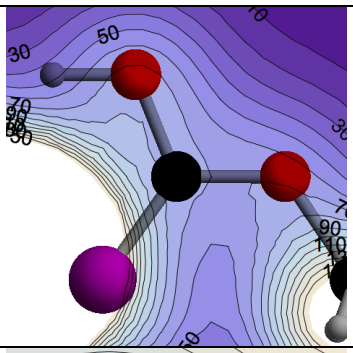
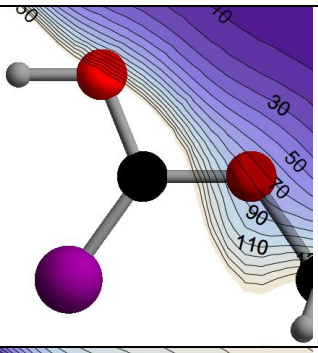
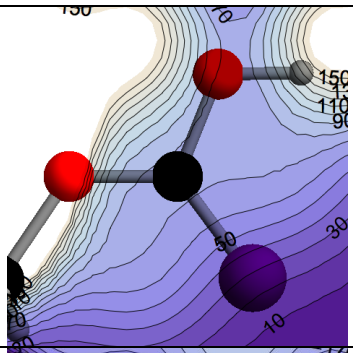
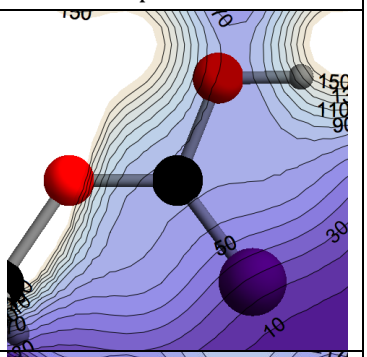
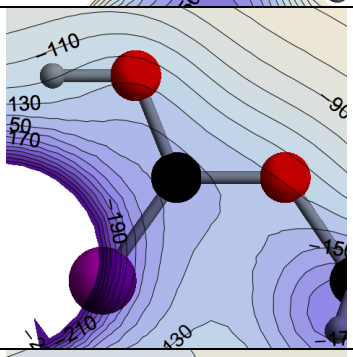
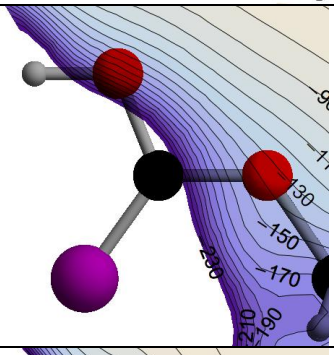
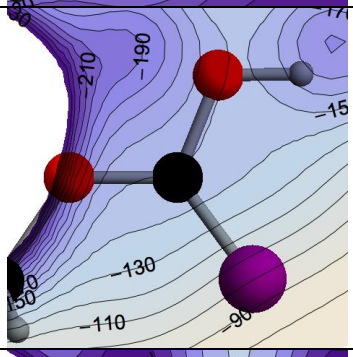
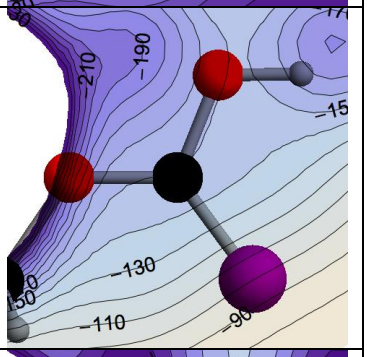
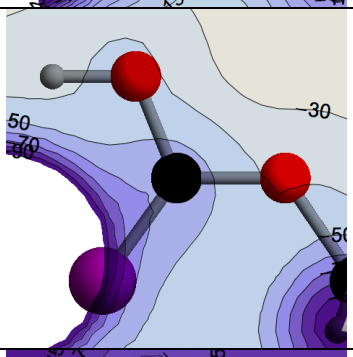
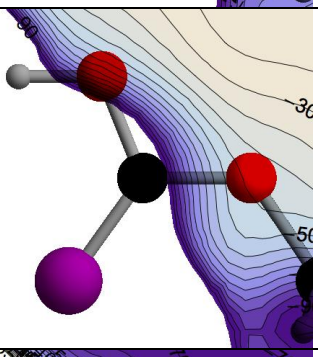
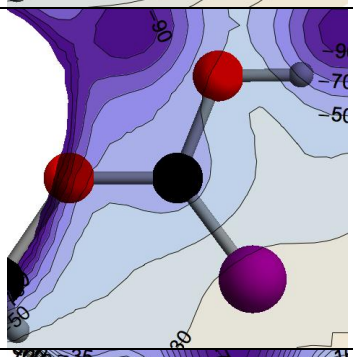
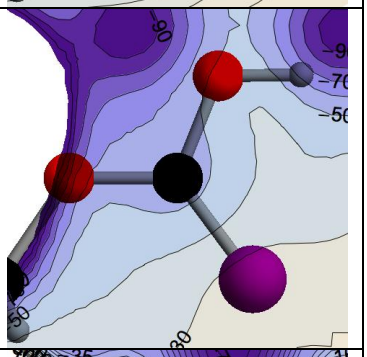
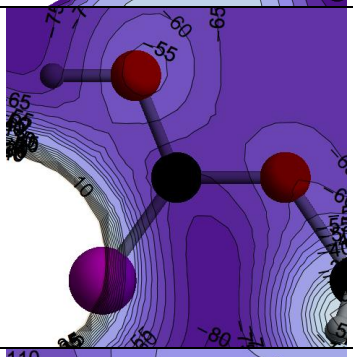
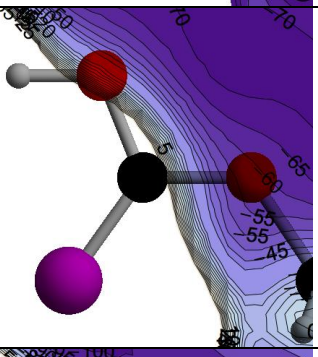
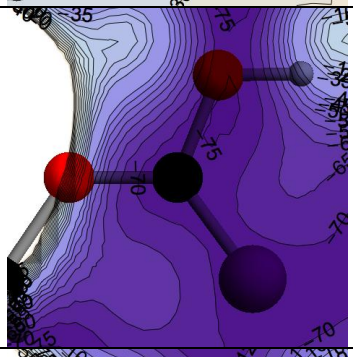
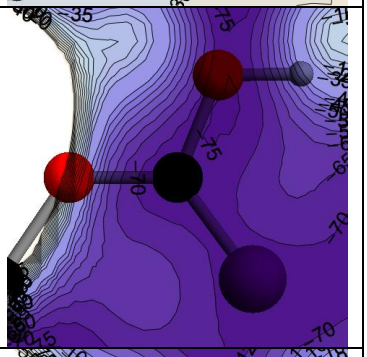
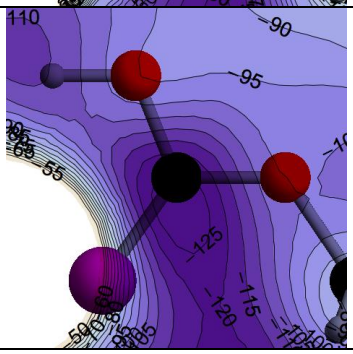
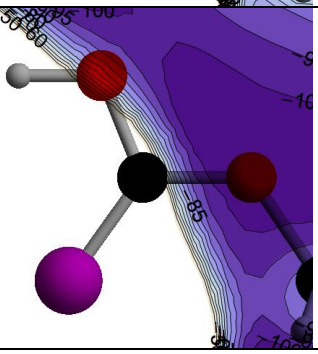
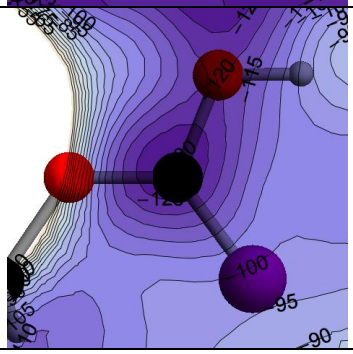
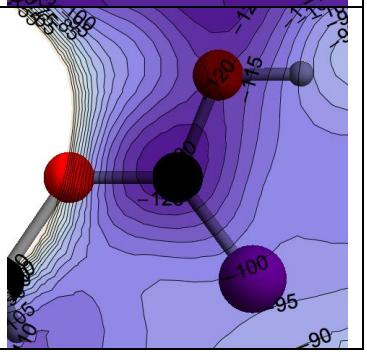
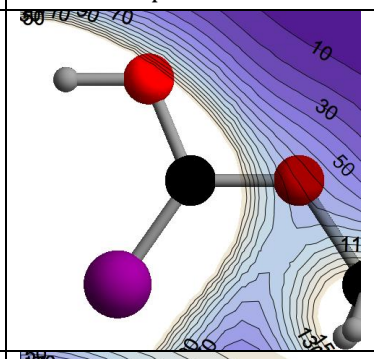
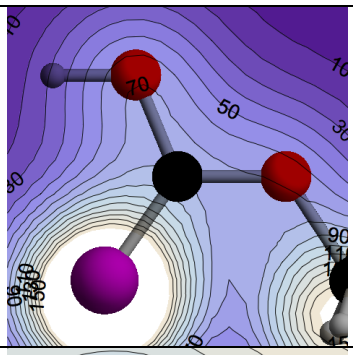
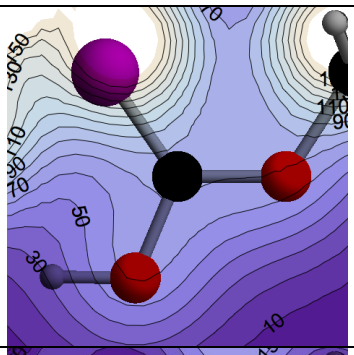
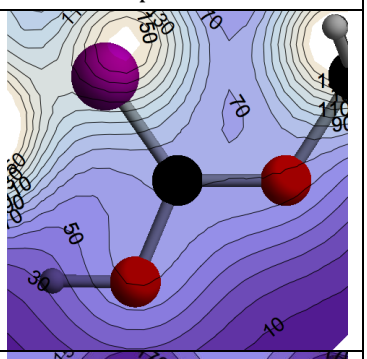
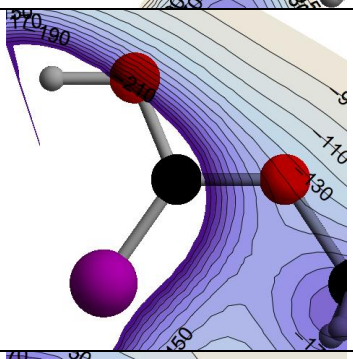
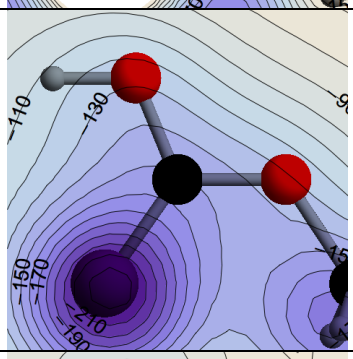
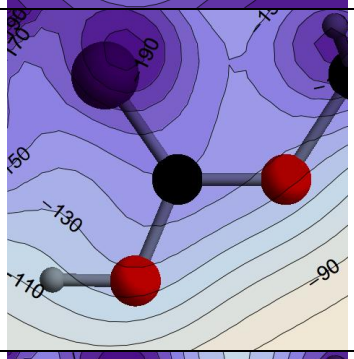
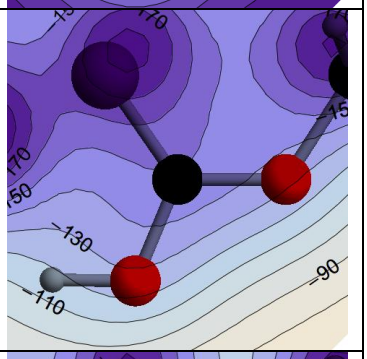
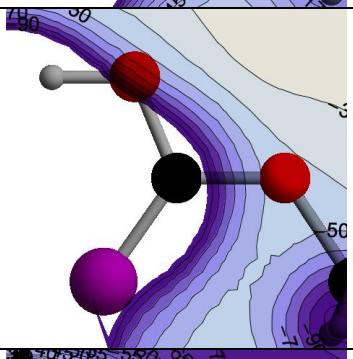
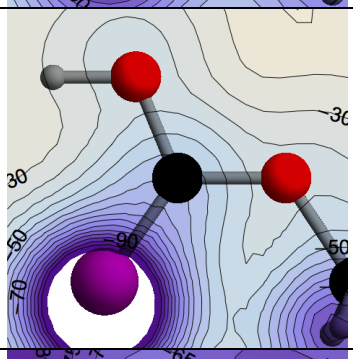
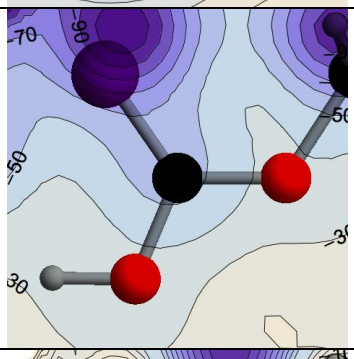
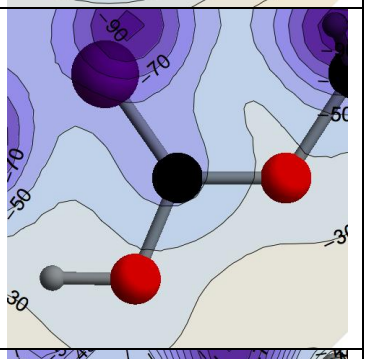
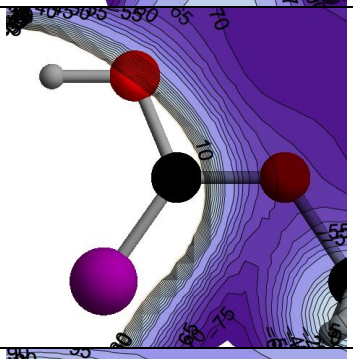
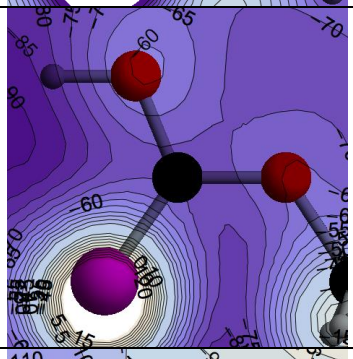
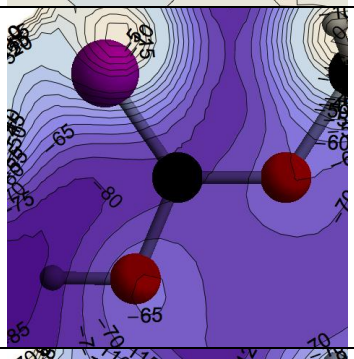
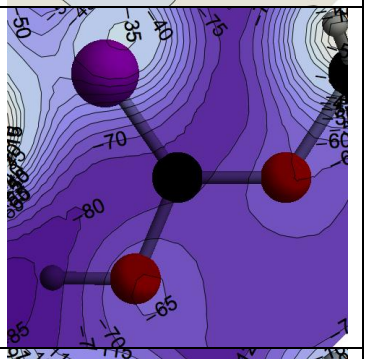
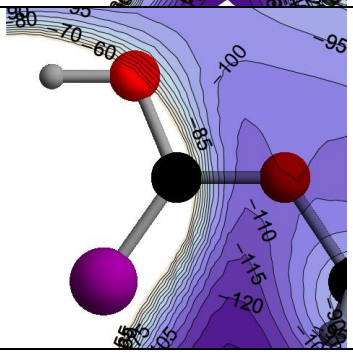
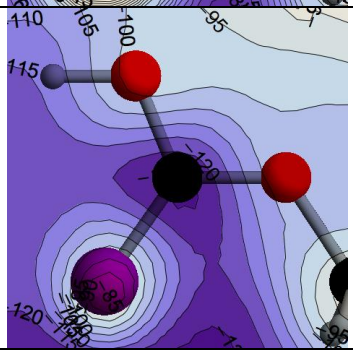
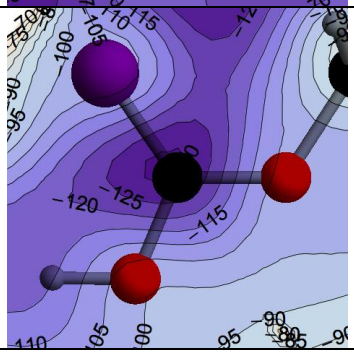
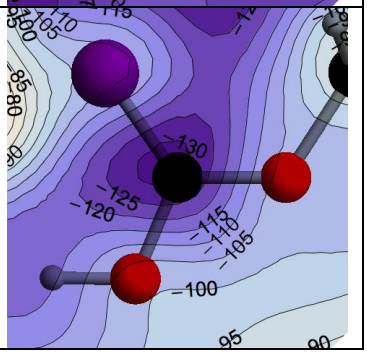
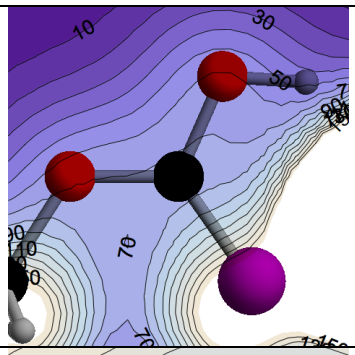
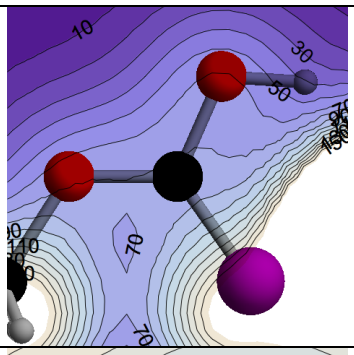
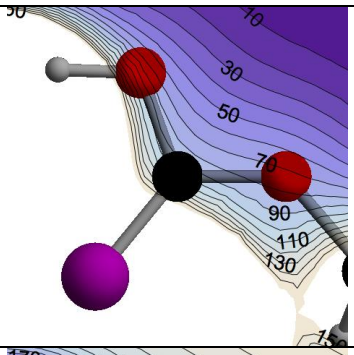
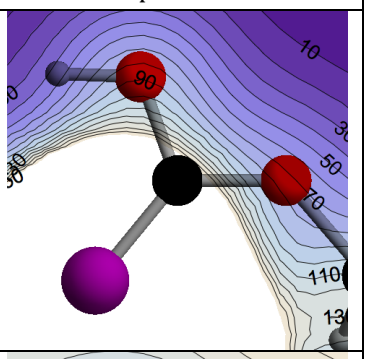
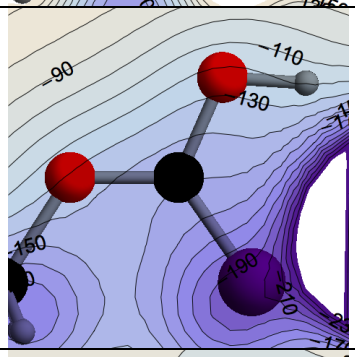
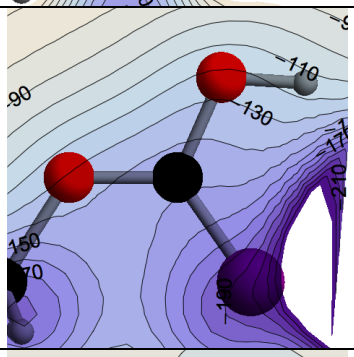
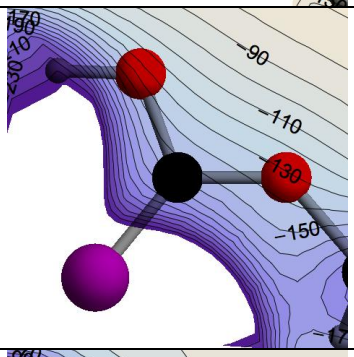
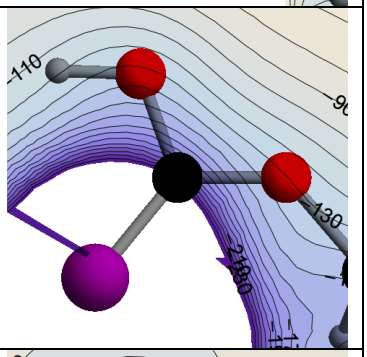
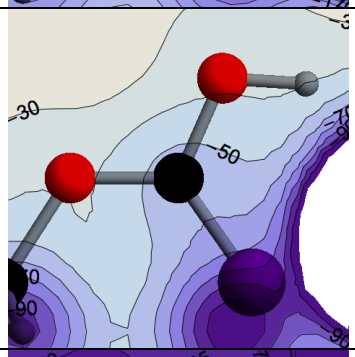
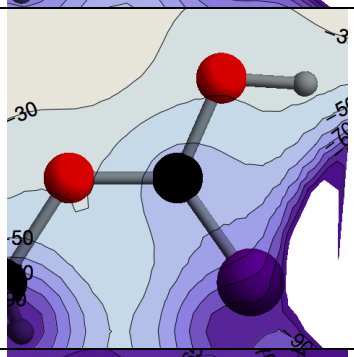
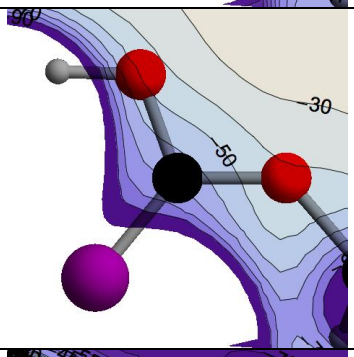
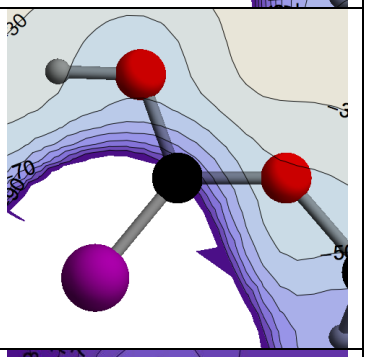
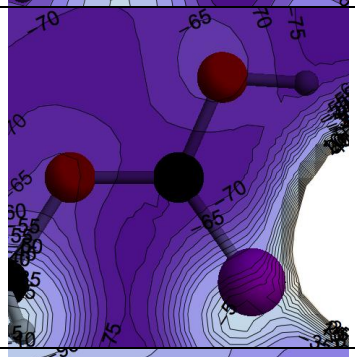
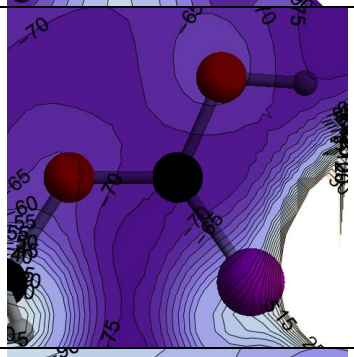
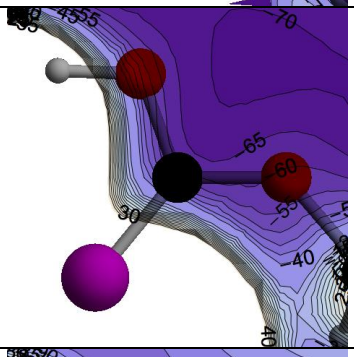
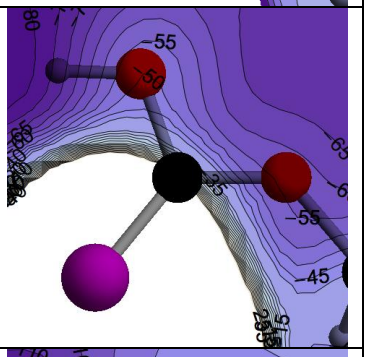
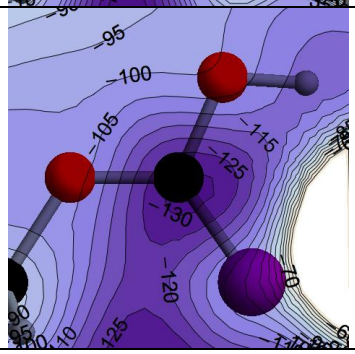
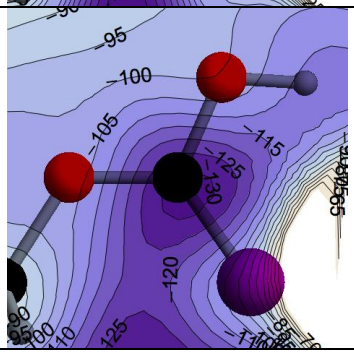
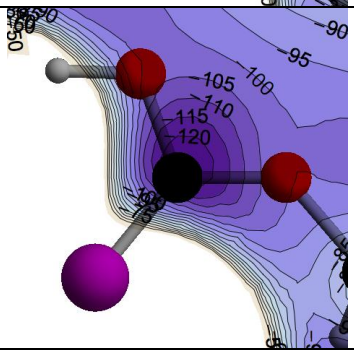
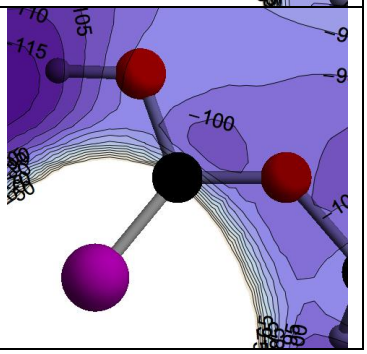
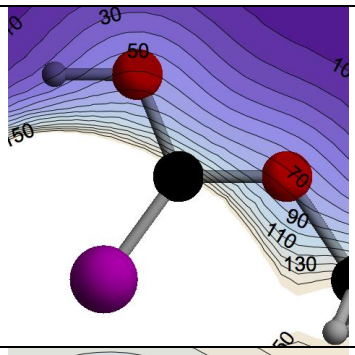
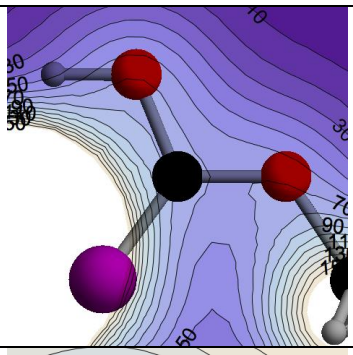
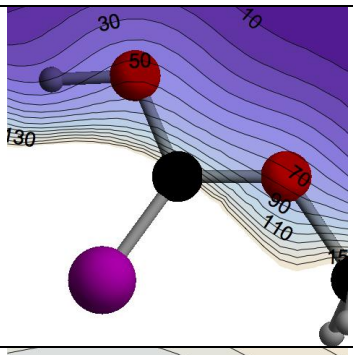
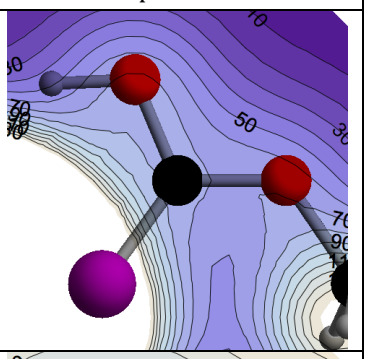
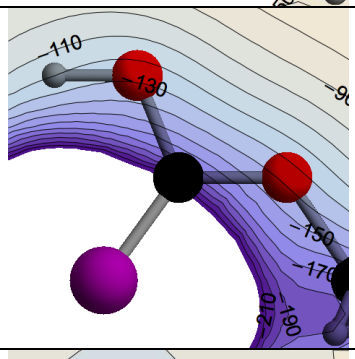
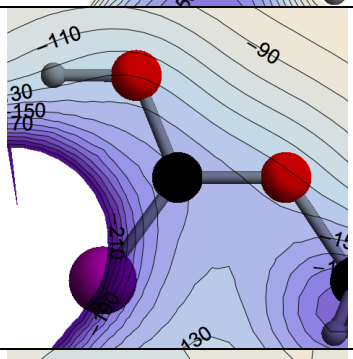
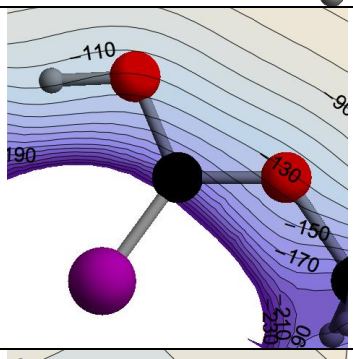
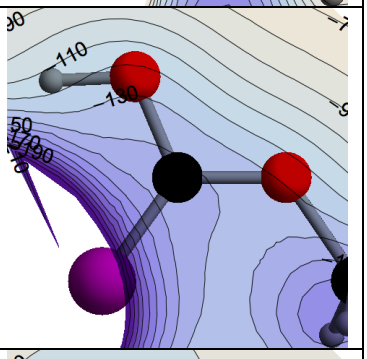
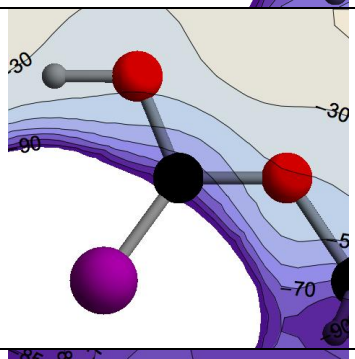
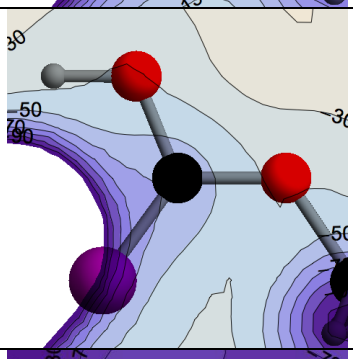
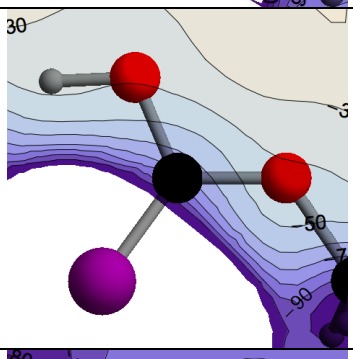
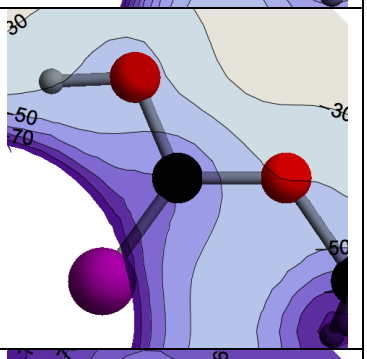
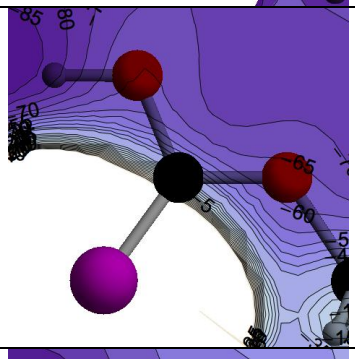
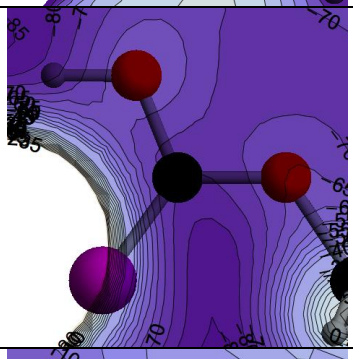
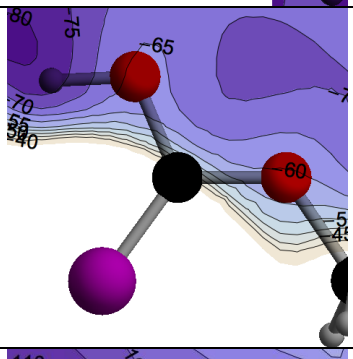
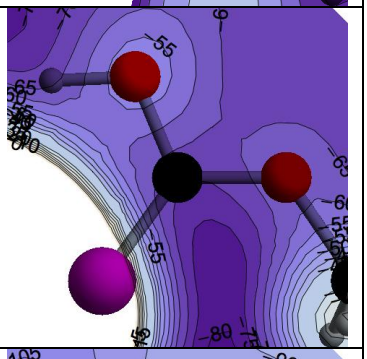
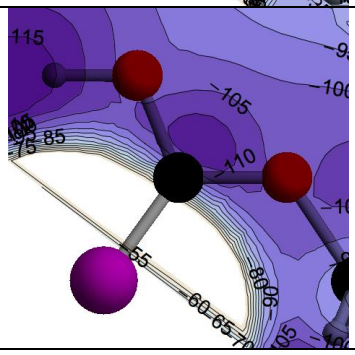
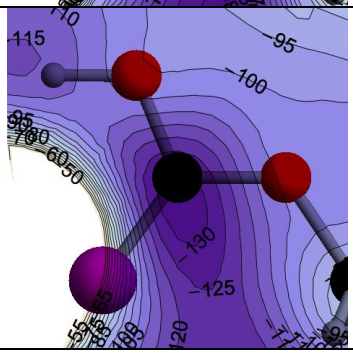
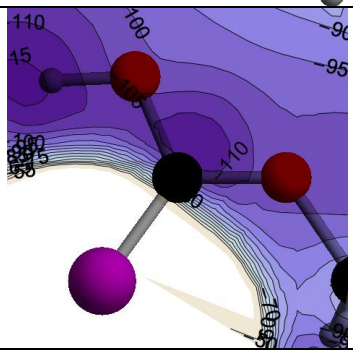
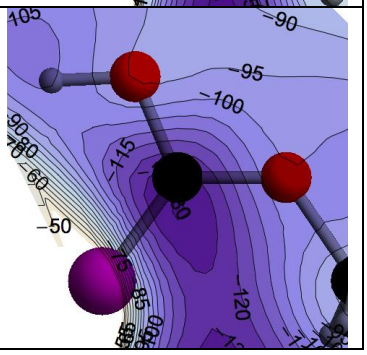
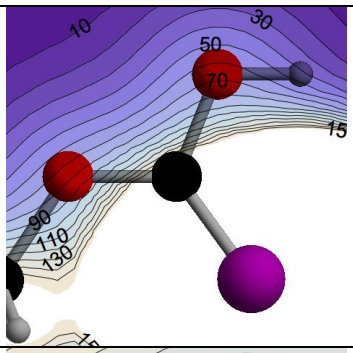
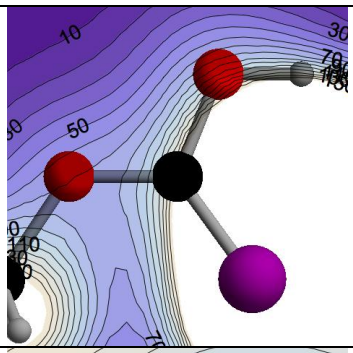
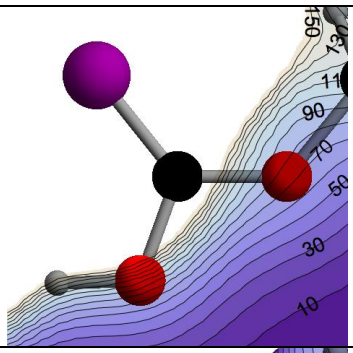
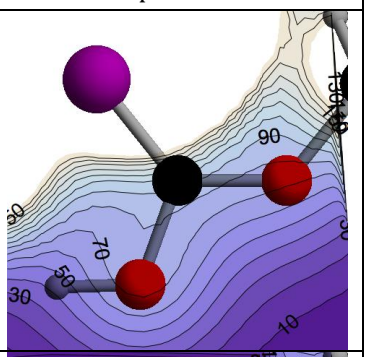
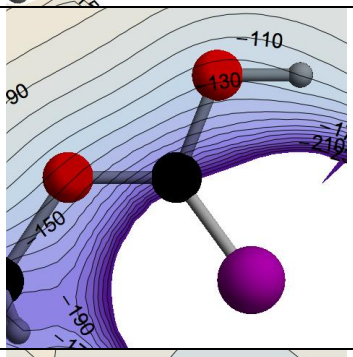
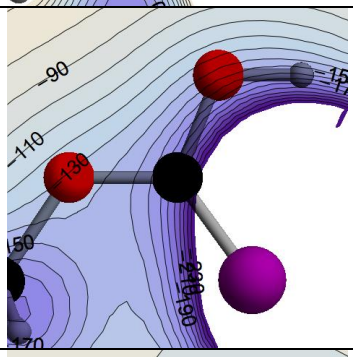
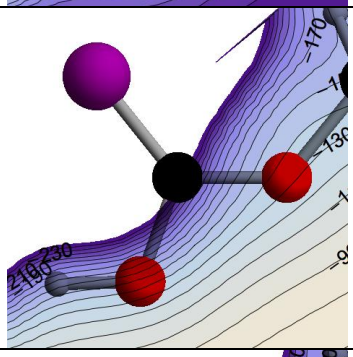
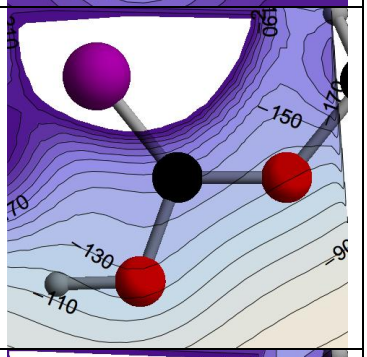
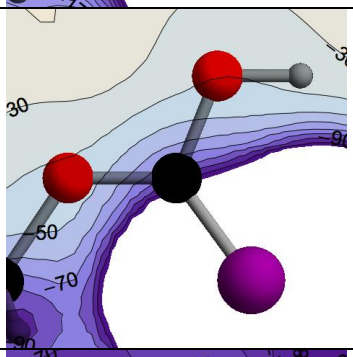
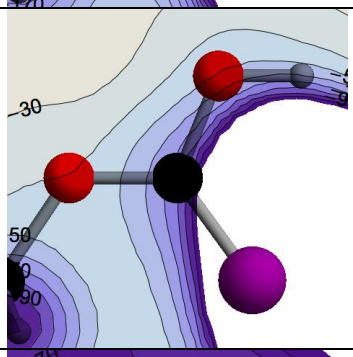
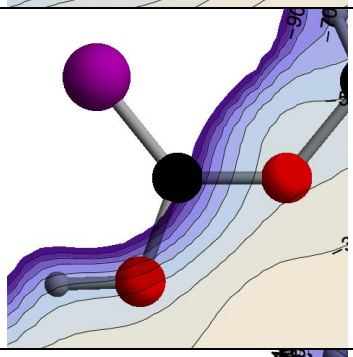
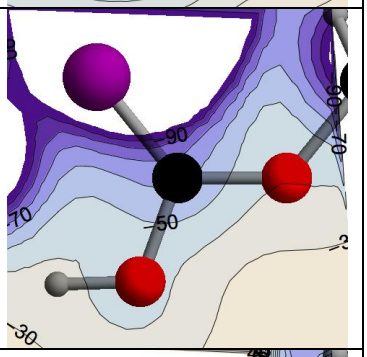
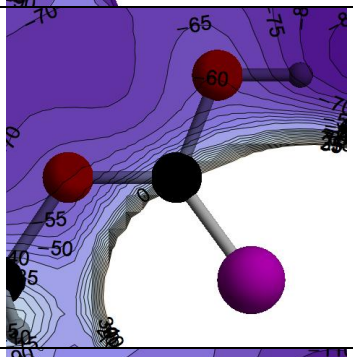
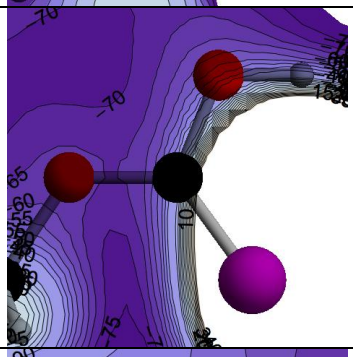
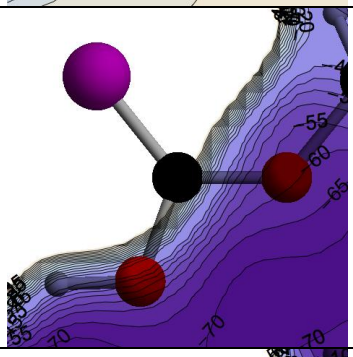
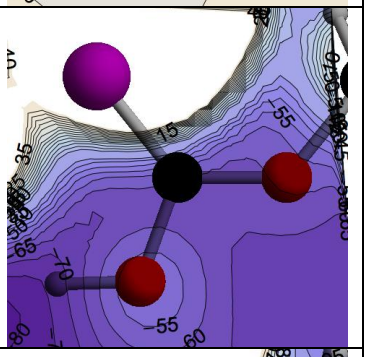
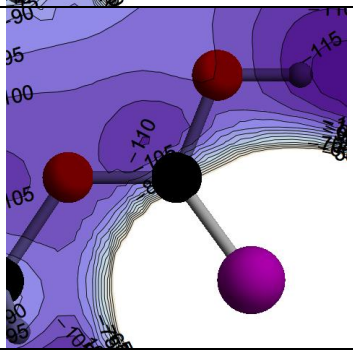
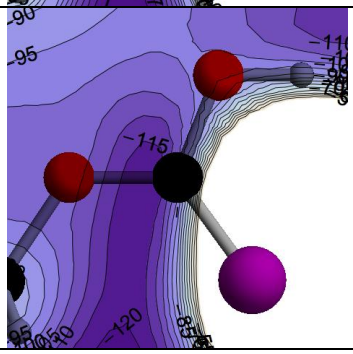
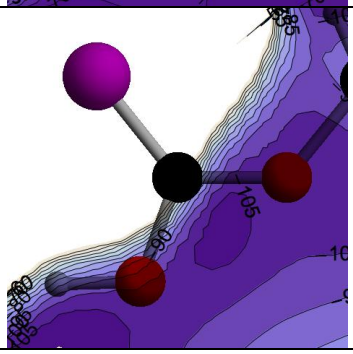
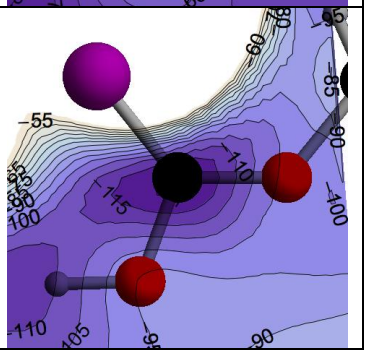
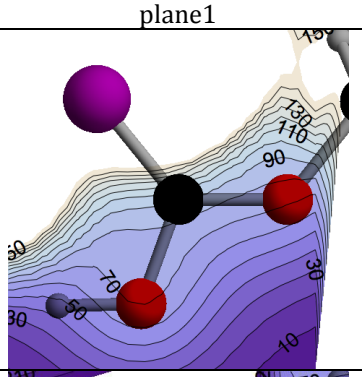
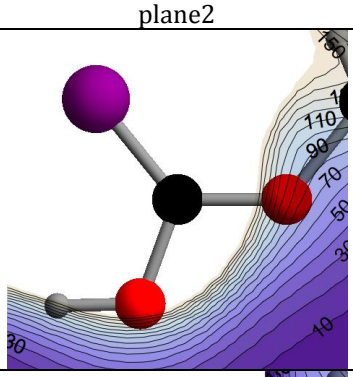
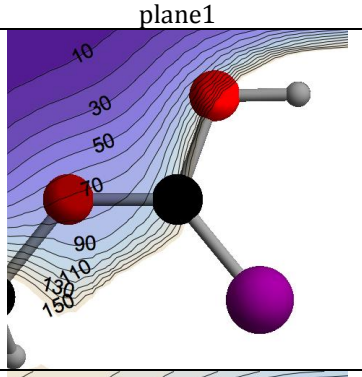
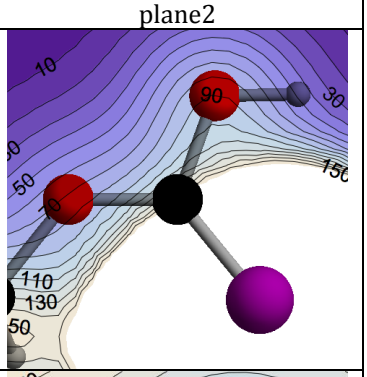
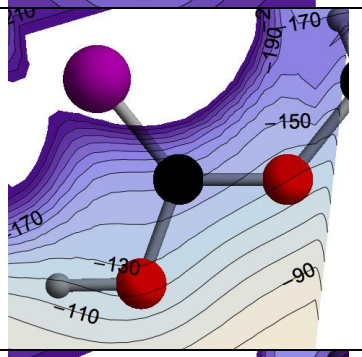
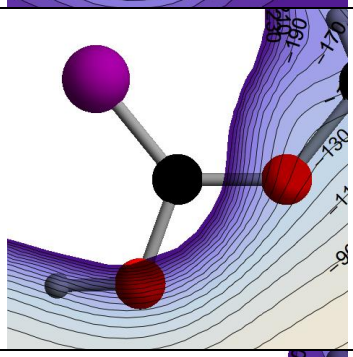
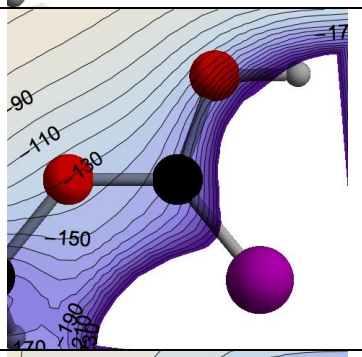
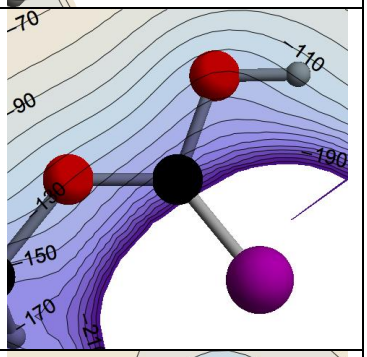
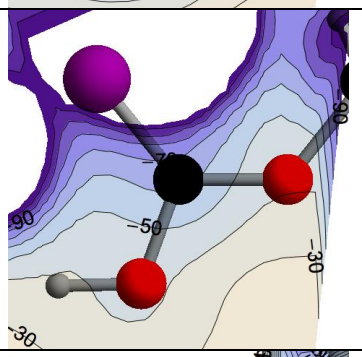
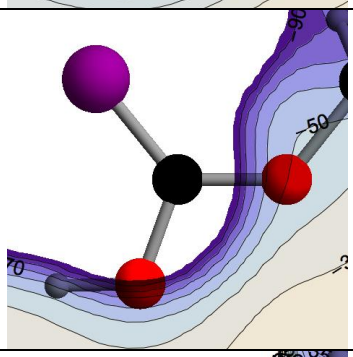
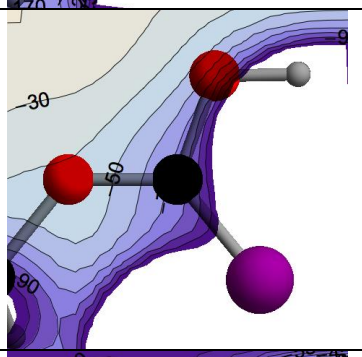
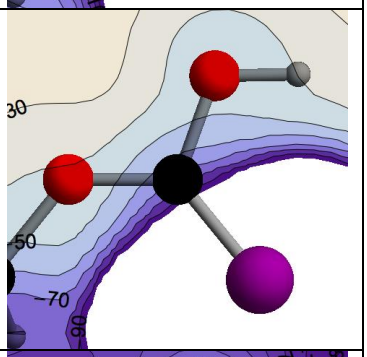
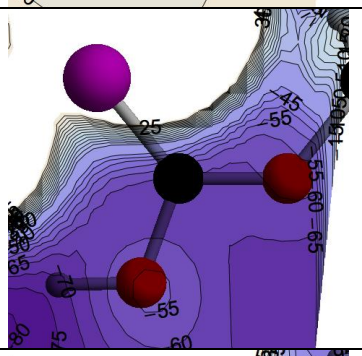
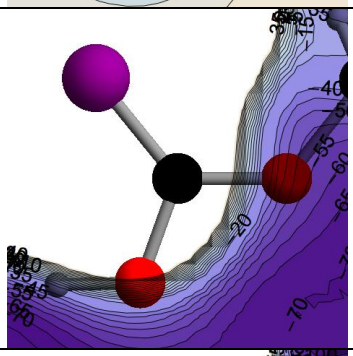
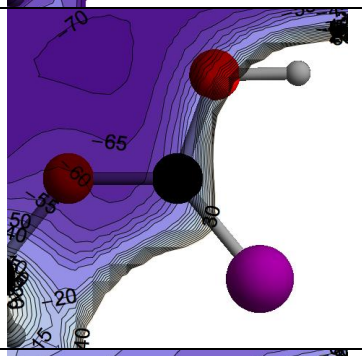
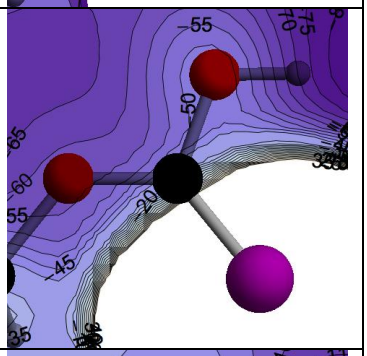
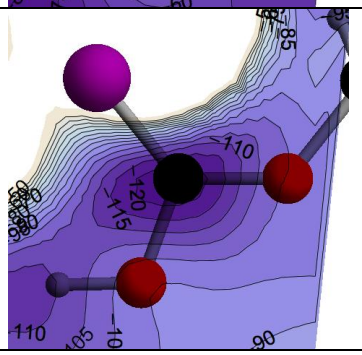
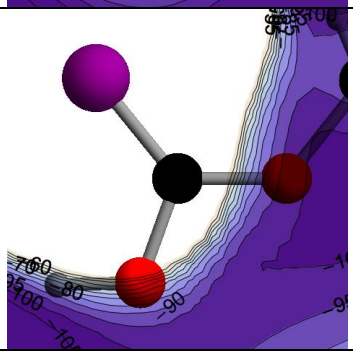
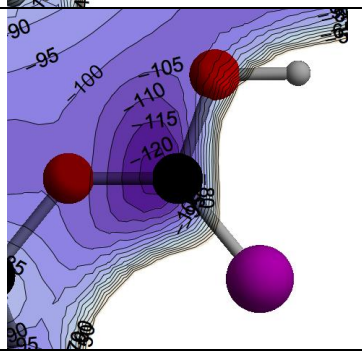
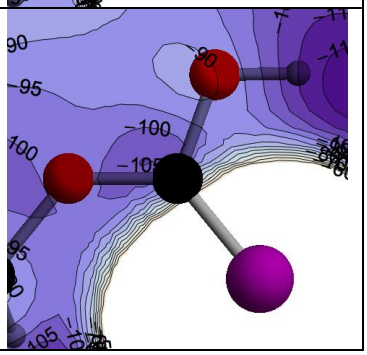
	12	**12**	**13**	**13**
	R= c-heptyl	R= c-heptyl	R=–$CH_2C(CH_3)_3$	R=–$CH_2C(CH_3)_3$
	plane1	plane2	plane1	plane2
ΔE_{Pauli}				
ΔE_{elst}				
ΔE_{oi}				
ΔE_{noi}				
ΔE_{int}				

	14'	**14'**	**14**	**14**
	R=–$(CH_2)CH(CH_3)_2$(2)	R=–$(CH_2)CH(CH_3)_2$(2)	R=–$(CH_2)CH(CH_3)_2$	R=–$(CH_2)CH(CH_3)_2$
	plane1	plane2	plane1	plane2
ΔE_{Pauli}				
ΔE_{elst}				
ΔE_{oi}				
ΔE_{noi}				
ΔE_{int}				

	15	**15**	**16**	**16**
	R=–CH_2(Ph)	R=–CH_2(Ph)	R=–$C(CH_2CH_3)_3$	R=–$C(CH_2CH_3)_3$
	plane1	plane2	plane1	plane2
ΔE_{Pauli}				
ΔE_{elst}				
ΔE_{oi}				
ΔE_{noi}				
ΔE_{int}				

	17	**17**	**18**	**18**
	R=–CH(CH$_3$)(CH$_2$CH$_3$)	R=–CH(CH$_3$)(CH$_2$CH$_3$)	R=–CH(CH$_3$)(Ph)	R=–CH(CH$_3$)(Ph)
	plane1	plane2	plane1	plane2
ΔE_{Pauli}				
ΔE_{elst}				
ΔE_{oi}				
ΔE_{noi}				
ΔE_{int}				

	19	**19**	**20**	**20**
	R=–CH(CH_2CH_3)$_2$	R=–CH(CH_2CH_3)$_2$	R=–(1-CH_3–c-hexyl)	R=–(1-CH_3–c-hexyl)
	plane1	plane2	plane1	plane2
ΔE_{Pauli}				
ΔE_{elst}				
ΔE_{oi}				
ΔE_{noi}				
ΔE_{int}				

	21	**21**	**21'**	**21'**
	R=–C(CH$_3$)$_2$(c-hexyl)	R=–C(CH$_3$)$_2$(c-hexyl)	R=–C(CH$_3$)$_2$(c-hexyl)(2)	R=–C(CH$_3$)$_2$(c-hexyl)(2)
	plane1	plane2	plane1	plane2
ΔE_{Pauli}				
ΔE_{elst}				
ΔE_{noi}				
ΔE_{oi}				
ΔE_{int}				

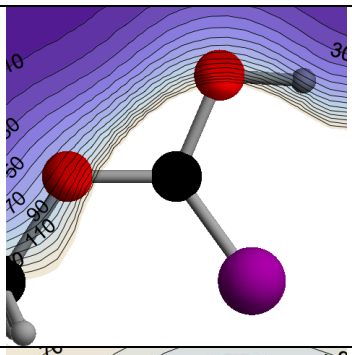
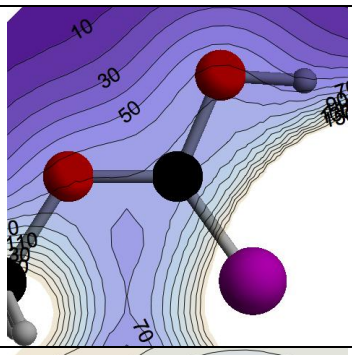
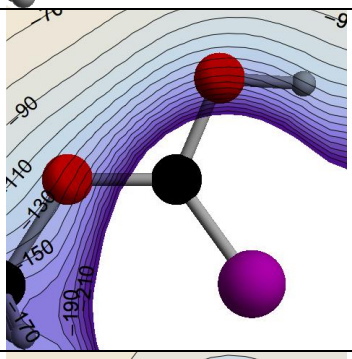
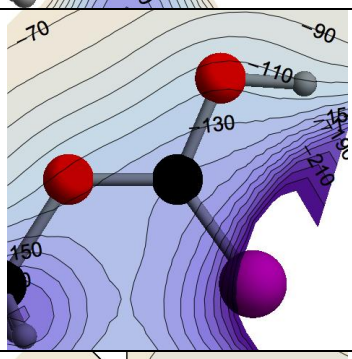
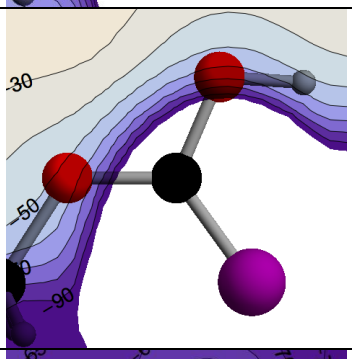
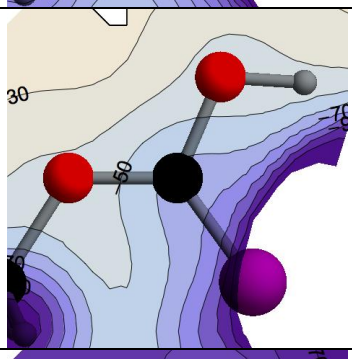
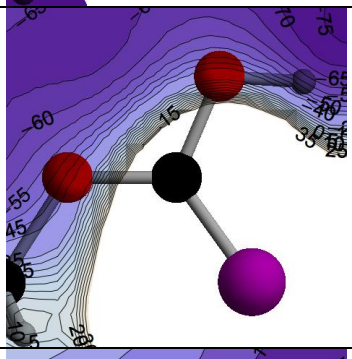
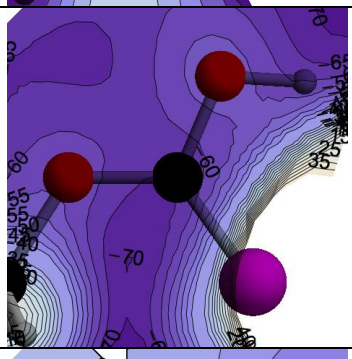
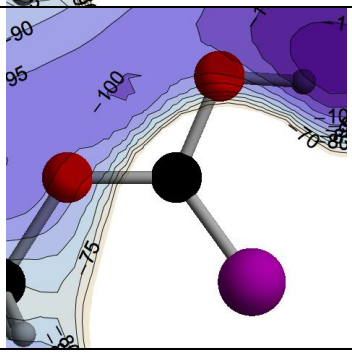
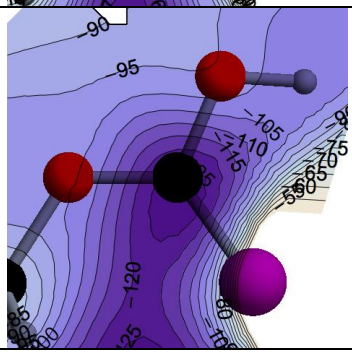
	22	**22**
	R=–CH(Ph)$_2$	R=–CH(Ph)$_2$
	plane1	plane2
ΔE_{Pauli}		
ΔE_{elst}		
ΔE_{oi}		
ΔE_{noi}		
ΔE_{int}		

Table S2. Cartesian coordinates of the optimized structures **1-22**. (Values are in Å.)

1 R=CH_3

C	-0.031944	0.047497	-0.054807
O	0.163001	-0.418682	1.326424
C	1.266797	-0.318318	1.941509
H	0.142464	1.118749	-0.097212
H	0.633333	-0.502889	-0.713807
O	1.211911	-0.790650	3.140145
H	2.048716	-0.721974	3.625887
H	-1.067714	-0.185415	-0.266828
C	2.495974	0.273707	1.363281
H	2.298626	1.305610	1.064874
H	3.322931	0.256030	2.067777
H	2.777609	-0.276729	0.462990

2 R=CH_2CH_3

C	-0.009296	0.006690	-0.073907
O	0.172339	-0.475178	1.300907
C	1.244867	-0.303097	1.958805
H	0.081641	1.088968	-0.089698
H	0.719127	-0.472965	-0.721350
O	1.188452	-0.805389	3.143340
H	2.011003	-0.671611	3.643616
H	-1.015444	-0.300504	-0.329700
C	2.451916	0.399749	1.440343
H	2.741538	-0.110946	0.516054
H	2.125549	1.396459	1.125532
C	3.623025	0.483280	2.416449
H	3.997855	-0.504293	2.690532
H	4.447374	1.012263	1.943620
H	3.365358	1.042632	3.317457

3 R=n-propyl

C	0.000000	0.000000	0.000000
O	0.000000	0.000000	1.467757
C	1.063722	0.000000	2.163048
H	0.410992	0.940804	-0.354942
H	0.563681	-0.854090	-0.363412
O	0.825571	-0.023451	3.428704
H	1.641342	-0.013551	3.956765
H	-1.046792	-0.086384	-0.262813
C	2.443897	-0.012353	1.601467
H	2.564455	-1.007491	1.153779
H	2.470420	0.687808	0.763150
C	3.575442	0.281243	2.595175
H	3.515200	-0.400847	3.451626
H	4.506587	0.007624	2.099942
C	3.646354	1.741668	3.046836
H	2.739170	2.078605	3.553352
H	4.474695	1.882784	3.738453
H	3.810859	2.402406	2.195485

4 R=n-butyl

C	-0.059059	-0.436429	0.233662
O	-0.023558	0.209627	1.550418
C	1.057251	0.530813	2.137581
H	0.453934	0.188759	-0.491258
H	0.388100	-1.423502	0.308729
O	0.850387	1.106475	3.270981
H	1.681022	1.334983	3.720968
H	-1.114739	-0.508389	0.004209
C	2.421353	0.312603	1.580474
H	2.487866	0.977180	0.709480
C	3.588696	0.555110	2.544894
H	4.494598	0.603722	1.939973

H	3.511630	1.553341	2.994723
H	2.455811	-0.701033	1.172652
C	3.757941	-0.525274	3.620992
H	2.847543	-0.622861	4.222701
H	3.890760	-1.490794	3.126464
C	4.945834	-0.249530	4.540610
H	4.829148	0.695662	5.073258
H	5.049507	-1.037829	5.284130
H	5.876850	-0.200878	3.975022
5 R=n-pentyl			
C	0.000000	0.000000	0.000000
O	0.000000	0.000000	1.466516
C	1.066289	0.000000	2.159569
H	0.532506	0.874554	-0.362337
H	0.445248	-0.923951	-0.357873
O	0.832496	0.022874	3.425419
H	1.652661	0.001839	3.947623
H	-1.048961	0.049508	-0.263625
C	2.444194	0.010477	1.593351
H	2.538611	0.972814	1.074522
C	3.580537	-0.184077	2.603795
H	4.505157	0.106376	2.103915
H	3.478596	0.535395	3.424057
H	2.483358	-0.746380	0.805063
C	3.720262	-1.622097	3.123241
H	2.774312	-1.978688	3.549316
H	3.925176	-2.273664	2.270114
C	4.826602	-1.792131	4.171437
H	4.967277	-2.860511	4.340612
H	5.770213	-1.424868	3.759864
C	4.539055	-1.107747	5.507751
H	5.332290	-1.314222	6.224850
H	4.474753	-0.021623	5.417739
H	3.606874	-1.472018	5.946902
6 R=i-propyl			
C	-0.170252	0.335440	0.039798
O	0.106213	-0.389532	1.286054
C	1.241400	-0.416265	1.856884
H	-0.043954	1.399930	0.214028
H	0.478842	-0.029444	-0.749188
O	1.215538	-1.089915	2.957601
H	2.072871	-1.083870	3.414202
H	-1.205857	0.101378	-0.173064
C	2.499384	0.197556	1.331089
H	2.209482	1.071614	0.747818
C	3.448887	0.633887	2.454324
H	3.856932	-0.217979	3.005761
H	4.302989	1.143781	2.012914
H	2.975894	1.322219	3.153837
C	3.169216	-0.828999	0.376670
H	2.515140	-1.137078	-0.436824
H	4.051151	-0.361585	-0.056514
H	3.485086	-1.718575	0.920423
7 R=i-butyl			
C	-0.028714	-0.094731	0.053749
O	0.003646	-0.018437	1.518634
C	1.081708	0.054422	2.188622
H	0.486348	0.763962	-0.366599
H	0.417006	-1.032938	-0.263919
O	0.867525	0.137966	3.456332
H	1.696716	0.180643	3.962273
H	-1.083991	-0.069097	-0.187294
C	2.448744	0.087170	1.600317

H	2.540298	1.082692	1.144978
C	3.618972	-0.173076	2.568910
H	2.478455	-0.617714	0.766210
C	3.647736	-1.629994	3.046414
H	3.823444	-2.303512	2.206026
H	4.456749	-1.776983	3.759880
H	2.723046	-1.946237	3.534268
C	4.934423	0.215562	1.885941
H	5.771359	0.053799	2.562815
H	5.104562	-0.394389	0.997130
H	4.942336	1.264295	1.588181
H	3.510124	0.494047	3.436108
8 R=t-butyl			
C	0.000000	0.000000	0.000000
O	0.000000	0.000000	1.464600
C	0.979739	0.000000	2.274654
H	0.144725	1.021590	-0.335128
H	0.758102	-0.667643	-0.388296
O	0.554826	0.027678	3.495735
H	1.285838	0.039001	4.134976
H	-0.992972	-0.349906	-0.255789
C	2.465620	-0.058881	1.964131
C	3.272111	0.177420	3.256412
H	3.101483	-0.597381	4.009473
H	4.332561	0.130258	3.018541
H	3.087185	1.162940	3.687813
C	2.777745	-1.484984	1.435127
H	2.272218	-1.715376	0.500890
H	3.849657	-1.544328	1.252258
H	2.517288	-2.249850	2.166078
C	2.855304	1.023287	0.931612
H	2.456163	0.832784	-0.059420
H	2.546771	2.018357	1.252088
H	3.940485	1.026077	0.845334
9 R=c-butyl			
C	0.254692	-0.507302	0.026665
O	0.035437	-0.026564	1.394351
C	0.979257	0.389130	2.141276
H	0.638042	0.307454	-0.581176
H	0.931970	-1.354877	0.045469
O	0.554299	0.778032	3.296607
H	1.277172	1.110495	3.854184
H	-0.730316	-0.805852	-0.309472
C	2.409762	0.397893	1.775667
C	3.474557	0.976594	2.741537
C	3.171905	-0.988898	1.837655
H	2.506877	0.820400	0.775297
C	4.398401	-0.210654	2.369225
H	3.184143	0.916413	3.794110
H	3.818698	1.985562	2.532795
H	2.742271	-1.650559	2.587852
H	3.270393	-1.522264	0.897004
H	4.955003	-0.672679	3.178412
H	5.086375	0.052185	1.568897
10 R=c-pentyl			
C	0.239440	-0.405451	-0.074773
O	0.034580	-0.095170	1.342692
C	0.976226	0.241147	2.132130
H	0.557788	0.494098	-0.593900
H	0.960391	-1.210498	-0.172565
O	0.543380	0.462805	3.328852
H	1.254954	0.757797	3.920911
H	-0.738160	-0.719423	-0.418880

C	2.410296	0.324489	1.769624
C	3.283670	1.259339	2.631808
C	3.092459	-1.107140	1.878900
H	2.465475	0.649578	0.731803
C	4.685725	0.665269	2.461995
H	3.018911	1.204057	3.695268
H	3.197289	2.301062	2.328601
C	4.447227	-0.843355	2.577734
H	3.222399	-1.515126	0.879283
H	2.479016	-1.812061	2.438841
H	5.078291	0.922414	1.476343
H	5.387279	1.045081	3.201409
H	5.243326	-1.433655	2.129161
H	4.384608	-1.131321	3.627449

11 R=c-hexyl$_{eq}$

C	0.000000	0.000000	0.000000
O	0.000000	0.000000	1.465764
C	1.058779	0.000000	2.173338
H	0.422100	0.935797	-0.354599
H	0.548821	-0.859983	-0.369335
O	0.792573	0.034315	3.437197
H	1.599901	0.072284	3.976483
H	-1.048464	-0.070553	-0.261645
C	2.450538	-0.084925	1.660339
C	3.470667	0.661933	2.544240
C	2.835506	-1.596484	1.527599
H	2.461550	0.352644	0.661089
C	4.883673	0.514163	1.967674
H	3.474338	0.237754	3.557066
H	3.199838	1.715229	2.630426
C	4.254664	-1.723521	0.964112
H	2.781083	-2.060184	2.515716
H	2.122230	-2.120202	0.890484
C	5.278399	-0.954272	1.800951
H	5.587554	1.028228	2.621527
H	4.928258	1.025448	1.001944
H	4.513777	-2.781705	0.920676
H	4.266379	-1.357310	-0.066272
H	6.261198	-1.022638	1.335414
H	5.370366	-1.421932	2.785706

11' R=c-hexylax

C	-0.000118	-0.187875	0.011553
O	0.037518	-0.074744	1.471707
C	1.109347	0.066464	2.147745
H	0.338870	0.746376	-0.426783
H	0.603756	-1.029955	-0.310339
O	0.868943	0.184475	3.409512
H	1.689807	0.296464	3.924330
H	-1.046323	-0.357080	-0.211282
C	3.004777	-1.413833	1.489190
C	3.483546	0.956063	2.368721
C	3.471267	-1.977140	2.832373
H	3.843574	-1.383315	0.791766
H	2.248549	-2.057969	1.039211
C	4.013516	0.348136	3.676266
H	4.331868	1.108915	1.700007
H	3.053780	1.945063	2.537602
C	4.524292	-1.081119	3.487387
H	3.877468	-2.974675	2.664171
H	2.620398	-2.116136	3.507870
H	4.804928	0.994174	4.056448
H	3.263535	0.361071	4.484825
H	4.830281	-1.497793	4.446433

H	5.419458	-1.057786	2.859801
C	2.488366	0.064961	1.585422
H	2.402669	0.450288	0.569763

12 R=c-heptyl

C	0.102902	0.105268	-0.348403
O	-0.090132	0.145954	1.102525
C	0.861828	0.156377	1.951168
H	0.624519	1.003691	-0.665591
H	0.640633	-0.795759	-0.623565
O	0.424687	0.252165	3.159341
H	1.154558	0.268124	3.807652
H	-0.904181	0.088134	-0.746320
C	2.313015	0.049154	1.627787
C	3.240879	0.834158	2.587138
C	2.727411	-1.450520	1.451276
H	2.431777	0.509024	0.645377
C	3.435803	0.352012	4.033802
H	4.216362	0.817149	2.098891
H	2.934547	1.882744	2.597208
C	2.339783	-2.456793	2.541023
H	3.810838	-1.419428	1.333753
H	2.337937	-1.815422	0.500348
C	3.829807	-1.115612	4.242362
H	2.560621	0.572990	4.668330
H	4.207118	0.995697	4.460304
C	2.693059	-2.117816	4.008062
H	2.837045	-3.387225	2.263453
H	1.271407	-2.678091	2.475548
H	4.699053	-1.359031	3.625708
H	4.163869	-1.219717	5.275151
H	2.940196	-3.051716	4.512104
H	1.802449	-1.754668	4.531724

13 R=$CH_2C(CH_3)_3$

C	0.000000	0.000000	0.000000
O	0.000000	0.000000	1.464587
C	1.064469	0.000000	2.165171
H	0.491837	0.898403	-0.361836
H	0.487399	-0.900794	-0.361890
O	0.812369	0.001820	3.426642
H	1.625771	0.004001	3.959567
H	-1.050021	0.002531	-0.264172
C	2.434886	-0.000758	1.581992
C	3.682115	-0.012035	2.507509
C	4.895650	-0.007218	1.558992
H	5.819803	-0.016247	2.134982
H	4.900365	-0.885079	0.911299
H	4.906914	0.882758	0.928107
H	2.474972	0.871813	0.919533
H	2.469968	-0.863387	0.906691
C	3.747560	1.249944	3.387098
H	3.688480	2.159461	2.787964
H	2.966486	1.314084	4.150822
H	4.694005	1.270600	3.925308
C	3.738460	-1.289914	3.364103
H	3.682464	-2.187590	2.747124
H	4.680624	-1.323054	3.909214
H	2.949953	-1.365882	4.118700

14 R=$(CH_2)_2CH(CH_3)_2$

C	-0.034397	-0.431853	0.067112
O	-0.014043	-0.121351	1.500130
C	1.052388	0.173895	2.126912
H	0.321237	0.428205	-0.492991
H	0.570503	-1.314893	-0.117913

O	0.842610	0.414487	3.374792
H	1.665136	0.633821	3.845632
H	-1.077772	-0.627092	-0.146093
C	2.405453	0.245166	1.513774
H	2.345488	0.990454	0.713363
H	2.577106	-0.708758	1.003369
C	3.544771	0.560065	2.487881
H	3.561126	-0.196439	3.279236
C	4.935338	0.585852	1.821039
H	5.071218	-0.376131	1.315297
C	5.060212	1.702743	0.781407
H	4.906501	2.682991	1.238089
H	6.057302	1.699282	0.342998
H	4.354643	1.598026	-0.044903
C	6.017666	0.709986	2.896403
H	5.962886	-0.104140	3.620298
H	7.008723	0.685512	2.445535
H	5.926232	1.653165	3.439264
H	3.373095	1.535685	2.957460

14′ R=$(CH_2)_2CH(CH_3)_2$(2)

C	-0.822676	-1.274209	1.177498
O	-0.396278	0.045835	1.653949
C	0.800868	0.467817	1.568995
H	-0.724609	-1.311439	0.096481
H	-0.237132	-2.046063	1.667555
O	0.945535	1.638526	2.086668
H	1.852107	1.972616	1.978831
H	-1.863412	-1.335068	1.470242
C	1.944357	-0.309770	1.017147
H	1.574608	-0.985441	0.246578
H	2.254832	-0.951707	1.853437
C	3.150624	0.493771	0.499950
H	4.011090	-0.173597	0.544936
C	3.010522	1.030210	-0.935553
H	2.854941	0.159493	-1.581992
C	1.819545	1.972869	-1.122362
H	1.912775	2.870449	-0.505121
H	1.759364	2.305393	-2.157707
H	0.857767	1.502392	-0.897909
C	4.318360	1.701706	-1.363661
H	5.166931	1.024431	-1.264630
H	4.265329	2.017725	-2.404565
H	4.523162	2.588297	-0.759680
H	3.409770	1.311018	1.187574

15 R=CH_2(Ph)

C	-0.003748	-0.492475	0.089128
O	-0.017334	-0.159111	1.517264
C	1.027581	0.198010	2.148320
H	0.288494	0.384167	-0.481857
H	0.667097	-1.329624	-0.080945
O	0.820504	0.449235	3.388328
H	1.661628	0.715871	3.819549
H	-1.027809	-0.769124	-0.127699
C	2.394150	0.324564	1.546179
H	2.654115	-0.658166	1.138780
H	2.307427	0.987517	0.680531
C	3.431408	0.818031	2.528137
C	4.092788	-0.084321	3.367059
C	3.726254	2.181273	2.614002
C	5.035098	0.374318	4.280251
H	3.889981	-1.146030	3.295727
C	4.670508	2.634193	3.526832
H	3.231636	2.888395	1.959854

C	5.323518	1.732009	4.359773
H	5.549130	-0.329313	4.919515
H	4.900000	3.688837	3.582142
H	6.061346	2.086242	5.065743

16 R=C(CH_2CH_3)$_3$

C	-0.142530	-1.773008	1.515267
O	-0.065128	-0.365687	1.906501
C	0.908411	0.455160	1.866094
H	-0.250367	-1.829689	0.437921
H	0.726066	-2.314798	1.868466
O	0.551910	1.578566	2.402527
H	1.263459	2.237375	2.359632
H	-1.041183	-2.122811	2.009493
C	2.331076	0.241362	1.375278
C	2.979588	-0.566371	2.576752
C	4.504917	-0.522579	2.699671
H	4.796544	-1.151297	3.540493
H	5.011128	-0.901539	1.816166
H	4.875504	0.479580	2.905372
H	2.564247	-0.192621	3.516834
H	2.660467	-1.605344	2.494345
C	3.027304	1.617537	1.205692
H	3.072534	2.134897	2.173367
H	4.070963	1.409886	0.986482
C	2.478502	2.548703	0.116761
H	3.041837	3.480502	0.117677
H	2.581268	2.109433	-0.873321
H	1.426132	2.809617	0.243470
C	2.318952	-0.551681	0.030752
H	1.979640	-1.566059	0.221116
H	1.580376	-0.097188	-0.633541
C	3.648227	-0.651560	-0.723553
H	4.060474	0.318290	-0.993125
H	4.401804	-1.199360	-0.163330
H	3.478351	-1.196707	-1.651312

17 R=CH(CH_3)(CH_2CH_3)

C	0.021637	-0.977858	0.206289
O	-0.021438	-0.190357	1.443603
C	0.995310	0.371893	1.960959
H	0.409457	-0.368907	-0.603642
H	0.623107	-1.866531	0.373031
O	0.703006	0.982752	3.060326
H	1.484402	1.383241	3.476034
H	-1.013376	-1.242471	0.029203
C	2.371953	0.396474	1.382956
H	2.483355	-0.501986	0.775026
C	3.455846	0.388292	2.484407
H	3.232636	-0.403455	3.203081
H	3.437095	1.339348	3.030396
C	2.460464	1.635206	0.449294
H	1.673122	1.646662	-0.302712
H	2.400468	2.559998	1.022336
H	3.415216	1.612552	-0.069304
C	4.865392	0.173201	1.932783
H	5.577112	0.116959	2.754323
H	4.930792	-0.761330	1.374543
H	5.181890	0.985980	1.281741

18 R=CH(CH_3)(Ph)

C	-0.084791	-0.394449	0.177605
O	0.047635	0.041679	1.569552
C	1.159970	0.262880	2.149607
H	0.211420	0.412550	-0.484203
H	0.507549	-1.290152	0.016298

O	1.021495	0.585971	3.384944
H	1.902484	0.677897	3.812744
H	-1.140667	-0.609724	0.070133
C	2.520150	0.206877	1.505358
H	2.497271	-0.614740	0.788503
C	3.586853	-0.090402	2.549013
C	4.090212	0.910050	3.388990
C	4.042059	-1.400625	2.705678
C	5.027066	0.596513	4.370812
H	3.795230	1.944239	3.262731
C	4.984505	-1.706743	3.678566
H	3.668911	-2.185154	2.059456
C	5.473923	-0.710120	4.516235
H	5.415070	1.378531	5.008133
H	5.336429	-2.723489	3.782027
H	6.206462	-0.950689	5.273573
C	2.747575	1.523368	0.712559
H	2.016352	1.653462	-0.082118
H	2.703696	2.397408	1.358146
H	3.736090	1.476324	0.261682

19 R=CH(CH_2CH_3)$_2$

C	-2.178108	-1.129459	-1.088795
O	-2.026708	-0.266817	0.087157
C	-0.914888	0.221278	0.468815
H	-1.911865	-0.569866	-1.980317
H	-1.569270	-2.020031	-0.969646
O	-1.048738	0.952780	1.525403
H	-0.207459	1.352822	1.800344
H	-3.231368	-1.381122	-1.093923
C	0.417859	-0.049563	-0.142161
C	1.011413	-1.287690	0.616442
H	0.250868	-0.338394	-1.180073
C	2.196824	-1.912948	-0.115901
H	2.546804	-2.782209	0.439016
H	1.916947	-2.247190	-1.115403
H	3.035215	-1.225185	-0.207373
H	1.306488	-0.969690	1.618553
H	0.234554	-2.043450	0.750691
C	1.337680	1.185596	-0.112349
H	1.527789	1.490978	0.924382
H	2.310230	0.865777	-0.482503
C	0.836759	2.365389	-0.945004
H	1.543206	3.191888	-0.893581
H	0.734618	2.087905	-1.994576
H	-0.128427	2.744448	-0.602345

20 R=(1-CH_3-c-hexyl)

C	-0.208686	-0.458053	0.145517
O	0.033466	-0.068211	1.538610
C	1.145438	0.167145	2.129779
H	-0.204622	0.450172	-0.462522
H	0.530441	-1.184341	-0.192948
O	0.921064	0.547431	3.349575
H	1.754946	0.668831	3.842514
H	-1.207004	-0.898397	0.174728
C	2.892972	-1.458549	1.341207
C	3.597460	0.640703	2.577915
C	3.070110	-2.259005	2.638426
H	3.834566	-1.460937	0.773102
H	2.146256	-1.934403	0.694637
C	3.871056	-0.184524	3.853297
H	4.539499	0.693405	2.017223
H	3.345835	1.686529	2.814848
C	4.164225	-1.654247	3.526244

H	3.322798	-3.294933	2.378421
H	2.117929	-2.309923	3.193200
H	4.720667	0.274015	4.375402
H	3.045446	-0.147232	4.590462
H	4.267733	-2.231912	4.453358
H	5.131156	-1.719191	3.003632
C	2.556734	0.051518	1.576287
C	2.647028	0.855962	0.252540
H	2.111465	0.384501	-0.575131
H	2.283951	1.884956	0.373158
H	3.702205	0.908719	-0.038029

21 R=C(CH$_3$)$_2$(c-hexyl)

C	-0.217196	-0.246583	0.386472
O	0.030873	-0.213669	1.832330
C	1.143825	-0.059176	2.446415
H	-0.172806	0.776208	0.005738
H	0.496956	-0.904653	-0.109643
O	0.938930	-0.048660	3.729711
H	1.773341	0.067154	4.218187
H	-1.230740	-0.644229	0.313628
C	2.543673	0.071296	1.871072
C	3.492188	0.566230	2.988465
H	3.594262	-0.142016	3.824435
H	4.497919	0.693752	2.578681
H	3.182149	1.547450	3.373797
C	2.546296	1.128980	0.733409
H	2.159914	0.738367	-0.211987
H	1.977216	2.026084	1.010365
H	3.577631	1.447967	0.555184
C	2.954955	-1.366042	1.335462
C	4.375425	-1.374136	0.734034
C	2.809041	-2.493754	2.377309
H	2.266686	-1.596614	0.508471
C	4.695130	-2.744251	0.111555
H	5.113970	-1.165001	1.521643
H	4.483233	-0.592308	-0.028533
C	3.141172	-3.864648	1.762954
H	3.490038	-2.310264	3.222592
H	1.788666	-2.528131	2.790204
C	4.537570	-3.878833	1.130119
H	5.717895	-2.724639	-0.287646
H	4.027313	-2.920045	-0.747006
H	3.060477	-4.637141	2.539068
H	2.386504	-4.109103	0.998003
H	4.721861	-4.848300	0.648676
H	5.298781	-3.770642	1.919508

21′ R=C(CH$_3$)$_2$(c-hexyl)(2)

C	0.040693	0.611797	0.056347
O	0.043550	0.383083	1.505782
C	1.015430	0.031193	2.262283
H	0.555781	1.549457	-0.159849
H	0.493323	-0.238970	-0.457128
O	0.578922	-0.175839	3.467040
H	1.317851	-0.401655	4.063719
H	-1.021693	0.687391	-0.181222
C	2.474366	-0.229562	1.903267
C	2.986626	0.720126	0.796003
H	2.728156	1.767837	0.984638
H	4.077925	0.651407	0.762296
H	2.626256	0.435738	-0.195711
C	2.467800	-1.703139	1.386867
H	2.269600	-2.416144	2.196661
H	1.722254	-1.860748	0.597986

H	3.449736	-1.925539	0.957111
C	3.354145	-0.096277	3.203295
C	4.794334	-0.632290	3.044099
C	3.393804	1.341659	3.765699
H	2.919299	-0.767456	3.974855
C	5.552906	-0.571022	4.381829
H	5.333555	-0.028854	2.299581
H	4.788947	-1.666863	2.680821
C	4.140456	1.400435	5.107347
H	3.912010	1.988269	3.043135
H	2.382123	1.760836	3.884960
C	5.562837	0.842528	4.975618
H	6.578808	-0.929506	4.225877
H	5.084800	-1.268940	5.094962
H	4.164649	2.438204	5.465013
H	3.583987	0.822224	5.863665
H	6.057988	0.836082	5.955548
H	6.155783	1.508457	4.328354

22 R=CH(Ph)$_2$

C	-0.140197	-0.479949	0.244567
O	-0.051654	-0.060435	1.650433
C	1.060909	0.223207	2.213197
H	0.294668	0.295276	-0.391928
H	0.369665	-1.441611	0.129584
O	0.927741	0.563472	3.451027
H	1.819400	0.719138	3.842722
H	-1.211552	-0.587494	0.071077
C	2.419529	0.193274	1.550540
H	2.442449	-0.738960	0.967859
C	3.523142	0.116926	2.608103
C	4.028045	-1.138232	2.984853
C	4.011757	1.273747	3.240431
C	5.006568	-1.236669	3.976288
H	3.665875	-2.044134	2.496050
C	4.984361	1.169151	4.242332
H	3.669916	2.260254	2.927629
C	5.481844	-0.083511	4.610481
H	5.399550	-2.214619	4.252793
H	5.362983	2.071271	4.721847
H	6.245366	-0.161818	5.383902
C	2.535197	1.356890	0.554433
C	3.282619	1.160368	-0.616409
C	1.951955	2.608878	0.799908
C	3.454199	2.207930	-1.523291
H	3.743580	0.192326	-0.816456
C	2.120118	3.654297	-0.114480
H	1.364229	2.792745	1.701074
C	2.872616	3.456273	-1.274721
H	4.042530	2.048426	-2.426465
H	1.662926	4.623150	0.083778
H	3.004534	4.271537	-1.985396