Electronic Supplementary Material (ESI) for RSC Advances.

Self-assembled supramolecular structures of *O*,*N*,*N'* tridentate imidazole-phenol Schiff base compounds

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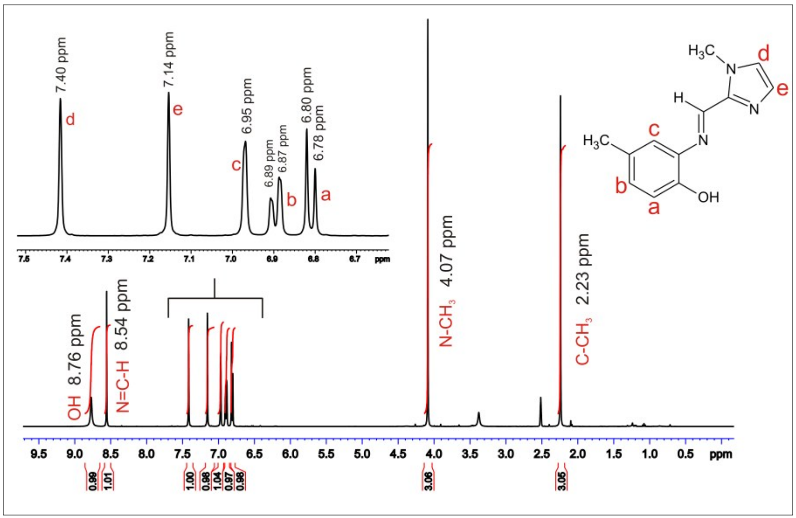


Figure S1: ^{1}H NMR spectrum of (1) in DMSO-d_6.

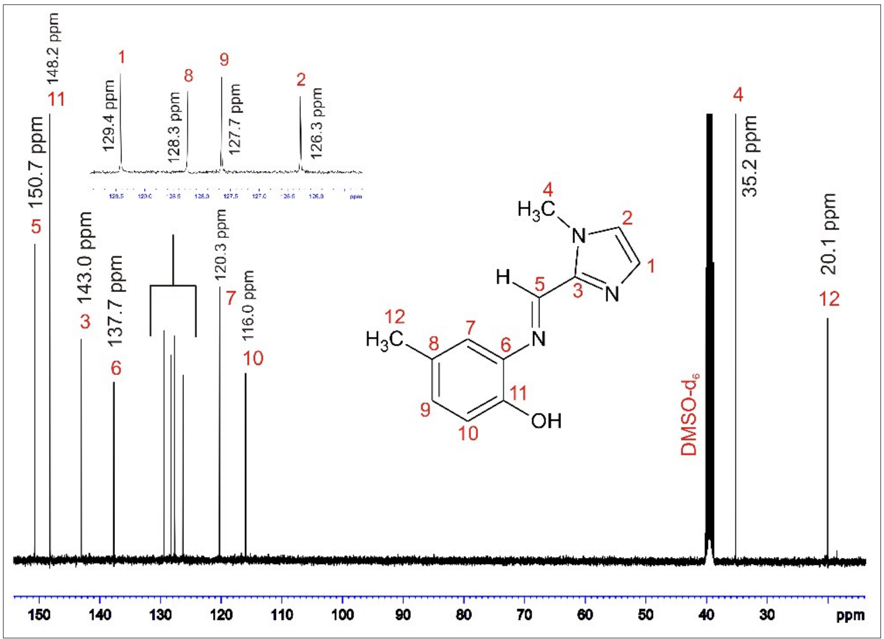


Figure S2: ^{13}C NMR spectrum of (1) in DMSO-d_6.

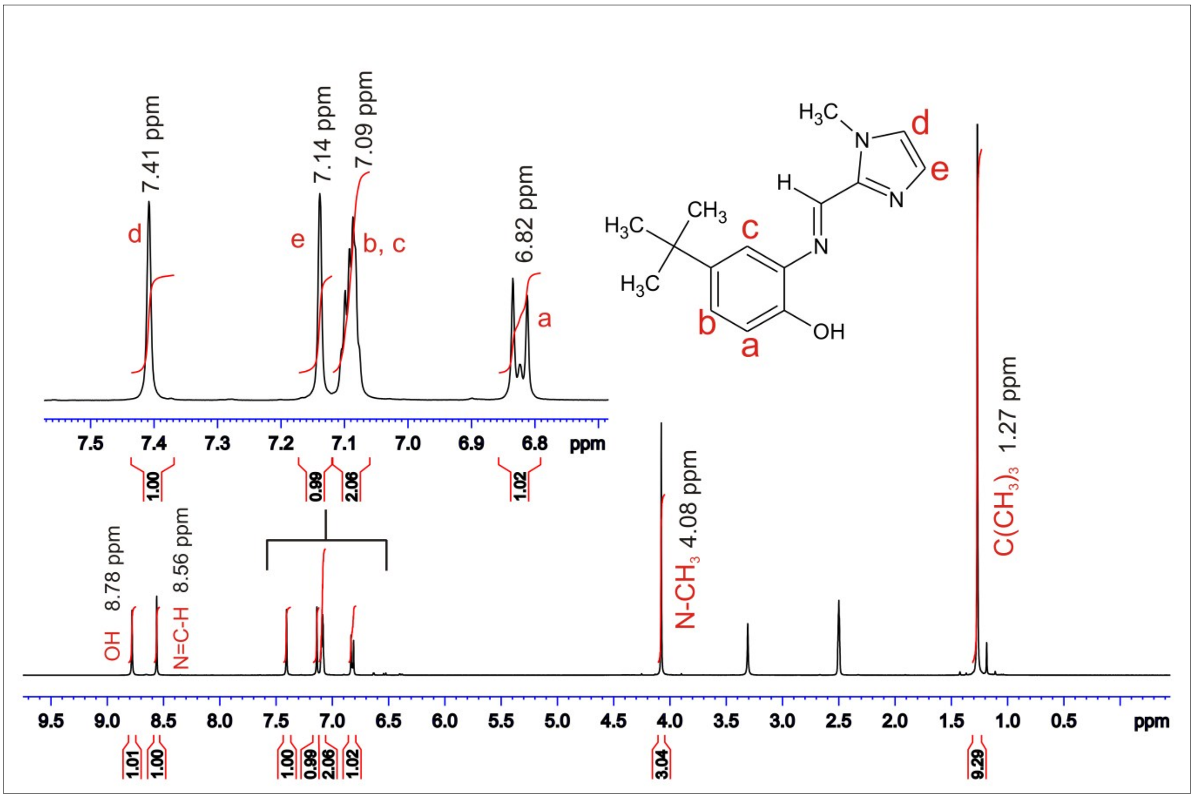


Figure S3: ^{1}H NMR spectrum of (2) in DMSO-d_6.

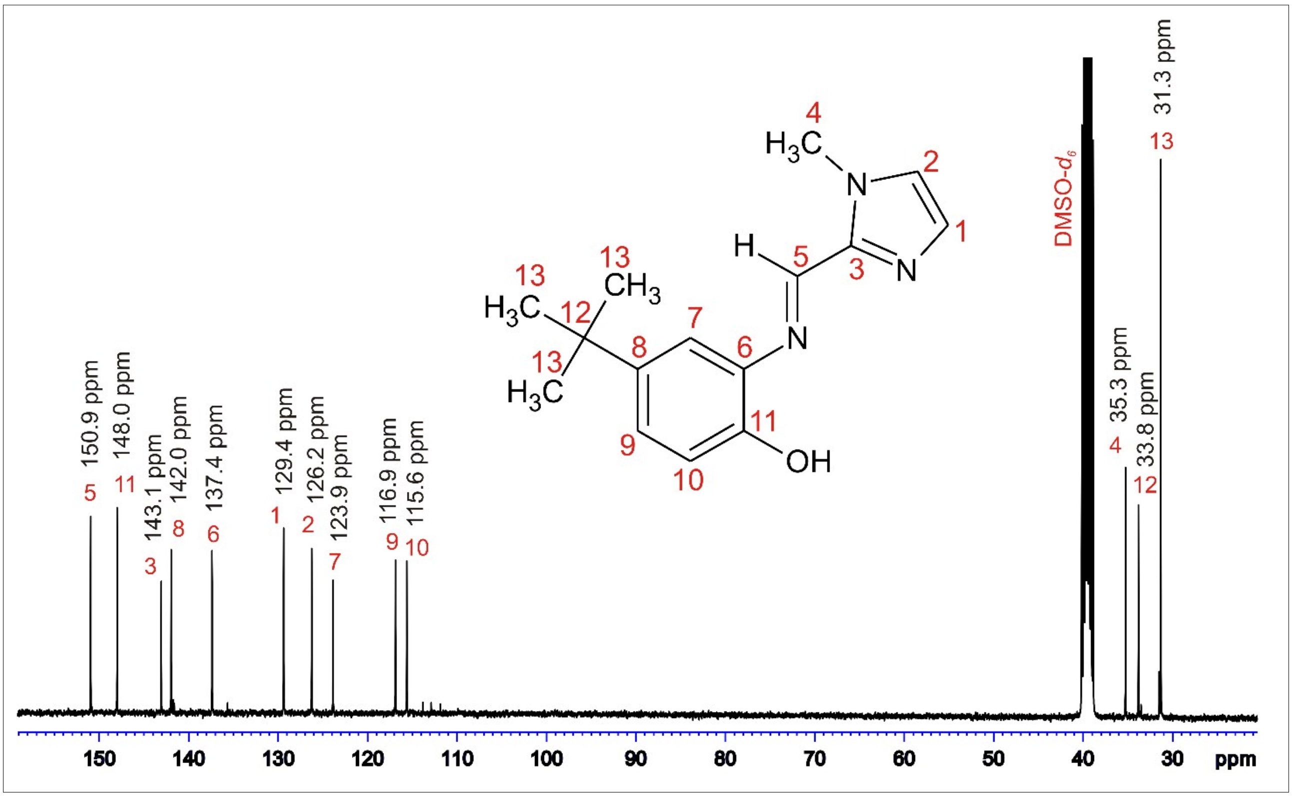


Figure S4: ^{13}C NMR spectrum of (2) in DMSO-d_6.

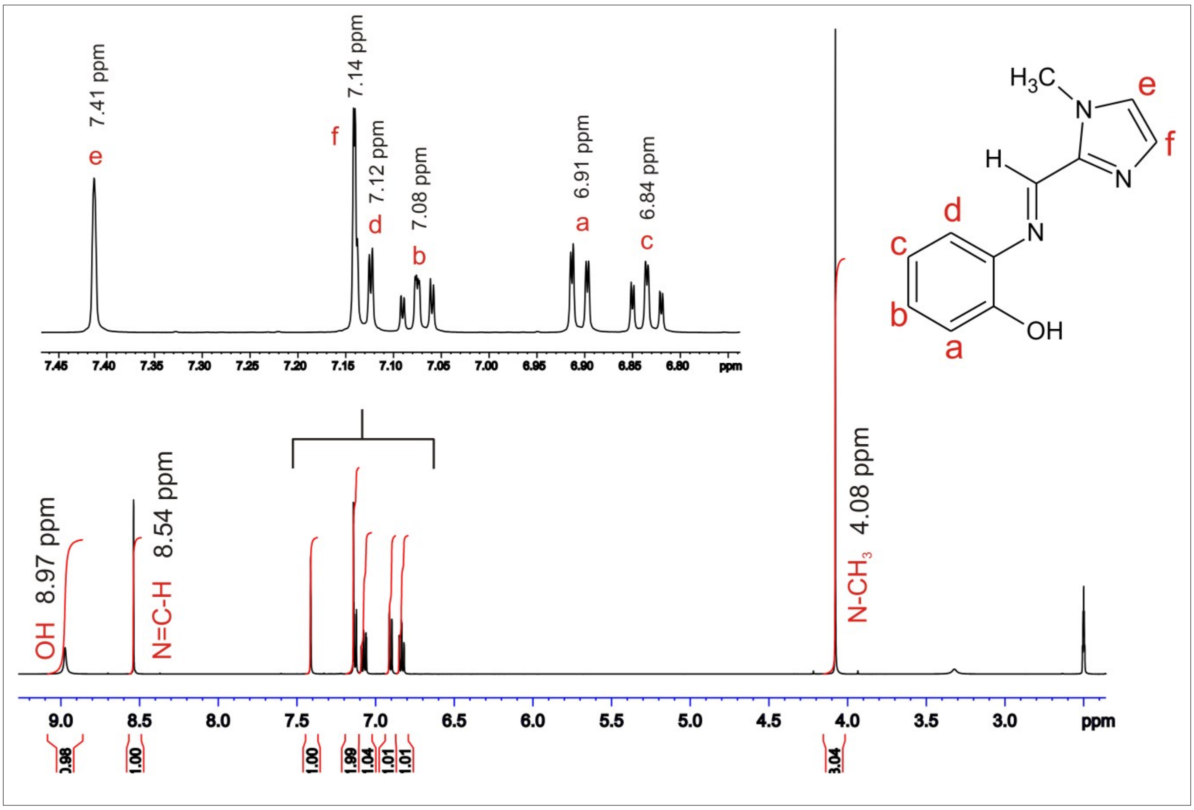


Figure S5: ^{1}H NMR spectrum of (3) in DMSO-d_6.

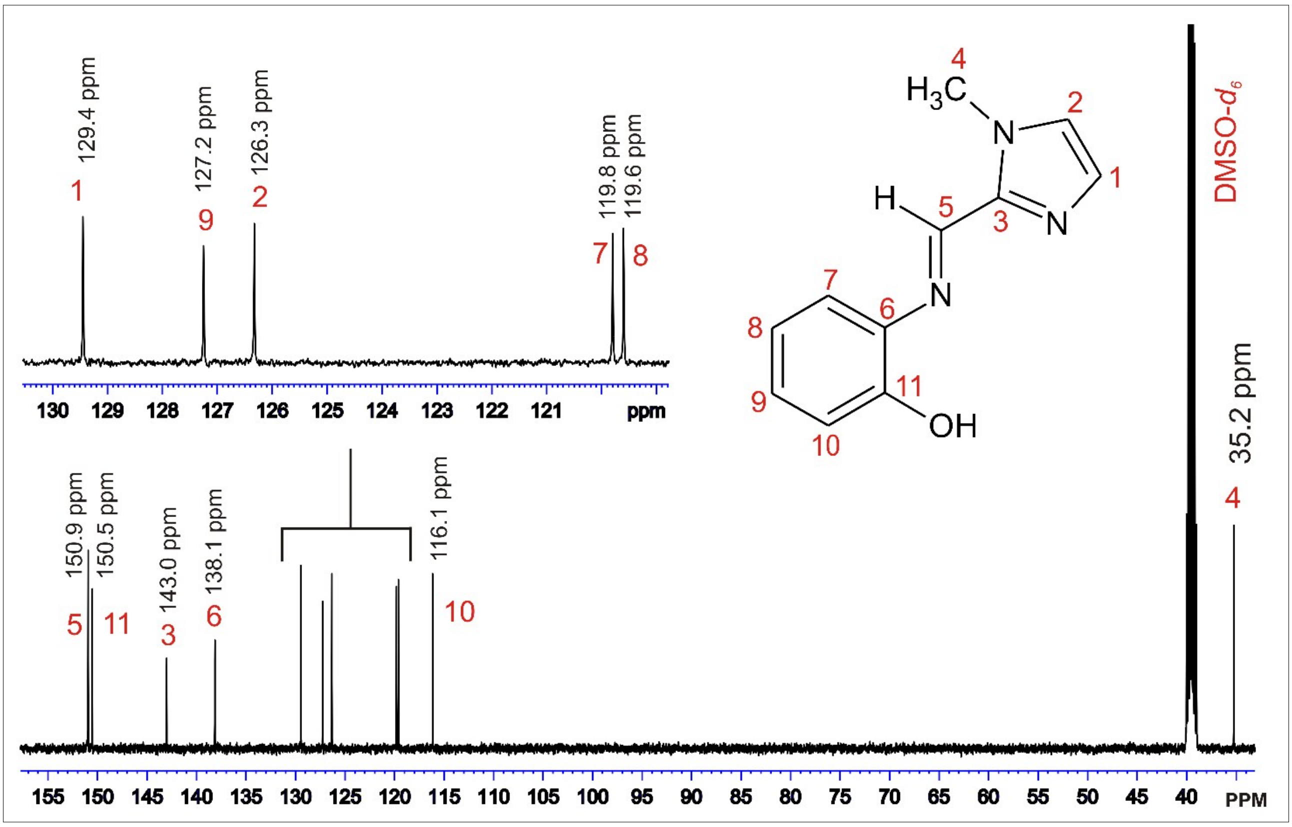


Figure S6: ^{13}C NMR spectrum of (3) in DMSO-d_6.

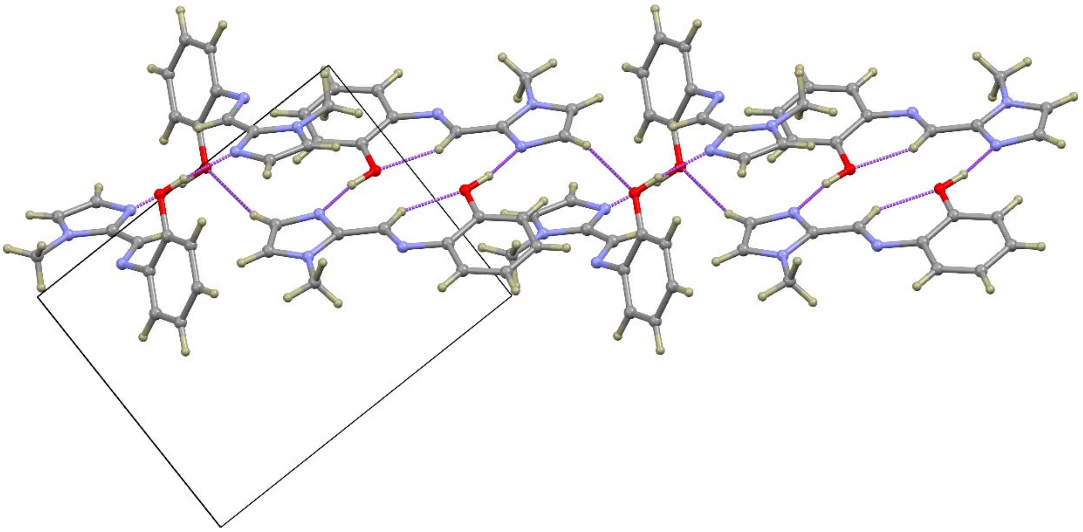
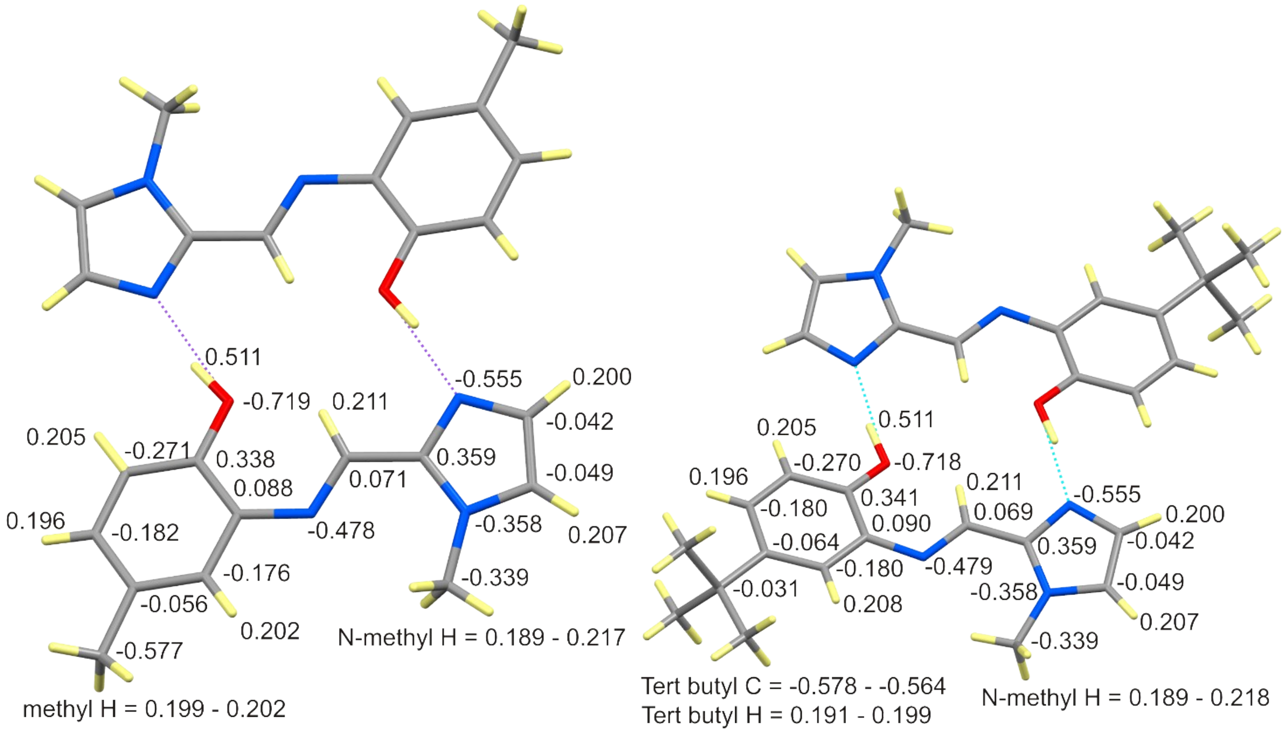
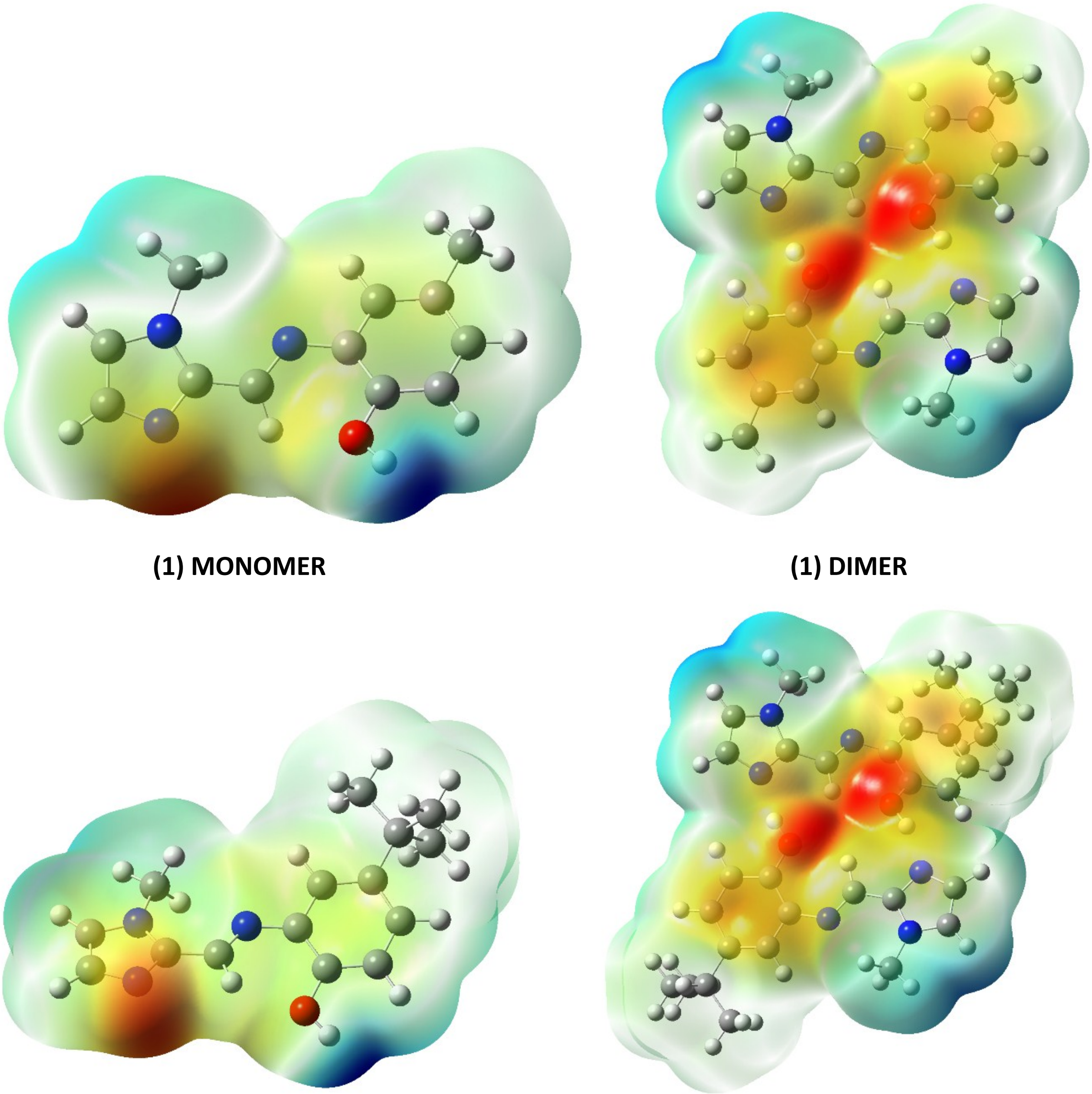


Figure S7: One-dimensional column of (3) viewed down the c-axis. All atoms are shown as spheres of arbitrary radius. The column comprises alternating dimers units of (3a) and (3b) linked by C–H···O interactions between the OH group and imidazole C–H.



(1) **(2)**

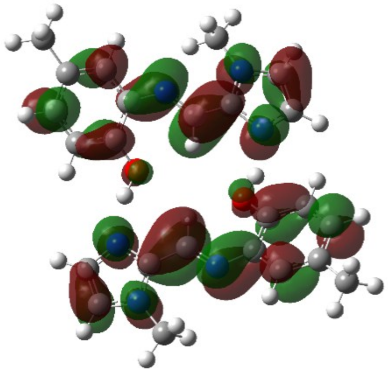
Figure S8: DFT calculated partial charges (e) for the dimeric structures of (1) and (2). The hydroxy proton and oxygen have the most positive and negative charges respectively.



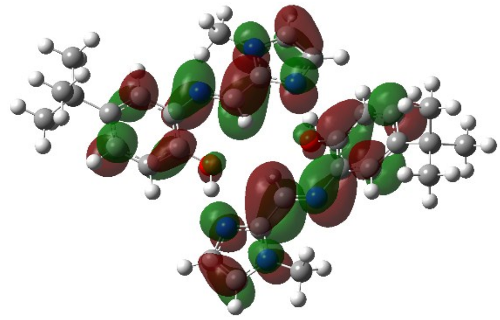
(1) MONOMER **(1) DIMER**

(2) MONOMER **(2) DIMER**

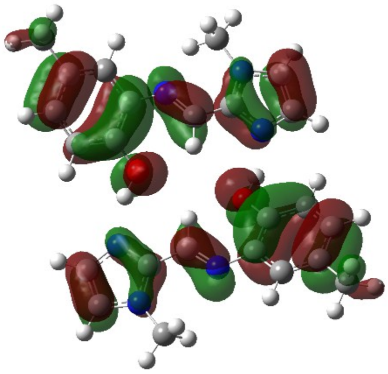
Fig. S9: Total SCF density molecular electrostatic potential maps of the monomer and dimer species of Ligands (1) and (2). Red regions indicate the most electron dense area and blue the most electropositive.



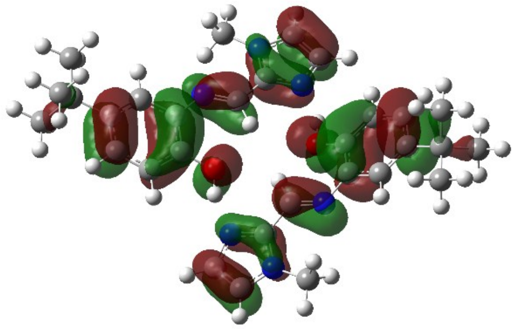
(1) LUMO



(2) LUMO



(1) HOMO



(2) HOMO

Figure S10: The HOMO and LUMO plots for geometry optimised dimer of (1) and (2) illustrating how the orbitals span both molecules.

Table S1: Summary of the major TD-DFT calculated electronic transitions for the monomeric and dimeric forms of (1) and the corresponding molecular orbitals (CH_3CN solvent continuum).

Wavelength (nm)[a]	Oscillator Strength, f	Molecular orbitals[b]	Contribution (%)[c]	Assignment[d]
Monomer				
346.80	0.5703	57 → 58	91	π(Imd, Im, Phenol, Me) → π*(Imd, Im, Phenol)
294.23	0.3213	54 → 58 55 → 58 56 → 58	11 45 32	π(N-Me, Imd, Im, Phen) → π*(Imd, Im, Phenol) π(N-Me, Imd, Im, Phen) → π*(Imd, Im, Phenol)* π(Imd, Im, Phenol, Me) → π*(Imd, Im, Phenol)
237.07	0.1371	54 → 58 55 → 58 57 → 59	36 12 34	π(N-Me, Imd, Im, Phen) → π*(Imd, Im, Phenol) π(N-Me, Imd, Im, Phen) → π*(Imd, Im, Phenol) π(Imd, Im, Phenol, Me) → π*(Phenol, Me)
Dimer				
356.28	0.6102	113 → 115 114 → 116	83 10	π(Imd, Im, Phenol, Me) → π*(Imd, Im, Phenol) π(Imd, Im, Phenol, Me) → π*(Imd, Im, Phenol)
295.18	0.7446	109 → 116 110 → 115 112 → 115	16 20 45	π(Imd, Im, Phenol) → π*(Imd, Im, Phenol) π(N-Me, Imd, Im, Phen) → π*(Imd, Im, Phenol) π(Imd, Im, Phenol, Me) → π*(Imd, Im, Phenol)
238.57	0.2213	107 → 116 108 → 115 113 → 117 114 → 118	13 19 11 33	π(Imd, Im, Phenol) → π*(Imd, Im, Phenol) π(Imd, Im, Phenol) → π*(Imd, Im, Phenol) π(Imd, Im, Phenol, Me) → π*(Phenol) π(Imd, Im, Phenol, Me) → π*(Phenol)

[a] Three of the 24 calculated excited states with the highest oscillator strengths are listed.

[b] For the monomer, the HOMO is orbital 57 and LUMO is 58; these are 114 and 115 for the dimer.

[c] Only orbitals with contributions >10% are listed.

[d] Imd = imidazole; Im = imine; Phenol = benzene ring + OH; Phen = benzene ring; N-Me = imidazole N-CH_3; Me = phenolic methyl substituent.