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Table S1: Calculated energies of the neutral minima and transition states to imine formation with zero, one and two waters.

Structure	MP2/ 6-31G(d)[a]	ΔMP2[b,c]	ΔQCI[b,d]	ZPVE[b]	$\Delta H_{298,0}$[b]	ST[b]	ΔG_{solv}[b]	H_{298}[a]	G_{298}(aq)[a]
1	-209.68237	-283.27	-57.69	89.47	8.65	41.38	-9.45	-209.99436	-210.04519
2	-209.63265	-291.69	-53.87	89.87	5.91	33.44	-28.33	-209.95158	-210.01335
3	-209.69878	-288.66	-56.08	94.53	6.25	33.78	-11.32	-210.01189	-210.05699
4	-285.89630	-400.54	-67.90	113.41	11.87	49.16	-15.08	-286.32990	-286.39414
5	-285.87987	-406.29	-62.08	115.49	7.60	37.41	-31.42	-286.31559	-286.38442
6	-285.91690	-404.10	-66.05	119.03	9.18	41.21	-16.79	-286.34928	-286.40728
7	-362.11396	-516.76	-77.71	142.89	13.31	53.23	-23.46	-362.66395	-362.74064
8	-362.11299	-516.73	-75.81	146.11	11.35	46.61	-28.72	-362.65978	-362.73511
9	-362.11339	-518.27	-74.56	144.53	11.55	47.49	-37.02	-362.66186	-362.74637
10	-362.10263	-523.65	-70.87	141.00	9.48	42.43	-38.30	-362.65837	-362.73910
11	-362.13624	-520.55	-75.80	147.27	11.17	46.37	-25.22	-362.68588	-362.75747
12	-209.69176	-290.77	-55.50	92.96	6.36	32.65	-11.10	-210.00787	-210.05162
13	-209.69914	-288.55	-56.00	94.44	6.31	33.87	-14.81	-210.01210	-210.06078
14	-209.59979	-293.22	-55.69	86.13	6.67	34.87	-15.07	-209.92407	-209.97401
15	-209.68895	-289.96	-57.80	89.24	8.41	39.62	-11.73	-210.00823	-210.05958
16	-285.91125	-405.65	-66.35	117.87	9.83	43.19	-15.08	-286.34609	-286.40436
17	-285.84897	-411.28	-63.11	111.82	8.82	40.12	-26.07	-286.29316	-286.35935
18	-285.90616	-405.91	-67.91	113.47	11.42	47.28	-19.94	-286.34553	-286.41275
19	-362.12960	-521.87	-76.30	145.97	12.00	48.50	-27.16	-362.68153	-362.75719
20	-362.07372	-529.26	-72.62	137.73	10.68	45.20	-35.96	-362.63892	-362.72008
21	-362.11820	-524.94	-77.91	140.79	13.80	53.24	-25.46	-362.67819	-362.75689
T^-	-209.07577	-308.47	-53.12	80.12	5.87	33.06	-142.96	-209.42053	-209.59655

[a] energies in hartree

[b] energy corrections in millihartree

[c] ΔMP2 = MP2/6-311+G(3df,2p) - MP2/6-31G(d)

[d] ΔQCI = QCISD(T)/6-31G(d) - MP2/6-31G(d)

Table S2: Calculated energies of the protonated minima and transition states to iminium ion formation with zero, one and two waters.

Structure	MP2/ 6-31G(d)[a]	ΔMP2[b,c]	ΔQCI[b,d]	ZPVE[b]	$\Delta H_{298,0}$ [b]	ST[b]	ΔG_{solv} [b]	H_{298} [a]	G_{298}(aq)[a]
22	-210.06359	-281.81	-58.47	108.01	6.90	36.48	-115.10	-210.35811	-210.50969
23	-210.00293	-283.48	-56.38	102.51	6.09	33.57	-109.40	-210.30336	-210.44633
24	-210.05357	-285.42	-60.64	102.41	8.89	41.23	-104.48	-210.35748	-210.50319
25	-286.29410	-397.43	-68.25	131.34	10.26	44.42	-107.88	-286.70862	-286.86092
26	-286.25609	-397.91	-66.37	127.11	8.59	39.74	-107.77	-286.67510	-286.82261
27	-286.28175	-401.84	-70.68	125.36	12.61	51.37	-99.38	-286.70673	-286.85748
28	-362.51565	-513.29	-77.94	159.17	12.20	49.35	-108.47	-363.04723	-363.20505
29	-362.48357	-514.05	-76.30	151.94	12.32	50.37	-108.88	-363.02138	-363.18063
30	-362.50216	-517.19	-81.10	154.54	14.01	52.58	-95.68	-363.04362	-363.19188

[a] energies in hartree

[b] energy corrections in millihartree

[c] ΔMP2 = MP2/6-311+G(3df,2p) - MP2/6-31G(d)

[d] ΔQCI = QCISD(T)/6-31G(d) - MP2/6-31G(d)