

## Electronic Supplementary Information

### Highly selective and sensitive determination of mercury ions by total-reflection X-ray fluorescence spectrometry

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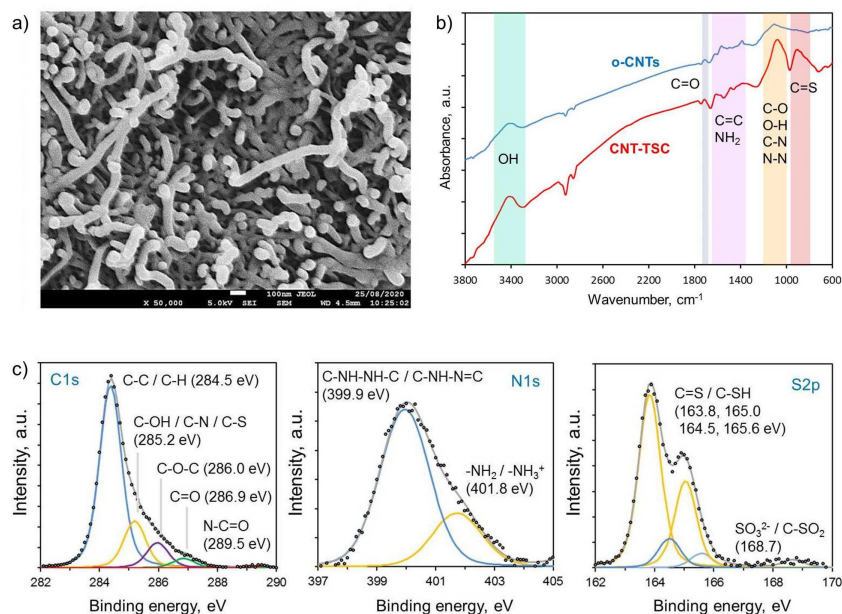
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The synthesized CNT-TSC was characterized by scanning electron microscopy (SEM), Fourier-transform infrared spectroscopy (FT-IR), and X-ray photoelectron spectroscopy (XPS). The SEM image in Fig. S1a indicates that the oxidation of CNTs and further modification with TSC molecules did not cause damage to CNTs structure. The FT-IR spectra of o-CNTs and CNT-TSC presented in Fig. S1b reveals the broad bands at 3300-3500  $\text{cm}^{-1}$  and 2850-2950  $\text{cm}^{-1}$  corresponding to stretching vibration of O-H and the vibration of  $-\text{CH}_2-$  bonds in the lattice<sup>1</sup>. The FT-IR spectra also show the stretching vibration at 1720  $\text{cm}^{-1}$  corresponding to C=O of carboxyl and amide groups and several bands at 1350-1650 attributed to C=C and N-H<sup>1,2</sup>. The broad band at 980-1200  $\text{cm}^{-1}$  corresponds to C-O, O-H of o-CNTs and C-N, N-N of TSC molecule<sup>1,3,4</sup>. The FT-IR spectrum of CNT-TSC also reveals a band at 800-950  $\text{cm}^{-1}$  corresponding to C=S, confirming successful grafting of the TSC molecules to the CNTs<sup>4,5</sup>. The high-resolution C1s, N1s, S2p spectra of CNT-TSC are presented in Fig. S1c. The C1s spectrum shows the five peaks at 284.5, 285.2, 286.0, 286.9, and 289.5 eV assigned to C-C, C-OH, C-O-C, C=O, and N-C=O<sup>1,2,6,7</sup>. The N1s spectrum of CNT-TSC shows two peaks at 399.9 and 401.8 eV assigned to C-NH-NH-C/C-NH-N=C and  $-\text{NH}_2/-\text{NH}_3^+$ , respectively<sup>8,9</sup>. The S2p spectrum of CNT-TSC shows two doublets at 163.8/165.0 and 164.5/165.6 eV corresponding to the contributions of the 2p<sub>3/2</sub> and 2p<sub>1/2</sub> levels of sulfur in the thione/thiol form (C=S/C-SH)<sup>9</sup>, the small peak at 168.7 eV assigned to some impurities ( $\text{SO}_4^{2-}/\text{C-SO}_3$ ,  $\text{SO}_3^{2-}/\text{C-SO}_2$ )<sup>10</sup>.



**Fig. S1** The SEM image of CNT-TSC (a), the FT-IR spectra of o-CNTs and CNT-TSC (b), the XPS high-resolution C1s, N1s and S2p spectra of CNT-TSC (c).

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