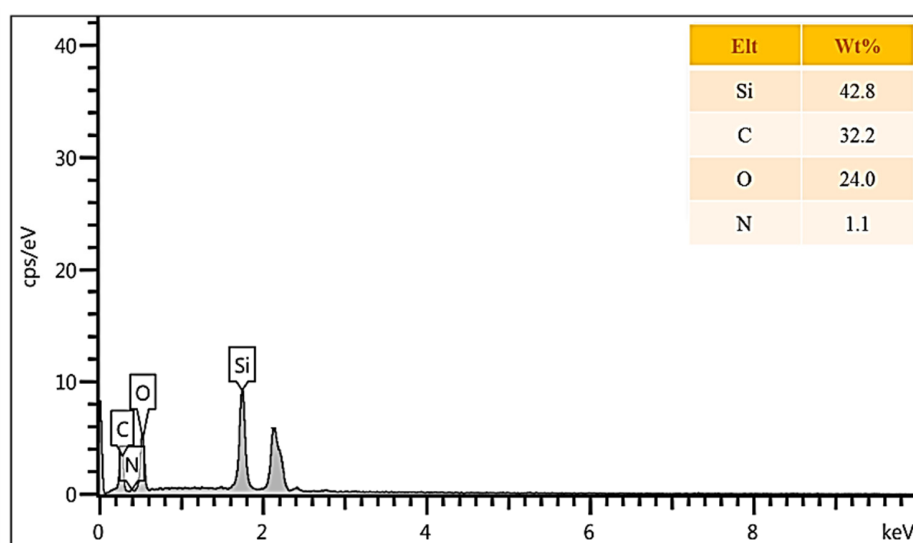


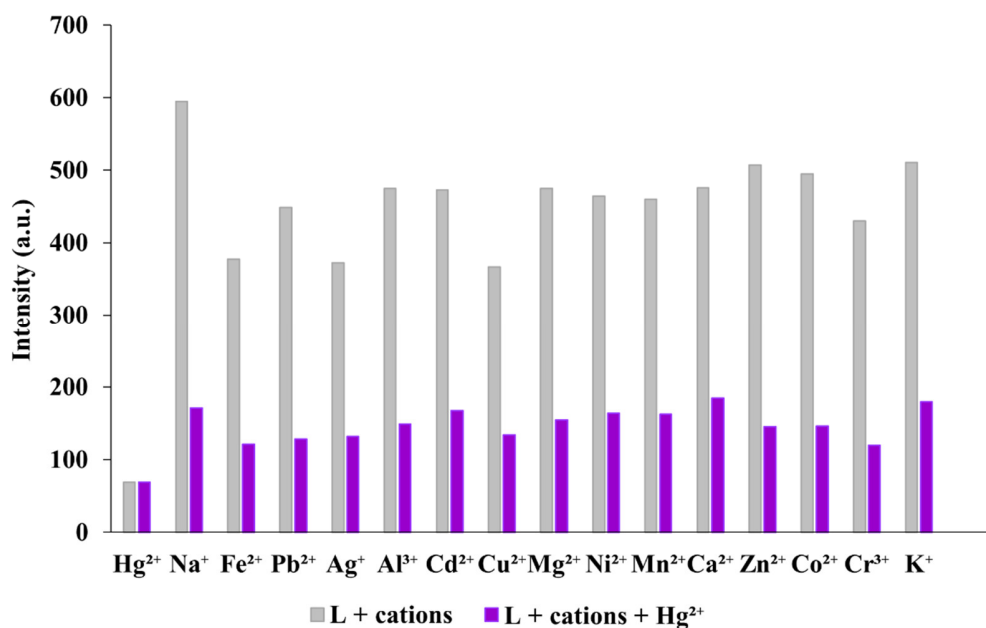
## Supplementary Materials

# Fumed-Si-Pr-Ald-Barb as a Fluorescent Chemosensor for the $\text{Hg}^{2+}$ Detection and $\text{Cr}_2\text{O}_7^{2-}$ Ions: A Combined Experimental and Computational Perspective

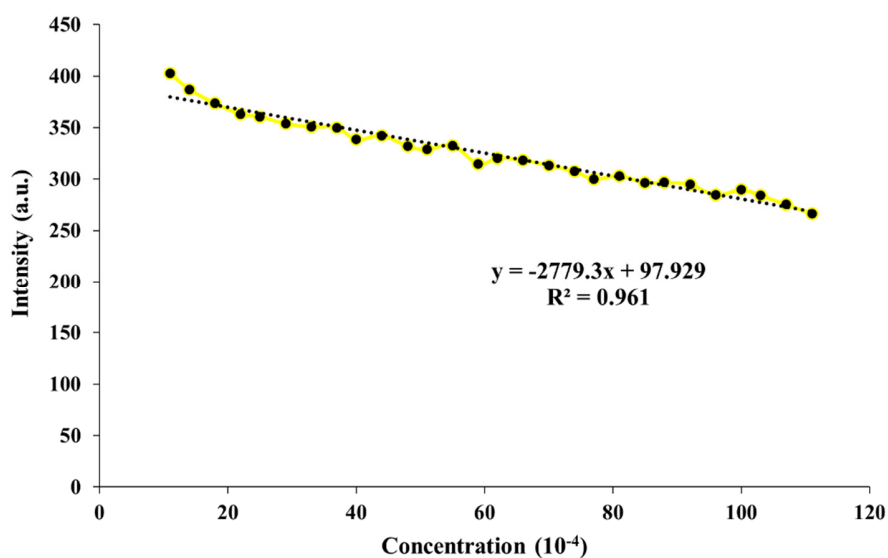
Ghodsi Mohammadi Ziarani <sup>1,\*</sup>, Mahtab Rezakhani<sup>1</sup>, Mehran Feizi-Dehnayebi <sup>1,\*</sup>, and Stoyanka Nikolova<sup>2,\*</sup>



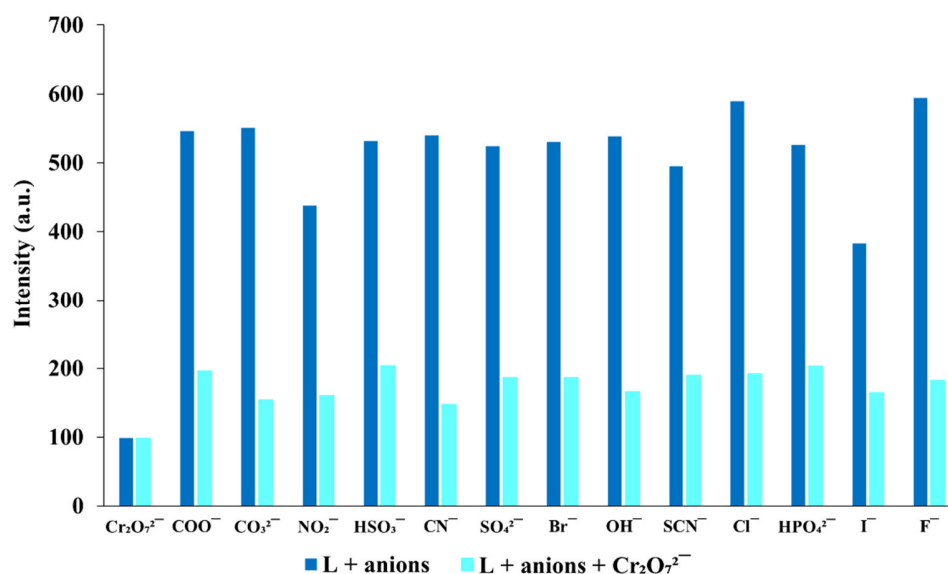
**Figure S1.** EDX of fumed-Si-Pr-Ald-Barb.



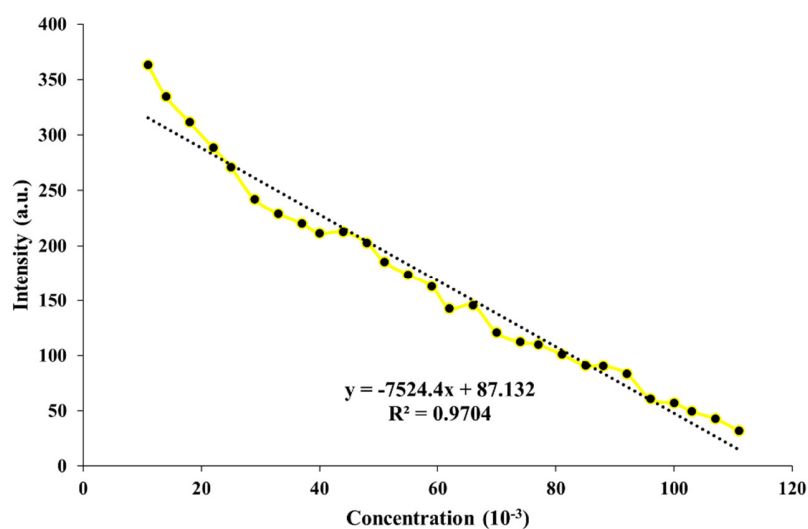
**Figure S2.** Competition test of fumed-Si-Pr-Ald-Barb (2.5 mL, 0.02 g in 100 mL (H<sub>2</sub>O:EtOH/2:3)) for Hg<sup>2+</sup> (200  $\mu$ L,  $1 \times 10^{-2}$  M) in the presence of other cations ( $\lambda_{em}$  = 300 nm,  $\lambda_{ex}$  = 375 nm).



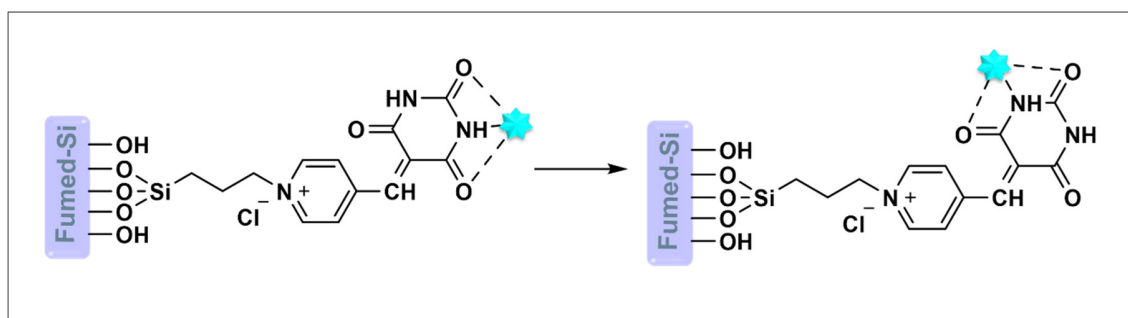
**Figure S3.** The plot of fluorescence intensity of fumed-Si-Pr-Ald-Barb against different concentrations of Hg<sup>2+</sup>.



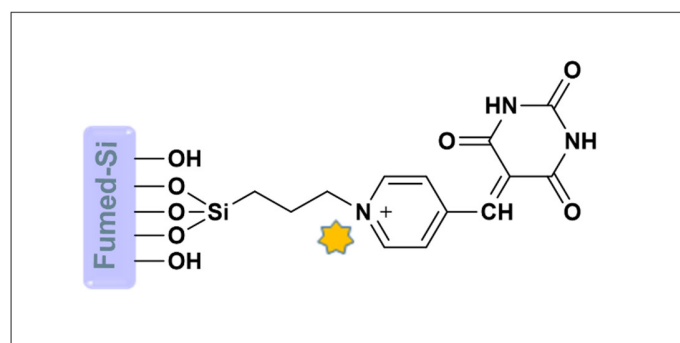
**Figure S4.** Competition test of fumed-Si-Pr-Ald-Barb (2.5 mL, 0.02 g in 100 mL (H<sub>2</sub>O:EtOH/2:3)) for Cr<sub>2</sub>O<sub>7</sub><sup>2-</sup> (200  $\mu$ L,  $1 \times 10^{-2}$  M) in the presence of other anions ( $\lambda_{em}$ = 300 nm,  $\lambda_{ex}$ = 380 nm).



**Figure S5.** The plot of fluorescence intensity of fumed-Si-Pr-Ald-Barb against different concentrations of Cr<sub>2</sub>O<sub>7</sub><sup>2-</sup>.



**Scheme S1.** Proposed binding mode between fumed-Si-Pr-Ald-Barb and  $\text{Hg}^{2+}$ .



**Scheme S2.** Proposed binding mode between fumed-Si-Pr-Ald-Barb and  $\text{Cr}_2\text{O}_7^{2-}$ .

**Table S1.** Mulliken charge distribution of selected atoms in Pr-Ald-Barb.

Atom	Charge
O1	-0.481
O2	-0.472
O3	-0.463
N1	-0.336
N2	-0.340
N3	+0.414
H-N1	+0.280
H-N2	+0.282

**Table S2.** Estimated Mulliken atomic charges, Fukui functions and dual descriptor of selected atoms for Pr-Ald-Barb.

Atom	$q^{(N)}$	$q^{(N+1)}$	$q^{(N-1)}$	$ f^+ $	$ f^- $	$\Delta f$
O1	-0.481	-0.498	-0.446	0.017	0.035	-0.018
O2	-0.472	-0.487	-0.441	0.015	0.031	-0.016
O3	-0.463	-0.478	-0.433	0.015	0.030	-0.015
N1	-0.336	-0.349	-0.313	0.013	0.023	-0.010
N2	-0.340	-0.354	-0.314	0.014	0.026	-0.012
N3	+0.414	+0.444	+0.403	0.030	0.011	0.019
H-N1	+0.280	+0.294	+0.273	0.014	0.007	0.007
H-N2	+0.282	+0.295	+0.275	0.013	0.007	0.006

**Table S3.** Quantum reactivity parameters of Pr-Ald-Barb, Pr-Ald-Barb+Hg<sup>2+</sup>, and Pr-Ald-Barb+Cr<sub>2</sub>O<sub>7</sub><sup>2-</sup> obtained from DFT.

parameter	Pr-Ald-Barb	Pr-Ald-Barb+Cr <sub>2</sub> O <sub>7</sub> <sup>2-</sup>	Pr-Ald-Barb+Hg <sup>2+</sup>
E <sub>HOMO</sub>	-5.31	-3.82	-5.31
E <sub>LUMO</sub>	-4.61	-3.53	-4.68
ΔE <sub>(LUMO-HOMO)</sub>	0.70	0.29	0.63
χ	4.96	3.67	4.99
η	0.35	0.14	0.31
σ	2.85	7.14	3.22
P <sub>i</sub>	-4.96	-3.67	-4.99
ω	35.14	48.10	40.16