Table S1. Total electronic energies (Hartrees) for model compounds **1-4**, and their oxygen protonated forms, **1Ha-4Ha**.

dihedral	**1**	**1Ha**	**2**	**2Ha**	**3**	**3Ha**	**4**	**4Ha**
-180	-248.53733	-248.88237	-287.8429	-288.1949	-365.26892	-365.62416	-553.84950	-554.20297
-160	-248.53691	-248.87982	-287.8424	-288.1933	-365.26776	-365.62176	-553.84745	-554.20139
-140	-248.53407	-248.87168	-287.8395	-288.1864	-365.26360	-365.61332	-553.84150	-554.19365
-120	-248.52751	-248.85854	-287.8336	-288.1741	-365.25646	-365.59957	-553.83271	-554.18172
-100	-248.51916	-248.84219	-287.826	-288.1577	-365.24911	-365.58221	-553.82221	-554.17047
-90	-248.51495	-248.83679	-287.8225	-288.1479	-365.24567	-365.57951	-553.81739	-554.16461
-80	-248.51228	-248.83949	-287.8195	-288.1547	-365.24275	-365.58626	-553.81982	-554.15975
-60	-248.52120	-248.85548	-287.8282	-288.1718	-365.25106	-365.60218	-553.82675	-554.17408
-40	-248.52886	-248.86834	-287.8365	-288.1849	-365.26095	-365.61443	-553.83438	-554.18599
-20	-248.53305	-248.87645	-287.8416	-288.1927	-365.26716	-365.62190	-553.83934	-554.19296
0	-248.53369	-248.87907	-287.8429	-288.1949	-365.26892	-365.62420	-553.83903	-554.19529
20	-248.53305	-248.87645	-287.8416	-288.1927	-365.26713	-365.62195	-553.83357	-554.19299
40	-248.52886	-248.86834	-287.8364	-288.1849	-365.26095	-365.61442	-553.82439	-554.18473
60	-248.52120	-248.85548	-287.8281	-288.1718	-365.25115	-365.60218	-553.81794	-554.17146
80	-248.51228	-248.83949	-287.8195	-288.1547	-365.24273	-365.58692	-553.82013	-554.15620
90	-248.51495	-248.83679	-287.8225	-288.1479	-365.24567	-365.57951	-553.82248	-554.15197
100	-248.51916	-248.84219	-287.826	-288.1577	-365.24915	-365.58221	-553.82531	-554.15901
120	-248.52751	-248.85854	-287.8336	-288.1741	-365.25649	-365.59793	-553.83174	-554.17552
140	-248.53407	-248.87168	-287.8395	-288.1864	-365.26360	-365.61334	-553.84105	-554.19030
160	-248.53691	-248.87982	-287.8424	-288.1933	-365.26777	-365.62176	-553.84733	-554.19943
180	-248.53733	-248.88237	-287.8429	-288.1949	-365.2689	-365.6242	-553.84950	-554.20297

Table S2. Total electronic energies (Hartrees) for optimized structures **1Hb-4Hb.**

structure	Energy
1Hb	-248.95911
2Hb	-288.17671
3Hb	-365.60659
4Hb	-554.18540

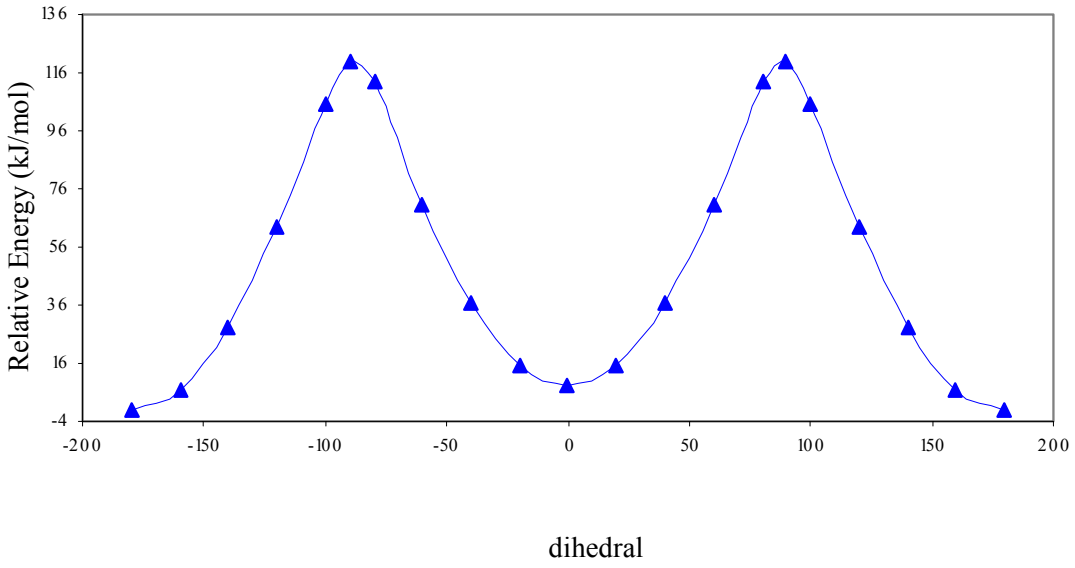

Figure S1 Composite scan (Relative E_{elec} (kJ/mol) vs. dihedral angle) of forward and reverse dihedral scans for **1Ha**.

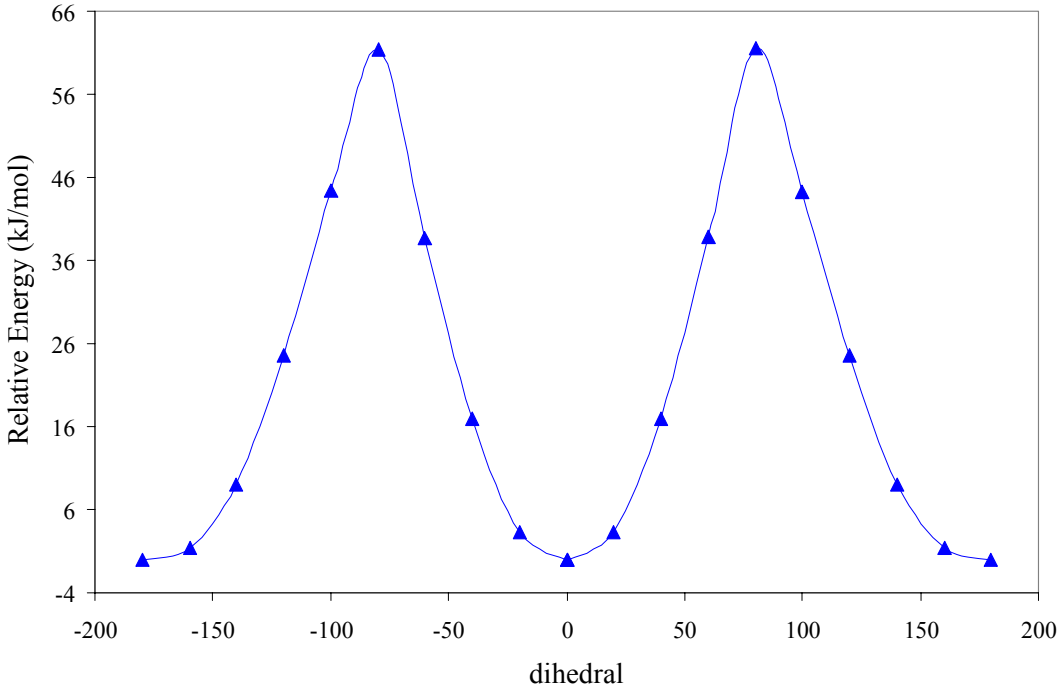

Figure S2 Composite scan (Relative E_{elec} (kJ/mol) vs. dihedral angle) of forward and reverse dihedral scans for **2**.

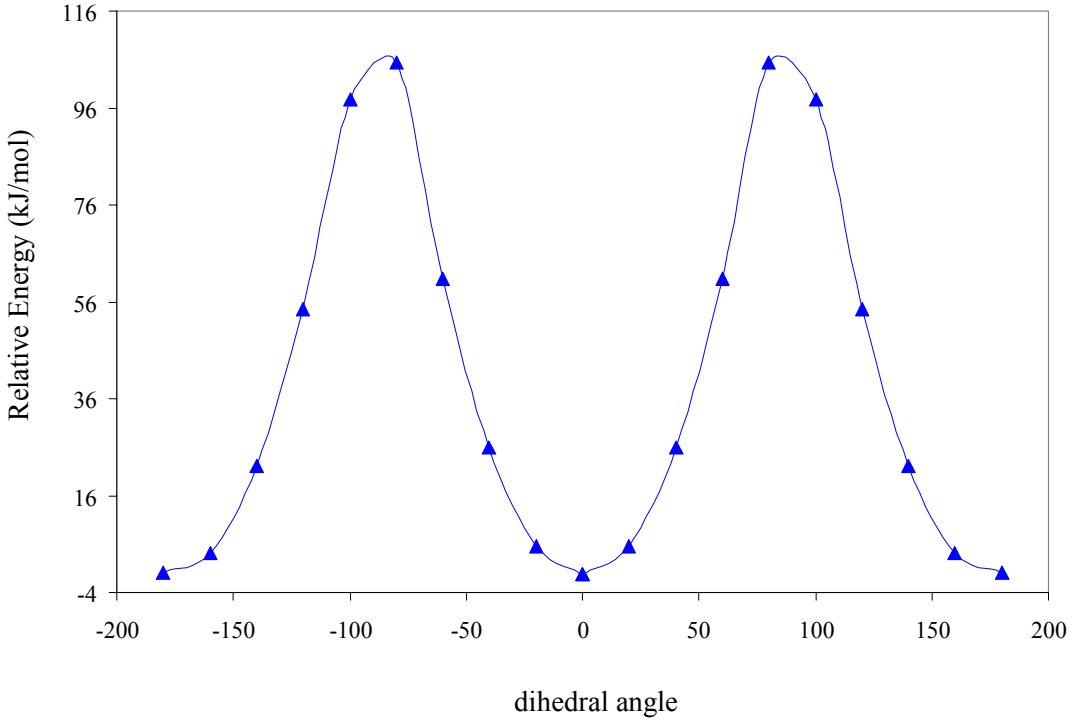

Figure S3 Composite scan (Relative E_{elec} (kJ/mol) vs. dihedral angle) of forward and reverse dihedral scans for **2Ha**.

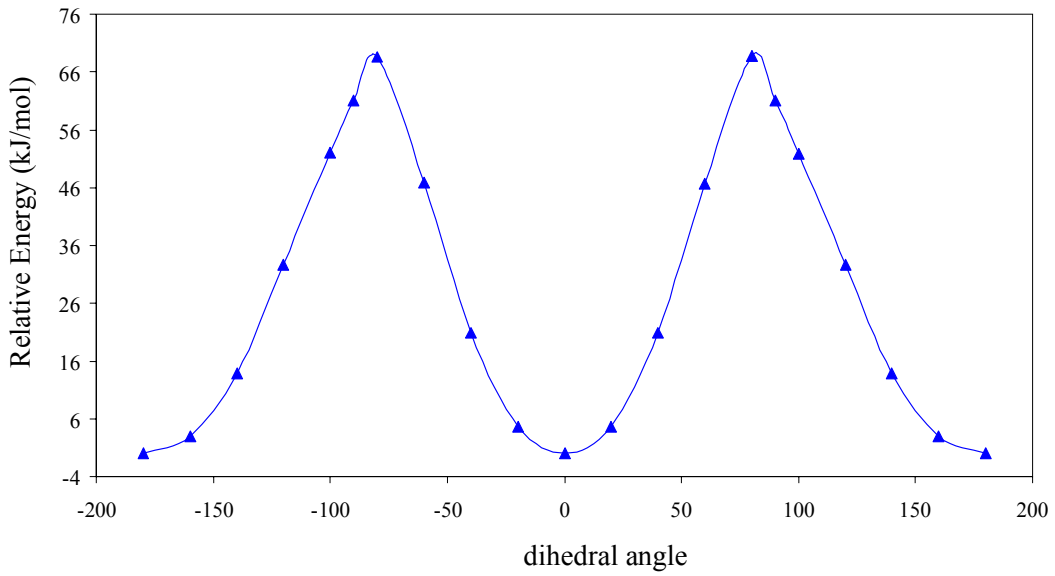

Figure S4 Composite scan (Relative E_{elec} (kJ/mol) vs. dihedral angle) of forward and reverse dihedral scans for **3**.

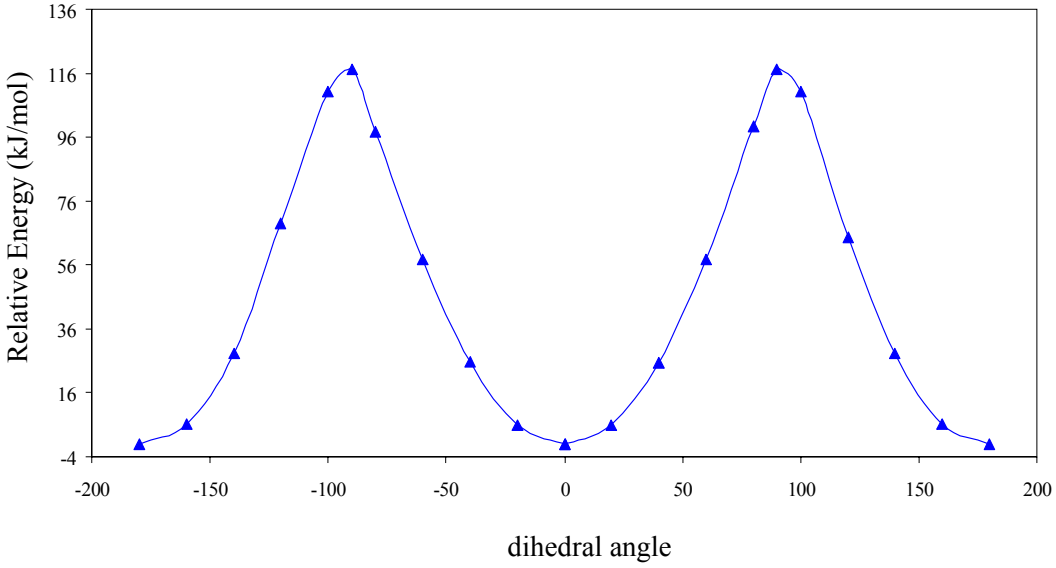

Figure S5 Composite scan (Relative E_{elec} (kJ/mol) vs. dihedral angle) of forward and reverse dihedral scans for **3Ha**.

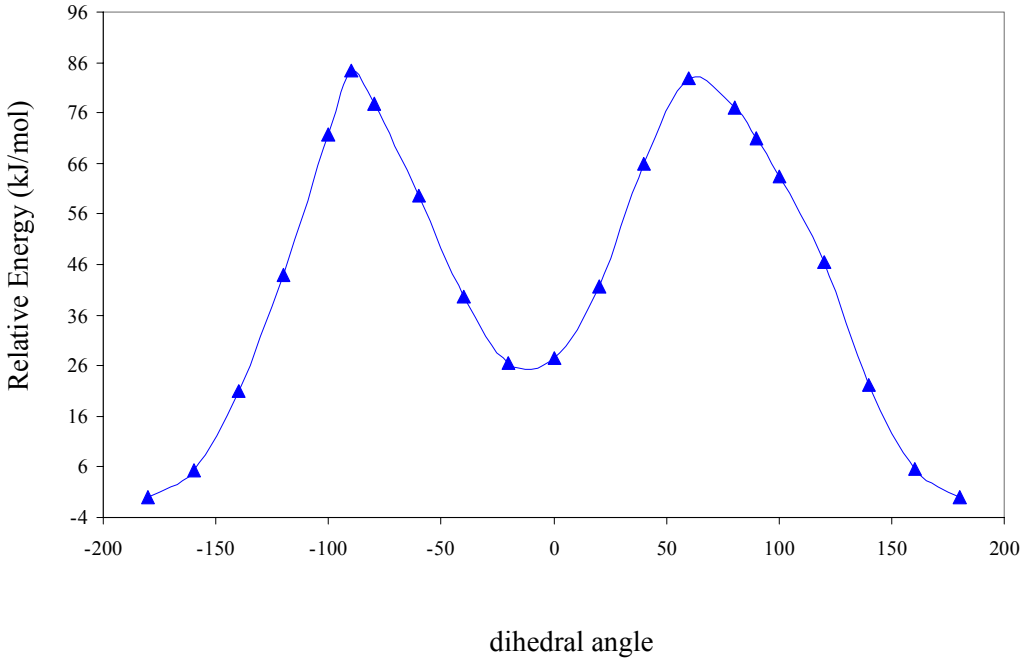

Figure S6 Composite scan (Relative E_{elec} (kJ/mol) vs. dihedral angle) of forward and reverse dihedral scans for **4**.

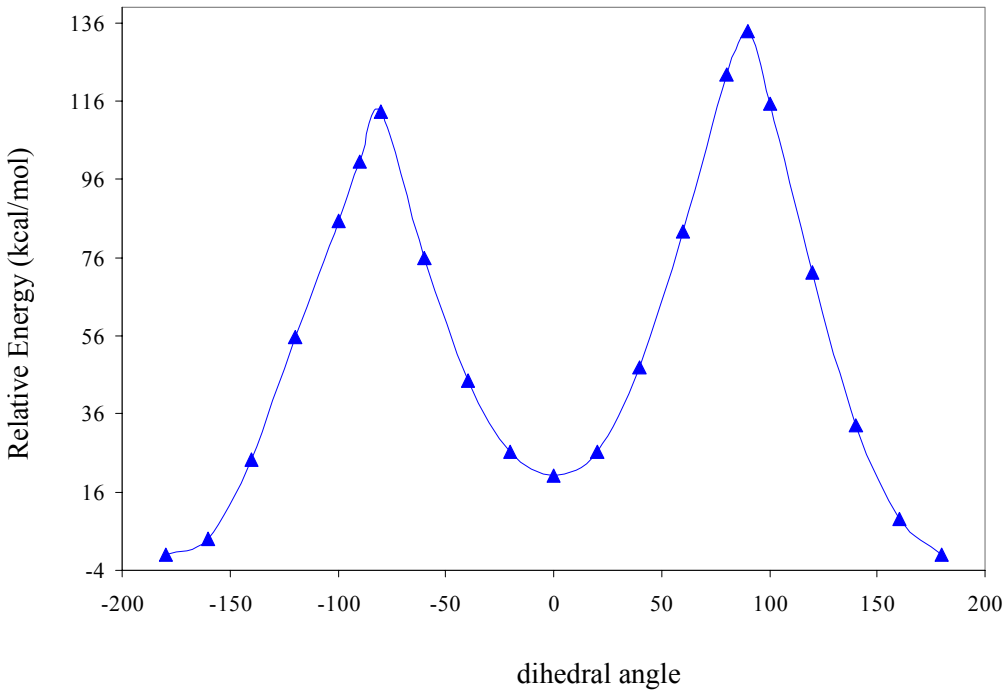

Figure S7 Composite scan (Relative E_{elec} (kJ/mol) vs. dihedral angle) of forward and reverse dihedral scans for **4Ha**.

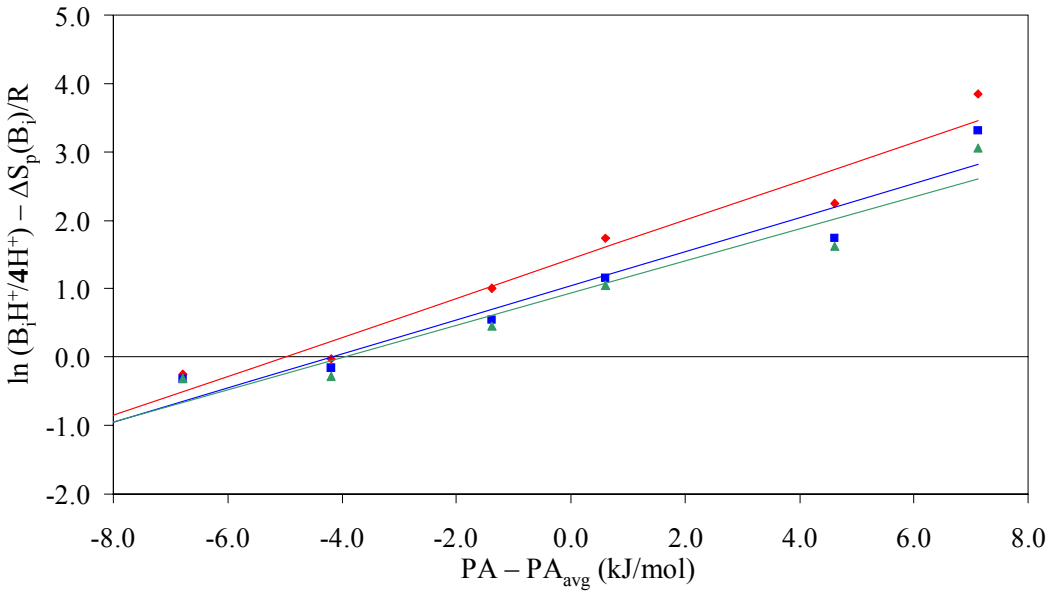

Figure S8 Plot of ln (B_iH^+/**4**H^+) vs. $\Delta H_{Bi} - \Delta H_{avg}$ at activation amplitudes 15% (♦) and 50% (■) and 85% (▲).

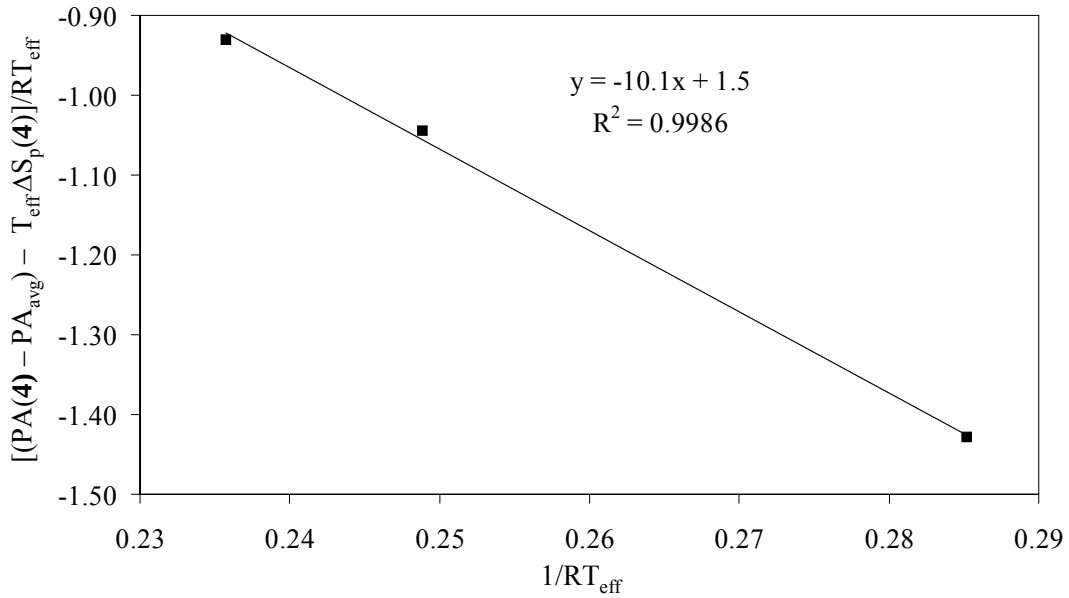

Figure S9 Plot of $[(PA(\mathbf{4}) - PA_{avg}) - T_{eff}\Delta S_p(\mathbf{4})]/RT_{eff}$ vs. $1/RT_{eff}$.