Supporting Information

Enormous Hydrogen Bond Strength Enhancement Through π-Conjugation Gain: Implications for Enzyme Catalysis

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Supplementary Methods

All XH…YH and XH…Y^- complexes, XH = **Im**, **Ph**, **Ac In**, **Cyc**, **Ae**, YH = **1'-4'**, Y^- = **1-4**, and the individual monomers were optimized in the gas-phase at ωB97X-D/6-311+G(2d,p) using a pruned (99, 590) ultrafine grid employing the Gaussian09[1] program. Vibrational frequency analyses verified the nature of the stationary points.

Block-localized wavefunction (BLW) analyses

BLW[2,3] computations quantified the π-electron delocalization energies (DE_π) of the hydrogen-bonded acids (XH = **Im**, **Ph**, **Ac**). The DE_π value of XH is calculated by its π-electron-localized Lewis reference state (Ψ^{loc}) minus the energy of its fully delocalized wavefunction□□Ψ^{deloc}); $DE_\pi = E(\Psi^{loc}) - \square\square\square\Psi^{deloc})$. Both Ψ^{loc} and Ψ^{deloc} were optimized self-consistently. Ψ_{loc} is constructed by restricting the expansion of molecular orbitals over basis functions within a selected molecular subspace. All subspaces with π-type symmetry (i.e., "π-blocks") were assigned two π-electrons and the p_z, p_z, d_{xz}, d_{yz} basis functions belonging to the heavy atoms included in the specific π-block. In **Im**, three separate π-blocks were assigned to the C=C π-bond, the C=N π-bond, and the N π-lone pair. In **Ph**, four separate π-blocks were assigned to the three C=C π-bonds and the exocyclic O π-lone pair. In **Ac**, two separate π-blocks were assigned to the C=O π-bond and the N π-lone pair. This BLW localization scheme effectively disables all π-conjugation interactions in XH while leaving the σ-framework intact, and the resulting DE_π value provides a measure of the amount of π-conjugation in XH. ΔDE_π is the computed DE_π difference of XH before and after forming a hydrogen bond to Y^- or YH. This quantity measures the amount of π-conjugation *gain* in XH upon hydrogen bonding to Y^- or YH, and provides a lower bound estimate of the RAHB effect for the enzymatic models considered (since H^+ moves even more towards Y^- at the $[X^-\ldots H^+\ldots Y^-]$ transition state (TS). For example, the ΔDE_π value for XH = imidazole in $\mathbf{Im_1}$ (15.3 kcal/mol) is 4.0 kcal/mol stronger at the $\mathbf{Im_1}$**-TS** (19.3 kcal/mol). Since its introduction in 1998, the reliability of the BLW method for quantifying π-electron delocalization energies in molecules has been documented extensively by computed energetic and structural parameters consistent with experimental evidence.[3]

All BLW computations were performed at HF/6-31G(d)//ωB97X-D/6-311+G(2d,p) using GAMESS 2013-R1.[4] Applications of the BLW method for quantifying π-electron delocalization energies have been tested extensively at the 6-31G(d), 6-31+G(d), 6-311+G(d,p) and cc-pVTZ levels to show insignificant basis set dependency. Benchmark results at the HF/6-31G(d), 6-31+G(d), and 6-311+G(d,p) levels are listed in the **Table S2**.

Nucleus-Independent Chemical Shifts (NICS)

Dissected nucleus independent chemical shifts, $NICS(0)_{\pi zz}$,[5,6] were computed at PW91/IGLOIII. $NICS(0)_{\pi zz}$ computed at the ring heavy atom centers "0" include

magnetic tensor components in the out-of-plane (*zz*) direction (perpendicular to the ring plane) and only contributions from each π-orbital (a localized molecular orbital analysis based on the NBO dissection is applied here). Negative $NICS(0)_{\pi zz}$ computed at ring centers denote aromaticity. The computed $\Delta NICS(0)_{\pi zz}$ for a π-conjugated ring, before and after forming a hydrogen bond, quantifies its change in aromatic character upon hydrogen bonding.

Details of the natural bond orbital (NBO) deletion procedure

Natural bond orbital (NBO)[7] computations were performed at HF/6-31G(d)//ωB97X-D/6-311+G(2d,p) to quantify the effects of $\pi \rightarrow \pi^*$ interactions (DEL_π) in XH (**Im**, **Ph**, **Ac**) before and after forming a hydrogen bond to Y^- or YH (**Table S4**). For **Im**, six $\pi \rightarrow \pi^*$ interactions were deleted (C=C → C=N*, C=C → N π-orbital*, C=N → C=C*, C=N → N π-orbital pair*, N π-lone pair → C=C*, and N π-lone pair → C=N*). For **Ph**, 12 $\pi \rightarrow \pi^*$ interactions were deleted (three C=C → O π-long pair*, three O π-long pair→ C=C*, and six C=C → C=C* interactions). For **Ac**, two $\pi \rightarrow \pi^*$ interactions were deleted (C=O → N π-orbital* and N π-lone pair → C=O*).

XH…Y models derived from protein data bank (PDB) structures

To ensure that our XH…Y^-models properly reflect the acid residue-substrate interactions for the enzymes considered, we also evaluated His-substrate and Tyr-substrate interactions derived from selected PDB structures (PDB entry in parenthesis) of the triosephosphate isomerase (1NEY), citrate synthase (4CSC), ketosteroid isomerase (1OHP), and photoactive yellow protein (3PYP). Large computed hydrogen bonding interaction energies (ΔE_{HB}), comparable to those of $\mathbf{Im_1}$, $\mathbf{Im_2}$, $\mathbf{Ph_3}$, $\mathbf{Ph_4}$, were obtained for all PDB-based XH…Y models (**Table S6**). The PDB-based models were derived by extracting the Cartesian coordinates of the catalytic His or Tyr residue and a truncated version of the substrate from the PDB archive, followed by partial geometry optimization. During geometry optimization, the Cartesian coordinates of the amino acid N–C–C backbone as well as selected atoms in the substrate (see atoms in asterisk * in the **Table S8**) were fixed to their original spacial positions in the PDB file considered.

Full Citation for Methods

S1. Gaussian 09, Revision D. 01, Frisch, M.J., Trucks, G.W., Schlegel, H.B., Scuseria, G. E., Robb, M.A., Cheeseman, J.R., Scalmani, G., Barone, V., Mennucci, B., Petersson, G.A., Nakatsuji, H., Caricato, M., Li, X., Hratchian, H.P., Izmaylov, A. F., Bloino, J., Zheng, G., Sonnenberg, J. L., Hada, M., Ehara, M., Toyota, K., Fukuda, R., Hasegawa, J., Ishida, M., Nakajima, T., Honda, Y., Kitao, O., Nakai, H., Vreven, T., Montgomery, Jr., J.A., Peralta, J.E., Ogliaro, F., Bearpark, M., Heyd, J.J., Brothers, E., Kudin, K.N., Staroverov, V.N., Kobayashi, R., Normand, J., Raghavachari, K., Rendell, A., Burant, J.C., Iyengar, S.S., Tomasi, J., Cossi, M., Rega, N., Millam, J.M., Klene, M., Knox, J.E., Cross, J.B., Bakken, V., Adamo, C., Jaramillo, J., Gomperts, R., Stratmann, R.E., Yazyev, O., Austin, A.J., Cammi, R., Pomelli, C., Ochterski, J.W., Martin, R.L., Morokuma, K., Zakrzewski, V.G., Voth, G.A., Salvador, P., Dannenberg, J.J., Dapprich, S., Daniels, A.D., Farkas, Ö., Foresman, J.B., Ortiz, J.V., Cioslowski, J. & Fox, D.J. (Gaussian, Inc., Wallingford CT, 2009).

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Figure S1. Schematic illustrations of all model complexes studied. Blue dashed lines indicate short, strong hydrogen bonding interactions.

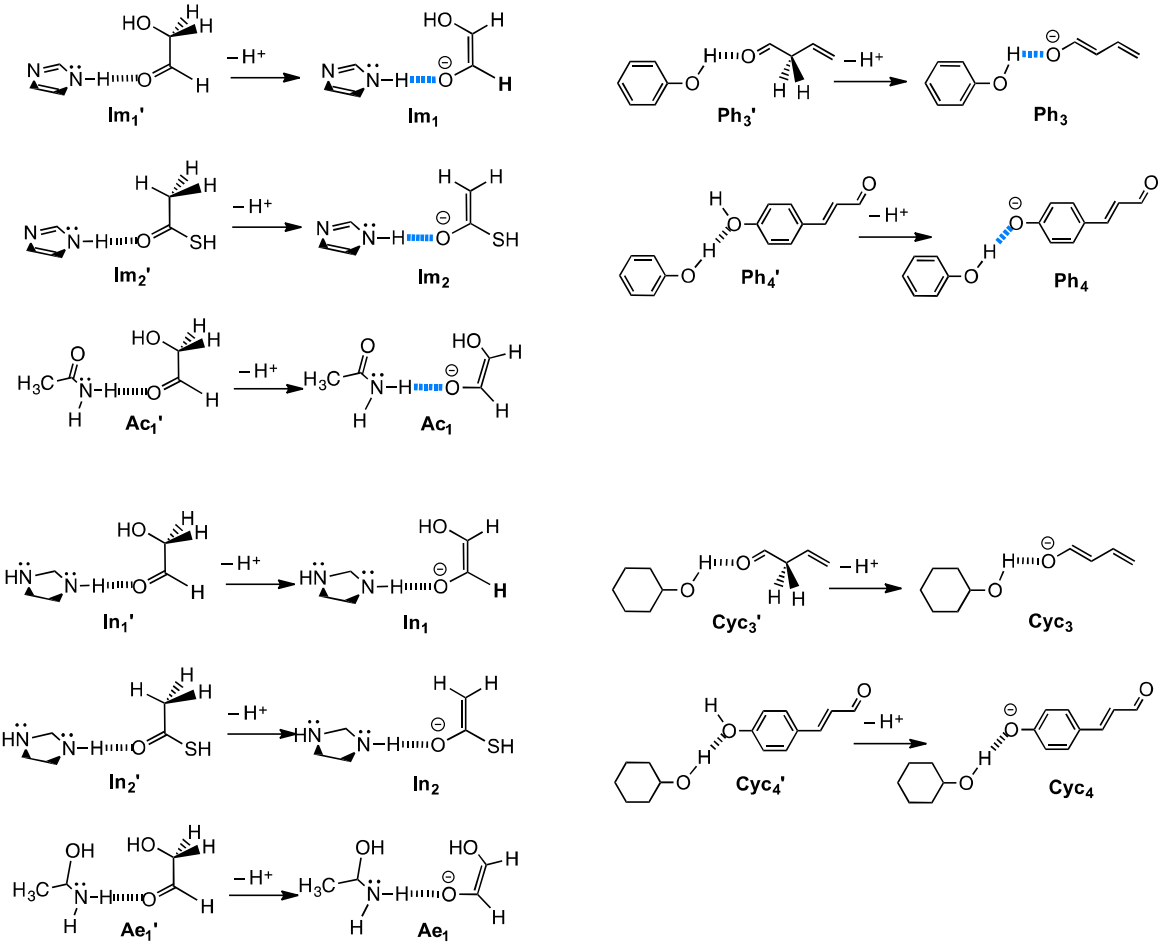
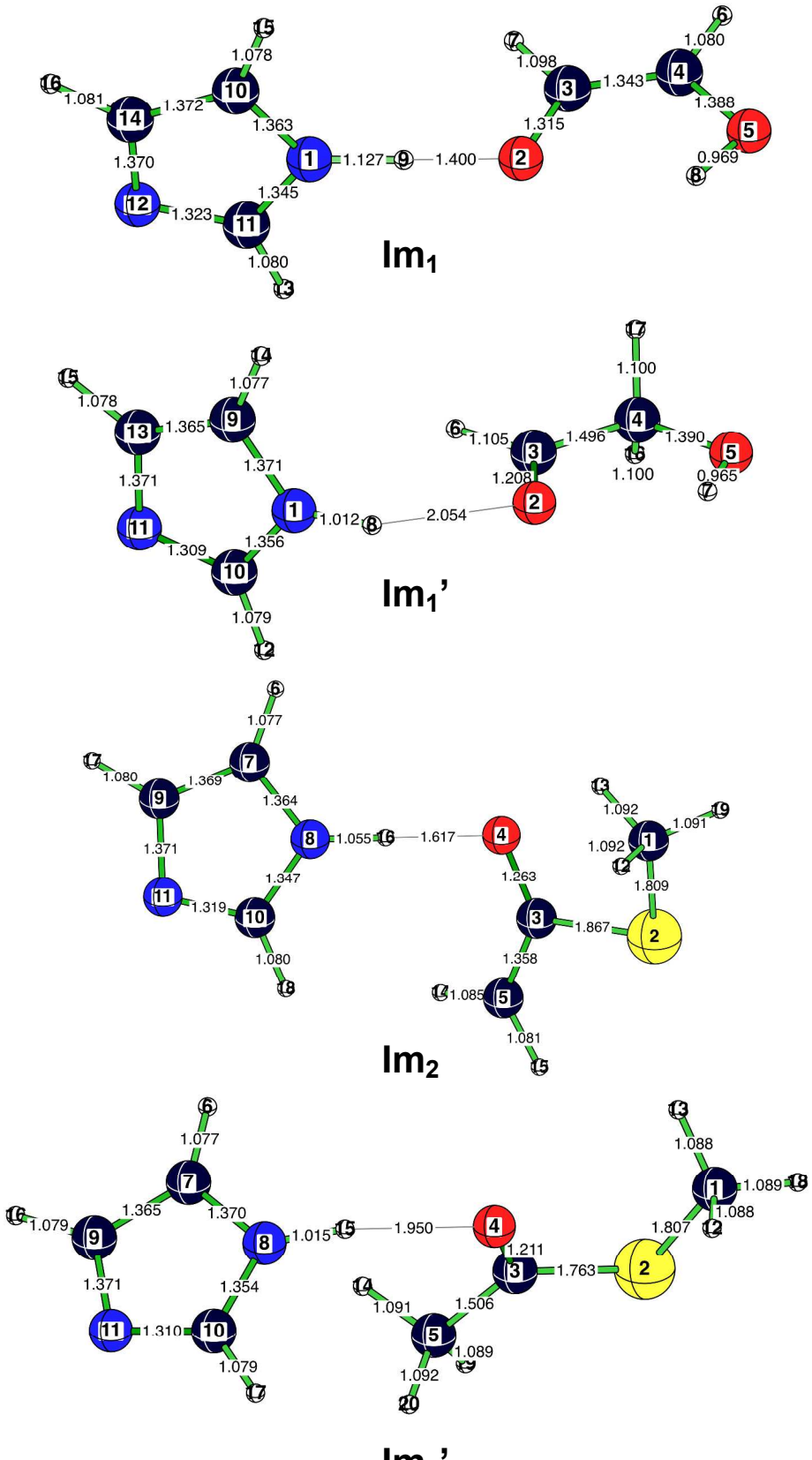
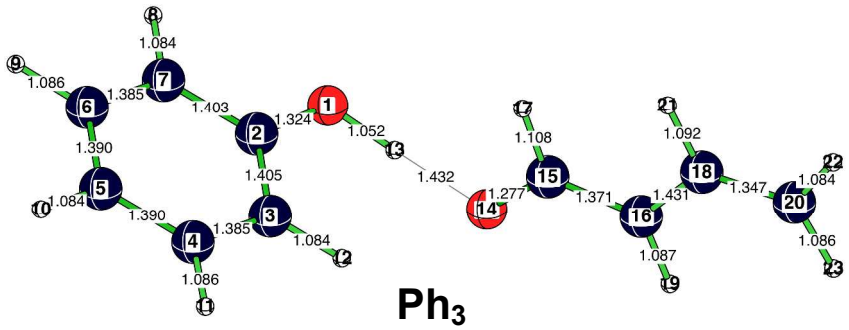


Figure S2. Optimized geometries (all values in Å) at ωB97X-D/6-311+G(2d,p) for all model complexes studied.





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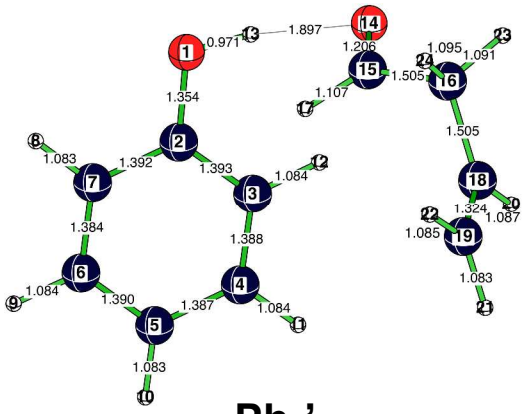

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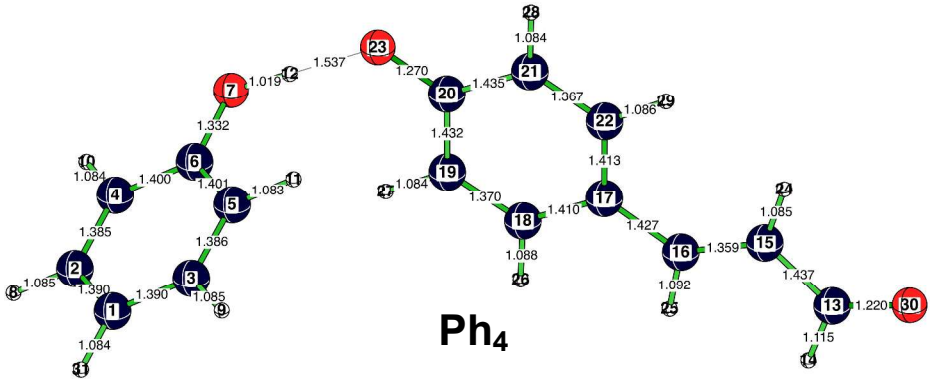

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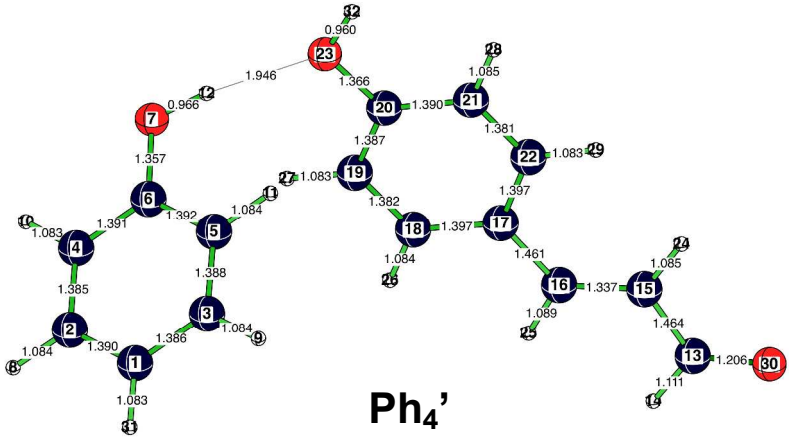

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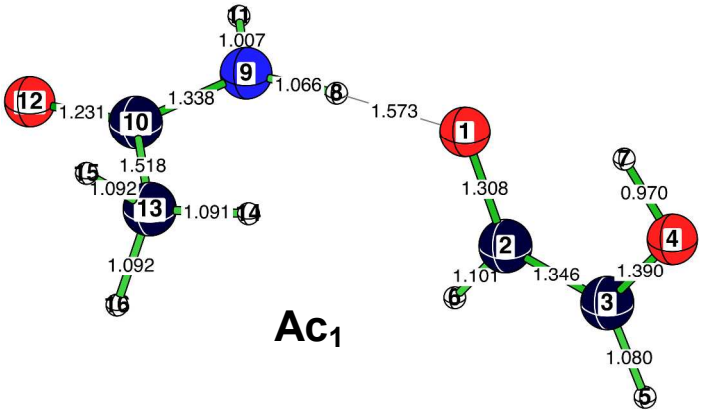
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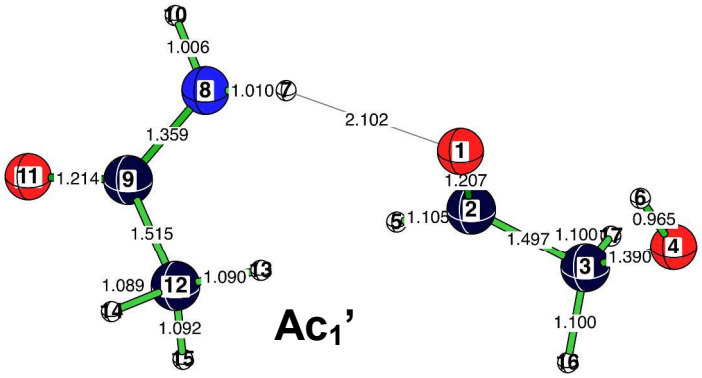
Ac1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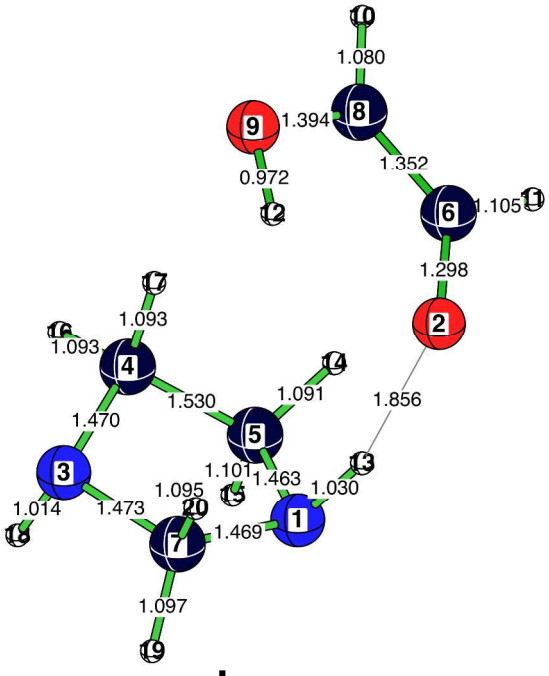
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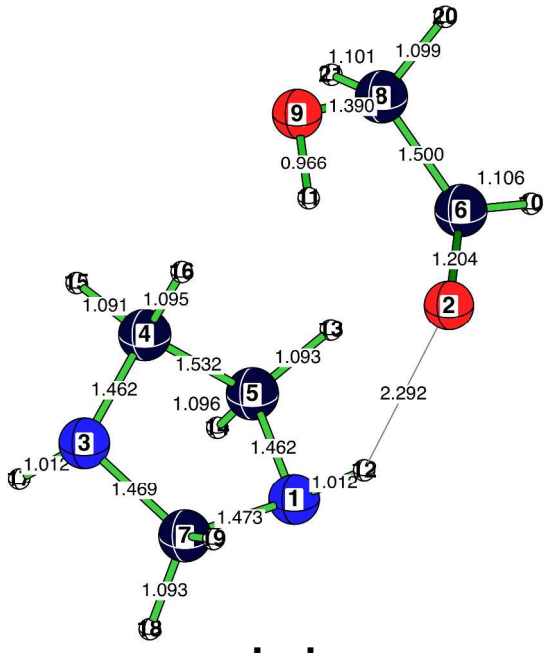
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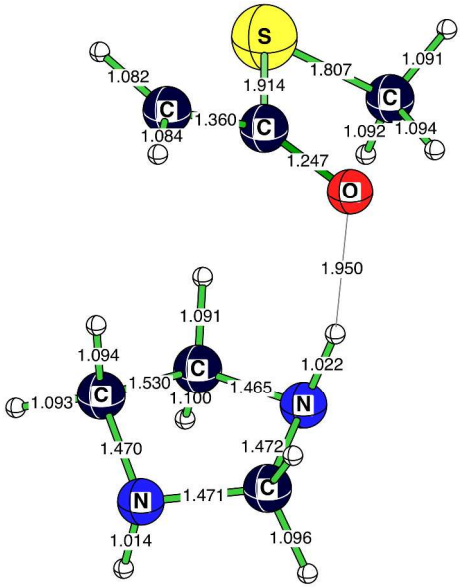
In1'



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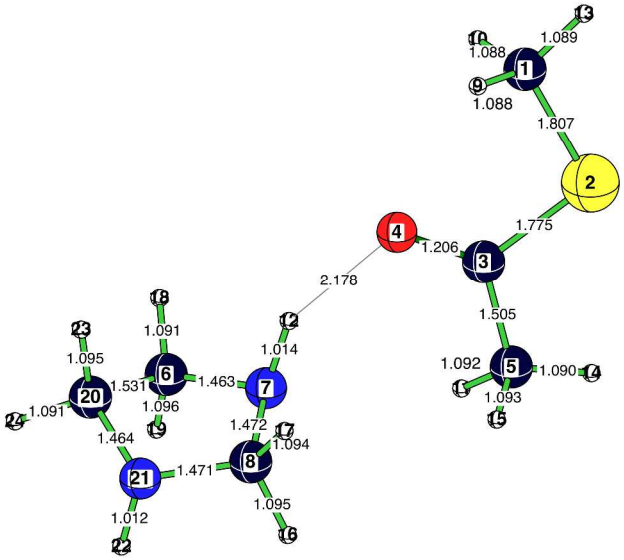

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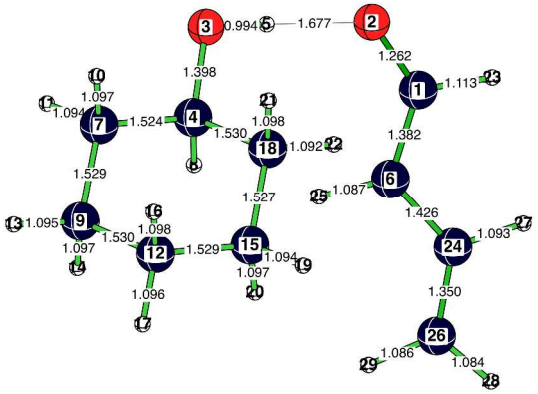
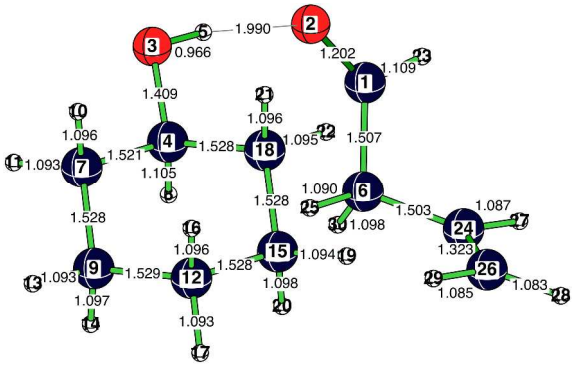


Cyc_3



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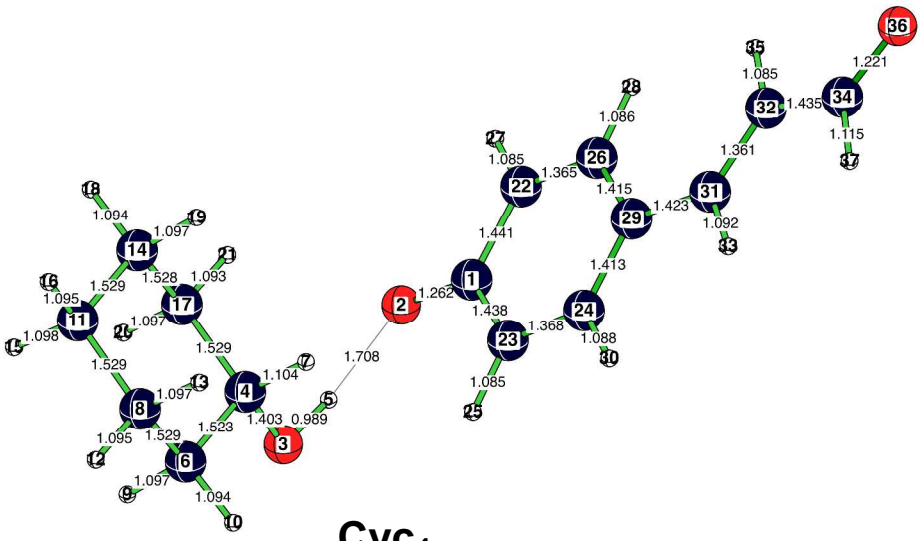
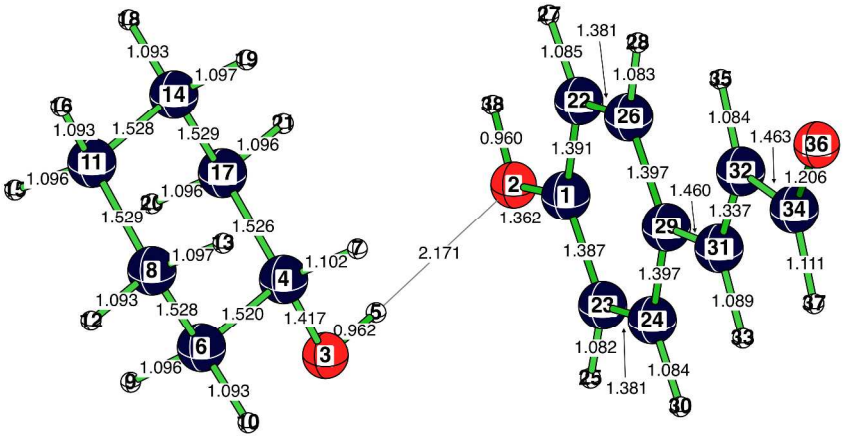


Cyc$_4$



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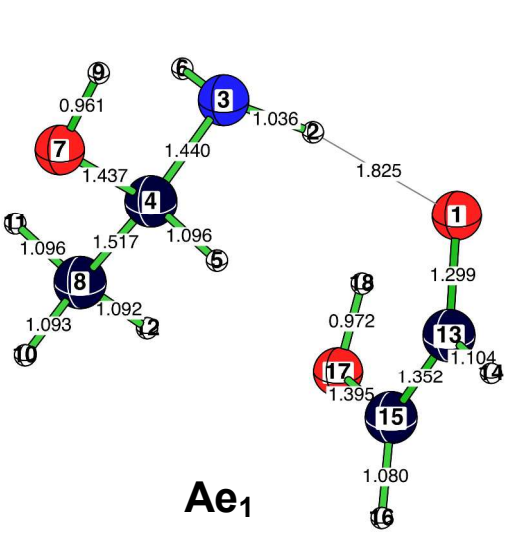
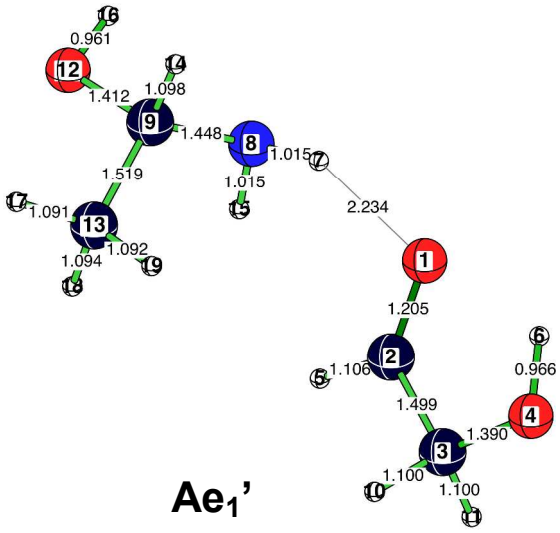


Ae$_1$



Ae$_1$'

Figure S3. Plot for computed ΔE_{HB} vs. Δd_{D-H} at ωB97X-D/6-311+G(2d,p) for **Im$_1$**, **Im$_2$**, **Ph$_3$**, **Ph$_4$**, **Im$_1$'**, **Im$_2$'**, **Ph$_3$'**, **Ph$_4$**,'

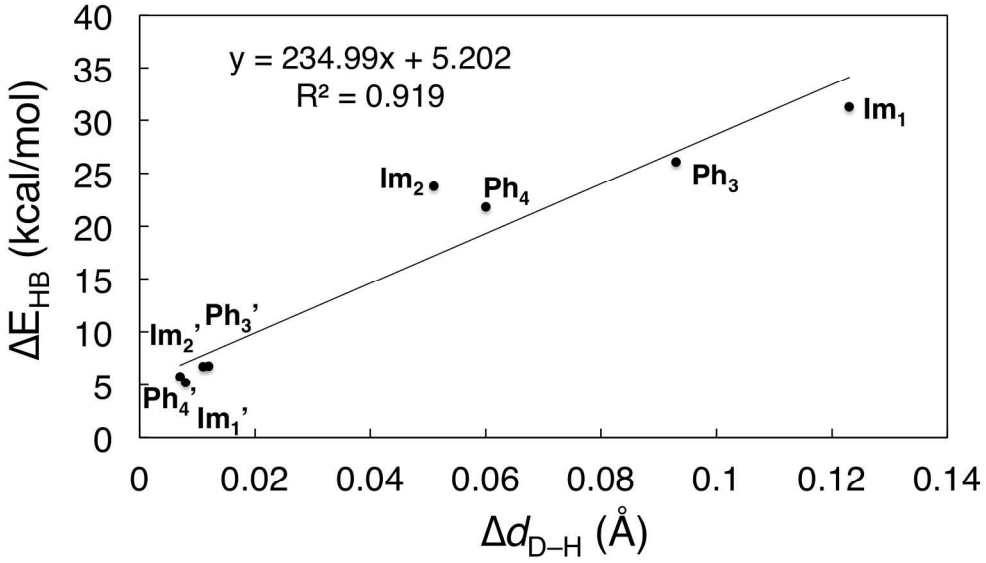


Table S1. Benchmark results at the ωB97X-D/6-311+G(2d,p) and composite (c~)CCSD(T)/aug-cc-pVTZ//ωB97XD/6-311+G(2d,p) levels.

	XH…Y model	ΔE_{HB} (kcal/mol)	XH…Y model	ΔE_{HB} (kcal/mol)	$\Delta\Delta E_{HB}$ (kcal/mol)
ωB97X-D	**Im$_1$**	31.27	**In$_1$**	15.73	15.54
(c~)CCSD(T)[†]	**Im$_1$**	31.89	**In$_1$**	16.58	15.31
ωB97X-D	**Ph$_3$**	26.09	**Cyc$_3$**	17.99	8.10
(c~)CCSD(T)[†]	**Ph$_3$**	27.22	**Cyc$_3$**	19.12	8.10

ΔE_{HB} is the computed hydrogen bonding interaction energy with zero-point energy (ZPE) correction.

[†]Composite (c~)CCSD(T)/aug-cc-pVTZ energies were derived by: E[c~CCSD(T)/aug-cc-pVTZ] = E[MP2/aug-cc-pVTZ] + E[(CCSD(T) – MP2)/aug-cc-pVDZ].

Table S2. Benchmark results for BLW computed π-electron delocalization energies.

XH…Y model	HF/6-31G(d)		HF/6-31+G(d)		HF/6-311+G(d,p)	
	DE_π (kcal/mol)	ΔDE_π[†] (kcal/mol)	DE_π (kcal/mol)	ΔDE_π[‡] (kcal/mol)	DE_π (kcal/mol)	ΔDE_π[§] (kcal/mol)
Im$_1$	94.36	15.31	97.66	15.66	100.02	15.27
Im$_2$	89.98	10.93	93.22	11.22	95.63	10.88
Ph$_3$	107.59	8.19	110.59	8.41	113.97	8.44
Ph$_4$	106.05	6.65	108.66	6.48	111.98	6.45
Ac$_1$	35.46	7.74	36.08	7.62	37.14	7.79

DE_π is the π-electron delocalization energy of XH in the XH…Y model considered.
ΔDE_π is the computed DE_π difference of XH before and after forming a hydrogen bond to Y.

[†]Based on comparisons to the DE_π value of **Im (**79.05 kcal/mol**)**, **Ph** (99.40 kcal/mol), or **Ac** (27.72 kcal/mol) at HF/6-31G(d).
[‡]Based on comparisons to the DE_π value of **Im (**82.00kcal/mol**)**, **Ph** (102.18 kcal/mol), or **Ac** (28.46 kcal/mol) at HF/6-31+G(d).
[§]Based on comparisons to the DE_π value of **Im (**84.75 kcal/mol**)**, **Ph** (105.53 kcal/mol), or **Ac** (29.35kcal/mol) at HF/6-311+G(d,p).

Table S3. Computed gas-phase hydrogen bonding interaction energies.

XH…Y model	ΔE_{HB} (kcal/mol)	XH…Y model	ΔE_{HB} (kcal/mol)	$\Delta\Delta E_{HB}$ (kcal/mol)
Im_1	31.27	**In_1**	15.73	15.54
Im_2	23.78	**In_2**	13.52	10.26
Ph_3	26.09	**Cyc_3**	17.99	8.10
Ph_4	21.84	**Cyc_4**	15.32	6.52
Ac_1	25.83	**Ae_1**	17.17	8.66
Im_1'	5.19	**In_1'**	2.85	2.34
Im_2'	6.72	**In_2'**	4.45	2.27
Ph_3'	6.75	**Cyc_3'**	5.61	1.14
Ph_4'	5.75	**Cyc_4'**	5.02[†]	0.73
Ac_1'	4.29	**Ae_1'**	2.53	1.75

ΔE_{HB} is the computed gas-phase hydrogen bonding interaction energy at ωB97X-D/6-311+G(2d,p) with ZPE correction.
$\Delta\Delta E_{HB}$ is the interaction energy of the [XH…Y^-] and [XH…YH] complexes minus that of their analogs with an unconjugated XH (XH = **In**, **Cyc**, or **Ae_1**).

[†]A constrained geometry optimization was carried out for **Cyc_4'** to avoid stacking interactions (C-O-O-C dihedral angle fixed to 64.6°, according to the optimized geometry of **Cyc_4**).

Table S4. Computed natural bond orbital (NBO) deletion energies.

XH…Y model	DEL_π (kcal/mol)	ΔDEL_π[†‡] (kcal/mol)
Im_1	179.24	35.49
Im_2	168.42	25.67
Ph_3	206.05	18.69
Ph_4	201.83	14.47
Im_1'	145.08	5.47
Im_2'	146.01	6.40
Ph_3'	188.48	1.91
Ph_4'	188.32	1.74

DEL_π is the computed NBO deletion energy, at HF/6-31G(d)//ωB97X-D/6-311+G(2d,p), by removing all of the $\pi \rightarrow \pi^*$ interactions in XH (see Supplementary Methods).
ΔDEL_π is the computed DEL_π difference in XH before and after forming a hydrogen bond to Y.

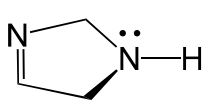
[†]Based on comparisons to the computed DEL_π values of the **Im** (143.75 kcal/mol) and **Ph** (187.36 kcal/mol) monomers.
[‡]Correlation coefficient $R^2 = 0.994$ for ΔDEL_π vs. $\Delta\Delta E_{HB}$ (see **Table S3**) values.

Table S5. Computed ΔE_{HB} and $\Delta\Delta E_{HB}$ based on alternative unconjugated XH references (XH = **Id** or **Cyd**).

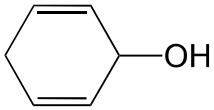
XH…Y model	ΔE_{HB} (kcal/mol)	$\Delta\Delta E_{HB}$[†] (kcal/mol)	XH…Y model	$\Delta\Delta E_{HB}$[‡] (kcal/mol)
Id$_1$	18.48	12.79	**In$_1$**	15.54
Id$_2$	15.24	8.54	**In$_2$**	10.26
Cyd$_3$	19.11	6.97	**Cyc$_3$**	8.10
Cyd$_4$	15.41	5.43	**Cyc$_4$**	6.52
Id$_1$'	4.76	0.43	**In$_1$'**	2.34
Id$_2$'	4.75	1.97	**In$_2$'**	2.27
Cyd$_3$'	5.05	1.70	**Cyc$_3$'**	1.14
Cyd$_4$'	4.76	0.99	**Cyc$_4$'**	0.73

ΔE_{HB} is the computed gas-phase hydrogen bonding interaction energy at ωB97X-D/6-311+G(2d,p) with ZPE correction.
$\Delta\Delta E_{HB}$ is the interaction energy of the [XH…Y$^-$] and [XH…YH] complexes minus that of their analogs with an unconjugated XH (XH = **Id** or **Cyd**).

[†]ΔE_{HB} values for [XH…Y$^-$] and [XH…YH] complexes based on alternative unconjugated XH references (XH = **Id** or **Cyd**).
[‡]ΔE_{HB} values for [XH…Y$^-$] and [XH…YH] complexes based on unconjugated XH references (XH = **In** or **Cyc**).



Imidazoline (**Id**)



Cyclohexadieneol (**Cyd**)

Table S6. Computed hydrogen bonding interaction energies in implicit water solvation.

XH…Y model	$\Delta E_{HB(sol)}$ (kcal/mol)	XH…Y model	$\Delta E_{HB(sol)}$ (kcal/mol)	$\Delta\Delta E_{HB(sol)}$ (kcal/mol)
Im$_1$	12.01	**In$_1$**	3.47	8.54
Im$_2$	8.91	**In$_2$**	5.06	3.86
Ph$_3$	13.01	**Cyc$_3$**	9.02	3.99
Ph$_4$	12.46	**Cyc$_4$**	8.65	3.81
Ac$_1$	8.95	**Ae$_1$**	5.26	3.69

$\Delta E_{HB(sol)}$ is the computed hydrogen bonding interaction energy, in implicit water solvation, at IEFPCM-ωB97X-D/6-311+G(2d,p) with ZPE correction.
$\Delta\Delta E_{HB(sol)}$ is the interaction energy of the **Im$_{1,2}$**, **Ph$_{1,2}$**, or **Ac$_1$** complex minus that of its "unconjugated" analog, **In$_{1,2}$**, **Cyc$_{1,2}$**, or **Ae$_1$**.

Table S7. Computed hydrogen bonding interaction energies for protein structure database (PDB)-derived XH…Y models.

Enzyme	ΔE_{HB} XH…Y models[†] (kcal/mol)	ΔE_{HB} PDB-derived models[‡] (kcal/mol)
Triosephosphate Isomerase	31.19 (**Im$_1$**)	31.87 (1NEY)
Citrate Synthase	24.75 (**Im$_2$**)	27.99 (4CSC)
Ketosteroid Isomeras	26.79 (**Ph$_3$**)	27.02 (1OHP)
Photoactive Yellow Protein	22.84 (**Ph$_4$**)	24.25 (3PYP)

[†]ΔE_{HB} computed at ωB97X-D/6-311+G(2d,p) without ZPE correction.
[‡]ΔE_{HB} computed at ωB97X-D/6-311+G(2d,p)//ωB97X-D/6-31+G(d) without ZPE correction.

Table S8. Optimized Cartesian coordinates and energies at ωB97X–D/6–311+G(2d,p) for all structures computed in the gas phase.

Im_1

	X	Y	Z
N	1.184286	–0.156933	–0.161603
O	–1.314531	–0.155925	–0.534235
C	–1.938792	0.556116	0.378076
C	–3.271636	0.719464	0.373503
O	–4.030343	0.121306	–0.623192
H	–3.837156	1.290186	1.095159
H	–1.354349	1.036000	1.174004
H	–3.359973	–0.332677	–1.154946
H	0.071167	–0.167751	–0.335692
C	2.079263	0.753962	–0.638341
C	1.903861	–1.029003	0.566748
N	3.196994	–0.752964	0.595718
H	1.442844	–1.866888	1.069394
C	3.311722	0.378175	–0.168082
H	1.770681	1.578385	–1.261112
H	4.266900	0.855188	–0.335398

Total electronic energy = –454.71263 a.u.
ZPE = 0.12008 a.u.
Number of imaginary frequency (NIm) = 0

Im_1–TS

	X	Y	Z
N	1.153599	–0.159029	–0.146299
O	–1.281944	–0.220183	–0.561349
C	–1.901402	0.544000	0.325451
C	–3.230570	0.699150	0.317337
O	–4.005786	0.055487	–0.632362
H	–3.786718	1.307388	1.014855
H	–1.302326	1.058311	1.081609
H	–3.359180	–0.433289	–1.159537
H	–0.075556	–0.205554	–0.369713
C	2.051625	0.736625	–0.648075
C	1.877510	–0.963540	0.651390
N	3.168538	–0.663049	0.703980
H	1.425416	–1.782027	1.195061
C	3.281707	0.420726	–0.123775
H	1.752173	1.518073	–1.330107
H	4.231706	0.908340	–0.294716

Total electronic energy = –454.71230 a.u.
ZPE = 0.11758 a.u.
NIm = 1 (ω_{Im} = 620*i* cm^{-1})

Im_2

	X	Y	Z
C	–0.614401	3.268994	–1.782187
S	0.236339	3.731926	–0.254336
C	0.993880	2.086797	0.197275
O	1.184864	1.279088	–0.755108
C	1.288660	1.964883	1.517375
H	1.300162	–2.318957	–1.782775
C	0.930455	–2.369147	–0.772001
N	0.762923	–1.251070	–0.009194
C	0.546168	–3.423262	0.012740
C	0.292636	–1.665734	1.182803
N	0.144780	–2.975048	1.244220
H	–1.658985	3.008934	–1.601053
H	–0.081736	2.403331	–2.181942
H	1.854029	1.105515	1.860888
H	0.993184	2.722736	2.229956
H	0.955975	–0.254506	–0.294927
H	0.536831	–4.473577	–0.239052
H	0.074286	–0.965817	1.975190
H	–0.560470	4.098955	–2.487752

Total electronic energy = –817.01378 a.u.
ZPE = 0.14515 a.u.
NIm = 0

Im_1'

	X	Y	Z
N	1.285675	–0.397286	–0.479845
O	–1.628673	–0.348902	–0.856475
C	–1.809664	0.370628	0.096840
C	–3.180191	0.812960	0.502343
O	–4.179262	0.313319	–0.325048
H	–0.962505	0.730307	0.708491
H	–3.751265	–0.230114	–0.998303
H	0.405254	–0.623599	–0.924914
C	2.067838	0.699171	–0.734290
C	1.845995	–1.049555	0.568037
N	2.931854	–0.453692	0.990822
H	1.424255	–1.955530	0.976156
C	3.079177	0.642582	0.180326
H	1.846324	1.392233	–1.528077
H	3.905777	1.325142	0.298382
H	–3.331489	0.497373	1.545192
H	–3.182032	1.912864	0.508732

Total electronic energy = –455.262634 a.u.
ZPE = 0.134718 a.u. (NIm = 0)

Im_2'

	X	Y	Z
C	–0.301207	3.963603	–1.754287
S	0.788298	3.745516	–0.329301
C	0.601853	2.012730	–0.061259
O	–0.106435	1.323413	–0.760869
C	1.383689	1.476326	1.108242
H	1.857271	–2.021093	–1.182573
C	1.233092	–2.253329	–0.336257
N	0.154585	–1.483403	0.009958
C	1.260666	–3.271581	0.573048
C	–0.403323	–2.054758	1.103095
N	0.232853	–3.139312	1.470600
H	–1.316563	3.672125	–1.494998
H	0.054004	3.364996	–2.590103
H	1.974433	0.618972	0.781240
H	–0.105579	–0.593333	–0.403217
H	1.957429	–4.093001	0.629029
H	–1.275761	–1.642967	1.587441
H	–0.268539	5.021478	–2.010273
H	2.034841	2.227672	1.553105
H	0.679194	1.118403	1.862087

Total electronic energy = –817.5798738 a.u.
ZPE = 0.158992 a.u.
NIm = 0

In_1

	X	Y	Z
N	–1.378299	–1.650786	0.744245
O	1.202418	–0.497119	1.168946
N	–2.929784	0.154635	0.488839
C	–2.044296	0.105968	–0.683395
C	–1.527204	–1.334286	–0.676723
C	1.711201	–0.131929	0.031803
C	–2.270760	–0.731572	1.463741
C	1.578852	1.117625	–0.468248
O	0.870252	2.055168	0.281339
H	1.984464	1.482822	–1.400740
H	2.282622	–0.857999	–0.573780
H	0.644345	1.536717	1.071833
H	–0.411982	–1.394731	0.993107
H	–0.567128	–1.443204	–1.183353
H	–2.257968	–2.003583	–1.157080
H	–2.591749	0.387856	–1.586903
H	–1.211407	0.799850	–0.542746
H	–3.806247	–0.282351	0.224242

H	–3.045483	–1.262989	2.030205
H	–1.678217	–0.137612	2.166820

Total electronic energy = –457.09701 a.u.
ZPE = 0.16986 a.u.
NIm = 0

In_2

	X	Y	Z
C	1.009506	1.746528	–2.386706
S	–0.149887	2.438692	–1.185771
C	0.665075	1.826119	0.433685
O	1.785350	1.291061	0.319532
C	–0.119784	2.062969	1.519159
C	–0.178774	–1.445738	–0.586701
N	1.271836	–1.520235	–0.392994
C	1.483829	–2.246421	0.869825
H	1.884573	1.431952	–1.809719
H	1.297174	2.507328	–3.113746
H	1.601622	–0.562888	–0.255309
H	0.588880	0.883339	–2.906377
H	–1.091406	2.528411	1.417546
H	2.060893	–3.167017	0.723191
H	2.031965	–1.603583	1.565280
H	–0.452909	–0.487186	–1.030890
H	–0.524415	–2.252662	–1.249415
C	–0.748322	–1.634938	0.820377
N	0.173493	–2.598403	1.438044
H	–0.072642	–3.519634	1.092035
H	–0.704563	–0.684414	1.360002
H	–1.773234	–2.013363	0.847315
H	0.245680	1.798194	2.504727

Total electronic energy = –819.40485 a.u.
ZPE = 0.19321 a.u.
NIm = 0

In_1'

	X	Y	Z
N	–1.496124	–1.762763	0.776522
O	1.292567	–0.265348	1.142712
N	–2.943929	0.120029	0.546595
C	–1.982530	0.124736	–0.555380
C	–1.502198	–1.328732	–0.619507
C	1.750175	–0.088052	0.043049
C	–2.482153	–0.920187	1.475238
C	1.687231	1.248242	–0.635054
O	1.075223	2.217838	0.151037

H	2.232106	–0.908490	–0.519889
H	0.808455	1.789410	0.975018
H	–0.580261	–1.586239	1.168962
H	–0.512239	–1.455999	–1.064719
H	–2.204917	–1.934818	–1.202067
H	–2.451305	0.483088	–1.473133
H	–1.153657	0.797803	–0.313556
H	–3.852582	–0.140393	0.185761
H	–3.341101	–1.507359	1.811264
H	–2.013683	–0.473032	2.356679
H	2.713590	1.540862	–0.899010
H	1.148074	1.107105	–1.584438

Total electronic energy = –457.666194 a.u.
ZPE = 0.182642 a.u.
NIm = 0

In_2'

	X	Y	Z
C	–0.586702	3.730863	–1.879608
S	0.430091	3.820472	–0.388583
C	0.519934	2.095880	0.019718
O	–0.006467	1.246487	–0.655718
C	1.283825	1.801393	1.282753
C	1.434663	–2.676734	–0.450702
N	1.274700	–1.420758	0.281358
C	0.344561	–1.706775	1.385588
H	–1.555997	3.296066	–1.645517
H	–0.086298	3.129955	–2.635803
H	1.904083	0.917457	1.122874
H	0.840292	–0.732386	–0.323711
H	–0.710438	4.752835	–2.234869
H	1.890061	2.646903	1.607005
H	0.560548	1.565064	2.067552
H	0.852582	–1.677366	2.354640
H	–0.442438	–0.947031	1.390897
H	1.639987	–2.481693	–1.504315
H	2.275015	–3.248351	–0.040693
C	0.117966	–3.415204	–0.194853
N	–0.222862	–3.048004	1.180635
H	0.231498	–3.696093	1.810930
H	–0.658061	–3.050974	–0.875829
H	0.181629	–4.499417	–0.298897

Total electronic energy = –819.983542 a.u.
ZPE = 0.206908 a.u.
NIm = 0

Ph_3

	X	Y	Z
O	–0.762048	–1.468426	1.255253
C	–1.677045	–0.780271	0.590168
C	–1.502234	0.562254	0.215108
C	–2.496221	1.227507	–0.483460
C	–3.685005	0.593971	–0.828295
C	–3.862594	–0.734046	–0.457289
C	–2.878577	–1.414364	0.239972
H	–3.012908	–2.450570	0.529587
H	–4.782661	–1.249459	–0.716083
H	–4.456229	1.123870	–1.375620
H	–2.336712	2.263880	–0.764425
H	–0.578185	1.060090	0.484724
H	0.102058	–0.901597	1.453377
O	1.292479	–0.144269	1.698161
C	2.106919	–0.163260	0.714760
C	3.322217	0.463987	0.624504
H	1.801878	–0.749945	–0.174615
C	4.137206	0.359482	–0.546806
H	3.672256	1.052917	1.468690
C	5.344028	0.913278	–0.773219
H	3.712963	–0.248690	–1.348561
H	5.866876	0.760487	–1.710458
H	5.832381	1.531774	–0.025472

Total electronic energy = –538.14256 a.u.
ZPE = 0.18260 a.u.
NIm = 0

Ph_4

	X	Y	Z
C	2.288436	–2.826372	0.320005
C	2.695008	–2.160288	1.470241
C	1.267493	–2.275709	–0.444966
C	2.095287	–0.971538	1.850656
C	0.659332	–1.085549	–0.079630
C	1.066818	–0.414727	1.081406
O	0.516735	0.727895	1.487850
H	3.490314	–2.573573	2.082513
H	0.933939	–2.781446	–1.345167
H	2.406013	–0.449076	2.748179
H	–0.134167	–0.657746	–0.680446
H	–0.246305	1.017750	0.877158
C	–8.549302	–1.848239	–0.474975
H	–8.392962	–2.640579	0.293417

C	–7.408294	–0.999581	–0.685236
C	–6.269574	–1.202361	0.027389
C	–5.030549	–0.494716	–0.011629
C	–3.972796	–0.889547	0.833204
C	–2.760822	–0.251186	0.842859
C	–2.502159	0.862770	–0.018188
C	–3.585166	1.256296	–0.873564
C	–4.786614	0.605141	–0.864396
O	–1.388526	1.472535	–0.045060
H	–7.503313	–0.210060	–1.422771
H	–6.298919	–2.029344	0.739490
H	–4.131213	–1.734116	1.499832
H	–1.968370	–0.579435	1.506158
H	–3.411557	2.098278	–1.534565
H	–5.573528	0.942794	–1.531916
O	–9.624879	–1.772455	–1.044850
H	2.757422	–3.758304	0.026402

Total electronic energy = –805.12603 a.u.
ZPE = 0.24177 a.u.
NIm = 0

Ph_3'

	X	Y	Z
O	–0.889010	–1.130656	1.959626
C	–1.500328	–0.671845	0.842473
C	–1.336587	0.631117	0.376833
C	–1.986843	1.037284	–0.780130
C	–2.805064	0.161798	–1.477595
C	–2.970194	–1.133638	–1.002284
C	–2.324370	–1.553509	0.147994
H	–2.445276	–2.561599	0.525291
H	–3.610022	–1.827851	–1.534977
H	–3.312037	0.484613	–2.378351
H	–1.854379	2.053800	–1.132859
H	–0.712629	1.324907	0.928987
H	–0.236518	–0.484209	2.275287
O	1.432849	0.416429	2.323882
C	2.034798	0.021683	1.355686
C	3.427713	0.459210	0.989034
H	1.556866	–0.690061	0.654898
C	3.400485	1.185375	–0.329351
C	3.857568	0.688689	–1.467877
H	2.944394	2.171544	–0.317464
H	3.794021	1.250473	–2.391841
H	4.317398	–0.293256	–1.516568
H	3.819284	1.089249	1.789521

H	4.045810	–0.440418	0.901964

Total electronic energy = –538.680969 a.u.
ZPE = 0.197325 a.u.
NIm = 0

Ph_4'

	X	Y	Z
C	4.644522	–2.201047	–0.340811
C	5.157087	–1.695509	0.847755
C	3.855316	–1.385864	–1.137641
C	4.884939	–0.395740	1.239826
C	3.577616	–0.080392	–0.758027
C	4.091729	0.416910	0.436062
O	3.847577	1.679804	0.867723
H	5.776659	–2.321423	1.479551
H	3.448511	–1.764837	–2.068063
H	5.277958	0.007457	2.165073
H	2.961097	0.553339	–1.385711
H	3.238000	2.127343	0.266306
C	–5.017792	–1.470507	–1.041984
H	–4.839462	–2.172049	–0.198977
C	–3.951992	–0.492864	–1.268602
C	–2.865319	–0.488861	–0.489570
C	–1.710103	0.402474	–0.564829
C	–0.671909	0.248930	0.356880
C	0.445223	1.061798	0.334524
C	0.537576	2.053319	–0.630244
C	–0.479273	2.229163	–1.561733
C	–1.590928	1.410371	–1.524127
O	1.661207	2.830750	–0.631468
H	–4.103326	0.203741	–2.085911
H	–2.819556	–1.234452	0.303270
H	–0.739757	–0.529063	1.109147
H	1.246843	0.932679	1.050854
H	–0.401540	3.006047	–2.315519
H	–2.373667	1.561475	–2.257108
O	–6.027712	–1.542086	–1.697725
H	4.859568	–3.218751	–0.641663
H	1.620069	3.482447	–1.335110

Total electronic energy = –805.638052 a.u.
ZPE = 0.255571 a.u.
NIm = 0

Cyc_3

	X	Y	Z
C	1.334453	–2.031110	0.052642

O	0.438336	–2.847875	0.403986
O	–2.024916	–2.249378	1.240165
C	–2.270195	–0.938130	0.820875
H	–1.095624	–2.481715	0.973221
C	1.405344	–0.667002	0.265367
C	–3.671193	–0.534423	1.264425
H	–1.557211	–0.244776	1.302224
C	–4.008608	0.892946	0.833064
H	–4.385296	–1.239606	0.820749
H	–3.748009	–0.642576	2.350243
C	–3.837145	1.078363	–0.675581
H	–5.029893	1.149972	1.134279
H	–3.342799	1.592447	1.354020
C	–2.438765	0.657464	–1.128885
H	–4.582334	0.463110	–1.196616
H	–4.035335	2.119102	–0.954369
C	–2.118606	–0.770711	–0.691900
H	–2.347098	0.752194	–2.215290
H	–1.695456	1.337789	–0.695747
H	–2.800671	–1.478836	–1.179814
H	–1.100812	–1.043152	–0.978772
H	2.194407	–2.450892	–0.515568
C	2.493136	0.112879	–0.227416
H	0.614821	–0.177171	0.828826
C	2.700617	1.441860	–0.108461
H	3.250528	–0.455079	–0.773638
H	3.577805	1.914915	–0.535398
H	1.995961	2.080630	0.416758

Total electronic energy = –808.76169 a.u.
ZPE = 0.31244 a.u.
NIm = 0

Cyc_4

	X	Y	Z
C	1.489598	–1.567943	0.019250
O	0.586979	–2.445215	–0.066088
O	–1.640747	–1.908158	1.329421
C	–2.060365	–0.764000	0.634318
H	–0.809327	–2.216453	0.890595
C	–3.233503	–0.143387	1.380908
H	–1.243874	–0.021444	0.605366
C	–3.762197	1.100152	0.666243
H	–4.026320	–0.898013	1.456695
H	–2.922097	0.096127	2.401472
C	–4.135528	0.796309	–0.785355
H	–4.624955	1.507859	1.202968

H	–2.989001	1.878325	0.678673
C	–2.962413	0.164975	–1.535596
H	–4.984248	0.100463	–0.797920
H	–4.467350	1.709400	–1.290690
C	–2.446769	–1.078158	–0.811824
H	–3.256846	–0.085155	–2.559597
H	–2.150643	0.898446	–1.614722
H	–3.224536	–1.852120	–0.793494
H	–1.578201	–1.501707	–1.321572
C	2.530066	–1.453531	–0.970920
C	1.554662	–0.616502	1.094951
C	2.540661	0.329829	1.150781
H	0.793517	–0.677111	1.865649
C	3.504004	–0.500327	–0.892115
H	2.507328	–2.161405	–1.792509
H	4.263044	–0.457400	–1.667568
C	3.552177	0.433896	0.169816
H	2.554752	1.033162	1.980822
C	4.549489	1.442723	0.286369
C	5.604461	1.726273	–0.526147
H	4.446942	2.084158	1.164113
C	6.490973	2.806854	–0.201907
H	5.813871	1.161969	–1.428439
O	7.468756	3.164988	–0.839625
H	6.224252	3.348512	0.735689

Total electronic energy = –541.77631 a.u.
ZPE = 0.25389 a.u.
NIm = 0

Cyc_3'

	X	Y	Z
C	–1.105290	–2.127417	1.409540
O	–2.093416	–1.476261	1.622244
O	–2.601261	1.427828	1.593107
C	–1.470341	1.943786	0.929226
H	–2.527361	0.465425	1.615946
C	0.249778	–1.554839	1.084153
C	–1.523694	3.461311	1.016138
H	–0.551285	1.610737	1.443952
C	–0.338851	4.105537	0.297160
H	–2.464737	3.793084	0.562966
H	–1.552733	3.758988	2.066903
C	–0.241890	3.639483	–1.155492
H	–0.422589	5.194406	0.341272
H	0.589144	3.843167	0.820036
C	–0.198692	2.114156	–1.241577

H	–1.114671	4.003426	–1.710213
H	0.640451	4.072034	–1.635024
C	–1.396640	1.489398	–0.527455
H	–0.168582	1.790026	–2.285710
H	0.730556	1.760427	–0.774850
H	–2.327008	1.788090	–1.022780
H	–1.354372	0.396312	–0.575810
H	–1.159445	–3.234247	1.444852
C	0.828466	–2.201742	–0.143111
H	0.171163	–0.472671	0.976516
C	1.088665	–1.556634	–1.268906
H	1.025510	–3.269360	–0.079992
H	1.502895	–2.072076	–2.127007
H	0.902116	–0.492810	–1.370792
H	0.893010	–1.767935	1.948540

Total electronic energy = –542.324732 a.u.
ZPE = 0.26755 a.u.
NIm = 0

Cyc_4'

	X	Y	Z
C*	1.410000	–2.053740	0.052020
O*	0.569570	–3.122920	–0.024450
O*	–1.496570	–1.627100	1.634920
C*	–1.670150	–0.646270	0.627730
H	–1.021140	–2.367930	1.246170
C	–2.447340	0.510510	1.233360
H	–0.683810	–0.267360	0.313430
C	–2.683280	1.615390	0.204110
H	–3.405840	0.125680	1.599820
H	–1.902820	0.893500	2.099670
C	–3.380580	1.076590	–1.044980
H	–3.272210	2.420820	0.649840
H	–1.720230	2.054440	–0.083090
C	–2.610320	–0.099710	–1.643980
H	–4.391010	0.744480	–0.778530
H	–3.495140	1.870630	–1.787680
C	–2.384870	–1.196050	–0.602820
H	–3.143130	–0.504610	–2.508360
H	–1.639250	0.255740	–2.010470
H	–3.344360	–1.619150	–0.284600
H	–1.801520	–2.017630	–1.032980
C	1.832220	–1.365360	–1.081140
C	1.808120	–1.637140	1.313270
C	2.623610	–0.528350	1.429900
H	1.456550	–2.169970	2.186830

C	2.649750	–0.260570	–0.949130
H	1.511630	–1.690060	–2.065900
H	2.964640	0.264510	–1.842470
C	3.061150	0.183000	0.309690
H	2.926020	–0.199600	2.418090
C	3.918490	1.350020	0.498430
C	4.445910	2.143670	–0.440030
H	4.146750	1.589660	1.536340
C	5.287280	3.278180	–0.057520
H	4.287080	1.998100	–1.502910
O	5.799530	4.042020	–0.838390
H	5.435500	3.404120	1.036560
H	0.372830	–3.322800	–0.942730

*Constrained geometry optimization (C-O-O-C dihedral angle fixed to 64.6°, according to the optimized geometry of **Cyc$_4$**).
Total electronic energy = –809.282042 a.u.
ZPE = 0.325372 a.u.
NIm = 1 (ω_{Im} = 14*i* cm^{-1})

Ac$_1$

	X	Y	Z
O	–1.158211	1.394370	–0.419602
C	–1.601172	0.992684	0.744186
C	–2.714150	0.247222	0.879477
O	–3.427071	–0.108700	–0.259913
H	–3.127911	–0.112203	1.810255
H	–1.048054	1.264654	1.656581
H	–2.900302	0.302737	–0.962802
H	0.232351	2.122999	–0.313465
N	1.207646	2.542202	–0.212427
C	2.306527	1.789288	–0.085781
H	1.351571	3.538798	–0.193449
O	3.445283	2.241825	0.035998
C	2.057871	0.292309	–0.096432
H	1.007898	0.051613	–0.268664
H	2.681296	–0.158117	–0.871264
H	2.376858	–0.117362	0.864372

Total electronic energy = –437.71969 a.u.
ZPE = 0.12429 a.u.
NIm = 0

Ac$_1$'

	X	Y	Z
O	–1.377375	1.201463	–0.656302
C	–1.547551	0.945001	0.510940
C	–2.763161	0.214746	0.989874

O	–3.635705	–0.116842	–0.040194
H	–0.804453	1.242274	1.272951
H	–3.248288	0.211005	–0.861495
H	0.435266	2.264889	–0.684148
N	1.263997	2.606778	–0.219957
C	2.305476	1.790849	0.091226
H	1.403816	3.598027	–0.117533
O	3.340828	2.210019	0.566481
C	2.080567	0.314131	–0.160078
H	1.179317	0.106079	–0.737547
H	2.949846	–0.083149	–0.682981
H	2.017673	–0.194807	0.803999
H	–2.418225	–0.683026	1.523813
H	–3.255839	0.851012	1.739752

Total electronic energy = –438.275071 a.u.
ZPE = 0.13708 a.u.
NIm = 0

Ae_1

	X	Y	Z
O	1.471132	–4.155582	2.015357
H	1.242142	–2.853248	0.757448
N	0.935669	–2.145520	0.065981
C	–0.358535	–1.633492	0.435170
H	–0.395138	–1.626284	1.530193
H	0.886657	–2.601231	–0.839492
O	–0.487015	–0.285518	–0.045945
C	–1.543916	–2.418593	–0.093622
H	0.420825	0.029100	–0.065516
H	–2.484420	–1.946318	0.202568
H	–1.505876	–2.448235	–1.188204
H	–1.512445	–3.436493	0.300674
C	0.434567	–4.259400	2.791365
H	0.435330	–3.765046	3.778465
C	–0.672265	–4.957114	2.451074
H	–1.562885	–5.085222	3.048844
O	–0.689023	–5.596130	1.210836
H	0.205086	–5.395525	0.885653

Total electronic energy = –438.89342 a.u.
ZPE = 0.14867 a.u.
NIm = 0

Ae_1'

	X	Y	Z
O	–1.389602	1.251333	–0.558359
C	–1.692840	0.926749	0.561440

C	–2.925676	0.124315	0.848706
O	–3.645067	–0.183654	–0.300381
H	–1.066797	1.207640	1.428979
H	–3.170592	0.205455	–1.046184
H	0.485130	2.447150	–0.341201
N	1.327346	2.784779	0.113733
C	2.338176	1.750603	0.188288
H	–2.610677	–0.787615	1.376975
H	–3.537479	0.699918	1.558797
O	3.582665	2.344671	0.489816
C	2.105978	0.675070	1.236191
H	2.375130	1.282356	–0.804613
H	1.087050	3.120288	1.040612
H	3.631928	3.149041	–0.033891
H	2.939597	–0.028920	1.256639
H	2.017060	1.131721	2.225989
H	1.191519	0.122282	1.010345

Total electronic energy = –439.459281 a.u.
ZPE = 0.16094 a.u.
NIm = 0

Imidazole (**Im**)

	X	Y	Z
C	0.005569	0.035331	0.000000
C	1.368483	0.018602	0.000000
N	1.744316	1.338083	0.000000
N	–0.460141	1.326152	0.000000
C	0.607297	2.079393	0.000000
H	–0.667107	–0.807390	0.000000
H	2.084348	–0.785385	0.000000
H	2.684955	1.690372	0.000000
H	0.620081	3.158533	0.000000

Total electronic energy = –226.20616 a.u.
ZPE = 0.07182 a.u.
NIm = 0

Imidazolidine (**In**)

	X	Y	Z
N	–0.307231	0.244214	0.126895
N	–2.466492	–0.583969	0.714108
C	–2.552120	0.108710	–0.572301
C	–1.110534	0.096013	–1.087490
C	–1.104288	–0.342951	1.215468
H	–0.171264	1.229303	0.311368
H	–0.880900	0.889691	–1.799807
H	–0.886973	–0.864005	–1.565114

H	–3.268413	–0.386884	–1.229085
H	–2.890239	1.138897	–0.416959
H	–2.591346	–1.575859	0.560861
H	–0.671243	–1.288613	1.553204
H	–1.114848	0.343943	2.066312

Total electronic energy = –228.61349 a.u.
ZPE = 0.11979 a.u.
NIm = 0

Phenol (**Ph**)

	X	Y	Z
H	0.188776	0.144423	0.000000
O	1.138649	0.009957	0.000000
C	1.771443	1.214888	0.000000
C	3.161178	1.207469	0.000000
C	3.851285	2.407861	0.000000
C	3.170395	3.619095	0.000000
C	1.784085	3.617163	0.000000
C	1.080696	2.420949	0.000000
H	3.681336	0.257691	0.000000
H	4.934966	2.396250	0.000000
H	3.716159	4.554193	0.000000
H	1.238604	4.553557	0.000000
H	–0.005071	2.425615	0.000000

Total electronic energy = –307.45396 a.u.
ZPE = 0.10539 a.u.
NIm = 0

Cyclohexanol (**Cyc**)

	X	Y	Z
O	–1.082812	1.686476	0.855975
C	–2.107666	1.247494	–0.022750
H	–0.241844	1.635477	0.397564
C	–3.415258	1.284965	0.750555
H	–2.186979	1.945610	–0.871246
C	–4.581020	0.794224	–0.107393
H	–3.305630	0.647228	1.634986
H	–3.593346	2.301705	1.108496
C	–4.313051	–0.602209	–0.667867
H	–5.502018	0.797902	0.480798
H	–4.739235	1.491333	–0.939133
C	–2.992681	–0.644416	–1.436173
H	–4.270164	–1.320210	0.159724
H	–5.136653	–0.915585	–1.314942
C	–1.834413	–0.150450	–0.568858
H	–2.788402	–1.657804	–1.790797

H	–3.074226	–0.011332	–2.327971
H	–1.687296	–0.826005	0.281468
H	–0.902046	–0.148972	–1.144646

Total electronic energy = –311.09980 a.u.
ZPE = 0.17586 a.u.
NIm = 0

Acetamide (**Ac**)

	X	Y	Z
N	1.037608	–0.229586	–0.095325
H	0.071463	–0.062185	–0.319951
C	1.972837	0.615555	–0.610767
C	3.395369	0.377249	–0.153349
O	1.678101	1.509657	–1.374400
H	3.566893	–0.639879	0.202238
H	1.268892	–0.939697	0.574539
H	4.068265	0.595384	–0.980385
H	3.619971	1.073353	0.657760

Total electronic energy = –209.21959 a.u.
ZPE = 0.07373 a.u.
NIm = 0

1–Aminoethanol (**Ae**)

	X	Y	Z
H	0.928010	–3.050340	0.130370
N	0.869540	–2.054060	–0.039070
C	–0.436750	–1.532190	0.319250
H	–0.702930	–1.996350	1.279020
H	1.066740	–1.888430	–1.020470
O	–0.342730	–0.133180	0.470800
C	–1.542620	–1.790290	–0.688340
H	0.482820	0.036710	0.932420
H	–2.480350	–1.345850	–0.350850
H	–1.277850	–1.344750	–1.650820
H	–1.690490	–2.863770	–0.822710

Total electronic energy = – 210.40728 a.u.
ZPE = 0.09827 a.u.
NIm = 0

1

	X	Y	Z
O	0.004276	0.016053	–0.002768
C	1.292594	0.009223	–0.000828
C	2.050065	1.136167	–0.000508
O	1.378673	2.365809	–0.002409
H	3.129314	1.194353	0.001063

H	1.842566	–0.954261	0.000695
H	0.455052	2.060175	–0.003574

Total electronic energy = –228.45675 a.u.
ZPE = 0.04838 a.u.
NIm = 0

2

	X	Y	Z
C	–0.603766	3.274007	–1.831406
S	–0.199663	3.587477	–0.099961
C	0.898073	2.024931	0.247398
O	1.052717	1.250933	–0.703098
C	1.347608	2.020212	1.535752
H	–1.680805	3.164088	–1.974840
H	–0.098627	2.331504	–2.074807
H	1.975631	1.203772	1.874323
H	1.088169	2.815471	2.222284
H	–0.230368	4.071296	–2.477605

Total electronic energy = –590.76816 a.u.
ZPE = 0.07177 a.u.
NIm = 0

3

	X	Y	Z
O	1.262897	–0.105510	1.617749
C	2.105096	–0.129945	0.697047
C	3.355723	0.485147	0.627389
H	1.853040	–0.722177	–0.221705
C	4.190916	0.347901	–0.510784
H	3.688351	1.082919	1.473746
C	5.421834	0.868019	–0.749222
H	3.767118	–0.271911	–1.306645
H	5.944111	0.672481	–1.679515
H	5.924513	1.496157	–0.018450

Total electronic energy = – 230.64589 a.u.
ZPE = 0.07608 a.u.
NIm = 0

4

	X	Y	Z
C	–2.591424	–1.961155	–0.063407
O	–3.507016	–2.804529	–0.104049
C	–1.559155	–1.878443	–1.083040
C	–2.466267	–0.984385	0.999544
C	–1.454204	–0.070638	1.021825
H	–3.216159	–1.009379	1.783356

C	–0.559354	–0.955362	–1.035984
H	–1.619167	–2.594303	–1.896478
H	0.184514	–0.942144	–1.827691
C	–0.456108	–0.006790	0.016125
H	–1.399819	0.644709	1.840762
C	0.568016	0.966178	0.097989
C	1.620146	1.214162	–0.740398
H	0.504500	1.620696	0.970319
C	2.539453	2.267898	–0.445557
H	1.793820	0.634376	–1.640651
O	3.518423	2.599214	–1.102192
H	2.304452	2.824475	0.492828

Total electronic energy = –497.63567 a.u.
ZPE = 0.13479 a.u.
NIm = 0

1'

	X	Y	Z
O	–1.634410	–0.349490	–0.858964
C	–1.809382	0.366152	0.091224
C	–3.181601	0.815319	0.505836
O	–4.177752	0.311519	–0.324234
H	–0.963998	0.727966	0.706075
H	–3.736463	–0.226844	–0.994466
H	–3.335548	0.498713	1.547763
H	–3.185917	1.915105	0.508538

Total electronic energy = –229.04702 a.u.
ZPE = 0.06171 a.u.
NIm = 0

2'

	X	Y	Z
C	–0.451051	3.291305	–1.911531
S	0.410733	3.688797	–0.374122
C	0.635721	2.046844	0.273734
O	0.251748	1.064071	–0.300958
C	1.346844	2.006735	1.603035
H	–1.386658	2.780920	–1.693386
H	0.175241	2.658964	–2.537098
H	2.235833	1.382155	1.501380
H	–0.648438	4.237300	–2.413629
H	1.633826	2.996686	1.956702
H	0.686791	1.535814	2.333574

Total electronic energy = –591.361432 a.u.

ZPE = 0.08560 a.u.
NIm = 0

3'

	X	Y	Z
O	1.446534	0.369207	2.357543
C	2.025546	0.023580	1.366184
C	3.422104	0.467602	0.985632
H	1.543676	–0.661371	0.636742
C	3.403496	1.186267	–0.333961
C	3.861223	0.684773	–1.470890
H	2.951864	2.174933	–0.329241
H	3.802111	1.243232	–2.397403
H	4.319886	–0.298173	–1.514388
H	3.812182	1.100664	1.784689
H	4.042569	–0.431814	0.906972

Total electronic energy = –231.214199 a.u.
ZPE = 0.08989 a.u.
NIm = 0

4'

	X	Y	Z
C	–5.491770	–1.018282	–1.084531
H	–5.372486	–1.819285	–0.323295
C	–4.315045	–0.171693	–1.277539
C	–3.204568	–0.390257	–0.563869
C	–1.943093	0.341399	–0.615921
C	–0.893634	–0.048635	0.220591
C	0.321905	0.606922	0.214040
C	0.513596	1.682868	–0.643753
C	–0.517843	2.090503	–1.487329
C	–1.727685	1.425660	–1.469922
O	1.720188	2.297398	–0.618371
H	–4.404184	0.618416	–2.014993
H	–3.229028	–1.213476	0.149464
H	–1.036378	–0.887879	0.892854
H	1.130839	0.299875	0.864483
H	–0.370199	2.930777	–2.158225
H	–2.515101	1.760008	–2.134349
O	–6.531627	–0.891986	–1.683855
H	1.734262	3.020777	–1.249042

Total electronic energy = –498.173064 a.u.
ZPE = 0.14833 a.u.

NIm = 0

Table S9. Partially optimized PDB–based models computed at ωB97X–D/6–311+G(2d,p)//ωB97X–D/6–31+G(d). Asterisks (*) denote atoms with fixed coordinates during optimization (based on the PDB file considered).

1NEY model: complex

	X	Y	Z
N*	4.932513	0.572552	–2.786535
C*	4.040333	–0.174818	–1.927308
C*	4.788603	–0.543714	–0.634750
C*	–4.016710	–2.487489	0.903343
O	5.829219	–0.011694	–0.304280
C	3.384461	–1.403430	–2.591990
C	2.362479	–2.045094	–1.696693
N	2.685554	–3.112855	–0.888977
C	1.066228	–1.648986	–1.440516
C	1.592797	–3.338743	–0.175397
N	0.589162	–2.488131	–0.470686
H	4.429316	1.259150	–3.336845
H	3.201909	0.443406	–1.548171
H	2.921387	–1.060063	–3.525266
H	4.157739	–2.130463	–2.862566
H	0.448315	–0.859817	–1.848274
H	1.487308	–4.112227	0.573034
H	–0.350870	–2.404530	0.037008
C	–2.766490	–1.702637	0.560151
O	–1.611489	–2.185717	0.966034
C	–2.854973	–0.520318	–0.096204
H	–3.957417	–3.500047	0.481772
H	–4.102017	–2.594621	1.992999
H	4.309372	–1.310743	–0.003747
H	5.632265	1.049148	–2.223241
H	–4.926135	–2.001385	0.526095
O	–1.698884	0.227089	–0.330473
H	–1.038319	–0.208404	0.236835
H	–3.763364	–0.042785	–0.443111

Total electronic energy = –741.33522 a.u.

1NEY model: residue

	X	Y	Z
N*	4.932090	0.572770	–2.786520
C*	4.041170	–0.175060	–1.927440
C*	4.788340	–0.543700	–0.634690
O	5.831145	–0.017500	–0.313845

C	3.505603	–1.430556	–2.652991
C	2.353561	–2.102570	–1.972646
N	2.488336	–2.754711	–0.763746
C	1.051080	–2.177609	–2.395494
C	1.295576	–3.213079	–0.468066
N	0.385572	–2.892035	–1.424832
H	4.439421	1.269307	–3.333419
H	3.165814	0.408384	–1.582621
H	3.193036	–1.114347	–3.654177
H	4.333315	–2.135047	–2.794944
H	0.555376	–1.805896	–3.279788
H	1.036835	–3.779983	0.415515
H	–0.591806	–3.139001	–1.427413
H	4.310035	–1.311433	–0.003862
H	5.649874	1.033755	–2.233018

Total electronic energy = –473.50680 a.u.

1NEY model: substrate

	X	Y	Z
C*	–4.016860	–2.487480	0.903400
C	–2.917139	–2.205324	–0.106813
O	–1.713271	–2.613468	0.159747
C	–3.210824	–1.537369	–1.259779
H	–4.108250	–3.570453	1.069526
H	–3.764964	–2.033454	1.872518
H	–4.992717	–2.098897	0.576805
O	–2.155459	–1.306073	–2.153684
H	–1.417267	–1.725929	–1.665632
H	–4.172163	–1.154468	–1.581720

Total electronic energy = –267.77764 a.u.

4CSC model: complex

	X	Y	Z
N*	2.346320	1.775620	0.200790
C*	0.869070	1.968380	0.379010
C*	0.196000	2.654030	–0.872590
N*	1.862520	–2.528730	0.495390
C*	0.417850	–2.490040	0.592610
C*	–0.092520	–1.900040	1.904170
S	–1.619610	2.624410	–0.731360
C	–1.949440	0.818590	–0.363280
O	–1.285100	–0.051550	–1.019100
C	–2.925370	0.642110	0.573590
O	0.634590	–1.634860	2.840210
C	–0.253700	–3.819550	0.228960
C	–1.734050	–3.695870	0.019020

N	–2.334490	–2.605930	–0.571810
C	–2.759290	–4.575920	0.270920
C	–3.661940	–2.874690	–0.632300
N	–3.964820	–4.060220	–0.141850
H	0.081750	–1.753780	–0.156470
H	2.216550	–1.576090	0.498910
H	2.252440	–2.964210	1.329700
H	0.239790	–4.167200	–0.686900
H	–0.063880	–4.577750	1.000040
H	–1.912360	–1.677450	–0.807450
H	–4.366710	–2.156610	–1.028780
H	–2.690250	–5.556220	0.726450
H	–3.290750	–0.357050	0.800300
H	–3.353420	1.481670	1.108370
H	2.496700	1.108580	–0.553560
H	2.719450	1.348790	1.045410
H	0.351900	1.021420	0.563690
H	0.721810	2.612230	1.251700
H	0.505390	3.699700	–0.953510
H	0.500690	2.121610	–1.780270
H	–1.178050	–1.695460	1.958230

Total electronic energy = –1158.98308 a.u.

4CSC model: residue

	X	Y	Z
N*	–2.153540	–3.482750	–1.532310
C*	–2.133210	–3.569010	–0.086540
C*	–0.868450	–2.993510	0.544280
O	0.050008	–2.545426	–0.103076
C	–2.332977	–5.036594	0.356966
C	–2.555298	–5.215886	1.822775
N	–3.724295	–4.840810	2.454526
C	–1.764172	–5.702520	2.831394
C	–3.583579	–5.122461	3.781405
N	–2.409685	–5.641195	4.044032
H	–4.550032	–4.469898	2.008746
H	–0.759881	–6.096343	2.748080
H	–4.367124	–4.929862	4.501285
H	–3.178298	–5.429446	–0.219998
H	–1.455002	–5.624587	0.063427
H	–2.973966	–2.977504	0.306803
H	–2.037927	–2.516493	–1.826000
H	–1.354235	–3.980460	–1.918706
H	–0.823602	–3.007508	1.651305

Total electronic energy = –473.50512 a.u.

4CSC model: substrate

	X	Y	Z
N*	1.988130	1.733340	1.319270
C*	0.576360	1.928480	0.850100
C*	0.499700	2.706280	–0.520660
S	–1.183291	2.784523	–1.170012
C	–1.248591	1.007795	–1.941172
O	–0.142571	0.478178	–2.154095
C	–2.537598	0.598360	–2.160441
H	–2.714289	–0.354811	–2.653301
H	–3.383920	1.201158	–1.847974
H	2.473847	1.177785	0.617247
H	1.972835	1.167878	2.165010
H	0.048770	0.976492	0.707904
H	0.047680	2.505779	1.616563
H	0.890411	3.721658	–0.399521
H	1.098194	2.167026	–1.264510

Total electronic energy = –685.43334 a.u.

1OHP model: complex

	X	Y	Z
N*	–10.350780	1.462690	–0.978180
C*	–9.032040	1.278360	–0.393360
C*	–8.017910	2.165650	–1.105770
C*	7.325900	–0.583950	–1.114980
C*	8.267230	0.661890	–1.224300
O	–7.636699	3.228570	–0.674013
C	–8.596984	–0.190388	–0.534810
C	–7.200632	–0.463761	–0.018600
C	–6.902853	–0.364857	1.346389
C	–6.157504	–0.827481	–0.876857
C	–5.627349	–0.615311	1.831903
C	–4.871555	–1.088129	–0.410592
C	–4.583614	–0.986361	0.962565
O	–3.383276	–1.225101	1.478064
C	–0.469536	–1.569086	–0.161170
C	0.618724	–2.169106	–0.753957
C	1.984843	–1.683129	–0.682837
C	2.276273	–0.542333	0.299407
C	1.065910	0.415472	0.280039
C	–0.255179	–0.276006	0.609742
C	2.982579	–2.227809	–1.417876
C	4.407391	–1.752045	–1.464797
C	4.755757	–0.733038	–0.375282
C	3.560688	0.223971	–0.134760
C	5.984560	0.088554	–0.761883

C	6.359953	1.165699	0.274126
C	3.918303	1.390191	0.811102
C	7.636607	1.731624	–0.330574
C	6.778456	0.587633	1.645527
O	–1.676411	–2.025456	–0.209494
C	5.198302	2.143166	0.421520
O	8.096903	2.838722	–0.144707
H	–5.408728	–0.538053	2.893287
H	–7.689148	–0.090349	2.049548
H	–4.075577	–1.379962	–1.090668
H	–6.354072	–0.919268	–1.944783
H	–9.331297	–0.812718	–0.001653
H	–8.667323	–0.466164	–1.595576
H	–8.991684	1.562846	0.669811
H	–7.665973	1.793190	–2.089941
H	–10.981076	0.729728	–0.666977
H	–10.749958	2.355530	–0.704826
C	2.420939	–1.139970	1.717124
H	2.392739	–0.360144	2.489099
H	1.603199	–1.838323	1.914937
H	3.355392	–1.700943	1.824776
H	7.035104	1.410599	2.321644
H	5.969843	0.008383	2.098590
H	7.652754	–0.068878	1.573417
H	–1.093771	0.396039	0.391271
H	–0.322731	–0.492169	1.685830
H	1.221234	1.237620	0.990148
H	0.997484	0.862568	–0.721993
H	3.330297	0.668794	–1.118526
H	2.731450	–3.041888	–2.099197
H	5.104954	–2.601919	–1.398905
H	4.608358	–1.290583	–2.450226
H	4.969406	–1.281026	0.552701
H	3.093482	2.109089	0.832678
H	5.431657	2.916839	1.163027
H	5.044829	2.659434	–0.536347
H	5.690862	0.646132	–1.670516
H	7.655162	–1.267746	–0.324363
H	7.276784	–1.151923	–2.048127
H	9.307542	0.482946	–0.933863
H	8.281077	1.051265	–2.249915
H	0.436983	–3.075756	–1.329746
H	–2.681798	–1.527280	0.766193
H	4.018972	1.017596	1.837872

Total electronic energy = –1444.35151 a.u.

1OHP model: residue

	X	Y	Z
N*	–9.247440	2.026670	–4.540080
C*	–8.211490	1.389530	–3.742630
C*	–7.461290	2.438240	–2.929810
O	–7.272823	2.372426	–1.739408
C	–7.204100	0.707710	–4.694442
C	–6.097104	–0.029137	–3.980674
C	–6.326379	–1.286587	–3.411376
C	–4.828383	0.530511	–3.837181
C	–5.330827	–1.964164	–2.721259
C	–3.816622	–0.134207	–3.147555
C	–4.069081	–1.384110	–2.586239
O	–3.126270	–2.090557	–1.899944
H	–5.513358	–2.939504	–2.281687
H	–7.306711	–1.748382	–3.510078
H	–2.835221	0.325136	–3.048480
H	–4.617386	1.506734	–4.268179
H	–7.768245	0.008729	–5.326614
H	–6.791503	1.471586	–5.365529
H	–8.589144	0.640610	–3.029938
H	–7.083752	3.295907	–3.527537
H	–9.599143	1.397215	–5.254569
H	–10.034241	2.316871	–3.967817
H	–2.305908	–1.584980	–1.852267

Total electronic energy = –554.74870 a.u.

1OHP model: substrate

	X	Y	Z
C*	–2.325410	3.703830	–5.367430
C*	–3.309380	3.469520	–6.561930
C	0.868434	–0.438080	0.545257
C	1.077144	0.701286	–0.236128
C	0.228771	1.160414	–1.305386
C	–1.145288	0.485189	–1.449225
C	–0.956579	–1.020014	–1.165902
C	–0.358391	–1.295008	0.212424
C	0.585286	2.174943	–2.140363
C	–0.204572	2.666020	–3.317697
C	–1.650743	2.169534	–3.319623
C	–1.706437	0.685018	–2.888866
C	–2.286924	2.325012	–4.695204
C	–3.737418	1.816266	–4.764746
C	–3.105866	0.057657	–3.086808
C	–4.135071	2.237081	–6.172328
C	–4.707894	2.577853	–3.831899

O	1.594795	–0.830657	1.501191
C	–3.742280	0.321194	–4.462156
O	–4.964848	1.707893	–6.882643
C	–2.099186	1.079140	–0.386523
H	–2.996430	0.459700	–0.254394
H	–1.587252	1.142059	0.577181
H	–2.415980	2.094433	–0.649645
H	–5.719247	2.173852	–3.953978
H	–4.419059	2.472430	–2.783352
H	–4.746272	3.650081	–4.055406
H	–0.057008	–2.346390	0.295069
H	–1.112539	–1.133633	0.997268
H	–1.917956	–1.545510	–1.254763
H	–0.290951	–1.431696	–1.938428
H	–1.016200	0.151258	–3.565322
H	1.570388	2.623594	–2.004414
H	–0.206831	3.767802	–3.360143
H	0.271144	2.343181	–4.266051
H	–2.216186	2.776253	–2.598844
H	–3.040723	–1.025799	–2.943585
H	–4.761709	–0.083118	–4.496029
H	–3.169582	–0.199097	–5.242489
H	–1.710460	1.671224	–5.375324
H	–2.709768	4.467299	–4.680481
H	–1.337218	4.031749	–5.701571
H	–3.970954	4.314279	–6.781207
H	–2.770999	3.233631	–7.487622
H	1.981965	1.274434	–0.032679
H	–3.786251	0.420768	–2.307262

Total electronic energy = –889.55974 a.u.

3PYP model: complex

	X	Y	Z
N*	6.635547	–3.451894	–1.842915
C*	5.642513	–2.516543	–1.280767
C*	6.454683	–1.459843	–0.545667
C*	–9.309420	–1.042713	–0.457897
O*	–9.679199	–1.950255	0.281190
C*	–7.984752	–0.516032	–0.569653
O	7.611442	–1.606925	–0.216313
C	4.616586	–3.170423	–0.319992
C	3.508330	–2.269958	0.174986
C	3.539170	–1.711021	1.456398
C	2.393312	–1.991782	–0.623957
C	2.497578	–0.921519	1.929428
C	1.340659	–1.203927	–0.171115

C	1.374609	–0.665258	1.127080
O	0.385204	0.071593	1.637291
H	7.415966	–3.542756	–1.198245
H	5.096056	–2.016073	–2.091113
H	4.180533	–4.017057	–0.867604
H	5.169697	–3.598747	0.526573
H	4.390149	–1.909635	2.107405
H	2.334034	–2.418339	–1.625089
H	2.523985	–0.502919	2.931368
H	0.476246	–1.004277	–0.798638
H	–0.384815	0.173751	0.985577
C	–6.925585	–0.989936	0.155776
C	–5.549058	–0.603028	0.081892
C	–4.602724	–1.172081	0.970245
C	–3.265245	–0.845100	0.936319
C	–2.748533	0.090434	–0.021961
C	–3.716060	0.658809	–0.923479
C	–5.046478	0.326759	–0.865793
O	–1.516073	0.408865	–0.096956
H	–7.846521	0.277814	–1.301438
H	–7.163764	–1.771483	0.879880
H	–4.954060	–1.893364	1.708159
H	–2.564322	–1.295595	1.635026
H	–3.347904	1.368266	–1.660326
H	–5.731092	0.785192	–1.576590
H	–10.059549	–0.560084	–1.124931
H	6.226910	–4.370165	–1.987444
H	5.910968	–0.534638	–0.277854

Total electronic energy = –1052.41864 a.u.

3PYP model: residue

	X	Y	Z
N*	6.617130	–3.470150	–1.874580
C*	5.629670	–2.529240	–1.311890
C*	6.449050	–1.465230	–0.595570
O	7.561881	–1.663022	–0.165241
C	4.606822	–3.149089	–0.326912
C	3.604639	–2.152034	0.207043
C	3.749112	–1.585381	1.477850
C	2.526961	–1.733704	–0.575450
C	2.855276	–0.634672	1.955301
C	1.621599	–0.781649	–0.113655
C	1.786878	–0.229001	1.156181
O	0.938484	0.704954	1.671623
H	7.364800	–3.620126	–1.202530
H	5.081505	–2.041791	–2.128623

H	4.087063	–3.954482	–0.861037
H	5.160685	–3.616855	0.496144
H	4.579842	–1.892320	2.109677
H	2.382657	–2.160785	–1.565869
H	2.970829	–0.200399	2.943186
H	0.787100	–0.475862	–0.741601
H	0.241691	0.906359	1.035364
H	6.191101	–4.365924	–2.092083
H	5.956806	–0.486316	–0.441472

Total electronic energy = –554.74870 a.u.

3PYP model: substrate

	X	Y	Z
C*	–9.309410	–1.042720	–0.457900
O*	–9.679210	–1.950250	0.281190
C*	–7.984750	–0.516030	–0.569650
C	–6.939446	–1.003597	0.182878
C	–5.578509	–0.608332	0.203829
C	–4.662179	–1.263995	1.075973
C	–3.335663	–0.929516	1.143669
C	–2.767722	0.126084	0.323368
C	–3.719263	0.784818	–0.561696
C	–5.039604	0.431557	–0.610145
O	–1.558302	0.448334	0.368988
H	–7.838652	0.293976	–1.281882
H	–7.207155	–1.815698	0.862312
H	–5.044912	–2.064038	1.711315
H	–2.659318	–1.448016	1.819564
H	–3.329536	1.581475	–1.191888
H	–5.702196	0.961612	–1.292865
H	–10.061118	–0.557468	–1.124381

Total electronic energy = –497.63130 a.u.

Table S10. Optimized Cartesian coordinates and energies at IEF-PCM-ωB97X-D/6-311+G(2d,p) for all structures computed in implicit water solvation.

$Im_{1(sol)}$

	X	Y	Z
N	1.205543	–0.160540	–0.182360
O	–1.357733	–0.191677	–0.589184
C	–1.946760	0.506001	0.360496
C	–3.273049	0.712560	0.400844
O	–4.086993	0.179293	–0.591344
H	–3.796844	1.275823	1.158891
H	–1.333313	0.942621	1.159377

H	–3.469761	–0.281564	–1.177222
H	0.141455	–0.186766	–0.367587
C	2.098685	0.754659	–0.663381
C	1.908664	–1.013628	0.584848
N	3.194811	–0.715560	0.631833
H	1.444880	–1.844652	1.095637
C	3.319895	0.402585	–0.156328
H	1.798807	1.561724	–1.311716
H	4.272652	0.885763	–0.312805

Total electronic energy = –454.79300 a.u.
ZPE = 0.12085 a.u.
NIm = 0

$In_{1(sol)}$

	X	Y	Z
N	–1.401452	–1.024875	0.533843
O	1.112628	0.318986	1.155431
N	–3.713134	–0.894742	0.613947
C	–3.332127	–0.559315	–0.770819
C	–1.782120	–0.539780	–0.796279
C	1.725102	0.156107	0.012034
C	–2.512701	–0.608585	1.386019
C	2.924711	0.701667	–0.272129
O	3.556972	1.482283	0.695616
H	3.469128	0.596860	–1.199081
H	1.251022	–0.454105	–0.773051
H	2.930636	1.459480	1.435081
H	–0.521835	–0.581915	0.832633
H	–1.424185	0.482144	–0.980262
H	–1.370400	–1.181802	–1.578052
H	–3.755167	–1.288997	–1.461441
H	–3.730460	0.421922	–1.037779
H	–3.866404	–1.895877	0.660190
H	–2.520073	–1.149102	2.334168
H	–2.486512	0.472125	1.602082

Total electronic energy = –457.18295 a.u.
ZPE = 0.16930 a.u.
NIm = 0

$Im_{2(sol)}$

	X	Y	Z
C	–0.582177	3.043963	–1.822333
S	0.184401	3.642240	–0.293981
C	1.085636	2.123111	0.260615
O	1.522556	1.356261	–0.651793
C	1.221230	2.013350	1.607972

H	1.043243	–2.176461	–1.885916
C	0.782533	–2.253433	–0.843502
N	0.857089	–1.185788	0.006725
C	0.341210	–3.304226	–0.088971
C	0.464338	–1.622446	1.219514
N	0.142351	–2.901052	1.209809
H	–1.440546	2.406587	–1.610729
H	0.156289	2.489726	–2.398673
H	1.841674	1.224823	2.021170
H	0.733970	2.703923	2.282887
H	1.149843	–0.213764	–0.238840
H	0.157149	–4.319856	–0.404560
H	0.428221	–0.969089	2.078017
H	–0.909430	3.916171	–2.387291

Total electronic energy = –817.09180 a.u.
ZPE = 0.14532 a.u.
NIm = 0

$In_{2(sol)}$

	X	Y	Z
C	1.135384	1.642399	–2.301062
S	0.037386	2.555404	–1.189421
C	0.623737	1.938301	0.491566
O	1.749480	1.384208	0.528210
C	–0.263321	2.211171	1.487372
C	–0.259406	–1.423074	–0.560864
N	1.203726	–1.420470	–0.464255
C	1.528867	–2.306796	0.663484
H	2.069958	1.463418	–1.769251
H	1.321712	2.254662	–3.182360
H	1.482559	–0.474374	–0.203827
H	0.702034	0.688832	–2.602257
H	–1.225356	2.660310	1.277021
H	1.961959	–3.251720	0.322854
H	2.263709	–1.808549	1.302224
H	–0.611707	–0.479421	–0.980334
H	–0.599932	–2.241984	–1.204467
C	–0.712883	–1.657617	0.879947
N	0.286738	–2.594997	1.409951
H	–0.011191	–3.533227	1.171122
H	–0.672477	–0.713652	1.432378
H	–1.715753	–2.076878	0.972571
H	–0.011282	1.962163	2.512488

Total electronic energy = –819.488913 a.u.
ZPE = 0.19347 a.u.
NIm = 0

$Ph_{3(sol)}$

	X	Y	Z
C	2.170112	–2.868567	0.306744
C	2.616747	–2.207938	1.446005
C	1.158306	–2.292734	–0.451372
C	2.063278	–0.994418	1.824057
C	0.596398	–1.077532	–0.085526
C	1.045940	–0.414888	1.061459
O	0.538031	0.761802	1.461843
H	3.405687	–2.642505	2.049895
H	0.797990	–2.793992	–1.343019
H	2.409241	–0.479028	2.712910
H	–0.191567	–0.631790	–0.681014
H	–0.236309	1.057984	0.871891
C	–8.456753	–1.921292	–0.502034
H	–8.319005	–2.696423	0.278392
C	–7.328224	–1.052962	–0.702692
C	–6.209583	–1.225421	0.042284
C	–4.982714	–0.481670	0.008339
C	–3.936332	–0.832354	0.881171
C	–2.739396	–0.157508	0.894875
C	–2.499230	0.939608	0.017080
C	–3.568201	1.287193	–0.864689
C	–4.755823	0.602860	–0.863985
O	–1.390562	1.584853	0.004199
H	–7.418003	–0.278187	–1.456835
H	–6.234694	–2.037109	0.769717
H	–4.083769	–1.663736	1.564859
H	–1.953343	–0.453027	1.580980
H	–3.413455	2.117915	–1.544897
H	–5.534850	0.908123	–1.554770
O	–9.516384	–1.862633	–1.111569
H	2.604250	–3.817117	0.015103

Total electronic energy = –805.19657 a.u.
ZPE = 0.24199 a.u.
NIm = 0

$Cyc_{3(sol)}$

	X	Y	Z
C	1.454374	–1.956358	0.459858
O	0.664337	–2.950915	0.579479
O	–1.862648	–2.209189	1.201084
C	–2.033267	–0.867731	0.781318
H	–0.933883	–2.481152	1.011925
C	–3.462730	–0.442955	1.081844

H	–1.356037	–0.216252	1.356346
C	–3.718425	1.000369	0.647006
H	–4.143088	–1.117121	0.547134
H	–3.661100	–0.564248	2.150614
C	–3.383465	1.206532	–0.830173
H	–4.759578	1.270292	0.842517
H	–3.100153	1.674141	1.252360
C	–1.953374	0.764834	–1.138018
H	–4.079402	0.619502	–1.441658
H	–3.525393	2.254897	–1.106972
C	–1.713592	–0.679745	–0.699919
H	–1.741716	0.873380	–2.205066
H	–1.251159	1.421945	–0.610308
H	–2.353865	–1.356570	–1.279041
H	–0.676897	–0.970236	–0.889991
C	2.382727	–1.854367	–0.626957
C	1.459580	–0.867989	1.386058
C	2.292105	0.210387	1.221470
H	0.777643	–0.912896	2.228421
C	3.207082	–0.770465	–0.775235
H	2.408000	–2.665288	–1.347288
H	3.884944	–0.741591	–1.622260
C	3.190865	0.303756	0.140285
H	2.260772	1.021393	1.944081
C	4.028678	1.458483	0.016740
C	4.947139	1.746741	–0.939851
H	3.903054	2.203366	0.803041
C	5.682574	2.978088	–0.871389
H	5.156515	1.080889	–1.770497
O	6.532425	3.347275	–1.672741
H	5.433569	3.625187	–0.006217

Total electronic energy = –808.83491 a.u.
ZPE = 0.31239 a.u.
NIm = 0

$Ph_{4(sol)}$

	X	Y	Z
O	–0.796782	–1.482458	1.378910
C	–1.670742	–0.786821	0.638544
C	–1.422219	0.520341	0.204192
C	–2.364603	1.190753	–0.563307
C	–3.564702	0.584148	–0.912360
C	–3.812144	–0.714078	–0.479297
C	–2.879797	–1.395442	0.287334
H	–3.071939	–2.407828	0.624501
H	–4.743381	–1.204152	–0.741556

H	–4.295488	1.113462	–1.511587
H	–2.154689	2.203004	–0.891295
H	–0.489483	1.000793	0.474823
H	0.067022	–0.953801	1.566794
O	1.359050	–0.268946	1.850394
C	2.076009	–0.170082	0.787561
C	3.314762	0.393352	0.669058
H	1.642662	–0.584400	–0.142160
C	4.009351	0.438018	–0.590684
H	3.791830	0.818532	1.549978
C	5.223266	0.960302	–0.831631
H	3.475878	–0.005778	–1.432918
H	5.656373	0.941656	–1.824768
H	5.810605	1.418025	–0.040525

Total electronic energy = –538.21857 a.u.
ZPE = 0.18307 a.u.
NIm = 0

$Cyc_{4(sol)}$

	X	Y	Z
C	1.387419	–2.105555	–0.042586
O	0.491846	–2.935647	0.330797
O	–1.885113	–2.161005	1.258763
C	–2.214001	–0.854335	0.834575
H	–0.982135	–2.391838	0.916980
C	1.453522	–0.757066	0.208048
C	–3.607920	–0.510106	1.338397
H	–1.509245	–0.133002	1.281453
C	–4.027686	0.894072	0.902738
H	–4.312554	–1.248386	0.936173
H	–3.633437	–0.599277	2.428321
C	–3.935422	1.059273	–0.614300
H	–5.043777	1.104204	1.247134
H	–3.374155	1.631708	1.383946
C	–2.540258	0.700493	–1.124747
H	–4.671809	0.401967	–1.092502
H	–4.192877	2.083215	–0.899290
C	–2.133678	–0.705013	–0.682836
H	–2.501441	0.777555	–2.214682
H	–1.815436	1.424958	–0.733197
H	–2.803180	–1.446463	–1.136323
H	–1.116258	–0.933813	–1.012317
H	2.219991	–2.514126	–0.648254
C	2.520311	0.057748	–0.301589
H	0.670013	–0.286611	0.798363
C	2.686785	1.383480	–0.142575

H	3.274151	–0.474908	–0.884706
H	3.535529	1.899801	–0.575590
H	1.976218	1.979898	0.423185

Total electronic energy = –541.85702 a.u.
ZPE = 0.25386 a.u.
NIm = 0

$Ac_{1(sol)}$

	X	Y	Z
O	-1.240862	1.485759	-0.487547
C	-1.556398	0.960501	0.673441
C	-2.647667	0.197379	0.863256
O	-3.497561	-0.057833	-0.208707
H	-2.948038	-0.254477	1.797079
H	-0.903516	1.141469	1.539315
H	-3.078431	0.411345	-0.945214
H	0.254806	2.173145	-0.372009
N	1.222055	2.564421	-0.259707
C	2.290623	1.787004	-0.059481
H	1.373807	3.561158	-0.274194
O	3.433410	2.231394	0.090494
C	2.028131	0.298559	-0.023272
H	0.978781	0.058453	-0.190693
H	2.641920	-0.185781	-0.784464
H	2.339369	-0.088177	0.948774

Total electronic energy = –437.80357 a.u.
ZPE = 0.12416 a.u.
NIm = 0

$Ae_{1(sol)}$

	X	Y	Z
O	1.536824	-4.125340	2.177842
H	1.160909	-2.930440	0.753833
N	0.901945	-2.229889	0.046574
C	-0.355615	-1.613756	0.396727
H	-0.369865	-1.528111	1.490120
H	0.832069	-2.695746	-0.852742
O	-0.428345	-0.305457	-0.173285
C	-1.591432	-2.363556	-0.063428
H	0.451513	0.071119	-0.079531
H	-2.501573	-1.832659	0.224614
H	-1.579447	-2.466961	-1.152725
H	-1.600425	-3.357142	0.387557
C	0.436046	-4.290183	2.864529
H	0.343675	-3.832807	3.861396
C	-0.620811	-4.998057	2.417602

H	-1.548804	-5.153979	2.948224
O	-0.559456	-5.596370	1.160937
H	0.312683	-5.330516	0.832605

Total electronic energy = –438.98049 a.u.
ZPE = 0.14805 a.u.
NIm = 0

Imidazole (**Im$_{(sol)}$**)

	X	Y	Z
C	0.003193	0.031695	0.000000
C	1.366992	0.020248	0.000000
N	1.739349	1.337930	0.000000
N	–0.463329	1.326284	0.000000
C	0.611050	2.081202	0.000000
H	–0.666612	–0.813864	0.000000
H	2.085822	–0.781004	0.000000
H	2.681833	1.691275	0.000000
H	0.629501	3.159923	0.000000

Total electronic energy = –226.21784 a.u.
ZPE = 0.07207 a.u.
NIm = 0

Imidazolidine (**In$_{(sol)}$**)

	X	Y	Z
N	–0.304818	0.247588	0.128452
N	–2.467890	–0.587961	0.715414
C	–2.550126	0.115493	–0.570040
C	–1.111618	0.088675	–1.087206
C	–1.103275	–0.343573	1.218319
H	–0.204796	1.238803	0.310158
H	–0.880465	0.875606	–1.805487
H	–0.897303	–0.878659	–1.552604
H	–3.270331	–0.371890	–1.227598
H	–2.872622	1.149089	–0.408983
H	–2.567030	–1.579715	0.536183
H	–0.673306	–1.290348	1.554340
H	–1.112309	0.345380	2.066511

Total electronic energy = –228.62082 a.u.
ZPE = 0.11994 a.u.
NIm = 0

Phenol (**Ph$_{(sol)}$**)

	X	Y	Z
H	0.183667	0.140985	0.000000
O	1.136235	0.010514	0.000000
C	1.770556	1.215030	0.000000

C	3.161477	1.207044	0.000000
C	3.853691	2.408278	0.000000
C	3.171968	3.619848	0.000000
C	1.783752	3.617425	0.000000
C	1.078440	2.421560	0.000000
H	3.686113	0.259121	0.000000
H	4.937405	2.395757	0.000000
H	3.717570	4.555242	0.000000
H	1.237993	4.553699	0.000000
H	–0.006368	2.424608	0.000000

Total electronic energy = –307.46101 a.u.
ZPE = 0.10534 a.u.
NIm = 0

Cyclohexanol (**Cyc$_{(sol)}$**)

	X	Y	Z
O	–1.073650	1.683842	0.855696
C	–2.108629	1.242902	–0.021110
H	–0.241245	1.660851	0.376717
C	–3.415283	1.282340	0.753165
H	–2.183465	1.941152	–0.867537
C	–4.581003	0.794581	–0.107516
H	–3.312574	0.640194	1.635957
H	–3.597577	2.299432	1.110059
C	–4.313863	–0.601545	–0.668957
H	–5.502018	0.799225	0.480572
H	–4.734495	1.493507	–0.938202
C	–2.992536	–0.644191	–1.435400
H	–4.273211	–1.320486	0.157976
H	–5.137174	–0.911073	–1.318156
C	–1.834196	–0.154281	–0.565518
H	–2.788355	–1.657492	–1.789935
H	–3.070767	–0.008806	–2.325523
H	–1.693537	–0.833145	0.283749
H	–0.901163	–0.151577	–1.138246

Total electronic energy = –311.10520 a.u.
ZPE = 0.17553 a.u.
NIm = 0

Acetamide (**Ac$_{(sol)}$**)

	X	Y	Z
N	1.045034	–0.249920	–0.137027
H	0.077959	–0.112254	–0.381939
C	1.959994	0.655818	–0.531785
C	3.389859	0.388266	–0.130995

O	1.651577	1.648020	–1.183315
H	3.512467	–0.528570	0.443964
H	1.295596	–1.063469	0.396793
H	3.998243	0.329454	–1.034284
H	3.748672	1.232505	0.458948

Total electronic energy = –209.23183 a.u.
ZPE = 0.07393 a.u.
NIm = 0

1-Aminoethanol (**Ae$_{(sol)}$**)

	X	Y	Z
H	0.918286	–3.048921	0.134016
N	0.873549	–2.053858	–0.052931
C	–0.428492	–1.527846	0.313906
H	–0.691356	–1.983078	1.276293
H	1.041605	–1.926528	–1.046283
O	–0.333824	–0.120225	0.465569
C	–1.535843	–1.788306	–0.689805
H	0.457566	0.050056	0.984933
H	–2.477344	–1.352594	–0.350149
H	–1.274874	–1.348551	–1.656252
H	–1.675883	–2.862650	–0.819698

Total electronic energy = –210.41473 a.u.
ZPE = 0.09789 a.u.
NIm = 0

1$_{(sol)}$

	X	Y	Z
O	–0.001164	–0.002604	–0.002761
C	1.302516	0.001176	–0.000809
C	2.043265	1.130562	–0.000518
O	1.384180	2.362135	–0.002399
H	3.121826	1.189912	0.001057
H	1.851904	–0.954271	0.000709
H	0.450013	2.100609	–0.003610

Total electronic energy = –228.55565 a.u.
ZPE = 0.04842 a.u.
NIm = 0

2$_{(sol)}$

	X	Y	Z
C	–0.594477	3.266843	–1.828557
S	0.237695	3.724027	–0.287068
C	0.981932	2.061848	0.218117
O	1.186844	1.237894	–0.699354
C	1.248629	1.998744	1.555020

H	–1.631500	2.979821	–1.654209
H	–0.046339	2.426657	–2.256546
H	1.772067	1.137301	1.956767
H	0.955711	2.795963	2.225433
H	–0.561593	4.114592	–2.511562

Total electronic energy = –590.85851 a.u.
ZPE = 0.07200 a.u.
NIm = 0

3$_{(sol)}$

	X	Y	Z
O	1.271822	–0.090254	1.638787
C	2.113193	–0.127739	0.693025
C	3.352195	0.478867	0.618472
H	1.840362	–0.721774	–0.207694
C	4.192401	0.337497	–0.533001
H	3.699007	1.080484	1.457699
C	5.414560	0.867403	–0.742884
H	3.776995	–0.279917	–1.332675
H	5.954869	0.685478	–1.664640
H	5.898195	1.493036	0.002520

Total electronic energy = –230.73563 a.u.
ZPE = 0.07652 a.u.
NIm = 0

4$_{(sol)}$

	X	Y	Z
C	–2.579720	–1.954477	–0.067905
O	–3.506843	–2.811971	–0.113380
C	–1.556774	–1.874805	–1.081161
C	–2.467190	–0.990772	0.992709
C	–1.454239	–0.069235	1.023585
H	–3.215393	–1.012690	1.778458
C	–0.554018	–0.946785	–1.031255
H	–1.606065	–2.585594	–1.900026
H	0.188167	–0.935420	–1.823414
C	–0.460531	–0.006212	0.021640
H	–1.407069	0.641522	1.844720
C	0.568348	0.976910	0.110802
C	1.609941	1.210252	–0.734108
H	0.504757	1.630288	0.981811
C	2.534990	2.264223	–0.445215
H	1.775555	0.624811	–1.632542
O	3.509352	2.572740	–1.124835
H	2.321382	2.831796	0.483418

Total electronic energy = –497.71403 a.u.

ZPE = 0.13498 a.u.
NIm = 0