**Supplementary Information**

![Graph](image1.png)

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

![Graph](image2.png)

**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 ($\Delta E_{\text{HB}}$ 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 $\Delta E_{\text{HB}} = -0.37 \times V(r_{\text{cp}}) + 3.1118$ and $\Delta E_{\text{HB}} = (-5.554 \times 10^5) \times \exp(-4.12 \times d(ON))$ equations, respectively.

Electronic Supplementary Material (ESI) for RSC Advances
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