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Supplementary Information

A facile water-stable MOF-based "off-on" fluorescent switch for label-free detection of dopamine in biological fluid

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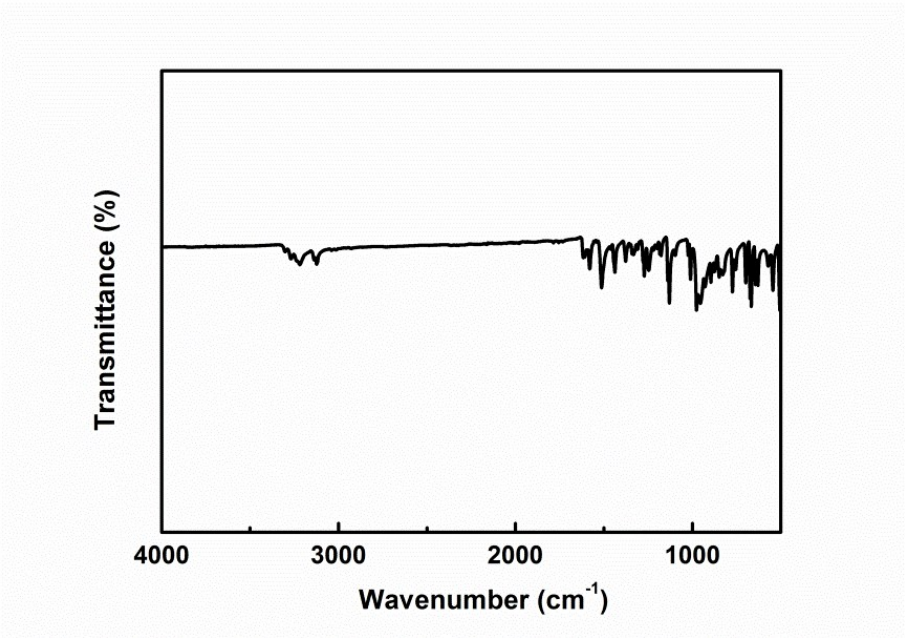

Fig. S1 Fourier transform infrared (FT-IR) spectra of Abtz-CdI_2-MOF.

As shown in Figure S1, the bands around ca. 3124 cm^{-1} and bands in the 1100-1300 cm^{-1} range can be related to ν(C-H) and ν(C-N) or ν(N-N) of triazole moieties. The triazole out of plane ring absorption also can be observed at around 630 cm^{-1}.[1-5]

X-ray crystallography. Diffraction intensities for complex Abtz-CdI_2-MOF were collected on a Bruker SMART 1000 CCD diffractometer with graphite-monochromated Mo-Kα radiation (λ = 0.71073 Å) by using the ω-φ scan technique. Lorentz polarization and absorption corrections were applied. The structures were solved by direct methods and refined with the full-matrix least-squares technique using the SHELXS-97 and SHELXL-97 programs. Anisotropic thermal parameters were assigned to all non-hydrogen atoms. The organic hydrogen atoms were generated geometrically; the hydrogen atoms of the water molecules were located from difference maps and refined with isotropic temperature factors. Analytical expressions of neutral-atom scattering factors were employed, and anomalous dispersion corrections were incorporated. The crystallographic data and details of refinements for Abtz-CdI_2-MOF are summarized in Table S1, selected bond lengths and angles are listed in Table S2. CCDC-1031671 (Abtz-CdI_2-MOF) contains the supplementary crystallographic data for this paper. These data can be obtained free of charge from The Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/data_request/cif.

Table S1 Crystallographic data and details of refinements for complex Abtz-CdI_2-MOF [a,b]

	Abtz-CdI_2-MOF
Formula	$C_{18}H_{20}CdI_2N_8$
M (g mol^{-1})	714.62
crystal system	Orthorhombic
space group	*Pbca*
a (Å)	14.468(4)
b (Å)	13.931(4)
c (Å)	22.740(7)
α (º)	90
β (º)	90
γ (º)	90
V (Å^3)	4583(2)
Z	8
F (000)	2704
ρ_{calc} (Mg m^{-3})	2.071
μ (mm^{-1})	3.668
data/restraints/params	4039 / 0 / 263
GOF on F^2	1.070
R_1[a] (I=2σ(I))	0.0177
ωR_2[a] (all data)	0.0368

[a] $R_1 = \Sigma||F_o| - |F_c||/|F_o|$. [b] $\omega R_2 = [\Sigma w(|F_o|^2 - |F_c^2|^2/w|F_o^2|^2]^{1/2}$.

Table S2 Selected bond lengths /Å and bond angles /° for Abtz-CdI_2-MOF

Cd(1)-N(7)	2.360(2)	Cd(1)-N(3)	2.370(2)
Cd(1)-N(4)	2.402(2)	Cd(1)-N(8)	2.415(2)
N(7)-Cd(1) -N(3)	153.55(15)	N(7)-Cd(1) -N(4)	96.16(11)
N(3)-Cd(1) -N(4)	96.85(10)	N(7)-Cd(1) -N(8)	103.99(11)
N(3)-Cd(1) -N(8)	97.44(10)	N(4)-Cd(1) -N(8)	95.985(16)
N(3)-Cd(1) -N(8)	97.44(10)	N(4)-Cd(1) -N(8)	95.985(16)

Table S3 Analytical figures of merit for the detection of DA

Content	Value
LOD (nM)	57
Linear range (μM)	0.25-50
Calibration function	$\Delta I = 4.951C - 5.314$
Correlation coefficient R^2	0.995
RSD (n = 3) (%)	1.4

References

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