Electronic Supplementary Informations for

# Aggregation-induced emission polydithioacetal with pendant tetraphenylethtlene groups for $Hg^{2+}$ detection and removal

Yu Gu, Jianjian Zhu, Xinyu Yuan, Siyong Li, Zhongxiang Zhao, and Yanbing Lu*

Advanced Catalytic Engineering Research Center of the Ministry of Education, College of Chemistry and Chemical Engineering, Hunan University, Changsha 410082, P. R. China

***Contents:***

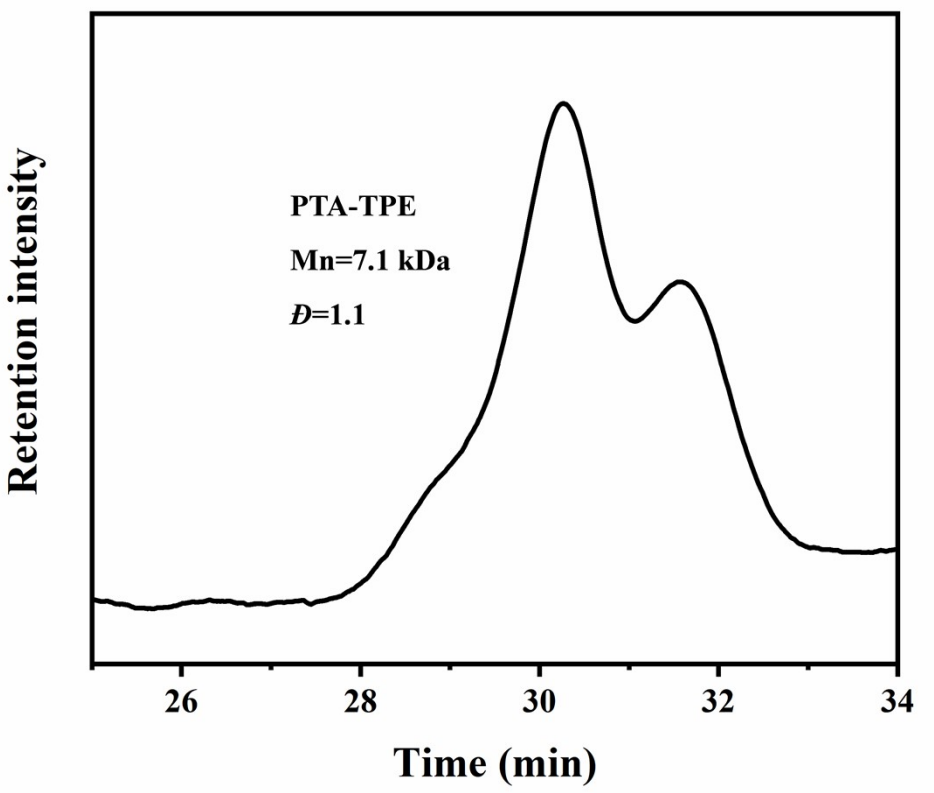



**Figure S1**. The GPC trace of polymer PTA-TPE.

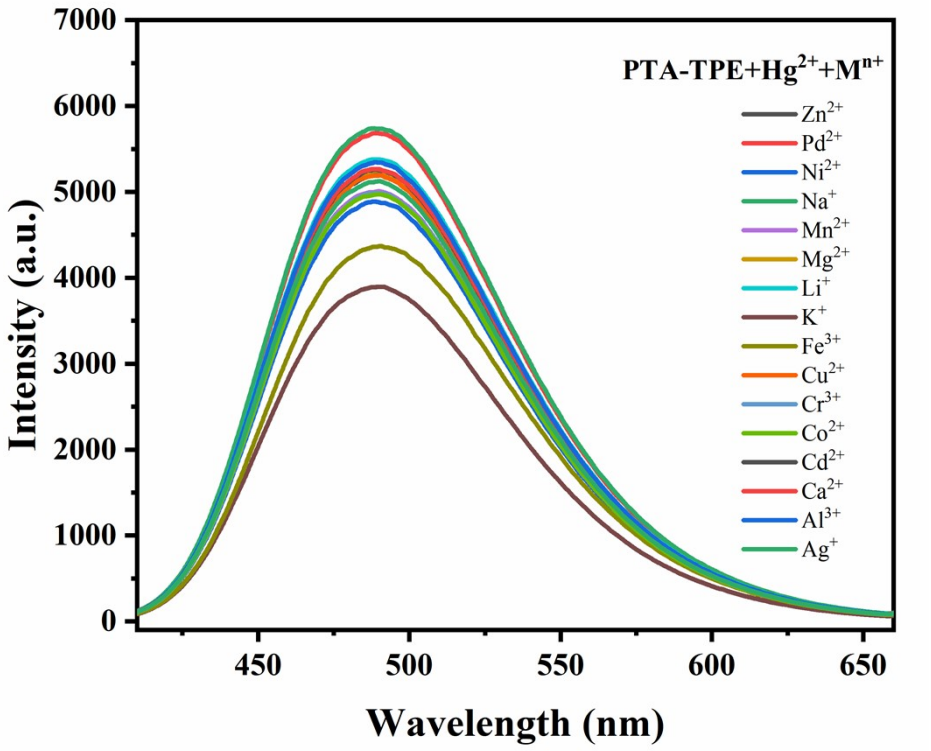



**Figure S2**. Photoluminescence spectra of PTA-PTE (10 μM) in the presence of $Hg^{2+}$ and various metal ions in PBS solution.

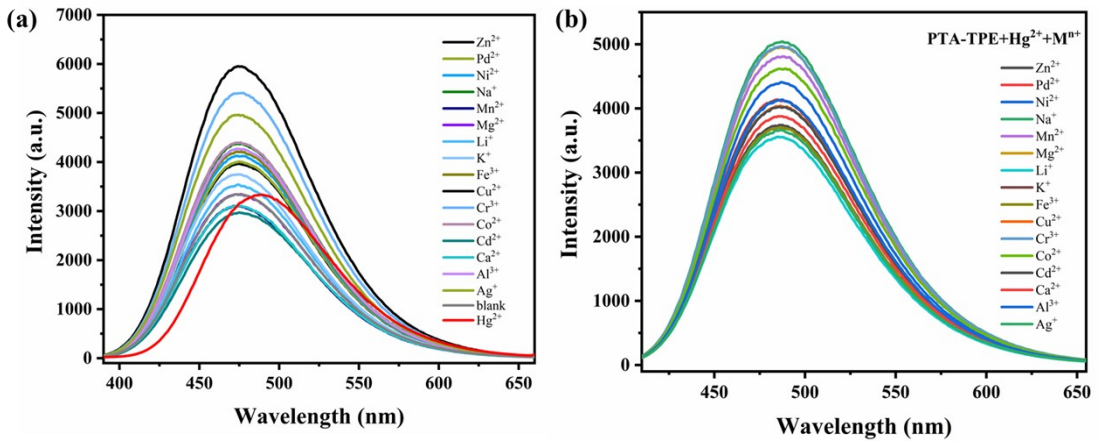



**Figure S3.** (A) Photoluminescence spectra of PTA-PTE (10 μM) in the presence of $Hg^{2+}$ in PBS (pH 5.0). (B) Photoluminescence spectra of PTA-PTE (10 μM) in the presence of $Hg^{2+}$ and various metal ions in PBS (pH 5.0).

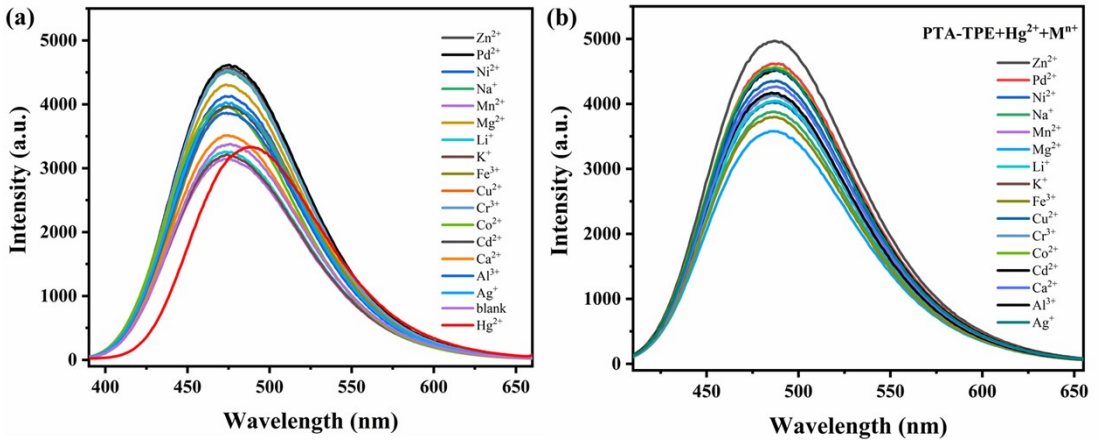
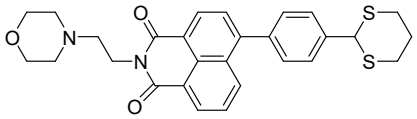
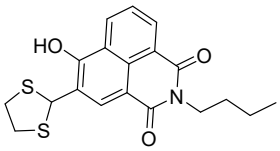
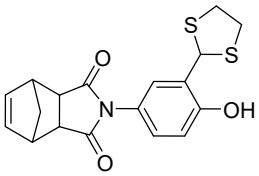
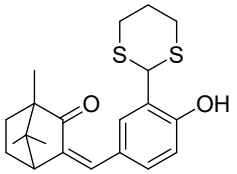
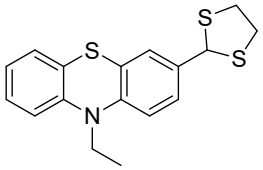
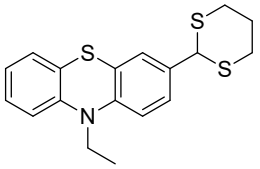
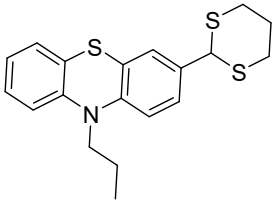
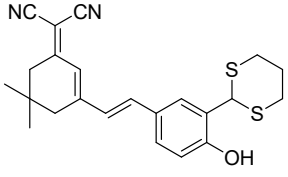
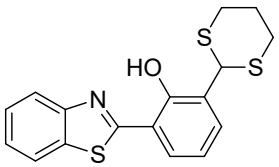
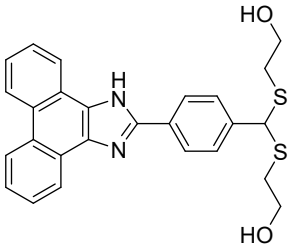
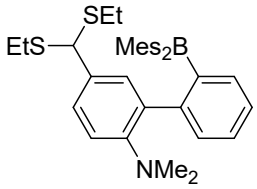
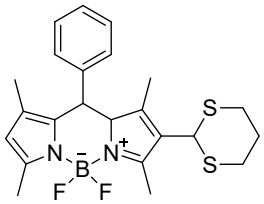
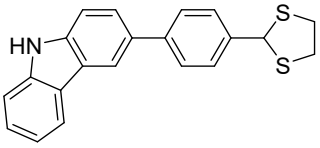
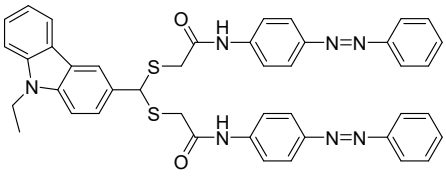
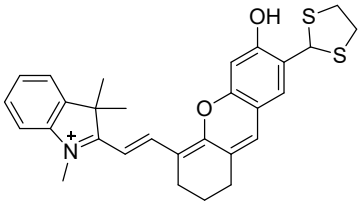
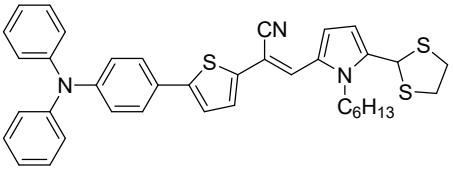
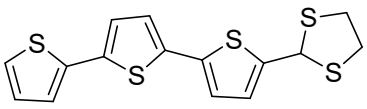
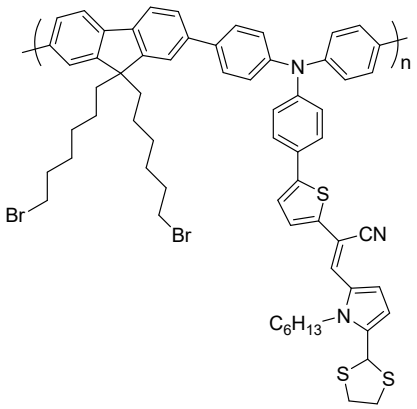
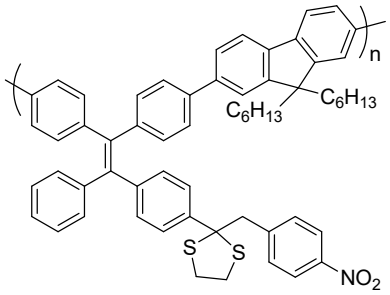
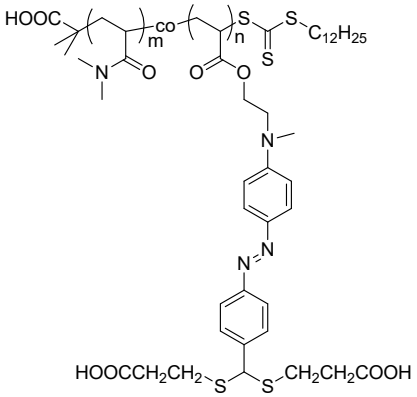
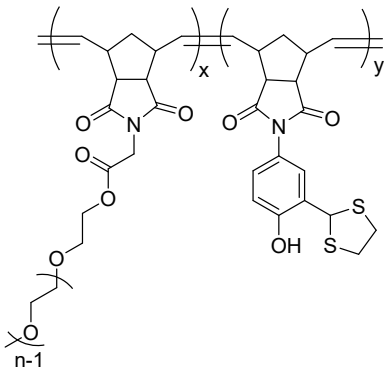
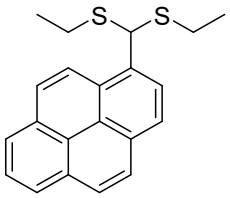



**Figure S4.** (A) Photoluminescence spectra of PTA-PTE (10 μM) in the presence of $Hg^{2+}$ in PBS (pH 9.0). (B) Photoluminescence spectra of PTA-PTE (10 μM) in the presence of $Hg^{2+}$ and various metal ions in PBS (pH 9.0).

**Table S1.** Comparison between various sensing parameters of thioacetal based detection systems.

| Probes | Media | Response time | Detection limit | Ref. |
|---|---|---|---|---|
|  | ACN/$H_2O$ (8:2) | 10 s | 3.3 nM | S1 |
|  | EtOH/$H_2O$ (2:8, v/v; pH7.4) | 10 min | 40 nM | S2 |
|  | DMSO/$H_2O$ (3:2,) | < 1 min | 8.2 nM | S3 |
|  | 99% PBS buffer | 15 min | 19.3nM | S4 |
|  | EtOH/$H_2O$ (1/1, v/v) | 5 min | 18.7 nM | S5 |
|  | EtOH/$H_2O$ (1/1, v/v) | 5 min | 20.7 nM | S5 |
|  | DMSO/$H_2O$ (1:3, v/v) | < 1 min | 12.5 nM | S6 |
|  | DMF/PBS buffer (10 mM, pH 7.4, 5: 5, v/v) | 15 min | 297nM | S7 |

| | | | | |
|---|---|---|---|---|
|  | $CH_3CN/H_2O$ (1:1,v/v) | 15 min | 200 nM | S8 |
|  | PBS (2 mM Triton X-100) | ~1 min | 1.16 nM | S9 |
|  | $H_2O$ | - | 72.7 nM | S10 |
|  | HEPES buffer/$CH_3CN$ (4 : 1, v/v) | - | 0.9 nM | S11 |
|  | THF/$H_2O$ ($f_w$ = 5%) | - | 205 nM | S12 |
|  | $CH_3CN/H_2O$ (1:1,v/v) | 30 s | 18 nM | S13 |
|  | HEPES buffer (10 mM, pH 7.4) | 5 min | 320 nM | S14 |
|  | THF | 6 min | 800 nM | S15 |
|  | EtOH/$H_2O$ (1/1, v/v) | 1 min | 10.3 nM | S16 |

| | | | | |
|---|---|---|---|---|
|  | THF | 10 min | 1000 nM | S17 |
|  | THF/$H_2O$ (2:98, v/v) | 5 min | 230 nM | S18 |
|  | HEPES buffer (pH 7.4) | 15 min | - | S19 |
|  | Water | < 1 min | 107 nM | S3 |
|  | $CH_3CN/H_2O$ (1:1,v/v) | < 1 min | 55 nM | S20 |

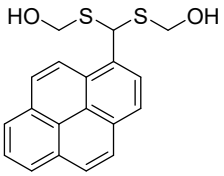
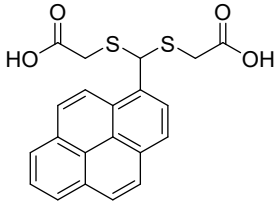
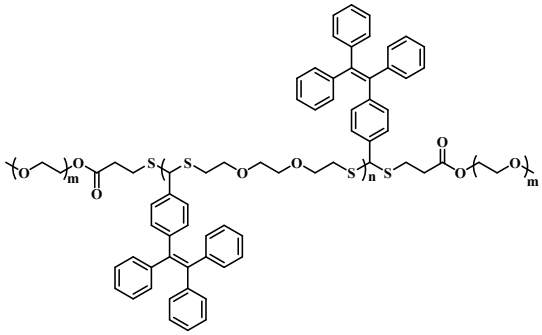
| | | | | |
|---|---|---|---|---|
|  | PBS buffer | 30 min | 1.74 nM | S21 |
|  | PBS buffer | 30 min | 1.53 nM | S21 |
|  | Water | < 1 min | 10.81 nM | This work |

**Table S2.** Comparative table of various $Hg^{2+}$-specific polymer receptors with the present system.

| Materials | Adsorption time | Detection limit | Detection specificity | Removal Rate (%) | Ref. |
|---|---|---|---|---|---|
| Tryptophan-fluorescent polymer | / | 1.5 nM | $Hg^{2+}$ & $HSO_4^-$ | 93.5 | S22 |
| Cysteamine-functionalized hydrogel | 3 h | 0.3 nM | $Hg^{2+}$ | 90.7 | S23 |
| Thiol-amine functionalized polymer | 0.5 h | / | $Hg^{2+}$ | / | S24 |
| Fluorescence probe on mesoporous silica | 3 h | 0.19 μM | $Hg^{2+}$ & $Cu^{2+}$ | 96.3 | S25 |
| AIE fluorescent polymer | 12 h | 0.30 μM | $Hg^{2+}$ | 90.0 | S26 |
| AIE thioacetal polymer | 0.5 h | 10.81 nM | $Hg^{2+}$ | 80.6 | This work |

## References


S1. D. Jothi, S. K. Iyer, *Inorg. Chem. Commun.* **2022**, *143*, 109735.

S2. M. Tian, C. Wang, Q. Ma, Y. Bai, J. Sun, C. Ding, *ACS Omega* **2020**, *5*, 18176-18184.

S3. T. Samanta, N. Das, D. Patra, P. Kumar, B. Sharmistha, R. Shunmugam, *ACS Sustain. Chem. Eng.* **2021**, *9*, 5196-5203..

S4. Z. Wang, Y. Zhang, J. Yin, Y. Yang, H. Luo, J. Song, X. Xu, S. Wang, *ACS Sustain. Chem. Eng.* **2020**, *8*, 12348-12359.

S5. C. Wang, L. Wang, S. Fang, D. Qin, J. Zhou, G. Yang, S. Jin, H. Duan, *Res. Chem. Intermediat.* **2019**, *45*, 2045-2063.

S6. J. Wang, Q. Niu, T. Hu, T. Li, T. *J.* Wei, *Photochem. Photobiol. A Chem.* **2019**, *384*, 112036.

S7. S. C. Pei, C. Z. Li, X. Y. Pei, W. H. Zeng, Y. Y. Zhang, K. X. Jiang, X. Huang, X. L. Liao, Chen, J. *Spectrochim. Acta A* **2023**, *285*, 121886.

S8. I. J. Chang, K. S. Hwang, S. K. Chang, Selective $Hg^{2+}$ signaling via dithiane to aldehyde conversion of an ESIPT fluorophore. *Dyes Pigments* **2017**, *137*, 69-74.

S9. Y. Gao, N. Yi, Z. Ou, Z . Li, T. Ma, H. Jia, W. Xing, G. Yang, Y. Li, *Sensor. Actuat. B: Chem.* **2018**, *267*, 136-144.

S10. Q. W. Xu, C. Wang, Z. B. Sun, C. H. Zhao, *Org. Biomol. Chem.* **2015**, *13*, 3032-3039.

S11. S. Saha, H. Agarwalla, H. Gupta, M. Baidya, E. Suresh, S. K. Ghosh, Das, *Dalton Trans.* **2013**, *42*, 15097–15105.

S12. Pan, J.; Ma, J.; Liu, L.; Li, D.; Huo, Y.; Liu, H. *J. Photochem. Photobiol. A Chem.* **2021**, *416*, 113322.

S13. Z. Yu, Z. Tian, Z. Li, Z. Luo, Y. Li, Y. Li, J. Ren, *Sensor. Actuat. B: Chem.* **2016**, *223*, 172-177.

S14. Y. Wang, X. Hou, Z. Li, C. Liu, S. Hu, C. Li, Z. Xu, Y. Wang, *Dyes Pigments* **2020**, *173*, 107951.

S15. J. Ding, H. Li, C. Wang, J. Yang, Y. Xie, Q. Peng, Q. Li, Z. Li, *ACS Appl. Mater. Inter.* **2015**, *7*, 11369-11376.

S16. L. Lan, Q. Niu, T. Li, *Anal. Chim. Acta* **2018**, *1023*, 105-114.

S17. J. Ding, H. Li, Y. Xie, Q. Peng, Q. Li, Z. Li, *Polym. Chem.* **2017**, *8*, 2221-2226.

S18. Y. Shan, W. Yao, Z. Liang, L. Zhu, S. Yang, Z. Ruan, *Dyes Pigments* **2018**, *156*, 1-7.

S19. A. Balamurugan, H. I. Lee, *Macromolecules* **2015**, *48*, 1048-1054.

S20. Y. Y. Liu, S. Naha, N. Thirumalaivasan, S. Velmathi, S. P. Wu, *Sensor. Actuat. B: Chem.* **2018**, *277*, 673-678.

S21. Y. Gao, T. Ma, Z. Ou, W. Cai, G. Yang, Y. Li, M. Xu, Q. Li, *Talanta* **2018**, *178*, 663-669.

S22. N. Choudhury, B. Saha, B. Ruidas and P. De, *ACS Appl. Polym. Mater.* 2019, 1, 461-471.

S23. M. Bansal, B. Ram, G. S. Chauhan and A. Kaushik, *Int J Biol Macromol*. 2018, 112, 728-736.

S24. S. Chatterjee, H. Gohil, I. Raval, S. Chatterjee and A. R. Paital, *Small* **2019**, 15, 1804749.

S25. D. Dai, Z. Li, J. Yang, C. Wang, J.-R. Wu, Y. Wang, D. Zhang and Y.-W. Yang, *J. Am. Chem. Soc* **2019**, 141, 4756-4763.

S26. B. Liu, F. Zhao, Y. Qiu, W. Liu and Z. Wu, J Mater Chem C **2023**, 11, 1499-1508.