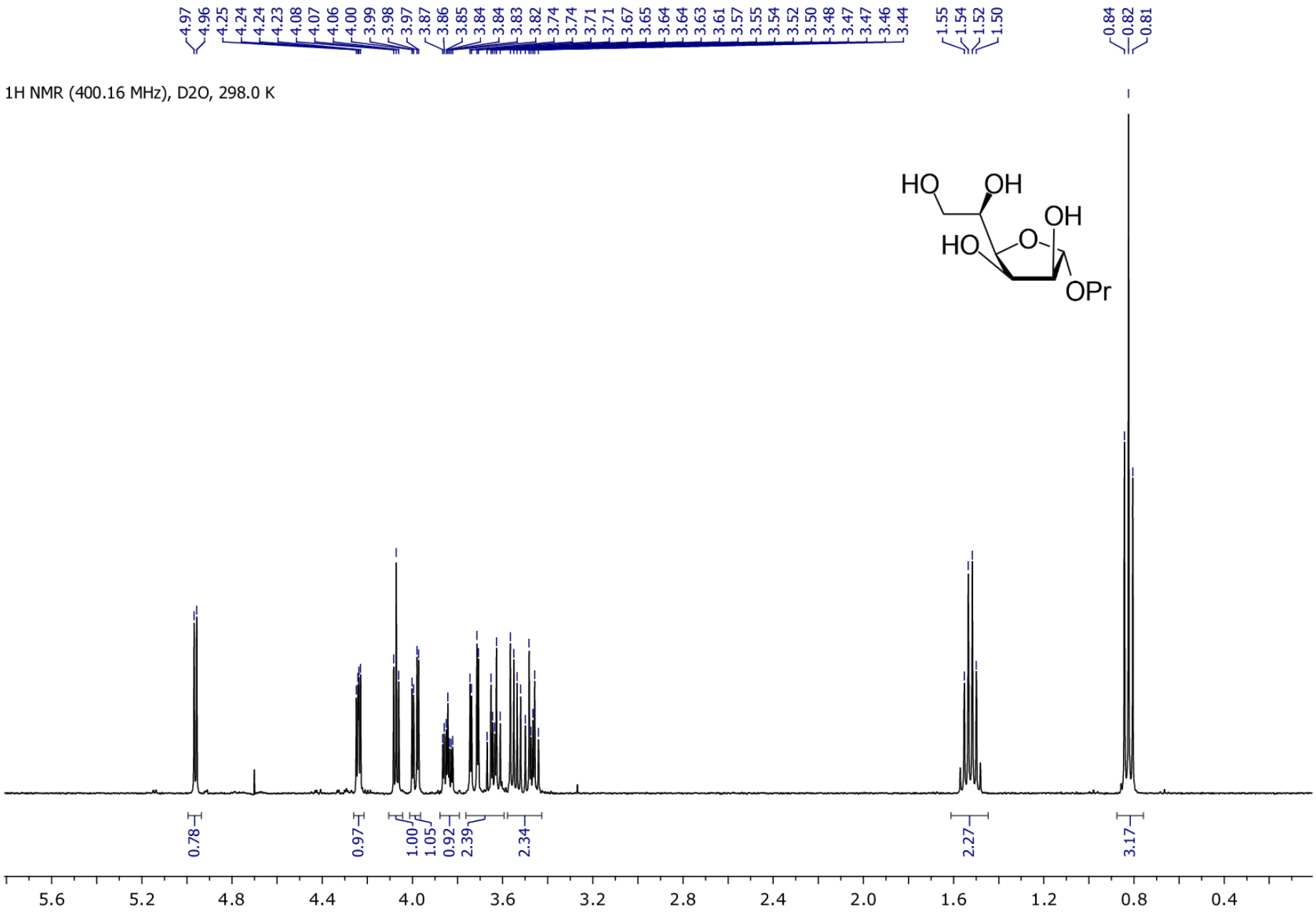
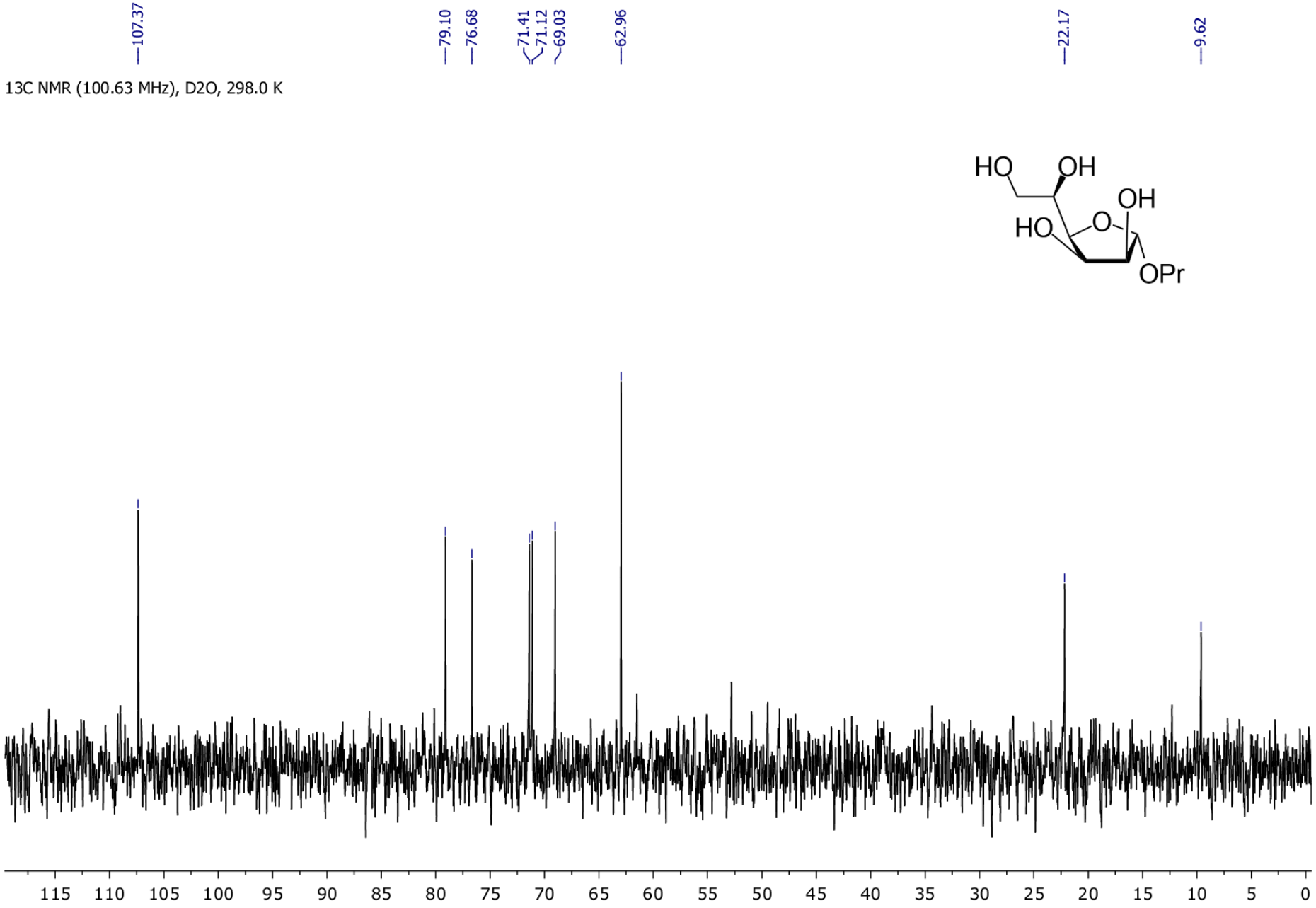
Copies of ^{1}H and ^{13}C NMR spectra of compounds 1–3 and 1s–3s and computational details for all found conformers

Propyl α-D-mannofuranoside (1)

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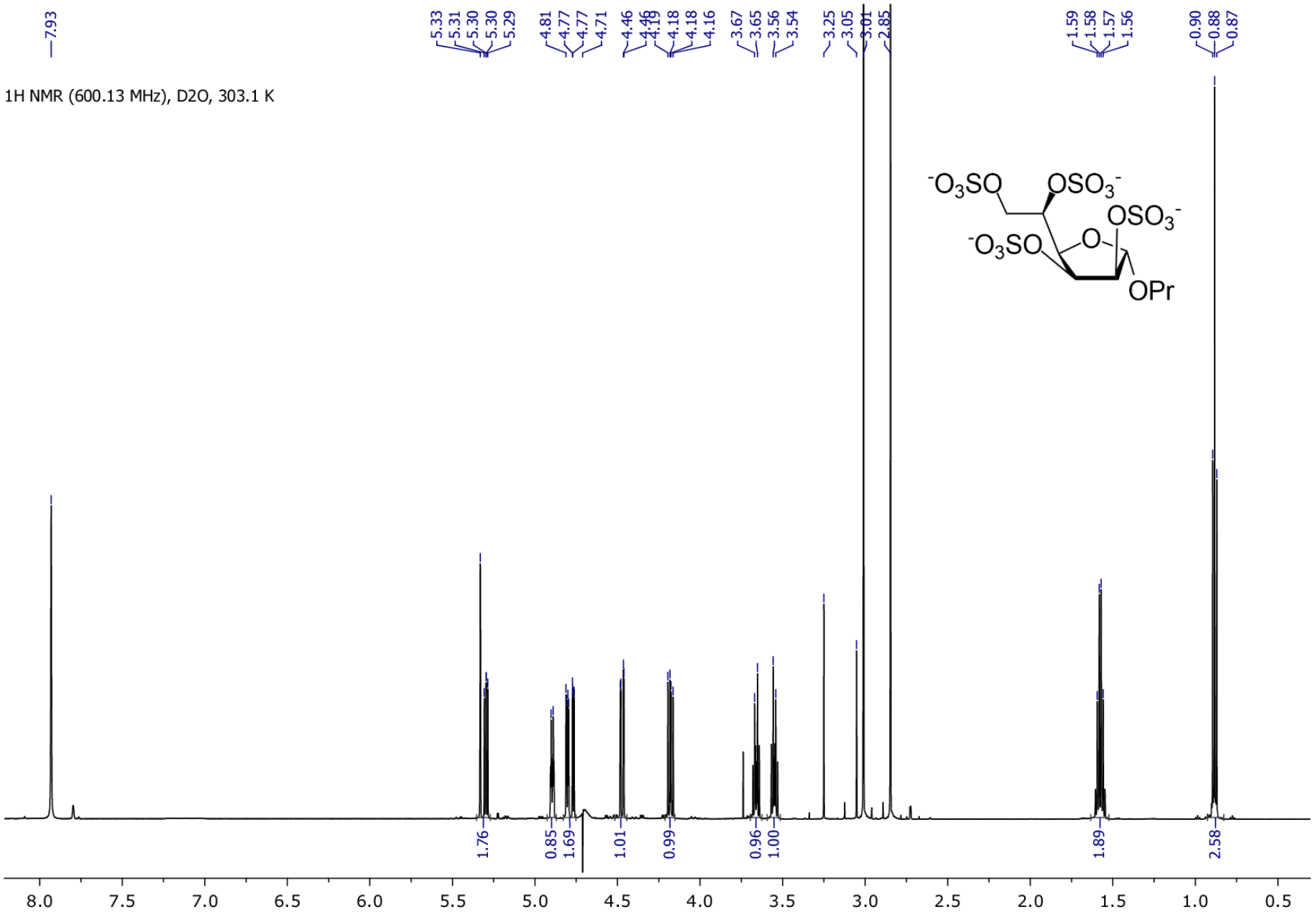
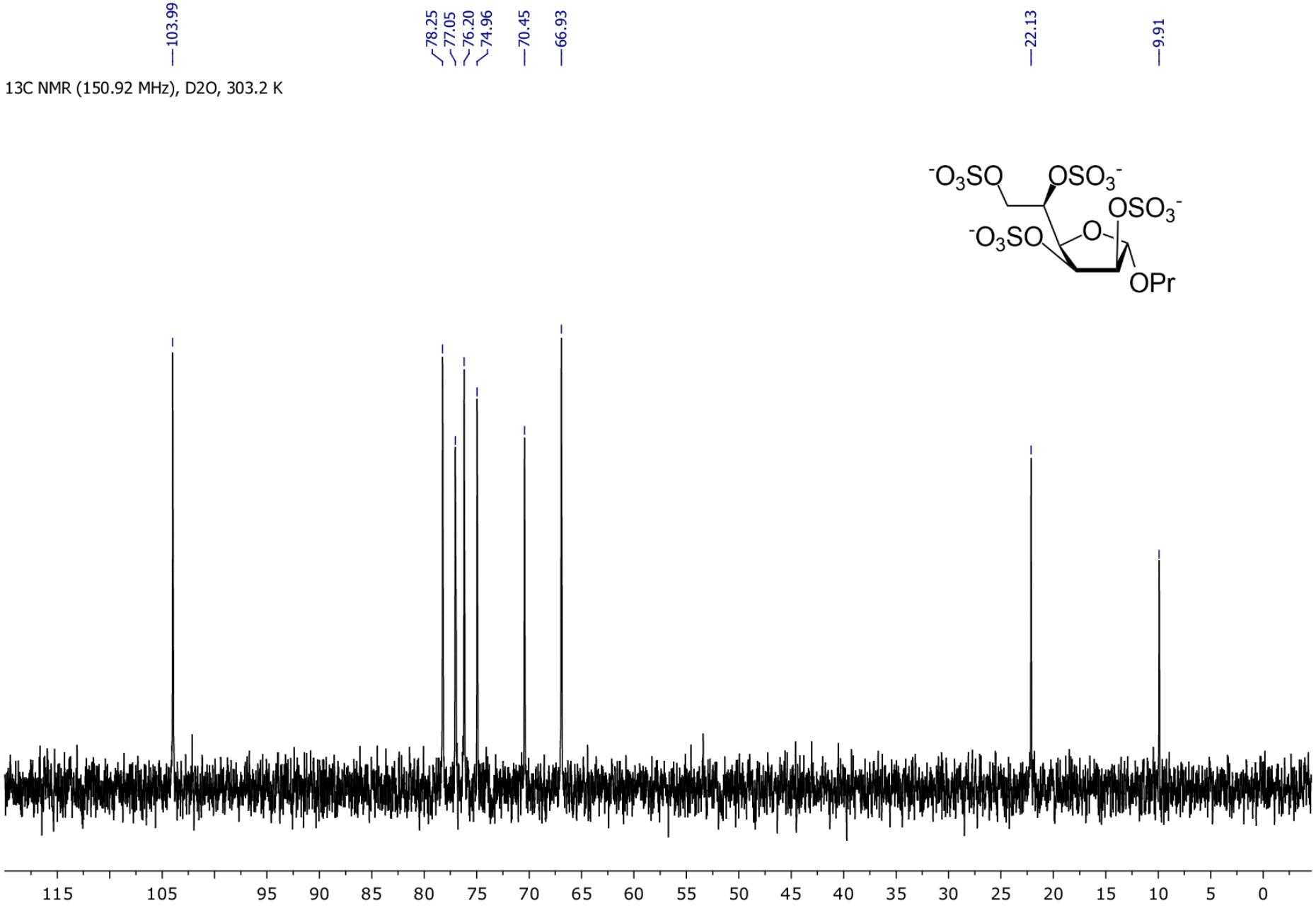
79.10
76.68
71.41
71.12
69.03
62.96
22.17
9.62
13C NMR (100.63 MHz), D2O, 298.0 K
HO
OH
OH
HO
O
OPr
115 110 105 100 95 90 85 80 75 70 65 60 55 50 45 40 35 30 25 20 15 10 5 0

Per-O-sulfated propyl α-D-mannofuranoside (1s)

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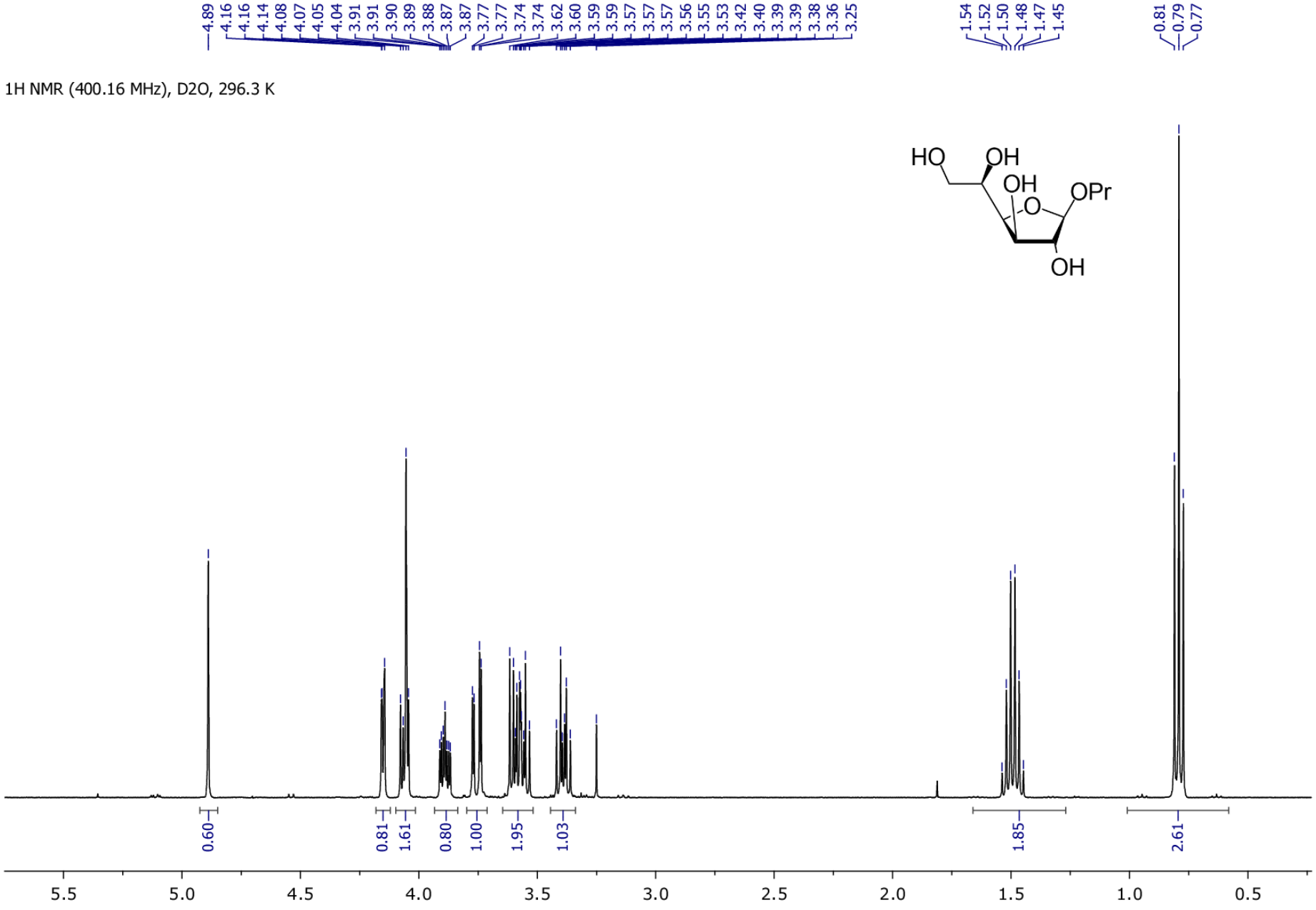
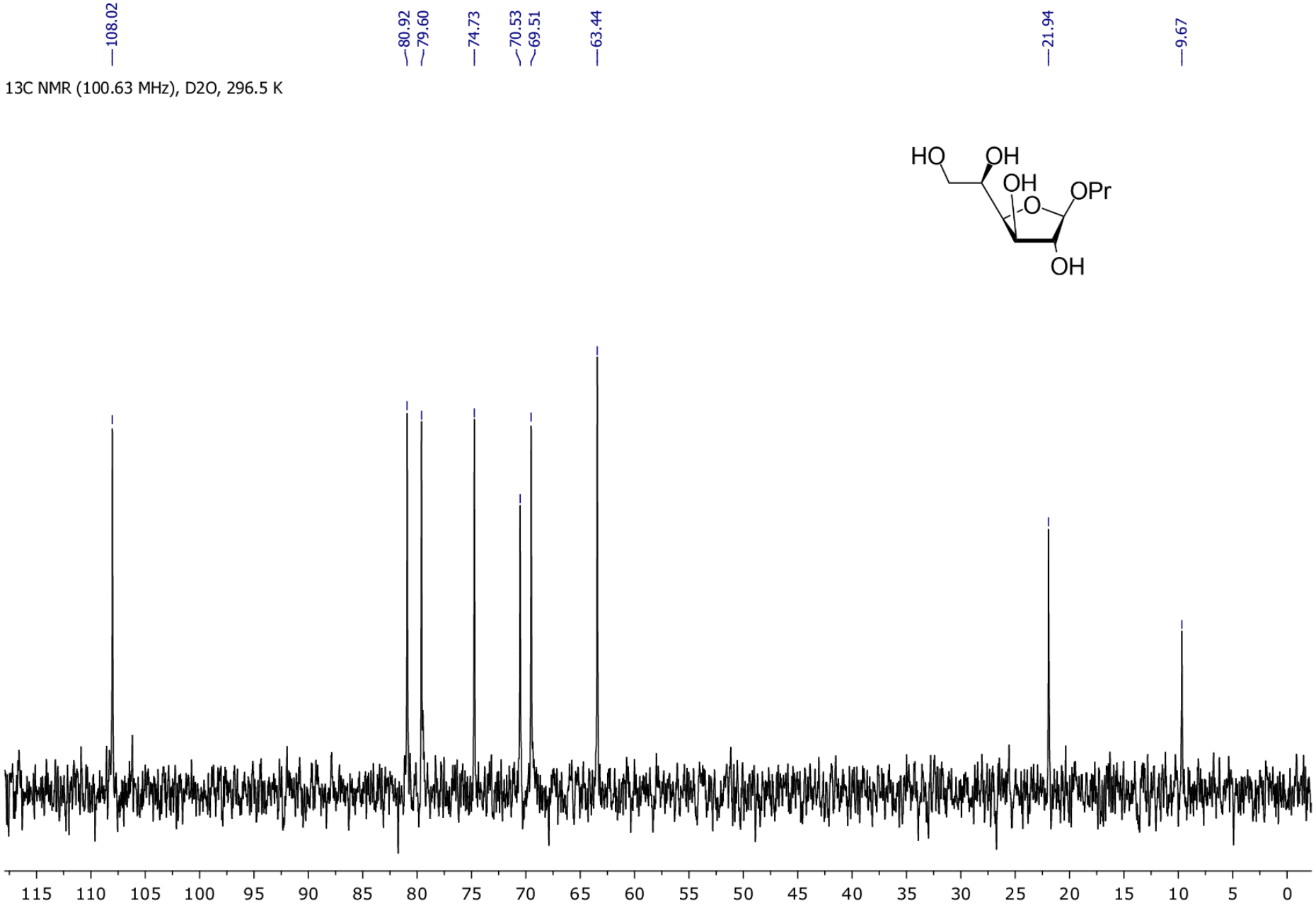
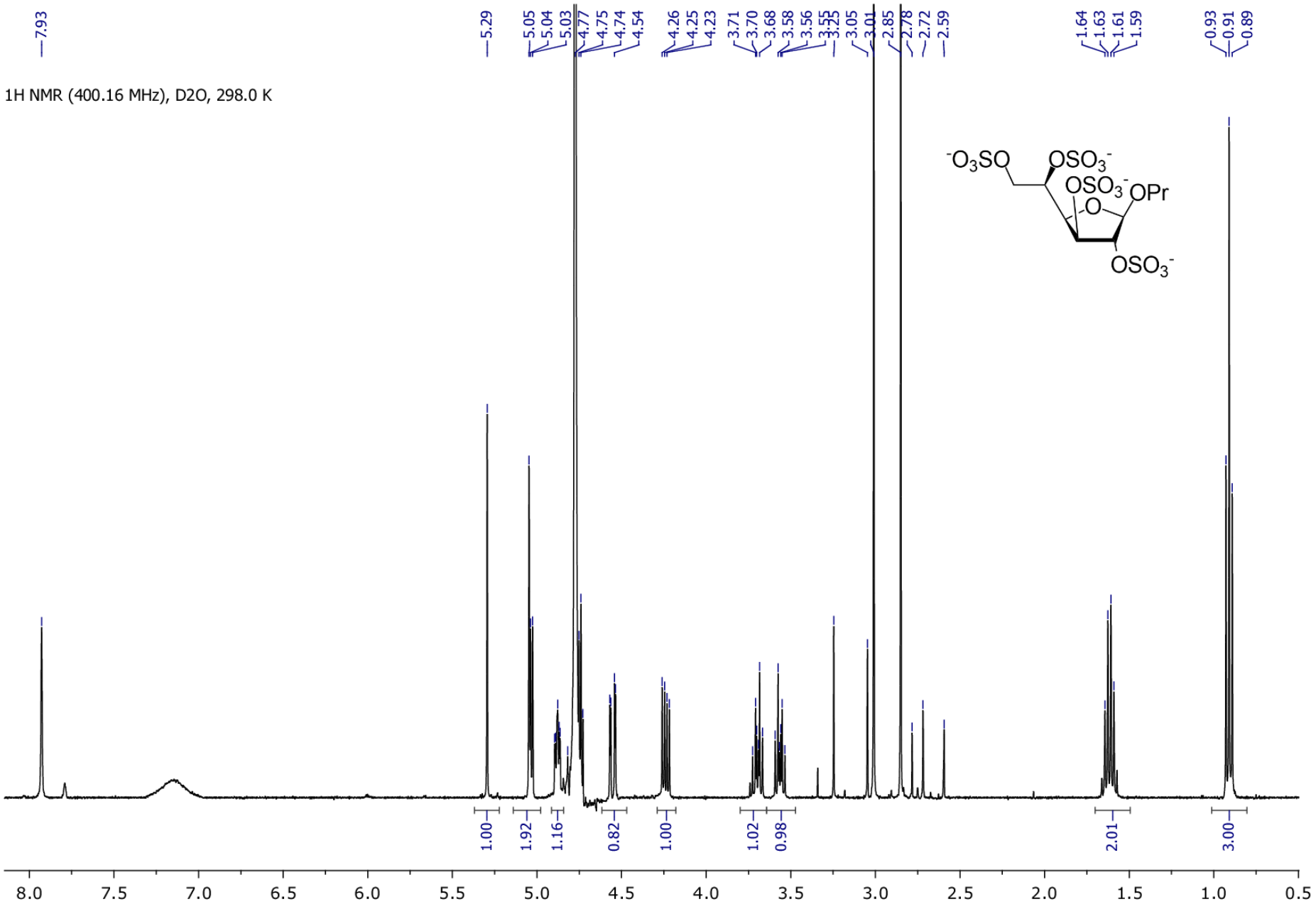
78.25
77.05
76.20
74.96
70.45
66.93
22.13
9.91
13C NMR (150.92 MHz), D2O, 303.2 K
$^{-}O_3SO$
OSO_3^{-}
OSO_3^{-}
$^{-}O_3SO$
O
OPr
115
105
95
90
85
80
75
70
65
60
55
50
45
40
35
30
25
20
15
10
5
0

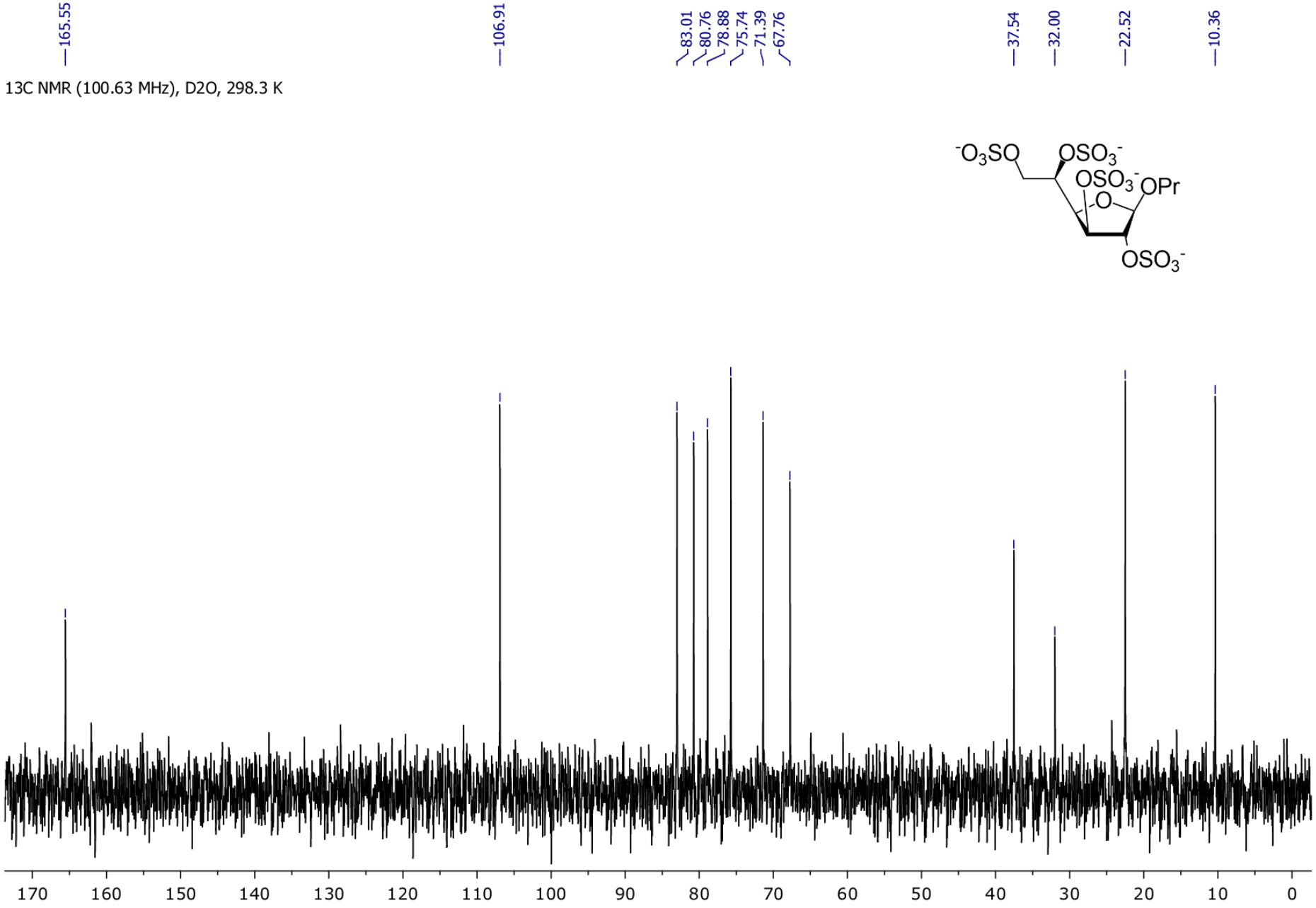
Propyl β-D-glucofuranoside (2)



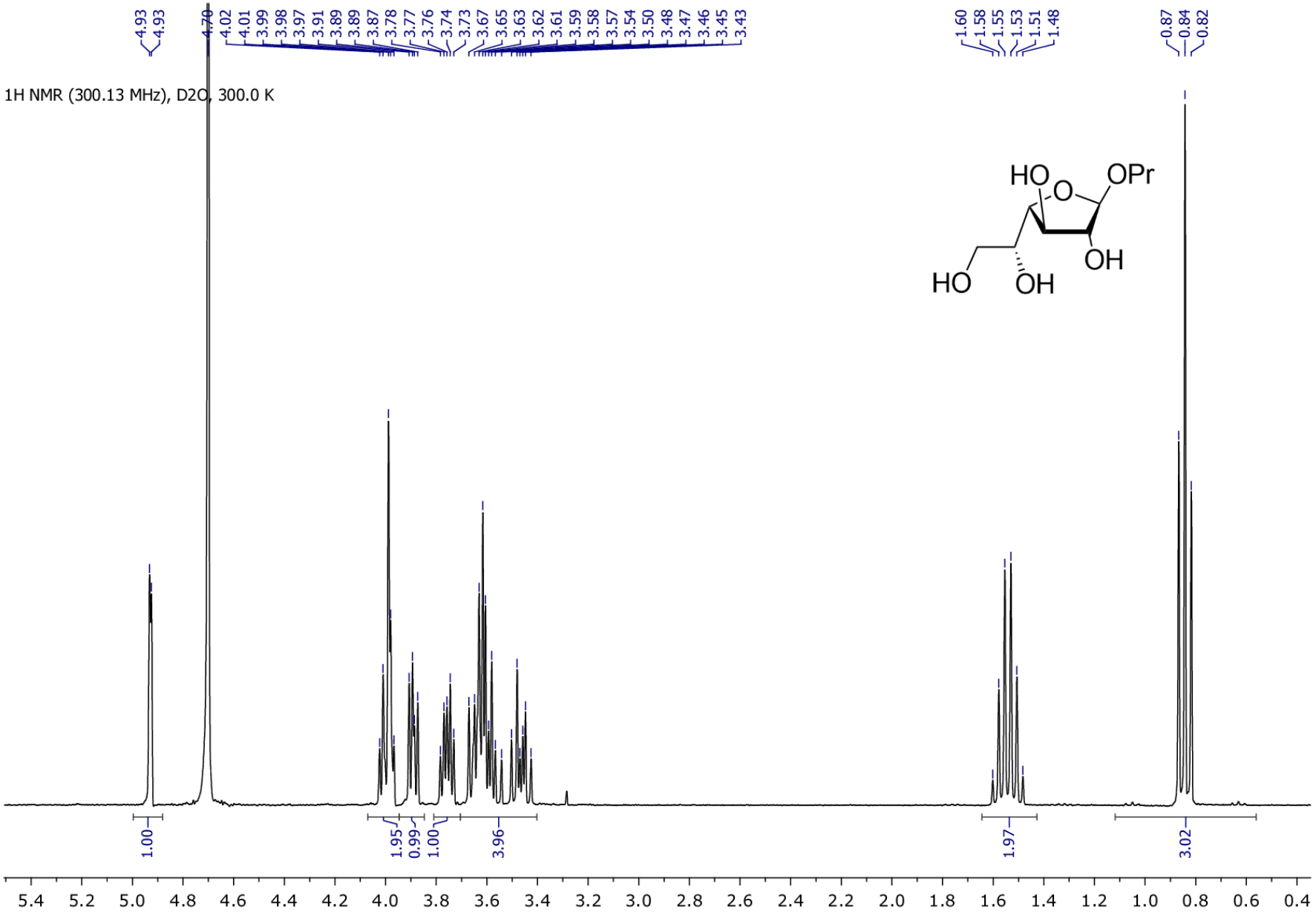

108.02
80.92
79.60
74.73
70.53
69.51
63.44
21.94
9.67
13C NMR (100.63 MHz), D2O, 296.5 K
HO
OH
OH
O
OPr
OH
115 110 105 100 95 90 85 80 75 70 65 60 55 50 45 40 35 30 25 20 15 10 5 0

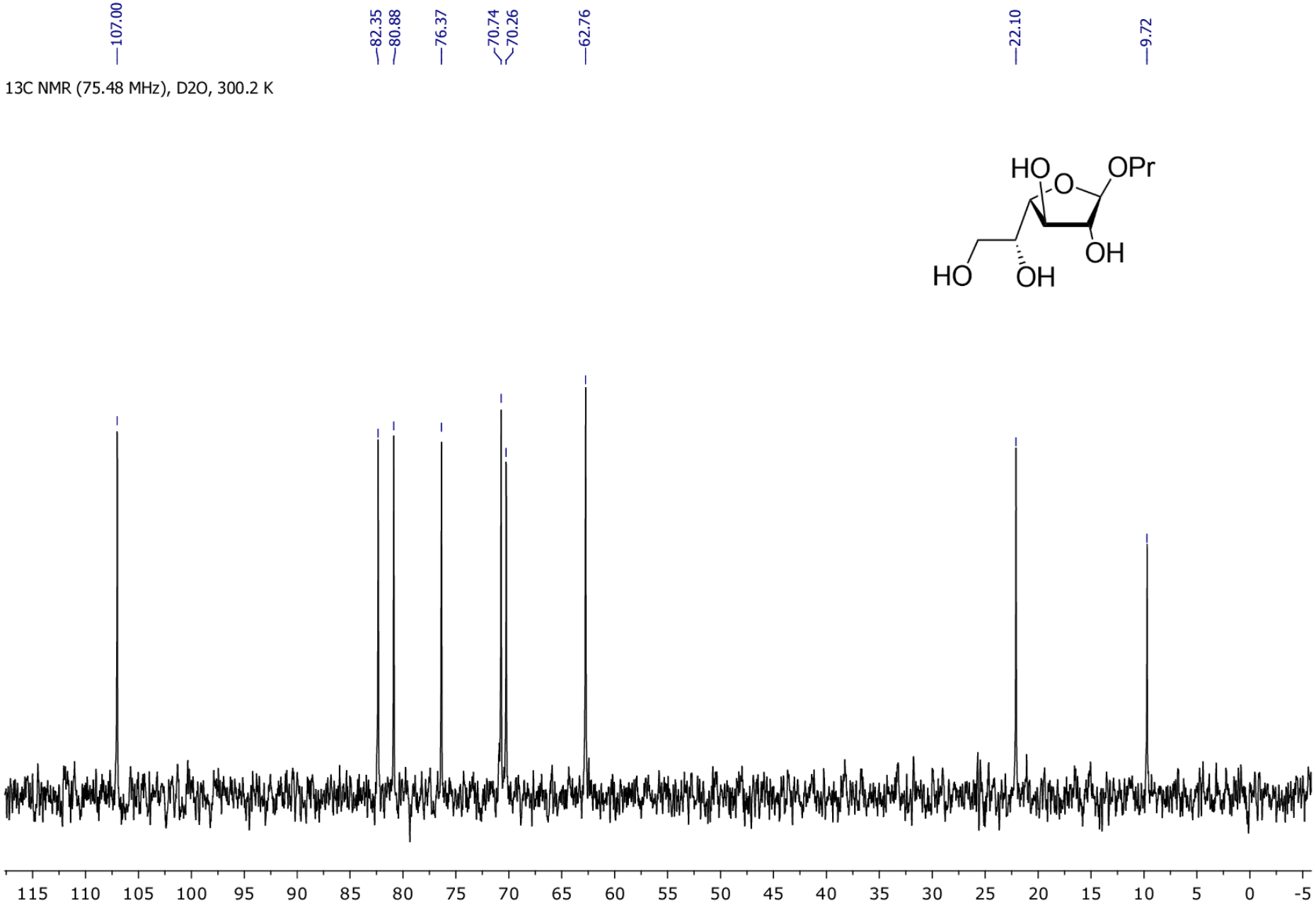
Per-O-sulfated propyl β-D-glucofuranoside (2s)



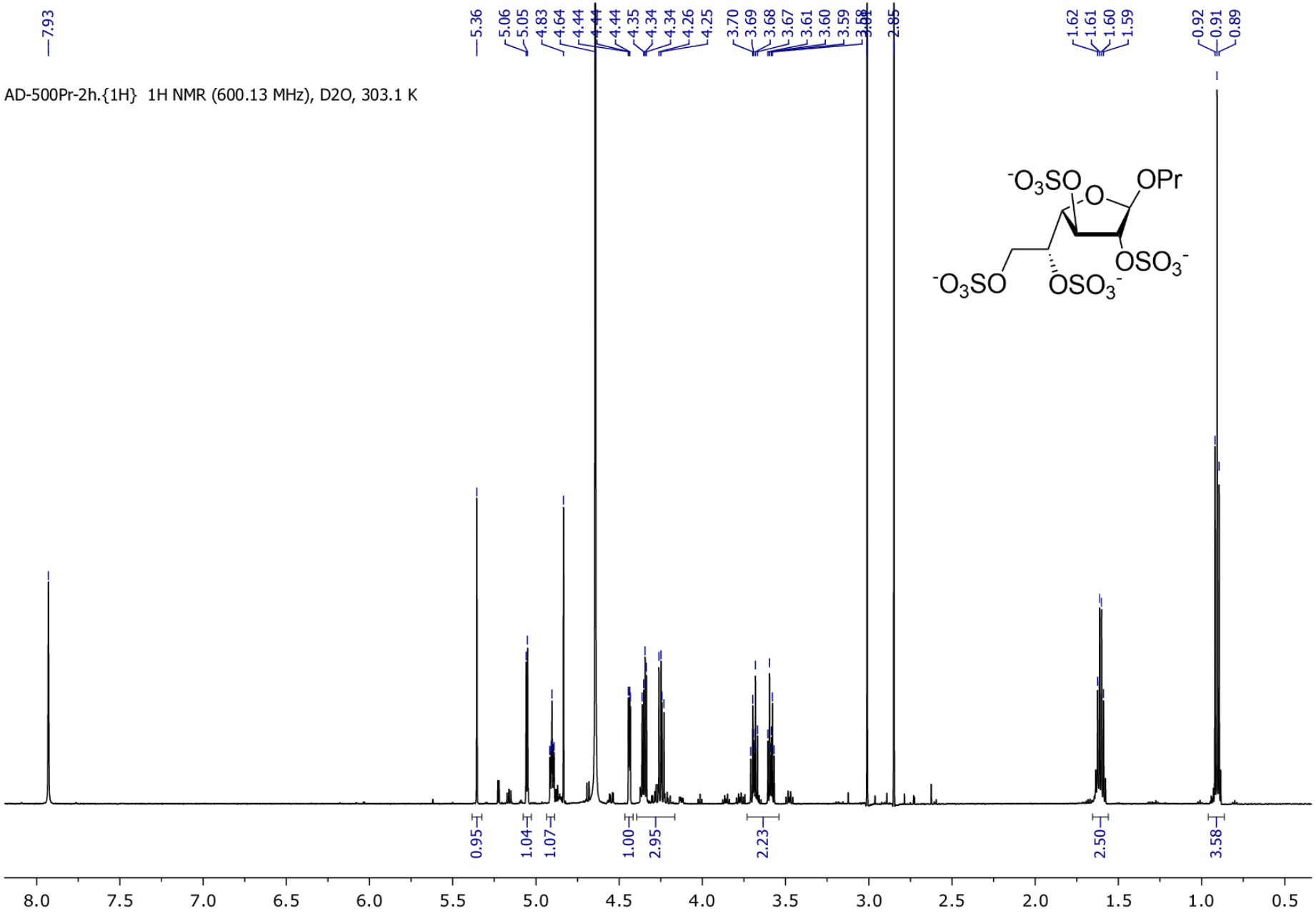

165.55
106.91
83.01
80.76
78.88
75.74
71.39
67.76
37.54
32.00
22.52
10.36
13C NMR (100.63 MHz), D2O, 298.3 K
-O3SO
OSO3-
OSO3-
OPr
-O
OSO3-
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0

Propyl β-D-galactofuranoside (3)




107.00
82.35
80.88
76.37
70.74
70.26
62.76
22.10
9.72
13C NMR (75.48 MHz), D2O, 300.2 K
HO
O
OPr
OH
HO
OH
115 110 105 100 95 90 85 80 75 70 65 60 55 50 45 40 35 30 25 20 15 10 5 0 -5

Per-O-sulfated propyl β-D-galactofuranoside (3s)



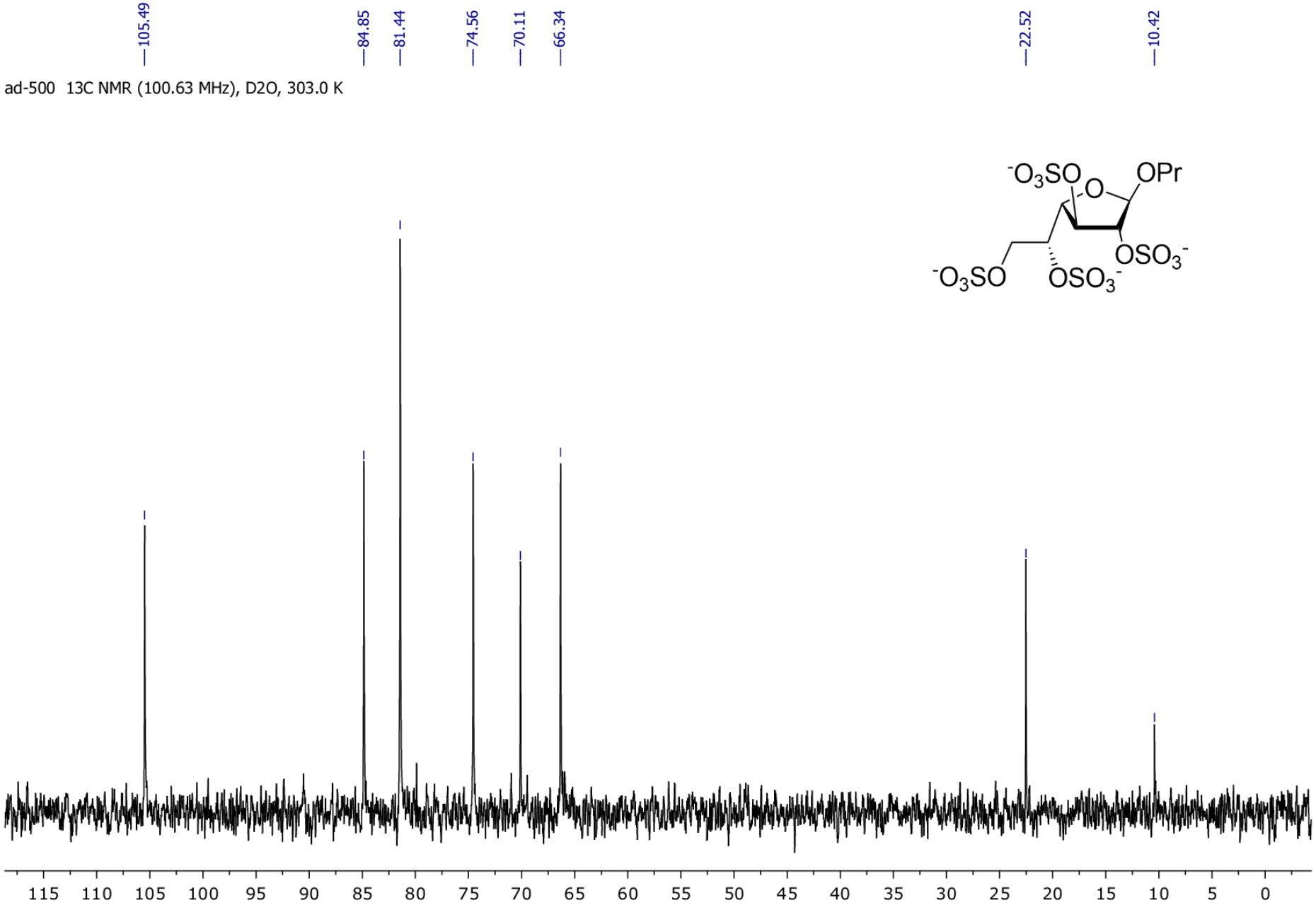

105.49
84.85
81.44
74.56
70.11
66.34
22.52
10.42
ad-500 13C NMR (100.63 MHz), D2O, 303.0 K
-O3SO
O
OPr
OSO3-
-O3SO
OSO3-
115 110 105 100 95 90 85 80 75 70 65 60 55 50 45 40 35 30 25 20 15 10 5 0

Table S1. Starting and final conformations with their energies for structure **1s**.

Starting conformer	Absolute energy, hartree	Energy relative to the lowest found conformation, kcal/mole	Final conformer
C1-endo_-60	-3287.431410778	7.2	C2-exo/C3-endo
C1-endo_+60	-3287.441204100	1.0	C2-exo/**C3-endo**
C1-exo_-60	-3287.434707545	5.1	C1-exo
C1-exo_+60	-3287.442860602	0.0	C1-exo
C2-endo_-60	-3287.434681089	5.1	C1-exo
C2-endo_+60	-3287.442815659	0.0	C1-exo
C2-exo_-60	-3287.441222255	1.0	C2-exo/**C3-endo**
C2-exo_+60	-3287.431381399	7.2	C2-exo/**C3-endo**
C3-endo_-60	-3287.431428682	7.2	C2-exo/**C3-endo**
C3-endo_+60	-3287.441426069	0.9	C2-exo/**C3-endo**
C3-exo_-60	-3287.432478471	6.5	C2-endo
C3-exo_+60	-3287.442816477	0.0	C1-exo
C4-endo_-60	-3287.432491076	6.5	C2-endo
C4-endo_+60	-3287.442776143	0.1	C1-exo
C4-exo_-60	-3287.431424486	7.2	C4-exo
C4-exo_+60	-3287.440999657	1.2	C4-exo
O4-endo_-60	-3287.434632933	5.2	C1-exo
O4-endo_+60	-3287.442822636	0.0	C1-exo
O4-exo_-60	-3287.432335961	6.6	C2-endo
O4-exo_+60	-3287.442825355	0.0	C1-exo

Table S2. Starting and final conformations with their energies for structure **1**.

Starting conformer	Absolute energy, hartree	Energy relative to the lowest found conformation, kcal/mole	Final conformer
C1-endo_-60	-800.697596820	4.1	C3-endo
C1-endo_+60	-800.700791611	2.1	C3-endo
C1-endo_180	-800.704085847	0.0	C3-endo
C1-exo_-60	-800.691467457	7.9	C1-exo
C1-exo_+60	-800.696711940	4.6	C1-exo
C1-exo_180	-800.699386724	2.9	C1-exo
C2-endo_-60	-800.692123482	7.5	C1-exo
C2-endo_+60	-800.696701951	4.6	C1-exo
C2-endo_180	-800.699403766	2.9	C1-exo
C2-exo_-60	-800.700506479	2.2	C3-endo
C2-exo_+60	-800.698252725	3.7	C3-endo
C2-exo_180	-800.703141067	0.6	C3-endo
C3-endo_-60	-800.700508978	2.2	C3-endo
C3-endo_+60	-800.698275031	3.6	C3-endo
C3-endo_180	-800.703163472	0.6	C3-endo
C3-exo_-60	-800.699947556	2.6	C2-endo
C3-exo_+60	-800.699741055	2.7	C1-exo
C3-exo_180	-800.703138229	0.6	C1-exo
C4-endo_-60	-800.699920198	2.6	C2-endo
C4-endo_+60	-800.699737988	2.7	C1-exo
C4-endo_180	-800.703163029	0.6	C1-exo
C4-exo_-60	-800.700502528	2.2	C3-endo
C4-exo_+60	-800.698257524	3.7	C3-endo
C4-exo_180	-800.703128644	0.6	C3-endo
O4-endo_-60	-800.703097903	0.6	C3-endo
O4-endo_+60	-800.699868677	2.6	C1-exo
O4-endo_180	-800.703133682	0.6	C1-exo
O4-exo_-60	-800.699183006	3.1	C2-endo
O4-exo_+60	-800.699838525	2.7	C1-exo
O4-exo_180	-800.703117696	0.6	C3-endo

Table S3. Starting and final conformations with their energies for structure **2s**.

Starting conformer	Absolute energy, hartree	Energy relative to the lowest found conformation, kcal/mole	Final conformer
C1-endo_-60	-3287.434834474	6.1	C2-exo/C3-endo
C1-endo_+60	-3287.444516980	0.1	**C2-exo**/C3-endo
C1-endo_180	-3287.437815713	4.3	C2-exo/C3-endo
C1-exo_-60	-3287.435433086	5.8	C4-endo/C3-exo
C1-exo_+60	-3287.433049873	7.3	C4-endo/C3-exo
C1-exo_180	-3287.429713775	9.4	C4-endo
C2-endo_-60	-3287.433182646	7.2	C4-endo/C3-exo
C2-endo_+60	-3287.439092049	3.5	C4-endo/C3-exo
C2-endo_180	-3287.429654903	9.4	C4-endo/C3-exo
C2-exo_-60	-3287.434875084	6.1	C2-exo/C3-endo
C2-exo_+60	-3287.444623266	0.0	C2-exo/C3-endo
C2-exo_180	-3287.437747850	4.3	C2-exo/C3-endo
C3-endo_-60	-3287.434859978	6.1	C2-exo/C3-endo
C3-endo_+60	-3287.444628043	0.0	C2-exo/C3-endo
C3-endo_180	-3287.437876406	4.2	C2-exo/C3-endo
C3-exo_-60	-3287.435391621	5.8	C4-endo/C3-exo
C3-exo_+60	-3287.439094383	3.5	C4-endo/C3-exo
C3-exo_180	-3287.430638553	8.8	C4-endo/C3-exo
C4-endo_-60	-3287.432996891	7.3	C4-endo/C3-exo
C4-endo_+60	-3287.439119103	3.5	C4-endo/C3-exo
C4-endo_180	-3287.430032129	9.2	C4-endo/C3-exo
C4-exo_-60	-3287.434828508	6.1	C2-exo/C3-endo
C4-exo_+60	-3287.444542571	0.1	C2-exo/C3-endo
C4-exo_180	-3287.437850169	4.3	C2-exo/C3-endo
O4-endo_-60	-3287.435453272	5.8	C4-endo/C3-exo
O4-endo_+60	-3287.433147687	7.2	C4-endo/C3-exo
O4-endo_180	-3287.438058189	4.1	C2-exo/C3-endo
O4-exo_-60	-3287.432986486	7.3	C4-endo/C3-exo
O4-exo_+60	-3287.439078389	3.5	C4-endo/C3-exo
O4-exo_180	-3287.437845892	4.3	C2-exo/C3-endo

Table S4. Starting and final conformations with their energies for structure **2**.

Starting conformer	Absolute energy, hartree	Energy relative to the lowest found conformation, kcal/mole	Final conformer
C1-endo_-60	-800.699803925	2.1	C2-exo
C1-endo_+60	-800.698775680	2.7	C2-exo
C1-endo_180	-800.702939349	0.1	C2-exo
C1-exo_-60	-800.696925869	3.9	C4-endo
C1-exo_+60	-800.691869147	7.0	C3-exo
C1-exo_180	-800.696230240	4.3	C2-endo
C2-endo_-60	-800.696377241	4.2	C3-exo
C2-endo_+60	-800.698152879	3.1	C2-exo
C2-endo_180	-800.702689639	0.2	O4-endo
C2-exo_-60	-800.699829914	2.0	C2-exo
C2-exo_+60	-800.698784061	2.7	C2-exo/C3-endo
C2-exo_180	-800.702907234	0.1	C2-exo
C3-endo_-60	-800.700689790	1.5	C2-exo
C3-endo_+60	-800.696355567	4.2	C2-exo
C3-endo_180	-800.703067297	0.0	C2-exo
C3-exo_-60	-800.696384827	4.2	C3-exo
C3-exo_+60	-800.698245183	3.0	C2-endo
C3-exo_180	-800.699952461	2.0	C3-exo
C4-endo_-60	-800.696357505	4.2	C3-exo
C4-endo_+60	-800.698244268	3.0	C2-endo
C4-endo_180	-800.700001707	1.9	C3-exo
C4-exo_-60	-800.699880111	2.0	C2-exo
C4-exo_+60	-800.698047689	3.2	C2-exo
C4-exo_180	-800.703087386	0.0	C2-exo
O4-endo_-60	-800.696928753	3.9	C4-endo/C3-exo
O4-endo_+60	-800.691877399	7.0	C3-exo
O4-endo_180	-800.696216494	4.3	C2-exo
O4-exo_-60	-800.696346302	4.2	C3-exo
O4-exo_+60	-800.698099176	3.1	C2-endo
O4-exo_180	-800.703098738	0.0	C2-exo

Table S5. Starting and final conformations with their energies for structure **3s**.

Starting conformer	Absolute energy, hartree	Energy relative to the lowest found conformation, kcal/mole	Final conformer
C1-endo_-60	-3287.462577288	2.2	C1-endo
C1-endo_+60	-3287.460456548	3.5	C1-endo
C1-endo_180	-3287.460664733	3.4	C1-endo
C1-exo_-60	-3287.462506805	2.2	C1-endo
C1-exo_+60	-3287.458028624	5.0	C1-exo
C1-exo_180	-3287.457152559	5.6	C3-endo
C2-endo_-60	-3287.462538150	2.2	C1-endo
C2-endo_+60	-3287.457976681	5.1	C1-exo
C2-endo_180	-3287.460416586	3.5	C1-endo
C2-exo_-60	-3287.456152731	6.2	C1-endo
C2-exo_+60	-3287.458663355	4.6	C1-endo
C2-exo_180	-3287.456739561	5.8	C1-endo
C3-endo_-60	-3287.462511036	2.2	C1-endo
C3-endo_+60	-3287.460471777	3.5	C1-endo
C3-endo_180	-3287.457115711	5.6	C3-endo
C3-exo_-60	-3287.462513615	2.2	C1-endo
C3-exo_+60	-3287.458651441	4.6	C1-exo
C3-exo_180	-3287.460655387	3.4	C1-endo
C4-endo_-60	-3287.458337015	4.8	O4-exo
C4-endo_+60	-3287.466057720	0.0	C1-endo
C4-endo_180	-3287.458441313	4.8	C1-endo
C4-exo_-60	-3287.456323521	6.1	C1-endo
C4-exo_+60	-3287.458079244	5.0	C1-exo
C4-exo_180	-3287.456717075	5.9	C1-endo/C2-exo
O4-endo_-60	-3287.456468019	6.0	C1-endo
O4-endo_+60	-3287.456965412	5.7	C1-exo
O4-endo_180	-3287.456989096	5.7	C3-endo
O4-exo_-60	-3287.452654291	8.4	C1-endo
O4-exo_+60	-3287.462089579	2.5	C1-endo
O4-exo_180	-3287.456760122	5.8	C1-endo

Table S6. Starting and final conformations with their energies for structure **3**.

Starting conformer	Absolute energy, hartree	Energy relative to the lowest found conformation, kcal/mole	Final conformer
C1-endo_-60	-800.702714639	1.8	C1-endo/O4-exo
C1-endo_+60	-800.703644764	1.2	O4-exo
C1-endo_180	-800.701461245	2.6	C1-endo/O4-exo
C1-exo_-60	-800.703938468	1.0	C3-exo
C1-exo_+60	-800.705606279	0.0	C3-exo
C1-exo_180	-800.703380269	1.4	C3-exo
C2-endo_-60	-800.703948654	1.0	C3-exo
C2-endo_+60	-800.705603785	0.0	C3-exo
C2-endo_180	-800.703246722	1.5	C3-exo
C2-exo_-60	-800.702716147	1.8	O4-exo
C2-exo_+60	-800.703637788	1.2	O4-exo
C2-exo_180	-800.701427620	2.6	O4-exo
C3-endo_-60	-800.702714091	1.8	O4-exo
C3-endo_+60	-800.703664558	1.2	O4-exo
C3-endo_180	-800.701457153	2.6	O4-exo
C3-exo_-60	-800.703947849	1.0	C3-exo
C3-exo_+60	-800.705592316	0.0	C3-exo
C3-exo_180	-800.703292763	1.5	C3-exo
C4-endo_-60	-800.698709341	4.3	C4-endo/C3-exo
C4-endo_+60	-800.703611569	1.3	C3-exo
C4-endo_180	-800.703927481	1.1	C3-exo
C4-exo_-60	-800.702612882	1.9	O4-exo
C4-exo_+60	-800.705590826	0.0	C3-exo
C4-exo_180	-800.701438249	2.6	O4-exo
O4-endo_-60	-800.703928620	1.1	C3-exo
O4-endo_+60	-800.705607657	0.0	C3-exo
O4-endo_180	-800.703345536	1.4	C3-exo
O4-exo_-60	-800.702732610	1.8	O4-exo
O4-exo_+60	-800.703718598	1.2	O4-exo
O4-exo_180	-800.701518924	2.6	O4-exo