

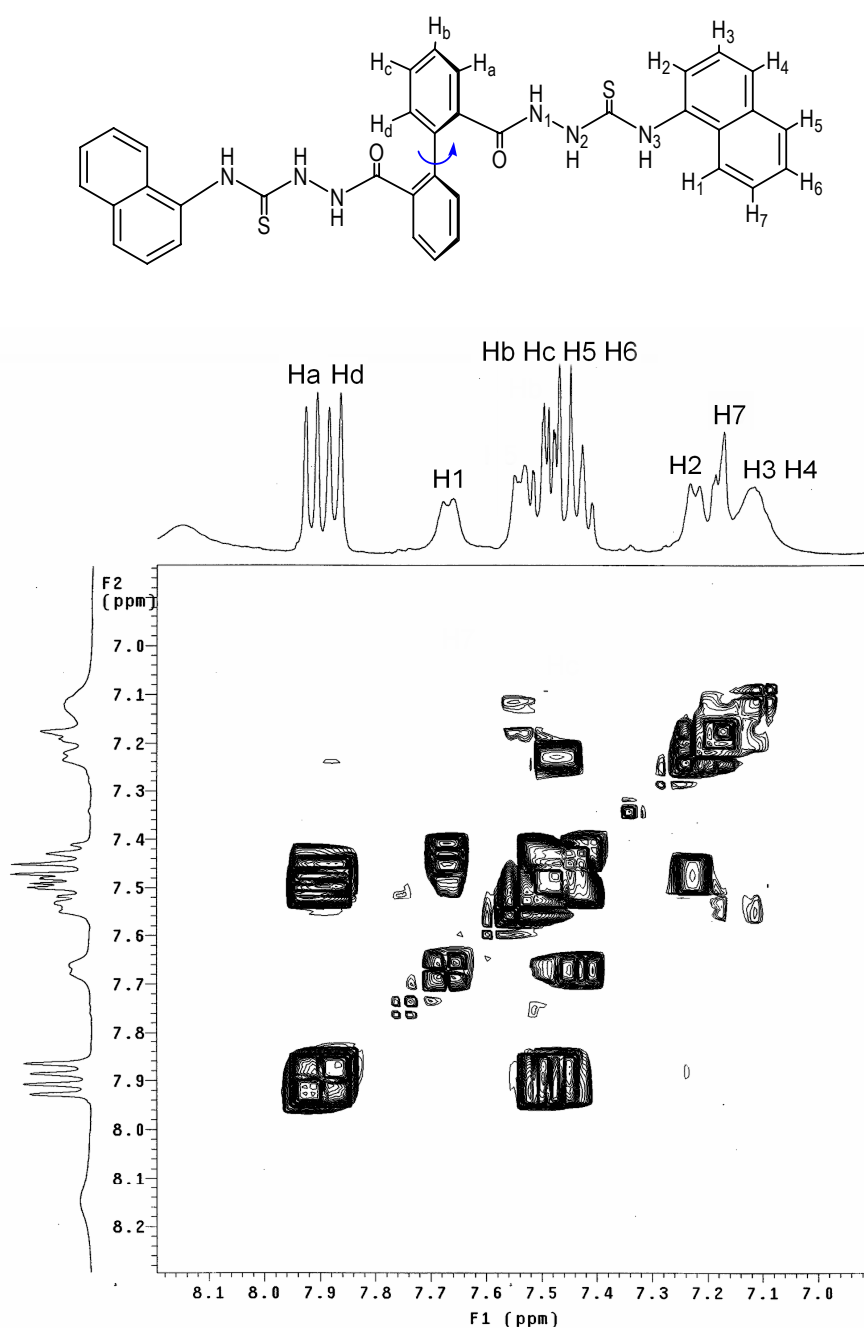
Supporting Materials

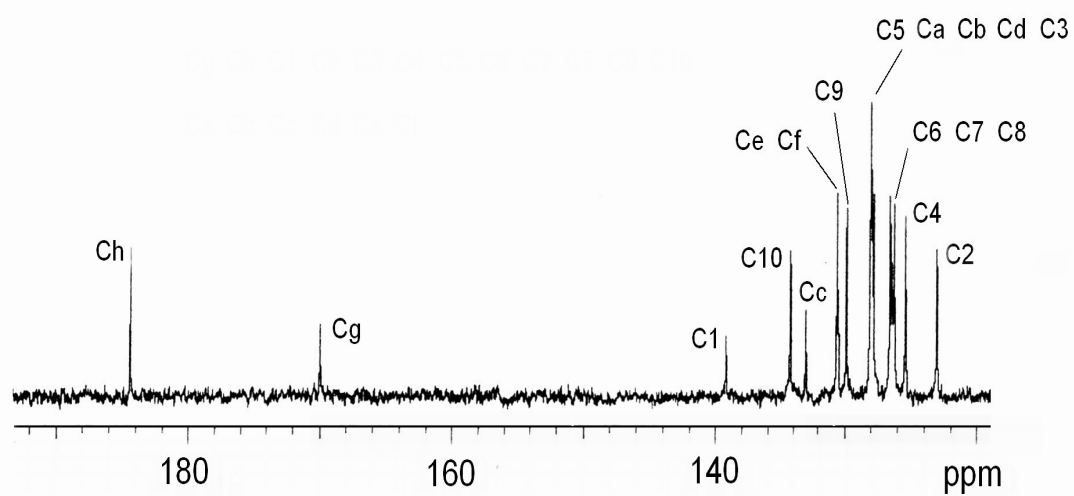
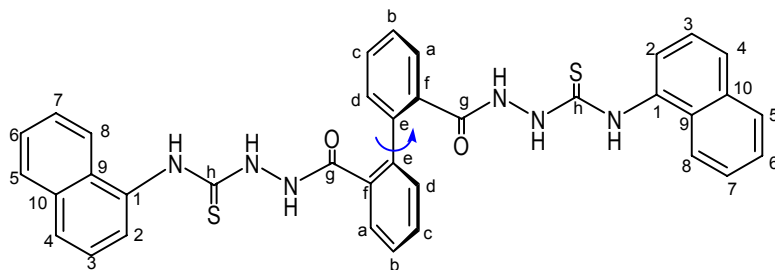
Thiourea-based Molecular Clips for Fluorescent Discrimination of Isomeric Dicarboxylates

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Spectrum of SN

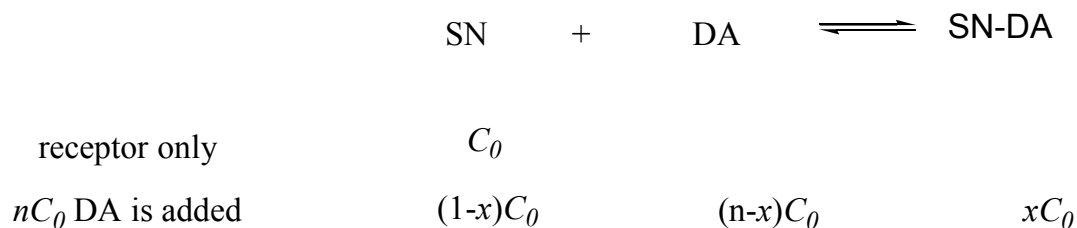
^1H gCOSY NMR (400 MHz, CD_3CN)



^{13}C NMR (100 MHz, CD_3CN)

Association Constant Calculation:

Generally, for the formation of 1: 1 complexed species formed by the receptor SN and the guest anion (DA), if we assume $x C_0$ to the concentration of complexes species SN-DA, when the concentration of the added guest anion is a $n C_0$ with the original concentration of the receptor SN being fixed at C_0 :



$$K = \frac{[\text{SN-DA}]}{[\text{SN}][\text{DA}]} \quad (1)$$

The measurements are performed under the conditions where the fluorescent intensity of the free receptor in such a concentration is A_0 ; after addition of a given amount ($n C_0$) of DA, the fluorescent intensity becomes:

$$A = A_I x + A_0 (1-x) \quad (2)$$

where A_I is the fluorescent intensity of the saturated value in the presence of excess guest anions.

It is easy to derive the usual equation:

$$\frac{A-A_0}{A_I-A_0} = x \quad (3)$$

From eqs (1) and (3), we can obtain the equation:

$$\frac{n}{A-A_0} = \frac{I}{K C_0} \cdot \frac{I}{A_I-A} + \frac{I}{A_I-A_0} \quad (4)$$

K_s can be obtained by a linear analysis of $\frac{I}{A_I-A}$ (X) versus $\frac{n}{A-A_0}$ (Y).

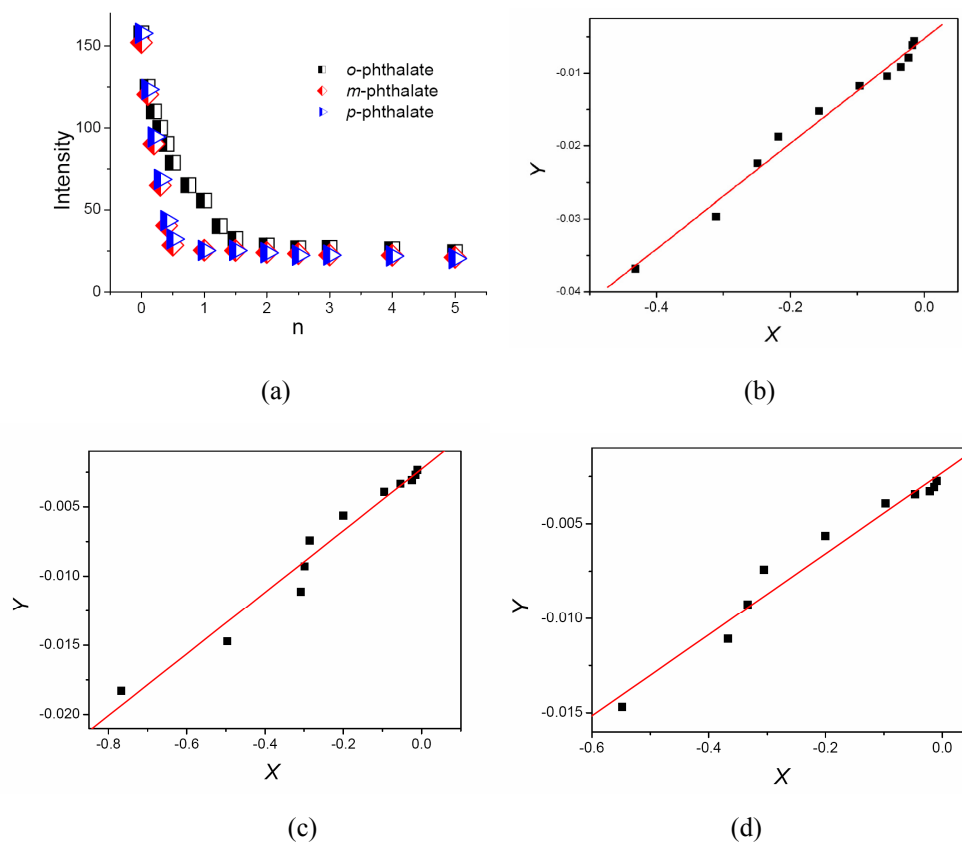


Figure S1. Plot for SN (a) versus number of equivalents of phthalate ions (n) added and (b) *o*- (c) *m*- (d) *p*-phthalate ion system with $\log K_{ass}$ being calculated as 5.14 ± 0.02 , 5.65 ± 0.02 , 5.67 ± 0.03 , respectively. Emission intensity is recorded at 420nm (Excitation at 340 nm).

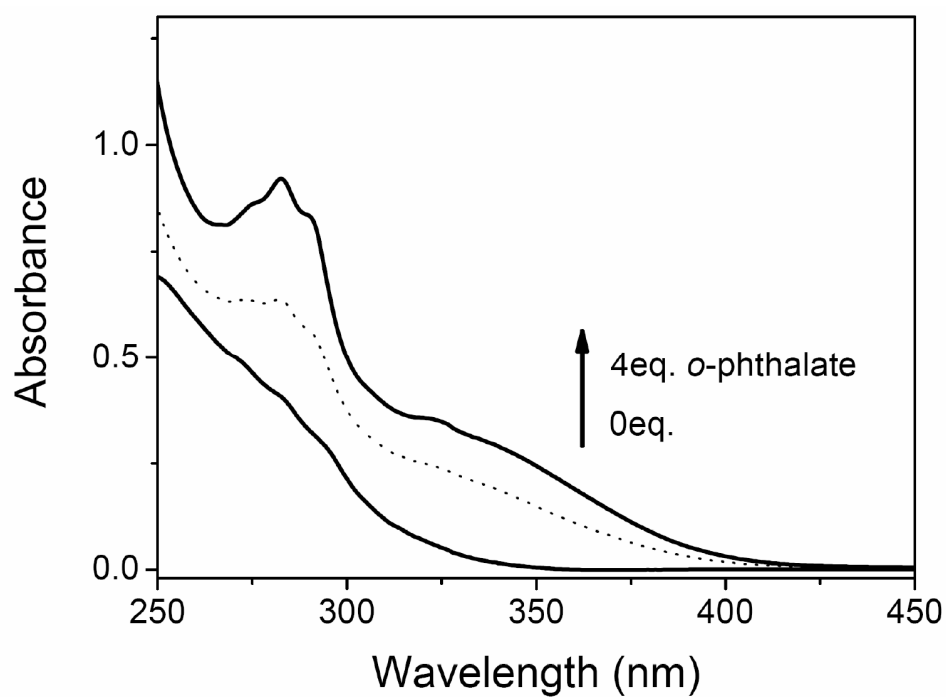


Figure S2 Absorption spectra of SN ($2 \times 10^{-5} \text{ M}$) in MeCN upon the addition of *o*-phthalate ion.

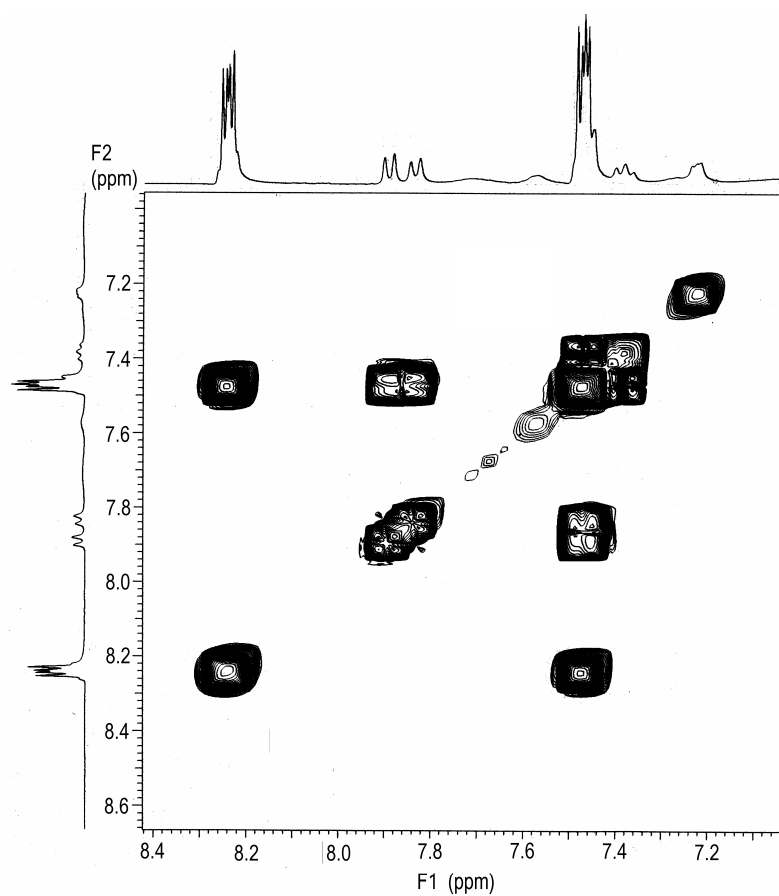


Figure S3 ^1H gCOSY NMR (400 MHz, CD_3CN) of SN upon the addition of 2.0 equivalent molar ratio of *o*-phthalate anion.