

Electronic Supplementary Information (ESI)

Novel AIE-active ratiometric fluorescent probes for mercury(II) based on the Hg²⁺-promoted deprotection of thioketal, and good mechanochromic properties

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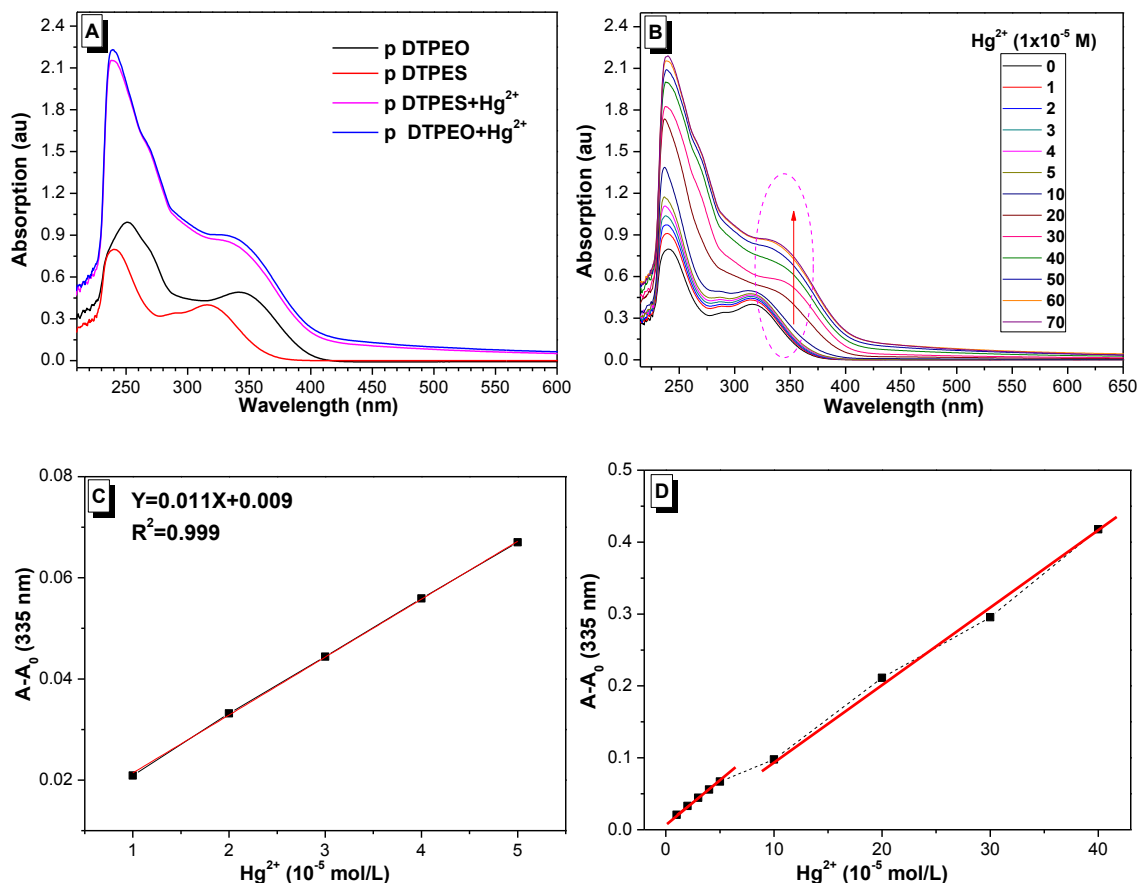


Fig. S1 (A) UV-Vis spectra of *pDTPEO* and *pDTPEs* (20 μM in THF) in presence of Hg^{2+} (6.0×10^{-4} M). (B) UV-Vis spectra of *pDTPEs* (20 μM) in the presence of different amounts of Hg^{2+} . (C) and (D) the plot of UV-Vis titration of *pDTPEs* with Hg^{2+} ions.

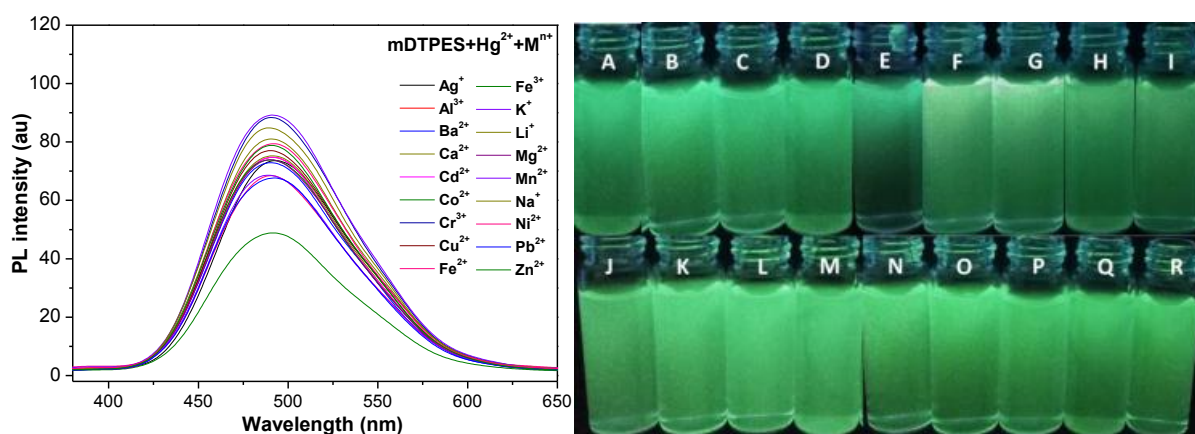


Fig. S2 Photoluminescence spectra of *mDTPEs* (20 μM) in the presence of Hg^{2+} and various metal ions (6×10^{-4} M) in THF/ H_2O (2/98, v/v) solution. And the corresponding fluorescence photos of *mDTPEs* reacted with Hg^{2+} in the presence of various metal ions. (A-R) Ag^+ , Cu^{2+} , Pb^{2+} , Co^{2+} , Fe^{3+} , Cr^{3+} , Al^{3+} , Cd^{2+} , Fe^{2+} , Mn^{2+} , Mg^{2+} , Ba^{2+} , Ca^{2+} , Ni^{2+} , Zn^{2+} , Li^+ , K^+ , Na^+ .

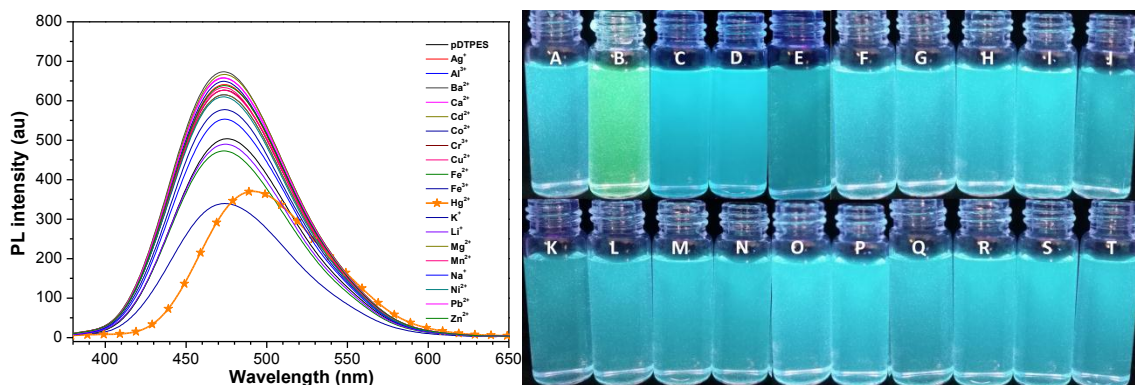


Fig. S3 Photoluminescence spectra of **pDTPES** (20 μ M) in the presence of various metal ions (6×10^{-4} M) excited at 354 nm in THF-H₂O mixtures with the water fraction of 98%. And the corresponding fluorescence photos of **pDTPES** in the presence of different metal ions. (A) **pDTPES**; (B) **pDTPES** + Hg²⁺; (C-T) **pDTPES** + Ag⁺, Cu²⁺, Fe³⁺, Pb²⁺, Co²⁺, Cr³⁺, Al³⁺, Mn²⁺, Fe²⁺, Cd²⁺, Mg²⁺, Ba²⁺, Ca²⁺, Ni²⁺, Zn²⁺, Li⁺, K⁺, Na⁺.

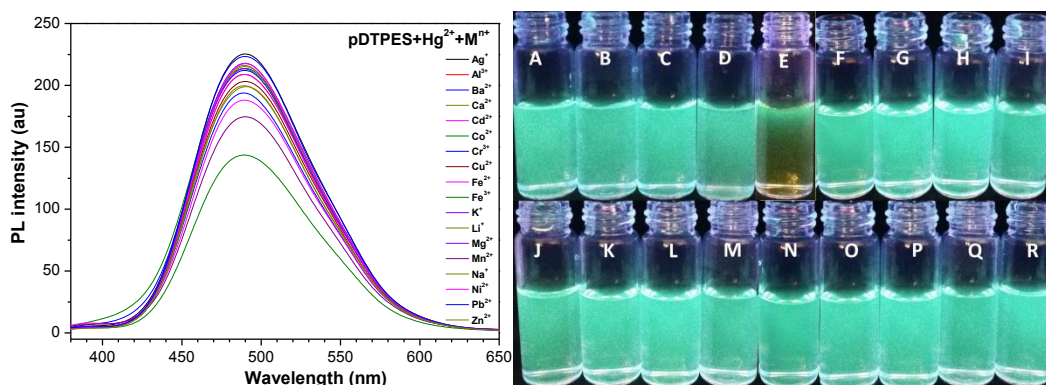


Fig. S4 Photoluminescence spectra of **pDTPES** (20 μ M) in the presence of Hg²⁺ and various metal ions (6×10^{-4} M) in THF/H₂O (2/98, v/v) solution. And the corresponding fluorescence photos of **pDTPES** reacted with Hg²⁺ in the presence of various metal ions. (A-R) Ag⁺, Cu²⁺, Pb²⁺, Co²⁺, Fe³⁺, Cr³⁺, Al³⁺, Cd²⁺, Fe²⁺, Mn²⁺, Mg²⁺, Ba²⁺, Ca²⁺, Ni²⁺, Zn²⁺, Li⁺, K⁺, Na⁺.

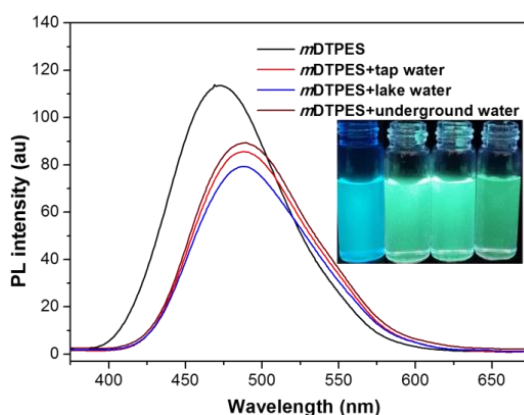


Fig. S5 Photoluminescence spectra and the corresponding fluorescence photos of **mDTPES** (20 μ M) and **mDTPES** reacted with Hg²⁺ (50 μ M) in tap water, lake water and underground water (from left to right).

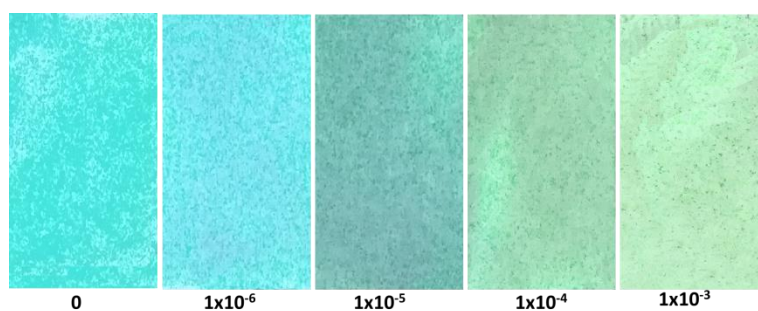


Fig. S6 Photos of fluorescence response of **pDTPES** test strips exposed to different concentrations of Hg^{2+} ions in water. From left to right: single **pDTPES** test strip; **pDTPES** test strips with different concentration of Hg^{2+} ions: 1×10^{-6} , 1×10^{-5} , 1×10^{-4} , 1×10^{-3} M.

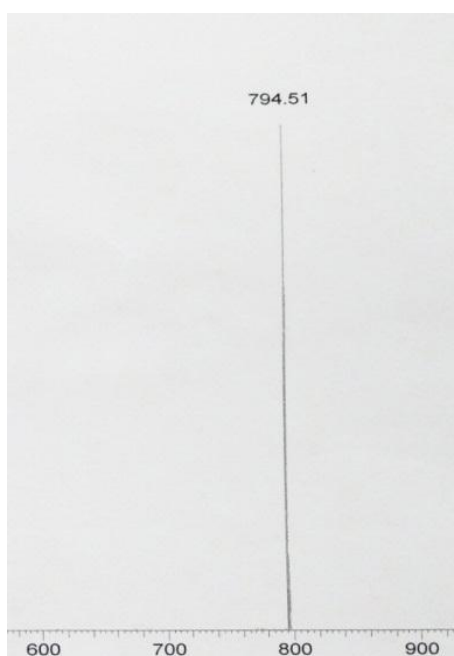


Fig. S7 MS spectrum of **mDTPES+Hg²⁺**, the same value as the formula mass of **mDTPEO**.

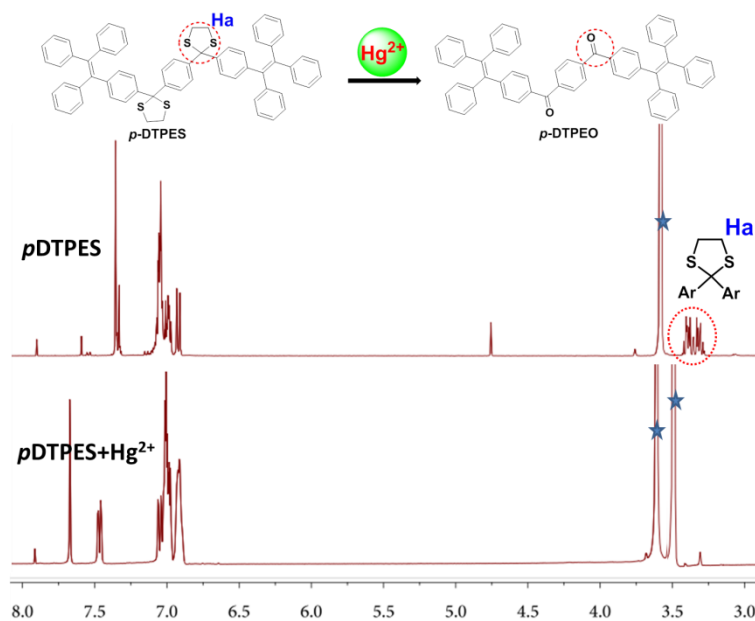


Fig. S8 ^1H NMR spectra of **pDTPES** ($\text{THF-}d_8$) before and after the addition of Hg^{2+} ions, the solvent peak is marked with asterisk.

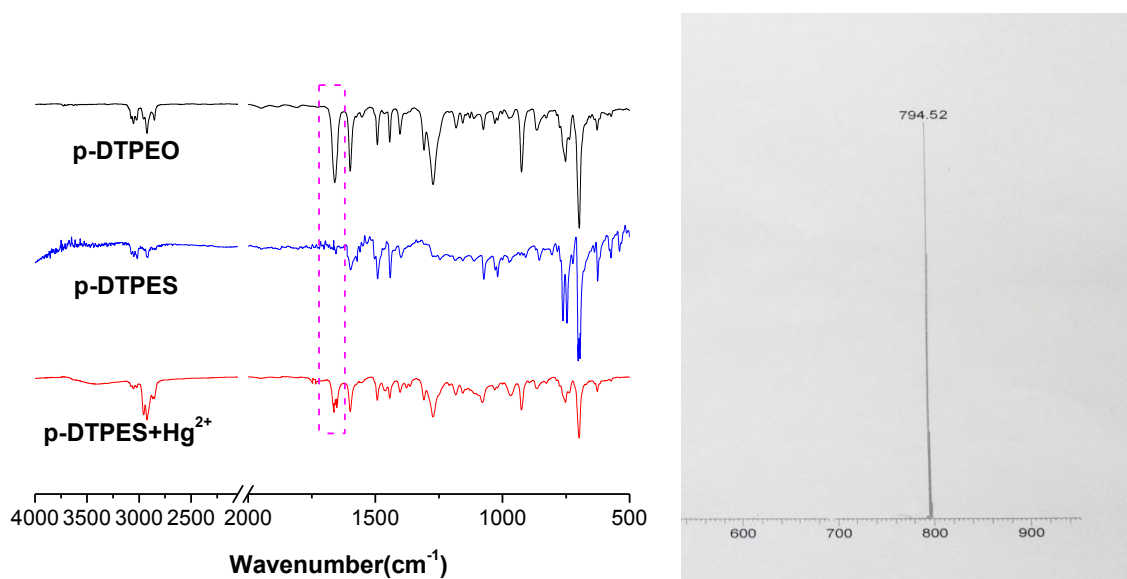


Fig. S9 IR spectra of **pDTPEO**, **pDTPES** and the reaction product of **pDTPES** with Hg^{2+} . MS spectrum of the reaction product of **pDTPES** with Hg^{2+} , the same value as the formula mass of **pDTPEO**.

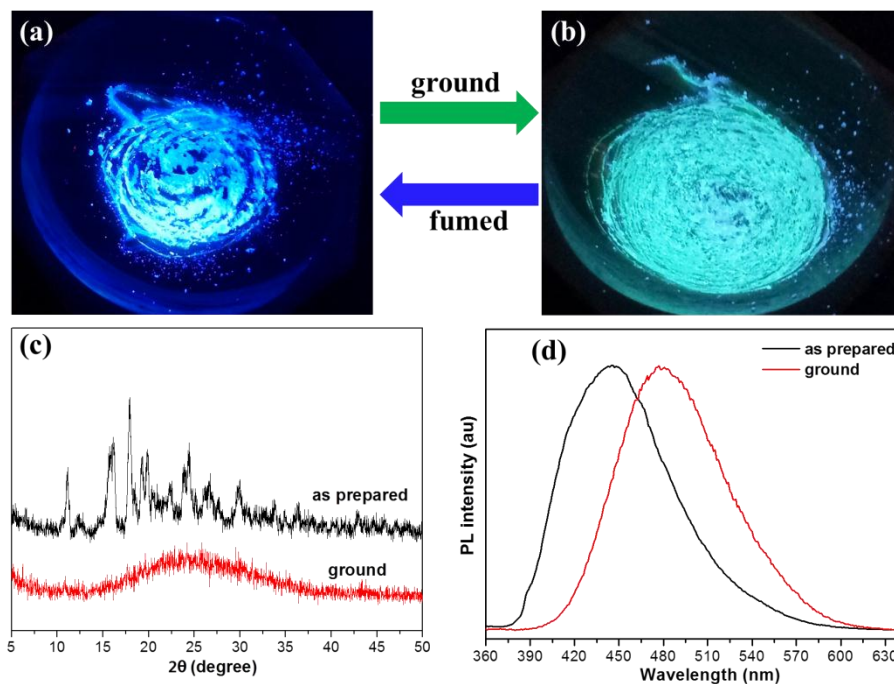


Fig. S10 Fluorescent photos of a) as prepared and b) ground samples of *pDTPES* taken under UV illumination, c) XRD diffractograms of as prepared and ground powders of *pDTPES*, d) PL spectra of as prepared and ground powders of *pDTPES*.

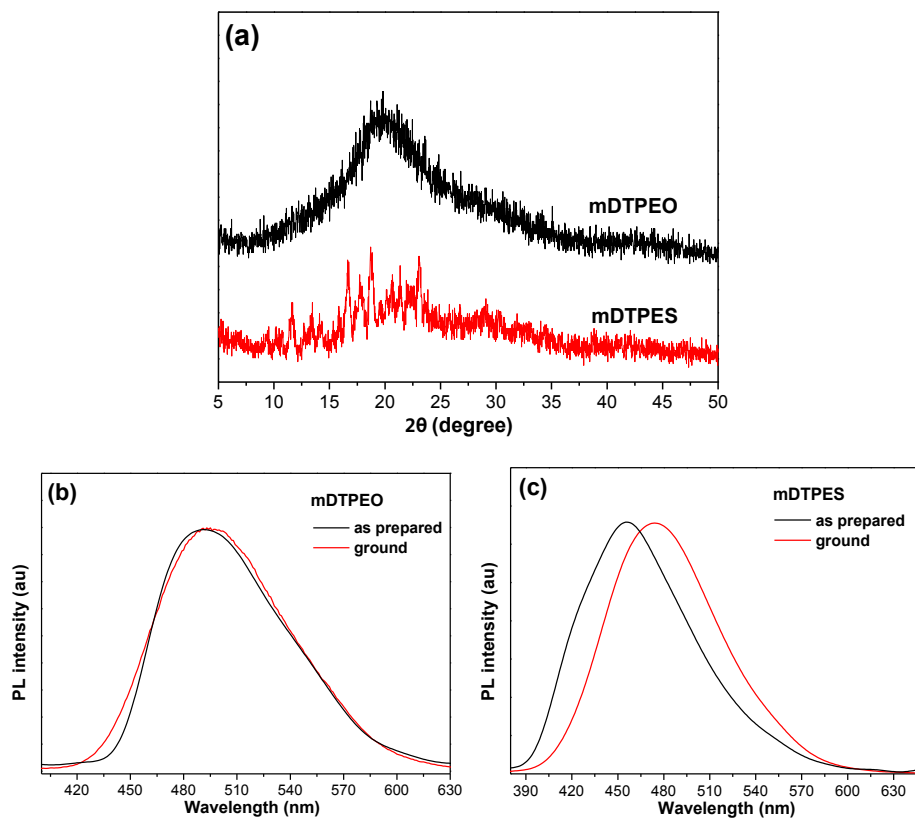


Fig. S11. (a) XRD diffractograms of as prepared powders of *mDTPEO* and *mDTPES*; PL spectra of as prepared and ground powders of *mDTPEO* (b) and *mDTPES* (c).

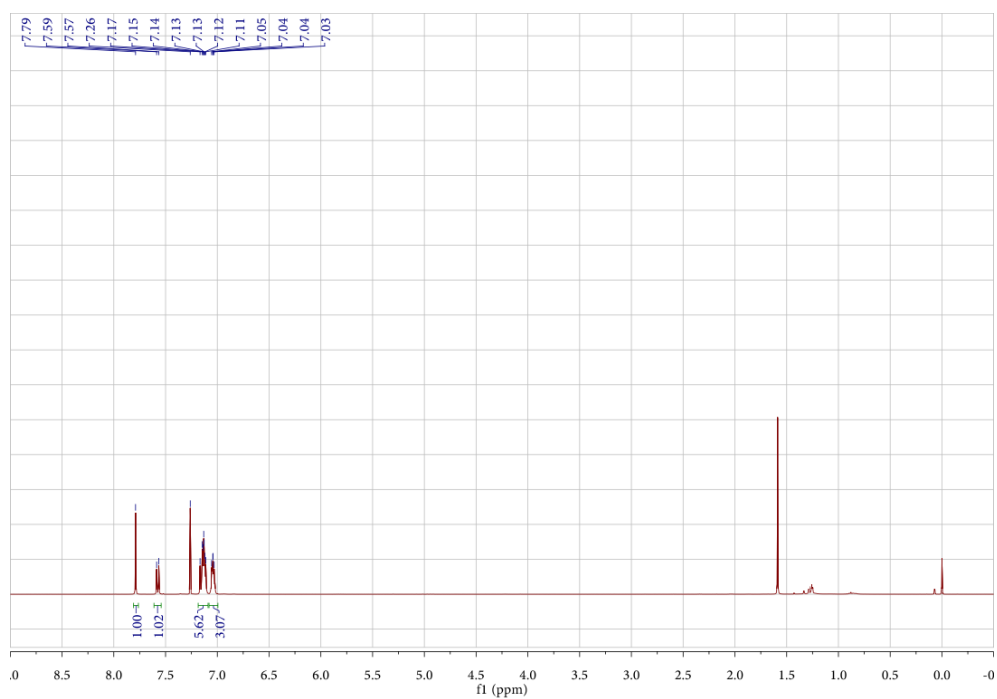


Figure S12. ¹H NMR of *p*DTPEO in CDCl₃.

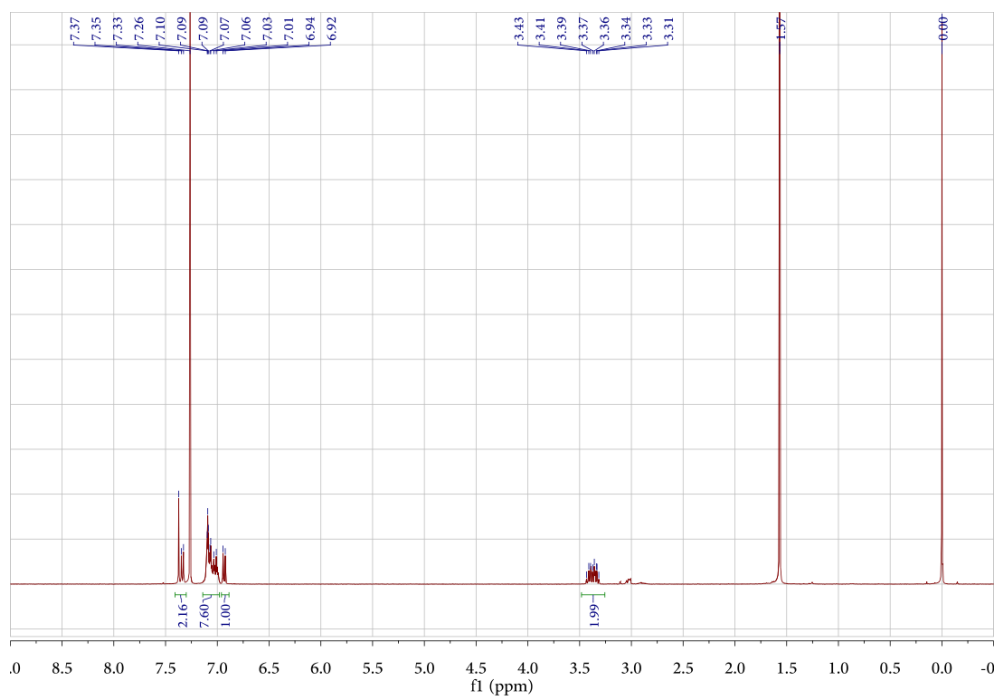


Figure S13. ¹H NMR of *p*DTPES in CDCl₃.

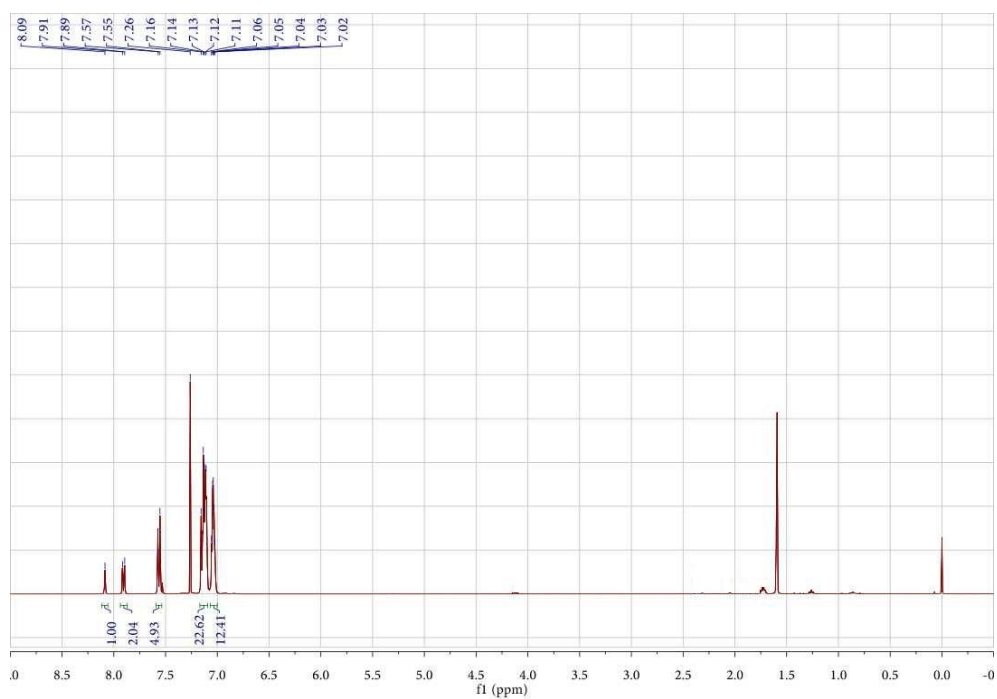


Figure S14. ¹H NMR of *m*DTPEO in CDCl₃.

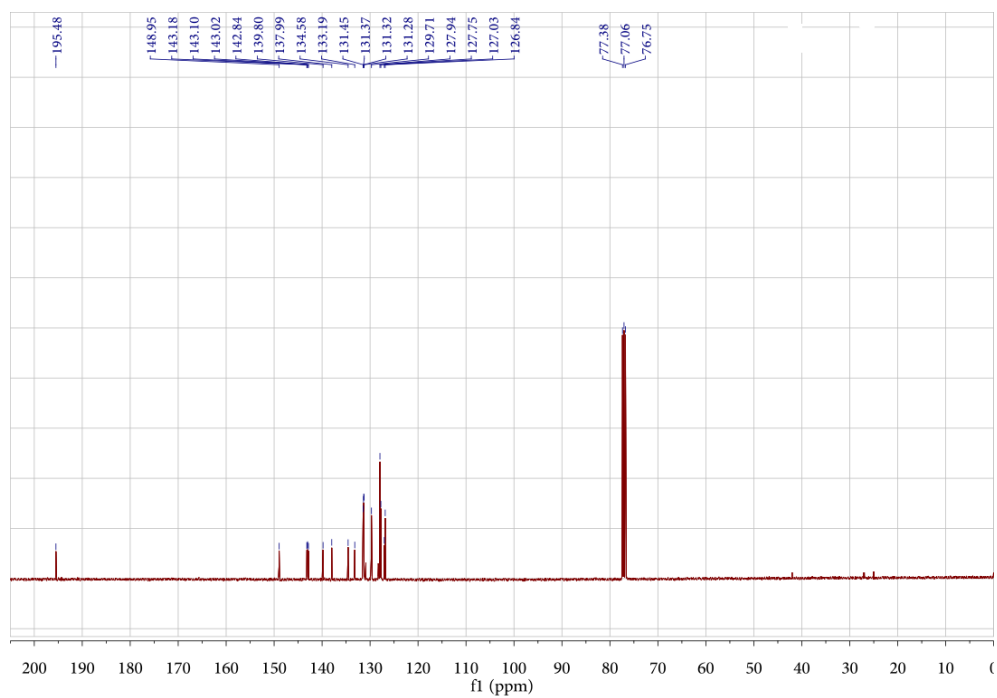


Figure S15. ¹³C NMR of *m*DTPEO in CDCl₃.

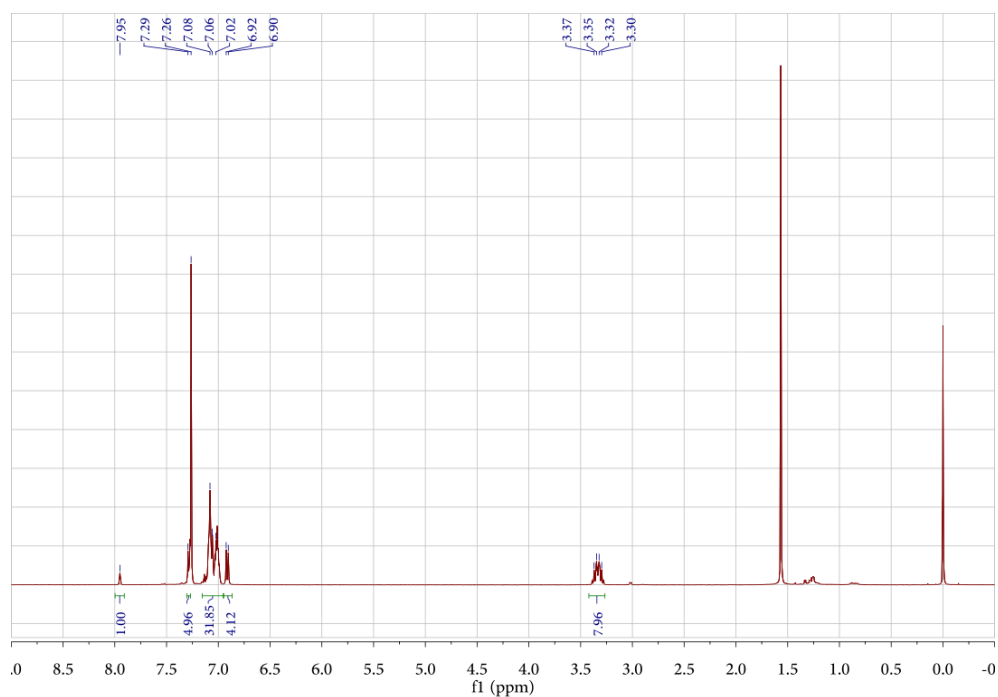


Figure S16. ¹H NMR of *m*DTPES in CDCl₃.

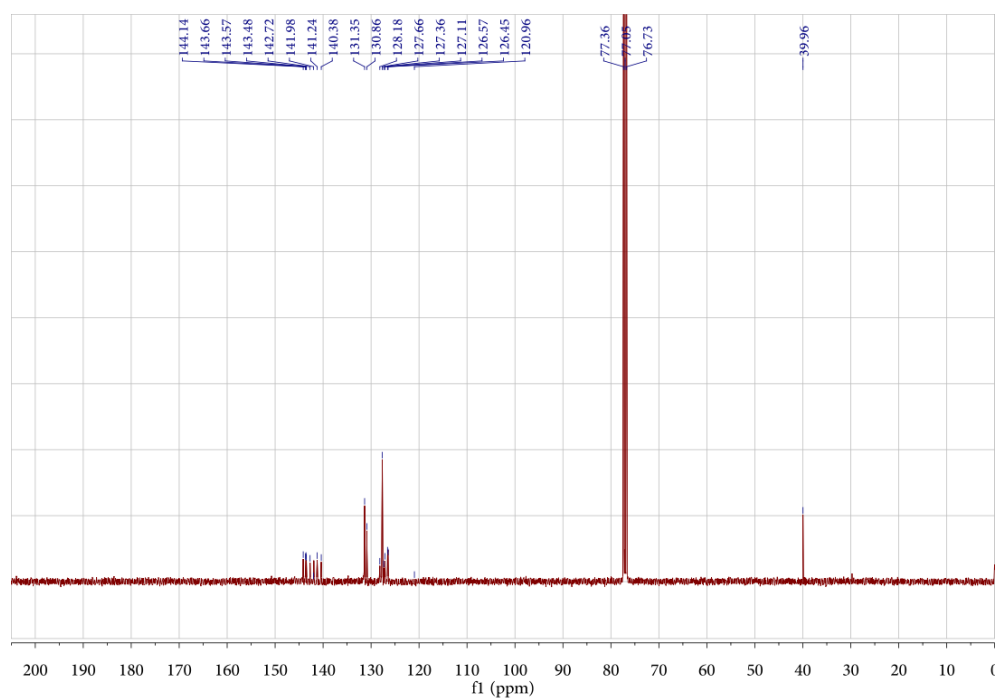


Figure S17. ¹³C NMR of *m*DTPES in CDCl₃.