

Electronic Supplementary Information

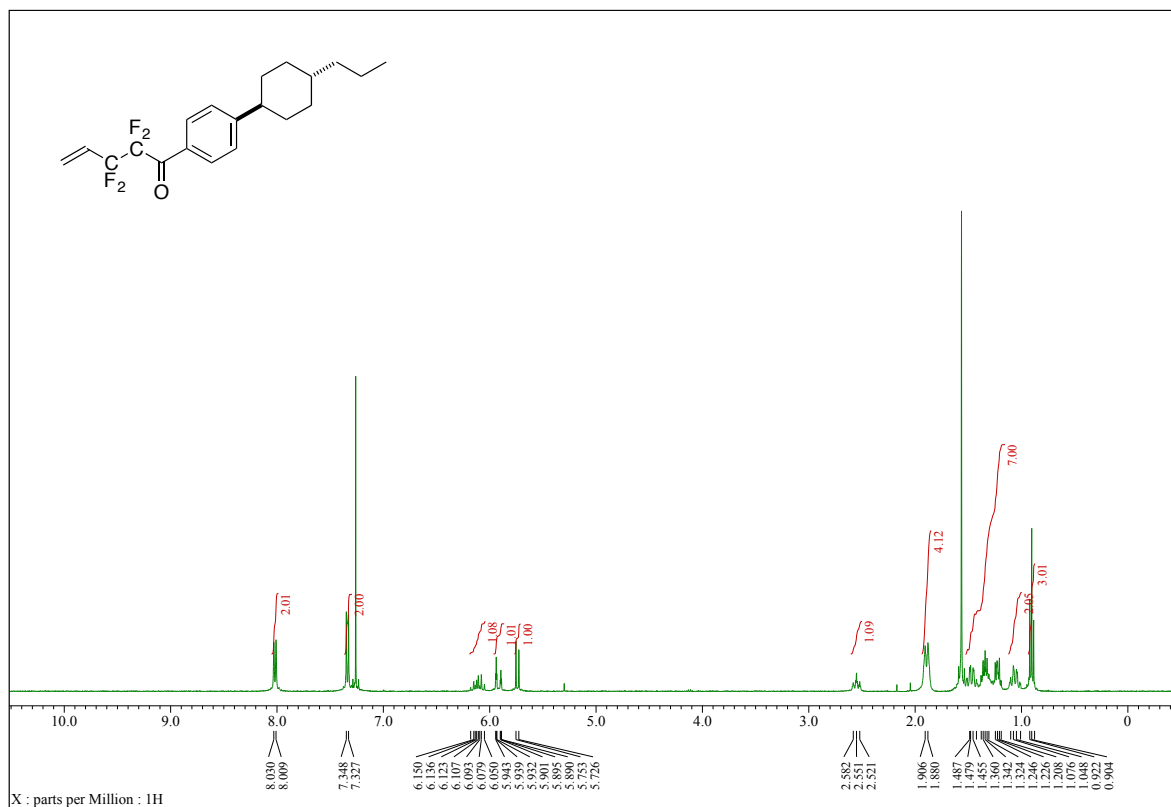
Rational design and synthesis of a novel laterally-tetrafluorinated tricyclic mesogen with large negative dielectric anisotropy

Shigeyuki Yamada,^a Ken Tamamoto,^a Takumi Kida,^a Tomoyuki Asai,^b Takashi Ishihara,^a Tsutomu Konno^a

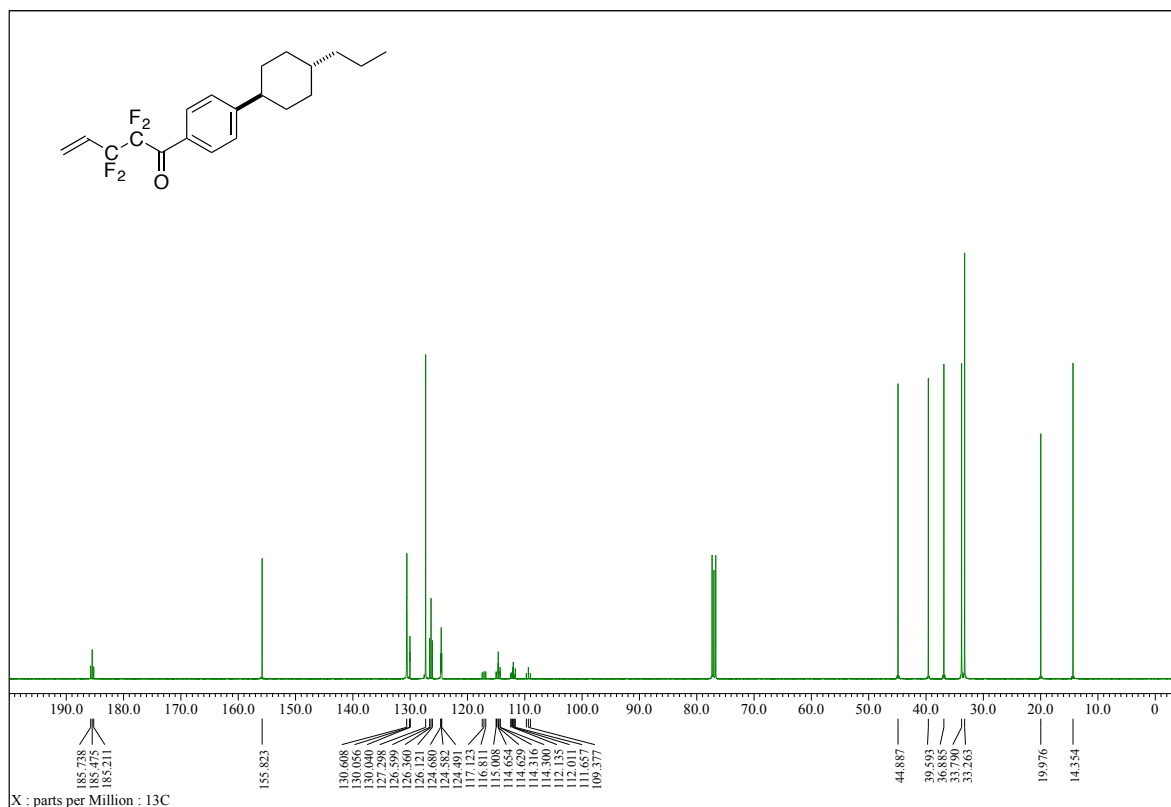
^a *Faculty of Molecular Chemistry and Engineering, Kyoto Institute of Technology,
Matsugasaki, Sakyo-ku, Kyoto 606-8585, Japan*

^b *AGC Seimi Chemical Co., Ltd., Chigasaki 3-2-10, Chigasaki-city, Kanagawa 253-0041, Japan*

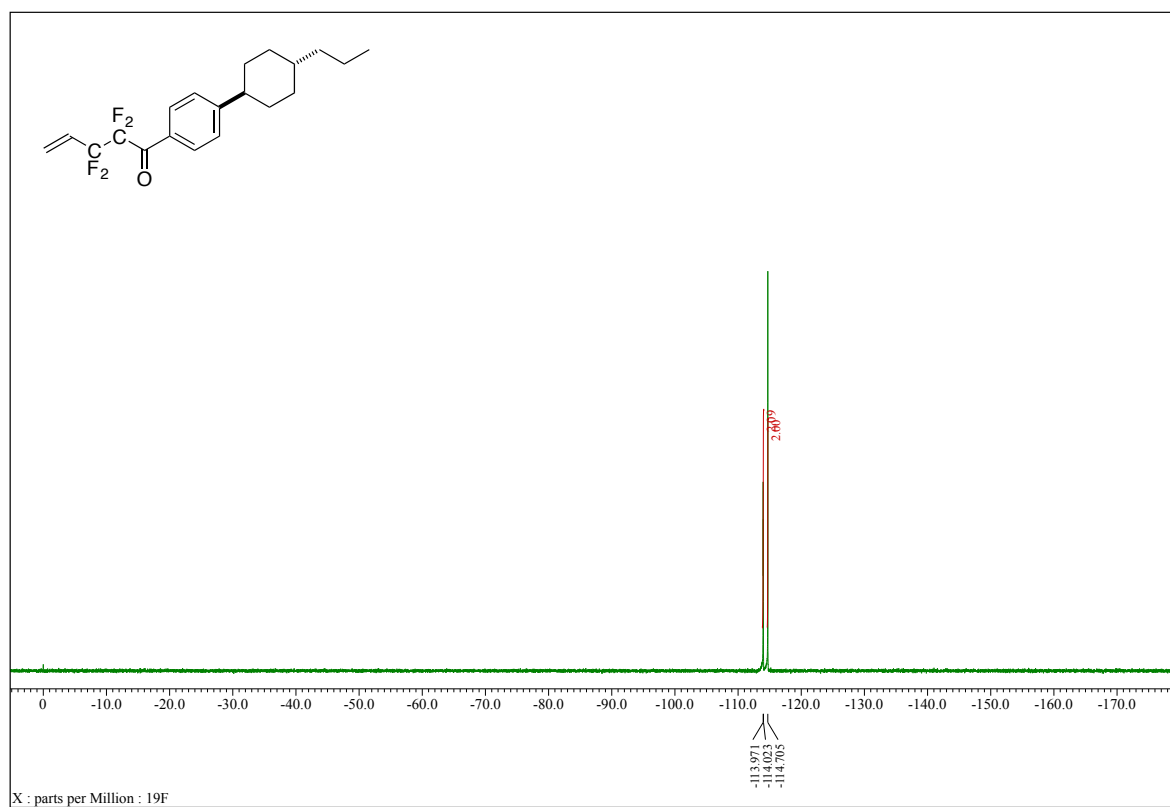
^1H NMR spectrum of 2,2,3,3-tetrafluoro-1-[4-(trans-4-n-propylcyclohexyl)phenyl]pent-4-en-1-one (10)



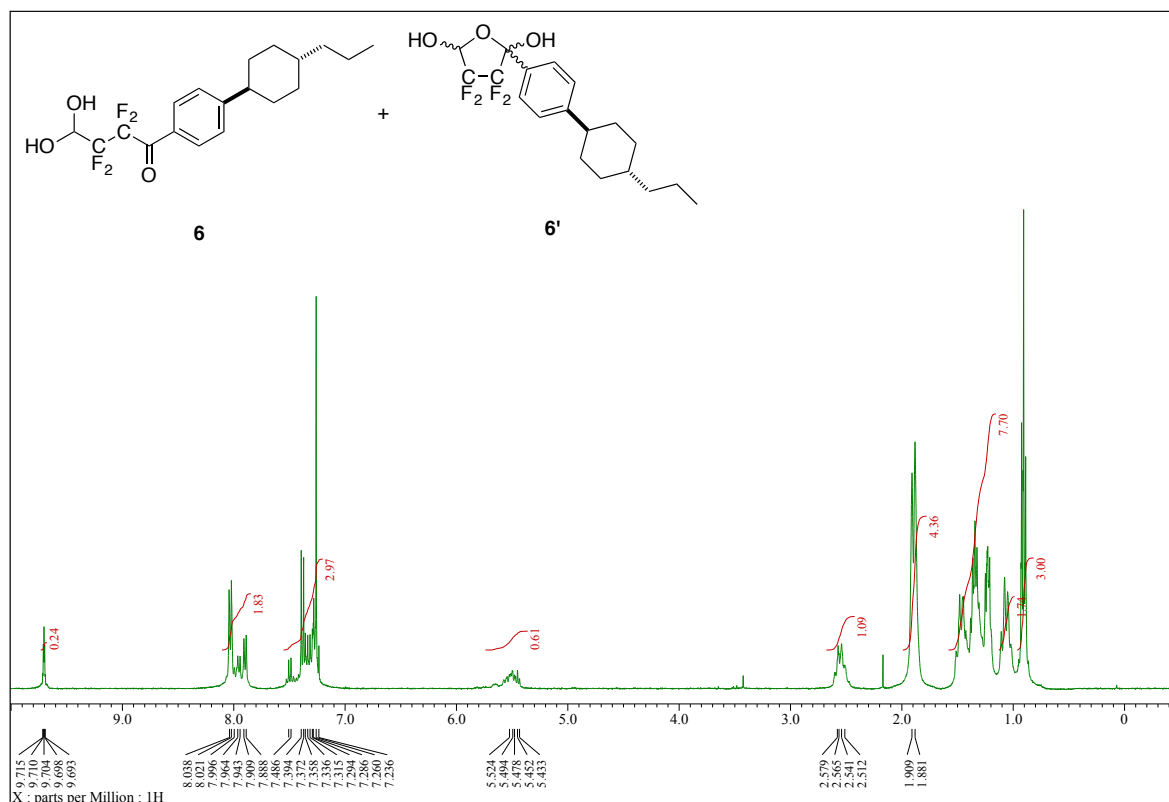
^{13}C NMR spectrum of 2,2,3,3-tetrafluoro-1-[4-(trans-4-n-propylcyclohexyl)phenyl]pent-4-en-1-one (10)



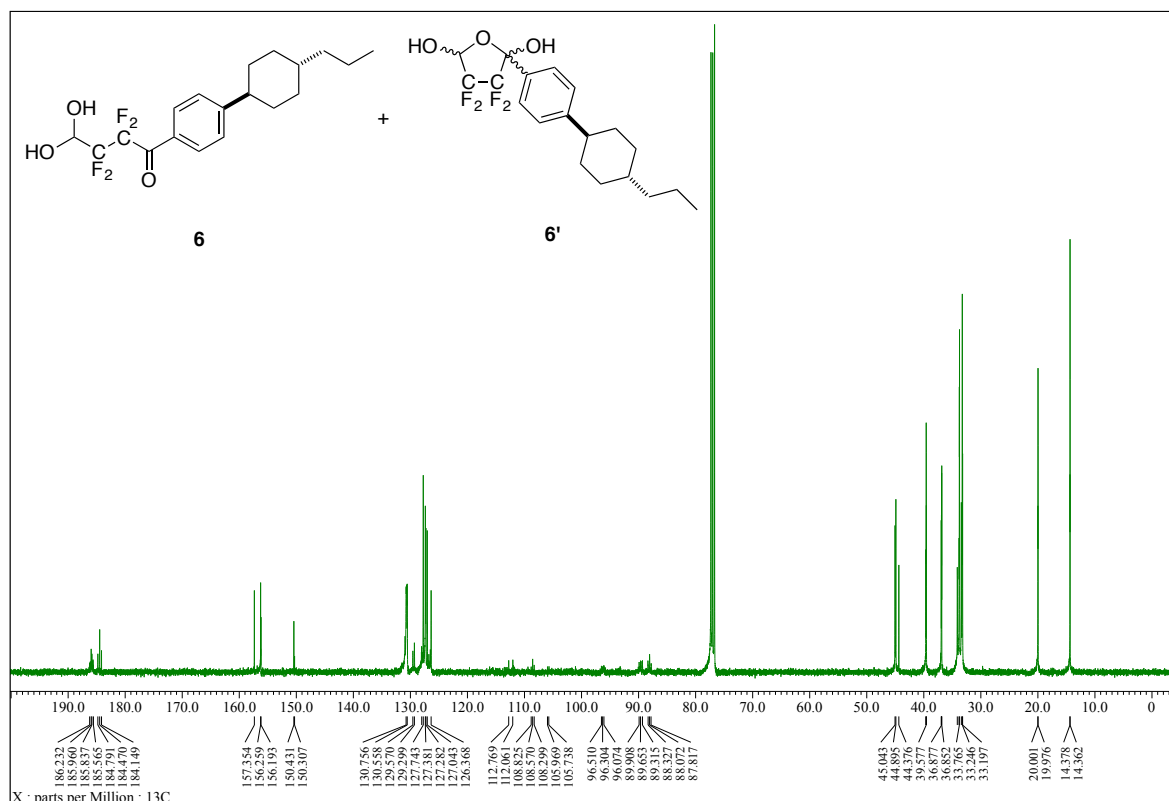
^{19}F NMR spectrum of 2,2,3,3-tetrafluoro-1-[4-(trans-4-n-propylcyclohexyl)phenyl]pent-4-en-1-one (**10**)



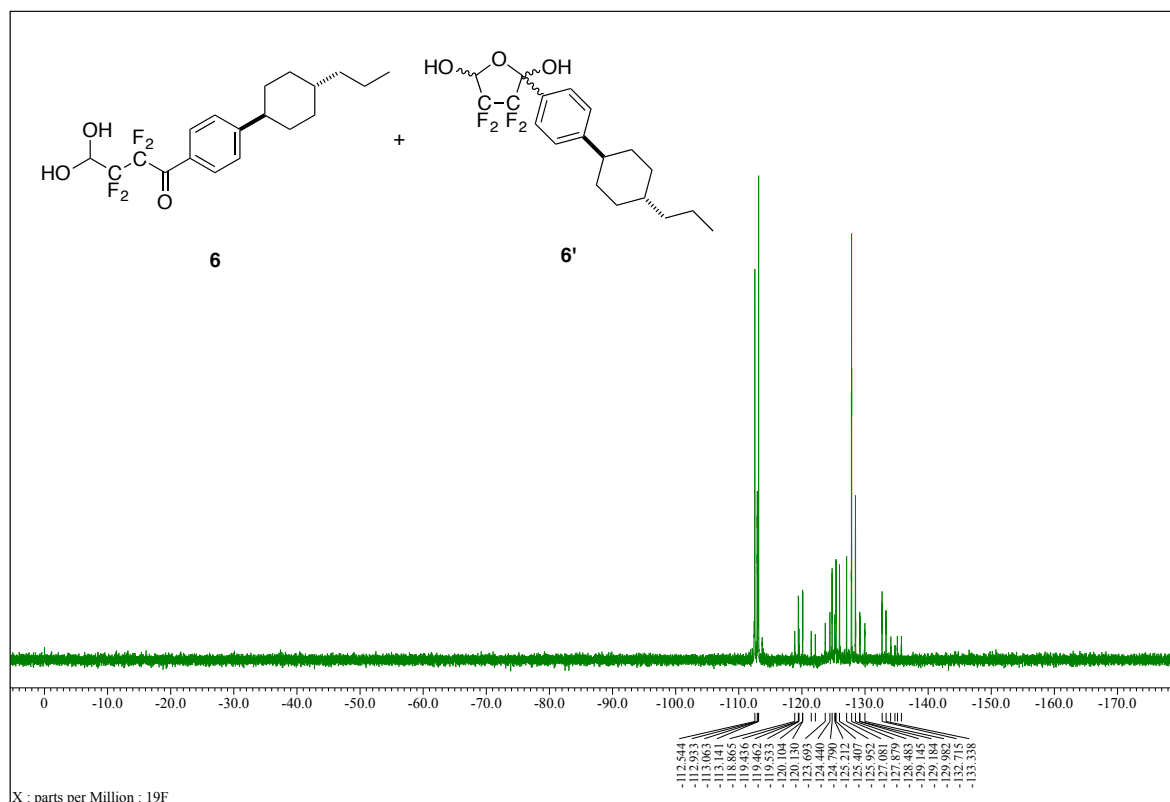
¹H NMR spectrum of a mixture of
 2,2,3,3-tetrafluoro-4-oxo-4-[4-(trans-n-propylcyclohexyl)phenyl]butanal-monohydrate (**11**) and
 2,2,3,3-tetrafluoro-4-hydroxy-1-[4-(trans-4-n-propylcyclohexyl)phenyl]furanose (**11'**)



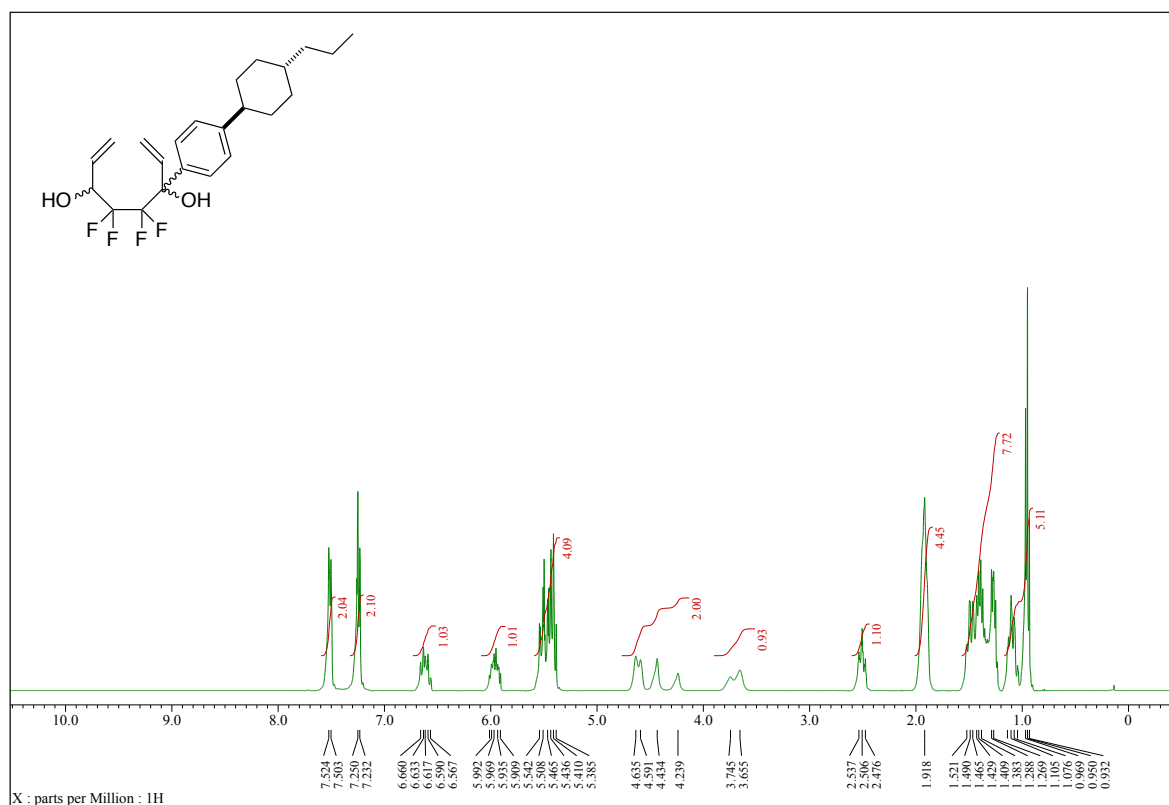
¹³C NMR spectrum of a mixture of
 2,2,3,3-tetrafluoro-4-oxo-4-[4-(trans-n-propylcyclohexyl)phenyl]butanal-monohydrate (**11**) and
 2,2,3,3-tetrafluoro-4-hydroxy-1-[4-(trans-4-n-propylcyclohexyl)phenyl]furanose (**11'**)



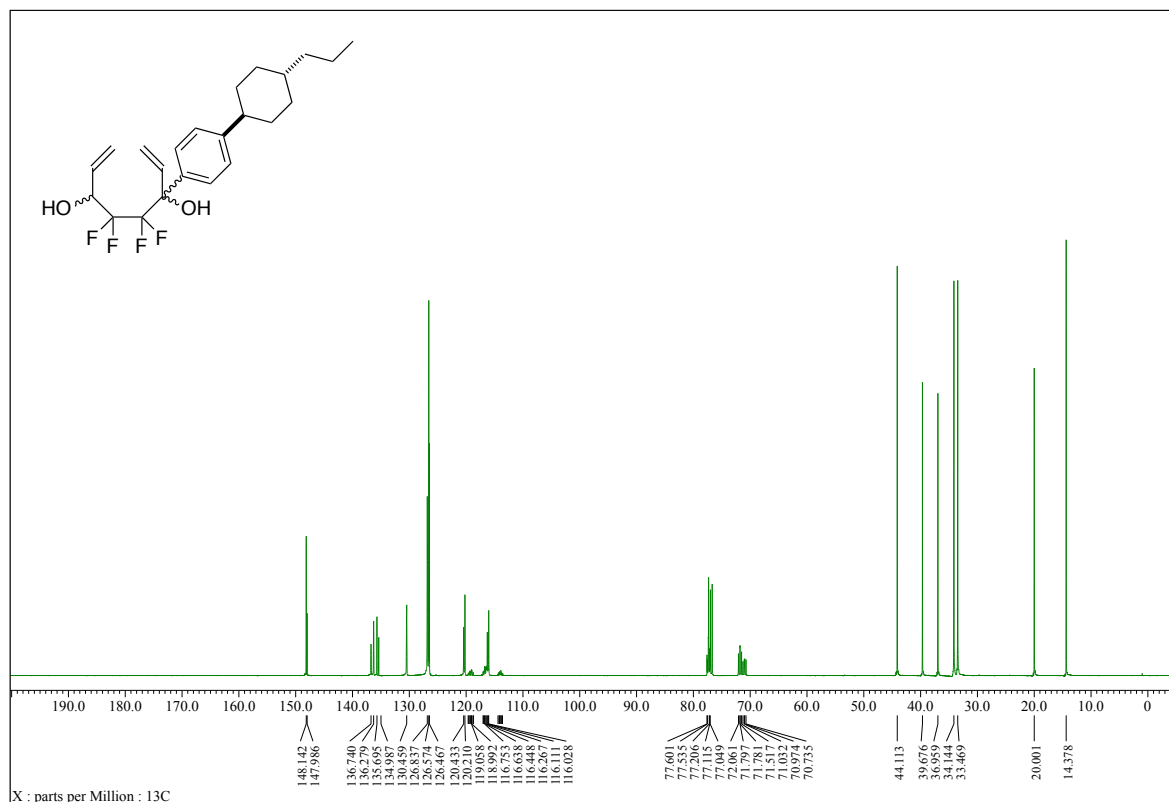
¹⁹F NMR spectrum of a mixture of
 2,2,3,3-tetrafluoro-4-oxo-4-[4-(trans-n-propylcyclohexyl)phenyl]butanal monohydrate (**11**) and
 2,2,3,3-tetrafluoro-4-hydroxy-1-[4-(trans-4-n-propylcyclohexyl)phenyl]furanose (**11'**)



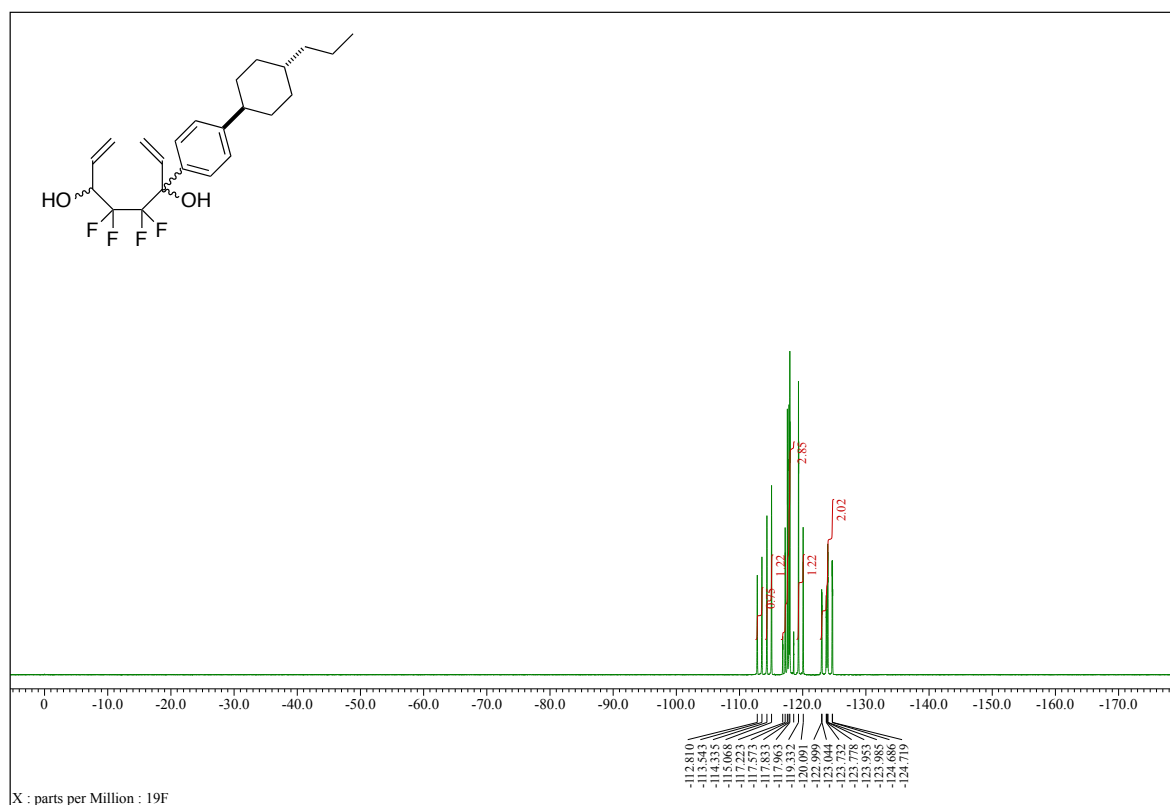
^1H NMR spectrum of 4,4,5,5-tetrafluoro-3-[4-(trans-4-n-propylcyclohexyl)phenyl]octa-1,7-dien-3,6-diol (7)



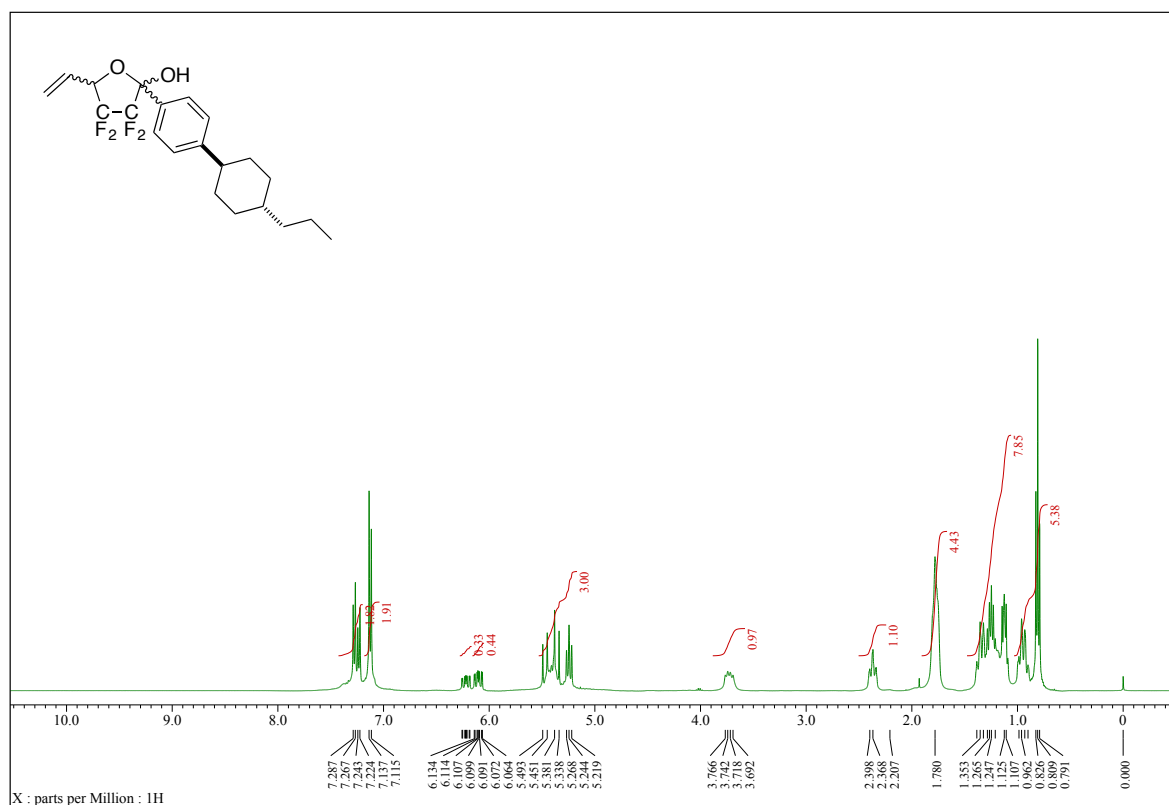
^{13}C NMR spectrum of 4,4,5,5-tetrafluoro-3-[4-(trans-4-n-propylcyclohexyl)phenyl]octa-1,7-dien-3,6-diol (7)



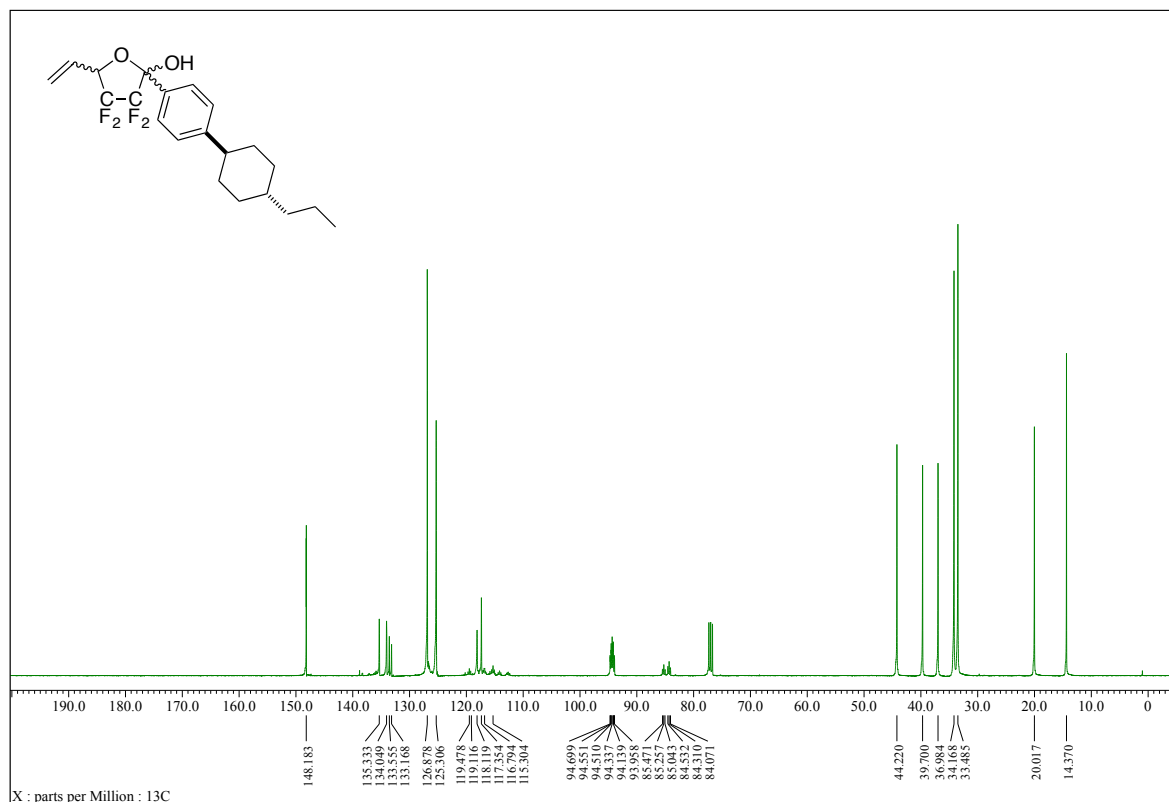
^{19}F NMR spectrum of 4,4,5,5-tetrafluoro-3-[4-(trans-4-n-propylcyclohexyl)phenyl]octa-1,7-dien-3,6-diol (7)



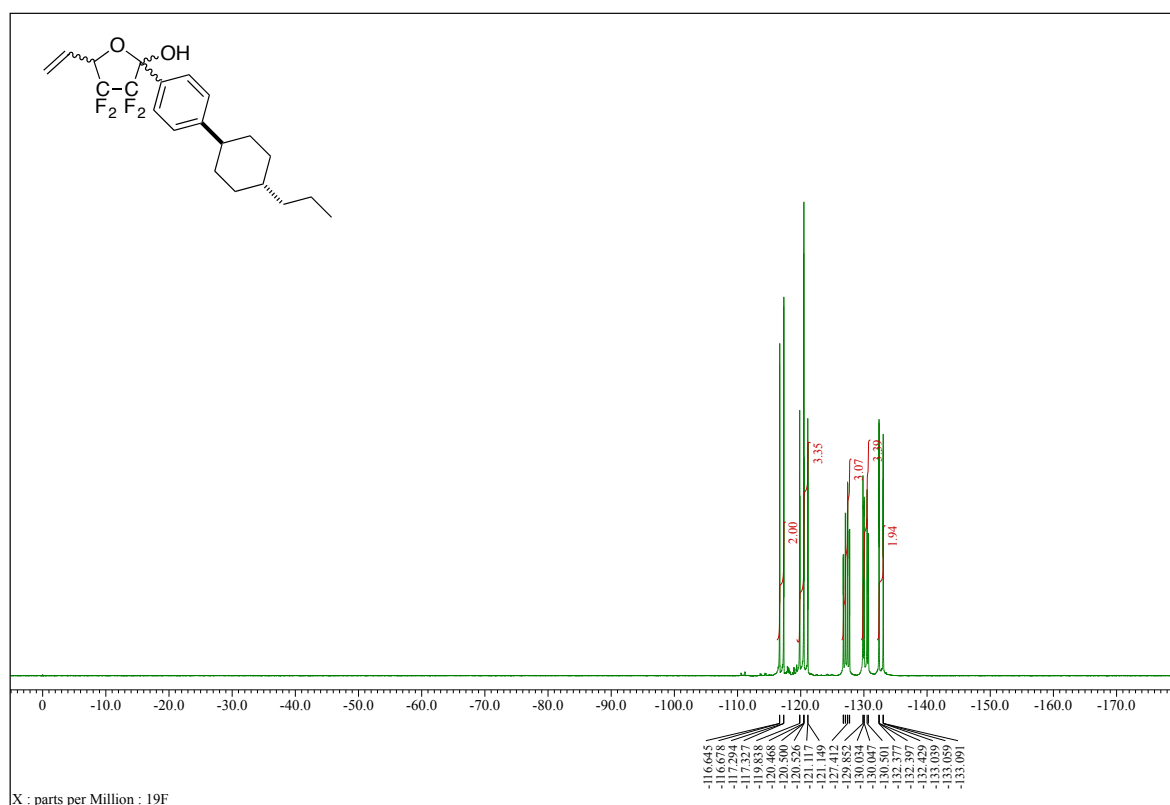
^1H NMR spectrum of 2,2,3,3-tetrafluoro-4-(ethen-1-yl)-1-[4-(trans-4-n-propylcyclohexyl)phenyl]furanose (**12**)



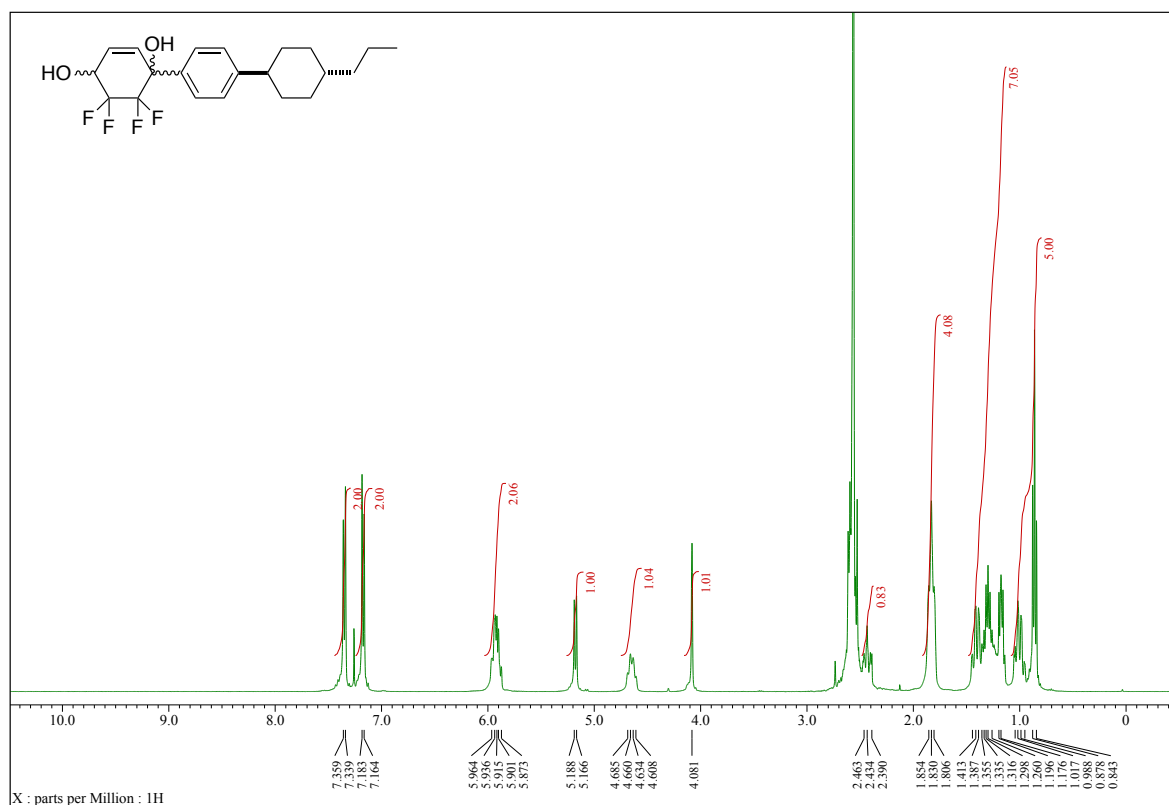
^{13}C NMR spectrum of 2,2,3,3-tetrafluoro-4-(ethen-1-yl)-1-[4-(trans-4-n-propylcyclohexyl)phenyl]furanose (**12**)



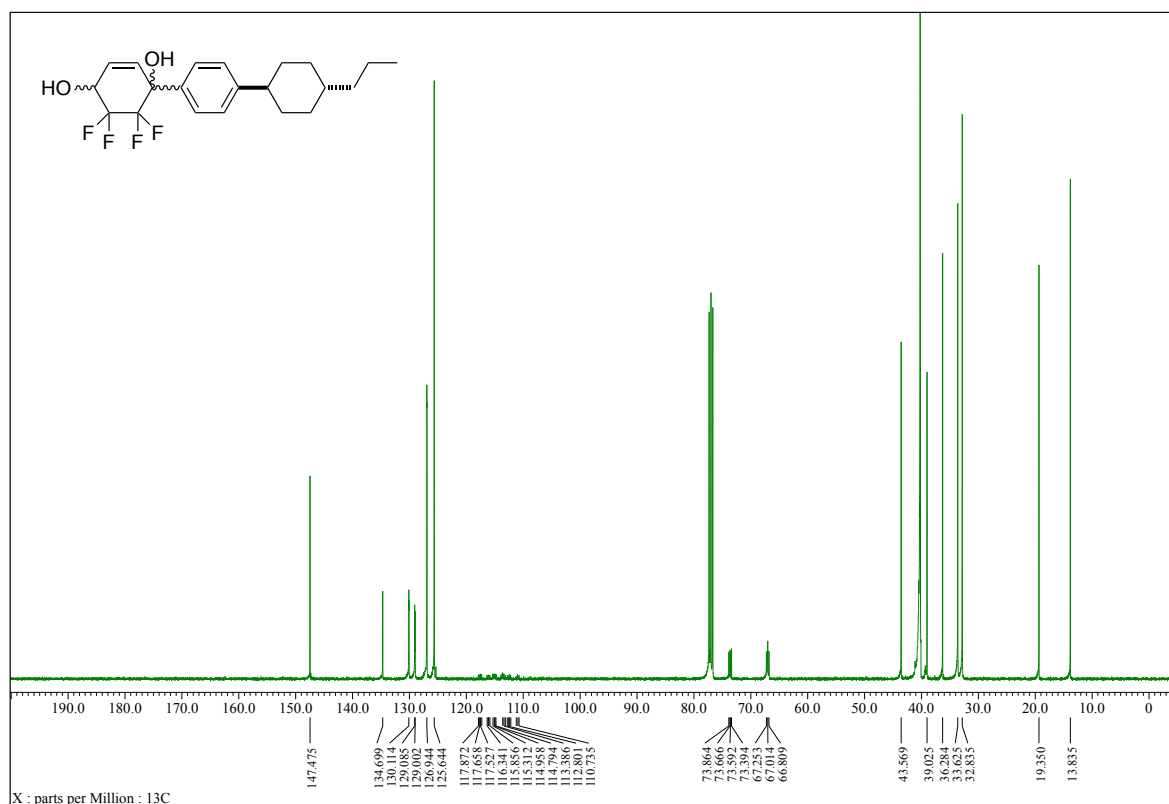
¹⁹F NMR spectrum of 2,2,3,3-tetrafluoro-4-(ethen-1-yl)-1-[4-(trans-4-n-propylcyclohexyl)phenyl]furanose (**12**)



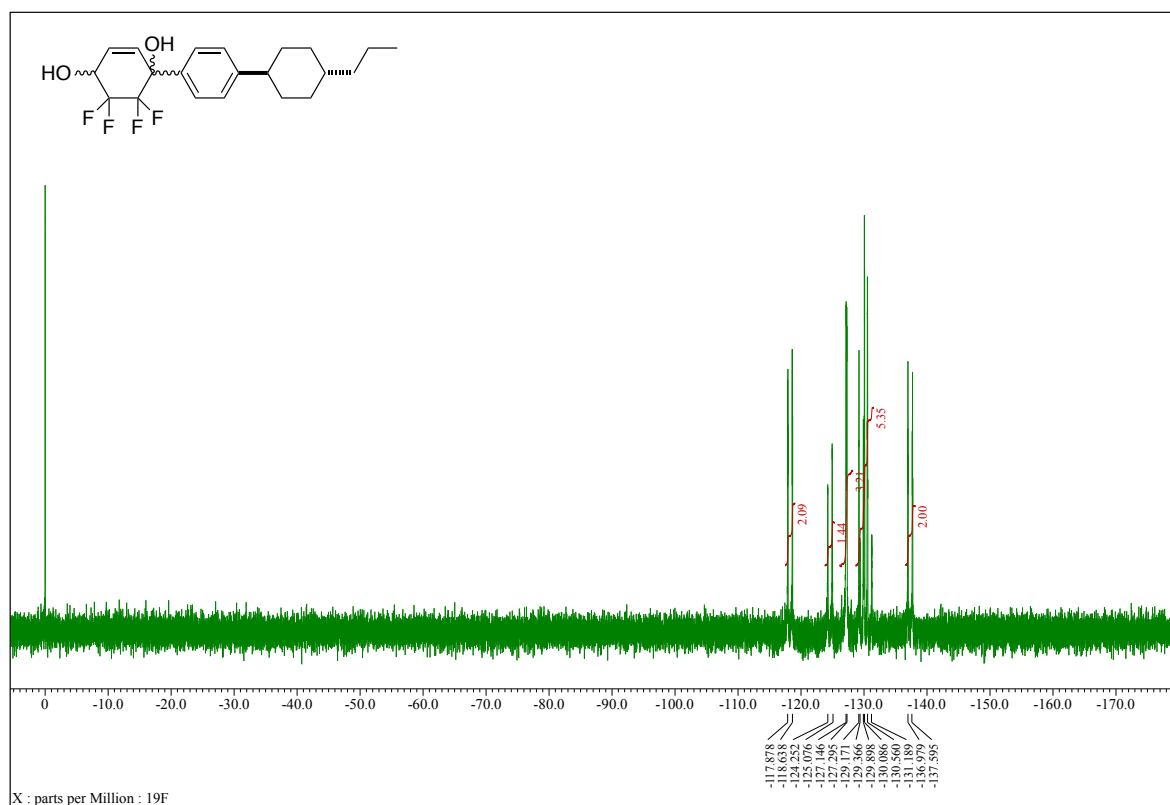
^1H NMR spectrum of 5,5,6,6-tetrafluoro-1-[4-(trans-4-n-propylcyclohexyl)phenyl]cyclohex-2-en-1,4-diol (**13**)



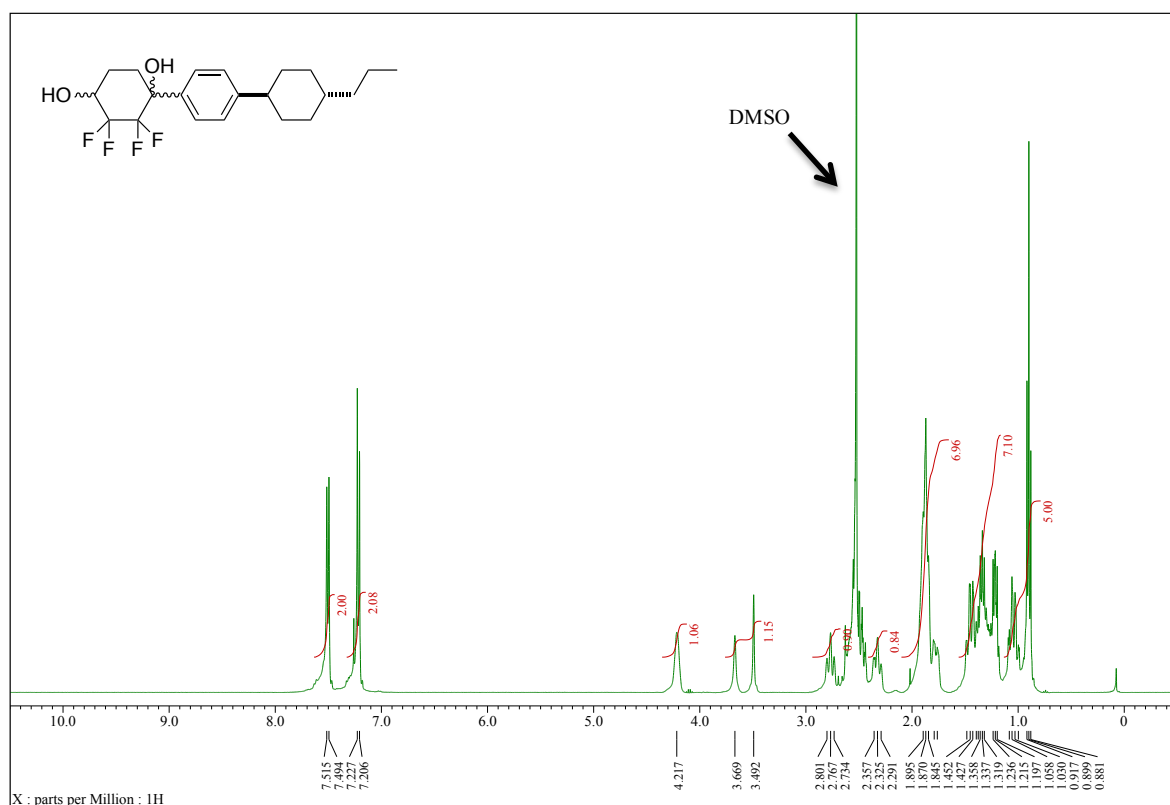
^{13}C NMR spectrum of 5,5,6,6-Tetrafluoro-1-[4-(trans-4-n-propylcyclohexyl)phenyl]cyclohex-2-en-1,4-diol (**13**)



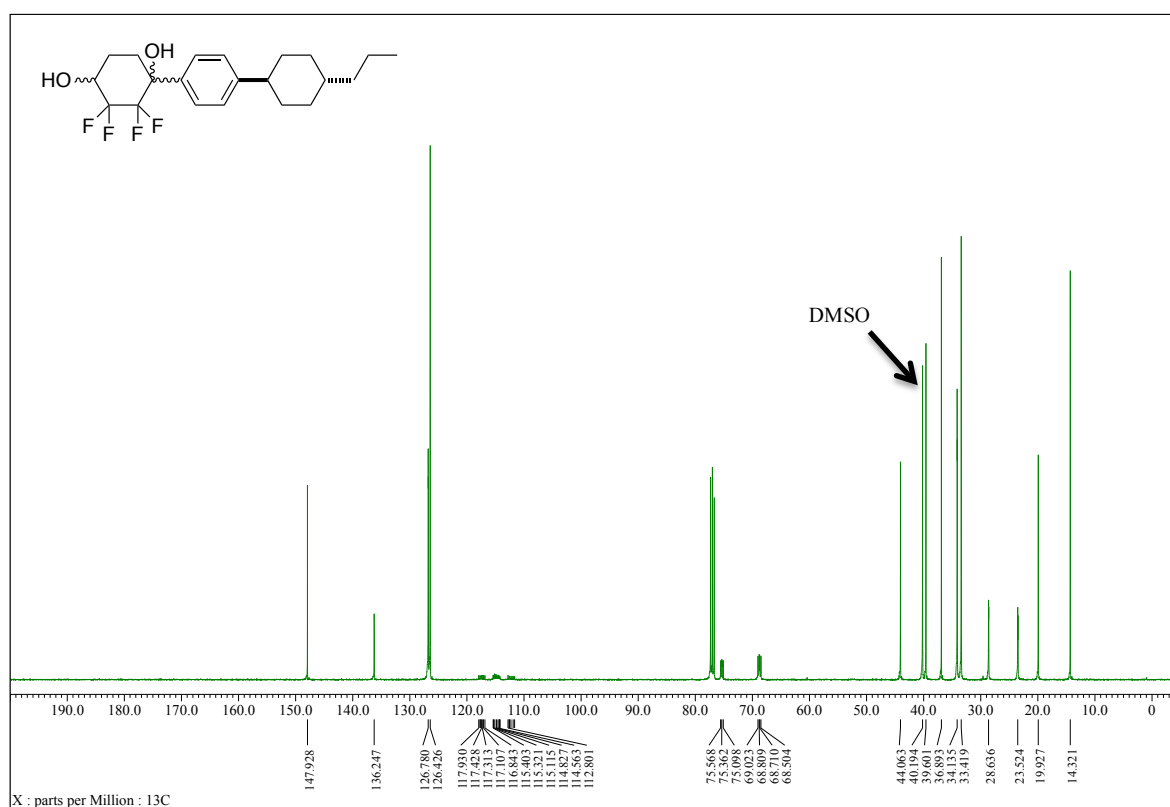
^{19}F NMR spectrum of 5,5,6,6-tetrafluoro-1-[4-(trans-4-n-propylcyclohexyl)phenyl]cyclohex-2-en-1,4-diol (**13**)



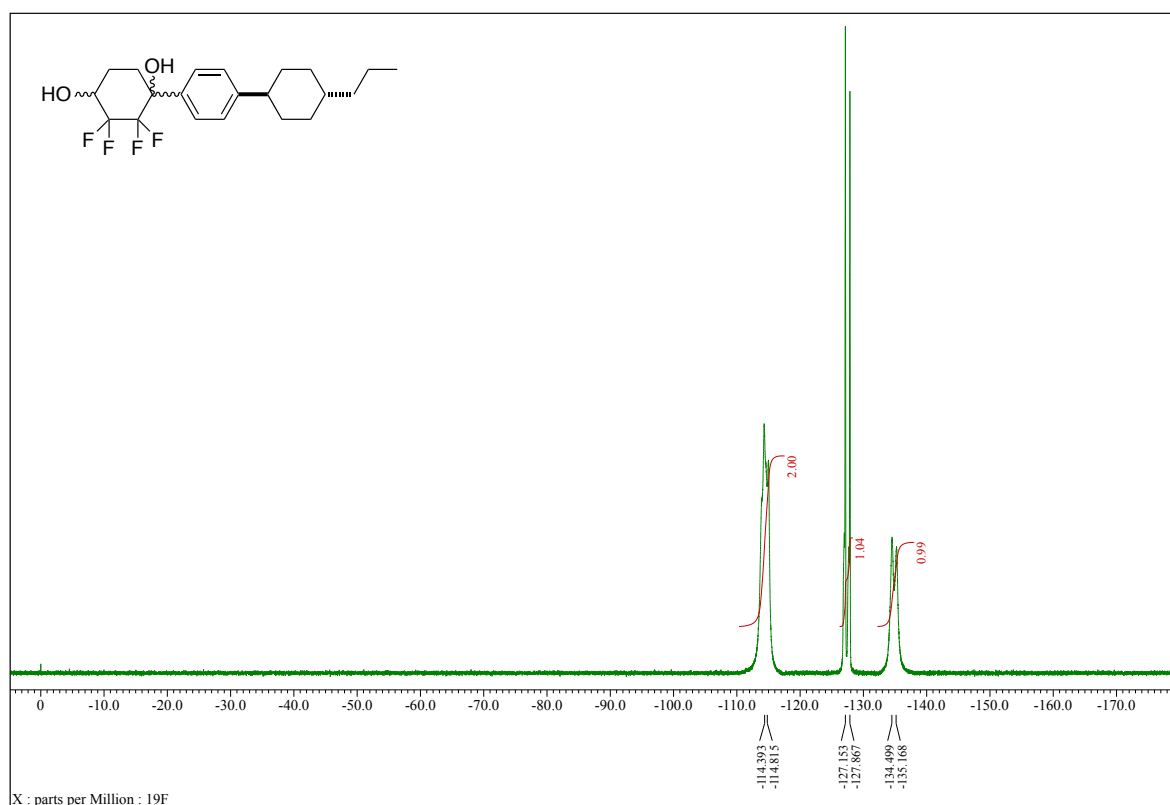
^1H NMR spectrum of 2,2,3,3-tetrafluoro-1-[4-(trans-4-n-propylcyclohexyl)phenyl]cyclohexan-1,4-diol (**6**) (Less Polar)



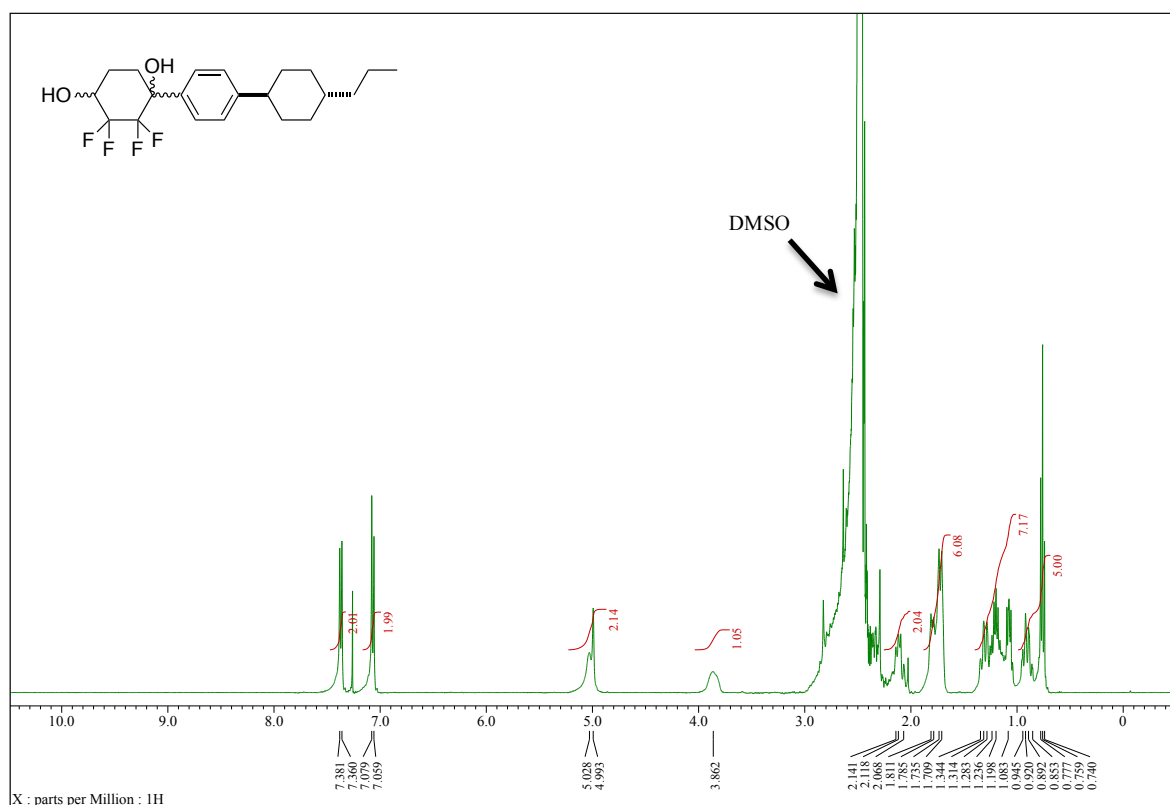
^{13}C NMR spectrum of 2,2,3,3-tetrafluoro-1-[4-(trans-4-n-propylcyclohexyl)phenyl]cyclohexan-1,4-diol (**6**) (Less Polar)



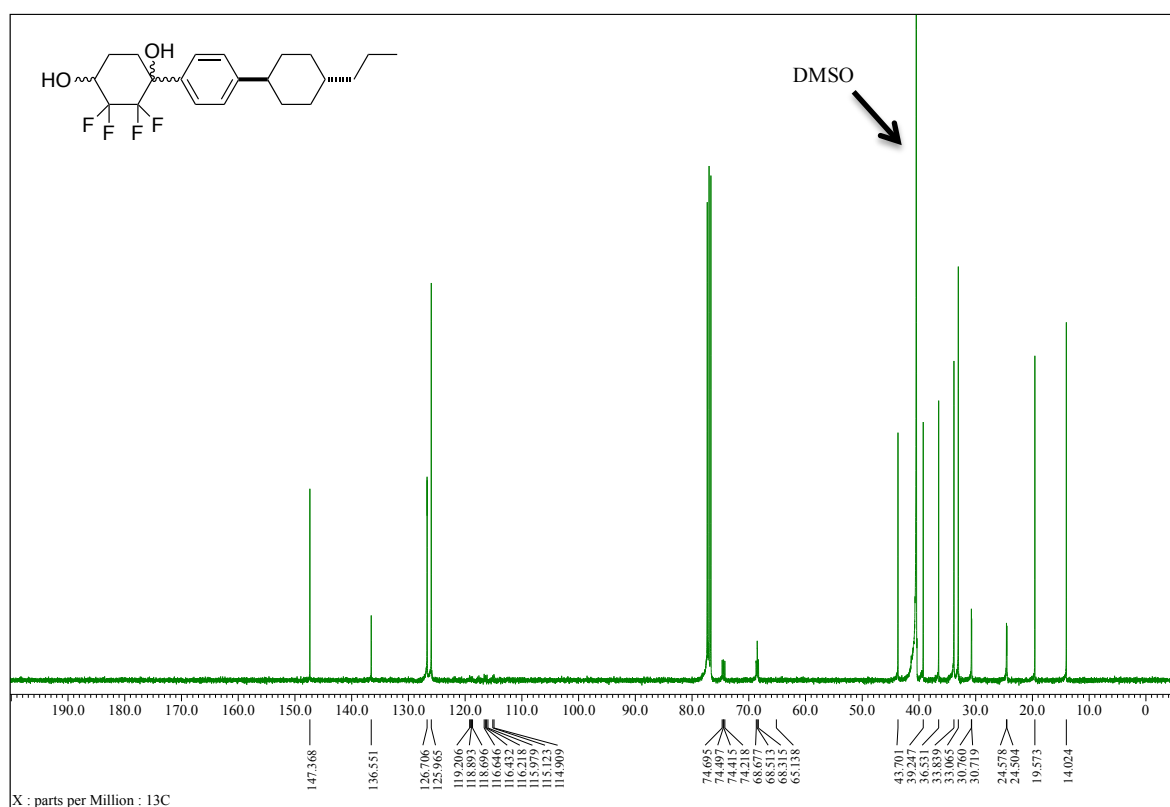
^{19}F NMR spectrum of 2,2,3,3-tetrafluoro-1-[4-(trans-4-n-propylcyclohexyl)phenyl]cyclohexan-1,4-diol (**6**)
(Less Polar)



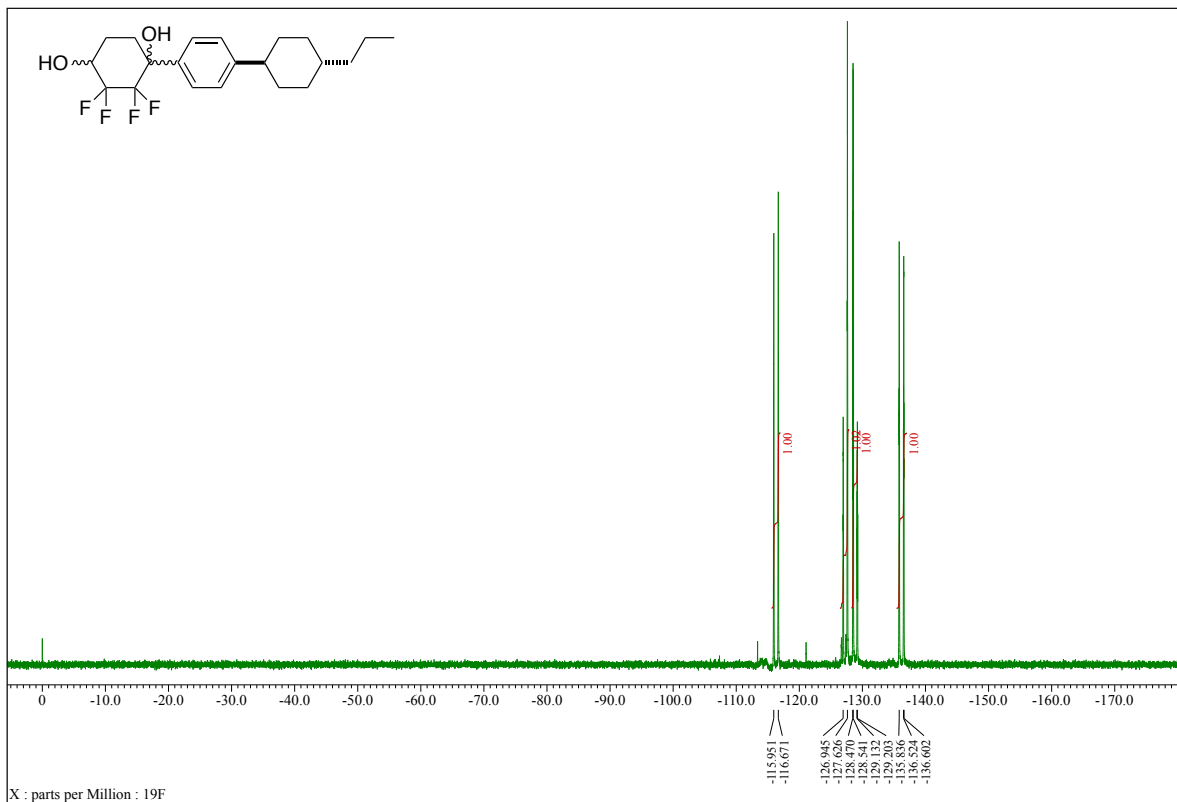
^1H NMR spectrum of 2,2,3,3-tetrafluoro-1-[4-(trans-4-n-propylcyclohexyl)phenyl]cyclohexan-1,4-diol (**6**)
(More Polar)



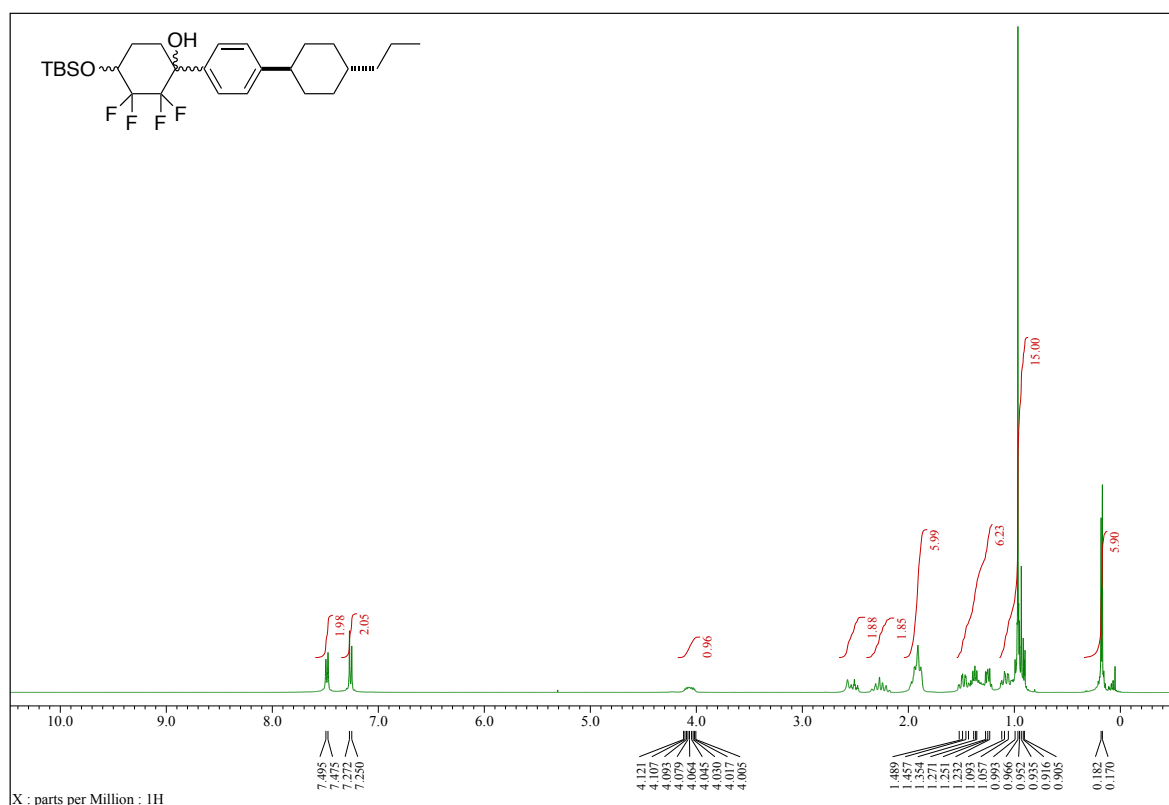
^{13}C NMR spectrum of 2,2,3,3-tetrafluoro-1-[4-(trans-4-n-propylcyclohexyl)phenyl]cyclohexan-1,4-diol (**6**)
(More Polar)



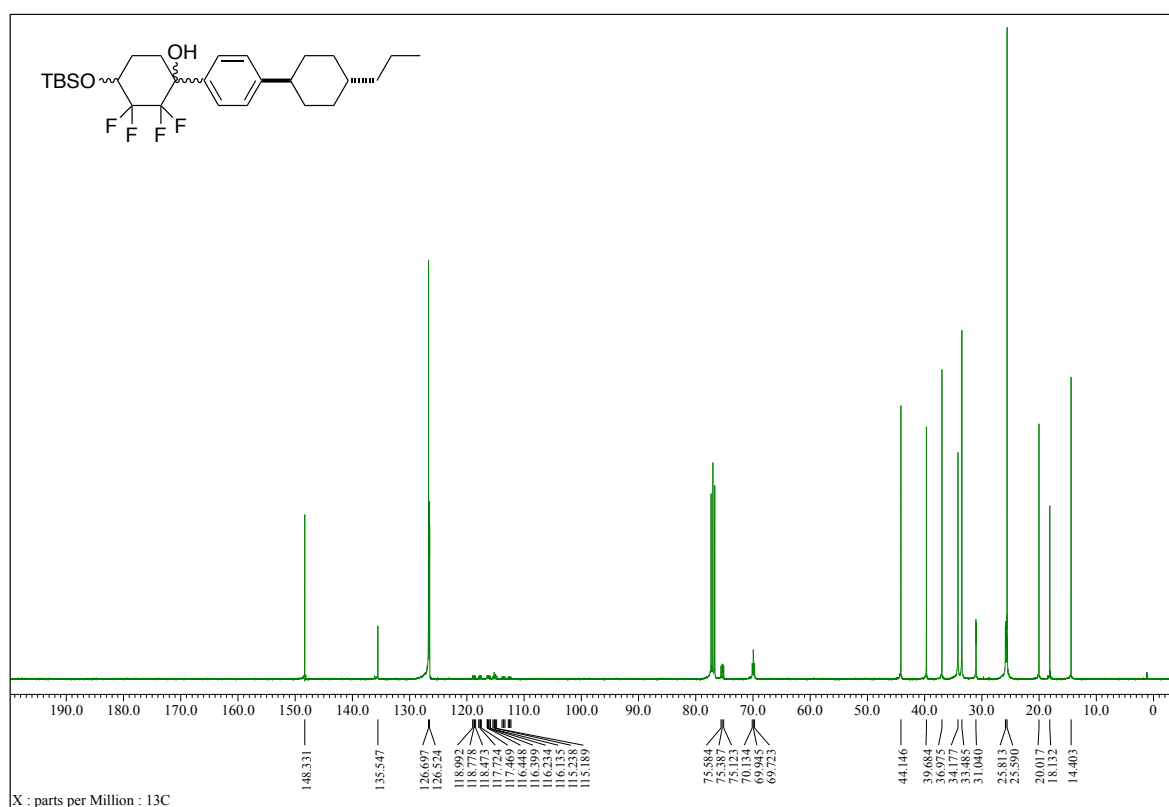
¹⁹F NMR spectrum of 2,2,3,3-tetrafluoro-1-[4-(trans-4-n-propylcyclohexyl)phenyl]cyclohexan-1,4-diol (**6**)
(More Polar)



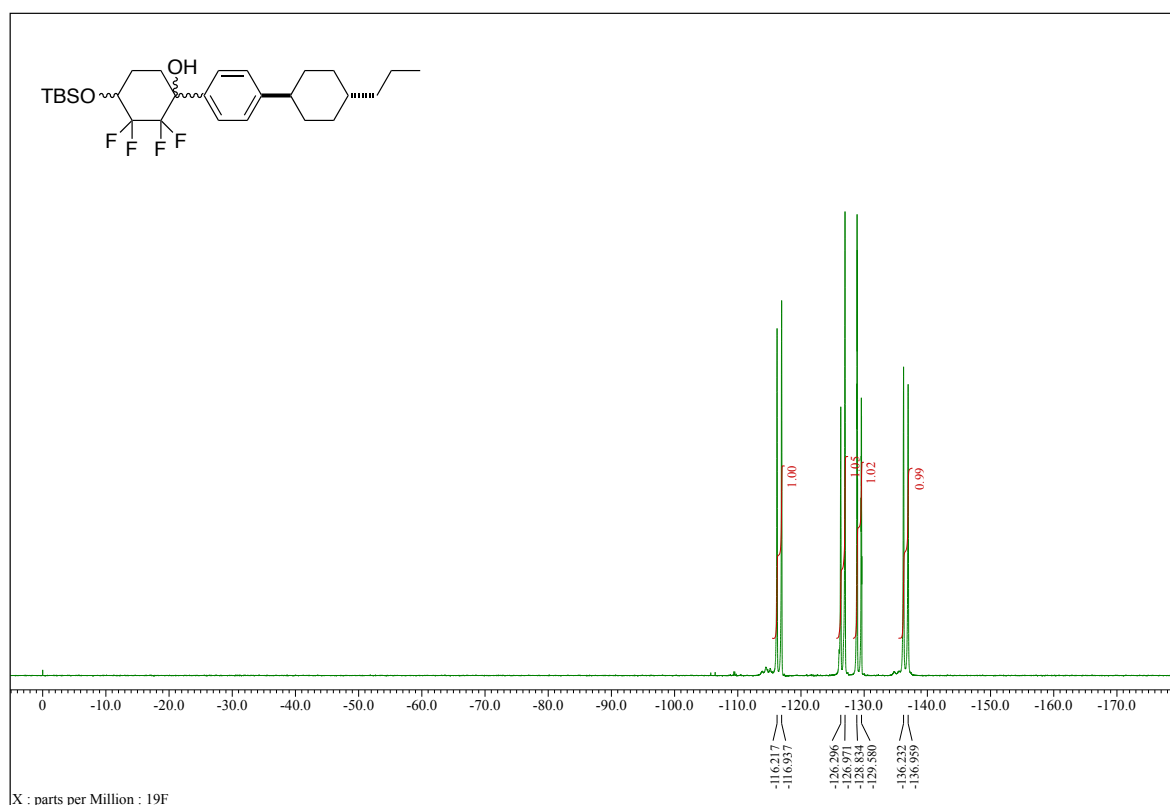
¹H NMR spectrum of
4-tert-butyltrimethylsilyloxy-2,2,3,3-tetrafluoro-1-[4-(trans-4-n-propylcyclohexyl)phenyl]cyclohexan-1-ol (**14**)



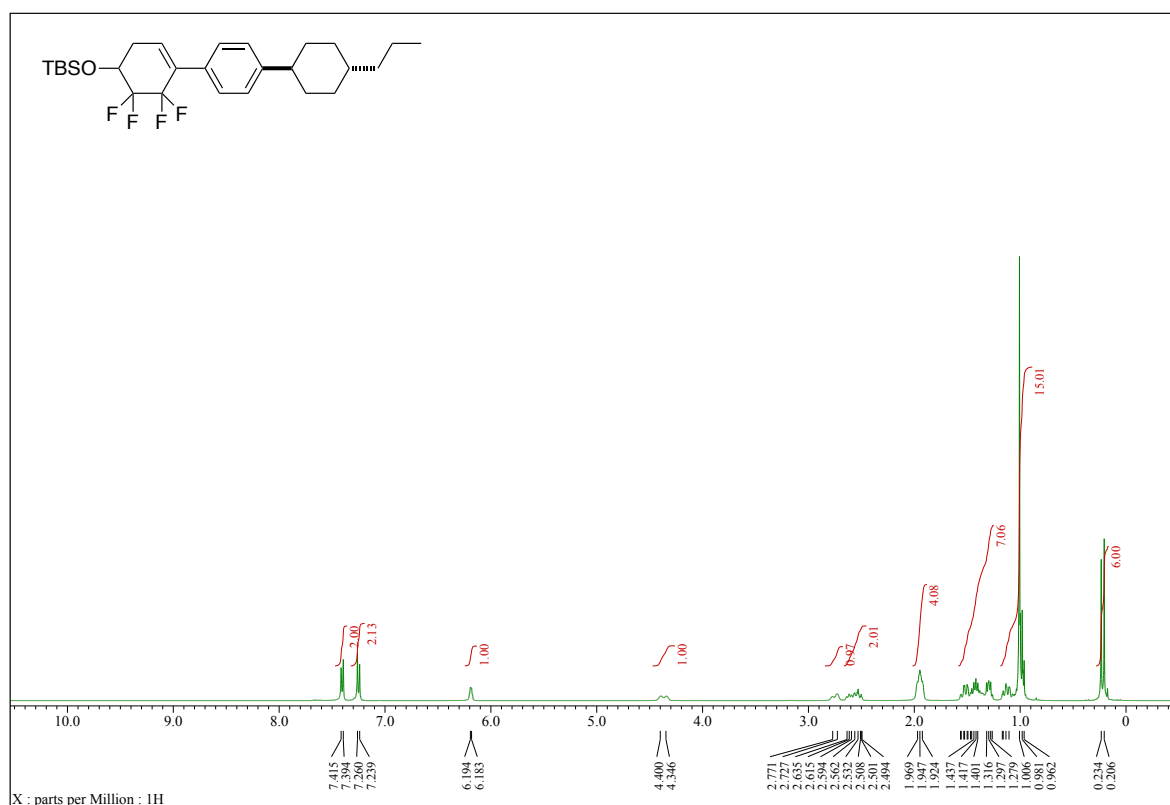
¹³C NMR spectrum of
4-tert-butyltrimethylsilyloxy-2,2,3,3-tetrafluoro-1-[4-(trans-4-n-propylcyclohexyl)phenyl]cyclohexan-1-ol (**14**)



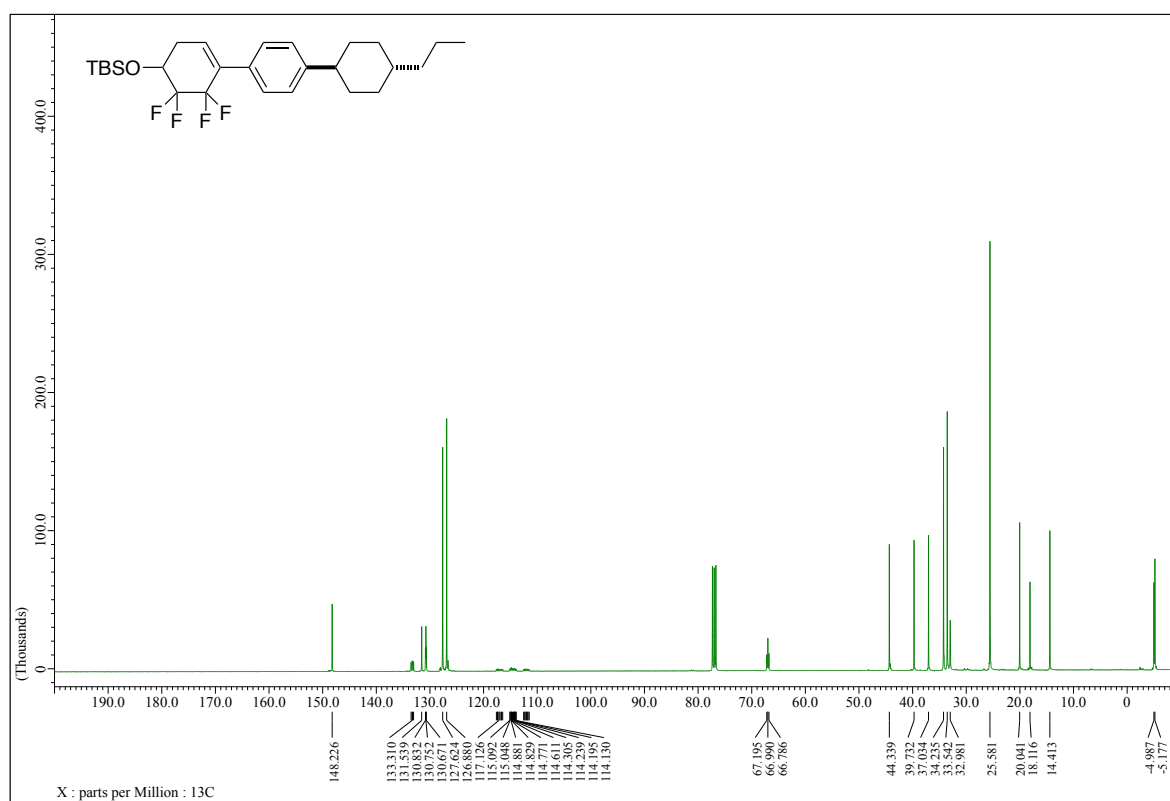
¹⁹F NMR spectrum of
4-tert-butyltrimethylsilyloxy-2,2,3,3-tetrafluoro-1-[4-(trans-4-n-propylcyclohexyl)phenyl]cyclohexan-1-ol (**14**)



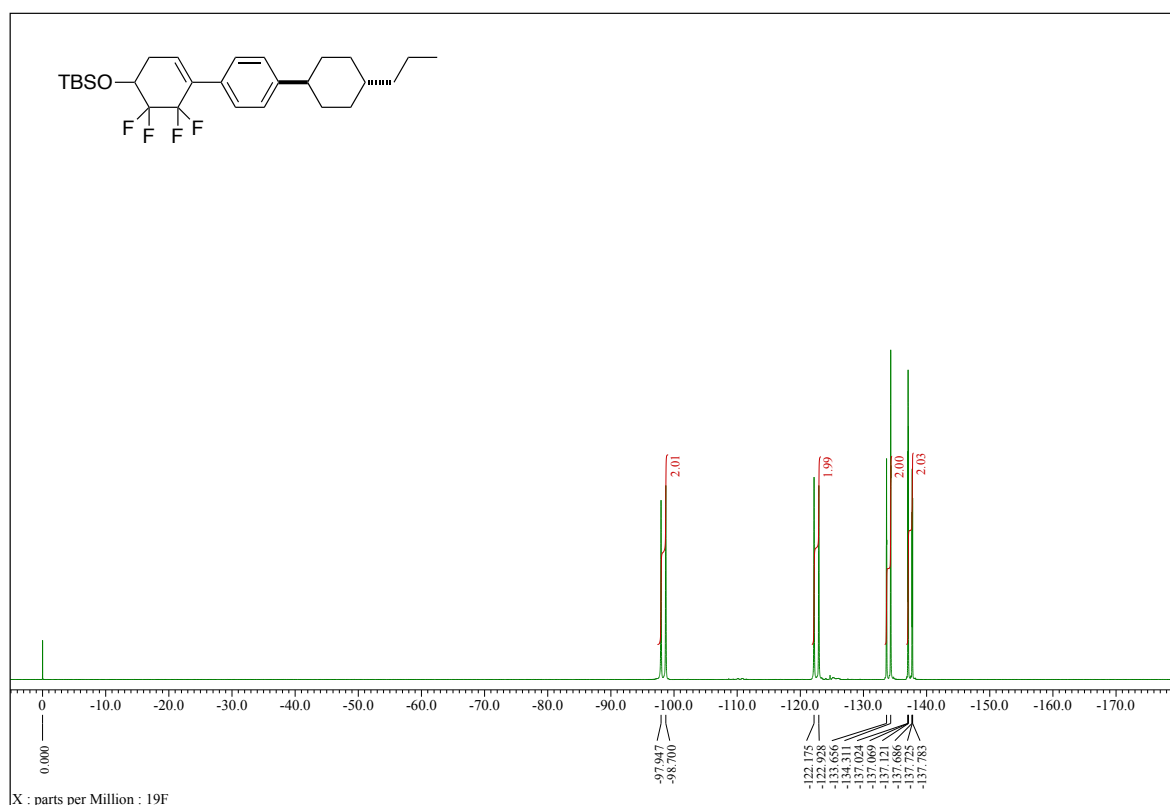
¹H NMR spectrum of
4-tert-Butyldimethylsilyloxy-5,5,6,6-tetrafluoro-1-[4-(trans-4-n-propylcyclohexyl)phenyl]cyclohex-1-ene (**5**)



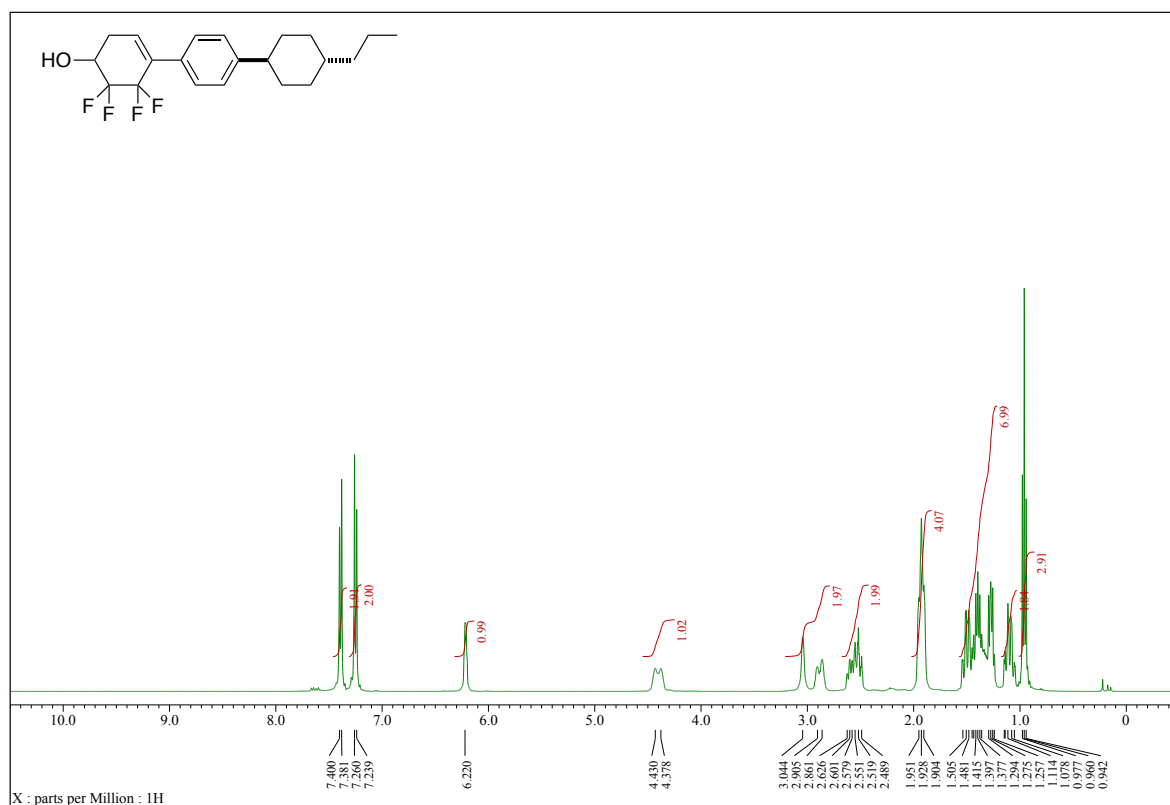
¹³C NMR spectrum of
4-tert-Butyldimethylsilyloxy-5,5,6,6-tetrafluoro-1-[4-(trans-4-n-propylcyclohexyl)phenyl]cyclohex-1-ene (**5**)



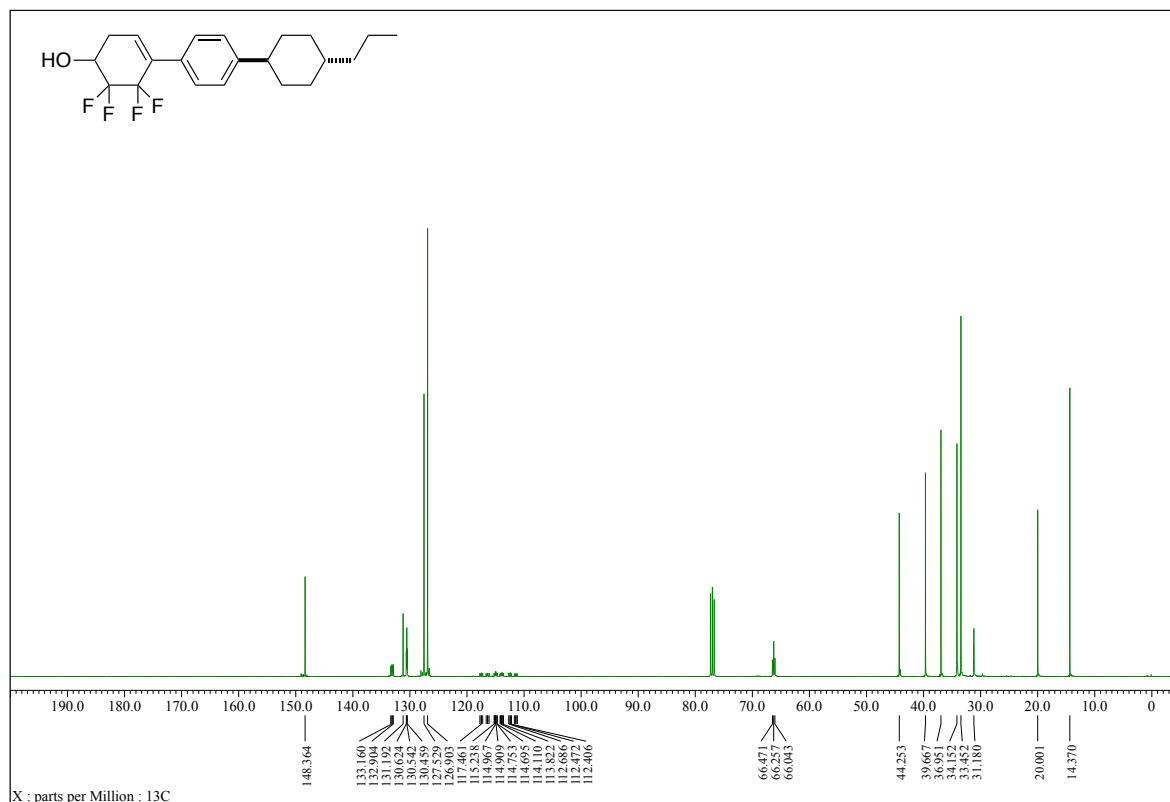
¹⁹F NMR spectrum of
4-tert-Butyldimethylsilyloxy-5,5,6,6-tetrafluoro-1-[4-(trans-4-n-propylcyclohexyl)phenyl]cyclohex-1-ene (**5**)



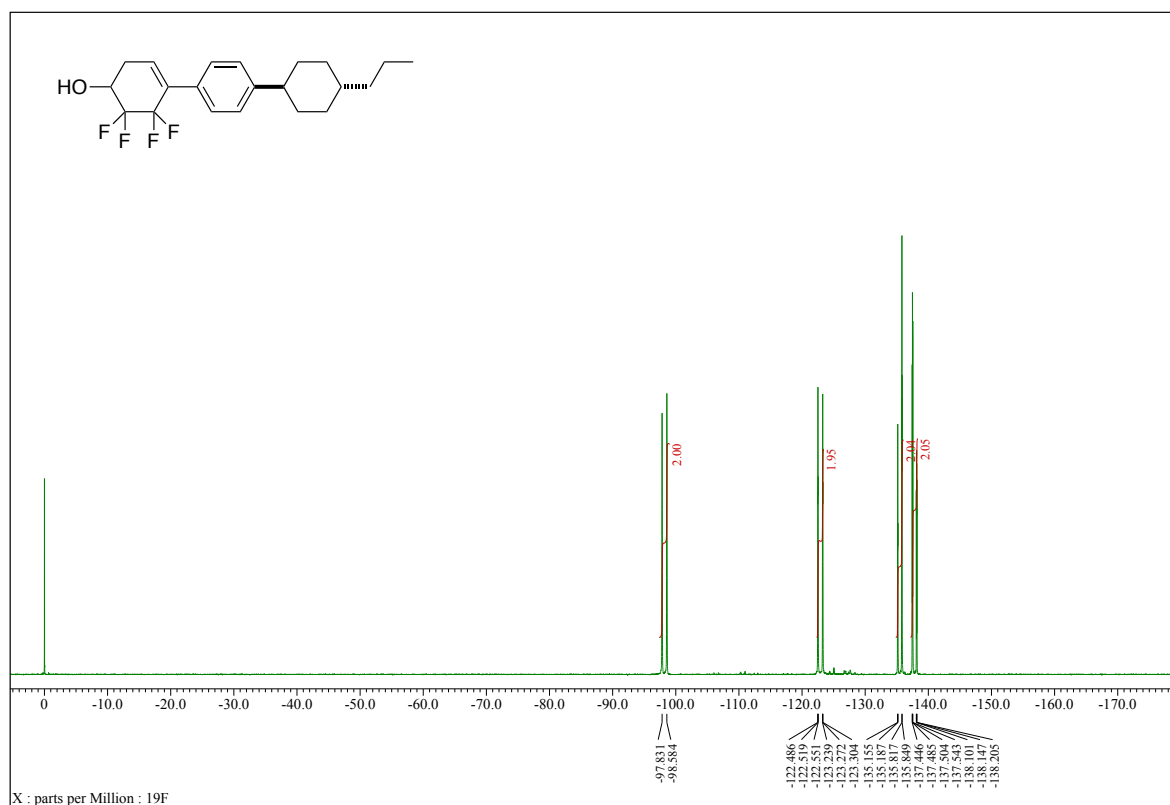
^1H NMR spectrum of 5,5,6,6-tetrafluoro-4-[4-(trans-4-n-propylcyclohexyl)phenyl]cyclohex-3-en-1-ol (**4**)



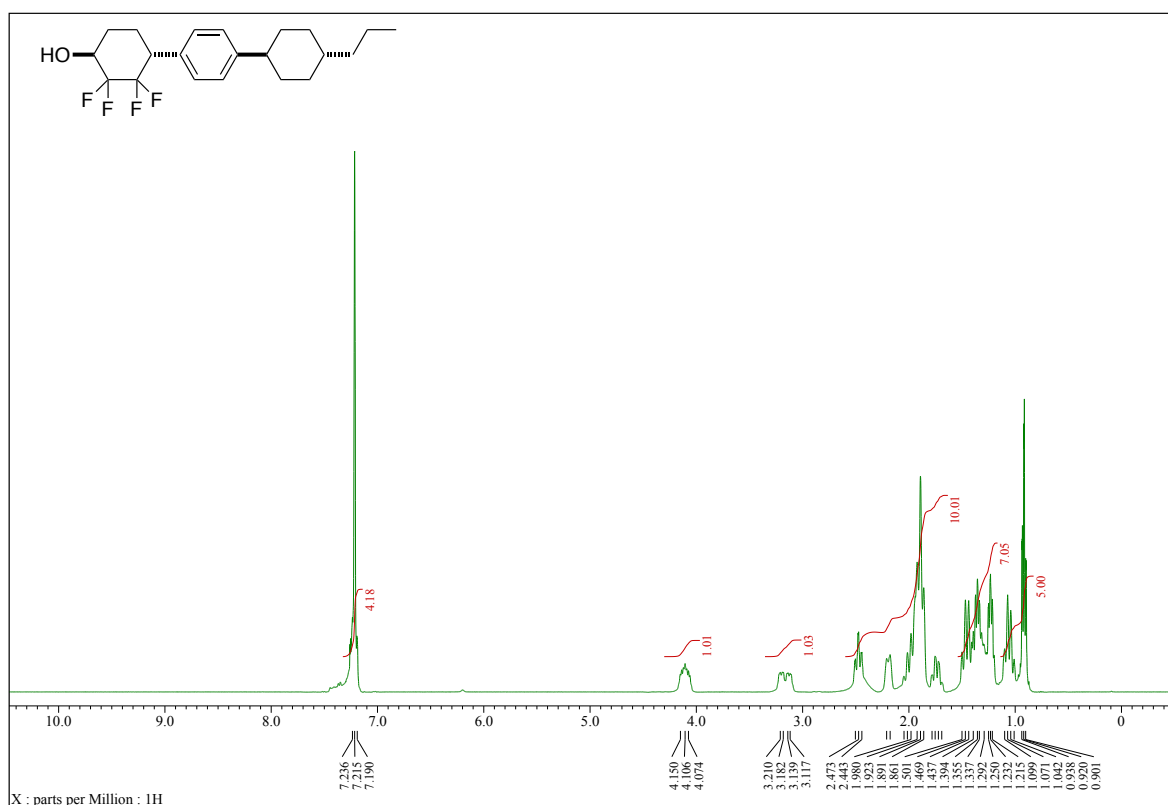
^{13}C NMR spectrum of 5,5,6,6-tetrafluoro-4-[4-(trans-4-n-propylcyclohexyl)phenyl]cyclohex-3-en-1-ol (**4**)



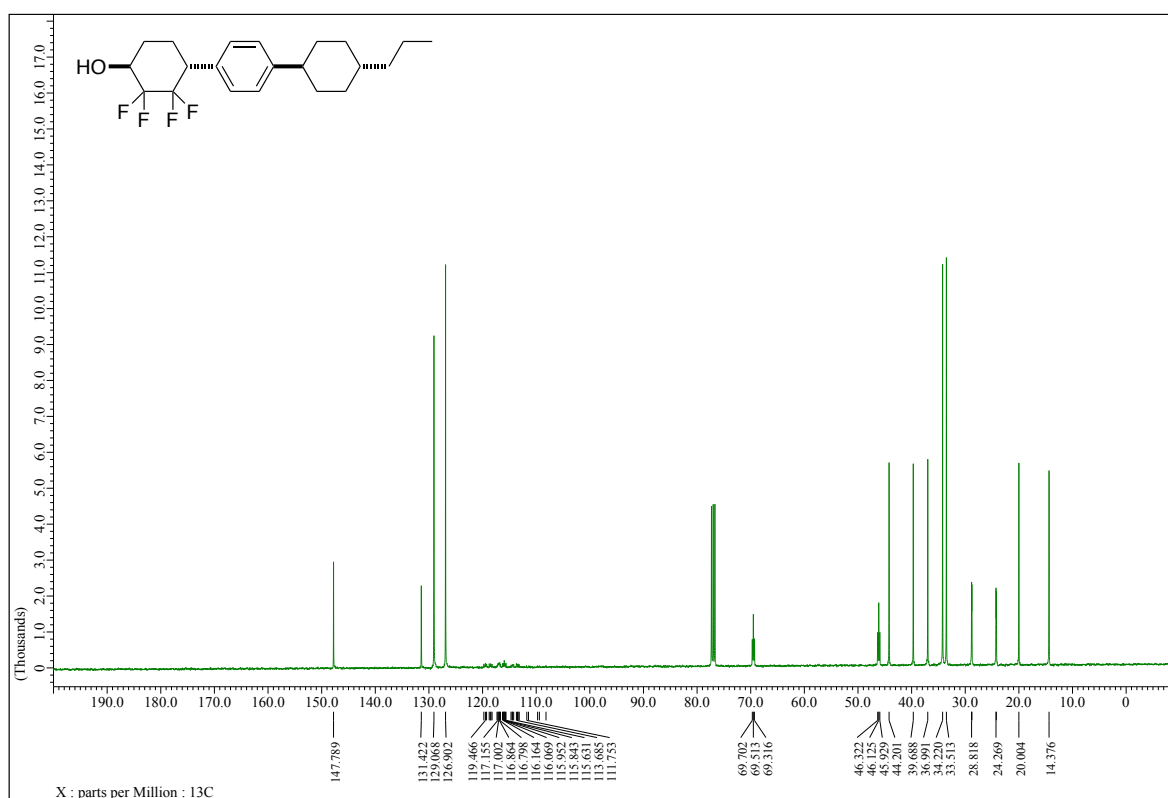
¹⁹F NMR spectrum of 5,5,6,6-tetrafluoro-4-[4-(trans-4-n-propylcyclohexyl)phenyl]cyclohex-3-en-1-ol (4)



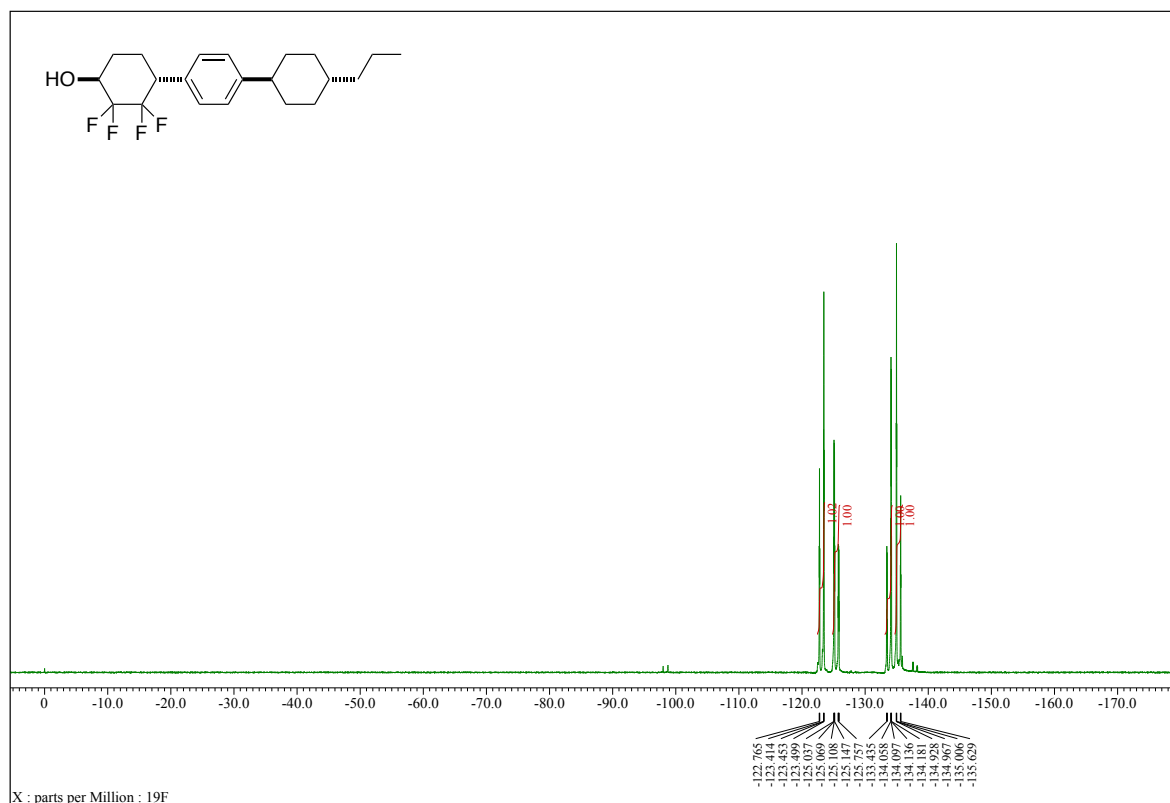
^1H NMR spectrum of *trans*-2,2,3,3-Tetrafluoro-4-[4-(*trans*-4-*n*-propylcyclohexyl)phenyl]cyclohexan-1-ol (*trans*-15) (More Polar)



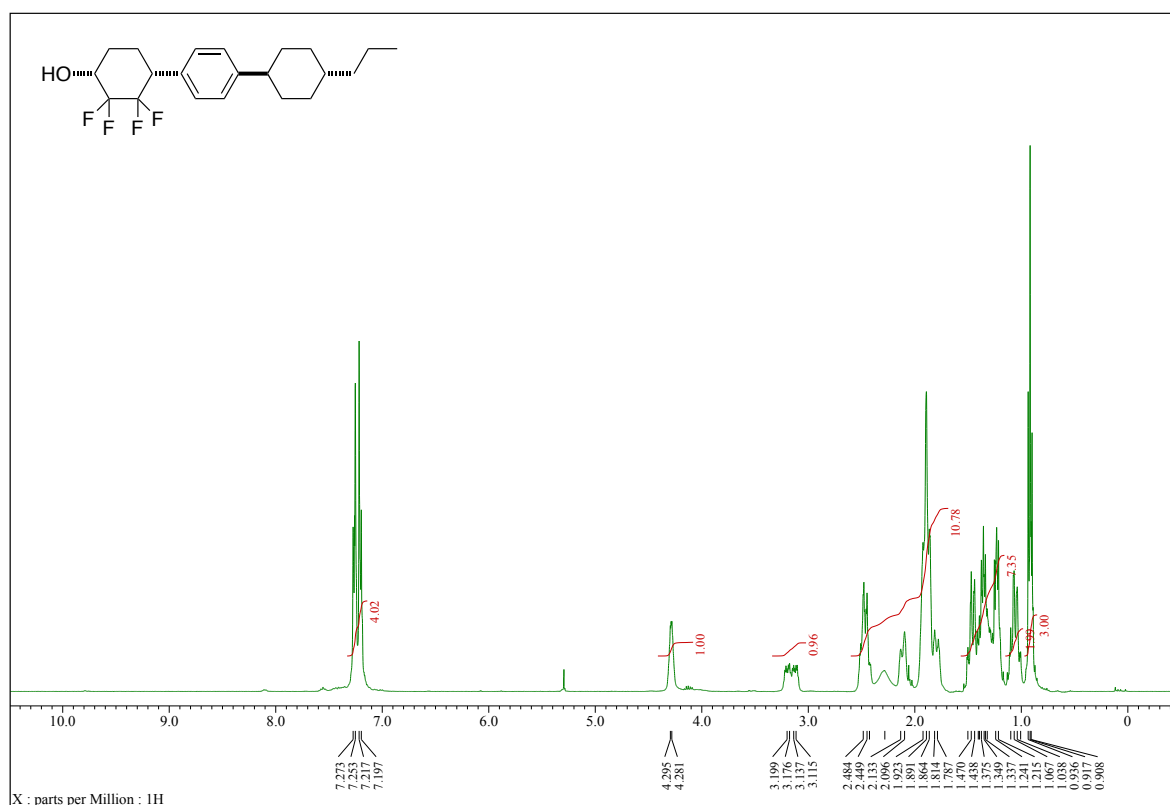
^{13}C NMR spectrum of *trans*-2,2,3,3-Tetrafluoro-4-[4-(*trans*-4-*n*-propylcyclohexyl)phenyl]cyclohexan-1-ol (*trans*-15) (More Polar)



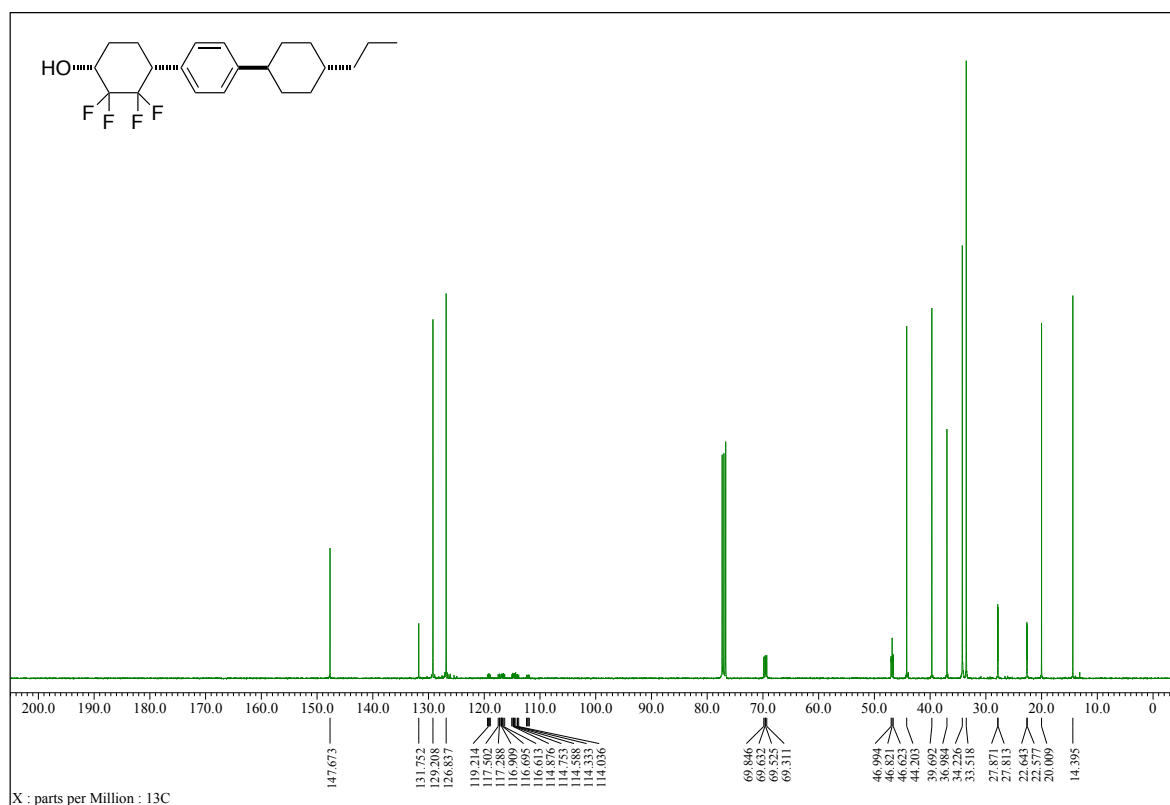
¹⁹F NMR spectrum of *trans*-2,2,3,3-Tetrafluoro-4-[4-(*trans*-4-*n*-propylcyclohexyl)phenyl]cyclohexan-1-ol (***trans*-15**) (More Polar)



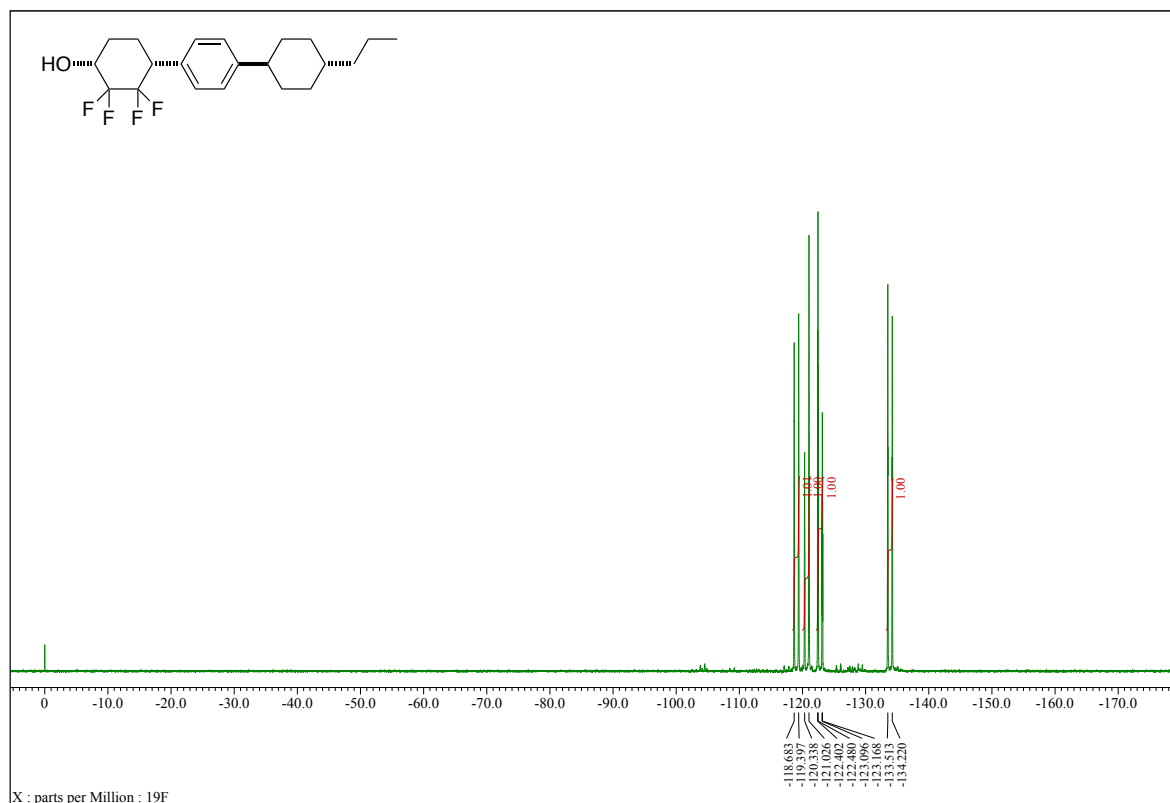
^1H NMR spectrum of *cis*-2,2,3,3-Tetrafluoro-4-[4-(*trans*-4-*n*-propylcyclohexyl)phenyl]cyclohexan-1-ol (**cis-15**) (Less Polar)



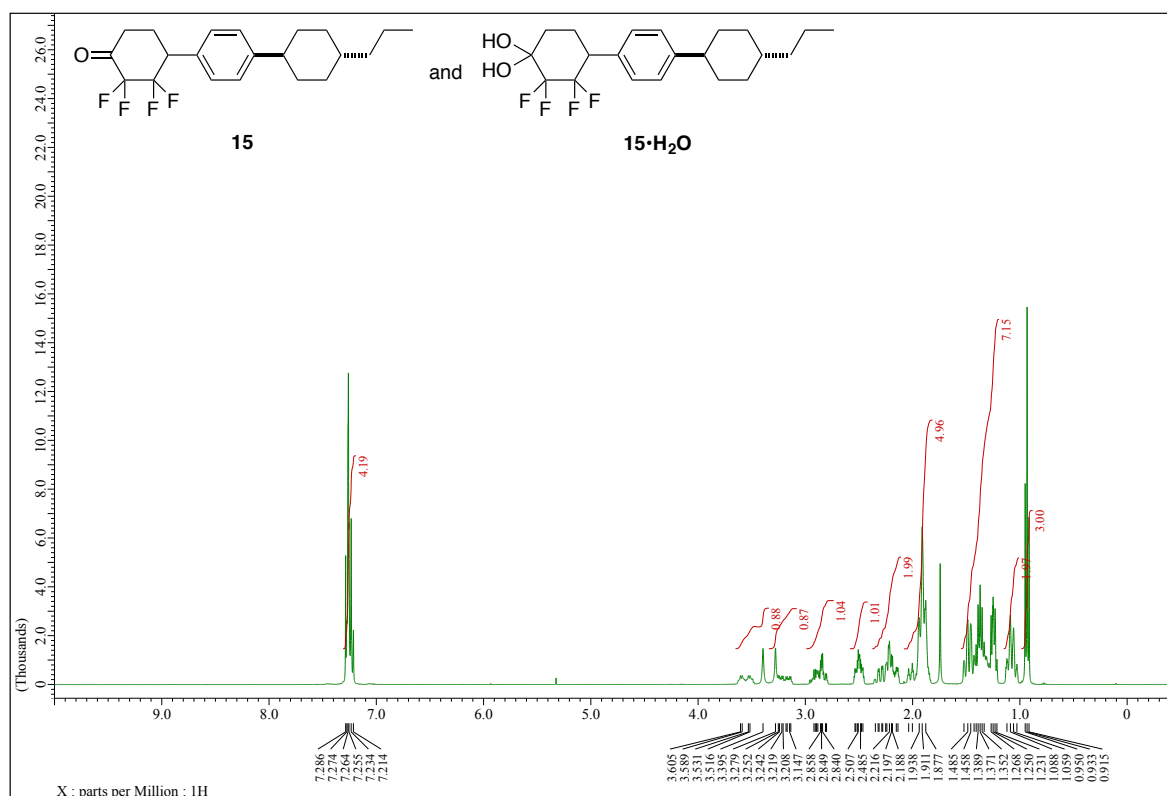
^{13}C NMR spectrum of *cis*-2,2,3,3-Tetrafluoro-4-[4-(*trans*-4-*n*-propylcyclohexyl)phenyl]cyclohexan-1-ol (**cis-15**) (Less Polar)



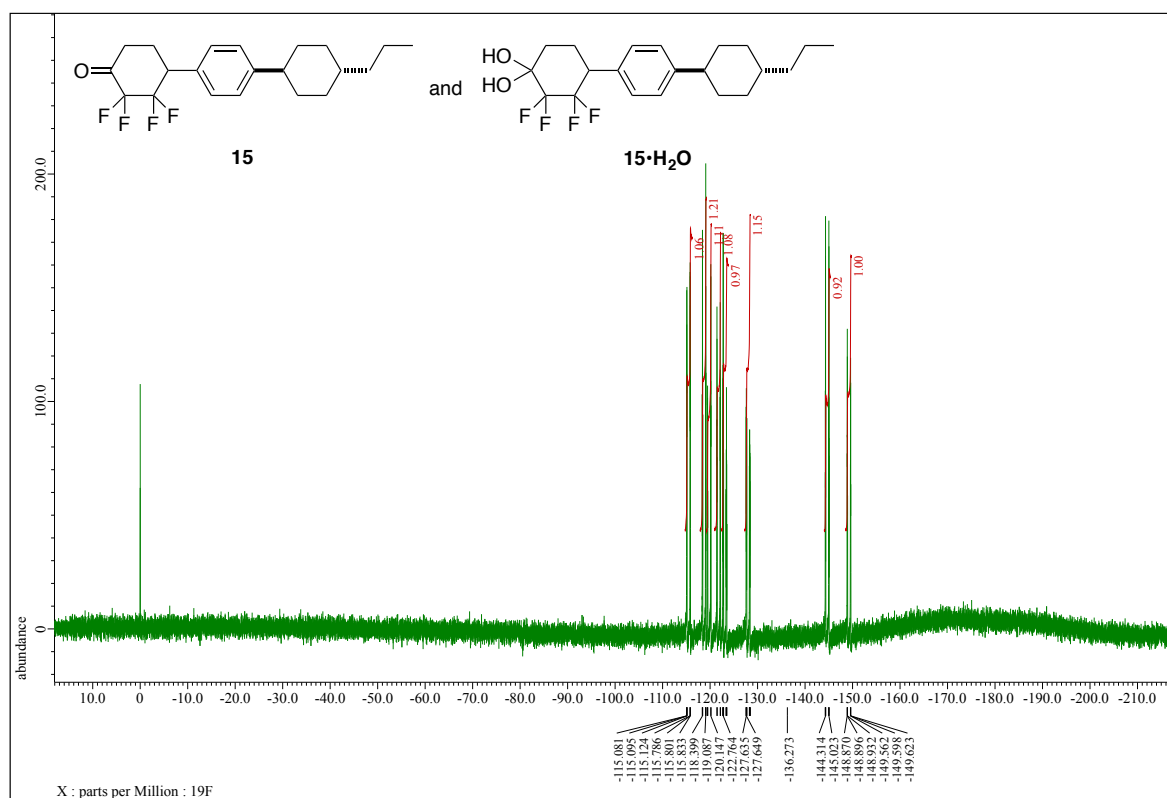
¹⁹F NMR spectrum of *cis*-2,2,3,3-Tetrafluoro-4-[4-(*trans*-4-*n*-propylcyclohexyl)phenyl]cyclohexan-1-ol (*cis*-15)
(Less Polar)



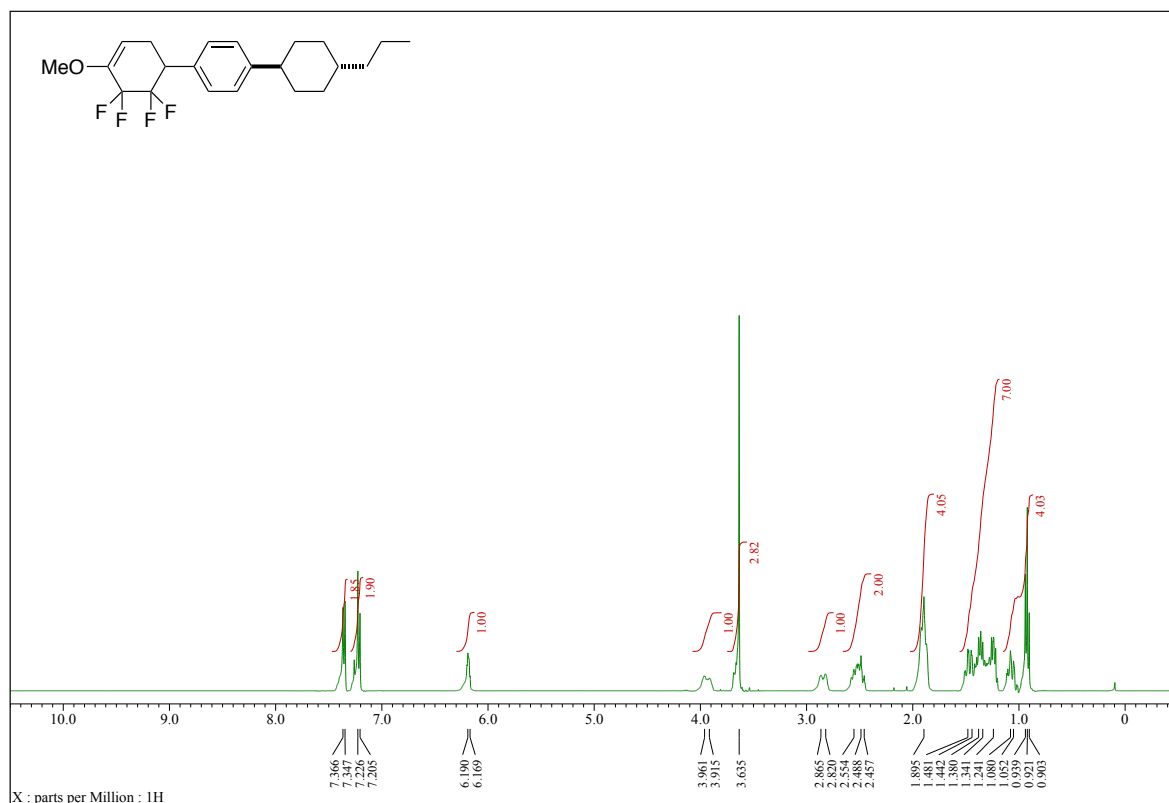
^1H NMR spectrum of a mixture of 2,2,3,3-tetrafluoro-4-[4-(trans-n-propylcyclohexyl)phenyl]cyclohexan-1-one (**3**) and the hydrate (**3**• H_2O)



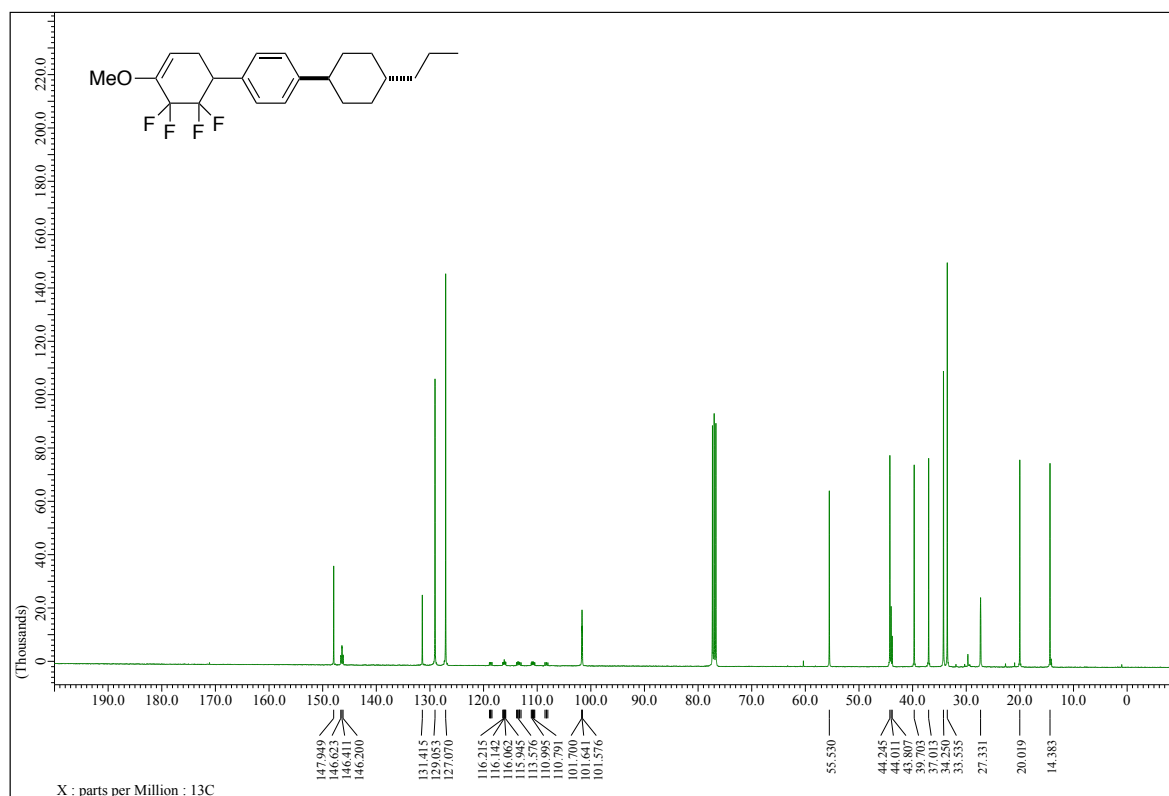
^{19}F NMR spectrum of a mixture of 2,2,3,3-tetrafluoro-4-[4-(trans-n-propylcyclohexyl)phenyl]cyclohexan-1-one (**3**) and the hydrate (**3**• H_2O)



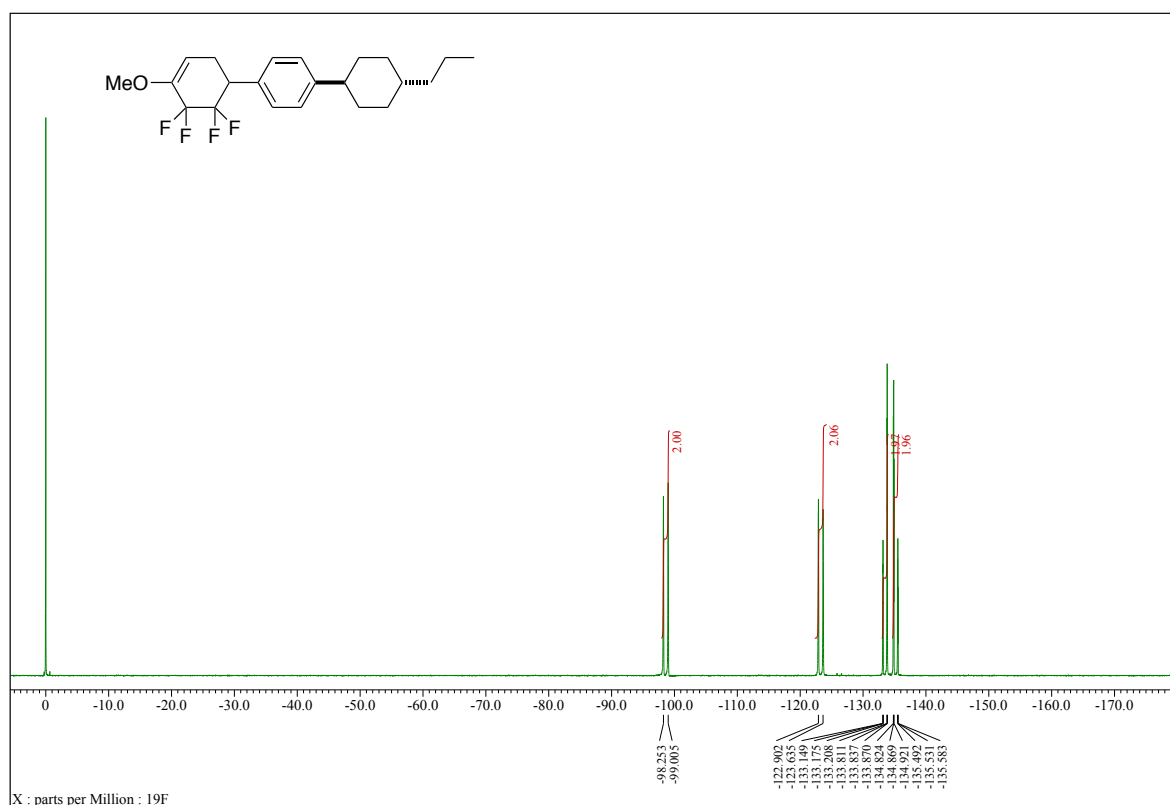
^1H NMR spectrum of 5,5,6,6-tetrafluoro-1-methoxy-4-[4-(trans-4-n-propylcyclohexyl)phenyl]cyclohex-1-ene (**2b**)



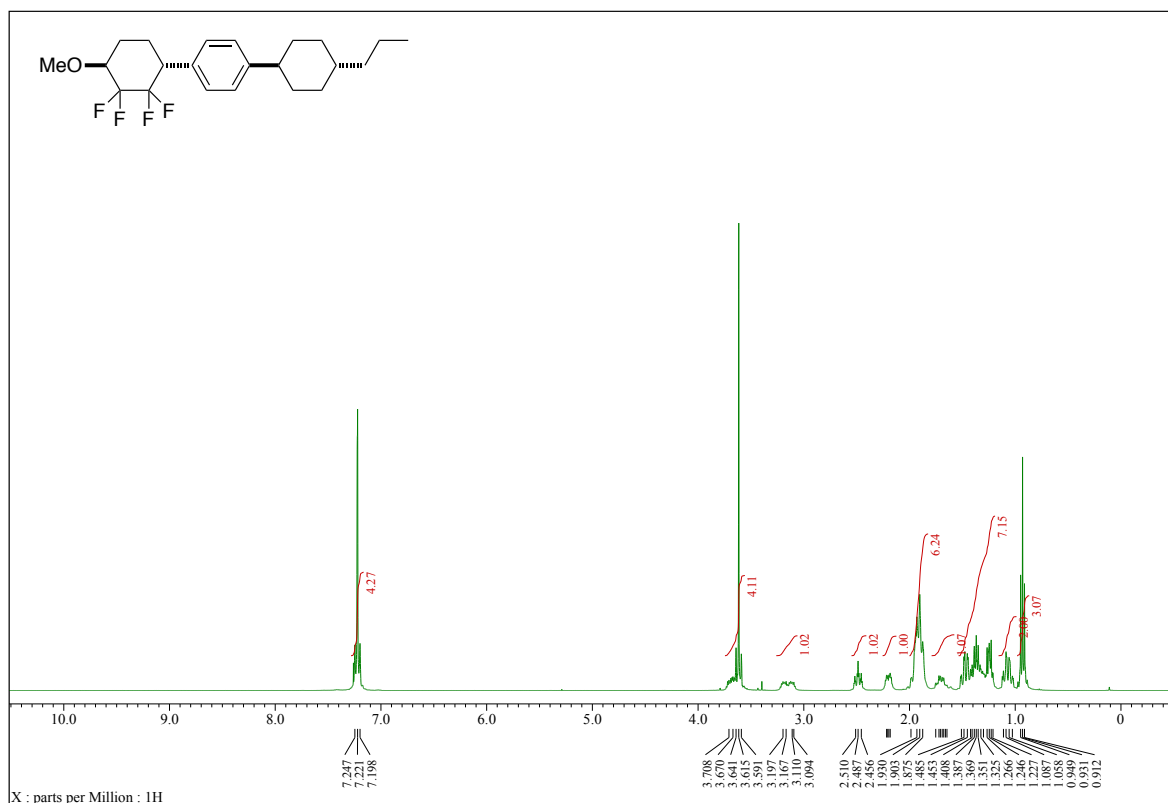
^{13}C NMR spectrum of 5,5,6,6-tetrafluoro-1-methoxy-4-[4-(trans-4-n-propylcyclohexyl)phenyl]cyclohex-1-ene (**2b**)



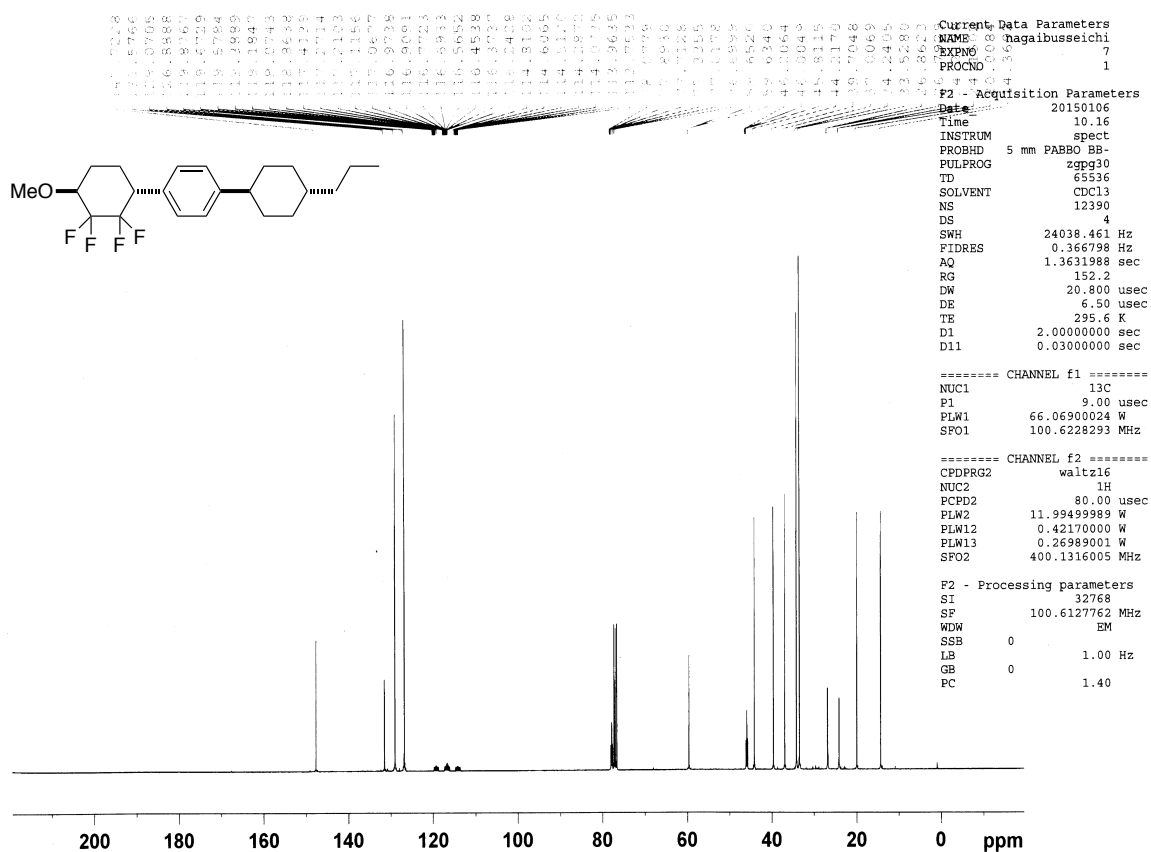
^{19}F NMR spectrum of 5,5,6,6-tetrafluoro-1-methoxy-4-[4-(trans-4-n-propylcyclohexyl)phenyl]cyclohex-1-ene (**2b**)



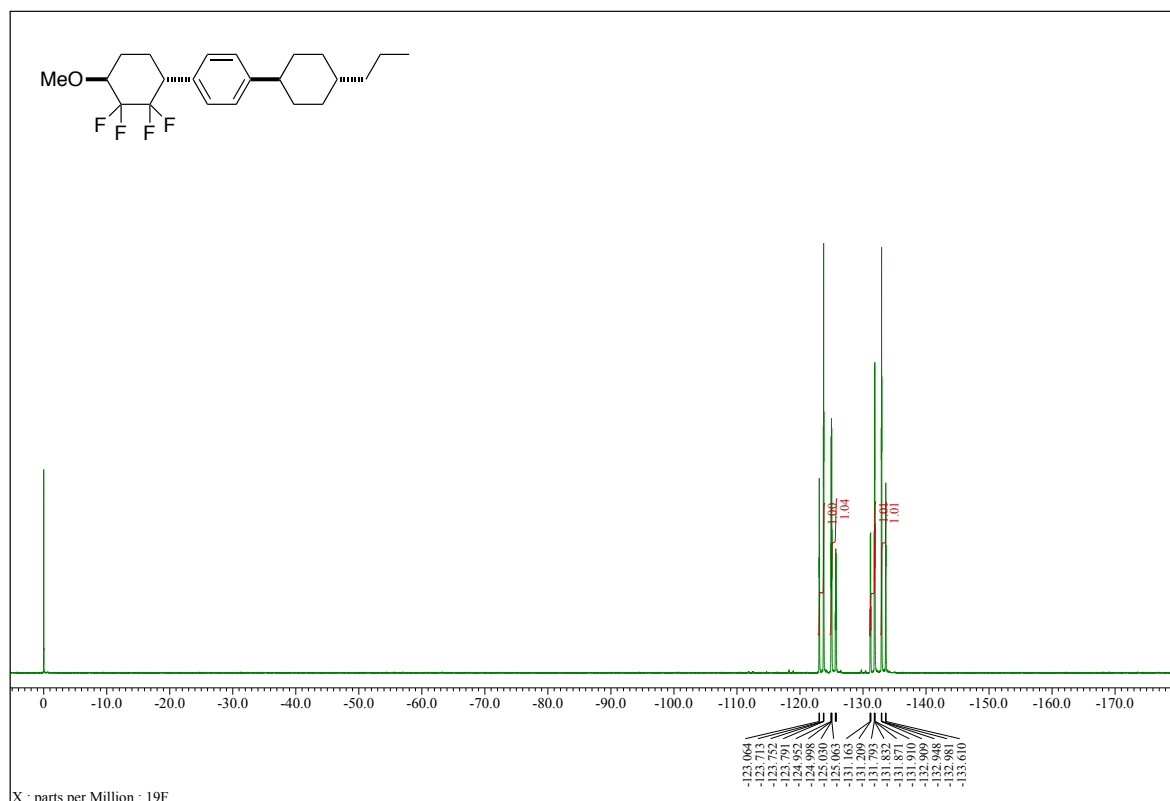
¹H NMR spectrum of
trans-2,2,3,3-tetrafluoro-4-[4-(*trans*-4-*n*-propylcyclohexyl)phenyl]-1-methoxycyclohexane (*trans*-2c)



¹³C NMR spectrum of
trans-2,2,3,3-tetrafluoro-4-[4-(*trans*-4-*n*-propylcyclohexyl)phenyl]-1-methoxycyclohexane (*trans*-2c)

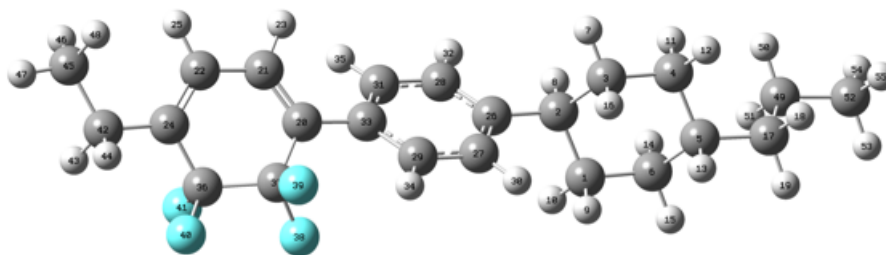


¹⁹F NMR spectrum of
trans-2,2,3,3-tetrafluoro-4-[4-(*trans*-4-*n*-propylcyclohexyl)phenyl]-1-methoxycyclohexane (***trans*-2c**)



Theoretical calculation

Cartesian coordinate (Å) and absolute energy of the optimized structure for **1a^a**



Center	Atomic	Atomic	Coordinates (Angstroms)			28	6	0	-0.913883	1.262534	0.951345
Number	Number	Type	X	Y	Z	29	6	0	0.404146	-0.568597	-0.660713
-----						30	1	0	-1.533915	-1.284670	-1.187647
1	6	0	-3.793387	-0.961407	0.749142	31	6	0	0.475736	1.265461	0.890778
2	6	0	-3.190625	0.377024	0.271170	32	1	0	-1.416879	1.972555	1.600364
3	6	0	-3.820437	0.796328	-1.076365	33	6	0	1.163885	0.357148	0.073486
4	6	0	-5.352642	0.8439361	-1.000113	34	1	0	0.899305	-1.286834	-1.301723
5	6	0	-5.946360	-0.495830	-0.531782	35	1	0	1.034362	1.962255	1.505428
6	6	0	-5.326199	-0.903197	0.816593	36	6	0	4.888538	-0.791772	0.291974
7	1	0	-3.424501	1.771346	-1.378323	37	6	0	3.419927	-0.874341	-0.210621
8	1	0	-3.470815	1.139706	1.009853	38	9	0	2.825687	-1.936038	0.401043
9	1	0	-3.491651	-1.762153	0.063176	39	9	0	3.468001	-1.181907	-1.557853
10	1	0	-3.379446	-1.220734	1.728805	40	9	0	5.570038	-1.863505	-0.209784
11	1	0	-5.650649	1.642269	-0.309310	41	9	0	4.867493	-0.959231	1.661471
12	1	0	-5.763754	1.111655	-1.980208	42	6	0	7.090128	0.469101	-0.096888
13	1	0	-5.633799	-1.253796	-1.265530	43	1	0	7.464733	0.009740	0.826821
14	1	0	-5.621868	-0.185447	1.591758	44	1	0	7.378439	-0.225560	-0.894506
15	1	0	-5.719408	-1.877256	1.129415	45	6	0	7.771493	1.819696	-0.315066
16	1	0	-3.515797	0.083922	-1.852998	46	1	0	7.553520	2.518629	0.497102
17	6	0	-7.488490	-0.515762	-0.529547	47	1	0	8.854993	1.688809	-0.357289
18	1	0	-7.836470	-0.317113	-1.551858	48	1	0	7.457800	2.281801	-1.255112
19	1	0	-7.819582	-1.535776	-0.294047	49	6	0	-8.196955	0.458054	0.423452
20	6	0	2.635067	0.406465	-0.019666	50	1	0	-7.896489	1.487120	0.198889
21	6	0	3.351387	1.548399	-0.027872	51	1	0	-7.885277	0.265227	1.455590
22	6	0	4.806991	1.594201	-0.130694	52	6	0	-9.723178	0.352361	0.334256
23	1	0	2.827821	2.497102	0.007070	53	1	0	-10.065289	-0.656185	0.587551
24	6	0	5.587730	0.507678	-0.027085	54	1	0	-10.213109	1.050724	1.018537
25	1	0	5.257989	2.566529	-0.289997	55	1	0	-10.076483	0.575469	-0.677568
26	6	0	-1.675132	0.354763	0.207560	-----					
27	6	0	-0.983531	-0.561107	-0.596366						

Absolute energy: E(RB3LYP) = -1293.04210901 a.u.

The number of imaginary frequencies = 0

Dipole moment (field-independent basis, Debye):

X = -0.7760

Y = 3.6603

Z = -0.2892

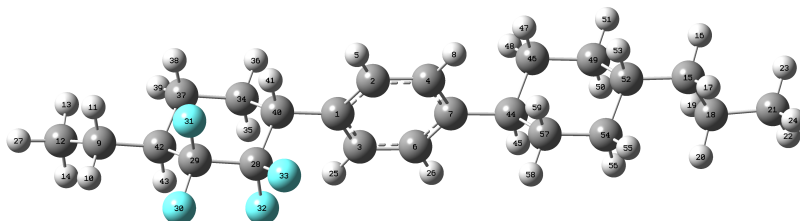
Tot = 3.7537

Exact polarizability (α_{xx} , α_{xy} , α_{yy} , α_{xz} , α_{yz} , α_{zz}) [a.u.]:

452.271 13.518 230.846 -3.473 9.010 202.055

^a Computation was carried out by using Gaussian 09W (rev. C.01) using the B3LYP/6-311++G(d,p) level of theory.

Cartesian coordinate (Å) and absolute energy of the optimized structure for **1b**^a



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	1.076434	-0.258536	0.270702
2	6	0	0.228911	0.046413	1.340265
3	6	0	0.490951	-0.549705	-0.965020
4	6	0	-1.153937	0.057666	1.185336
5	1	0	0.656874	0.282546	2.309442
6	6	0	-0.893838	-0.533731	-1.117175
7	6	0	-1.745511	-0.232075	-0.049715
8	1	0	-1.774840	0.298746	2.041361
9	6	0	7.012448	-0.435009	0.019596
10	1	0	7.428372	0.500766	-0.362582
11	1	0	7.150026	-0.416337	1.105204
12	6	0	7.789525	-1.609081	-0.585337
13	1	0	7.476659	-2.571407	-0.172259
14	1	0	7.660552	-1.652129	-1.671463
15	6	0	-7.623934	0.174780	0.570502
16	1	0	-8.039757	-0.528152	1.304421
17	1	0	-7.966352	1.170309	0.882576
18	6	0	-8.230271	-0.140641	-0.804487
19	1	0	-7.917271	-1.138099	-1.131485
20	1	0	-7.846501	0.561548	-1.552288
21	6	0	-9.761283	-0.075143	-0.796931
22	1	0	-10.175664	-0.305477	-1.782455
23	1	0	-10.184716	-0.789407	-0.083485
24	1	0	-10.113686	0.921711	-0.513358
25	1	0	1.112135	-0.780491	-1.821839
26	1	0	-1.321057	-0.759072	-2.089457
27	1	0	8.858492	-1.502294	-0.384522
28	6	0	3.311287	0.864561	-0.206501
29	6	0	4.833361	0.851246	0.078522
30	9	0	5.410158	1.901692	-0.581073
31	9	0	4.994255	1.105836	1.425185
32	9	0	3.163499	0.787379	-1.574962
33	9	0	2.799686	2.070074	0.172264
34	6	0	3.246906	-1.622051	0.091082
35	1	0	3.072108	-1.815739	-0.971448
36	1	0	2.755668	-2.428707	0.640754
37	6	0	4.753964	-1.629782	0.381970
38	1	0	4.923818	-1.577782	1.463466
39	1	0	5.180847	-2.576488	0.043744
40	6	0	2.579660	-0.287047	0.487892
41	1	0	2.762210	-0.123977	1.554968
42	6	0	5.504924	-0.467318	-0.296920
43	1	0	5.377984	-0.554762	-1.382803
44	6	0	-3.251877	-0.218228	-0.237233
45	1	0	-3.447450	-0.477468	-1.286159
46	6	0	-3.966736	-1.274985	0.632780
47	1	0	-3.745722	-1.082822	1.689850
48	1	0	-3.563915	-2.267889	0.407756
49	6	0	-5.487242	-1.256758	0.421352
50	1	0	-5.708898	-1.569205	-0.606630
51	1	0	-5.961200	-1.994861	1.078646
52	6	0	-6.086246	0.136811	0.681174
53	1	0	-5.851049	0.392509	1.725274
54	6	0	-5.382930	1.184027	-0.200103
55	1	0	-5.782365	2.181796	0.014974
56	1	0	-5.599575	0.983953	-1.256715
57	6	0	-3.861985	1.179202	0.007739
58	1	0	-3.385142	1.907949	-0.655459
59	1	0	-3.634451	1.498203	1.032318

Absolute energy: E(RB3LYP) = -1295.50237337 a.u.

The number of imaginary frequencies = 0

Dipole moment (field-independent basis, Debye):

X = -0.5947

Y = -3.7878

Z = 0.3677

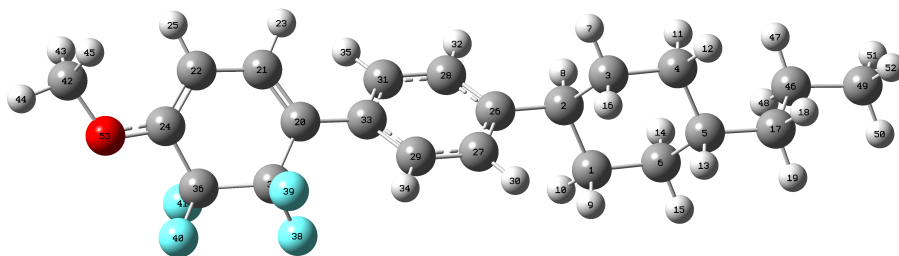
Tot = 3.8518

Exact polarizability (α_{xx} , α_{xy} , α_{yy} , α_{xz} , α_{yz} , α_{zz}) [a.u.]:

381.045 -8.729 216.660 0.549 5.023 225.455

^a Computation was carried out by using Gaussian 09W (rev. C.01) using the B3LYP/6-311++G(d,p) level of theory.

Cartesian coordinate (Å) and absolute energy of the optimized structure for **2a^a**



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	3.782837	-0.966179	-0.748913
2	6	0	3.182443	0.373269	-0.265391
3	6	0	3.817832	0.786614	1.083420
4	6	0	5.351594	0.832885	1.002849
5	6	0	5.943004	-0.507565	0.528106
6	6	0	5.317216	-0.909887	-0.821221
7	1	0	3.422917	1.762181	1.392238
8	1	0	3.464805	1.138915	-1.003392
9	1	0	3.482248	-1.769111	-0.061745
10	1	0	3.364303	-1.224047	-1.729267
11	1	0	5.648657	1.634179	0.311810
12	1	0	5.767029	1.097914	1.984189
13	1	0	5.630415	-1.268721	1.261655
14	1	0	5.611376	-0.187905	-1.595947
15	1	0	5.709056	-1.884955	-1.139954
16	1	0	3.514655	0.069046	1.858779
17	6	0	7.486839	-0.530963	0.522213
18	1	0	7.838211	-0.333216	1.545682
19	1	0	7.815669	-1.553267	0.284215
20	6	0	-2.655925	0.418079	0.029650
21	6	0	-3.367667	1.569946	0.042968
22	6	0	-4.821974	1.647453	0.126649
23	1	0	-2.831660	2.514040	0.017757
24	6	0	-5.587467	0.541540	0.009354
25	1	0	-5.269955	2.622629	0.275356
26	6	0	1.665334	0.355432	-0.199595
27	6	0	0.969241	-0.563858	0.602402
28	6	0	0.903471	1.270814	-0.939514
29	6	0	-0.421944	-0.566466	0.669777
30	1	0	1.518522	-1.293387	1.191030
31	6	0	-0.489780	1.275675	-0.879300
32	1	0	1.408259	1.984079	-1.586950
33	6	0	-1.182650	0.365250	-0.062354
34	1	0	-0.918779	-1.286572	1.310766
35	1	0	-1.047677	1.975665	-1.494540
36	6	0	-4.912605	-0.778166	-0.307066
37	6	0	-3.448424	-0.857026	0.214622
38	9	0	-2.858308	-1.931172	-0.386421
39	9	0	-3.525166	-1.162482	1.565257
40	9	0	-5.613798	-1.829997	0.189328
41	9	0	-4.876972	-0.929214	-1.676762
42	6	0	-7.678087	1.613024	0.335297
43	1	0	-7.504080	2.379842	-0.428667
44	1	0	-8.723820	1.307541	0.323988
45	1	0	-7.414721	2.006352	1.324080
46	6	0	8.197183	0.442585	-0.432192
47	1	0	7.898823	1.474257	-0.206734
48	1	0	7.883811	0.250284	-1.466112
49	6	0	9.724872	0.333723	-0.344703
50	1	0	10.065047	-0.677439	-0.598552
51	1	0	10.216157	1.032254	-1.030873
52	1	0	10.080219	0.556457	0.668580
53	8	0	-6.926668	0.433961	0.045954

Absolute energy: E(RB3LYP) = -1328.94386772 a.u.

The number of imaginary frequencies = 0

Dipole moment (field-independent basis, Debye):

X = 0.0755

Y = 4.8555

Z = 0.4913

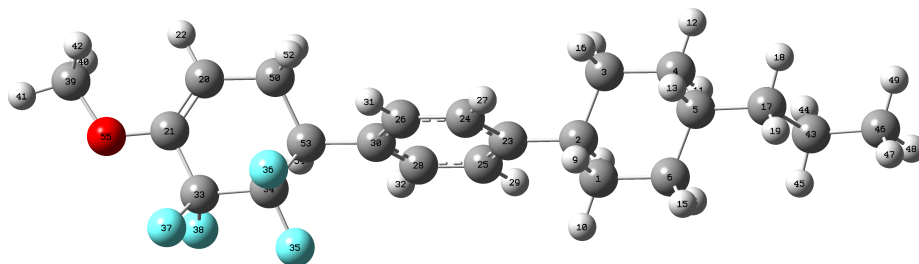
Tot = 4.8809

Exact polarizability (α_{xx} , α_{xy} , α_{yy} , α_{xz} , α_{yz} , α_{zz}) [a.u.]:

444.824 -17.645 223.766 -4.153 -9.061 196.248

^a Computation was carried out by using Gaussian 09W (rev. C.01) using the B3LYP/6-311++G(d,p) level of theory.

Cartesian coordinate (Å) and absolute energy of the optimized structure for **2b**^a



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)					
			X	Y	Z			
1	6	0	-3.761221	-1.068943	-0.506080	28	6	0
2	6	0	-3.204256	0.009598	0.450956	29	1	0
3	6	0	-3.842831	1.382138	0.136658	30	6	0
4	6	0	-5.378196	1.319402	0.162755	31	1	0
5	6	0	-5.926974	0.247761	-0.798174	32	1	0
6	6	0	-5.297222	-1.120138	-0.474862	33	6	0
7	1	0	-3.480502	2.129151	0.853523	34	6	0
8	1	0	-3.518590	-0.267860	1.468218	35	9	0
9	1	0	-3.426106	-0.854730	-1.530435	36	9	0
10	1	0	-3.342414	-2.047301	-0.241345	37	9	0
11	1	0	-5.708802	1.101994	1.187950	38	9	0
12	1	0	-5.793734	2.302378	-0.096176	39	6	0
13	1	0	-5.584265	0.523667	-1.809098	40	1	0
14	1	0	-5.621683	-1.451841	0.521457	41	1	0
15	1	0	-5.657568	-1.875068	-1.186167	42	1	0
16	1	0	-3.509261	1.716469	-0.855834	43	6	0
17	6	0	-7.469118	0.213700	-0.867804	44	1	0
18	1	0	-7.820993	1.198506	-1.208951	45	1	0
19	1	0	-7.761881	-0.498447	-1.653356	46	6	0
20	6	0	4.742122	1.659903	-0.049994	47	1	0
21	6	0	5.509290	0.558397	-0.088369	48	1	0
22	1	0	5.205423	2.638187	-0.126488	49	1	0
23	6	0	-1.686167	0.067522	0.455497	50	6	0
24	6	0	-0.952615	0.350304	-0.708372	51	1	0
25	6	0	-0.964165	-0.152127	1.635662	52	1	0
26	6	0	0.440241	0.415331	-0.692315	53	6	0
27	1	0	-1.471949	0.522903	-1.647086	54	1	0
						55	8	0

Absolute energy: E(RB3LYP) = -1330.17070706 a.u.

The number of imaginary frequencies = 0

Dipole moment (field-independent basis, Debye):

X = -1.0735

Y = 5.0404

Z = 0.5687

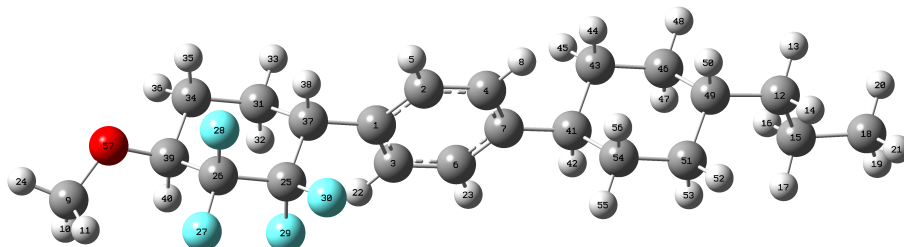
Tot = 5.1848

Exact polarizability (α_{xx} , α_{xy} , α_{yy} , α_{xz} , α_{yz} , α_{zz}) [a.u.]:

376.541 5.031 212.047 -0.669 -4.580 214.615

^a Computation was carried out by using Gaussian 09W (rev. C.01) using the B3LYP/6-311++G(d,p) level of theory.

Cartesian coordinate (Å) and absolute energy of the optimized structure for *trans*-**2c**^a



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-1.071107	-0.145017	-0.426129
2	6	0	-0.245531	0.729383	-1.145692
3	6	0	-0.510514	-1.036180	0.498796
4	6	0	1.140646	0.712565	-0.940387
5	1	0	-0.673562	1.409841	-1.851855
6	6	0	0.875661	-1.052983	0.704116
7	6	0	1.701245	-0.178634	-0.015499
8	1	0	1.770995	1.380173	-1.489805
9	6	0	-7.288887	-1.801625	0.372667
10	1	0	-6.836696	-2.497979	-0.302251
11	1	0	-7.081166	-2.095373	1.380369
12	6	0	7.495286	0.169863	-0.563692
13	1	0	7.947312	-0.526648	-1.238559
14	1	0	7.893832	1.147119	-0.739851
15	6	0	7.794385	-0.252724	0.886672
16	1	0	7.395837	-1.229979	1.062833
17	1	0	7.342362	0.443789	1.561538
18	6	0	9.317669	-0.271251	1.112191
19	1	0	9.525488	-0.564863	2.119913
20	1	0	9.769690	-0.967766	0.437326
21	1	0	9.716215	0.706004	0.936027
22	1	0	-1.140864	-1.703775	1.048227
23	1	0	1.303686	-1.733401	1.410321
24	1	0	-8.347255	-1.788852	0.215839
25	6	0	-3.245165	0.875671	0.319532
26	6	0	-4.768426	0.894063	0.093820
27	9	0	5.338939	1.772674	0.945325
28	9	0	-5.030501	1.264642	-1.177592
29	9	0	-2.983086	0.505097	1.590945
30	9	0	-2.742428	2.108737	0.097485
31	6	0	-3.167860	-1.533209	-0.398506
32	1	0	-2.960142	-1.826918	0.609208
33	1	0	-2.715676	-2.229595	-1.073395
34	6	0	-4.691113	-1.514816	-0.624228
35	1	0	-4.898826	-1.221100	-1.631942
36	1	0	-5.089579	-2.492134	-0.448239
37	6	0	-2.594368	-0.126605	-0.651812
38	1	0	-2.802097	0.167106	-1.659523
39	6	0	-5.341921	-0.512548	0.347111
40	1	0	-5.134207	-0.806266	1.354823
41	6	0	3.224522	-0.197156	0.210067
42	1	0	3.432317	-0.490780	1.217791
43	6	0	3.875117	-1.199606	-0.761231
44	1	0	3.667315	-0.905988	-1.768953
45	1	0	3.476569	-2.176864	-0.585079
46	6	0	5.398397	-1.218131	-0.535688
47	1	0	5.606203	-1.511749	0.472035
48	1	0	5.850430	-1.914641	-1.210551
49	6	0	5.972003	0.188387	-0.789219
50	1	0	5.764191	0.482006	-1.796940
51	6	0	5.321419	1.190837	0.182088
52	1	0	5.719966	2.168095	0.005938
53	1	0	5.529227	0.897215	1.189808
54	6	0	3.798135	1.209365	-0.043449
55	1	0	3.346104	1.905869	0.631421
56	1	0	3.590331	1.502991	-1.051169
57	8	0	-6.756373	-0.495474	0.137509

Absolute energy: E(RB3LYP) = -1331.40087979 a.u.
The number of imaginary frequencies = 0

Dipole moment (field-independent basis, Debye):
X = 1.3276 Y = -2.9851

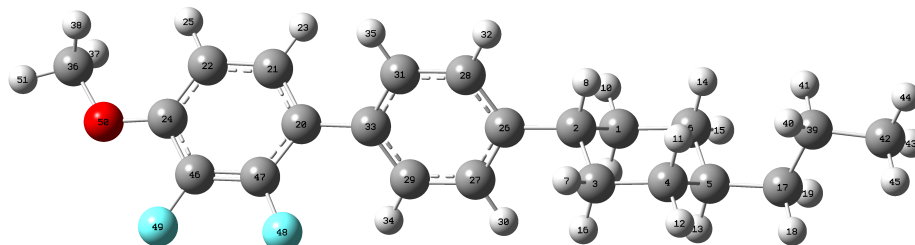
Z = 1.0482

Tot = 3.4310

Exact polarizability (α_{xx} , α_{xy} , α_{yy} , α_{xz} , α_{yz} , α_{zz}) [a.u.]:
372.938 6.398 208.137 -1.276 -2.428 220.808

^a Computation was carried out by using Gaussian 09W (rev. C.01) using the B3LYP/6-311++G(d,p) level of theory.

Cartesian coordinate (Å) and absolute energy of the optimized structure for **2d^a**



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	3.375219	-0.743770	1.100663
2	6	0	2.753091	-0.341799	-0.257183
3	6	0	3.375449	0.981499	-0.758175
4	6	0	4.909245	0.904732	-0.819027
5	6	0	5.520220	0.515294	0.540709
6	6	0	4.908880	-0.810788	1.030550
7	1	0	2.966771	1.228917	-1.745369
8	1	0	3.027474	-1.122778	-0.981999
9	1	0	3.077753	-0.011704	1.864498
10	1	0	2.965903	-1.709665	1.420906
11	1	0	5.199401	0.167136	-1.580406
12	1	0	5.315945	1.869654	-1.149813
13	1	0	5.211223	1.291127	1.260279
14	1	0	5.200189	-1.625325	0.352663
15	1	0	5.314721	-1.067256	2.018179
16	1	0	3.079602	1.798746	-0.085895
17	6	0	7.064199	0.520857	0.546028
18	1	0	7.406294	1.535061	0.292469
19	1	0	7.406084	0.337334	1.575332
20	6	0	-3.095559	-0.237718	-0.045339
21	6	0	-3.823385	-1.434396	0.035799
22	6	0	-5.219187	-1.467381	0.088943
23	1	0	-3.276795	-2.370720	0.081582
24	6	0	-5.954819	-0.276519	0.063651
25	1	0	-5.724965	-2.422089	0.163270
26	6	0	1.235654	-0.294531	-0.204715
27	6	0	0.552381	0.624499	0.608493
28	6	0	0.462079	-1.177385	-0.970424
29	6	0	-0.839769	0.659780	0.655958
30	1	0	1.112134	1.326213	1.220944
31	6	0	-0.932929	-1.148583	-0.928012
32	1	0	0.958096	-1.895404	-1.619459
33	6	0	-1.611523	-0.231329	-0.110181
34	1	0	-1.332170	1.379053	1.301992
35	1	0	-1.500376	-1.832864	-1.552514
36	6	0	-8.073439	-1.368355	0.199402
37	1	0	-7.840391	-1.925317	1.115082
38	1	0	-7.906940	-2.008967	-0.675070
39	6	0	7.770206	-0.477405	-0.385769
40	1	0	7.464257	-0.301953	-1.424897
41	1	0	7.460623	-1.501610	-0.142283
42	6	0	9.298386	-0.381662	-0.291686
43	1	0	9.645931	-0.587942	0.727768
44	1	0	9.786597	-1.098237	-0.961227
45	1	0	9.649832	0.620987	-0.563258
46	6	0	-5.244033	0.930467	-0.019066
47	6	0	-3.857117	0.940777	-0.071303
48	9	0	-3.255646	2.147814	-0.175581
49	9	0	-5.914269	2.098717	-0.058915
50	8	0	-7.307751	-0.170010	0.114799
51	1	0	-9.115457	-1.048796	0.223417

Absolute energy: E(RB3LYP) = -1129.21338712 a.u.

The number of imaginary frequencies = 0

Dipole moment (field-independent basis, Debye):

X = 0.2186

Y = -3.9089

Z = 0.3116

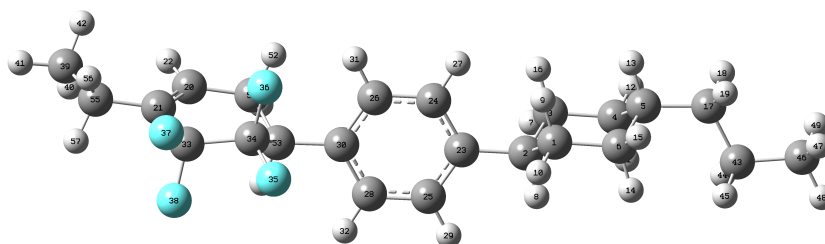
Tot = 3.9273

Exact polarizability (α_{xx} , α_{xy} , α_{yy} , α_{xz} , α_{yz} , α_{zz}) [a.u.]:

424.458 10.110 225.651 -3.374 9.038 186.811

^a Computation was carried out by using Gaussian 09W (rev. C.01) using the B3LYP/6-311++G(d,p) level of theory.

Cartesian coordinate (Å) and absolute energy of the optimized structure for ethylated cyclohexene derivatives^a



-----						29	1	0	-1.518355	-0.437085	2.547745
Center	Atomic	Atomic	Coordinates (Angstroms)			30	6	0	1.138196	0.165390	0.507292
Number	Number	Type	X	Y	Z	31	1	0	0.956493	0.630705	-1.591538
-----						32	1	0	0.936158	-0.339650	2.587663
1	6	0	-3.775331	-1.057789	-0.529368	33	6	0	4.889434	-0.830863	0.033081
2	6	0	-3.215149	-0.005767	0.451962	34	6	0	3.360696	-0.862803	-0.205156
3	6	0	-3.842611	1.376381	0.167843	35	9	0	2.886880	-2.093172	0.138925
4	6	0	-5.376734	1.323762	0.186769	36	9	0	3.151783	-0.726607	-1.558064
5	6	0	-5.928745	0.278824	-0.798586	37	9	0	5.482376	-1.726031	-0.816257
6	6	0	-5.310145	-1.098902	-0.505019	38	9	0	5.121918	-1.317232	1.308699
7	1	0	-3.478951	2.102141	0.902572	39	6	0	7.659943	1.935316	-0.295755
8	1	0	-3.531637	-0.303816	1.460432	40	1	0	7.468613	2.495986	0.623562
9	1	0	-3.435088	-0.824700	-1.545743	41	1	0	8.742472	1.835644	-0.403152
10	1	0	-3.365339	-2.042769	-0.284336	42	1	0	7.299862	2.531795	-1.138590
11	1	0	-5.712561	1.086399	1.203659	43	6	0	-8.221946	-0.128276	0.411080
12	1	0	-5.783790	2.313204	-0.051482	44	1	0	-7.967293	0.567854	1.217470
13	1	0	-5.582786	0.574684	-1.800465	45	1	0	-7.902553	-1.119826	0.749358
14	1	0	-5.640730	-1.450806	0.480083	46	6	0	-9.741829	-0.132514	0.215464
15	1	0	-5.672192	-1.833077	-1.233814	47	1	0	-10.038642	-0.845630	-0.560250
16	1	0	-3.502669	1.731309	-0.813072	48	1	0	-10.262562	-0.408463	1.136702
17	6	0	-7.469227	0.256049	-0.871213	49	1	0	-10.104919	0.854503	-0.088423
18	1	0	-7.813709	1.247520	-1.193784	50	6	0	3.223893	1.604528	0.115290
19	1	0	-7.764746	-0.437519	-1.669499	51	1	0	2.926060	2.369068	0.839716
20	6	0	4.719163	1.615003	-0.044176	52	1	0	2.764377	1.902288	-0.833846
21	6	0	5.506597	0.537441	-0.105949	53	6	0	2.652991	0.245136	0.570290
22	1	0	5.173966	2.597033	-0.127511	54	1	0	2.953438	0.086938	1.610630
23	6	0	-1.698236	0.044381	0.460389	55	6	0	7.010851	0.552185	-0.262415
24	6	0	-0.963545	0.344874	-0.694262	56	1	0	7.265628	0.004588	-1.176145
25	6	0	-0.981483	-0.198097	1.635034	57	1	0	7.443239	-0.036337	0.555529
26	6	0	0.425952	0.405881	-0.673960	-----					
27	1	0	-1.479770	0.535424	-1.628969						
28	6	0	0.410827	-0.140144	1.658991						

Absolute energy: E(RB3LYP) = -1294.27029778 a.u.

The number of imaginary frequencies = 0

Dipole moment (field-independent basis, Debye):

X = -0.9404

Y = 3.9380

Z = 0.6291

Tot = 4.0973

Exact polarizability (α_{xx} , α_{xy} , α_{yy} , α_{xz} , α_{yz} , α_{zz}) [a.u.]:

383.969 3.148 219.887 -0.818 -4.690 220.179

^a Computation was carried out by using Gaussian 09W (rev. C.01) using the B3LYP/6-311++G(d,p) level of theory.

Plots of destabilization energy and dipole moment along the short molecular axis as functions of the C1-C2-C3-C4 dihedral angle

