

## *Supporting information*

Driving Force to Detect Alzheimer's Disease Biomarkers: The Application Of A Thioflavine T@Er-MOF Ratiometric Fluorescent Sensor for Smart Detection of Presenilin 1, amyloid  $\beta$ -protein and Acetyl Choline

Xing Ze Wang<sup>a</sup>, Jing Du<sup>a</sup>, Nan Nan Xiao<sup>c</sup>, Yan Zhang<sup>c</sup>, Ling Fei<sup>d</sup>, Jed D. LaCoste<sup>d</sup>, Zhuo Huang<sup>a</sup>, Qian Wang<sup>a</sup>, Xin Rui Wang<sup>a\*</sup> and Bin Ding<sup>a,b\*</sup>

<sup>a</sup>Key Laboratory of Inorganic-Organic Hybrid Functional Material Chemistry (Tianjin Normal University), Ministry of Education, Tianjin Key Laboratory of Structure and Performance for Functional Molecule, College of Chemistry, Tianjin Normal University, 393 Binshui West Road, Tianjin 300387, PR China

<sup>b</sup>Key Laboratory of Advanced Energy Materials Chemistry (Ministry of Education), Collaborative Innovation Center of Chemical Science and Engineering (Tianjin), College of Chemistry, Nankai University, Tianjin 300071, PR China

<sup>c</sup>State Key Laboratory of Medicinal Chemical Biology, Nankai University, Tianjin, 300350, China.

<sup>d</sup>Chemical Engineering Department, University of Louisiana at Lafayette, Madison Hall, Room 218 C, Lafayette, LA, 70504, United States

\*To whom correspondence should be addressed.

E-mail: [wangxinrui-tjnu@outlook.com](mailto:wangxinrui-tjnu@outlook.com); [hxydb@tjnu.edu.cn](mailto:hxydb@tjnu.edu.cn) Received Date (automatically inserted by publisher)

**Table S1.** Crystallographic Data and Details of Refinements for **Er-MOF**<sup>a,b</sup>

<b>Er-MOF</b>	
Formula	C <sub>24.82</sub> H <sub>21.38</sub> ErN <sub>1.27</sub> O <sub>7.27</sub>
M (g mol <sup>-1</sup> )	621.0195
Crystal system	monoclinic
Space group	I <sub>2</sub> /a
<i>a</i> (Å)	13.9072(6)
<i>b</i> (Å)	13.7531(9)
<i>c</i> (Å)	32.8737(12)
$\alpha$ (deg)	90
$\beta$ (deg)	102.000(4)
$\gamma$ (deg)	90
<i>V</i> (Å <sup>3</sup> )	6150.2(5)
Z	8
F (000)	2490.0
$\rho_{calc}$ (Mg m <sup>-3</sup> )	1.367
$\mu$ (mm <sup>-1</sup> )	2.769
data/restraints/parameters	5424/127/367
GOF on F <sup>2</sup>	1.033
R <sub>1</sub> <sup>a</sup> (I = 2 $\sigma$ (I))	0.0524
$\omega$ R <sub>2</sub> <sup>b</sup> (all data)	0.1461

$${}^a R_1 = \sum ||F_0| - |F_c||/|F_0|; {}^b \omega R_2 = [\sum w(|F_0|^2 - |F_c|^2/w|F_o^2|^2)]^{1/2}.$$

**Table S2.** Selected Bond Lengths [ $\text{\AA}$ ] and Angles [ $^\circ$ ] for **Er-MOF<sup>a</sup>**.

Er-MOF					
Er(1)-O(1)	2.304(6)	Er(1)-O(1) <sup>1</sup>	2.687(5)	Er(1)-O(2) <sup>1</sup>	2.379(6)
Er(1)-O(3) <sup>2</sup>	2.338(5)	Er(1)-O(4) <sup>3</sup>	2.323(6)	Er(1)-O(5) <sup>4</sup>	2.372(5)
Er(1)-O(6) <sup>4</sup>	2.481(6)	O(4)-Er(1) <sup>6</sup>	2.323(6)	Er(1)-O(7)	2.32(2)
Er(1)-O(8)	2.405(10)	O(5)-Er(1) <sup>4</sup>	2.372(5)	O(6)-Er(1) <sup>4</sup>	2.481(6)
O(1)-Er(1) <sup>1</sup>	2.687(5)	O(2)-Er(1) <sup>1</sup>	2.379(6)	O(3)-Er(1) <sup>5</sup>	2.338(5)
O(1)-Er(1)-O(1) <sup>1</sup>	75.7(2)	O(1)-Er(1)-O(2) <sup>1</sup>	124.58(18)	O(1)-Er(1)-O(3) <sup>2</sup>	80.76(19)
O(1)-Er(1)-O(4) <sup>3</sup>	74.47(19)	O(1)-Er(1)-O(5) <sup>4</sup>	133.8(2)	O(1)-Er(1)-O(6) <sup>4</sup>	82.10(19)
O(1) <sup>1</sup> -Er(1)-C(21) <sup>4</sup>	138.0(2)	O(1)-Er(1)-C(21) <sup>4</sup>	107.7(2)	O(1)-Er(1)-O(7)	84.2(4)
O(1)-Er(1)-O(8)	147.1(5)	O(1)-Er(1)-O(7)	75.9(8)	O(1)-Er(1)-O(8)	142.1(15)
O(2) <sup>1</sup> -Er(1)-O(1) <sup>1</sup>	50.55(17)	O(2) <sup>1</sup> -Er(1)-O(6) <sup>4</sup>	126.57(19)	O(3) <sup>2</sup> -Er(1)-O(1) <sup>1</sup>	66.95(17)
O(2) <sup>1</sup> -Er(1)-O(8)	72.6(4)	O(3) <sup>2</sup> -Er(1)-O(5) <sup>4</sup>	141.9(2)	O(3) <sup>2</sup> -Er(1)-O(6) <sup>4</sup>	144.2(2)
O(3) <sup>2</sup> -Er(1)-O(2) <sup>1</sup>	88.9(2)	O(3) <sup>2</sup> -Er(1)-O(8)	71.1(5)	O(4) <sup>3</sup> -Er(1)-O(2) <sup>1</sup>	74.4(2)
O(4) <sup>3</sup> -Er(1)-O(3) <sup>2</sup>	133.40(18)	O(4) <sup>3</sup> -Er(1)-O(1) <sup>1</sup>	68.99(17)	O(4) <sup>3</sup> -Er(1)-O(6) <sup>4</sup>	70.1(2)
O(4) <sup>3</sup> -Er(1)-O(5) <sup>4</sup>	79.6(2)	O(4) <sup>3</sup> -Er(1)-O(8)	137.9(5)	O(5) <sup>4</sup> -Er(1)-O(2) <sup>1</sup>	82.6(2)
O(5) <sup>4</sup> -Er(1)-O(6) <sup>4</sup>	53.0(2)	O(5) <sup>4</sup> -Er(1)-O(1) <sup>1</sup>	128.4(2)	O(5) <sup>4</sup> -Er(1)-O(8)	70.9(5)

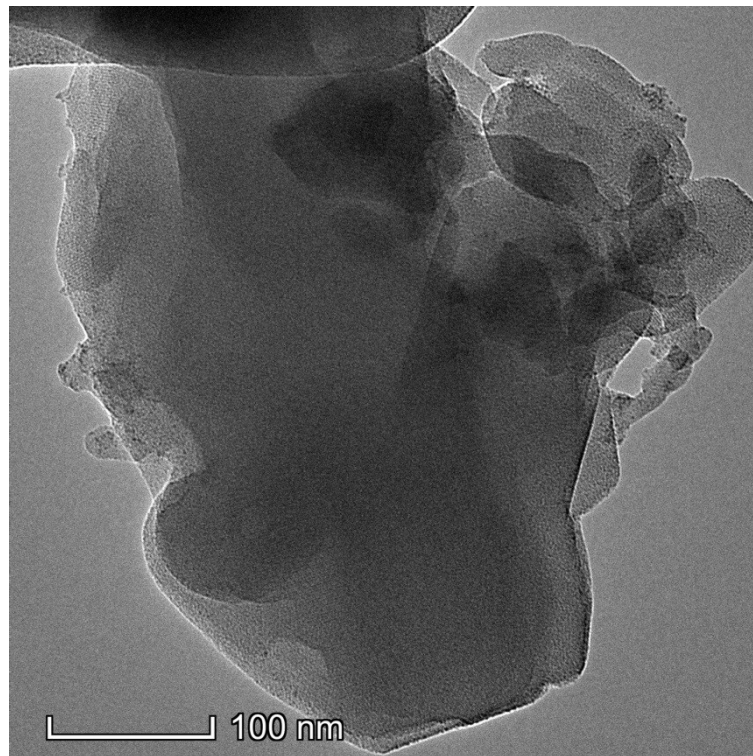
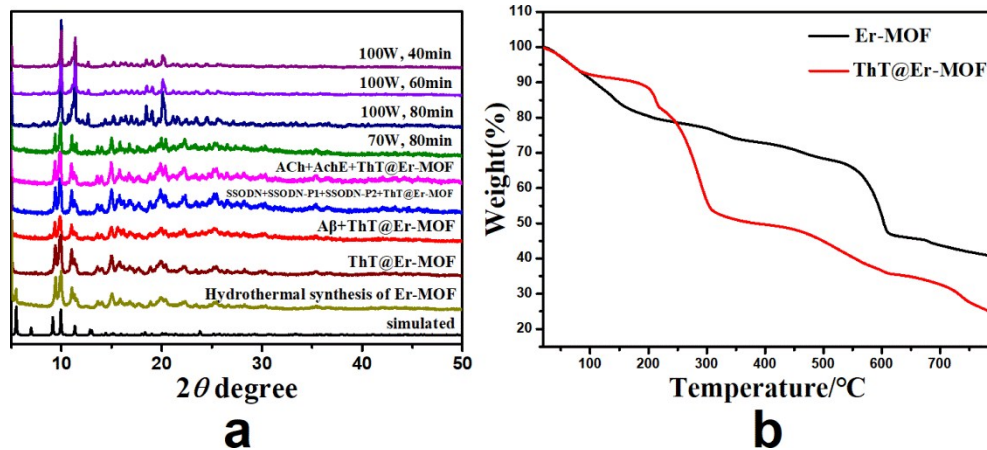
Symmetry code: <sup>1</sup>1/2 -x, 1/2 -y, 1/2 -z; <sup>2</sup>-x, -1/2 +y, 1/2 -z; <sup>3</sup>1/2 +x, 1 -y, +z; <sup>4</sup>1-x, 1-y, 1-z**Table S3.** Hydrogen bonds for **Er-MOF** [ $\text{\AA}$  and  $^\circ$ ]<sup>a</sup>

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
O(8)-H(8B)...O(2) <sup>1</sup>	0.86	2.49	2.833(19)	105
C(5)-H(5)...O(4)	0.93	2.44	2.763(9)	100
C(7)-H(7)...O(6) <sup>2</sup>	0.93	2.46	3.351(10)	160

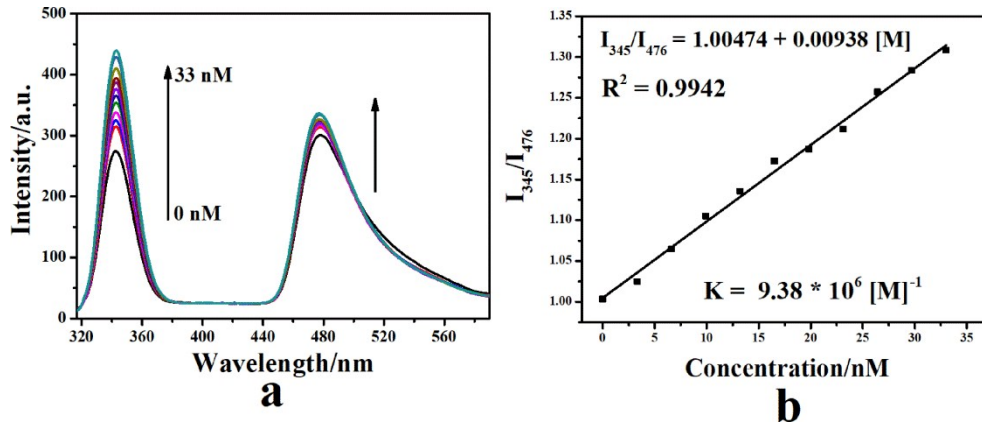
Symmetry code: <sup>1</sup> 1/2-x, 1/2-y, 1/2-z; <sup>2</sup> 1-x, 1-y, 1-z

**Table S4.** Fluorescent lifetime of **Er-MOF** and **ThT@Er-MOF** in different solutions

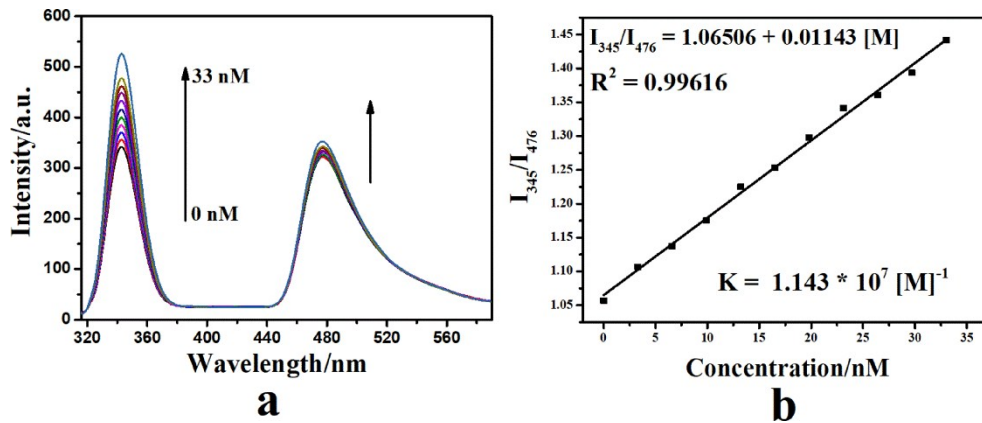
Sample	B1	T1/ns	B2	T2/ns	T/ns
Er-MOF	1384.7318	21.7982	5.99E+10	1.1847	1.1846
ThT@Er-MOF	1.67E+08	0.5847	1.67E+08	0.5847	0.5847
ThT@Er-MOF+ACh(50nM)	1.53E+03	19.5573	1.35E+09	1.3893	1.3896
ThT@Er-MOF+ACh(100nM)	1.13E+07	2.1309	2000.33364	25.1301	2.1789
ThT@Er-MOF+A $\beta$ (50nM)	1.75E+07	0.7167	1.75E+07	0.7167	0.7167
ThT@Er-MOF+A $\beta$ (100nM)	2.27E+11	1.0063	1045.04781	12.4681	1.0063

**Fig. S1** TEM image of **Er-MOF** synthesized by ultrasonic method.**Fig. S2** (a) Experimental PXRD patterns of **Er-MOF** and **ThT@Er-MOF** under

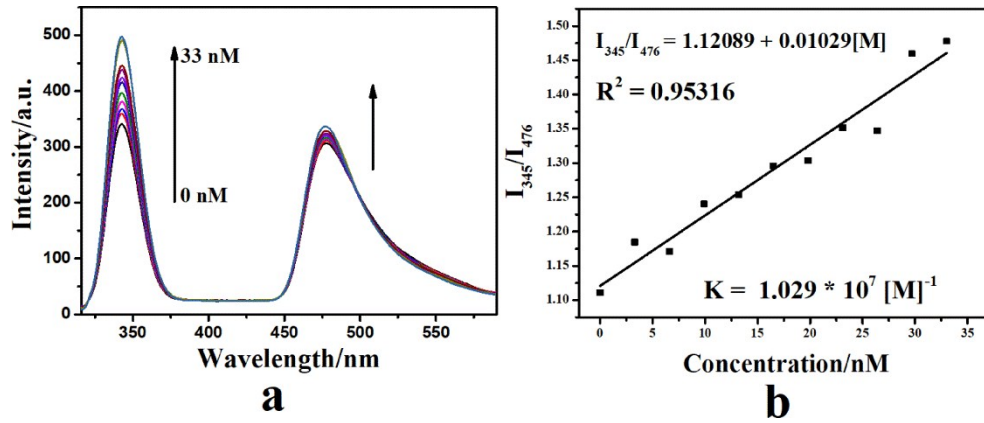
different conditions; (b) TG analysis curves of **Er-MOF** and **ThT@Er-MOF**.



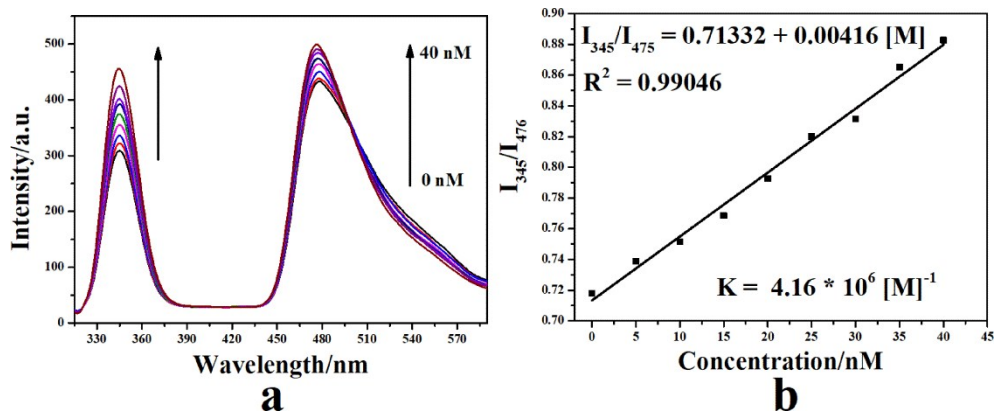
**Fig. S3** (a) Fluorescence emission spectra of **ThT@Er-MOF** (0.1 g/L, 3 mL) by the addition of 2 pM SSODN-P and different concentrations of SSODN solution when excited at 310 nm; (b) The linear relation between fluorescence intensity ratio and different concentrations of SSODN solution added into **ThT@Er-MOF**.



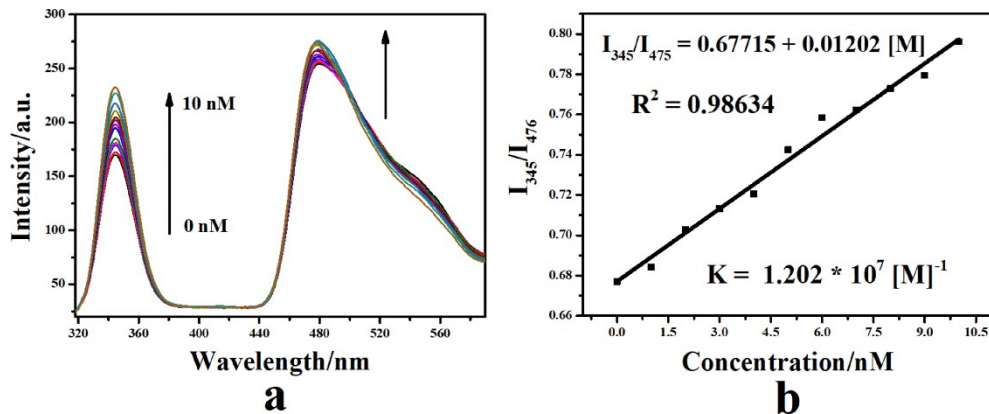
**Fig. S4** (a) Fluorescence emission spectra of **ThT@Er-MOF** (0.1 g/L, 3 mL) by the addition of 2 pM SSODN-P1 and 2 pM SSODN-P2 and different concentrations of SSODN solution when excited at 310 nm; (b) The linear relation between fluorescence intensity ratio and different concentrations of SSODN solution added into **ThT@Er-MOF**.



**Fig. S5** (a) Fluorescence emission spectra of **ThT@MOF1** (0.1 g/L, 3 mL) by the addition of 2 pM SSODN-P and different concentrations of SSODN-X solution when excited at 310 nm; (b) The linear relation between fluorescence intensity ratio and different concentrations of SSODN-X solution added into **ThT@Er-MOF**.

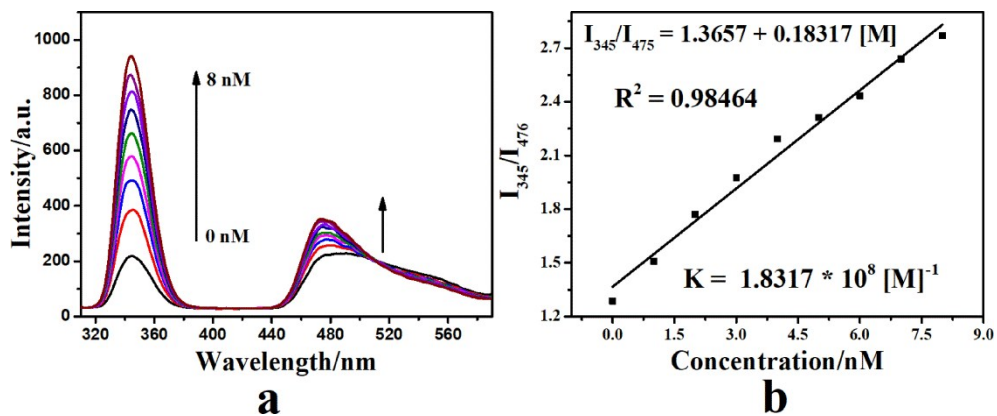


**Fig. S6** (a) Fluorescence emission spectra of **ThT@Er-MOF** (0.1 g/L, 3 mL) by the addition of different concentrations of A $\beta$  solution when excited at 310 nm; (b) The linear relation between fluorescence intensity ratio and different concentrations of A $\beta$  solution added into **ThT@Er-MOF**.



**Fig. S7** (a) Fluorescence emission spectra of **ThT@Er-MOF** (0.1 g/L, 3 mL) by the

addition of different concentrations of ACh solution when excited at 310 nm; (b) The linear relation between fluorescence intensity ratio and different concentrations of ACh solution added into **ThT@Er-MOF**.



**Fig. S8** (a) Fluorescence emission spectra of **ThT@Er-MOF** (0.1 g/L, 3 mL) by the addition of AchE (1U/mL, 0.5 μL) and different concentrations of ACh solution when excited at 310 nm; (b) The linear relation between fluorescence intensity ratio and different concentrations of ACh solution added into **ThT@Er-MOF**.