## Supplementary Information for

## Replacement of quinoline with isoquinoline affords target metal ion switching from Zn<sup>2+</sup> to Cd<sup>2+</sup> in fluorescent sensor TQLN (*N*,*N*,*N'*,*N'*-tetrakis(2quinolylmethyl)-2,6-bis(aminomethyl)pyridine)

Yuji Mikata,<sup>a,b,c,\*</sup> Ayaka Takekoshi,<sup>c</sup> Minori Kaneda,<sup>c</sup> Hideo Konno,<sup>d</sup> Keiko Yasuda,<sup>a</sup> Masato Aoyama<sup>a</sup> and Satoshi Tamotsu<sup>a</sup>

<sup>a</sup>Department of Chemistry, Biology, and Environmental Science, Faculty of Science, Nara Women's University, Nara 630-8506, Japan

<sup>b</sup>KYOUSEI Science Center, Nara Women's University, Nara 630-8506, Japan

<sup>c</sup>Department of Chemistry, Faculty of Science, Nara Women's University, Nara 630-8506, Japan

<sup>*d*</sup>National Institute of Advanced Industrial Science and Technology (AIST), 1-1-1 Higashi, Tsukuba, Ibaraki 305-8565, Japan

## Experimental

**General.** All reagents and solvents used for synthesis were from commercial sources and used as received. *N*,*N*-Dimethylformamide (DMF, Dojin) was spectral grade (Spectrosol). All aqueous solution was prepared using Milli-Q water (Millipore). <sup>1</sup>H NMR (300 MHz) and <sup>13</sup>C NMR (75.5 MHz) spectra were recorded on a Varian GEMINI 2000 spectrometer and referenced to internal Si(CH<sub>3</sub>)<sub>4</sub> or solvent signals. UV-vis and fluorescence spectra were measured on a Jasco V-660 spectrophotometer and Jasco FP-6300 spectrofluorometer, respectively. Fluorescence quantum yields were measured on a HAMAMATSU photonics C9920-02 absolute PL quantum yield measurement system. Fluorescence lifetimes were measured on a HORIBA fluorescence lifetime system DeltaFlex. *CAUTION: Perchlorate salts of metal complexes* with organic ligands are potentially explosive. All due precautions should be taken.

*N,N,N',N'*-tetrakis(2-quinolylmethyl)-2,6-bis(aminomethyl)pyridine (TQLN). To the mixture of bis(2-aminomethyl)pyridine (228 mg, 1.66 mmol) and potassium carbonate (2.30 g, 16.6 mmol) in dry CH<sub>3</sub>CN (50 mL) was added 2-chloromethylquinoline hydrochloride (1.18 g, 6.64 mmol) and potassium iodide (287 mg, 1.73 mmol), then refluxed for 2 days under N<sub>2</sub>. The resultant reaction mixture was cooled to r.t. and the solvent was evaporated. After extraction with CHCl<sub>3</sub>/water, the organic layer was dried and evaporated. The residue was washed with ethyl acetate to give TQLN as yellow-white powder (588 mg, 0.838 mmol, 50%). <sup>1</sup>H NMR (CDCl<sub>3</sub>, Me<sub>4</sub>Si, 300 MHz):  $\delta$  (ppm) 8.05 (d, *J* = 8.7 Hz, 4H), 8.02 (d, *J* = 9.9 Hz, 4H), 7.59-7.77 (m, 13H), 7.41-7.49 (m, 6H), 4.08 (s, 8H), 3.92 (s, 4H).

<sup>13</sup>C NMR (CDCl<sub>3</sub>, Me<sub>4</sub>Si, 75.5 MHz): δ (ppm) 159.9, 158.3, 147.2, 136.4, 136.1, 129.1,

128.8, 127.2, 127.1, 125.9, 121.2, 120.9, 61.1, 60.4.

Anal. Calcd for C<sub>47</sub>H<sub>39</sub>N<sub>7</sub> (TQLN): H, 5.60; C, 79.63; N, 13.91. Found: H, 5.55; C, 79.95; N, 13.97.

N,N,N',N'-tetrakis(1-isoquinolylmethyl)-2,6-bis(aminomethyl)pyridine (1isoTQLN). To the mixture of bis(2-aminomethyl)pyridine (73.0 mg, 0.531 mmol) and potassium carbonate (880 mg, 6.37 mmol) in dry CH<sub>3</sub>CN (13 mL) was added 1chloromethylisoquinoline (377 mg, 2.12 mmol) in CH<sub>3</sub>CN (15 mL) and potassium iodide (352 mg, 2.12 mmol), then refluxed for 3 days under N<sub>2</sub>. The resultant reaction mixture was cooled to r.t. and the solvent was evaporated. After extraction with CHCl<sub>3</sub>/water, the organic layer was dried and evaporated. The residue was washed

with ethyl acetate to give 1-isoTQLN as yellow-white powder (235 mg, 0.335 mmol, 63%).

<sup>1</sup>H NMR (CDCl<sub>3</sub>, Me<sub>4</sub>Si, 300 MHz): δ (ppm) 8.40 (d, *J* = 5.5 Hz, 4H), 7.85 (d, *J* = 8.5, 4H), 7.67 (d, *J* = 8.2, 4H), 7.47-7.52 (m, 8H), 7.33 (t, *J* = 7.6 Hz, 1H), 7.08 (ddd, *J* = 8.4, 6.9, 1.2 Hz, 4H), 6.91 (d, *J* = 7.8, 2H), 4.30 (s, 8H), 3.90 (s, 4H).

<sup>13</sup>C NMR (CDCl<sub>3</sub>, Me<sub>4</sub>Si, 75.5 MHz): δ (ppm) 158.1, 157.7, 141.1, 135.9, 135.6, 129.5, 127.3, 126.6, 126.4, 126.1, 122.0, 120.4, 60.8, 60.1.

Anal. Calcd for C<sub>47</sub>H<sub>41</sub>N<sub>7</sub>O (1-isoTQLN·H<sub>2</sub>O): H, 5.74; C, 78.41; N, 13.91. Found: H, 5.43; C, 79.03; N, 13.91.

*N*,*N*,*N*',*N*'-tetrakis(2-quinolylmethyl)-1,3-bis(aminomethyl)benzene (*m*-TQXN). To the mixture of *m*-xylylenediamine (0.38 mL, 3.0 mmol) and potassium carbonate (6.63 g, 48.0 mmol) in dry CH<sub>3</sub>CN (120 mL) was added 2-chloromethylquinoline hydrochloride (2.57 g, 12.0 mmol) in CH<sub>3</sub>CN (50 mL) and potassium iodide (1.99 g, 12.00 mmol), then refluxed for 2 days under N<sub>2</sub>. The resultant reaction mixture was cooled to r.t. and the solvent was evaporated. After extraction with CHCl<sub>3</sub>/water, the organic layer was dried and evaporated. The residue was washed with acetonitrile to give *m*-TQXN as white powder (1.19 mg, 1.70 mmol, 57%).

<sup>1</sup>H NMR (CDCl<sub>3</sub>, Me<sub>4</sub>Si, 300 MHz): δ (ppm) 8.04 (d, *J* = 8.2 Hz, 4H), 7.98 (d, *J* = 8.5 Hz, 4H), 7.72 (d, *J* = 8.5 Hz, 4H), 7.69 (br. d, 4H), 7.65 (ddd, *J* = 8.2, 7.0, 1.2 Hz, 4H), 7.56 (s, 1H), 7.46 (ddd, *J* = 0.6, 7.0, 7.0 Hz, 4H), 7.25-7.28 (m, 3H), 4.00 (s, 8H), 3.74 (s, 4H). <sup>13</sup>C NMR (CDCl<sub>3</sub>, Me<sub>4</sub>Si, 75.5 MHz): δ (ppm) 160.0, 147.2, 138.7, 136.0, 129.4, 129.2, 128.7, 128.0, 127.7, 127.2, 127.1, 125.9, 120.7, 60.9, 58.9.

Anal. Calcd for C<sub>48</sub>H<sub>40</sub>N<sub>6</sub> (*m*-TQXN): H, 5.75; C, 82.26; N, 11.99. Found: H, 5.73; C, 82.00; N, 11.83.

*N,N,N',N'*-tetrakis(1-isoquinolylmethyl)-1,3-bis(aminomethyl)benzene (*m*-1isoTQXN). To the mixture of *m*-xylylenediamine (0.13 mL, 1.0 mmol) and potassium carbonate (2.21 g, 16.0 mmol) in dry CH<sub>3</sub>CN (50 mL) was added 1chloromethylisoquinoline (710 mg, 4.00 mmol) in CH<sub>3</sub>CN (50 mL) and potassium iodide (664 mg, 4.00 mmol), then refluxed for 1.5 days under N<sub>2</sub>. The resultant reaction mixture was cooled to r.t. and the solvent was evaporated. After extraction with CHCl<sub>3</sub>/water, the organic layer was dried and evaporated. The residue was washed with acetonitrile to give *m*-1-isoTQXN as white powder (258 mg, 0.370 mmol, 37%). <sup>1</sup>H NMR (CDCl<sub>3</sub>, Me<sub>4</sub>Si, 300 MHz): δ (ppm) 8.40 (d, *J* = 5.5 Hz, 4H), 7.70 (d, *J* = 8.5 Hz, 4H), 7.70 (d, *J* = 8.5 Hz, 4H), 7.49-7.55 (m, 8H), 6.96-7.07 (m, 8H), 4.15 (s, 8H), 3.56 (s, 4H).

<sup>13</sup>C NMR (CDCl<sub>3</sub>, Me<sub>4</sub>Si, 75.5 MHz): δ (ppm) 158.2, 141.2, 138.4, 136.0, 131.0, 129.6, 128.4, 127.5, 127.3, 126.6, 126.5, 126.1, 120.4, 60.2, 59.4.

Anal. Calcd for C<sub>48</sub>H<sub>40</sub>N<sub>6</sub> (*m*-1-isoTQXN): H, 5.75; C, 82.26; N, 11.99. Found: H, 5.71; C, 82.29; N, 11.93.

*N,N,N',N'*-tetrakis(7-methoxy-1-isoquinolylmethyl)-2,6-bis(aminomethyl)pyridine (7-MeO-1-isoTQLN). To the mixture of bis(2-aminomethyl)pyridine (32.0 mg, 0.23 mmol) and potassium carbonate (510 mg, 3.69 mmol) in dry CH<sub>3</sub>CN (20 mL) was added 7-methoxy-1-chloromethylisoquinoline (192 mg, 0.926 mmol) in CH<sub>3</sub>CN (20 mL) and potassium iodide (154 mg, 0.926 mmol), then refluxed for 1.5 days under N<sub>2</sub>. The resultant reaction mixture was cooled to r.t. and the solvent was evaporated. After extraction with CHCl<sub>3</sub>/water, the organic layer was dried and evaporated. The residue was washed with ethanol to give 7-MeO-1-isoTQLN as brown-white powder (35 mg, 0.0426 mmol, 18%).

<sup>1</sup>H NMR (CDCl<sub>3</sub>, Me<sub>4</sub>Si, 300 MHz): δ (ppm) 8.33 (d, *J* = 5.5 Hz, 4H), 7.59 (d, *J* = 8.9, 4H), 7.42 (d, *J* = 5.5, 4H), 7.26-7.27 (m, 5H), 7.15 (dd, *J* = 8.9, 2.7 Hz, 4H), 6.98 (d, *J* = 7.6 Hz, 2H), 4.37 (s, 8H), 3.87 (s, 4H), 3.28 (s, 12H).

<sup>13</sup>C NMR (CDCl<sub>3</sub>, Me<sub>4</sub>Si, 75.5 MHz): δ (ppm) 158.3, 157.6, 156.2, 139.6, 136.0, 131.6,
128.6, 128.1, 122.5, 121.7, 119.9, 103.9, 61.1, 60.6, 55.1.

Anal. Calcd for C<sub>47</sub>H<sub>41</sub>N<sub>7</sub>O (7-MeO-1-isoTQLN·H<sub>2</sub>O): H, 5.88; C, 72.82; N, 11.67. Found: H, 5.59; C, 72.82; N, 11.41.

[Zn<sub>2</sub>( $\mu$ -OH)(1-isoTQLN)(H<sub>2</sub>O)](ClO<sub>4</sub>)<sub>3</sub>. To the acetonitrile solution (0.3 mL) of 1isoTQLN (14.4 mg, 20.5 µmol) was added Zn(ClO<sub>4</sub>)<sub>2</sub>·6H<sub>2</sub>O (8.3 mg, 22.3 µmol) in acetonitrile (0.5 mL), and the solution was kept at 4 °C under ether diffusion condition to give [Zn<sub>2</sub>( $\mu$ -OH)(1-isoTQLN)(H<sub>2</sub>O)](ClO<sub>4</sub>)<sub>3</sub> as yellow-white powder (3.8 mg, 3.1 µmol, 15%). Single crystals suitable for X-ray crystallography were obtained by crystallization from acetone.

X-ray Crystallography. A single crystal of [Zn<sub>2</sub>(µ-OH)(1-isoTQLN)(H<sub>2</sub>O)](ClO<sub>4</sub>)<sub>3</sub> was covered by Paratone-N oil and mounted on a glass fiber. All data were collected at 153 K on a Rigaku Mercury CCD detector, with monochromatic MoKα radiation, operating at 50 kV/40 mA. Data were processed on a PC using CrystalClear Software (Rigaku). Structures were solved by direct methods (SHELXS version 2013/1) and refined by full-matrix least-squares methods on  $F^2$  (SHELXL version 2016/6). The disordered solvents were removed by PLATON/SQUEEZE (total potential solvent accessible void volume = 437 Å; electron count/cell = 111). Crystal data are CCDC-1507448 summarized in Table S1. 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/datarequest/cif.

Formula	CH. ClaN-Q. Zna	
	1166.01	
Crystal system	triclinic	
Space group	P-1	
<i>a,</i> Å	11.020(4)	
<i>b,</i> Å	12.924(5)	
<i>c,</i> Å	19.504(8)	
α, deg	93.355(6)	
β, deg	97.139(5)	
γ, deg	99.558(5)	
<i>V</i> , Å <sup>3</sup>	2708.9(18)	
Ζ	2	
$D_{\text{calc}}$ g cm <sup>-3</sup>	1.429	
μ, mm <sup>-1</sup>	1.101	
$2\theta_{max}$ , deg	55	
temp, K	153	
no. reflns collected	19433	
no. reflns used	11530	
no. of params	658	
R <sub>int</sub>	0.0325	
Final $R1 (I > 2\sigma(I))^a$	0.0762	
wR2 (all data) <sup>b</sup>	0.2110	
GOF	1.123	

Table S1 Crystallographic Data for  $[Zn_2(\mu-OH)(1-isoTQLN)](ClO_4)_3$ 

 ${}^{a}R1 = \Sigma ||F_{o}| - |F_{c}|| / \Sigma |F_{o}|. \quad {}^{b}wR2 = [\Sigma w[(F_{o}{}^{2} - F_{c}{}^{2})^{2}] / \Sigma [w(F_{o}{}^{2})^{2}]]^{1/2}.$ 

 $[Zn_2(\mu\text{-}OH)(1\text{-}isoTQLN)(H_2O)](ClO_4)_3$ 

Table S2 Selected Bond Distances (Å) and Angles (°) for  $[Zn_2(\mu-OH)(1-isoTQLN)-$ 

$(H_2O)](ClO_4)_3$ in the	Crystal Structure
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	Zn1	Zn2
Zn-N1(pyridine)	2.195(5)	_
Zn-Nx(aliphatic)	2.175(4)	2.203(4)
Zn-Ny(isoquinoline1)	2.088(4)	2.061(4)
Zn-Nz(isoquinoline2)	2.058(4)	2.070(5)
Zn-O1(hydroxide)	1.947(4)	1.934(4)
Zn-O2(water)	_	2.094(3)
N1-Zn-Nx	77.51(16)	_
N1-Zn-Ny	130.58(16)	_
N1-Zn-Nz	107.51(16)	_
N1-Zn-O1	100.73(15)	_
Nx-Zn-Ny	77.96(16)	78.26(15)
Nx-Zn-Nz	79.63(17)	78.78(16)
Nx-Zn-O1	173.05(15)	95.08(15)
Nx-Zn-O2	_	164.43(16)
Ny-Zn-Nz	109.32(17)	120.77(18)
Ny-Zn-O1	98.58(16)	109.19(17)
Ny-Zn-O2	_	91.43(15)
Nz-Zn-O1	107.27(17)	126.66(17)
Nz-Zn-O2	_	97.02(16)
O1-Zn-O2	-	99.35(15)



**Fig. S1** (a) Absorbance and (b) fluorescence intensity plots of TQLN in the presence of increasing amount of Zn<sup>2+</sup>. (c) Absorption spectra, (d) absorbance plot and (e) fluorescence intensity plot of TQLN in the presence of increasing amount of Cd<sup>2+</sup>. (f) Fluorescence spectra of TQLN in the presence of 1 equiv. of metal ions. All measurements were performed on 34  $\mu$ M TQLN in DMF-H<sub>2</sub>O (1:1) at 25 °C ( $\lambda_{ex}$  = 317 nm).



**Fig. S2** (a) Absorbance and (b) fluorescence intensity plots of 1-isoTQLN in the presence of increasing amount of Cd<sup>2+</sup>. (c) Absorption spectra, (d) absorbance plot and (e) fluorescence intensity plot of 1-isoTQLN in the presence of increasing amount of Zn<sup>2+</sup>. (f) Fluorescence spectra of 1-isoTQLN in the presence of 1 equiv. of metal ions. All measurements were performed on 34  $\mu$ M 1-isoTQLN in DMF-H<sub>2</sub>O (1:1) at 25 °C ( $\lambda_{ex}$  = 323 nm).



**Fig. S3** Partial <sup>1</sup>H NMR spectra of TQLN in the presence of increasing amount of  $Zn^{2+}$  in CD<sub>3</sub>CN-CDCl<sub>3</sub> (1:1).



**Fig. S4** Partial <sup>1</sup>H NMR spectra of TQLN in the presence of increasing amount of Cd<sup>2+</sup> in CD<sub>3</sub>CN-CDCl<sub>3</sub> (1:1).



**Fig. S5** Partial <sup>1</sup>H NMR spectra of 1-isoTQLN in the presence of increasing amount of  $Cd^{2+}$  in  $CD_3CN-CDCl_3$  (1:1).



**Fig. S6** Partial <sup>1</sup>H NMR spectra of 1-isoTQLN in the presence of increasing amount of  $Zn^{2+}$  in CD<sub>3</sub>CN-CDCl<sub>3</sub> (1:1).



Metal	TQLNZn	TQLNCd	1-isoTQLNCd	7-MeO-1-isoTQLNCd
0.000000	0.0000	0.0000	0.0000	0.0000
0.000007	46.7080	16.2030	18.5640	27.5350
0.000014	102.4300	36.1350	39.2160	52.8910
0.000021	161.3600	55.3830	60.2630	78.1990
0.000027	218.7500	74.1600	81.6390	101.6000
0.000034	266.2300	82.0730	101.1000	110.9800
0.000041	280.7500	81.3790	102.7500	112.0900
0.000051	284.8400	81.6290	103.1800	111.8900
0.000068	291.3900	80.9390	103.9200	112.3700

	TQLNZn	TQLNCd	1-isoTQLNCd	7-MeO-1-isoTQLNCd
zinc binding 2/7/2008				
Best-fit values				
BMAX	284.8	84.12	102.4	116.9
KD	1.8852e-007	1.1438e-008	5.4764e-009	5.3683e-008
LO	3.4000e-005	3.4000e-005	3.4000e-005	3.4000e-005
Std. Error				
BMAX	6.998	2.009	0.8505	3.895
KD	2.2081e-007	6.5572e-008	1.6285e-008	1.8965e-007
95% Confidence Intervals	and the second se			
BMAX	268.2 to 301.3	79.37 to 88.87	100.4 to 104.4	107.7 to 126.1
KD	-3.3371e-007 to 7.1074e-007	-1.4364e-007 to 1.6652e-007	-3.3037e-008 to 4.3990e-008	-3.9484e-007 to 5.0220e-007
Goodness of Fit				
Degrees of Freedom	7	7	7	7
R squared	0.9954	0.9886	0.9986	0.9839
Absolute Sum of Squares	452.9	91.72	17.91	232.3
Sy.x	8.044	3.620	1.599	5.761
Constraints				
LO	L0 = 3.4000e-005	L0 = 3.4000e-005	L0 = 3.4000e-005	L0 = 3.4000e-005
Data				
Number of X values	9	9	9	9
Number of Y replicates	1	1	1	1
Total number of values	9	9	9	9
Number of missing values	0	0	0	0

**Fig. S7** Estimation of dissociation constants ( $K_d$ ) for TQLN-Zn<sup>2+</sup>, TQLN-Cd<sup>2+</sup>, 1isoTQLN-Cd<sup>2+</sup> and 7-MeO-1-isoTQLN-Cd<sup>2+</sup> in DMF-H<sub>2</sub>O (1:1) at 25°C.



Wavelength (nm)

**Fig. S8** Fluorescence spectra of (a) TQLN-Zn<sup>2+</sup>, (b) TQLN-Cd<sup>2+</sup> and (c) 1-isoTQLN-Cd<sup>2+</sup> complexes in the absence (blue squares) and presence (red circles) of 1 equiv. of TPEN. All measurements were performed on 34  $\mu$ M ligand in DMF-H<sub>2</sub>O (1:1) at 25 °C.



**Fig. S9** (a) Fluorescence spectra and (b) fluorescence intensity at 353 nm ( $\lambda_{ex}$  = 317 nm) of *m*-TQXN in the presence of 1 equiv. of metal ions in DMF-H<sub>2</sub>O (1:1) at 25 °C.  $I_0$  is the emission intensity of free ligand.



Wavelength (nm)

**Fig. S10** Comparison of fluorescence spectra of 34  $\mu$ M of 1-isoTQLN (red circles) and *m*-1-isoTQXN (blue squares) in the absence (dotted lines with open marks) and presence (solid lines with filled marks) of 1 equiv. of Cd<sup>2+</sup> in DMF-H<sub>2</sub>O (1:1) at 25 °C.



**Fig. S11** (a) Fluorescence spectra and (b) fluorescence intensity at 357 nm ( $\lambda_{ex}$  = 323 nm) of *m*-1-isoTQXN in the presence of 1 equiv. of metal ions and (c, e) fluorescence spectra and (d, f) intensity plot of *m*-1-isoTQXN in the presence of increasing amount of (c, d) Zn<sup>2+</sup> and (e, f) Cd<sup>2+</sup>. All measurements were performed on 34 µM ligand in DMF-H<sub>2</sub>O (1:1) at 25 °C.



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Calculated using 2 exponentials
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Prompt data : Prompt
Decay data : Decay
The initial parameters are:
     Shift Value = 0
                                                                                             ch;
                                                                                                                                                                                                           sec
                                                                                                                                              2.743484E-10
    Shift Limit = 10
                                                                                              ch;
                                                                                                                                                                                                         sec
    Tl Estimate = 184.5032 ch;
T2 Estimate = 738.0129 ch;
                                                                                                                                               5.061817E-09
                                                                                                                                                                                                         sec
                                                                                                                                              2.024727E-08
                                                                                                                                                                                                         sec
   A Free
B1 Free
B2 Free
    Prompt and decay LO = 200
Prompt and decay HI = 3800
                                                                                                                     ch;
                                                                                                                                           5.486969E-09
                                                                                                                                                                                                       sec
                                                                                                                                            1.042524E-07
                                                                                                                  ch;
                                                                                                                                                                                                        sec
   Background on prompt = 0.1490066
Time calibration = 2.743484E-11 sec/ch
The fitted parameters are:
    Hi reduced to: 3790 ch
    SHIFT = 0.2467207
                                                                                                                                                                                                        S.Dev = 1.379891E-12 sec
                                                                                                             6.768744E-12 sec
                                                                                        ch;
                         = 0.2467207 ch; 0.7667442-12 sec S.Dev = 1.3795912-12 sec

= 53.24297 ch; 1.460712E-09 sec S.Dev = 1.402607E-10 sec

= 383.4688 ch; 1.05204E-08 sec S.Dev = 9.309877E-12 sec

= -0.3773081 S.Dev = 3.955138E-02

= 4.099279E-03 [1.42 Rel.Ampl][0.09 Alpha] S.Dev = 1.263955E-04

= 3.944981E-02 [98.58 Rel.Ampl][0.91 Alpha] S.Dev = 3.302527E-05

contained and the second s
     Τ1
                                                                                                                                                                                                                                                                                               sec
     T2
                                                                                                                                                                                                                                                                                               sec
     A
    B1
     B2
    Average Life Time = 9.667615E-09 sec
CHISQ = 0.9776787 [ 3585 degrees of freedom ]
      Chi-squared Probability =
                                                                                                                   82.74514 percent
     Durbin-Watson Parameter = Negative residuals =
                                                                                                                      1.949922
                                                                                                                        41.38123 percent
     Residuals < 1 s.dev
Residuals < 2 s.dev
Residuals < 3 s.dev
                                                                                                     =
                                                                                                                        69.45141 percent
                                                                                                                      96.12921 percent
99.44305 percent
                                                                                                =
      Residuals < 4 s.dev
                                                                                                   =
                                                                                                                     99.88861 percent
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**Fig. S12** Fluorescence lifetime measurement for TQLN-Zn<sup>2+</sup> complex at 428 nm in DMF-H<sub>2</sub>O (1:1) at 25 °C.



**Fig. S13** Fluorescence lifetime measurement for 1-isoTQLN-Cd<sup>2+</sup> complex at 365 nm in DMF-H<sub>2</sub>O (1:1) at 25 °C.



Wavelength (nm)

**Fig. S14** (a) Fluorescence spectra of TQLN-Zn<sup>2+</sup> complex in various solvents ( $\lambda_{ex}$  = 317 nm). (b) Fluorescence spectra of TQLN-Zn<sup>2+</sup> complex in different concentrations ( $\lambda_{ex}$  = 317 nm). (c) Excitation spectra of TQLN-Zn<sup>2+</sup> complex in various solvents ( $\lambda_{em}$  = 428 nm). All measurements were performed at 25 °C.



**Fig. S15** (a) Absorbance and (b) fluorescence intensity plots of 7-MeO-1-isoTQLN in the presence of increasing amount of Cd<sup>2+</sup>. (c) Absorption spectra, (d) absorbance plot and (e) fluorescence intensity plot of 7-MeO-1-isoTQLN in the presence of increasing amount of Zn<sup>2+</sup>. (f) Fluorescence spectra of 7-MeO-1-isoTQLN in the presence of 1 equiv. of metal ions. All measurements were performed on 34  $\mu$ M 7-MeO-1-isoTQLN in DMF-H<sub>2</sub>O (1:1) at 25 °C ( $\lambda_{ex}$  = 323 nm).





**Fig. S16** Effect of pH on fluorescence intensity of (a) TQLN, (b) 1-isoTQLN and (c) 7-MeO-1-isoTQLN in the absence (blue squares) and presence (red circles) of 1 equiv. of (a)  $Zn^{2+}$  or (b, c)  $Cd^{2+}$  in DMF-H<sub>2</sub>O (1:1) at 25 °C.



Fig. S17 <sup>1</sup>H NMR spectrum for TQLN in CDCl<sub>3</sub>.



Fig. S18 <sup>13</sup>C NMR spectrum for TQLN in CDCl<sub>3</sub>.



Fig. S19 <sup>1</sup>H NMR spectrum for 1-isoTQLN in CDCl<sub>3</sub>.



Fig. S20 <sup>13</sup>C NMR spectrum for 1-isoTQLN in CDCl<sub>3</sub>.



**Fig. S21** <sup>1</sup>H NMR spectrum for *m*-TQXN in CDCl<sub>3</sub>.



**Fig. S22** <sup>13</sup>C NMR spectrum for *m*-TQXN in CDCl<sub>3</sub>.



**Fig. S23** <sup>1</sup>H NMR spectrum for *m*-1-isoTQXN in CDCl<sub>3</sub>.



**Fig. S24** <sup>13</sup>C NMR spectrum for *m*-1-isoTQXN in CDCl<sub>3</sub>.

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Fig. S25 <sup>1</sup>H NMR spectrum for 7-MeO-1-isoTQLN in CDCl<sub>3</sub>.



Fig. S26 <sup>13</sup>C NMR spectrum for 7-MeO-1-isoTQLN in CDCl<sub>3</sub>.