

Supplementary Information for

**Effect of methoxy substituents on fluorescent Zn<sup>2+</sup>/Cd<sup>2+</sup> selectivity of  
bisquinoline derivatives with a N,N'-dimethylalkanediamine skeleton**

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**Table S1.** Crystallographic Data for  $[(\mu\text{-Cl})_2\text{Cd}_2(\text{BQDMEN})_2](\text{ClO}_4)_2$  and  $[\text{Zn}(\text{BQDMEN})\text{Cl}]\text{ClO}_4$

	$[(\mu\text{-Cl})_2\text{Cd}_2(\text{BQ-})$ $\text{DMEN})_2](\text{ClO}_4)_2$	$[\text{Zn}(\text{BQDMEN})\text{Cl}]\text{-}$ $\text{ClO}_4$
Formula	$\text{C}_{48}\text{H}_{52}\text{Cd}_2\text{Cl}_4\text{N}_8\text{O}_8$	$\text{C}_{24}\text{H}_{26}\text{Cl}_2\text{N}_4\text{O}_4\text{Zn}$
FW	1235.62	570.78
Crystal system	monoclinic	trigonal
Space group	$C2/c$	$R3c$
$a$ , Å	45.845(14)	30.1327(13)
$b$ , Å	13.759(4)	30.1327(13)
$c$ , Å	26.417(8)	14.7905(7)
$\alpha$ , deg	90	90
$\beta$ , deg	107.426(3)	90
$\gamma$ , deg	90	120
$V$ , Å <sup>3</sup>	15899(8)	11630.3(9)
Z	12	18
$D_{\text{calc}}$ , g cm <sup>-3</sup>	1.549	1.467
$\mu$ , mm <sup>-1</sup>	1.0632	1.1942
$2\theta_{\text{max}}$ , deg	61.5	55
temp, K	153	153
no. reflns collected	91605	39478
no. reflns used	23213	5925
no. of params	998	318
$R_{\text{int}}$	0.0311	0.0371
Final $R1$ ( $I > 2\sigma(I)$ ) <sup>a</sup>	0.0543	0.0248
$wR2$ (all data) <sup>b</sup>	0.1588	0.0559
GOF	1.064	1.098
Flack parameter	-	0.028(4)

<sup>a</sup> $R1 = \sum ||F_o| - |F_c|| / \sum |F_o|$ .    <sup>b</sup> $wR2 = [\sum w[(F_o^2 - F_c^2)^2] / \sum [w(F_o^2)^2]]^{1/2}$ .

**Table S2.** Interatomic Distances ( $\text{\AA}$ ) for  $[(\mu\text{-Cl})_2\text{Cd}_2(\text{BQDMEN})_2](\text{ClO}_4)_2$  and  $[\text{Zn}(\text{BQDMEN})\text{Cl}]\text{ClO}_4$

Bonds <sup>a</sup>	$[(\mu\text{-Cl})_2\text{Cd}_2(\text{BQDMEN})_2](\text{ClO}_4)_2$	$[\text{Zn}(\text{BQDMEN})\text{Cl}]\text{ClO}_4$			
	Cd1 <sup>b</sup>	Cd2 <sup>b</sup>	Cd3 <sup>c</sup>	Cd4 <sup>c</sup>	Zn1
M-Cl1	2.5924(12)	2.5660(12)	2.5849(10)	2.5696(10)	2.2623(7)
M-Cl2	2.5646(12)	2.5823(11)	2.5849(10) <sup>d</sup>	2.5696(10) <sup>d</sup>	-
M-N1	2.345(3)	2.333(3)	2.334(3)	2.346(4)	2.136(2)
M-N2	2.334(3)	2.329(3)	2.334(3) <sup>d</sup>	2.346(4) <sup>d</sup>	2.195(3)
M-N3	2.484(3)	2.527(3)	2.503(3)	2.486(3)	2.218(3)
M-N4	2.464(3)	2.496(3)	2.503(3) <sup>d</sup>	2.486(3) <sup>d</sup>	2.1205(19)
M...O1 (pechlorate)	-	-	-	-	3.588(2)

<sup>a</sup> N1 and N2 denote aliphatic nitrogen and N3 and N4 denote aromatic (quinoline) nitrogen atoms.

<sup>b</sup> See Fig. 4.

<sup>c</sup> See Fig. S10a.

<sup>d</sup> Generated by symmetry operation (-X+1, Y, -Z+1/2).

**Table S3.** Bond Angles ( $^{\circ}$ ) for  $[(\mu\text{-Cl})_2\text{Cd}_2(\text{BQDMEN})_2](\text{ClO}_4)_2$  and  $[\text{Zn}(\text{BQDMEN})\text{Cl}]\text{ClO}_4$

Angle <sup>a</sup>	$[(\mu\text{-Cl})_2\text{Cd}_2(\text{BQDMEN})_2](\text{ClO}_4)_2$		$[\text{Zn}(\text{BQDMEN})\text{Cl}]\text{ClO}_4$	
	Cd1 <sup>b</sup>	Cd2 <sup>b</sup>	Cd3 <sup>c</sup>	Cd4 <sup>c</sup>
Cl1-M-Cl2	91.18(4)	91.38(4)	88.19(4)	88.86(4)
Cl1-M-N1	168.16(10)	95.67(8)	96.93(8)	169.91(8)
Cl1-M-N2	93.25(9)	170.90(7)	169.67(9)	96.94(10)
Cl1-M-N3	100.29(7)	90.35(7)	99.22(7)	93.41(7)
Cl1-M-N4	93.34(8)	101.21(7)	93.64(7)	100.27(7)
Cl2-M-N1	96.98(8)	168.38(7)	169.67(9) <sup>d</sup>	96.94(10) <sup>d</sup>
Cl2-M-N2	173.78(10)	94.56(8)	96.93(8) <sup>d</sup>	169.91(8) <sup>d</sup>
Cl2-M-N3	89.82(7)	100.13(6)	93.64(7) <sup>d</sup>	100.27(7) <sup>d</sup>
Cl2-M-N4	103.15(8)	94.28(8)	99.22(7) <sup>d</sup>	93.41(7) <sup>d</sup>
N1-M-N2	79.31(11)	79.64(10)	79.48(10)	78.58(14)
N1-M-N3	71.29(11)	70.67(9)	94.38(11)	93.67(12)
N1-M-N4	93.13(11)	93.40(10)	71.59(11)	71.24(11)
N2-M-N3	93.67(11)	95.38(10)	71.59(11) <sup>d</sup>	71.24(11) <sup>d</sup>
N2-M-N4	72.26(12)	71.50(10)	94.38(11) <sup>d</sup>	93.67(12) <sup>d</sup>
N3-M-N4	161.01(10)	161.31(9)	162.09(10)	160.83(10)
Zn1				

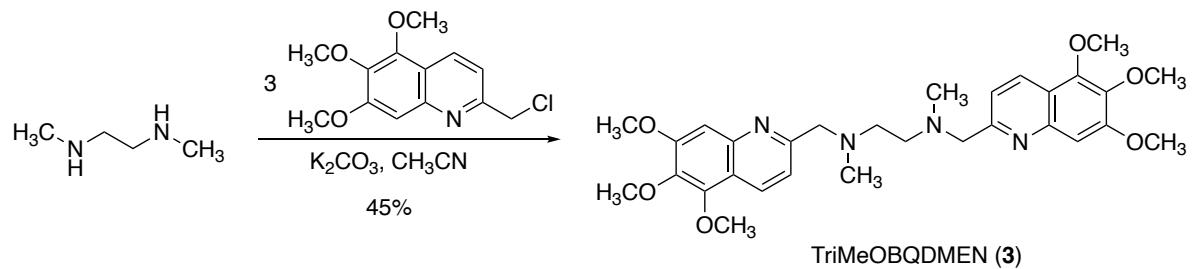
<sup>a</sup> N1 and N2 denote aliphatic nitrogen and N3 and N4 denotes aromatic (quinoline) nitrogen atoms.

<sup>b</sup> See Fig. 4.

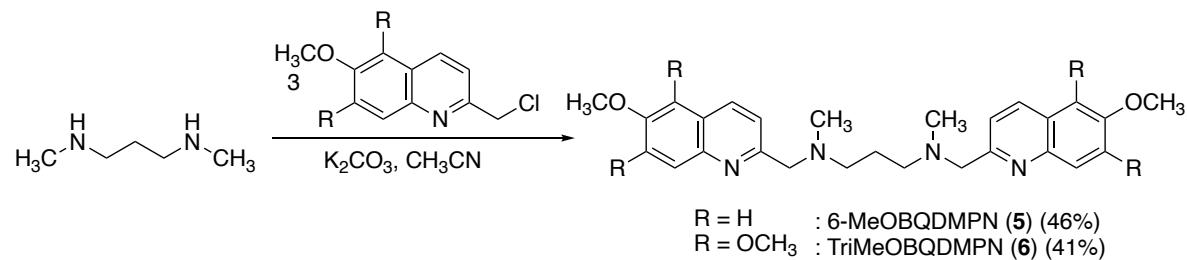
<sup>c</sup> See Fig. S10a.

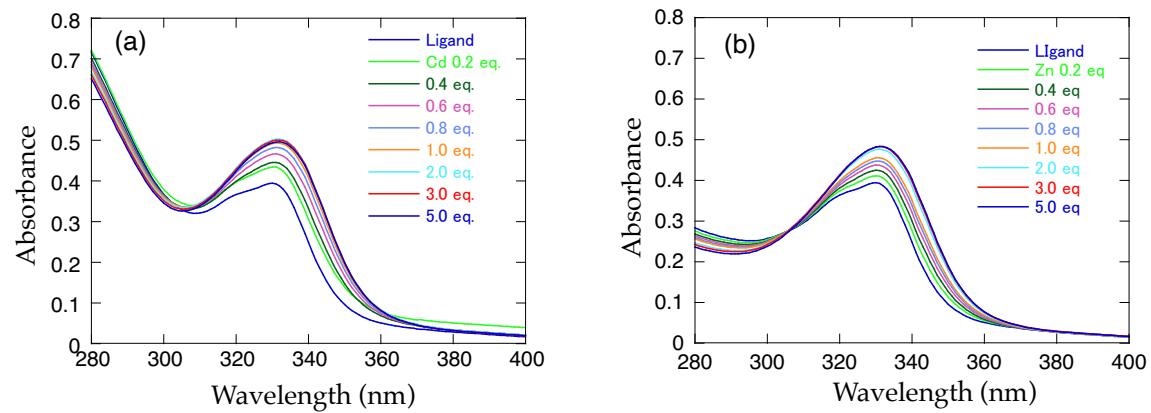
<sup>d</sup> Generated by symmetry operation (-X+1, Y, -Z+1/2).

Scheme S1



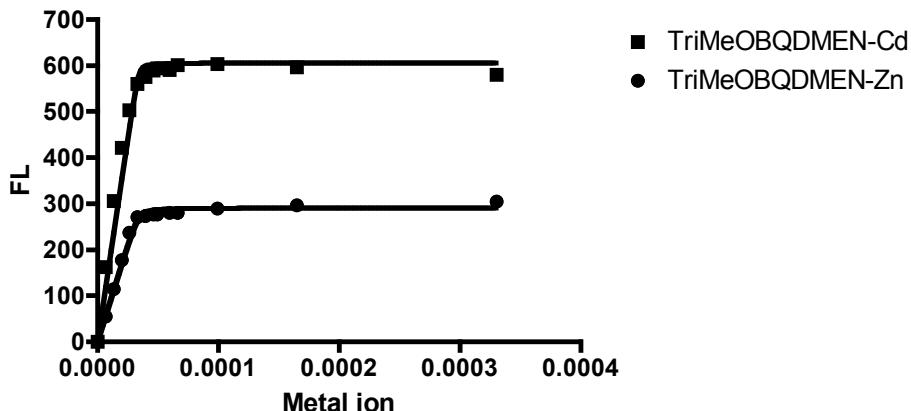
Scheme S2





**Fig. S1.** UV-vis absorption spectra of 34  $\mu\text{M}$  TriMeOBQDMEN (**3**) in DMF- $\text{H}_2\text{O}$  (1:1) at 25  $^\circ\text{C}$  in the presence of (a)  $\text{Cd}^{2+}$  and (b)  $\text{Zn}^{2+}$ .

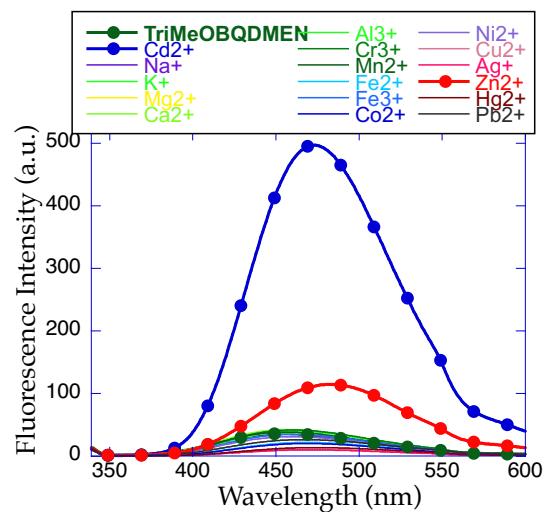
### Binding Constants for TriMeOBQDMEN



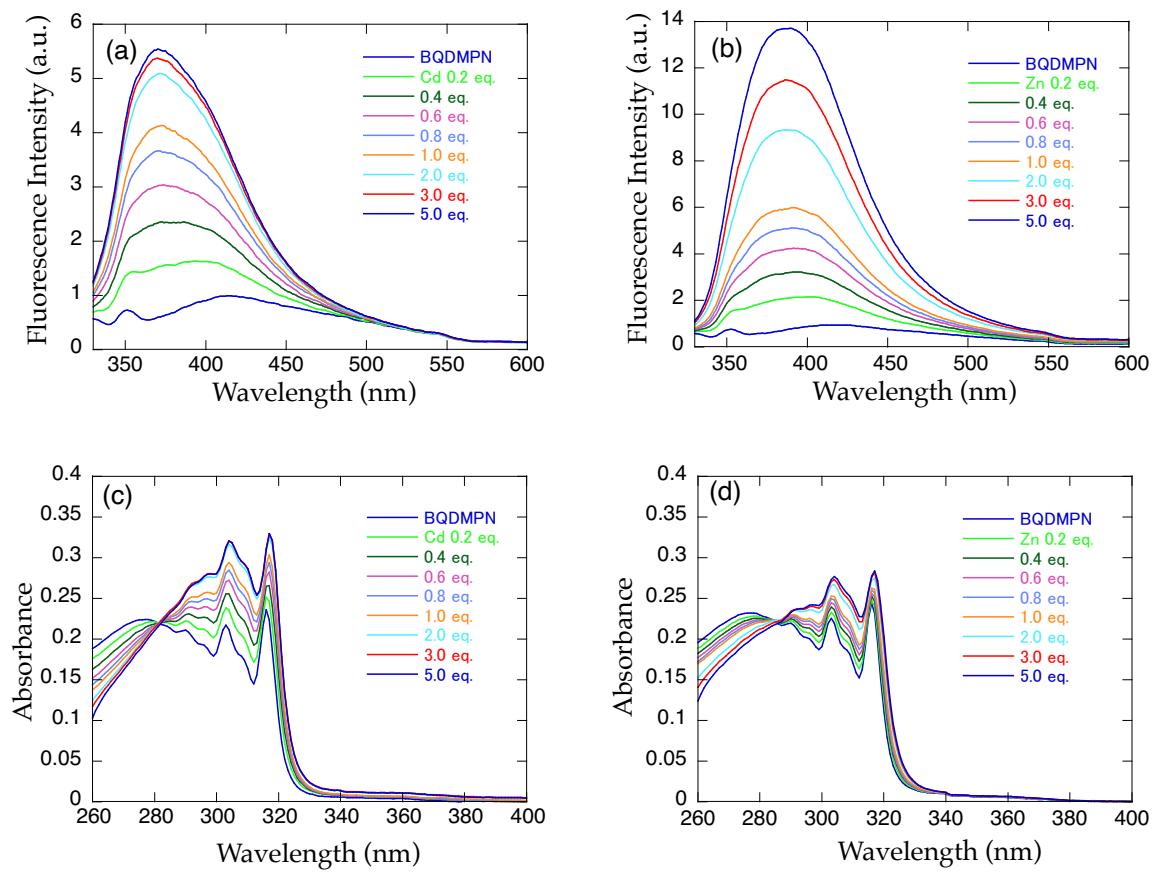
metal ion	TriMeOBQDMEN-Cd	TriMeOBQDMEN-Zn
0.000000	0.0000	0.0000
6.600000e-06	162.3400	54.3300
1.320000e-05	306.0500	114.8000
1.980000e-05	420.6200	177.6800
2.640000e-05	503.2000	236.3700
3.300000e-05	560.2800	270.9100
3.960000e-05	575.2000	272.7600
4.620000e-05	588.7300	275.9200
4.950000e-05	593.8900	276.6700
0.000059	590.6200	279.7100
0.000066	600.9500	280.5400
0.000099	602.7300	289.4500
0.000165	596.5700	296.8500
0.000330	579.5900	304.1100

	TriMeOBQDMEN-Cd	TriMeOBQDMEN-Zn
zinc binding 2/7/2008		
Best-fit values		
BMAX	605.8	290.7
KD	7.7459e-008	2.0873e-007
L0	3.4000e-005	3.4000e-005
Std. Error		
BMAX	15.29	4.609
KD	2.2370e-007	1.9566e-007
95% Confidence Intervals		
BMAX	572.5 to 639.1	280.6 to 300.7
KD	-4.0999e-007 to 5.6490e-007	-2.1762e-007 to 6.3508e-007
Goodness of Fit		
Degrees of Freedom	12	12
R squared	0.9677	0.9913
Absolute Sum of Squares	15225	1098
Sy.x	35.62	9.566
Constraints		
L0	L0 = 3.4000e-005	L0 = 3.4000e-005
Data		
Number of X values	14	14
Number of Y replicates	1	1
Total number of values	14	14
Number of missing values	0	0

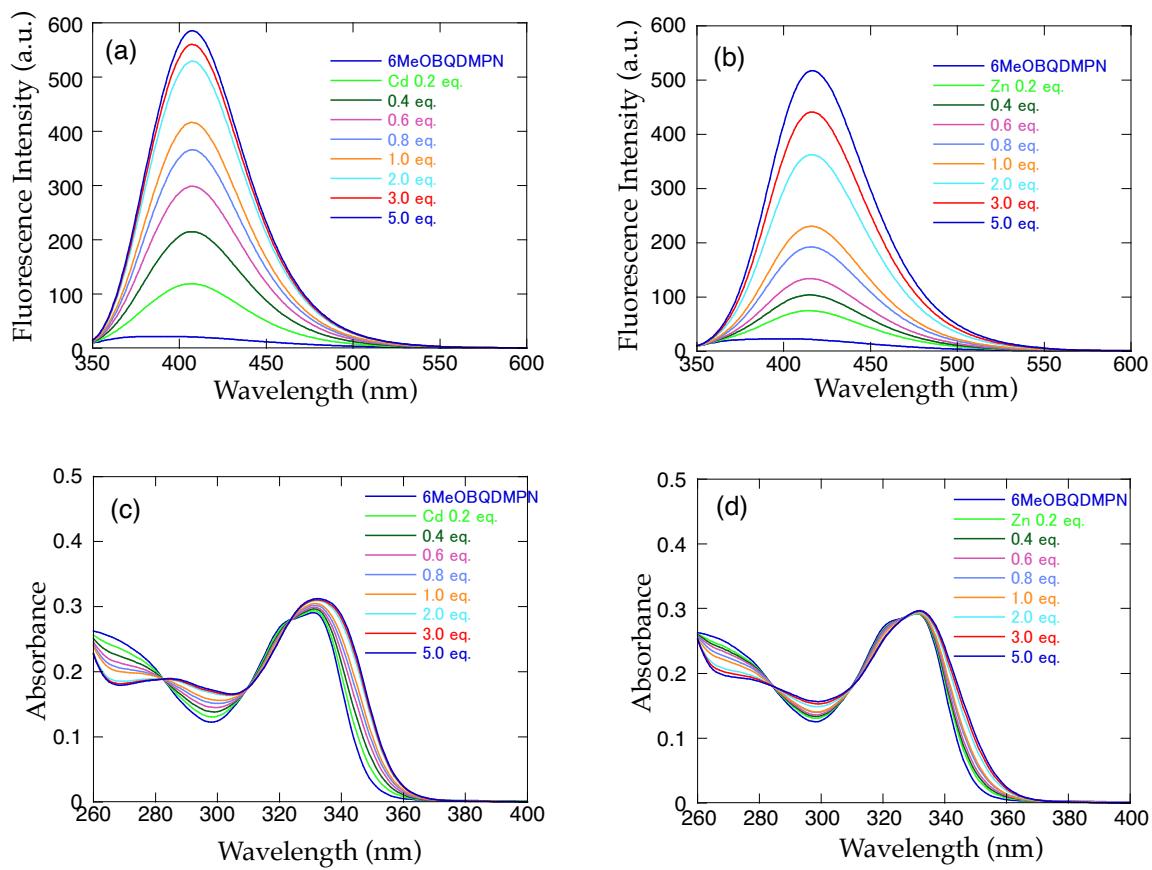
**Fig. S2.** Estimation of dissociation constants ( $K_d$ ) for TriMeOBQDMEN (3) with  $\text{Cd}^{2+}$  and  $\text{Zn}^{2+}$  in DMF- $\text{H}_2\text{O}$  (1:1) at 25°C.



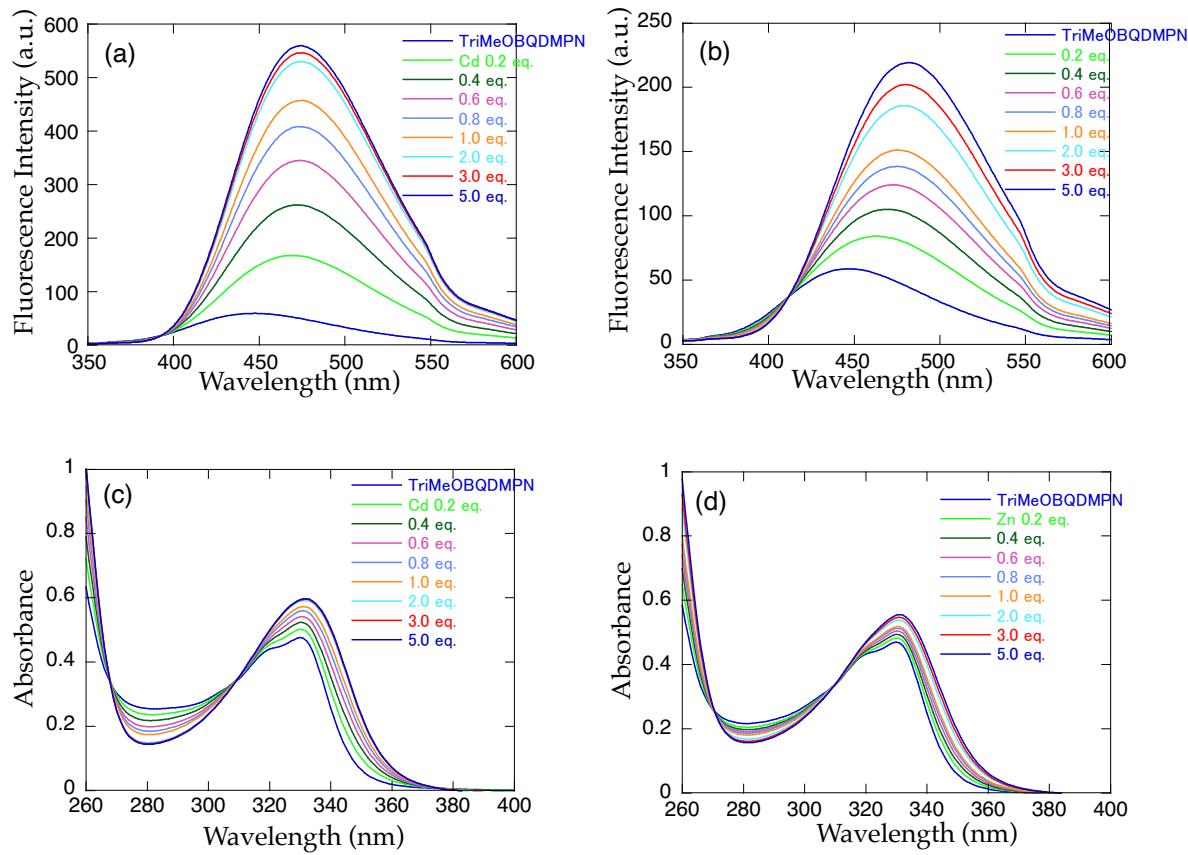
**Fig. S3.** Fluorescence spectra of 34  $\mu$ M TriMeOBQDMEN (**3**) in the presence of 1 equiv. of various metal ions in DMF-H<sub>2</sub>O (1:1) at 25 °C ( $\lambda_{\text{ex}} = 339$  nm).



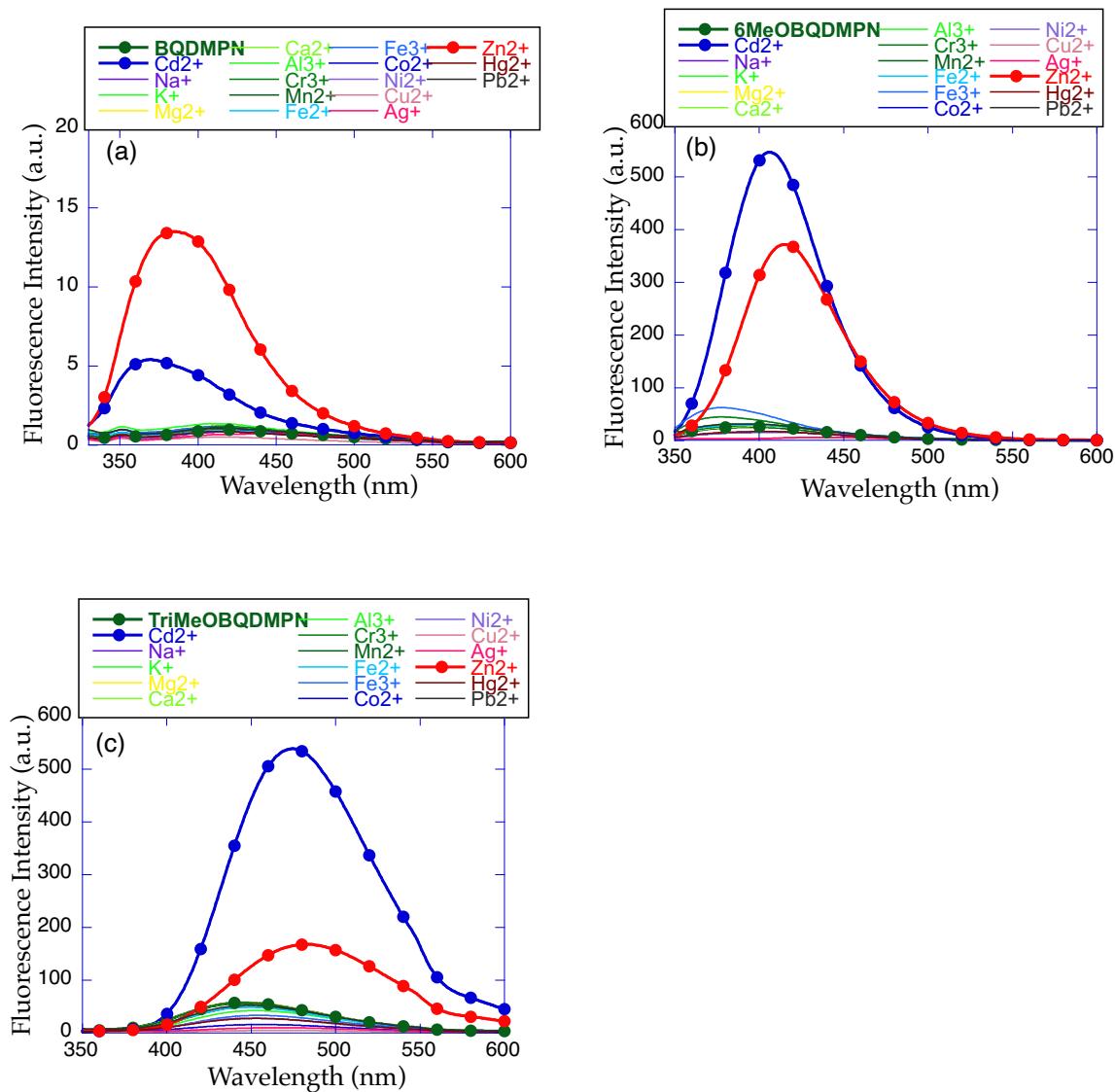
**Fig. S4.** (a,b) Fluorescence and (c,d) UV-vis spectra of 34  $\mu\text{M}$  BQDMPN (**4**) in DMF-H<sub>2</sub>O (1:1) at 25 °C in the presence of increasing amount of (a,c) Cd<sup>2+</sup> and (b,d) Zn<sup>2+</sup> ( $\lambda_{\text{ex}} = 317 \text{ nm}$ ).



**Fig. S5.** (a,b) Fluorescence and (c,d) UV-vis spectra of 34  $\mu$ M 6-MeOBQDMPN (**5**) in DMF-H<sub>2</sub>O (1:1) at 25 °C in the presence of increasing amount of (a,c) Cd<sup>2+</sup> and (b,d) Zn<sup>2+</sup> ( $\lambda_{\text{ex}} = 341$  nm).

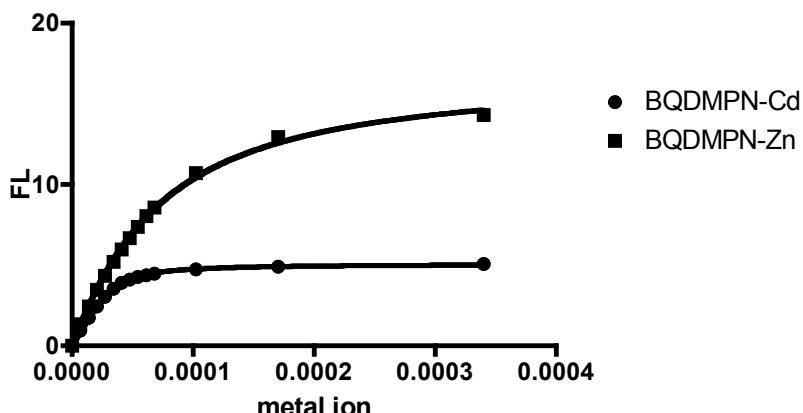


**Fig. S6.** (a,b) Fluorescence and (c,d) UV-vis spectra of  $34 \mu\text{M}$  **TriMeOBQDMPN (6)** in  $\text{DMF-H}_2\text{O}$  (1:1) at  $25^\circ\text{C}$  in the presence of (a,c)  $\text{Cd}^{2+}$  and (b,d)  $\text{Zn}^{2+}$  ( $\lambda_{\text{ex}} = 337 \text{ nm}$ ).



**Fig. S7.** Fluorescence spectra of 34  $\mu\text{M}$  (a) BQDMPN (**4**) ( $\lambda_{\text{ex}} = 317 \text{ nm}$ ), (b) 6-MeOBQDMPN (**5**) ( $\lambda_{\text{ex}} = 341 \text{ nm}$ ) and (c) TriMeOBQDMPN (**6**) ( $\lambda_{\text{ex}} = 337 \text{ nm}$ ) in the presence of 1 equiv. of various metal ions in DMF-H<sub>2</sub>O (1:1) at 25 °C.

### Binding Constants for BQDMPN

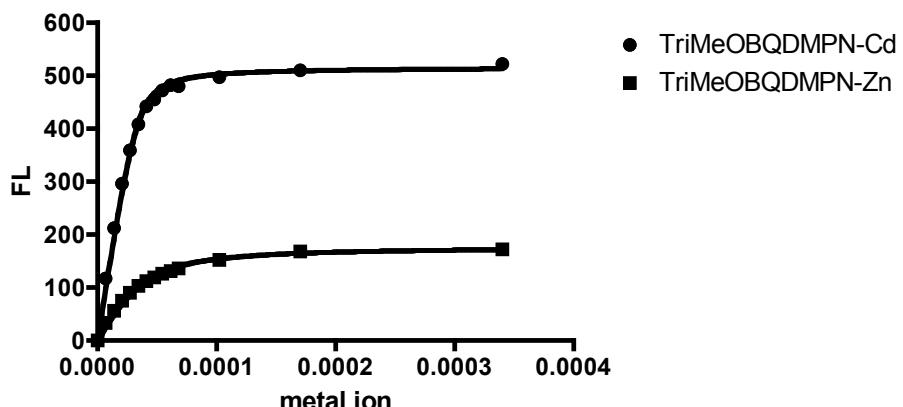


metal ion	BQDMPN-Cd	BQDMPN-Zn
0.000000	0.00000	0.00000
0.000007	0.92822	1.3360
0.000014	1.73550	2.4308
0.000020	2.42120	3.4558
0.000027	3.02550	4.3261
0.000034	3.51830	5.1843
0.000041	3.89020	5.9545
0.000048	4.10260	6.6661
0.000054	4.27730	7.3535
0.000061	4.36640	8.0314
0.000068	4.46490	8.5568
0.000102	4.72370	10.6990
0.000170	4.89050	12.9330
0.000340	5.06100	14.2960

	BQDMPN-Cd	BQDMPN-Zn
zinc binding 2/7/2008		
Best-fit values		
BMAX	5.073	17.02
KD	4.7108e-006	5.1306e-005
L0	3.4000e-005	3.4000e-005
Std. Error		
BMAX	0.02865	0.2715
KD	2.2418e-007	2.2804e-006
95% Confidence Intervals		
BMAX	5.010 to 5.135	16.43 to 17.61
KD	4.2224e-006 to 5.1993e-006	4.6337e-005 to 5.6275e-005
Goodness of Fit		
Degrees of Freedom	12	12
R squared	0.9994	0.9983
Absolute Sum of Squares	0.01777	0.3965
Sy.x	0.03849	0.1818
Constraints		
L0	L0 = 3.4000e-005	L0 = 3.4000e-005
Data		
Number of X values	14	14
Number of Y replicates	1	1
Total number of values	14	14
Number of missing values	0	0

**Fig. S8.** Estimation of dissociation constants ( $K_d$ ) for BQDMPN (4) with  $\text{Cd}^{2+}$  and  $\text{Zn}^{2+}$  in DMF- $\text{H}_2\text{O}$  (1:1) at 25°C.

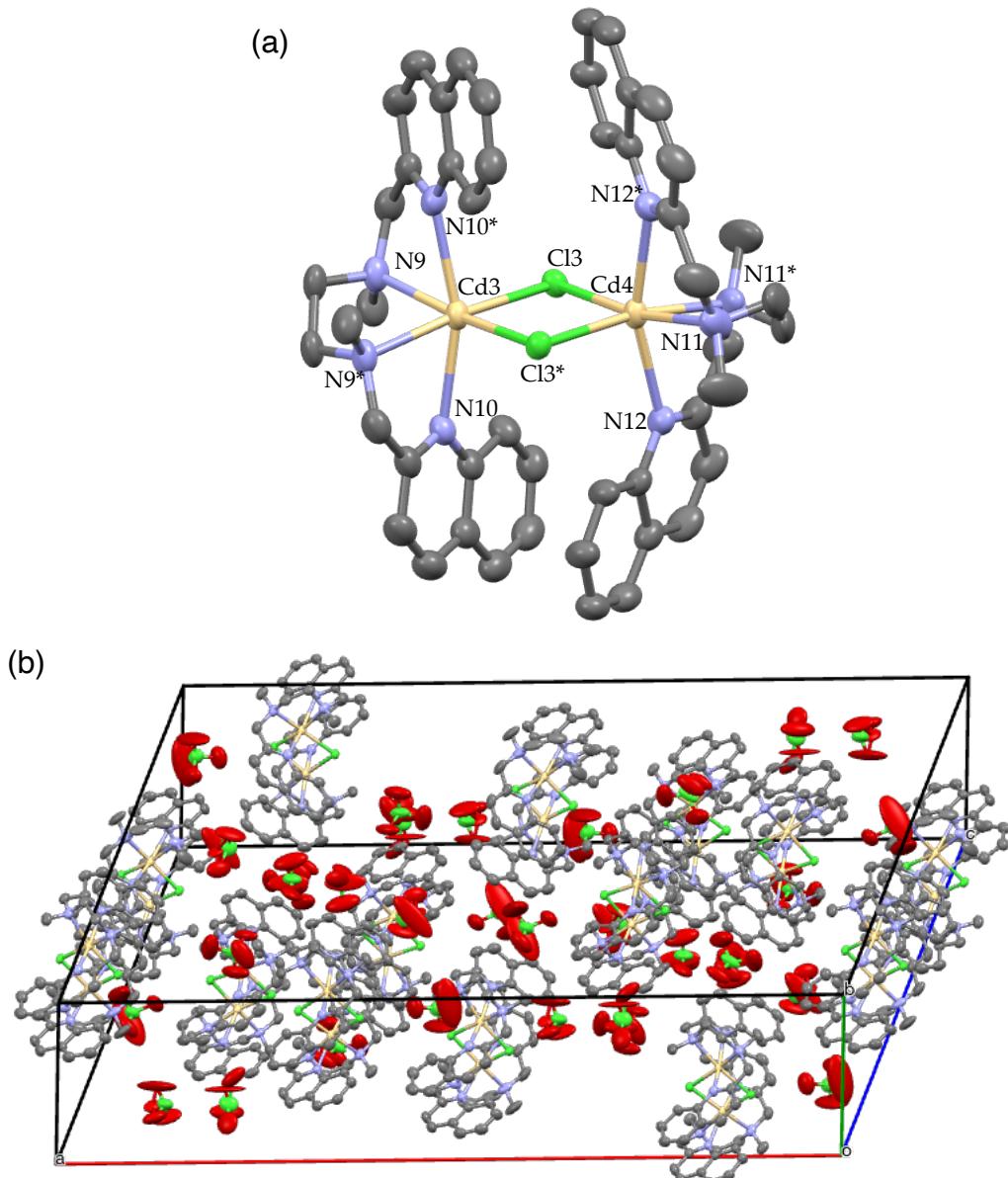
### Binding Constants for TriMeOBQDMPN



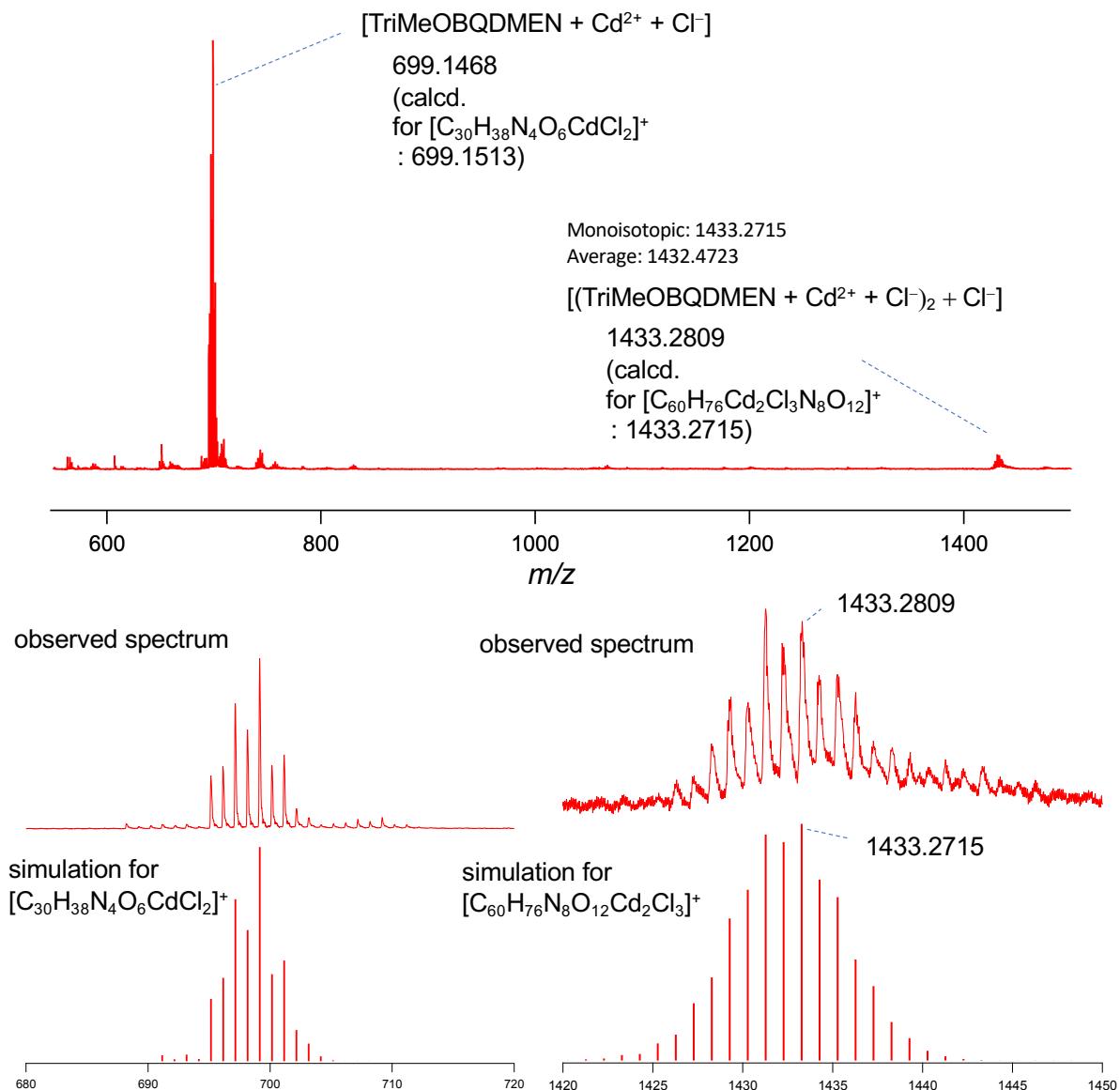
metal ion	TriMeOBQDMPN-Cd	TriMeOBQDMPN-Zn
0.000000	0.0000	0.0000
0.000007	116.9500	32.9210
0.000014	212.1400	55.7840
0.000020	295.5500	75.4120
0.000027	358.8000	89.8850
0.000034	408.0700	102.7200
0.000041	442.4900	111.7100
0.000048	455.1700	118.9300
0.000054	472.2800	125.8000
0.000061	482.0400	131.1000
0.000068	480.3600	136.4300
0.000102	497.0900	152.1600
0.000170	510.4000	168.1900
0.000340	522.0100	172.3400

	TriMeOBQDMPN-Cd	TriMeOBQDMPN-Zn
zinc binding 2/7/2008		
Best-fit values		
BMAX	515.7	177.6
KD	1.8164e-006	1.1125e-005
L0	3.4000e-005	3.4000e-005
Std. Error		
BMAX	7.412	3.770
KD	3.8540e-007	1.2650e-006
95% Confidence Intervals		
BMAX	499.6 to 531.9	169.4 to 185.8
KD	9.7658e-007 to 2.6562e-006	8.3684e-006 to 1.3881e-005
Goodness of Fit		
Degrees of Freedom	12	12
R squared	0.9952	0.9934
Absolute Sum of Squares	1642	215.7
Sy.x	11.70	4.240
Constraints		
L0	L0 = 3.4000e-005	L0 = 3.4000e-005
Data		
Number of X values	14	14
Number of Y replicates	1	1
Total number of values	14	14
Number of missing values	0	0

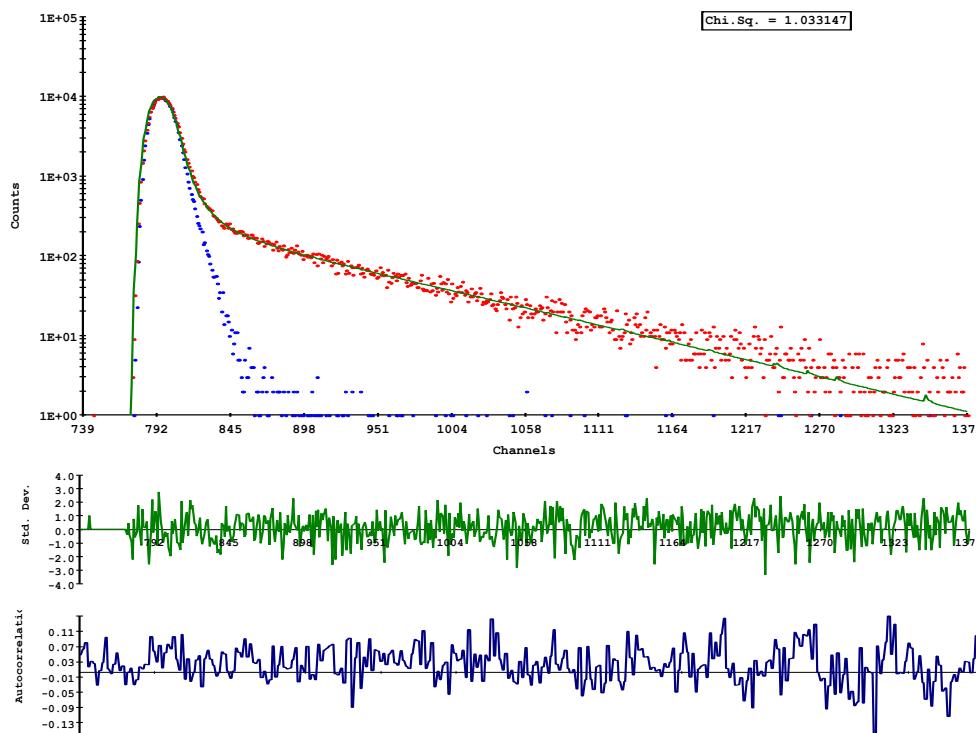
**Fig. S9.** Estimation of dissociation constants ( $K_d$ ) for TriMeOBQDMPN (6) with  $\text{Cd}^{2+}$  and  $\text{Zn}^{2+}$  in DMF-H<sub>2</sub>O (1:1) at 25°C.



**Fig. S10.** (a) Perspective view of crystallographically independent molecule showing atom numbering (See also Fig. 4) for  $[(\mu\text{-Cl})_2\text{Cd}_2(\text{BQDMEN})_2](\text{ClO}_4)_2$  with 50% probability. Hydrogen atoms and counter anions were omitted for clarity. Atoms with asterisks were generated by symmetry operation  $(-\text{X}+1, \text{Y}, -\text{Z}+1/2)$ . (b) Unit cell packing.



**Fig. S11.** ESI-MS spectrum of 34 μM TriMeOBQDMEN (**3**) in DMF-H<sub>2</sub>O (1:1) in the presence of 3 equiv. of Cd(ClO<sub>4</sub>)<sub>2</sub>.



Calculated using 3 exponentials

Prompt data : Prompt  
Decay data : BQDMEN(370)

The initial parameters are:

Shift Value = 0	ch;	0	sec
Shift Limit = 40	ch;	2.194787E-09	sec
T1 Estimate = 6.321533	ch;	3.468605E-10	sec
T2 Estimate = 12.64307	ch;	6.937211E-10	sec
T3 Estimate = 25.28613	ch;	1.387442E-09	sec

A Free  
B1 Free  
B2 Free  
B3 Free

Prompt and decay LO = 739 ch; 4.05487E-08 sec  
Prompt and decay HI = 1416 ch; 7.769547E-08 sec

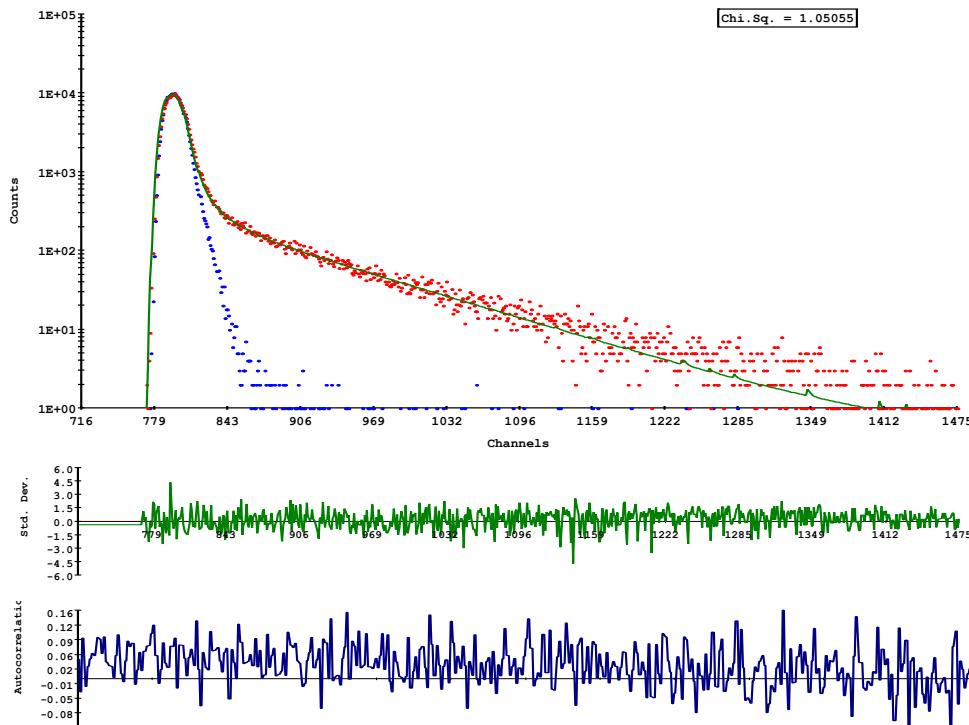
Background on prompt = 0  
Time calibration = 5.486969E-11 sec/ch

The fitted parameters are:

Hi reduced to: 1376 ch

SHIFT = -2.058854	ch;	-1.129687E-10	sec	S.Dev = 1.083906E-12	sec
T1 = 19.9895	ch;	1.096817E-09	sec	S.Dev = 1.420633E-10	sec
T2 = 2.572635	ch;	1.411597E-10	sec	S.Dev = 2.84237E-12	sec
T3 = 106.7898	ch;	5.859523E-09	sec	S.Dev = 7.624264E-11	sec
A = -2.183464E-02				S.Dev = 9.720971E-02	
B1 = 2.991585E-03	[ 4.25 Rel.Ampl] [ 0.01 Alpha]	S.Dev = 1.158314E-04			
B2 = 0.4696873	[ 85.97 Rel.Ampl] [ 0.99 Alpha]	S.Dev = 1.470682E-03			
B3 = 1.286851E-03	[ 9.78 Rel.Ampl] [ 0.00 Alpha]	S.Dev = 1.215098E-05			
Average Life Time = 1.627174E-10 sec					
CHISQ = 1.033147 [ 630 degrees of freedom ]					
Chi-squared Probability = 27.40336 percent					
Durbin-Watson Parameter = 1.906936					
Negative residuals = 41.37931 percent					
Residuals < 1 s.dev = 65.04702 percent					
Residuals < 2 s.dev = 95.76803 percent					
Residuals < 3 s.dev = 99.84326 percent					
Residuals < 4 s.dev = 100 percent					

**Fig. S12.** Fluorescence lifetime measurement of 34  $\mu$ M BQDMEN (**1**) in DMF-H<sub>2</sub>O (1:1) with 370 nm bandpath filter (BPF) at 25 °C ( $\lambda_{\text{ex}} = 331$  nm).



Calculated using 3 exponentials

Prompt data : Prompt  
Decay data : BQDMEN-Cd(370)

The initial parameters are:

Shift Value = 0	ch;	0	sec
Shift Limit = 40	ch;	2.194787E-09	sec
T1 Estimate = 6.396973	ch;	3.509999E-10	sec
T2 Estimate = 12.79395	ch;	7.019997E-10	sec
T3 Estimate = 25.58789	ch;	1.403999E-09	sec

A Free  
B1 Free  
B2 Free  
B3 Free

Prompt and decay LO = 716 ch; 3.928669E-08 sec  
Prompt and decay HI = 1515 ch; 8.312757E-08 sec

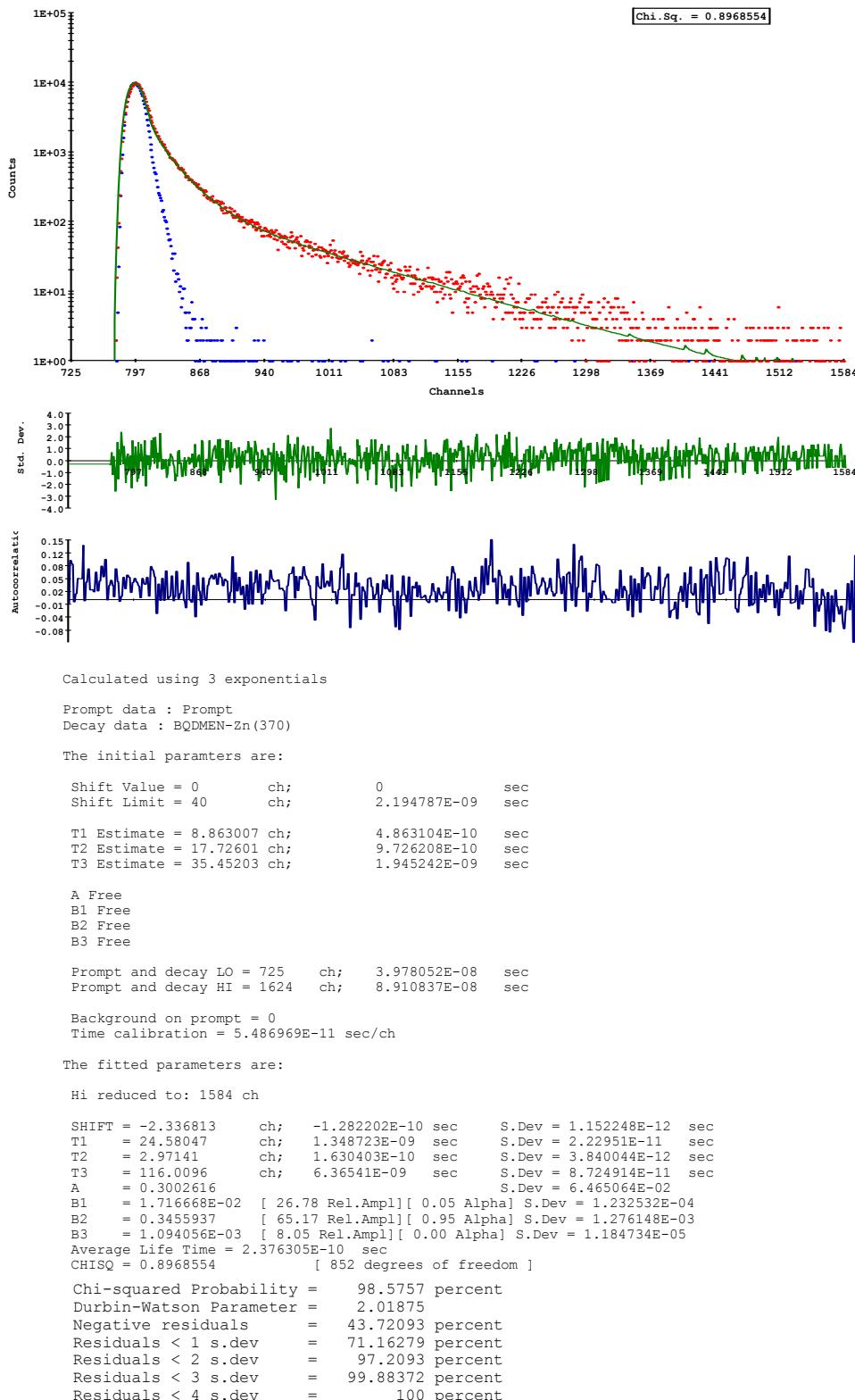
Background on prompt = 0  
Time calibration = 5.486969E-11 sec/ch

The fitted parameters are:

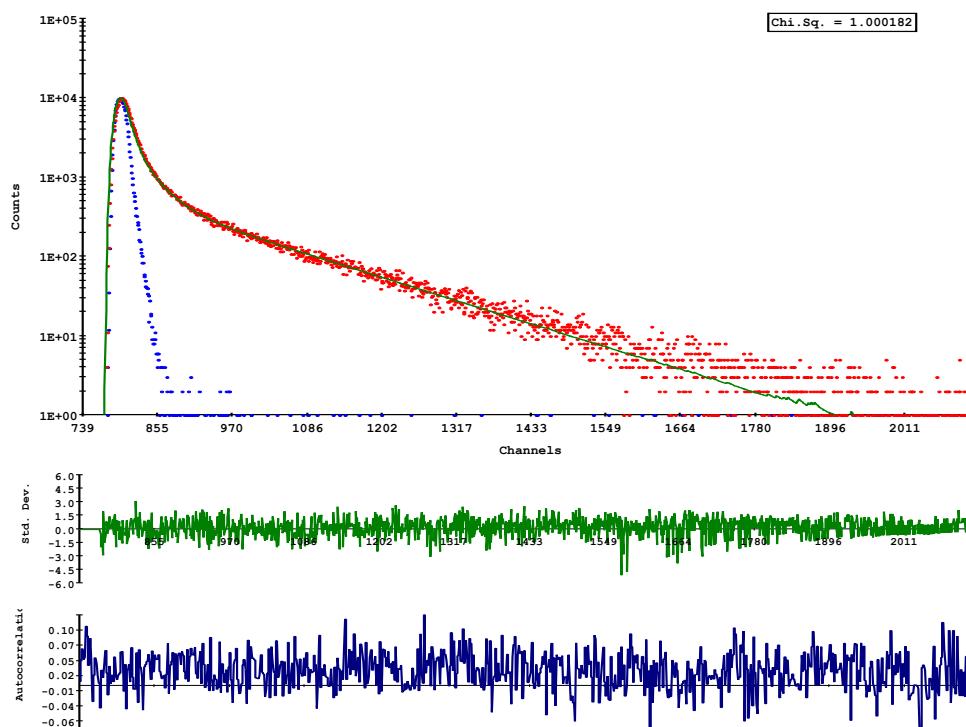
Hi reduced to: 1475 ch

SHIFT = -2.154608	ch;	-1.182227E-10	sec	S.Dev = 1.090123E-12	sec
T1 = 20.25125	ch;	1.11118E-09	sec	S.Dev = 1.446477E-10	sec
T2 = 2.629027	ch;	1.442539E-10	sec	S.Dev = 3.138603E-12	sec
T3 = 98.0094	ch;	5.377745E-09	sec	S.Dev = 6.644517E-11	sec
A = 0.3654477				S.Dev = 6.951313E-02	
B1 = 3.433938E-03	[ 5.02 Rel.Ampl][ 0.01 Alpha]	S.Dev = 1.193745E-04			
B2 = 0.4459012	[ 84.67 Rel.Ampl][ 0.99 Alpha]	S.Dev = 1.427966E-03			
B3 = 1.455953E-03	[ 10.31 Rel.Ampl][ 0.00 Alpha]	S.Dev = 1.356757E-05			
Average Life Time = 1.685225E-10 sec					
CHISQ = 1.05055 [ 752 degrees of freedom ]					
Chi-squared Probability = 16.32303 percent					
Durbin-Watson Parameter = 1.91					
Negative residuals = 43.55263 percent					
Residuals < 1 s.dev = 67.89474 percent					
Residuals < 2 s.dev = 95.26316 percent					
Residuals < 3 s.dev = 99.47369 percent					
Residuals < 4 s.dev = 99.73684 percent					

**Fig. S13.** Fluorescence lifetime measurement of 34  $\mu\text{M}$  BQDMEN (**1**) in the presence of 3 equiv. of  $\text{Cd}^{2+}$  in DMF- $\text{H}_2\text{O}$  (1:1) with 370 nm bandpath filter (BPF) at 25 °C ( $\lambda_{\text{ex}} = 331$  nm).



**Fig. S14.** Fluorescence lifetime measurement of 34  $\mu\text{M}$  BQDMEN (**1**) in the presence of 3 equiv. of  $\text{Zn}^{2+}$  in DMF- $\text{H}_2\text{O}$  (1:1) with 370 nm bandpath filter (BPF) at 25 °C ( $\lambda_{\text{ex}} = 331$  nm).



Calculated using 3 exponentials

Prompt data : Prompt  
Decay data : 6MeOBQDMEN(400)

The initial parameters are:

Shift Value = 0	ch;	0	sec
Shift Limit = 40	ch;	2.194787E-09	sec
T1 Estimate = 26.065	ch;	1.430179E-09	sec
T2 Estimate = 52.13	ch;	2.860357E-09	sec
T3 Estimate = 104.26	ch;	5.720714E-09	sec

A Free  
B1 Free  
B2 Free  
B3 Free

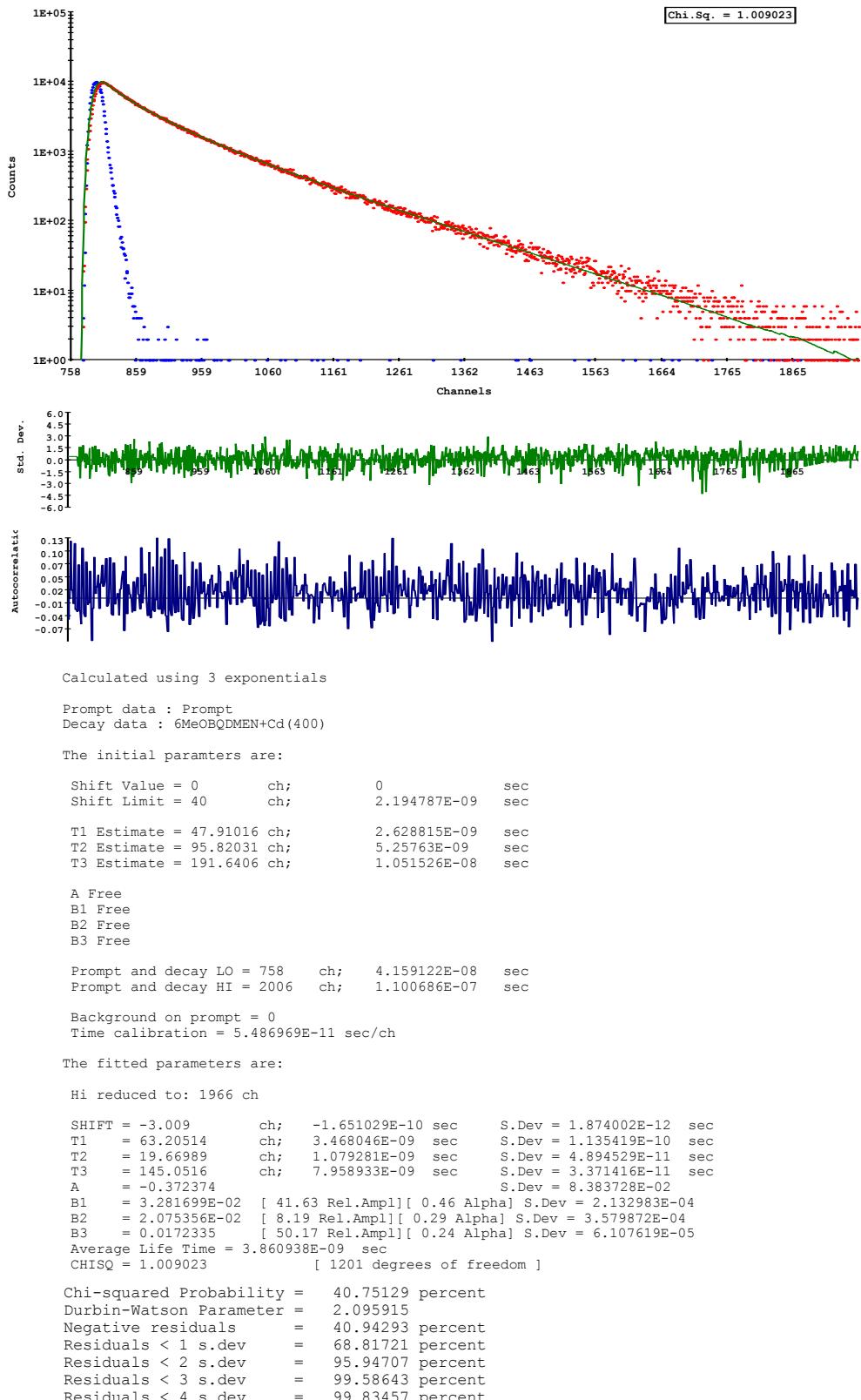
Prompt and decay LO = 739	ch;	4.05487E-08	sec
Prompt and decay HI = 2167	ch;	1.189026E-07	sec

Background on prompt = 0  
Time calibration = 5.486969E-11 sec/ch

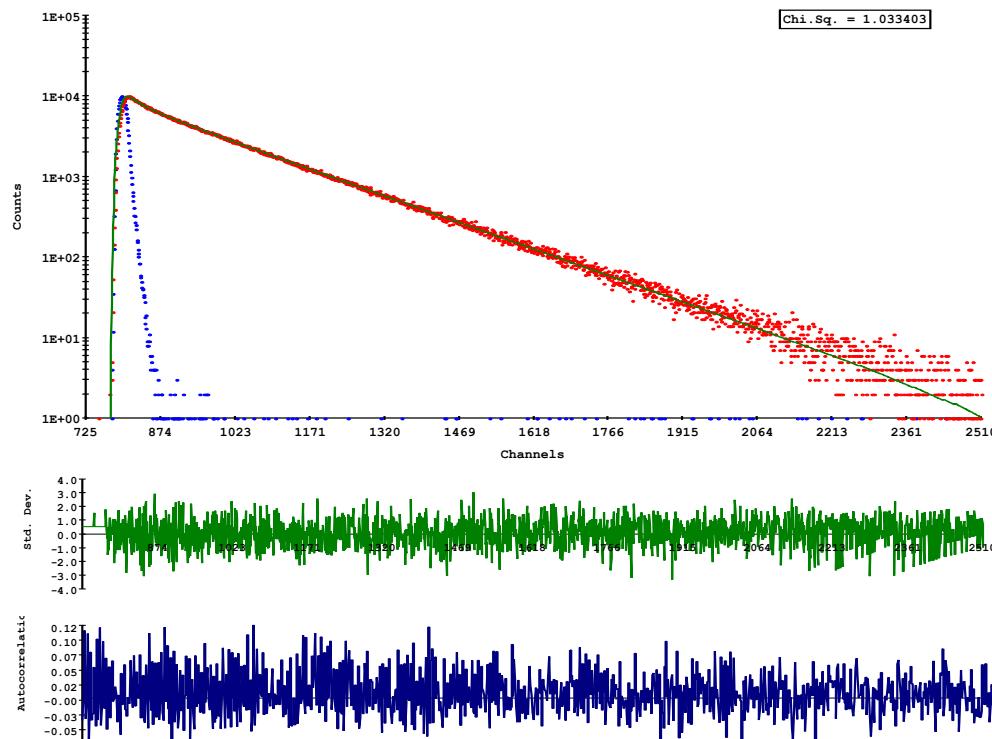
The fitted parameters are:

Hi reduced to: 2127 ch					
SHIFT = -3.890543	ch;	-2.134729E-10	sec	S.Dev = 1.494274E-12	sec
T1 = 30.32877	ch;	1.66413E-09	sec	S.Dev = 4.721755E-11	sec
T2 = 8.101191	ch;	4.445098E-10	sec	S.Dev = 6.387385E-12	sec
T3 = 170.5184	ch;	9.356294E-09	sec	S.Dev = 5.271822E-11	sec
A = 6.281438E-02				S.Dev = 5.216248E-02	
B1 = 0.0187077	[ 27.18 Rel.Ampl]	[ 0.13 Alpha]	S.Dev = 1.543823E-04		
B2 = 0.1252533	[ 48.62 Rel.Ampl]	[ 0.85 Alpha]	S.Dev = 5.516689E-04		
B3 = 2.962186E-03	[ 24.20 Rel.Ampl]	[ 0.02 Alpha]	S.Dev = 1.38906E-05		
Average Life Time = 7.794783E-10 sec					
CHISQ = 1.000182 [ 1381 degrees of freedom ]					
Chi-squared Probability = 49.30325 percent					
Durbin-Watson Parameter = 1.986441					
Negative residuals = 41.82866 percent					
Residuals < 1 s.dev = 69.11447 percent					
Residuals < 2 s.dev = 95.89633 percent					
Residuals < 3 s.dev = 99.42405 percent					
Residuals < 4 s.dev = 99.85601 percent					

**Fig. S15.** Fluorescence lifetime measurement of 34  $\mu\text{M}$  6-MeOBQDMEN (**2**) in DMF-H<sub>2</sub>O (1:1) with 400 nm bandpath filter (BPF) at 25 °C ( $\lambda_{\text{ex}} = 331$  nm).



**Fig. S16.** Fluorescence lifetime measurement of 34  $\mu\text{M}$  6-MeOBQDMEN (**2**) in the presence of 3 equiv. of  $\text{Cd}^{2+}$  in DMF- $\text{H}_2\text{O}$  (1:1) with 400 nm bandpath filter (BPF) at 25 °C ( $\lambda_{\text{ex}} = 331$  nm).



Calculated using 3 exponentials

Prompt data : Prompt  
Decay data : 6MeOBQDMEN+Zn(400)

The initial parameters are:

Shift Value = 0	ch;	0	sec
Shift Limit = 40	ch;	2.194787E-09	sec
T1 Estimate = 90.2103	ch;	4.949811E-09	sec
T2 Estimate = 180.4206	ch;	9.899622E-09	sec
T3 Estimate = 360.8412	ch;	1.979924E-08	sec

A Free  
B1 Free  
B2 Free  
B3 Free

Prompt and decay LO = 725 ch; 3.978052E-08 sec  
Prompt and decay HI = 2550 ch; 1.399177E-07 sec

Background on prompt = 0  
Time calibration = 5.486969E-11 sec/ch

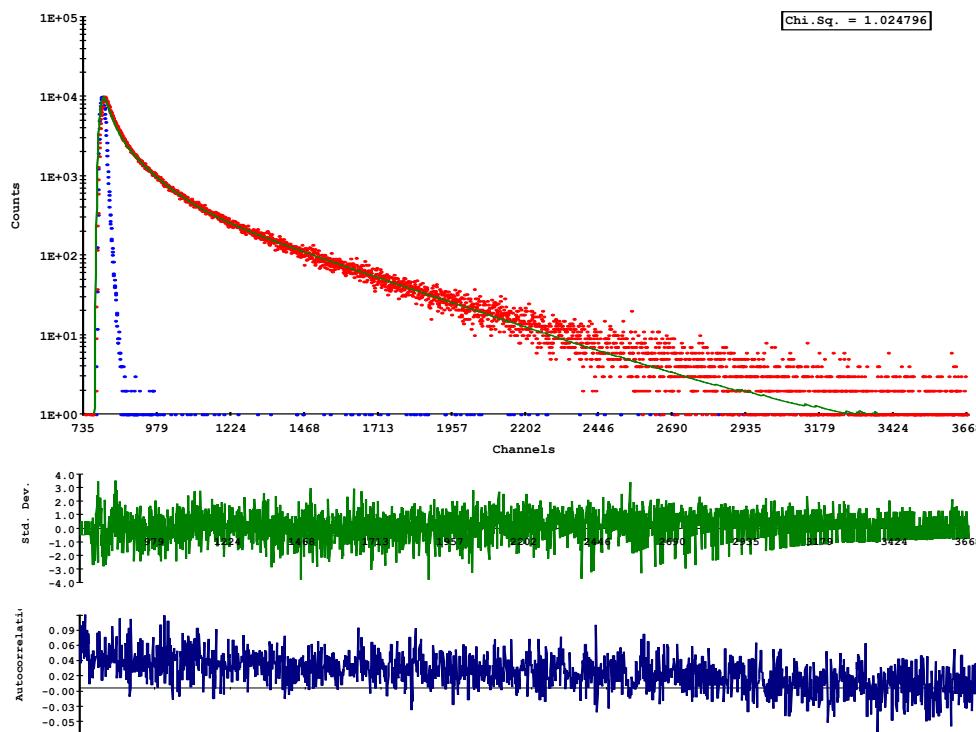
The fitted parameters are:

Hi reduced to: 2510 ch

SHIFT = -2.716218	ch;	-1.49038E-10	sec	S.Dev = 1.961694E-12	sec
T1 = 81.62655	ch;	4.478823E-09	sec	S.Dev = 7.581209E-10	sec
T2 = 196.2167	ch;	1.076635E-08	sec	S.Dev = 2.363335E-11	sec
T3 = 22.98573	ch;	1.26122E-09	sec	S.Dev = 5.844236E-11	sec
A = -0.5201862				S.Dev = 7.006758E-02	
B1 = 4.838324E-03	[ 4.39 Rel.Ampl][ 0.08 Alpha]	S.Dev = 2.137139E-04			
B2 = 4.181635E-02	[ 91.15 Rel.Ampl][ 0.65 Alpha]	S.Dev = 7.030841E-05			
B3 = 1.749571E-02	[ 4.47 Rel.Ampl][ 0.27 Alpha]	S.Dev = 3.323509E-04			
Average Life Time = 7.699802E-09 sec					
CHISQ = 1.033403 [ 1778 degrees of freedom ]					

Chi-squared Probability =	15.95741 percent
Durbin-Watson Parameter =	2.074491
Negative residuals =	42.94513 percent
Residuals < 1 s.dev =	65.84547 percent
Residuals < 2 s.dev =	95.35275 percent
Residuals < 3 s.dev =	99.60806 percent
Residuals < 4 s.dev =	100 percent

**Fig. S17.** Fluorescence lifetime measurement of 34  $\mu$ M 6-MeOBQDMEN (**2**) in the presence of 3 equiv. of  $Zn^{2+}$  in DMF-H<sub>2</sub>O (1:1) with 400 nm bandpath filter (BPF) at 25 °C ( $\lambda_{ex} = 331$  nm).



Calculated using 3 exponentials

Prompt data : Prompt  
Decay data : TriMeOBQDMEN(460)

The initial parameters are:

Shift Value = 0	ch;	0	sec
Shift Limit = 40	ch;	2.194787E-09	sec
T1 Estimate = 71.69888	ch;	3.934095E-09	sec
T2 Estimate = 143.3978	ch;	7.868191E-09	sec
T3 Estimate = 286.7955	ch;	1.573638E-08	sec

A Free  
B1 Free  
B2 Free  
B3 Free

Prompt and decay LO = 735 ch; 4.032922E-08 sec  
Prompt and decay HI = 3708 ch; 2.034568E-07 sec

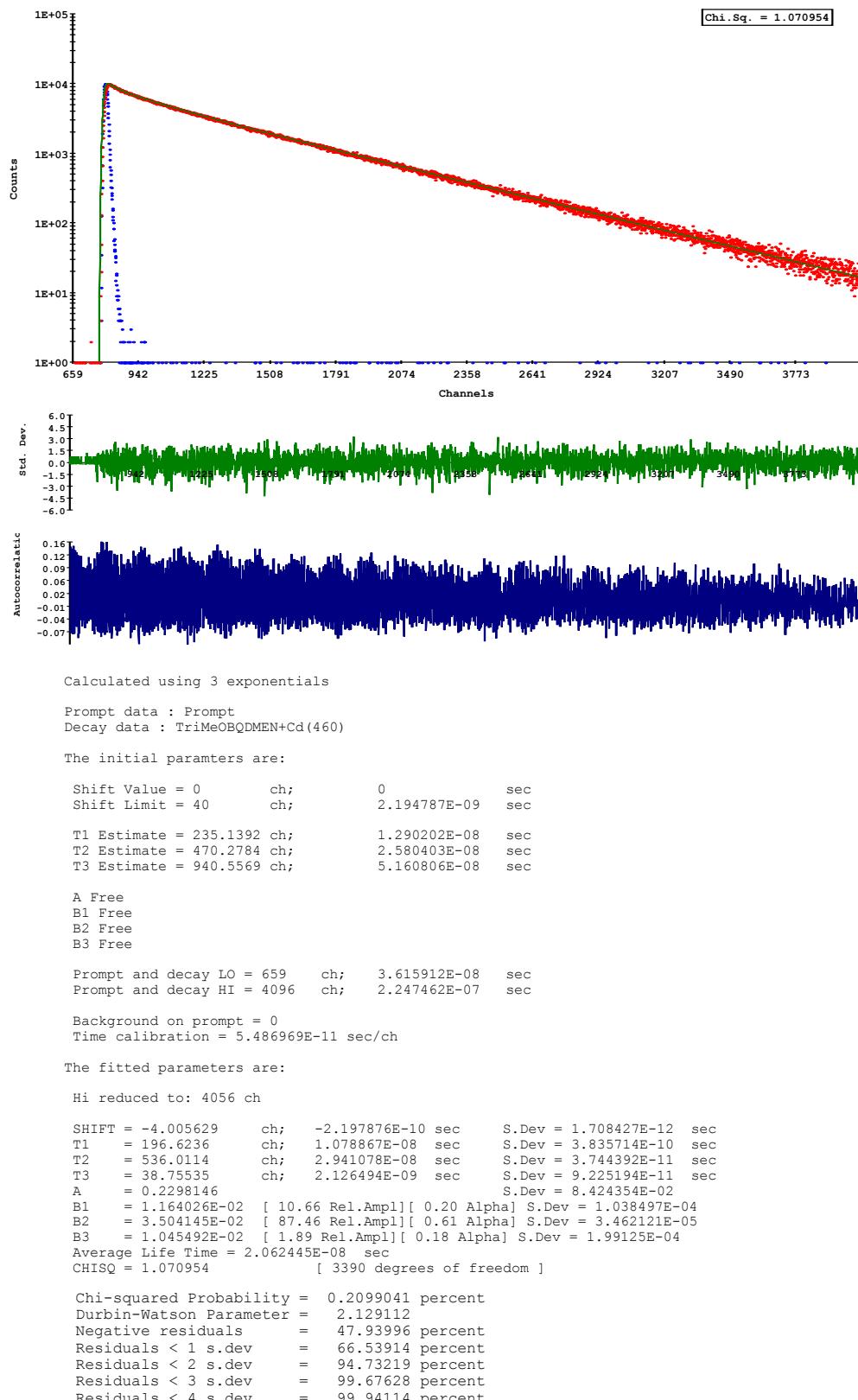
Background on prompt = 0  
Time calibration = 5.486969E-11 sec/ch

The fitted parameters are:

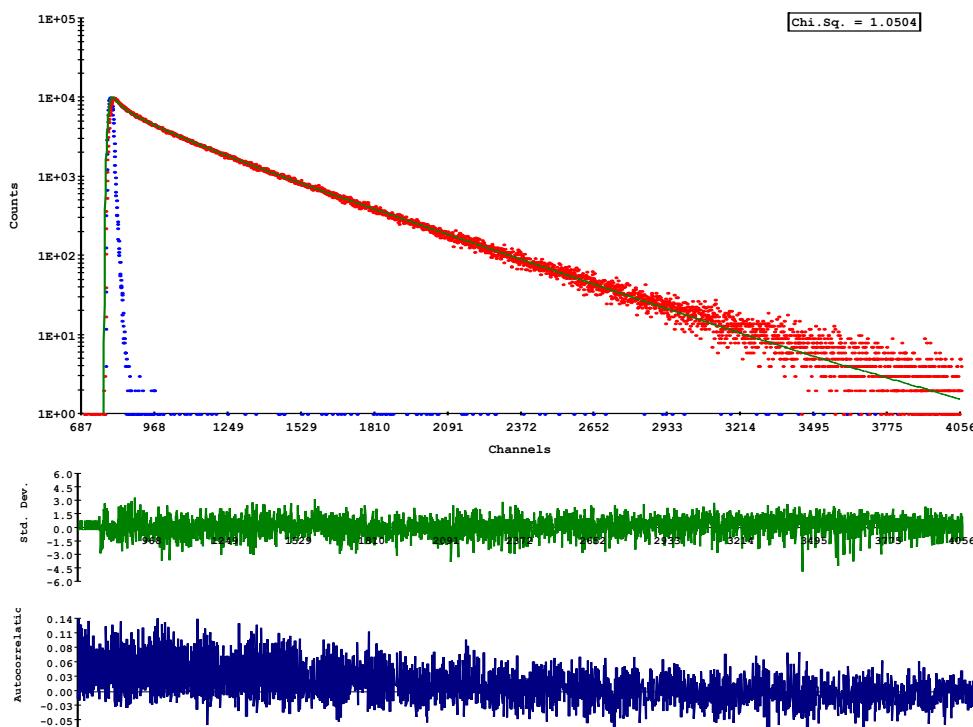
Hi reduced to: 3668 ch

SHIFT = -3.323519	ch;	-1.823605E-10	sec	S.Dev = 1.500537E-12	sec
T1 = 84.96255	ch;	4.661868E-09	sec	S.Dev = 6.951915E-11	sec
T2 = 21.45439	ch;	1.177195E-09	sec	S.Dev = 1.299422E-11	sec
T3 = 331.8786	ch;	1.821007E-08	sec	S.Dev = 7.218948E-11	sec
A = 0.5093214				S.Dev = 3.690384E-02	
B1 = 2.175961E-02	[ 42.48 Rel.Ampl][ 0.27 Alpha]	S.Dev = 8.823608E-05			
B2 = 5.341699E-02	[ 26.33 Rel.Ampl][ 0.67 Alpha]	S.Dev = 2.534038E-04			
B3 = 4.089027E-03	[ 31.18 Rel.Ampl][ 0.05 Alpha]	S.Dev = 1.343116E-05			
Average Life Time = 3.012455E-09 sec					
CHISQ = 1.024796 [ 2926 degrees of freedom ]					
Chi-squared Probability = 17.12076 percent					
Durbin-Watson Parameter = 1.872714					
Negative residuals = 41.95638 percent					
Residuals < 1 s.dev = 67.75732 percent					
Residuals < 2 s.dev = 95.60327 percent					
Residuals < 3 s.dev = 99.62508 percent					
Residuals < 4 s.dev = 100 percent					

**Fig. S18.** Fluorescence lifetime measurement of 34  $\mu$ M TriMeOBQDMEN (**3**) in DMF-H<sub>2</sub>O (1:1) with 460 nm bandpath filter (BPF) at 25 °C ( $\lambda_{\text{ex}} = 331$  nm).



**Fig. S19.** Fluorescence lifetime measurement of 34  $\mu\text{M}$  TriMeOBQDMEN (**3**) in the presence of 3 equiv. of  $\text{Cd}^{2+}$  in DMF- $\text{H}_2\text{O}$  (1:1) with 460 nm bandpath filter (BPF) at 25 °C ( $\lambda_{\text{ex}} = 331$  nm).



Calculated using 3 exponentials

Prompt data : Prompt  
Decay data : TriMeOBQDMEN+Zn(460)

The initial parameters are:

Shift Value = 0	ch;	0	sec
Shift Limit = 40	ch;	2.194787E-09	sec
T1 Estimate = 158.8361	ch;	8.715284E-09	sec
T2 Estimate = 317.6721	ch;	1.743057E-08	sec
T3 Estimate = 635.3442	ch;	3.486114E-08	sec

A Free  
B1 Free  
B2 Free  
B3 Free

Prompt and decay LO = 687 ch; 3.769548E-08 sec  
Prompt and decay HI = 4096 ch; 2.247462E-07 sec

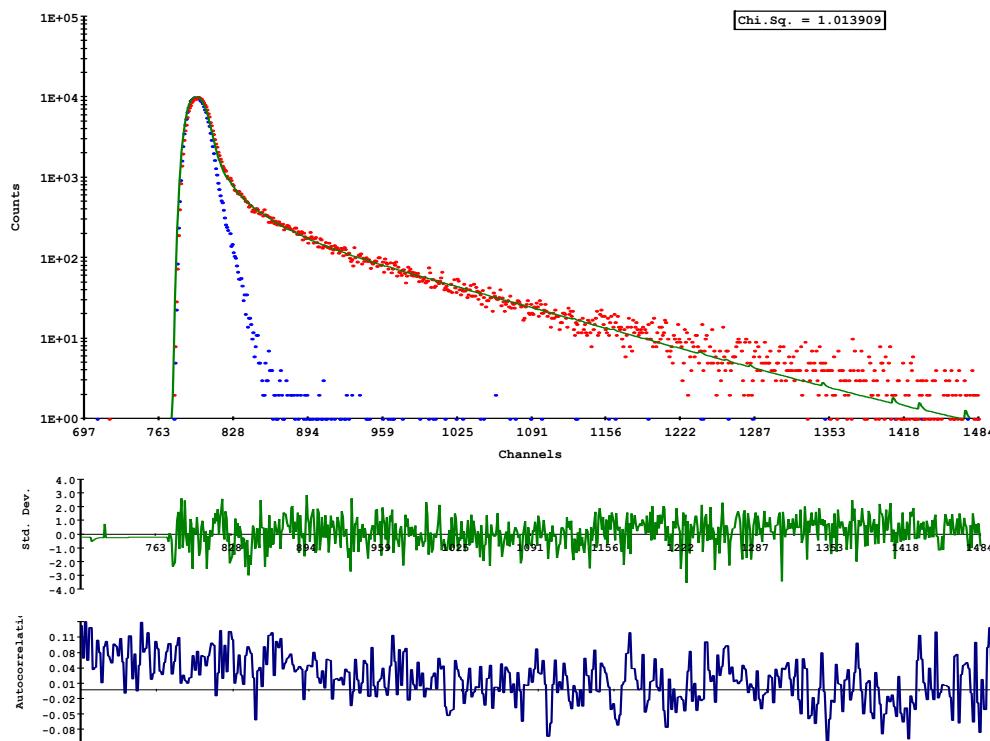
Background on prompt = 0  
Time calibration = 5.486969E-11 sec/ch

The fitted parameters are:

Hi reduced to: 4056 ch					
SHIFT = -3.575563	ch;	-1.9619E-10	sec	S.Dev = 1.766694E-12	sec
T1 = 157.0574	ch;	8.617693E-09	sec	S.Dev = 3.452446E-10	sec
T2 = 384.715	ch;	2.110919E-08	sec	S.Dev = 3.870911E-11	sec
T3 = 28.31529	ch;	1.553651E-09	sec	S.Dev = 4.039898E-11	sec
A = 0.2480554				S.Dev = 0.0529433	
B1 = 1.561505E-02	[ 18.44 Rel.Ampl]	[ 0.24 Alpha]	S.Dev = 1.075282E-04		
B2 = 2.660358E-02	[ 76.96 Rel.Ampl]	[ 0.42 Alpha]	S.Dev = 3.846521E-05		
B3 = 2.157576E-02	[ 4.59 Rel.Ampl]	[ 0.34 Alpha]	S.Dev = 2.260056E-04		
Average Life Time = 1.143779E-08 sec					
CHISQ = 1.0504 [ 3362 degrees of freedom ]					

Chi-squared Probability =	2.063783 percent
Durbin-Watson Parameter =	2.024117
Negative residuals =	44.33234 percent
Residuals < 1 s.dev =	67.12166 percent
Residuals < 2 s.dev =	95.04451 percent
Residuals < 3 s.dev =	99.52522 percent
Residuals < 4 s.dev =	99.94065 percent

**Fig. S20.** Fluorescence lifetime measurement of 34  $\mu$ M TriMeOBQDMEN (**3**) in the presence of 3 equiv. of  $Zn^{2+}$  in DMF-H<sub>2</sub>O (1:1) with 460 nm bandpath filter (BPF) at 25 °C ( $\lambda_{ex}$  = 331 nm).



Calculated using 3 exponentials

Prompt data : Prompt  
Decay data : BQDMPN(370)

The initial parameters are:

Shift Value = 0	ch;	0	sec
Shift Limit = 40	ch;	2.194787E-09	sec
T1 Estimate = 10.12097	ch;	5.553346E-10	sec
T2 Estimate = 20.24194	ch;	1.110669E-09	sec
T3 Estimate = 40.48389	ch;	2.221338E-09	sec

A Free  
B1 Free  
B2 Free  
B3 Free

Prompt and decay LO = 697 ch; 3.824417E-08 sec  
Prompt and decay HI = 1524 ch; 8.36214E-08 sec

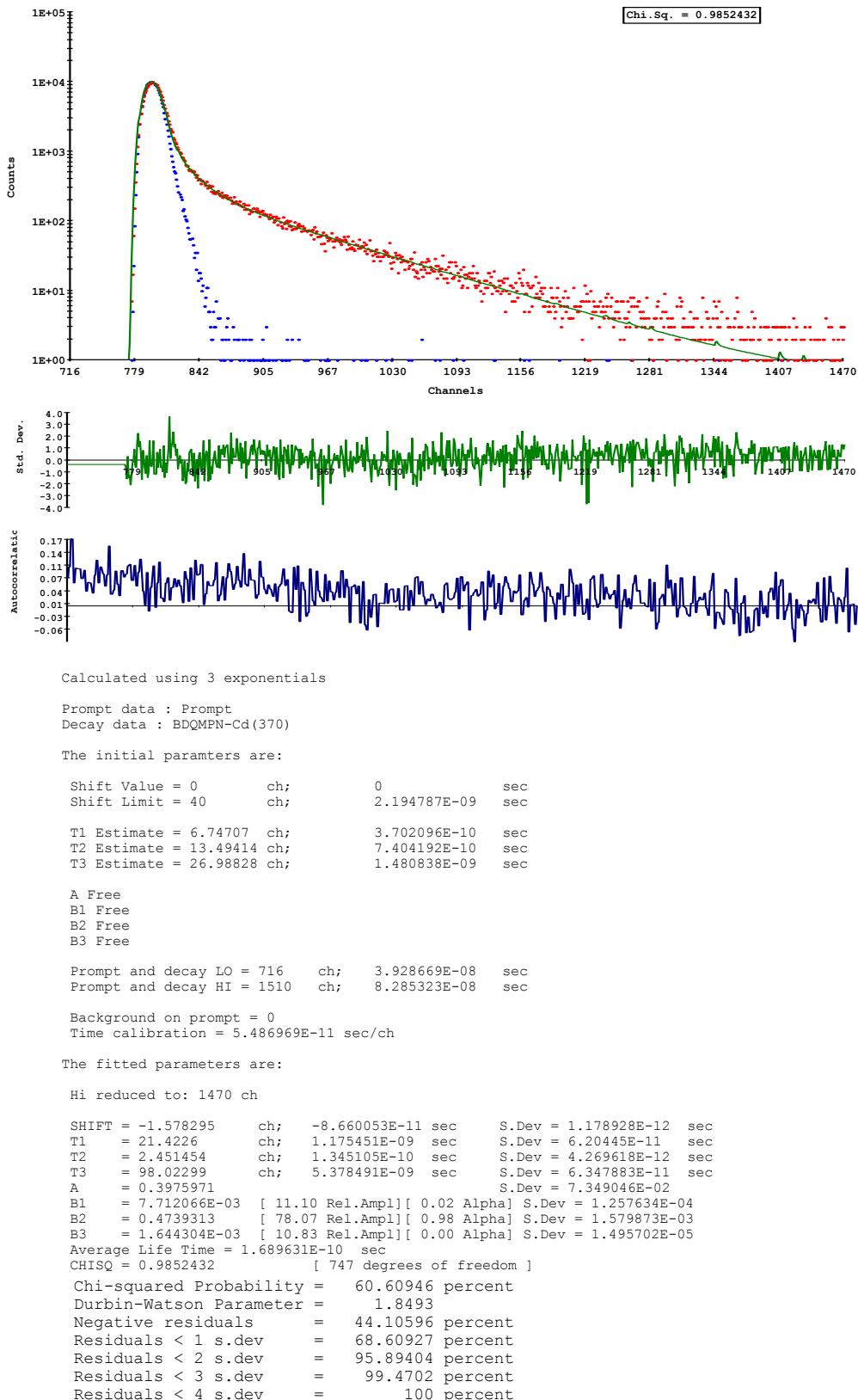
Background on prompt = 1.298701E-02  
Time calibration = 5.486969E-11 sec/ch

The fitted parameters are:

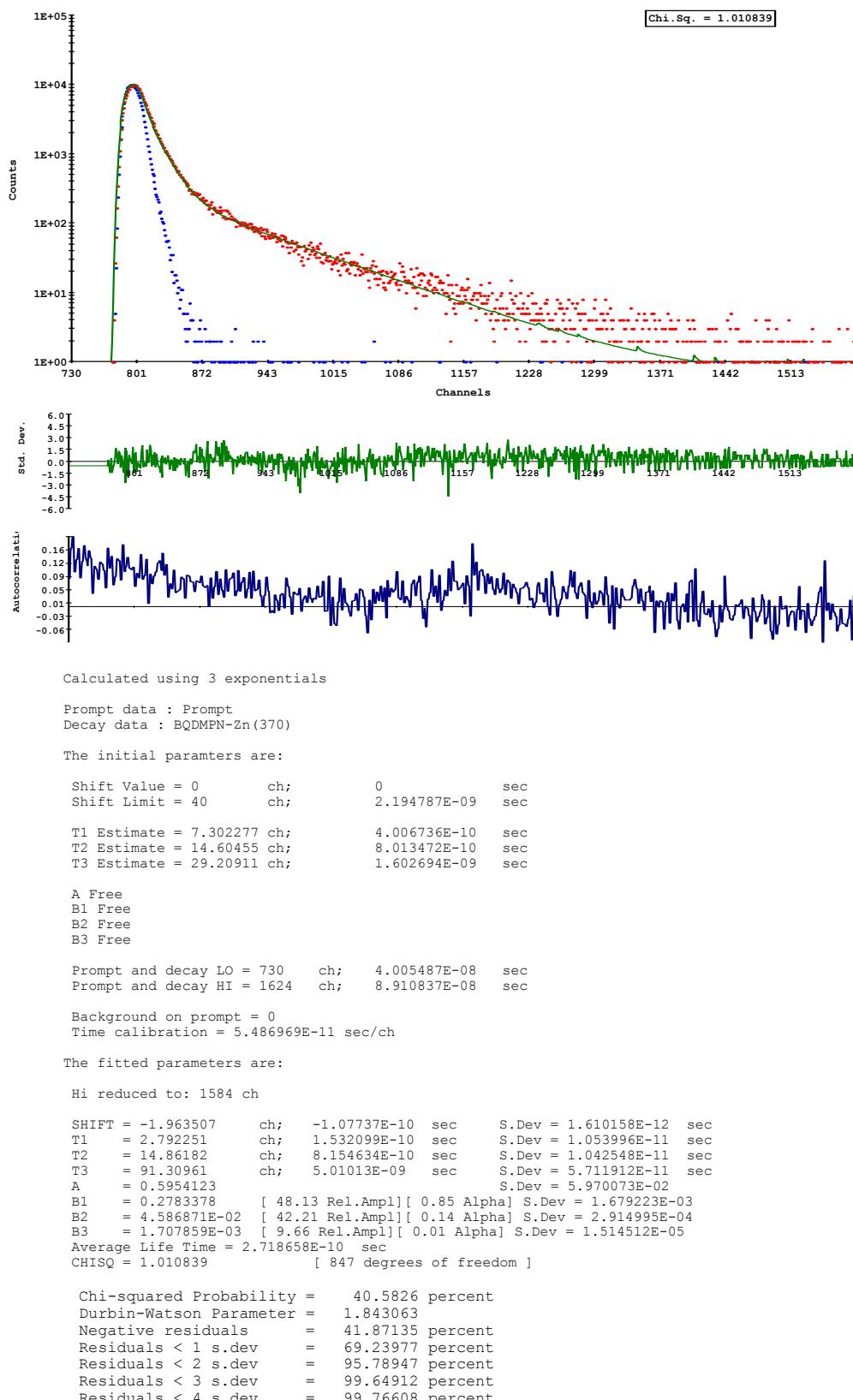
Hi reduced to: 1484 ch

SHIFT = -0.8064182	ch;	-4.424791E-11	sec	S.Dev = 1.210901E-12	sec
T1 = 25.43094	ch;	1.395388E-09	sec	S.Dev = 6.649837E-11	sec
T2 = 2.203921	ch;	1.209284E-10	sec	S.Dev = 5.048008E-12	sec
T3 = 109.8176	ch;	6.025657E-09	sec	S.Dev = 6.593334E-11	sec
A = 0.2356746				S.Dev = 7.477585E-02	
B1 = 6.829942E-03	[ 11.11 Rel.Ampl][ 0.01 Alpha]	S.Dev = 1.016135E-04			
B2 = 0.5451438	[ 76.82 Rel.Ampl][ 0.98 Alpha]	S.Dev = 0.0017402			
B3 = 1.720164E-03	[ 12.08 Rel.Ampl][ 0.00 Alpha]	S.Dev = 1.45503E-05			
Average Life Time = 1.549934E-10 sec					
CHISQ = 1.013909 [ 780 degrees of freedom ]					
Chi-squared Probability = 38.5802 percent					
Durbin-Watson Parameter = 1.741592					
Negative residuals = 46.5736 percent					
Residuals < 1 s.dev = 68.65482 percent					
Residuals < 2 s.dev = 95.17767 percent					
Residuals < 3 s.dev = 99.61929 percent					
Residuals < 4 s.dev = 100 percent					

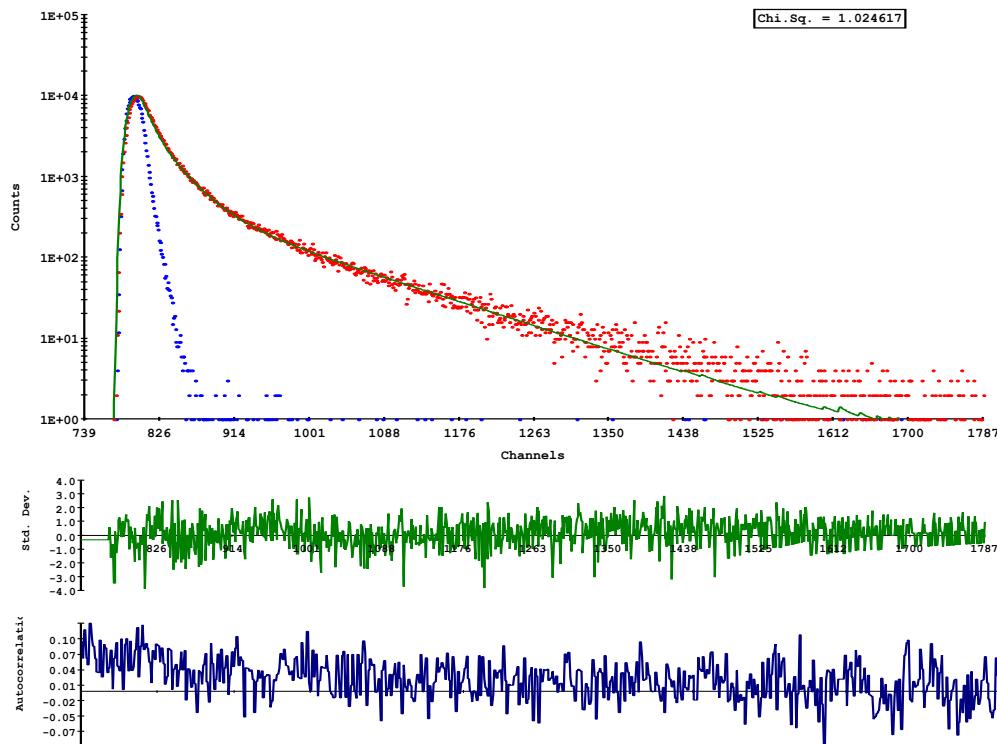
**Fig. S21.** Fluorescence lifetime measurement of 34  $\mu$ M BQDMPN (4) in DMF-H<sub>2</sub>O (1:1) with 370 nm bandpath filter (BPF) at 25 °C ( $\lambda_{\text{ex}} = 331$  nm).



**Fig. S22.** Fluorescence lifetime measurement of 34  $\mu$ M BQDMPN (**4**) in the presence of 3 equiv. of Cd<sup>2+</sup> in DMF-H<sub>2</sub>O (1:1) with 370 nm bandpath filter (BPF) at 25 °C ( $\lambda_{\text{ex}} = 331$  nm).



**Fig. S23.** Fluorescence lifetime measurement of 34  $\mu$ M BQDMPN (**4**) in the presence of 3 equiv. of Zn<sup>2+</sup> in DMF-H<sub>2</sub>O (1:1) with 370 nm bandpath filter (BPF) at 25 °C ( $\lambda_{\text{ex}} = 331$  nm).



Calculated using 3 exponentials

Prompt data : Prompt  
Decay data : 6MeOBQDMPN(400)

The initial parameters are:

```

Shift Value = 0      ch;      0      sec
Shift Limit = 40     ch;  2.194787E-09  sec

T1 Estimate = 17.15479 ch;  9.412776E-10  sec
T2 Estimate = 34.30957 ch;  1.882555E-09  sec
T3 Estimate = 68.61914 ch;  3.76511E-09  sec
  
```

```

A Free
B1 Free
B2 Free
B3 Free
  
```

```

Prompt and decay LO = 739      ch;  4.05487E-08  sec
Prompt and decay HI = 1827      ch;  1.002469E-07  sec
  
```

Background on prompt = 0  
Time calibration = 5.486969E-11 sec/ch

The fitted parameters are:

Hi reduced to: 1787 ch

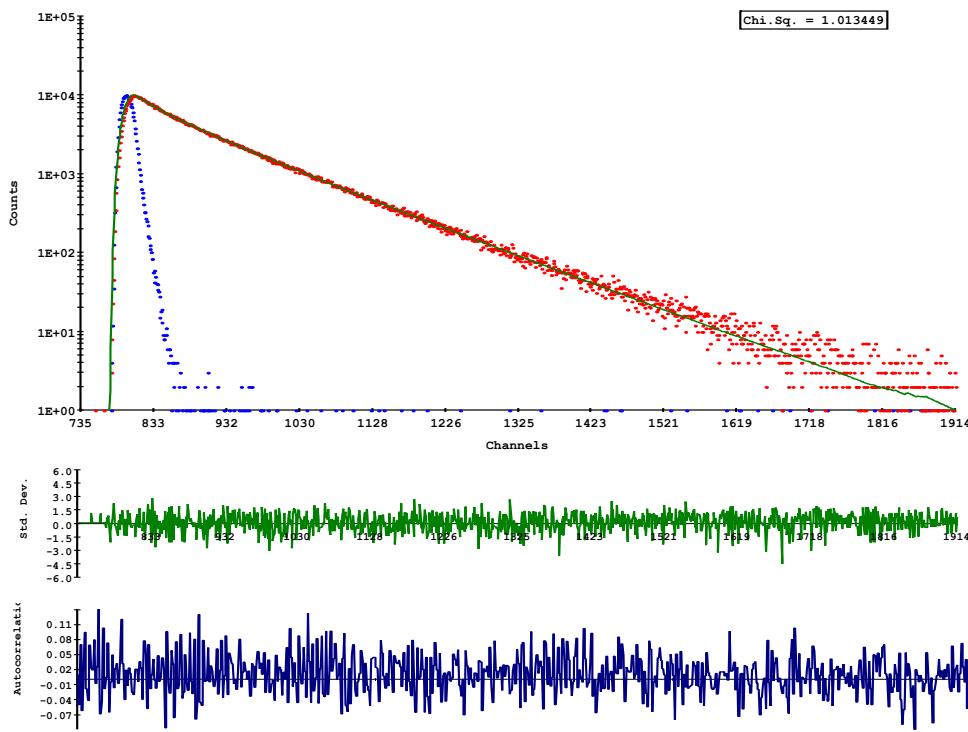
```

SHIFT = -2.44339      ch;  -1.34068E-10  sec  S.Dev = 1.46784E-12  sec
T1 = 8.192328      ch;  4.495105E-10  sec  S.Dev = 1.593177E-11  sec
T2 = 29.20401      ch;  1.602415E-09  sec  S.Dev = 2.156081E-11  sec
T3 = 125.4298      ch;  6.882292E-09  sec  S.Dev = 5.625533E-11  sec
A = 0.3542998      S.Dev = 6.170324E-02
B1 = 0.1029654      [ 40.13 Rel.Ampl] [ 0.75 Alpha] S.Dev = 5.797698E-04
B2 = 3.058379E-02  [ 42.49 Rel.Ampl] [ 0.22 Alpha] S.Dev = 1.852779E-04
B3 = 2.912044E-03  [ 17.38 Rel.Ampl] [ 0.02 Alpha] S.Dev = 1.879831E-05
Average Life Time = 8.451738E-10  sec
CHISQ = 1.024617      [ 1041 degrees of freedom ]
  
```

```

Chi-squared Probability = 28.3864 percent
Durbin-Watson Parameter = 1.812145
Negative residuals = 43.08866 percent
Residuals < 1 s.dev = 69.49476 percent
Residuals < 2 s.dev = 95.61487 percent
Residuals < 3 s.dev = 99.14204 percent
Residuals < 4 s.dev = 100 percent
  
```

**Fig. S24.** Fluorescence lifetime measurement of 34  $\mu\text{M}$  6-MeOBQDMPN (**5**) in DMF-H<sub>2</sub>O (1:1) with 400 nm bandpath filter (BPF) at 25 °C ( $\lambda_{\text{ex}} = 331$  nm).



Calculated using 3 exponentials

Prompt data : Prompt  
Decay data : 6MeOBQDMPN+Cd(400)

The initial parameters are:

```
Shift Value = 0      ch;      0      sec
Shift Limit = 40     ch;  2.194787E-09  sec
T1 Estimate = 50.9483 ch;  2.795517E-09  sec
T2 Estimate = 101.8966 ch; 5.591035E-09  sec
T3 Estimate = 203.7932 ch; 1.118207E-08  sec
```

```
A Free
B1 Free
B2 Free
B3 Free
```

```
Prompt and decay LO = 735    ch;  4.032922E-08  sec
Prompt and decay HI = 1954    ch;  1.072154E-07  sec
```

Background on prompt = 0  
Time calibration = 5.486969E-11 sec/ch

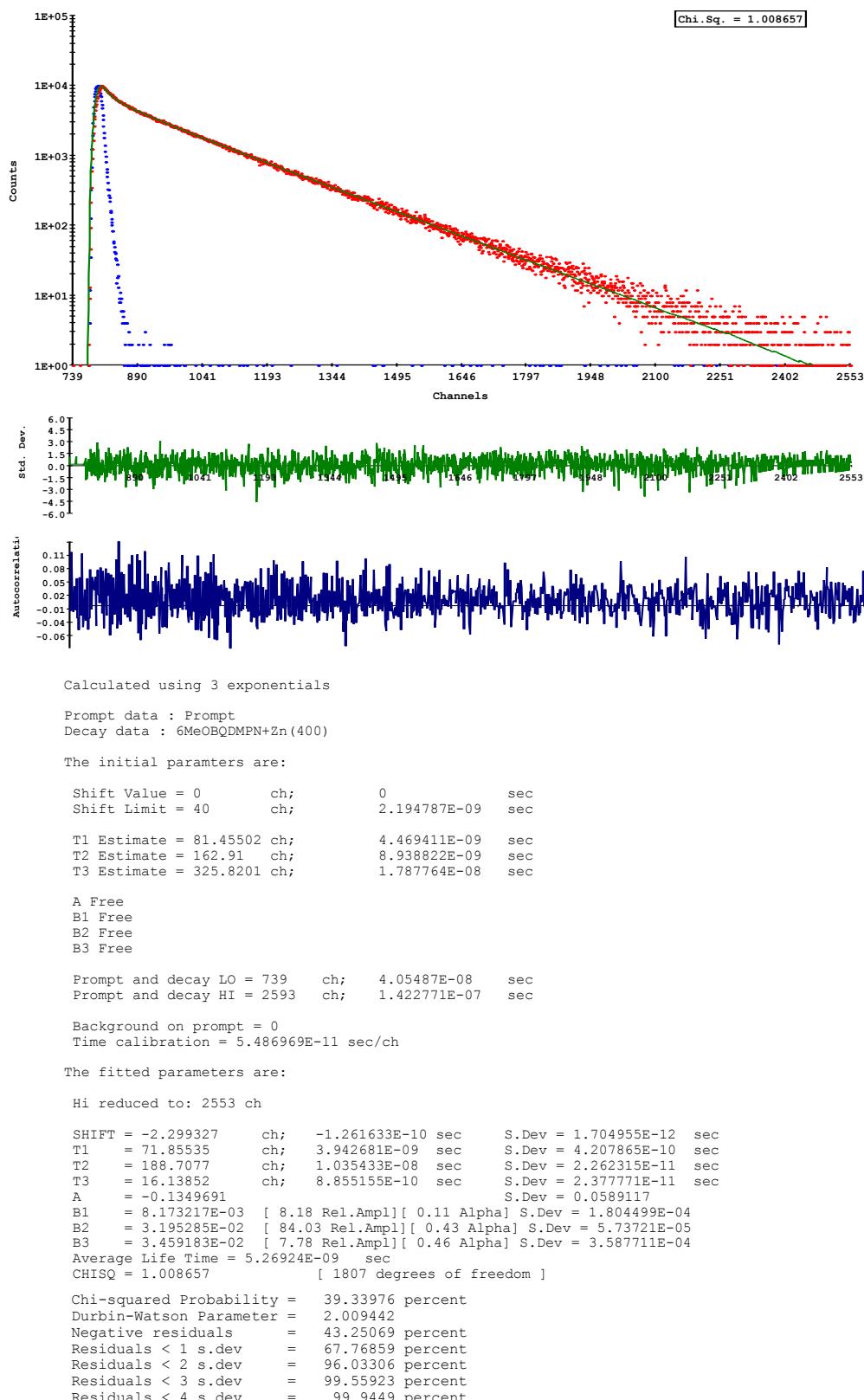
The fitted parameters are:

Hi reduced to: 1914 ch

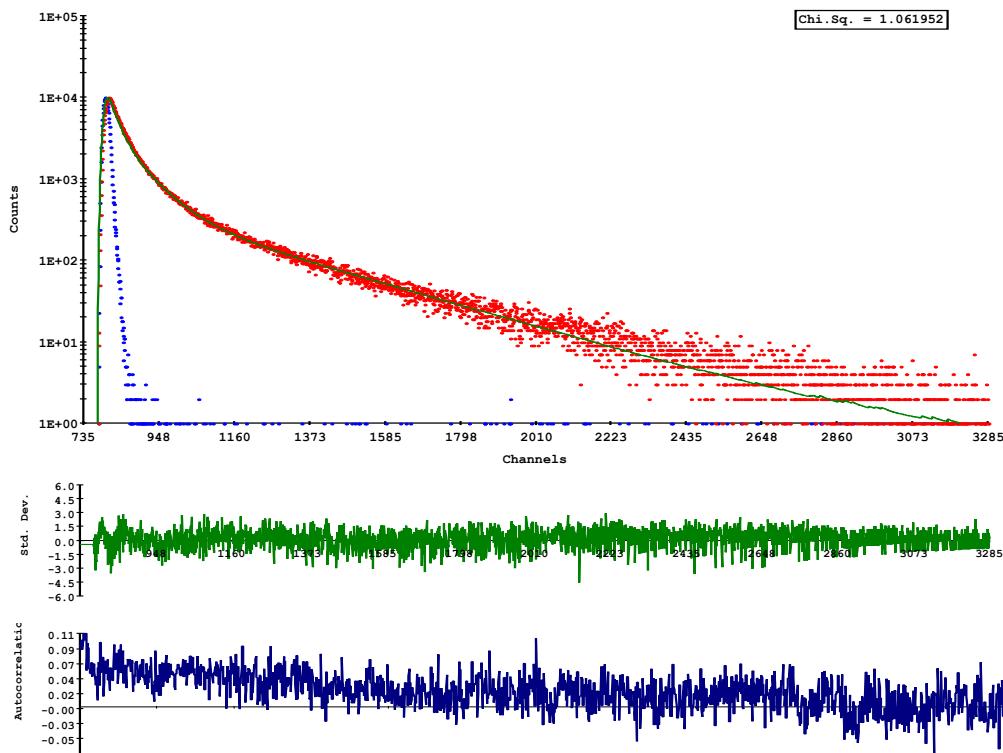
```
SHIFT = -2.324281    ch;  -1.275326E-10 sec  S.Dev = 1.74503E-12  sec
T1   = 76.03949     ch;  4.172263E-09 sec  S.Dev = 3.383254E-10  sec
T2   = 126.2669     ch;  6.928227E-09 sec  S.Dev = 4.088469E-11  sec
T3   = 20.19334     ch;  1.108002E-09 sec  S.Dev = 4.289861E-11  sec
A    = -0.1022718          S.Dev = 7.874002E-02
B1  = 1.934554E-02 [ 26.48 Rel.Ampl][ 0.28 Alpha] S.Dev = 2.573188E-04
B2  = 2.913029E-02 [ 66.21 Rel.Ampl][ 0.42 Alpha] S.Dev = 1.2183E-04
B3  = 2.011764E-02 [ 7.31 Rel.Ampl][ 0.29 Alpha] S.Dev = 3.391925E-04
Average Life Time = 4.443955E-09 sec
CHISQ = 1.013449 [ 1172 degrees of freedom ]
```

```
Chi-squared Probability = 36.77269 percent
Durbin-Watson Parameter = 1.981979
Negative residuals = 43.98305 percent
Residuals < 1 s.dev = 67.28814 percent
Residuals < 2 s.dev = 95.59322 percent
Residuals < 3 s.dev = 99.49152 percent
Residuals < 4 s.dev = 99.91525 percent
```

**Fig. S25.** Fluorescence lifetime measurement of 34  $\mu$ M 6-MeOBQDMPN (**5**) in the presence of 3 equiv. of Cd<sup>2+</sup> in DMF-H<sub>2</sub>O (1:1) with 400 nm bandpath filter (BPF) at 25 °C ( $\lambda_{\text{ex}} = 331$  nm).



**Fig. S26.** Fluorescence lifetime measurement of 34  $\mu\text{M}$  6-MeOBQDMPN (**5**) in the presence of 3 equiv. of  $\text{Zn}^{2+}$  in DMF-H<sub>2</sub>O (1:1) with 400 nm bandpath filter (BPF) at 25 °C ( $\lambda_{\text{ex}} = 331 \text{ nm}$ ).



Calculated using 3 exponentials

Prompt data : Prompt  
Decay data : TriMeOBQDMPN(460)

The initial parameters are:

Shift Value = 0	ch;	0	sec
Shift Limit = 40	ch;	2.194787E-09	sec
T1 Estimate = 58.95563	ch;	3.234877E-09	sec
T2 Estimate = 117.9113	ch;	6.469754E-09	sec
T3 Estimate = 235.8225	ch;	1.293951E-08	sec

A Free  
B1 Free  
B2 Free  
B3 Free

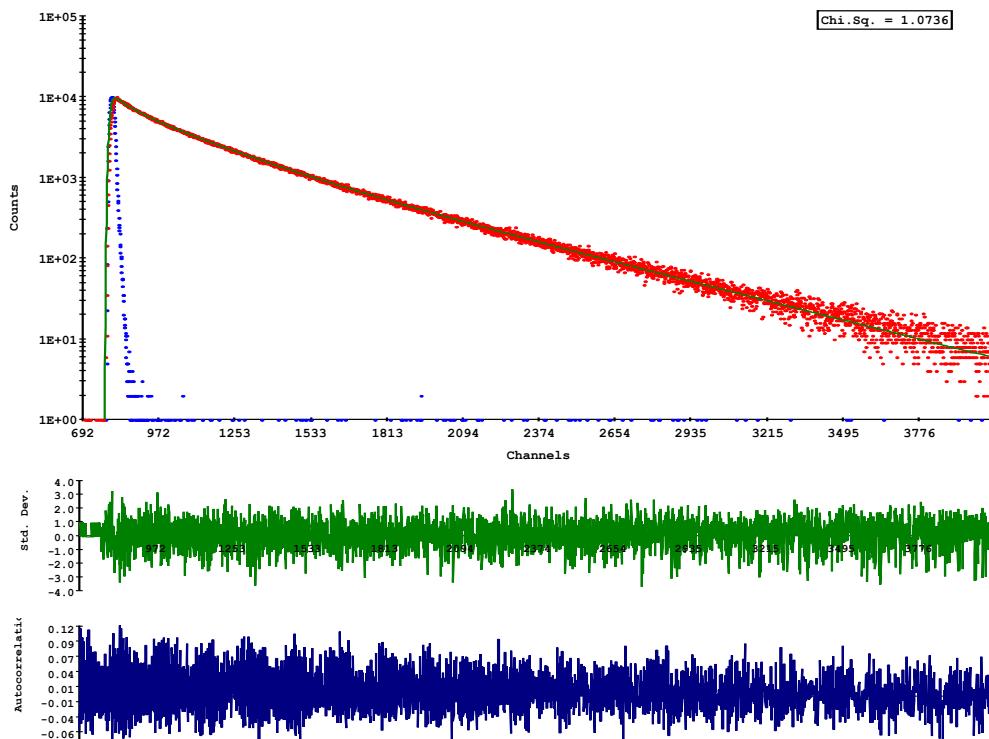
Prompt and decay LO = 735 ch; 4.032922E-08 sec  
Prompt and decay HI = 3325 ch; 1.824417E-07 sec

Background on prompt = 0  
Time calibration = 5.486969E-11 sec/ch

The fitted parameters are:

Hi reduced to: 3285 ch				
SHIFT = -1.852206	ch;	-1.016299E-10	sec	S.Dev = 1.630483E-12 sec
T1 = 73.86161	ch;	4.052763E-09	sec	S.Dev = 7.636283E-11 sec
T2 = 23.1508	ch;	1.270277E-09	sec	S.Dev = 1.330892E-11 sec
T3 = 345.2584	ch;	1.894422E-08	sec	S.Dev = 1.019326E-10 sec
A = 0.47133				S.Dev = 4.511932E-02
B1 = 2.146125E-02	[ 42.37 Rel.Ampl][ 0.27 Alpha]	S.Dev = 9.526328E-05		
B2 = 5.609271E-02	[ 34.71 Rel.Ampl][ 0.70 Alpha]	S.Dev = 2.533723E-04		
B3 = 2.484279E-03	[ 22.92 Rel.Ampl][ 0.03 Alpha]	S.Dev = 9.895746E-06		
Average Life Time = 2.564942E-09 sec				
CHISQ = 1.061952 [ 2543 degrees of freedom ]				
Chi-squared Probability = 1.485473 percent				
Durbin-Watson Parameter = 1.805697				
Negative residuals = 42.17954 percent				
Residuals < 1 s.dev = 65.77813 percent				
Residuals < 2 s.dev = 95.17836 percent				
Residuals < 3 s.dev = 99.56879 percent				
Residuals < 4 s.dev = 99.9608 percent				

**Fig. S27.** Fluorescence lifetime measurement of 34  $\mu$ M TriMeOBQDMPN (**6**) in DMF-H<sub>2</sub>O (1:1) with 460 nm bandpath filter (BPF) at 25 °C ( $\lambda_{\text{ex}} = 331$  nm).



Calculated using 3 exponentials

Prompt data : Prompt  
Decay data : TriMeOBQDMPN-Cd(460)

The initial parameters are:

```

Shift Value = 0      ch;      0      sec
Shift Limit = 40    ch;  2.194787E-09  sec

T1 Estimate = 184.4599 ch;  1.012126E-08  sec
T2 Estimate = 368.9199 ch;  2.024252E-08  sec
T3 Estimate = 737.8397 ch;  4.048503E-08  sec
  
```

```

A Free
B1 Free
B2 Free
B3 Free
  
```

```

Prompt and decay LO = 692      ch;  3.796982E-08  sec
Prompt and decay HI = 4096    ch;  2.247462E-07  sec
  
```

Background on prompt = 1.219512E-02  
Time calibration = 5.486969E-11 sec/ch

The fitted parameters are:

Hi reduced to: 4056 ch

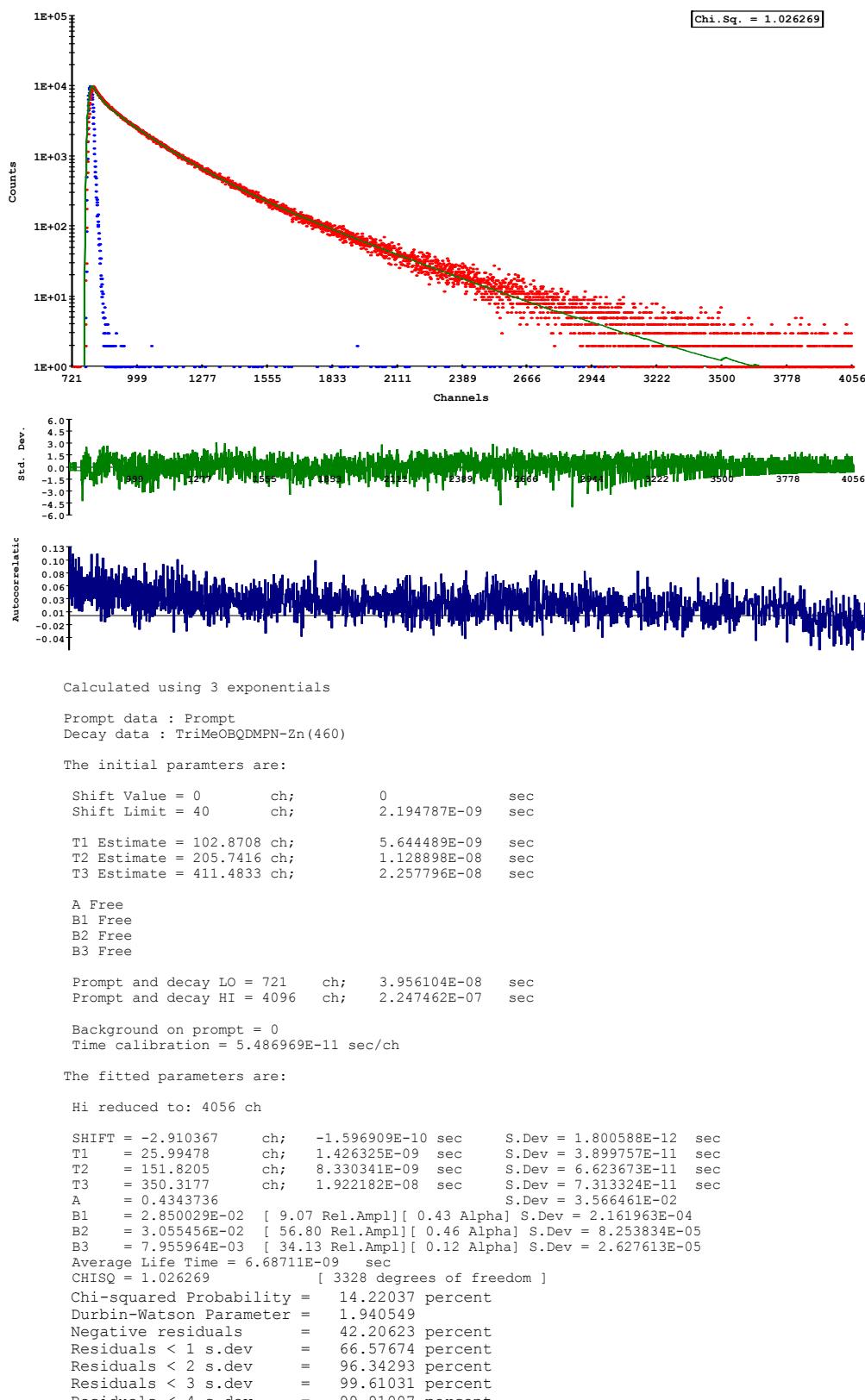
```

SHIFT = -2.609949      ch;  -1.432071E-10  sec  S.Dev = 1.775269E-12  sec
T1   = 244.7231      ch;  1.342788E-08  sec  S.Dev = 2.651276E-10  sec
T2   = 61.38607     ch;  3.368234E-09  sec  S.Dev = 9.448889E-11  sec
T3   = 511.4449     ch;  2.806282E-08  sec  S.Dev = 7.316742E-11  sec
A    = 3.668435E-02          S.Dev = 8.102692E-02
B1  = 2.517539E-02  [ 40.18 Rel.Ampl][ 0.46 Alpha] S.Dev = 9.35765E-05
B2  = 1.340181E-02  [ 5.37 Rel.Ampl][ 0.24 Alpha] S.Dev = 1.55628E-04
B3  = 1.632542E-02  [ 54.45 Rel.Ampl][ 0.30 Alpha] S.Dev = 3.42707E-05
Average Life Time = 1.532404E-08  sec
CHISQ = 1.0736          [ 3357 degrees of freedom ]
  
```

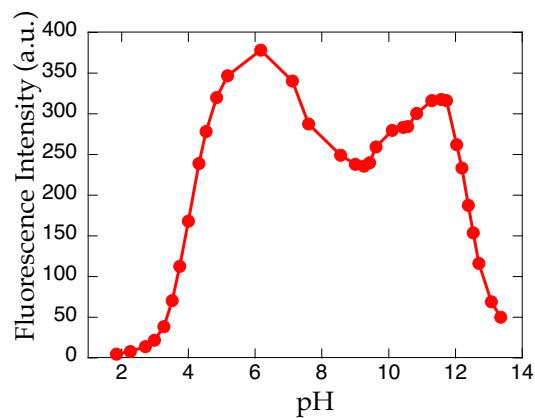
```

Chi-squared Probability = 0.1578351 percent
Durbin-Watson Parameter = 2.119035
Negative residuals = 46.18128 percent
Residuals < 1 s.dev = 66.86478 percent
Residuals < 2 s.dev = 94.44279 percent
Residuals < 3 s.dev = 99.52452 percent
Residuals < 4 s.dev = 100 percent
  
```

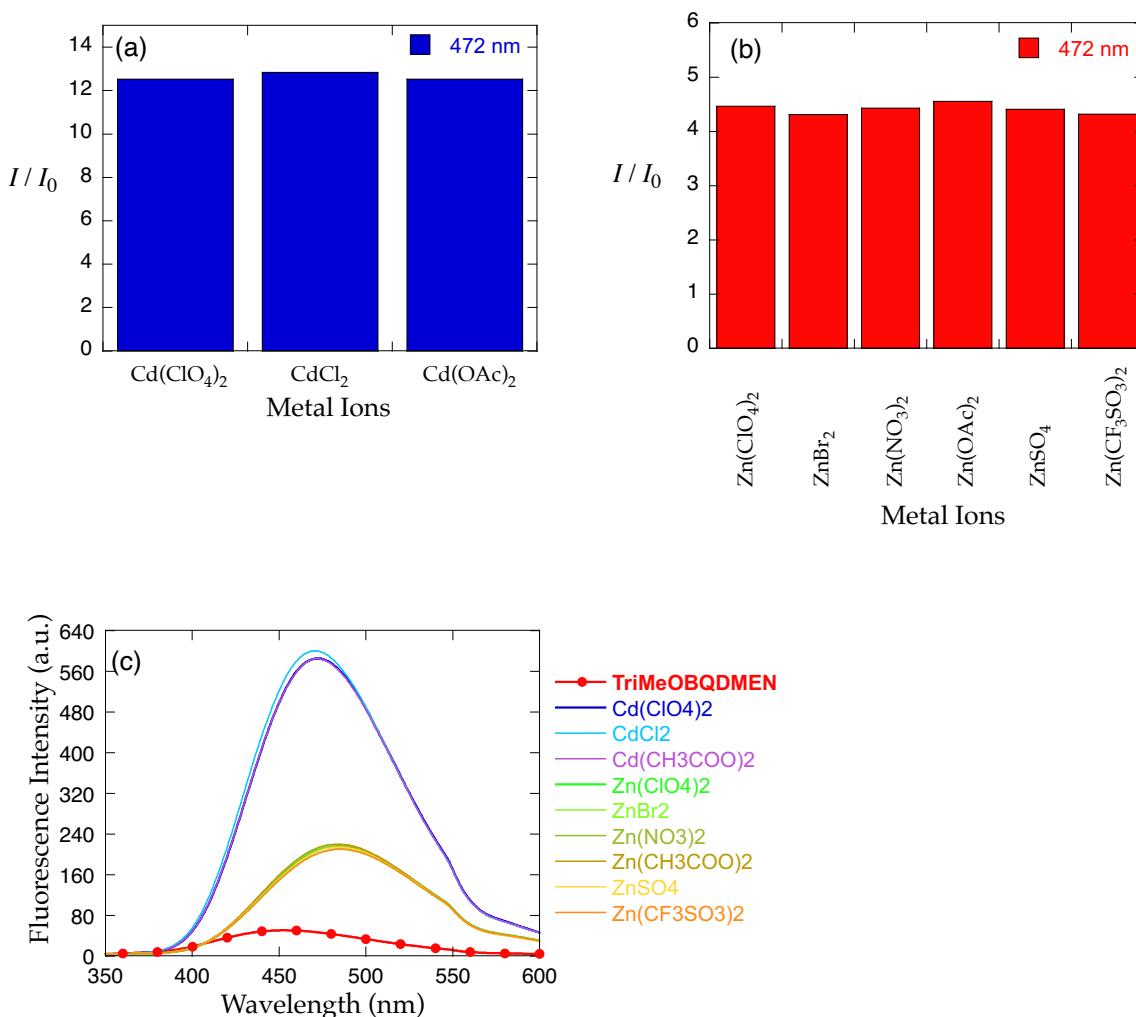
**Fig. S28.** Fluorescence lifetime measurement of 34  $\mu$ M TriMeOBQDMPN (**6**) in the presence of 3 equiv. of Cd<sup>2+</sup> in DMF-H<sub>2</sub>O (1:1) with 460 nm bandpath filter (BPF) at 25 °C ( $\lambda_{\text{ex}} = 331$  nm).



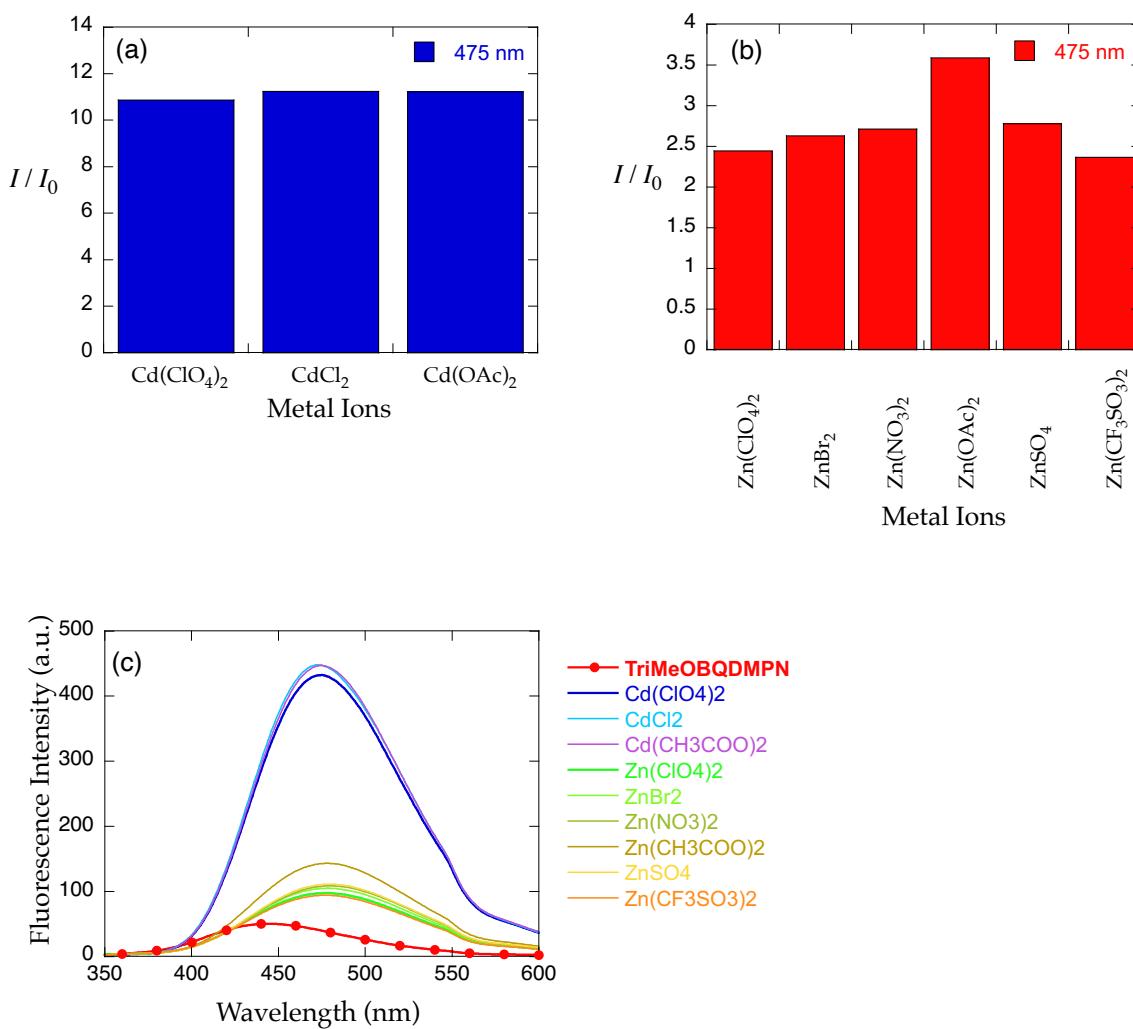
**Fig. S29.** Fluorescence lifetime measurement of 34  $\mu$ M TriMeOBQDMPN (**6**) in the presence of 3 equiv. of  $Zn^{2+}$  in DMF-H<sub>2</sub>O (1:1) with 460 nm bandpath filter (BPF) at 25 °C ( $\lambda_{ex} = 331$  nm).



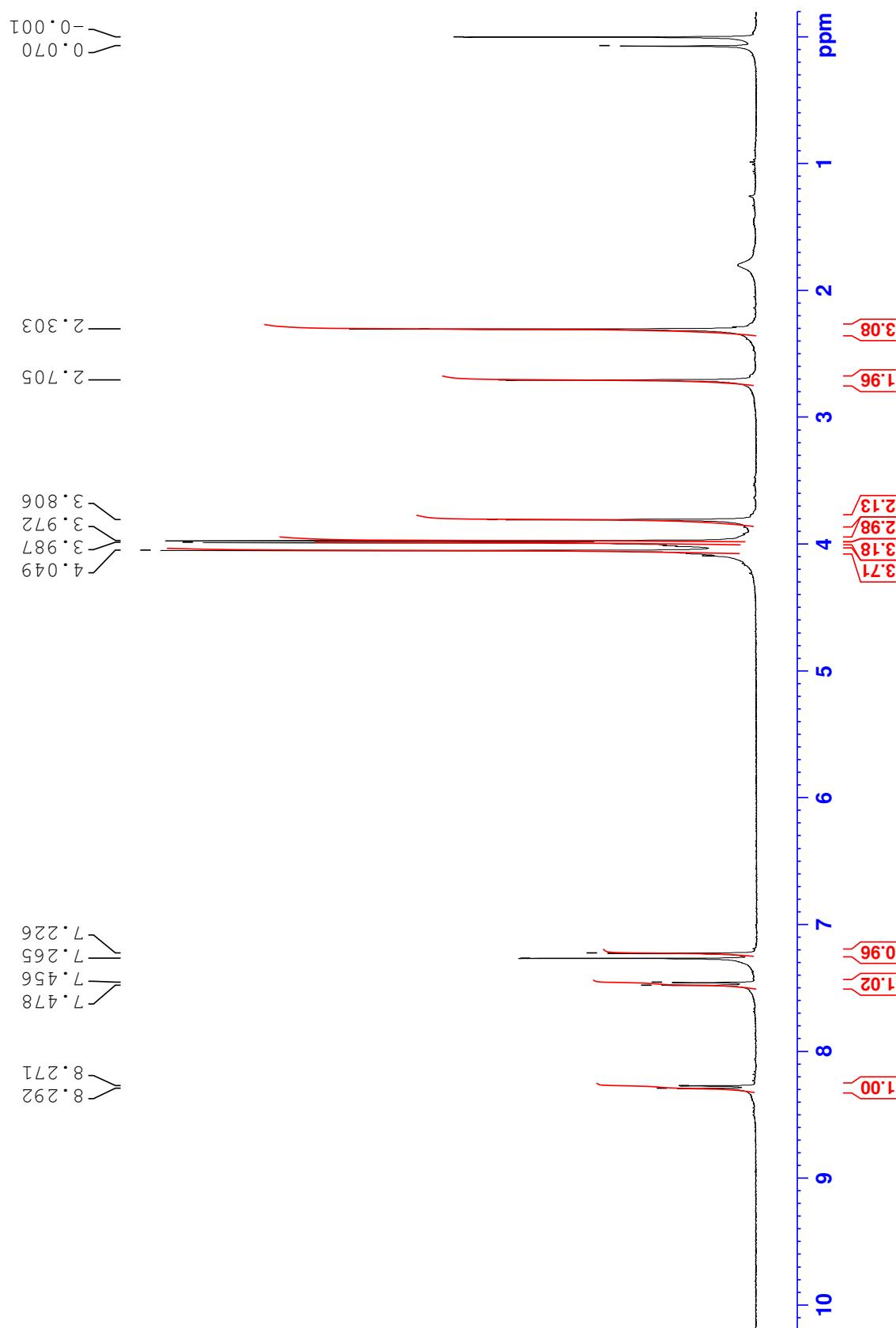
**Fig. S30.** Effect of pH on fluorescence intensity of TriMeOBQDMEN (**3**) at 485 nm in the presence of 1 equiv. of  $Zn^{2+}$  in DMF-H<sub>2</sub>O (1:1) at 25 °C. Condition: H<sub>2</sub>SO<sub>4</sub> or NaOH was added to the neutral solution.



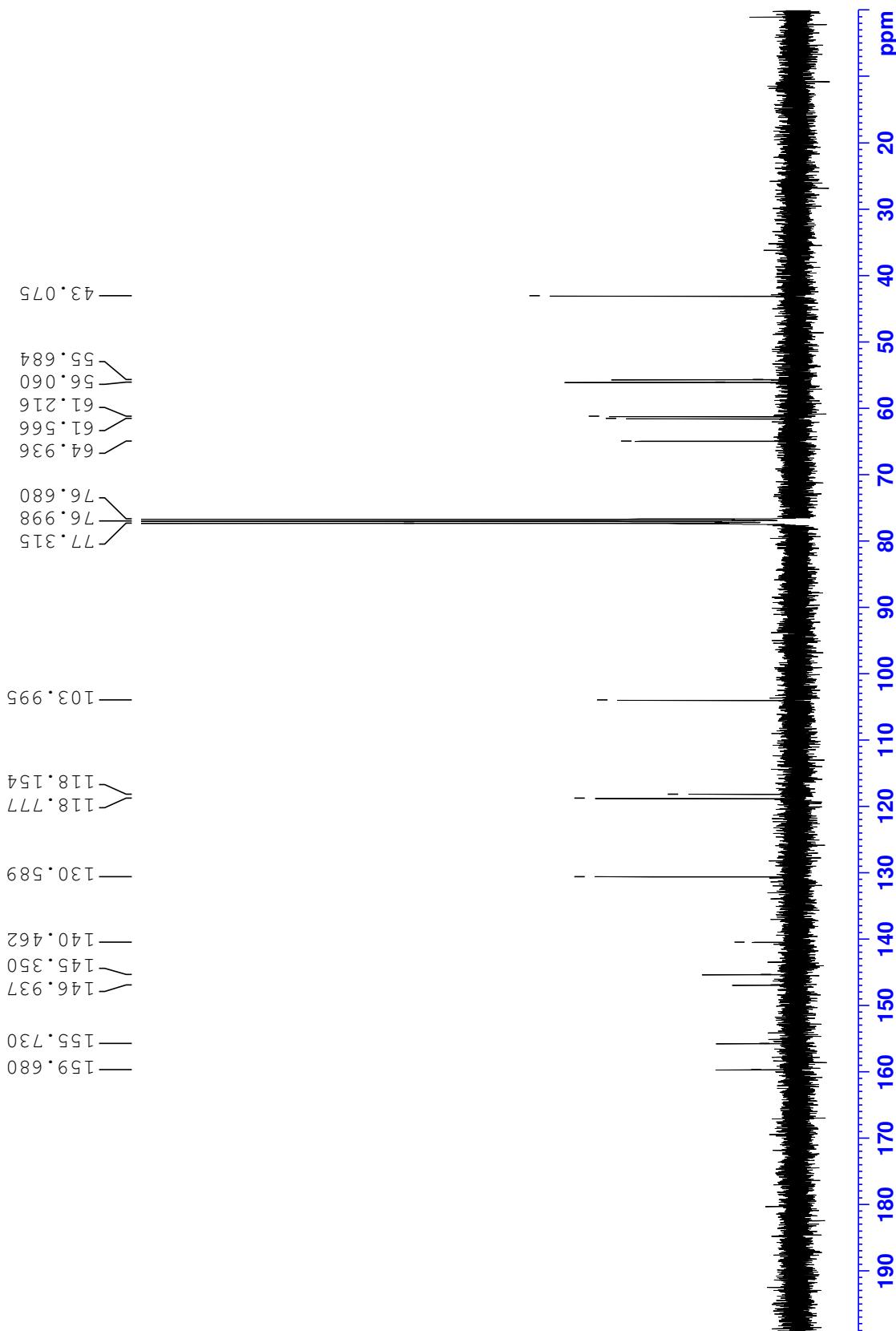
**Fig. S31.** Effect of counter anion on the fluorescence intensity of 34  $\mu\text{M}$  TriMeOBQDMEN (**3**) in the presence of 1 equiv. of various metal salts in DMF- $\text{H}_2\text{O}$  (1:1) at 25  $^\circ\text{C}$  ( $\lambda_{\text{ex}} = 339$  nm).  $I_0$  is the emission intensity of free ligand. (a) Effect of cadmium salt. (b) Effect of zinc salt. (c) Fluorescence spectra.



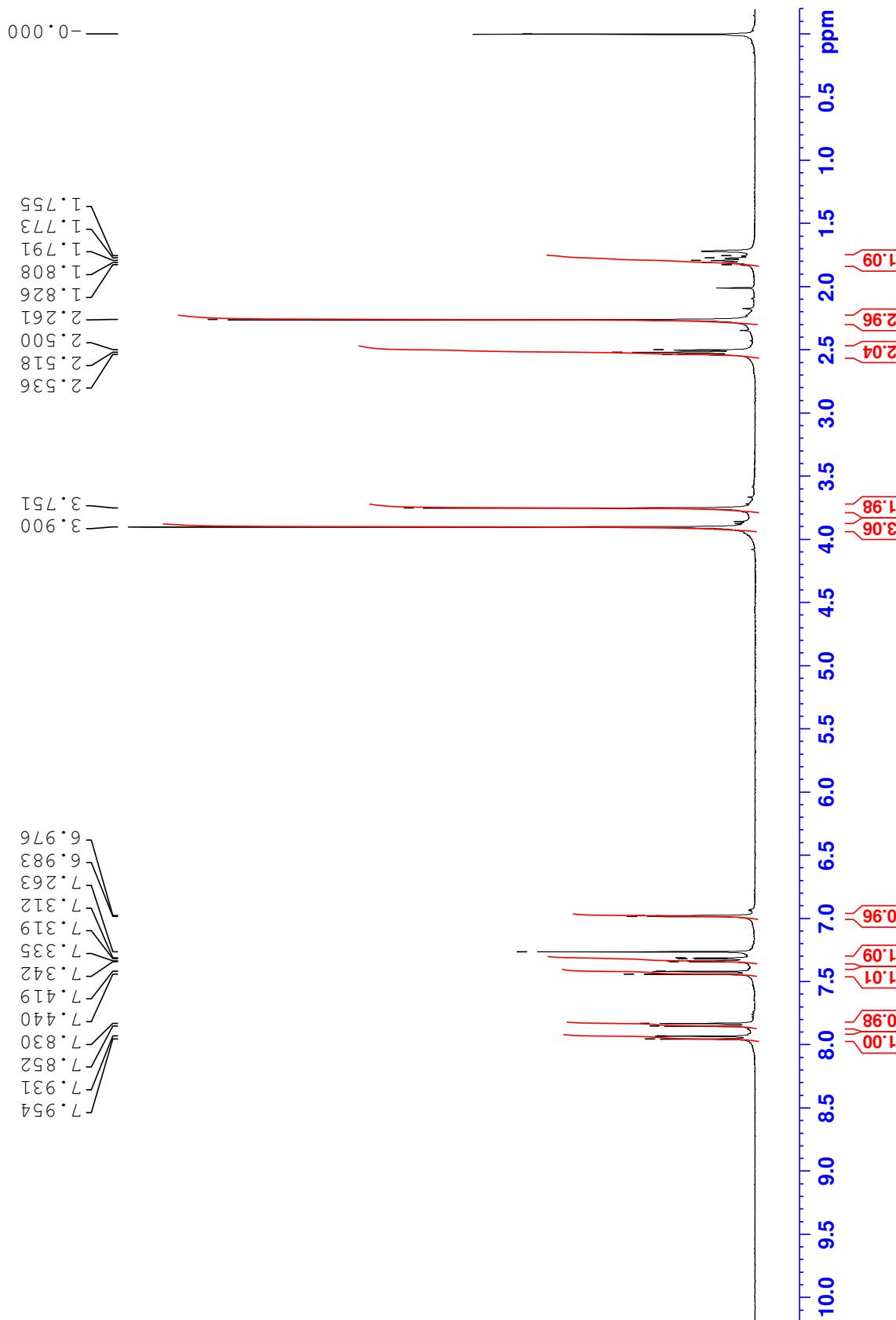
**Fig. S32.** Effect of counter anion on the fluorescence intensity of 34  $\mu\text{M}$  **TriMeOBQDMPN** (**6**) in the presence of 1 equiv. of various metal salts in DMF- $\text{H}_2\text{O}$  (1:1) at 25  $^{\circ}\text{C}$  ( $\lambda_{\text{ex}} = 337$  nm).  $I_0$  is the emission intensity of free ligand. (a) Effect of cadmium salt. (b) Effect of zinc salt. (c) Fluorescence spectra.



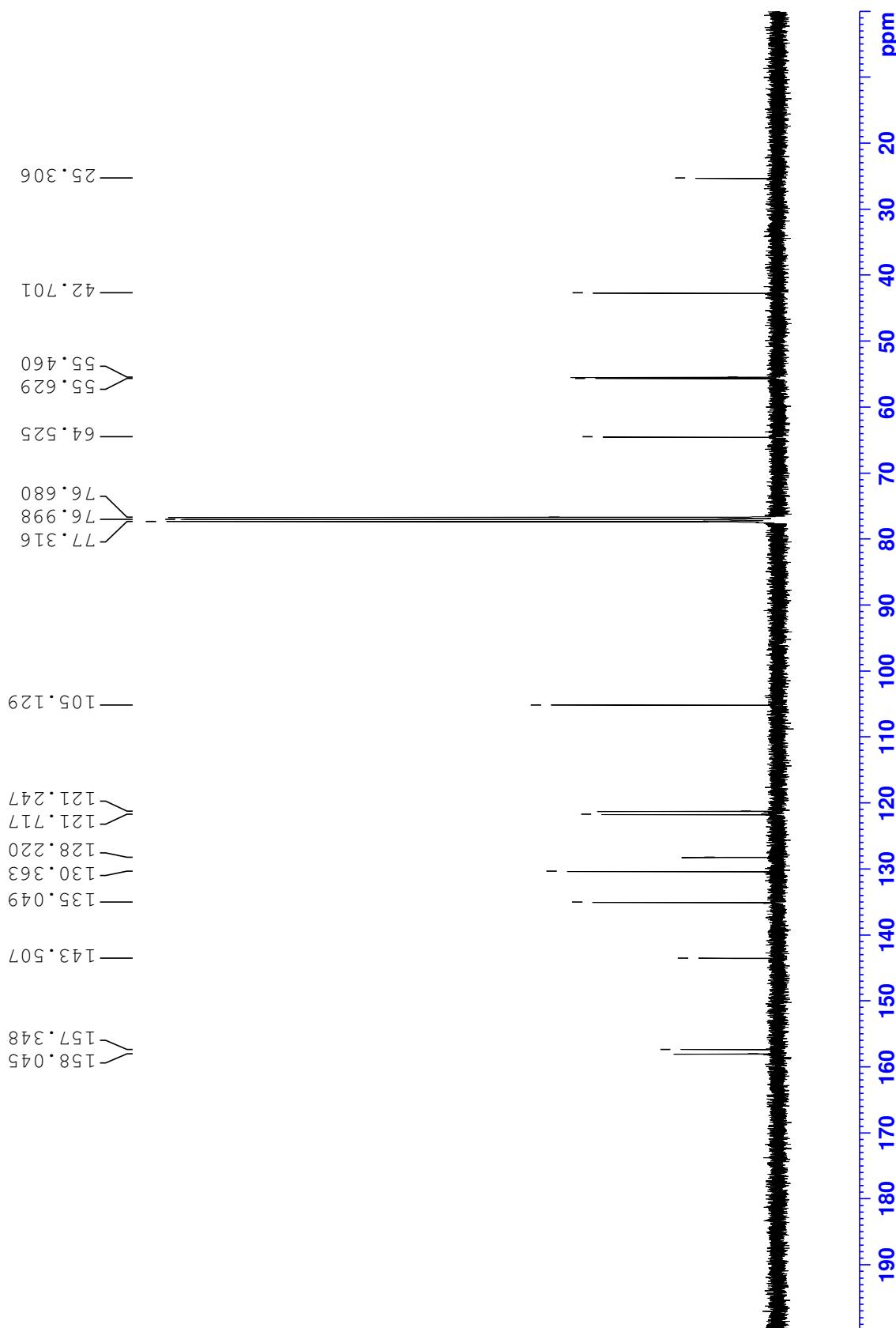
**Fig. S33.**  $^1\text{H}$  NMR spectrum for TriMeOBQDMEN (**3**) in  $\text{CDCl}_3$ .



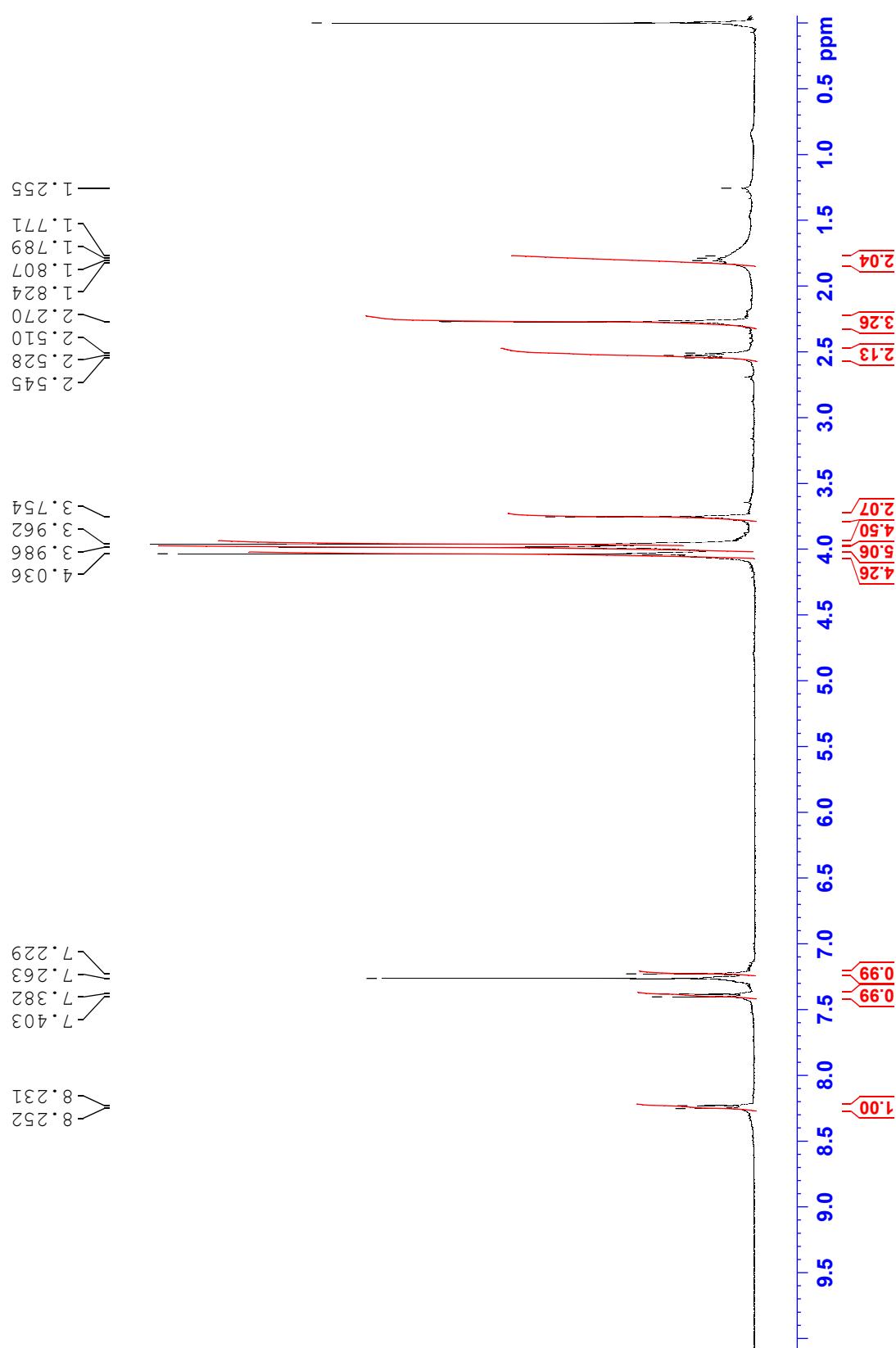
**Fig. S34.**  $^{13}\text{C}$  NMR spectrum for TriMeOBQDMEN (3) in  $\text{CDCl}_3$ .



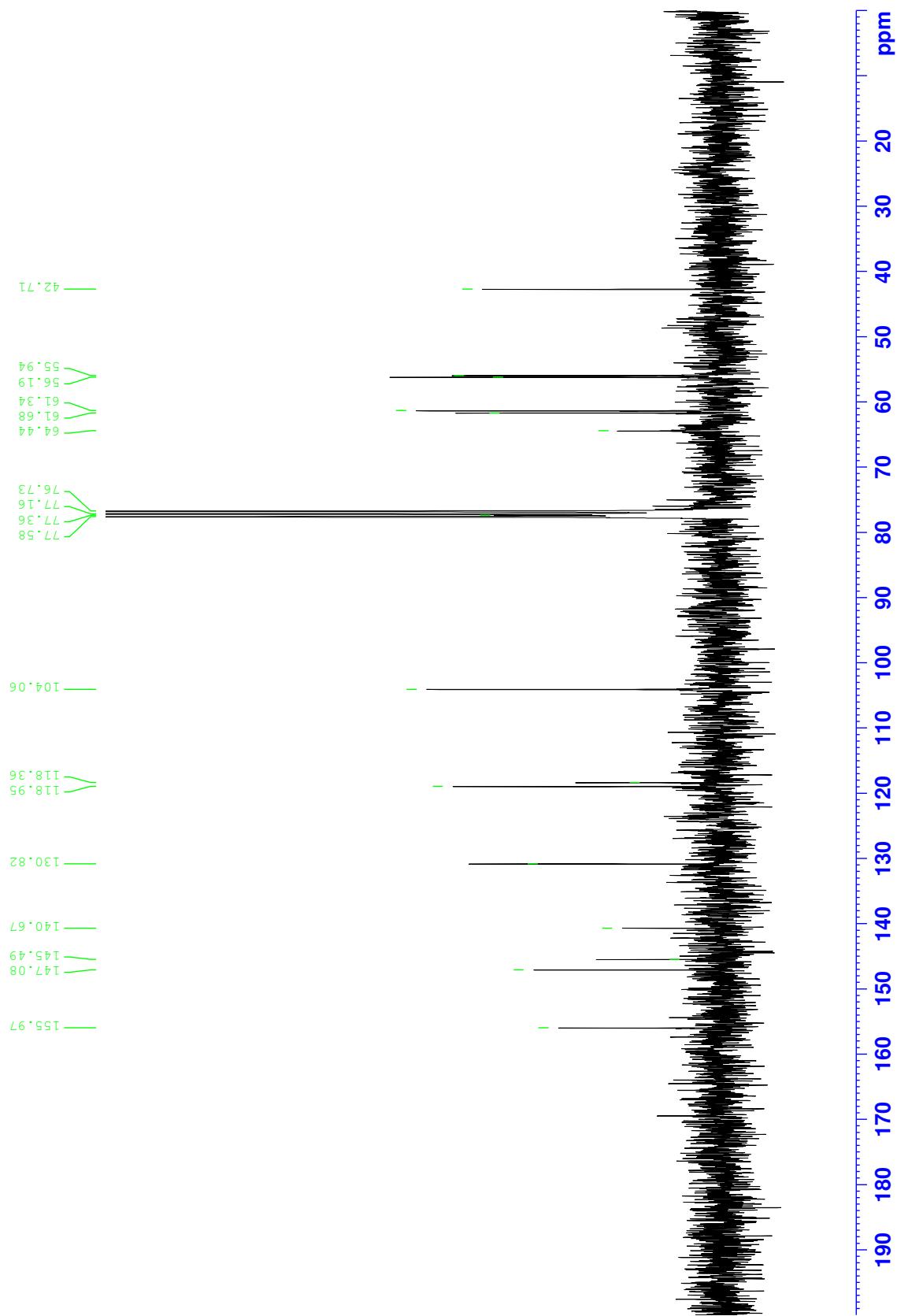
**Fig. S35.** <sup>1</sup>H NMR spectrum for 6-MeOBQDMPN (**5**) in  $\text{CDCl}_3$ .



**Fig. S36.**  $^{13}\text{C}$  NMR spectrum for 6-MeOBQDMPN (**5**) in  $\text{CDCl}_3$ .



**Fig. S37.**  $^1\text{H}$  NMR spectrum for TriMeOBQDMPN (6) in  $\text{CDCl}_3$ .



**Fig. S38.**  $^{13}\text{C}$  NMR spectrum for TriMeOBQDMPN (**6**) in  $\text{CDCl}_3$ .