Electronic Supplementary Material (ESI) for Environmental Science: Nano.

Electronic Supplementary Information

Thiolated Silica Nanoadsorbents Enable Ultrahigh and Fast Decontamination of Mercury (II): Understanding the Contribution of Thiol Moieties Density and Accessibility on Adsorption Performance

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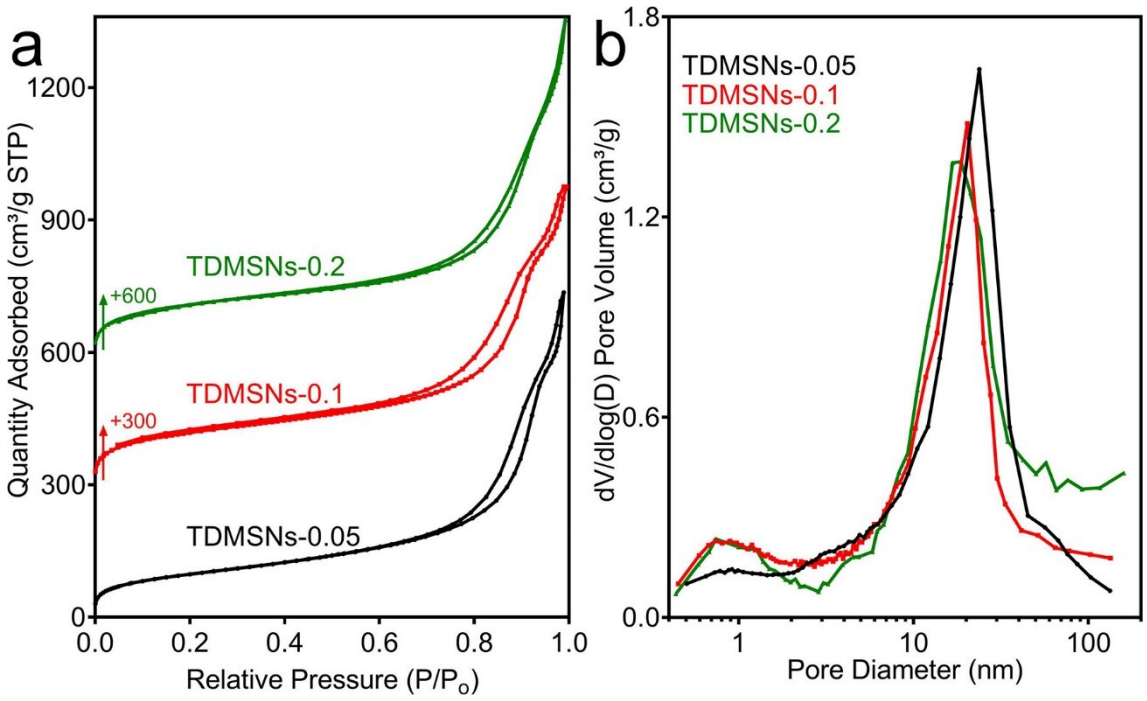

Fig. S1 (a) N_2 sorption isotherms and (b) pore size distribution curves of TDMSNs-*r*.

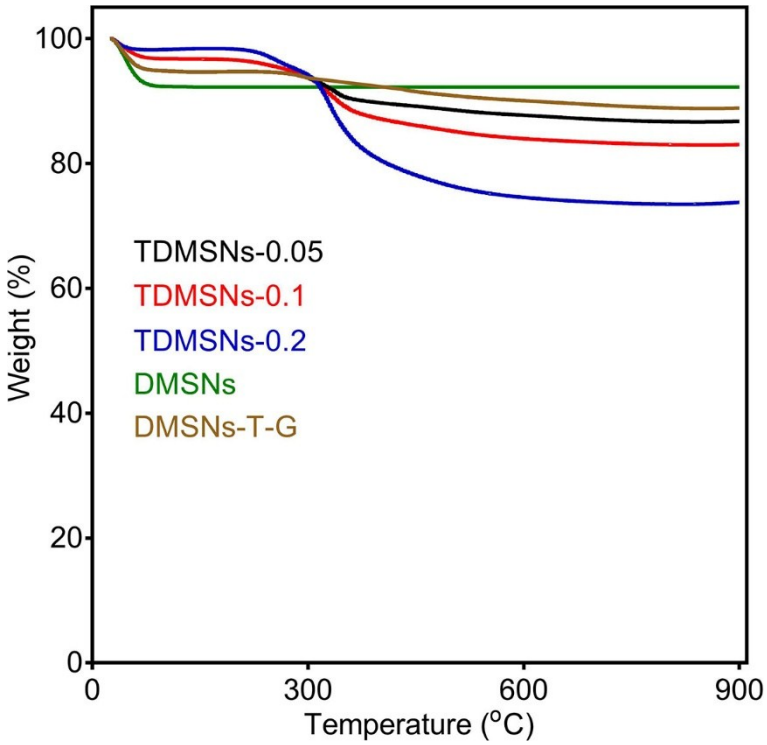

Fig. S2 TGA profiles of adsorbents.

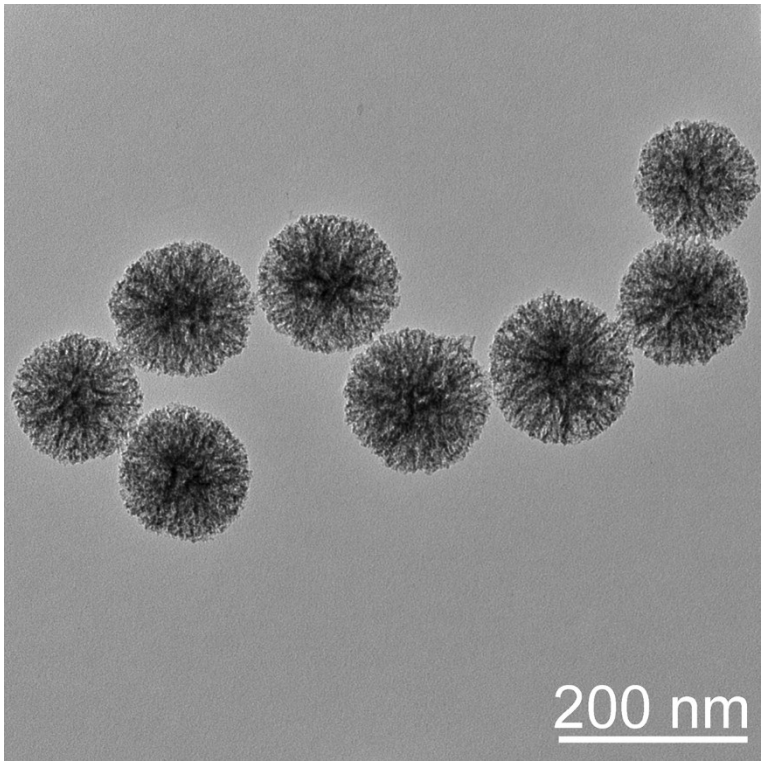

Fig. S3 TEM image of TDMSNs-0.2 after 5 cycle's mercury (II) adsorption.

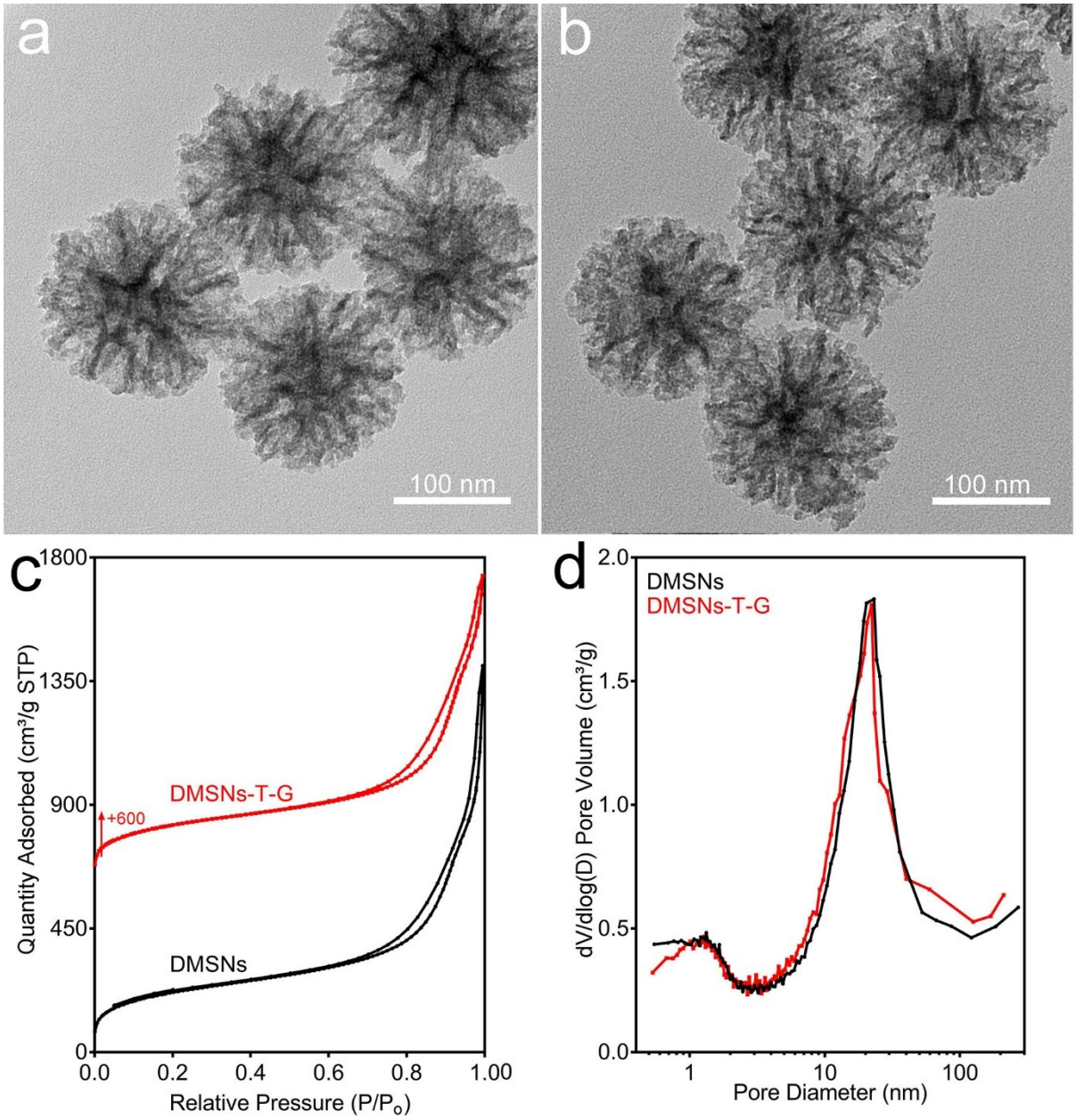

Fig. S4 TEM images of (a) DMSNs and (b) DMSNs-T-G. (c) N_2 sorption isotherms and (d) pore size distribution curves of DMSNs and DMSNs-T-G.

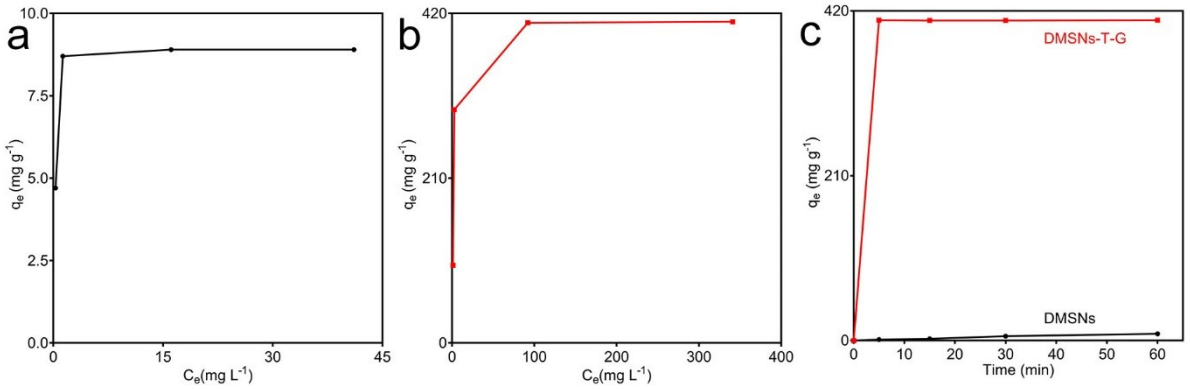

Fig. S5 Adsorption isotherms for mercury (II) adsorption on (a) DMSNs and (b) DMSNs-T-G. (c) The kinetic adsorption profiles for mercury (II) adsorption on DMSNs and DMSNs-T-G.

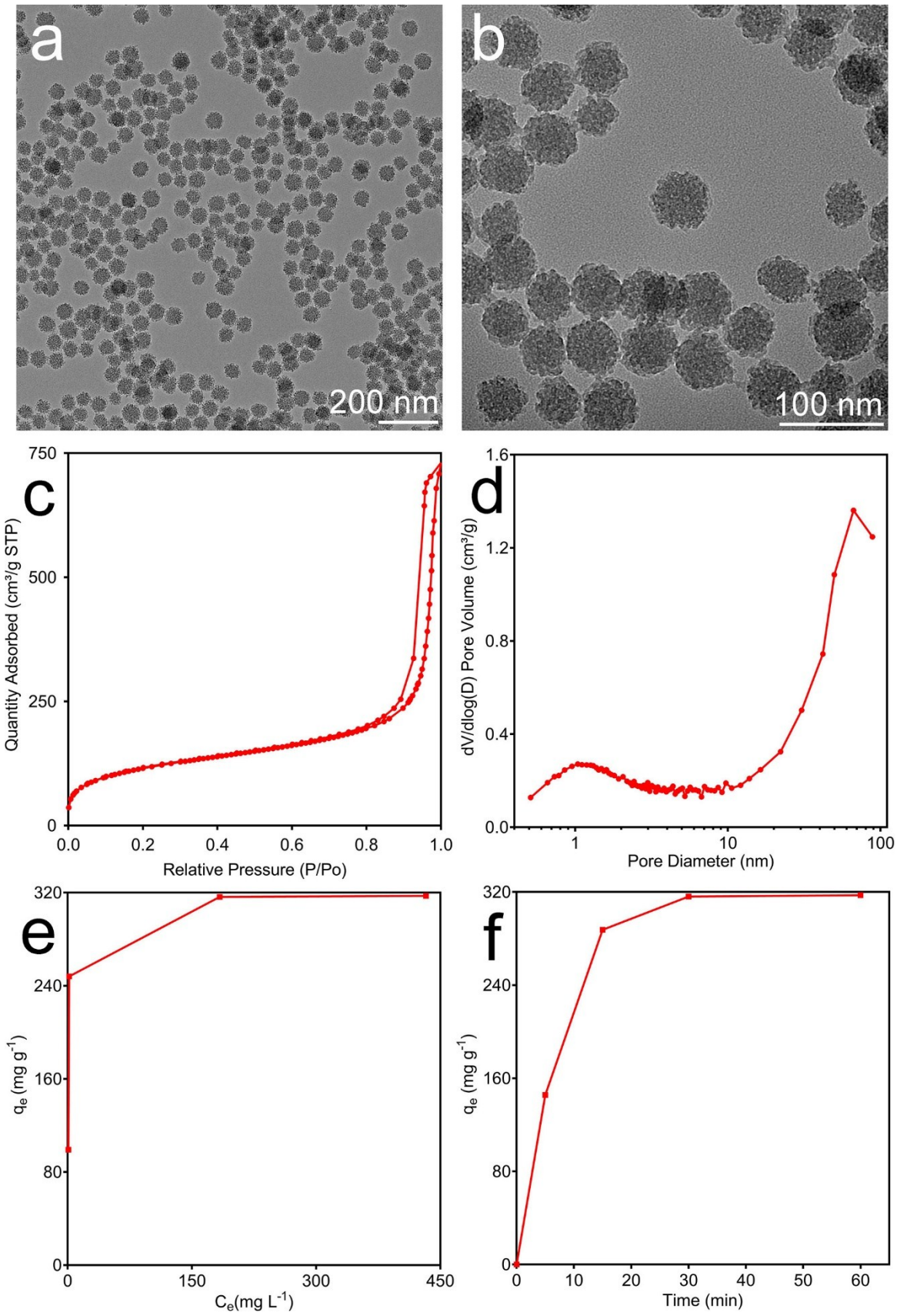

Fig. S6 TEM images (a and b), (c) N_2 sorption isotherms, and (d) pore size distribution curves, (e) adsorption isotherm for mercury (II) adsorption, and (f) the kinetic adsorption profile for mercury (II) adsorption for TMSNs-0.2.

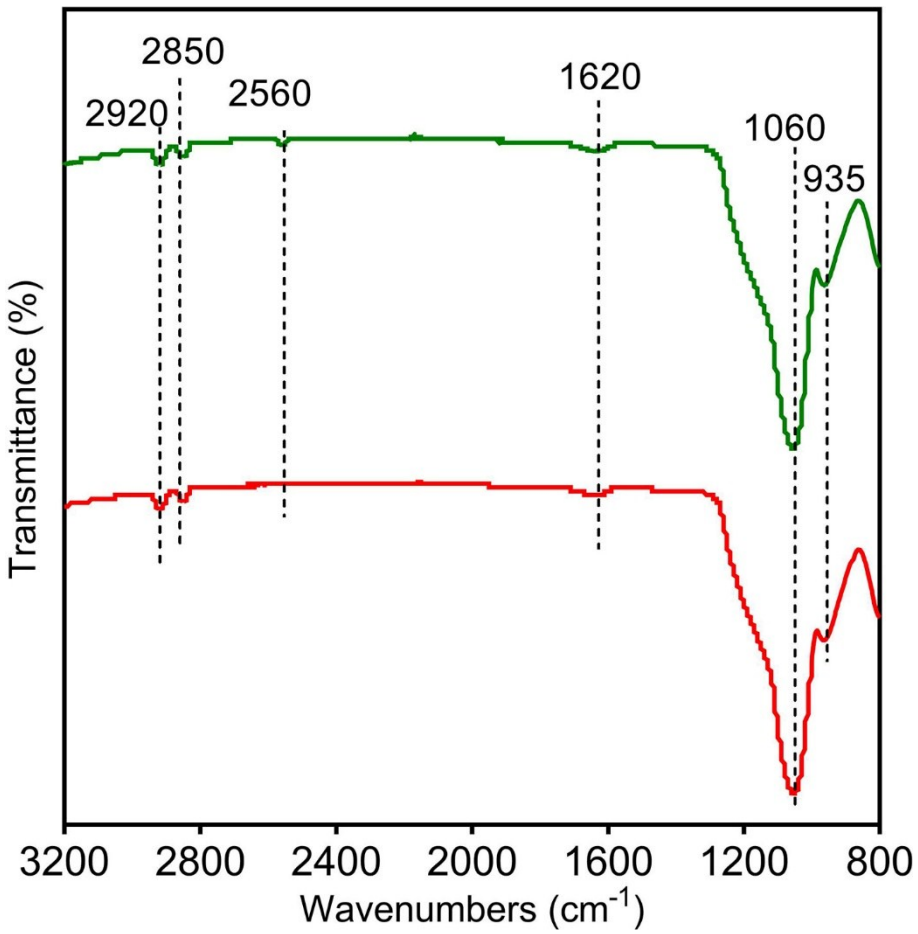

Fig. S7 FT-IR spectra of TDMSNs-0.2 before (red) and after (green) Hg (II) adsorption.

Table S1. Langmuir model parameters for TDMSNs-*r*.

Adsorbent	K_L (L mg^{-1})	q_{max} (mg g^{-1})	R^2
TDMSNs-0.05	0.405	707.4	0.99
TDMSNs-0.1	0.321	1033.1	0.99
TDMSNs-0.2	0.138	1502.4	0.99

Table S2. Detailed comparison of mercury adsorption performance for various adsorbents.

Adsorbent	Q [a]	M [b]	t [c]	R [d]	Ref
Thiol-functionalized MOF	1000	0.91	20	0.90 after 3 cycles	Nat. Commun., 2014, 5, 5537.
Thiolated porous organic polymer	1216	1.19	10	NA	Adv. Mater., 2017, 29, 1700665.
MCM-41	42	0.08	30	NA	Micropor. Mesopor. Mater., 2018, 258, 217.
SBA-15	429	3.71	5	NA	New J. Chem., 2014, 38, 248.
Mesoporous silica	600	NA	60	NA	Adv. Mater., 1998, 10, 161.
PMO	64.8	1	90	NA	Langmuir, 2010, 26, 10076.
Hierarchically porous silica	140	NA	720	NA	J. Mater. Chem., 2011, 21, 15567.
TDMSNs-0.2	1502.4	2.11	5	0.89 after 5 cycles	This work

[a] Adsorption capacity (mg g^{-1}); [c] Mercury to Sulphur molar ratio; [c] time to reach 99.9% of the equilibrium adsorption capacity (min); [d] Retention of initial adsorption capacity.

Table S3. Pseudo-second order kinetic parameters for TDMSNs-*r*.

Adsorbent	K_2 (g mg^{-1} min^{-1})	q_e (mg g^{-1})	R^2
TDMSNs-0.05	0.003	711.0	0.99
TDMSNs-0.1	0.004	1033.1	0.99
TDMSNs-0.2	0.002	1510.2	0.99

Table S4. Measured equilibrium concentration (C_e) after 5 min for TDMSNs-*r* at different initial concentration (C_i) of the mercury (II). For C_i of 10 ppm, atomic absorption spectrometer in its high sensitivity mode with the limit of detection of 0.001 ppm was used while for other concentrations, the limit of detection was increased to 0.1 ppm.

C_i (ppm)	TDMSNs-0.5	TDMSNs-0.1	TDMSNs-0.2
10	<LOD*	<LOD*	<LOD*
50	0.8	0.3	0.1
100	1.7	1.2	0.9
200	2.3	2.9	2.1
300	3.8	4.1	2.9
400	59.4	6.8	3.8
500	154.2	11.9	6.7
600	-	98.2	-
750	398.6	241.3	89.1
1000	-	487.2	296.7
1500	-	-	751.4

* Less than limit of detection