

Supporting Information

Ligand-doped Liquid Crystal Sensor System for Detecting Mercuric Ion in Aqueous Solutions

Chih-Hsin Chen, Yi-Cheng Lin, Hao-Hsiang Chang and Adam Shih-Yuan Lee**

Department of Chemistry, Tamkang University, New Taipei City 25137, Taiwan

* To whom correspondence should be addressed.

Phone: +886-2-26215656

Email: chc@mail.tku.edu.tw

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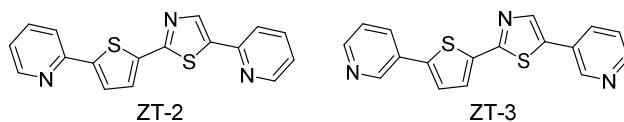


Figure S1. Structure of ZT-2 and ZT-3.

Synthesis of ZT-2. The mixture of 5-bromo-2-(5-bromothiophen-2-yl)thiazole (1.0 eq.) and 2-(tributylstannyl)pyridine (3.0 eq.) and tetrakis(triphenylphosphine) palladium (6.0%) were allowed to react in dry DMF at 120 °C for 48 h. After cooling, the solution was filtered and quenched by water. After that, the solution was extracted three times with dichloromethane. The combined organic extracted were washed with brine and dried over MgSO₄. The solvent was removed under reduced pressure and the crude product was further purified by column chromatography by using dichloromethane/hexane (1:1) as the eluent followed by recrystallization by dichloromethane and hexane to yield ZT-2 as an orange-yellow solid. ¹H NMR (300 MHz, CDCl₃): δ 8.59-8.65 (m, 2H), 8.22 (s, 1H), 7.69-7.78 (m, 5H), 7.60 (d, 1H, *J* = 3.6 Hz), 7.19-7.27 (m, 2H). ¹³C NMR (75.5 MHz, C₄D₂O): δ 163.7, 152.3, 151.6, 150.7, 150.4, 148.5, 141.5, 141.2, 140.2, 137.4, 137.3, 128.2, 125.9, 123.2, 120.1, 119.4, 117.5. FABMS (*m/z*): 321 [*M*⁺]; HRMS (*m/z*): calcd for C₁₇H₁₁N₃S₂: 321.0394; found: 321.0400.

Synthesis of ZT-3. The mixture of 5-bromo-2-(5-bromothiophen-2-yl)thiazole (1.0 eq.) and 3-(tributylstannyl)pyridine (3.0 eq.) and tetrakis(triphenylphosphine) palladium (6.0%) were allowed to react in dry DMF at 120 °C for 48 h. After cooling, the solution was filtered and quenched by water. After that, the solution was extracted three times with dichloromethane. The combined organic extracted were washed with brine and dried over MgSO₄. The solvent was removed under reduced pressure and the crude product was further purified by column chromatography by using dichloromethane/hexane (1:1) as the eluent followed by recrystallization by dichloromethane and hexane to yield ZT-3 as an orange-yellow solid. ¹H

NMR (300 MHz, CD₂Cl₂): δ 8.92 (d, 1H, J = 2.2 Hz), 8.85 (d, 1H, J = 2.2 Hz), 8.53-8.57 (m, 2H), 8.00 (s, 1H), 7.88-7.95 (m, 2H), 7.57 (d, 1H, J = 3.6 Hz), 7.34-7.41 (m, 3H). ¹³C NMR (75.5 MHz, CD₂Cl₂): δ 161.2, 149.2, 149.0, 147.3, 146.7, 142.7, 139.9, 137.2, 135.1, 133.4, 132.8, 129.5, 127.8, 127.3, 125.0, 123.8, 123.7. FABMS (m/z): 321 [M^+]; HRMS (m/z): calcd for C₁₇H₁₁N₃S₂: 321.0394; found: 321.0411.

Binding study of ZT-2 and ZT-3.

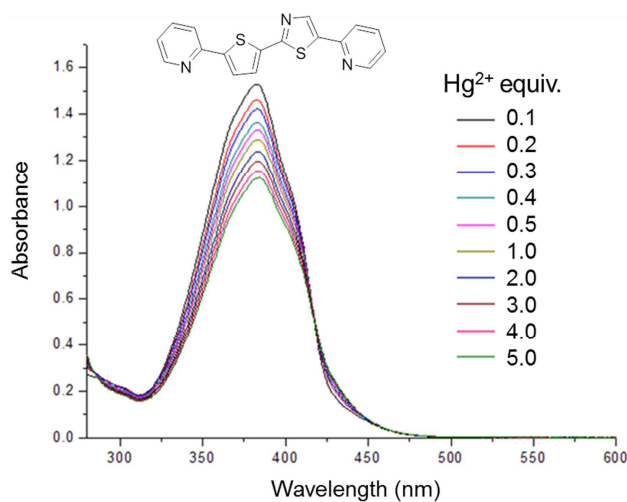


Figure S2. Absorbance response of ZT-2 (50.0 μM) to various equivalents of Hg²⁺ in methanol.

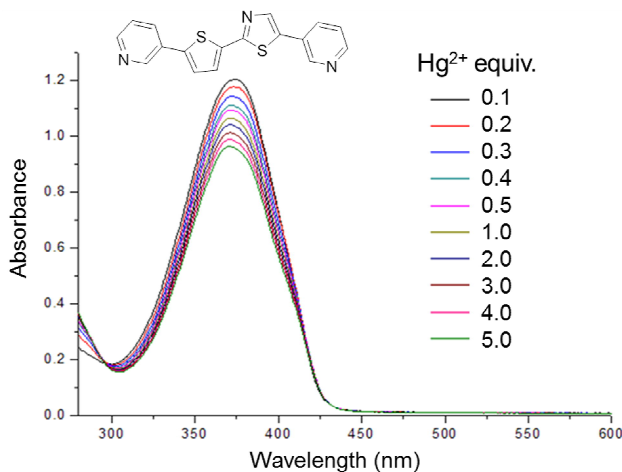


Figure S3. Absorbance response of ZT-3 (50.0 μM) to various equivalents of Hg²⁺ in methanol.