

## Supplementary Information for

### **Fluorescence signaling systems for sensing Hg(II) ion derived from A<sub>2</sub>B-corroles**

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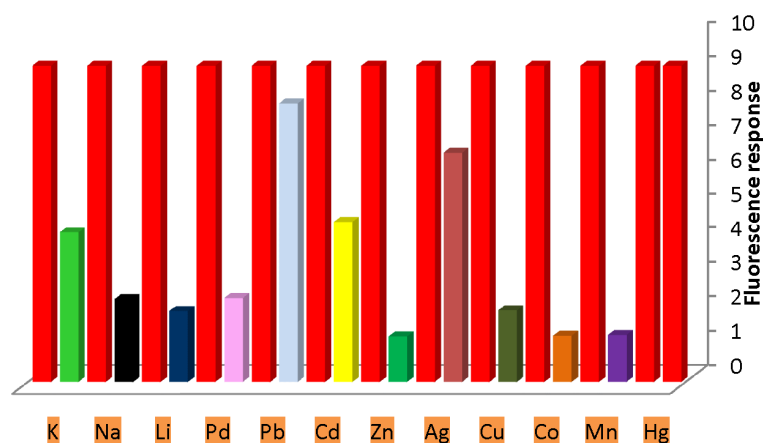
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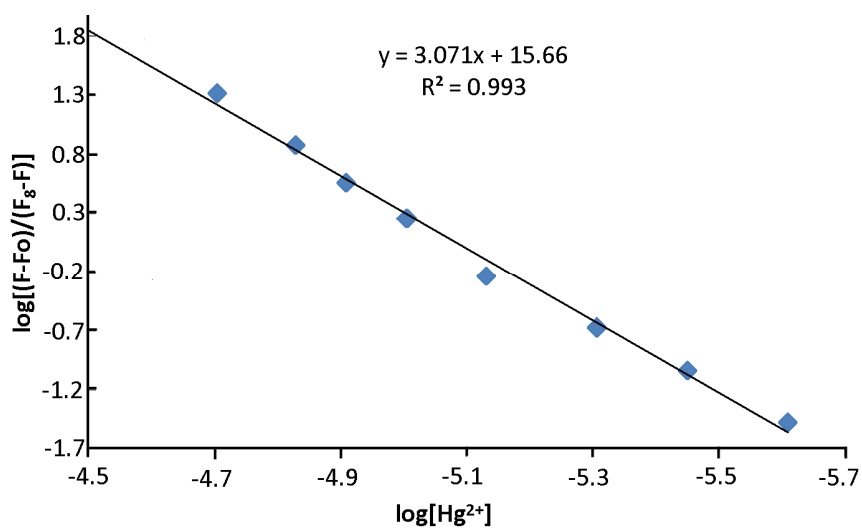
Fig S4. ESI-MS spectrum of the free base corrole **4**.

**Table S1:** UV-Visible absorption and the extinction coefficient of the corroles1-4 in toluene and dichloromethane.

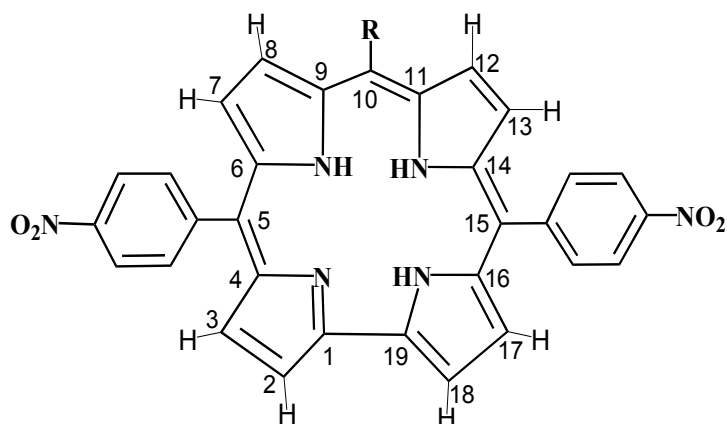
Corroles	Solvents	$\lambda_{\text{max}} / \text{nm} (\epsilon / \text{m}^{-1} \text{cm}^{-1})$
1	Toluene	448 (10,200), 595 (2,830)
	CH <sub>2</sub> Cl <sub>2</sub>	424 (15,800), 594 (3,150)
2	Toluene	448 (17,500), 596 (6,900)
	CH <sub>2</sub> Cl <sub>2</sub>	426 (54,950), 597 (12,800)
3	Toluene	445 (31,470), 599 (11,700), 638 <sup>sh</sup> (11,200)
	CH <sub>2</sub> Cl <sub>2</sub>	437 (40,800), 595 (13,400), 635 <sup>sh</sup> (12,550)
4	Toluene	448 (34,400), 591 (11,544), 662 (11,400)
	CH <sub>2</sub> Cl <sub>2</sub>	439 (60,100), 592 (20,300), 652 (19,400)



**Figure S1.**  $\text{Hg}^{2+}$  ion sensing in presence of other metal ion. The fluorescence response ( $F_0/F$ ) in presence of divalent metal ion is plotted.  $F_0$ =fluorescence intensity in absence of any metal ion &  $F$ = fluorescence intensity in the presence of metal ions. Initial red bar shows the extent of quenching by  $\text{Hg}^{2+}$  ion and respective coloured bar signifies  $\text{Hg}^{2+}$  ion quenching in presence of divalent metal ion.



**Figure S2.** A plot for the determination of association constant for **4** with  $\text{Hg}^{2+}$  ion ;  $\log$  of the ratio of  $(F-F_0)$  over  $(F_8-F)$  versus  $\log$  of the free  $\text{Hg}^{2+}$  ion concentration.  $F_0$ =fluorescence intensity in the absence of  $\text{Hg}^{2+}$  ion ;  $F_8$ =fluorescence intensity in the presence of excess  $\text{Hg}^{2+}$  ion.  $F$ = fluorescence intensity at a given amount of  $\text{Hg}^{2+}$  ion. For detail derivation please refer X. J. Zhu, S. T. Fu, W. K. Wong, J. P. Guo, W. Y. Wong, *Angew. Chem.*, 2006, **118**, 3222.



**Table S2.**  $^1\text{H}$  NMR chemical shifts (ppm) in  $\text{CDCl}_3$

Corrole	$^1\text{H}_a(2, 18)$	$^1\text{H}_c(7,13)$	$^1\text{H}_b(3,17)$	$^1\text{H}_d(8,12)$	Reference
<b>1</b>	9.102	8.899	8.650 (overlapped)		This work
<b>2</b>	9.054	8.862	8.695	8.374	This work
<b>3</b>	9.075	8.758	8.626 (overlapped with naphthyl-H)	8.352	This work
<b>4</b>	8.957	8.778	8.611 ( overlapped )		This work
$\text{H}_3(\text{tpfc})$	9.100	8.750	8.570 (2d overlapping, 4H)		<i>Magn. Reson. Chem.</i> 2004; <b>42</b> : 624–635.

The electronic communication within the whole corrole molecules is evident from the chemical shift value of the  $\beta$ -pyrrolic hydrogens. The higher deshielding of the 2, 18-hydrogen and its high resembles to that of free base 5,10,15-tris(pentafluorophenyl)corrole signifies that the electronic communication or electron withdrawl by the nitro-phenyl group in the studied A2B corroles. This effect further stabilise the macrocycle to a greater extent. In case of corrole **2** and **3** an appreciable overlap between the 3, 17, 8, 12 hydrogens with that of hydrogens from meso-dimethylphenyl and tridecyloxyphenyl group has been found. Chemical shift value for meso-phenyl hydrogens are given in the text in the experimental section. In all the cases the signals for the NH protons were not detected.

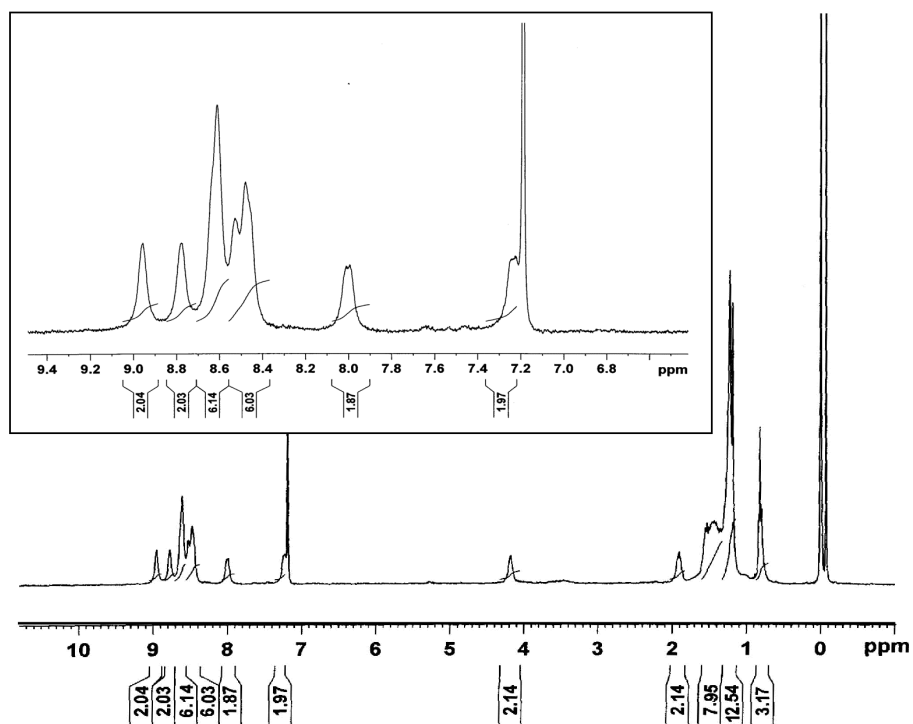


Figure S3.  $^1\text{H}$  NMR spectrum of 4. Inset shows the extended aromatic region.

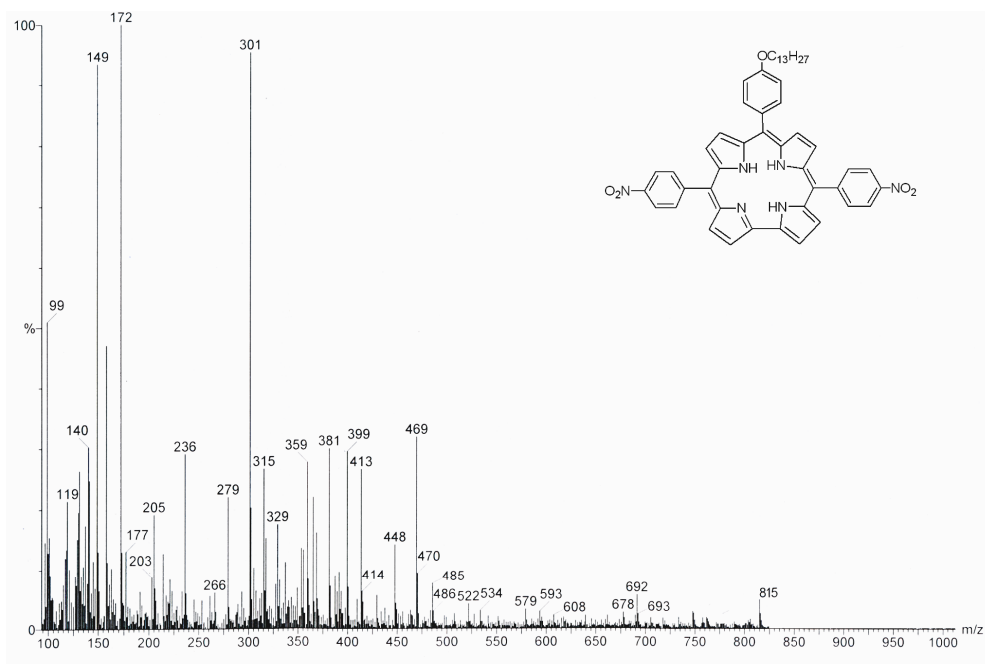


Figure S4. ESIMS spectrum of 4.