

Supplementary Material

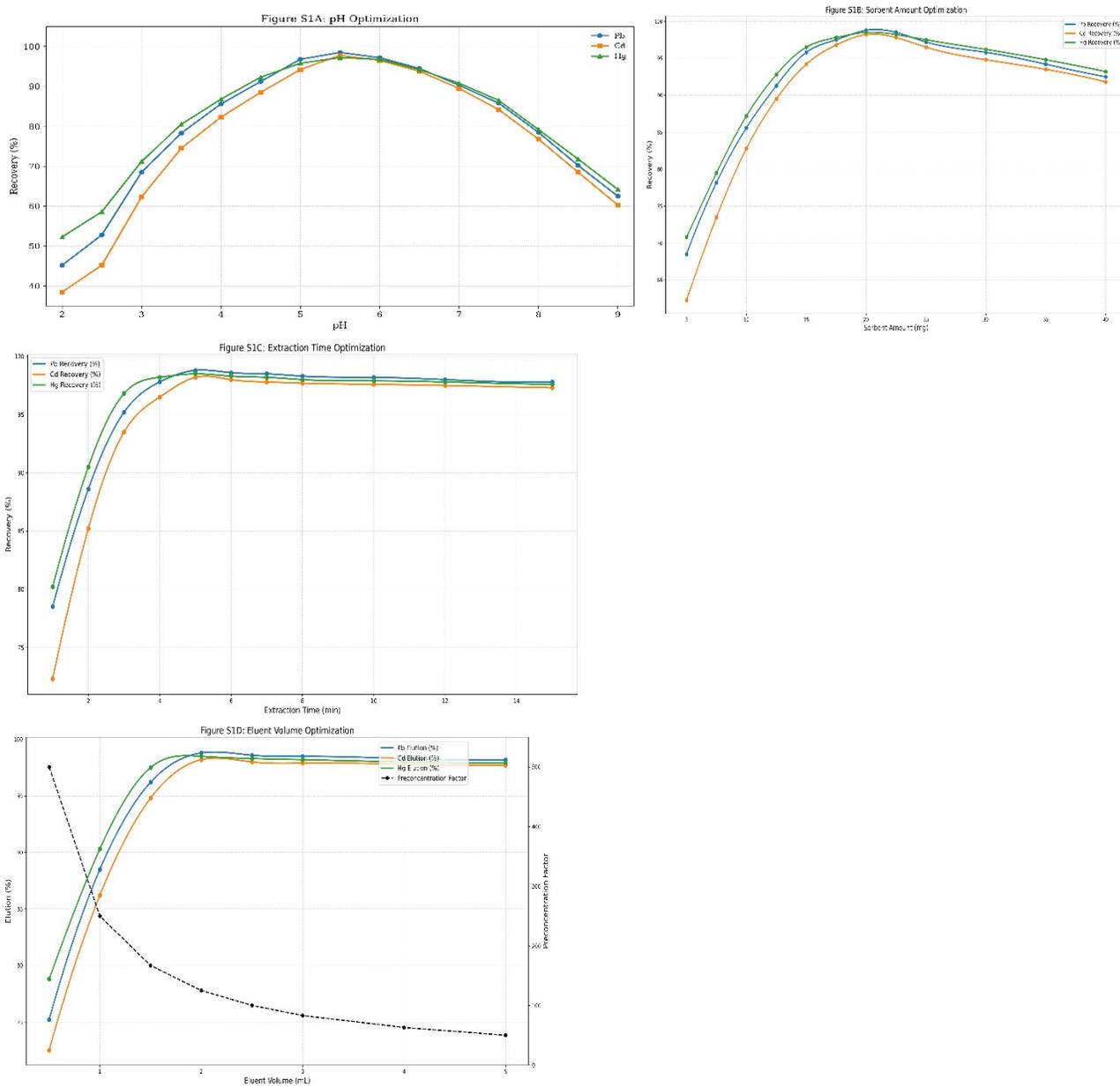


Figure S1. Optimization curves for (A) pH effect, (B) sorbent amount, (C) extraction time, and (D) eluent volume.

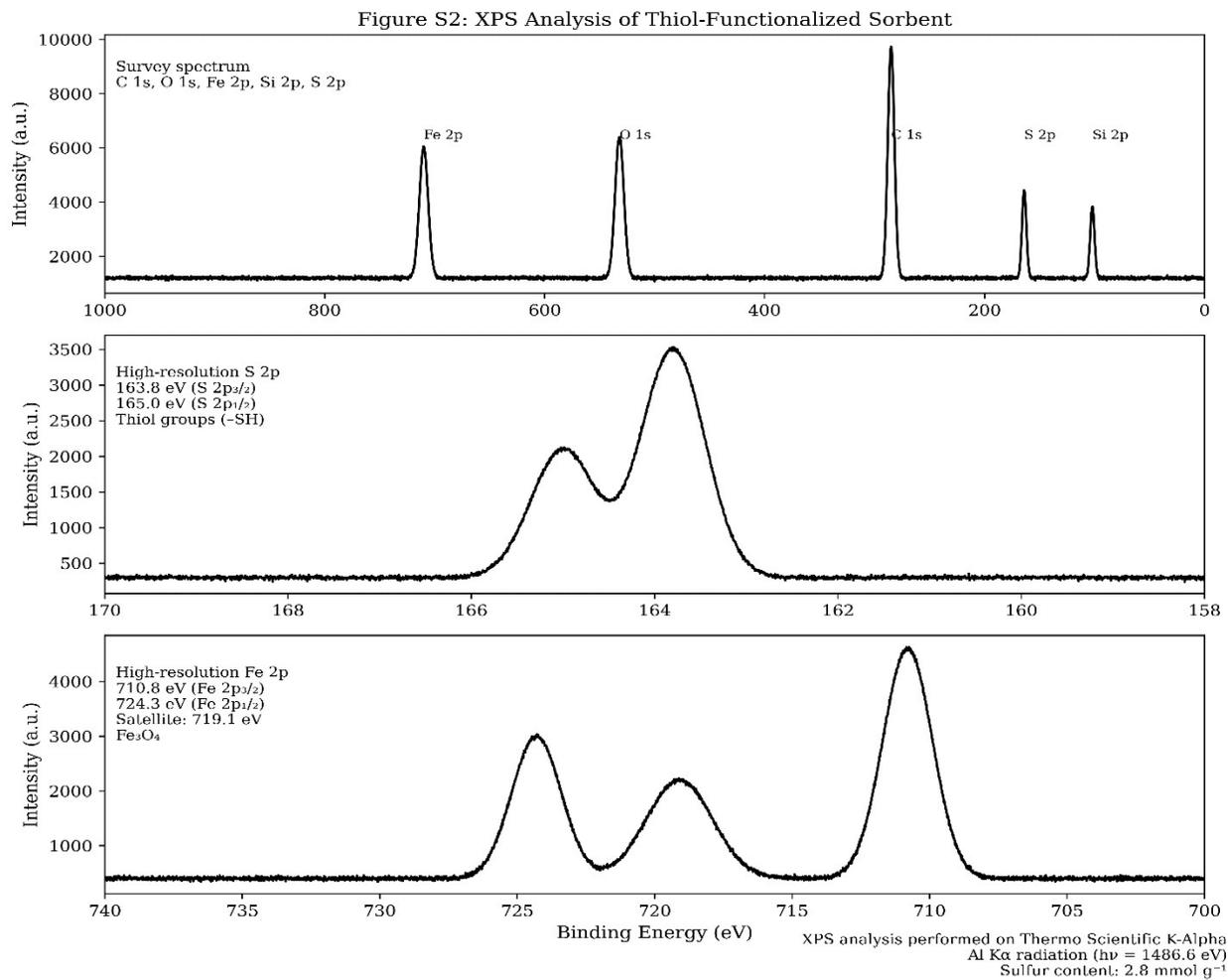


Figure S2. XPS survey spectrum and high-resolution spectra of S 2p, Fe 2p regions for MB-SH before and after metal adsorption.

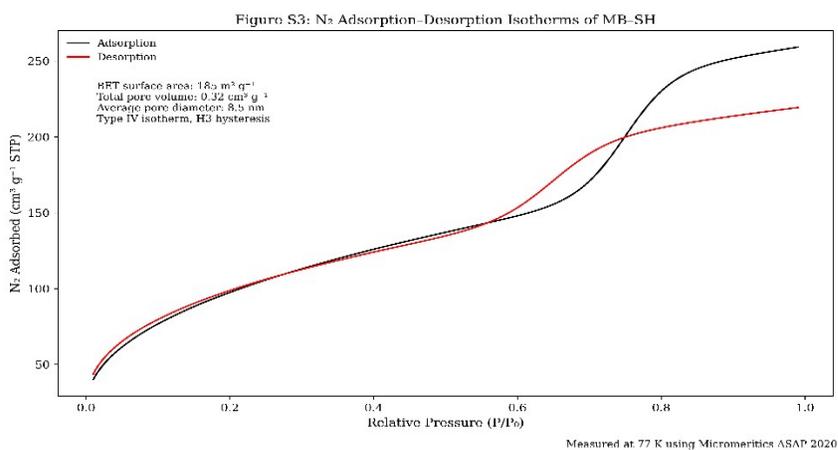


Figure S3. N₂ adsorption-desorption isotherms

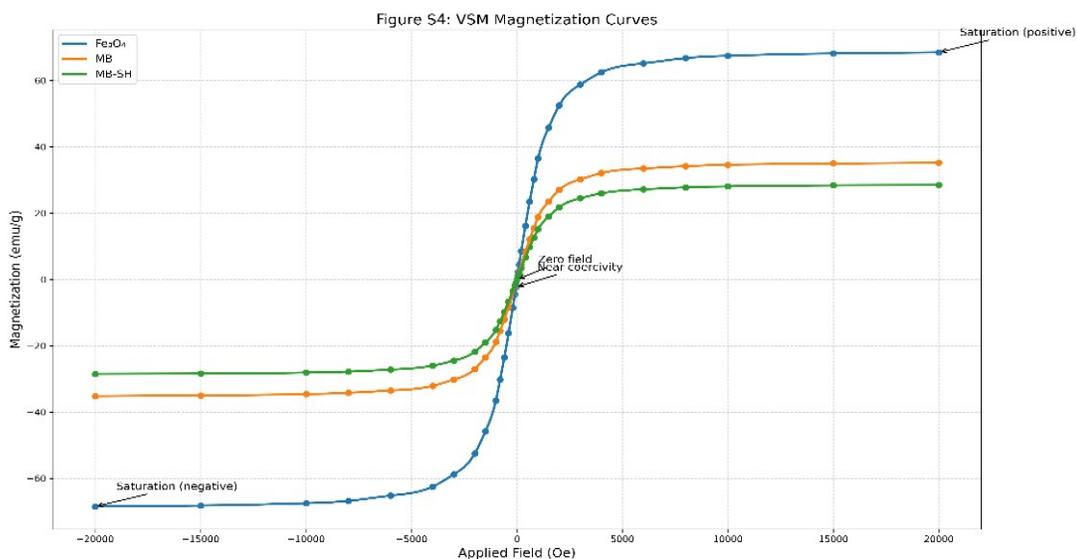


Figure S4. VSM magnetization curves of Fe₃O₄, MB, and MB-SH at room temperature.

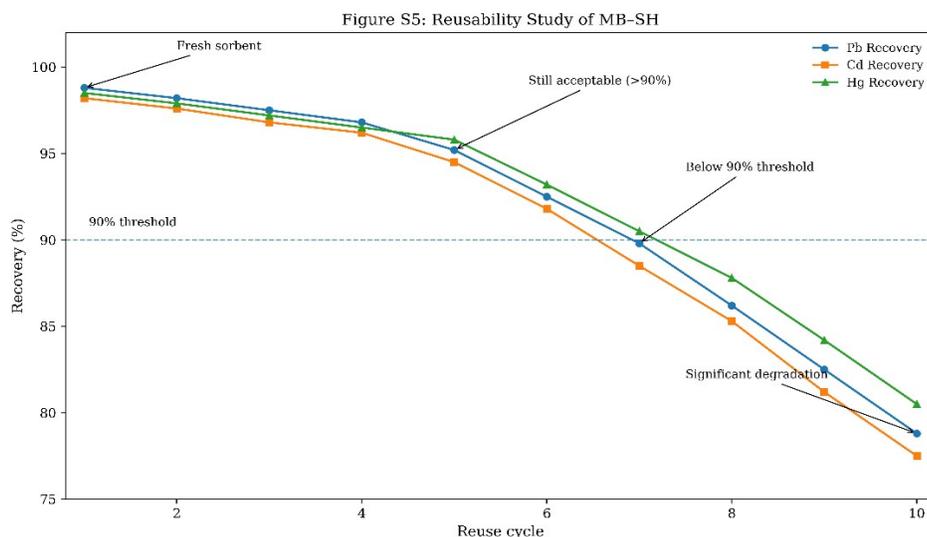


Figure S5. Reusability study showing recovery percentages over 10 consecutive adsorption-desorption cycles.

Table S1. Instrumental operating conditions for ICP-MS analysis.

Parameter	Value	Unit	Notes
RF Power	1550	W	Optimized daily
Plasma Gas Flow (Ar)	15.0	L/min	Outer gas
Auxiliary Gas Flow (Ar)	0.90	L/min	Intermediate gas
Nebulizer Gas Flow (Ar)	1.05	L/min	Carrier gas
Sampling Depth	8.0	mm	From the load coil
Spray Chamber	2	°C	Peltier cooled

Temperature			
Nebulizer Type	MicroMist		Glass concentric
Spray Chamber	Scott type		Double pass
Sample Uptake Rate	0.4	mL/min	Self-aspiration
Stabilization Time	30	s	Before measurement
Integration Time	0.1	s	Per mass
Replicates	3		Per sample
Acquisition Mode	Peak hopping		
Dwell Time	0.1	s	Per isotope
Sweeps per Replicate	100		
CRC Mode	He collision		For interference removal
He Gas Flow	4.5	mL/min	In the collision cell
Octopole Bias	-18	V	
Quadrupole Bias	-15	V	
Monitored Isotopes	208Pb, 111Cd, 202Hg		Main isotopes
Internal Standards	115In, 103Rh, 209Bi		At 10 µg/L
Internal Standard Mode	Online addition		Via T-piece
Rinse Time	60	s	Between samples
Rinse Solution	2% HNO ₃		Trace metal grade
Oxides (CeO/Ce)	<2	%	Daily check
Doubly Charged (Ce ⁺⁺ /Ce ⁺)	<3	%	Daily check

Table S2. Interference study results showing the effect of coexisting ions on the recovery of target analytes.

Interfering Ion	Concentration (mg/L)	Concentration Ratio (Ion: Metal)	Pb Recovery (%)	Cd Recovery (%)	Hg Recovery (%)	Notes
Na ⁺	100	10000	97.8	97.2	97.5	No interference
Na ⁺	200	20000	97.5	96.8	97.2	
K ⁺	100	10000	97.6	97.0	97.3	No interference
K ⁺	200	20000	97.3	96.7	97.0	
Ca ²⁺	250	25000	96.8	96.2	96.5	No interference
Ca ²⁺	500	50000	96.2	95.5	96.0	
Mg ²⁺	100	10000	97.2	96.8	97.0	No interference
Mg ²⁺	300	30000	96.5	96.0	96.3	
Al ³⁺	10	1000	96.8	96.2	96.5	Slight interference
Al ³⁺	50	5000	93.5	92.8	93.2	
Fe ³⁺	10	1000	96.2	95.5	96.0	Slight interference
Fe ³⁺	50	5000	92.8	91.5	92.5	

Cu ²⁺	5	500	96.5	95.8	96.2	Competing soft metal
Cu ²⁺	50	5000	88.5	87.2	89.2	Significant competition
Zn ²⁺	5	500	96.8	96.0	96.5	Competing soft metal
Zn ²⁺	50	5000	89.2	88.5	90.0	Significant competition
Cl ⁻	500	50000	97.5	97.0	97.2	No interference
Cl ⁻	1000	100000	97.2	96.5	96.8	
SO ₄ ²⁻	500	50000	97.3	96.8	97.0	No interference
SO ₄ ²⁻	1000	100000	96.8	96.2	96.5	
NO ₃ ⁻	500	50000	97.6	97.0	97.3	No interference
NO ₃ ⁻	1000	100000	97.2	96.6	96.9	
CO ₃ ²⁻	100	10000	96.5	95.8	96.2	Slight pH effect
CO ₃ ²⁻	500	50000	94.2	93.5	94.8	

Table S3. Comparison of the adsorption capacities of MB-SH with other thiol-functionalized sorbents reported in the literature.

Sorbent Material	Surface Area (m ² /g)	Pb Capacity (mg/g)	Cd Capacity (mg/g)	Hg Capacity (mg/g)	Synthesis Time (h)	Cost	Reference
Fe ₃ O ₄ -SiO ₂ -SH	245	85.2	62.5	105.8	48	High	[15]
MOF-SH	820	125.6	95.3	158.2	72	Very High	[22]
GO-Fe ₃ O ₄ -thiol	320	95.8	72.6	128.5	36	High	[28]
Mesoporous silica-MPTMS	580	105.3	82.5	145.6	60	Medium	[31]
Thiol-chitosan beads	125	68.5	52.3	88.6	24	Low	[37]
MB-SH (this work)	185	92.5	75.8	135.2	28	Low	This work