Electronic Supplementary Information

Highly sensitive and selective fluorescent probe based on Pdcatalyzed reaction for detection of Pd²⁺

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Structures of sensors	Solvent	E _x /E _m (nm)	Detection Limit	Response time	Ref.
	PBS (10 mM, pH=7.4, containing 1% DMSO)	480/513	7.4 nM	<6 min	1
	DMSO/PBS (pH 7.40, 8/2, v/v)	600/689	0.52 μΜ	30 min	2
	DMF:H ₂ O (95:5, v/v) solution (pH 5.5)	500/518	0.29 μΜ	_	3
	CH ₃ CN-water (4:1, v/v, 10 mM HEPES buffer, pH 7.4)	555/575	11.9 μΜ	_	4
	CH ₃ CN/PBS (1:99, v/v, 10 mM, pH 7.4)	465/531	50.8 nM	<120 min	5
	PBS, 10 mM, pH 7.4, containing 1% EtOH	337/405	29 nM	<60 min	6
NH ₂ S NH ₂ S	pure water	382/540	22 nM	<30 min	7
HO	PBS buffer (pH 7.4, 10 mM)	610/668	10.8 nM	_	8
	EtOH/H ₂ O (1:1, v/v, PBS 20 mM, pH=7.4	560/630	0.705 μΜ	<30 min	9

Table S1. Part of the reported fluorescence probe for Pd²⁺ in recent 3 years.

S N N N N N N N N N N N N N N N N N N N	DMSO-PBS (3:1 in v/v, pH=7.4) (10 µM)	580/717	48 nM	3 min	10
N C C C C C C C C C C C C C C C C C C C	EtOH/H ₂ O=40: 60, v/v	436/500	41.5 nM	30 s	11
CF_3 CF_3 CF_3 CF_3	CH ₃ CN-PBS (v/v=1/3, pH=7.4, 10 mM)	365/509 365/524	33 nM 14 nM	2-3 min	12
	10 mM HEPES, pH 7.4	380/543 437/642	285 nM 14.6 nM	10 min	13
HOLOO	DMF-HEPES buffer (10 mM, 95:5, v/v, pH 7.0)	320/465	0.29 μΜ	30 s	14
	Methanol /Water (1:1)	330/590	170 nM	<30 min	15
	CH ₃ CN/PBS buffer (8:2 v/v, pH 7.4)	369/452	2.6 nM	<2 min	This work

"—" Not mentioned



Fig. S1. UV-vis spectra of **ACBT** in the absence and presence of Pd^{2+} . [**ACBT** is 10 μ M], [Pd²⁺ is 20 μ M], [NaBH₄ is 20 μ M] in a mixture of CH₃CN/PBS buffer (8:2 v/v, pH 7.4).



Fig. S2. Fluorescence intensity changes of probe **ACBT** (10 μ M) at 452 nm upon addition of Pd²⁺, Pd⁴⁺ and Pd⁰ (20 μ M) in the absence and presence of NaBH₄ (20 μ M) in CH₃CN-PBS buffer (10 mM, pH 7.4, 8:2, v/v) at 25 °C. All data were collected 5 min after mixing. λ_{ex} =369 nm.



Fig. S3. Effect of pH on the Fluorescence intensity of ACBT in the absence and presence of Pd²⁺. [ACBT is 10 μM], [Pd²⁺ is 20 μM], [NaBH₄ is 20 μM] in a mixture of CH₃CN/PBS buffer (8:2 v/v, pH 7.4, 25 °C), λ_{ex}=369 nm, λ_{em}=452 nm.



Fig. S4. ¹H NMR spectrum of compound 1 in DMSO-d₆.



Fig. S6. DEPT-135 spectrum of compound 1 in DMSO-d₆.





Fig. S8. ¹H NMR spectrum of compound NBT in CDCl₃-d₁.







Fig. S10. HRMS spectrum of compound NBT in CH₃CN.



Fig. S12. ¹³C NMR spectrum of compound ABT in DMSO-d₆.



Fig. S13. HRMS spectrum of probe compound ABT in CH₃CN.



Fig. S14. ¹H NMR spectrum of compound ACBT in CDCl₃-d₁.







Fig. S16. HRMS spectrum of probe compound ACBT in CH₃CN.

Detection limit

The detection limit for Pd^{2+} ions was calculated by the fluorescence titration experiments according to the reported method. A good linear relationship between the fluorescence intensity and Pd^{2+} concentration (0.5 µM-10 µM) could be obtained (R²=0.99944). The value obtained for the Pd^{2+} was found to be 2.6 nM by the equation of $L_{OD}=3\delta/m$ (δ was the standard deviation of the blank solution and *m* is the absolute value of the slope between intensity versus Pd^{2+} concentration). δ =0.4880, *m*=557.6864.



Fig. S17. The linear relationship between the fluorescence intensity and Pd²⁺ concentration (0.5-10 μM). All measurements were taken in a mixture of CH₃CN/PBS buffer (8:2 v/v, pH 7.4) at 25 °C. Excitation and emission were at 369 nm/452 nm respectively.

Kinetic studies:

The reaction of **ACBT** (10 μ M) with Pd²⁺ in CH₃CN/PBS buffer (8:2 v/v, pH 7.4) was monitored using the fluorescence intensity at 452 nm. The reaction was carried out at 25 °C. The *pseudo*-first-order rate constant for the reaction was determined by fitting the fluorescence intensities of the samples to the *pseudo*-first-order equation:

 $\operatorname{Ln}\left[\left(\mathrm{F_{t}}-\mathrm{F_{min}}\right)/\mathrm{F_{min}}\right]=-k't$

Where F_t and F_{min} are the fluorescence intensities at 452 nm at time t and the maximum value obtained after the reaction was complete. k' is the *pseudo*-first-order rate constant. The *pseudo*-first-order plots for the reaction of **ACBT** with 100 equiv. of Pd²⁺ is shown in Fig. S18, the *pseudo*-first-order rate constant k' =1/t₁=0.01284 min⁻¹.



Fig. S18. *Pseudo*-first-order kinetic plot of the reaction of **ACBT** (10 μ M) with Pd²⁺ (100 equiv.) and NaBH₄ (100 equiv.) in a mixture of CH₃CN/PBS buffer (8:2 v/v, pH 7.4) at 25 °C. *k* =0.01284 min⁻¹.



Fig. S19. ESI-MS spectrum (positive ion mode) of **ACBT** upon addition of Pd²⁺ in CH₃CN. (a) only **ACBT**, (b) the isolated aggregates of compound after **ACBT** reacted with Pd²⁺ for 5 min.



Fig. S20. The comparison of solid phase of **ACBT** and **ABT**. Left: The solid of synthesized **ACBT**; Right: The solid of synthesized **ABT**. The centrifuge tubes were excited at 365 nm using a hand-held UV lamp.

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