Supporting Information

A chlorine-free microwave-assisted, ionic liquid-catalyzed esterification of arylsulfonic acids by alcohols; An experimental and theoretical study

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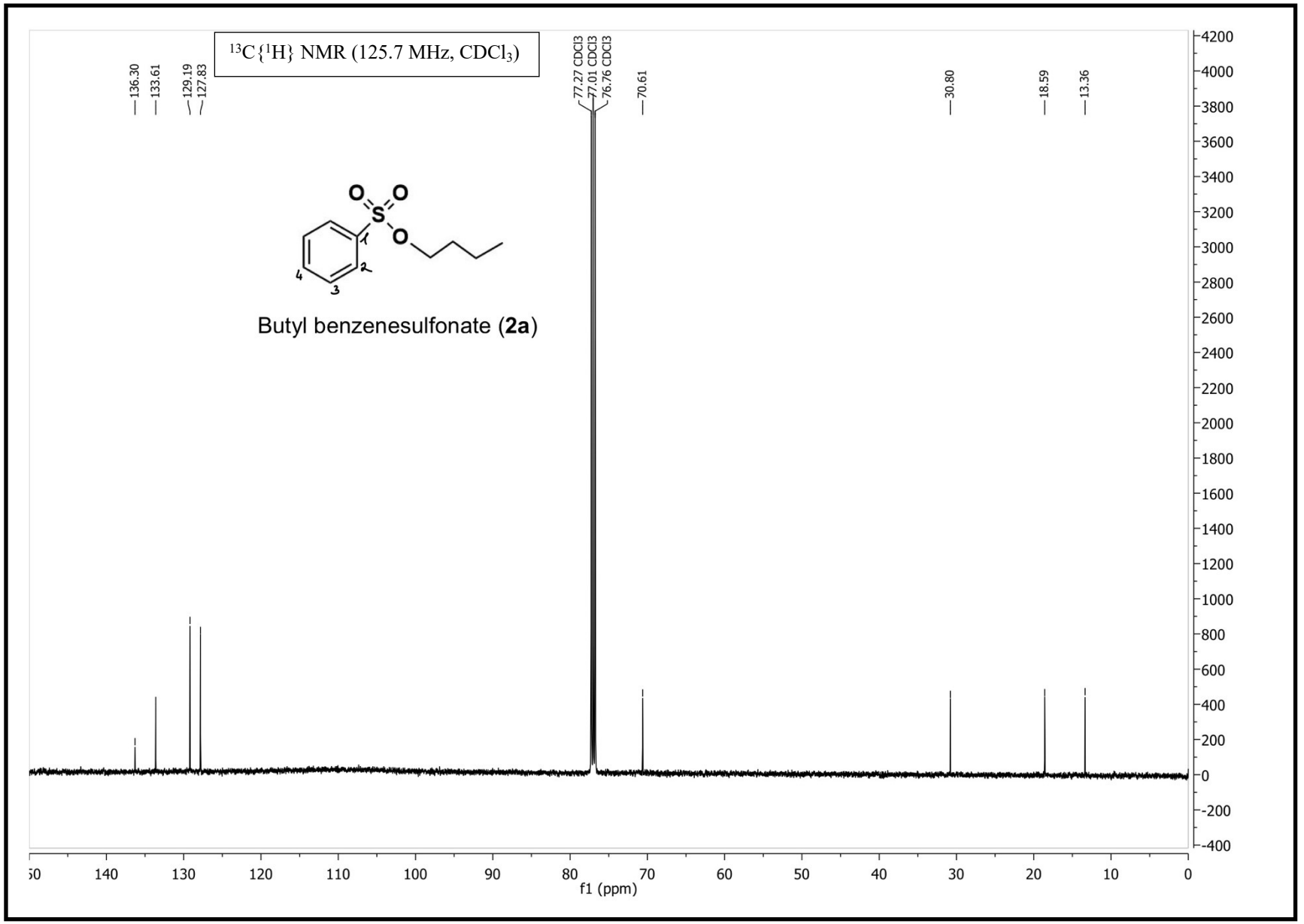
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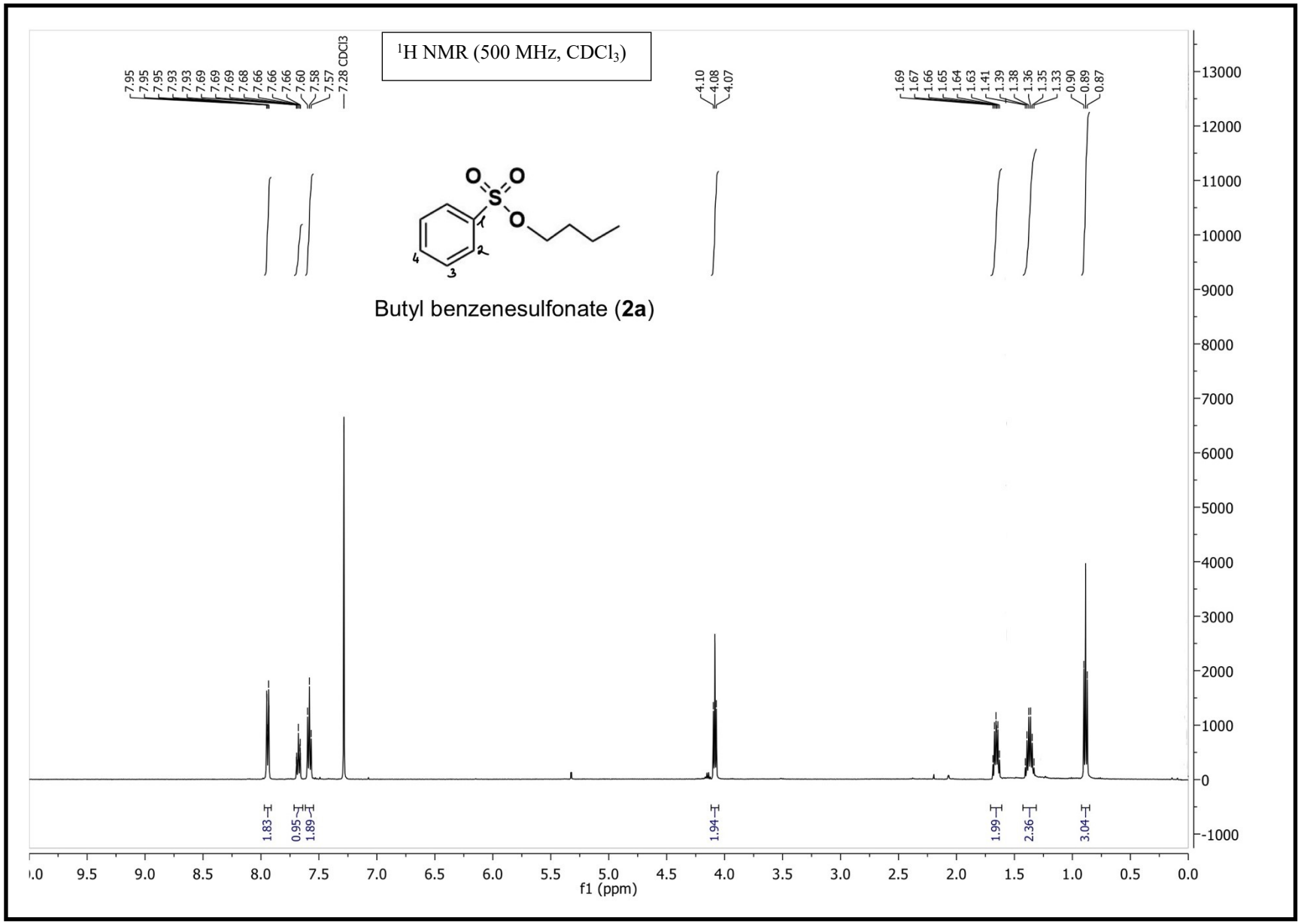
133.61
129.19
127.83
77.27 CDCl3
77.01 CDCl3
76.76 CDCl3
70.61
30.80
18.59
13.36
Butyl benzenesulfonate (2a)
f1 (ppm)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7.95
7.95
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7.69
7.69
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7.66
7.66
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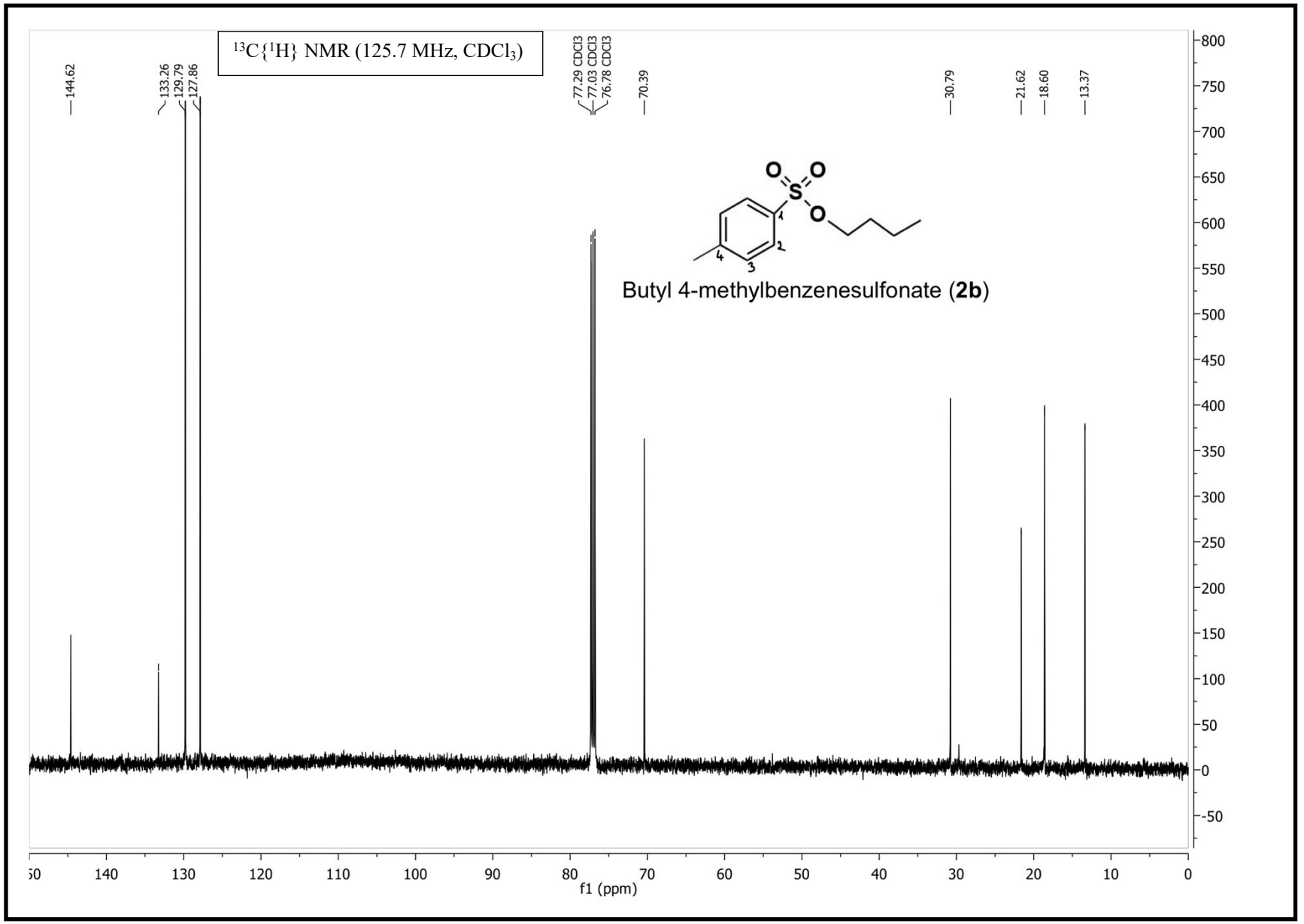
7.57
7.28 CDCl3
4.10
4.08
4.07
1.69
1.67
1.66
1.65
1.64
1.63
1.41
1.39
1.38
1.36
1.35
1.33
0.90
0.89
0.87
Butyl benzenesulfonate (**2a**)
1.83
0.95
1.89
1.94
1.99
2.36
3.04
f1 (ppm)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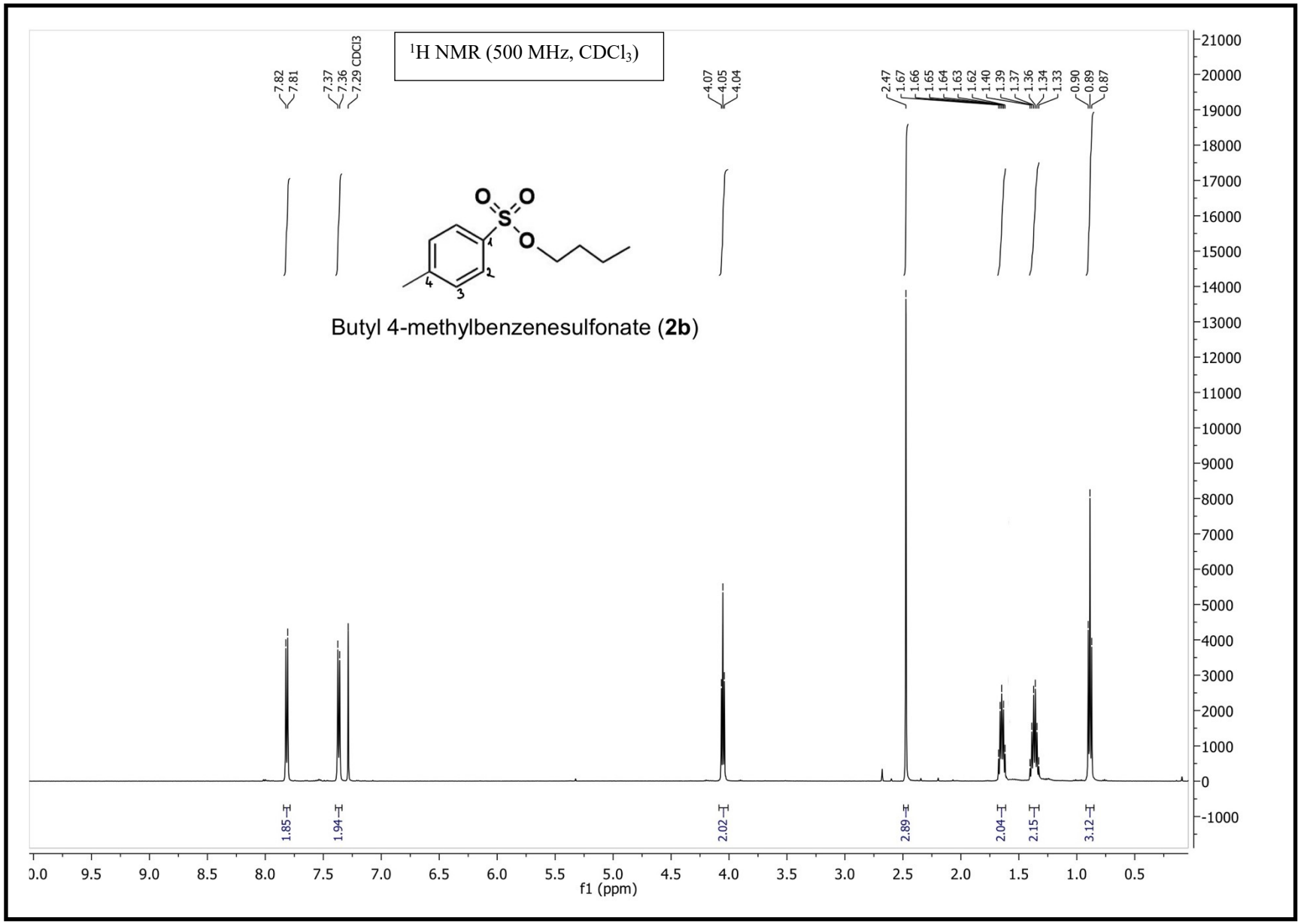
129.79
127.86
77.29 CDCl3
77.03 CDCl3
76.78 CDCl3
70.39
30.79
21.62
18.60
13.37
Butyl 4-methylbenzenesulfonate (**2b**)
f1 (ppm)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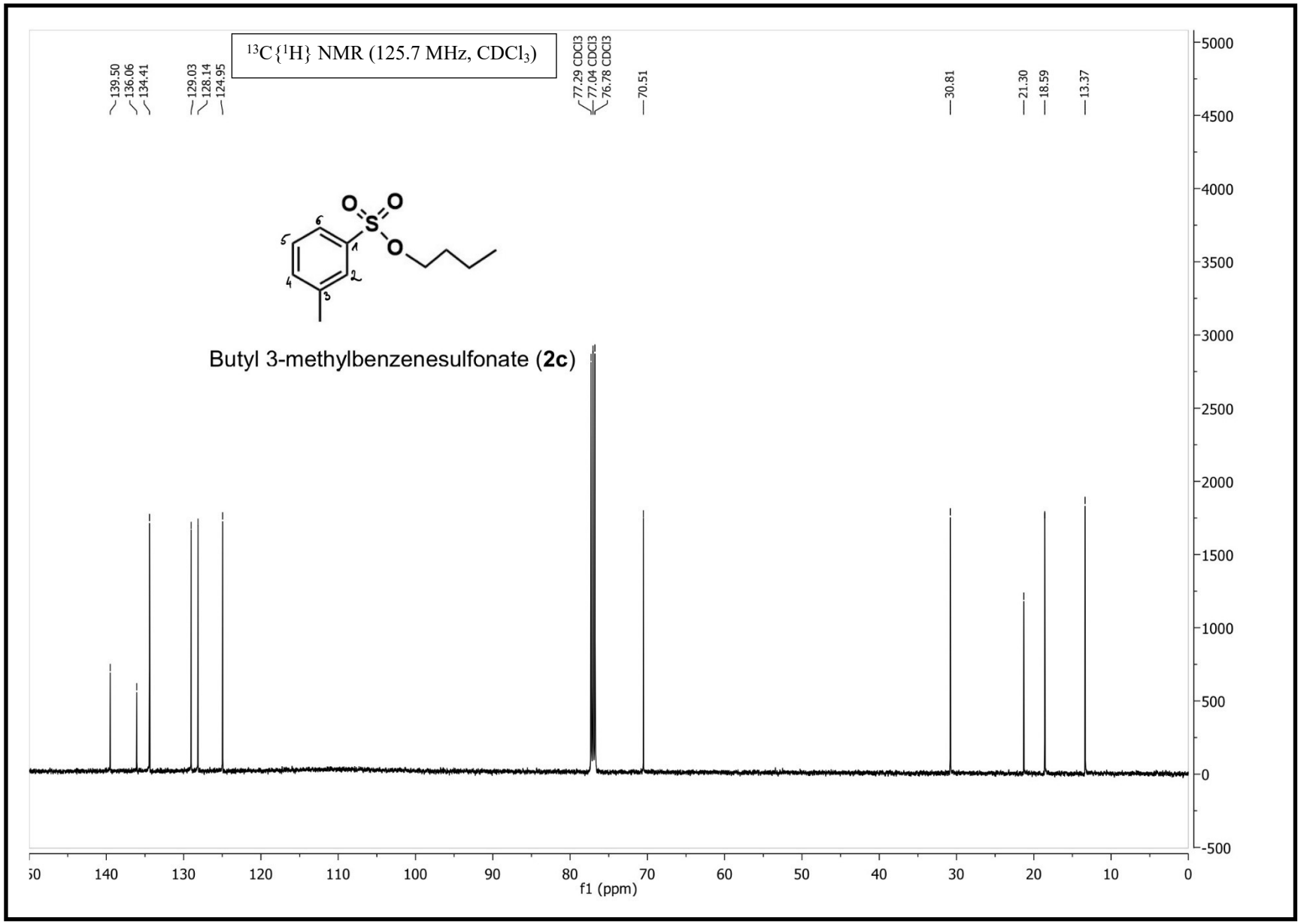
7.81
7.37
7.36
7.29 CDCl3
4.07
4.05
4.04
2.47
1.67
1.66
1.65
1.64
1.63
1.62
1.40
1.39
1.37
1.36
1.34
1.33
0.90
0.89
0.87
Butyl 4-methylbenzenesulfonate (2b)
1.85
1.94
2.02
2.89
2.04
2.15
3.12
f1 (ppm)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136.06
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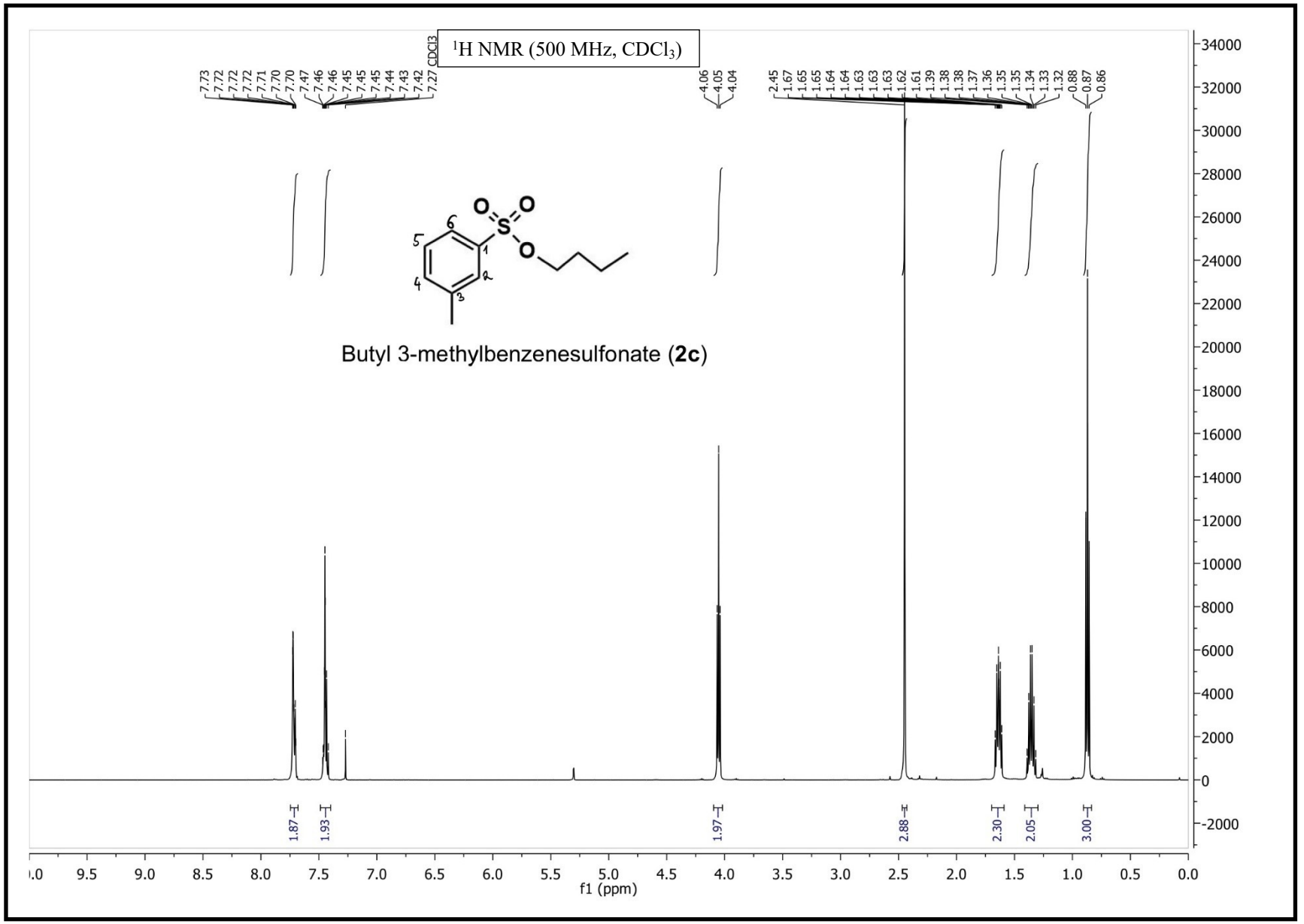
129.03
128.14
124.95
77.29 CDCl3
77.04 CDCl3
76.78 CDCl3
70.51
30.81
21.30
18.59
13.37
Butyl 3-methylbenzenesulfonate (2c)
f1 (ppm)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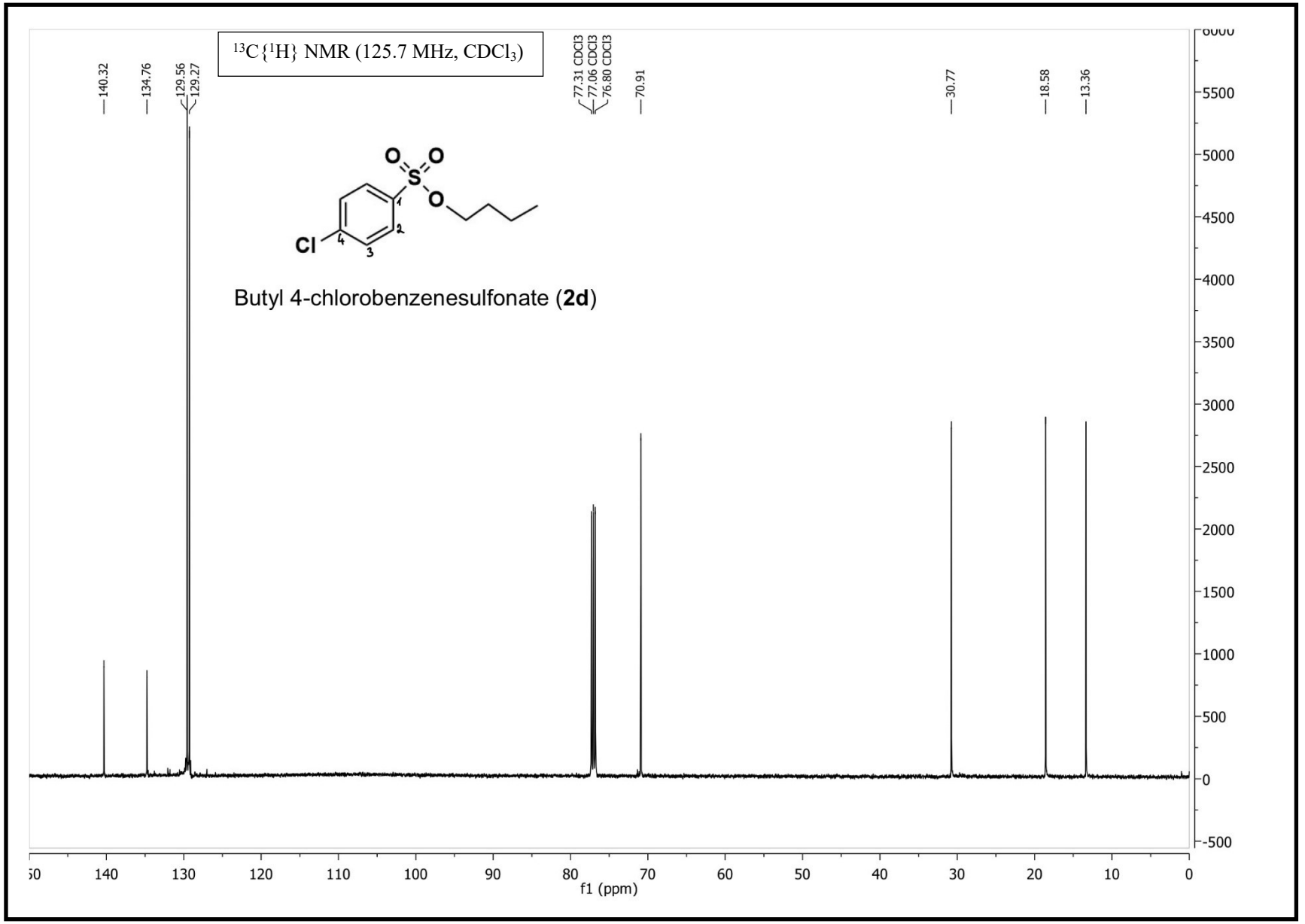
f1 (ppm)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134.76
129.56
129.27
77.31 CDCl3
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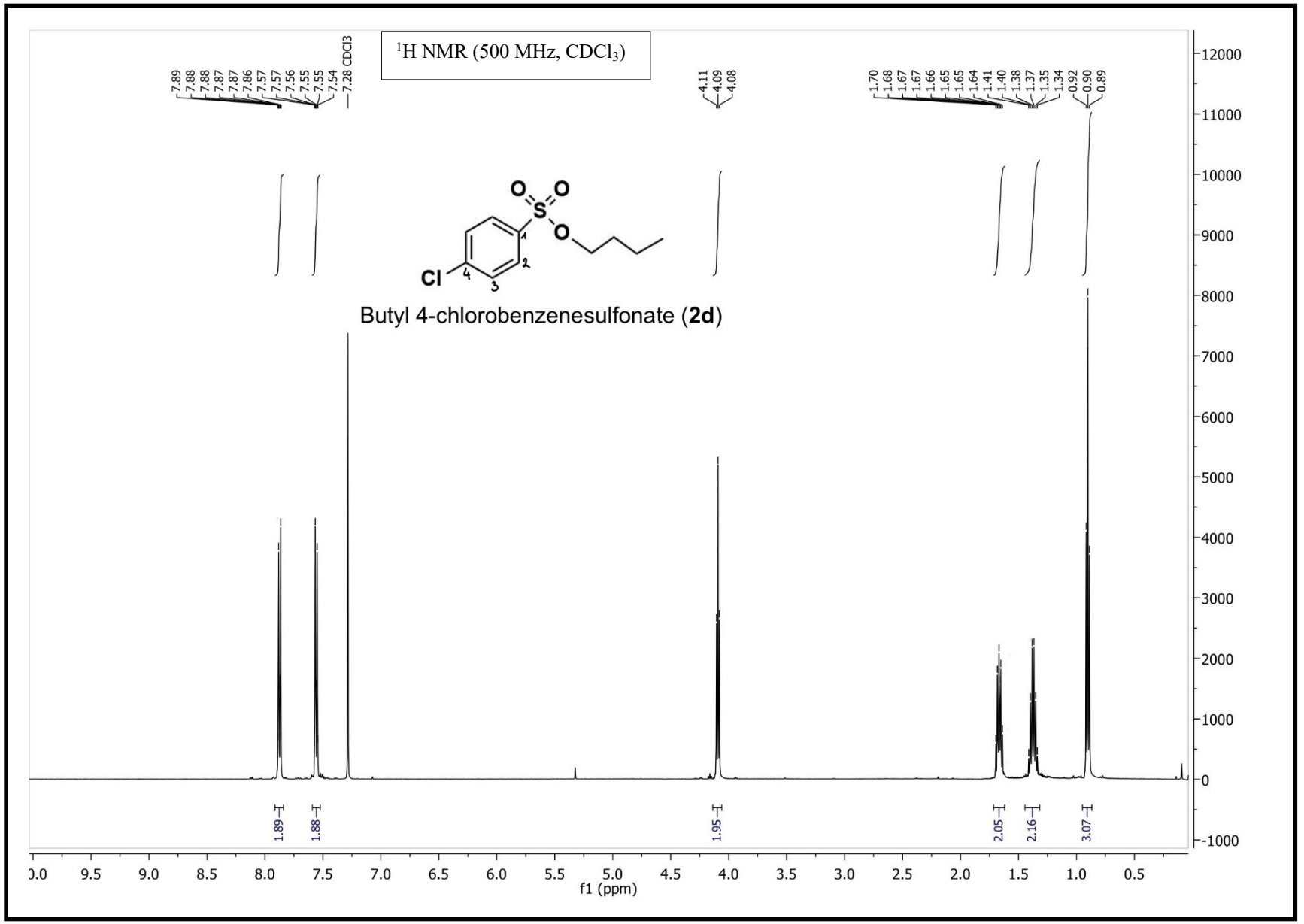
70.91
30.77
18.58
13.36
Butyl 4-chlorobenzenesulfonate (**2d**)
f1 (ppm)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7.88
7.88
7.87
7.87
7.86
7.57
7.57
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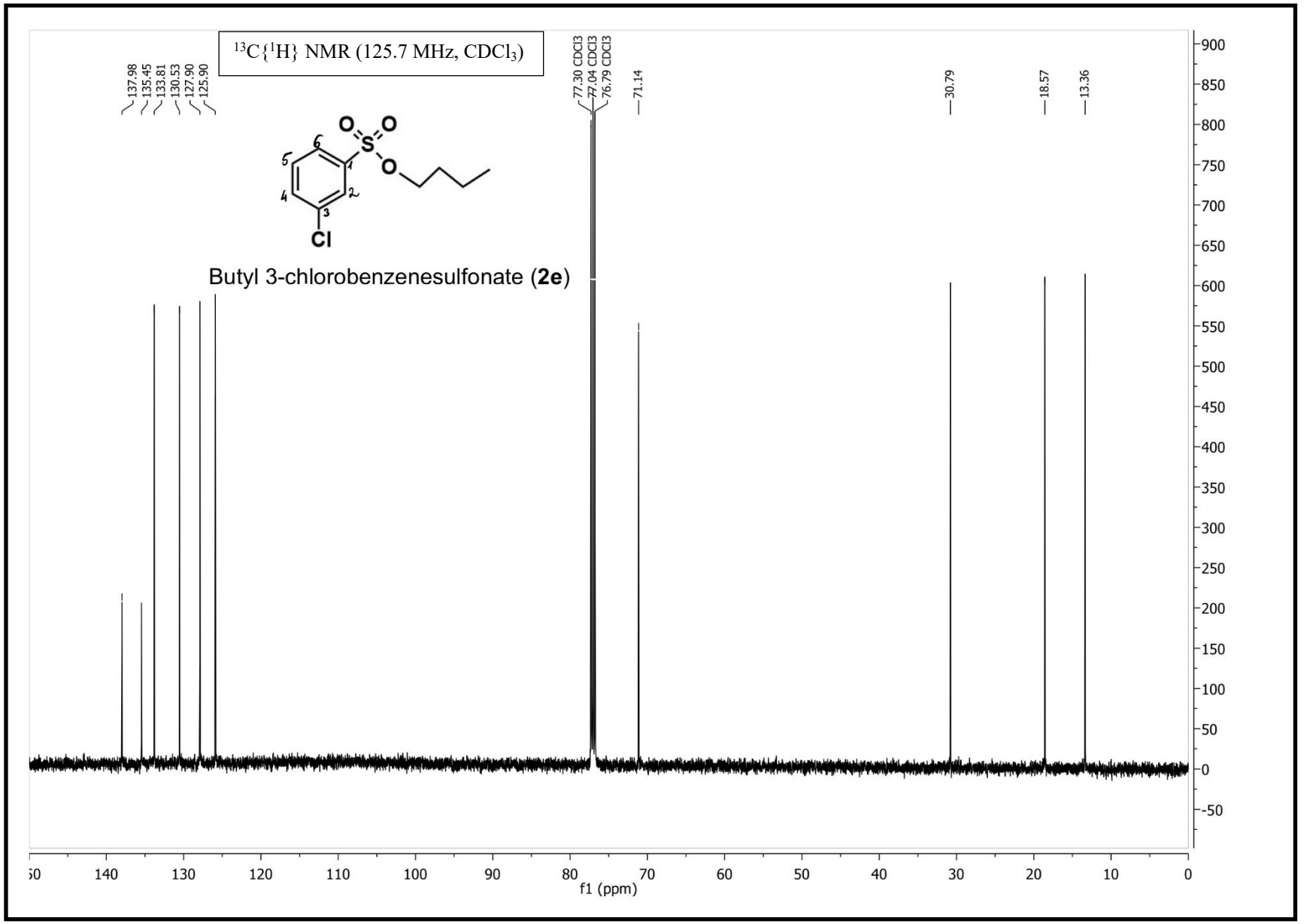
7.55
7.54
7.28 CDCl3
4.11
4.09
4.08
1.70
1.68
1.67
1.67
1.66
1.65
1.65
1.64
1.41
1.40
1.38
1.37
1.35
1.34
0.92
0.90
0.89
Butyl 4-chlorobenzenesulfonate (2d)
1.89
1.88
1.95
2.05
2.16
3.07
f1 (ppm)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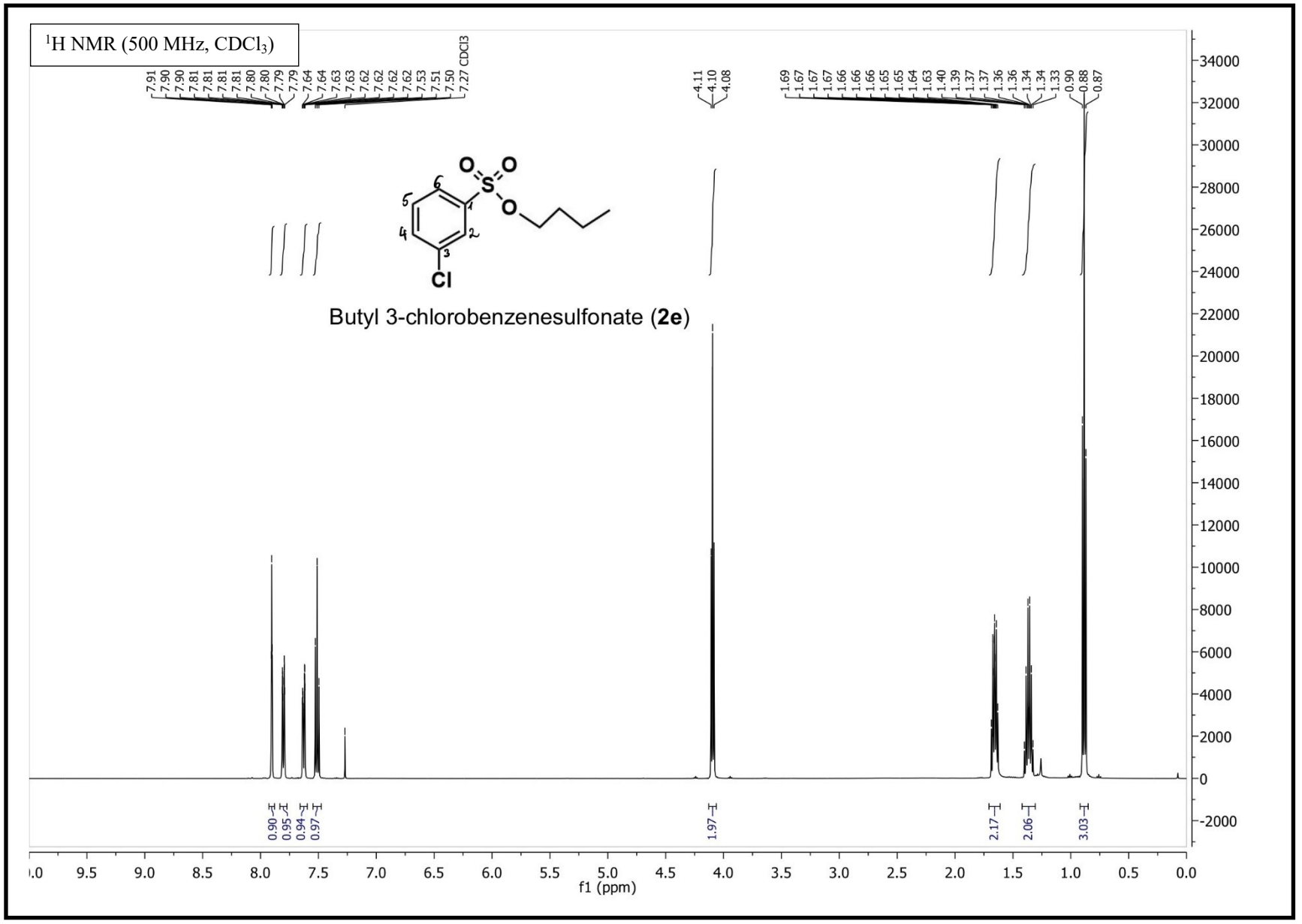
135.45
133.81
130.53
127.90
125.90
77.30 CDCl3
77.04 CDCl3
76.79 CDCl3
71.14
30.79
18.57
13.36
Butyl 3-chlorobenzenesulfonate (**2e**)
f1 (ppm)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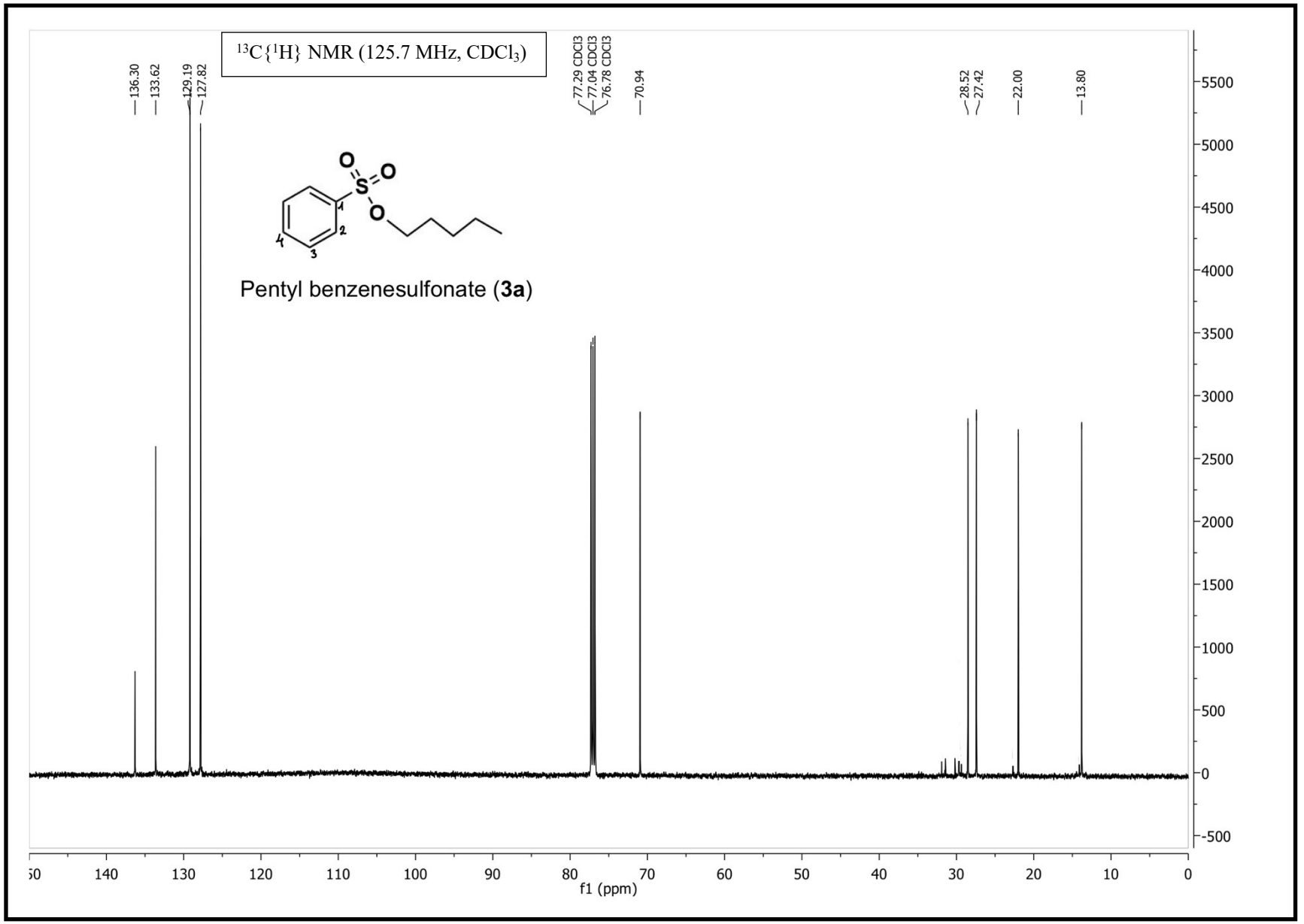
Butyl 3-chlorobenzenesulfonate (**2e**)
f1 (ppm)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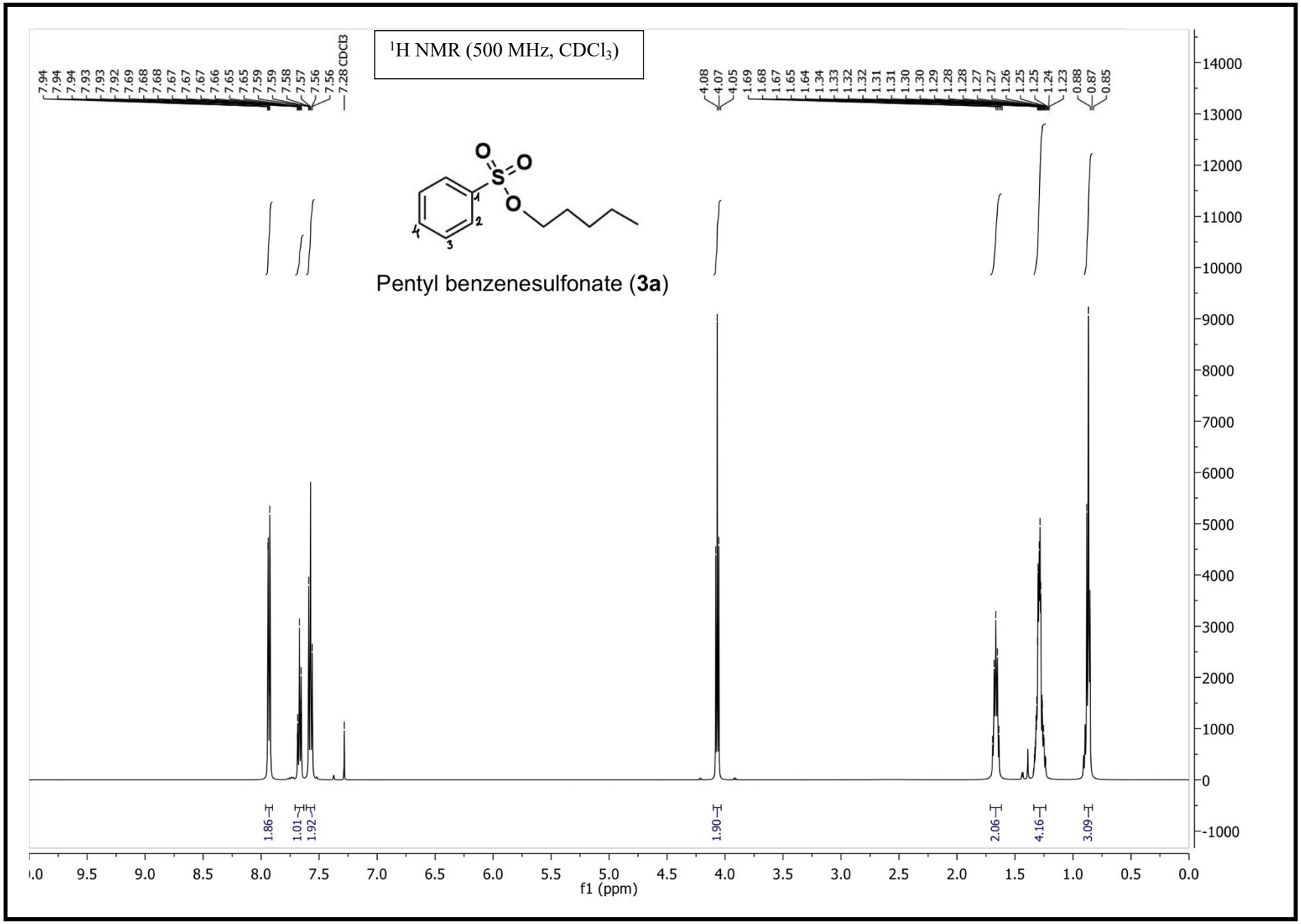
136.30
133.62
129.19
127.82
77.29 CDCl3
77.04 CDCl3
76.78 CDCl3
70.94
28.52
27.42
22.00
13.80
Pentyl benzenesulfonate (3a)
f1 (ppm)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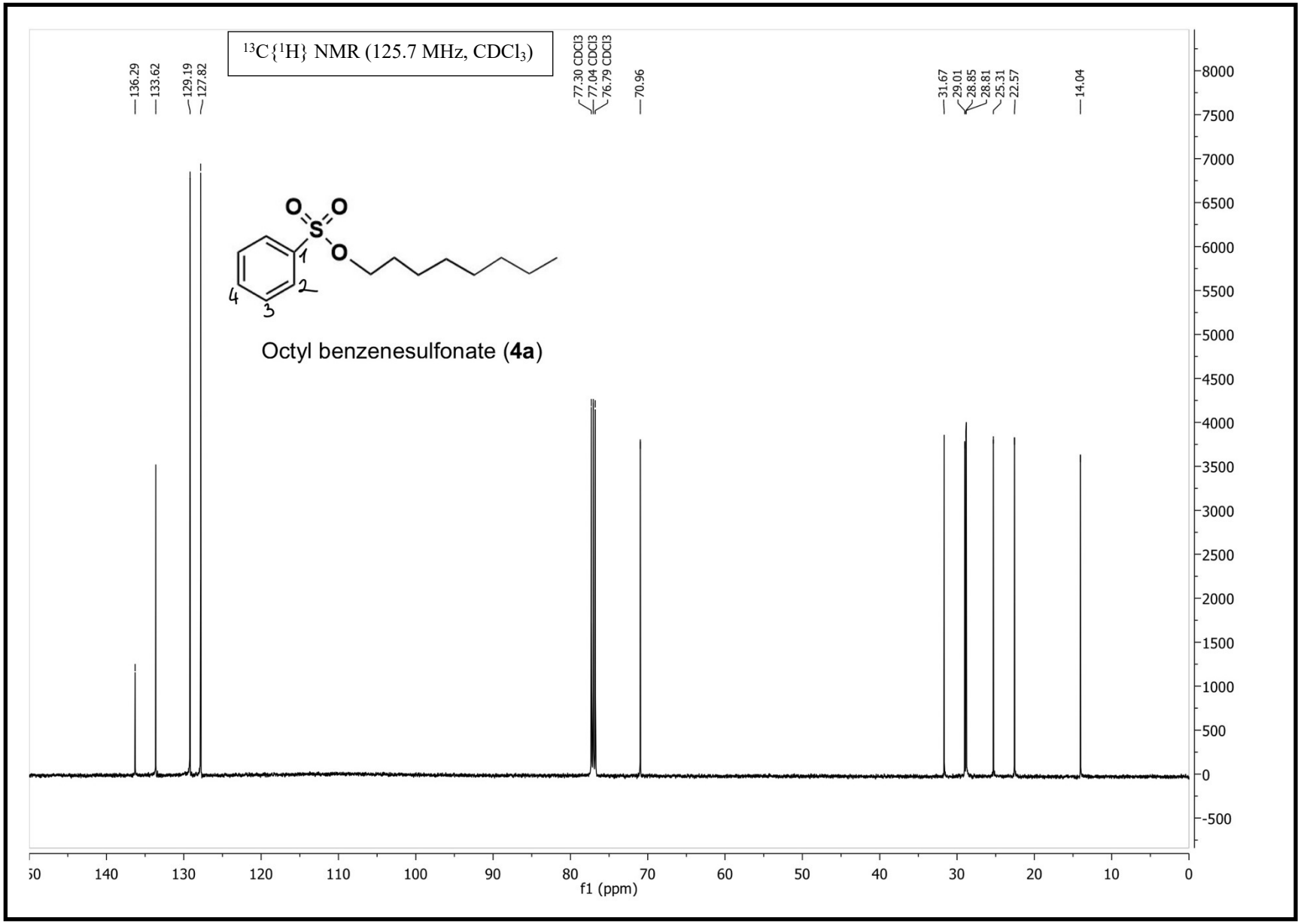
Pentyl benzenesulfonate (**3a**)
f1 (ppm)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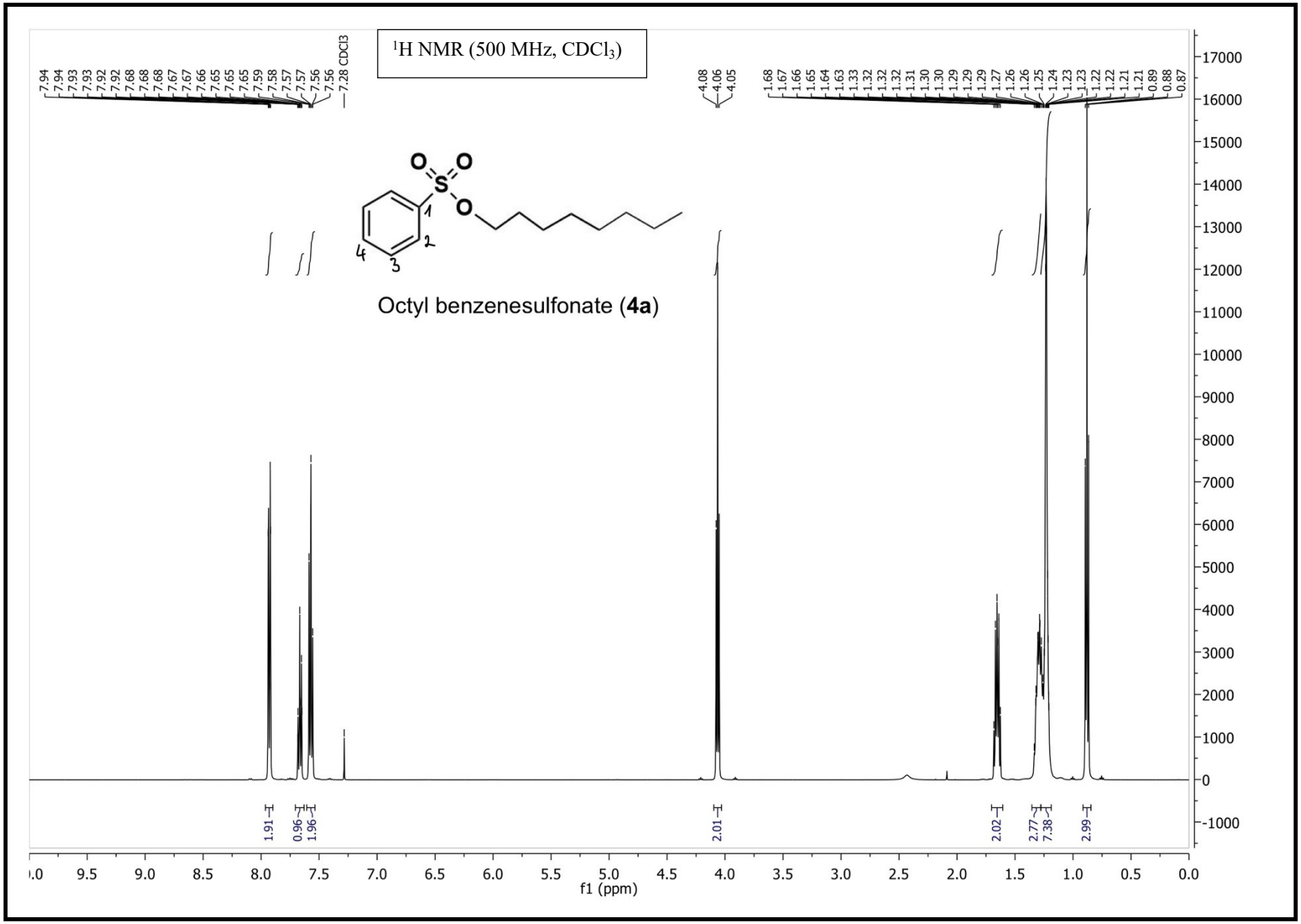
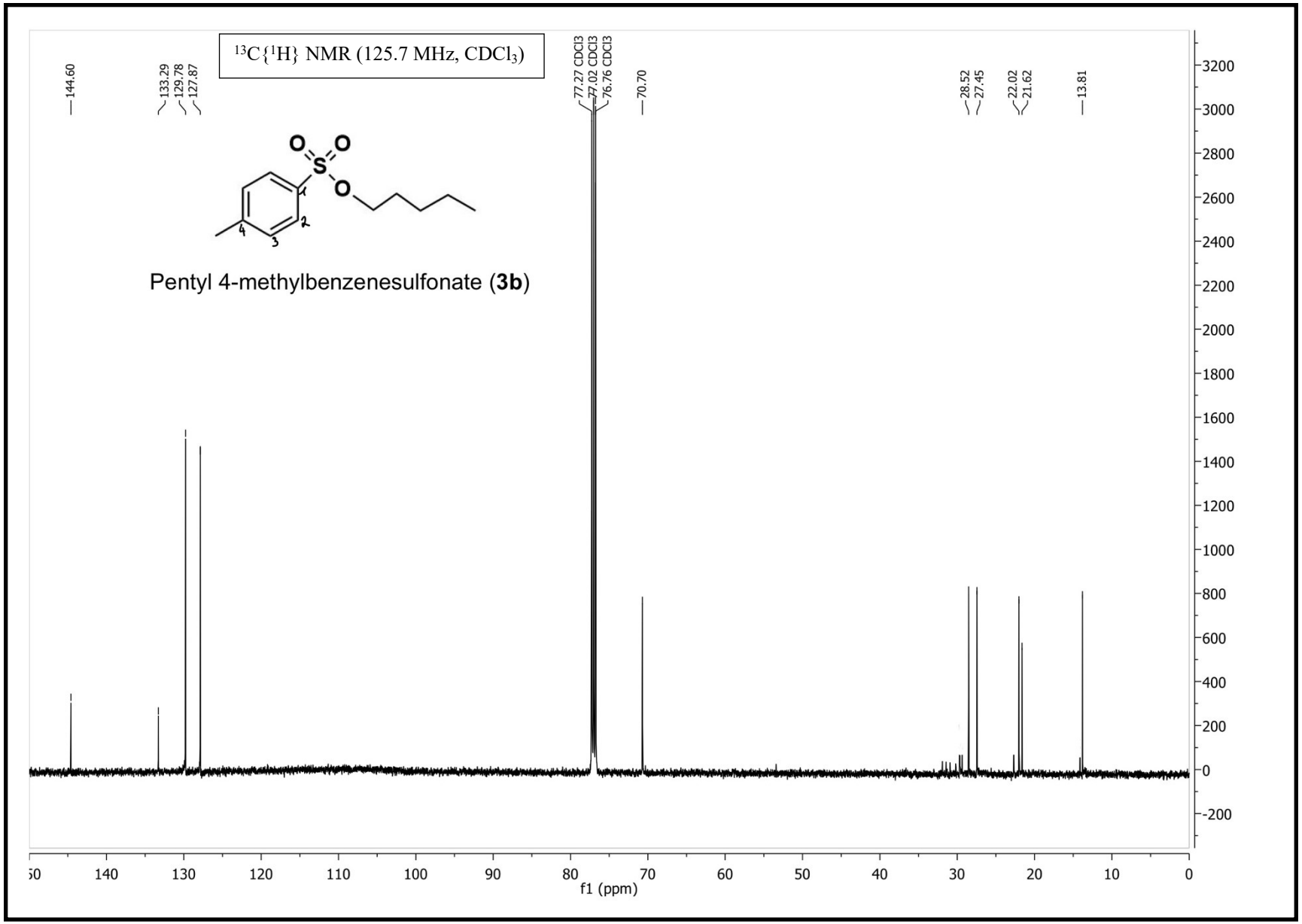
133.62
129.19
127.82
77.30 CDCl3
77.04 CDCl3
76.79 CDCl3
70.96
31.67
29.01
28.85
28.81
25.31
22.57
14.04
Octyl benzenesulfonate (4a)
f1 (ppm)


^{1}H NMR (500 MHz, $CDCl_3$)
Octyl benzenesulfonate (**4a**)
f1 (ppm)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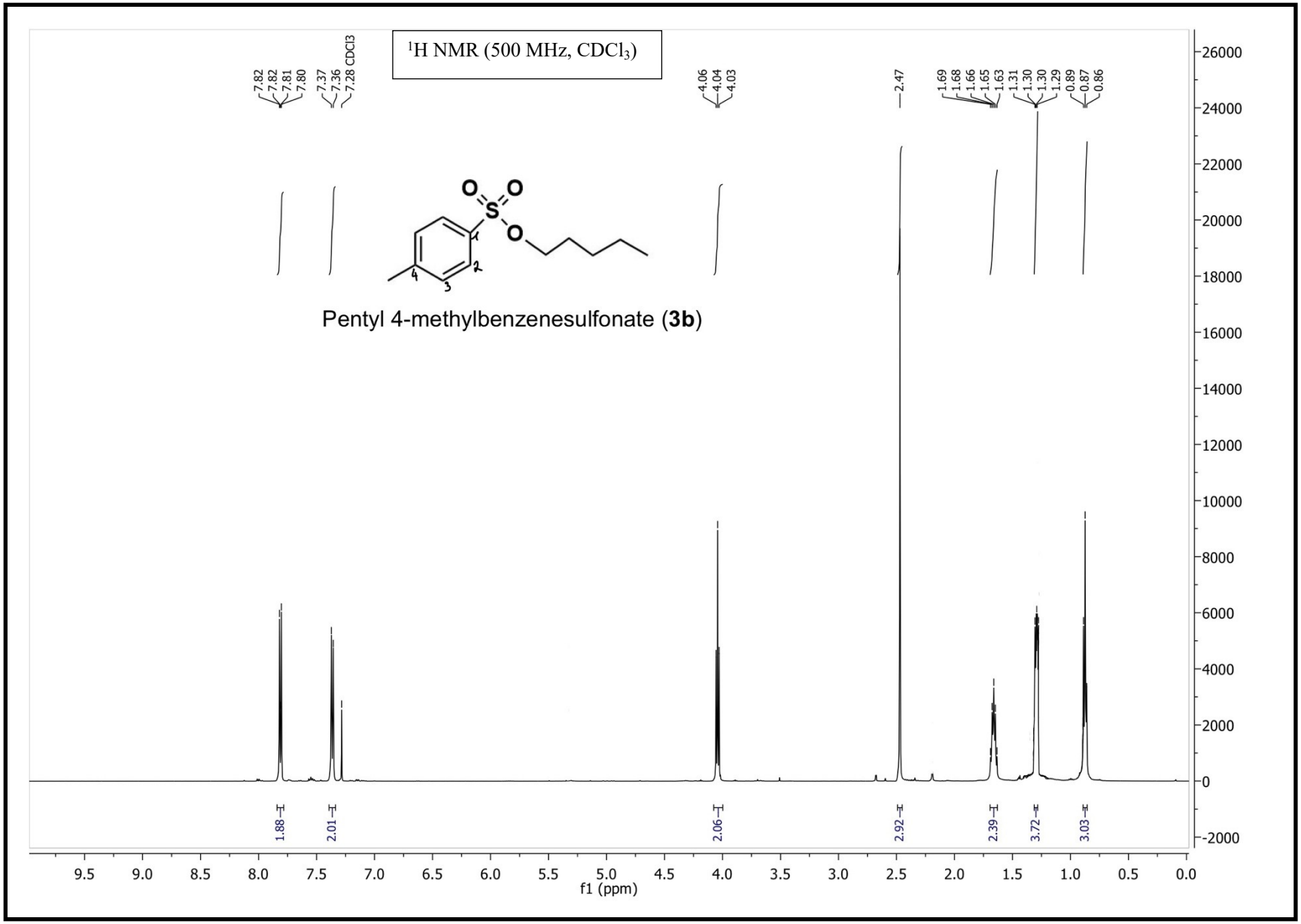
133.29
129.78
127.87
77.27 CDCl3
77.02 CDCl3
76.76 CDCl3
70.70
28.52
27.45
22.02
21.62
13.81
Pentyl 4-methylbenzenesulfonate (**3b**)
f1 (ppm)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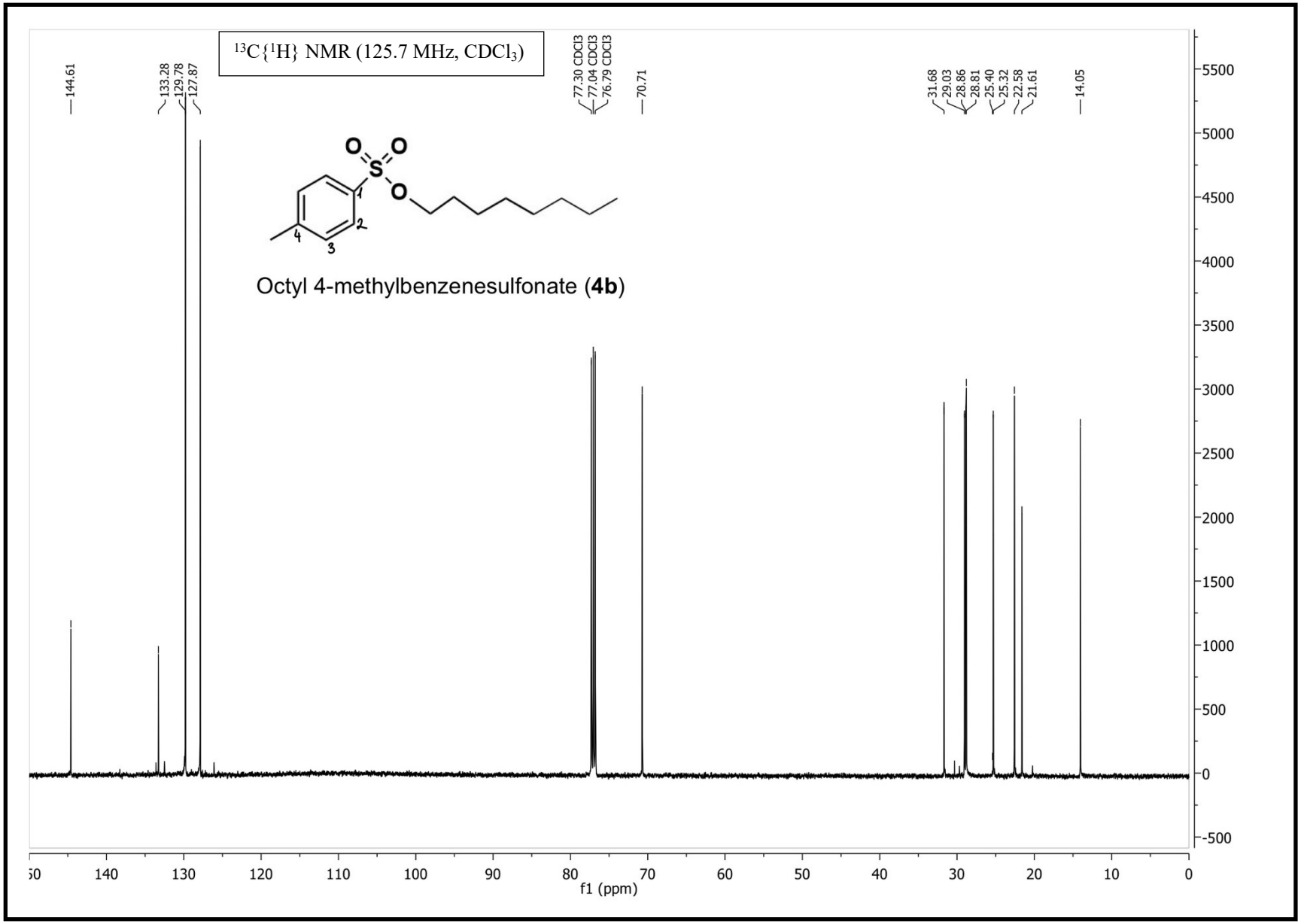
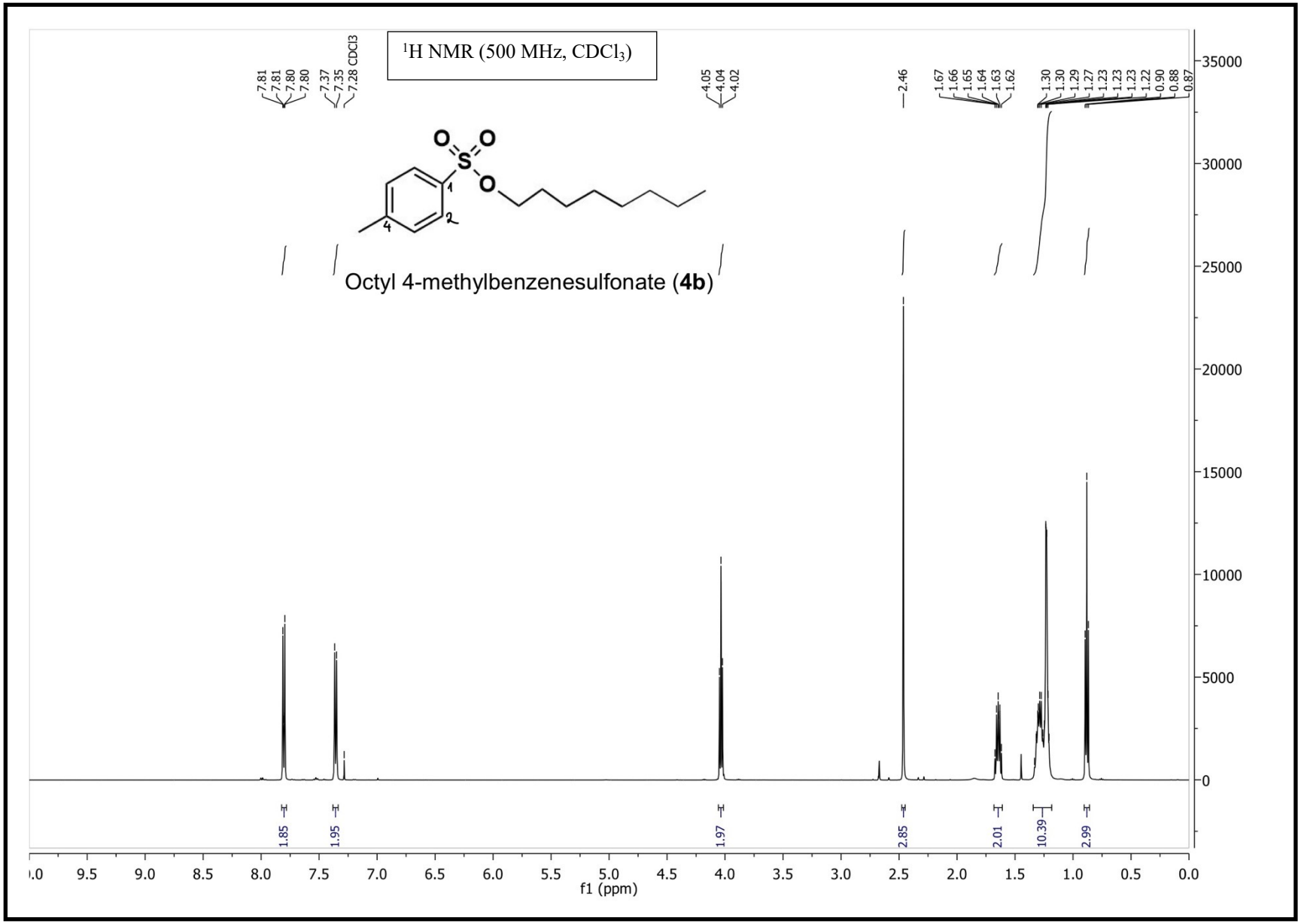
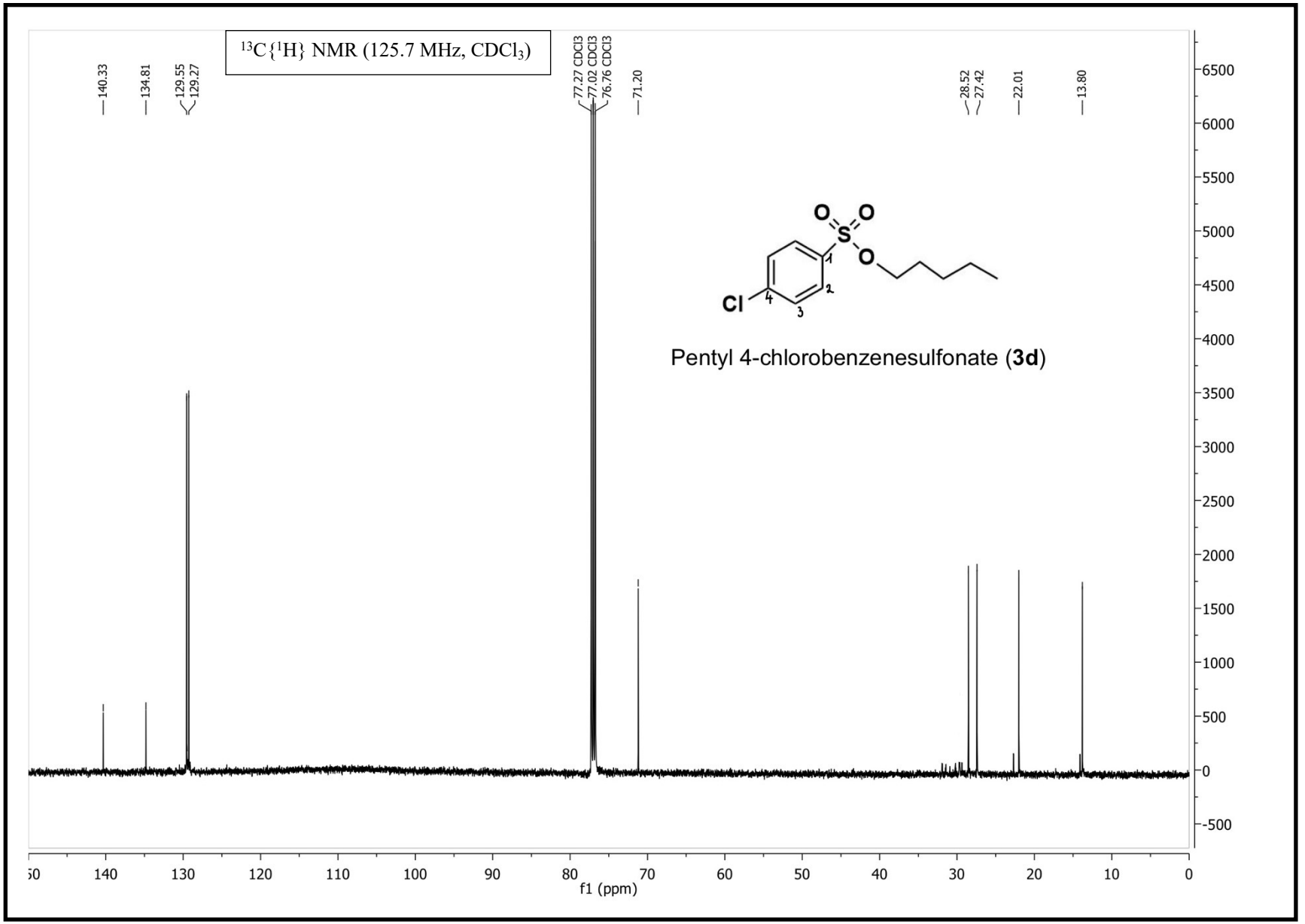
7.82
7.82
7.81
7.80
7.37
7.36
7.28 CDCl3
4.06
4.04
4.03
2.47
1.69
1.68
1.66
1.65
1.63
1.31
1.30
1.30
1.29
0.89
0.87
0.86
Pentyl 4-methylbenzenesulfonate (**3b**)
1.88
2.01
2.06
2.92
2.39
3.72
3.03
f1 (ppm)


$^{13}C\{^{1}H\}$ NMR (125.7 MHz, $CDCl_3$)
144.61
133.28
129.78
127.87
77.30 CDCl3
77.04 CDCl3
76.79 CDCl3
70.71
31.68
29.03
28.86
28.81
25.40
25.32
22.58
21.61
14.05
Octyl 4-methylbenzenesulfonate (**4b**)
f1 (ppm)


^{1}H NMR (500 MHz, $CDCl_3$)
Octyl 4-methylbenzenesulfonate (**4b**)
7.81
7.81
7.80
7.80
7.37
7.35
7.28 CDCl3
4.05
4.04
4.02
2.46
1.67
1.66
1.65
1.64
1.63
1.62
1.30
1.30
1.29
1.27
1.23
1.23
1.23
1.22
0.90
0.88
0.87
35000
30000
25000
20000
15000
10000
5000
0
1.85
1.95
1.97
2.85
2.01
10.39
2.99
f1 (ppm)


$^{13}C\{^{1}H\}$ NMR (125.7 MHz, $CDCl_3$)
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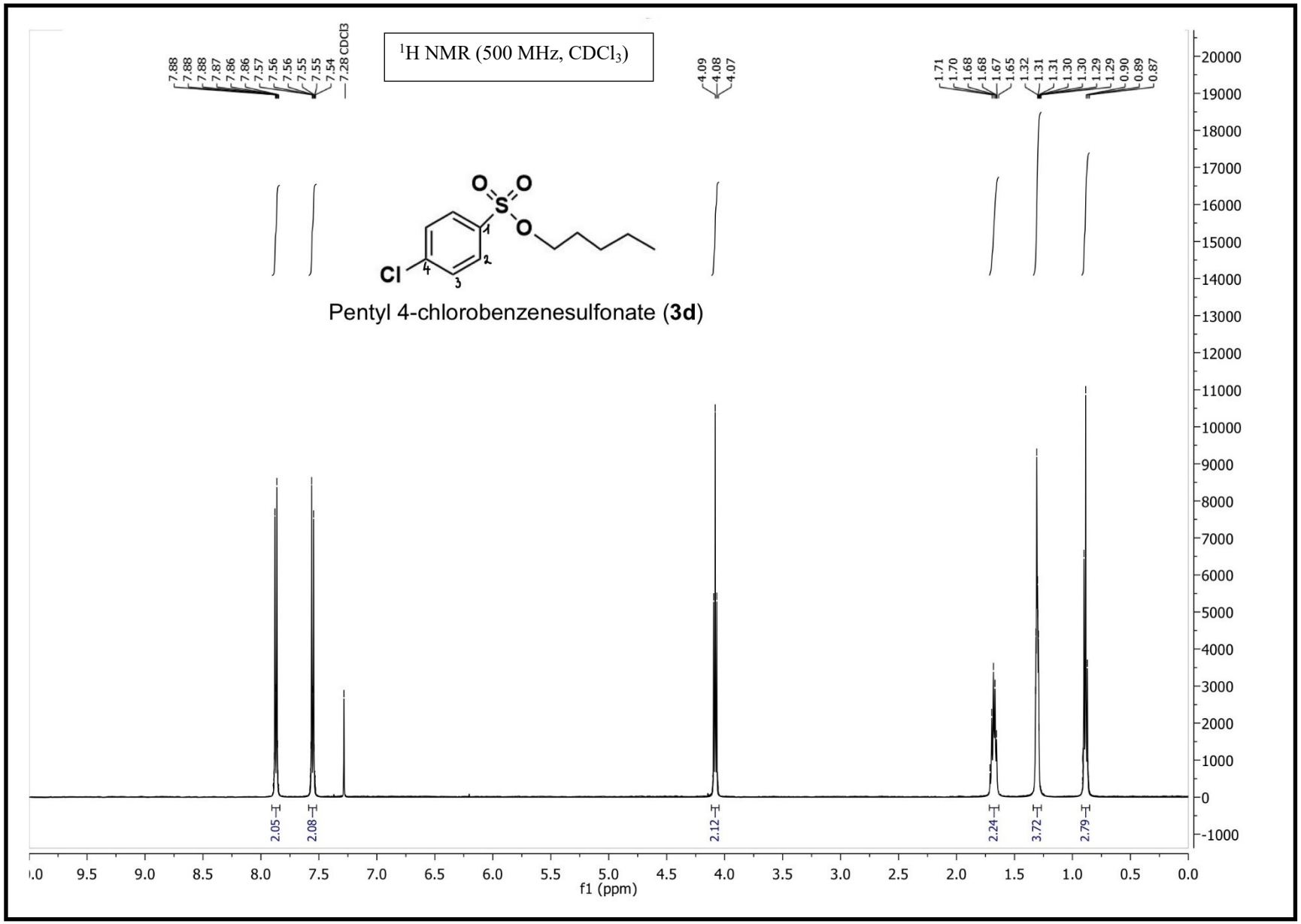
134.81
129.55
129.27
77.27 CDCl3
77.02 CDCl3
76.76 CDCl3
71.20
28.52
27.42
22.01
13.80
Pentyl 4-chlorobenzenesulfonate (**3d**)
f1 (ppm)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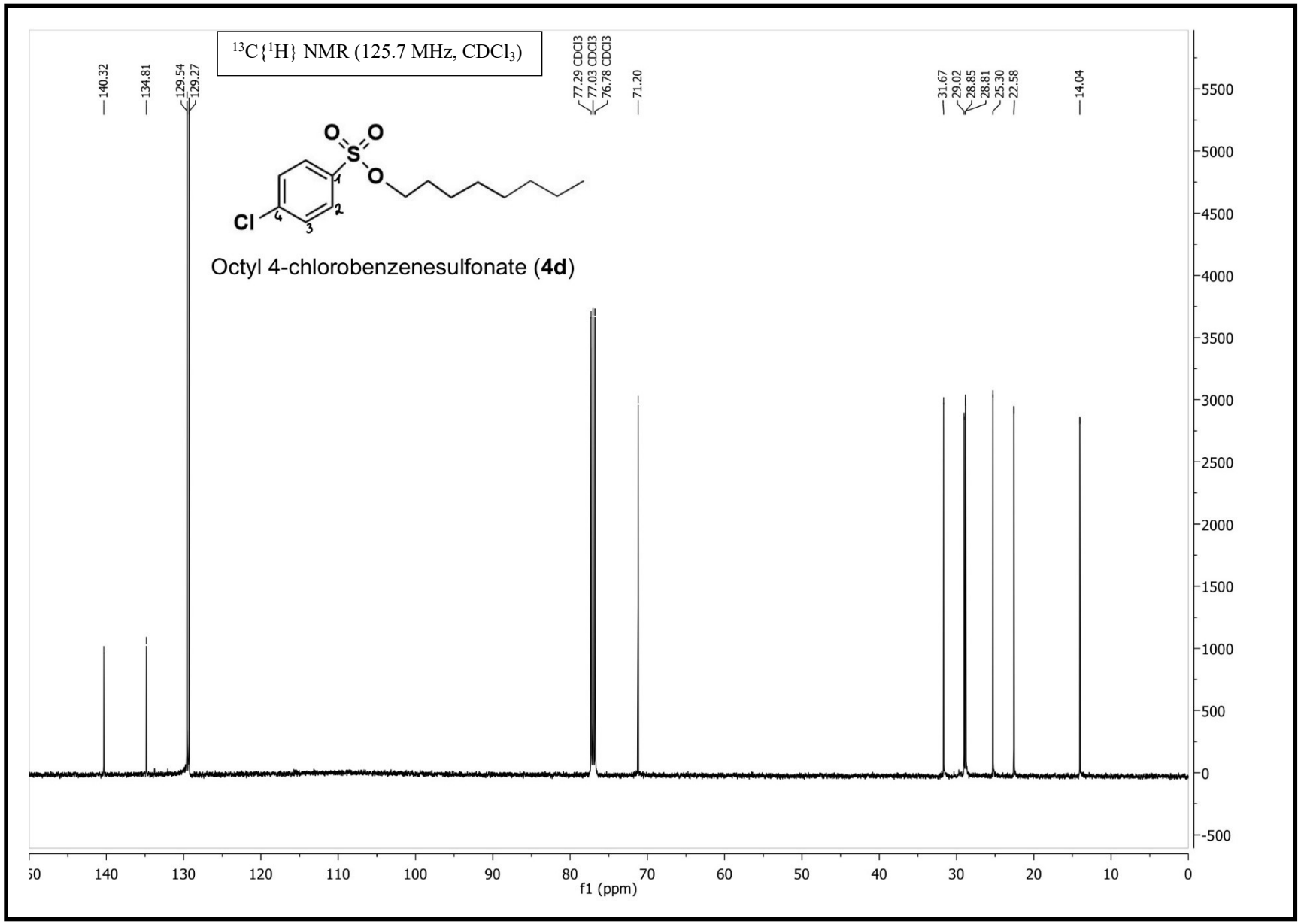
7.88
7.88
7.87
7.86
7.86
7.57
7.56
7.56
7.55
7.55
7.54
7.28 CDCl3
4.09
4.08
4.07
1.71
1.70
1.68
1.68
1.67
1.65
1.32
1.31
1.31
1.30
1.30
1.29
1.29
0.90
0.89
0.87
Cl
Pentyl 4-chlorobenzenesulfonate (3d)
2.05
2.08
2.12
2.24
3.72
2.79
f1 (ppm)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134.81
129.54
129.27
77.29 CDCl3
77.03 CDCl3
76.78 CDCl3
71.20
31.67
29.02
28.85
28.81
25.30
22.58
14.04
Cl
Octyl 4-chlorobenzenesulfonate (**4d**)
f1 (ppm)

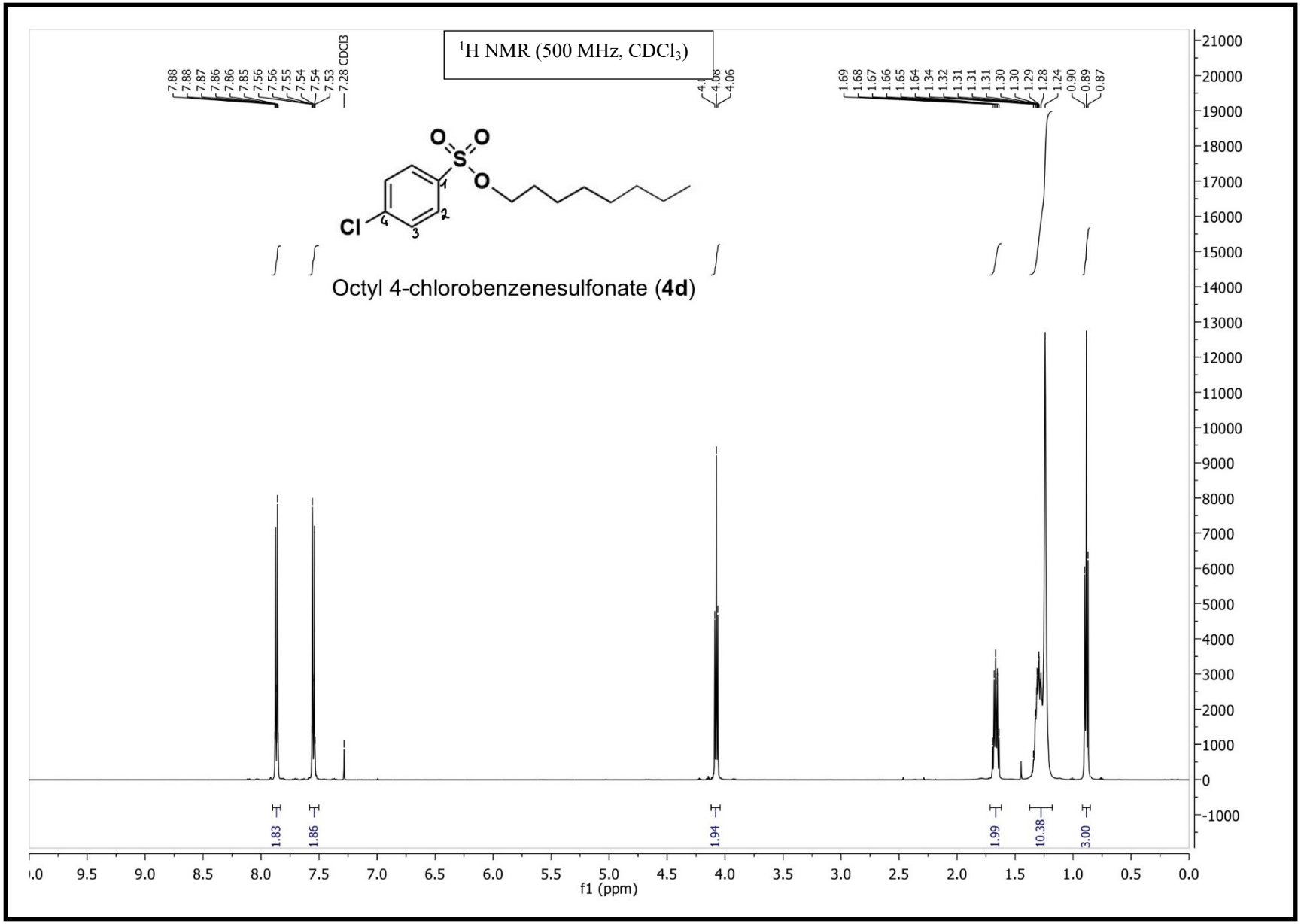
^{1}H NMR (500 MHz, $CDCl_3$)
Octyl 4-chlorobenzenesulfonate (**4d**)
f1 (ppm)

Table S1–S4 Containing the Computed Row Data

Table S1. Computed energies (*E*), zero-point energies, internal energies (*U*), enthalpies (*H*) and Gibbs free energies (*G*) given in Hartree as well as entropies (*S*) given in J mol^{-1} K^{-1} at B3LYPD3/def2TZVP[PCM(BuOH)] basis set with the consideration of PCM solvent method using the parameter set of butanol for **small molecules and ions**.

	Molecule	E	ZPE	U	H	G	S
	HOH	-76.47002852	-76.448938	-76.446103	-76.445158	-76.467243	46.481
	BuOH	-233.77879561	-233.642284	-233.635414	-233.634470	-233.672421	79.876
	BuOH+H$^+$	-234.17910182	-234.029249	-234.022090	-234.021146	-234.059900	81.564
	5BuOH	-1168.95917431	-1168.267039	-1168.227893	-1168.226949	-1168.352029	263.253
	5BuOH+H$^+$	-1169.39423199	-1168.690827	-1168.652831	-1168.651887	-1168.769927	248.437
	Bu$^+$	-157.64978334	-157.533424	-157.527979	-157.527035	-157.561394	72.315

Table S2. Computed energies (*E*), zero-point energies, internal energies (*U*), enthalpies (*H*) and Gibbs free energies (*G*) given in Hartree as well as entropies (*S*) given in J mol^{-1} K^{-1} at B3LYPD3/def2TZVP[PCM(BuOH)] basis set with the consideration of PCM solvent method using the parameter set of butanol for **substituent study of 1a-c**.

	Molecule	E	ZPE	U	H	G	S
1a	p-H-PhSO$_3$H	-856.33906897	-856.223810	-856.215175	-856.214231	-856.258200	92.542
8a	p-H-PhSO$_3^-$	-855.90123433	-855.797675	-855.789542	-855.788598	-855.832457	92.309
2a	p-H-PhSO$_3$Bu	-1013.65327916	-1013.424843	-1013.410436	-1013.409492	-1013.469584	126.475
1b	p-Me-PhSO$_3$H	-895.67468792	-895.532229	-895.521717	-895.520773	-895.569654	102.879
8b	p-Me-PhSO$_3^-$	-895.23560004	-895.104915	-895.095782	-895.094838	-895.140684	96.491
2b	p-Me-PhSO$_3$Bu	-1052.98889064	-1052.733180	-1052.716938	-1052.715994	-1052.780488	135.739
1d	p-Cl-PhSO$_3$H	-1315.96544124	-1315.859770	-1315.849946	-1315.849002	-1315.896264	99.472
8d	p-Cl-PhSO$_3^-$	-1315.52948510	-1315.435449	-1315.426110	-1315.425166	-1315.472262	99.122
2d	p-Cl-PhSO$_3$Bu	-1473.27975384	-1473.060888	-1473.045277	-1473.044332	-1473.107946	133.886

Table S3. Computed energies (*E*), zero-point energies, internal energies (*U*), enthalpies (*H*) and Gibbs free energies (*G*) given in Hartree as well as entropies (*S*) given in J mol^{-1} K^{-1} at B3LYPD3/def2TZVP[PCM(BuOH)] basis set with the consideration of PCM solvent method using the parameter set of butanol for **implicit solvent model for 1**. The imaginary frequency is listed for the TS in cm^{-1}.

	Molecule	E	ZPE	U	H	G	S	im FRQ
	17	-1090.45264513	-1090.185593	-1090.169575	-1090.168631	-1090.230053	129.273	
	18	-1090.43516200	-1090.173529	-1090.157416	-1090.156472	-1090.218374	130.283	-269
	19	-1090.45662842	-1090.189285	-1090.173346	-1090.172402	-1090.233158	127.873	
	24	-856.72039994	-856.594181	-856.585030	-856.584086	-856.628745	93.994	
	25	-856.71008496	-856.584022	-856.574299	-856.573355	-856.619041	96.155	
	26	-780.05039743	-779.965297	-779.943659	-779.942871	-779.992098	87.305	
	26	-1090.05023638	-1089.796989	-1089.781505	-1089.780561	-1089.840709	126.592	–324
	9	-1090.05337231	-1089.799976	-1089.783620	-1089.782676	-1089.845780	132.813	
	10	-1090.05325349	-1089.799519	-1089.783355	-1089.782411	-1089.844516	130.710	
	11	-1090.45264513	-1090.185593	-1090.169575	-1090.168631	-1090.230053	129.273	

Table S4. Computed energies (*E*), zero point energies, internal energies (*U*), enthalpies (*H*) and Gibbs free energies (*G*) given in Hartree as well as entropies (*S*) given in J mol^{-1} K^{-1} at B3LYPD3/def2TZVP[PCM(BuOH)] basis set with the consideration of PCM solvent method using the parameter set of butanol for **explicit-implicit solvent model for 1**. The imaginary frequency is listed for the TS in cm^{-1}.

	Molecule	E	ZPE	U	H	G	S	im FRQ
	Route I							
	12	-2958.02808679	-2958.026926	-2958.027406	-2958.027384	-2958.025664	333.909	
	13[a,b]	-2957.95235679	-2957.950719	-2957.951199	-2957.951177	-2957.949457	236.909	-440[b]
	14	-2958.02887779	-2958.027717	-2958.028197	-2958.028175	-2958.026455	234.909	
	15	-2958.02418679	-2958.023026	-2958.023506	-2958.023484	-2958.021764	205.909	
	16	-2958.02418679	-2958.023026	-2958.023506	-2958.023484	-2958.021764	246.909	
	Route II							
	20	-2872.34445615	-2871.547413	-2871.486399	-2871.485433	-2871.660617	365.235	
	22[a,b]	-2872.28839679	-2871.489885	-2871.431383	-2871.430416	-2871.596317	345.696	–260[b]
	23	-2872.34179317	-2871.542744	-2871.481005	-2871.480039	-2871.656103	367.087	
	Route III							
	28	-2988.06532972	-2987.213649	-2987.146575	-2987.145609	-2987.335424	396.029	
	29[a,b]	-2988.04557611	-2988.044415	-2988.044895	-2988.044873	-2988.043153	391.110	-298[b]
	31	-2988.04604020	-2988.044879	-2988.045359	-2988.045337	-2988.043617	395.919	

[a]Estimated TS; [b]Computed as a single point frequency calculation at B3LYPD3/631(d,p)[PCM(BuOH)] obtained at B3LYPD3/def2TZVP[PCM(BuOH)].

Table S5. Computed energies (*E*), zero point energies, internal energies (*U*), enthalpies (*H*) and Gibbs free energies (*G*) given in Hartree as well as entropies (*S*) given in J mol^{-1} K^{-1} at B3LYPD3/631(d,p)[PCM(BuOH)] basis set computed as single point frequency calculation at the geometries obtained at B3LYPD3/def2TZVP[PCM(BuOH)] with the consideration of PCM solvent method using the parameter set of butanol for **explicit-implicit solvent model for 1**.

	Molecule	E	ZPE	U	H	G	S
	Route I						
	12	-2957.53646744	-2957.531279	-2957.531920	-2957.530611	-2957.526942	388.943
	13[a]	-2957.45563392	-2957.423223	-2957.422733	-2957.425038	-2957.417354	292.489
	14	-2957.53898840	-2957.529596	-2957.535092	-2957.536009	-2957.531044	290.186
	15	-2957.52565726	-2957.529118	-2957.525912	-2957.525413	-2957.527901	261.683
	16	-2957.53206539	-2957.527563	-2957.525958	-2957.525357	-2957.520860	301.997
	Route II						
	20	-2871.84571020	-2871.046712	-2870.993774	-2870.988028	-2871.168951	421.032
	22[a]	-2871.78871798	-2870.989029	-2870.931760	-2870.935628	-2871.101302	401.593
	23	-2871.84370694	-2871.045125	-2870.981876	-2870.988366	-2871.157745	422.813
	Route III						
	28	-2987.56796970	-2986.718340	-2986.649230	-2986.652651	-2986.835487	451.678
	29[a]	-2987.54552801	-2987.543393	-2987.549772	-2987.549408	-2987.543401	447.046
	31	-2987.55234926	-2987.548026	-2987.553497	-2987.551341	-2987.546544	451.175

[a]It has multiply imaginary frequences.

Table S6. Computed energies (*E*), zero point energies, internal energies (*U*), enthalpies (*H*) and Gibbs free energies (*G*) given in Hartree as well as entropies (*S*) given in J mol^{-1} K^{-1} at B3LYPD3/def2-SVP(d,p)[PCM(BuOH)] basis set computed as single point frequency calculation at the geometries obtained at B3LYPD3/def2TZVP[PCM(BuOH)] with the consideration of PCM solvent method using the parameter set of butanol for **explicit-implicit solvent model for 1**.

	Molecule	E	ZPE	U	H	G	S
	Route I						
	12	-2957.47254810	-2957.472631	-2957.473081	-2957.473353	-2957.473364	344.299
	13	-2957.58373925	-2957.583837	-2957.584130	-2957.583523	-2957.583982	247.263
	Route II						
	20	-2871.78967710	-2870.993885	-2870.932354	-2870.930566	-2871.107676	375.544
	22	-2871.73360348	-2870.935821	-2870.876519	-2870.875722	-2871.043846	356.007
	Route III						
	28	-2987.50991108	-2986.659337	-2986.592103	-2986.591671	-2986.782968	406.406
	29*	-2987.49002926	-2987.490716	-2987.490310	-2987.490550	-2987.490272	401.501

Additional Tables containing XYZ coordinates of computed species at B3LYPD3/def2TZVP[PCM(BuOH)]

Water molecule

008aaa_HOH_b3lypG3_Def2TZVP_PCMbu.log

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	0.000009	-0.112619	-0.000003
2	1	0	-0.762978	0.476795	0.000042
3	1	0	0.763108	0.476647	-0.000015

Oxonium molecule

008aba_HOH+H+_b3lypG3_Def2TZVP_PCMbu.log

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-0.000001	0.117876	-0.000003
2	1	0	0.905530	-0.404949	0.000045
3	1	0	-0.905522	-0.404942	-0.000023
4	1	0	-0.000011	1.163487	-0.000032

Butanol molecule

009aaa_BuOH_b3lypG3_Def2TZVP_PCMbu.log

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.514415	-0.294135	0.000002
2	1	0	-3.398125	0.347004	-0.000013
3	1	0	-2.567229	-0.937093	0.882235
4	1	0	-2.567225	-0.937129	-0.882206
5	6	0	-1.228181	0.529965	-0.000013
6	1	0	-1.215233	1.186643	0.876046
7	1	0	-1.215229	1.186607	-0.876098
8	6	0	0.028980	-0.339300	0.000008
9	1	0	0.028161	-0.991956	0.879004
10	1	0	0.028167	-0.991989	-0.878963
11	6	0	1.306792	0.477140	-0.000003
12	1	0	1.338346	1.123781	0.885792
13	1	0	1.338354	1.123744	-0.885825
14	8	0	2.421247	-0.423269	0.000021
15	1	0	3.233680	0.094827	0.000010

Protonated butanol molecule

009baa_BuOH+H+_b3lypG3_Def2TZVP_PCMbu.log

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.566864	-0.332959	-0.007781
2	1	0	-3.460796	0.291697	0.015523
3	1	0	-2.602172	-1.004153	0.852971
4	1	0	-2.605982	-0.943492	-0.912386
5	6	0	-1.305258	0.526944	0.017993
6	1	0	-1.304971	1.157461	0.911131
7	1	0	-1.300974	1.200684	-0.843107
8	6	0	-0.030666	-0.329690	0.003177
9	1	0	-0.007274	-0.965357	0.891939
10	1	0	-0.033745	-0.979470	-0.875786
11	6	0	1.182895	0.558451	-0.023015
12	1	0	1.287878	1.197405	0.848446
13	1	0	1.290613	1.140551	-0.933317
14	8	0	2.481546	-0.252097	0.004499
15	1	0	2.595318	-0.766954	0.825849
16	1	0	2.573475	-0.852606	-0.759692

Deprotonated butanol molecule

009daa_BuOH-H+_b3lypG3_Def2TZVP_PCMbu.log

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.523906	-0.282555	-0.000001
2	1	0	-3.401450	0.369551	-0.000018
3	1	0	-2.587871	-0.926595	0.881484
4	1	0	-2.587868	-0.926636	-0.881456
5	6	0	-1.220515	0.516499	-0.000016
6	1	0	-1.201200	1.176054	0.875333
7	1	0	-1.201197	1.176016	-0.875395
8	6	0	0.032786	-0.356450	0.000005
9	1	0	0.025501	-1.014919	0.878564
10	1	0	0.025508	-1.014952	-0.878530
11	6	0	1.368986	0.425047	-0.000004
12	1	0	1.298470	1.124548	0.882244
13	1	0	1.298476	1.124519	-0.882276
14	8	0	2.481301	-0.348795	0.000013

Butyl cation

009cab_Bu+_b3lypG3_Def2TZVP_PCMbu.log

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.119623	1.505465	-0.000000
2	1	0	-0.943887	2.580759	-0.000000
3	1	0	-1.712110	1.259801	0.883723
4	1	0	-1.712110	1.259801	-0.883723
5	6	0	0.206733	0.750008	-0.000000
6	1	0	0.797121	1.019368	0.877770
7	1	0	0.797121	1.019368	-0.877770
8	6	0	-0.000378	-0.754731	-0.000000
9	1	0	-0.661452	-1.137800	-0.817595
10	1	0	-0.661452	-1.137800	0.817595
11	6	0	1.089253	-1.639757	-0.000000
12	1	0	2.122986	-1.301637	-0.000000
13	1	0	0.920435	-2.712496	-0.000000

$PhSO_3H$ (1a)

000baa_pHPhSO3H_b3lypG3_Def2TZVP_PCMbu.log

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.933114	-1.189181	0.029777
2	6	0	0.547987	-1.239564	-0.047003
3	6	0	-0.165857	-0.044794	-0.099563
4	6	0	0.474723	1.190438	-0.081590
5	6	0	1.861637	1.225414	-0.004728
6	6	0	2.587662	0.039837	0.052618
7	1	0	2.501017	-2.109143	0.068151
8	1	0	0.027762	-2.186694	-0.074113
9	1	0	-0.101591	2.103149	-0.134566
10	1	0	2.373041	2.178636	0.006757
11	16	0	-1.932303	-0.103269	-0.175365
12	8	0	-2.429789	1.164973	-0.635332
13	8	0	-2.346365	-1.322038	-0.807192
14	8	0	-2.369759	-0.290165	1.355612
15	1	0	-2.324754	0.558931	1.825892
16	1	0	3.667854	0.072712	0.110764

8a

000bba_pHPhSO3-_b3lypG3_Def2TZVP_PCMbu.log

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.959540	-1.204928	-0.031069
2	6	0	0.568161	-1.210017	-0.053921
3	6	0	-0.129391	-0.005826	-0.045740
4	6	0	0.563032	1.202566	-0.018604
5	6	0	1.953108	1.203966	0.004614
6	6	0	2.653972	0.000534	0.000147
7	1	0	2.500410	-2.143044	-0.041088
8	1	0	0.019737	-2.141493	-0.087416
9	1	0	0.011858	2.133363	-0.026490
10	1	0	2.489584	2.144476	0.022483
11	16	0	-1.928197	-0.000087	-0.008381
12	8	0	-2.333288	1.166138	-0.798878
13	8	0	-2.342721	-1.277785	-0.594603
14	8	0	-2.273707	0.121681	1.413291
15	1	0	3.736599	0.003149	0.015953

pMePhSO$_3$H (1b)
000aaa_pMePhSO3H_b3lypG3_Def2TZVP_PCMbu.log

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.929018	-1.206286	0.001191
2	6	0	0.545693	-1.244478	-0.072533
3	6	0	-0.162618	-0.045770	-0.110721
4	6	0	0.497191	1.178631	-0.078833
5	6	0	1.882703	1.195784	-0.005105
6	6	0	2.619331	0.009648	0.035914
7	1	0	2.483319	-2.136078	0.031196
8	1	0	0.020829	-2.189064	-0.105334
9	1	0	-0.064886	2.101141	-0.115913
10	1	0	2.399087	2.147233	0.019821
11	6	0	4.121422	0.036723	0.084255
12	1	0	4.488476	0.953076	0.546560
13	1	0	4.515940	-0.815998	0.637511
14	1	0	4.533950	-0.010398	-0.927457
15	16	0	-1.925025	-0.085061	-0.177377
16	8	0	-2.413035	1.194075	-0.618513
17	8	0	-2.357501	-1.291328	-0.821903
18	8	0	-2.363876	-0.287210	1.352904
19	1	0	-2.300751	0.553768	1.835218

8b
000aba_pMePhSO3-_b3lypG3_Def2TZVP_PCMbu.log

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.957087	-1.202639	-0.019021
2	6	0	0.565869	-1.208221	-0.051198
3	6	0	-0.134780	-0.007969	-0.045859
4	6	0	0.565711	1.196037	-0.009830
5	6	0	1.953206	1.191888	0.022376
6	6	0	2.673790	-0.006531	0.018382
7	1	0	2.492167	-2.145239	-0.024632
8	1	0	0.021582	-2.142209	-0.086781
9	1	0	0.021453	2.131142	-0.015114
10	1	0	2.487938	2.134604	0.049554
11	16	0	-1.930921	0.001785	-0.018009
12	8	0	-2.330502	1.161133	-0.822302
13	8	0	-2.346261	-1.280874	-0.593968
14	8	0	-2.288818	0.138520	1.399778
15	6	0	4.179412	0.003924	0.027337
16	1	0	4.572039	0.279287	-0.955541
17	1	0	4.565459	0.731942	0.743442
18	1	0	4.583886	-0.975720	0.283066

3b

000aca_pMePhSO3Bu_b3lypG3_Def2TZVP_PCMbu_f.log

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.188868	-0.636995	-1.201557
2	6	0	1.999344	0.075651	-1.211891
3	6	0	1.412489	0.427110	-0.000048
4	6	0	1.999603	0.076357	1.211858
5	6	0	3.189140	-0.636298	1.201684
6	6	0	3.802195	-1.002914	0.000109
7	1	0	3.649004	-0.913058	-2.142118
8	1	0	1.533158	0.360497	-2.144684
9	1	0	1.533619	0.361738	2.144588
10	1	0	3.649472	-0.911804	2.142312
11	16	0	-0.100969	1.326113	-0.000156
12	8	0	-0.248219	2.053758	1.235984
13	8	0	-0.248295	2.053311	-1.236551
14	8	0	-1.115594	0.098339	0.000091
15	6	0	-2.547616	0.414667	0.000110
16	1	0	-2.769409	1.004881	-0.890359
17	1	0	-2.769377	1.004858	0.890601
18	6	0	-3.294270	-0.900341	0.000101
19	1	0	-2.997849	-1.477568	0.880187
20	1	0	-2.997881	-1.477539	-0.880014
21	6	0	-4.809474	-0.690039	0.000133
22	1	0	-5.094105	-0.099715	-0.876371
23	1	0	-5.094070	-0.099712	0.876647
24	6	0	-5.577921	-2.009984	0.000152
25	1	0	-5.332500	-2.605689	0.882713
26	1	0	-6.655917	-1.839100	0.000166
27	1	0	-5.332525	-2.605701	-0.882410
28	6	0	5.108782	-1.746241	0.000133
29	1	0	5.945150	-1.041576	-0.000666
30	1	0	5.209709	-2.373125	0.886345
31	1	0	5.209048	-2.374293	-0.885334

pClPhSO$_3$H (1d)

000caa_pClPhSO3H_b3lypG3_Def2TZVP_PCMbu.log

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.931546	-1.201431	0.024302
2	6	0	0.547953	-1.238714	-0.050051
3	6	0	-0.165287	-0.043911	-0.098280
4	6	0	0.482729	1.186768	-0.078899
5	6	0	1.867624	1.225413	-0.004744
6	6	0	2.576963	0.031052	0.048287

7	1	0	2.503863	-2.117163	0.059514
8	1	0	0.030191	-2.186983	-0.078453
9	1	0	-0.085380	2.104624	-0.128607
10	1	0	2.389704	2.171242	0.008255
11	16	0	-1.931396	-0.096166	-0.175244
12	8	0	-2.419900	1.176399	-0.630893
13	8	0	-2.343621	-1.311424	-0.813571
14	8	0	-2.369866	-0.288206	1.352989
15	1	0	-2.337199	0.560676	1.824897
16	17	0	4.316378	0.077802	0.140997

8d

000cba_pClPhSO3-_b3lypG3_Def2TZVP_PCMbu.log

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.960244	-1.211561	-0.030257
2	6	0	0.570222	-1.207869	-0.051745
3	6	0	-0.129007	-0.005566	-0.043721
4	6	0	0.565489	1.200724	-0.017960
5	6	0	1.954206	1.210362	0.004227
6	6	0	2.637388	0.000267	-0.000206
7	1	0	2.509598	-2.142665	-0.040269
8	1	0	0.026581	-2.141830	-0.084605
9	1	0	0.019527	2.134215	-0.026279
10	1	0	2.499584	2.143697	0.020824
11	16	0	-1.928100	-0.000173	-0.008894
12	8	0	-2.327360	1.168056	-0.797745
13	8	0	-2.336298	-1.276986	-0.599328
14	8	0	-2.273183	0.118193	1.412111
15	17	0	4.389728	0.004568	0.024527

2d
000cca_pClPhSO3Bu_b3lypG3_Def2TZVP_PCMbu.log

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.447409	-1.149957	1.214224
2	6	0	-2.342315	-0.312163	1.213367
3	6	0	-1.799079	0.097977	0.000090
4	6	0	-2.342743	-0.311248	-1.213303
5	6	0	-3.447841	-1.149039	-1.214400
6	6	0	-3.987169	-1.560447	-0.000148
7	1	0	-3.886928	-1.478358	2.145007
8	1	0	-1.912019	0.024416	2.145844
9	1	0	-1.912776	0.026034	-2.145678
10	1	0	-3.887690	-1.476737	-2.145275
11	16	0	-0.393774	1.165691	0.000251
12	8	0	-0.336147	1.903066	-1.236239
13	8	0	-0.335878	1.902332	1.237166
14	8	0	0.744829	0.056885	-0.000196
15	6	0	2.137327	0.522734	-0.000142
16	1	0	2.294363	1.132616	0.890688
17	1	0	2.294343	1.132847	-0.890818
18	6	0	3.016815	-0.707144	-0.000305
19	1	0	2.782330	-1.311828	-0.880577
20	1	0	2.782356	-1.312036	0.879831
21	6	0	4.501703	-0.339208	-0.000283
22	1	0	4.722964	0.277441	0.876340
23	1	0	4.722942	0.277634	-0.876776
24	6	0	5.403887	-1.571632	-0.000430
25	1	0	5.222145	-2.189597	-0.883092
26	1	0	6.458047	-1.288761	-0.000415
27	1	0	5.222170	-2.189788	0.882102
28	17	0	-5.377001	-2.612166	-0.000298

3b+H$^+$

005aaa_PhSO3H-BuOH_+H+_b3lypG3_Def2TZVP_PCMbu.log

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-1.811833	-2.211484	0.146621
2	1	0	-1.558270	-3.149317	0.152322
3	8	0	0.003527	-1.675525	1.526782
4	1	0	-0.644518	-2.281434	1.925922
5	8	0	0.049668	-1.797725	-1.228049
6	1	0	-0.556833	-2.471986	-1.578566
7	6	0	-1.662101	0.210131	0.038638
8	6	0	-1.494596	1.272529	0.921317
9	6	0	-2.695095	0.167220	-0.891864
10	6	0	-2.407645	2.316778	0.872810
11	1	0	-0.680910	1.285123	1.630074
12	6	0	-3.575202	1.239592	-0.944851
13	1	0	-2.813039	-0.669102	-1.563276
14	6	0	-3.438220	2.305476	-0.061640
15	1	0	-2.302841	3.143577	1.561912
16	1	0	-4.373881	1.232543	-1.673916
17	1	0	-4.137064	3.130416	-0.101913
18	8	0	0.732431	-0.101349	0.081506
19	6	0	2.134845	-0.491882	0.248754
20	1	0	2.296766	-0.713123	1.302705
21	1	0	2.331870	-1.384366	-0.344634
22	16	0	-0.491954	-1.141678	0.115076
23	6	0	2.969335	0.680486	-0.217453
24	1	0	2.741401	0.885131	-1.266782
25	1	0	2.685579	1.568196	0.354388
26	6	0	4.465448	0.408723	-0.049391
27	1	0	4.679754	0.193987	1.002083
28	1	0	4.736973	-0.490502	-0.611041
29	6	0	5.322538	1.583079	-0.517298
30	1	0	6.385379	1.371232	-0.388616
31	1	0	5.148566	1.798000	-1.574358
32	1	0	5.089552	2.487781	0.049349

Butanol claster
000daa_4BuOH_ b3lypG3_Def2TZVP_PCMbu.log

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.675897	-3.981130	3.289956
2	1	0	4.223247	-3.901185	4.234567
3	1	0	4.147127	-4.771920	2.696865
4	1	0	2.654910	-4.303690	3.522145
5	6	0	3.674710	-2.648885	2.532563
6	1	0	4.709966	-2.334290	2.344847
7	1	0	3.228256	-1.869453	3.164339
8	6	0	2.916637	-2.720453	1.201603
9	1	0	3.363361	-3.489124	0.557716
10	1	0	1.877399	-3.026051	1.382157
11	6	0	2.915426	-1.397208	0.449210
12	1	0	3.947652	-1.079823	0.243361
13	1	0	2.445611	-0.613434	1.061809
14	8	0	2.206173	-1.565254	-0.785723
15	1	0	2.180988	-0.703395	-1.256934
16	8	0	-0.479202	-1.191330	-0.887099
17	1	0	0.431108	-1.536855	-0.716158
18	8	0	1.251247	0.708585	-2.033734
19	1	0	0.418677	0.270556	-1.764985
20	8	0	-2.015281	-0.546876	1.378981
21	1	0	-1.418065	-0.783735	0.641217
22	6	0	1.311155	1.997927	-1.410769
23	6	0	2.625812	2.665992	-1.788159
24	1	0	1.233712	1.903996	-0.317152
25	1	0	0.465694	2.614898	-1.747869
26	6	0	2.776934	4.068428	-1.186694
27	1	0	3.455820	2.028050	-1.456236
28	1	0	2.689370	2.719879	-2.882741
29	6	0	4.100086	4.740105	-1.566037
30	1	0	1.939739	4.697734	-1.516862
31	1	0	2.699227	4.006000	-0.093014
32	1	0	4.180774	5.738354	-1.124026
33	1	0	4.956392	4.151068	-1.218719
34	1	0	4.191431	4.847731	-2.652713
35	6	0	-2.117914	0.870902	1.407533
36	6	0	-3.115200	1.274675	2.487221
37	1	0	-2.451033	1.265185	0.433232
38	1	0	-1.139712	1.335698	1.620197
39	6	0	-3.292002	2.792098	2.611439
40	1	0	-4.081705	0.803225	2.264246
41	1	0	-2.779336	0.858722	3.446601
42	6	0	-4.296160	3.191627	3.696943
43	1	0	-2.319443	3.255459	2.825835
44	1	0	-3.617421	3.200970	1.645272
45	1	0	-4.401415	4.279422	3.763345
46	1	0	-5.287754	2.772546	3.491598
47	1	0	-3.980732	2.826362	4.680897
48	6	0	-1.204000	-2.143046	-1.687309

49	6	0	-2.603579	-1.604498	-1.947701
50	1	0	-1.258831	-3.103692	-1.157238
51	1	0	-0.671895	-2.313542	-2.633063
52	6	0	-3.471194	-2.572488	-2.760867
53	1	0	-3.076222	-1.393337	-0.980302
54	1	0	-2.520995	-0.645595	-2.476485
55	6	0	-4.878625	-2.029404	-3.025522
56	1	0	-2.977175	-2.789627	-3.717310
57	1	0	-3.543140	-3.530691	-2.229363
58	1	0	-5.476849	-2.739864	-3.604933
59	1	0	-5.409021	-1.833282	-2.086940
60	1	0	-4.840495	-1.089122	-3.586990

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005aab_PhSO3H-BuOH_+H+_b3lypG3_Def2TZVP_PCMbu.log

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-1.622890	-2.306426	0.407868
2	1	0	-2.052037	-2.222068	1.272643
3	8	0	0.057001	-1.457078	1.637383
4	1	0	0.751840	-0.827363	1.899372
5	8	0	-0.052812	-1.924384	-1.119769
6	1	0	-0.577466	-2.743551	-1.190825
7	6	0	-1.680235	0.202113	0.038835
8	6	0	-1.414913	1.436379	0.630055
9	6	0	-2.862658	-0.046853	-0.653810
10	6	0	-2.375257	2.433145	0.535886
11	1	0	-0.491362	1.620400	1.155855
12	6	0	-3.792556	0.977862	-0.766082
13	1	0	-3.056433	-1.008374	-1.103098
14	6	0	-3.555557	2.209576	-0.166225
15	1	0	-2.191905	3.389461	1.006316
16	1	0	-4.706749	0.803890	-1.316833
17	1	0	-4.292357	2.997838	-0.245220
18	8	0	0.735318	-0.063249	-0.110238
19	6	0	2.109533	-0.490142	-0.394429
20	1	0	2.351199	-1.380189	0.190431
21	1	0	2.159951	-0.744342	-1.451567
22	16	0	-0.478652	-1.118337	0.172103
23	6	0	3.016474	0.669491	-0.045511
24	1	0	2.686275	1.553743	-0.597035
25	1	0	2.918938	0.898870	1.019231
26	6	0	4.477663	0.362163	-0.379304
27	1	0	4.794238	-0.533743	0.163550
28	1	0	4.563839	0.126423	-1.444290
29	6	0	5.405602	1.525121	-0.034506
30	1	0	6.441957	1.288142	-0.280893
31	1	0	5.126419	2.425386	-0.587085
32	1	0	5.359378	1.760439	1.031493

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006abb_PhSO3H-BuOH_+H+_b3lypG3_Def2TZVP_PCMbu_TS_f.log

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-2.064246	-2.098315	0.824639
2	1	0	-1.898572	-2.773722	1.504678
3	8	0	-0.109028	-1.481657	1.942605
4	1	0	0.800332	-0.828901	1.611480
5	8	0	-0.310197	-1.897095	-0.735600
6	1	0	-0.965918	-2.578259	-0.978608
7	6	0	-1.679282	0.314537	0.305694
8	6	0	-2.710767	0.623454	1.186147
9	6	0	-1.341985	1.121676	-0.774761
10	6	0	-3.420338	1.797463	0.970997
11	1	0	-2.955372	-0.023957	2.014672
12	6	0	-2.085401	2.272556	-0.987251
13	1	0	-0.534136	0.860747	-1.440455
14	6	0	-3.114130	2.613328	-0.112940
15	1	0	-4.218671	2.065064	1.649298
16	1	0	-1.852567	2.906343	-1.831683
17	1	0	-3.680154	3.520231	-0.278647
18	8	0	0.849127	-0.203392	0.476165
19	6	0	1.922939	-0.415924	-0.475882
20	1	0	2.221288	-1.465407	-0.459948
21	1	0	1.548219	-0.177205	-1.471171
22	16	0	-0.754166	-1.176366	0.588046
23	6	0	3.069997	0.495802	-0.086426
24	1	0	2.716639	1.530325	-0.084755
25	1	0	3.381841	0.259818	0.935072
26	6	0	4.257924	0.348911	-1.039460
27	1	0	4.593107	-0.692791	-1.044088
28	1	0	3.933402	0.574788	-2.059901
29	6	0	5.422575	1.260406	-0.658313
30	1	0	6.258667	1.141417	-1.349677
31	1	0	5.119904	2.310151	-0.675028
32	1	0	5.784084	1.033837	0.347613

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007aaa_PhSO3H-BuOH_+H+_B_b3lypG3_Def2TZVP_PCMbu.log

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-0.889042	-3.994549	-0.634947
2	1	0	-0.439849	-4.450271	0.096350
3	8	0	-0.377768	-1.270821	1.624475
4	1	0	-1.845524	-4.149105	-0.559198

5	8	0	-0.310636	-1.649740	-0.811895
6	1	0	-0.640158	-2.901661	-0.666807
7	6	0	-1.723405	0.392091	0.062057
8	6	0	-2.374515	0.908446	1.178926
9	6	0	-2.108483	0.710530	-1.238717
10	6	0	-3.444075	1.770974	0.980052
11	1	0	-2.055276	0.635999	2.174752
12	6	0	-3.178773	1.574587	-1.416606
13	1	0	-1.588478	0.288212	-2.086831
14	6	0	-3.842290	2.102593	-0.311486
15	1	0	-3.965966	2.180763	1.833954
16	1	0	-3.496218	1.833213	-2.417553
17	1	0	-4.677460	2.774565	-0.459070
18	8	0	0.828560	0.287346	0.109940
19	6	0	2.209819	-0.254270	0.193984
20	1	0	2.337248	-0.675588	1.190521
21	1	0	2.301236	-1.037111	-0.558264
22	16	0	-0.368354	-0.688448	0.315727
23	6	0	3.144153	0.902489	-0.065448
24	1	0	2.921474	1.326939	-1.047618
25	1	0	2.960896	1.682879	0.677330
26	6	0	4.607678	0.457620	-0.007498
27	1	0	4.816181	0.020056	0.973415
28	1	0	4.776421	-0.334104	-0.743675
29	6	0	5.570611	1.613922	-0.268817
30	1	0	6.608020	1.278439	-0.223694
31	1	0	5.400756	2.049014	-1.256478
32	1	0	5.441163	2.406439	0.471949

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008aaa_PhSO3H-BuOH_+H+_B_-H2O_b3lypG3_Def2TZVP_PCMbu.log

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	0.987900	3.971457	-0.544427
2	1	0	0.229302	4.578684	-0.547126
3	8	0	0.352590	1.257728	1.648213
4	1	0	1.603849	4.235989	-1.247770
5	8	0	0.287534	1.664283	-0.785009
6	1	0	0.668389	2.899853	-0.641994
7	6	0	1.714290	-0.377207	0.070952
8	6	0	2.373949	-0.892048	1.183410
9	6	0	2.096954	-0.688017	-1.232410
10	6	0	3.449763	-1.745141	0.977368
11	1	0	2.056471	-0.625352	2.181321
12	6	0	3.173420	-1.542743	-1.417557
13	1	0	1.570054	-0.267167	-2.077017
14	6	0	3.845557	-2.069113	-0.316808
15	1	0	3.978431	-2.153464	1.827800
16	1	0	3.489052	-1.795445	-2.420594
17	1	0	4.685595	-2.733736	-0.469980
18	8	0	-0.838748	-0.289683	0.110952

19	6	0	-2.223253	0.242112	0.201822
20	1	0	-2.350605	0.658632	1.200407
21	1	0	-2.322203	1.027473	-0.546820
22	16	0	0.351374	0.691384	0.333117
23	6	0	-3.150857	-0.919654	-0.059375
24	1	0	-2.927406	-1.339912	-1.043200
25	1	0	-2.961485	-1.701086	0.680766
26	6	0	-4.616979	-0.483861	0.002455
27	1	0	-4.826341	-0.050199	0.984913
28	1	0	-4.791837	0.308880	-0.731238
29	6	0	-5.573426	-1.645202	-0.260284
30	1	0	-6.612754	-1.316091	-0.212426
31	1	0	-5.402718	-2.076652	-1.249403
32	1	0	-5.437915	-2.438888	0.478136

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013aaa_PhSO3H+H+_A_b3lypG3_Def2TZVP_PCMbu.log

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-1.943250	0.796685	1.113872
2	1	0	-1.944596	0.366739	1.991506
3	8	0	-1.911552	-1.451835	0.031978
4	8	0	-1.776977	0.713218	-1.243488
5	1	0	-2.739649	0.866867	-1.334672
6	6	0	0.338490	-0.042935	-0.006821
7	6	0	1.047716	-1.242842	-0.036689
8	6	0	0.957627	1.208737	0.039339
9	6	0	2.433098	-1.176945	-0.023146
10	1	0	0.532011	-2.191466	-0.068564
11	6	0	2.340931	1.244688	0.049686
12	1	0	0.377505	2.120269	0.066662
13	6	0	3.072749	0.057834	0.018717
14	1	0	3.009912	-2.090806	-0.045311
15	1	0	2.849364	2.198011	0.083409
16	1	0	4.153752	0.098587	0.028964
17	16	0	-1.390548	-0.133970	-0.009927

25

015aaa_PhSO3H+H+_B_b3lypG3_Def2TZVP_PCMbu.log

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-1.838071	0.101067	1.634603
2	1	0	-2.616336	0.671316	1.770315
3	8	0	-1.908724	-1.293858	-0.646639

4	8	0	-1.924471	1.224029	-0.739206
5	6	0	0.345634	-0.003961	-0.152873
6	6	0	1.012766	-1.229721	-0.052425
7	6	0	0.998562	1.232730	-0.104575
8	6	0	2.388527	-1.202320	0.089889
9	1	0	0.470395	-2.162839	-0.093102
10	6	0	2.374355	1.226569	0.037090
11	1	0	0.445318	2.156926	-0.183483
12	6	0	3.062276	0.017385	0.135237
13	1	0	2.935850	-2.131339	0.163943
14	1	0	2.911571	2.163799	0.070412
15	1	0	4.138169	0.026022	0.247760
16	16	0	-1.361438	-0.018884	-0.355126
17	1	0	-2.033809	-0.769939	2.024182

26

017aaa_PhSO3H+H+_B_-H2O_b3lyp631dp_PCMbu.log

Standard orientation

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-2.266020	1.289988	0.000197
2	8	0	-2.265914	-1.290031	-0.000224
3	6	0	0.096742	0.000004	-0.000201
4	6	0	0.760183	1.248140	-0.000085
5	6	0	0.760172	-1.248139	0.000101
6	6	0	2.144351	1.225040	-0.000103
7	1	0	0.206457	2.178617	0.000136
8	6	0	2.144345	-1.225023	0.000064
9	1	0	0.206440	-2.178608	0.000676
10	6	0	2.828632	0.000005	0.000081
11	1	0	2.694663	2.158340	-0.000226
12	1	0	2.694649	-2.158329	0.000026
13	1	0	3.913344	0.000007	-0.000040
14	16	0	-1.616664	0.000009	0.000031

27

018aaa_PhSO3H-BuOH_+H+_+BuOH_b3lypG3_Def2TZVP_PCMbu.log

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	0.197723	1.534679	1.506377
2	8	0	0.717591	2.291303	-0.834432
3	6	0	1.869326	0.086504	0.053923
4	6	0	2.024858	-0.813223	1.111383
5	6	0	2.663384	0.057214	-1.094754
6	6	0	3.020589	-1.768941	1.005950
7	1	0	1.391356	-0.757784	1.984671

8	6	0	3.653761	-0.908189	-1.172323
9	1	0	2.512839	0.771957	-1.890393
10	6	0	3.828432	-1.815015	-0.129417
11	1	0	3.168976	-2.476583	1.809510
12	1	0	4.289925	-0.950755	-2.045205
13	1	0	4.604376	-2.565530	-0.200725
14	8	0	-0.829803	0.231742	-0.441225
15	6	0	-2.192234	0.463313	0.145871
16	1	0	-2.030105	0.381214	1.215866
17	1	0	-2.490455	1.476187	-0.117401
18	16	0	0.638372	1.296411	0.177568
19	6	0	-3.125308	-0.595679	-0.390361
20	1	0	-3.183029	-0.519504	-1.479865
21	1	0	-2.727157	-1.583121	-0.147130
22	6	0	-4.527042	-0.429478	0.208531
23	1	0	-4.465401	-0.504838	1.297806
24	1	0	-4.901801	0.572912	-0.016502
25	6	0	-5.500909	-1.476328	-0.327776
26	1	0	-6.491331	-1.346406	0.110863
27	1	0	-5.600674	-1.399129	-1.412778
28	1	0	-5.158461	-2.486685	-0.093379
29	1	0	-0.865374	0.273893	-1.415231

9

021aaa_PhSO3H+BuOH_b3lypG3_Def2TZVP_PCMbu_SCAN_begins_FRQ.log

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-0.432174	-2.624233	-0.492998
2	1	0	0.439861	-2.141648	-0.709967
3	8	0	-2.216234	-2.935233	1.076939
4	1	0	1.861968	-1.237180	-2.019362
5	8	0	-0.127150	-1.801036	1.804915
6	6	0	-1.772028	-0.483308	0.252466
7	6	0	-2.818774	-0.470857	-0.667386
8	6	0	-1.228842	0.697017	0.746763
9	6	0	-3.320316	0.748051	-1.100876
10	1	0	-3.234151	-1.399673	-1.034000
11	6	0	-1.741852	1.912680	0.307018
12	1	0	-0.422241	0.661912	1.464390
13	6	0	-2.782009	1.938207	-0.615240
14	1	0	-4.132519	0.770151	-1.815347
15	1	0	-1.327408	2.837019	0.687080
16	1	0	-3.177928	2.886232	-0.955610
17	8	0	1.781827	-1.430562	-1.076426
18	6	0	2.116272	-0.245242	-0.314144
19	1	0	1.426564	0.561755	-0.577221
20	1	0	1.934223	-0.520940	0.723840
21	16	0	-1.123082	-2.045147	0.790863
22	6	0	3.556451	0.178060	-0.527768
23	1	0	4.213740	-0.658325	-0.272893
24	1	0	3.714202	0.397461	-1.589655
25	6	0	3.923529	1.406027	0.307072
26	1	0	3.249953	2.230946	0.053766
27	1	0	3.755509	1.185037	1.365916
28	6	0	5.371293	1.845805	0.099339
29	1	0	5.610208	2.721472	0.705737
30	1	0	6.065759	1.048111	0.374077
31	1	0	5.556267	2.101896	-0.946832

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022aab_PhSO3H+BuOH_b3lypG3_Def2TZVP_PCMbu.log

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	2.241253	-2.214752	0.167533
2	1	0	2.032378	-3.163162	0.238540
3	8	0	0.343032	-2.008183	-1.242952
4	1	0	-0.510365	-1.361334	-1.304403
5	8	0	0.189773	-1.749612	1.426311

6	6	0	1.673446	0.201612	0.042656
7	6	0	2.390557	0.516755	-1.108938
8	6	0	1.611865	1.044441	1.149619
9	6	0	3.069679	1.735583	-1.146152
10	1	0	2.420476	-0.164310	-1.951567
11	6	0	2.306041	2.253651	1.094795
12	1	0	1.042874	0.762974	2.028321
13	6	0	3.029250	2.599512	-0.049236
14	1	0	3.632759	2.004801	-2.033789
15	1	0	2.277911	2.923770	1.947749
16	1	0	3.563298	3.543548	-0.085690
17	8	0	-0.823243	-0.254363	-0.467066
18	6	0	-1.976330	-0.194566	0.351950
19	1	0	-2.268148	-1.193839	0.709723
20	1	0	-1.763336	0.411911	1.246218
21	16	0	0.801663	-1.367572	0.145785
22	6	0	-3.133611	0.432969	-0.427819
23	1	0	-2.823350	1.423866	-0.784249
24	1	0	-3.326574	-0.174790	-1.322226
25	6	0	-4.417269	0.555340	0.402681
26	1	0	-4.712348	-0.438819	0.764528
27	1	0	-4.214371	1.157584	1.298485
28	6	0	-5.578627	1.178631	-0.377821
29	1	0	-6.479964	1.253618	0.239323
30	1	0	-5.326310	2.187499	-0.723591
31	1	0	-5.828075	0.579538	-1.260959

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022aab_PhSO3H+BuOH_b3lypG3_Def2TZVP_PCMbu.log

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	2.241253	-2.214752	0.167533
2	1	0	2.032378	-3.163162	0.238540
3	8	0	0.343032	-2.008183	-1.242952
4	1	0	-0.510365	-1.361334	-1.304403
5	8	0	0.189773	-1.749612	1.426311
6	6	0	1.673446	0.201612	0.042656
7	6	0	2.390557	0.516755	-1.108938
8	6	0	1.611865	1.044441	1.149619
9	6	0	3.069679	1.735583	-1.146152
10	1	0	2.420476	-0.164310	-1.951567
11	6	0	2.306041	2.253651	1.094795
12	1	0	1.042874	0.762974	2.028321
13	6	0	3.029250	2.599512	-0.049236
14	1	0	3.632759	2.004801	-2.033789
15	1	0	2.277911	2.923770	1.947749
16	1	0	3.563298	3.543548	-0.085690
17	8	0	-0.823243	-0.254363	-0.467066
18	6	0	-1.976330	-0.194566	0.351950
19	1	0	-2.268148	-1.193839	0.709723
20	1	0	-1.763336	0.411911	1.246218

21	16	0	0.801663	-1.367572	0.145785
22	6	0	-3.133611	0.432969	-0.427819
23	1	0	-2.823350	1.423866	-0.784249
24	1	0	-3.326574	-0.174790	-1.322226
25	6	0	-4.417269	0.555340	0.402681
26	1	0	-4.712348	-0.438819	0.764528
27	1	0	-4.214371	1.157584	1.298485
28	6	0	-5.578627	1.178631	-0.377821
29	1	0	-6.479964	1.253618	0.239323
30	1	0	-5.326310	2.187499	-0.723591
31	1	0	-5.828075	0.579538	-1.260959

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024aaa_PhSO3H+BuOH_b3lypG3_Def2TZVP_PCMbu.log

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-1.883570	2.225378	-0.561783
2	1	0	-1.977489	2.858781	0.160511
3	8	0	0.027916	1.537695	-1.626017
4	1	0	-0.567983	2.235342	-1.955482
5	8	0	-0.147661	1.983538	1.041334
6	6	0	-1.631865	-0.175093	-0.055452
7	6	0	-1.864121	-0.957094	-1.176251
8	6	0	-2.265806	-0.409386	1.155350
9	6	0	-2.769268	-2.008361	-1.075637
10	1	0	-1.350287	-0.754804	-2.105532
11	6	0	-3.161615	-1.469495	1.241854
12	1	0	-2.064922	0.218866	2.012647
13	6	0	-3.415697	-2.266011	0.129371
14	1	0	-2.963789	-2.627912	-1.941330
15	1	0	-3.660705	-1.669643	2.180954
16	1	0	-4.115931	-3.087895	0.201954
17	8	0	0.745783	0.066813	-0.040156
18	6	0	2.104358	0.512719	0.122173
19	1	0	2.374173	1.182393	-0.699341
20	1	0	2.193630	1.063915	1.061001
21	16	0	-0.484870	1.201188	-0.139771
22	6	0	2.995071	-0.714803	0.126203
23	1	0	2.670759	-1.384431	0.928507
24	1	0	2.859897	-1.256439	-0.814708
25	6	0	4.469910	-0.357907	0.312655
26	1	0	4.782329	0.322217	-0.486379
27	1	0	4.593889	0.192224	1.250997
28	6	0	5.374770	-1.588480	0.318560
29	1	0	6.422093	-1.311043	0.452948
30	1	0	5.102283	-2.270508	1.127882
31	1	0	5.292125	-2.139511	-0.621633

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C -1.60298200 -4.02654500 -2.15861300
C -1.42458700 -2.91086500 -1.39321500
C -1.75858500 -1.66328700 -1.86347300
C -2.27202700 -1.52415600 -3.14001100
C -2.44482900 -2.64462700 -3.93239100
C -2.10975600 -3.89432800 -3.44154300
H -1.35637900 -4.99731100 -1.77710900
H -1.03550000 -2.99952500 -0.36783000
H -2.53685200 -0.54998900 -3.49480700
H -2.84168200 -2.54181300 -4.92213900
S -1.50774400 -0.24024400 -0.88544000
O -2.38786500 0.78779600 -1.41647300
O -1.81246400 -0.62203400 0.48632800
O -0.07718400 0.10256400 -1.04778000
H 1.10153100 -1.12905500 -1.42844100
O 1.73144600 -1.85536800 -1.62019400
H 1.98388400 -2.91766000 -0.56762100
C 1.99629600 -1.97146700 -3.04715400
H 1.14527800 -2.40986500 -3.55147900
H 2.21714500 -0.99696800 -3.44459500
H 2.85348300 -2.61860900 -3.15582900
O 2.09768400 -3.61180400 0.16217700
H 0.81010200 -3.36321900 1.15764600
O 0.73241800 1.24238400 1.84726300
H -0.10723300 1.83953900 1.50328700
C 2.38832100 -4.92120200 -0.38036400
H 1.57234100 -5.27327900 -0.99971200
H 3.29702200 -4.89890600 -0.96732900
H 2.52540800 -5.59739200 0.44946300
C 1.91417300 1.96754500 2.26770300
H 1.72844300 2.48371300 3.19963200
H 2.71897900 1.26092900 2.38506600
H 2.16051900 2.66443400 1.48698200
O -2.97233200 -2.24646200 2.33937400
H -2.31507300 -1.91839600 1.70673100
C -4.21548000 -2.49030300 1.63914700
H -4.48411600 -1.65493600 1.00681900
H -4.15981100 -3.38759000 1.03061100
H -4.97965700 -2.63211000 2.38969500
O 4.04554400 -2.74851400 1.92120400
H 3.39364800 -3.07107300 1.27067300
C 3.40752900 -2.52625200 3.19289300
H 2.49430000 -1.94992800 3.10546300
H 3.17667500 -3.46305900 3.69352000
H 4.10512400 -1.97893700 3.80987300
H -2.24801400 -4.76344200 -4.05357800
S 2.61498300 2.17610600 -1.91165000
O 2.42620200 1.14266700 -2.88882300
O 2.87475700 3.51417700 -2.33742500
C 3.88206600 1.69926500 -0.81712900
C 3.93110700 0.39710200 -0.34631700
C 4.80006100 2.64246500 -0.39484800
C 4.88387300 0.04300000 0.59180000
H 3.23624000 -0.33508600 -0.70548200

C 5.76973000 2.28067300 0.52317400
H 4.74684000 3.63622500 -0.78772600
C 5.80287000 0.98962000 1.02116000
H 4.87750100 -0.94969000 0.99887400
H 6.48954400 3.00441000 0.84965600
H 6.54605800 0.71599000 1.74398400
O 1.37046600 2.19337600 -0.99032000
H 0.74381700 1.39134800 -0.98824000
C -0.51848000 -4.21382600 2.47501900
H -0.61353900 -5.11149600 1.87503900
H -1.49037400 -3.89682400 2.80763400
H 0.12831100 -4.42078300 3.31921900
O 0.00097700 -3.12000600 1.67536100
H 0.10351800 -1.70450000 2.38857800
O -1.19528000 2.53059300 1.22458600
H -2.01982300 2.12711500 1.62088900
C -1.40382400 3.51058600 0.16807100
H -0.43298400 3.68506600 -0.26493800
H -2.04494600 3.07432400 -0.58163500
O -3.08167400 1.12974000 2.18835700
H -2.92798300 0.30787900 1.69182800
C -4.47524800 1.32357600 2.55480100
H -5.09836500 1.17941100 1.68877400
H -4.75298400 0.63275100 3.33944200
H -4.56032800 2.33374700 2.92548800
C -1.99358800 4.79469500 0.74765400
H -2.94877300 4.57329200 1.21511800
H -1.32872300 5.16688000 1.51929600
C -2.18839900 5.86488800 -0.34145900
H -2.84528300 5.47698100 -1.11392300
H -1.23272600 6.07821400 -0.80985100
C -2.78181300 7.16636900 0.23025800
H -2.12747500 7.58223400 0.98896500
H -2.91144500 7.90882300 -0.54913500
H -3.74929100 6.97788800 0.68360900
O 0.23217500 -0.86271000 2.91905800
H 0.54296200 0.27374700 2.27292600
C -0.78795200 -0.64731400 3.94169400
H -1.53614200 0.03216900 3.56921200
H -1.26322500 -1.58423900 4.18299700
H -0.30038600 -0.24005400 4.81440100
O -4.93060600 0.26478700 -0.39503400
H -4.09285700 0.60800800 -0.75279300
C -5.83881400 -0.06253500 -1.46272500
H -6.73006800 -0.46850100 -1.00880500
H -6.11332100 0.81297200 -2.04164500
H -5.42135700 -0.80543100 -2.13358100

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C 2.94123100 3.34520200 -1.83205600
C 2.53909000 2.21606100 -1.13470000
C 2.46164600 0.98472100 -1.76741500
C 2.79323000 0.90471000 -3.11108000
C 3.17980400 2.03300000 -3.81337800
C 3.25867700 3.25892800 -3.17563800
H 3.02085500 4.28638600 -1.32366000
H 2.28648600 2.28288300 -0.09884700
H 2.76531000 -0.04786800 -3.59379000
H 3.43356600 1.95154800 -4.85241000
S 1.90538400 -0.52394400 -0.84645700
O 2.71120600 -1.42395800 -1.70963900
O 2.35441000 0.00402500 0.47232300
O 0.40603100 -0.06869100 -1.30902500
H -0.10812300 1.21988500 -1.63188400
O -0.63776100 2.11129100 -1.69148800
H -0.51516200 2.79199800 -0.92166100
C -1.32333300 2.43351300 -2.94889500
H -0.59367100 2.77297400 -3.66613600
H -1.81638700 1.52901300 -3.25607400
H -2.04130600 3.20794500 -2.73027400
O -0.36031500 3.60336100 0.26071100
H 0.19521800 3.15616700 0.99124400
O -1.70078300 -0.73594200 2.25686600
H -1.78198700 -0.77840800 1.27578200
C -0.08630400 5.02489900 0.13716700
H 0.92214300 5.18710600 -0.21331000
H -0.78641900 5.43080400 -0.57584700
H -0.23092800 5.51071000 1.09165500
C -2.74765600 -1.49349100 2.91496100
H -2.70488400 -2.53392200 2.62566000
H -2.58163200 -1.41070600 3.97826000
H -3.71667100 -1.08526800 2.66968200
O 4.36024300 0.88831200 1.94660400
H 3.65681800 0.61016500 1.31934200
C 5.60084200 1.10717900 1.24669100
H 5.96231000 0.19874300 0.77736300
H 5.50148000 1.87029800 0.48335900
H 6.32897700 1.43288300 1.97524300
O -2.83124300 3.36603500 1.51914200
H -2.04866000 3.46526000 0.95340100
C -2.45650400 2.67341900 2.72857600
H -2.29426800 1.61872200 2.55169900
H -1.55405500 3.09161900 3.16358900
H -3.27019700 2.79213200 3.42840800
H 3.57358600 4.13085700 -3.71503400
S -2.88304300 -1.10897800 -1.58899400
O -2.50708100 -0.41287700 -2.79930100
O -3.27228000 -2.48840200 -1.74346700
C -4.24090600 -0.27704000 -0.86681700
C -4.05941500 0.95264600 -0.25734600
C -5.50000500 -0.84305500 -0.93802700
C -5.14030800 1.62386500 0.28084000
H -3.08392800 1.38452900 -0.18392800

C -6.58469700 -0.16724300 -0.40721100
H -5.61115300 -1.80404200 -1.39522500
C -6.40515500 1.06415000 0.19930600
H -4.96118900 2.56226200 0.76099800
H -7.56221200 -0.60331600 -0.46332300
H -7.24703000 1.58375100 0.61301800
O -1.80070100 -0.93679200 -0.56261200
H -0.42121100 -0.57231500 -0.97827100
C 2.15953500 3.08475600 2.75136000
H 2.32821400 4.05091500 2.29918000
H 3.02668500 2.45854000 2.61725800
H 1.94312400 3.22361900 3.80325400
O 1.01016700 2.49341100 2.07571500
H 0.92109500 1.54005800 2.28842400
O 1.20951300 -1.72668500 -0.11500500
H 1.55509600 -1.86983400 1.25222400
C 0.69555700 -2.95247500 -0.77061900
H 0.12626300 -2.65551800 -1.63597300
H 1.54551600 -3.54032600 -1.05639600
O 1.81183400 -1.91280600 2.26549400
H 1.39427800 -1.11017400 2.73670500
C 3.26420800 -2.14132000 2.47842800
H 3.59397200 -2.72012800 1.63039900
H 3.75870200 -1.18696800 2.51622300
H 3.36327900 -2.69173000 3.39901100
C -0.18473400 -3.66845200 0.24921200
H 0.43858100 -4.08213000 1.03410600
H -0.85185200 -2.94082400 0.68544400
C -1.01416200 -4.77839700 -0.42499600
H -0.35988500 -5.43603900 -0.99027300
H -1.71230400 -4.31357500 -1.10951600
C -1.79446400 -5.60588700 0.61366600
H -2.46896000 -4.96638100 1.17382900
H -2.38786200 -6.37285100 0.12883700
H -1.11859500 -6.08767400 1.31299300
O 0.50697700 0.01595400 3.21569600
H -0.40319500 -0.25864100 2.85089700
C 0.46011500 0.31865200 4.63435500
H 0.10833400 -0.53575000 5.19805400
H 1.46253000 0.56492400 4.94703400
H -0.19017000 1.16312900 4.81494500
O 3.84200300 -3.47488300 -0.38062300
H 3.51268100 -2.72907600 -0.92704700
C 4.97032000 -4.11754400 -0.99390500
H 5.24755500 -4.95196000 -0.36608700
H 4.73304200 -4.49575400 -1.98268900
H 5.82331200 -3.45149200 -1.07863800

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C -1.14132500 -1.16545200 3.98001800
C -1.46997000 -1.03602700 2.64277300
C -0.46266800 -1.09585200 1.69433300
C 0.85170500 -1.29937400 2.06873900
C 1.17054400 -1.44000800 3.40584900
C 0.17448900 -1.37076300 4.36276400
H -1.91432800 -1.10508500 4.71996000
H -2.48235500 -0.87995100 2.34378800
H 1.64179900 -1.33115800 1.35340700
H 2.20131600 -1.56194500 3.66577100
S -0.81453000 -0.87913400 -0.02227200
O -1.79400000 0.24509400 -0.35387900
O 0.41330800 0.34892200 -0.07602400
O -0.12226900 -1.69643700 -1.01361900
H 0.16779800 1.49540400 0.71832400
O -0.07409000 2.33535900 1.28011200
H -1.04710800 2.69245700 1.25953200
C 0.86520200 2.82673100 2.30616000
H 0.69688500 2.27448400 3.21886400
H 1.85806300 2.64450900 1.93164900
H 0.63744000 3.86957100 2.43605800
O -2.39416900 3.17653900 1.27942400
H -2.84279400 3.16595900 0.36537900
O 0.10222900 1.61894200 -2.39822700
H 0.12293600 1.23373500 -1.49327500
C -3.20460200 2.47468600 2.27140800
H -3.55148700 1.53324300 1.87409400
H -2.57796800 2.30381600 3.13355000
H -4.04229800 3.09518100 2.55811600
C 1.29205900 1.23339700 -3.13808900
H 2.04019300 0.87373600 -2.44751800
H 1.05238900 0.45044400 -3.84578800
H 1.66428300 2.09942500 -3.66537200
O -4.34259800 -0.53743600 1.05729800
H -3.61484500 -1.02183700 0.61876200
C -5.40234800 -1.43500900 1.44357600
H -5.92175900 -1.83884800 0.58102000
H -5.03057500 -2.25983400 2.04162500
H -6.10561400 -0.86810500 2.03409100
O -1.02245700 5.42369000 2.19235600
H -1.63106000 4.73366500 1.87285300
C -0.85328800 6.45097100 1.20212100
H -0.44773400 6.06423200 0.27190800
H -1.78497200 6.96397800 0.98308100
H -0.15558400 7.16898000 1.60607900
H 0.42065000 -1.46535700 5.40171200
S 3.85154700 0.28306800 0.66077200
O 3.65116400 1.65005100 1.10499800
O 3.90004900 -0.72768400 1.69825900
C 5.40559800 0.24459400 -0.14369100
C 5.90593300 1.39113000 -0.73209600
C 6.12239900 -0.93693700 -0.19146500
C 7.11683900 1.34873300 -1.39836400
H 5.35373200 2.30362500 -0.64387400

C 7.33270000 -0.97888600 -0.85806400
H 5.73391000 -1.80014900 0.30769600
C 7.82769600 0.16264500 -1.46591500
H 7.50806600 2.23715000 -1.85284500
H 7.89051400 -1.89332700 -0.89547400
H 8.76815700 0.13057200 -1.97991500
O 2.86881700 -0.08663200 -0.38986600
H 1.39586800 0.09011400 -0.21624100
C -4.86545800 2.36400800 -0.90445100
H -4.79705900 1.38855100 -0.45000200
H -5.27895100 2.27373900 -1.90086400
H -5.50890600 3.00279400 -0.31830800
O -3.56186100 3.00493900 -0.95762000
H -3.04321300 2.74153200 -1.75014600
O -2.17670700 -1.90814400 0.10516300
H -2.58929600 0.07276300 -1.15516800
C -2.16562700 -3.33630900 -0.21170600
H -3.20799400 -3.62324500 -0.16830500
H -1.80362800 -3.46770300 -1.21587300
O -3.27029900 0.05020300 -2.20818700
H -2.95385600 0.80844500 -2.77474700
C -3.63864700 -1.18172700 -2.89986400
H -4.27560200 -1.73528300 -2.23039300
H -4.19323600 -0.92171400 -3.79037900
H -2.76169100 -1.75702900 -3.15080500
C -1.35430900 -4.17699600 0.77411900
H -0.30713100 -3.91383400 0.69408200
H -1.67357400 -3.96466700 1.78712900
C -1.52701800 -5.67910700 0.47559400
H -1.22024300 -5.88169700 -0.54561900
H -2.57619700 -5.94792100 0.55835300
C -0.69837400 -6.54913100 1.44047400
H -1.00274500 -6.37538100 2.46691300
H -0.82729700 -7.60326200 1.22131400
H 0.35608500 -6.31061500 1.35601000
O -2.21885300 2.16035300 -3.14479800
H -1.23843500 1.97582600 -2.88391800
C -2.33374900 2.93330900 -4.36321600
H -1.93452500 2.38280800 -5.20537600
H -3.38088300 3.13343600 -4.53224000
H -1.80497200 3.87163500 -4.26608800
O -0.92279700 -2.92160800 -3.31239300
H -0.45308300 -2.52247400 -2.55945400
C -0.07858300 -3.81730700 -4.05634800
H -0.67811300 -4.23122900 -4.85334800
H 0.77043600 -3.30310900 -4.49370600
H 0.29121300 -4.63170900 -3.44281200

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1001aaa_2PhSO3H_1BuOH_8MeOH_b3lyp631dp_PCMbu_f3.log

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-6.985477	0.295285	-2.427118
2	6	0	-5.675364	0.514129	-2.012380
3	6	0	-5.358717	0.379741	-0.658681
4	6	0	-6.331853	0.035830	0.282694
5	6	0	-7.642639	-0.182039	-0.143952
6	6	0	-7.970592	-0.054661	-1.496081
7	1	0	-7.246534	0.401761	-3.476312
8	1	0	-4.906999	0.797124	-2.722925
9	1	0	-6.067924	-0.045135	1.331136
10	1	0	-8.406993	-0.444769	0.580583
11	1	0	-8.991996	-0.222700	-1.823322
12	16	0	-3.660964	0.601918	-0.124410
13	8	0	-3.042017	1.567572	-1.077750
14	8	0	-3.707548	1.082997	1.285006
15	8	0	-3.022202	-0.768509	-0.236959
16	1	0	-1.385227	-0.914912	-0.012216
17	8	0	-1.494322	3.707194	-0.364667
18	1	0	-1.971595	2.895693	-0.646977
19	8	0	-2.698098	-0.364643	3.515161
20	1	0	-3.005751	0.134451	2.735202
21	6	0	-2.292087	4.371802	0.617287
22	1	0	-1.671474	5.134859	1.092504
23	1	0	-3.156199	4.863818	0.154100
24	1	0	-2.649719	3.674833	1.381960
25	6	0	-3.714457	-1.302911	3.844389
26	1	0	-3.919321	-2.004480	3.024513
27	1	0	-3.366539	-1.879157	4.707491
28	1	0	-4.658500	-0.813150	4.128227
29	8	0	-0.407838	-1.085283	0.095105
30	1	0	-0.103738	-2.492845	-0.206483
31	6	0	0.004862	-0.676737	1.432104
32	6	0	0.136140	0.835073	1.551172
33	1	0	0.969579	-1.162064	1.603425
34	1	0	-0.726498	-1.053323	2.154476
35	6	0	0.581485	1.251891	2.960465
36	1	0	0.863448	1.188511	0.812136
37	1	0	-0.826388	1.305368	1.317176
38	6	0	0.649242	2.771827	3.139008
39	1	0	-0.114388	0.827232	3.694816
40	1	0	1.566024	0.813191	3.170164
41	1	0	1.033933	3.038570	4.128937
42	1	0	1.297126	3.232540	2.385947
43	1	0	-0.344036	3.223245	3.036170
44	8	0	-0.040319	-0.109046	-2.588680
45	1	0	-0.001240	-0.295863	-1.634157
46	6	0	0.570114	-1.206190	-3.260335
47	1	0	0.089674	-2.162009	-3.009733

48	1	0	0.455240	-1.039501	-4.335158
49	1	0	1.642018	-1.285521	-3.034860
50	8	0	0.148326	-3.475122	-0.446407
51	1	0	1.242698	-3.609557	-0.400354
52	6	0	-0.559695	-4.428834	0.395365
53	1	0	-1.604689	-4.118226	0.454849
54	1	0	-0.478593	-5.405334	-0.081482
55	1	0	-0.112440	-4.458310	1.391711
56	6	0	3.220051	-4.209152	-1.505302
57	1	0	2.587213	-4.954414	-1.989003
58	1	0	3.377984	-3.361188	-2.176386
59	1	0	4.182014	-4.663531	-1.253761
60	8	0	2.554916	-3.792531	-0.296987
61	1	0	3.001643	-2.974539	0.065201
62	6	0	6.334827	-0.422079	1.462051
63	6	0	7.692897	-0.236009	1.717435
64	6	0	8.569997	0.063241	0.670770
65	6	0	8.091471	0.173804	-0.636211
66	6	0	6.733406	-0.009678	-0.903481
67	6	0	5.866890	-0.305161	0.150022
68	1	0	5.649039	-0.666855	2.265701
69	1	0	8.066619	-0.328203	2.732373
70	1	0	9.626777	0.205656	0.874597
71	1	0	8.773545	0.399750	-1.449866
72	1	0	6.347783	0.063606	-1.913936
73	16	0	4.112617	-0.491451	-0.180874
74	8	0	3.953742	-0.737959	-1.632330
75	8	0	3.651453	-1.616312	0.698115
76	8	0	3.470254	0.806294	0.269426
77	1	0	3.069720	1.845305	-0.674622
78	8	0	2.775404	2.630810	-1.293174
79	1	0	1.990787	3.231787	-0.851072
80	8	0	1.084671	4.078299	-0.281187
81	1	0	0.110540	3.834801	-0.306943
82	6	0	2.434213	2.166698	-2.631215
83	1	0	3.282819	1.591730	-2.998061
84	1	0	1.536053	1.544151	-2.607608
85	1	0	2.284036	3.052302	-3.248314
86	6	0	1.239170	5.448527	-0.684776
87	1	0	0.777911	6.110721	0.052940
88	1	0	2.308592	5.660265	-0.732048
89	1	0	0.790478	5.628352	-1.666917
90	8	0	-3.748334	-3.281022	0.808671
91	1	0	-3.549476	-2.378721	0.492563
92	6	0	-4.818889	-3.784304	0.019769
93	1	0	-5.055617	-4.788477	0.382559
94	1	0	-5.723714	-3.167147	0.105374
95	1	0	-4.554816	-3.859638	-1.044526

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1003aaa_2PhSO3H_1BuOH_8MeOH_b3lyp631dp_PCMbu_SCAN_CO_fine_cont_FRQ.log

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	7.085597	-0.102401	1.222456
2	6	0	5.826364	0.310413	0.785447
3	6	0	5.319070	-0.201160	-0.411875
4	6	0	6.053029	-1.109690	-1.177202
5	6	0	7.312296	-1.514840	-0.731009
6	6	0	7.826571	-1.014131	0.467018
7	1	0	7.488752	0.293812	2.149496
8	1	0	5.248953	1.028423	1.357306
9	1	0	5.646249	-1.479169	-2.111595
10	1	0	7.891474	-2.217382	-1.322039
11	1	0	8.806899	-1.330430	0.809907
12	16	0	3.677469	0.289811	-0.948515
13	8	0	3.478978	1.699973	-0.539156
14	8	0	3.622385	0.036755	-2.414351
15	8	0	2.724563	-0.636627	-0.194556
16	1	0	1.536139	0.002875	0.532656
17	8	0	0.212945	4.431998	-0.507443
18	1	0	0.535577	3.961369	0.318831
19	8	0	1.297648	-1.141650	-3.502671
20	1	0	2.079054	-0.697475	-3.121293
21	6	0	1.197409	4.330468	-1.553693
22	1	0	0.678225	4.345578	-2.513937
23	1	0	1.877978	5.185905	-1.503630
24	1	0	1.770052	3.404117	-1.460781
25	6	0	1.541262	-2.540502	-3.457928
26	1	0	1.725091	-2.905666	-2.438384
27	1	0	0.650864	-3.045769	-3.845119
28	1	0	2.393992	-2.836353	-4.088347
29	8	0	0.784690	0.360283	1.130530
30	1	0	0.864889	-0.138643	2.042052
31	6	0	-0.768547	-0.070179	0.584200
32	6	0	-0.694756	0.454935	-0.844357
33	1	0	-1.264056	0.516836	1.334465
34	1	0	-0.661809	-1.128578	0.744876
35	6	0	-1.929306	0.335557	-1.749472
36	1	0	-0.412417	1.512487	-0.782289
37	1	0	0.131847	-0.064157	-1.342939
38	6	0	-1.641791	0.914386	-3.139626
39	1	0	-2.218324	-0.715536	-1.838119
40	1	0	-2.777006	0.856801	-1.297229
41	1	0	-2.512516	0.803408	-3.794527
42	1	0	-1.407245	1.983262	-3.078920
43	1	0	-0.793398	0.404169	-3.606787
44	8	0	0.970563	3.125435	1.619277
45	1	0	0.986675	2.165476	1.426425
46	6	0	2.216883	3.491840	2.229280
47	1	0	3.063635	3.209530	1.596209

48	1	0	2.207465	4.575410	2.361763
49	1	0	2.320129	3.018213	3.211737
50	8	0	0.812780	-0.970883	3.276226
51	1	0	-0.091943	-1.389890	3.290259
52	6	0	1.800759	-2.016620	3.280072
53	1	0	1.801132	-2.580228	2.339997
54	1	0	2.776605	-1.544678	3.412995
55	1	0	1.623782	-2.698629	4.117188
56	6	0	-2.378922	-2.099631	4.381488
57	1	0	-1.768558	-2.579486	5.149582
58	1	0	-2.637044	-1.087444	4.714912
59	1	0	-3.302403	-2.670317	4.247525
60	8	0	-1.608220	-2.086432	3.176242
61	1	0	-2.146723	-1.700602	2.456901
62	6	0	-4.308336	-2.833033	-0.819242
63	6	0	-4.929371	-3.593643	-1.810040
64	6	0	-6.093689	-3.127322	-2.426390
65	6	0	-6.638251	-1.895859	-2.055600
66	6	0	-6.024303	-1.126555	-1.065738
67	6	0	-4.861813	-1.602190	-0.455850
68	1	0	-3.397954	-3.180416	-0.343022
69	1	0	-4.501882	-4.547637	-2.102509
70	1	0	-6.573182	-3.721649	-3.198098
71	1	0	-7.539291	-1.530359	-2.538362
72	1	0	-6.430027	-0.163816	-0.776552
73	16	0	-4.108947	-0.666260	0.880771
74	8	0	-4.610418	-1.229141	2.157621
75	8	0	-2.611859	-0.859612	0.743641
76	8	0	-4.519567	0.759125	0.650417
77	1	0	-3.702567	2.173139	0.831263
78	8	0	-3.340175	3.095749	0.922841
79	1	0	-2.641330	3.583963	-0.170807
80	8	0	-2.138317	4.004610	-1.019495
81	1	0	-1.089626	4.179122	-0.806527
82	6	0	-2.736426	3.277322	2.214388
83	1	0	-3.284218	2.696580	2.960088
84	1	0	-1.682806	2.977218	2.214254
85	1	0	-2.802753	4.336679	2.471196
86	6	0	-2.806293	5.209021	-1.472067
87	1	0	-2.343668	5.515860	-2.409603
88	1	0	-3.854806	4.965112	-1.640012
89	1	0	-2.717278	6.003940	-0.728038
90	8	0	2.342267	-3.423377	0.026598
91	1	0	2.533614	-2.476167	-0.111924
92	6	0	3.586199	-4.092681	0.184109
93	1	0	3.377624	-5.161261	0.289637
94	1	0	4.246890	-3.958706	-0.683614
95	1	0	4.128788	-3.762349	1.081409

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1005aaa_2PhSO3H_1BuOH_8MeOH_b3lyp631dp_PCMbu_SCAN_CO_end.log

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	7.526817	-0.922147	-0.281229
2	6	0	6.349747	-0.189420	-0.128478
3	6	0	5.229467	-0.530767	-0.892252
4	6	0	5.274005	-1.581595	-1.810152
5	6	0	6.459033	-2.306829	-1.955811
6	6	0	7.581302	-1.979785	-1.192737
7	1	0	8.401229	-0.662462	0.307342
8	1	0	6.303578	0.642243	0.566438
9	1	0	4.396890	-1.823987	-2.399221
10	1	0	6.503272	-3.124504	-2.668404
11	1	0	8.500334	-2.545639	-1.310362
12	16	0	3.715221	0.411395	-0.678578
13	8	0	4.086698	1.844277	-0.658759
14	8	0	2.798987	0.021403	-1.788353
15	8	0	3.171143	-0.038196	0.676004
16	1	0	1.842495	0.652545	1.104185
17	8	0	0.720313	4.608725	-0.684120
18	1	0	1.083005	3.963863	0.741568
19	8	0	1.770621	-2.523905	-2.495487
20	1	0	2.099814	-1.661760	-2.179221
21	6	0	1.411701	4.010811	-1.784287
22	1	0	1.057034	2.993070	-1.985149
23	1	0	1.291712	4.611751	-2.693922
24	1	0	2.472267	3.955212	-1.532250
25	6	0	2.066248	-3.501918	-1.507040
26	1	0	1.866232	-3.151967	-0.486218
27	1	0	1.437118	-4.376828	-1.700104
28	1	0	3.116399	-3.830046	-1.546985
29	8	0	0.972954	1.086730	1.406347
30	1	0	0.620108	0.624791	2.275912
31	6	0	-1.776572	-0.189979	-0.247463
32	6	0	-0.916988	-0.286967	-1.492262
33	1	0	-1.923904	0.845160	0.068447
34	1	0	-1.364514	-0.772424	0.579055
35	6	0	-1.426409	0.542746	-2.678132
36	1	0	0.081622	0.059480	-1.199392
37	1	0	-0.798623	-1.338326	-1.779124
38	6	0	-0.493151	0.457510	-3.889974
39	1	0	-2.428225	0.197815	-2.960804
40	1	0	-1.535875	1.588879	-2.362946
41	1	0	-0.868607	1.059649	-4.723658
42	1	0	0.512382	0.813987	-3.641104
43	1	0	-0.394585	-0.575844	-4.240996
44	8	0	1.282004	3.543859	1.635137
45	1	0	1.112428	2.126514	1.526187
46	6	0	2.591675	3.946704	2.064153
47	1	0	3.367747	3.551879	1.399719

48	1	0	2.657251	5.038377	2.095889
49	1	0	2.747371	3.555284	3.071729
50	8	0	0.097525	-0.039451	3.460442
51	1	0	-0.425935	-0.842633	3.194500
52	6	0	1.124708	-0.444785	4.382895
53	1	0	1.823573	-1.142348	3.909314
54	1	0	1.659221	0.454760	4.694807
55	1	0	0.674500	-0.911581	5.264200
56	6	0	-0.728882	-3.337755	2.123045
57	1	0	0.354957	-3.277992	2.236194
58	1	0	-1.095204	-4.266860	2.575522
59	1	0	-0.968705	-3.345462	1.053736
60	8	0	-1.293584	-2.194871	2.777953
61	1	0	-2.216964	-2.082118	2.488492
62	6	0	-5.845672	-2.720923	-0.437511
63	6	0	-6.949957	-3.149515	-1.172576
64	6	0	-7.799702	-2.215666	-1.771229
65	6	0	-7.556310	-0.846048	-1.638693
66	6	0	-6.456817	-0.398154	-0.908140
67	6	0	-5.616426	-1.347740	-0.321802
68	1	0	-5.182142	-3.431371	0.041495
69	1	0	-7.147342	-4.211427	-1.273504
70	1	0	-8.658376	-2.556905	-2.340547
71	1	0	-8.223035	-0.125352	-2.100078
72	1	0	-6.258684	0.660481	-0.787494
73	16	0	-4.207588	-0.787686	0.601638
74	8	0	-3.833360	-1.812877	1.592965
75	8	0	-3.108225	-0.754054	-0.580694
76	8	0	-4.444103	0.579180	1.097111
77	1	0	-3.429349	2.162861	1.260778
78	8	0	-2.790440	2.896357	1.279029
79	1	0	-2.176178	3.557523	-0.189526
80	8	0	-1.859730	3.985463	-1.019716
81	1	0	-0.251793	4.457704	-0.818978
82	6	0	-2.115094	2.905868	2.540153
83	1	0	-2.771748	3.274916	3.337351
84	1	0	-1.747125	1.910785	2.814131
85	1	0	-1.256681	3.573623	2.446326
86	6	0	-2.793367	5.003313	-1.379228
87	1	0	-2.424936	5.487508	-2.286461
88	1	0	-3.782652	4.579049	-1.588771
89	1	0	-2.896061	5.763351	-0.594453
90	8	0	2.692055	-2.510569	1.963675
91	1	0	2.864981	-1.703739	1.441578
92	6	0	3.926236	-3.202039	2.106290
93	1	0	3.742060	-4.087720	2.720429
94	1	0	4.330838	-3.533989	1.140195
95	1	0	4.690067	-2.591222	2.607051

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1021aaa_2PhSO3H_1BuOH_9MeOH_SN1_b3lyp631dp_PCMbu.log

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.329205	0.067402	4.109306
2	6	0	0.841691	0.155392	2.805524
3	6	0	1.582854	-0.434579	1.775973
4	6	0	2.794952	-1.085688	2.015717
5	6	0	3.266038	-1.158127	3.328827
6	6	0	2.534155	-0.589054	4.372040
7	1	0	0.763490	0.517422	4.919851
8	1	0	-0.088113	0.683566	2.611212
9	1	0	3.365542	-1.509818	1.196363
10	1	0	4.207469	-1.658697	3.531968
11	1	0	2.905393	-0.650747	5.390423
12	16	0	0.978133	-0.335878	0.094886
13	8	0	0.683446	1.106393	-0.171812
14	8	0	1.959063	-0.957371	-0.806303
15	8	0	-0.345934	-1.146508	0.078838
16	1	0	4.154071	1.171932	-1.603483
17	8	0	2.671364	2.052444	-2.002470
18	1	0	2.006612	1.720540	-1.369659
19	8	0	3.526942	-4.213796	-1.028862
20	1	0	3.894744	-3.308805	-0.922756
21	6	0	2.645371	3.482240	-1.953569
22	1	0	3.033485	3.868826	-1.002289
23	1	0	3.279133	3.850988	-2.763355
24	1	0	1.625653	3.853206	-2.098431
25	6	0	3.378852	-4.763837	0.270368
26	1	0	2.583049	-4.274597	0.852193
27	1	0	3.111081	-5.819859	0.161883
28	1	0	4.308527	-4.710525	0.854992
29	8	0	4.951913	0.697447	-1.272074
30	6	0	5.439703	1.405252	-0.127863
31	6	0	6.321861	2.591553	-0.513028
32	1	0	6.016936	0.685548	0.464068
33	1	0	4.602096	1.739870	0.500773
34	6	0	6.894702	3.329124	0.703510
35	1	0	7.139058	2.226725	-1.148892
36	1	0	5.736519	3.290240	-1.126179
37	6	0	7.783406	4.516681	0.321234
38	1	0	6.069646	3.679633	1.338236
39	1	0	7.471646	2.623638	1.316632
40	1	0	8.177497	5.022142	1.208862
41	1	0	8.636939	4.192501	-0.284807
42	1	0	7.224871	5.256358	-0.263462
43	8	0	-3.071959	3.782654	-0.937965
44	1	0	-2.286673	3.346204	-1.335920
45	6	0	-3.147167	5.095837	-1.468233
46	1	0	-3.317766	5.102235	-2.555153
47	1	0	-3.991065	5.604802	-0.993075

48	1	0	-2.239580	5.681916	-1.264007
49	8	0	-2.124705	1.667130	2.919402
50	1	0	-2.545586	1.080190	2.273764
51	6	0	-2.486473	3.005344	2.583374
52	1	0	-1.840784	3.672792	3.160830
53	1	0	-2.355372	3.224018	1.516600
54	1	0	-3.530227	3.225246	2.850751
55	6	0	-3.260610	-2.844722	-3.733078
56	1	0	-2.560278	-3.219418	-4.479554
57	1	0	-4.250386	-3.267334	-3.919077
58	1	0	-3.304945	-1.753735	-3.775530
59	8	0	-2.785903	-3.290487	-2.442720
60	1	0	-3.330843	-2.876423	-1.731967
61	6	0	-5.363592	1.703976	0.099606
62	6	0	-6.482017	2.311433	0.671146
63	6	0	-7.418144	1.551667	1.377953
64	6	0	-7.247028	0.173017	1.523921
65	6	0	-6.134878	-0.455841	0.965294
66	6	0	-5.211634	0.323712	0.264497
67	1	0	-4.632608	2.295991	-0.446747
68	1	0	-6.622300	3.381672	0.559633
69	1	0	-8.285876	2.035706	1.815032
70	1	0	-7.977661	-0.414615	2.069734
71	1	0	-5.986017	-1.524553	1.063104
72	16	0	-3.799428	-0.472279	-0.462853
73	8	0	-4.006844	-1.940223	-0.424364
74	8	0	-3.473822	0.117994	-1.764801
75	8	0	-2.661150	-0.088535	0.606265
76	1	0	-1.748700	-0.470141	0.349943
77	8	0	-0.763568	2.702051	-1.967439
78	1	0	-0.398175	2.104921	-1.287618
79	8	0	4.960156	-1.924202	-0.573560
80	1	0	4.795249	-1.000927	-0.882600
81	6	0	-0.764058	1.988425	-3.207674
82	1	0	-1.123510	2.673573	-3.978777
83	1	0	0.250251	1.665844	-3.468610
84	1	0	-1.427803	1.117126	-3.172918
85	6	0	6.293608	-2.277747	-0.924003
86	1	0	6.492876	-2.125229	-1.992629
87	1	0	7.033611	-1.705863	-0.348628
88	1	0	6.425990	-3.339197	-0.699330
89	8	0	-0.510587	-3.654038	1.594037
90	1	0	-0.418461	-2.755226	1.237354
91	6	0	-1.762963	-3.722056	2.267173
92	1	0	-1.893947	-4.750521	2.614430
93	1	0	-1.799708	-3.059262	3.143413
94	1	0	-2.605814	-3.470409	1.609221
95	1	0	-0.353668	-2.168115	-1.210587
96	8	0	-0.439704	-2.836337	-1.958403
97	1	0	-1.497777	-3.015495	-2.182983
98	6	0	0.250579	-4.085458	-1.618560
99	1	0	1.322683	-3.885600	-1.596061
100	1	0	-0.101423	-4.436869	-0.647419
101	1	0	0.008721	-4.792877	-2.410182

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1023aaa_2PhSO3H_1BuOH_9MeOH_SN1_b3lyp631dp_PCMbu_SCAN_SO_TS_FRQ.log
0 1
C 1.80483800 -2.09979300 4.33492000
C 1.19306200 -1.49108000 3.24067600
C 1.97853800 -1.26269900 2.10607100
C 3.33143600 -1.60446200 2.02239800
C 3.91636100 -2.20395800 3.13867700
C 3.15711300 -2.45392900 4.28395100
H 1.22305500 -2.29732000 5.22905500
H 0.13969300 -1.21528700 3.27133800
H 3.91100800 -1.38726700 1.12975300
H 4.96684900 -2.47357600 3.10988200
H 3.62120900 -2.92612900 5.14405500
S 1.24190200 -0.45513600 0.70994400
O 0.47279800 0.71967500 1.10302400
O 2.13553800 -0.44552900 -0.43683900
O -0.09059400 -1.79161300 0.20905400
H 3.13233000 1.85007500 -1.67942500
O 1.59145600 2.04209000 -2.48321100
H 0.73423200 2.17703300 -2.02420800
O 4.20793100 -2.92330100 -1.95335300
H 4.43953900 -2.05653800 -1.55221400
C 1.56406200 2.73761700 -3.72445300
H 1.42824200 3.81959700 -3.59460600
H 2.52495300 2.57094600 -4.21760800
H 0.76958700 2.36198600 -4.38224100
C 4.75288800 -3.93102200 -1.11989400
H 4.35848300 -3.89482200 -0.09324700
H 4.48606000 -4.90332800 -1.54581500
H 5.85097700 -3.88087200 -1.06074800
O 4.01950100 1.83553700 -1.24797700
C 3.93323100 2.64089500 -0.06949200
C 3.80303900 4.12796300 -0.39550600
H 4.84992200 2.45667400 0.50239700
H 3.08839300 2.31906900 0.55721000
C 3.73978900 5.01251400 0.85536600
H 4.65308500 4.42593000 -1.02323100
H 2.89786400 4.27506600 -0.99978400
C 3.61357500 6.50376600 0.52908500
H 2.88975400 4.70158200 1.47792600
H 4.63929900 4.84660000 1.46358700
H 3.56891700 7.10933500 1.44012100
H 4.46785800 6.85266500 -0.06200400
H 2.70589700 6.70580200 -0.05083200
O -1.74711800 3.12755900 1.28224400
H -1.27958000 2.82449100 0.47949300
C -1.32109400 4.45109200 1.56965200
H -1.54250200 5.15216600 0.75218200
H -1.86026100 4.78851800 2.45930900
H -0.24413300 4.50530500 1.78455800
O -2.04421100 -0.74681900 3.45484700
H -2.35968100 -0.80815200 2.53684200
C -2.30886000 0.58223000 3.89741900

H -1.82269900 0.70878900 4.86910700
H -1.91656300 1.33786900 3.20598800
H -3.38580100 0.76193100 4.03134800
C -2.44687300 -1.84338900 -4.32610000
H -1.66099300 -2.06127700 -5.04992500
H -3.41580400 -2.11278000 -4.75264800
H -2.43469900 -0.78158400 -4.06778600
O -2.19673600 -2.65584800 -3.15867000
H -2.84222200 -2.39342600 -2.44269700
C -4.69904400 1.54207800 0.58643600
C -5.85336100 2.19486000 1.01855700
C -7.10915300 1.60615800 0.84136400
C -7.21807500 0.35647900 0.22962400
C -6.07241700 -0.31115000 -0.20848700
C -4.82636200 0.28943600 -0.02483900
H -3.72675300 2.00566000 0.73256500
H -5.77080500 3.16682600 1.49497600
H -8.00157900 2.12287000 1.18091700
H -8.19217200 -0.10201800 0.09157100
H -6.13705300 -1.28150000 -0.68613800
S -3.34991400 -0.55274600 -0.58905300
O -3.80403400 -1.83637400 -1.21614400
O -2.65839500 0.33619100 -1.56995300
O -2.51248100 -0.78757500 0.64324400
H -0.97910700 -1.36394300 0.39913200
O -0.93278400 2.44459400 -1.34099000
H -1.45174200 1.60843300 -1.36921900
O 5.10771000 -0.60217300 -0.73987200
H 4.60961100 0.23099400 -0.93362500
C -1.70199000 3.43782100 -2.03524400
H -1.11583900 4.35871100 -2.04479400
H -1.90566400 3.13502700 -3.06786500
H -2.65085000 3.62588000 -1.52209300
C 6.47572400 -0.37713500 -1.06488500
H 6.61167000 -0.11771700 -2.12301000
H 6.91102100 0.42365500 -0.45314900
H 7.02604800 -1.29985900 -0.86342100
O -0.39010700 -4.62559800 0.59339900
H -0.19895500 -3.67500000 0.67383400
C -1.79723700 -4.78540300 0.72984400
H -2.02660200 -5.84161100 0.56324700
H -2.15140500 -4.51477000 1.73501400
H -2.36247200 -4.19176000 -0.00158200
H 0.02808800 -2.08255700 -1.32963100
O 0.06167400 -2.38813200 -2.29978100
H -0.97223900 -2.51756400 -2.68928100
C 0.86897600 -3.60339400 -2.40695700
H 1.91360400 -3.32121400 -2.26010400
H 0.54019700 -4.32296400 -1.65431900
H 0.71879800 -3.99306600 -3.41309700

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1025aaa_2PhSO3H_1BuOH_9MeOH_SN1_b3lyp631dp_PCMbu_SCAN_SO_vege_f3.log

C -2.85586100 -1.05259200 3.60582300
C -1.97155500 -1.05293300 2.52339100
C -2.51374700 -1.08674700 1.23699000
C -3.88988500 -1.10689000 0.99729500
C -4.75226700 -1.10870800 2.09189000
C -4.23609500 -1.08923900 3.39200200
H -2.45906200 -1.01686000 4.61412500
H -0.89576600 -0.98510200 2.68077800
H -4.27317800 -1.07371200 -0.01646300
H -5.82644000 -1.11699800 1.92878800
H -4.91076100 -1.08867300 4.24289100
S -1.42238100 -1.12600200 -0.16545700
O -0.04332300 -0.85168500 0.23090500
O -2.01738900 -0.44942000 -1.32322500
O -1.21886100 2.08835000 0.71835700
H -0.53477300 -2.47163800 -2.28143100
O 0.08678600 -2.19931600 -2.99035100
H 1.04467100 -1.70640400 -2.54995600
O -5.48738700 3.07886200 -0.79894100
H -5.15325000 2.22166300 -1.13128900
C 0.31203400 -3.28640200 -3.93747200
H 0.85268100 -4.10334600 -3.46368200
H -0.66002200 -3.62031600 -4.29975200
H 0.88673500 -2.86158400 -4.76218200
C -5.47980100 3.01944800 0.61898300
H -4.46393700 3.01520800 1.05061500
H -5.99362700 3.91303100 0.98816100
H -6.02082500 2.14164400 1.00664900
O -1.47184600 -2.70735900 -0.67454600
C -0.86725100 -3.71640200 0.21956100
C -1.23437300 -5.08758200 -0.32296700
H -1.28493900 -3.57300300 1.22260300
H 0.21322200 -3.55511400 0.25155500
C -0.67865400 -6.21519100 0.56181500
H -2.32515700 -5.16807100 -0.38629500
H -0.84403500 -5.19725500 -1.34295600
C -1.03708800 -7.60279800 0.02405000
H 0.41158000 -6.11762200 0.63640500
H -1.06856700 -6.10139000 1.58236800
H -0.63233300 -8.39058100 0.66894400
H -2.12102000 -7.73726500 -0.02925500
H -0.63067200 -7.75827600 -0.98251300
O 2.63495500 -2.98181100 0.24608300
H 2.36935400 -2.36388200 -0.44841100
C 3.63413300 -3.83596600 -0.31115600
H 4.53446300 -3.27997400 -0.60613300
H 3.91462900 -4.55876200 0.45948400
H 3.26591600 -4.38968100 -1.18417300
O 1.05092400 -0.18671200 3.24301100
H 1.26380800 0.33307400 2.44899300
C 2.08692300 -1.14058000 3.43340600
H 1.80421900 -1.76342600 4.28860300

H 2.22083300 -1.79398000 2.56019200
H 3.05163500 -0.66560500 3.66263200
C 1.57313300 3.87031800 -3.45878800
H 0.86791400 4.08357200 -4.26555500
H 2.52124500 4.37596900 -3.68504000
H 1.75253400 2.78967500 -3.42150400
O 1.00496800 4.35042200 -2.24206300
H 1.59564800 4.06513800 -1.51175800
C 4.51842900 0.12257400 0.78837800
C 5.77131600 -0.25020400 1.26694600
C 6.73544600 0.71935900 1.55743900
C 6.44192900 2.07273000 1.37411400
C 5.18710600 2.45997500 0.89879600
C 4.23410300 1.48024100 0.61190500
H 3.77812200 -0.63880100 0.56581800
H 5.99954100 -1.30170400 1.40886900
H 7.70970800 0.42023800 1.92758200
H 7.18890300 2.82869600 1.59749100
H 4.94065500 3.50704500 0.74897000
S 2.61068700 1.97169300 0.02949000
O 2.70922600 3.42291900 -0.30465200
O 2.33612700 1.14591400 -1.19480300
O 1.65267500 1.69693000 1.14627600
H -0.26645600 1.93800800 0.86305900
O 2.08288900 -1.23490300 -2.05552800
H 1.98724100 -0.32359600 -1.62782400
O -4.54471300 0.63245000 -1.76885000
H -3.60051500 0.53683000 -1.56155400
C 3.20706000 -1.17101200 -2.97915800
H 3.42456700 -2.19216000 -3.29718900
H 2.96007200 -0.54707000 -3.84019800
H 4.06531500 -0.75744000 -2.45046400
C -4.71614300 0.41720600 -3.17264300
H -4.18257700 1.16832100 -3.76992900
H -4.37143900 -0.58152000 -3.46801100
H -5.78485800 0.49480100 -3.38544100
O -2.42608400 3.52645700 2.68846000
H -1.99654000 2.97676100 1.99066200
C -1.82048900 4.80427300 2.63487200
H -2.28032000 5.43436500 3.40407000
H -0.73737200 4.77059700 2.83588800
H -1.96435200 5.30723300 1.66453300
H -1.28605400 2.51551900 -0.16614300
O -1.43599100 3.31429200 -1.74320100
H -0.53922400 3.67308300 -1.94243200
C -2.32954100 4.41883600 -1.63032400
H -3.30809000 4.00360700 -1.37269600
H -2.02702200 5.13722000 -0.85449300
H -2.41187200 4.96325300 -2.58089000