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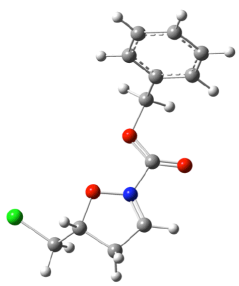
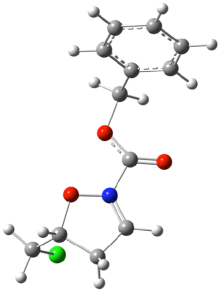
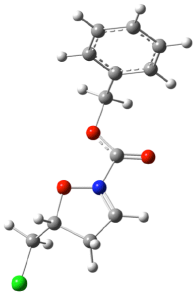
(a) R = Cl



Cl-ROT1
(2.9)

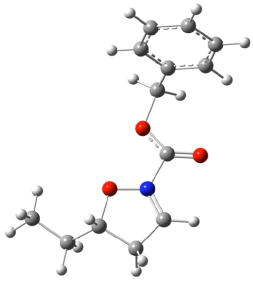


Cl-ROT2
(0.0)

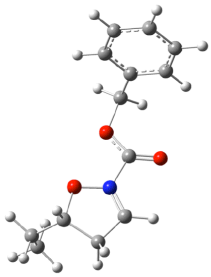


Cl-ROT3
(1.6)

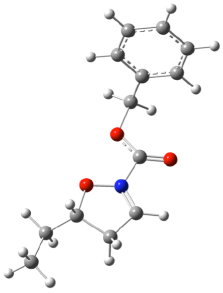
(b) R = CH_3



CH_3-ROT1
(0.0)



CH_3-ROT2
(0.7)



CH_3-ROT3
(0.2)

Figure S1. Geometry and relative energy (in kcal/mol, in parentheses) of rotamers, as determined at the B3LYP/6-31G* + ZPE level.

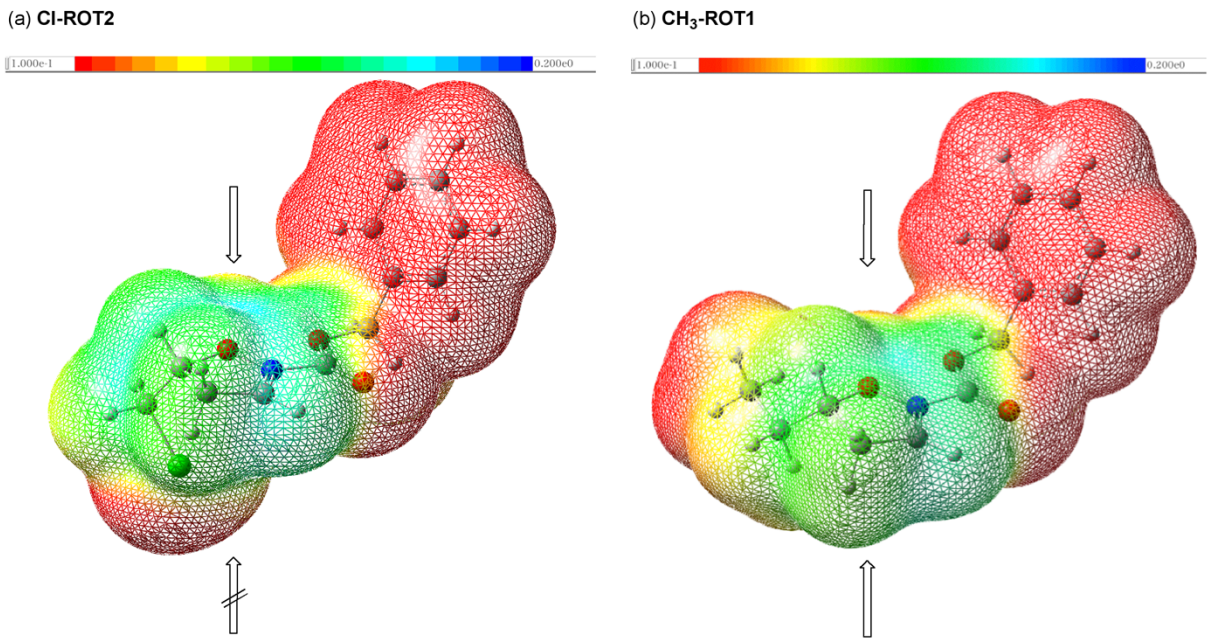


Figure S2. Electrostatic potential maps for (a) **Cl-ROT2** and (b) **CH_3-ROT1**.

Table S1. Raw energy data

(a) Cl

	E (au)	ZPE (au)	ΔE (kcal/mol)	Δ (E+ZPE) (kcal/mol)
Cl-ROT1	-1205.414579	0.236988	2.9	2.7
Cl-ROT2	-1205.419133	0.237250	0.0	0.0
Cl-ROT3	-1205.416513	0.237168	1.6	1.6

(b) CH_3

	E (au)	ZPE (au)	ΔE (kcal/mol)	Δ (E+ZPE) (kcal/mol)
CH3-ROT1	-785.146894	0.274512	0.0	0.0
CH3-ROT2	-785.146005	0.274668	0.6	0.7
CH3-ROT3	-785.146661	0.274548	0.1	0.2

XYZ coordinates of optimized geometries

=== Cl-ROT1 ===

C	-2.582344	0.916823	0.668539
O	-1.095747	0.851194	0.623918
C	-1.699323	1.244170	-1.505582
C	-3.009418	1.137265	-0.810109
H	-2.894884	-0.053786	1.056320
H	-1.478920	1.430053	-2.551002
H	-3.602310	2.049391	-0.960547
H	-3.596692	0.306572	-1.220204
N	-0.734802	1.083595	-0.671534
C	-3.001185	2.039683	1.602373
H	-4.092857	2.109905	1.602700
H	-2.582790	2.996335	1.278698
C	0.743521	1.130938	-1.028576
O	1.005375	1.333833	-2.177943
O	1.426702	0.938627	0.044646
C	2.943679	0.867426	-0.105844
H	3.210008	1.628800	-0.839267
H	3.258792	1.164770	0.892883
C	3.371840	-0.509090	-0.487151
C	3.649818	-0.819108	-1.826852
C	3.502172	-1.501024	0.496864
C	4.053086	-2.107180	-2.176399
H	3.559172	-0.051000	-2.590274
C	3.900825	-2.788121	0.143903
H	3.298957	-1.261045	1.537783
C	4.176278	-3.090847	-1.192639
H	4.278360	-2.340823	-3.212591
H	4.007402	-3.551144	0.909010
H	4.495980	-4.092339	-1.465528
Cl	-2.463893	1.731910	3.283695

=== Cl-ROT2 ===

C	-2.625015	0.925404	0.639751
O	-1.149779	0.757363	0.602056
C	-1.713562	1.256660	-1.514021
C	-3.032864	1.120792	-0.844003
H	-3.003918	-0.011616	1.055521
H	-1.478306	1.493618	-2.545639
H	-3.644655	2.015292	-1.008828
H	-3.579353	0.264524	-1.259365
N	-0.761412	1.046594	-0.677501
C	-2.962356	2.065163	1.585940
H	-2.499293	1.897127	2.559850
H	-4.046622	2.127350	1.711712
C	0.717395	1.109804	-1.004693
O	1.001710	1.347892	-2.142110
O	1.385602	0.887511	0.074115
C	2.903056	0.840398	-0.056765
H	3.169660	1.620579	-0.769992
H	3.203148	1.120300	0.951644
C	3.356502	-0.522041	-0.461123
C	3.641609	-0.804543	-1.805358
C	3.503295	-1.528173	0.505784
C	4.066976	-2.079524	-2.176179
H	3.538684	-0.025215	-2.555678
C	3.924824	-2.802078	0.131898
H	3.295703	-1.309164	1.550515
C	4.206340	-3.077551	-1.209183
H	4.297160	-2.291609	-3.215930
H	4.044403	-3.575824	0.884254
H	4.543560	-4.068615	-1.498573
Cl	-2.379962	3.656300	0.970738

=== Cl-ROT3 ===

C	-2.621947	0.904917	0.662394
O	-1.140938	0.757699	0.628555
C	-1.711743	1.236516	-1.491726
C	-3.028924	1.070314	-0.824748
H	-2.993094	-0.021994	1.100561
H	-1.478270	1.465806	-2.525770
H	-3.685962	1.931541	-0.995579
H	-3.547713	0.194935	-1.237003
N	-0.755027	1.055692	-0.651547
C	-2.935177	2.097455	1.560470
H	-2.526748	3.026059	1.154206
H	-2.536066	1.934875	2.562621
C	0.724818	1.128247	-0.982074
O	1.004458	1.373444	-2.119047
O	1.395534	0.904416	0.094371
C	2.914729	0.846070	-0.041983
H	3.184017	1.630227	-0.749827
H	3.218559	1.115446	0.968129
C	3.355284	-0.516181	-0.458650
C	3.638743	-0.788564	-1.805430
C	3.492097	-1.532599	0.499138
C	4.052904	-2.063778	-2.187780
H	3.543778	-0.001326	-2.548527
C	3.902119	-2.806676	0.113529
H	3.285724	-1.321595	1.545747
C	4.182231	-3.071987	-1.229960
H	4.282151	-2.268260	-3.229235
H	4.013873	-3.588585	0.858566
H	4.510568	-4.063331	-1.528400
Cl	-4.719836	2.273179	1.684357

=== CH3-ROT1 ===

C	-2.668184	0.726163	-0.056925
O	-1.229649	0.725352	0.372828
C	-1.480635	2.657992	-0.745946
C	-2.866771	2.123825	-0.700477
H	-2.727096	-0.068696	-0.806062
H	-1.100533	3.582285	-1.166504
H	-3.498522	2.790698	-0.095456
H	-3.312785	2.083049	-1.700259
N	-0.673099	1.855924	-0.145988
C	-3.537895	0.421032	1.150992
H	-4.579703	0.481731	0.807460
H	-3.403518	1.219281	1.892193
C	-3.267874	-0.952269	1.774297
H	-2.241413	-1.027542	2.146024
H	-3.943430	-1.120369	2.617438
H	-3.430872	-1.757961	1.049851
C	0.809296	2.099756	0.035551
O	1.245756	3.119955	-0.413184
O	1.315481	1.102255	0.677474
C	2.820182	1.125083	0.898522
H	3.076766	2.156931	1.139705
H	2.906772	0.490819	1.779268
C	3.542005	0.593928	-0.294805
C	4.104114	1.472661	-1.232578
C	3.667075	-0.791273	-0.480146
C	4.783119	0.970021	-2.341890
H	4.016270	2.546119	-1.088396
C	4.341520	-1.290727	-1.591893
H	3.243725	-1.475675	0.251236

C	4.899926	-0.409825	-2.522490
H	5.226369	1.653594	-3.059758
H	4.442096	-2.363304	-1.727923
H	5.433848	-0.799936	-3.384126

=== CH3-ROT2 ===

C	-2.677478	0.792943	-0.109932
O	-1.250794	0.814487	0.351089
C	-1.495889	2.719894	-0.813277
C	-2.883172	2.191323	-0.749977
H	-2.705246	0.013418	-0.876449
H	-1.114236	3.633293	-1.255748
H	-3.502522	2.867072	-0.143556
H	-3.341265	2.144614	-1.743718
N	-0.688657	1.929713	-0.196674
C	-3.561670	0.420521	1.073186
H	-3.277965	-0.588734	1.392403
H	-4.584715	0.337640	0.682387
C	-3.512178	1.381499	2.264723
H	-3.866361	2.387714	2.011970
H	-4.159117	1.009012	3.063639
H	-2.498719	1.462745	2.670036
C	0.793689	2.173648	-0.021445
O	1.235010	3.176252	-0.504166
O	1.294873	1.197376	0.656114
C	2.798936	1.223198	0.881442
H	3.059923	2.264053	1.074288
H	2.879903	0.630655	1.791284
C	3.521314	0.632311	-0.283040
C	4.079522	1.462104	-1.266673
C	3.650530	-0.760303	-0.395162
C	4.758451	0.903561	-2.348939
H	3.989000	2.541450	-1.179065
C	4.325592	-1.315788	-1.479673
H	3.229906	-1.406338	0.371804
C	4.879764	-0.483578	-2.456351
H	5.198679	1.549516	-3.102616
H	4.429566	-2.393729	-1.558789
H	5.413990	-0.916937	-3.296876

=== CH3-ROT3 ===

C	-2.665252	0.807364	-0.027312
O	-1.233268	0.800870	0.413054
C	-1.464125	2.725905	-0.721042
C	-2.858786	2.215561	-0.649684
H	-2.722965	0.029354	-0.794551
H	-1.075517	3.641305	-1.153201
H	-3.461073	2.888247	-0.021224
H	-3.330507	2.195619	-1.637714
N	-0.661387	1.915983	-0.125256
C	-3.533477	0.468927	1.173037
H	-3.420905	1.256638	1.928115
H	-3.155404	-0.458782	1.616561
C	-5.007935	0.298460	0.780553
H	-5.137715	-0.500944	0.042808
H	-5.597548	0.034776	1.662485
H	-5.434956	1.218629	0.365160
C	0.826286	2.137969	0.038745
O	1.273735	3.147459	-0.423333
O	1.323230	1.138274	0.684190
C	2.829670	1.141081	0.893848
H	3.103083	2.171430	1.122656
H	2.913588	0.514431	1.780265
C	3.534788	0.587521	-0.299284
C	4.100142	1.448540	-1.251448
C	3.641061	-0.801124	-0.469868
C	4.763758	0.924943	-2.360362
H	4.026883	2.524582	-1.118791
C	4.300306	-1.321513	-1.581159
H	3.215104	-1.471823	0.272598
C	4.862024	-0.458223	-2.526128
H	5.209632	1.594741	-3.089509
H	4.386466	-2.396735	-1.705718
H	5.384110	-0.864651	-3.387479