

Supplementary Materials: A Computational Study of the Mechanism of Succinimide Formation in the Asn–His Sequence: Intramolecular Catalysis by the His Side Chain

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Cartesian coordinates (in Å), total energies (in au), zero-point energies (in kJ mol⁻¹), and SM8 hydration free energies (in kJ mol⁻¹) of the B3LYP/6-31+G(d,p) optimized geometries.

Geometry: R

Total energy: -1136.999684

Zero-point energy: 920.3961

Hydration free energy: -94.4271731

Cartesian coordinates:

6	-5.023267737	0.347721433	2.158811172
6	-4.075648744	-0.102801669	1.064569563
8	-4.403945115	-0.958843962	0.232100541
7	-2.855529810	0.492231680	1.039447469
1	-2.541298583	1.109665462	1.780998167
6	-1.829224048	0.065632579	0.108341611
6	-0.495749007	0.689480417	0.549593118
8	-0.428379550	1.380061854	1.581142910
7	0.555529818	0.425442051	-0.241806909
1	0.410518212	-0.138217688	-1.080244826
6	1.938426088	0.739316795	0.136634615
6	-2.192681021	0.408303338	-1.371665927
6	-1.829924336	-0.766483816	-2.268552478
8	-0.704332676	-0.882692624	-2.758698735
7	-2.819502778	-1.682084281	-2.431690994
1	-2.582058313	-2.553362228	-2.885429023
6	2.325383663	2.183944444	-0.278600444
8	3.217148218	2.424190530	-1.090723167
7	1.613643182	3.150885343	0.351976745
1	0.888977099	2.864321436	1.003345851
6	1.829112620	4.561663223	0.068544193
6	2.899836906	-0.295962103	-0.467686257
6	2.843823508	-1.636237206	0.205439633
6	3.866319029	-2.297299185	0.848575958
7	3.321894522	-3.488332044	1.288969829
6	2.012163427	-3.499761631	0.902785334
7	1.691588268	-2.402676509	0.249638658
1	-1.714926594	-1.023464443	0.195170614
1	1.984023024	0.690724603	1.231153525
1	-1.645741994	1.288817185	-1.715496396
1	-3.261716509	0.616174445	-1.427101830
1	3.912477175	0.108729863	-0.401568401
1	2.689223147	-0.394213041	-1.539916028
1	4.899458642	-2.036599377	1.021150414
1	3.805175772	-4.216282959	1.793342812
1	1.349224315	-4.325949345	1.119202071
1	-5.948848476	0.705389160	1.699339278
1	-4.607314411	1.135125460	2.792420555
1	-5.277197589	-0.516593418	2.779470300
1	1.190572173	5.151412841	0.729154410
1	2.874691218	4.835724911	0.239887263
1	1.587038356	4.800694939	-0.972817927
1	-3.620988177	-1.657187580	-1.809117328

Geometry: TS1

Total energy: -1136.953376

Zero-point energy: 906.8741

Hydration free energy: -117.8530274

Cartesian coordinates:

6	5.534172005	0.597853581	1.091921339
6	4.262741491	1.085799949	0.416154931
8	4.241739460	2.126792055	-0.244197406
7	3.166787893	0.292310917	0.565502776
1	3.150017486	-0.450408836	1.258980139
6	1.841118696	0.687789404	0.130157462
6	0.820982568	-0.316201345	0.701923333
8	1.125204193	-1.027994285	1.701622320
7	-0.295252741	-0.303212359	-0.000553835
1	-1.331472606	1.926152616	-0.874131337
6	-1.398353007	-1.153003701	0.423680793
6	1.672629845	0.706505046	-1.399195647
6	0.221621011	0.882570973	-1.780419135
8	-0.367838204	2.004884547	-1.513800529
7	-0.245403317	0.151557885	-2.825061042
1	-1.200381164	0.320668409	-3.110745784
1	0.074994511	-0.801675874	-2.925862536
6	-1.185193546	-2.589140490	-0.109173746
8	-1.766701978	-3.020373943	-1.111053298
7	-0.287147372	-3.308223358	0.609296059
1	0.280076774	-2.777228857	1.273892703
6	0.163378240	-4.619959501	0.173956486
6	-2.746067509	-0.609079984	-0.090181050
6	-3.054336989	0.777183920	0.380634883
6	-3.996776448	1.201344528	1.285363910
7	-3.868279325	2.576811091	1.370911694
6	-2.875297446	2.958682015	0.537446909
7	-2.373288869	1.897058060	-0.071514011
1	1.612716657	1.690433906	0.516121177
1	-1.424889987	-1.196347580	1.523749043
1	2.061120432	-0.227795129	-1.817236585
1	2.237458688	1.539347378	-1.831262046
1	-3.546862045	-1.279439772	0.235774457
1	-2.747658490	-0.647020127	-1.183871914
1	-4.729127127	0.655977579	1.859156540
1	-4.414182297	3.191691589	1.956307304
1	-2.548656333	3.978873767	0.403105402
1	6.304937357	0.455092329	0.328963286
1	5.403061396	-0.334996537	1.647319858
1	5.888383605	1.376390041	1.773868790
1	0.590640139	-5.152554028	1.027011656
1	-0.686130421	-5.183786846	-0.216490985
1	0.921098314	-4.556023034	-0.618912156

Geometry: INT1

Total energy: -1136.973842

Zero-point energy: 921.2655

Hydration free energy: -105.3594879

Cartesian coordinates:

6	5.630716824	0.749923190	1.104356899
6	4.379963045	1.183570747	0.357710882
8	4.384422158	2.133288780	-0.421900753
7	3.256365916	0.440015656	0.592832477
1	3.230768080	-0.188160340	1.387395659
6	1.960527981	0.843157210	0.080968061
6	0.878494712	-0.010816093	0.733476109
8	0.974738329	-0.554084618	1.842065093
7	-0.163677468	-0.137179081	-0.130031407
1	-1.255378471	1.867604183	-1.127602189
6	-1.277950870	-1.023302958	0.253254690
6	1.683441752	0.611080540	-1.409986250
6	0.147396709	0.509158776	-1.485905001
8	-0.358760833	1.808451424	-1.545341841
7	-0.309966235	-0.254701962	-2.615447693
1	-1.175917095	0.112629171	-2.989765602
1	-0.376706654	-1.257376444	-2.467489200
6	-0.924242972	-2.474444500	-0.155629170
8	-1.279470396	-2.962562661	-1.231277517
7	-0.181612251	-3.142385692	0.761430776
1	0.208101475	-2.595463983	1.523440630
6	0.354545254	-4.469806261	0.492149128
6	-2.680201817	-0.642909496	-0.263002551
6	-3.215756954	0.648674071	0.275998978
6	-4.186043604	0.853519133	1.229439735
7	-4.307777967	2.224846149	1.352052842
6	-3.425275810	2.795115369	0.486957492
7	-2.757514993	1.872071024	-0.175633170
1	1.778153812	1.899720892	0.319709442
1	-1.299482420	-0.977115257	1.346494258
1	2.129225009	-0.335964887	-1.730768089
1	2.038461771	1.414425521	-2.054272457
1	-3.348633575	-1.455448766	0.039695072
1	-2.696357721	-0.637555977	-1.355083417
1	-4.785848262	0.167899719	1.807906968
1	-4.939538030	2.715350960	1.967545477
1	-3.309967070	3.863845385	0.377586342
1	6.417109146	0.535535385	0.375521222
1	5.480956937	-0.129006803	1.737850504
1	5.974930387	1.583806677	1.723184695
1	0.638285301	-4.936309053	1.437730805
1	-0.410798914	-5.075622839	0.003882132
1	1.230797719	-4.429717977	-0.166482906

Geometry: INT2

Total energy: -1137.371933

Zero-point energy: 958.9732

Hydration free energy: -243.9719846

Cartesian coordinates:

6	5.550528947	-0.071522073	0.518343334
6	4.324770853	0.781497984	0.274822080
8	4.371173924	1.920544493	-0.160347598
7	3.095979087	0.175811484	0.570871870
1	3.149704720	-0.586787672	1.240308347
6	1.914222716	1.040884504	0.735353500
6	0.763610898	0.137740996	1.198362791
8	0.646128444	-0.367066428	2.300612057
7	-0.096892512	-0.067561556	0.129440641
1	-1.227433858	1.561419881	-1.518369282
6	-1.249451878	-0.962101052	0.310673724
6	1.391399171	1.607182495	-0.589310512
6	0.402815043	0.551868311	-1.107004986
8	-0.540572545	0.974724420	-1.994986782
6	-0.925938829	-2.393280675	-0.158493309
8	-0.244455719	-2.611023899	-1.181646582
7	-1.463111301	-3.391923697	0.552146140
1	-1.919756405	-3.174323767	1.427184677
6	-1.297257650	-4.801550805	0.188447144
6	-2.577959093	-0.491328990	-0.352237010
6	-3.023029077	0.889164365	0.032121148
6	-4.032946708	1.286160505	0.875346741
7	-4.039028808	2.665028468	0.827036265
6	-3.058868182	3.061049672	-0.023471395
7	-2.427274299	2.011964997	-0.518176300
1	2.106847427	1.824481836	1.474805439
1	-1.392492183	-0.974229941	1.395741629
1	2.176935788	1.848448068	-1.305887925
1	0.820463915	2.520288964	-0.401257345
1	-3.347451753	-1.209157405	-0.052005063
1	-2.489043999	-0.558153561	-1.439966531
1	-4.735905618	0.729320307	1.475477694
1	-4.671944334	3.275058398	1.326055821
1	-2.850957359	4.096103254	-0.252260818
1	6.290042255	0.139843618	-0.255995830
1	5.333016849	-1.142778582	0.541311912
1	5.988260263	0.215278818	1.481191231
1	-2.028521110	-5.391051596	0.741916797
1	-1.464004037	-4.924822196	-0.882608670
1	-0.289511931	-5.151538430	0.430942387
7	1.166456812	-0.525278979	-1.900667704
1	2.100828904	-0.664937172	-1.498854632
1	0.607060108	-1.433870933	-1.802682167
1	1.241389415	-0.226896996	-2.876372313

Geometry: TS2

Total energy: -1137.361052

Zero-point energy: 950.5377

Hydration free energy: -252.9538712

Cartesian coordinates:

6	5.623272563	0.418485158	0.225593931
6	4.308036815	1.165817215	0.293288992
8	4.222379462	2.380640788	0.180464057
7	3.172510425	0.383342921	0.470305536
1	3.314506219	-0.527758485	0.893522328
6	1.914817238	1.048244109	0.822859641
6	0.879343540	-0.038540759	1.112484754
8	0.951025788	-0.876929355	1.999445146
7	-0.147436468	0.036524410	0.187315680
1	-2.109330727	1.855351233	-0.871775883
6	-1.167022059	-1.030326571	0.248134078
6	1.282246601	1.861403027	-0.314049741
6	0.128698679	1.014933668	-0.858472182
8	-0.807631258	1.511074288	-1.542907048
6	-0.587833568	-2.346718763	-0.329390510
8	-0.363460594	-2.450348114	-1.541492002
7	-0.405486689	-3.344556539	0.554982312
1	-0.402975635	-3.101501594	1.537406670
6	0.136198834	-4.645717899	0.166494266
6	-2.510624115	-0.767259414	-0.473288915
6	-3.323042343	0.383971990	0.035003379
6	-4.462167587	0.443207818	0.795774659
7	-4.795472707	1.782931089	0.901678453
6	-3.894830916	2.520072448	0.230654912
7	-3.004827019	1.688582744	-0.295823459
1	2.054473556	1.662945509	1.720356303
1	-1.364538537	-1.163167596	1.315857948
1	1.988468956	2.158117143	-1.086843055
1	0.835983531	2.779925738	0.080465529
1	-3.103929059	-1.678349987	-0.348120895
1	-2.335537524	-0.650427341	-1.545268824
1	-5.058436350	-0.333187947	1.248290462
1	-5.594762670	2.156126782	1.397957205
1	-3.902685119	3.595409068	0.139376373
1	6.200059953	0.797254153	-0.621314671
1	5.504254752	-0.664050879	0.130944289
1	6.196301968	0.634494129	1.133356195
1	-0.195323696	-5.395871002	0.886340453
1	-0.234027270	-4.903000922	-0.826183171
1	1.231224550	-4.630302467	0.139824324
7	1.085337647	-0.056819860	-2.180062922
1	2.060148092	-0.260182110	-1.960046092
1	0.568962993	-0.937815296	-2.293456699
1	1.033716412	0.495025493	-3.034062813

Geometry: PC

Total energy: -1137.375655

Zero-point energy: 947.1483

Hydration free energy: -267.1979077

Cartesian coordinates:

6	5.684947062	1.194806743	0.714555357
6	4.276360356	1.589083450	0.329904776
8	3.991668875	2.685419049	-0.141124408
7	3.297588538	0.636268469	0.514998638
1	3.487949049	-0.189264806	1.067437754
6	1.922542251	1.004572616	0.284813412
6	0.956252222	0.019697520	0.921232739
8	1.102270660	-0.609666082	1.951837470
7	-0.192688489	-0.048747665	0.113449474
1	-2.283907956	1.703620769	-1.380855218
6	-1.295176019	-0.943243430	0.533066868
6	1.441293746	1.063719020	-1.176826538
6	0.004638390	0.617721165	-1.104294604
8	-0.874592660	0.826499771	-1.933490298
6	-0.951402477	-2.408258217	0.119587405
8	-1.293329432	-2.836063509	-0.981366491
7	-0.299594098	-3.125308856	1.057974991
1	0.078287988	-2.625331750	1.854406232
6	0.125332190	-4.505240929	0.834116746
6	-2.699774281	-0.630960782	-0.026604031
6	-3.255318191	0.736633748	0.220657559
6	-4.144345415	1.215396360	1.148019106
7	-4.362253535	2.549142424	0.845724737
6	-3.640839508	2.890048226	-0.230159857
7	-2.972326507	1.806024622	-0.615511711
1	1.738328115	1.986861691	0.747826116
1	-1.312979596	-0.867220295	1.623990322
1	1.958749415	0.310905936	-1.786108467
1	1.540657527	2.043450871	-1.644034972
1	-3.372130814	-1.354968361	0.443407930
1	-2.712794615	-0.851434226	-1.095929615
1	-4.643554589	0.726363316	1.969543760
1	-4.980011079	3.175377383	1.347577466
1	-3.610546699	3.863696078	-0.694959006
1	6.325414293	1.281316527	-0.167471140
1	5.761853125	0.180138020	1.113683524
1	6.055905862	1.905146273	1.458537941
1	0.103270020	-5.044503039	1.783127953
1	-0.563266330	-4.975197878	0.131748165
1	1.138528118	-4.551088244	0.419613125
7	1.323015265	-2.014172676	-2.647375141
1	0.453581980	-2.499113180	-2.424639980
1	2.068803079	-2.705413446	-2.604360075
1	1.256473394	-1.729152631	-3.622632562

Geometry: P

Total energy: -1080.410361

Zero-point energy: 816.3417

Hydration free energy: -81.3119773

Cartesian coordinates:

6	5.686530427	0.445161297	0.525708954
6	4.340491890	0.972273764	0.068873389
8	4.218176870	2.021655935	-0.555896885
7	3.249729070	0.195061647	0.373846090
1	3.334596188	-0.536667172	1.068736001
6	1.913738753	0.698030786	0.129281611
6	0.881958837	-0.253139153	0.722129958
8	1.007430862	-0.905771733	1.747858114
7	-0.229575813	-0.273241281	-0.106449852
1	-2.314518323	2.064889791	-1.549840468
6	-1.459424191	-0.989297574	0.304053682
6	1.473590139	0.824062424	-1.337224186
6	0.026963771	0.357184899	-1.341170223
8	-0.780050107	0.486416872	-2.238744191
6	-1.408310256	-2.467465046	-0.174067008
8	-2.129316525	-2.889818941	-1.071564012
7	-0.515698330	-3.242812964	0.492788600
6	-0.338121063	-4.651069082	0.162448787
6	-2.773232251	-0.312330459	-0.132712919
6	-2.901247527	1.125367660	0.268740223
6	-3.287442891	1.740229771	1.441542203
7	-3.260856339	3.112102514	1.315791374
6	-2.867484560	3.337645974	0.078437206
7	-2.634666755	2.172042158	-0.596020276
1	1.784655535	1.671902657	0.625837760
1	-1.410364387	-0.983856478	1.397217189
1	2.055121379	0.152914351	-1.979211999
1	1.563222495	1.832211461	-1.741903370
1	-3.573351176	-0.889984832	0.340993548
1	-2.905566460	-0.434877536	-1.208006541
1	-3.594852011	1.267208351	2.364684850
1	-2.739370613	4.308998747	-0.378708523
1	6.342833388	0.358915725	-0.344411152
1	5.628598198	-0.524215452	1.027916702
1	6.135632682	1.176023486	1.204479524
1	0.402730854	-5.077315437	0.840939111
1	-1.281387678	-5.194608962	0.270786138
1	0.004354779	-4.772642942	-0.870189233
1	0.047147050	-2.820748905	1.221514629

Geometry: NH₃

Total energy: -56.566977

Zero-point energy: 90.1855

Hydration free energy: -19.4912509

Cartesian coordinates:

7	0.000000000	0.000000000	0.108262171
1	0.949447645	0.000000000	-0.252611733
1	-0.474723823	-0.822245780	-0.252611733
1	-0.474723823	0.822245780	-0.252611733