Turn-off fluorescence of imidazole-based sensor probe by mercury ions

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SI Figure S1¹H and ¹³C NMR spectra of probe 3



SI Figure S2 ¹H and ¹³C NMR spectra of probe 5

SI Figure S3 HRMS spectra of probe 5



SI Figure S4 Calibration plot of 5+Hg²⁺(Concentration of Hg²⁺Vs. Fluorescence Intensity)



SI Figure S5 ¹H NMR spectrum of compound 5 (1 mM) with different concentration of Hg^{2+} (1 mM) in DMSO-d₆ solvent



SI Figure S6 AAS spectrum of probe 5 with absorption of Hg²⁺



Method: Hg (Flame)

SI Figure S7 FTIR spectrum of probe 5 and 5+Hg²⁺



SI Figure S8 ESI-MS spectra of probe 5+Hg²⁺



SI Figure S9 MTT assay of Hela cells treated with different concentrations of the probe 5





SI Figure S10 GC-MS spectra of probe 3



Name of the probe	Method	solvent	Analyte	LOD	Application	Reference journals
Mono -					Test strips and	Journal of
thiosemicarbazone	Absorbance	DMSO/ Tris Hcl		31 nM	real samples	photochemistry and
	and	(8/2, v/v, pH = 7.0)	Hg^{2+}			photobiology A:
	Fluorescence					Chemistry. 2017, 338,
						1-7.
	Absorbance	$H_2O-acetonitrile$	Hg ²⁺	57 nM	Bio imaging	Sensors and actuators
Bisethylsulfane moiety	and	(v/v = 50/50)				B: Chemical. 2018,
	Fluorescence					277, 673 – 678.
A new phenothiazine	Absorbance	DMSO/H ₂ O	Hg ²⁺	12.5 nM	Paper strip and	Journal of
based	and	(1:3, v/v)			living cells	photochemistry and
	Fluorescence					photobiology A:
						Chemistry. 2019, 384,
						112036
2,6 -diformylphenol	Absorbance	Buffer solution	Hg ²⁺	6.82 nM	living cells and	Chem. Res. Toxicol.
based	and				real samples	2019, 32, 1144-1150
	Fluorescence					
A novel camphor-	Colorimetric		Hg ²⁺	19.3 nM	Bio imaging	ACS sustainable
based probe	and	PBS buffer solution			and test strip	chemistry and
	fluorescence					Engineering. 2020, 8
						(33) 12348-12359
Anthraquinone based	Absorbance	CH ₃ OH/HEPES	Hg ²⁺	8.2 nM	living cells and	Inorganic chemistry
	and	(10mM, pH 7.4, 1/1,			real samples	communications.
	Fluorescence	v/v)				2021, 130, 108753
A novel coumarin	Absorbance	THF-H ₂ O	Hg ²⁺	27.8 n M	Bio imaging	RSC Adv., 2021,11,
based	and	(1;1, v/v)			and paper strip	23597
	Fluorescence					
A naphthylamide	Colorimetric	DMSO/ PBS buffer	Hg ²⁺	13 nM	Bio imaging	~ .
based	and	(1:9, v/v, pH = 7.4)				Chemistry open.
	fluorescence					2021, 10(11, 1116-
						1122
Pyridyl styryl	Colorimetric	THF-H ₂ O	Hg^{2+}	205 nM	Real sample	Journal of
pyrazoles	and				and paper strip	photochemistry and
	fluorescence					photobiology A:
						Chemistry. 2021, 416,
						113322
Diphenyl imidazole-	absorbance and	CH ₃ CN-H ₂ O (8:2,	Hg ²⁺	5.3 nM	Bio imaging,	This work
based chemo sensor	turn-off	v/v)			paper strips and	

SI Table S1 Comparison of present sensor compound 5 with previous reports for Hg^{2+} detection.

fluorescence		real samples	

SI Table S2 density surfaces of the frontier orbitals involved in electronic transitions of chromophores probe 5 and $(5+Hg^{2+})$ which is derived from B3LYP/6-31G** level of theory









SI Table S3. HOMO and LUMO energy difference between 5 and $5+Hg^{2+}$

Fluorophore	HOMO(eV)	LUMO(eV)	Energy gap(ΔE)
5	-5.4860	-5.7873	3.96
$5 + Hg^{2+}$	-1.5186	-2.3845	3.40

SI Table S4 Selected transitions achieved from TD-DFT calculation with B3LYP/6-31G** level of theory

•	$\lambda \max(nM)$	Oscillatory	ΔΕ,	Selected major
		strength	Energy(eV)	transitions
	347	0.6827	3.5716	H
	317	0.2802	3.9013	H —→L+1 (47%)
Probe 5	304	0.0238	4.0781	HL+2 (47%)
	289	0.0137	4.2811	H → L+3 (43%)
	265	0.1564	4.6621	H-3→L (57%)
	262	0.2184	4.7301	H —▶L+7 (50%)
	263	0.0125	4.7036	H-1 → L +1(64%)
	255	0.0157	4.8593	H-1L+3(76%)
	258	0.0223	4.7920	H-4 — L(76%)
	253	0.0129	4.8849	H -2 → L+1(38%)
	245	0.0121	50589	H-1 → L+5(49%)
	397	0.2056	3.8900	H—▶ L+1(48%)
Probe 3 (5+Hg ²⁺)	298	0.0736	4.1508	H-1 → L (41%)
	297	0.0278	4.1745	H→ L+2(41%)
	291	0.1356	4.2534	H-2 → L (40%)
	270	0.1389	4.5869	H-4 ──► L (49%)
	266	0.0246	4.6603	H-6→ L (36%)
	265	0.0151	4.6780	H-5 → L (40%)
	260	0.0460	4.7580	H
	260	0.0880	4.9389	H-6 → L (56%)