

Supplementary Information

Table S1. Cartesian coordinates of optimized transition states of Phe + OH reaction.

TS-Ra	N	2.909296	-0.084005	-1.244712
	H	2.985316	-1.023650	-1.621062
	C	1.680926	0.094575	-0.514959
	H	1.598309	1.203207	-0.260088
	C	1.630676	-0.672913	0.809080
	O	1.977472	-1.818342	0.940659
	C	0.482540	-0.286145	-1.409638
	H	0.551913	0.346743	-2.298335
	H	0.636123	-1.320089	-1.738774
	O	1.148472	0.070690	1.833482
	H	3.723196	0.095158	-0.667549
	H	1.101985	-0.508651	2.609878
	O	1.396799	2.632539	0.339822
	H	1.055234	2.286412	1.183777
	C	-0.884585	-0.166695	-0.770239
	C	-1.629494	-1.311330	-0.471708
	C	-1.435979	1.087227	-0.477633
	C	-2.895898	-1.211793	0.102764
	H	-1.216723	-2.290037	-0.694735
	C	-2.700087	1.187881	0.096133
H	-0.860478	1.983155	-0.679707	
C	-3.435703	0.039373	0.386607	
H	-3.459907	-2.111460	0.322898	
H	-3.113980	2.166437	0.313737	
TS-Rb	N	2.752774	-1.274386	-0.448224
	H	3.561387	-0.745357	-0.756907
	C	1.525292	-0.530110	-0.733312
	H	1.187430	-0.622123	-1.779947
	C	1.847157	0.952910	-0.558077
	O	2.954265	1.384998	-0.360063
	C	0.400210	-1.091310	0.165118
	H	0.400275	-2.177992	0.036587
	H	0.817285	-0.936497	1.289618
	O	0.772551	1.741053	-0.730991
	H	2.749155	-2.177877	-0.906796
	H	1.076534	2.655357	-0.625134
	O	1.679522	-0.638003	2.262550
	H	2.466383	-0.904070	1.747389
	C	-0.995238	-0.548484	0.093309
	C	-1.416578	0.483195	0.940441
	C	-1.921534	-1.104649	-0.797882
	C	-2.722843	0.957872	0.884085
	H	-0.714219	0.898320	1.653391
	C	-3.225574	-0.620456	-0.865133
H	-1.619673	-1.922920	-1.444439	
C	-3.629939	0.413037	-0.023335	
H	-3.035339	1.751353	1.553819	
H	-3.927239	-1.057835	-1.566773	
H	-4.647821	0.783921	-0.066488	
TS-Ria	N	2.825718	1.439206	0.619270
	H	3.183915	1.634864	-0.311927
	C	1.667146	0.534645	0.530003
	H	1.360824	0.294168	1.550803
	C	2.086675	-0.763951	-0.157589
	O	2.082469	-0.970090	-1.346521

	C	0.526729	1.243728	-0.211870
	H	0.433555	2.244024	0.211695
	H	0.791153	1.354792	-1.264943
	C	-0.809462	0.537546	-0.107980
	C	-1.562158	0.640240	1.099876
	H	-1.316706	1.437050	1.792889
	C	-1.127680	-0.543697	-0.982457
	H	-0.534682	-0.668366	-1.879409
	C	-2.609467	-0.222500	1.369046
	H	-3.184023	-0.107127	2.281173
	C	-2.179540	-1.400787	-0.704928
	H	-2.418938	-2.200073	-1.397230
	C	-2.925573	-1.247889	0.469019
	H	-3.744940	-1.924468	0.683792
	O	2.578811	-1.660822	0.732346
	H	2.892181	-2.420304	0.217514
	H	3.576480	1.003850	1.146633
	O	-1.734502	2.002512	-1.137995
	H	-2.633094	1.640336	-1.167246
TS-R _{is}	N	2.801621	1.594255	-0.585559
	H	3.024064	1.243793	-1.513806
	C	1.738065	0.778754	0.027702
	H	1.627889	1.089369	1.063500
	C	2.143922	-0.688816	0.017154
	O	1.878868	-1.496487	-0.843078
	C	0.429453	1.046060	-0.727559
	H	0.313629	2.131511	-0.738756
	H	0.564039	0.733490	-1.768542
	C	-0.866067	0.416616	-0.220218
	C	-1.226470	-0.908031	-0.621914
	H	-0.444829	-1.557784	-0.993066
	C	-1.932217	1.277911	0.183479
	H	-1.693101	2.302601	0.443321
	C	-2.531983	-1.353621	-0.527552
	H	-2.774440	-2.367821	-0.824480
	C	-3.235026	0.820084	0.278533
	H	-4.019419	1.490067	0.611918
	C	-3.544480	-0.497851	-0.076466
	H	-4.567677	-0.850937	-0.015123
	O	2.967488	-0.982616	1.048739
	H	3.229347	-1.908852	0.936704
	H	3.649516	1.533397	-0.030736
	O	-0.253694	-0.031535	1.655600
	H	-1.112845	-0.260148	2.038942
TS-R _{oa}	N	2.972409	1.549953	-0.152049
	H	3.378075	1.151902	-0.995705
	C	1.837899	0.727457	0.259306
	H	1.535731	1.025204	1.265350
	C	2.173366	-0.763900	0.280003
	O	2.822439	-1.327232	-0.566634
	C	0.663727	0.974066	-0.721393
	H	0.460774	2.047333	-0.708917
	H	1.008976	0.710042	-1.725523
	C	-0.607112	0.229956	-0.405248
	C	-1.073545	-0.799116	-1.214947
	H	-0.503272	-1.084917	-2.092504
	C	-1.388778	0.618801	0.721178
	C	-2.260113	-1.475917	-0.912066
	H	-2.601247	-2.276763	-1.558505
	C	-2.561597	-0.105519	1.043914

	H	-3.123458	0.176740	1.925693
	C	-3.005087	-1.125933	0.218970
	H	-3.919670	-1.658453	0.453261
	O	1.654951	-1.400640	1.352696
	H	1.879784	-2.339673	1.259908
	H	3.700467	1.522206	0.555534
	O	-2.184509	2.349468	0.004285
	H	-2.691080	1.967372	-0.729210
	H	-0.947547	1.257209	1.473897
TS-Ros	N	-2.997274	-1.204377	-0.744519
	H	-3.471930	-0.458751	-1.247781
	C	-1.769741	-0.679458	-0.156573
	H	-1.388760	-1.372094	0.594000
	C	-1.981625	0.684467	0.499017
	O	-2.745864	1.526871	0.098429
	C	-0.695659	-0.551078	-1.277250
	H	-0.674975	-1.526838	-1.768209
	H	-1.057762	0.175003	-2.012190
	C	0.684780	-0.166276	-0.809128
	C	1.134630	1.147530	-0.877685
	H	0.482107	1.912159	-1.286846
	C	1.549601	-1.155294	-0.250240
	H	1.324640	-2.197982	-0.428496
	C	2.420745	1.496724	-0.452685
	H	2.748522	2.527639	-0.525712
	C	2.870093	-0.794746	0.125880
	H	3.530243	-1.565326	0.503713
	C	3.288493	0.521158	0.050836
	H	4.288995	0.794319	0.365661
	O	-1.202188	0.880486	1.592563
	H	-1.384853	1.779058	1.909329
	H	-3.632764	-1.505420	-0.012228
	O	0.779595	-1.480522	1.583195
	H	0.557215	-0.563979	1.813870
TS-Rma	N	-1.891803	1.756724	-0.205761
	H	-2.497473	1.985175	0.578994
	C	-1.818752	0.307618	-0.333897
	H	-1.527290	0.050399	-1.355648
	C	-3.161128	-0.371307	-0.054393
	O	-4.088763	0.144794	0.516089
	C	-0.748421	-0.282092	0.627035
	H	-0.954345	0.104637	1.631150
	H	-0.872439	-1.366307	0.667657
	C	0.671754	0.040795	0.218833
	C	1.473416	-0.937291	-0.354583
	H	1.090437	-1.941951	-0.493588
	C	1.204304	1.332613	0.390318
	H	0.576327	2.105947	0.812895
	C	2.820031	-0.671641	-0.715404
	C	2.511300	1.629159	-0.010122
	H	2.895169	2.634593	0.122041
	C	3.309468	0.652703	-0.582444
	H	4.322730	0.873953	-0.893705
	O	-3.191196	-1.648248	-0.498864
	H	-4.055074	-2.013231	-0.253426
	H	-2.330149	2.161319	-1.026558
	H	3.338910	-1.367199	-1.359401
	O	3.807180	-1.582714	0.781532
	H	3.466210	-1.038404	1.507798

TS-Rms	N	3.295080	-1.252119	-0.126779
	H	3.708970	-0.862828	0.717033
	C	1.984274	-0.644244	-0.335874
	H	1.632887	-0.898831	-1.338308
	C	2.019412	0.879539	-0.206708
	O	2.728030	1.477081	0.563777
	C	0.988965	-1.227509	0.704041
	H	1.141334	-2.309076	0.680010
	H	1.292052	-0.882186	1.697444
	C	-0.463115	-0.893729	0.450852
	C	-1.104659	0.136965	1.123472
	H	-0.568803	0.717421	1.866638
	C	-1.197543	-1.643174	-0.487532
	H	-0.712154	-2.463044	-1.007535
	C	-2.450822	0.483998	0.828463
	C	-2.541174	-1.361773	-0.747631
	H	-3.087663	-1.964761	-1.463732
	C	-3.176790	-0.327618	-0.082686
	H	-4.216594	-0.098028	-0.276386
	O	1.154628	1.505632	-1.039742
	H	1.221152	2.455004	-0.849357
H	3.921196	-1.003893	-0.887033	
H	-2.989117	1.118199	1.518055	
O	-2.287128	2.108227	-0.324227	
H	-1.524348	1.814601	-0.846223	
TS-Rpa	N	-3.208188	-1.533176	-0.326405
	H	-3.530386	-1.194647	-1.229327
	C	-2.042261	-0.753709	0.115285
	H	-1.802287	-1.064388	1.134119
	C	-2.387180	0.735069	0.134750
	O	-2.352257	1.473515	-0.819044
	C	-0.847847	-1.040297	-0.811556
	H	-0.788816	-2.126579	-0.911890
	H	-1.073026	-0.625248	-1.797790
	C	0.463727	-0.488061	-0.304223
	C	0.926315	0.776834	-0.707717
	H	0.326622	1.362383	-1.394988
	C	1.238987	-1.229624	0.606300
	H	0.891135	-2.207111	0.925578
	C	2.118448	1.285937	-0.221448
	H	2.466832	2.261276	-0.538281
	C	2.431533	-0.733020	1.100204
	H	3.021984	-1.313749	1.798057
	C	2.927602	0.518827	0.654220
	H	3.727725	0.998982	1.198677
	O	-2.843076	1.129712	1.346404
H	-3.103495	2.059777	1.258689	
H	-3.977297	-1.425810	0.327892	
O	4.383472	-0.086154	-0.607985	
H	3.817261	-0.560978	-1.235799	
TS-Rps	N	3.368861	-1.162255	-0.450910
	H	3.817693	-0.937309	0.433800
	C	2.051832	-0.528546	-0.491398
	H	1.655856	-0.602992	-1.506008
	C	2.111408	0.947670	-0.098077
	O	2.724695	1.369554	0.851585
	C	1.108073	-1.284678	0.478916
	H	1.217384	-2.343310	0.231613
	H	1.492098	-1.145541	1.494296
	C	-0.344149	-0.879959	0.412687

C	-0.886799	0.047899	1.318884
H	-0.247043	0.479056	2.082252
C	-1.192417	-1.444470	-0.556665
H	-0.789049	-2.172143	-1.253632
C	-2.228681	0.388398	1.275365
H	-2.639360	1.086344	1.995328
C	-2.532535	-1.113305	-0.613996
H	-3.178240	-1.564303	-1.356898
C	-3.078919	-0.154196	0.278000
H	-4.149639	-0.095144	0.406437
O	1.404073	1.745241	-0.927126
H	1.492256	2.650226	-0.588467
H	3.965043	-0.782981	-1.180480
O	-3.354478	1.377796	-1.006384
H	-2.460232	1.750273	-0.968766

Table S2. Entropies of reaction and entropy barriers at 298.15 K, all in kcal/mol, for the modeled channels of Phe + OH reaction in gas phase ($-T\Delta S_{gas}$, $-T\Delta S_{gas}^\ddagger$) and in solution ($-T\Delta S_{sol}$, $-T\Delta S_{sol}^\ddagger$).

	$-T\Delta S_{gas}^\ddagger$	$-T\Delta S_{gas}$	$-T\Delta S_{sol}^\ddagger$	$-T\Delta S_{sol}$
<i>Ra</i>	10.01	-0.26	5.58	-0.26
<i>Rb</i>	10.50	-0.22	6.07	-0.22
<i>Ria</i>	10.50		6.07	
<i>Ris</i>	11.12	11.30	6.69	6.87
<i>Roa</i>	9.91	10.96	5.48	6.53
<i>Ros</i>	11.38	11.84	6.95	7.41
<i>Rma</i>	9.89	10.48	5.46	6.05
<i>Rms</i>	9.96	10.37	5.53	5.94
<i>Rpa</i>	9.94		5.51	
<i>Rps</i>	9.08	10.31	4.65	5.88

Table S3. Cartesian coordinates of optimized transition states of GFG + OH reaction.

GFG-TS _a	C	4.799271	-0.950529	-0.221538
	H	4.694660	-1.422981	-1.203755
	H	4.885310	-1.765016	0.519762
	C	3.517750	-0.205934	0.134102
	O	3.531900	0.745619	0.911297
	N	2.382556	-0.690949	-0.425694
	H	2.401222	-1.534871	-0.989364
	C	1.058528	-0.206351	-0.137515
	H	0.952128	-0.090815	1.028407

	C	0.081812	-1.306565	-0.576460
	O	0.447012	-2.203960	-1.329213
	C	0.810045	1.187411	-0.772549
	H	1.601159	1.838292	-0.393107
	H	0.975825	1.077191	-1.849179
	C	-0.544297	1.816315	-0.526730
	C	-1.422012	2.039387	-1.592605
	H	-1.127578	1.747615	-2.595810
	C	-0.938466	2.207986	0.760125
	H	-0.275058	2.027210	1.598504
	C	-2.663746	2.636651	-1.385061
	H	-3.327487	2.805998	-2.225833
	C	-2.183980	2.796311	0.968594
	H	-2.476906	3.086055	1.971445
	C	-3.049493	3.015073	-0.101588
	H	-4.016266	3.476872	0.064101
	N	-1.169281	-1.224669	-0.083752
	H	-1.439180	-0.482982	0.550712
	C	-2.178146	-2.195932	-0.441610
	H	-2.502042	-2.086606	-1.483147
	H	-1.787604	-3.212945	-0.347267
	C	-3.384082	-2.030787	0.455138
	O	-3.507202	-1.187688	1.304416
	O	1.166950	0.259420	2.400799
	H	2.056924	0.638295	2.249223
	O	-4.323031	-2.953794	0.171984
	H	-5.069456	-2.792747	0.768556
	N	5.917287	-0.015554	-0.228190
	H	5.802664	0.623273	0.553693
	H	6.793630	-0.508636	-0.101573
GFG-TSb	N	3.886396	-3.469032	-1.007298
	H	4.100860	-2.674400	-1.603500
	C	3.067390	-2.995878	0.101759
	H	2.519167	-3.828738	0.553716
	H	3.633659	-2.505602	0.913989
	C	2.086579	-1.945346	-0.408384
	O	2.381467	-1.183267	-1.322430
	H	4.761290	-3.851093	-0.667464
	N	0.887928	-1.895360	0.229056
	H	0.711790	-2.423109	1.078622
	C	-0.100415	-0.865446	-0.086618
	H	-0.000239	-0.643792	-1.151741
	C	0.263096	0.398273	0.720341
	O	-0.115208	0.588200	1.876038
	C	-1.497438	-1.432860	0.180240
	H	-1.550797	-2.400630	-0.324076
	H	-1.509946	-1.746576	1.325970
	C	-2.697634	-0.603429	-0.151311
	C	-3.004072	0.595344	0.512737
	H	-2.363189	0.939887	1.313810
	C	-3.573462	-1.052673	-1.152076
	H	-3.361872	-1.986175	-1.663024
	C	-4.134742	1.327194	0.164225
	H	-4.358609	2.248159	0.690964
	C	-4.700026	-0.316256	-1.503583
	H	-5.357683	-0.678126	-2.285878
	C	-4.983762	0.879050	-0.846529
	H	-5.864658	1.451968	-1.113307
	N	1.082539	1.251446	0.073565
	H	1.490251	0.980273	-0.815432

	C	1.611277	2.427868	0.727187
	H	0.808289	2.990749	1.208798
	H	2.325946	2.176219	1.520435
	C	2.311154	3.306149	-0.285841
	O	2.485192	3.029385	-1.443177
	O	2.737089	4.449925	0.285040
	H	3.189138	4.960292	-0.403631
	O	-0.913050	-2.061899	2.576894
	H	-0.663011	-1.129364	2.742691
GFG-TSo	C	-4.274464	-2.078749	0.049289
	H	-4.001971	-2.753502	0.868269
	H	-4.327678	-2.692789	-0.866995
	C	-3.148951	-1.075395	-0.190262
	O	-3.365775	0.028442	-0.673107
	N	-1.901316	-1.501847	0.131058
	H	-1.725336	-2.445204	0.451204
	C	-0.731401	-0.713622	-0.192314
	H	-0.913993	-0.213142	-1.147615
	C	0.443101	-1.689010	-0.339873
	O	0.370843	-2.847459	0.039492
	C	-0.439607	0.383948	0.886271
	H	-1.402775	0.684930	1.300774
	H	0.155036	-0.047670	1.695194
	C	0.219959	1.620337	0.332385
	C	1.569167	1.906069	0.520131
	H	2.188555	1.217389	1.084513
	C	-0.594140	2.557197	-0.372498
	H	-1.584694	2.250588	-0.683892
	C	2.135760	3.066599	-0.024522
	H	3.188661	3.272293	0.133907
	C	0.007012	3.696322	-0.960964
	H	-0.613100	4.379152	-1.528494
	C	1.354265	3.958581	-0.766018
	H	1.803053	4.849206	-1.190947
	N	1.561488	-1.173482	-0.926675
	H	1.608477	-0.175082	-1.071951
	C	2.786275	-1.933169	-0.968426
	H	2.535437	-2.994251	-1.003280
	H	3.355595	-1.697983	-1.871207
	C	3.682542	-1.699469	0.241284
	O	3.467599	-0.936558	1.146129
	O	-1.529023	3.418284	1.204814
	H	-0.746012	3.789847	1.640758
	O	4.786205	-2.470032	0.162350
	H	5.319095	-2.288753	0.951203
	N	-5.503906	-1.362139	0.365912
	H	-5.513066	-0.503586	-0.178566
	H	-6.315049	-1.908406	0.100728
GFG-TSm	N	-5.980060	0.374612	0.148782
	H	-5.713637	1.115613	-0.494199
	C	-5.026758	-0.717724	-0.009961
	H	-5.029408	-1.358067	0.878638
	H	-5.221883	-1.372145	-0.877785
	C	-3.631577	-0.139411	-0.231081
	O	-3.464577	0.912728	-0.837288
	H	-6.915029	0.070561	-0.097272
	N	-2.602958	-0.876450	0.253645
	H	-2.746603	-1.765315	0.715974
	C	-1.223037	-0.515085	0.002605
	H	-1.129246	-0.203774	-1.042002

	C	-0.385035	-1.780513	0.238403
	O	-0.852604	-2.766790	0.793180
	C	-0.760167	0.674834	0.903467
	H	-1.634020	1.316255	1.027267
	H	-0.487171	0.298859	1.893084
	C	0.363398	1.492132	0.306605
	C	1.654486	1.455664	0.814142
	H	1.883435	0.840498	1.676423
	C	0.097456	2.313116	-0.808849
	H	-0.913332	2.350891	-1.202647
	C	2.685619	2.257670	0.259790
	H	3.712743	2.044267	0.516897
	C	1.111232	3.071483	-1.399307
	H	0.885179	3.690045	-2.260498
	C	2.401896	3.029012	-0.893775
	H	3.194878	3.610586	-1.346741
	N	0.897744	-1.730055	-0.191191
	H	1.289782	-0.888868	-0.594975
	C	1.802327	-2.835326	0.035866
	H	1.803628	-3.139556	1.087399
	H	1.510270	-3.722841	-0.535689
	C	3.202750	-2.434274	-0.367014
	O	3.515916	-1.355479	-0.802234
	O	4.068677	-3.445871	-0.178827
	H	4.943137	-3.130243	-0.452588
	O	2.818486	3.725031	1.647329
	H	1.921474	4.080071	1.547449
GFG-TSp	C	-5.097351	-0.448936	-0.108965
	H	-5.161745	-0.937203	0.869499
	H	-5.272837	-1.230529	-0.869073
	C	-3.675481	0.051856	-0.349316
	O	-3.445258	0.990836	-1.100758
	N	-2.693281	-0.633079	0.287864
	H	-2.890472	-1.403948	0.912729
	C	-1.291303	-0.338858	0.074135
	H	-1.137363	-0.136146	-0.988896
	C	-0.506000	-1.586356	0.499313
	O	-0.970751	-2.392171	1.295794
	C	-0.850207	0.923607	0.880640
	H	-1.620616	1.675436	0.694792
	H	-0.870859	0.680166	1.946131
	C	0.494734	1.473436	0.478585
	C	1.612418	1.374924	1.323888
	H	1.503186	0.900120	2.293468
	C	0.651022	2.094354	-0.776425
	H	-0.209819	2.185097	-1.431416
	C	2.846940	1.867928	0.935510
	H	3.702162	1.788397	1.595145
	C	1.879177	2.587514	-1.178230
	H	1.989599	3.063016	-2.144871
	C	2.997972	2.530722	-0.308039
	H	3.988347	2.706528	-0.701783
	N	0.723850	-1.722575	-0.045901
	H	1.094912	-1.040511	-0.693979
	C	1.590962	-2.821282	0.314130
	H	1.904553	-2.771191	1.363089
	H	1.079849	-3.780893	0.193863
	C	2.823448	-2.793378	-0.561198
	O	3.057503	-1.959225	-1.397730
	O	3.094103	4.451879	0.313952

H	2.210769	4.506700	0.710546
N	-6.021216	0.677280	-0.175936
H	-5.699505	1.300474	-0.911895
H	-6.952320	0.360959	-0.421031
O	3.640484	-3.824244	-0.280965
H	4.410065	-3.747637	-0.865023

Table S4. Entropies of reaction and entropy barriers at 298.15 K, all in kcal/mol, for the modeled channels of GFG + OH reaction in gas phase ($-T\Delta S_{gas}$, $-T\Delta S_{gas}^\ddagger$) and in solution ($-T\Delta S_{sol}$, $-T\Delta S_{sol}^\ddagger$).

	$-T\Delta S_{gas}^\ddagger$	$-T\Delta S_{gas}$	$-T\Delta S_{sol}^\ddagger$	$-T\Delta S_{sol}$
<i>alpha</i>	11.34	26.50	6.91	-0.32
<i>beta</i>	11.47	-0.53	7.04	-0.53
<i>ortho</i>	10.76	11.04	6.33	6.61
<i>meta</i>	9.84	10.75	5.41	6.32
<i>para</i>	9.25	10.65	4.82	6.22

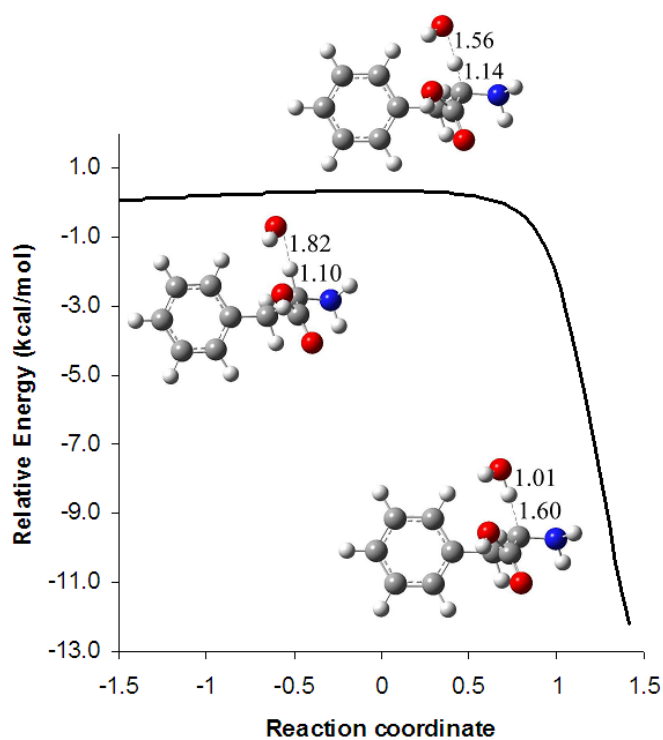


Figure S1. Intrinsic reaction coordinate calculation for the *Ra* reaction path.

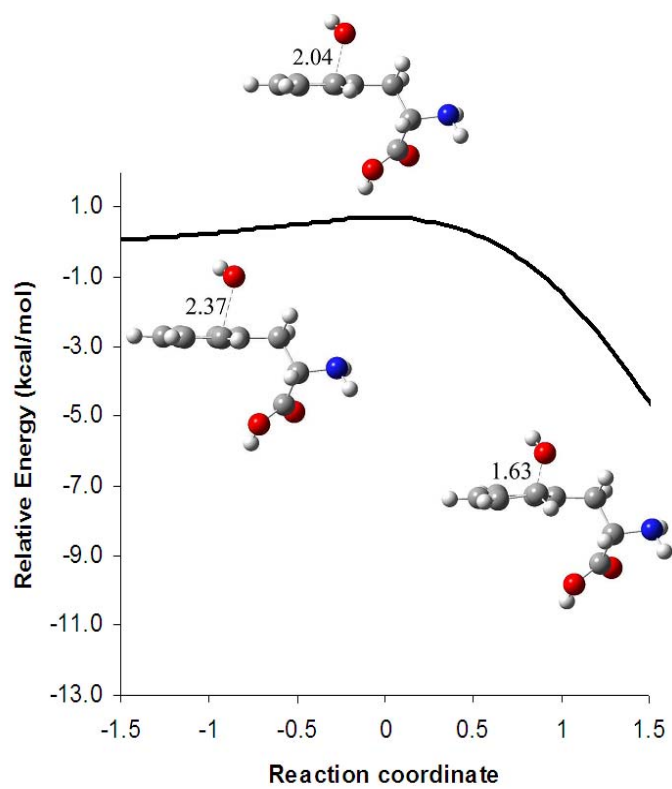


Figure S1. Intrinsic reaction coordinate calculation for the *Roa* reaction path.