Supplementary Materials: Racemization of Serine Residues Catalyzed by Dihydrogen Phosphate Ion: A Computational Study

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Table S1. Total energies (au), zero-point energies (kJ mol^{-1}), and SM8 hydration Gibbs energies (kJ mol^{-1}) of the B3LYP/6-31+G(d,p) optimized geometries.

Geometry	Total energy	Zero-point energy	SM8 hydration Gibbs energy (6-31G(d))
RC1	−1214.796707	608.9651	−296.1826227
TS1	−1214.766347	592.5568	−254.6472538
PC1	−1214.769463	603.3364	−264.7760431
RC2	−1214.793672	608.7317	−293.0041047
TS2	−1214.765673	593.5349	−251.8666249
PC2	−1214.771689	603.2522	−260.0603910
RC3	−1214.792629	608.6808	−292.1551194
TS3	−1214.765384	595.2807	−253.4428643
PC3	−1214.772209	602.7276	−259.7720172

Table S2. Cartesian coordinates (Å) of RC1 (reactant complex of pathway 1).

Atom	*x*	*y*	*z*
6	1.855418700	-0.144259477	1.884547663
6	0.862506711	0.083382408	0.734358779
6	1.224594369	1.183379009	-0.287230600
8	0.400594001	1.553379806	-1.132684213
7	2.450701802	1.750339723	-0.182078617
6	2.875902951	2.795628013	-1.096290403
1	3.054331982	2.406857699	-2.107283728
1	3.798179523	3.242935662	-0.716883827
7	0.454545282	-1.141467566	0.029443151
6	1.267724096	-2.060576541	-0.514325386
8	2.514242761	-2.056167427	-0.413098088
6	0.581559207	-3.168459414	-1.293524033
1	1.494954552	-0.998042514	2.474016897
1	0.952906562	-4.132667086	-0.935132204
1	-0.506684394	-3.134445314	-1.208615791
1	0.862915776	-3.075218972	-2.347586061
1	1.836935576	0.737693559	2.532772523
15	-2.961391081	0.326263653	0.270778612
8	-2.518565152	1.256736827	-1.013844103
1	-1.550008637	1.392769452	-1.029224301
1	2.102690728	3.564957316	-1.167400170
8	-2.057234361	0.620987571	1.446744212
1	-0.078939648	0.435434287	1.191400944
1	3.132652848	1.259948303	0.394487286
8	3.220749232	-0.333844509	1.502377651
1	-0.554634817	-1.239901713	-0.124387822
1	3.197891956	-1.037427126	0.808364984
8	-4.460007841	0.275537039	0.314295709
8	-2.422470153	-1.211401831	-0.259778007
1	-3.083759466	-1.555337246	-0.875081055

Table S3. Cartesian coordinates (Å) of TS1 (transition state of pathway 1).

Atom	*x*	*y*	*z*
6	-1.862508679	-0.058242986	1.728822258
6	-0.920816313	-0.056812340	0.559039572
6	-0.960973320	-1.137652260	-0.366999483
8	-0.195409381	-1.255947207	-1.398156541
7	-1.827549866	-2.175433854	-0.107868521
6	-1.868291143	-3.356041913	-0.949347921
1	-2.330171818	-3.167464490	-1.929873655
1	-2.437978495	-4.137475851	-0.435657765
7	-0.570301509	1.242079308	0.015571905
6	-1.466810705	2.129167054	-0.469190628
8	-2.700016464	1.959664260	-0.457397168
6	-0.885003626	3.417817354	-1.033323744
1	-1.664750891	0.826145029	2.350513151
1	-1.260740692	4.265063307	-0.450296614
1	0.208278357	3.432391749	-1.033410956
1	-1.245941446	3.537596957	-2.059102394
1	-1.710202881	-0.946870944	2.352323354
15	2.752449461	-0.171221044	0.155481299
8	2.122074991	-0.570974539	-1.210501802
1	1.031703047	-0.843398709	-1.289646369
1	-0.852838626	-3.716266971	-1.127860995
8	1.812890407	-0.728281921	1.342461299
1	0.826476072	-0.567388156	1.175752708
1	-2.675851574	-1.900922558	0.376889990
8	-3.279421067	-0.097466588	1.386446527
1	0.405623222	1.522073888	-0.010371260
1	-3.373607719	0.588464742	0.693458853
8	4.194025575	-0.446395027	0.408500446
8	2.463697339	1.477063886	0.181857741
1	3.021912667	1.879137134	0.861454437

Table S4. Cartesian coordinates (Å) of PC1 (product complex of pathway 1).

Atom	*x*	*y*	*z*
6	-1.963559929	0.067819071	1.652393389
6	-1.050820656	-0.021667774	0.463841659
6	-1.109526162	-1.140775956	-0.355418736
8	-0.347978309	-1.365190455	-1.418071577
7	-2.006814343	-2.144593135	-0.070152664
6	-2.046518367	-3.382719934	-0.827175686
1	-2.456916993	-3.256206028	-1.839687061
1	-2.665161241	-4.104317203	-0.284206921
7	-0.510026495	1.205210099	-0.060074264
6	-1.290780984	2.228793068	-0.474402753
8	-2.534836456	2.217925992	-0.429593883
6	-0.552746012	3.449463367	-1.000696290
1	-1.689695393	0.942985050	2.256891923
1	-0.811174032	4.316132957	-0.383594320
1	0.532529835	3.320542949	-1.012685589
1	-0.904146912	3.652164537	-2.016848048
1	-1.871392990	-0.822721755	2.284526735
15	2.791120961	-0.268002018	0.116188293

8	2.016626863	-0.591419270	-1.156270692
1	0.614208672	-0.977841478	-1.320739370
1	-1.038197689	-3.789982614	-0.926439197
8	1.965409423	-0.878545565	1.405500089
1	1.000317906	-0.778449134	1.274012112
1	-2.871041943	-1.812302691	0.342475626
8	-3.374945984	0.132915736	1.313997137
1	0.496399967	1.351110709	-0.081468155
1	-3.419040626	0.844693263	0.643512622
8	4.245860083	-0.551102190	0.301165688
8	2.509611789	1.382768590	0.294090465
1	3.080116287	1.725609188	0.995226423

Table S5. Cartesian coordinates (Å) of RC2 (reactant complex of pathway 2).

Atom	x	y	z
6	1.776772672	-0.119314343	1.879104488
6	0.865880902	0.108522277	0.664814053
6	1.293208967	1.201712888	-0.338537243
8	0.526640938	1.549187915	-1.245728908
7	2.506532462	1.776197900	-0.150148459
6	2.998519442	2.808758278	-1.044673617
1	3.327725510	2.396495375	-2.007978697
1	3.840447990	3.319476497	-0.569748477
7	0.502632297	-1.111167830	-0.073958416
6	1.322242945	-2.088010869	-0.494545139
8	2.538957378	-2.166731470	-0.217176283
6	0.673480298	-3.165966466	-1.344776286
1	1.374920127	-0.969604413	2.446058230
1	0.804936174	-4.130727338	-0.845421973
1	-0.390202455	-2.991644237	-1.521299230
1	1.199738175	-3.215079555	-2.302916141
1	1.714343915	0.764664561	2.521357963
15	-2.946986148	0.164974979	0.278623933
8	-3.739304563	-1.108816753	0.392519073
8	-1.962491174	-0.033097318	-1.068710797
1	-1.354103683	0.723425429	-1.187250631
8	-2.084248253	0.743016560	1.376339540
1	-0.099293892	0.464564766	1.068007376
1	3.147298908	1.285173791	0.472289319
8	3.164001536	-0.311201868	1.590646692
1	-0.453730106	-1.086740909	-0.438453123
1	3.181956717	-1.057799827	0.943057093
8	-3.970184404	1.379943079	-0.230178667
1	2.201992068	3.529351081	-1.244259325
1	-4.722993566	0.945997864	-0.654055985

Table S6. Cartesian coordinates (Å) of TS2 (transition state of pathway 2).

Atom	x	y	z
6	-1.851171010	-0.369214207	1.688307930
6	-0.965362749	-0.130348872	0.501840735
6	-0.722303169	-1.182022080	-0.426926295
8	0.048038758	-1.071630476	-1.454196282
7	-1.269672336	-2.418102669	-0.166602604
6	-0.994977916	-3.559899215	-1.017682430
1	-1.515601385	-3.508159989	-1.985687551

1	-1.305571299	-4.473075777	-0.499203307
7	-0.940207701	1.210302103	-0.050383307
6	-2.029534584	1.921213741	-0.412535018
8	-3.204726430	1.549276572	-0.232123810
6	-1.754353550	3.280340703	-1.039808414
1	-1.859565132	0.530126533	2.318951153
1	-2.165013992	4.062206701	-0.392554035
1	-0.690454460	3.474140294	-1.202694992
1	-2.281784250	3.333213229	-1.996846679
1	-1.465161890	-1.197899146	2.292539361
15	2.717878491	0.385088858	0.228906480
8	3.640440160	1.518543531	0.534764033
8	1.783418318	0.600207654	-1.027002584
1	1.025754391	-0.168422976	-1.262738695
8	1.762560999	-0.079122254	1.428568431
1	0.778479156	-0.165244125	1.172825842
1	-2.158215916	-2.386603638	0.321673369
8	-3.220615898	-0.756627898	1.380483733
1	-0.035826734	1.577572732	-0.328850719
1	-3.520677961	-0.063067341	0.758411295
8	3.592685636	-0.982302422	-0.061848554
1	4.510025165	-0.709582232	-0.197387692
1	0.076402715	-3.614111247	-1.221471956

Table S7. Cartesian coordinates (Å) of PC2 (product complex of pathway 2).

Atom	***x***	***y***	***z***
6	-2.405609832	-0.129333753	1.463336330
6	-1.380567717	-0.117325923	0.370698852
6	-1.056926179	-1.263574419	-0.308830476
8	-0.110003233	-1.371687290	-1.253361215
7	-1.722578217	-2.455215201	-0.042605677
6	-1.371913495	-3.678624180	-0.745803804
1	-1.603586454	-3.648838593	-1.820993572
1	-1.922617674	-4.507428900	-0.289396519
7	-0.880373856	1.143638474	-0.088071695
6	-1.677397650	2.177575663	-0.433438020
8	-2.921187336	2.162709263	-0.340222324
6	-0.958906870	3.423349848	-0.925415620
1	-2.264943375	0.755103391	2.099140741
1	-1.099062179	4.228550703	-0.196125352
1	0.111481348	3.265959688	-1.081057018
1	-1.423839321	3.743316868	-1.862363566
1	-2.285213472	-1.020694361	2.088869502
15	2.917590379	0.217663269	0.168369181
8	4.023444040	1.219056605	0.275466614
8	1.713974730	0.399386397	-0.764069008
1	0.631281036	-0.692431271	-1.124794958
8	2.296982833	-0.049275706	1.678323191
1	1.393012965	-0.392410589	1.612188676
1	-2.708682435	-2.321082108	0.140688148
8	-3.773020212	-0.180103460	0.995083169
1	0.124679113	1.204794248	-0.282242925
1	-3.830796787	0.590886828	0.395390360
8	3.551469106	-1.260757423	-0.235714325
1	-0.302357597	-3.874092706	-0.643340464

1	4.492104703	-1.242575646	-0.014091557

Table S8. Cartesian coordinates (Å) of RC3 (reactant complex of pathway 3).

Atom	*x*	*y*	*z*
6	1.813881834	-0.146365857	1.876761840
6	0.881034506	0.105245392	0.682957032
6	1.321864771	1.184398126	-0.330061165
8	0.559906695	1.545650301	-1.235753160
7	2.546422965	1.737572072	-0.149412222
6	3.045801636	2.763652086	-1.047643644
1	3.301281134	2.357180872	-2.035070886
1	3.936776347	3.217482371	-0.605974605
7	0.462276235	-1.100874935	-0.046495040
6	1.244772346	-2.094454291	-0.495320023
8	2.462203129	-2.217314896	-0.236488451
6	0.552628745	-3.131951291	-1.361869362
1	1.399013654	-0.981235897	2.456647611
1	0.698306988	-4.119203636	-0.913554447
1	-0.515274172	-2.940538725	-1.487962642
1	1.036673246	-3.139608636	-2.343602281
1	1.793286018	0.742624186	2.514579341
15	-2.955819334	0.415798211	0.227874443
8	-1.946934907	0.018923046	-1.064252179
1	-1.324226449	0.749425228	-1.250411510
8	-2.062148700	0.644466587	1.425412403
1	-0.066159341	0.484735698	1.106311651
1	3.185735115	1.226209821	0.457471577
8	3.187712894	-0.380909921	1.557922802
1	-0.500759496	-1.035444368	-0.393456001
1	3.170254680	-1.129756262	0.912784563
8	-4.013366845	1.387586417	-0.223855593
1	2.280850303	3.530669477	-1.190588449
8	-3.659467522	-1.085764262	0.384849339
1	-4.502503395	-1.040636424	-0.085569085

Table S9. Cartesian coordinates (Å) of TS3 (transition state of pathway 3).

Atom	*x*	*y*	*z*
6	-1.758985924	-0.189233292	1.748116227
6	-0.879394006	-0.089736219	0.532111072
6	-0.879315837	-1.166102308	-0.433239022
8	-0.151060070	-1.166025736	-1.480385385
7	-1.618692562	-2.285567869	-0.144863049
6	-1.585601043	-3.456289219	-0.999761938
1	-2.167175416	-3.325418831	-1.924501004
1	-1.987189398	-4.313460117	-0.449411633
7	-0.745113515	1.235545243	-0.058363465
6	-1.762143720	2.041675282	-0.426487706
8	-2.966768807	1.797473645	-0.221743260
6	-1.363261003	3.347295267	-1.100112478
1	-1.616987892	0.710077715	2.363558338
1	-1.711260222	4.184882505	-0.486996341
1	-0.285254861	3.442449901	-1.257601769
1	-1.875196168	3.409540113	-2.065084531
1	-1.469984903	-1.054374178	2.355690444
15	2.752497169	-0.035636097	0.165848895

8	1.877066058	0.290961689	-1.127222563
1	1.071365800	-0.346814597	-1.325258866
8	1.730201288	-0.482374946	1.293820897
1	0.693425564	-0.347862180	1.063822716
1	-2.444604970	-2.117830085	0.420469426
8	-3.178082193	-0.384154044	1.494434720
1	0.184477002	1.512829809	-0.353951779
1	-3.401269801	0.327598784	0.858567106
8	3.955525757	-0.907109527	0.007413334
1	-0.553070563	-3.666862196	-1.285740594
8	3.233417919	1.487017958	0.583021773
1	4.191720409	1.457973810	0.702817597

Table S10. Cartesian coordinates (Å) of PC3 (product complex of pathway 3).

Atom	***x***	***y***	***z***
6	-2.283168660	0.048702006	1.493880464
6	-1.318802038	-0.055498665	0.351983938
6	-1.169639329	-1.230460050	-0.342180457
8	-0.287973241	-1.447479843	-1.329023694
7	-1.960769549	-2.331019854	-0.043258664
6	-1.768667877	-3.602716853	-0.720286733
1	-2.031565307	-3.575076015	-1.788247268
1	-2.390086631	-4.354827865	-0.223695286
7	-0.708186741	1.141703746	-0.144001833
6	-1.399046190	2.260954652	-0.448471446
8	-2.629651581	2.388719679	-0.288686705
6	-0.571149611	3.416911059	-0.985325532
1	-2.014751522	0.912409304	2.117283762
1	-0.632636849	4.254595656	-0.282586772
1	0.479126391	3.156059944	-1.138904669
1	-1.010478410	3.747981448	-1.931135367
1	-2.232174190	-0.850620314	2.117404367
15	2.876577965	-0.146184389	0.112045477
8	1.752890838	0.073193304	-0.908132298
1	0.543367533	-0.872837529	-1.227962550
8	2.199918288	-0.946269617	1.390033516
1	1.247355415	-0.765985361	1.433833574
1	-2.915754317	-2.085907405	0.184235027
8	-3.669745849	0.150898725	1.095205797
1	0.284286709	1.087632571	-0.394077816
1	-3.672368808	0.926090671	0.498506488
8	4.186121981	-0.789170676	-0.215899944
1	-0.723784383	-3.911097466	-0.644115365
8	3.149296277	1.373279729	0.726621819
1	4.059477442	1.396837647	1.051053871