Supplementary data

An ESIPT-based fluorescent probe for highly selective and ratiometric detection of mercury (II) in solution and in cells

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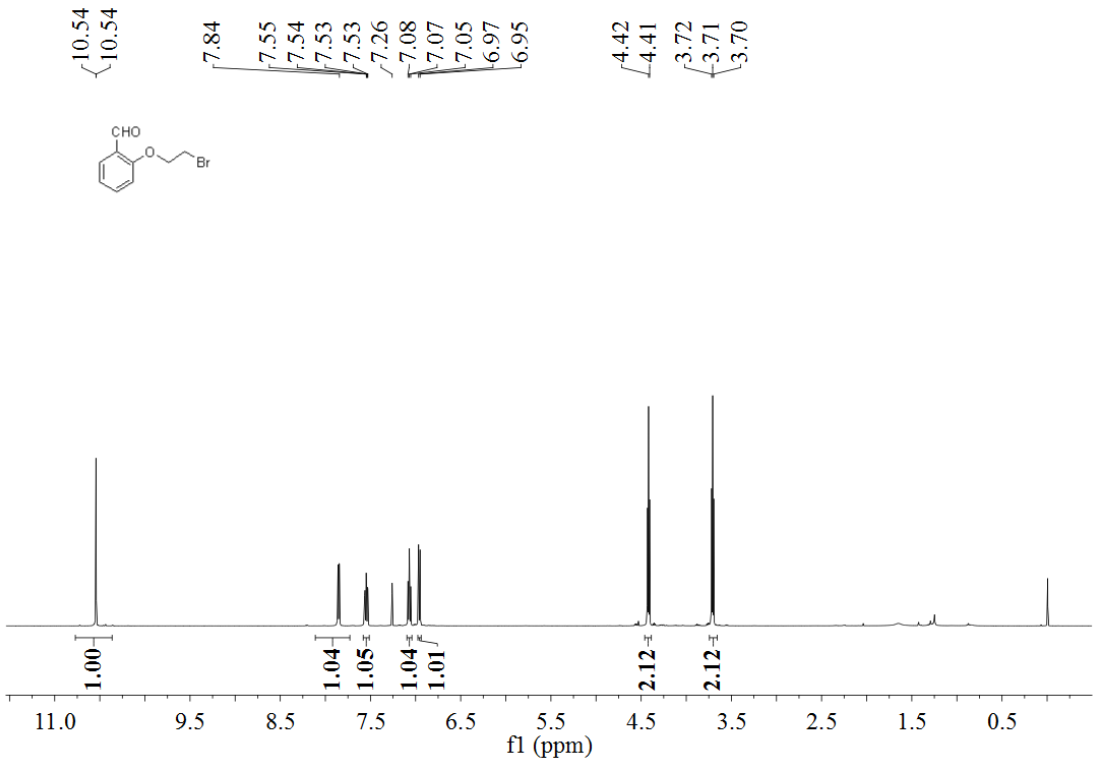

Fig. S1. ^{1}H NMR of compound **M1** (500 MHz, $CDCl_3$).

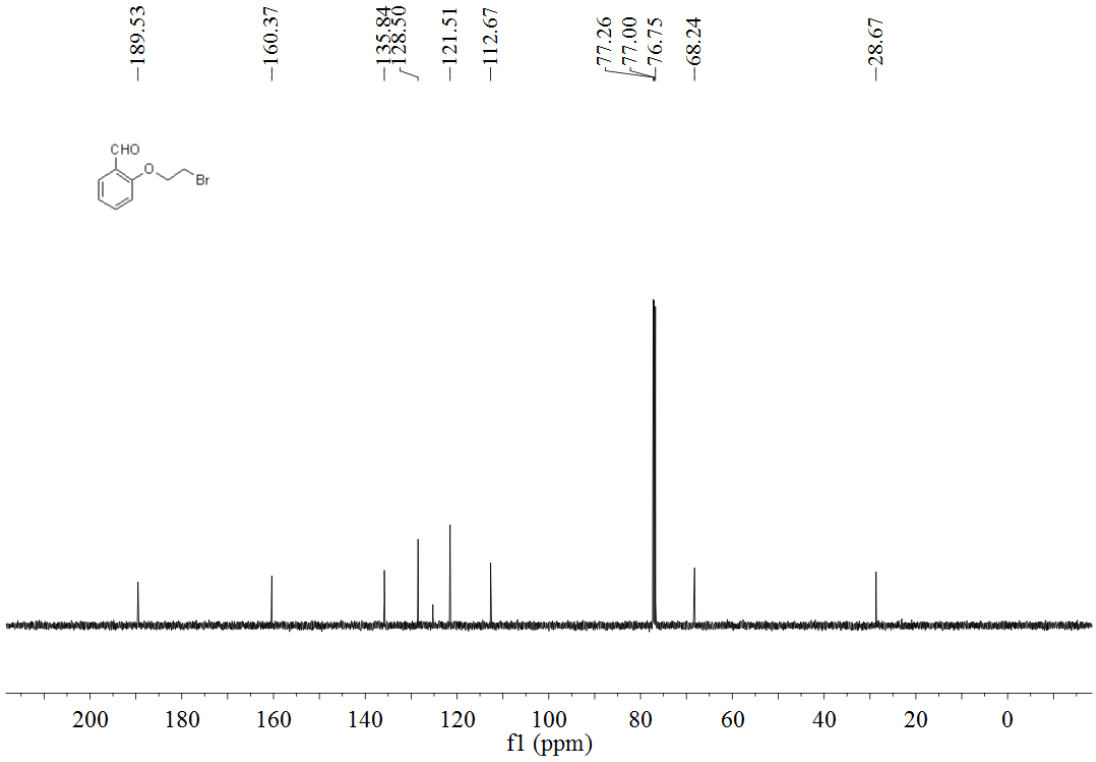

Fig. S2. ^{13}C NMR of compound **M1** (126 MHz, $CDCl_3$).

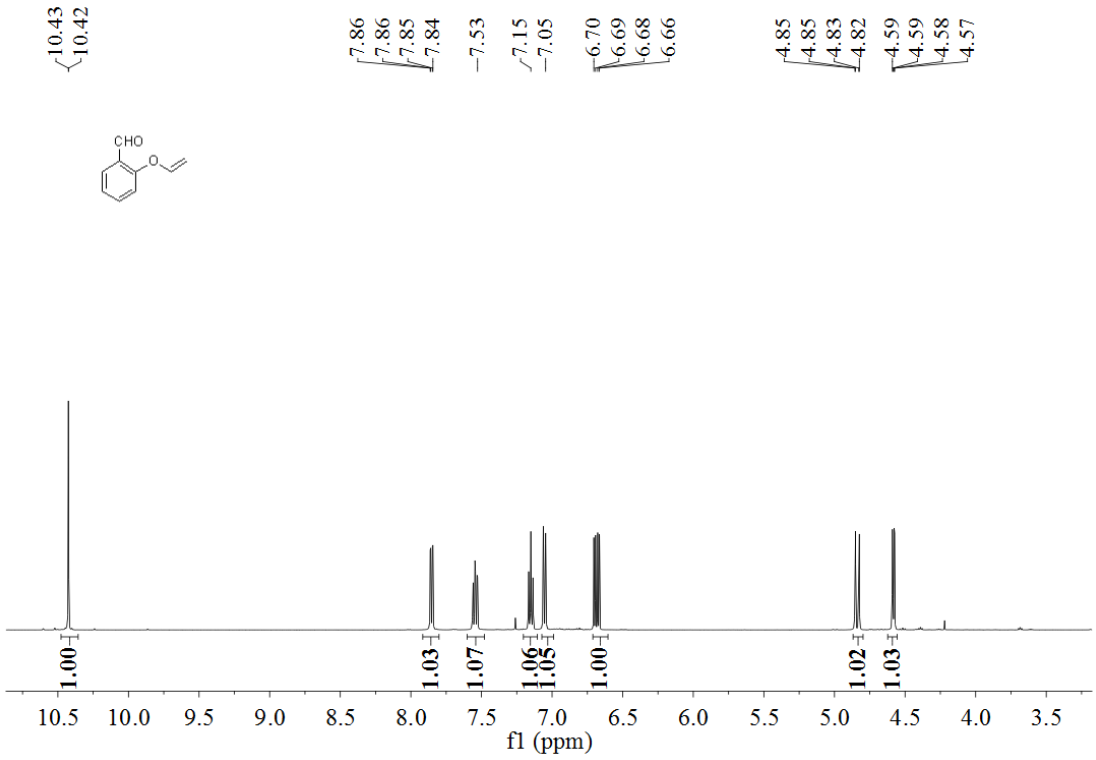

Fig. S3. ^{1}H NMR of compound **M2** (500 MHz, $CDCl_3$).

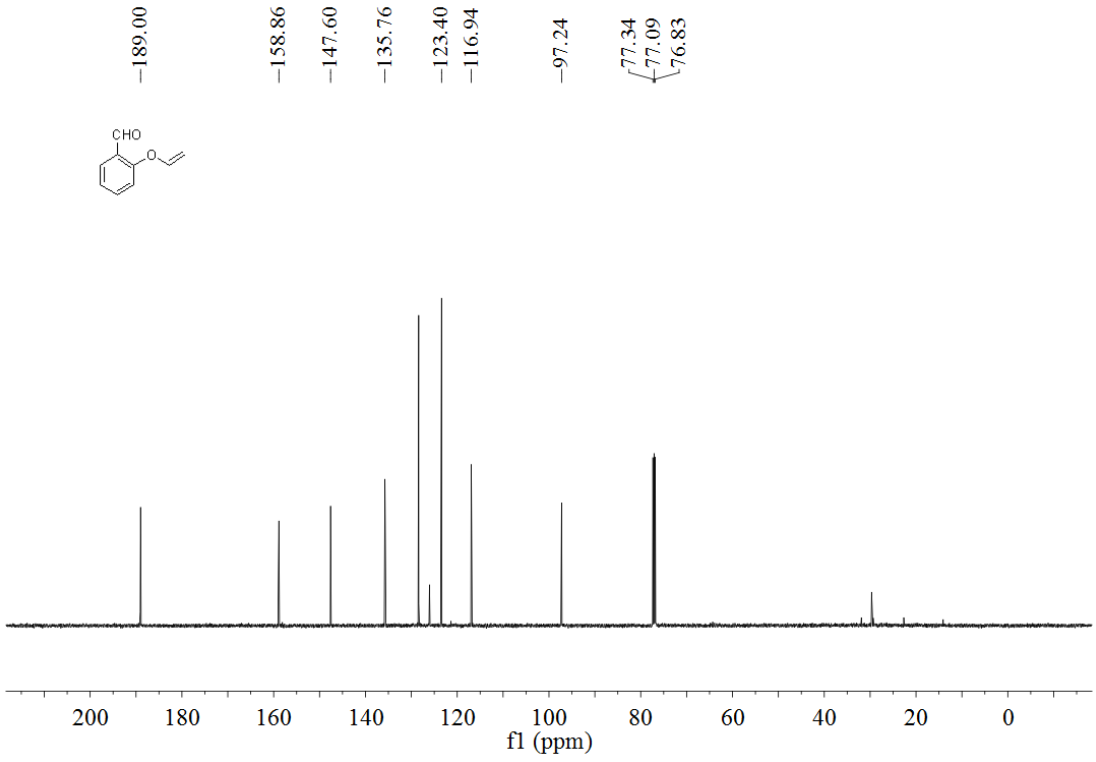

Fig. S4. ^{13}C NMR of compound **M2** (126 MHz, $CDCl_3$).

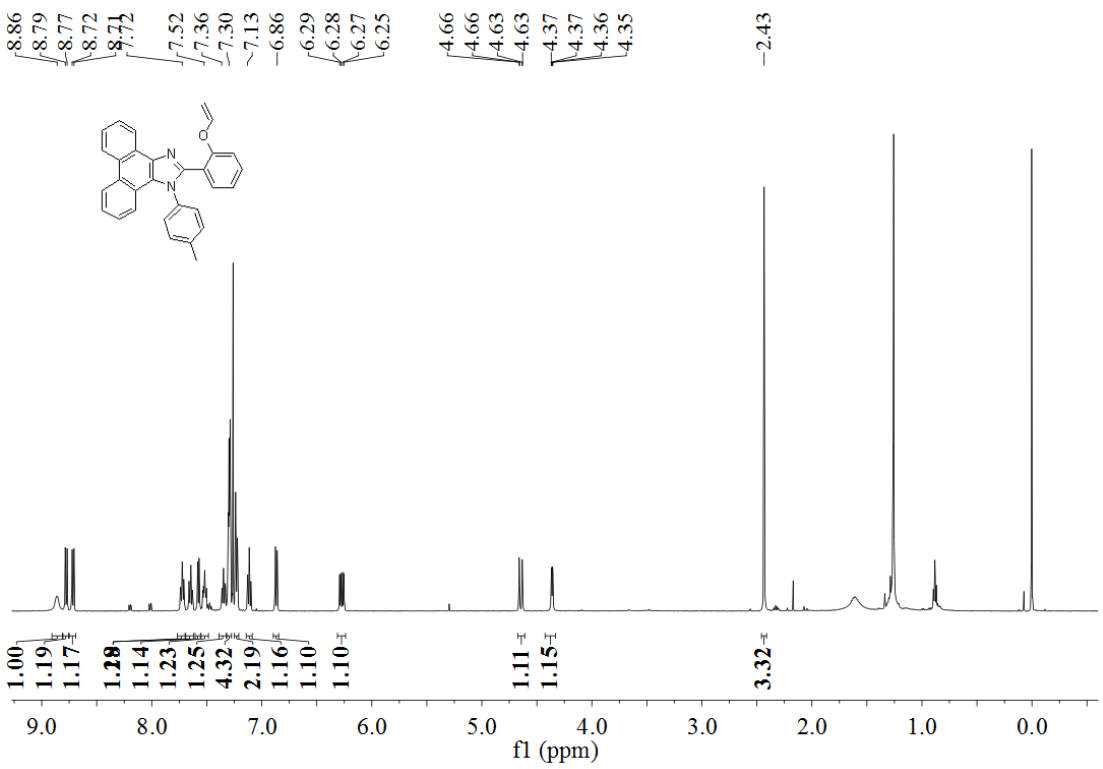

Fig. S5. ^{1}H NMR of probe **Pvi** (500 MHz, $CDCl_3$).

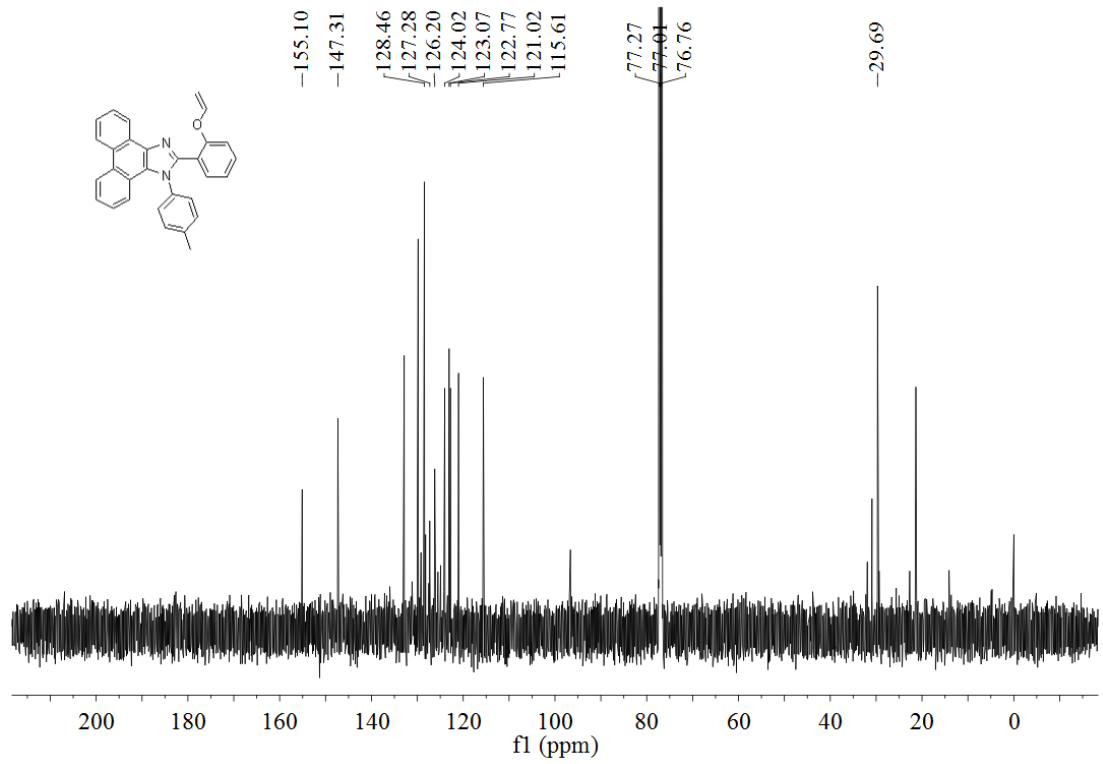

Fig. S6. ^{13}C NMR of probe **Pvi** (126 MHz, $CDCl_3$).

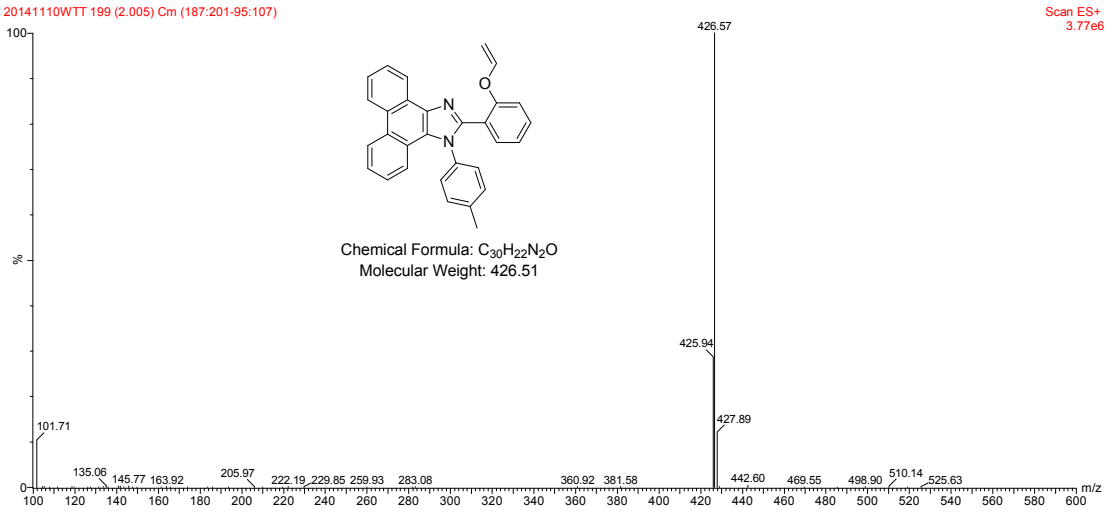

Fig. S7. Mass spectrometry spectrum of probe **Pvi**.

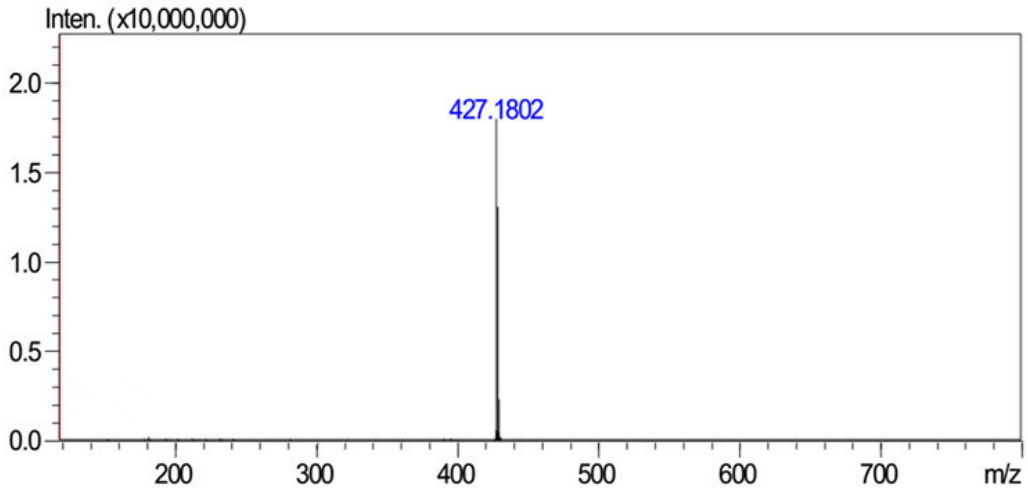

Fig. S8. HR-MS spectrum of probe **Pvi**.

The detailed investigation for the reaction of probe Pvi with $HgCl_2$.

Pvi (42.6 mg, 0.10 mmol) was dissolved in 5 mL of CH_3CN-PBS (1:1, v/v, pH 7.4) solution, and $HgCl_2$ (13.6 mg, 0.05 mmol) was then added into the solution. After stirring overnight at room temperature, the mixture was washed with water, and extracted by ethyl acetate. The organic layer was evaporated under reduced pressure,

and the crude product was purified by silica gel chromatography (petroleum ether/ethyl acetate, 20:1, v/v) to give the fluorophore **Pol**. ^{1}H NMR (500 MHz, $CDCl_3$): δ 13.93 (s, 1H), 8.76 (d, *J* = 8.3 Hz, 1H), 8.71 (dd, *J* = 12.9, 4.8 Hz, 2H), 7.82–7.73 (m, 1H), 7.67 (ddd, *J* = 8.4, 7.1, 1.4 Hz, 1H), 7.57–7.45 (m, 5H), 7.29–7.26 (m, 1H), 7.22 (ddd, *J* = 8.5, 7.2, 1.5 Hz, 1H), 7.13 (ddd, *J* = 15.4, 8.3, 1.0 Hz, 2H), 6.80 (dd, *J* = 8.1, 1.5 Hz, 1H), 6.54 (ddd, *J* = 8.3, 7.2, 1.3 Hz, 1H), 2.63 (s, 3H). ^{13}C NMR (126 MHz, $CDCl_3$): δ 159.25, 148.56, 140.79, 136.39, 134.37, 131.44, 130.62, 129.46, 128.71, 128.43, 127.43, 127.11, 126.46, 126.12, 125.91, 125.17, 124.11, 123.17, 122.73, 122.56, 120.92, 117.99, 113.23, 21.57. MS (EI) m/z: 400.62 (M^+). HR-MS (ESI) calculated for $C_{28}H_{21}N_2O^+$ (M + H^+): 401.1648, found 401.1640.

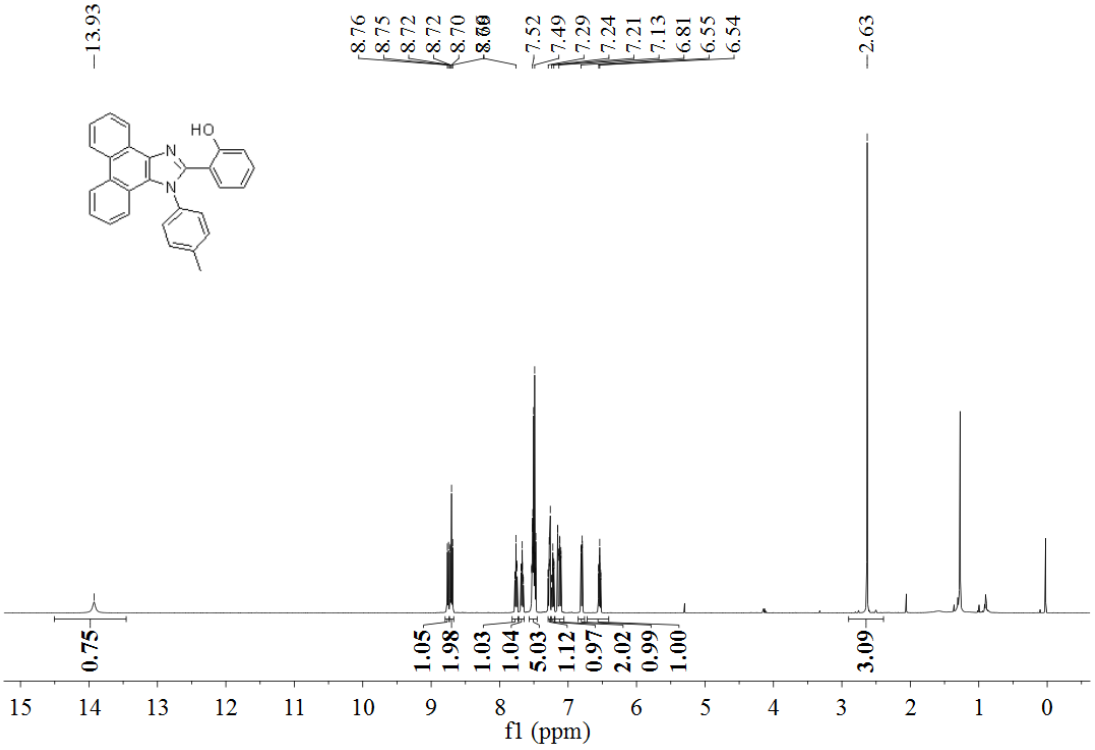

Fig. S9. ^{1}H NMR of fluorophore **Pol** (500 MHz, $CDCl_3$).

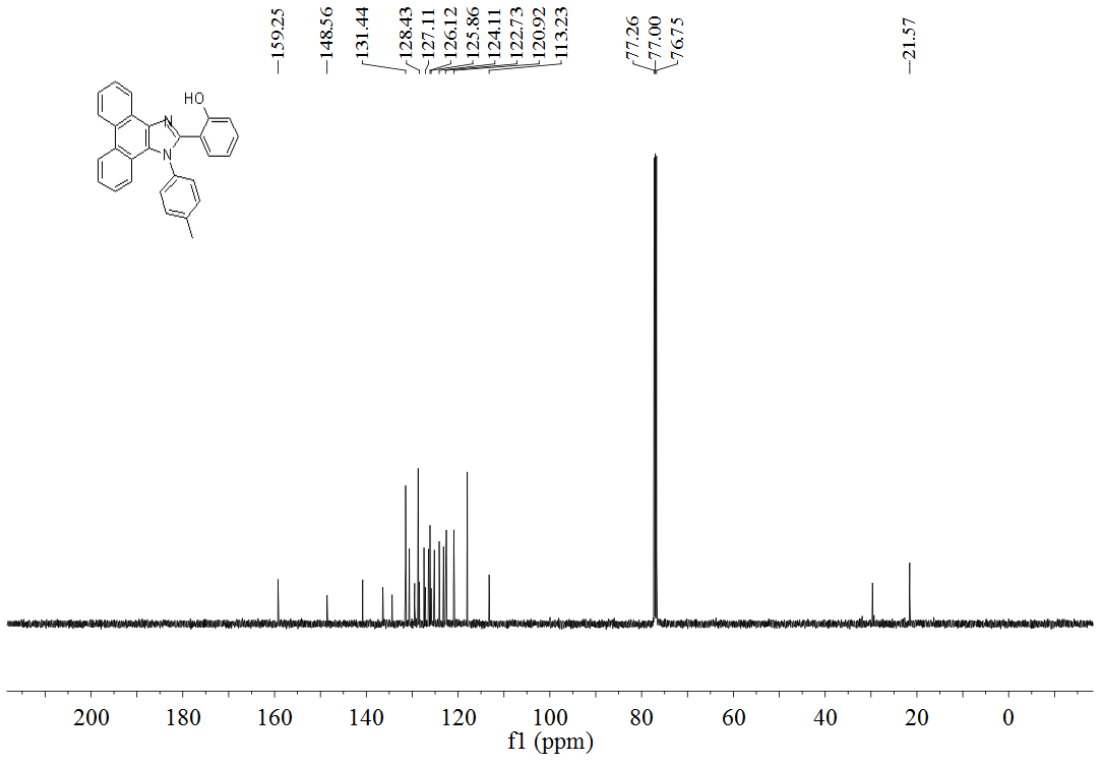

Fig. S10. ^{13}C NMR of fluorophore **Pol** (126 MHz, $CDCl_3$).

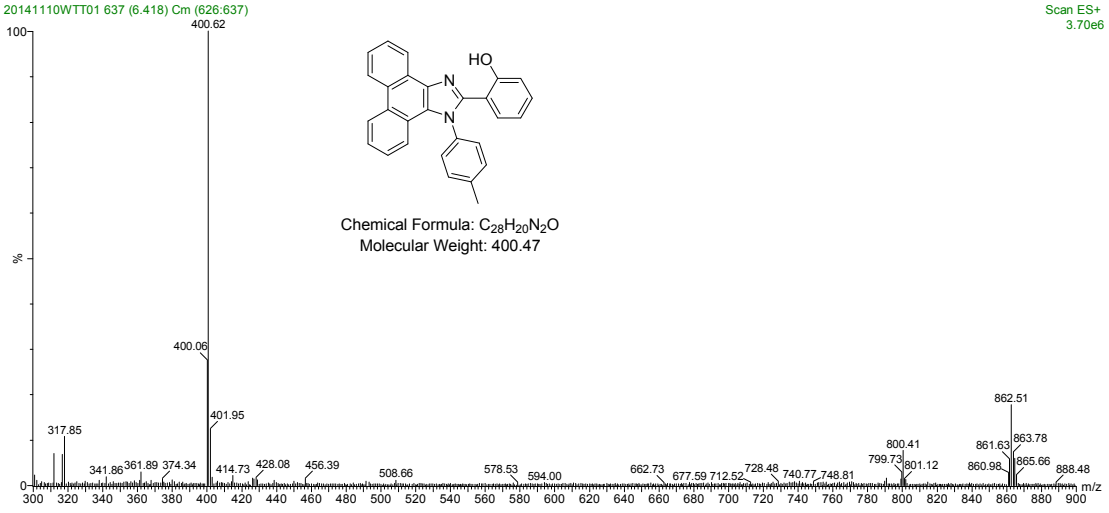

Fig. S11. Mass spectrometry spectrum of fluorophore **Pol**.

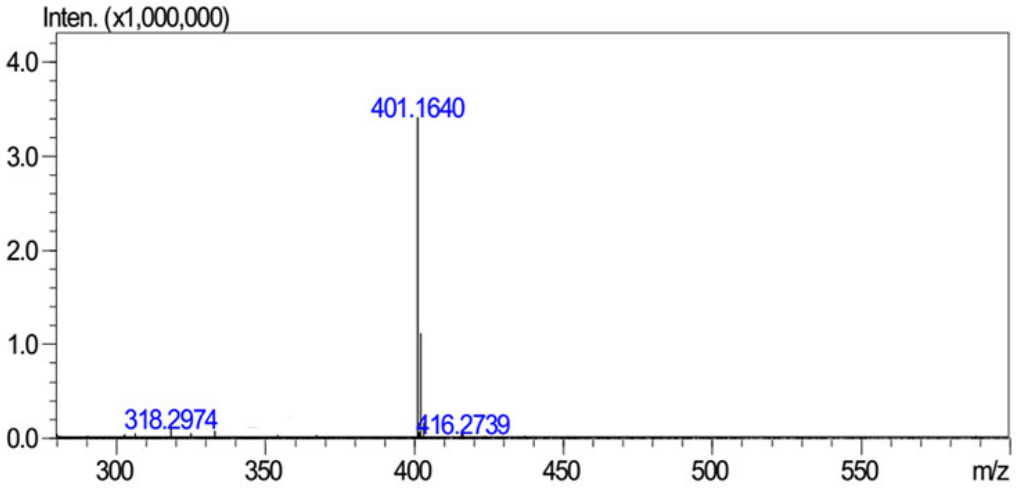

Fig. S12. HR-MS spectrum of fluorophore **Pol**.

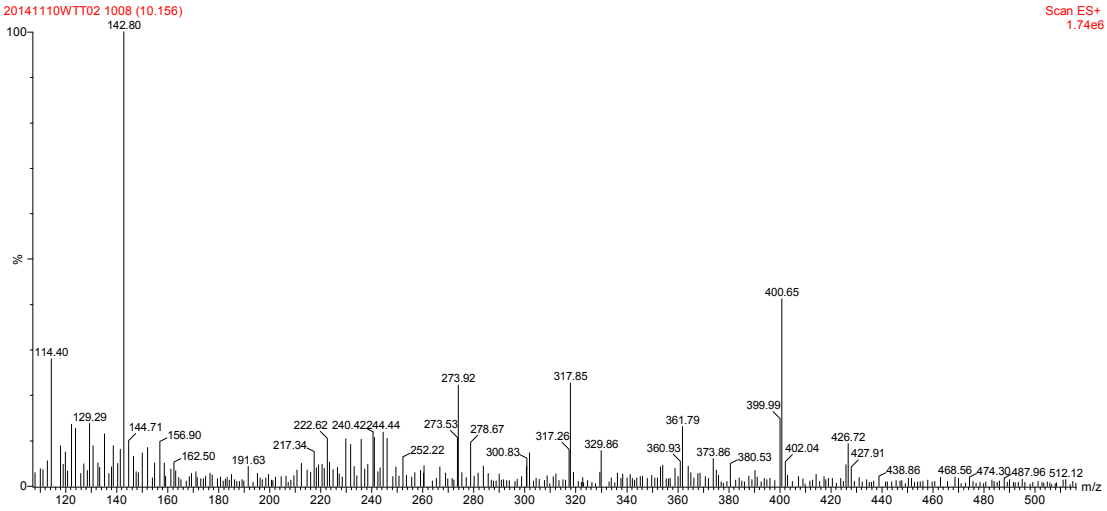

Fig. S13. Mass spectrometry spectrum of probe **Pvi** after addition of 0.5 equiv. of Hg^{2+}.