Supplementary Materials: Nonenzymatic Deamidation Mechanism on a Glutamine Residue with a C-Terminal Adjacent Glycine Residue: A Computational Mechanistic Study

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Table S1. Coordinates of all atoms in RC-A at B3LYP/6-31+G(d,p).

Atom	Coordinate			Atom	Coordinate		
	X	Y	Z		X	Y	Z
N	3.326727	0.638011	−0.46016	O	−2.36153	−2.76428	0.113149
C	2.10785	−0.04537	−0.04962	H	−1.80997	−2.39821	0.850122
H	1.608992	−0.42805	−0.94315	C	4.063757	0.278139	−1.5382
C	2.442004	−1.24286	0.880888	O	3.754082	−0.67853	−2.26614
C	1.216919	0.991173	0.649103	C	5.296814	1.11561	−1.8138
H	3.165384	−1.85607	0.335816	H	6.17416	0.462425	−1.81385
H	2.966689	−0.86696	1.766553	H	5.209038	1.553418	−2.81246
C	1.249504	−2.14712	1.249848	H	5.448494	1.916019	−1.08612
H	0.642461	−2.34348	0.363028	H	3.608177	1.424907	0.112003
H	1.644204	−3.11328	1.590431	C	−1.97469	2.410836	0.229094
C	0.29428	−1.68698	2.343387	O	−2.68869	1.851992	−0.62645
N	−0.10396	0.822172	0.457085	N	−1.94396	3.744379	0.369353
C	−1.09967	1.59599	1.181708	H	−1.3297	4.145428	1.063715
H	−0.58268	2.23185	1.901066	C	−2.74165	4.645279	−0.45723
O	−0.93534	−1.87401	2.256267	H	−2.44775	4.570268	−1.50823
N	0.824906	−1.12214	3.44513	H	−3.80408	4.401412	−0.37337
H	1.818668	−1.00271	3.57041	H	−2.57815	5.66532	−0.11035
H	0.215818	−0.86385	4.20952	O	1.723345	1.874448	1.361425
P	−2.27262	−1.88398	−1.26524	H	−0.43066	0.07663	−0.18651
O	−3.43374	−0.73959	−1.07236	H	−3.07094	0.155467	−0.86312
O	−0.91433	−1.18172	−1.3155	H	−1.75997	0.913399	1.729456
O	−2.70075	−2.79447	−2.3938				

Table S2. Coordinates of all atoms in TS1-A at B3LYP/6-31+G(d,p).

Atom	Coordinate			Atom	Coordinate		
	X	Y	Z		X	Y	Z
N	3.399226	0.294874	−0.33211	O	−2.45963	−2.21926	−0.03785
C	2.105495	−0.29949	−0.04185	H	−1.76462	−1.84116	1.16839
H	1.649076	−0.61544	−0.98885	C	4.254106	−0.20268	−1.25752
C	2.2187	−1.54351	0.863567	O	4.033843	−1.2651	−1.86108
C	1.19853	0.777073	0.572886	C	5.510356	0.606722	−1.51105
H	2.826723	−2.2856	0.340479	H	6.382775	−0.01568	−1.29171
H	2.766653	−1.28117	1.776651	H	5.550472	0.872122	−2.5715
C	0.853474	−2.15699	1.184126	H	5.564772	1.51849	−0.91201
H	0.318394	−2.40135	0.262853	H	3.540626	1.227461	0.039603
H	0.987804	−3.09341	1.738281	C	−1.63427	2.216406	0.567428
C	−0.05273	−1.28747	2.037861	O	−2.82046	1.989347	0.24252
N	−0.02975	0.334031	0.93629	N	−0.93825	3.247687	0.068605
C	−0.89773	1.331822	1.578462	H	0.050066	3.281087	0.303503
H	−0.33019	1.963834	2.271601	C	−1.47426	4.152876	−0.94056
O	−1.34577	−1.57126	2.088852	H	−1.64968	3.633288	−1.88856
N	0.429475	−0.93045	3.274682	H	−2.42014	4.582073	−0.60093
H	1.383373	−0.6037	3.337163	H	−0.75467	4.956019	−1.10102
H	−0.21573	−0.42816	3.871774	O	1.606791	1.953411	0.681895
P	−2.61429	−1.38533	−1.32227	H	−0.8136	−0.26892	−0.68022
O	−3.73768	−0.22326	−1.08206	H	−3.4243	0.519059	−0.51024
O	−1.22531	−0.54486	−1.53882	H	−1.6686	0.791782	2.131217
O	−2.96174	−2.10931	−2.5953				

Table S3. Coordinates of all atoms in INT1-A at B3LYP/6-31+G(d,p).

Atom	Coordinate			Atom	Coordinate		
	X	Y	Z		X	Y	Z
N	3.728009	0.151306	−0.50526	O	−2.10401	−1.69662	−0.17183
C	2.43001	−0.36845	−0.10194	H	−1.42854	−1.22282	1.22945
H	1.928912	−0.76147	−0.99929	C	4.519106	−0.48555	−1.40522
C	2.501111	−1.50261	0.923253	O	4.234131	−1.60326	−1.86126
C	1.56649	0.805104	0.374257	C	5.785837	0.239847	−1.81251
H	3.017508	−2.35619	0.478063	H	6.647612	−0.38209	−1.55344
H	3.089174	−1.18628	1.792966	H	5.784041	0.368351	−2.89875
C	1.074354	−1.88166	1.312825	H	5.897883	1.216743	−1.33685
H	0.507975	−2.15573	0.415977	H	3.907362	1.125633	−0.29785
H	1.057686	−2.73739	1.991146	C	−1.359	2.109405	0.609626
C	0.328616	−0.74239	2.016969	O	−2.56906	1.897781	0.83339
N	0.52849	0.552574	1.210944	N	−0.92326	2.72066	−0.49948
C	−0.2859	1.706377	1.632603	H	0.083755	2.811615	−0.60757
H	0.372046	2.556513	1.8328	C	−1.81863	3.173205	−1.55838
O	−1.03454	−0.98491	2.119633	H	−2.35251	2.332261	−2.01076
N	0.799784	−0.58947	3.379527	H	−2.55488	3.878348	−1.16229
H	1.742164	−0.21273	3.416886	H	−1.22229	3.671041	−2.32313
H	0.189349	0.030272	3.905167	O	1.802142	1.951212	−0.05652
P	−3.33981	−1.29572	−0.97508	H	−1.85911	−0.33061	−2.27325
O	−4.13609	−0.09072	−0.21485	H	−3.54461	0.615277	0.13919
O	−2.79021	−0.57939	−2.36643	H	−0.81617	1.436774	2.542106
O	−4.36904	−2.32246	−1.37007				

Table S4. Coordinates of all atoms in RC-B at B3LYP/6-31+G(d,p).

Atom	Coordinate			Atom	Coordinate		
	X	Y	Z		X	Y	Z
N	−3.58882	−0.189569	−0.439722	O	2.4017	3.870281	−0.25536
C	−2.238212	−0.128889	0.109313	H	0.06957	0.39023	−0.857243
H	−1.883961	0.900795	0.019531	O	2.315516	1.947834	1.35709
C	−2.248295	−0.528168	1.608022	H	1.918772	1.082948	1.639532
C	−1.376233	−1.069129	−0.753705	C	−4.463908	0.84399	−0.394354
H	−3.056224	0.045349	2.071887	O	−4.174814	1.937073	0.117889
H	−2.53642	−1.582221	1.696209	C	−5.826121	0.594348	−1.010537
C	−0.962215	−0.217129	2.395004	H	−6.000261	1.339303	−1.792256
H	−0.687638	0.833578	2.270697	H	−5.932242	−0.404402	−1.439967
H	−1.171351	−0.360499	3.462998	H	−6.591759	0.734767	−0.241893
C	0.285637	−1.032983	2.089264	H	−3.864399	−1.07365	−0.849445
N	−0.171007	−0.585966	−1.101275	C	1.895897	−1.992876	−1.123444
C	0.777349	−1.316071	−1.936597	O	1.74621	−3.138414	−0.656559
H	0.240701	−2.097835	−2.475779	N	3.024284	−1.279197	−0.973596
H	1.204899	−0.612501	−2.656025	H	3.017574	−0.273821	−1.189262
O	1.414255	−0.503695	2.07043	C	4.134909	−1.773993	−0.170527
N	0.142744	−2.3595	1.902348	H	4.961885	−1.067464	−0.254608
H	−0.771486	−2.780524	1.827225	H	3.853533	−1.872637	0.883735
H	0.916528	−2.873057	1.493227	H	4.463132	−2.751299	−0.534341
P	2.032084	2.270142	−0.218805	O	−1.815313	−2.186046	−1.075216
O	3.049883	1.585423	−1.113769	H	1.731983	4.403164	0.198859
O	0.551642	2.061628	−0.516995				

Table S5. Coordinates of all atoms in TS1-B at B3LYP/6-31+G(d,p).

Atom	Coordinate			Atom	Coordinate		
	X	Y	Z		X	Y	Z
N	−3.67238	−0.30328	−0.51601	O	1.932685	3.947065	0.001872
C	−2.35067	−0.11162	0.057588	H	0.238516	1.060184	−0.5956
H	−2.13018	0.964	0.064468	O	1.93505	1.748354	1.367108
C	−2.25911	−0.61749	1.50807	H	1.602539	0.270464	1.586706
C	−1.32237	−0.79879	−0.86138	C	−4.72626	0.501251	−0.24321
H	−3.00472	−0.08422	2.102931	O	−4.66889	1.409832	0.602015
H	−2.52904	−1.67994	1.546888	C	−5.99816	0.224533	−1.02064
C	−0.87505	−0.36345	2.103903	H	−6.29094	1.134207	−1.55295
H	−0.61279	0.69444	2.013687	H	−5.89717	−0.59282	−1.7383
H	−0.8752	−0.60368	3.173842	H	−6.79826	−0.01883	−0.31535
C	0.253195	−1.17783	1.500526	H	−3.70365	−0.93188	−1.31154
N	−0.03852	−0.75619	−0.42211	C	2.250886	−1.84995	−0.78976
C	0.90343	−1.40135	−1.36949	O	2.379954	−2.9901	−0.29606
H	0.450297	−2.30129	−1.79506	N	3.289152	−1.00943	−0.93622
H	1.084137	−0.71206	−2.20359	H	3.118267	−0.02503	−1.16265
O	1.493839	−0.74281	1.695992	C	4.608589	−1.33756	−0.41311
N	0.165966	−2.54124	1.603024	H	5.298721	−0.54126	−0.69497
H	−0.74739	−2.94192	1.436272	H	4.596707	−1.4317	0.678911
H	0.918535	−3.03765	1.125174	H	4.962398	−2.28209	−0.83455
P	1.930143	2.314257	−0.05773	O	−1.70393	−1.30434	−1.93672
O	3.032019	1.899029	−1.00844	H	1.345943	4.287108	0.694418
O	0.462356	2.023542	−0.71186				

Table S6. Coordinates of all atoms in INT1-B at B3LYP/6-31+G(d,p).

Atom	Coordinate			Atom	Coordinate		
	X	Y	Z		X	Y	Z
N	4.133178	−0.03517	−0.50209	O	−4.64674	−1.94523	0.828981
C	2.829318	−0.43353	0.011506	H	−3.23015	−3.76225	−1.07896
H	2.638278	−1.46746	−0.31529	O	−2.10583	−1.91909	0.376095
C	2.73939	−0.41161	1.538832	H	−1.28985	−0.65722	1.1695
C	1.750546	0.391008	−0.7128	C	5.21314	−0.8552	−0.46892
H	3.384778	−1.19474	1.943296	O	5.190618	−1.95652	0.102038
H	3.125182	0.541569	1.918787	C	6.462927	−0.34341	−1.15729
C	1.288003	−0.63854	1.959506	H	6.749464	−1.05239	−1.93959
H	0.934752	−1.60424	1.580031	H	6.338881	0.647178	−1.60067
H	1.18795	−0.654	3.047806	H	7.277548	−0.30681	−0.4283
C	0.356959	0.455336	1.428401	H	4.140752	0.753606	−1.13648
N	0.562529	0.598599	−0.08088	C	−1.32733	2.261445	−0.47723
C	−0.58065	1.001315	−0.91165	O	−0.73711	3.289132	−0.09235
H	−0.18245	1.19756	−1.90938	N	−2.66051	2.187579	−0.625
H	−1.27944	0.165984	−0.98445	H	−3.08635	1.271859	−0.80448
O	−0.98962	0.161004	1.648689	C	−3.53186	3.317877	−0.33569
N	0.604949	1.70255	2.125495	H	−4.55217	3.04676	−0.6103
H	1.596594	1.922272	2.121113	H	−3.50794	3.581689	0.72771
H	0.134769	2.463863	1.63623	H	−3.22968	4.196421	−0.9128
P	−3.46033	−1.72531	−0.29169	O	1.968275	0.748291	−1.8823
O	−3.80395	−0.45266	−1.02723	H	−4.38851	−2.59071	1.504005
O	−3.69329	−2.95774	−1.35683				

Table S7. Coordinates of all atoms in RC-C at B3LYP/6-31+G(d,p).

Atom	Coordinate			Atom	Coordinate		
	X	Y	Z		X	Y	Z
N	3.528144	−0.37817	0.837352	H	3.402862	−0.70204	1.788609
C	2.373328	−0.5113	−0.04082	N	0.057537	0.365002	0.362486
H	2.474218	0.252883	−0.81116	H	−0.82643	0.215392	0.885689
C	2.377632	−1.90899	−0.72012	C	−0.06773	1.117103	−0.88236
C	1.120421	−0.32292	0.829552	C	−0.61853	2.51676	−0.59942
H	3.341396	−1.99573	−1.23012	H	0.891931	1.182471	−1.39086
H	2.372902	−2.67243	0.06523	H	−0.76707	0.607908	−1.55389
C	1.272262	−2.17234	−1.76471	O	−1.80325	2.682662	−0.24976
O	1.099601	−0.87182	1.945374	N	0.23097	3.544124	−0.74548
H	1.201034	−1.34364	−2.47335	H	1.186972	3.353004	−1.01037
H	1.566293	−3.05555	−2.34538	C	−0.15742	4.929936	−0.49962
C	−0.13893	−2.44069	−1.25388	H	−1.03364	5.190405	−1.09866
O	−1.12063	−1.84171	−1.7341	H	−0.39658	5.085963	0.556551
N	−0.28087	−3.38023	−0.29975	H	0.674717	5.575614	−0.77899
H	0.505302	−3.87662	0.092099	P	−3.7277	−0.41647	0.685123
H	−1.20208	−3.60227	0.052639	O	−2.44813	−0.27126	1.506638
C	4.713695	0.145383	0.44009	O	−3.89112	0.928546	−0.24216
O	4.905985	0.55147	−0.71698	O	−3.54513	−1.62011	−0.41704
C	5.800183	0.212381	1.494146	H	−2.66369	−1.64347	−0.86094
H	5.488208	−0.18212	2.463706	O	−5.04655	−0.68192	1.375963
H	6.668374	−0.35194	1.141765	H	−3.08417	1.500416	−0.22792
H	6.10876	1.254796	1.61552				

Table S8. Coordinates of all atoms in TS1-C at B3LYP/6-31+G(d,p).

Atom	Coordinate			Atom	Coordinate		
	X	Y	Z		X	Y	Z
N	−3.83646	−0.56674	−0.54862	H	−3.69612	−1.48715	−0.94792
C	−2.6719	0.043502	0.059805	N	−0.19714	0.06434	−0.20667
H	−2.72605	1.121645	−0.10074	H	1.210006	−0.97485	−0.89238
C	−2.59496	−0.24593	1.593366	C	−0.19148	1.530312	−0.36438
C	−1.39102	−0.5665	−0.50909	C	1.214076	2.079049	−0.6028
H	−3.43261	0.26193	2.078813	H	−0.75806	1.806934	−1.26274
H	−2.74831	−1.32123	1.742408	H	−0.64854	2.068366	0.472489
C	−1.28541	0.214739	2.25078	O	1.978882	1.568247	−1.4433
O	−1.42507	−1.71448	−0.96631	N	1.538781	3.191424	0.075077
H	−1.20949	1.303871	2.23559	H	0.908014	3.526143	0.789777
H	−1.29169	−0.07524	3.307425	C	2.806925	3.889087	−0.10903
C	−0.00217	−0.36213	1.660886	H	3.639323	3.315855	0.311673
O	1.090873	0.342137	1.97513	H	2.995754	4.048925	−1.17309
N	0.137232	−1.73611	1.741606	H	2.747189	4.853767	0.395049
H	−0.63277	−2.28927	1.385536	P	3.337603	−1.4241	−0.37486
H	1.039632	−2.07343	1.415534	O	1.927005	−1.61561	−1.16836
C	−5.04102	0.046855	−0.64364	O	4.041609	−0.13916	−1.10295
O	−5.24372	1.183243	−0.18698	O	3.013104	−1.0585	1.088034
C	−6.13562	−0.73318	−1.34316	H	1.923008	−0.15658	1.631585
H	−5.81169	−1.7169	−1.69023	O	4.212214	−2.6266	−0.62003
H	−6.97607	−0.85701	−0.65413	H	3.394905	0.598252	−1.211
H	−6.49102	−0.15183	−2.19891				

Table S9. Coordinates of all atoms in INT1-C at B3LYP/6-31+G(d,p).

Atom	Coordinate			Atom	Coordinate		
	X	Y	Z		X	Y	Z
N	4.10914	−0.26957	0.492042	H	4.015966	0.305992	1.318282
C	2.928411	−0.95832	0.007034	N	0.577373	−0.23041	−0.445
H	3.261314	−1.55179	−0.85239	H	−3.06846	1.132678	0.655568
C	2.326292	−1.89256	1.055806	C	−0.35793	0.741455	−1.03872
C	1.90376	0.04874	−0.5477	C	−0.64901	1.978829	−0.17387
H	3.050041	−2.67492	1.301564	H	0.053616	1.070428	−1.99687
H	2.121756	−1.34435	1.984424	H	−1.30831	0.245199	−1.22484
C	1.055961	−2.50477	0.479673	O	−1.77887	2.174196	0.326338
O	2.309149	1.095262	−1.08741	N	0.353985	2.850137	−0.01958
H	1.287142	−3.00863	−0.46505	H	1.24401	2.598286	−0.44485
H	0.625943	−3.24915	1.152932	C	0.229596	4.068198	0.771812
C	−0.04557	−1.4801	0.190671	H	−0.53614	4.727358	0.352411
O	−0.91142	−2.06514	−0.72932	H	−0.04271	3.835811	1.805725
N	−0.7613	−1.14173	1.40953	H	1.189584	4.584552	0.761651
H	−0.15372	−0.66444	2.070796	P	−4.42658	−0.49801	−0.04171
H	−1.55725	−0.5329	1.230801	O	−3.78045	0.54903	1.03028
C	5.302955	−0.27536	−0.15699	O	−5.41583	0.439594	−0.97935
O	5.489358	−0.9078	−1.20661	O	−3.31065	−1.01932	−0.94796
C	6.411292	0.534124	0.485033	H	−1.83037	−1.67244	−0.70905
H	6.126251	0.980924	1.440213	O	−5.31794	−1.44197	0.720981
H	7.278789	−0.11376	0.637298	H	−4.92244	0.859673	−1.69944
H	6.70808	1.330175	−0.20445				

Table S10. Coordinates of all atoms in INT2 at B3LYP/6-31+G(d,p).

Atom	Coordinate			Atom	Coordinate		
	X	Y	Z		X	Y	Z
N	−3.97444	−0.37852	−0.71376	H	−3.74722	−0.11561	−1.66345
C	−2.89977	−0.856	0.134827	N	−0.61274	−0.02973	0.730839
H	−3.36825	−1.10612	1.094296	H	2.457104	−1.76623	−1.05579
C	−2.23204	−2.10991	−0.433	C	0.212168	1.056786	1.262218
C	−1.91697	0.283663	0.470201	C	0.712898	2.044165	0.206018
H	−2.95046	−2.93462	−0.42516	H	−0.35431	1.577423	2.036669
H	−1.95879	−1.9424	−1.48228	H	1.096253	0.615094	1.725589
C	−1.00828	−2.46613	0.405913	O	1.224381	1.6482	−0.86525
O	−2.33284	1.442872	0.587413	N	0.642017	3.342071	0.521901
H	−1.30126	−2.65619	1.443409	H	0.162347	3.607403	1.370759
H	−0.52322	−3.37349	0.034228	C	1.161463	4.398971	−0.34117
C	0.047121	−1.3589	0.421695	H	2.214754	4.219494	−0.57017
O	0.948458	−1.6555	1.441587	H	0.601606	4.445904	−1.28004
N	0.737663	−1.27032	−0.87853	H	1.064404	5.349621	0.18276
H	0.853998	−0.28676	−1.13933	P	4.148548	−0.69329	−0.17517
H	0.1884	−1.71292	−1.61073	O	3.453609	−1.81826	−1.13701
C	−5.2468	−0.18385	−0.27818	O	3.923531	0.725155	−0.9806
O	−5.60001	−0.43335	0.883528	O	3.344882	−0.63011	1.129594
C	−6.22595	0.349394	−1.30409	H	1.862742	−1.28009	1.259789
H	−7.07287	−0.33879	−1.37421	O	5.634339	−0.94708	−0.13977
H	−6.60899	1.312964	−0.95527	H	3.002638	1.055654	−0.91275
H	−5.78855	0.479873	−2.2965				

Table S11. Coordinates of all atoms in TS2 at B3LYP/6-31+G(d,p).

Atom	Coordinate			Atom	Coordinate		
	X	Y	Z		X	Y	Z
N	−3.98724	−0.36997	−0.6943	H	−3.77843	−0.10847	−1.6486
C	−2.89308	−0.81718	0.144091	N	−0.61532	0.050837	0.721748
H	−3.343	−1.06406	1.113455	H	1.720404	−1.56343	−0.99509
C	−2.20906	−2.06659	−0.41544	C	0.19878	1.145543	1.249754
C	−1.92778	0.344127	0.452561	C	0.777152	2.069753	0.177603
H	−2.91366	−2.90256	−0.39192	H	−0.40025	1.712917	1.963421
H	−1.95508	−1.9101	−1.47174	H	1.042872	0.7028	1.783173
C	−0.97357	−2.39854	0.417585	O	1.20435	1.62098	−0.91195
O	−2.35474	1.498561	0.543889	N	0.868179	3.3648	0.492536
H	−1.25859	−2.59784	1.45538	H	0.481534	3.678866	1.372169
H	−0.4694	−3.29471	0.044049	C	1.490742	4.3525	−0.38572
C	0.061934	−1.27223	0.462776	H	2.534968	4.09213	−0.57772
O	1.014285	−1.53101	1.378973	H	0.960553	4.406115	−1.34046
N	0.706924	−1.13188	−0.93822	H	1.446906	5.32413	0.10516
H	0.831465	−0.11996	−1.14189	P	4.031054	−0.87061	−0.20522
H	0.120078	−1.53066	−1.67114	O	3.202125	−1.83211	−1.10515
C	−5.25608	−0.19225	−0.23916	O	4.040321	0.618866	−0.95924
O	−5.58434	−0.43671	0.930477	O	3.237605	−0.62363	1.137043
C	−6.26108	0.313526	−1.25347	H	2.072204	−1.09061	1.220867
H	−7.09363	−0.39345	−1.30718	O	5.494562	−1.22482	−0.01747
H	−6.65997	1.270419	−0.90419	H	3.147508	1.010607	−0.985
H	−5.84124	0.447526	−2.25293				

Table S12. Coordinates of all atoms in PC at B3LYP/6-31+G(d,p).

Atom	Coordinate			Atom	Coordinate		
	X	Y	Z		X	Y	Z
N	3.573704	−0.86186	0.641598	H	3.28379	−0.8296	1.609842
C	2.54463	−0.89664	−0.37244	N	0.659322	0.524626	−1.21309
H	3.050652	−1.10986	−1.32263	H	−1.14508	−1.11344	2.287346
C	1.485157	−1.96695	−0.09764	C	0.104289	1.852391	−1.48343
C	1.890774	0.48067	−0.53958	C	−0.59246	2.440517	−0.25155
H	1.967842	−2.9455	−0.03643	H	0.90616	2.502919	−1.83285
H	1.000019	−1.7687	0.865158	H	−0.63796	1.741006	−2.27519
C	0.451774	−1.9636	−1.22216	O	−1.14045	1.714241	0.595068
O	2.406292	1.5156	−0.14949	N	−0.60896	3.779593	−0.18064
H	0.885552	−2.368	−2.147	H	−0.10023	4.312674	−0.87238
H	−0.41289	−2.58184	−0.97202	C	−1.30405	4.503953	0.879718
C	−0.08908	−0.59881	−1.57211	H	−2.35304	4.200542	0.924632
O	−1.15023	−0.45692	−2.17848	H	−0.84119	4.310439	1.851975
N	−0.43752	−0.61416	2.835421	H	−1.24716	5.570163	0.661478
H	−0.42414	0.335212	2.46615	P	−3.68036	−1.29401	0.341157
H	−0.77846	−0.55348	3.792465	O	−2.4285	−1.94637	0.906671
C	4.90027	−0.76145	0.353699	O	−3.60293	0.331196	0.604505
O	5.323971	−0.73004	−0.80949	O	−3.65284	−1.4148	−1.30489
C	5.835907	−0.70673	1.54299	H	−2.76865	−1.19565	−1.66459
H	6.549814	−1.53173	1.467316	O	−5.05917	−1.73964	0.77256
H	6.402431	0.227958	1.500336	H	−2.69129	0.6906	0.575287
H	5.320897	−0.76711	2.504259				

Table S13. Electronic and zero-point energies for all structures in $CH_3COGlnNH_3CH_3$ at MP2/6-311+G(2d,2p)//B3LYP/6-31+G(d,p).

	Zero-point correction at B3LYP/6-31+G(d,p)	Single-point Energy at MP2/6-311+G(2d,2p)	Sum of single-point and zero-point energies
RC	0.279893	−1345.1288275	−1344.848935
TS1	0.278436	−1345.0904735	−1344.812038
INT1	0.281998	−1345.1104289	−1344.828431
INT2	0.282645	−1345.1128434	−1344.830198
TS2	0.277784	−1345.0984595	−1344.820676
PC	0.277820	−1345.1123404	−1344.83452

Table S14. Electronic and zero-point energies for all structures in $CH_3COGlnNH_3CH_3$ at MP2/6-311+G(2d,2p)//B3LYP/6-31+G(d,p).

	Zero-point correction at B3LYP/6-31+G(d,p)	Single-point Energy at MP2/6-311+G(2d,2p)	Sum of single-point and zero-point energies
RC	0.337248	−1552.7146803	−1552.377432
TS1	0.335963	−1552.6808827	−1552.344920
INT1	0.33754	−1552.6937447	−1552.356205
INT2	0.339362	−1552.6990823	−1552.359720
TS2	0.33455	−1552.6846848	−1552.350135
PC	0.335014	−1552.7011125	−1552.366099