Supporting Information

An Alternative Route to the Anticancer Agent: 2-Fluorofucose from Readily Available L-(—)Rhamnose and Mechanistic Insights into a Zinc/Ammonium Iodide-Mediated Elimination Reaction

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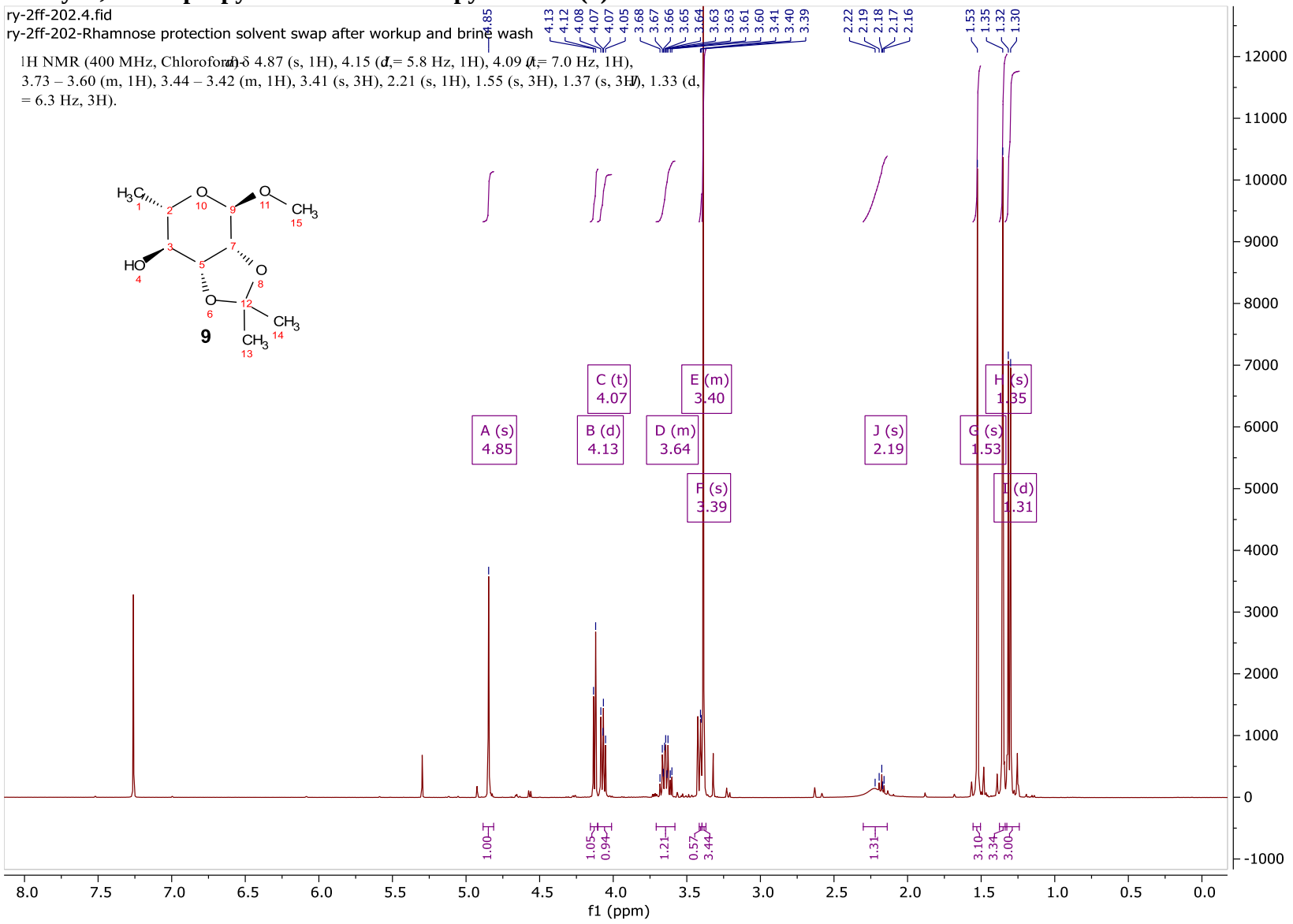
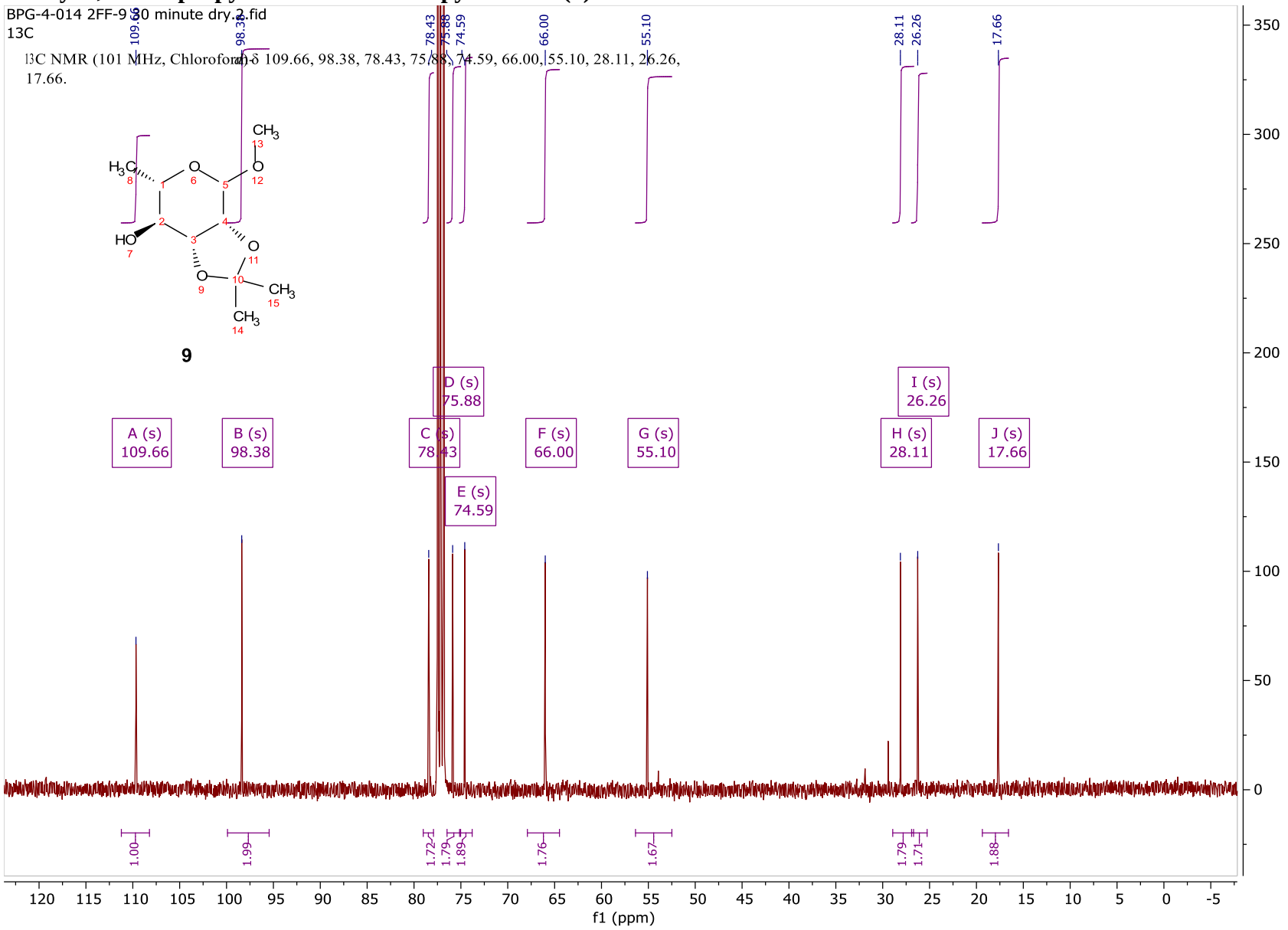
NMR Spectra:

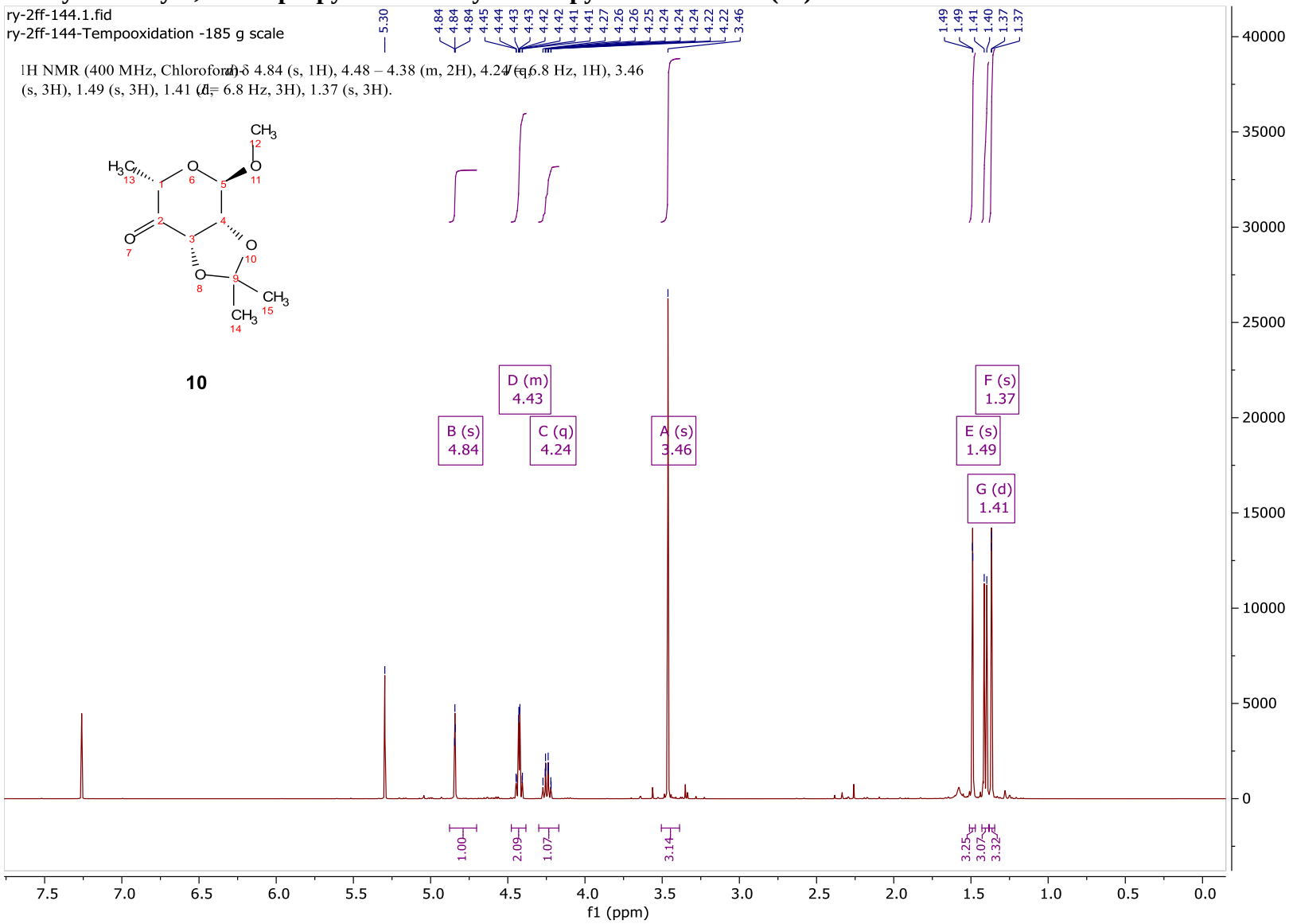
Methyl 2,3-*O*-isopropylidene-α-L-rhamnopyranoside (9) ^{1}H



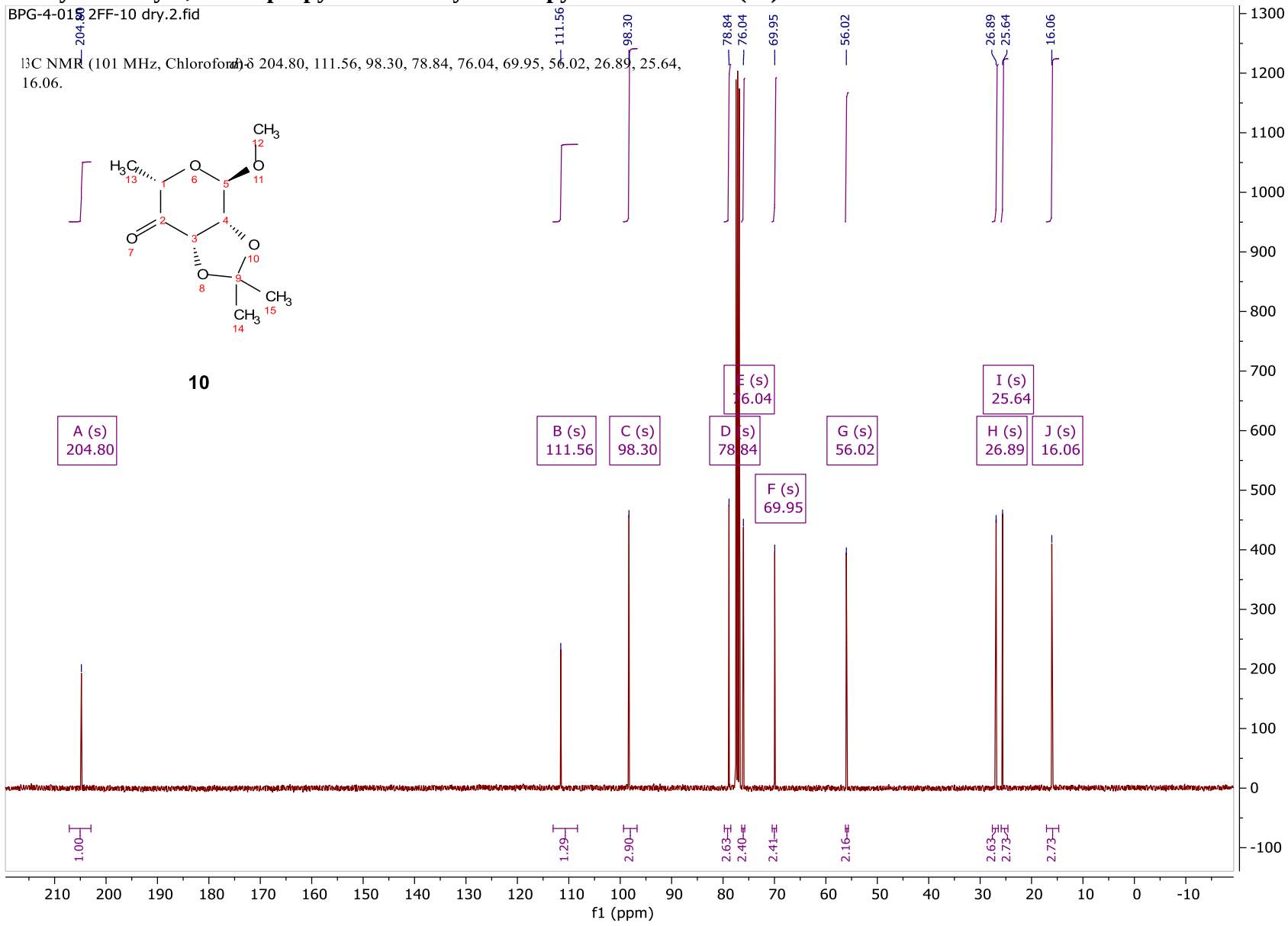
Methyl 2,3-*O*-isopropylidene-α-L-rhamnopyranoside (9) ^{13}C



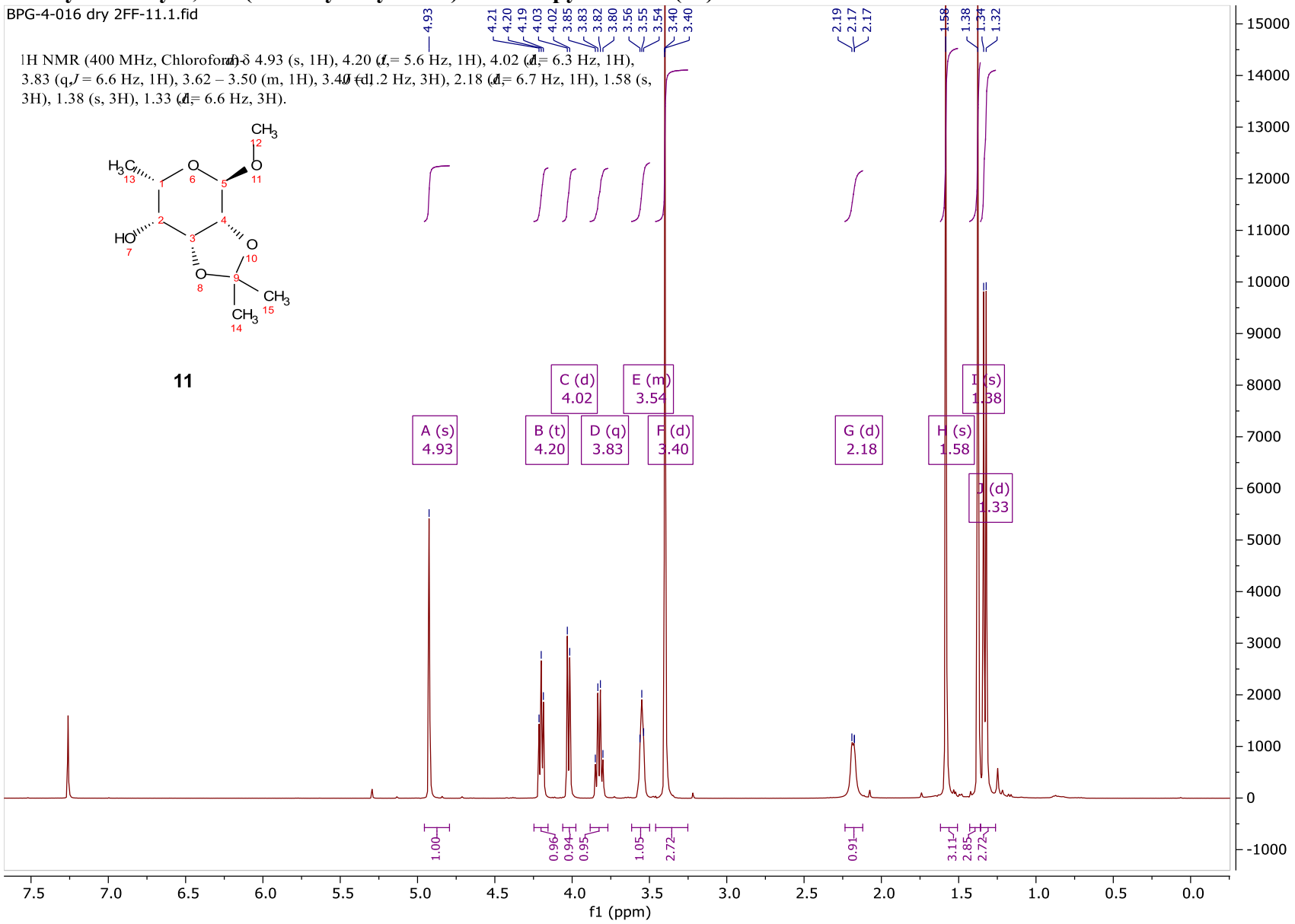
Methyl 6-deoxy-2,3-*O*-isopropylidene-α-L-lyxo-hexopyranosid-4-ulose (10) ^{1}H



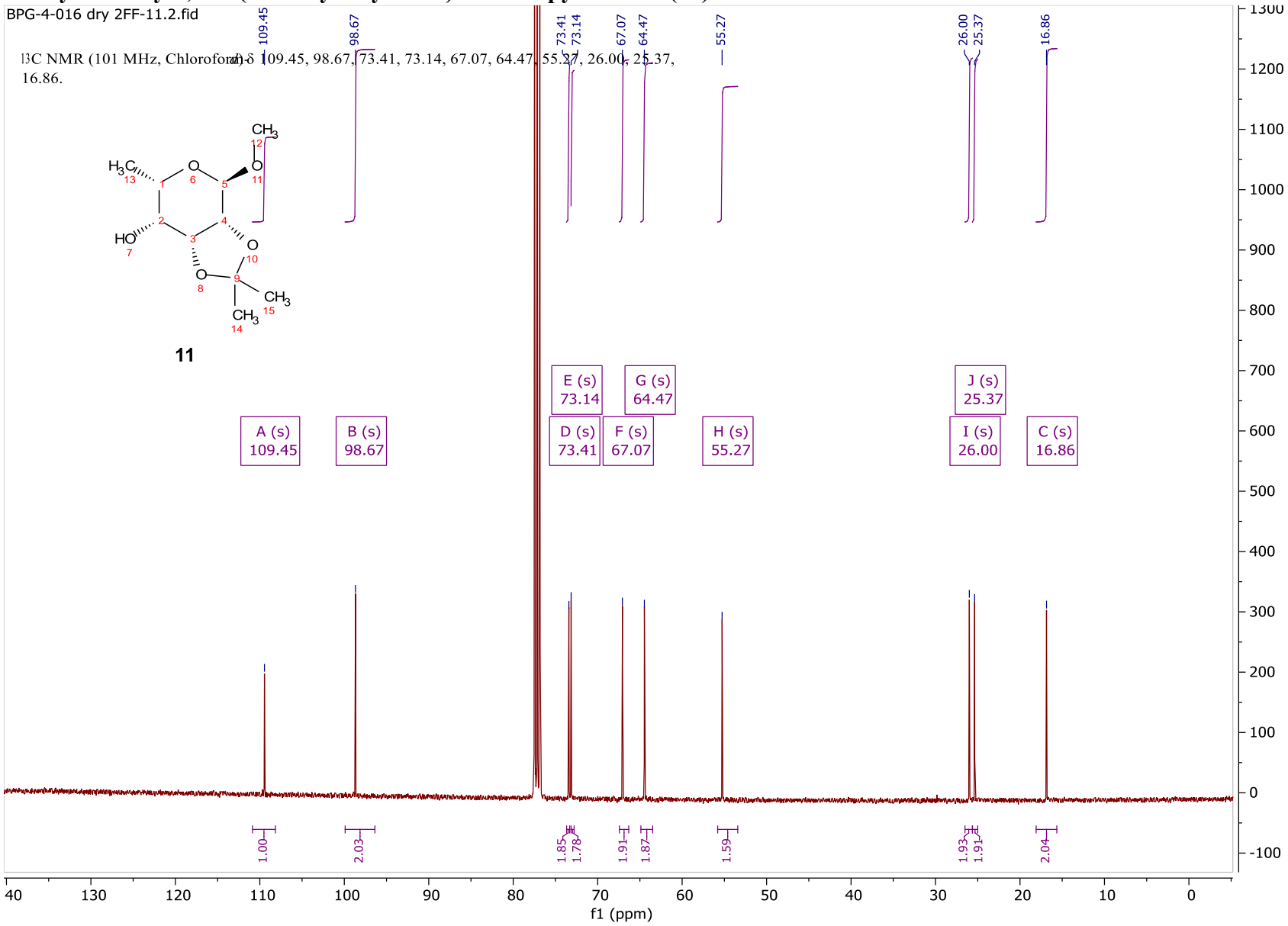
Methyl 6-deoxy-2,3-*O*-isopropylidene-α-L-lyxo-hexopyranosid-4-ulose (10) ^{13}C



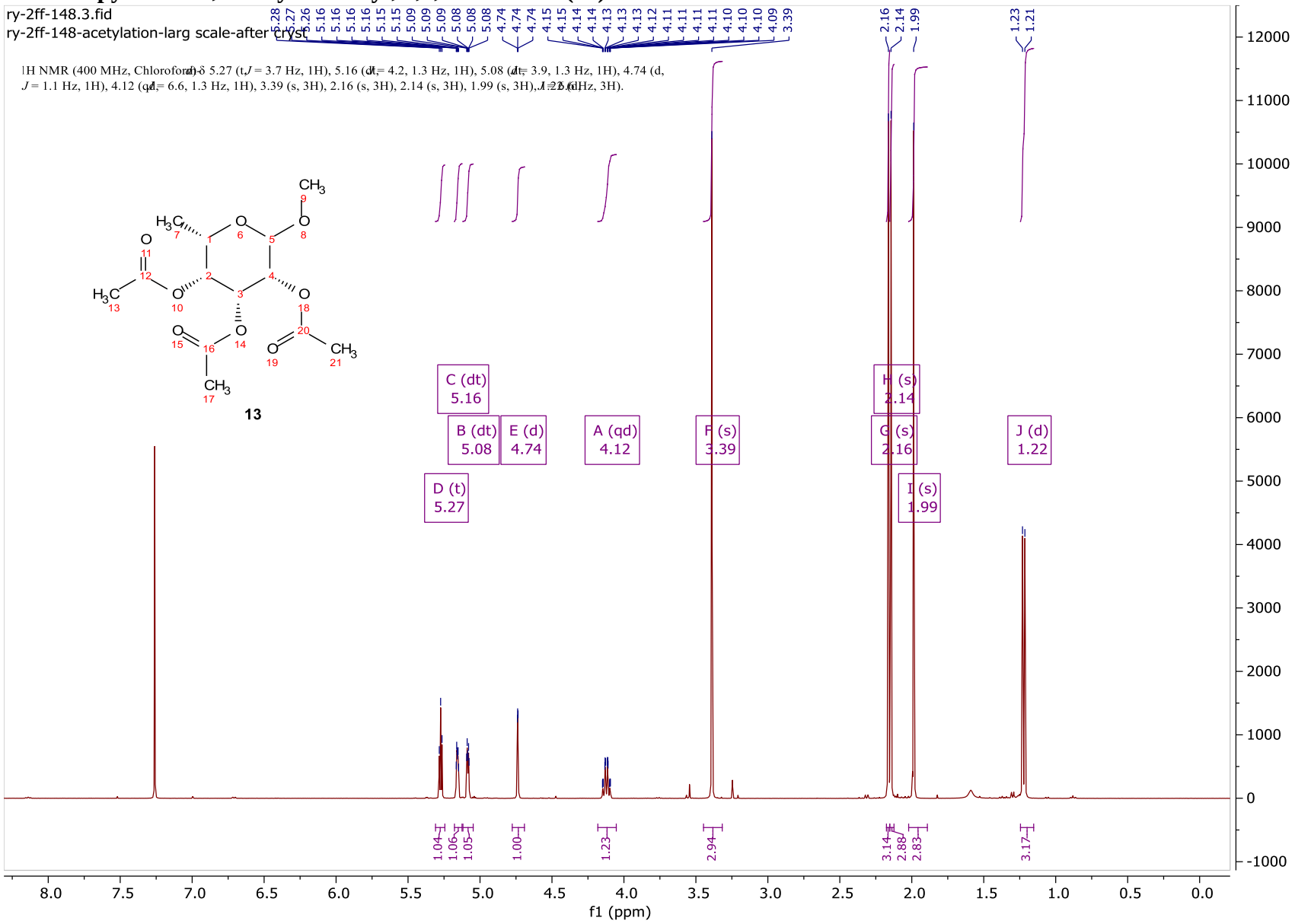
Methyl 6-deoxy-2,3-*O*-(1-methylethylidene)-α-L-talopyranoside (11) ^{1}H



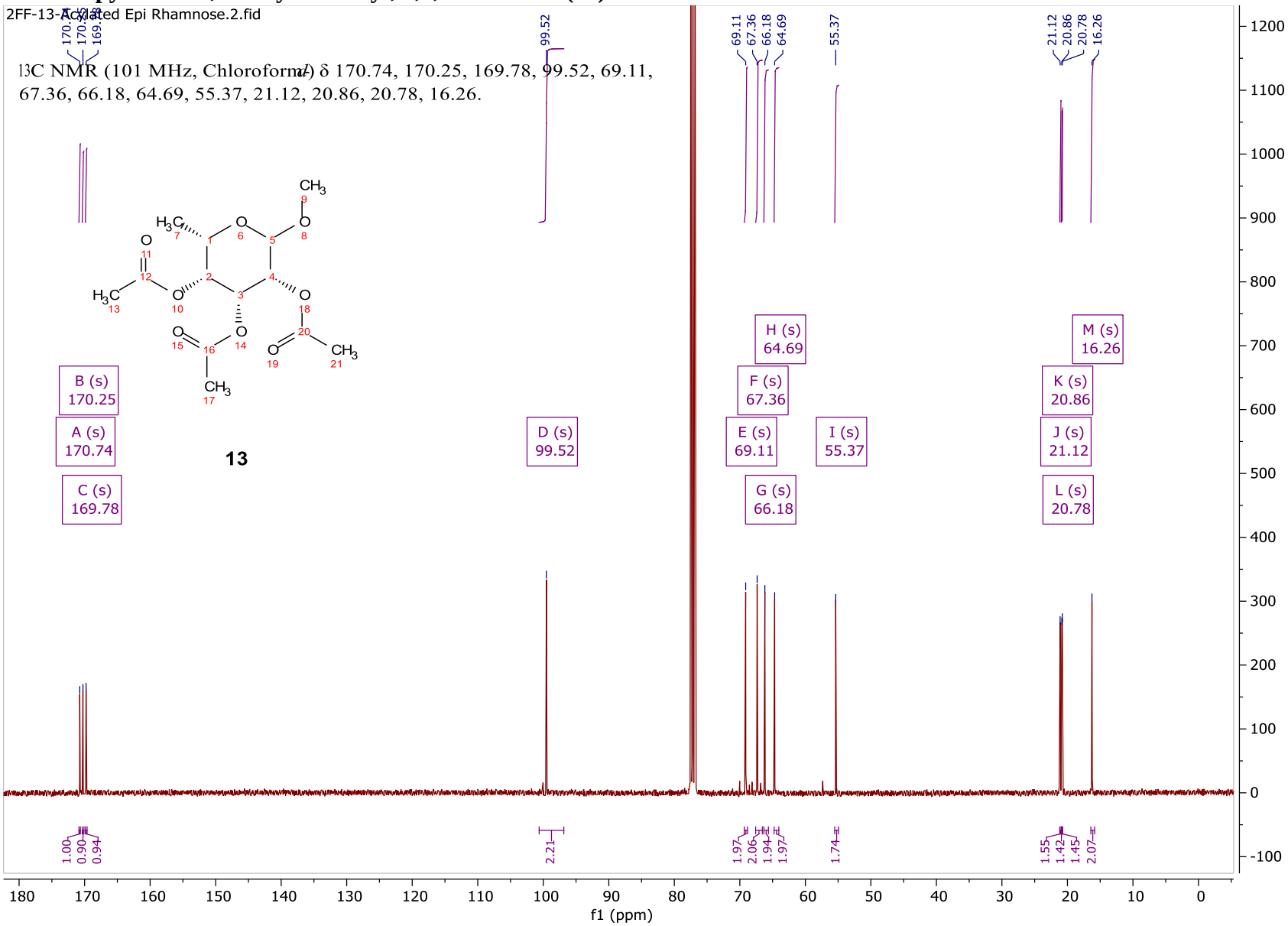
Methyl 6-deoxy-2,3-*O*-(1-methylethylidene)-α-L-talopyranoside (11) ^{13}C



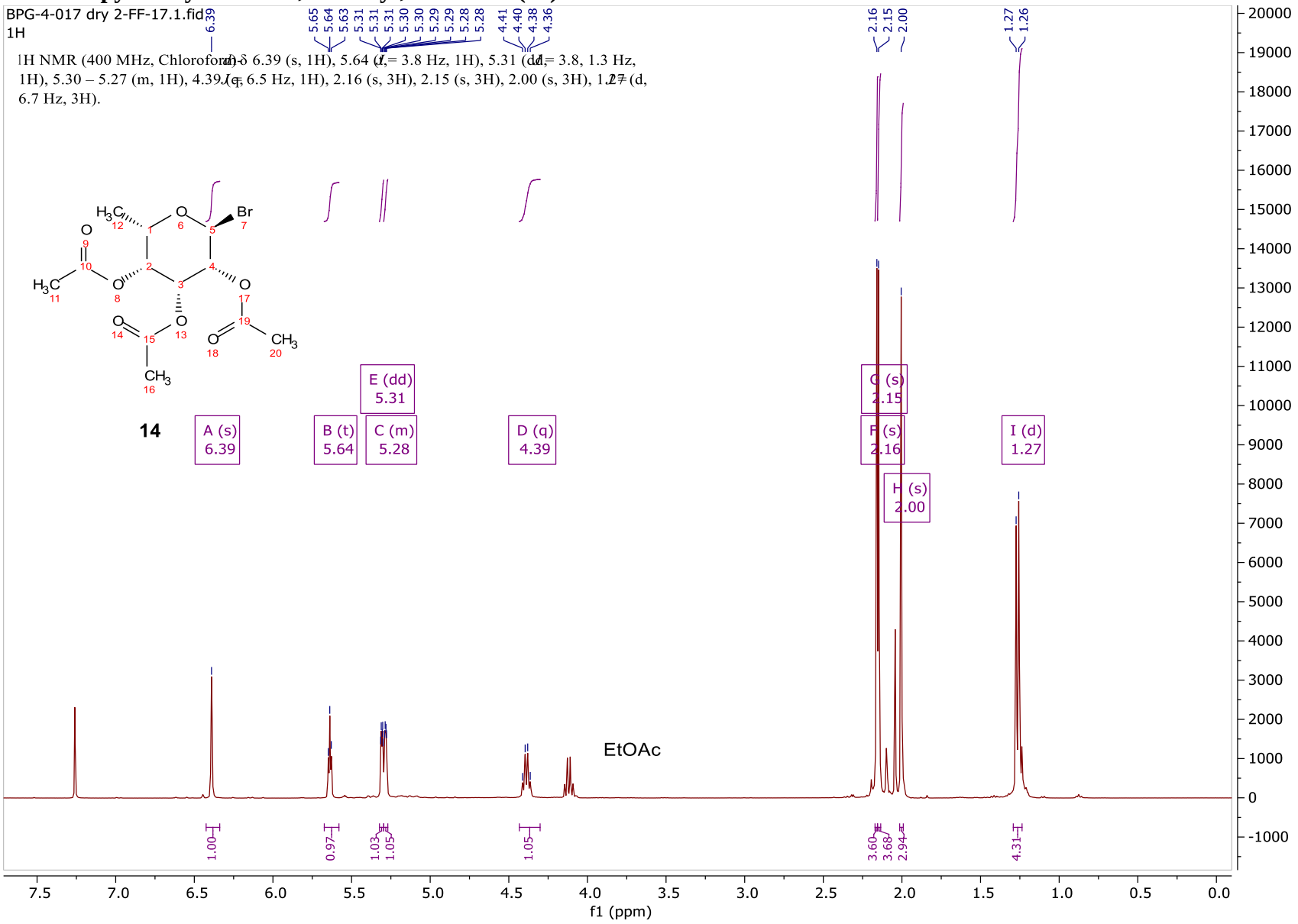
α-L-Talopyranoside, methyl 6-deoxy-, 2,3,4-triacetate (13) ^{1}H



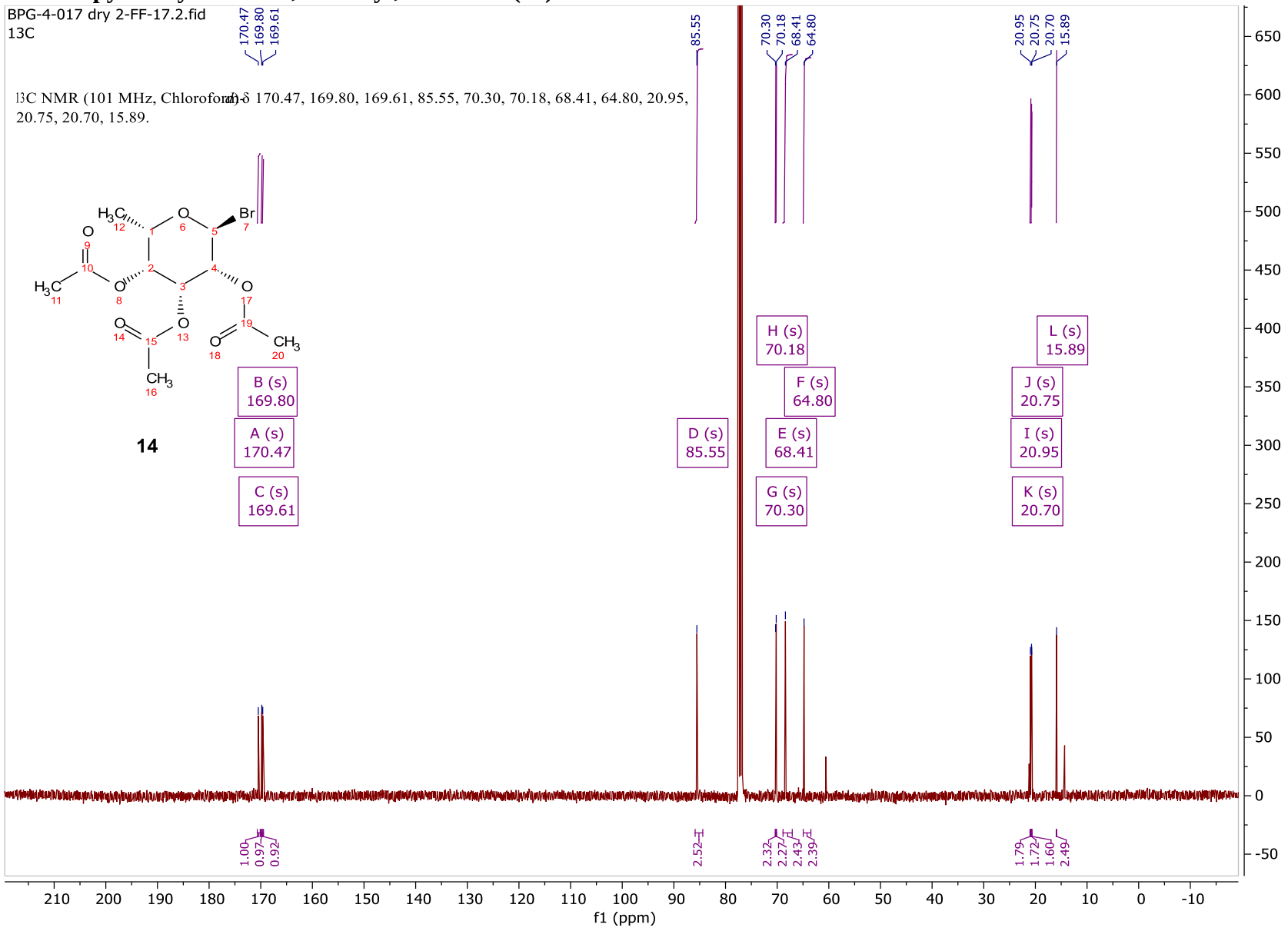
α-L-Talopyranoside, methyl 6-deoxy-, 2,3,4-triacetate (13) ^{13}C



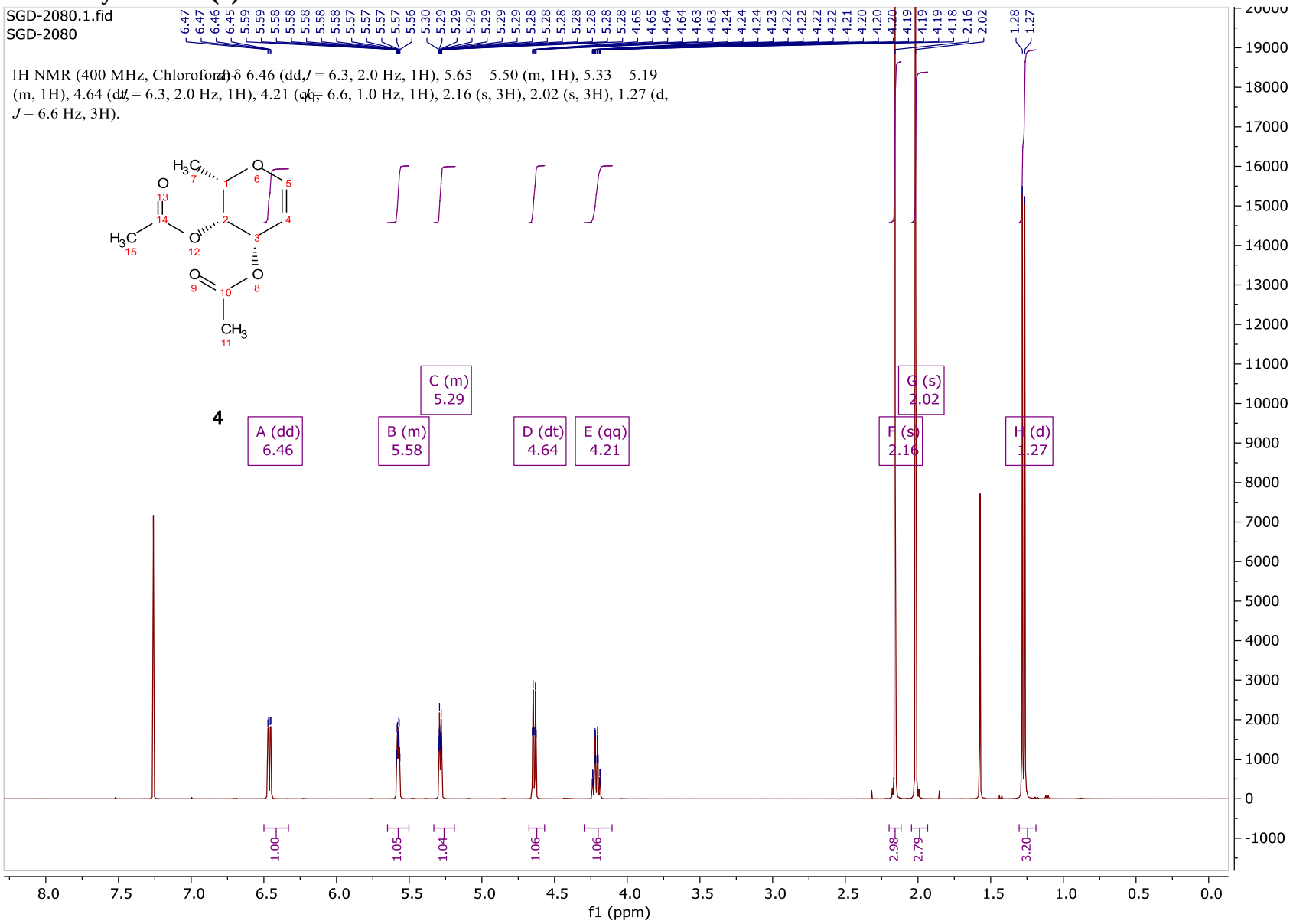
α-L-Talopyranosyl bromide, 6-deoxy-, triacetate (14) ^{1}H



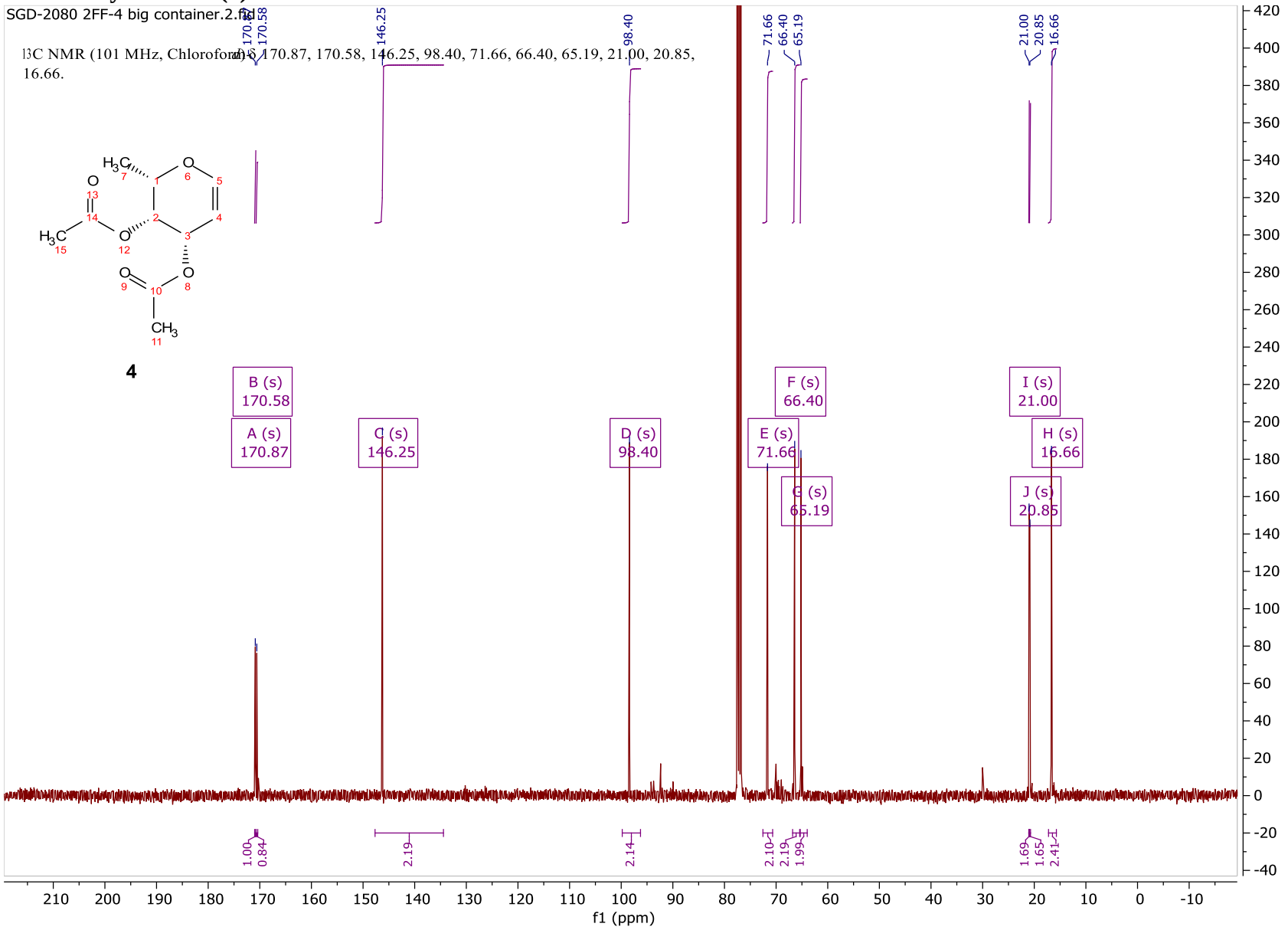
α-L-Talopyranosyl bromide, 6-deoxy-, triacetate (14) ^{13}C



Di-*O*-Acetyl-L-fucal (4) ^{1}H



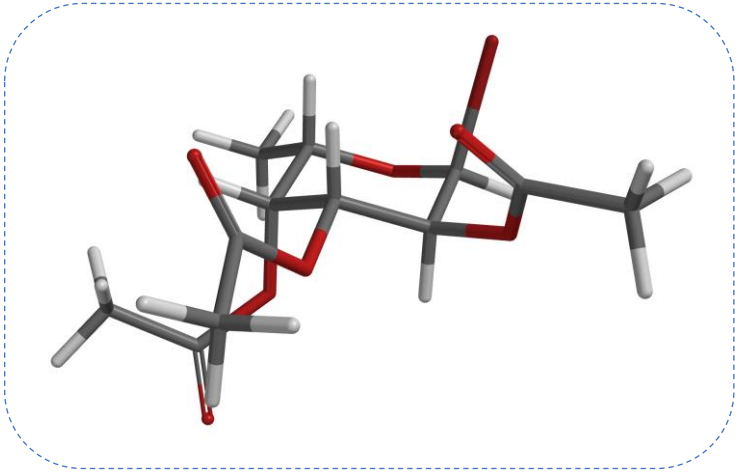
Di-*O*-Acetyl-L-fucal (4) ^{13}C



Quantum mechanical modeling studies:

Geometry optimizations for all conformations of **3**, **14** and **18** and the resulting elimination products were performed using density functional calculations at the RB3LYP/6-31G*/C-PCM (implicit non-polar solvent, **ε** = 7.43) level and the corresponding radical intermediates were subjected to the UB3LYP/6-31G*/C-PCM (implicit non-polar solvent, **ε** = 7.43) level in the Spartan-20 software running on Macintosh and Linux platforms. True minimum for all structures was confirmed by performing vibrational analyses. Convergence and consistency of the optimizations was verified by re-optimization of several examples from multiple starting points; energetic variations of 0.01 kcal/mol or less were found among these calculated structures. Relative enthalpies $\Delta H°_{rel}$ were calculated by including zero-point and thermal corrections to 298.15 K. All values are in kcal/mol as also depicted in Scheme 3 in the manuscript. Importantly, neither the vibration nor the solvation corrections introduced differences between relative E° and relative H° values that were large enough to reorder the relative energy structures; thus, either set of data led to the same conclusions.

Cartesian coordinates for geometry minimized 3:

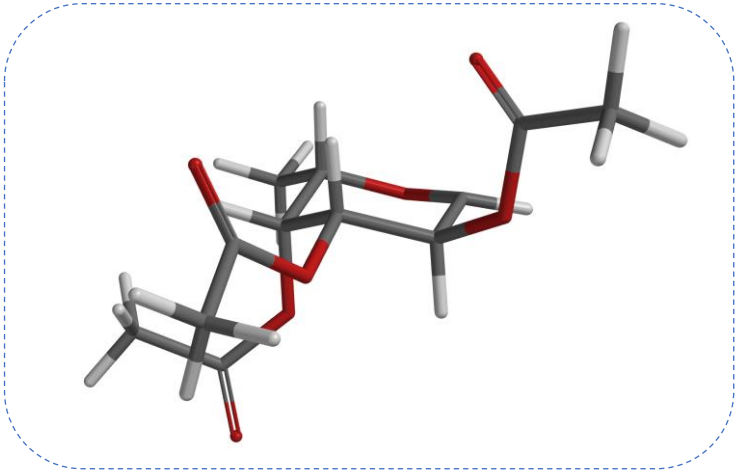


	Atom		X	Y	Z
1	C	C13	-0.7214715	-1.1326584	0.7804204
2	C	C3	0.1832665	1.1791296	0.5892093
3	O	O1	-1.2515440	0.5280328	2.4684487
4	C	C4	-0.8717116	1.6318615	1.6045324
5	C	C1	-1.6824387	-0.6106934	1.8618425
6	C	C2	-0.3405753	-0.0301251	-0.2086744
7	H	H7	-1.7644452	1.9326163	1.0418919
8	H	H3	-1.1889429	0.2924808	-0.8078198
9	H	H5	0.3791491	2.0008848	-0.1005493
10	O	O2	-1.1883367	-2.3913162	0.2806203
11	O	O3	0.6782240	-0.5649659	-1.0676339
12	O	O4	1.3757649	0.7885144	1.2931317
13	C	C5	-0.4183282	2.7595611	2.5150632
14	H	H8	0.4474831	2.4560726	3.1100127
15	H	H9	-1.2310601	3.0411791	3.1902804
16	C	C7	-1.7623750	-2.5933618	-0.9375075

17	C	C8	2.6252475	1.2506629	0.9994442
18	C	C9	0.7479111	-0.0571151	-2.3287021
19	O	O5	0.1109365	0.9107224	-2.6890308
20	O	O6	-1.9039765	-1.7472078	-1.7925108
21	O	O7	3.5528840	0.7413765	1.5887951
22	C	C10	1.6987099	-0.8573621	-3.1766180
23	H	H2	1.2340448	-1.8204766	-3.4173115
24	H	H4	2.6245696	-1.0613605	-2.6315079
25	H	H6	1.9111463	-0.3171998	-4.0999360
26	C	C11	-2.1907036	-4.0337900	-1.0566749
27	H	H11	-2.5895070	-4.2125031	-2.0557703
28	H	H14	-2.9595185	-4.2498338	-0.3070556
29	H	H15	-1.3437360	-4.6996395	-0.8644701
30	C	C12	2.7826558	2.3756521	0.0035725
31	H	H13	2.4197827	2.0959231	-0.9902237
32	H	H16	3.8436297	2.6180957	-0.0602409
33	H	H17	2.2281265	3.2639845	0.3250495
34	H	H20	0.1861652	-1.3984196	1.3339340
35	H	H12	-1.8737531	-1.3643373	2.6218757
36	Br	Br1	-3.6003193	-0.3581551	1.0693038
37	H	H1	-0.1469540	3.6337706	1.9148091

Cartesian coordinates for geometry minimized radical $3^{\cdot eq}$:

$\Delta H_{(rel)}$ = 6.0 kcal/mol



	Atom		X	Y	Z
1	C	C13	-0.5847580	-1.3192192	0.7629720
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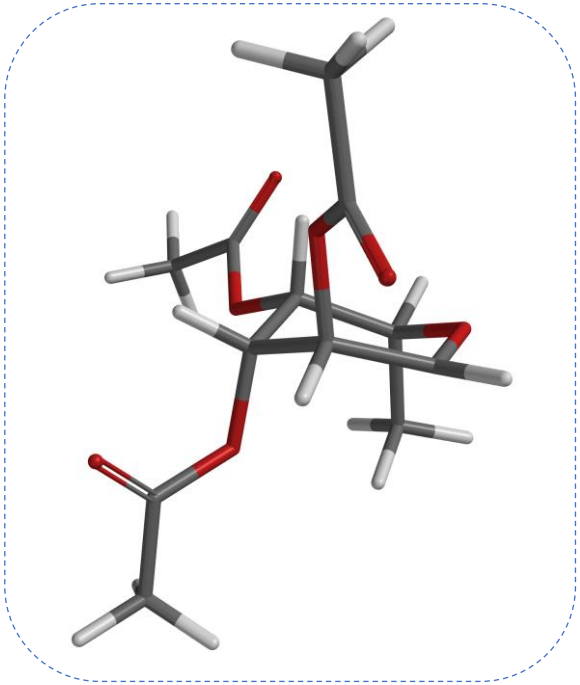
3	O	O1	-1.2940508	0.4065174	2.4032310
4	C	C4	-0.9929152	1.4735153	1.4790131
5	C	C6	-1.4726657	-0.8411535	1.8769740
6	C	C2	-0.2458211	-0.2018830	-0.2254913
7	H	H7	-1.8793274	1.6441329	0.8529051
8	H	H3	-1.1025462	0.0291590	-0.8569125
9	H	H5	0.3328833	1.8761234	-0.1691419
10	H	H12	-1.7920934	-1.5580244	2.6279389
11	O	O2	-1.1471702	-2.4940775	0.1203323
12	O	O3	0.8374537	-0.6762468	-1.0508591
13	O	O4	1.3256636	0.7783826	1.3206778
14	C	C5	-0.6942763	2.7074629	2.3137037
15	H	H8	0.1850932	2.5451234	2.9437375
16	H	H9	-1.5492427	2.9352817	2.9567684

17	H	H10	-0.5111475	3.5677656	1.6620355
18	C	C7	-2.3529186	-2.4212494	-0.4960635
19	C	C8	2.5355328	1.3739378	1.1328258
20	C	C9	0.9064471	-0.2004364	-2.3212598
21	O	O5	0.1523201	0.6451422	-2.7587430
22	O	O6	-3.0060338	-1.4034235	-0.6105833
23	O	O7	3.4623370	0.9655407	1.7988125
24	C	C10	2.0280093	-0.8600411	-3.0795382
25	H	H2	1.8410672	-1.9366105	-3.1541152
26	H	H4	2.9734299	-0.7261178	-2.5441757
27	H	H6	2.0996319	-0.4270280	-4.0777856
28	C	C11	-2.7571404	-3.7775491	-1.0177980
29	H	H11	-3.6912996	-3.6911659	-1.5740472
30	H	H14	-2.8889829	-4.4719810	-0.1809043
31	H	H15	-1.9718836	-4.1837726	-1.6630800
32	C	C12	2.6566734	2.5085752	0.1422176
33	H	H13	2.4398494	2.1759676	-0.8780431
34	H	H16	3.6806011	2.8807693	0.1842243
35	H	H17	1.9652285	3.3223208	0.3846842
36	H	H20	0.3621038	-1.7122547	1.1570597

Cartesian coordinates for geometry minimized radical $3^{\cdot ax}$:

$\Delta H_{(rel)}$ = 0.0 kcal/mol



	Atom		X	Y	Z
1	H	H1	-0.1836608	-1.3496810	-0.7436864
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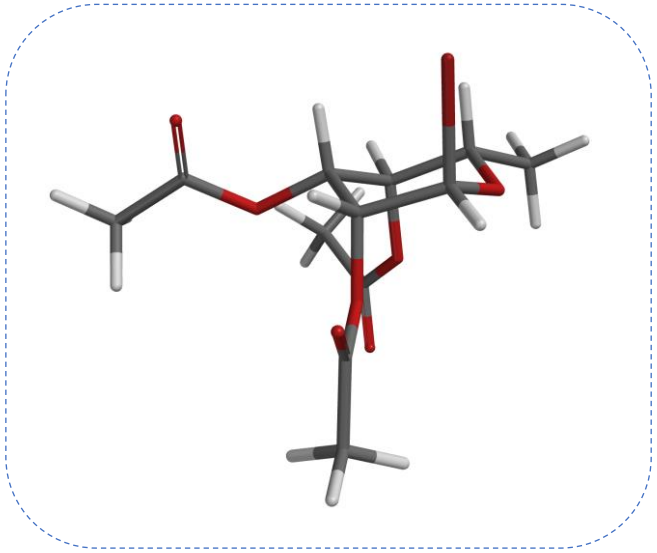
3	C	C14	0.3902202	1.9119742	0.4224868
4	C	C15	-1.6359148	0.9619910	1.3306656
5	O	O8	-0.9660444	2.0752540	0.9142688
6	C	C17	-1.5574907	-0.2998323	0.5567523
7	C	C18	0.4378658	0.7099804	-0.5449796
8	H	H23	-0.1604632	0.9665407	-1.4230340
9	H	H25	0.5620088	2.8125780	-0.1724754
10	H	H26	-2.5305955	1.2086460	1.8911173

11	H	H28	-1.9216508	-1.1381958	1.1511574
12	C	C16	1.3695932	1.8893046	1.5925470
13	H	H18	2.3955088	1.7934393	1.2244338
14	H	H21	1.1624621	1.0585087	2.2696469
15	H	H27	1.2871769	2.8298469	2.1460482
16	O	O9	1.7891852	0.4477904	-0.9648035
17	O	O10	0.6935864	-1.0407849	1.1052838
18	O	O11	-2.3906862	-0.2416385	-0.6737062
19	C	C2	2.2387341	1.1041397	-2.0677799
20	C	C3	0.7153337	-2.3796191	1.3402597
21	C	C4	-3.7064280	-0.5129722	-0.5241134
22	O	O1	-4.2182151	-0.7880991	0.5440666
23	O	O2	1.5695831	1.9054118	-2.6869730
24	O	O3	0.0534472	-3.1774163	0.7090721
25	C	C5	1.6572301	-2.7081758	2.4681656
26	H	H2	2.6664572	-2.3596819	2.2257900
27	H	H4	1.6649824	-3.7855526	2.6362934
28	H	H5	1.3394762	-2.1918338	3.3800774
29	C	C6	-4.4313674	-0.4228144	-1.8439728
30	H	H6	-5.4814968	-0.6814722	-1.7030363
31	H	H7	-3.9737647	-1.0997987	-2.5724413
32	H	H8	-4.3506346	0.5943113	-2.2420963
33	C	C7	3.6529288	0.6993640	-2.3900578
34	H	H3	3.7101559	-0.3848380	-2.5302668
35	H	H9	4.3130318	0.9593670	-1.5557263
36	H	H10	3.9823203	1.2110885	-3.2948341

Cartesian coordinates for geometry minimized 13:

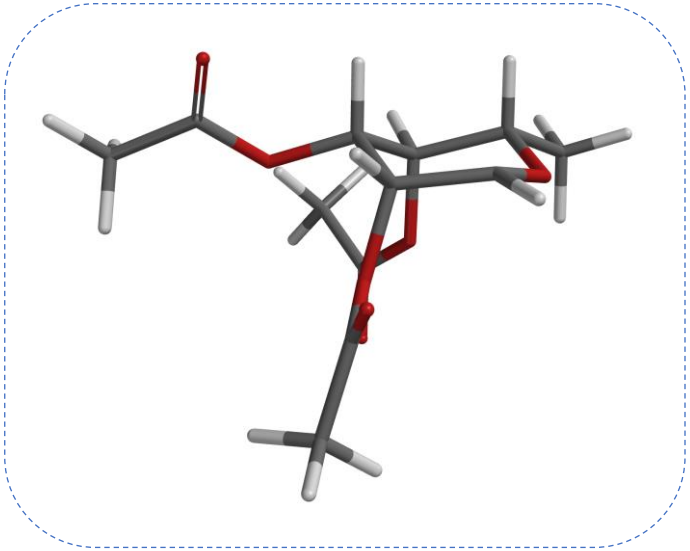


	Atom		X	Y	Z
1	H	H1	-0.7257712	-1.7334645	-1.7162723
2	C	C1	-0.7852974	-1.2177229	-0.7583564
3	C	C3	-0.7922985	1.0984048	0.3281765
4	O	O1	-2.4501837	-0.6189802	0.9302358
5	C	C4	-2.2328651	0.8084665	0.7716056
6	C	C6	-2.1739989	-1.4155119	-0.1345958
7	C	C2	-0.4653857	0.2710464	-0.9201353
8	H	H7	-2.8999839	1.1548625	-0.0278347
9	H	H3	-1.0767867	0.6466797	-1.7449872
10	H	H5	-0.7246022	2.1599682	0.0810021
11	H	H12	-2.3468204	-2.4500388	0.1497156
12	Br	Br1	-3.5850866	-1.1750733	-1.6630453
13	O	O2	0.1771054	-1.7941013	0.1472073
14	O	O3	0.9213784	0.4666182	-1.2367103

15	O	O4	0.0936905	0.7657724	1.4079718
16	C	C5	-2.6179416	1.4571155	2.0895959
17	H	H8	-1.9813753	1.0967056	2.9016915
18	H	H9	-3.6610787	1.2279354	2.3247469
19	H	H10	-2.5102557	2.5438516	2.0115419
20	C	C7	0.4386220	-3.1229447	-0.0001984
21	C	C8	1.1820411	1.5107547	1.7488531
22	C	C9	1.2763153	0.3979162	-2.5514070
23	O	O5	0.4817476	0.1737375	-3.4393811
24	O	O6	-0.1286434	-3.8238429	-0.8119925
25	O	O7	1.9091348	1.0622789	2.6088951
26	C	C10	2.7537283	0.6296167	-2.7174326
27	H	H2	3.3117239	-0.1420553	-2.1765546
28	H	H4	3.0330794	1.5986850	-2.2916255
29	H	H6	3.0117650	0.5987504	-3.7764345
30	C	C11	1.4974567	-3.5668705	0.9723840
31	H	H11	1.7030095	-4.6281474	0.8294176
32	H	H14	1.1561819	-3.3873990	1.9973062
33	H	H15	2.4117162	-2.9835511	0.8230080
34	C	C12	1.4048653	2.8470090	1.0805082
35	H	H13	1.5200442	2.7361376	-0.0012018
36	H	H16	2.3118041	3.2840388	1.4992070
37	H	H17	0.5629657	3.5233521	1.2650951

Cartesian coordinates for geometry minimized radical $13^{\cdot ax}$:

$\Delta H_{(rel)}$ = 1.5 kcal/mol



	Atom		X	Y	Z
1	H	H1	-0.8313249	-1.9991061	-1.4565215
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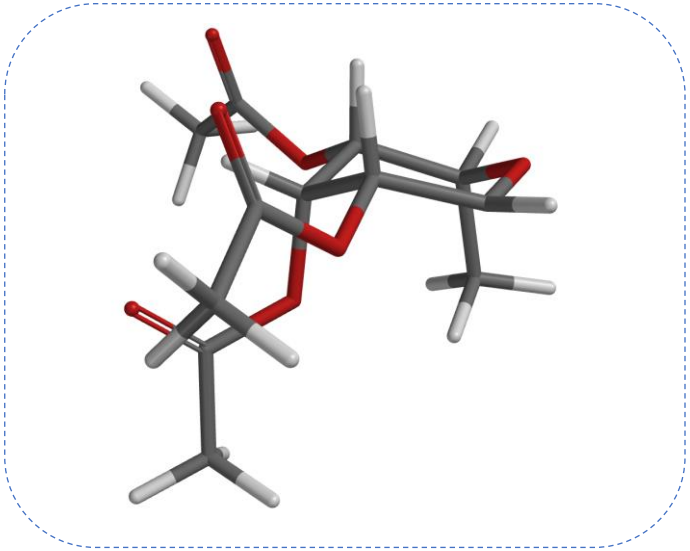
3	C	C3	-0.9330590	1.1007588	0.1225156
4	O	O1	-2.6487813	-0.4806822	0.9102514
5	C	C4	-2.4002942	0.8898675	0.5225426
6	C	C6	-2.2054488	-1.4531566	0.0638949
7	C	C2	-0.5605975	0.0979764	-0.9721691
8	H	H7	-3.0048428	1.0957656	-0.3711620
9	H	H3	-1.1650344	0.3269817	-1.8549086
10	H	H5	-0.8324021	2.1162483	-0.2667340
11	H	H12	-2.6203524	-2.4268071	0.2996081
12	O	O2	0.2122405	-1.7993474	0.3246673
13	O	O3	0.8273517	0.2912930	-1.2944517
14	O	O4	-0.1110990	0.9105351	1.2862429

15	C	C5	-2.8535045	1.7685836	1.6756918
16	H	H8	-2.2636534	1.5640733	2.5731671
17	H	H9	-3.9083724	1.5790106	1.8941198
18	H	H10	-2.7378553	2.8240724	1.4084939
19	C	C7	0.4520838	-3.1272371	0.3660024
20	C	C8	0.9621200	1.6883880	1.5922722
21	C	C9	1.2330507	-0.0713384	-2.5403852
22	O	O5	0.4826839	-0.5371858	-3.3727157
23	O	O6	-0.1773150	-3.9492092	-0.2736915
24	O	O7	1.6291067	1.3586610	2.5499113
25	C	C10	2.7054762	0.1850665	-2.7202551
26	H	H2	3.2740810	-0.3848365	-1.9780631
27	H	H4	2.9250983	1.2458630	-2.5602707
28	H	H6	3.0081834	-0.1086689	-3.7258782
29	C	C11	1.5909686	-3.4386402	1.3055068
30	H	H11	1.3459453	-3.0915311	2.3147275
31	H	H14	2.4951301	-2.9096193	0.9868942
32	H	H15	1.7741988	-4.5137786	1.3169829
33	C	C12	1.2453130	2.9187416	0.7628514
34	H	H13	1.4133318	2.6597652	-0.2860805
35	H	H16	2.1373172	3.3976540	1.1675168
36	H	H17	0.4080521	3.6239606	0.8094301

Cartesian coordinates for geometry minimized radical 13$^{\cdot eq}$:

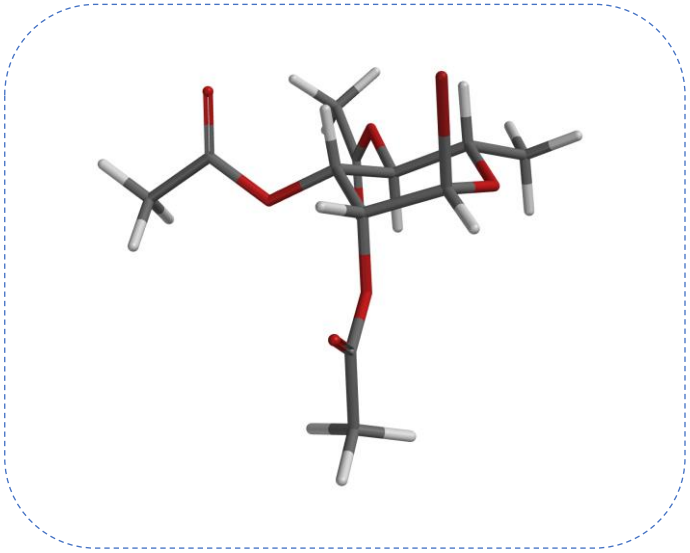
$\Delta H_{(rel)}$ = 0.0 kcal/mol



	Atom		X	Y	Z
1	H	H1	-1.6504114	-1.8936744	-2.5970153
2	C	C1	-1.4339950	-1.3733688	-1.6682273
3	C	C3	-0.2462696	0.3749491	-0.2990263
4	C	C5	-2.2518228	-0.9925096	0.5675134
5	C	C4	-1.5198975	0.3643147	0.5492245
6	O	O1	-2.4921479	-1.4099122	-0.7995691
7	C	C2	-0.6100968	-0.1205767	-1.7106110
8	H	H7	-2.1933076	1.1101778	0.1170703
9	H	H3	-1.1459546	0.6964017	-2.2151302
10	H	H5	0.1718343	1.3807944	-0.3470100
11	H	H9	-3.2545553	-0.8117321	0.9645796
12	O	O2	0.5819592	-0.4126510	-2.4671240
13	O	O3	0.7291607	-0.4996181	0.3020303
14	O	O4	-1.2394131	0.7263620	1.9126658

15	C	C6	-1.5997953	-2.1225058	1.3601640
16	H	H8	-0.6498907	-2.4231111	0.9145062
17	H	H10	-2.2752330	-2.9836653	1.3743639
18	H	H11	-1.4189852	-1.8049233	2.3910657
19	C	C7	1.1231080	0.6012942	-3.1939131
20	C	C8	-1.2628765	2.0493372	2.2279636
21	C	C9	2.0315405	-0.1200498	0.2739646
22	C	C10	2.8964938	-1.1478016	0.9559794
23	H	H14	2.5634221	-1.2907775	1.9890968
24	H	H15	3.9361325	-0.8190155	0.9421039
25	H	H16	2.8040637	-2.1106883	0.4427289
26	C	C11	-0.9969186	2.2509042	3.6963744
27	H	H13	-0.9467655	3.3177280	3.9164767
28	H	H17	-0.0586664	1.7635901	3.9789243
29	H	H18	-1.7989664	1.7897057	4.2829011
30	C	C12	2.4138386	0.1685224	-3.8364910
31	H	H12	2.6646459	0.8486257	-4.6519611
32	H	H19	2.3482554	-0.8599443	-4.2002256
33	H	H20	3.2073389	0.2109568	-3.0810746
34	O	O5	0.6269525	1.7056814	-3.2781209
35	O	O6	-1.4784097	2.9250533	1.4161489
36	O	O7	2.4256329	0.9121267	-0.2303469

Cartesian coordinates for geometry minimized 17:

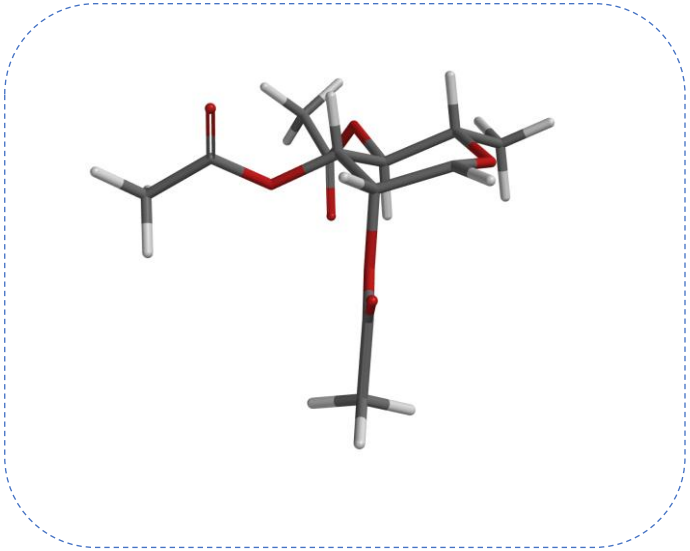


	Atom		X	Y	Z
1	H	H1	-2.0608544	0.6668668	-1.6907752
2	C	C1	-1.5701915	0.7002219	-0.7184726
3	C	C3	0.6022803	0.5811983	0.5259864
4	O	O1	-1.0915463	2.2491286	1.1029233
5	C	C4	0.3383375	2.0025092	1.0581291
6	C	C13	-1.8058839	2.0523215	-0.0375505
7	C	C2	-0.0787541	0.3901070	-0.8276506
8	H	H7	0.7785930	2.7286024	0.3631519
9	H	H3	0.3744566	1.0499729	-1.5704932
10	O	O2	-2.1518321	-0.3006244	0.1464557
11	O	O3	0.0804293	-0.9721245	-1.2544754
12	O	O4	2.0222458	0.4426316	0.3413209
13	C	C5	0.8587752	2.2316342	2.4659073
14	H	H8	0.4100538	1.5196472	3.1664386

15	H	H9	0.6188351	3.2482040	2.7910462
16	H	H10	1.9452023	2.1102579	2.4853197
17	C	C7	-3.4367167	-0.6763491	-0.1129406
18	C	C8	2.6615986	-0.5865928	0.9663729
19	C	C9	0.8075592	-1.2098104	-2.3831084
20	O	O5	1.3066034	-0.3363455	-3.0594723
21	O	O6	-4.1066672	-0.1803115	-0.9933248
22	O	O7	2.1045072	-1.3916850	1.6810708
23	C	C10	0.8912151	-2.6894910	-2.6479593
24	H	H2	-0.1151136	-3.1117372	-2.7346769
25	H	H4	1.3867308	-3.1878712	-1.8080509
26	H	H6	1.4506881	-2.8665806	-3.5670296
27	C	C11	-3.8727056	-1.7631718	0.8317713
28	H	H11	-4.9090335	-2.0319462	0.6251610
29	H	H14	-3.7736996	-1.4194473	1.8664779
30	H	H15	-3.2282537	-2.6403213	0.7119155
31	C	C12	4.1315593	-0.5624694	0.6407884
32	H	H13	4.2749922	-0.6236693	-0.4427659
33	H	H16	4.6291845	-1.3995492	1.1314886
34	H	H17	4.5712083	0.3818378	0.9788183
35	H	H18	0.2551502	-0.1669589	1.2404666
36	H	H12	-2.8577335	2.2194699	0.1803769
37	Br	Br1	-1.4412199	3.5424458	-1.4526408

Cartesian coordinates for geometry minimized radical $17^{\cdot ax}$:

$\Delta H_{(rel)}$ = 0.0 kcal/mol

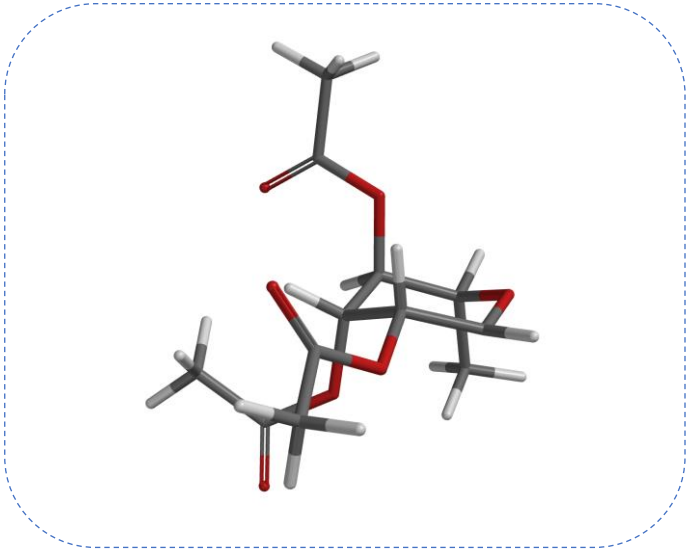


	Atom		X	Y	Z
1	H	H1	-0.7547131	-1.9425542	-1.7442715
2	C	C1	-0.7799793	-1.5019725	-0.7474874
3	C	C3	-0.7156587	0.6300211	0.5704624
4	O	O1	-2.4309716	-1.0624864	1.0270596
5	C	C4	-2.1567011	0.3573053	1.0390430
6	C	C6	-2.0901610	-1.7587647	-0.0949568
7	C	C2	-0.4851820	-0.0009889	-0.7994578
8	H	H7	-2.8427530	0.8338507	0.3260654
9	H	H3	-1.1542262	0.4541067	-1.5347890
10	H	H12	-2.5195825	-2.7545877	-0.1090153
11	O	O2	0.3247805	-2.1029725	0.0336429
12	O	O3	0.8770139	0.2646176	-1.1787359
13	O	O4	-0.5726335	2.0575750	0.4469101
14	C	C5	-2.4361044	0.8473468	2.4498014

15	H	H8	-1.7570709	0.3726301	3.1660975
16	H	H9	-3.4664444	0.6074999	2.7294757
17	H	H10	-2.3070533	1.9317110	2.5047522
18	C	C7	0.6351401	-3.3895775	-0.2383384
19	C	C8	0.4834963	2.6591171	1.0590711
20	C	C9	1.1510575	0.3398772	-2.5063259
21	O	O5	0.3167087	0.1669507	-3.3713058
22	O	O6	0.0561002	-4.0621353	-1.0699799
23	O	O7	1.3033392	2.0685639	1.7294070
24	C	C10	2.6062590	0.6559628	-2.7327659
25	H	H2	3.2272315	-0.1443824	-2.3164329
26	H	H4	2.8734716	1.5828615	-2.2154932
27	H	H6	2.7981677	0.7543728	-3.8016550
28	C	C11	1.7779205	-3.8618523	0.6258284
29	H	H11	2.0280967	-4.8924807	0.3712929
30	H	H14	1.4943739	-3.7989914	1.6817980
31	H	H15	2.6512800	-3.2180329	0.4801507
32	C	C12	0.4723416	4.1405979	0.7860045
33	H	H13	0.5458680	4.3212262	-0.2914828
34	H	H16	1.3097579	4.6139792	1.2996243
35	H	H17	-0.4711582	4.5770762	1.1297890
36	H	H18	0.0079884	0.2545297	1.2962172

Cartesian coordinates for geometry minimized radical $17^{\cdot eq}$:

$\Delta H_{(rel)}$ = 8.98 kcal/mol



	Atom		X	Y	Z
1	H	H5	0.7519739	-0.7209737	0.2785472
2	C	C13	0.1480022	0.1576744	0.0611033
3	C	C14	-1.1209893	1.2994864	-1.8736909
4	C	C15	-2.2118879	1.0211411	0.2531821
5	O	O8	-2.3386496	1.1546531	-1.1014865
6	C	C17	-1.2113291	0.0311123	0.7692400
7	C	C18	-0.0661882	0.2673920	-1.4619655
8	H	H22	-1.5529729	-1.0034074	0.6178849
9	H	H26	-3.1651316	1.1175751	0.7652285
10	H	H29	0.8854693	0.4931415	-1.9476762
11	O	O9	-1.1018844	0.2658050	2.1889935
12	O	O10	0.7975401	1.3481177	0.5331204
13	O	O11	-0.5411544	-1.0187917	-1.9322322
14	H	H28	-1.4295087	1.0491380	-2.8922608

15	C	C16	-0.6401166	2.7494878	-1.8330587
16	H	H19	0.2288954	2.8781751	-2.4873362
17	H	H24	-0.3630963	3.0536683	-0.8215550
18	H	H25	-1.4421372	3.4012362	-2.1925054
19	C	C1	-0.5965809	-0.7336230	2.9506511
20	C	C2	2.1282840	1.3999012	0.8322482
21	C	C3	0.3950479	-1.9398714	-2.2804803
22	C	C4	-0.2552347	-3.2018227	-2.7812877
23	H	H7	-0.9182817	-3.6095435	-2.0111991
24	H	H8	0.5123009	-3.9328715	-3.0367860
25	H	H9	-0.8684746	-2.9802368	-3.6609356
26	C	C5	2.9541598	0.1393713	0.7318044
27	H	H4	3.9924971	0.4023749	0.9354504
28	H	H10	2.8793794	-0.3222382	-0.2580857
29	H	H11	2.6219784	-0.5988772	1.4709513
30	C	C6	-0.6052018	-0.3545865	4.4084800
31	H	H3	-0.0286698	0.5640546	4.5586062
32	H	H12	-0.1761540	-1.1639824	5.0000601
33	H	H13	-1.6312176	-0.1568685	4.7361108
34	O	O1	-0.1938566	-1.7855466	2.4927950
35	O	O2	1.5906378	-1.7424707	-2.1921486
36	O	O3	2.5725514	2.4722056	1.1802330