Supplementary Information

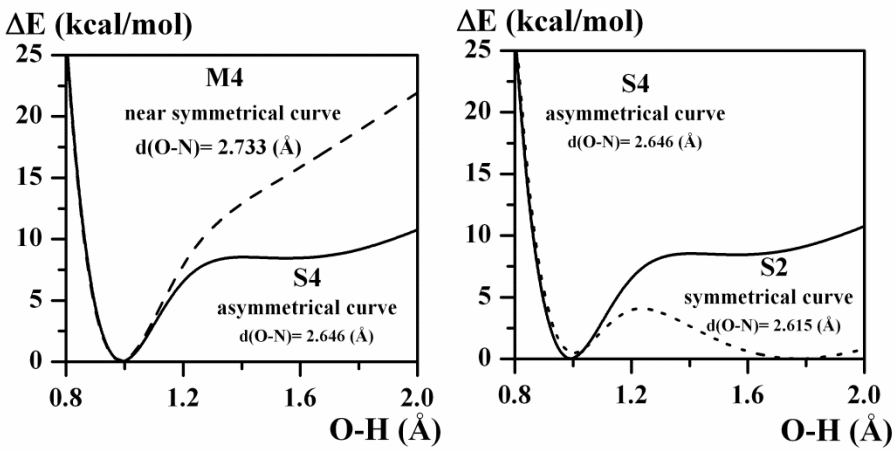
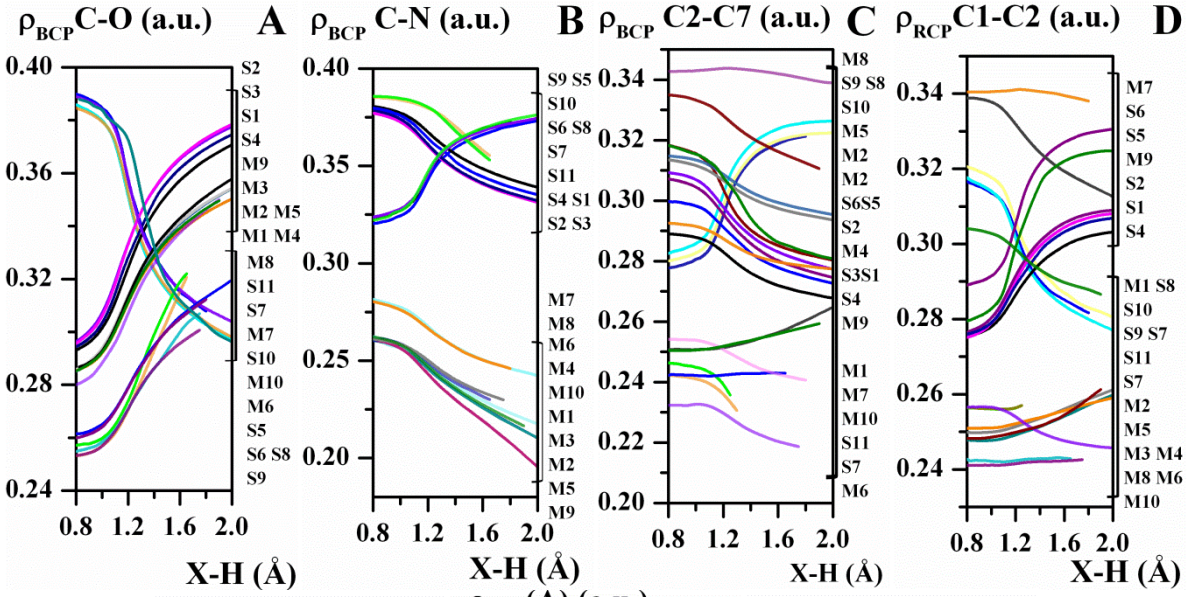


Fig. S1 Calculated (B3LYP/6-311++G(d,p)) nonadiabatic potential functions for proton transfer displacement for the M4, S4 and S2 compounds.



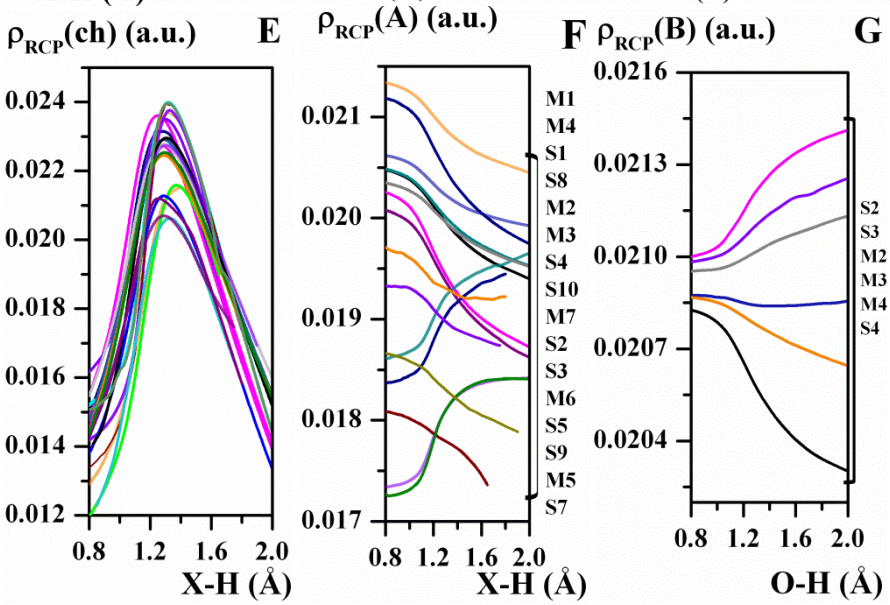


Fig. S2 Correlations between the electron density at (A) the CO bond, (B) the CN bond, (C) the C2C7 bond, (D) the C1C2 bond, (E) the chelate ring, (F) the A formation and (G) the B formation, and the XH bond length (d(XH), Å, where X = O or N).

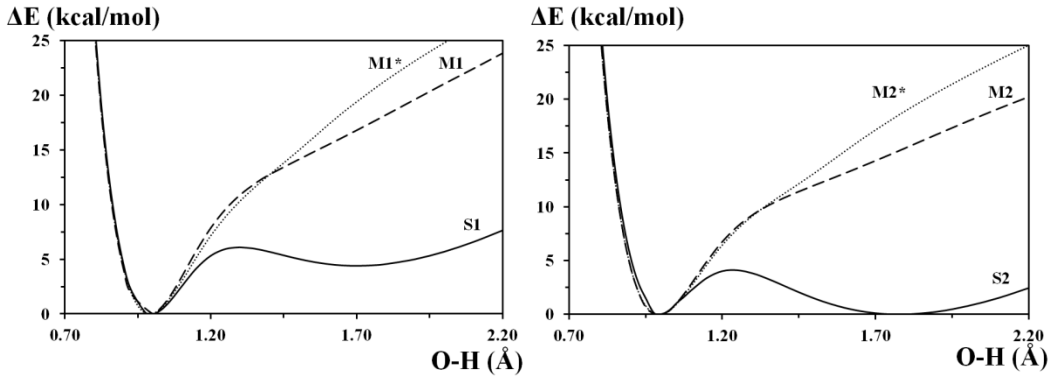


Fig. S3 Calculated (B3LYP/6-311++G(d,p)) nonadiabatic potential functions for proton transfer displacement for the M1, M1* unconjugated and S1 conjugated compounds (A); the M2 and M2* unconjugated and S2 conjugated compounds (B).

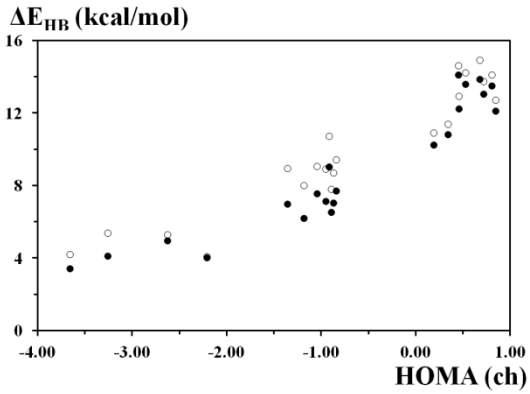


Fig. S4 Scatter plot of the hydrogen bond energy (ΔE_{HB}, kcal/mol) versus the aromaticity of chelate chain (HOMA(ch)) for the OH tautomeric form. The open and filled circles correspond to data obtained by the $\Delta E_{HB} = -0.37 \times V(r_{cp}) + 3.1$[118] and $\Delta E_{HB} = (-5.554 \times 10^5) \times \exp(-4.12 \times d(ON))$[119] equations, respectively.