Electronic Supplementary Information

A water-soluble highly sensitive and selective fluorescent probe for Hg^{2+} based on 2-(2-(8-hydroxyquinolin)-yl)benzimidazole via ligand to metal charge transfer (LMCT)

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1. Characterization data

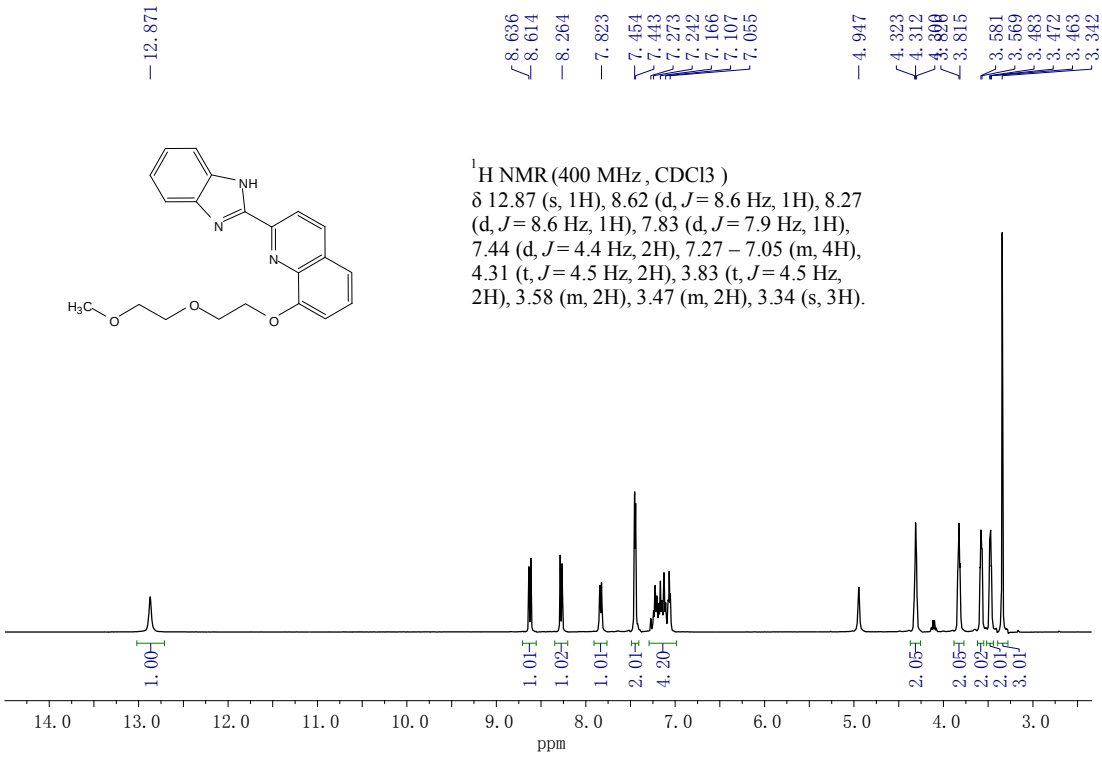

Figure S1. ^{1}H NMR spectrum of compound **L** in $CDCl_3$

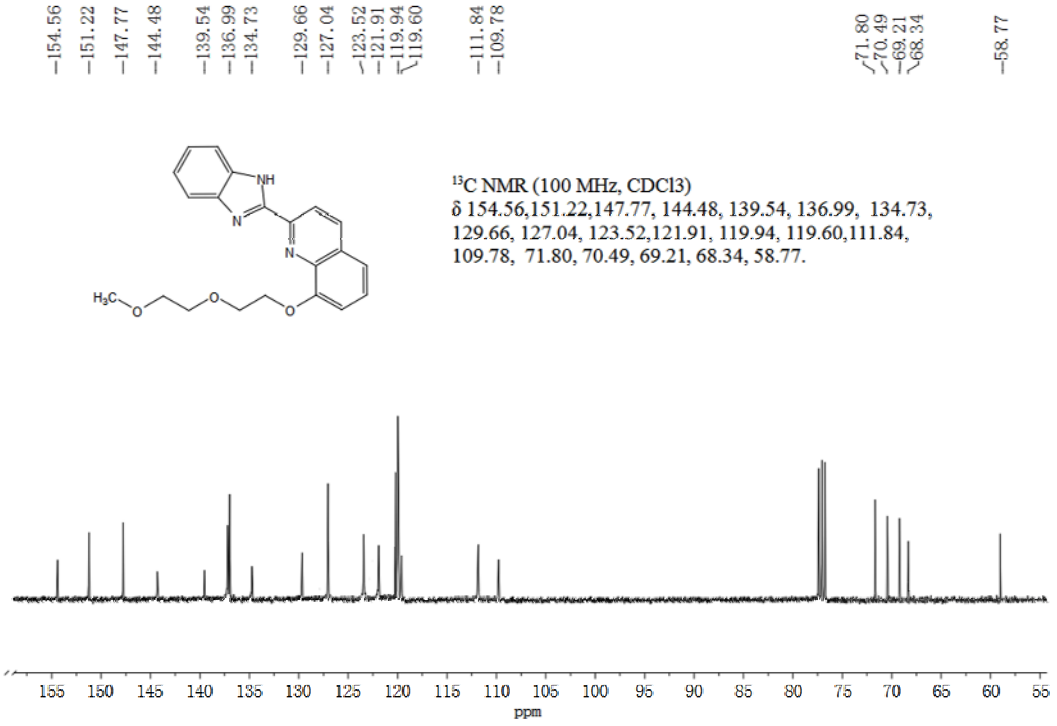

Figure S2. ^{13}C NMR spectrum of compound **L** in $CDCl_3$

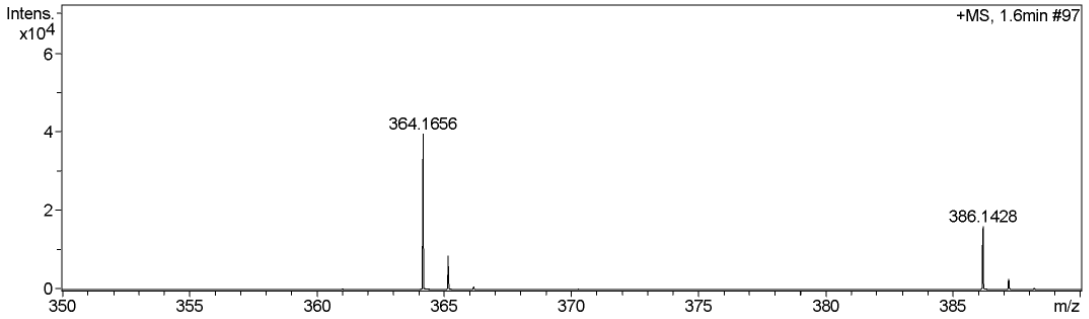

Figure S3. HRMS spectrum of compound **L** ($[M]^+$ =363.1583, Found: 364.1656 $[M+H]^+$ and 386.1428 $[M+Na]^+$).

2. Spectral data

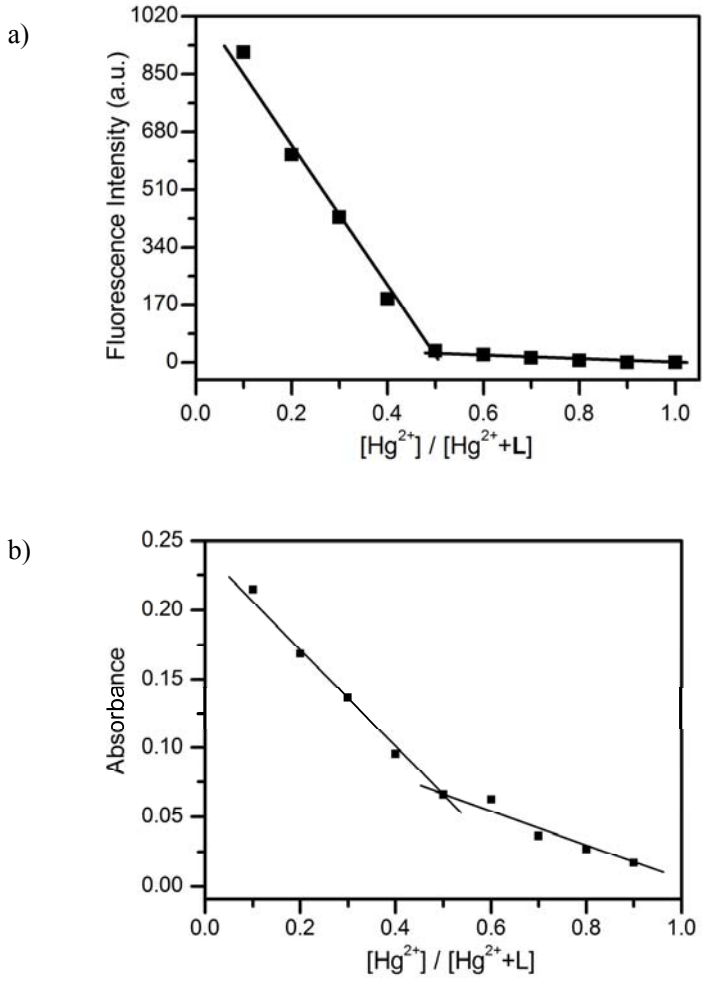

Figure S4. a) Job's plot based on the fluorescence spectrum monitored at 475 nm; b) Job's plot based on the absorption spectrum monitored at 348 nm, the total concentration of $[Hg^{2+}$+**L**] was 10 μM.

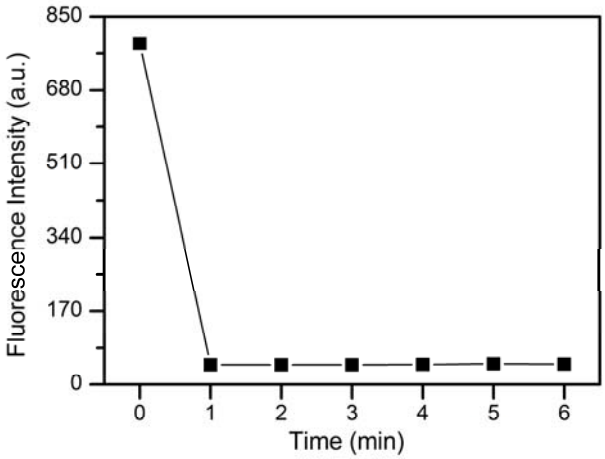

Figure S5. Fluorescence intensity changes of **L** (10 μM) in aqueous solution (1% DMSO, Tris-HCl 10 mM, pH = 7.4) in the presence of Hg^{2+} (1.0 equiv) against time. λ_{ex} = 348 nm, λ_{em} = 475 nm.

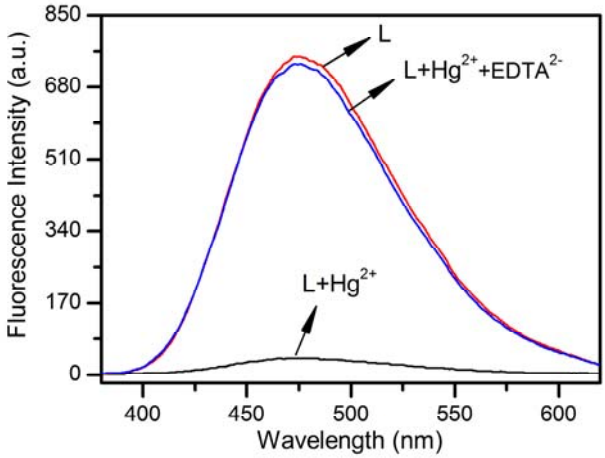

Figure S6. Fluorescence spectra of **L**, **L** + Hg^{2+}, **L** + Hg^{2+} + $EDTANa_2$ in aqueous solution (1% DMSO, Tris-HCl 10 mM, pH = 7.4).

3. Crystallographic original data

Crystallographic data (excluding structure factors) for the structures **L**-Hg^{2+} and **L** in this paper have been deposited with the Cambridge Crystallographic Data Center as supplementary publication Nos.CCDC-971509 and 971510, respectively. Copies of the data can be obtained, free of charge, on application to CCDC, 12 Union Road, Cambridge CB2 1EZ, UK. Fax: +44 (0)1223 336033 or e-mail: deposit@ccdc.cam.ac.uk.

Table S1 Crystal data and structure refinement of **L** and **L–Hg^{2+}**

Compd.	**L**	**L**-Hg^{2+}
Empirical formula	$C_{21}H_{21}N_3O_3$	$C_{21}H_{21}Cl_2HgN_3O_3$
Temperature	296(2)K	296(2)K
Formula weight	363.42	634.90
Crystal system	Orthorhombic	Triclinic
Space group	*Pbcn*	*P*-1
a (Å)	15.625 (4)	9.9298 (4)
b (Å)	9.194 (2)	11.1960 (5)
c (Å)\	27.403 (7)	12.2592 (5)
α(°)	90.00	90.6200 (10)
β(°)	90.00	92.7180 (10)
γ(°)	90.00	105.5080 (10)
V (Å^3)	3936.7 (17)	1311.42 (10)
Z	8	2
$D_{calc.}$(g cm^{-3})	1.230	1.608
	0.08	6.10
	1544.0	612.0
Abs coeff. (mm^{-1})	0.101	0.013
	1.049	1.008
	0.089	0.0263
F(000)	0.287	0.0731
R(int)	1.05	1.06
GOOF on F^2	-0.44	-1.04
R [I >2σ(I)][a]		
R_w (all data)[b]		
(Residues)max (e Å^{-3})		
(Residues)min (e Å^{-3})		

[a]$R_1 = ||Fo| - |Fc||/|Fo|$. [b]$R_w = [w(Fo^2 - Fc^2)2/w(Fo^2)^2]^{1/2}$