

Supporting Information

A computational investigation of the solvent-dependent enantioselective intramolecular Morita-Baylis-Hillman Reaction of enones

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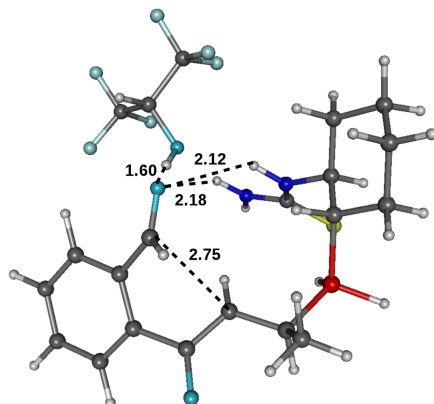
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Contents: Cartesian coordinates, energy and structure of optimized intermediates and transition states

SE 1

E(B3LYP) = -2490.308575 a.u.



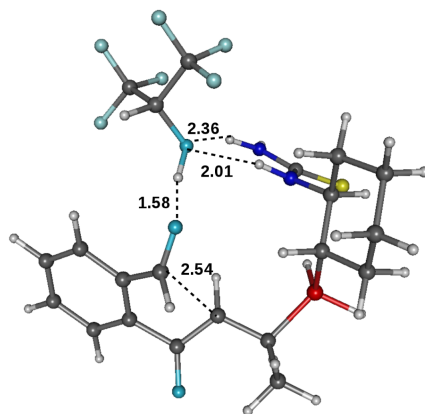
C	-3.907262	0.618297	-0.163645
C	-2.676075	1.493416	-0.103698
O	-4.015177	3.444037	0.057888
C	-2.887034	2.887735	-0.014670
C	-0.592774	2.100888	1.588789
C	-0.478874	3.226242	0.649058
C	-1.630097	3.707073	-0.014172
C	0.749125	3.903705	0.509247
C	-1.557445	4.911980	-0.725175
C	0.813857	5.079300	-0.231597
C	-0.345428	5.590556	-0.837056
H	1.629078	3.529659	1.025315
H	-2.458762	5.285368	-1.202727
H	1.757106	5.611546	-0.323265
H	-0.293316	6.516180	-1.405330
H	-1.734472	1.119375	-0.493890
O	0.309895	1.265896	1.812875
H	-1.485981	2.083084	2.224491
P	-3.393027	-1.043941	-0.718431
H	-2.715760	-1.000516	-1.950646
N	-0.294495	-1.746597	-0.827560
C	-0.093803	-1.705226	-2.178701
H	0.409496	-1.280157	-0.255771
N	0.934293	-0.923417	-2.570401
S	-1.072809	-2.513788	-3.306831
H	1.522744	-0.430223	-1.904225
H	1.100299	-0.811063	-3.559320
H	-4.524641	-1.838428	-0.977159
C	-2.377948	-1.978051	0.519125
C	-1.161177	-2.693810	-0.133380
C	-3.261443	-2.965764	1.318433
C	-0.361142	-3.453748	0.941818
H	-1.519912	-3.403102	-0.886302
C	-2.434406	-3.714013	2.374975
H	-4.091598	-2.431339	1.795753
H	-3.707437	-3.694422	0.625685
C	-1.238461	-4.431488	1.736525

H	0.095806	-2.729134	1.631201
H	0.461027	-3.984167	0.447551
H	-3.079468	-4.430829	2.897648
H	-2.077366	-3.000250	3.131327
H	-0.633623	-4.922801	2.507996
H	-1.600961	-5.226988	1.068979
H	-1.994932	-1.201456	1.196806
O	1.944062	0.117079	0.159185
C	3.230309	0.096905	0.707517
C	3.596301	-1.348756	1.102007
C	4.206717	0.733006	-0.303504
H	1.338294	0.674251	0.746674
F	4.816395	-1.426291	1.670148
F	3.570151	-2.192379	0.050203
F	2.698139	-1.801365	2.007632
F	3.875335	2.029590	-0.485724
F	5.484765	0.694271	0.124063
F	4.152849	0.126417	-1.508928
H	3.293757	0.693053	1.626209
C	-4.722949	0.546947	1.149092
H	-4.123419	0.151940	1.976686
H	-5.011000	1.572719	1.394009
H	-5.635877	-0.054514	1.043201
H	-4.593705	0.981535	-0.951566

SE 2

E(B3LYP) = -2490.308220 a.u.

Frequency = -36.52 cm⁻¹



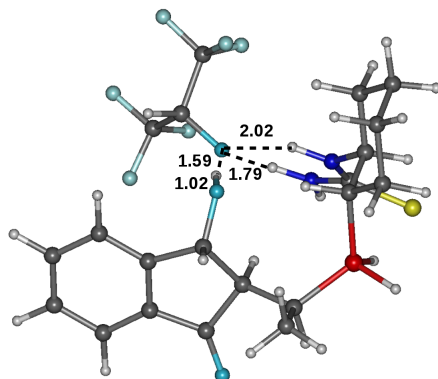
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C	-2.445171	3.356267	-0.331987
C	-0.651457	2.130472	1.472047
C	-0.161181	3.243233	0.628336
C	-1.081202	3.948833	-0.173433
C	1.175210	3.673847	0.705277
C	-0.683903	5.126091	-0.817764
C	1.569878	4.827789	0.031894
C	0.637377	5.560078	-0.719522

H	1.882243	3.132530	1.328085
H	-1.414761	5.671084	-1.408612
H	2.598829	5.170858	0.104106
H	0.951638	6.464074	-1.235469
H	-1.571366	1.425377	-0.738402
O	0.012243	1.093658	1.728271
H	-1.529803	2.345612	2.090884
P	-3.494697	-0.539860	-0.700176
H	-2.778604	-0.737284	-1.892514
N	-0.614439	-1.870155	-0.650526
C	-0.435718	-2.073090	-1.986497
H	0.163667	-1.440083	-0.149330
N	0.717918	-1.572507	-2.482063
S	-1.570420	-2.840419	-2.990811
H	1.390670	-1.084690	-1.898844
H	0.882628	-1.640487	-3.475164
H	-4.721517	-1.186008	-0.934790
C	-2.671280	-1.445657	0.687936
C	-1.644624	-2.494442	0.170168
C	-3.722635	-2.092014	1.623069
C	-0.997405	-3.225194	1.362637
H	-2.158327	-3.222157	-0.466368
C	-3.045818	-2.819803	2.795056
H	-4.415787	-1.331265	2.000292
H	-4.322479	-2.813929	1.049730
C	-2.040587	-3.862804	2.290631
H	-0.386421	-2.511850	1.933244
H	-0.314092	-3.985825	0.967298
H	-3.814928	-3.294173	3.416946
H	-2.530808	-2.086481	3.431548
H	-1.534429	-4.343635	3.136218
H	-2.575994	-4.658180	1.751633
H	-2.118157	-0.667743	1.234328
O	1.695869	-0.205023	0.265730
C	2.965029	-0.259922	0.843753
C	3.205634	-1.662440	1.441695
C	4.001193	0.143360	-0.225513
H	1.089410	0.410289	0.802982
F	4.399116	-1.751999	2.063330
F	3.145553	-2.636564	0.510370
F	2.249169	-1.922165	2.362834
F	3.797906	1.428373	-0.582044
F	5.269187	0.038199	0.221357
F	3.892099	-0.610325	-1.343132
H	3.074002	0.450750	1.672744
C	-4.691896	1.462217	0.834694
H	-4.217343	1.108416	1.756473
H	-4.850296	2.540055	0.923048
H	-5.669805	0.976050	0.722551
H	-4.346615	1.582605	-1.284286

SE 3

E(B3LYP) = -2490.353264 a.u.

C	-3.352363	0.672581	-0.317747
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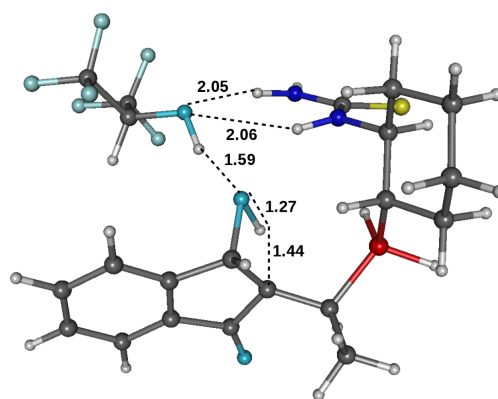
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C	-2.143210	2.839869	-0.891616
C	-1.282302	1.655668	1.081863
C	-0.602689	3.002750	0.870738
C	-1.139208	3.688282	-0.227307
C	0.391002	3.595018	1.648441
C	-0.715420	4.978378	-0.569087
C	0.827318	4.878025	1.304881
C	0.278790	5.567745	0.208492
H	0.817555	3.068224	2.497696
H	-1.145297	5.488372	-1.426647
H	1.606894	5.353541	1.894888
H	0.641234	6.562837	-0.034465
H	-1.269496	0.917597	-0.929734
O	-0.455666	0.608273	1.514394
H	-2.033669	1.783176	1.872424
P	-3.165771	-1.154376	-0.514628
H	-2.695139	-1.505753	-1.811272
N	-0.277824	-2.036359	-0.820275
C	-0.234472	-2.052074	-2.180253
H	0.433307	-1.438067	-0.363655
N	0.699053	-1.240990	-2.708947
S	-1.318553	-2.941791	-3.160700
H	1.266903	-0.648390	-2.094205
H	0.757678	-1.158425	-3.712552
H	-4.476007	-1.665670	-0.477734
C	-2.178454	-2.071574	0.753270
C	-1.083410	-2.904850	0.021830
C	-3.048004	-2.938688	1.688372
C	-0.217100	-3.636040	1.063025
H	-1.559333	-3.642163	-0.633657
C	-2.158269	-3.676574	2.703739
H	-3.786085	-2.318026	2.212945
H	-3.611032	-3.674466	1.095581
C	-1.070239	-4.502733	2.002429
H	0.347951	-2.896738	1.646571
H	0.518472	-4.249383	0.530074
H	-2.785327	-4.321618	3.331687
H	-1.688509	-2.941286	3.372188
H	-0.424305	-4.981998	2.747838
H	-1.540736	-5.314745	1.428316
H	-1.665421	-1.286365	1.328682

O	1.419053	0.052973	-0.208307
C	2.671922	0.378075	0.214375
C	3.481748	-0.883044	0.608291
C	3.399943	1.224940	-0.859078
H	0.301843	0.453735	0.849203
F	4.704909	-0.600193	1.119401
F	3.662690	-1.740824	-0.421748
F	2.806392	-1.562502	1.573624
F	2.727108	2.384672	-1.053051
F	4.668853	1.560342	-0.518998
F	3.460857	0.598910	-2.061140
H	2.689263	1.009643	1.125271
C	-4.318518	1.011895	0.833165
H	-3.969886	0.637441	1.801246
H	-4.422121	2.099601	0.911440
H	-5.317104	0.602092	0.645817
H	-3.830760	0.972596	-1.263623

SE 4

E(B3LYP) = -2490.279726 a.u.

Frequency = -1745.55 cm⁻¹



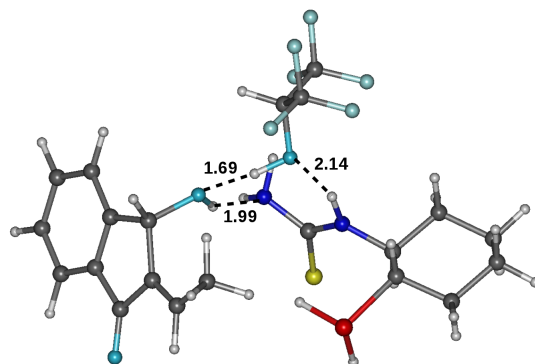
C	1.402706	3.147311	0.265756
C	0.033967	2.516169	0.122085
O	-1.100754	4.297489	1.313113
C	-1.100816	3.368893	0.501620
C	-0.388755	1.597951	-1.026104
C	-1.871217	1.892521	-1.186529
C	-2.278749	2.889738	-0.290144
C	-2.796923	1.290192	-2.036503
C	-3.605466	3.313578	-0.227159
C	-4.133170	1.712420	-1.979860
C	-4.534729	2.714605	-1.084233
H	-2.496092	0.511038	-2.733567
H	-3.896645	4.092526	0.472518
H	-4.867334	1.259559	-2.641850
H	-5.575700	3.026752	-1.060030
H	-0.046673	1.149995	0.583551
O	-0.132384	0.316315	-0.368584
H	0.158681	1.651786	-1.977286
P	2.686590	1.888435	0.698058

H	2.296887	1.163873	1.832898
N	2.204644	-1.201502	0.508611
C	2.129951	-1.501501	1.837861
H	1.327449	-1.082902	0.000202
N	0.934640	-1.973479	2.246913
S	3.412841	-1.266966	2.931213
H	0.139274	-2.107661	1.621524
H	0.814270	-2.161813	3.231249
H	3.861578	2.549497	1.103559
C	3.190171	0.749169	-0.669306
C	3.389458	-0.711506	-0.171527
C	4.444514	1.274284	-1.406297
C	3.755119	-1.612504	-1.367560
H	4.202915	-0.738799	0.560465
C	4.808152	0.351903	-2.581550
H	4.280161	2.296973	-1.767589
H	5.287399	1.315585	-0.701700
C	4.993356	-1.099125	-2.117180
H	2.897121	-1.666193	-2.054017
H	3.922365	-2.627108	-0.989026
H	5.721883	0.722770	-3.061932
H	4.012201	0.399163	-3.338992
H	5.201847	-1.747478	-2.976732
H	5.871252	-1.162236	-1.457740
H	2.333054	0.754180	-1.355680
O	-1.346152	-1.865083	0.233339
C	-2.735392	-1.959513	0.231114
C	-3.180149	-2.945767	-0.870588
C	-3.206447	-2.359093	1.643422
H	-1.037476	-0.960803	-0.106347
F	-4.527188	-3.031411	-0.960874
F	-2.698666	-4.188818	-0.686442
F	-2.726849	-2.504343	-2.068011
F	-2.861068	-1.387797	2.519678
F	-4.546573	-2.508440	1.712068
F	-2.639577	-3.506109	2.070818
H	-3.221457	-1.002217	0.001488
C	1.863717	4.041955	-0.904978
H	1.906100	3.489103	-1.849506
H	1.132291	4.847762	-1.023610
H	2.843664	4.503303	-0.726287
H	1.345893	3.767604	1.174667

SE 5

E(B3LYP) = -2490.360659 a.u.

C	0.678756	3.917959	-1.466394
C	-0.173242	3.794510	-0.435698
O	0.755535	5.517230	1.019317
C	-0.090367	4.668299	0.779258
C	-1.378109	2.873509	-0.306964
C	-2.017542	3.316254	0.999866
C	-1.269420	4.324241	1.620117
C	-3.179640	2.831517	1.599997
C	-1.658167	4.873820	2.844125

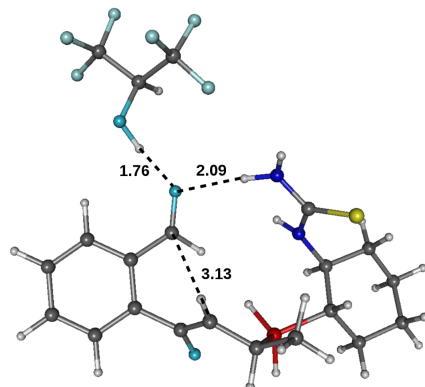


C	-3.574776	3.378105	2.825806
C	-2.821280	4.390659	3.444182
H	-3.766660	2.046001	1.130260
H	-1.059917	5.654875	3.304968
H	-4.479925	3.016649	3.307346
H	-3.151248	4.798085	4.396099
H	-0.577981	1.210441	0.534097
O	-1.063506	1.461926	-0.289182
H	-2.067426	2.979821	-1.151545
P	3.812131	0.934187	-1.233290
H	2.640857	1.256291	-0.495808
N	1.856279	-1.057517	0.537751
C	1.491004	-0.492370	1.704630
H	1.143684	-1.161244	-0.184200
N	0.113315	-0.185936	1.765354
S	2.501567	-0.098250	2.981614
H	-0.492638	-0.920419	1.398546
H	-0.150268	0.059731	2.715091
H	4.671731	1.097988	-0.110466
C	3.679722	-0.949391	-1.150953
C	3.197118	-1.538878	0.195735
C	5.046159	-1.554077	-1.548070
C	3.195011	-3.082728	0.171812
H	3.856927	-1.192298	0.996922
C	5.027701	-3.089836	-1.570796
H	5.346781	-1.163961	-2.528560
H	5.809626	-1.216837	-0.830607
C	4.563408	-3.654991	-0.222240
H	2.433804	-3.427037	-0.544593
H	2.891336	-3.446957	1.161023
H	6.027354	-3.467974	-1.821586
H	4.351138	-3.436083	-2.366446
H	4.510618	-4.750533	-0.260269
H	5.301587	-3.403417	0.553674
H	2.950307	-1.224799	-1.929347
O	-0.345497	-0.701256	-1.651962
C	-1.490564	-1.361293	-2.108038
C	-1.404831	-1.533860	-3.639525
C	-1.632284	-2.688902	-1.338269
H	-0.595546	0.198284	-1.313275
F	-2.506833	-2.137683	-4.135286
F	-0.330846	-2.246794	-4.021525
F	-1.317855	-0.312761	-4.213057
F	-1.768756	-2.414643	-0.011530

F	-2.720507	-3.384930	-1.714756
F	-0.555502	-3.483450	-1.472065
H	-2.406314	-0.790754	-1.910486
C	0.656644	3.170247	-2.760674
H	-0.195565	2.491359	-2.852200
H	0.634443	3.875991	-3.602245
H	1.578640	2.584221	-2.876755
H	1.473976	4.654982	-1.342528

RE 1

E(B3LYP) = -2490.306136 a.u.



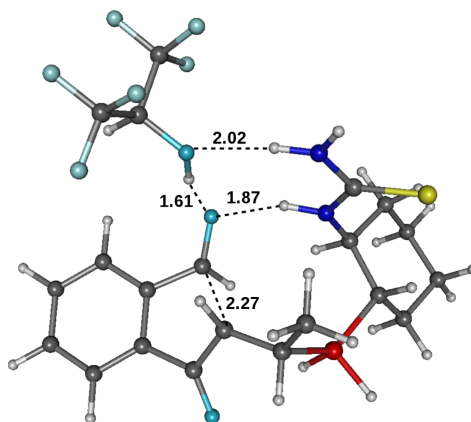
C	-3.115456	1.614524	1.708820
C	-1.702974	2.069235	1.473356
O	-2.599151	3.297319	-0.270726
C	-1.566427	2.975085	0.443391
C	0.568602	1.280010	-0.523088
C	0.855023	2.683965	-0.244575
C	-0.222809	3.539077	0.101823
C	2.147072	3.214351	-0.449786
C	0.001630	4.920466	0.151251
C	2.355400	4.583877	-0.359279
C	1.276838	5.437099	-0.073236
H	2.966794	2.549813	-0.706477
H	-0.828046	5.579222	0.390811
H	3.347555	4.994741	-0.523962
H	1.440276	6.510405	-0.015061
H	-0.900997	1.738727	2.123861
O	1.390365	0.355010	-0.631448
H	-0.490809	1.046022	-0.689181
P	-3.762224	1.133621	0.007360
H	-2.808525	1.133229	-1.007745
N	-2.190710	-1.495387	-0.830479
C	-1.568751	-2.176957	0.189554
H	-1.589432	-1.302282	-1.624212
N	-0.209253	-2.161569	0.107619
S	-2.350650	-2.981906	1.449307
H	0.298752	-1.406955	-0.356801
H	0.277326	-2.585114	0.887092
H	-4.831791	1.934560	-0.423267
C	-4.442296	-0.610320	-0.103164

C	-3.633457	-1.436498	-1.146898
C	-5.947412	-0.573069	-0.462922
C	-4.258069	-2.821346	-1.418638
H	-3.666256	-0.879086	-2.094367
C	-6.526151	-1.977539	-0.685386
H	-6.500421	-0.054839	0.331711
H	-6.095748	0.018626	-1.379731
C	-5.746518	-2.718011	-1.779237
H	-4.132249	-3.447939	-0.531418
H	-3.695765	-3.297325	-2.232630
H	-7.586533	-1.895685	-0.955536
H	-6.477877	-2.548115	0.252421
H	-6.155798	-3.724892	-1.926685
H	-5.869815	-2.187760	-2.736522
H	-4.317058	-1.093668	0.870679
O	4.042087	0.106072	0.028699
C	4.475962	-1.059892	-0.597615
C	5.904714	-0.810515	-1.117323
C	4.368300	-2.261284	0.369124
H	3.083593	0.241637	-0.159314
F	6.421712	-1.916763	-1.700723
F	6.750429	-0.420162	-0.148862
F	5.874642	0.161762	-2.056275
F	3.080217	-2.365356	0.790925
F	4.681033	-3.429157	-0.235536
F	5.142103	-2.136163	1.459185
H	3.872525	-1.322076	-1.477041
C	-3.295097	0.549256	2.793750
H	-4.346385	0.275540	2.939306
H	-2.726689	-0.362386	2.589309
H	-2.932423	0.968149	3.739778
H	-3.759474	2.481283	1.934408

RE 2

E(B3LYP) = -2490.303944 a.u.

Frequency = -152.88 cm⁻¹



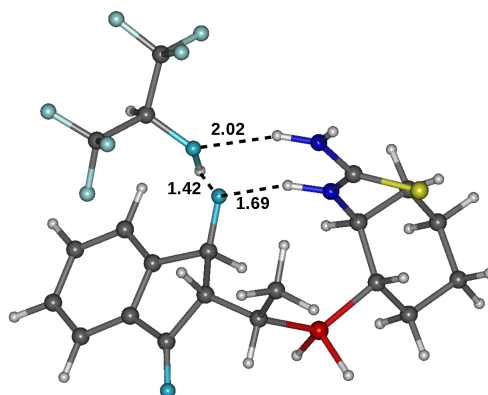
C	-2.253621	1.355872	1.710202
C	-1.125516	1.950105	0.900856
O	-2.484448	3.848912	0.428316

C	-1.380451	3.262651	0.360733
C	-0.188096	1.386541	-1.089134
C	0.460012	2.726496	-1.101149
C	-0.233201	3.757806	-0.444124
C	1.639807	3.005674	-1.804420
C	0.195310	5.083766	-0.555009
C	2.084256	4.326484	-1.883877
C	1.360230	5.362021	-1.271180
H	2.171829	2.206433	-2.313810
H	-0.363742	5.872804	-0.059604
H	2.989296	4.558343	-2.439783
H	1.717443	6.385811	-1.347759
H	-0.133392	1.727480	1.282393
O	0.469420	0.297787	-1.100840
H	-1.185124	1.374552	-1.555637
P	-3.604050	0.705007	0.602649
H	-3.704811	1.630077	-0.447253
N	-1.373676	-1.644381	-0.089437
C	-1.165656	-2.533641	0.922154
H	-0.569662	-1.111297	-0.440312
N	0.106073	-2.579579	1.383585
S	-2.363372	-3.499862	1.650619
H	0.872544	-2.008210	1.028357
H	0.292040	-3.194636	2.162432
H	-4.820643	0.889342	1.286042
C	-3.801447	-0.983609	-0.145010
C	-2.564728	-1.501432	-0.928923
C	-5.075231	-0.904275	-1.027507
C	-2.889614	-2.788923	-1.721963
H	-2.285993	-0.735673	-1.664397
C	-5.348445	-2.233112	-1.749993
H	-5.940829	-0.628557	-0.411507
H	-4.958344	-0.113819	-1.784339
C	-4.140008	-2.645254	-2.597182
H	-3.024912	-3.613054	-1.015338
H	-2.011192	-3.026064	-2.334112
H	-6.243271	-2.118470	-2.374382
H	-5.568954	-3.015394	-1.011329
H	-4.338890	-3.594480	-3.109267
H	-3.971962	-1.894204	-3.384714
H	-3.967003	-1.668504	0.696895
O	2.241043	-0.599733	0.555530
C	3.596616	-0.519784	0.243952
C	4.360136	-0.119159	1.522246
C	4.074291	-1.851948	-0.374763
H	1.678686	-0.124022	-0.129528
F	5.693551	-0.050596	1.309602
F	4.147306	-0.974721	2.540055
F	3.950810	1.104529	1.921762
F	3.339295	-2.112442	-1.479584
F	5.369829	-1.799601	-0.755248
F	3.929991	-2.895497	0.465810
H	3.810688	0.258586	-0.499686
C	-1.849000	0.392634	2.830788
H	-1.261507	-0.448504	2.460660
H	-1.232667	0.947916	3.546765
H	-2.713274	-0.007245	3.373409

H	-2.822057	2.201134	2.138935
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RE 3

E(B3LYP) = -2490.327498 a.u.



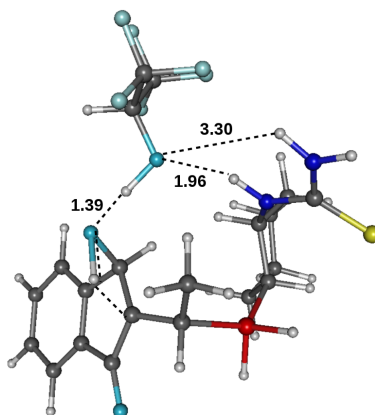
C	-1.340976	1.090422	2.016737
C	-0.248784	1.691117	1.109896
O	-0.593862	3.864123	2.205374
C	-0.154553	3.222968	1.259063
C	-0.229209	1.464722	-0.454060
C	0.516678	2.714570	-0.922489
C	0.507880	3.728223	0.045076
C	1.126544	2.930112	-2.157132
C	1.075497	4.985282	-0.198021
C	1.706502	4.178794	-2.402388
C	1.678944	5.201075	-1.435452
H	1.149791	2.139001	-2.901385
H	1.058903	5.754966	0.568809
H	2.189010	4.367239	-3.358555
H	2.141486	6.159583	-1.655138
H	0.713126	1.292843	1.465021
O	0.249782	0.276164	-0.922907
H	-1.285493	1.608350	-0.797967
P	-3.028171	0.999340	1.248023
H	-3.235241	2.225510	0.593243
N	-1.725781	-1.526597	-0.456219
C	-1.606901	-2.639074	0.312533
H	-0.868041	-0.981537	-0.706384
N	-0.332750	-3.046840	0.524316
S	-2.895637	-3.491286	1.043613
H	0.491334	-2.518960	0.231351
H	-0.198182	-3.822539	1.156530
H	-3.903406	1.099872	2.343279
C	-3.821199	-0.322601	0.208031
C	-2.950274	-0.901032	-0.941197
C	-5.159124	0.285393	-0.286210
C	-3.780246	-1.828040	-1.858982
H	-2.602360	-0.066847	-1.563095
C	-5.934025	-0.715924	-1.158917
H	-5.776629	0.594851	0.567851
H	-4.961984	1.188535	-0.883446

C	-5.078426	-1.172787	-2.345555
H	-4.010795	-2.748971	-1.315947
H	-3.139745	-2.101757	-2.705673
H	-6.860321	-0.239264	-1.503067
H	-6.223580	-1.584776	-0.552959
H	-5.637971	-1.885026	-2.963963
H	-4.855061	-0.307893	-2.989624
H	-4.013235	-1.148982	0.907754
O	1.951088	-1.116165	0.199472
C	3.213405	-1.008688	-0.358720
C	4.163115	-0.283776	0.621122
C	3.711782	-2.409873	-0.763911
H	1.285186	-0.428370	-0.259505
F	5.383847	-0.058249	0.080944
F	4.343820	-0.951932	1.777200
F	3.637418	0.927460	0.931355
F	2.881025	-2.926686	-1.698903
F	4.952288	-2.376963	-1.304105
F	3.739098	-3.273855	0.271576
H	3.215400	-0.407180	-1.279810
C	-0.955503	-0.199701	2.757655
H	-1.763366	-0.567477	3.400870
H	-0.666144	-0.999884	2.077738
H	-0.096544	0.024202	3.399527
H	-1.547792	1.868928	2.772062

RE 4

E(B3LYP) = -2490.268482 a.u.

Frequency = -1808.15 cm^{-1}

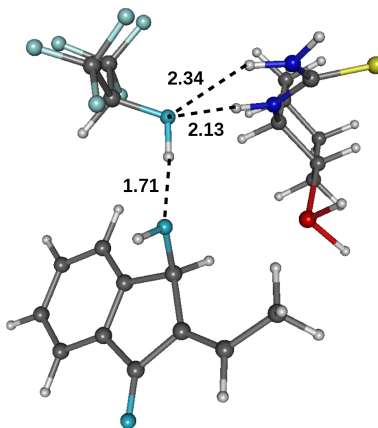


C	-1.494979	-0.811049	2.189943
C	-2.172980	0.362334	1.525298
O	-4.367244	-0.243688	2.358691
C	-3.642078	0.392975	1.586145
C	-1.716641	1.107658	0.272186
C	-2.996825	1.747864	-0.239073
C	-4.099164	1.334262	0.519974
C	-3.163373	2.650374	-1.286603
C	-5.388133	1.789102	0.241723
C	-4.454844	3.112746	-1.571808

C	-5.558611	2.685037	-0.817770
H	-2.311419	2.996175	-1.867182
H	-6.228780	1.450323	0.841499
H	-4.605007	3.814954	-2.388370
H	-6.550591	3.058624	-1.059050
H	-1.438379	1.536954	1.887106
O	-0.802620	2.062629	0.876845
H	-1.203815	0.545853	-0.518678
P	-1.486884	-2.394626	1.183019
H	-2.819137	-2.839913	1.186669
N	1.347197	-1.715503	0.009590
C	2.108119	-2.690048	0.575175
H	1.639319	-0.743264	0.146263
N	3.174643	-2.228956	1.278161
S	1.769308	-4.351745	0.520865
H	3.494920	-1.268939	1.214712
H	3.780716	-2.909361	1.712899
H	-0.801451	-3.386776	1.908717
C	-0.947553	-2.641524	-0.576626
C	0.307963	-1.849111	-1.013430
C	-2.082139	-2.450292	-1.606858
C	0.800881	-2.388716	-2.371286
H	-0.005005	-0.814475	-1.182491
C	-1.611221	-2.943194	-2.988009
H	-2.976483	-3.006578	-1.300537
H	-2.369018	-1.391641	-1.664318
C	-0.307298	-2.261410	-3.431105
H	1.113884	-3.432756	-2.257540
H	1.683494	-1.812513	-2.672646
H	-2.403931	-2.763779	-3.724601
H	-1.460212	-4.031378	-2.944785
H	0.037043	-2.692369	-4.378941
H	-0.502168	-1.196436	-3.625991
H	-0.670311	-3.704558	-0.541640
O	1.459156	1.193991	0.382104
C	2.349510	2.197222	0.040021
C	3.559377	2.143798	0.996033
C	2.742437	2.060246	-1.446889
H	0.484474	1.609939	0.634058
F	4.500777	3.064689	0.708640
F	4.169464	0.925343	0.978902
F	3.148011	2.360736	2.261300
F	1.633112	2.156823	-2.214431
F	3.597971	3.022530	-1.851941
F	3.313086	0.862375	-1.718425
H	1.912523	3.200282	0.151433
C	-0.134965	-0.564812	2.867482
H	0.254794	-1.470790	3.346105
H	0.621227	-0.181380	2.183578
H	-0.288348	0.188996	3.647584
H	-2.207909	-1.133341	2.968125

RE 5

$E(\text{B3LYP}) = -2490.354612 \text{ a.u.}$

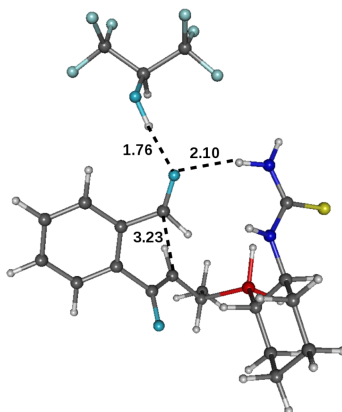


C	-3.260861	2.533095	-2.565515
C	-3.394772	2.021003	-1.330128
O	-5.665589	2.770925	-0.856514
C	-4.642851	2.193983	-0.516481
C	-2.381226	1.227780	-0.524564
C	-3.089340	0.994139	0.799468
C	-4.380794	1.536715	0.791918
C	-2.606590	0.345183	1.936136
C	-5.221212	1.440155	1.904068
C	-3.444228	0.242631	3.052171
C	-4.741508	0.783292	3.037436
H	-1.598963	-0.062527	1.966471
H	-6.217344	1.872883	1.873955
H	-3.083628	-0.255468	3.948552
H	-5.369045	0.693276	3.920017
H	-2.795459	-0.436424	-1.550186
O	-2.000166	-0.021518	-1.174874
H	-1.429288	1.753122	-0.394340
P	1.354995	2.999055	-0.470537
H	1.602532	4.396827	-0.579936
N	2.596478	0.152082	-0.407693
C	3.216265	-0.058032	-1.599395
H	1.790794	-0.437081	-0.221381
N	2.586330	-0.976376	-2.392231
S	4.602226	0.733396	-2.154505
H	1.851540	-1.575658	-2.031729
H	3.067926	-1.258558	-3.233053
H	1.711950	2.729222	-1.819767
C	2.994458	2.533876	0.344918
C	2.990300	1.030771	0.706989
C	3.246542	3.372921	1.613626
C	4.303495	0.605182	1.392132
H	2.180904	0.884365	1.436775
C	4.552762	2.958825	2.313321
H	3.286044	4.437398	1.349921
H	2.404838	3.254403	2.314877
C	4.563761	1.459114	2.643075
H	5.129885	0.708159	0.680930
H	4.236513	-0.457296	1.659946
H	4.687778	3.551598	3.227751
H	5.402184	3.192773	1.655614
H	5.523849	1.174680	3.092305

H	3.791197	1.249103	3.399506
H	3.799679	2.716064	-0.372574
O	0.057864	-1.642911	-0.533604
C	-0.492651	-2.758717	0.108422
C	-0.757005	-3.877842	-0.922195
C	0.459746	-3.164053	1.247862
H	-0.671659	-1.024164	-0.800666

SZ 1

E(B3LYP) = -2490.319039 a.u.



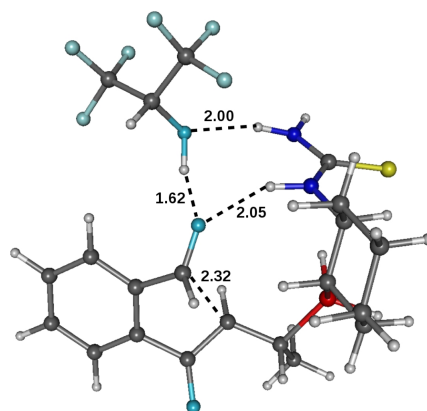
C	-3.391166	1.409389	-2.167716
C	-2.090937	1.859715	-1.579303
O	-3.066076	2.696612	0.414029
C	-2.066528	2.525675	-0.352379
C	0.228694	0.872695	0.447086
C	0.386282	2.317737	0.416400
C	-0.744121	3.114267	0.096087
C	1.602799	2.926046	0.804296
C	-0.639789	4.505700	0.230664
C	1.692569	4.306363	0.891551
C	0.563039	5.095489	0.611904
H	-4.211948	1.988019	-1.722589
H	2.458314	2.304515	1.051545
H	-1.512540	5.117176	0.020958
H	2.626992	4.774377	1.188258
H	0.629742	6.177907	0.691213
H	-1.193832	1.759742	-2.184380
O	1.113533	0.022570	0.653127
H	-0.796346	0.516832	0.285975
P	-3.621510	-0.329130	-1.541181
H	-2.485481	-1.059468	-1.907534
N	-1.923880	-1.835081	0.743604
C	-1.330553	-2.767950	-0.061481
H	-1.324846	-1.389330	1.431334
N	0.023031	-2.783381	0.007459
S	-2.192174	-3.811083	-1.079477
H	0.544326	-1.979456	0.360696
H	0.505271	-3.404241	-0.627131
H	-4.680870	-1.074089	-2.122935

C	-3.907894	-0.387086	0.280333
C	-3.361157	-1.675150	0.955630
C	-5.415730	-0.184841	0.567327
C	-3.659816	-1.638251	2.466779
H	-3.839836	-2.555029	0.514104
C	-5.678597	-0.154380	2.080607
H	-5.754836	0.754911	0.115307
H	-5.996482	-1.000753	0.111887
C	-5.152070	-1.425003	2.760138
H	-3.081656	-0.822553	2.928128
H	-3.307471	-2.576697	2.911677
H	-6.755184	-0.043292	2.259422
H	-5.190962	0.731219	2.510080
H	-5.307682	-1.370957	3.844422
H	-5.720749	-2.296770	2.404620
H	-3.378014	0.496514	0.663336
C	-3.460117	1.446841	-3.701823
H	-4.419493	1.085032	-4.090482
H	-3.328290	2.484266	-4.028059
H	-2.657008	0.854903	-4.157176
O	3.818554	-0.034158	1.105058
C	4.409256	-0.484397	-0.073112
C	5.757152	0.244962	-0.229289
C	4.536765	-2.025003	-0.060973
H	2.841395	0.013432	0.983229
F	6.429164	-0.183895	-1.322414
F	6.559359	0.090094	0.837022
F	5.532217	1.568908	-0.388737
F	3.302959	-2.562000	0.136211
F	4.990201	-2.505098	-1.240718
F	5.338316	-2.484801	0.912508
H	3.821945	-0.236409	-0.967861

SZ 2

E(B3LYP) = -2490.312349 a.u.

Frequency = -116.89 cm^{-1}



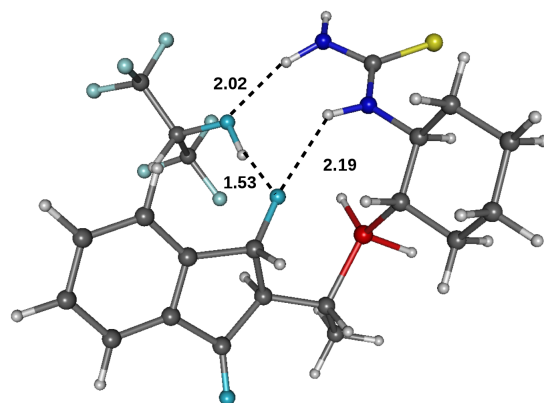
C	-3.790032	0.717395	-0.648191
C	-2.587792	1.624284	-0.472612
O	-3.993771	3.231977	0.606896

C	-2.879101	2.889090	0.166550
C	-0.681384	1.478679	0.840776
C	-0.483690	2.929349	0.575187
C	-1.642881	3.696195	0.360125
C	0.767812	3.558785	0.637128
C	-1.571245	5.090866	0.298784
C	0.840043	4.948795	0.539015
C	-0.326014	5.714329	0.383551
H	-4.421680	0.806548	0.246640
H	1.669589	2.974385	0.791799
H	-2.482161	5.665821	0.156292
H	1.806843	5.442223	0.597512
H	-0.254707	6.796947	0.315833
H	-1.889611	1.642969	-1.308417
O	0.171972	0.588056	0.532214
H	-1.345142	1.268651	1.690948
P	-3.235805	-1.027899	-0.741826
H	-2.351667	-1.171081	-1.817620
N	-0.371652	-2.211620	-0.346422
C	-0.184968	-2.609000	-1.635758
H	0.125321	-1.387286	-0.005626
N	0.831369	-2.002091	-2.285217
S	-1.185441	-3.735989	-2.428456
H	1.484881	-1.363563	-1.830961
H	1.007516	-2.281291	-3.239055
H	-4.310862	-1.864214	-1.091839
C	-2.502367	-1.684250	0.813941
C	-1.388988	-2.736634	0.548265
C	-3.593174	-2.228732	1.765069
C	-0.774156	-3.174449	1.890601
H	-1.824022	-3.607869	0.049864
C	-2.962869	-2.691535	3.089755
H	-4.353519	-1.461348	1.958996
H	-4.103819	-3.076823	1.286929
C	-1.842815	-3.714970	2.853095
H	-0.255905	-2.319060	2.347545
H	-0.013730	-3.936785	1.687213
H	-3.743688	-3.117803	3.731378
H	-2.559948	-1.817977	3.622073
H	-1.377100	-3.990372	3.806998
H	-2.273211	-4.637654	2.437269
H	-2.031744	-0.805457	1.271281
C	-4.655359	1.051652	-1.887544
H	-5.541290	0.408364	-1.970183
H	-4.994469	2.086068	-1.781725
H	-4.076137	0.974266	-2.815143
O	2.332970	0.158115	-0.849710
C	3.440470	0.204838	-0.001816
C	3.952404	-1.229812	0.243233
C	4.502641	1.145654	-0.608821
H	1.519951	0.508135	-0.373790
F	5.029322	-1.256871	1.055649
F	4.275867	-1.864140	-0.899832
F	2.974507	-1.949677	0.844983
F	3.973384	2.382333	-0.744108
F	5.586841	1.257897	0.191754
F	4.921752	0.742600	-1.821527

H 3.190939 0.613443 0.985593

SZ 3

E(B3LYP) = -2490.346032 a.u.

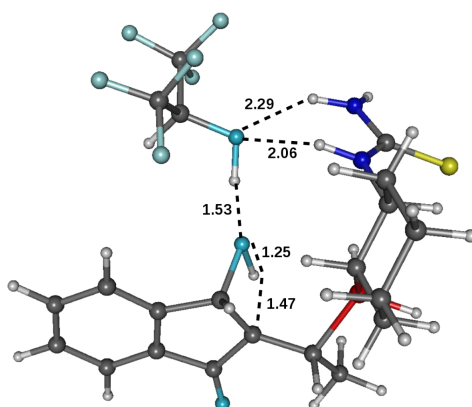


C	-2.859201	1.299877	-0.923658
C	-1.668981	2.155404	-0.526750
O	-2.667358	4.418459	-0.548754
C	-1.798313	3.641772	-0.188173
C	-0.949745	1.558225	0.706621
C	-0.055758	2.713544	1.132033
C	-0.618149	3.923942	0.679920
C	1.092600	2.724207	1.919772
C	-0.066126	5.158566	1.030588
C	1.661034	3.961297	2.253011
C	1.085443	5.166943	1.821118
H	-3.680401	1.434977	-0.204992
H	1.534447	1.796391	2.274198
H	-0.517772	6.081801	0.677501
H	2.560297	3.988961	2.863417
H	1.545706	6.111123	2.099493
H	-0.925961	2.109238	-1.339138
O	-0.458459	0.309073	0.392342
H	-1.708846	1.464977	1.517114
P	-2.368926	-0.513485	-0.750955
H	-1.296701	-0.910659	-1.553022
N	-0.531909	-2.656990	0.456605
C	0.191786	-3.608159	-0.201890
H	-0.068179	-1.807518	0.770495
N	1.487643	-3.272241	-0.438092
S	-0.445647	-5.098950	-0.685765
H	1.787578	-2.296891	-0.443363
H	2.008939	-3.915250	-1.017378
H	-3.435836	-1.075089	-1.506707
C	-2.630748	-1.418123	0.850858
C	-1.932445	-2.800849	0.827115
C	-4.133407	-1.573365	1.170031
C	-2.118585	-3.488964	2.194472
H	-2.395574	-3.435755	0.061809
C	-4.326848	-2.281988	2.522812
H	-4.625823	-0.592017	1.190393

H	-4.622174	-2.159655	0.379386
C	-3.604144	-3.636101	2.554859
H	-1.598769	-2.897560	2.962627
H	-1.630699	-4.467864	2.146942
H	-5.399815	-2.411612	2.711842
H	-3.941439	-1.637909	3.326829
H	-3.704894	-4.095004	3.546062
H	-4.082773	-4.323849	1.842614
H	-2.152084	-0.797155	1.614125
C	-3.381292	1.570358	-2.343759
H	-4.256498	0.957802	-2.584932
H	-3.669498	2.624318	-2.411017
H	-2.608700	1.383410	-3.099242
O	1.833071	-0.280056	-0.537712
C	2.649777	0.715782	-1.054231
C	4.099068	0.422222	-0.620554
C	2.472690	0.812895	-2.586464
H	0.936062	0.091204	-0.193836
F	4.973917	1.313241	-1.137936
F	4.504200	-0.811125	-0.980931
F	4.188774	0.504453	0.726115
F	1.160211	1.042317	-2.860109
F	3.171635	1.837692	-3.120628
F	2.825988	-0.313541	-3.231173
H	2.407636	1.711209	-0.656007

SZ 4

E(B3LYP) = -2490.279420 a.u.
Frequency = -1747.98 cm⁻¹

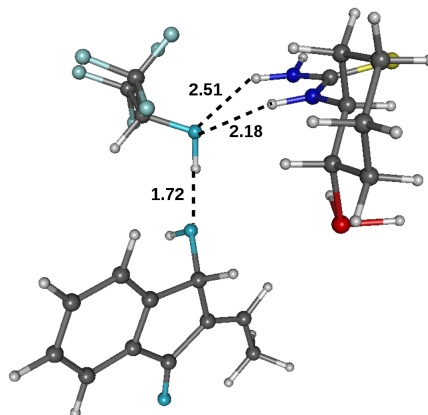


C	3.381064	-0.828673	-0.722403
C	2.257865	-1.847288	-0.694148
O	3.427694	-3.839690	-1.503312
C	2.507602	-3.281435	-0.898409
C	1.106662	-1.682785	0.290505
C	0.557089	-3.084639	0.450734
C	1.371479	-4.000755	-0.225687
C	-0.553335	-3.514493	1.171912
C	1.101083	-5.367819	-0.188886
C	-0.834431	-4.887281	1.208255

C	-0.014329	-5.804614	0.534884
H	4.033444	-0.905771	0.165486
H	-1.181438	-2.802247	1.701471
H	1.750651	-6.068898	-0.706151
H	-1.693138	-5.246258	1.770537
H	-0.248171	-6.865449	0.581899
H	1.104031	-1.241943	-1.362328
O	0.306571	-0.767063	-0.517988
H	1.315898	-1.228126	1.269431
P	2.723633	0.923878	-0.678794
H	1.831833	1.120324	-1.730393
N	0.181131	2.816845	-0.071170
C	0.187621	3.258556	-1.357071
H	-0.642596	2.303363	0.240117
N	-0.961224	3.016948	-2.041055
S	1.501801	4.060195	-2.071672
H	-1.579582	2.268372	-1.734638
H	-0.946287	3.226394	-3.029177
H	3.825450	1.738679	-0.989505
C	2.080269	1.531106	0.933783
C	1.305004	2.882202	0.851702
C	3.243064	1.633712	1.952289
C	0.808058	3.300345	2.248398
H	1.973116	3.659294	0.467147
C	2.708661	2.026140	3.337180
H	3.802252	0.691526	2.010950
H	3.950126	2.405472	1.616194
C	1.946725	3.356400	3.279313
H	0.038057	2.592727	2.590135
H	0.321815	4.278534	2.152503
H	3.546154	2.094504	4.041933
H	2.043450	1.235450	3.712570
H	1.539194	3.606772	4.265976
H	2.641296	4.164654	3.010063
H	1.383762	0.748048	1.254148
C	4.266692	-0.916978	-1.984042
H	5.126499	-0.239427	-1.925933
H	4.626182	-1.945394	-2.078312
H	3.693490	-0.689971	-2.891004
O	-1.834734	0.614520	-0.340361
C	-2.979202	-0.174188	-0.231366
C	-3.469494	-0.184461	1.231592
C	-4.031387	0.340685	-1.231496
H	-1.005622	0.009251	-0.382488
F	-4.575952	-0.940654	1.391443
F	-3.734840	1.047738	1.705067
F	-2.500730	-0.716362	2.017987
F	-4.450535	1.592497	-0.944606
F	-3.488218	0.376439	-2.470344
F	-5.112674	-0.463022	-1.283441
H	-2.782813	-1.221999	-0.500286

SZ 5

$E(\text{B3LYP}) = -2490.355356 \text{ a.u.}$

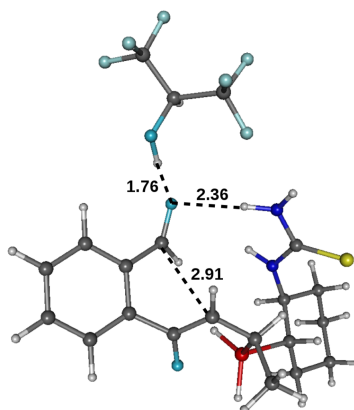


C	-3.404654	-2.320737	-2.252425
C	-3.674033	-1.628937	-1.128368
O	-6.095699	-1.859788	-0.830623
C	-5.007593	-1.429560	-0.470930
C	-2.611319	-0.911576	-0.306837
C	-3.391684	-0.298982	0.840148
C	-4.755405	-0.596672	0.736772
C	-2.915646	0.460028	1.909216
C	-5.676554	-0.143283	1.684871
C	-3.833054	0.921509	2.859347
C	-5.202461	0.624270	2.748853
H	-2.359443	-2.359219	-2.567125
H	-1.856108	0.680969	2.015474
H	-6.729444	-0.391614	1.584391
H	-3.481256	1.512384	3.701168
H	-5.892379	0.991748	3.503689
H	-2.504163	0.568832	-1.639033
O	-1.876354	0.078398	-1.081270
H	-1.831032	-1.594195	0.045610
P	0.808817	-3.111873	0.119999
H	1.019952	-2.435661	-1.112184
N	2.901690	-0.712056	-0.634494
C	3.408999	-0.662251	-1.891927
H	2.211920	-0.009332	-0.380701
N	2.844644	0.294545	-2.689503
S	4.601428	-1.696052	-2.494053
H	2.259087	1.025568	-2.301262
H	3.296210	0.470295	-3.574854
H	1.639664	-4.211735	-0.233270
C	2.076093	-2.183727	1.173163
C	3.310410	-1.640053	0.416376
C	2.503558	-3.091312	2.348617
C	4.305206	-0.958677	1.380491
H	3.819704	-2.467433	-0.088655
C	3.491884	-2.396387	3.297556
H	1.614976	-3.422702	2.901866
H	2.975979	-3.999017	1.944277
C	4.719581	-1.883140	2.533415
H	3.839795	-0.048150	1.788059
H	5.180196	-0.640225	0.801796
H	3.794558	-3.093763	4.089721
H	2.990484	-1.552525	3.795302

H	5.400096	-1.352093	3.211343
H	5.283317	-2.737844	2.131001
H	1.529675	-1.325088	1.597135
C	-4.373254	-3.048152	-3.130185
H	-4.302690	-2.669323	-4.159476
H	-4.097549	-4.111216	-3.178450
H	-5.401380	-2.959816	-2.779582
O	0.481387	1.303031	-0.555093
C	0.159991	2.584905	-0.093817
C	1.087147	2.906676	1.092501
C	0.252605	3.590598	-1.261475
H	-0.352000	0.811140	-0.769832
F	0.870466	4.145195	1.577302
F	2.388331	2.802334	0.767975
F	0.841608	2.028452	2.093799
F	1.473759	3.607665	-1.829458
F	-0.636579	3.222888	-2.217129
F	-0.054742	4.845803	-0.883361
H	-0.866777	2.646089	0.288006

RZ 1

$E(\text{B3LYP}) = -2490.313487 \text{ a.u.}$



C	-2.560033	0.897303	1.586339
C	-1.294724	1.621678	1.238497
O	-2.663377	3.027316	0.014452
C	-1.458748	2.718754	0.429164
C	0.623318	1.346473	-0.938152
C	0.830693	2.749359	-0.555039
C	-0.269742	3.476897	-0.037453
C	2.045129	3.403855	-0.836488
C	-0.169690	4.867481	0.087768
C	2.139576	4.781550	-0.668890
C	1.026396	5.512994	-0.225947
H	-2.394352	-0.177975	1.707315
H	2.887534	2.834540	-1.219163
H	-1.021285	5.427570	0.463060
H	3.070593	5.292734	-0.897642
H	1.102294	6.591253	-0.110315
H	-0.348798	1.325249	1.676902

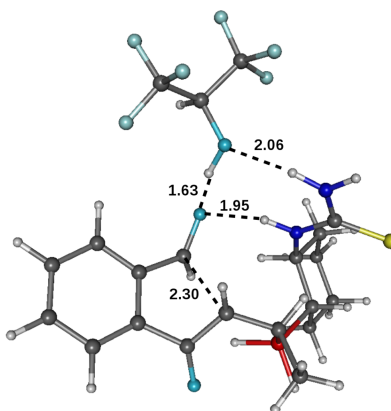
O	1.486218	0.460502	-1.014142
H	-0.400717	1.100966	-1.254265
P	-3.679872	1.091804	0.110028
H	-3.157169	1.186516	-1.186366
N	-2.297191	-1.528284	-0.888177
C	-1.634570	-2.197143	0.107367
H	-1.730586	-1.327367	-1.705027
N	-0.277343	-2.192362	-0.035062
S	-2.365974	-2.966855	1.417544
H	0.206865	-1.466763	-0.560482
H	0.247863	-2.585427	0.735037
H	-4.790638	1.930765	0.275060
C	-4.517926	-0.584648	-0.091778
C	-3.753626	-1.439259	-1.139148
C	-5.990351	-0.422154	-0.529815
C	-4.432642	-2.799448	-1.390089
H	-3.803881	-0.881149	-2.086205
C	-6.672549	-1.776165	-0.783992
H	-6.542141	0.137341	0.237005
H	-6.040932	0.182753	-1.450225
C	-5.896511	-2.607300	-1.814860
H	-4.377085	-3.404358	-0.480251
H	-3.873858	-3.334904	-2.168890
H	-7.703283	-1.611541	-1.123138
H	-6.734794	-2.332865	0.161958
H	-6.371644	-3.586743	-1.950120
H	-5.937126	-2.103304	-2.793218
H	-4.485959	-1.109187	0.870903
C	-3.280648	1.428738	2.849558
H	-4.212401	0.886523	3.057364
H	-2.617191	1.288339	3.709679
H	-3.499300	2.497230	2.757968
O	4.014496	0.319289	0.041735
C	4.488990	-0.941014	-0.311274
C	5.992057	-0.806206	-0.621229
C	4.178642	-1.968014	0.802165
H	3.097123	0.431577	-0.303803
F	6.548840	-2.005118	-0.912009
F	6.685411	-0.264511	0.394237
F	6.156628	-0.013266	-1.703640
F	2.838311	-1.964769	1.035692
F	4.511365	-3.226847	0.439079
F	4.790568	-1.694151	1.965181
H	4.021681	-1.333170	-1.224732

RZ 2

E(B3LYP) = -2490.309117 a.u.

Frequency = -123.78 cm⁻¹

C	-2.347632	1.060904	1.614550
C	-1.231549	1.904117	1.037885
O	-2.759231	3.574193	0.338624
C	-1.572949	3.168108	0.469034
C	-0.061125	1.509358	-0.900088
C	0.480624	2.888480	-0.757292

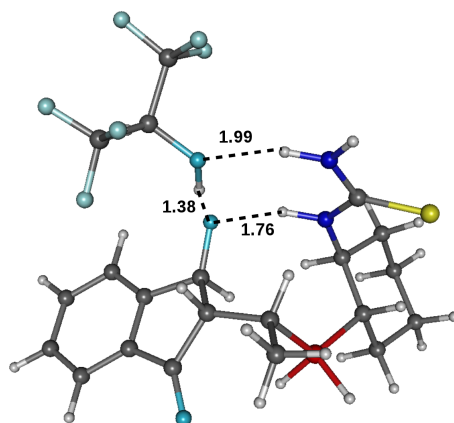


C	-0.394763	3.819752	-0.163654
C	1.713981	3.306927	-1.272331
C	-0.089376	5.182772	-0.171980
C	2.031953	4.666087	-1.241982
C	1.130041	5.600431	-0.709151
H	-1.976375	0.060159	1.849838
H	2.395614	2.586619	-1.715377
H	-0.782485	5.894555	0.268207
H	2.980991	5.005607	-1.648951
H	1.391440	6.655562	-0.701599
H	-0.266801	1.773540	1.518247
O	0.636010	0.449388	-0.907451
H	-1.012832	1.477697	-1.452229
P	-3.599414	0.786639	0.277141
H	-3.342259	1.570107	-0.852533
N	-1.380571	-1.546600	-0.112409
C	-1.209012	-2.239512	1.048548
H	-0.580710	-1.005191	-0.458995
N	0.031755	-2.153273	1.584217
S	-2.425324	-3.098848	1.871818
H	0.838001	-1.740333	1.116832
H	0.198154	-2.667168	2.437494
H	-4.868268	1.216723	0.697438
C	-3.840086	-0.939217	-0.333259
C	-2.556276	-1.533995	-0.989804
C	-5.032481	-0.932780	-1.322228
C	-2.844518	-2.915627	-1.616367
H	-2.266322	-0.863129	-1.810818
C	-5.285927	-2.328830	-1.913251
H	-5.936198	-0.573418	-0.813445
H	-4.832822	-0.230337	-2.146597
C	-4.025387	-2.874002	-2.594358
H	-3.044967	-3.631579	-0.812999
H	-1.931284	-3.246635	-2.125501
H	-6.117541	-2.270078	-2.626461
H	-5.599327	-3.012383	-1.112156
H	-4.211333	-3.880639	-2.988037
H	-3.775816	-2.241573	-3.460608
H	-4.080189	-1.552201	0.544620
C	-3.013885	1.645059	2.882415
H	-3.798609	0.984995	3.273008
H	-2.244102	1.739626	3.655800

H	-3.430161	2.635955	2.685194
O	2.478841	-0.622888	0.575633
C	3.625691	-0.948992	-0.147441
C	4.795563	-0.035112	0.280593
C	3.909093	-2.450433	0.048221
H	1.877318	-0.045200	0.019204
F	5.906648	-0.261728	-0.457572
F	5.123514	-0.173333	1.577072
F	4.438188	1.254900	0.080441
F	2.882044	-3.166425	-0.467433
F	5.033214	-2.840058	-0.590265
F	4.028728	-2.790570	1.345230
H	3.497570	-0.798556	-1.227638

RZ 3

E(B3LYP) = -2490.332034 a.u.



C	-1.549403	0.726774	1.593482
C	-0.575529	1.648358	0.838835
O	-1.734064	3.734407	1.459583
C	-0.911515	3.142432	0.768461
C	-0.257102	1.288519	-0.666942
C	0.320416	2.616089	-1.155196
C	-0.116300	3.682605	-0.353270
C	1.122064	2.856934	-2.268379
C	0.204766	5.010274	-0.657997
C	1.462814	4.180972	-2.566254
C	1.005791	5.249825	-1.774133
H	-1.166185	-0.292500	1.508446
H	1.470087	2.031004	-2.882496
H	-0.144602	5.821929	-0.025474
H	2.090776	4.391596	-3.428704
H	1.288761	6.267025	-2.031423
H	0.388419	1.563191	1.363416
O	0.461023	0.152526	-0.902251
H	-1.250581	1.210671	-1.177453
P	-3.205114	0.663639	0.754724
H	-3.377007	1.822848	-0.017891
N	-1.438428	-1.813071	-0.430449
C	-1.335294	-2.679533	0.611701

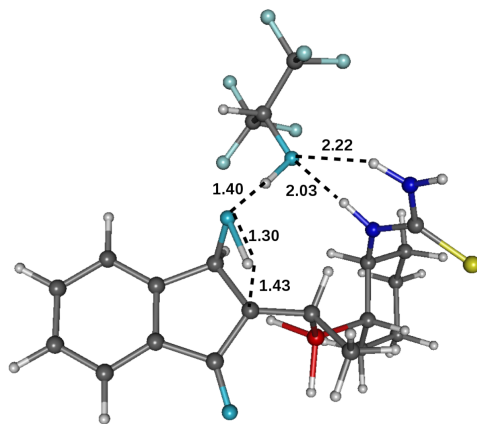
H	-0.607117	-1.231680	-0.674022
N	-0.088498	-2.810910	1.120424
S	-2.629969	-3.534020	1.328891
H	0.718542	-2.252554	0.833333
H	0.017715	-3.416521	1.921407
H	-4.192834	0.805624	1.743486
C	-3.745731	-0.786938	-0.260618
C	-2.644920	-1.427337	-1.158428
C	-4.988550	-0.354435	-1.075842
C	-3.246073	-2.579049	-1.993991
H	-2.297951	-0.664365	-1.866453
C	-5.549506	-1.534761	-1.886537
H	-5.765062	0.043333	-0.408168
H	-4.715829	0.456471	-1.767940
C	-4.472841	-2.132346	-2.800892
H	-3.513565	-3.401005	-1.322658
H	-2.456564	-2.947317	-2.659484
H	-6.409624	-1.187416	-2.472272
H	-5.920499	-2.306082	-1.198055
H	-4.879772	-2.987642	-3.353758
H	-4.178477	-1.385375	-3.554367
H	-4.023311	-1.543281	0.486702
C	-1.714168	1.058694	3.091389
H	-2.317642	0.299617	3.600798
H	-0.720183	1.052270	3.552261
H	-2.152043	2.047030	3.246458
O	2.024538	-0.756312	0.751128
C	3.360460	-0.586260	0.437068
C	4.021687	0.362191	1.461601
C	4.049577	-1.963313	0.351396
H	1.394327	-0.267149	0.028477
F	5.310220	0.638692	1.151642
F	3.997555	-0.118057	2.720612
F	3.353761	1.542963	1.466730
F	3.466629	-2.694306	-0.626939
F	5.364654	-1.862641	0.046715
F	3.948258	-2.670431	1.496160
H	3.505037	-0.114049	-0.546387

RZ 4

E(B3LYP) = -2490.274165 a.u.

Frequency = -1803.23 cm^{-1}

C	0.760120	-1.699744	-1.306195
C	2.116162	-1.110512	-1.013854
O	3.510694	-3.096467	-1.260628
C	3.323419	-1.939167	-0.868527
C	2.246849	0.113539	-0.106472
C	3.701235	0.073932	0.326605
C	4.312066	-1.108602	-0.111590
C	4.432929	1.020090	1.040175
C	5.650800	-1.384704	0.167577
C	5.779373	0.752730	1.319364
C	6.383603	-0.439476	0.890692
H	0.033270	-0.888931	-1.402624

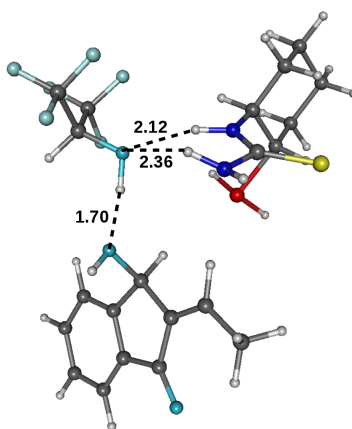


H	3.974702	1.948880	1.371059
H	6.100820	-2.311957	-0.177250
H	6.366111	1.478998	1.876690
H	7.430004	-0.623423	1.120993
H	2.130800	0.085209	-1.799589
O	1.950752	1.154812	-1.074946
H	1.564954	0.194541	0.754440
P	0.154049	-2.651667	0.191089
H	0.704970	-2.045143	1.332875
N	-2.166544	-0.558283	-0.191856
C	-2.644659	-0.634257	-1.472412
H	-1.734417	0.328634	0.061366
N	-2.384481	0.466607	-2.214638
S	-3.449442	-1.966398	-2.144486
H	-1.805289	1.229945	-1.865391
H	-2.672257	0.459372	-3.182046
H	0.755834	-3.921205	0.189211
C	-1.635025	-2.896235	0.599779
C	-2.321331	-1.529587	0.895304
C	-1.763876	-3.870581	1.794436
C	-3.784140	-1.731612	1.343701
H	-1.787156	-1.071382	1.739667
C	-3.234493	-4.048148	2.209191
H	-1.327115	-4.842333	1.532346
H	-1.194898	-3.486679	2.655264
C	-3.885975	-2.697496	2.532567
H	-4.365775	-2.109321	0.497272
H	-4.193316	-0.748749	1.606816
H	-3.282926	-4.718901	3.075926
H	-3.784455	-4.538686	1.394372
H	-4.940201	-2.840257	2.798479
H	-3.398405	-2.258879	3.416990
H	-2.105253	-3.325350	-0.293613
C	0.677591	-2.595144	-2.557601
H	0.977650	-1.989939	-3.419765
H	1.369207	-3.437661	-2.488803
H	-0.344400	-2.948272	-2.733746
O	-0.358322	1.930758	-0.613574
C	-0.287115	3.176028	-0.001383
C	-1.190244	4.176504	-0.751488
C	-0.648281	3.030696	1.492416
H	0.642471	1.598436	-0.872526

F	-1.122471	5.418804	-0.226043
F	-2.488191	3.797656	-0.748965
F	-0.795826	4.259173	-2.040289
F	0.272045	2.238512	2.099023
F	-0.664255	4.204148	2.153501
F	-1.853053	2.438008	1.673567
H	0.729302	3.593089	-0.035168

RZ 5

E(B3LYP) = -2490.353846 a.u.

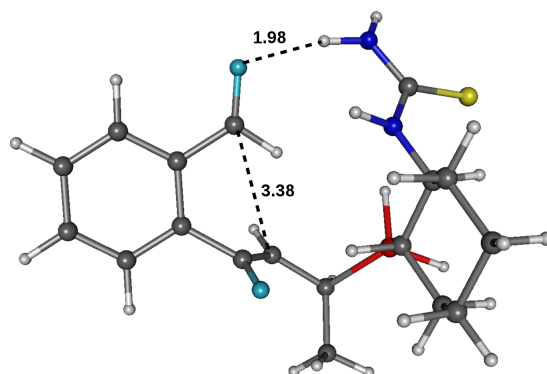


C	-2.279520	-1.854470	1.962580
C	-3.085225	-1.324488	1.020339
O	-5.245644	-2.432188	1.360307
C	-4.524899	-1.646171	0.757876
C	-2.623397	-0.287988	0.004206
C	-3.854916	-0.032531	-0.841213
C	-4.931566	-0.815417	-0.409467
C	-4.001929	0.834496	-1.923686
C	-6.175632	-0.759553	-1.043274
C	-5.245550	0.897294	-2.560990
C	-6.323814	0.106710	-2.126675
H	-1.243006	-1.511488	1.983834
H	-3.172458	1.447802	-2.266441
H	-6.995250	-1.379867	-0.691294
H	-5.380678	1.564461	-3.408551
H	-7.277853	0.172744	-2.643017
H	-2.721259	1.193671	1.333885
O	-2.119194	0.938533	0.614045
H	-1.777323	-0.644873	-0.591991
P	0.676792	-2.107063	-1.779092
H	0.956408	-1.348650	-2.956428
N	2.261171	-0.789116	0.611633
C	1.953691	-1.434666	1.760640
H	1.852502	0.135237	0.504246
N	1.182077	-0.684437	2.626320
S	2.359992	-3.020868	2.172121
H	1.191523	0.328010	2.542666
H	1.143803	-1.047384	3.569444
H	0.465554	-3.313700	-2.504924

C	2.470357	-2.454289	-1.294576
C	3.075526	-1.249323	-0.527353
C	3.369067	-2.834326	-2.489091
C	4.545940	-1.493185	-0.127638
H	3.066810	-0.389218	-1.211452
C	4.827143	-3.086635	-2.072395
H	2.956782	-3.722412	-2.984165
H	3.343917	-2.024370	-3.234589
C	5.406058	-1.867341	-1.342446
H	4.585215	-2.294095	0.617605
H	4.930611	-0.584038	0.352331
H	5.428729	-3.324949	-2.959724
H	4.873767	-3.964744	-1.412350
H	6.435253	-2.065754	-1.016926
H	5.457240	-1.016694	-2.040052
H	2.421041	-3.298777	-0.596581
C	-2.636646	-2.874416	2.996456
H	-2.430031	-2.475655	3.999994
H	-3.678955	-3.187446	2.938545
H	-1.981639	-3.749335	2.881567
O	0.454432	1.706288	0.775376
C	0.493729	3.014280	0.278209
C	1.202125	3.903421	1.319071
C	1.167848	3.010898	-1.109970
H	-0.474577	1.357220	0.730597
F	1.282233	5.186832	0.913063
F	2.447089	3.472598	1.596657
F	0.494029	3.883351	2.471062
F	0.429236	2.254726	-1.954603
F	1.253400	4.247161	-1.639195
F	2.408616	2.483098	-1.074428
H	-0.509137	3.434260	0.136102

SE* 1

E(B3LYP) = -1700.463409 a.u.



C	0.166312	-2.053176	1.904172
C	1.324457	-1.209297	1.450735
O	1.303544	-1.826123	-0.852521
C	1.807319	-1.212623	0.146283
C	1.755947	1.710194	-0.207659

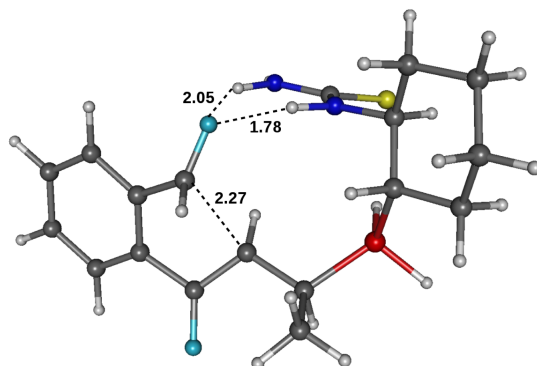
C	3.030208	1.003332	-0.336015
C	3.059722	-0.399831	-0.150600
C	4.199894	1.706202	-0.690763
C	4.275092	-1.069826	-0.348681
C	5.397964	1.026331	-0.857913
C	5.430897	-0.367574	-0.686902
H	4.138202	2.781861	-0.830705
H	4.304908	-2.149829	-0.233405
H	6.303116	1.565738	-1.124022
H	6.366593	-0.905447	-0.821075
H	1.823303	-0.608952	2.206162
O	1.563255	2.910800	-0.421223
H	0.912243	1.075939	0.106307
P	-1.391584	-1.181033	1.342795
H	-1.352497	0.102220	1.898621
N	-1.644376	1.424837	-0.520931
C	-2.019853	2.333821	0.427784
H	-0.905418	1.711507	-1.155473
N	-1.217778	3.422892	0.509478
S	-3.360621	2.127349	1.445075
H	-0.270428	3.421772	0.115560
H	-1.408396	4.062487	1.267769
H	-2.589682	-1.716060	1.885308
C	-1.666235	-1.076171	-0.481982
C	-2.389485	0.231411	-0.913200
C	-2.431840	-2.331845	-0.966136
C	-2.598472	0.232459	-2.440769
H	-3.362934	0.298481	-0.417110
C	-2.625763	-2.299052	-2.489670
H	-1.881305	-3.236104	-0.683346
H	-3.415313	-2.381397	-0.474649
C	-3.344248	-1.017344	-2.928937
H	-1.617342	0.284273	-2.937184
H	-3.147088	1.142607	-2.711784
H	-3.194789	-3.183514	-2.802376
H	-1.643275	-2.362462	-2.977102
H	-3.436915	-0.985791	-4.021476
H	-4.368217	-1.011725	-2.527031
H	-0.648957	-1.112138	-0.902373
C	0.191395	-3.541859	1.511127
H	1.043341	-4.008810	2.017626
H	-0.719839	-4.072420	1.817571
H	0.343339	-3.649984	0.435218
H	0.076617	-1.977933	2.997178

SE* 2

E(B3LYP) = -1700.449299 a.u.

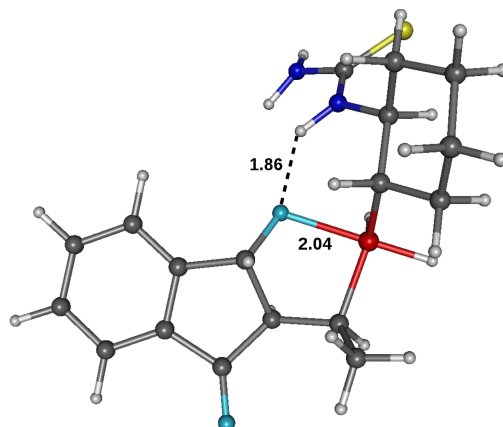
Frequency = -141.41 cm⁻¹

C	0.587749	-1.987538	0.967105
C	1.464080	-0.796574	0.603154
O	3.380080	-2.104420	1.204829
C	2.881395	-1.045679	0.771295
C	1.806329	0.310119	-1.356415



C	3.083794	0.824661	-0.773244
C	3.700188	0.078834	0.245081
C	3.704116	1.984536	-1.262397
C	4.970432	0.431706	0.715780
C	4.958479	2.349095	-0.771677
C	5.595897	1.569168	0.207239
H	3.218530	2.567160	-2.040707
H	5.436981	-0.173272	1.488523
H	5.453210	3.235754	-1.161131
H	6.575657	1.862090	0.576696
H	1.120363	0.175241	0.952462
O	0.884484	1.107178	-1.704286
H	1.894801	-0.656409	-1.874770
P	-1.182462	-1.522504	1.101436
H	-1.386765	-0.358759	1.874922
N	-1.573374	1.034020	-0.477559
C	-1.439770	1.967026	0.504254
H	-0.808486	0.985852	-1.168950
N	-0.370950	2.779447	0.344255
S	-2.475147	2.091492	1.850638
H	0.325090	2.563097	-0.374632
H	-0.139658	3.408370	1.098973
H	-1.827826	-2.540431	1.827394
C	-2.122837	-1.353770	-0.487316
C	-2.666831	0.093675	-0.618055
C	-3.235925	-2.412534	-0.645441
C	-3.395031	0.257051	-1.963886
H	-3.369728	0.296415	0.197055
C	-3.968887	-2.219661	-1.983967
H	-2.814589	-3.423947	-0.586008
H	-3.953789	-2.314621	0.181686
C	-4.507796	-0.789311	-2.134512
H	-2.665489	0.165688	-2.781908
H	-3.804143	1.272577	-2.013554
H	-4.786848	-2.947043	-2.055745
H	-3.277042	-2.442061	-2.809437
H	-4.983801	-0.668692	-3.115155
H	-5.291598	-0.613814	-1.383158
H	-1.371529	-1.502812	-1.275539
C	0.730373	-3.206373	0.026959
H	0.478888	-2.952429	-1.008364
H	1.777177	-3.518099	0.058056
H	0.112768	-4.055847	0.347263
H	0.842609	-2.335825	1.986128

SE* 3

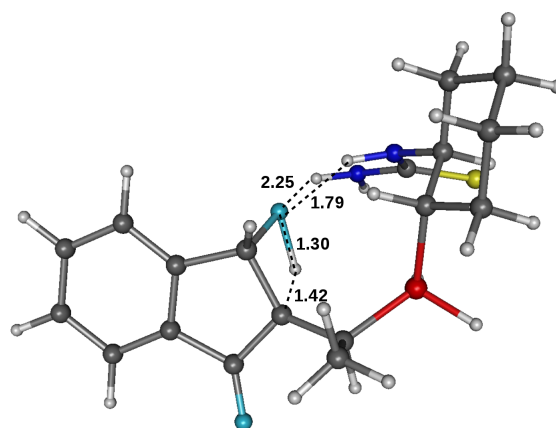
 $E(\text{B3LYP}) = -1700.481037 \text{ a.u.}$ 

C	-1.191530	-2.057312	-0.977824
C	-2.198304	-0.941247	-0.777466
O	-4.411349	-2.017929	-0.472114
C	-3.656936	-1.069283	-0.338960
C	-1.599875	0.054674	0.239103
C	-2.772525	0.982370	0.495049
C	-3.965335	0.267931	0.258556
C	-2.820564	2.284164	0.984201
C	-5.214182	0.826452	0.537900
C	-4.074460	2.854647	1.241898
C	-5.259697	2.132906	1.031163
H	-1.907824	2.844786	1.167772
H	-6.122097	0.257782	0.354758
H	-4.131253	3.872674	1.619647
H	-6.217505	2.599272	1.246047
H	-2.254408	-0.361619	-1.712659
O	-0.387788	0.480557	-0.273029
H	-1.440415	-0.486833	1.198915
P	0.530057	-1.217983	-0.929880
H	0.867464	-0.386179	-2.007964
N	2.226812	1.219833	-0.011552
C	2.871724	2.113590	-0.797184
H	1.218548	1.328862	0.127107
N	2.109413	3.198608	-1.154102
S	4.479881	1.978952	-1.293842
H	1.097430	3.125461	-1.142437
H	2.508433	3.797807	-1.863197
H	1.187769	-2.383229	-1.475097
C	1.630095	-1.109174	0.588404
C	2.771438	-0.070162	0.397184
C	2.230416	-2.475510	0.978101
C	3.592481	0.042544	1.698296
H	3.443264	-0.412876	-0.401190
C	3.073674	-2.371696	2.260636
H	1.432849	-3.214367	1.117107
H	2.859876	-2.844442	0.156689
C	4.174767	-1.312030	2.122801

H	2.940154	0.440119	2.489821
H	4.389016	0.774785	1.531806
H	3.507999	-3.353205	2.490107
H	2.418067	-2.113606	3.105928
H	4.721390	-1.204410	3.068053
H	4.909294	-1.641619	1.373400
H	0.977313	-0.755756	1.396046
C	-1.288142	-3.231121	0.007802
H	-0.499992	-3.970284	-0.170981
H	-1.223138	-2.903040	1.051259
H	-2.255730	-3.725691	-0.124534
H	-1.230807	-2.454919	-1.999196

SE* 4

E(B3LYP) = -1700.414671 a.u.
Frequency = -1748.05 cm⁻¹

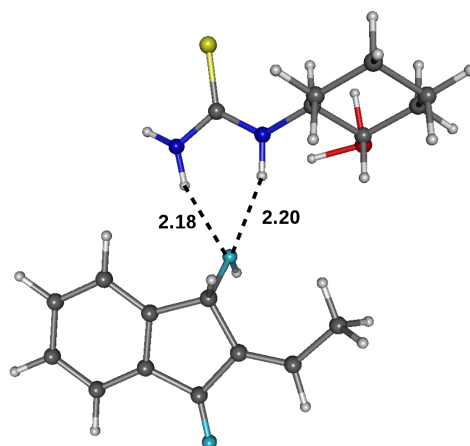


C	-0.613753	-1.490246	-1.474765
C	-1.562834	-0.518909	-0.810899
O	-3.318406	-0.848004	-2.452517
C	-2.941146	-0.530360	-1.320494
C	-1.573315	-0.202351	0.687519
C	-3.037565	0.113533	0.959302
C	-3.810690	-0.063086	-0.196498
C	-3.631594	0.565508	2.135291
C	-5.182920	0.186745	-0.202527
C	-5.010225	0.816477	2.138703
C	-5.781450	0.627156	0.981758
H	-3.039611	0.726659	3.033348
H	-5.760501	0.037374	-1.111077
H	-5.490610	1.163165	3.050751
H	-6.849728	0.827354	1.009356
H	-1.006108	0.765930	-0.582661
O	-0.731627	0.976985	0.666145
H	-1.179705	-0.959486	1.384232
P	1.137178	-0.889868	-1.437026
H	1.215898	0.429607	-1.902836
N	1.974480	1.362488	0.525661
C	2.072133	2.424806	-0.319228
H	1.028089	1.196447	0.912277

N	1.027816	3.290179	-0.230012
S	3.350160	2.682599	-1.405827
H	0.161961	2.998590	0.219329
H	0.987535	4.034506	-0.910830
H	1.882227	-1.624056	-2.379952
C	2.048952	-1.070729	0.165277
C	2.857771	0.213384	0.511212
C	2.940401	-2.334104	0.171071
C	3.567482	0.024857	1.865748
H	3.613293	0.394284	-0.262022
C	3.655189	-2.486964	1.524088
H	2.342593	-3.229217	-0.042479
H	3.690862	-2.251456	-0.628030
C	4.456393	-1.226971	1.880303
H	2.810242	-0.042168	2.660720
H	4.157381	0.926553	2.064523
H	4.312093	-3.364754	1.486439
H	2.909709	-2.685028	2.308134
H	4.922018	-1.342357	2.866595
H	5.277661	-1.100381	1.159827
H	1.257905	-1.184429	0.919735
C	-0.693561	-2.956673	-0.996045
H	-0.019435	-3.623408	-1.550103
H	-0.476280	-3.049582	0.073552
H	-1.717443	-3.307242	-1.159548
H	-0.861682	-1.463415	-2.548096

SE* 5

E(B3LYP) = -1700.50516554

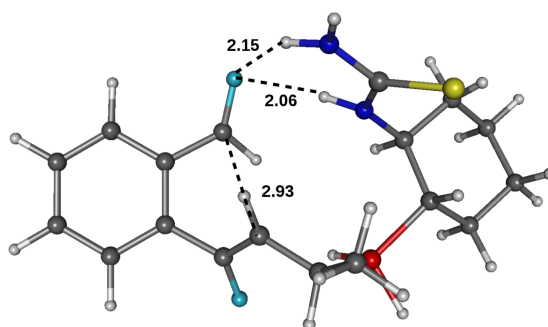


C	-2.216161	-2.945347	-0.482580
C	-2.775661	-1.764721	-0.170910
O	-5.071029	-2.268272	-0.816998
C	-4.241310	-1.497961	-0.355743
C	-2.114118	-0.527659	0.415949
C	-3.277110	0.435202	0.601417
C	-4.480745	-0.121432	0.149620
C	-3.254716	1.720799	1.142474
C	-5.684195	0.585839	0.217301
C	-4.456412	2.433947	1.211123

C	-5.661248	1.873758	0.752125
H	-2.329680	2.161080	1.506812
H	-6.604848	0.131060	-0.137608
H	-4.460367	3.436184	1.631876
H	-6.580022	2.449966	0.820964
H	-1.375759	0.007581	-1.344350
O	-1.064757	0.022552	-0.422755
H	-1.606291	-0.730287	1.364835
P	3.264712	-0.357684	-2.428672
H	2.191204	0.571219	-2.333010
N	1.878009	0.906946	0.275124
C	1.702447	2.240654	0.451932
H	1.042888	0.348452	0.114367
N	0.396355	2.650257	0.358721
S	2.934702	3.343415	0.788891
H	-0.295827	2.033691	-0.057791
H	0.255535	3.646487	0.269877
H	4.262406	0.652316	-2.312856
C	3.298318	-0.918941	-0.622494
C	3.138020	0.188077	0.444588
C	4.602360	-1.714661	-0.382312
C	3.239889	-0.387210	1.873764
H	3.930491	0.931655	0.309972
C	4.697430	-2.279117	1.043505
H	4.677533	-2.526483	-1.116729
H	5.462168	-1.051523	-0.561498
C	4.542585	-1.168581	2.090687
H	2.379017	-1.051078	2.052106
H	3.159363	0.442763	2.585463
H	5.656020	-2.798836	1.171606
H	3.909203	-3.033465	1.190241
H	4.563417	-1.588843	3.104504
H	5.395939	-0.478123	2.020833
H	2.454766	-1.623104	-0.523551
C	-0.786176	-3.345468	-0.305099
H	-0.339913	-3.610883	-1.273564
H	-0.178992	-2.558016	0.148188
H	-0.721769	-4.247251	0.318981
H	-2.887026	-3.694037	-0.907303

RE* 1

E(B3LYP) = -1700.453718 a.u.



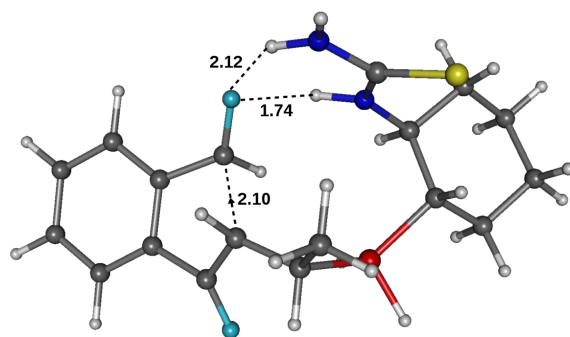
C	-0.381077	-1.070307	1.996488
C	-1.440727	-0.347047	1.242097
O	-2.302986	-2.387325	0.441383
C	-2.379654	-1.120900	0.548457
C	-1.855175	0.939894	-1.357771
C	-3.238765	0.743104	-0.913532
C	-3.516053	-0.373185	-0.092271
C	-4.281069	1.562775	-1.385336
C	-4.850625	-0.710534	0.163845
C	-5.600360	1.232350	-1.093259
C	-5.882680	0.086119	-0.331748
H	-4.041626	2.420939	-2.007563
H	-5.064014	-1.584663	0.772660
H	-6.412541	1.849660	-1.468337
H	-6.916027	-0.175305	-0.116271
H	-1.534206	0.725808	1.366009
O	-1.321694	2.012230	-1.668155
H	-1.283233	0.003097	-1.468331
P	0.783077	-1.884909	0.759328
H	-0.012041	-2.283088	-0.325224
N	1.336124	1.056064	-0.639133
C	1.676960	2.053013	0.229154
H	0.559496	1.290299	-1.256874
N	0.819995	3.103845	0.212046
S	3.005433	2.043629	1.283763
H	-0.017711	3.110623	-0.364576
H	0.975792	3.849824	0.873319
H	1.219212	-3.123785	1.277334
C	2.358935	-1.142941	0.088708
C	2.133359	-0.104533	-1.048212
C	3.236304	-2.329050	-0.395998
C	3.460218	0.307192	-1.725948
H	1.518861	-0.594947	-1.815829
C	4.548293	-1.857314	-1.041557
H	3.455842	-2.991703	0.449764
H	2.677720	-2.929857	-1.130696
C	4.273357	-0.900313	-2.205319
H	4.049833	0.896948	-1.017334
H	3.211181	0.966511	-2.566821
H	5.112457	-2.734571	-1.382353
H	5.166398	-1.352072	-0.286750
H	5.215489	-0.556050	-2.649031
H	3.729821	-1.434861	-2.999851
H	2.853013	-0.631729	0.923406
C	0.363359	-0.276052	3.072714
H	1.109391	-0.885291	3.598155
H	0.870136	0.603513	2.665950
H	-0.371241	0.063153	3.812037
H	-0.814158	-1.987830	2.429209

RE* 2

E(B3LYP) = -1700.443301 a.u.

Frequency = -214.43 cm⁻¹

C	-0.496031	0.050842	2.071222
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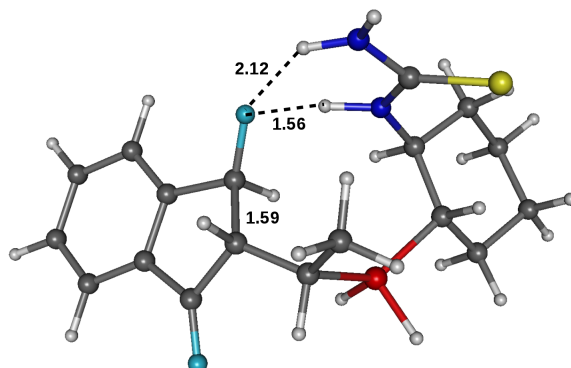


C	-1.638423	0.337106	1.119600
O	-2.655987	-1.717645	1.797309
C	-2.700515	-0.654840	1.142417
C	-1.664913	0.434722	-0.983339
C	-3.164300	0.358732	-0.968377
C	-3.724266	-0.334670	0.118067
C	-3.986442	0.850705	-1.987539
C	-5.092385	-0.620163	0.158217
C	-5.358291	0.592671	-1.931107
C	-5.907808	-0.147796	-0.871254
H	-3.550738	1.404203	-2.814600
H	-5.506087	-1.174249	0.996648
H	-6.007853	0.957639	-2.723229
H	-6.977294	-0.341955	-0.848250
H	-1.934630	1.383442	1.116424
O	-1.041258	1.414567	-1.505607
H	-1.216311	-0.575238	-1.097720
P	0.622301	-1.305516	1.441737
H	-0.159360	-2.175337	0.667404
N	1.551449	0.788259	-0.884376
C	2.093655	1.942351	-0.413999
H	0.614434	0.907896	-1.315122
N	1.314306	3.029256	-0.652962
S	3.561810	2.099769	0.430982
H	0.371519	2.922010	-1.025353
H	1.610648	3.914806	-0.271363
H	0.942635	-2.096550	2.559428
C	2.254666	-1.127576	0.570322
C	2.117765	-0.554706	-0.870028
C	2.912900	-2.532185	0.593183
C	3.439919	-0.663805	-1.662119
H	1.379664	-1.170984	-1.402370
C	4.234014	-2.552718	-0.192883
H	3.090329	-2.844593	1.629948
H	2.230853	-3.274277	0.149641
C	4.021190	-2.082139	-1.635562
H	4.162166	0.044089	-1.245490
H	3.231343	-0.345714	-2.690767
H	4.642684	-3.570726	-0.169916
H	4.965300	-1.901307	0.304580
H	4.970518	-2.099858	-2.184533
H	3.347393	-2.782306	-2.153901
H	2.854390	-0.418638	1.156293
C	0.277296	1.271300	2.584500
H	1.075174	0.999749	3.285890

H	0.720994	1.853221	1.775759
H	-0.428696	1.915395	3.121052
H	-0.922213	-0.496869	2.929754

RE* 3

E(B3LYP) = -1700.456227 a.u.

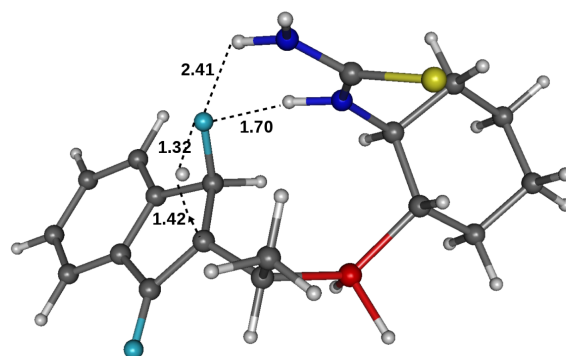


C	-0.470647	-0.062094	2.024064
C	-1.684348	0.345592	1.176590
O	-2.964508	-1.507858	2.158635
C	-2.837747	-0.663347	1.276956
C	-1.554519	0.624316	-0.385370
C	-2.989797	0.334521	-0.833979
C	-3.691371	-0.445970	0.096536
C	-3.604599	0.728974	-2.021167
C	-4.998285	-0.887736	-0.147769
C	-4.912611	0.300899	-2.266814
C	-5.604653	-0.505682	-1.343025
H	-3.069058	1.359782	-2.725029
H	-5.523065	-1.491452	0.588019
H	-5.409455	0.594939	-3.188704
H	-6.622046	-0.819713	-1.561606
H	-2.056514	1.297722	1.582402
O	-1.019511	1.793266	-0.773826
H	-0.959340	-0.263193	-0.766776
P	0.678432	-1.274283	1.200301
H	-0.113654	-2.220280	0.528655
N	1.524072	1.205894	-0.787054
C	2.155811	2.185997	-0.100479
H	0.488859	1.418811	-0.967692
N	1.402000	3.315925	0.005293
S	3.698522	2.107879	0.627757
H	0.407258	3.271310	-0.223884
H	1.747794	4.052472	0.601931
H	1.180457	-2.025065	2.278560
C	2.210398	-0.994641	0.180637
C	2.006528	-0.129060	-1.094987
C	2.771233	-2.406825	-0.126135
C	3.273724	-0.134267	-1.980265
H	1.205082	-0.587525	-1.689034
C	4.041938	-2.323593	-0.989159
H	2.987426	-2.943213	0.807154

H	2.019087	-2.998929	-0.669756
C	3.770122	-1.552129	-2.285499
H	4.059197	0.436762	-1.476940
H	3.025244	0.401198	-2.904251
H	4.388791	-3.342291	-1.203667
H	4.838277	-1.824596	-0.420791
H	4.682447	-1.499764	-2.892112
H	3.026200	-2.098522	-2.886386
H	2.898463	-0.445115	0.839308
C	0.292088	1.093403	2.690538
H	1.149324	0.746520	3.279613
H	0.646806	1.823802	1.963351
H	-0.395489	1.600668	3.376760
H	-0.867426	-0.724461	2.812059

RE* 4

E(B3LYP) = -1700.397651 a.u.
Frequency = -1791.98 cm⁻¹

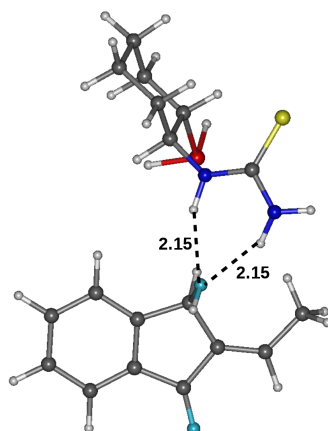


C	0.452657	-1.330957	1.346404
C	1.569579	-0.876493	0.413409
O	3.267066	-1.603625	1.983601
C	2.915238	-0.932199	1.007557
C	1.529106	0.269541	-0.601778
C	2.987331	0.693764	-0.703695
C	3.778172	-0.006470	0.215229
C	3.569916	1.609172	-1.576895
C	5.154881	0.202575	0.302376
C	4.951644	1.825623	-1.496161
C	5.738459	1.132254	-0.563058
H	2.969310	2.138023	-2.313213
H	5.746660	-0.349594	1.027802
H	5.423341	2.539769	-2.167179
H	6.808762	1.318259	-0.519518
H	1.372156	-1.376431	-0.896063
O	1.052888	-0.434374	-1.764241
H	0.888894	1.140665	-0.367318
P	-0.742365	-0.002898	1.831911
H	0.001823	1.163175	2.081373
N	-1.622406	-0.143299	-1.362964
C	-2.272626	-1.284243	-1.703819
H	-0.612478	-0.121090	-1.640072

N	-1.565715	-2.061426	-2.568236
S	-3.791021	-1.803694	-1.137381
H	-0.610122	-1.828432	-2.821752
H	-1.928386	-2.977008	-2.787966
H	-1.221108	-0.332870	3.114037
C	-2.294924	0.533445	0.960256
C	-2.102050	0.950794	-0.527297
C	-2.892410	1.667223	1.833921
C	-3.370417	1.624180	-1.098869
H	-1.302486	1.701976	-0.566264
C	-4.168082	2.254361	1.207928
H	-3.109068	1.291407	2.842331
H	-2.157741	2.479218	1.946828
C	-3.890164	2.760749	-0.211533
H	-4.147987	0.865128	-1.220960
H	-3.117668	1.993404	-2.099946
H	-4.533951	3.065881	1.849268
H	-4.952364	1.486054	1.181348
H	-4.803794	3.178511	-0.651435
H	-3.158880	3.583220	-0.170584
H	-2.959076	-0.342230	0.969400
C	-0.282883	-2.632364	0.970600
H	-1.006829	-2.941277	1.736228
H	-0.802513	-2.554378	0.014977
H	0.474201	-3.418321	0.887818
H	0.941815	-1.512848	2.321980

RE* 5

E(B3LYP) = -1700.501053 a.u.

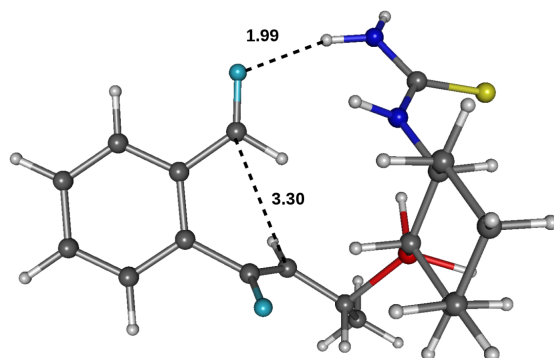


C	2.420726	-3.231468	1.167396
C	2.761374	-2.025261	0.684440
O	5.186652	-2.269878	0.762172
C	4.190359	-1.597232	0.537728
C	1.850618	-0.882495	0.262021
C	2.826266	0.237850	-0.062610
C	4.155234	-0.180669	0.084944
C	2.542563	1.537281	-0.482879
C	5.225923	0.678671	-0.174665
C	3.609946	2.402670	-0.744992

C	4.941221	1.979022	-0.591760
H	1.516822	1.874967	-0.606794
H	6.247294	0.329872	-0.049785
H	3.407555	3.420172	-1.069544
H	5.751279	2.673013	-0.799453
H	1.563651	-1.410632	-1.630279
O	0.995521	-1.198944	-0.869352
H	1.139819	-0.598534	1.044829
P	-1.597270	0.839925	2.104596
H	-0.819730	2.039105	2.147837
N	-1.911631	-0.121637	-0.868343
C	-2.607256	-1.287969	-0.837634
H	-0.911909	-0.219469	-1.020873
N	-1.836163	-2.388863	-1.107273
S	-4.262028	-1.466738	-0.542076
H	-0.826597	-2.337498	-1.001820
H	-2.281438	-3.281722	-0.951338
H	-2.326213	1.177256	3.279997
C	-2.885942	1.447837	0.862609
C	-2.379392	1.245729	-0.590085
C	-3.324152	2.908590	1.086382
C	-3.395445	1.746966	-1.638039
H	-1.472175	1.858116	-0.706229
C	-4.350528	3.380054	0.043138
H	-3.735044	3.014238	2.098270
H	-2.440687	3.564837	1.041195
C	-3.803589	3.204109	-1.379642
H	-4.278240	1.100673	-1.610665
H	-2.947872	1.640227	-2.634777
H	-4.610129	4.430973	0.228148
H	-5.277678	2.799485	0.152474
H	-4.552184	3.512142	-2.120765
H	-2.935237	3.867820	-1.519186
H	-3.749873	0.786600	1.001405
C	1.041468	-3.746727	1.427916
H	0.962263	-4.101808	2.464103
H	0.264445	-2.997421	1.258095
H	0.832115	-4.617686	0.790446
H	3.248662	-3.902643	1.402262

SZ* 1

E(B3LYP) = -1700.467255 a.u.

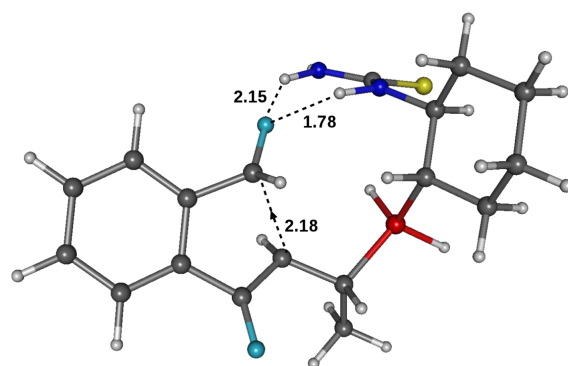


C	-0.167263	-1.869396	-2.033411
C	-1.248430	-0.918324	-1.633005
O	-1.603762	-1.903291	0.494914
C	-1.906950	-1.063726	-0.412308
C	-1.637869	1.835343	0.146970
C	-2.969975	1.231315	0.104838
C	-3.094645	-0.159387	-0.132749
C	-4.109043	2.016040	0.382358
C	-4.370116	-0.736515	-0.045217
C	-5.365540	1.430323	0.430059
C	-5.491494	0.046482	0.220598
H	-0.285382	-2.814345	-1.486225
H	-3.975318	3.078438	0.566230
H	-4.470584	-1.807963	-0.193488
H	-6.245164	2.033753	0.637980
H	-6.473422	-0.418823	0.266196
H	-1.560745	-0.166861	-2.353484
O	-1.382336	3.023412	0.366280
H	-0.811114	1.129908	-0.025683
P	1.404280	-1.110740	-1.365705
H	1.473105	0.197810	-1.856325
N	1.693623	1.321283	0.746831
C	2.228466	2.234135	-0.116409
H	0.930767	1.645108	1.332954
N	1.528284	3.391650	-0.210176
S	3.638709	1.959645	-1.016223
H	0.542691	3.439557	0.070220
H	1.845534	4.048213	-0.909407
H	2.632554	-1.676761	-1.804113
C	1.473745	-1.153053	0.477657
C	2.268069	0.027268	1.103580
C	2.035186	-2.524389	0.925811
C	2.296646	-0.117754	2.637884
H	3.293847	0.027580	0.721551
C	2.048929	-2.632753	2.457775
H	1.420858	-3.329674	0.505424
H	3.058276	-2.653745	0.541874
C	2.843188	-1.480634	3.086128
H	1.275282	0.006739	3.029692
H	2.902640	0.698325	3.049682
H	2.479686	-3.598674	2.749539
H	1.014257	-2.620127	2.826268
H	2.810264	-1.546081	4.180570
H	3.902021	-1.561826	2.798987
H	0.419149	-1.110451	0.786012
C	-0.043352	-2.119996	-3.543411
H	0.780637	-2.799349	-3.792639
H	-0.977768	-2.569842	-3.896603
H	0.099988	-1.184297	-4.097246

SZ* 2

E(B3LYP) = -1700.453041 a.u.
Frequency = -167.63 cm⁻¹

C	0.521699	-1.651296	1.547206
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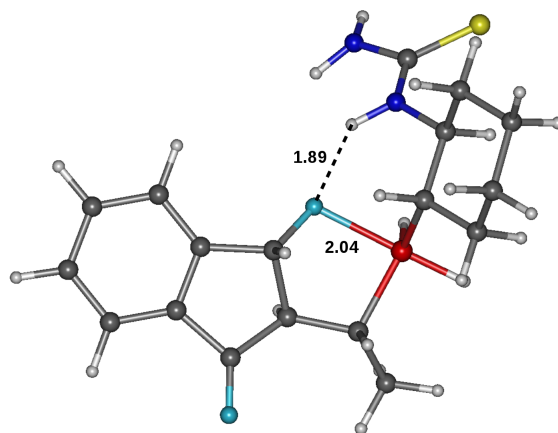


C	1.543533	-0.662746	1.013847
O	3.060982	-2.486703	0.641995
C	2.803609	-1.269914	0.607874
C	1.506667	0.627325	-0.746846
C	2.987989	0.804558	-0.607292
C	3.694567	-0.247821	-0.003014
C	3.678465	1.908475	-1.122621
C	5.092845	-0.251089	0.016744
C	5.074147	1.918186	-1.075183
C	5.779867	0.838975	-0.518708
H	0.592306	-2.575960	0.957341
H	3.126573	2.728548	-1.573509
H	5.621648	-1.084584	0.471334
H	5.621339	2.763881	-1.485044
H	6.866637	0.860787	-0.495026
H	1.625321	0.250900	1.602801
O	0.710770	1.616988	-0.698738
H	1.246946	-0.220654	-1.407442
P	-1.170601	-0.989404	1.283218
H	-1.242698	0.315594	1.784310
N	-2.022547	1.380412	-0.549579
C	-2.334533	2.229440	0.466302
H	-1.050564	1.459380	-0.899759
N	-1.420600	3.217825	0.650485
S	-3.710451	2.092602	1.453678
H	-0.485528	3.122659	0.256119
H	-1.554321	3.826998	1.444046
H	-2.096671	-1.693324	2.074821
C	-1.778687	-1.072934	-0.456279
C	-2.701239	0.128140	-0.817000
C	-2.457271	-2.432829	-0.742213
C	-3.123324	0.017083	-2.294011
H	-3.596243	0.106313	-0.186126
C	-2.896219	-2.512374	-2.214301
H	-1.776408	-3.261503	-0.507801
H	-3.337396	-2.543628	-0.092983
C	-3.797521	-1.329680	-2.596912
H	-2.236758	0.144757	-2.932498
H	-3.798300	0.850730	-2.517725
H	-3.415908	-3.463361	-2.383873
H	-2.004204	-2.522366	-2.857130
H	-4.057746	-1.384057	-3.660941
H	-4.743681	-1.396261	-2.040045

H	-0.864920	-0.999165	-1.062620
C	0.715550	-2.010153	3.039326
H	-0.003207	-2.762144	3.390435
H	1.722364	-2.423246	3.149043
H	0.638714	-1.123838	3.680353

SZ* 3

E(B3LYP) = -1700.483664 a.u.



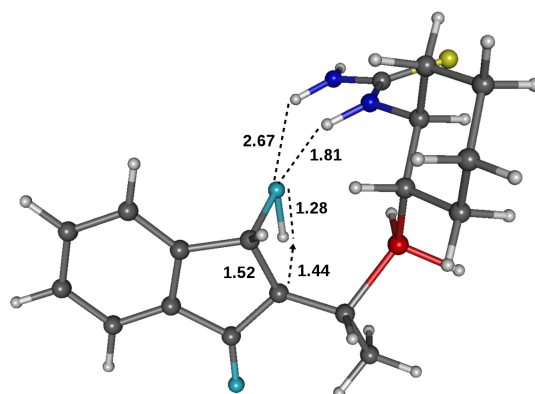
C	0.945485	-2.025159	1.160288
C	2.060730	-1.040697	0.883693
O	4.106203	-2.407821	0.592615
C	3.480022	-1.374577	0.428365
C	1.564313	-0.059089	-0.196437
C	2.829880	0.710831	-0.524567
C	3.935861	-0.122318	-0.253460
C	3.020318	1.962983	-1.099940
C	5.235748	0.266357	-0.582621
C	4.327459	2.364254	-1.408200
C	5.424260	1.523881	-1.161954
H	0.870692	-2.763345	0.347776
H	2.176102	2.613969	-1.311057
H	6.074499	-0.392121	-0.372505
H	4.495360	3.341857	-1.853635
H	6.425821	1.859573	-1.417310
H	2.197769	-0.417745	1.783150
O	0.407524	0.530524	0.279423
H	1.340321	-0.654944	-1.111437
P	-0.674699	-1.019940	1.040961
H	-0.952610	-0.063157	2.030091
N	-2.165761	1.411694	-0.182868
C	-2.784859	2.417539	0.479004
H	-1.147075	1.443299	-0.278423
N	-1.969847	3.483476	0.769076
S	-4.418994	2.431186	0.902654
H	-0.964665	3.351771	0.810240
H	-2.359624	4.174367	1.394955
H	-1.459537	-2.055411	1.670020
C	-1.691063	-0.985303	-0.532049
C	-2.776572	0.123251	-0.494450

C	-2.334120	-2.353936	-0.830783
C	-3.533666	0.152917	-1.837645
H	-3.500324	-0.100574	0.300843
C	-3.109485	-2.326061	-2.159055
H	-1.562756	-3.135058	-0.864018
H	-3.017872	-2.624134	-0.014611
C	-4.162185	-1.208539	-2.165743
H	-2.829019	0.445395	-2.630090
H	-4.300199	0.932200	-1.777471
H	-3.581467	-3.302668	-2.326220
H	-2.404142	-2.171815	-2.989228
H	-4.662826	-1.162843	-3.140968
H	-4.942642	-1.436570	-1.425005
H	-0.980488	-0.740676	-1.331465
C	1.042016	-2.762352	2.500975
H	0.197882	-3.442599	2.654849
H	1.965109	-3.352015	2.518444
H	1.075371	-2.061461	3.344170

SZ* 4

E(B3LYP) = -1700.412288 a.u.

Frequency = -1764.40 cm⁻¹

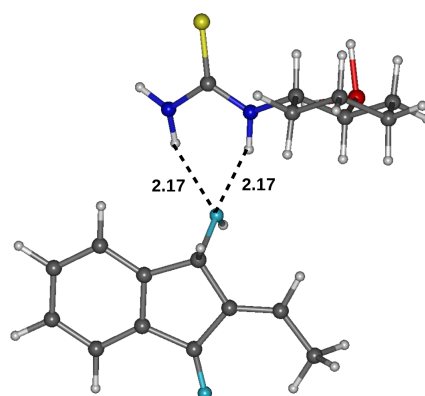


C	0.739234	2.186167	-0.319475
C	1.754639	1.065800	-0.325956
O	3.795632	2.261659	-0.959038
C	3.197944	1.306960	-0.452057
C	1.522397	-0.154061	0.558542
C	2.908169	-0.754008	0.705344
C	3.864240	0.097304	0.137475
C	3.295073	-1.957649	1.288814
C	5.221843	-0.219551	0.154771
C	4.657528	-2.285685	1.306634
C	5.613604	-1.423412	0.749033
H	0.705007	2.728371	0.642793
H	2.559313	-2.633788	1.718507
H	5.945786	0.460348	-0.286678
H	4.979291	-3.220205	1.760227
H	6.665251	-1.697837	0.777918
H	1.177667	-0.014322	-1.092999
O	0.627990	-0.876342	-0.326627

H	1.052189	0.008539	1.542598
P	-0.995016	1.506391	-0.513138
H	-1.110063	0.768491	-1.696423
N	-2.087890	-1.397624	-0.396177
C	-2.485605	-1.871446	-1.605948
H	-1.081583	-1.466463	-0.180469
N	-1.543784	-2.629211	-2.233718
S	-3.999512	-1.583673	-2.304997
H	-0.581513	-2.643708	-1.910568
H	-1.742938	-2.938788	-3.173352
H	-1.788143	2.641501	-0.777331
C	-1.864036	0.676613	0.897492
C	-2.830465	-0.431933	0.394893
C	-2.590294	1.718061	1.779089
C	-3.531293	-1.090836	1.599707
H	-3.598739	0.006548	-0.254536
C	-3.294003	1.033261	2.963073
H	-1.879410	2.470304	2.146125
H	-3.337841	2.251971	1.175454
C	-4.254381	-0.063059	2.481193
H	-2.779316	-1.632627	2.191670
H	-4.232421	-1.836986	1.210195
H	-3.831344	1.789833	3.548150
H	-2.538309	0.595873	3.631742
H	-4.713600	-0.566810	3.340452
H	-5.076855	0.394876	1.912386
H	-1.071481	0.198694	1.485353
C	0.934663	3.213233	-1.456248
H	0.231452	4.050553	-1.378692
H	1.958545	3.590673	-1.393174
H	0.828579	2.744397	-2.441680

SZ* 5

E(B3LYP) = -1700.503979 a.u.



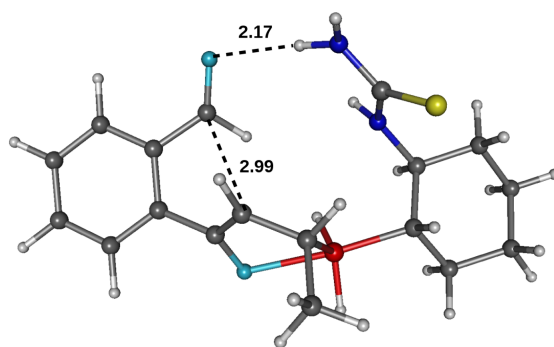
C	1.616767	2.759096	0.139481
C	2.412481	1.684403	0.295250
O	4.684971	2.595956	0.197708
C	3.913399	1.650345	0.296207
C	1.890271	0.263117	0.483921
C	3.152353	-0.577287	0.549363

C	4.297122	0.222088	0.449244
C	3.267022	-1.958181	0.709167
C	5.580437	-0.329574	0.501500
C	4.548644	-2.516590	0.757159
C	5.696349	-1.710929	0.654662
H	0.538953	2.580969	0.164927
H	2.385158	-2.587471	0.800222
H	6.453751	0.312067	0.424582
H	4.660324	-3.590563	0.882213
H	6.679364	-2.172023	0.699322
H	1.349860	0.093988	-1.413886
O	0.972795	-0.159208	-0.553486
H	1.300508	0.161146	1.401678
P	-3.352782	0.632368	-2.481156
H	-2.278410	-0.294513	-2.584558
N	-1.956077	-1.161278	-0.101761
C	-1.778204	-2.503521	-0.188016
H	-1.122852	-0.580345	-0.160876
N	-0.473197	-2.884913	-0.368497
S	-3.007372	-3.653380	-0.062547
H	0.220027	-2.197079	-0.649227
H	-0.330767	-3.844922	-0.647628
H	-4.349244	-0.381844	-2.567647
C	-3.374084	0.812115	-0.598100
C	-3.213325	-0.490961	0.218600
C	-4.672055	1.547683	-0.191950
C	-3.306433	-0.219937	1.735878
H	-4.009859	-1.188723	-0.060739
C	-4.757499	1.807952	1.319828
H	-4.745588	2.493235	-0.743890
H	-5.536679	0.939811	-0.498597
C	-4.604344	0.504879	2.115421
H	-2.441973	0.390551	2.041686
H	-3.226372	-1.178375	2.262009
H	-5.712370	2.295169	1.557108
H	-3.964043	2.512201	1.613913
H	-4.619182	0.707534	3.194129
H	-5.461609	-0.152616	1.908947
H	-2.525891	1.477297	-0.362056
C	2.031674	4.180463	-0.078176
H	1.586284	4.561911	-1.007736
H	1.634367	4.810017	0.730770
H	3.114694	4.294917	-0.120261

RZ* 1

E(B3LYP) = -1700.460926 a.u.

C	0.004645	-0.990804	1.478523
C	-1.384576	-0.465990	1.277170
O	-1.487639	-2.009457	-0.437914
C	-2.077957	-1.057777	0.257550
C	-2.344064	1.654077	-0.593304
C	-3.560097	0.832844	-0.416837
C	-3.418074	-0.549055	-0.145136
C	-4.832555	1.383998	-0.645832

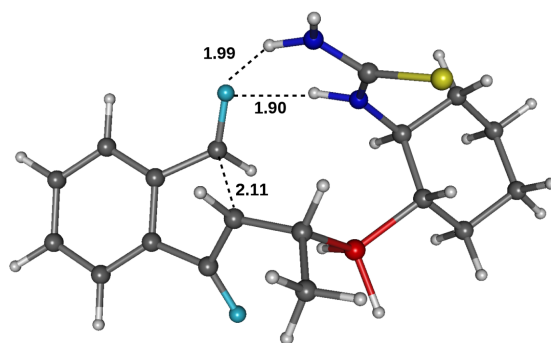


C	-4.548626	-1.372870	-0.199474
C	-5.951731	0.556320	-0.665263
C	-5.805039	-0.823600	-0.458962
H	0.690871	-0.205169	1.811102
H	-4.919034	2.450021	-0.837525
H	-4.438973	-2.436666	-0.008152
H	-6.936033	0.976189	-0.855222
H	-6.679412	-1.469188	-0.486739
H	-1.784024	0.319060	1.909029
O	-2.252391	2.868985	-0.433675
H	-1.467860	1.089267	-0.954792
P	0.580895	-1.518883	-0.217830
H	0.179011	-0.853346	-1.384561
N	1.578661	1.434514	-0.542548
C	1.596463	2.129348	0.636562
H	1.044480	1.879794	-1.280742
N	0.676942	3.134577	0.700844
S	2.632862	1.817462	1.933876
H	-0.177643	3.132403	0.140767
H	0.602158	3.591628	1.599652
H	0.732648	-2.896376	-0.436270
C	2.388569	-0.963305	-0.275236
C	2.509149	0.389861	-1.027475
C	3.279331	-2.017767	-0.967595
C	3.970676	0.862932	-1.146607
H	2.151865	0.203717	-2.051654
C	4.739715	-1.553805	-1.091394
H	3.232883	-2.961957	-0.408783
H	2.885225	-2.235774	-1.974075
C	4.837675	-0.208942	-1.824848
H	4.357935	1.090054	-0.148751
H	3.994537	1.797358	-1.722725
H	5.328108	-2.318516	-1.614836
H	5.172323	-1.453578	-0.085673
H	5.880444	0.130166	-1.861683
H	4.515838	-0.341416	-2.869731
H	2.742335	-0.817954	0.752365
C	0.116820	-2.189779	2.450532
H	1.147064	-2.558727	2.540815
H	-0.205848	-1.860922	3.444460
H	-0.532697	-3.013102	2.136885

RZ* 2

E(B3LYP) = -1700.450422 a.u.

Frequency = -187.81 cm^{-1}

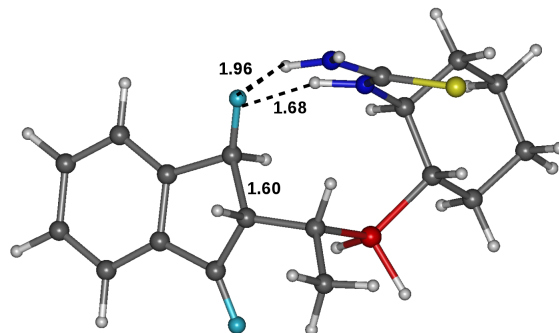


C	-0.164020	-0.580158	1.675860
C	-1.503532	-0.169269	1.098605
O	-2.030080	-2.425683	0.572164
C	-2.365744	-1.214862	0.617184
C	-1.722717	0.891321	-0.713233
C	-3.197405	0.597384	-0.686726
C	-3.538838	-0.626315	-0.077591
C	-4.182543	1.379036	-1.296935
C	-4.842585	-1.122954	-0.152802
C	-5.493951	0.896947	-1.339434
C	-5.820439	-0.350597	-0.783601
H	0.474218	0.299161	1.801162
H	-3.917613	2.331440	-1.747690
H	-5.088974	-2.078248	0.303304
H	-6.269063	1.487462	-1.822188
H	-6.845232	-0.710104	-0.833762
H	-1.956013	0.672147	1.617649
O	-1.230702	2.062853	-0.720229
H	-1.191848	0.116287	-1.306614
P	0.727901	-1.626610	0.436904
H	-0.013587	-1.834129	-0.730668
N	1.508345	1.332173	-0.428202
C	1.831237	2.066829	0.672816
H	0.608694	1.596056	-0.854956
N	0.922431	3.033049	0.955834
S	3.188304	1.826145	1.668150
H	0.014304	3.040327	0.486017
H	1.055047	3.559884	1.806303
H	0.935093	-2.916125	0.949143
C	2.383152	-1.023569	-0.120630
C	2.250836	0.230589	-1.039933
C	3.119461	-2.177778	-0.842683
C	3.624292	0.652223	-1.603099
H	1.632089	-0.063220	-1.899807
C	4.481138	-1.719869	-1.390765
H	3.257639	-3.021461	-0.154383
H	2.505416	-2.548376	-1.678582
C	4.327101	-0.508847	-2.319291
H	4.246088	1.024720	-0.783361
H	3.459711	1.490201	-2.291233
H	4.954459	-2.556297	-1.920101

H	5.140244	-1.459266	-0.551061
H	5.310018	-0.179150	-2.677253
H	3.753160	-0.804118	-3.211521
H	2.937073	-0.725455	0.778969
C	-0.248426	-1.311110	3.036395
H	0.744585	-1.559391	3.432759
H	-0.730933	-0.638656	3.753917
H	-0.849434	-2.220759	2.957544

RZ* 3

E(B3LYP) = -1700.461404 a.u.



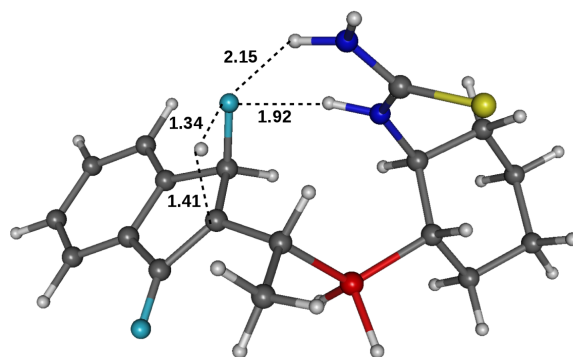
C	-0.230408	0.714772	1.632986
C	-1.585109	0.705789	0.910303
O	-2.564709	-0.997403	2.386963
C	-2.622896	-0.311565	1.366813
C	-1.567035	0.504285	-0.677144
C	-3.037861	0.137429	-0.894582
C	-3.612829	-0.393025	0.273787
C	-3.784957	0.220349	-2.067286
C	-4.919748	-0.894621	0.286817
C	-5.098237	-0.261714	-2.054359
C	-5.661338	-0.820876	-0.892171
H	0.407913	1.436302	1.115594
H	-3.345116	0.652618	-2.961684
H	-5.345096	-1.304927	1.199062
H	-5.698211	-0.208698	-2.960127
H	-6.684769	-1.186329	-0.914081
H	-2.012115	1.711276	1.037584
O	-1.021913	1.480689	-1.414842
H	-1.027499	-0.481999	-0.819430
P	0.654601	-0.902416	1.436322
H	-0.217834	-1.890211	0.956411
N	1.568551	0.824229	-1.131696
C	2.095102	1.972734	-0.631006
H	0.575963	0.948658	-1.468746
N	1.283485	3.043800	-0.824106
S	3.572307	2.133798	0.208484
H	0.306366	2.879914	-1.098672
H	1.565838	3.921617	-0.414226
H	0.984486	-1.371757	2.719311
C	2.224096	-1.010870	0.468644
C	2.087382	-0.531112	-1.009664

C	2.743984	-2.465208	0.567956
C	3.412180	-0.754276	-1.771650
H	1.329511	-1.161064	-1.494644
C	4.063162	-2.632163	-0.204477
H	2.888636	-2.748489	1.618982
H	1.997891	-3.158339	0.149848
C	3.902431	-2.204774	-1.668803
H	4.167348	-0.069102	-1.374304
H	3.239471	-0.474127	-2.817484
H	4.384960	-3.678989	-0.137557
H	4.843659	-2.025578	0.274760
H	4.857007	-2.309135	-2.198861
H	3.192111	-2.881077	-2.169642
H	2.918098	-0.321628	0.970907
C	-0.303051	1.108091	3.123238
H	0.696024	1.201977	3.564153
H	-0.784963	2.089636	3.194665
H	-0.896177	0.396266	3.702200

RZ* 4

E(B3LYP) = -1700.399342 a.u.

Frequency = -1780.83 cm⁻¹

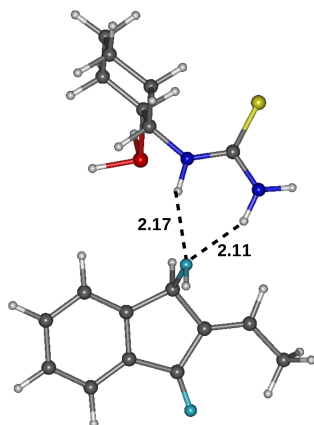


C	0.275318	-1.459737	0.972262
C	1.561700	-0.965914	0.347432
O	3.127530	-1.314418	2.195228
C	2.812354	-0.811312	1.111265
C	1.527708	0.088715	-0.761919
C	2.960220	0.598944	-0.790529
C	3.683180	0.094781	0.297559
C	3.575326	1.438181	-1.716392
C	5.022015	0.431281	0.502078
C	4.920100	1.777722	-1.520378
C	5.637104	1.284079	-0.418710
H	-0.409754	-1.770087	0.178737
H	3.028848	1.812103	-2.578917
H	5.562050	0.029582	1.355535
H	5.418275	2.431935	-2.232132
H	6.679908	1.562966	-0.288683
H	1.540219	-1.575744	-0.921602
O	1.135209	-0.722072	-1.874071
H	0.838959	0.946295	-0.621604

P	-0.685153	-0.052166	1.781468
H	0.182915	1.035413	1.980441
N	-1.629069	-0.139035	-1.334360
C	-2.223397	-1.346435	-1.543627
H	-0.666981	-0.090584	-1.699721
N	-1.487595	-2.161176	-2.342805
S	-3.699717	-1.868094	-0.885196
H	-0.517597	-1.925374	-2.554225
H	-1.810496	-3.109149	-2.468388
H	-1.068011	-0.375417	3.098880
C	-2.233202	0.615965	1.007923
C	-2.089336	0.972763	-0.504727
C	-2.712559	1.825226	1.847604
C	-3.386795	1.620132	-1.037605
H	-1.297002	1.727363	-0.593973
C	-4.007627	2.425314	1.276491
H	-2.868333	1.521250	2.890981
H	-1.934270	2.603463	1.855238
C	-3.824301	2.823237	-0.192789
H	-4.177491	0.863921	-1.054894
H	-3.202237	1.919165	-2.076266
H	-4.296428	3.293329	1.882165
H	-4.819264	1.690106	1.362318
H	-4.759411	3.232300	-0.594112
H	-3.076171	3.628152	-0.262792
H	-2.958372	-0.206622	1.079895
C	0.413264	-2.629914	1.966727
H	-0.570069	-3.004765	2.273708
H	0.942261	-3.441228	1.456155
H	1.007911	-2.362743	2.841989

RZ* 5

E(B3LYP) = -1700.499725 a.u.



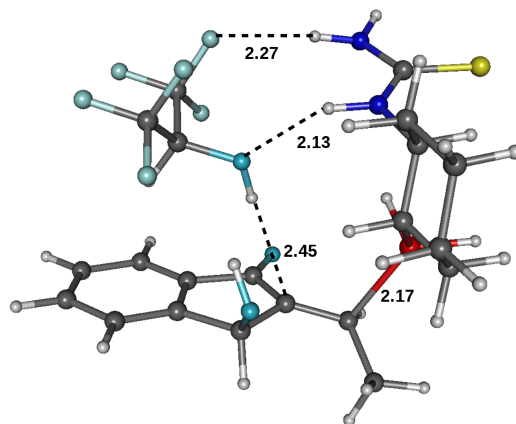
C	2.423525	-3.087761	0.127125
C	2.826212	-1.803947	0.086384
O	5.267847	-1.931809	0.268001
C	4.231791	-1.287326	0.161468
C	1.871030	-0.618316	-0.029187
C	2.793850	0.585969	-0.022880

C	4.133650	0.195594	0.089673
C	2.460666	1.937419	-0.114167
C	5.169024	1.133665	0.121325
C	3.492342	2.881562	-0.086626
C	4.835792	2.485069	0.031890
H	1.346738	-3.267485	0.083780
H	1.424922	2.254004	-0.203927
H	6.200283	0.804219	0.212690
H	3.252223	3.939612	-0.153788
H	5.616875	3.240302	0.054606
H	1.587727	-0.651166	-1.993779
O	1.020668	-0.664262	-1.203184
H	1.153869	-0.584993	0.798088
P	-1.538039	0.729879	2.188885
H	-1.011091	2.058236	2.238815
N	-2.011885	-0.112645	-0.805410
C	-2.470325	-1.391758	-0.814365
H	-1.035981	-0.000271	-1.063720
N	-1.554452	-2.295603	-1.281553
S	-4.009034	-1.914443	-0.346601
H	-0.570375	-2.047019	-1.336763
H	-1.802301	-3.269230	-1.183059
H	-2.174216	0.850210	3.457002
C	-3.059463	1.126434	1.138744
C	-2.696271	1.115850	-0.369879
C	-3.752229	2.449312	1.522629
C	-3.903811	1.461540	-1.265632
H	-1.943255	1.902372	-0.529653
C	-4.965505	2.757579	0.630740
H	-4.055290	2.407355	2.576340
H	-3.029530	3.276562	1.441665
C	-4.561475	2.784840	-0.849224
H	-4.632475	0.647206	-1.205409
H	-3.560301	1.510813	-2.307200
H	-5.407368	3.718429	0.926730
H	-5.738493	1.991132	0.784591
H	-5.436236	2.975498	-1.484135
H	-3.864300	3.620923	-1.019445
H	-3.751295	0.293171	1.312573
C	3.277651	-4.313002	0.223332
H	3.008968	-4.881384	1.125066
H	3.074126	-4.978122	-0.627869
H	4.341252	-4.076843	0.251721

SE^A 4 - Transition state mention in figure 7 in manuscript

E(B3LYP) = -2490.31027311 a.u.

C	-0.69573700	3.11185000	-1.27413000
C	0.49753300	2.46941500	-0.82044600
O	1.22305800	1.59033000	-2.96088800
C	1.41372100	1.87537800	-1.76653300
C	1.17308700	2.70189400	0.51813100
C	2.56936600	2.13260400	0.29355500
C	2.70999200	1.67655400	-1.02517200
C	3.62764900	2.02869700	1.19373500



C	3.91071600	1.13214000	-1.48019600
C	4.83570400	1.47173900	0.74606100
C	4.97865200	1.03369300	-0.57915500
H	3.52184000	2.36817600	2.22134100
H	3.99911800	0.79556900	-2.50989700
H	5.67365400	1.38407200	1.43310000
H	5.92689200	0.61410800	-0.90581500
H	0.67912000	0.06002400	-0.39430300
O	0.50828800	2.15338600	1.68324400
H	1.23803000	3.76987300	0.76499700
P	-2.35097300	1.70919800	-1.14643500
H	-1.88190500	0.66156000	-1.95473500
N	-2.38559200	-1.37490200	-0.29673100
C	-2.82743000	-1.99825900	-1.42377900
H	-1.40929400	-1.49228800	-0.03532000
N	-1.91291900	-2.81247800	-2.01672200
S	-4.35976600	-1.78104900	-2.10567800
H	-1.04597600	-3.08040700	-1.56639300
H	-2.21504400	-3.34161500	-2.82131800
H	-3.67042200	1.85667600	-1.65442700
C	-2.60633600	0.97610100	0.53774400
C	-3.17631200	-0.46952700	0.52582600
C	-3.49986200	1.89844500	1.40143200
C	-3.28750300	-1.00179000	1.96875400
H	-4.17323200	-0.45344000	0.07482400
C	-3.62402900	1.35906700	2.83579100
H	-3.08808800	2.91376500	1.42236400
H	-4.49961100	1.96466300	0.94762700
C	-4.14837300	-0.08341100	2.84913400
H	-2.27940600	-1.09291900	2.40054100
H	-3.71280200	-2.01165900	1.93125200
H	-4.28784700	2.01287800	3.41552200
H	-2.63793200	1.40039200	3.31976300
H	-4.17423500	-0.46975800	3.87564200
H	-5.18501700	-0.09947300	2.48203800
H	-1.60156500	0.96928800	0.98286500
O	0.57857300	-0.74638700	0.15645000
C	1.81795500	-1.38909000	0.34709100
C	1.82939300	-1.90949400	1.79595900
C	2.00023000	-2.49036100	-0.71731800
H	0.64784100	1.19083800	1.69927100
F	2.97256600	-2.55829200	2.08258600

F	0.79812900	-2.73932600	2.05222100
F	1.72573800	-0.86040800	2.64471600
F	1.96009700	-1.93761700	-1.94253400
F	3.17276400	-3.13515100	-0.58351400
F	1.00915400	-3.41976000	-0.66151900
H	2.65941400	-0.69472400	0.24633700
C	-1.17188000	4.38700700	-0.59356600
H	-1.25194000	4.27423100	0.49160400
H	-0.43665500	5.17854400	-0.79091200
H	-2.13782200	4.72422300	-0.98436800
H	-0.73126900	3.16832300	-2.36563400