

## Molecular tectonics: *p*-H-thiacalix[4]arene pyridyl appended positional isomers as tectons for the formation of 1D and 2D mercury coordination networks

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### ESI: NMR Spectra of compounds 2-4

#### 25,26,27,28-tetra[(2-pyridylmethyl)oxy]-2,8,14,20-tetrathiacycalix[4]arene (2)

<sup>1</sup>H-NMR (300 MHz, CDCl<sub>3</sub>): δ(ppm) = 5.30 (8H, s, ArOCH<sub>2</sub>), 6.37 (4H, t, Ar-H), 6.69 (4H, d, Py-H), 7.09 (8H, d, Ar-H), 7.22 (4H, m, Py-H), 7.43 (4H, m, Py-H), 8.59 (4H, d, Py-H).

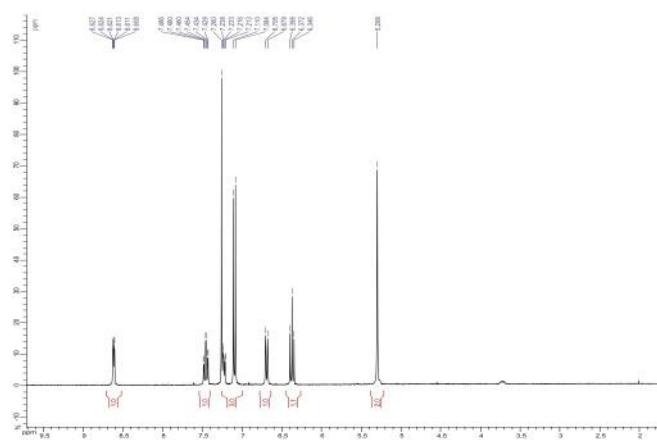


Figure S1: <sup>1</sup>H-NMR spectrum of 2

<sup>13</sup>C-NMR (75 MHz, CDCl<sub>3</sub>): δ(ppm) = 72.1, 122.1, 122.4, 123.9, 129.8, 134.7, 136.1, 149.0, 157.8, 159.7.

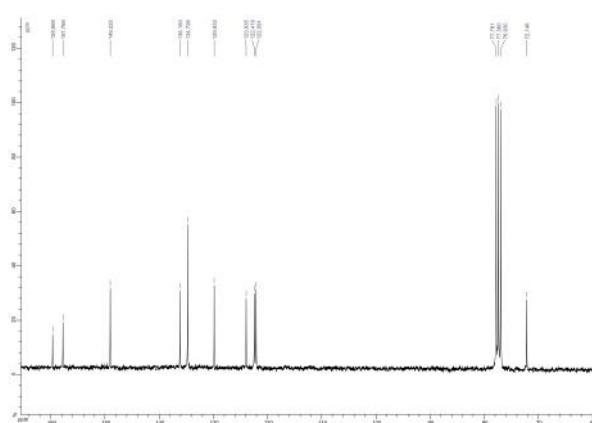
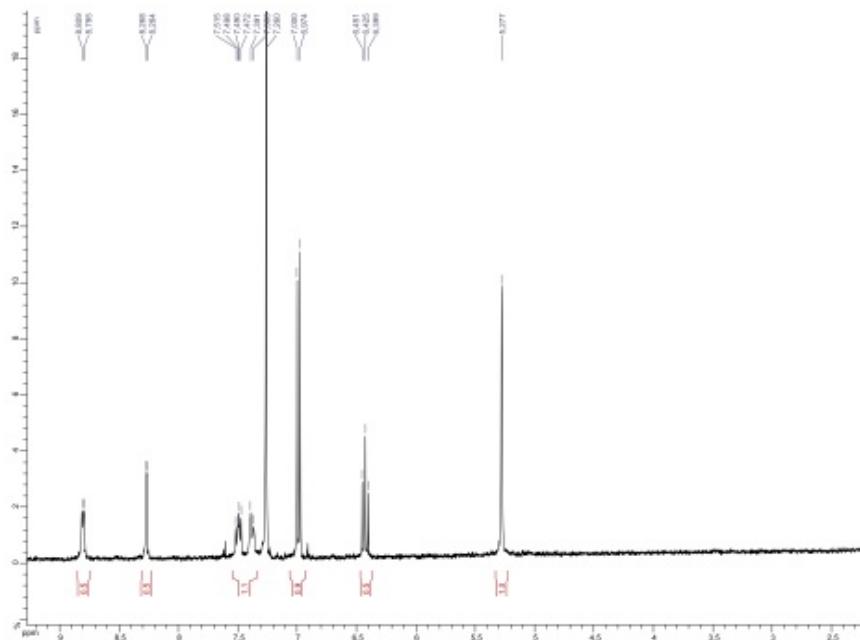


Figure S2: <sup>13</sup>C-NMR spectrum of 2

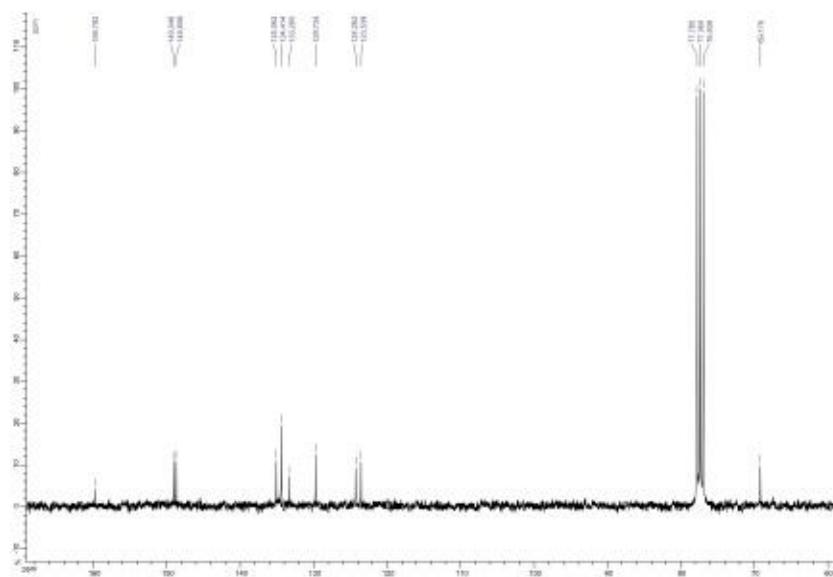
### 25,26,27,28-tetra[(3-pyridylmethyl)oxy]-2,8,14,20-tetrathiacyclo[4]arene (3)

**<sup>1</sup>H-NMR (300 MHz, CDCl<sub>3</sub>):** δ(ppm) = 55.28 (8H, s, ArOCH<sub>2</sub>), 6.42 (4H, t, Ar-H), 6.98 (8H, d, Ar-H), 7.38 (4H, d, Py-H), 7.48 (4H, m, Py-H), 8.27 (4H, s, Py-H), 8.79 (4H, d, Py-H).



**Figure S3 :**  $^1\text{H}$ -NMR spectrum of 3

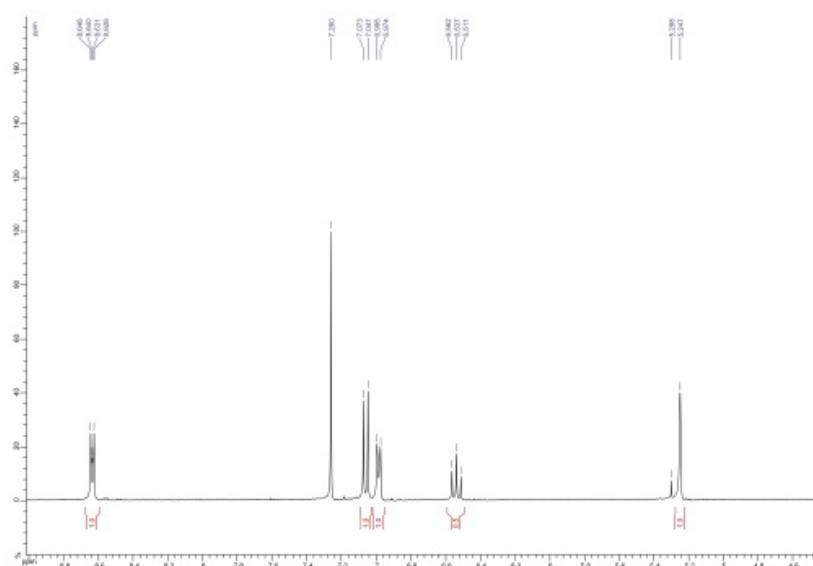
**<sup>13</sup>C-NMR (75 MHz, CDCl<sub>3</sub>):** δ(ppm) = 69.2, 123.5, 124.3, 129.7, 133.3, 134.4, 135.1, 148.7, 149.0, 159.8.



**Figure S4 :**  $^{13}\text{C}$ -NMR spectrum of 3

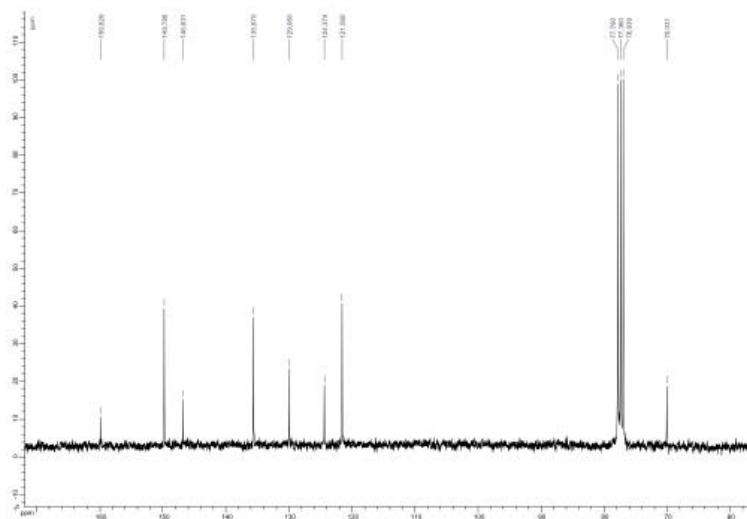
**25,26,27,28-tetra[(4-pyridylmethyl)oxy]-2,8,14,20-tetrathiacyclo[4]arene (4)**

**$^1\text{H-NMR}$  (300 MHz,  $\text{CDCl}_3$ ):**  $\delta$ (ppm) = 5.24 (8H, s, ArOCH<sub>2</sub>), 6.53 (4H, t, Ar-H), 6.98 (8H, d, Py-H), 7.06 (8H, d, Ar-H), 8.63 (8H, d, Py-H).



**Figure S5:**  $^1\text{H-NMR}$  spectrum of 4

**$^{13}\text{C-NMR}$  (75 MHz,  $\text{CDCl}_3$ ):**  $\delta$ (ppm) = 70.0, 121.6, 124.4, 129.9, 135.7, 146.8, 149.8, 159.8.



**Figure S6:**  $^{13}\text{C-NMR}$  spectrum of 4