

Supporting Information

An ultra-sensitive and ratiometric fluorescent probe based on the DTBET process for Hg²⁺ detection and imaging applications

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Supplementary Tables and Figures

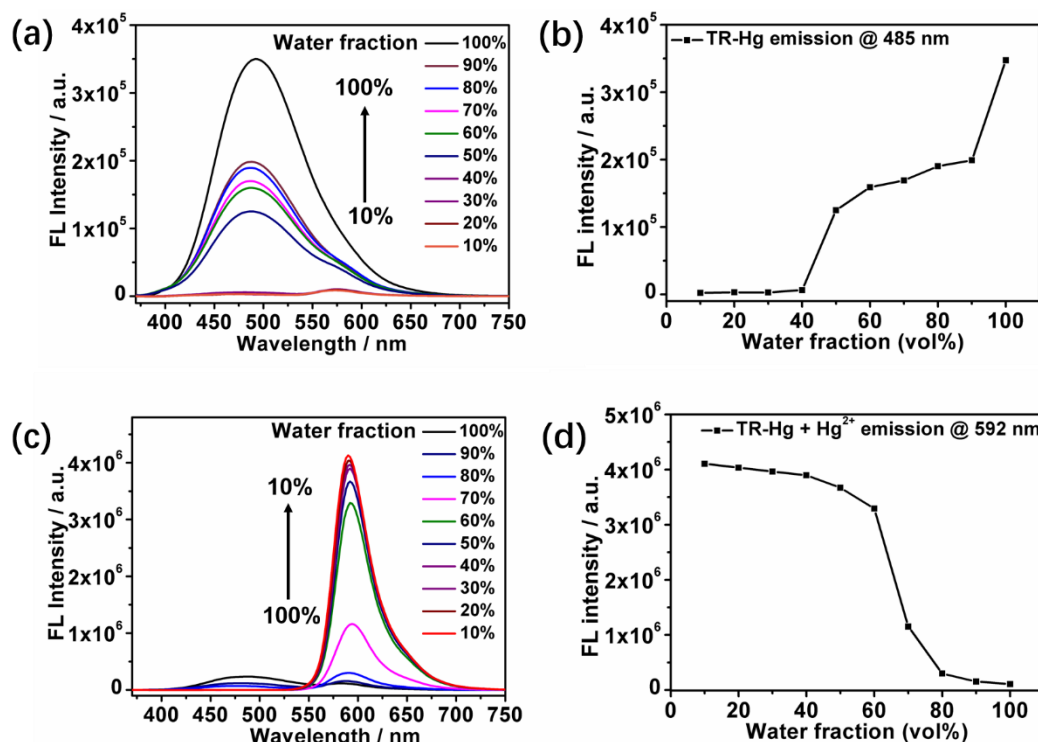
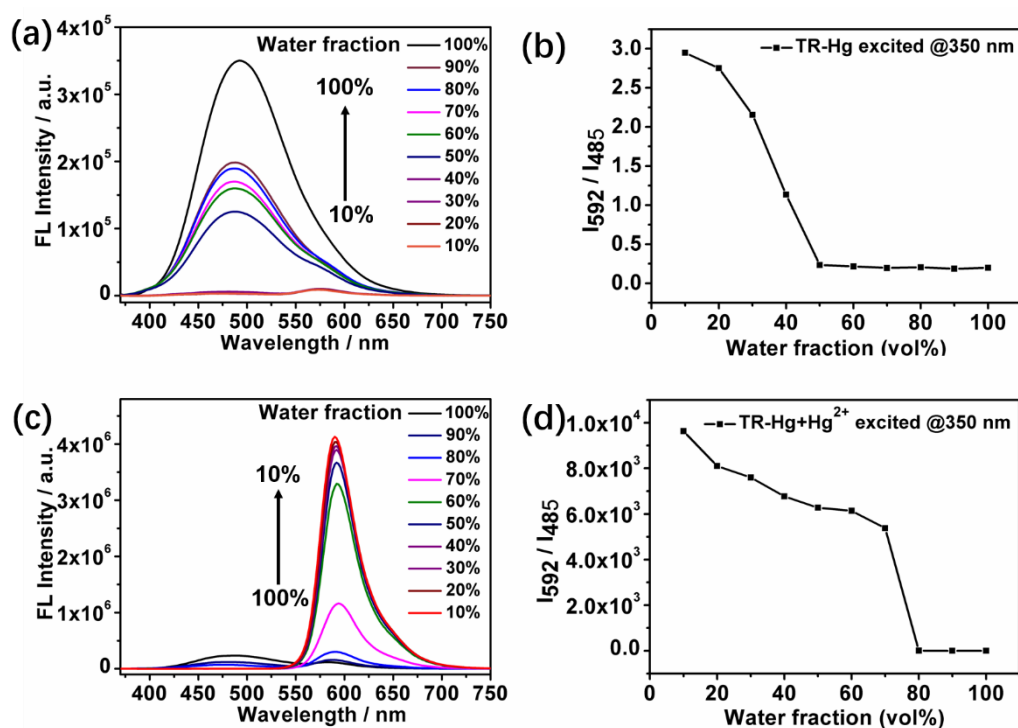


Fig. S1. (a) Fluorescence spectra of TR-Hg (10 μ M) in different water fraction; (b) fluorescence intensity of TR-Hg (10 μ M) at 485 nm in different water fraction; (c) fluorescence spectra of the reaction mixture of TR-Hg (10 μ M) and Hg^{2+} (10 μ M) in different water fraction; (d) fluorescence intensity of the reaction mixture of TR-Hg (10 μ M) and Hg^{2+} (10 μ M) at 592 nm in different water fraction. Ex: 350 nm.



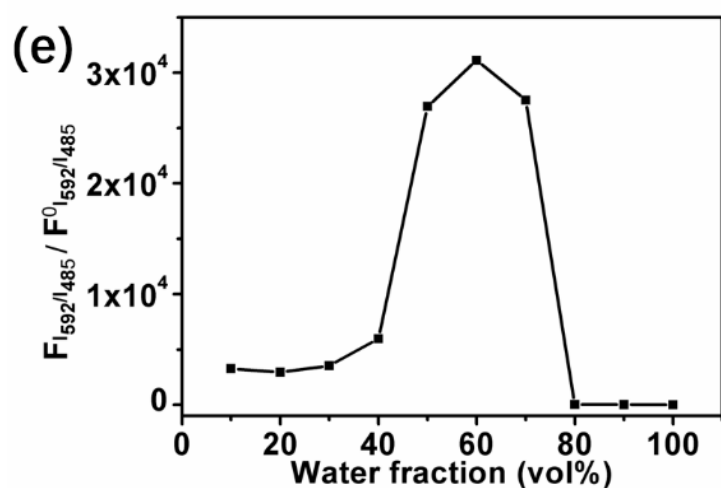


Fig. S2. (a) Fluorescence spectra of TR-Hg (10 μ M) in different water fraction; (b) fluorescence ratio (I_{592}/I_{485}) change of TR-Hg (10 μ M) in different water fraction; (c) fluorescence spectra of the reaction mixture of TR-Hg (10 μ M) and Hg^{2+} (10 μ M) in different water fraction; (d) fluorescence ratio (I_{592}/I_{485}) change of the reaction mixture of TR-Hg (10 μ M) and Hg^{2+} (10 μ M) in different water fraction; (e) the ratio change of TR-Hg (10 μ M) in the absence and presence of Hg^{2+} (10 μ M) in the different water fraction. Ex: 350 nm.

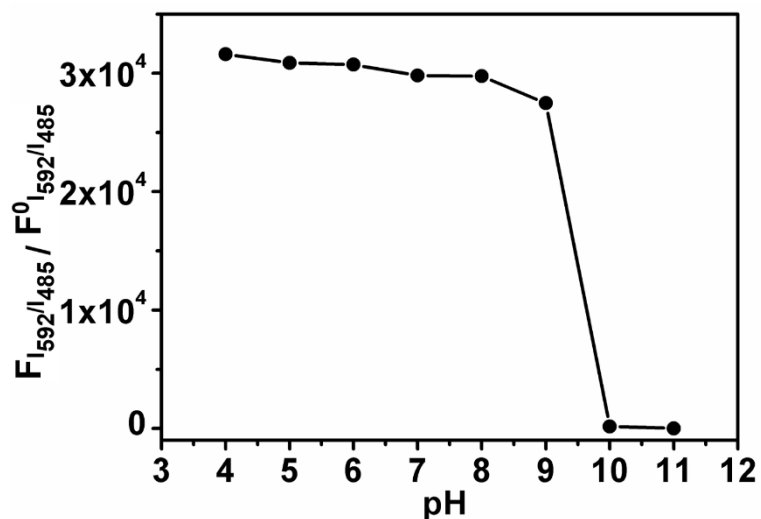


Fig. S3. The variation of enhanced fold of TR-Hg (10 μ M) in the presence of 10 μ M Hg^{2+} over a pH range of 4-11.

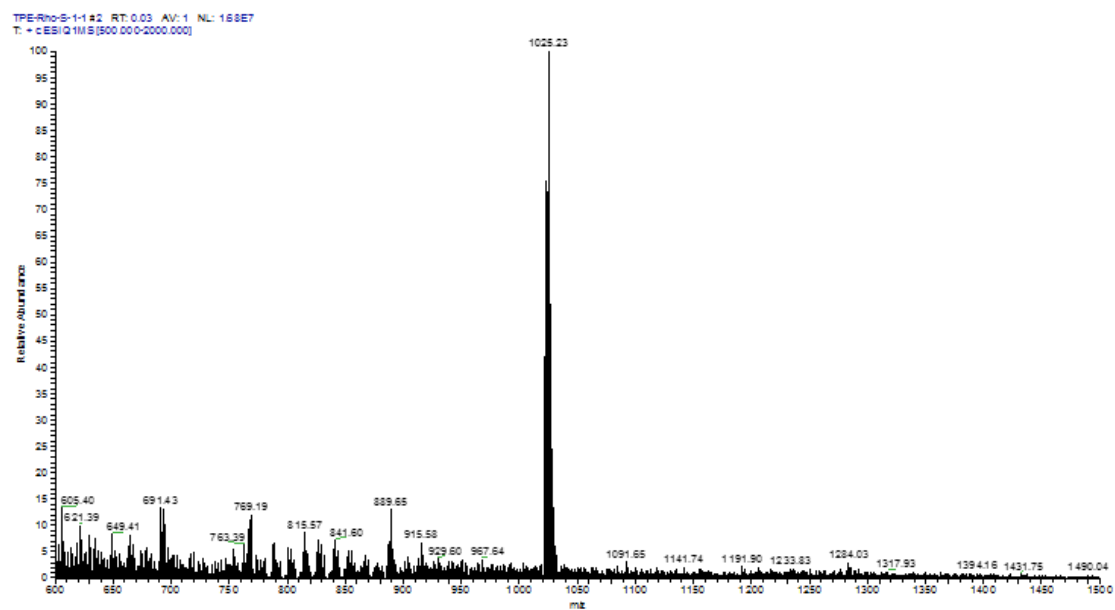


Fig. S4. Mass spectra of TR-Hg with 5 equiv. Hg^{2+} after 10 min incubation.

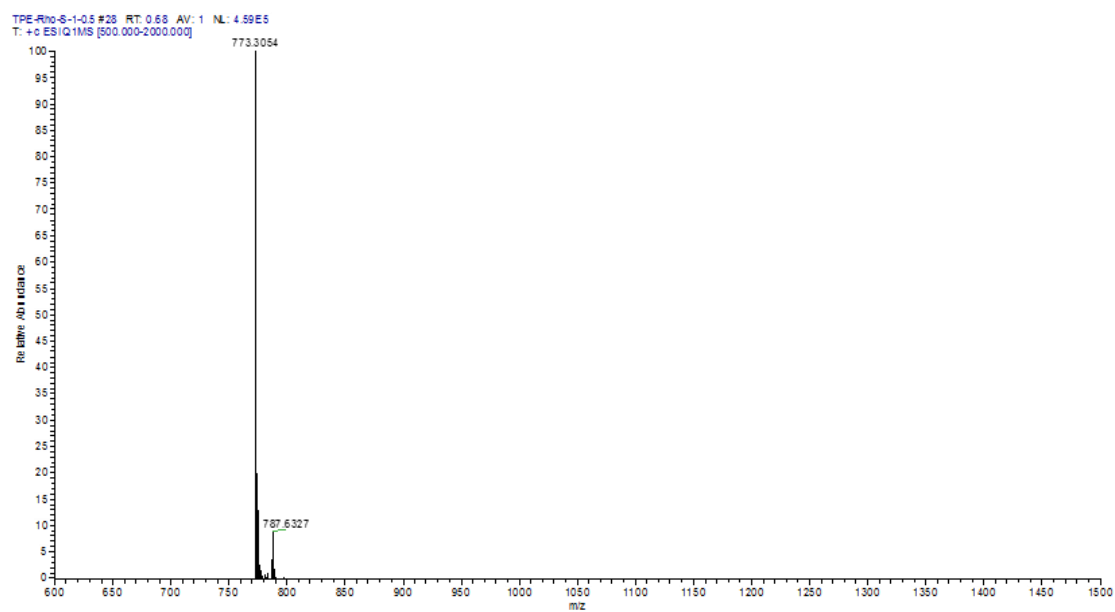


Fig. S5. Mass spectra of TR-Hg with 10 equiv. Hg^{2+} after 10 min incubation.

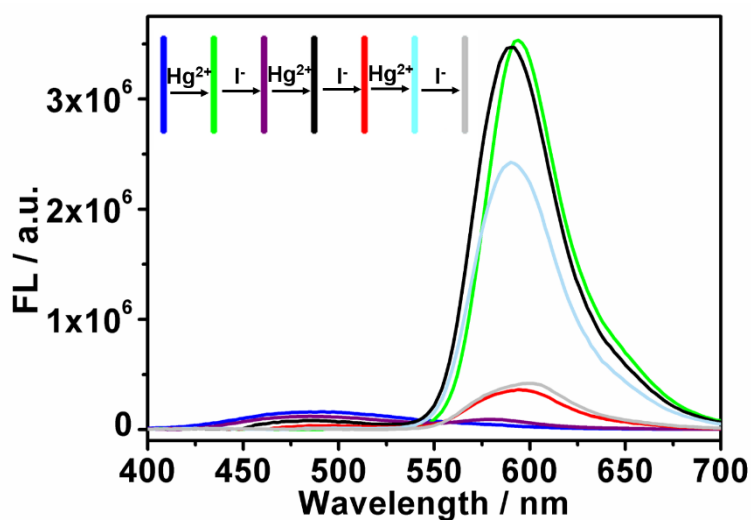


Fig. S6. Fluorescence spectra of TR-Hg (10 μM) using Hg²⁺ (20 μM) and I⁻ (50 μM) for the reversible test.

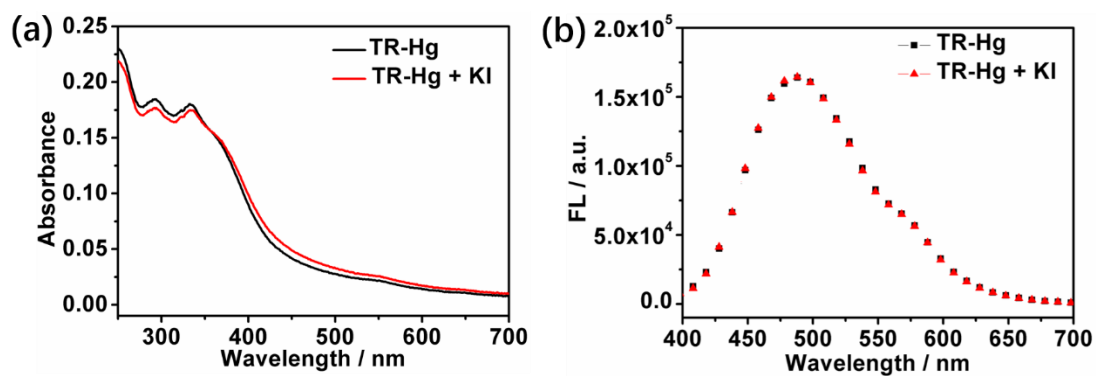


Fig. S7. Absorption (a) and emission (b) spectra of TR-Hg (10 μM) and the mixture and TR-Hg (10 μM) and KI (50 μM).

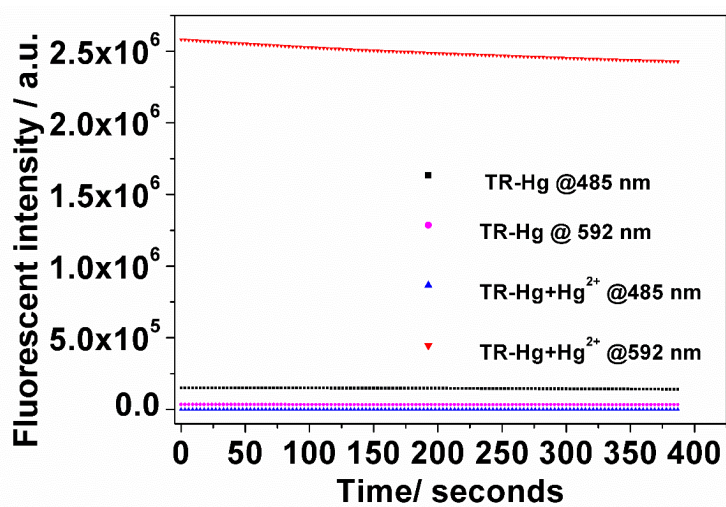


Fig. S8. Stability test of TR-Hg and the reaction product of TR-Hg and Hg²⁺ under the excitation at 355 nm.

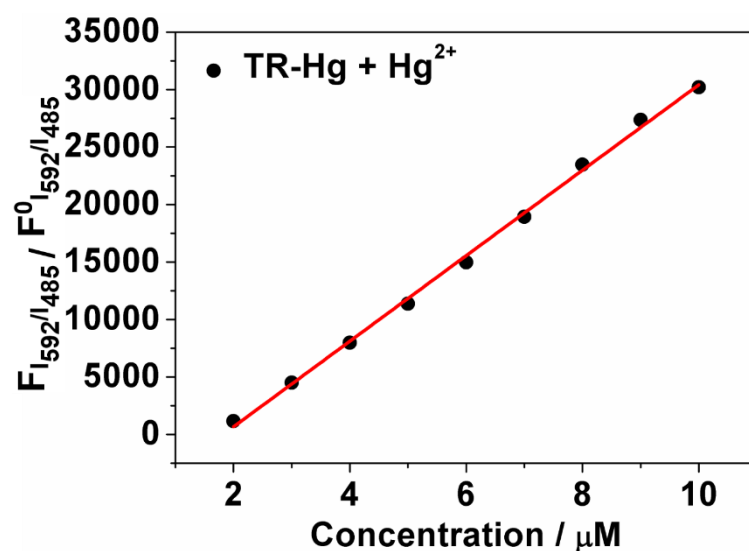


Fig. S9. The linear relationship between the enhanced fold of fluorescence (I_{592}/I_{485}) and Hg^{2+} at the concentration range from 2 to 10 μM .

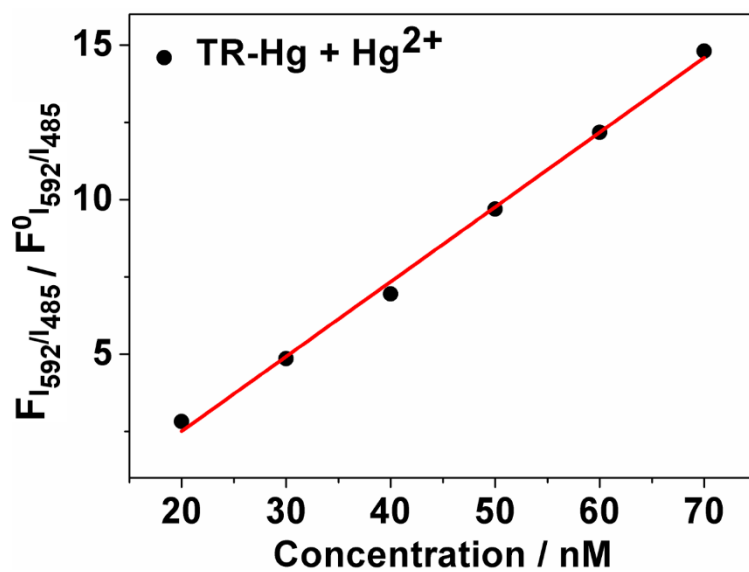


Fig. S10. The linear relationship between the enhanced fold of fluorescence (I_{592}/I_{485}) and Hg^{2+} at the concentration range from 20 to 70 nM.

Table S1. Properties of representative fluorescent ratiometric Hg²⁺ probes

probe	λ_{ex} /nm	λ_{em} /nm	FEF ^a /fold	Detection limit ^b /nM	Reaction time ^c	application
MS5 J. Am. Chem. Soc. 2007, 129, 5910-5918	499	524↑ 624↓	~	50	~	Charles River water, Newburyport water, Onondaga Lake water
3 Angew. Chem. Int. Ed. 2008, 47, 8025-8029	488	514↓ 589↑	~	~	~	In MCF-7 cells
4 Dyes and Pigments 2012, 92, 909-915	400	545↓ 585↑	65	30	~	~
3 J. Mater. Chem., 2012, 22, 4003-4008	330	475↑ 533↓		96	~	In living HeLa cells
Probe 1 Chem. Commun., 2012, 48, 8371-8373	408	472↓ 541↑	~	4.9	~	In Hep G2 cells
1 Dyes and Pigments 2015, 120, 208-212	440	478↓ 587↑	994	3.2	~	In Hela cells
ITR J Fluoresc 2015, 25, 1259-1266	390	490↓ 590↑	65	11	Within 5 min	In MCF-7 cells
Pvi Analyst, 2015, 140, 2778-2784	334	380↓ 477↑	~	7.8	within 80 min	In HeLa cells
BN-S Org. Biomol. Chem., 2015, 13, 3032-3039	320	503↓ 534↑	~	72.7	about 5 min	~
1 J Fluoresc 2015, 25, 319-325	380	515↓ 600↑	97	77	within 1 min	~
TMUHg-1 Dyes and Pigments 2017, 146, 136-142	380	466↓ 584↑	41.4	0.93	Within 5 min	In living cells
P-Hg Sensors and Actuators B 2017, 247, 626-631	350	465↓ 545↑	12.6	5.8	Within 10min	In bovine serum solution
TMUHg-3 Sensors and Actuators B 2017, 251, 410-415	380	464↓ 584↑	55.7	18.8	in 20 min	In living Glioma cells
3TS Analytica Chimica Acta 2018, 1023, 105-114	360	450↓ 550↑	14	10.3	Within 1 min	filter paper and TLC strips water, soil samples and seafood
M2 Sensors and Actuators B 2018, 255, 3074-3084	350	389↓ 560↑	None	91	Within 1.5min	Tap water samples; M2-doped agarose gels
ATC-Hg Chem. Commun., 2018, 54, 4955-4958	405	492↓ 572↑	24	27	within 3 min	In HeLa cells and E. coli; in the water samples from the Funan river
PYJO4 J. Mater. Chem. B, 2016, 4, 4934-4940	405	530↑ 665↓	6	5.7	~	In MCF-7 cells

Py-Met Org. Lett., 2011, 13, 5028-5031	342	383↓ 480↑	195	57.2	~	~
p-TPE-RNS Chem. Sci., 2017, 8, 2047-2055	355	485↓ 592↑	3,500	2 (1 ppb)	~	In HeLa cells
m-TPE-RNS Chem. Sci., 2017, 8, 2047-2055	355	480↓ 592↑	6,100	0.6 (0.3 ppb)	~	In HeLa cells
1 J Fluoresc 2014, 24, 473-480	468	529↓ 569↑	~	230	~	~
R1 Analyst, 2013, 138, 2654-2660	430	480↓ 695↑	~	28	within 10 s	In HeLa cells
L1 RSC Adv., 2014, 4, 14919-14927	330	440↓ 575↑	45	450	~	In HeLa cells
1 Tetrahedron Letters 2011, 52, 4775-4778	438	469↓ 492↑	~	2700	within 40 min	~
L2 J. Photochem. Photobio. A: Chem 2015, 311, 127-136	420	525↓ 580↑	30	5.7	~	In E. Coli and incubated bacteria
1 B. Kor. Chem. Soc. 2011, 32, 3959-3962	312	380↓ 445↑	~	17000	within 12 min	~
TR-Hg This work	355	485↓ 592↑	>30,000	0.043	within 10 s	Tap water samples Test-stripe for naked-eye test Onion tissues imaging

^a The fluorescence ratio changes before and after interaction with Hg²⁺;

^b The reported detection limit of corresponding probes;

^c The reaction time for responding to Hg²⁺;

~ Not mentioned.

Table S2. Application of TR-Hg to detect Hg²⁺ in tap water.

Sample	Added (nM)	Detect (nM)	Recovery	Relative error (%)
Tab water 1	50	49.05±0.17	98.1	1.9
	80	79.90±0.79	99.8	0.2
Tab water 2	50	50.25±0.71	100.5	0.5
	80	79.11±0.89	98.9	1.1
Tab water 3	50	48.88±0.11	97.8	2.2
	80	81.38±0.17	101.7	1.7

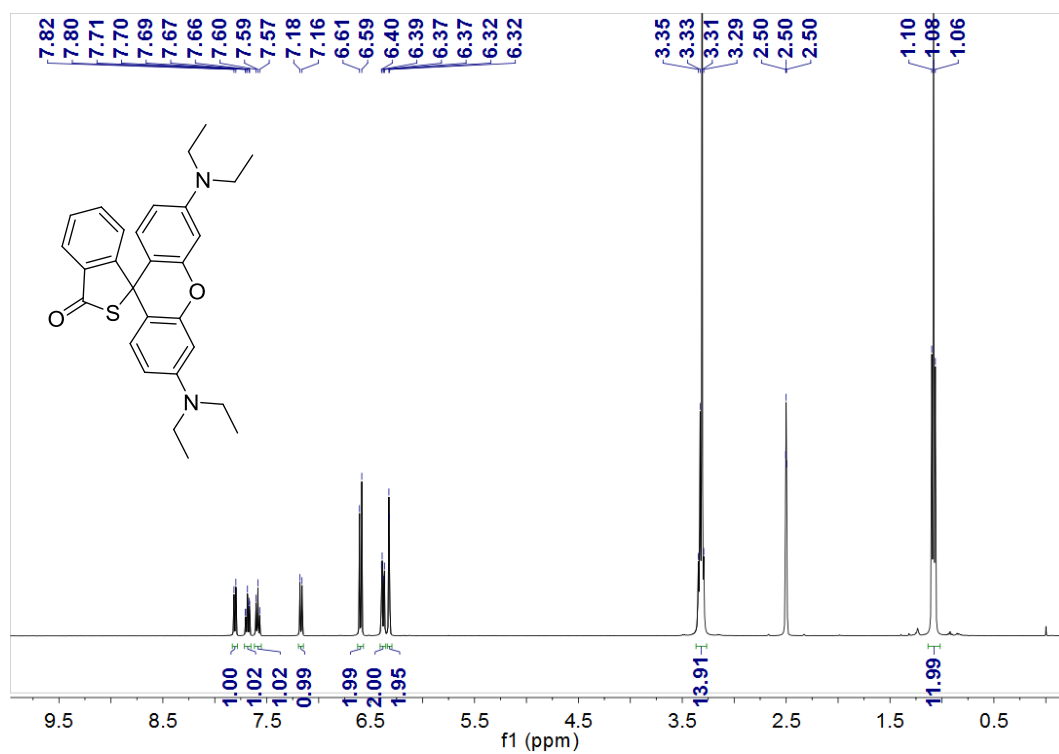


Fig. S11. ¹H NMR of compound Rhod-S (DMSO-d₆).

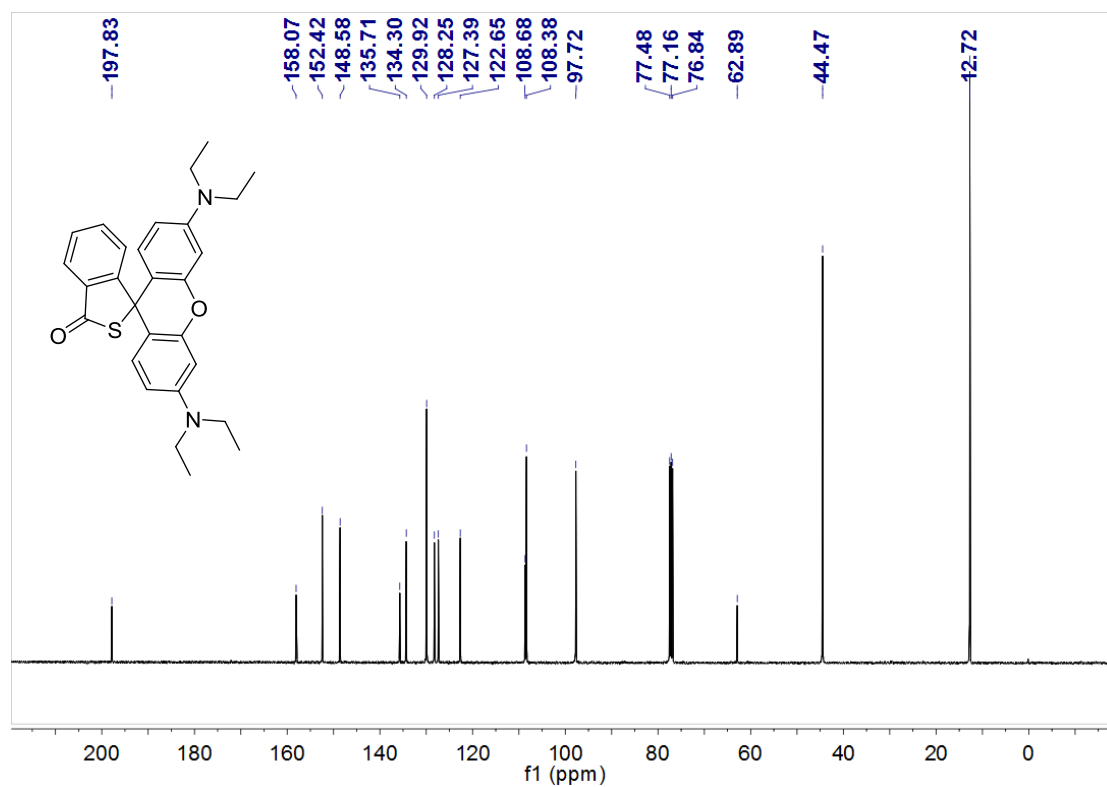


Fig. S12. ¹³C NMR of compound Rhod-S (CDCl₃).

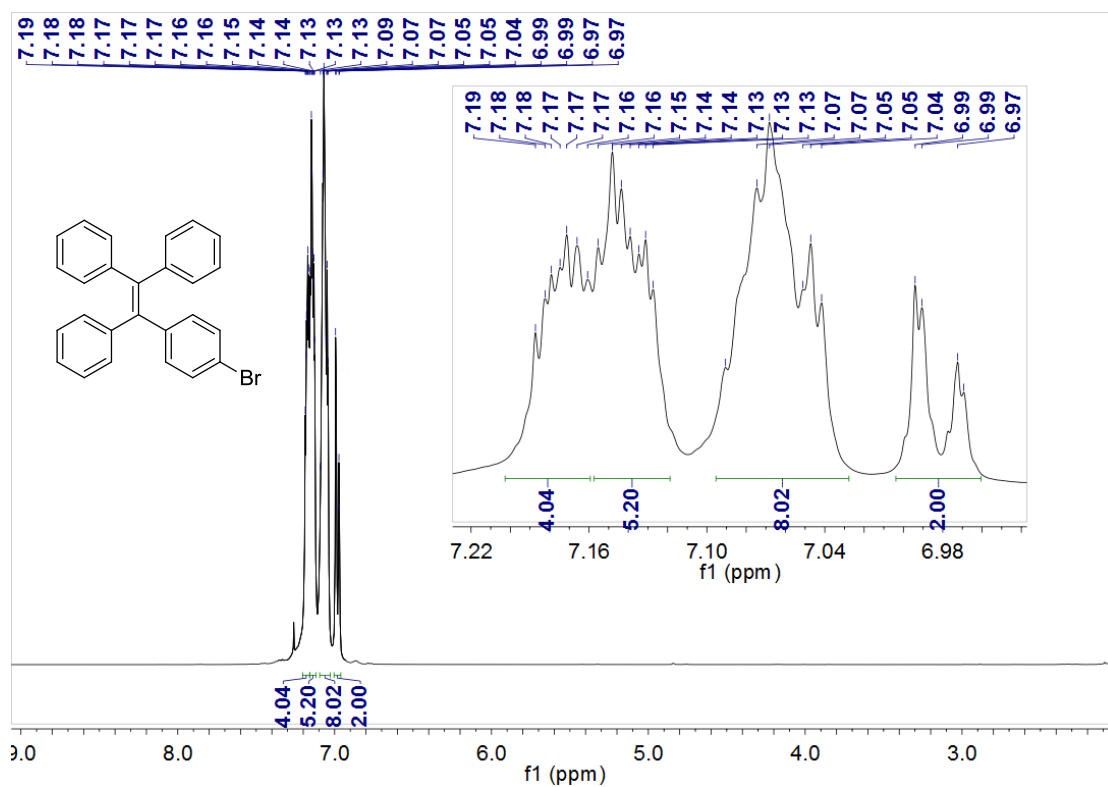


Fig. S13. ¹H NMR of compound TPE-Br (CDCl₃).

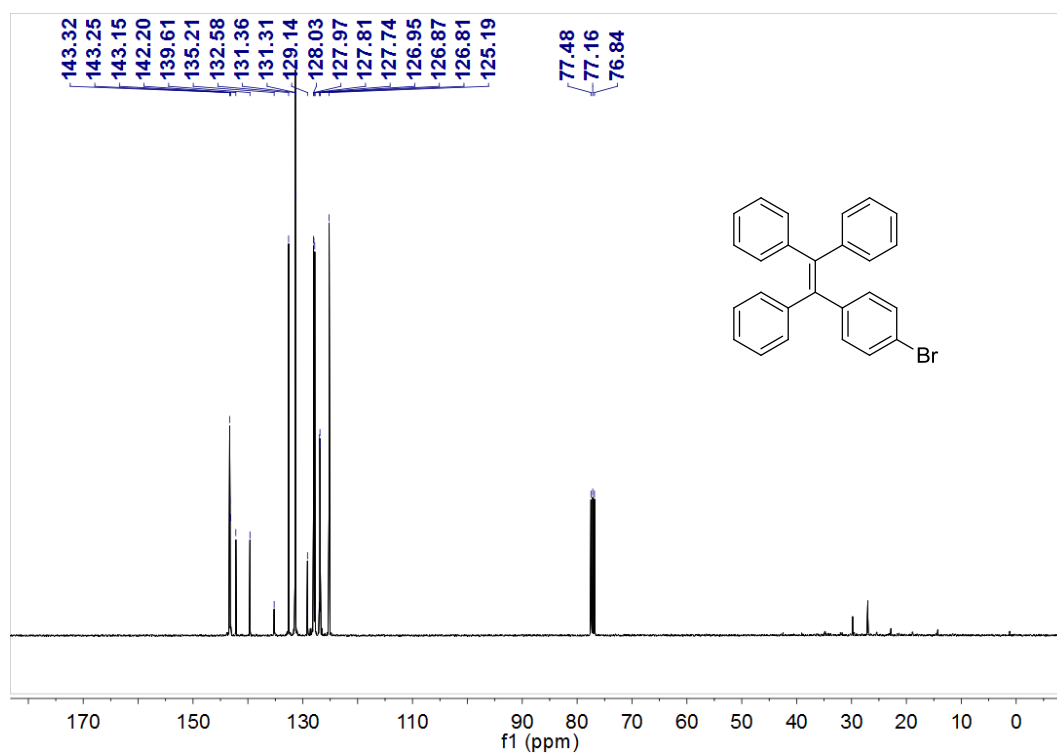


Fig. S14. ¹³C NMR of compound TPE-Br (CDCl₃).

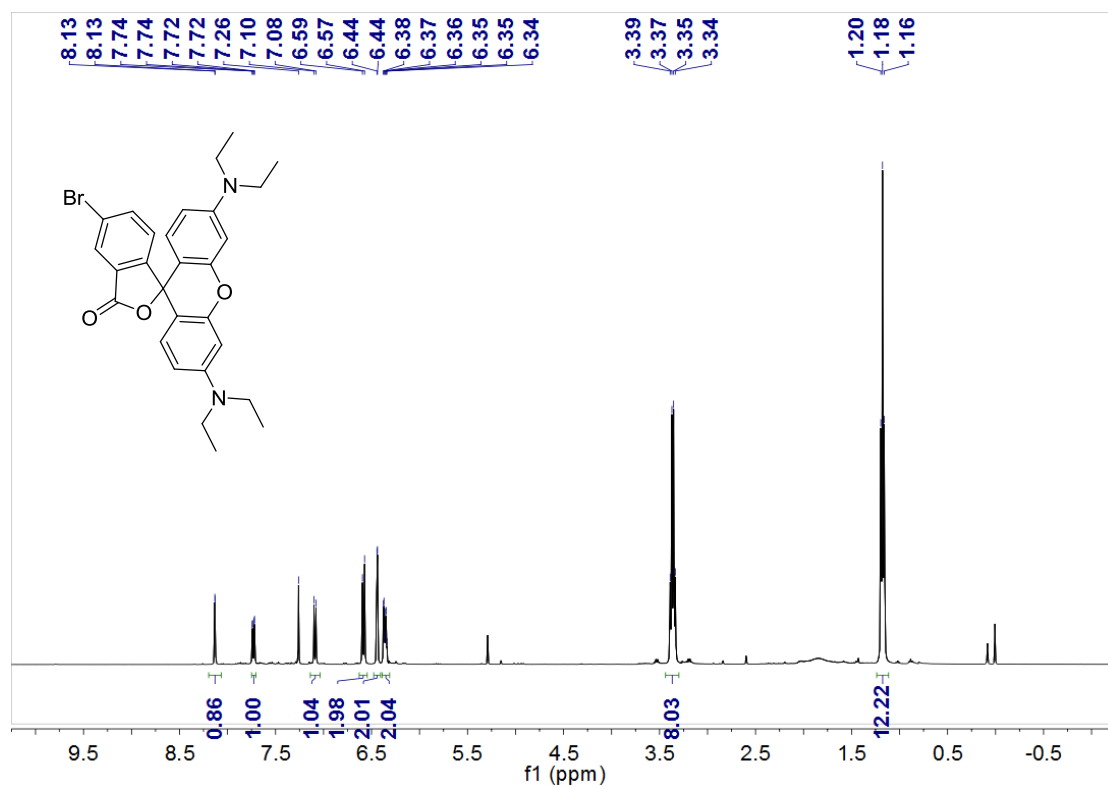


Fig. S15. ¹H NMR of compound Rhod-Br (CDCl₃).

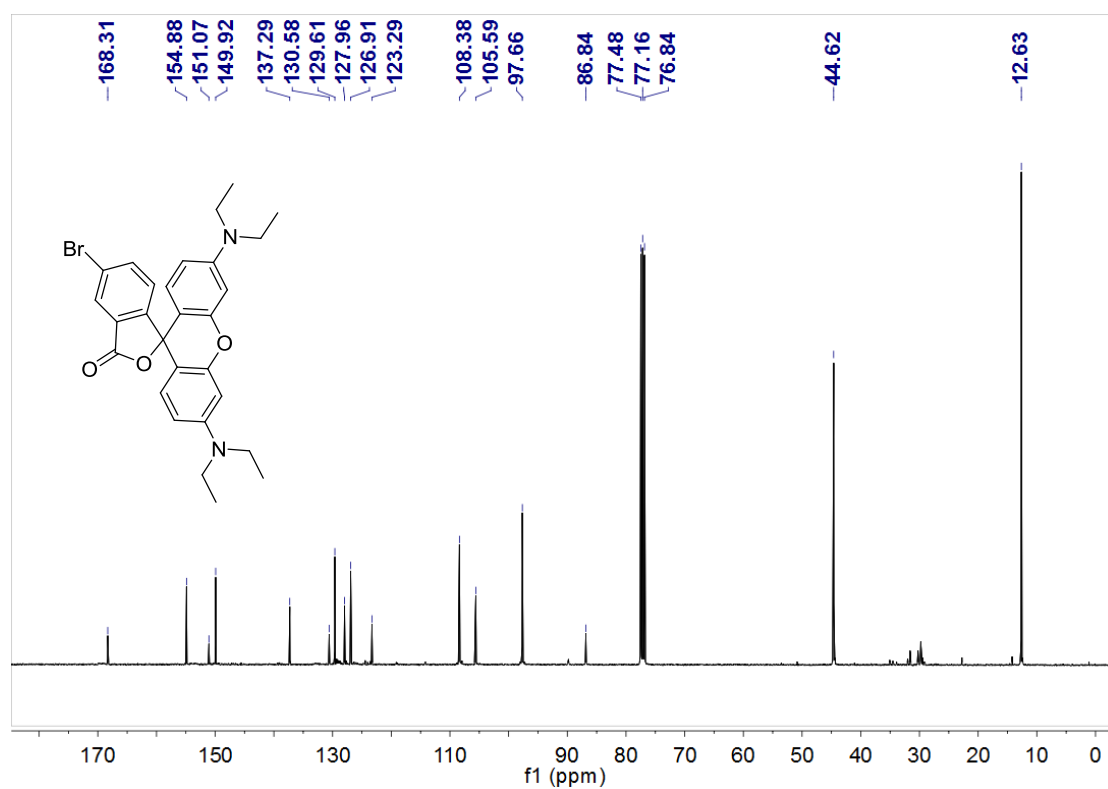


Fig. S16. ¹³C NMR of compound Rhod-Br (CDCl₃).

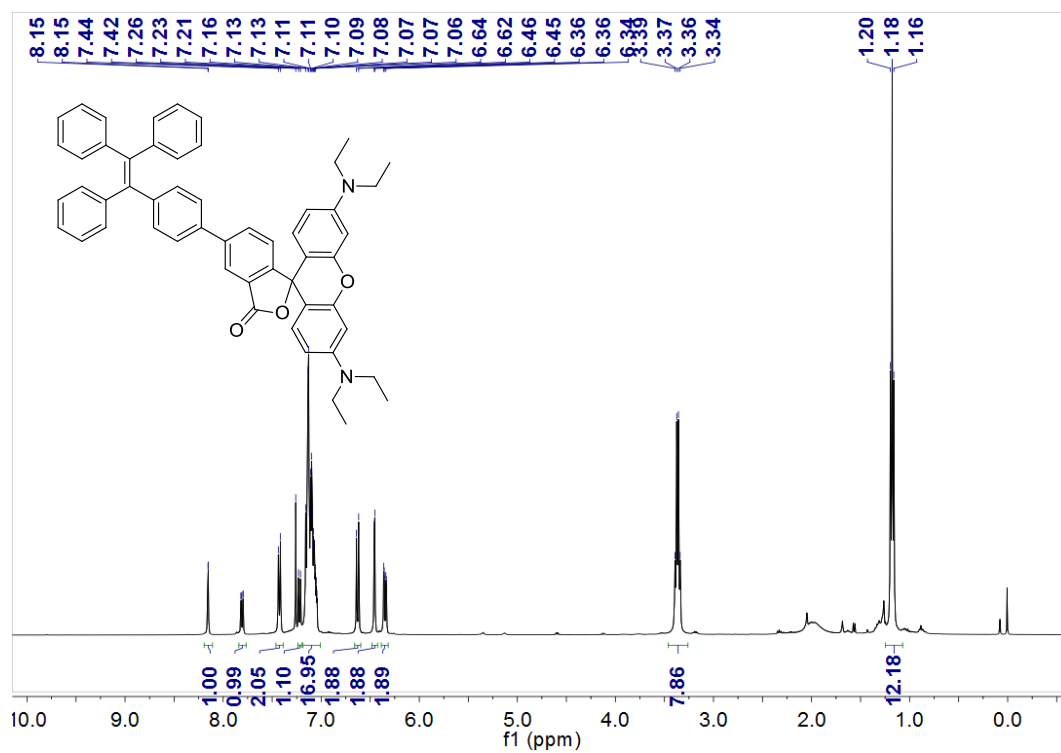


Fig. S17. ¹H NMR of compound TR (CDCl₃).

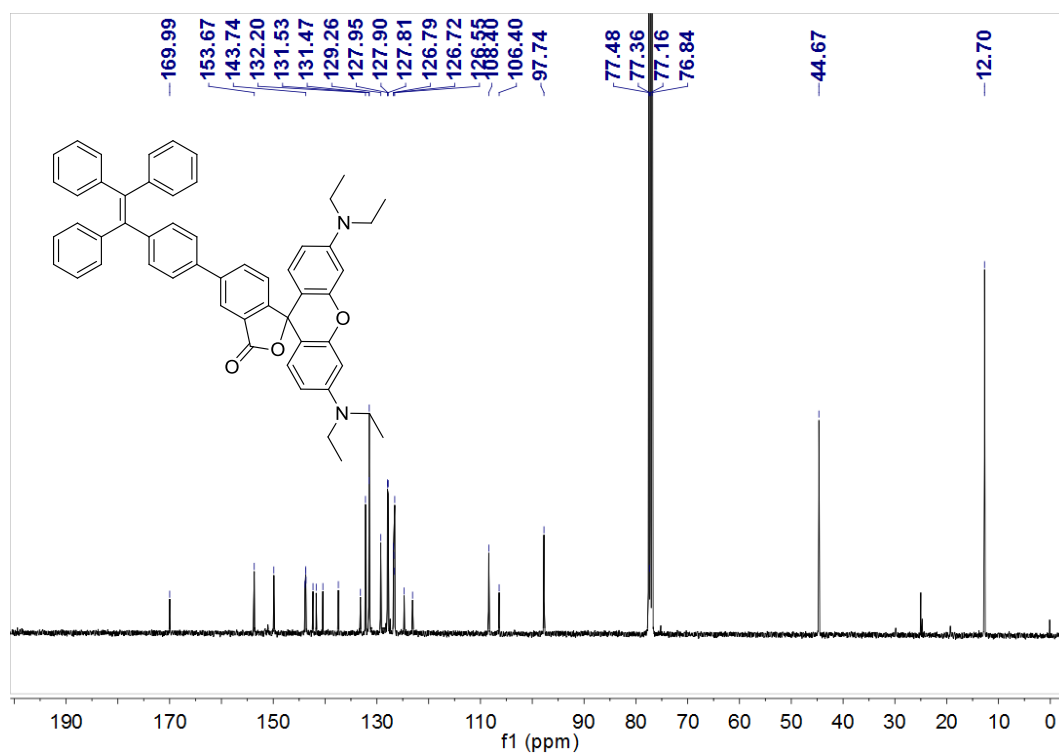


Fig. S18. ¹³C NMR of compound TR (CDCl₃).

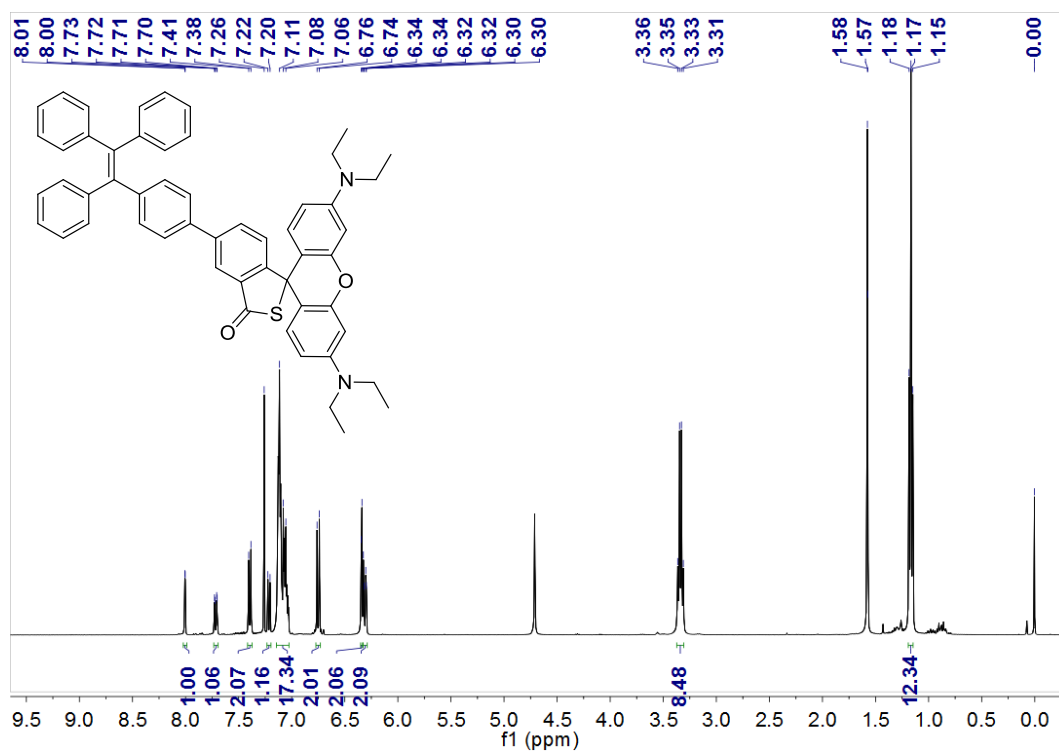


Fig. S19. ¹H NMR of compound TR-Hg (CDCl₃).

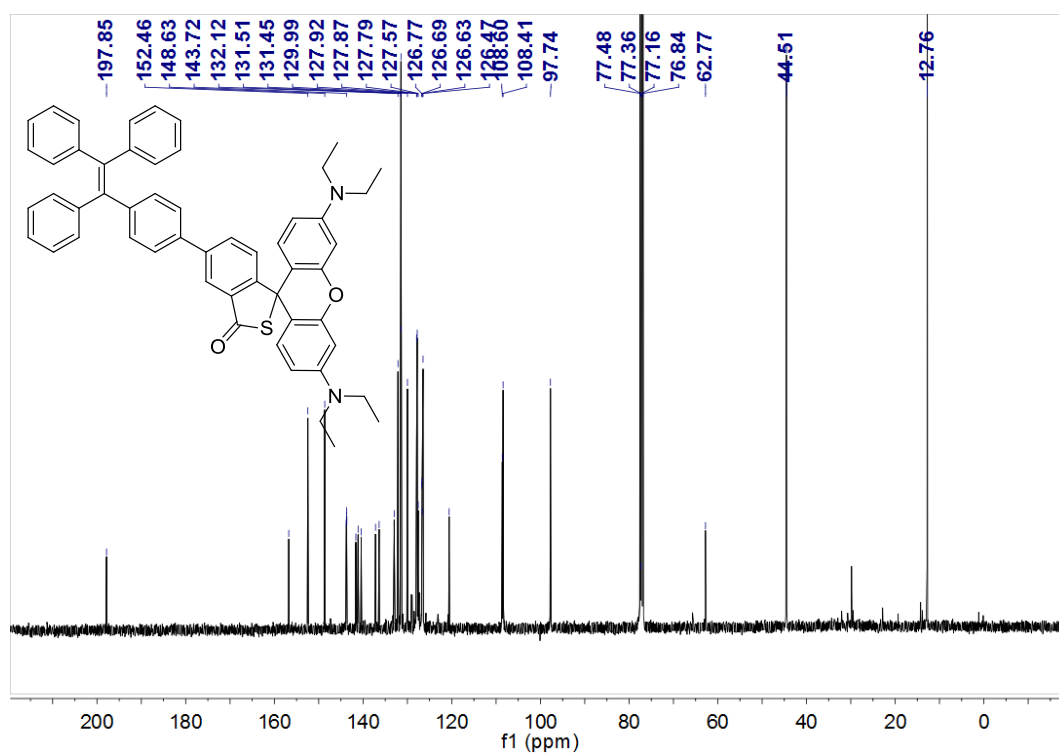


Fig. S20. ¹³C NMR of compound TR-Hg (CDCl₃).

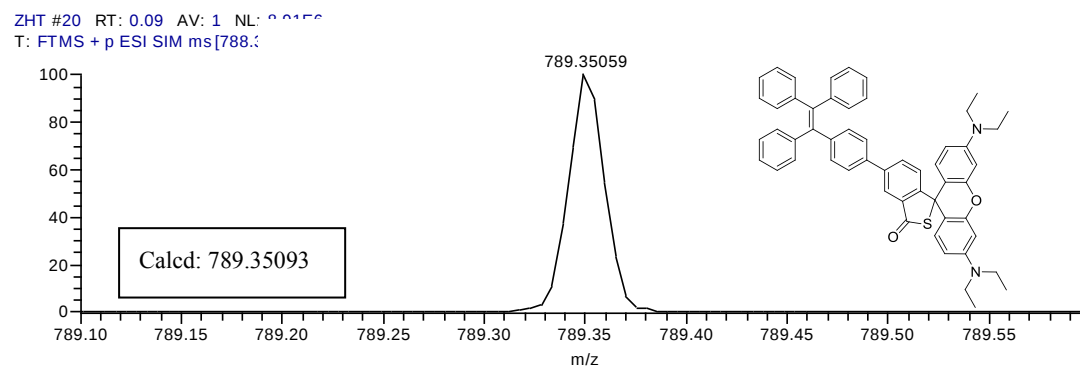


Fig. S21. High-resolution mass spectra of compound TR-Hg.