Table SM1. Total energies (E_{tot}), single point energies (E_{SP}), Zero-point energy corrections, ZPEC, thermal corrections of energies (TCE), enthalpies (TCH) and Gibbs-Free energies (TCG) of the studied derivatives in their neutral, protonated and hydrated forms of PDAH and its derivatives. All values are in Hartree. (w=water, P=H^+)

		E_{tot}	E_{sp}	ZPEC	TCE	TCH	TCG
PDAP-H	Neutral	-853.351236	-853.411385	0.257909	0.273826	0.274770	0.212697
	N1	-853.729121	-853.790368	0.270232	0.286883	0.287828	0.223566
	N2	-853.684232	-853.734852	0.269982	0.286298	0.287242	0.223797
	N3	-853.723806	-853.786119	0.271133	0.287267	0.288295	0.225493
	N4	-853.721458	-853.783621	0.270920	0.287350	0.288212	0.224953
	N5	-853.722840	-853.732952	0.271046	0.287347	0.288291	0.225040
PDAP-$H.H_2O$	N1@w	-929.82013	-929.88418	0.281992	0.30149	0.302434	0.23096
PDAP-CH_3	Neutral	-892.683973	-892.746519	0.285238	0.285238	0.303948	0.237782
	N1	-893.066803	-893.130336	0.297615	0.316150	0.317094	0.248118
	N3	-893.060524	-893.125138	0.298521	0.316448	0.317518	0.250718
	N4	-893.060524	-893.121326	0.298521	0.316574	0.317518	0.250718
PDAP-$CH_3.H_2O$	N1@w	-969.15321	-969.21965	0.309366	0.330677	0.331621	0.256228
PDAP-NH_2	Neutral	-908.734008	-908.798268	0.274703	0.274703	0.293072	0.227889
	N1	-909.120748	-909.185811	0.287455	0.305354	0.306298	0.239681
	N3	-909.105607	-909.171402	0.287800	0.305690	0.306634	0.240292
	N4	-909.114610	-909.180891	0.287670	0.305576	0.306520	0.240369
PDAP-$NH_2.H_2O$	N1@w	-985.20634	-985.2741	0.299311	0.319874	0.320818	0.248068
PDAP-Cl	Neutral	-1312.970589	-1313.036432	0.248325	0.265553	0.266497	0.201062
	N1	-1313.341874	-1313.409239	0.260890	0.278614	0.279559	0.212648
	N3	-1313.339182	-1313.407490	0.261561	0.278968	0.280006	0.213874
	N4	-1313.338837	-1313.407490	0.261252	0.279062	0.279912	0.213051
PDAP-$Cl.H_2O$	N1@w	-1389.4389	-1389.5084	0.27231	0.293144	0.294088	0.219525
PDAP-F	Neutral	-952.615648	-952.682478	0.250016	0.266825	0.267769	0.203647
	N1	-952.982150	-953.050528	0.262570	0.279857	0.280801	0.215278
	N3	-952.981225	-953.050357	0.262851	0.280202	0.281146	0.215302
	N4	-952.982895	-953.052301	0.263310	0.280406	0.281350	0.216506
PDAP-$F.H_2O$	N1@w	-1029.0838	-1029.1543	0.273965	0.294421	0.295365	0.221829
PDAP-CHO	Neutral	-966.704919	-966.772498	0.266761	0.284886	0.285831	0.218596
	N1	-967.069529	-967.138470	0.278796	0.297620	0.298565	0.229278
	N3	-967.071758	-967.155338	0.279858	0.298560	0.299279	0.231027
	N4	-967.085603	-967.155338	0.280192	0.298335	0.299504	0.231252
PDAP-$CHO.H_2O$	N1@w	-1043.1739	-1043.2448	0.291108	0.312717	0.313661	0.237885
PDAP-CN	Neutral	-945.613692	-945.680168	0.256293	0.274134	0.275078	0.208468
	N1	-945.975305	-946.042913	0.268588	0.287025	0.287970	0.219683
	N3	-945.974777	-946.043489	0.269046	0.287458	0.288402	0.219270

PDAP-CN.H_2O	N4	-945.973250	-946.042008	0.269365	0.287521	0.288465	0.221045
	W@N1	-1022.081606	-1022.151791	0.280345	0.301767	0.302711	0.227222
PDAP-NO_2	Neutral	-1057.901776	-1057.976557	0.259972	0.278670	0.279614	0.210507
	N1	-1058.261694	-1058.338728	0.271894	0.291211	0.292156	0.221397
	N3	-1058.273353	-1058.350802	0.272888	0.291920	0.292864	0.222809
	N4	-1058.258838	-1058.336408	0.272946	0.292023	0.292967	0.222620
	N1@w	-1134.3717	-1134.4497	0.283863	0.306221	0.307165	0.22933
PDAP-NO_2.H_2O	water	-76.458531	-76.463372	0.021289	0.024125	0.025069	0.003647