

Supplementary Information

New Hg(II) coordination polymers based on a thioimidazole ligand with good performance to detoxify Hg(II) and reversibly capture iodine

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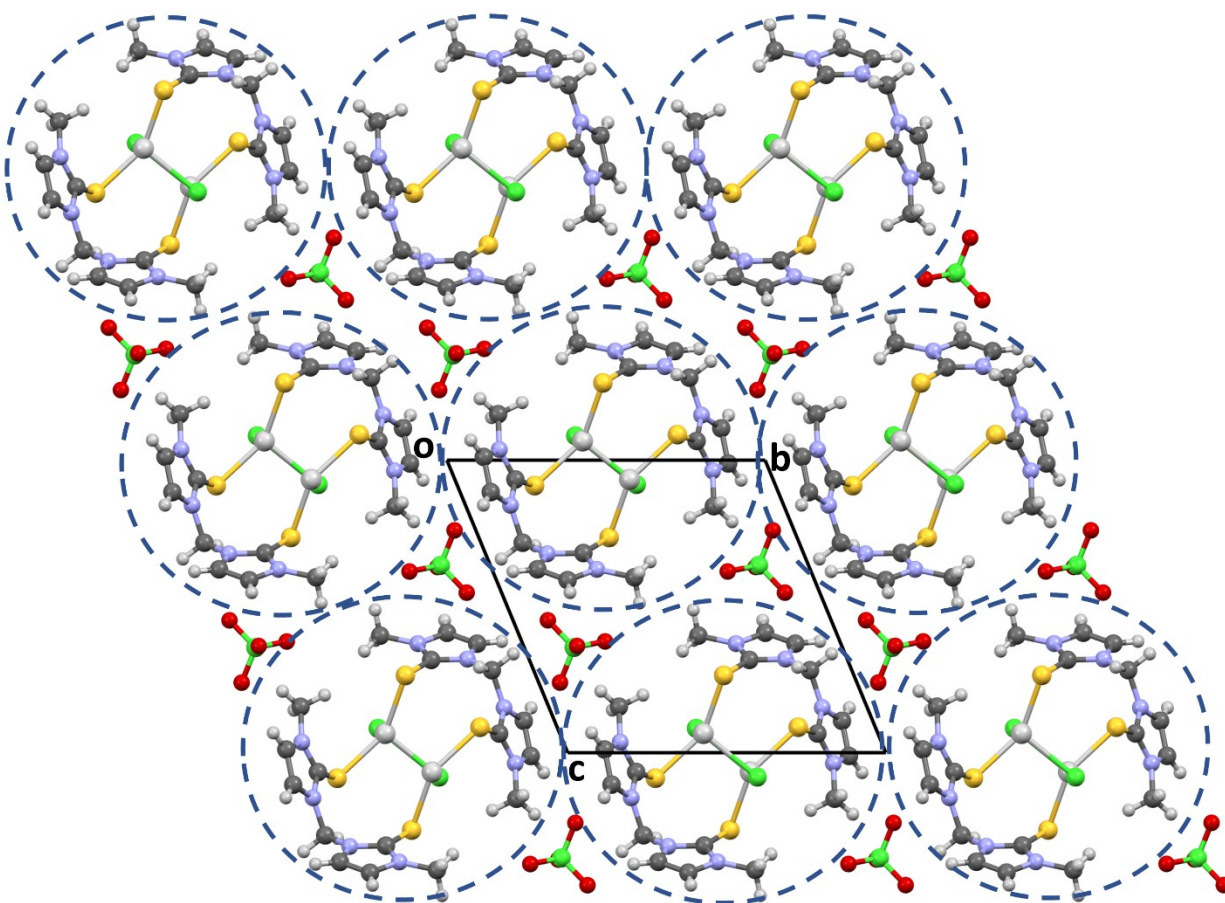


Figure S1: Packing of **2** viewed down *a*. Columnar chains are enclosed in dashed circles.

Search in CSD

We have searched in the Cambridge Structural Database, CSD version 5.43 updates (Jun 2022), for crystal structures of chlorocomplexes of Hg(II) with cyclic thioamides. The details of the search are shown in Figure S2.

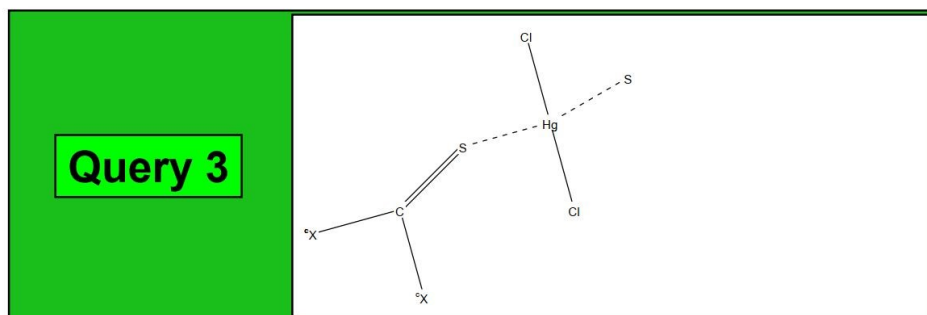


Figure S2: The structures searched in the CSD. X is any atom belonging to a cycle.

The only filter applied was “3D coordinates determined”. A total of 20 hits were found, whose refcodes are: BAPWAQ, BOPGOF, DEHWUL, DEJCUT, FUGXUD, FUYWON, FUZKET, KOXRAS, LOWGIP, MARRAY, NAKGOX, NAQQOL, NUYVIP, OKOWUG, RADZUV, RIMLEH, VEZYAC, VIGBUL, WODCUN, ZAWXUS. In the search we have also determined the distances Hg-S in all the structures. The histogram of the distances is reported below.

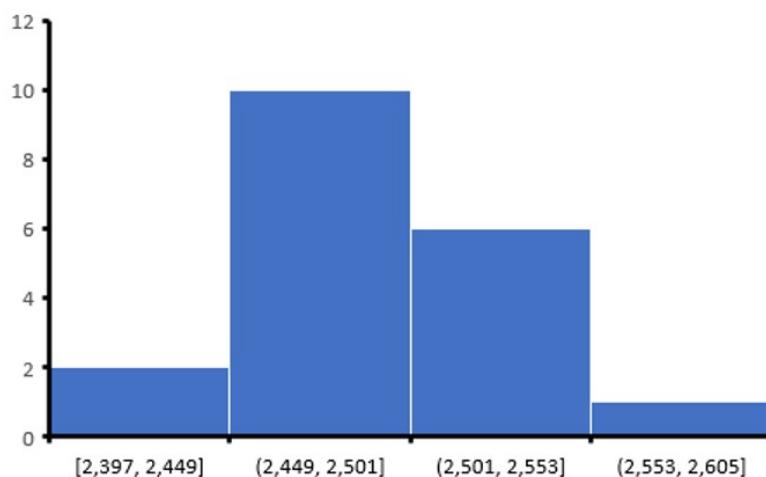


Figure S3: Histogram of the distances Hg-S in the 20 structures of the query of Figure S2.

We have also searched for thiocyanate complexes of Hg(II). In this case, only two hits were found, with CSD refcodes VITLES and WODDIC.

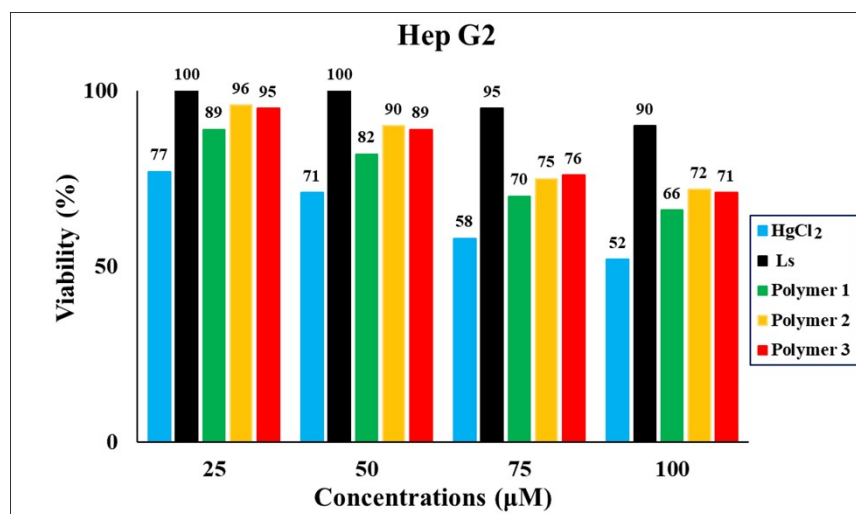


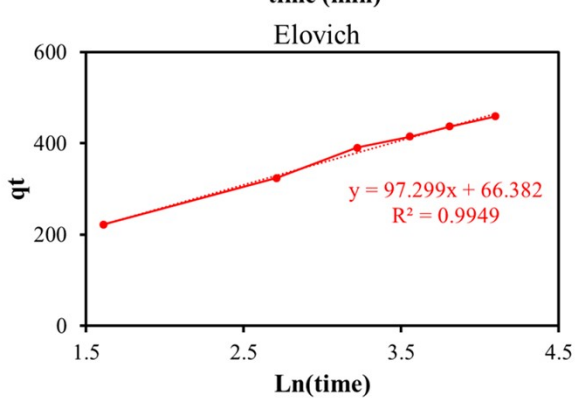
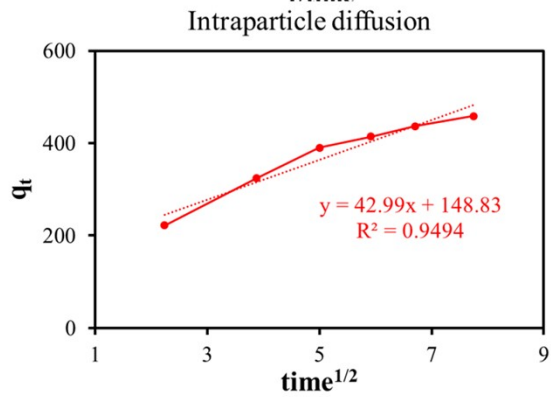
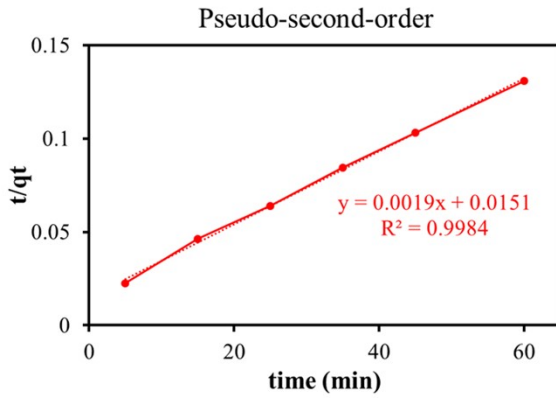
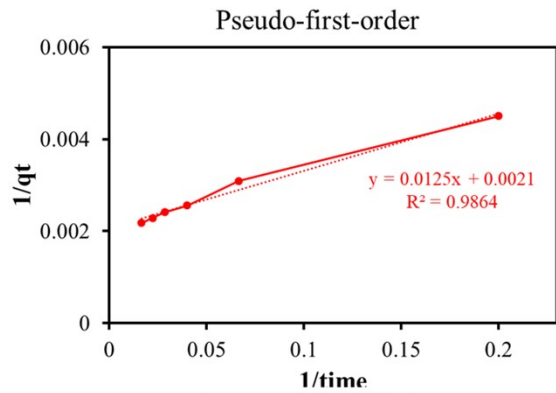
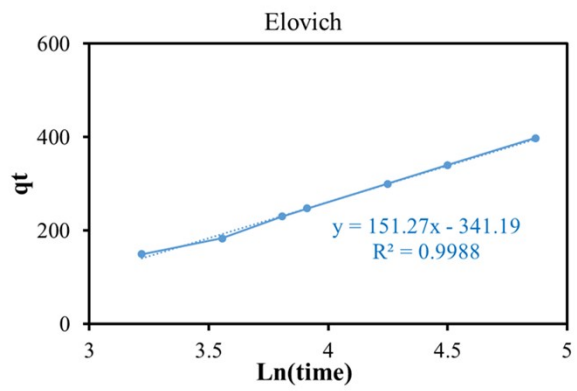
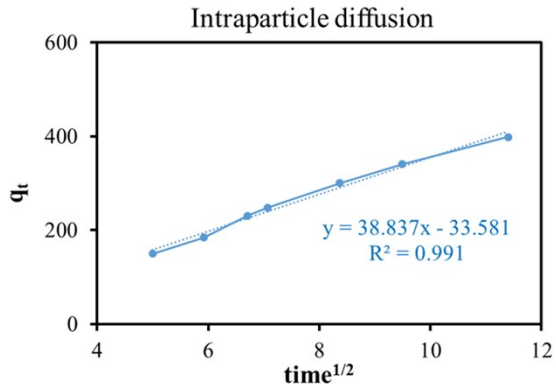
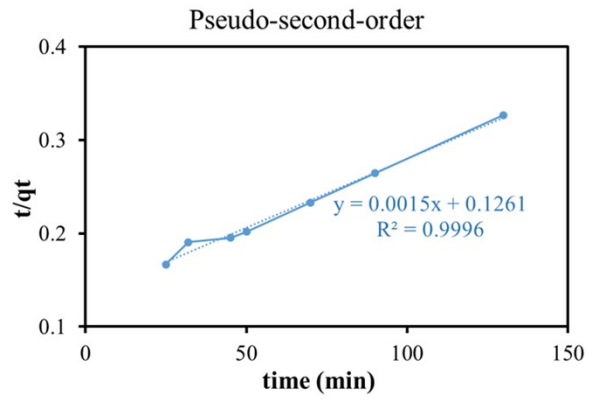
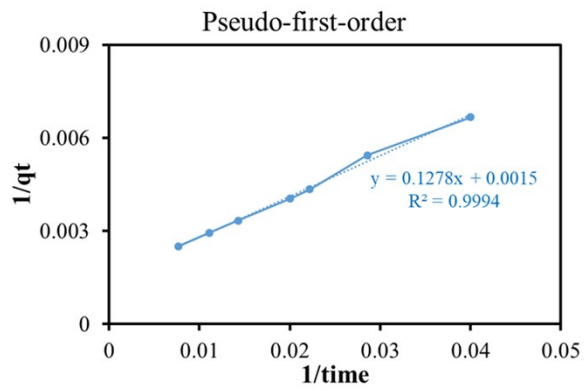
Figure S4: Evaluation of cell viability on treated HepG2 cells with HgCl₂, free ligand and polymers 1-3 with concentrations of 25, 50, 75, and 100 μM by MTT assay.

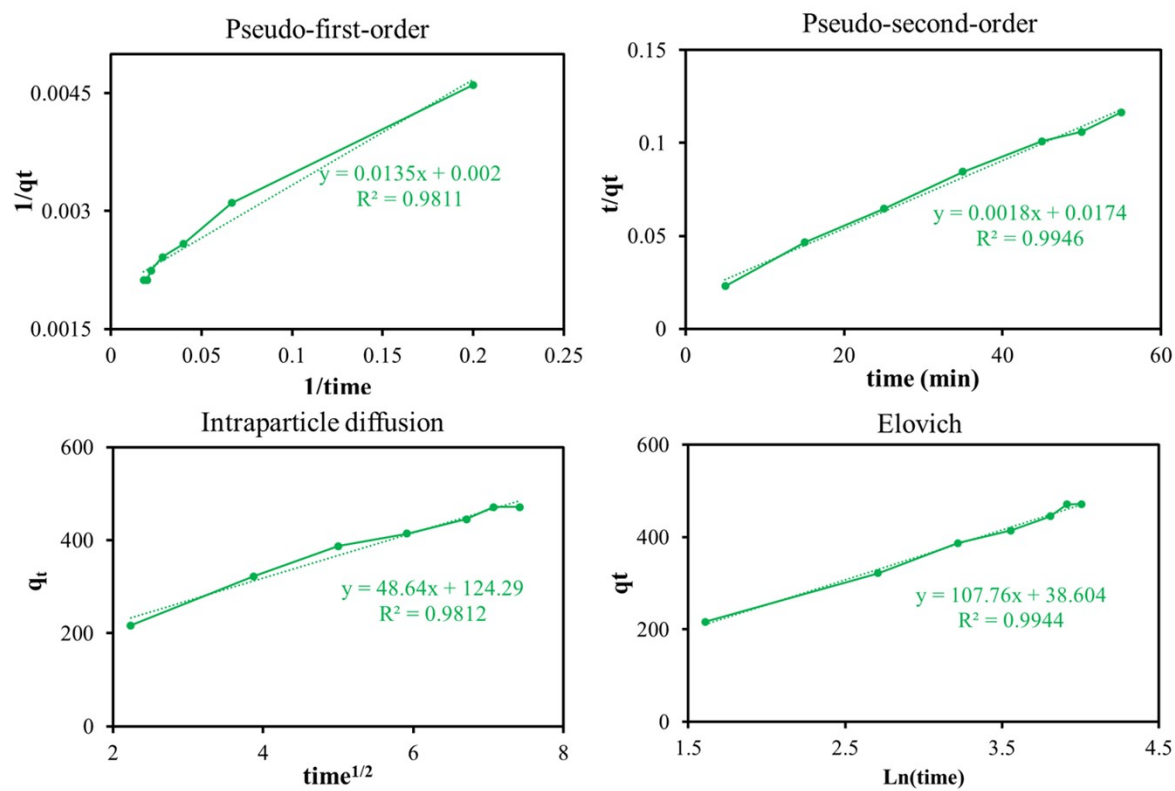
Table S1: Evaluation of cell viability on treated HepG2 cells with HgCl₂, free ligand, co-anions salts, and polymers **1-3** with concentrations of 25, 50, 75, and 100 μM by MTT assay, and IC50 values.

Concentration	HgCl ₂	Ls	NaBF ₄	NaClO ₄	KSCN	Polymer 1	Polymer 2	Polymer 3
100 μM	52	90	80	92	97	66	72	71
75 μM	58	95	88	96	99	70	75	76
50 μM	71	100	94	100	100	82	90	89
25 μM	77	100	100	100	100	89	96	95
IC 50	102.5	357	214.92	436.6	1083.5	142.4	152.29	155.87



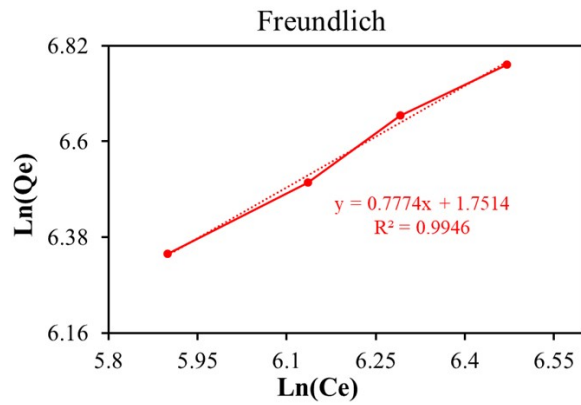
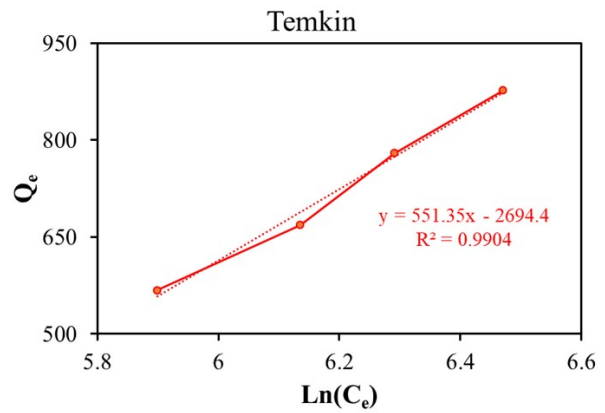
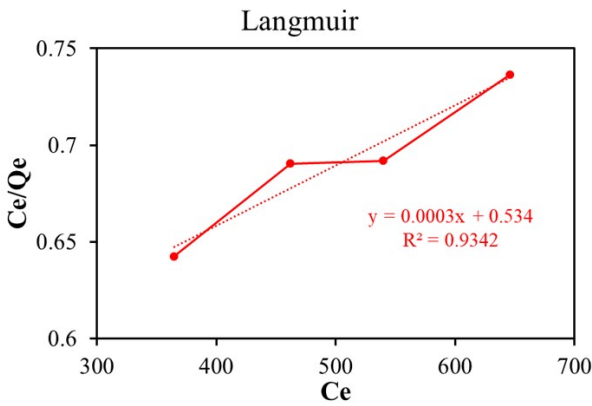
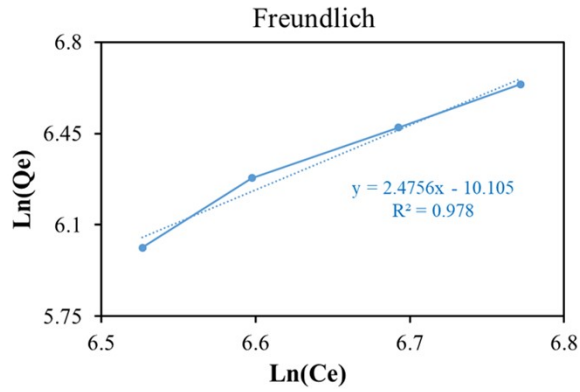
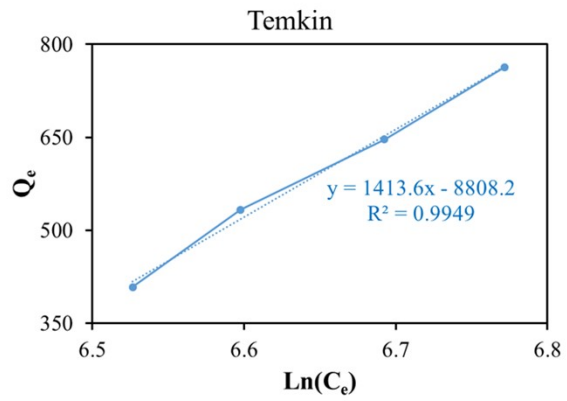
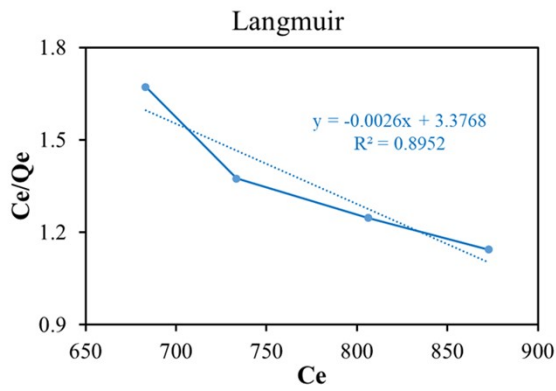
Figure S5: The precipitate of Hg-SCPs before and after iodine adsorption.





Fig

ure S6: The pseudo-first-order, pseudo-second-order, intraparticle diffusion, and Elovich models for the uptake of I₂ by polymers **1-3** at 0.005 M concentration of solution (**Polymer 1: blue, Polymer 2: red, Polymer 3: green**).



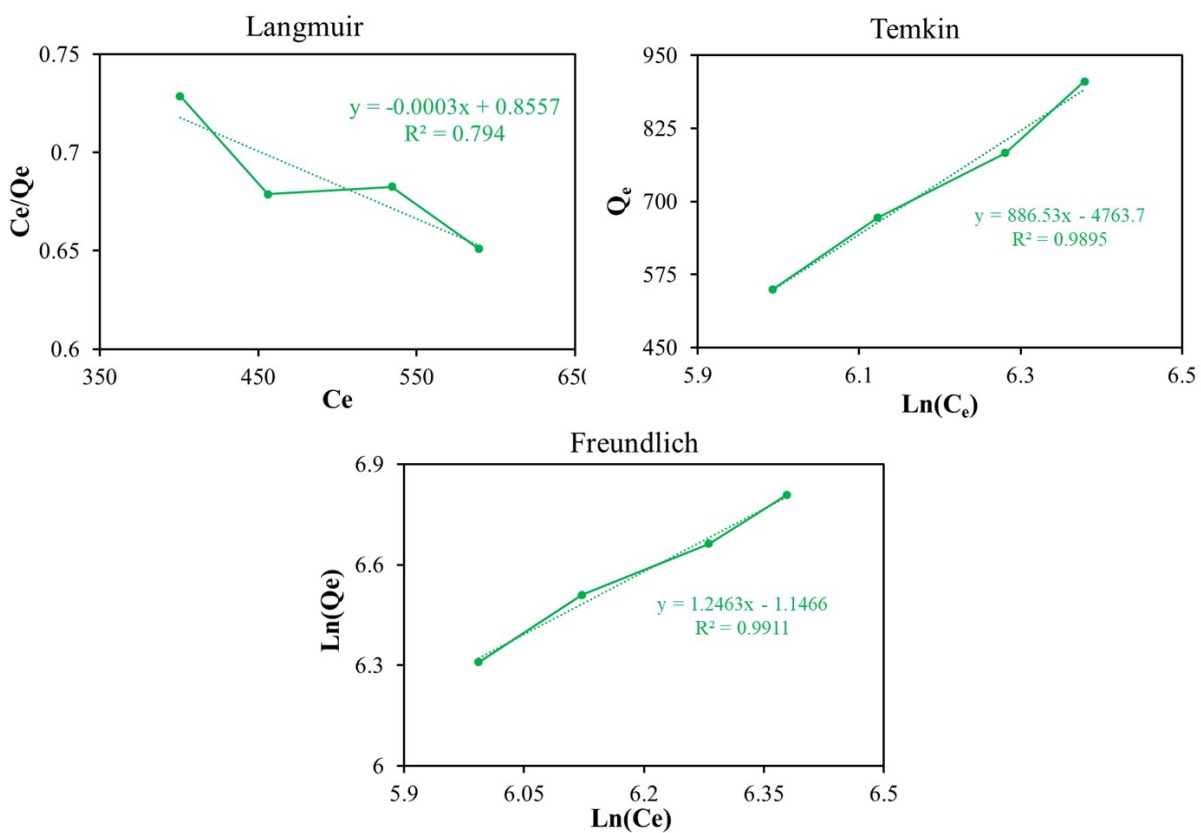


Figure S7: The Langmuir, Temkin, and Freundlich isotherm models for polymers 1-3 (**Polymer 1: blue, Polymer 2: red, Polymer 3: green**).

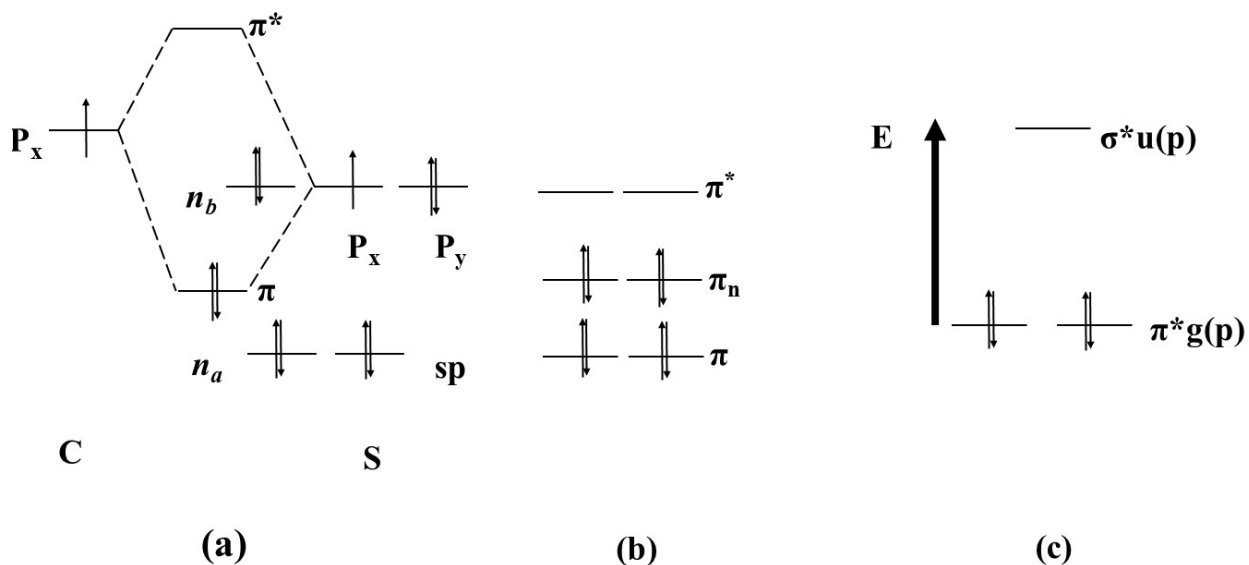


Figure S8: Simplified molecular orbital diagram of (a) $\text{C}=\text{S}$ bond as a Lewis base, (b) NCS^- as a Lewis base, and (c) I_2 as a Lewis acid.

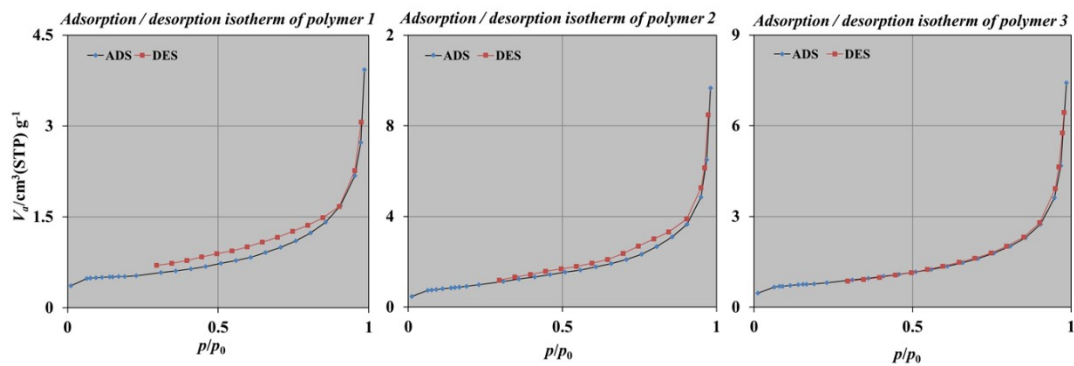


Figure S9: Nitrogen adsorption/ desorption isotherms at 77K of Hg-SCPs.

Table S2. The N_2 adsorption-desorption isotherm data of the synthesized Hg-SCPs polymers.

Data	Polymer 1	Polymer 2	Polymer 3	
V_m	0.4577	0.6491	0.723	[$\text{cm}^3(\text{STP}) \text{g}^{-1}$]
a_s, BET	1.9922	2.8251	3.1468	[$\text{m}^2 \text{g}^{-1}$]
C	447.3	365.34	248.36	
Total pore volume ($p/p_0=0.985$)	0.0060812	0.011473	0.014968	[$\text{cm}^3 \text{g}^{-1}$]
Average pore diameter	12.21	16.244	19.027	[nm]