

Electronic supplementary information (ESI)

Insights into H-aggregates and CH•••O hydrogen bonds mediated self-assembly of pyromellitic bisimide

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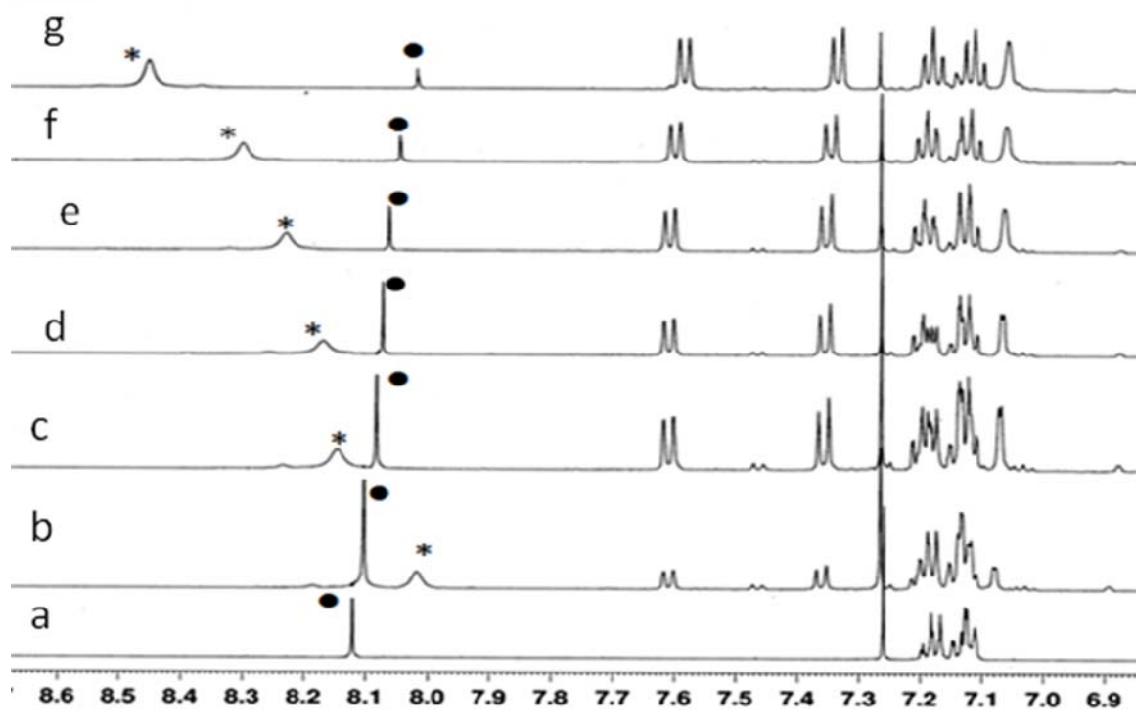


Fig. S1. NMR titration of bisimide receptor **1** in CDCl₃ at 14.80mM (500 MHz, 25 °C) with (a) 0.000, (b) 3.7, (c) 6.12, (d) 10.30, (e) 12.65 (f) 17.03 and (g) 44.32 mM of tryptophan methyl ester. The black circle indicate pyromelic ring protons, and * indicates Trp ring NH proton.

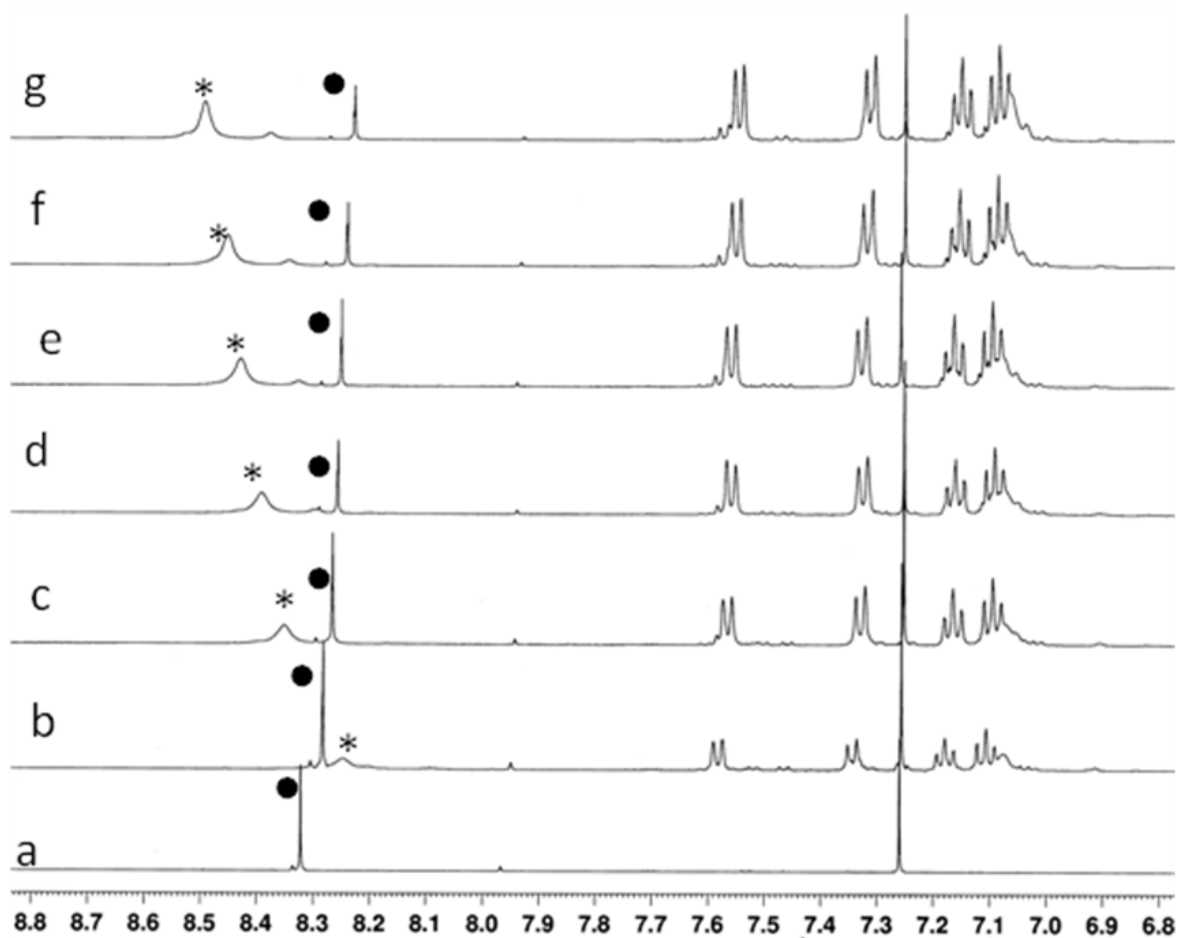


Fig. S2. NMR titration of bisimide receptor **2** in CDCl₃ at 16.93 mM (500 MHz, 25 °C) with (a) 0.000, (b) 8.06, (c) 13.43, (d) 18.45, (e) 21.03 (f) 28.59 and (g) 31.24 mM of tryptophan methyl ester. The black circle indicate pyromellitic ring protons, and * indicates Trp ring NH proton.

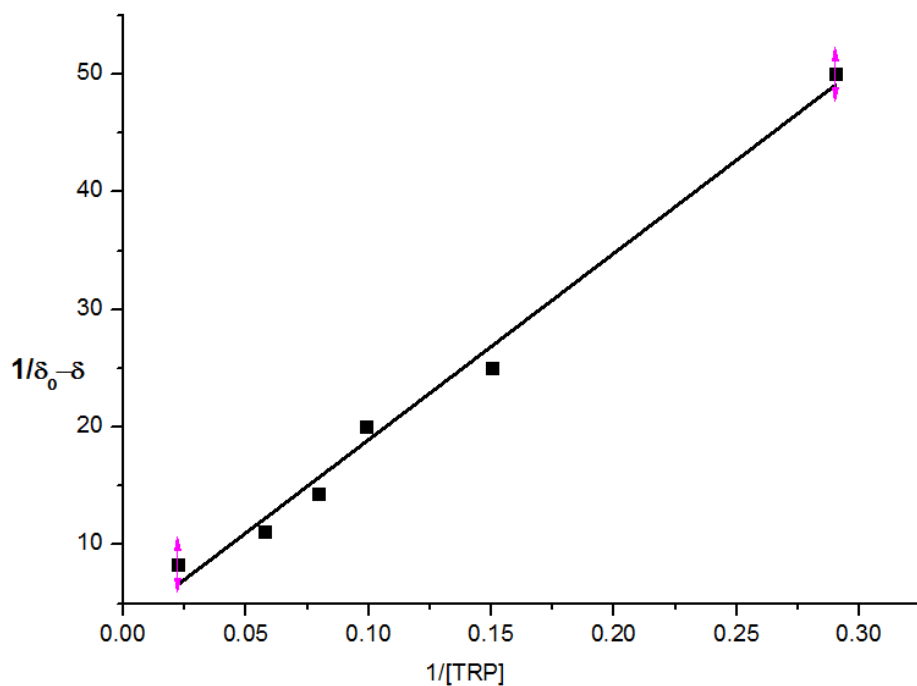


Fig. S3. B-H plot of bisimide 1-tryptophan complex from NMR titration experiments showing 1:1 complex formation.

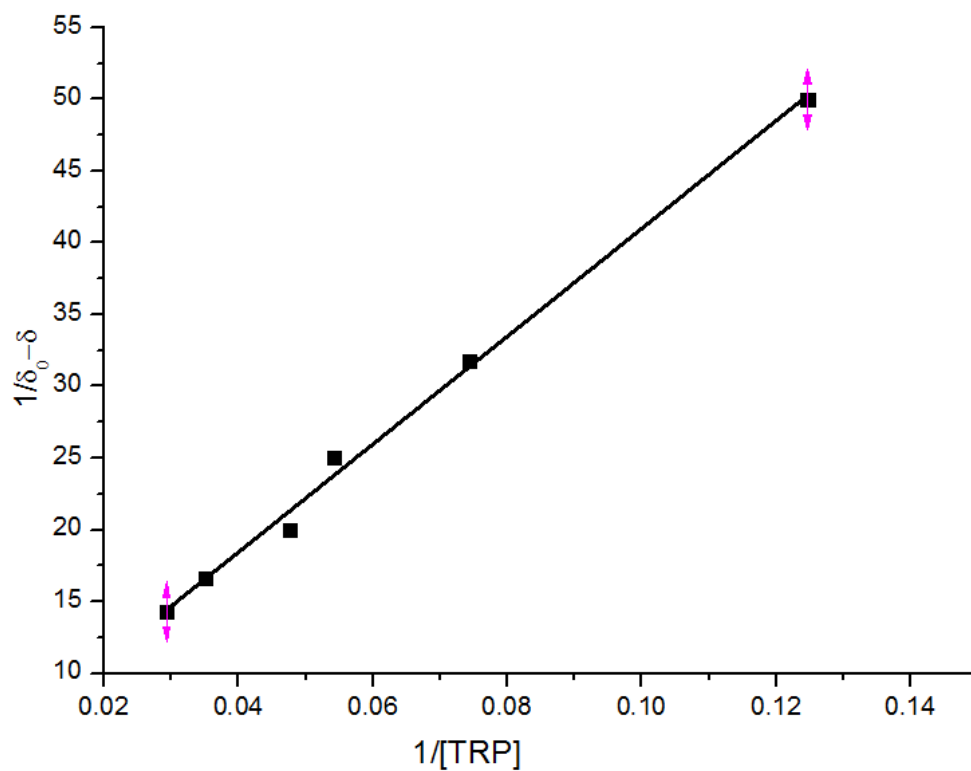


Fig. S4. B-H plot of bisimide 2-tryptophan complex.

Table S1: Binding constants of bisimides and tryptophan complexes.

Complex	$K_{\text{binding constant}} (M^{-1})$	stoichiometric ratio
Bisimide 1-tryptophan	2.94×10^2	1:1
Bisimide 2-tryptophan	9.06×10	1:1

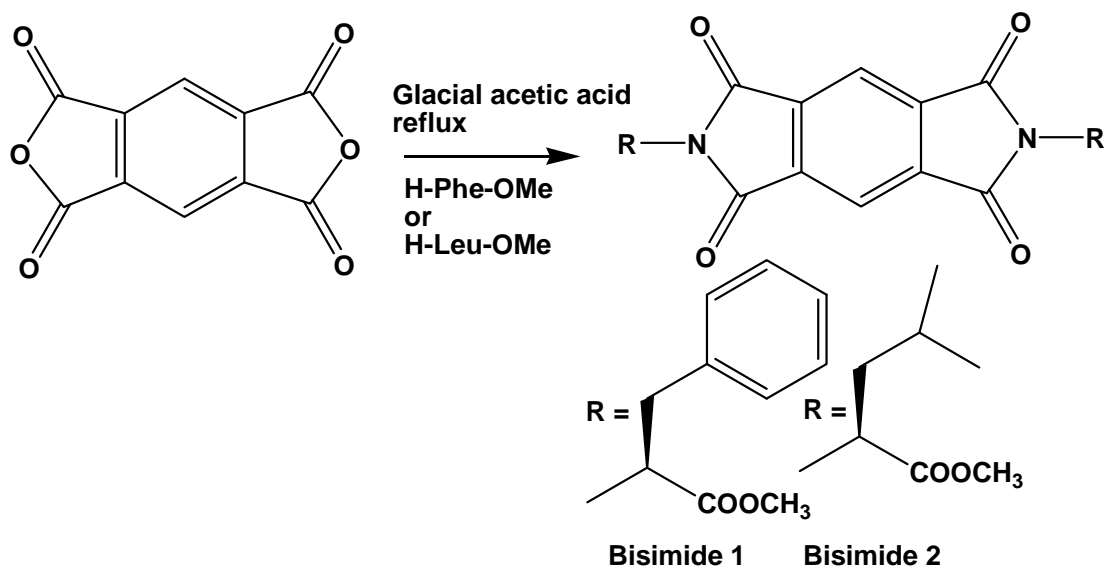


Fig. S5. Schematic presentation of synthesis of bisimides 1 and 2 .

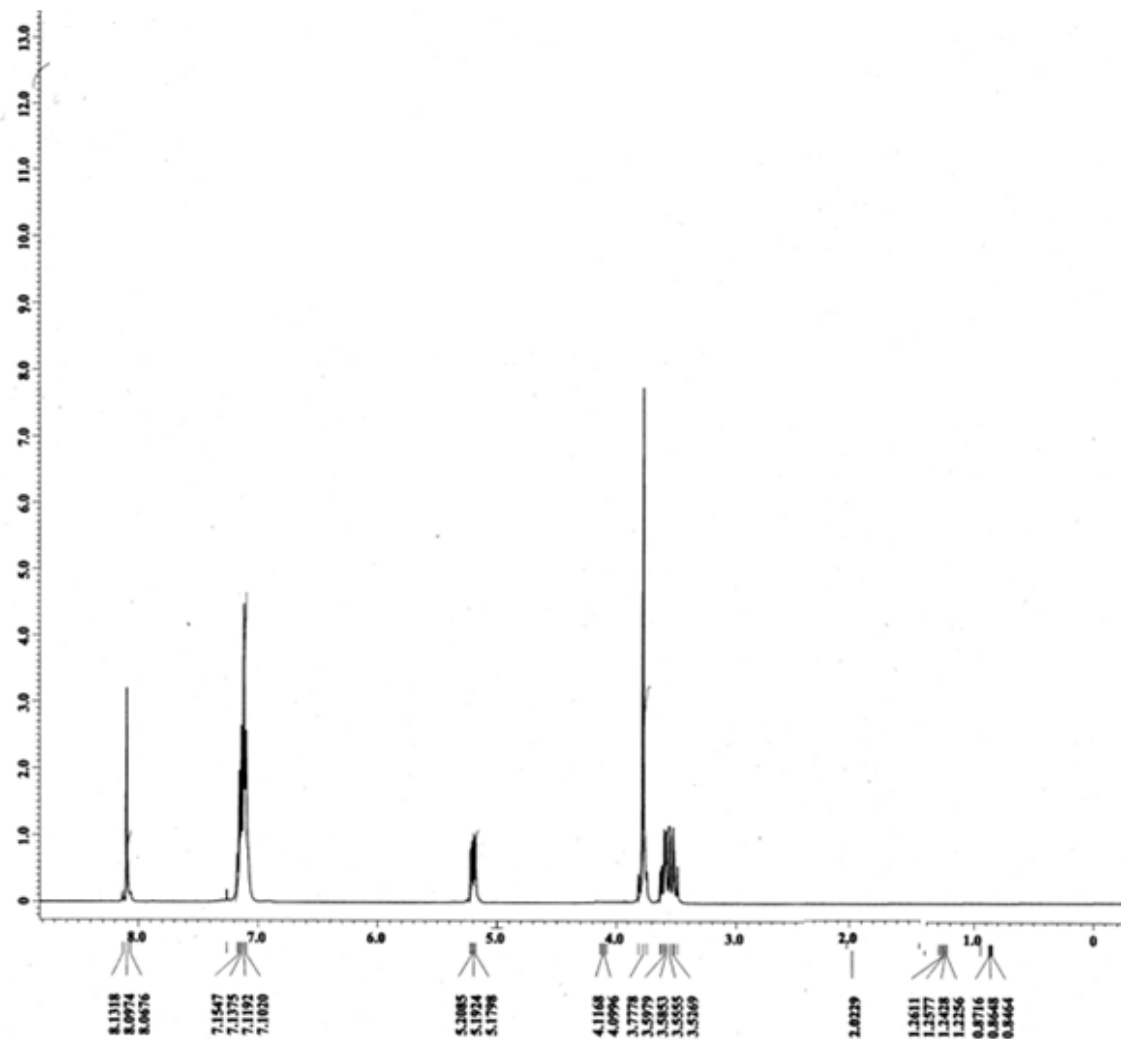


Fig. S6. ^1H NMR (400MHz, CDCl_3) spectra of bisimide 1.

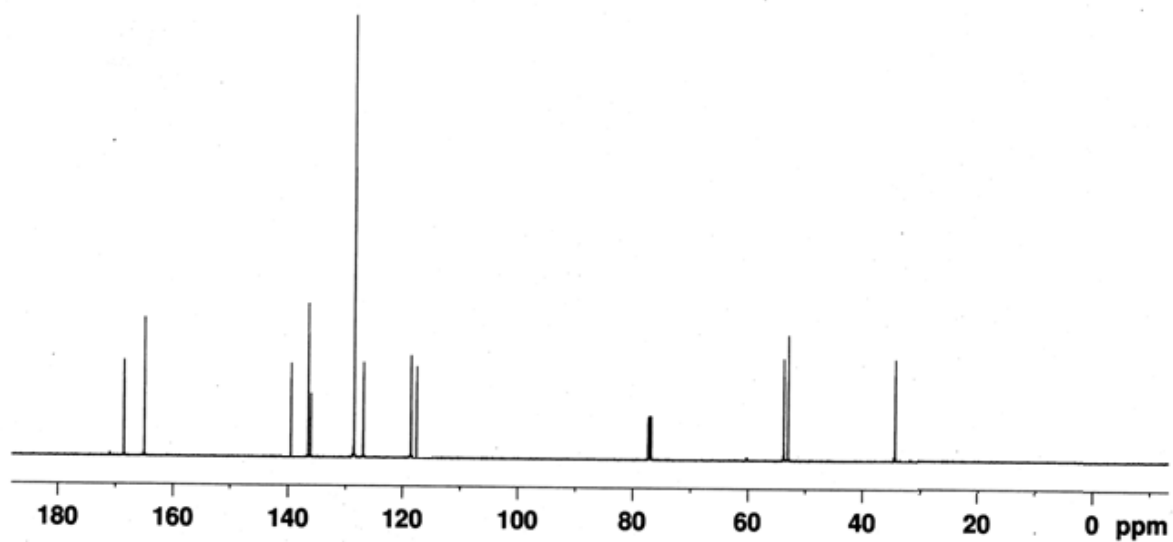


Fig. S7. ^{13}C NMR (125MHz, CDCl_3) spectra of bisimide 1.

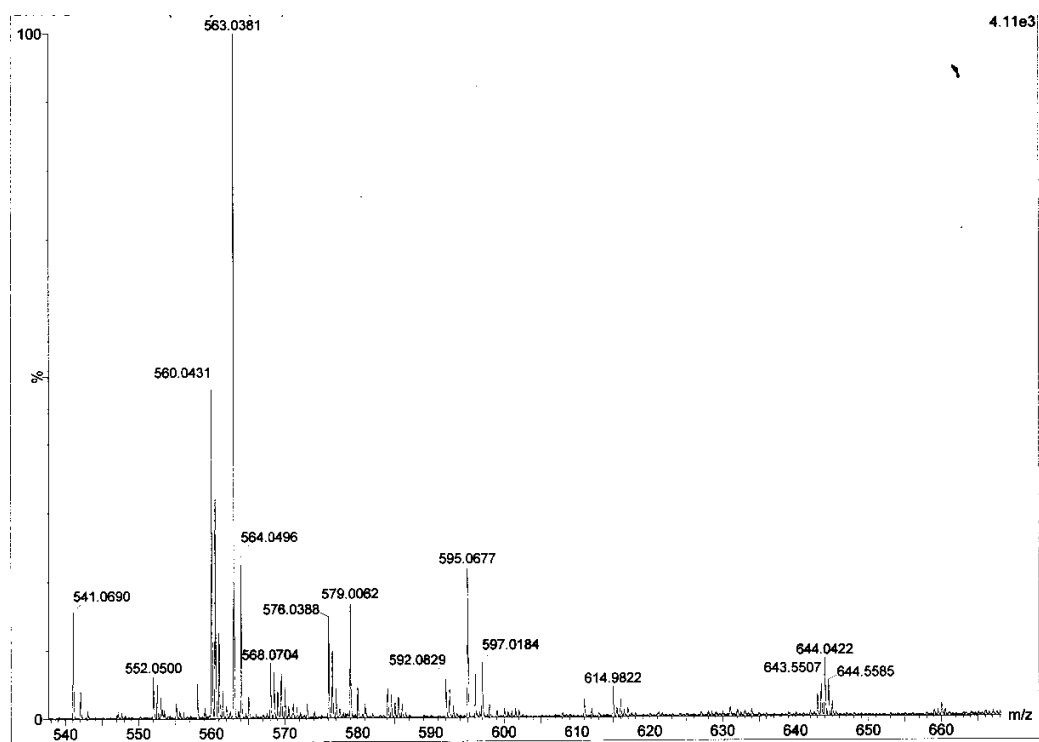


Fig. S8. Mass spectra of bisimide 1.

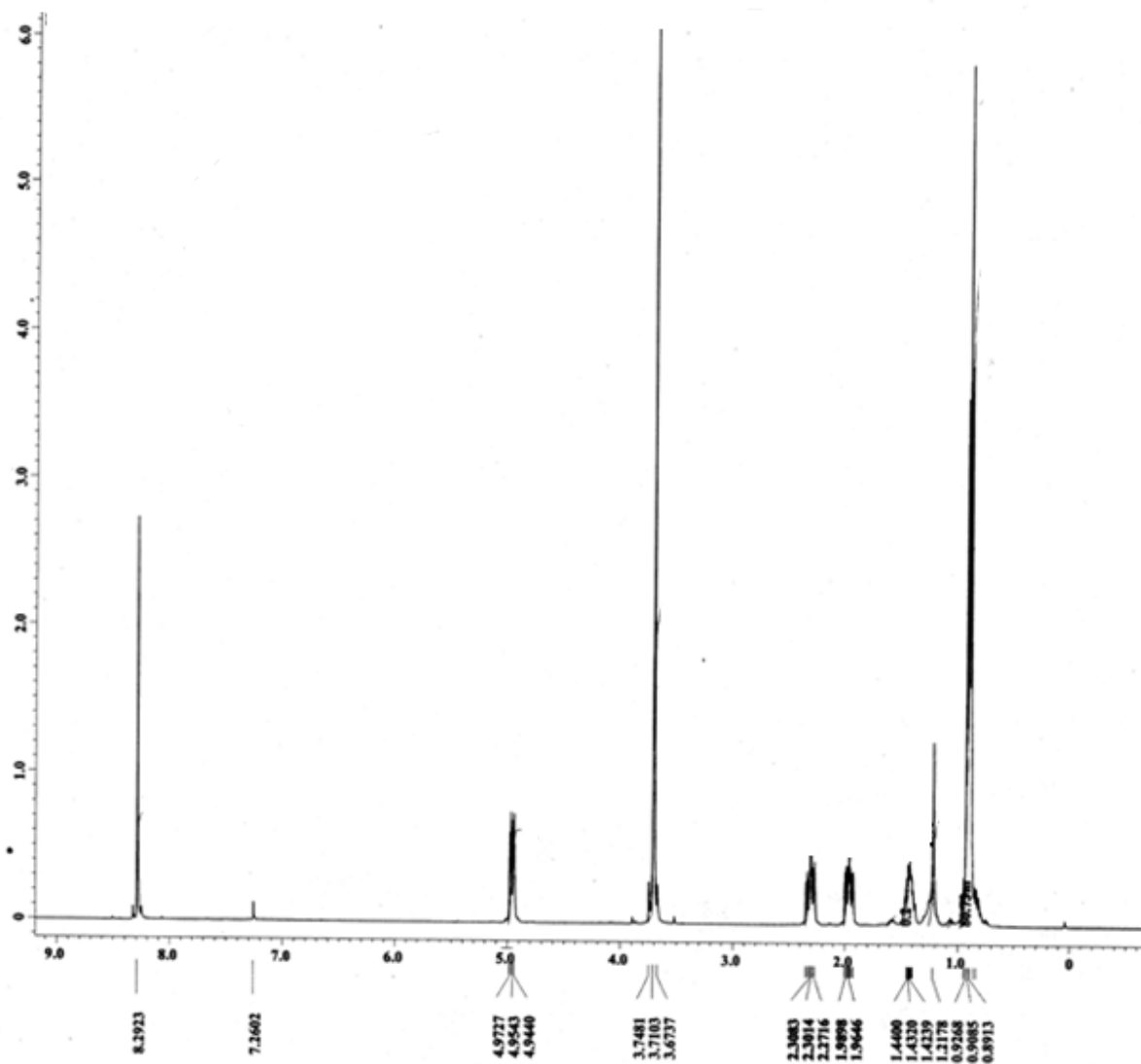


Fig. S9. ^1H NMR spectra of bisimide **2** in CDCl_3 .

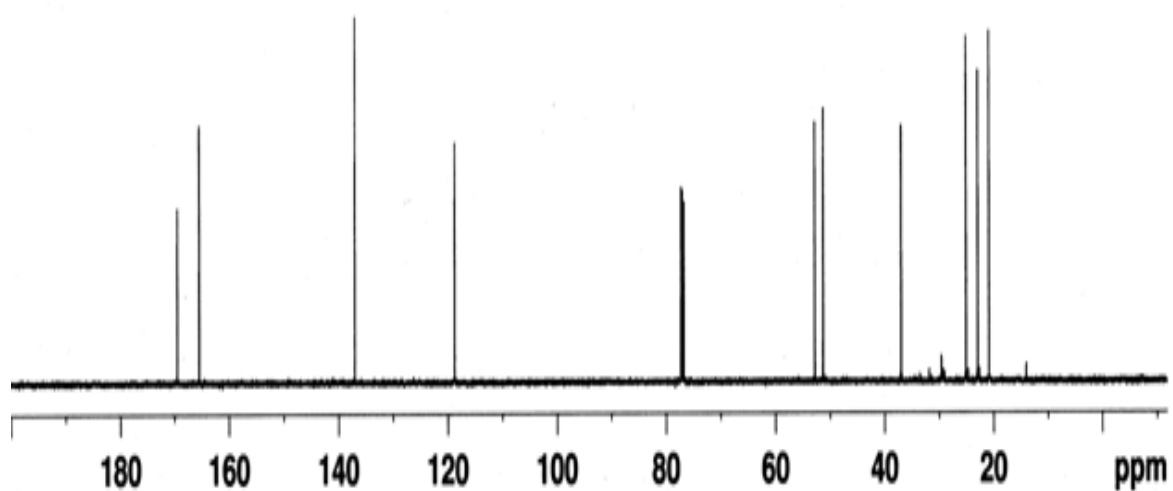


Fig. S10. ^{13}C NMR spectra of bisimide **2** in CDCl_3 .

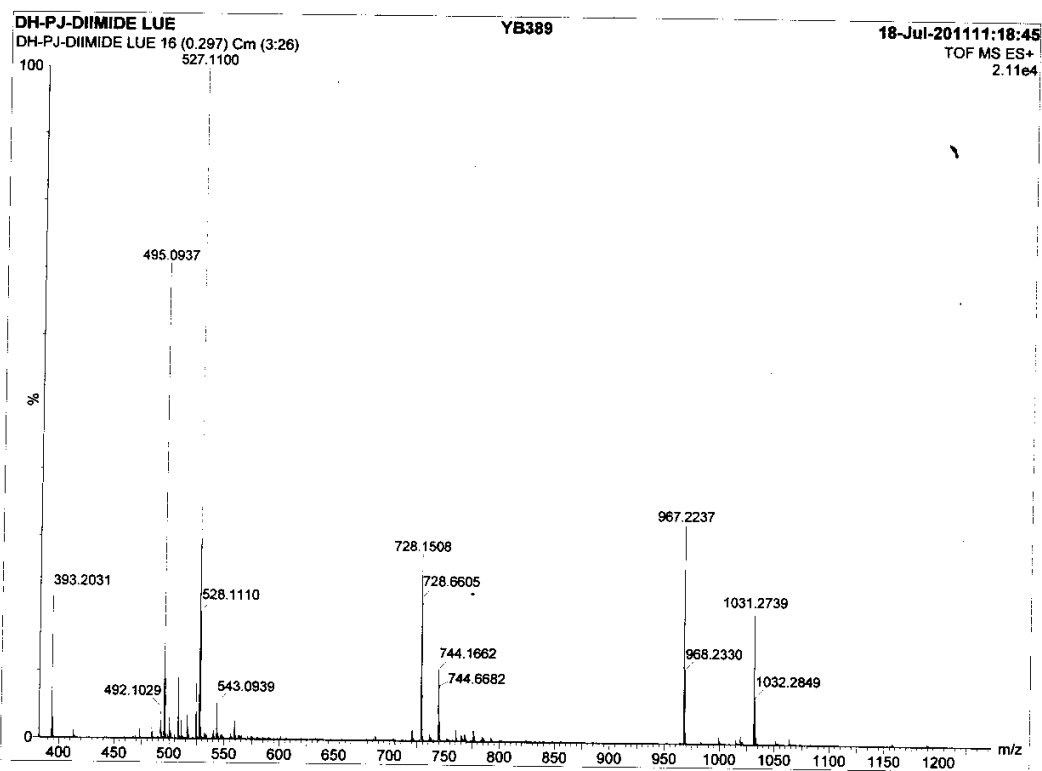


Fig. S11. Mass spectra of bisimide **2**.

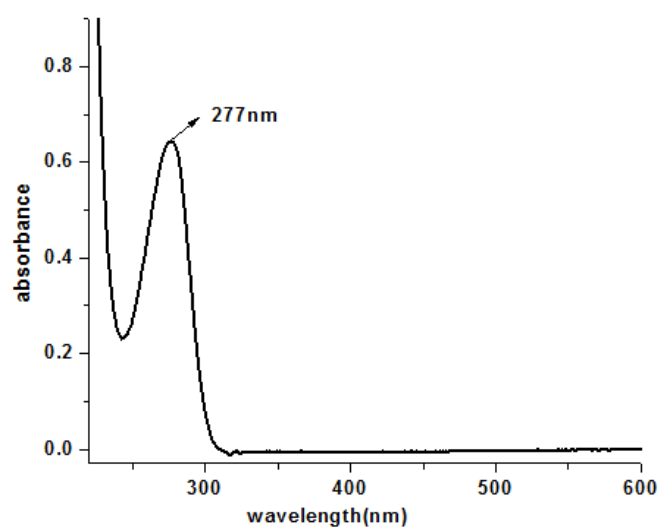


Fig. S12: absorption of Tryptophan methyl ester in chloroform, [0.00759mM].

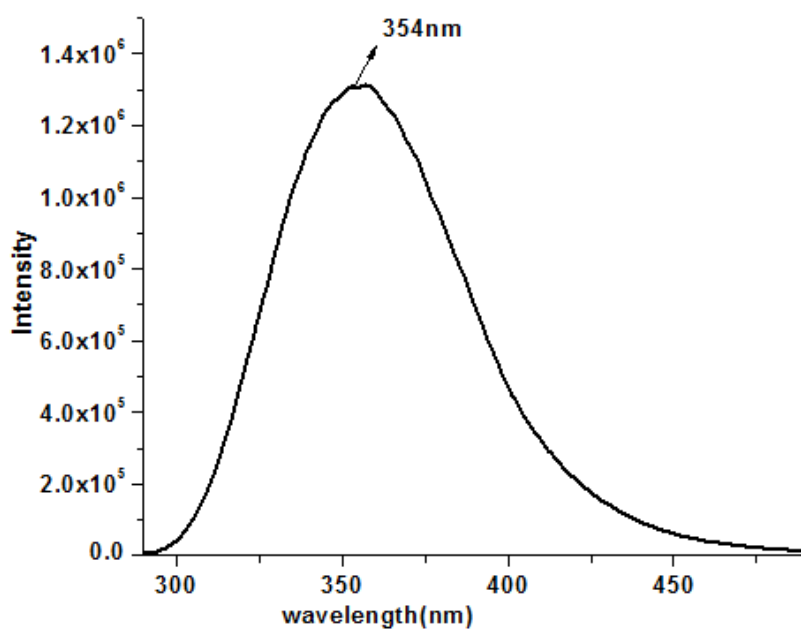


Fig. S13: Emission spectra of Tryptophan methyl ester in chloroform, [0.00759mM].

Optical rotation of bisimide **1** [α] = -0.765, bisimide **2** [α] = -1.952.

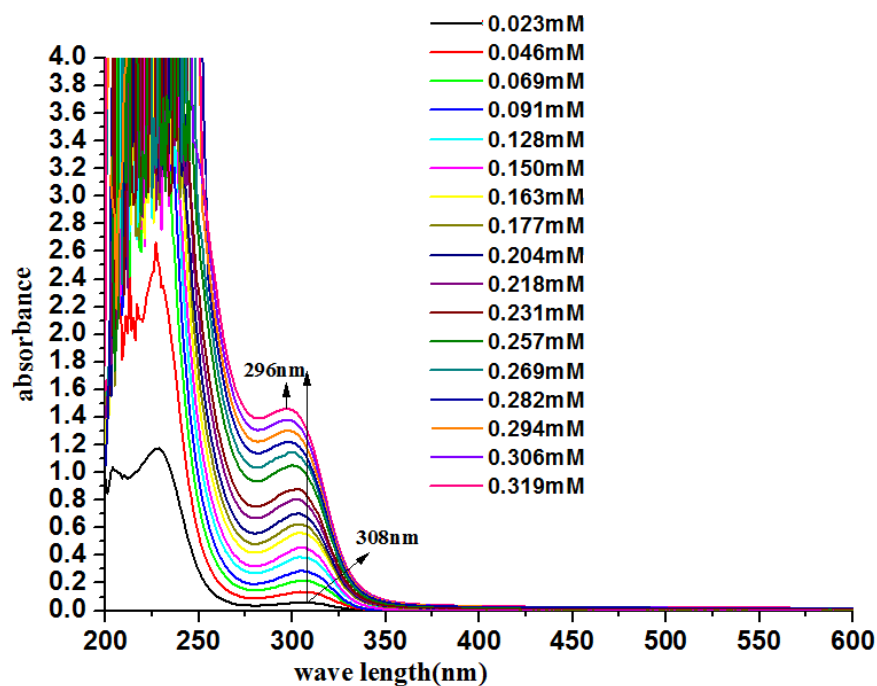


Fig. S14: Concentration dependent UV/vis spectra of bisimide 1 in full range.

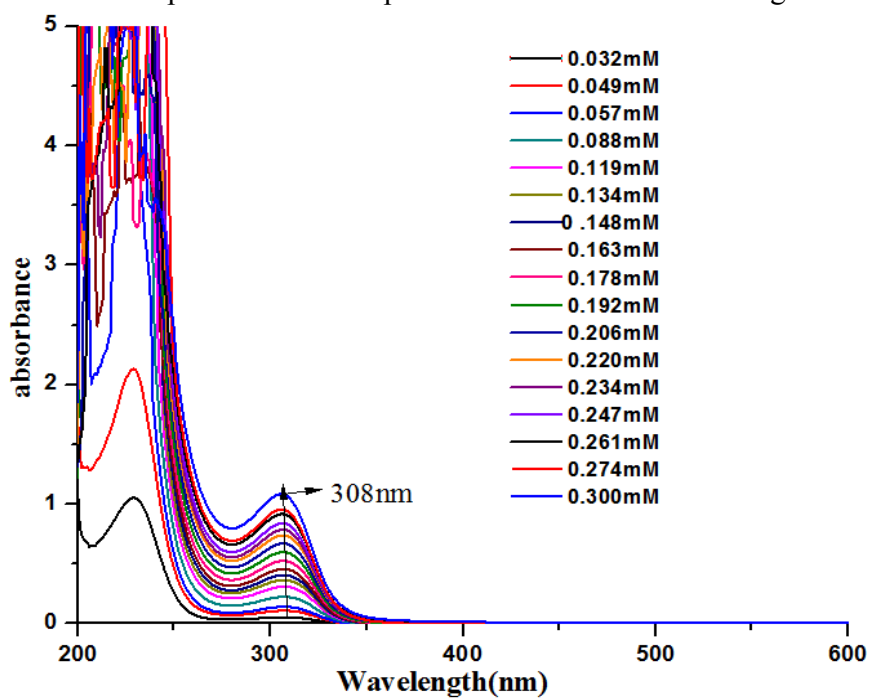


Fig. S15: Concentration dependent UV/vis spectra of bisimide 2 in full range.