Supplementary Information for

Methoxy-substituted tetrakisquinoline analogs of EGTA and BAPTA for fluorescent detection of Cd^{2+}

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Table S1. Crystallographic Data for BAPTQ

	BAPTQ
Formula	$C_{54}H_{44}N_6O_2$
FW	808.98
Crystal system	triclinic
Space group	*P*-1
a, Å	10.7273(18)
b, Å	11.8900(18)
c, Å	17.402(3)
α, deg	77.787(5)
β, deg	87.943(6)
γ, deg	73.552(4)
V, Å^3	2079.9(6)
Z	2
D_{calc}, g cm^{-3}	1.292
μ, mm^{-1}	0.0799
$2\theta_{max}$, deg	55
temp, K	153
no. reflns collected	16366
no. reflns used	9080
no. of params	735
R_{int}	0.0176
Final *R*1 ($I > 2\sigma(I)$)[a]	0.0470
*wR*2 (all data)[b]	0.1160
GOF	1.115

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

Table S2. Crystallographic Data for $[Cd(EGTQ)](ClO_4)_2 \cdot CH_3OH$ and $[Cd_2(\mu\text{-}OH)(EGTQ)(H_2O)_2](ClO_4)_3 \cdot 2CH_3CN$

	$[Cd(EGTQ)](ClO_4)_2 \cdot CH_3OH$	$[Cd_2(\mu\text{-}OH)(EGTQ)\text{-}(H_2O)_2](ClO_4)_3 \cdot 2CH_3CN$
Formula	$C_{47}H_{48}CdCl_2N_6O_{11}$	$C_{50}H_{55}Cd_2Cl_3N_8O_{17}$
FW	1056.25	1371.21
Crystal system	triclinic	monoclinic
Space group	*P*-1	$P2_1/c$
a, Å	11.0758(14)	22.6992(5)
b, Å	13.7776(16)	11.29840(10)
c, Å	14.882(2)	23.9600(5)
α, deg	87.257(3)	90
β, deg	89.363(4)	114.7039(9)
γ, deg	75.001(5)	90
V, Å^3	2191.1(5)	5582.51(18)
Z	2	4
D_{calc}, g cm^{-3}	1.601	1.631
μ, mm^{-1}	0.6925	0.9835
$2\theta_{max}$, deg	55	55
temp, K	153	153
no. reflns collected	21773	42577
no. reflns used	9852	12743
no. of params	609	723
R_{int}	0.0136	0.0174
Final $R1$ ($I > 2\sigma(I)$)[a]	0.0370	0.0387
$wR2$ (all data)[b]	0.0940	0.1040
GOF	1.025	1.042

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

Table S3. Crystallographic Data for $[Zn_2(\mu\text{-}OH)(EGTQ)](ClO_4)_3\cdot CH_3OH$ and $[Zn_4(\mu\text{-}CO_3)_2(EGTQ)_2](ClO_4)_4\cdot CH_3CN\cdot 2CHCl_3\cdot CH_3OH\cdot H_2O$

	$[Zn_2(\mu\text{-}OH)(EGTQ)]\text{-}(ClO_4)_3\cdot CH_3OH$	$[Zn_4(\mu\text{-}CO_3)_2(EGTQ)_2](ClO_4)_4\cdot CH_3CN\cdot 2CHCl_3\cdot CH_3OH\cdot H_2O$
Formula	$C_{47}H_{49}Cl_3N_6O_{16}Zn_2$	$C_{99}H_{99}Cl_{10}N_{13}O_{28}Zn_4$
FW	1191.05	2534.99
Crystal system	triclinic	monoclinic
Space group	*P*-1	$P2_1/n$
a, Å	11.91350(10)	23.6390(13)
b, Å	12.44190(10)	15.9622(9)
c, Å	17.5021(2)	30.6105(18)
α, deg	78.577(3)	90
β, deg	79.314(3)	112.100(2)
γ, deg	78.273(4)	90
V, Å^3	2461.18(6)	10701.6(11)
Z	2	4
D_{calc}, g cm^{-3}	1.607	1.573
μ, mm^{-1}	1.2159	1.2178
$2\theta_{max}$, deg	55	55
temp, K	153	153
no. reflns collected	24466	105545
no. reflns used	11062	24506
no. of params	673	1408
R_{int}	0.0153	0.0517
Final $R1$ ($I > 2\sigma(I)$)[a]	0.0405	0.0673
$wR2$ (all data)[b]	0.1108	0.1818
GOF	1.028	1.056

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

Table S4. Crystallographic Data for $[Cd(BAPTQ)](ClO_4)_2 \cdot H_2O$ and $[Cd_2(BAPTQ)(CH_3CN)_4(H_2O)_2](ClO_4)_4$

	$[Cd(BAPTQ)]$-$(ClO_4)_2 \cdot H_2O$	$[Cd_2(BAPTQ)(CH_3CN)_4(H_2O)_2]$-$(ClO_4)_4$
Formula	$C_{54}H_{46}CdCl_2N_6O_{11}$	$C_{62}H_{60}Cd_2Cl_4N_{10}O_{20}$
FW	1138.31	1631.84
Crystal system	monoclinic	triclinic
Space group	$P2_1/n$	P-1
a, Å	15.4421(8)	12.3738(8)
b, Å	15.5215(8)	17.9552(14)
c, Å	20.5748(10)	18.3514(13)
α, deg	90	103.789(3)
β, deg	92.922(3)	90.8895(10)
γ, deg	90	108.016(3)
V, Å^3	4925.1(4)	3747.9(5)
Z	4	2
D_{calc}, g cm^{-3}	1.535	1.446
μ, mm^{-1}	0.6226	0.7834
$2\theta_{max}$, deg	55	54.9
temp, K	153	153
no. reflns collected	50632	36976
no. reflns used	11303	16805
no. of params	703	887
R_{int}	0.0224	0.0387
Final $R1$ ($I > 2\sigma(I)$)[a]	0.0508	0.0584
$wR2$ (all data)[b]	0.1562	0.1653
GOF	1.049	1.061

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

Table S5. Crystallographic Data for $[Zn_2(\mu\text{-}OH)(BAPTQ)][Zn_2(\mu\text{-}OH)(BAPTQ)(CH_3CN)](ClO_4)_6\cdot 2CH_3CN\cdot C_2H_5OC_2H_5$ and $[Zn_2(\mu\text{-}OH)(6\text{-}MeOEGTQ)](ClO_4)_3$

	$[Zn_2(\mu\text{-}OH)(BAPTQ)][Zn_2(\mu\text{-}OH)(BAPTQ)(CH_3CN)](ClO_4)_6\cdot 2CH_3CN\cdot C_2H_5OC_2H_5$	$[Zn_2(\mu\text{-}OH)(6\text{-}MeOEGTQ)](ClO_4)_3$
Formula	$C_{126}H_{121}Cl_6N_{19}O_{31}Zn_4$	$C_{50}H_{53}Cl_3N_6O_{19}Zn_2$
FW	2871.69	1279.12
Crystal system	monoclinic	triclinic
Space group	$P2_1/c$	P-1
a, Å	23.1074(4)	13.244(3)
b, Å	28.4612(6)	14.742(3)
c, Å	19.2564(4)	17.352(3)
α, deg	90	91.076(3)
β, deg	91.4750(11)	96.137(2)
γ, deg	90	105.435(3)
V, Å^3	12660.0(4)	3242.9(11)
Z	4	2
D_{calc}, g cm^{-3}	1.507	1.310
μ, mm^{-1}	0.9609	0.9310
$2\theta_{max}$, deg	55	55
temp, K	153	153
no. reflns collected	128986	25309
no. reflns used	28808	14133
no. of params	1742	729
R_{int}	0.0294	0.0160
Final $R1$ ($I > 2\sigma(I)$)[a]	0.0695	0.0516
$wR2$ (all data)[b]	0.2282	0.1499
GOF	1.050	1.065

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

Table S6. Crystallographic Data for $[Cd_2Br_2(TriMeOBAPTQ)(CH_3OH)(H_2O)](ClO_4)_2$

	$[Cd_2Br_2(TriMeOBAPTQ)(CH_3OH)(H_2O)](ClO_4)_2$
Formula	$C_{67}H_{74}Br_2Cd_2Cl_2N_6O_{24}$
FW	1802.88
Crystal system	triclinic
Space group	*P*-1
a, Å	13.614(3)
b, Å	16.137(3)
c, Å	20.661(4)
α, deg	72.534(5)
β, deg	85.863(6)
γ, deg	76.622(6)
V, $Å^3$	4212.2(15)
Z	2
D_{calc}, g cm^{-3}	1.421
μ, mm^{-1}	1.5908
$2\theta_{max}$, deg	55
temp, K	153
no. reflns collected	44019
no. reflns used	19115
no. of params	941
R_{int}	0.0288
Final *R*1 ($I > 2\sigma(I)$)[a]	0.0555
*wR*2 (all data)[b]	0.1824
GOF	1.071

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

Table S7. Fluorescence Lifetimes for Cd^{2+} and Zn^{2+} Complexes of TQTACN, 6-MeOTQTACN and TriMeOTQTACN in DMF-H_2O (1:1)[a]

Ligand	Metal Ion	λ_{em} (nm)	BPF (nm)[b]	τ (nsec)[c]
TQTACN	Zn^{2+}	393	400	1.46 (48%), 6.94 (17%)
	Cd^{2+}	ND[d]	-	-
6-MeOTQTACN	Zn^{2+}	420	430	1.02 (27%), 3.68 (38%), 9.18 (35%)
	Cd^{2+}	420	430	0.99 (30%), 3.22 (49%), 8.62 (21%)
TriMeOTQTACN	Zn^{2+}	498	490	3.07 (3%), 8.76 (86%), 23.34 (11%)
	Cd^{2+}	489	490	2.72 (1%), 10.81 (87%), 22.78 (12%)

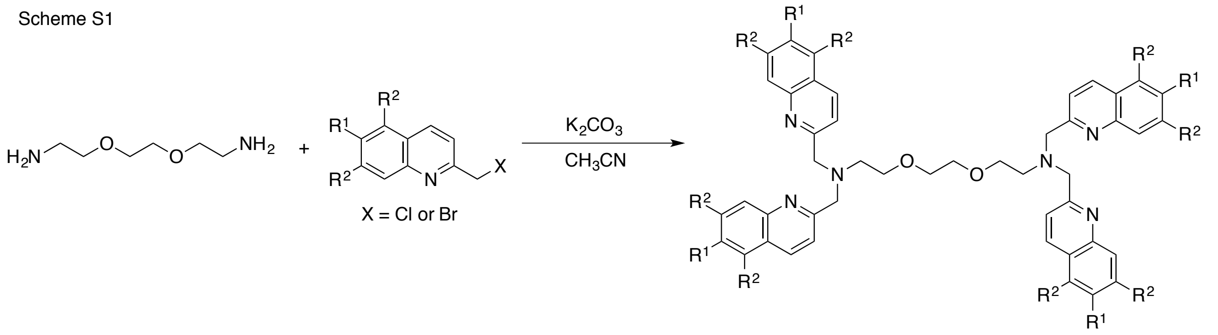
[a] Conditions: 34 μM solution in DMF-H_2O (1:1) at 25 °C in the presence of 2 equiv. of metal ion (λ_{ex} = 331 nm).

[b] Bandpath filter used (±10 nm).

[c] Components with extremely short lifetime (< 1 nsec) were omitted.

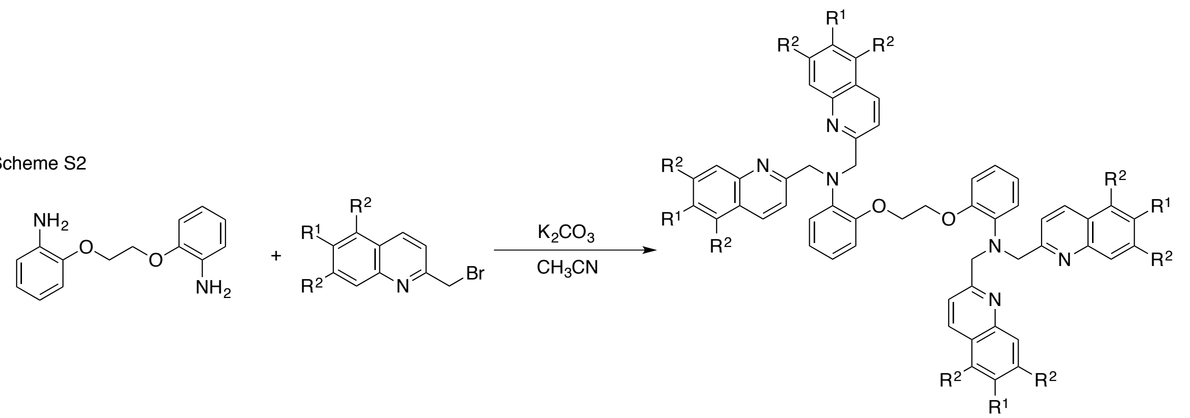
[d] No emission was observed.

Scheme S1



R^1 = H, R^2 = H	: EGTQ	quant.
R^1 = OCH_3, R^2 = H	: 6-MeOEGTQ	30%
R^1 = OCH_3, R^2 = OCH_3	: TriMeOEGTQ	68%

Scheme S2



R^1 = H, R^2 = H	: BAPTQ	71%
R^1 = OCH_3, R^2 = H	: 6-MeOBAPTQ	50%
R^1 = OCH_3, R^2 = OCH_3	: TriMeOBAPTQ	31%

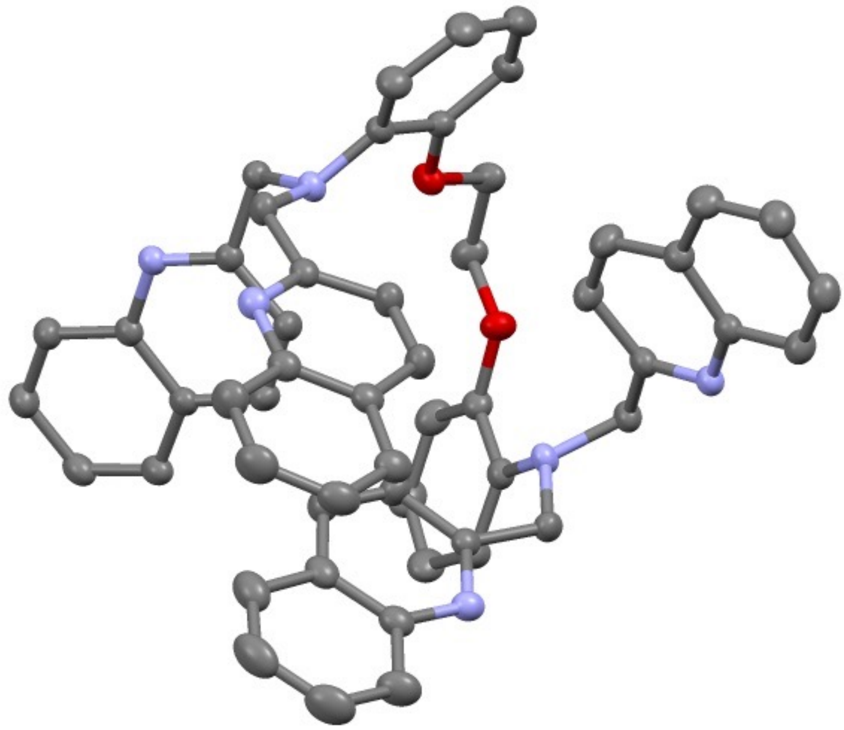


Fig. S1. Perspective view for BAPTQ in 50% probability. Hydrogen atoms are omitted for clarity.

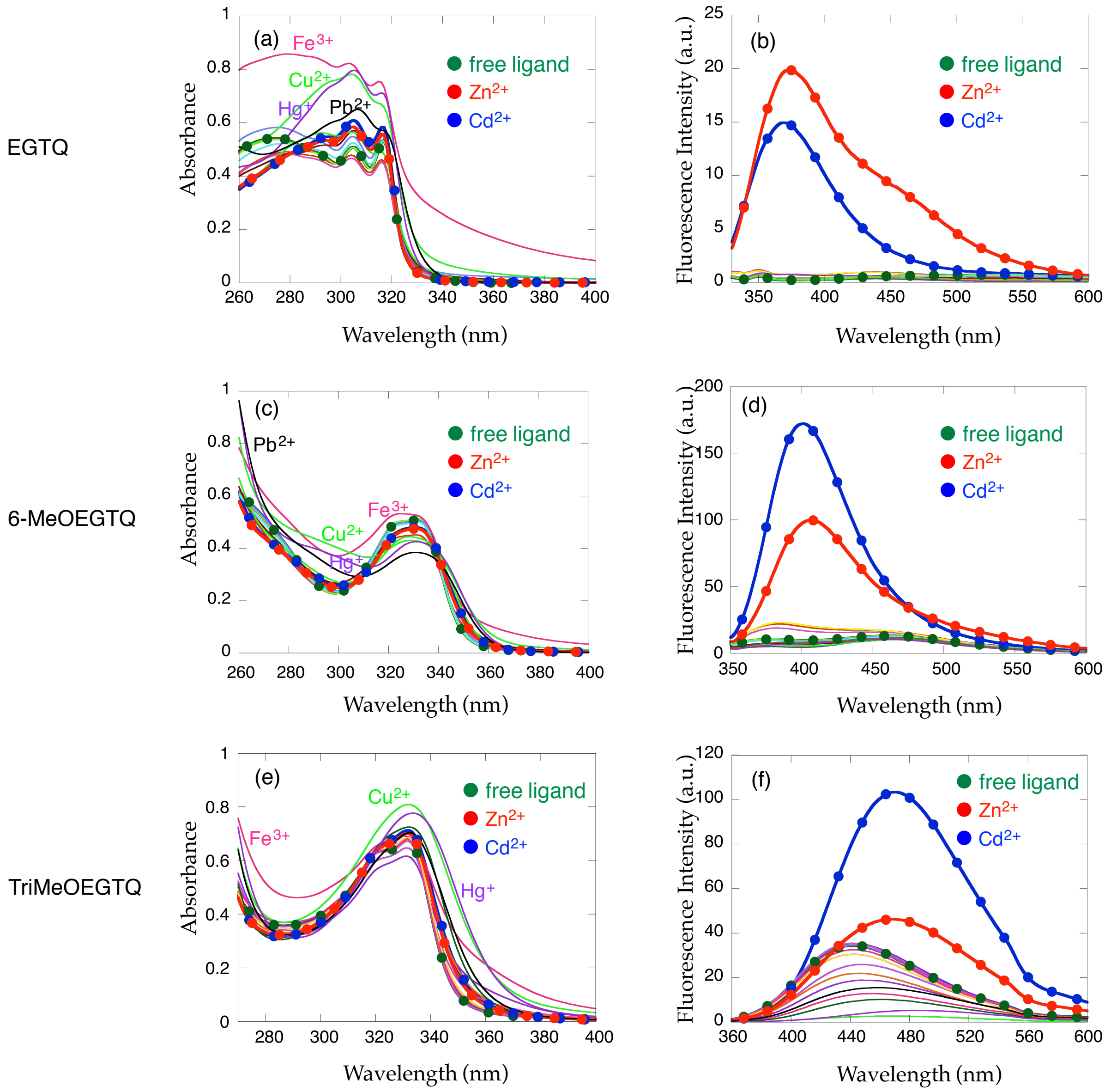


Fig. S2. (a, c, e) UV-vis absorption and (b, d, f) fluorescence spectral changes of 34 μM (a, b) EGTQ (λ_{ex} = 317 nm), (c, d) 6-MeOEGTQ (λ_{ex} = 342 nm) and (e, f) TriMeOEGTQ (λ_{ex} = 342 nm) in DMF-H_2O (1:1) at 25 °C in the presence of (a,b) 5 equiv. or (c-f) 2 equiv. of various metal ions.

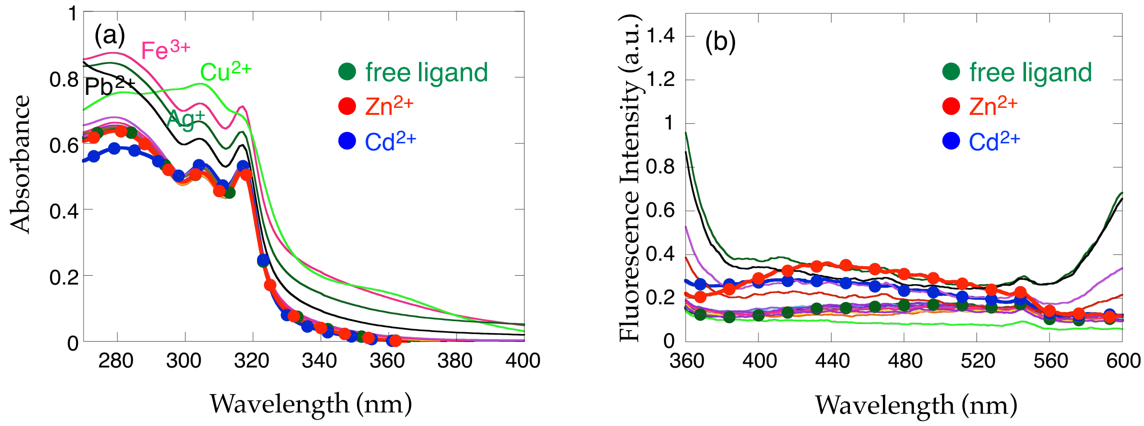


Fig. S3. (a) UV-vis absorption and (b) fluorescence spectral changes of 34 μM BAPTQ (λ_{ex} = 317 nm) in methanol-HEPES buffer (9:1, 50 mM HEPES, 0.1 M KCl, pH = 7.5) at 25 °C in the presence of 3 equiv. of various metal ions.

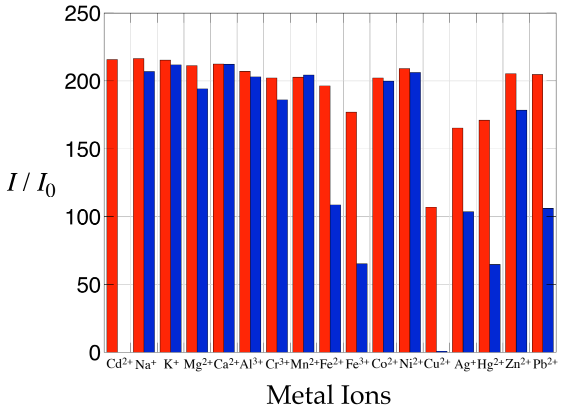


Fig. S4. Plot of fluorescence intensity of 34 μM TriMeOBAPTQ at 460 nm in methanol-HEPES buffer (9:1, 50 mM HEPES, 0.1 M KCl, pH = 7.5) at 25 °C in the presence of 3 equiv. of Cd^{2+} + 3 equiv. of metal ions (red bars) and 3 equiv. of Cd^{2+} + 30 equiv. of metal ions (blue bars) (λ_{ex} = 347 nm).

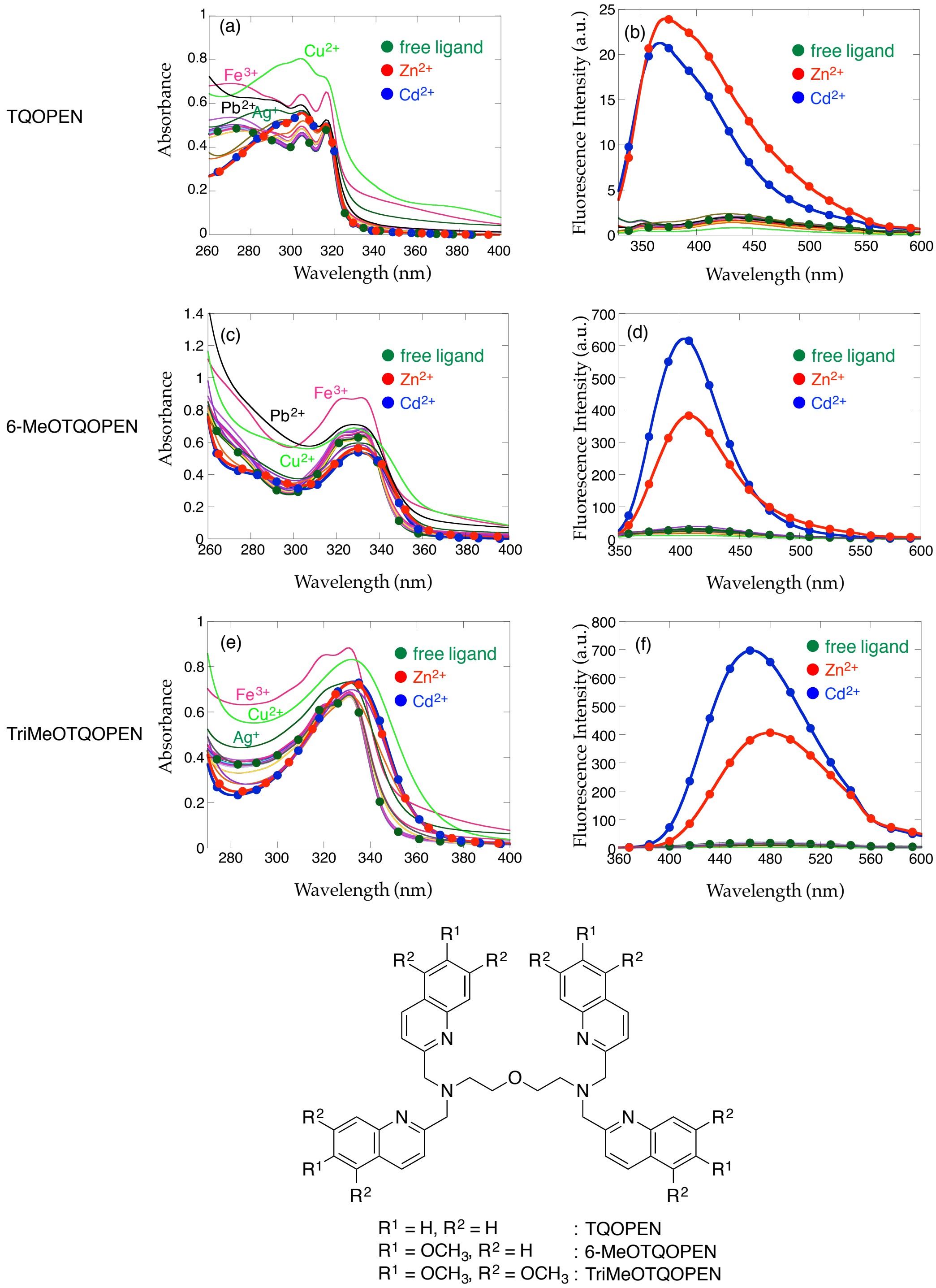


Fig. S5. (a, c, e) UV-vis absorption and (b, d, f) fluorescence spectral changes of 34 μM (a, b) TQOPEN (λ_{ex} = 317 nm), (c, d) 6-MeOTQOPEN (λ_{ex} = 342 nm) and (e, f) TriMeOTQOPEN (λ_{ex} = 342 nm) in methanol-HEPES buffer (9:1, 50 mM HEPES, 0.1 M KCl, pH = 7.5) at 25 °C in the presence of 3 equiv. of various metal ions.

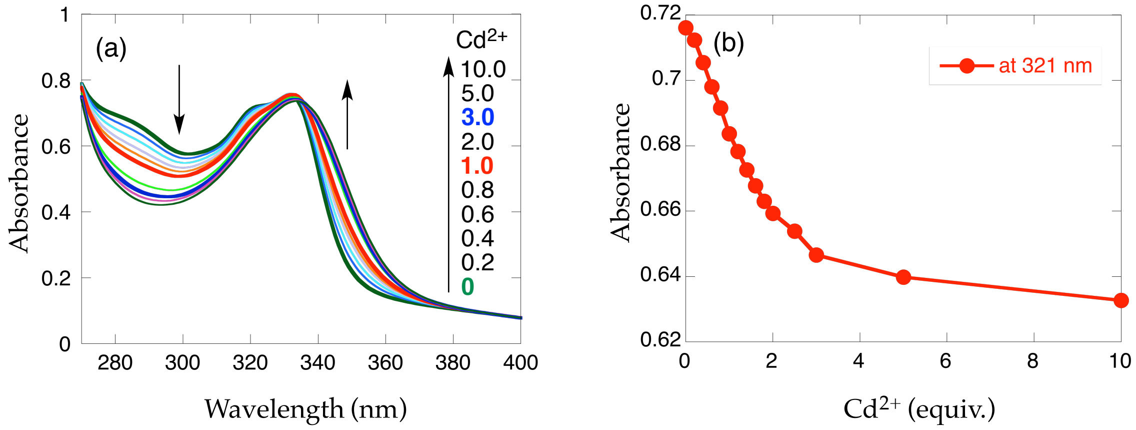


Fig. S6. (a) UV-vis absorption spectra and (b) plot of absorbance change at 321 nm of 34 μM TriMeOBAPTQ in methanol-HEPES buffer (9:1, 50 mM HEPES, 0.1 M KCl, pH = 7.5) at 25 °C in the presence of increasing amount of Cd^{2+}.

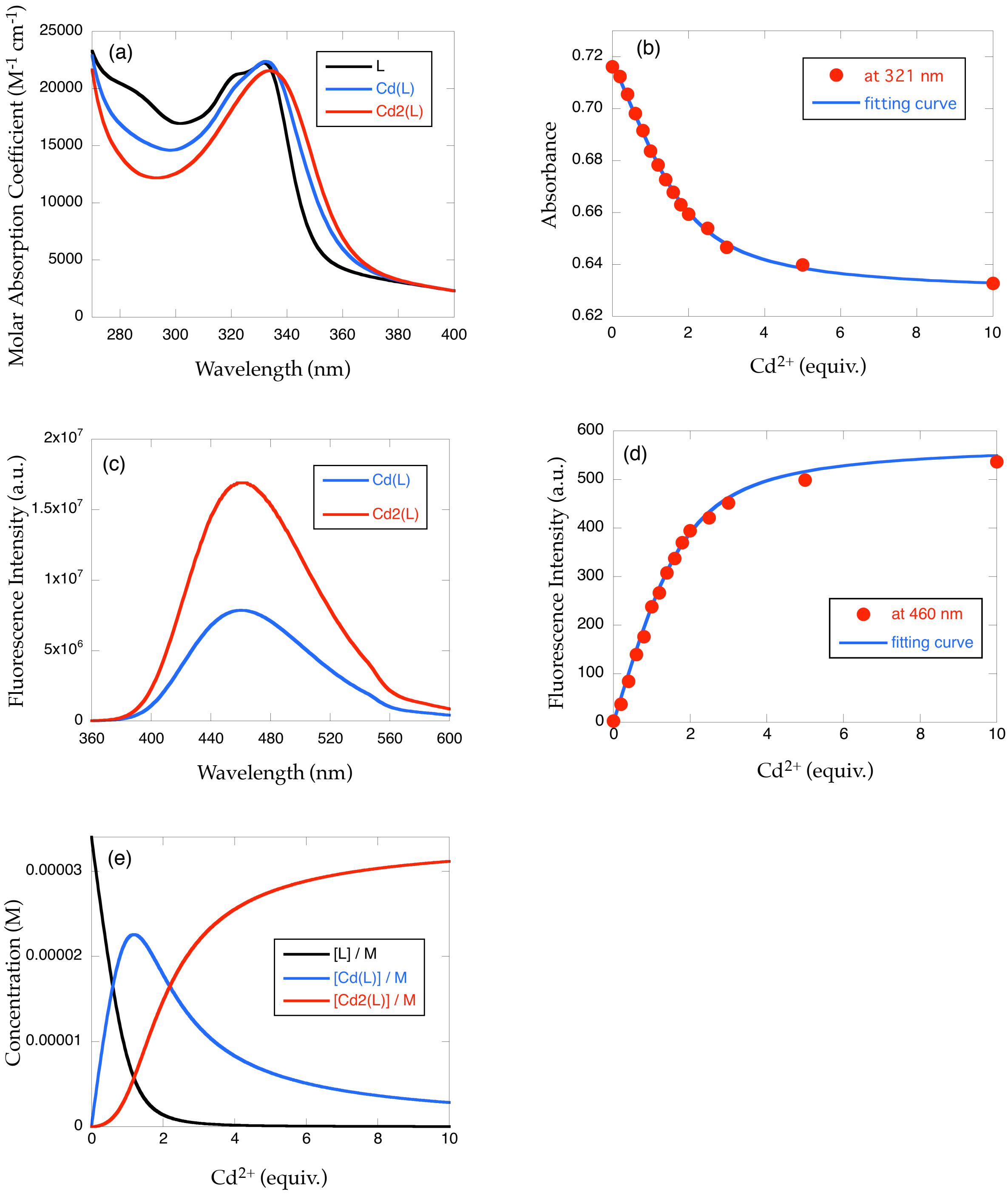


Fig. S7. (a) Separated UV-vis absorption spectra of free ligand (L), Cd(L) and Cd2(L), (b) simulated absorbance change at 321 nm, (c) separated fluorescence spectra of Cd(L) and Cd2(L), (d) simulated fluorescence intensity change at 460 nm and (e) distribution profile of L, Cd(L) and Cd2(L) during the titration of 34 μM TriMeOBAPTQ in methanol-HEPES buffer (9:1, 50 mM HEPES, 0.1 M KCl, pH = 7.5) at 25 °C in the presence of increasing amount of Cd^{2+}.

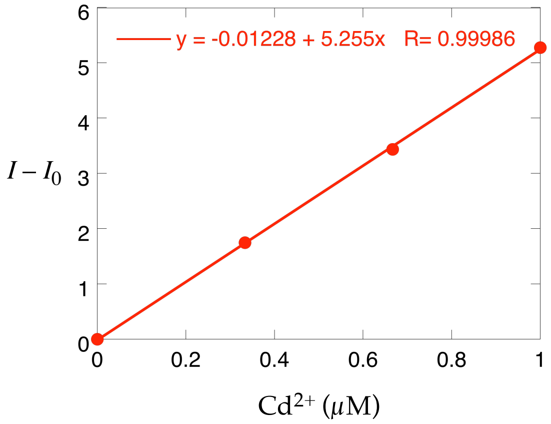


Fig. S8. Estimation of LOD (limit of detection) for Cd^{2+} with TriMeOBAPTQ in methanol-HEPES buffer (9:1, 50 mM HEPES, 0.1 M KCl, pH = 7.5) at 25 °C. The 3σ value (σ corresponds to standard deviation from 7 measurements) of blank solution (34 μM TriMeOBAPTQ) is 0.051831 in fluorescence intensity unit, which corresponds to 9.9 nM from the slope of the liner dynamic fluorescence intensity plot (*k*) shown above (LOD = 3σ/*k*).

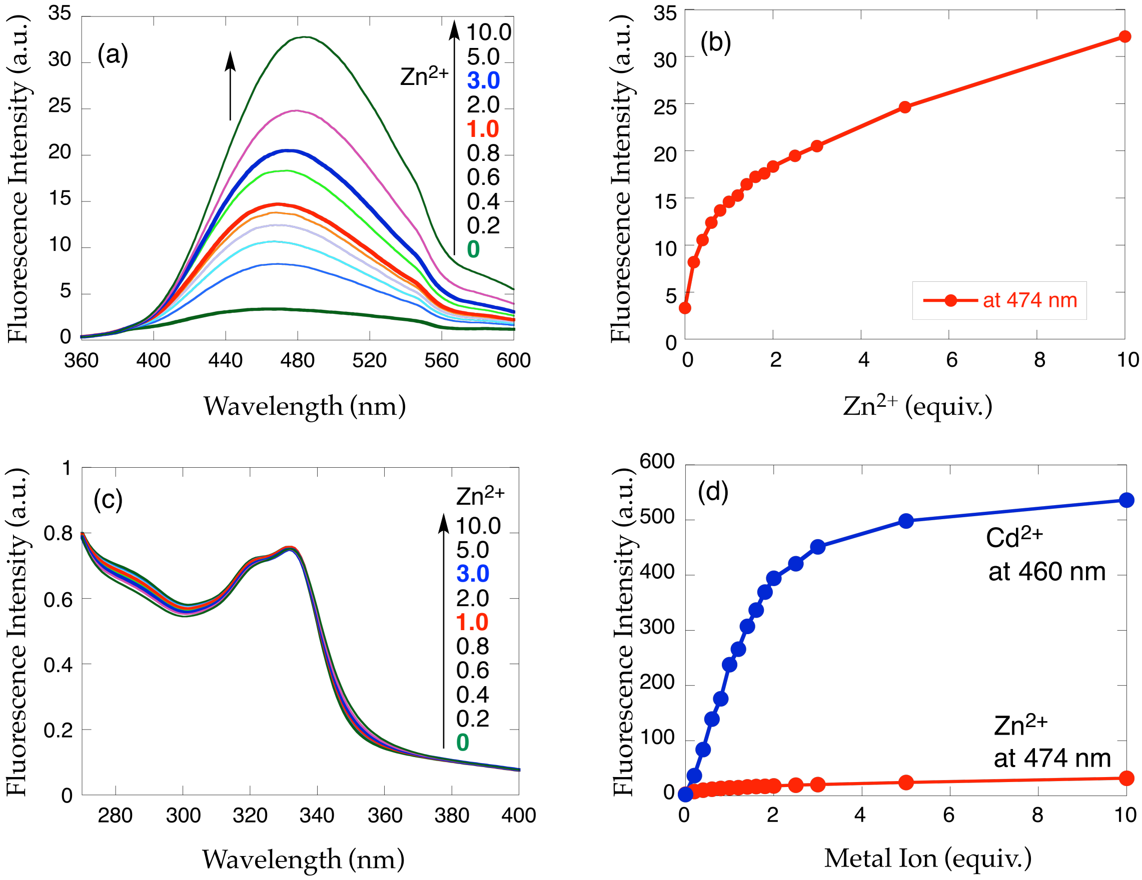


Fig. S9. (a) Fluorescence spectra (λ_{ex} = 347 nm), (b) plot of fluorescence intensity change at 474 nm and (c) UV-vis spectra of 34 μM TriMeOBAPTQ in methanol-HEPES buffer (9:1, 50 mM HEPES, 0.1 M KCl, pH = 7.5) at 25 °C in the presence of increasing amount of Zn^{2+}. (d) Comparison of fluorescence intensity changes of 34 μM TriMeOBAPTQ in methanol-HEPES buffer (9:1, 50 mM HEPES, 0.1 M KCl, pH = 7.5) at 25 °C in the presence of increasing amount of Cd^{2+} at 460 nm and Zn^{2+} at 474 nm (λ_{ex} = 347 nm).

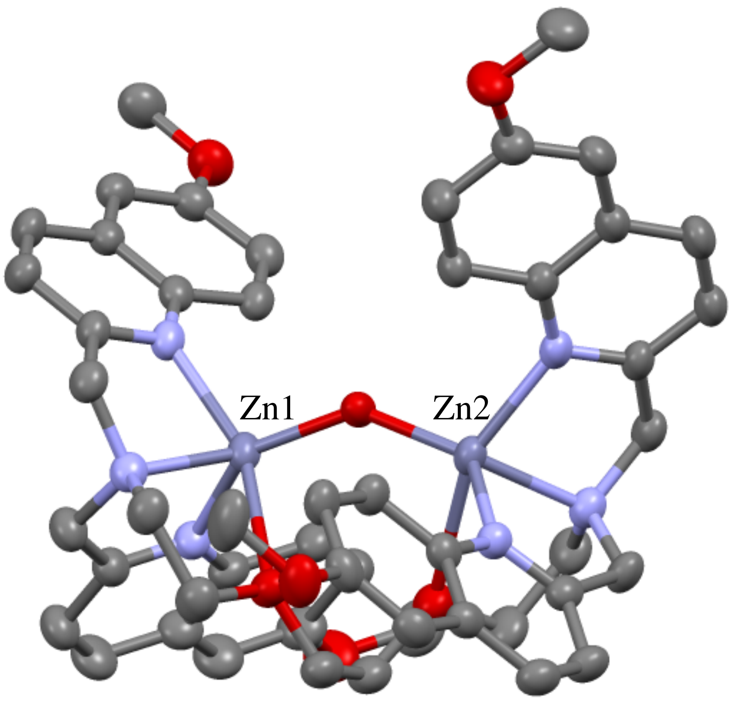


Fig. S10. Perspective view for $[Zn_2(\mu\text{-OH})(6\text{-MeOEGTQ})](ClO_4)_3$ in 50% probability. Hydrogen atoms, counteranions and solvents are omitted for clarity.

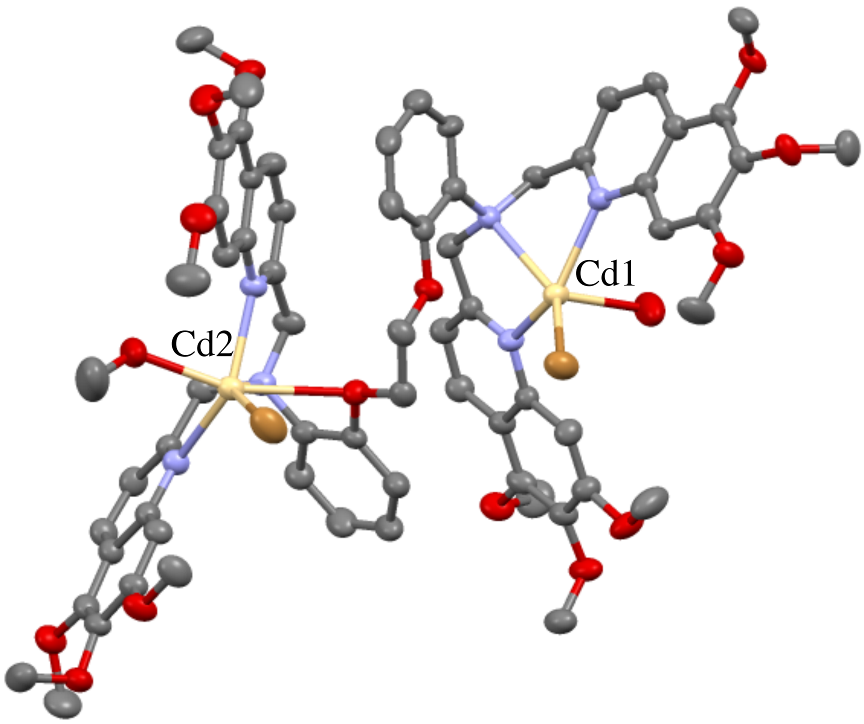
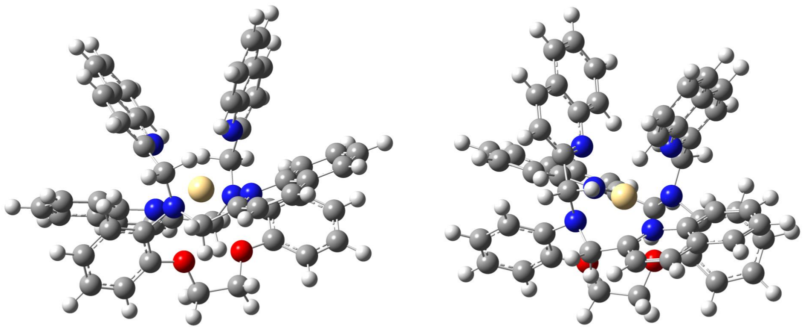


Fig. S11. Perspective view for $[Cd_2Br_2(TriMeOBAPTQ)(CH_3OH)(H_2O)](ClO_4)_2$ in 50% probability. Hydrogen atoms, counteranions and solvents are omitted for clarity.

(a)



(b)

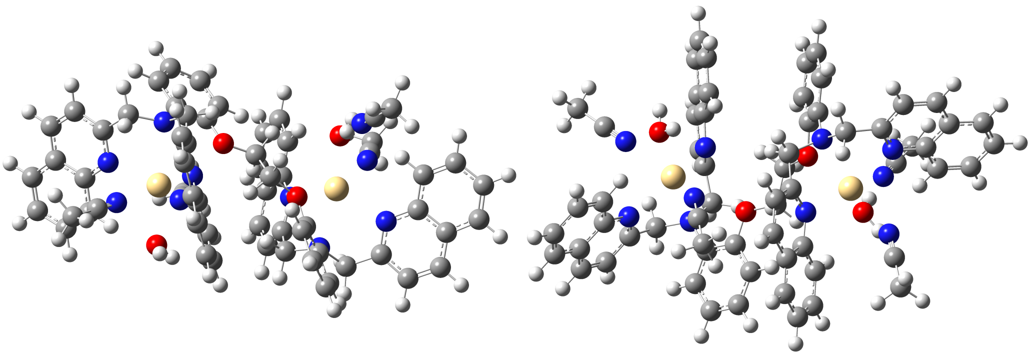


Figure S12. Optimized structures from different two directions for (a) $[Cd(BAPTQ)]^{2+}$ and (b) $[Cd_2(BAPTQ)(H_2O)_2(CH_3CN)_4]^{4+}$.

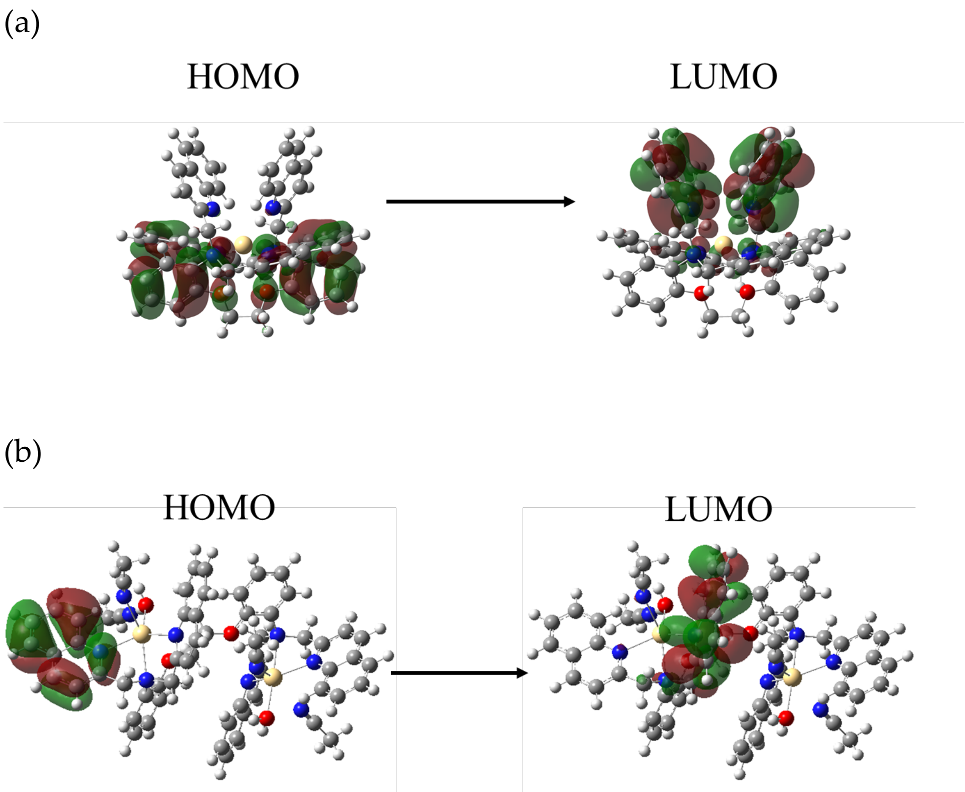
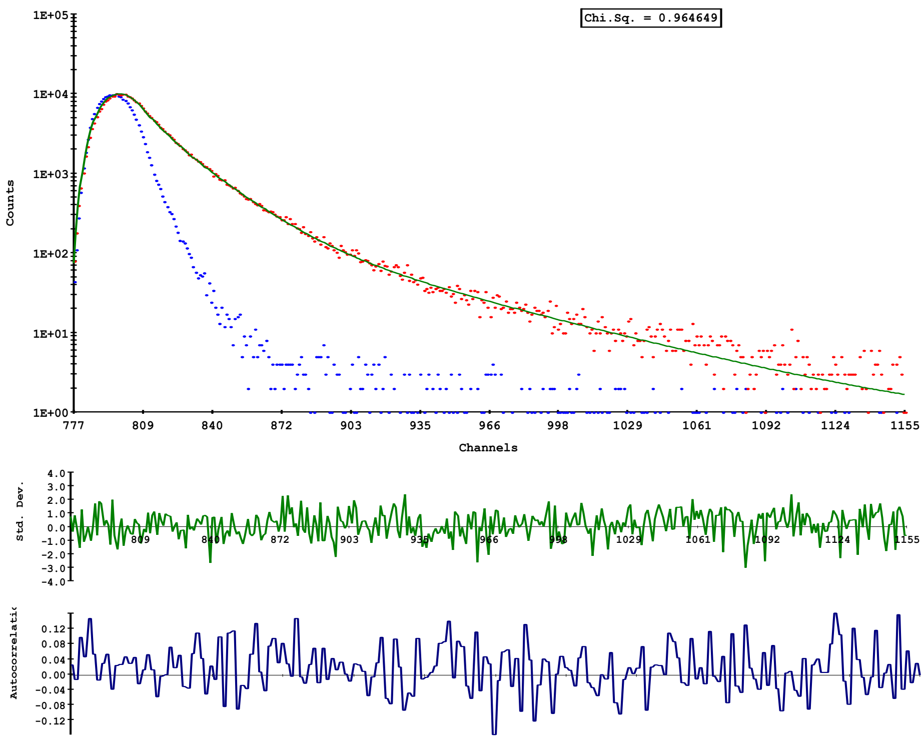


Figure S13. HOMO and LUMO for (a) $[Cd(BAPTQ)]^{2+}$ and (b) $[Cd_2(BAPTQ)(H_2O)_2(CH_3CN)_4]^{4+}$.

DAS6 v6.6. - HORIBA Jobin Yvon EGTQ-Zn3eq.das; EGTQ-Zn3eq [XSQ=0.964649] 28/11/2017

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Calculated using 3 exponentials

Prompt data : Prompt
Decay data : Decay

The initial paramters are:

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

 T1 Estimate = 6.813965 ch;          3.738801E-10   sec
 T2 Estimate = 13.62793 ch;          7.477602E-10   sec
 T3 Estimate = 27.25586 ch;          1.49552E-09    sec

 A Free
 B1 Free
 B2 Free
 B3 Free

 Prompt and decay LO = 777    ch;    4.263374E-08   sec
 Prompt and decay HI = 1195   ch;    6.556927E-08   sec

 Background on prompt = 44
 Time calibration = 5.486969E-11 sec/ch

The fitted parameters are:

 Hi reduced to: 1155 ch

 SHIFT = -2.279527     ch;   -1.250769E-10 sec     S.Dev = 1.489305E-12  sec
 T1    = 4.295159      ch;   2.35674E-10   sec     S.Dev = 1.255106E-11  sec
 T2    = 18.72869      ch;   1.027637E-09  sec     S.Dev = 1.561326E-11  sec
 T3    = 61.45101      ch;   3.371798E-09  sec     S.Dev = 9.510922E-11  sec
 A     = 0.6004243                                 S.Dev = 0.1754699
 B1    = 0.1583738     [ 40.32 Rel.Ampl][ 0.76 Alpha] S.Dev = 1.081974E-03
 B2    = 4.748077E-02  [ 52.71 Rel.Ampl][ 0.23 Alpha] S.Dev = 2.77062E-04
 B3    = 1.91202E-03   [ 6.96 Rel.Ampl][ 0.01 Alpha] S.Dev = 3.306427E-05
 Average Life Time = 4.455218E-10  sec
 CHISQ = 0.964649            [ 371 degrees of freedom ]

  Chi-squared Probability =    67.79879 percent
  Durbin-Watson Parameter =    1.944483
  Negative residuals      =    44.59103 percent
  Residuals < 1 s.dev     =    69.12929 percent
  Residuals < 2 s.dev     =    96.30607 percent
  Residuals < 3 s.dev     =    99.73615 percent
  Residuals < 4 s.dev     =         100 percent
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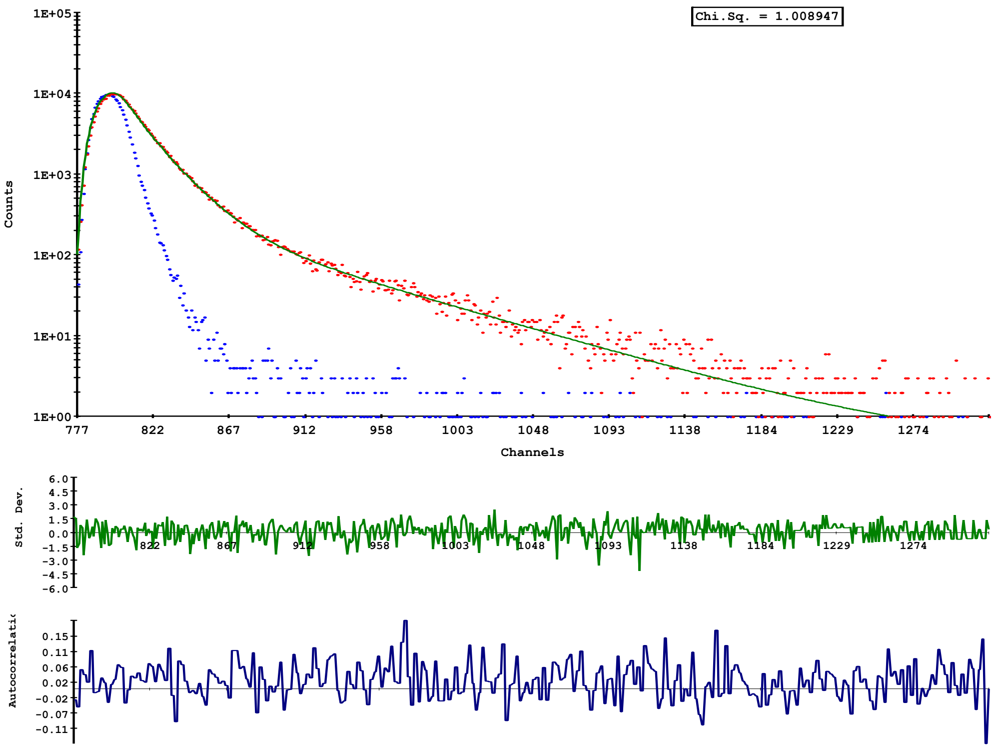
Fig. S14. Fluorescent lifetime measurement of 34 μM EGTQ in the presence of 3 equiv. of Zn^{2+} in methanol-HEPES buffer (9:1, 50 mM HEPES, 0.1 M KCl, pH = 7.5) at 370 nm at 25 °C (λ_{ex} = 331 nm).

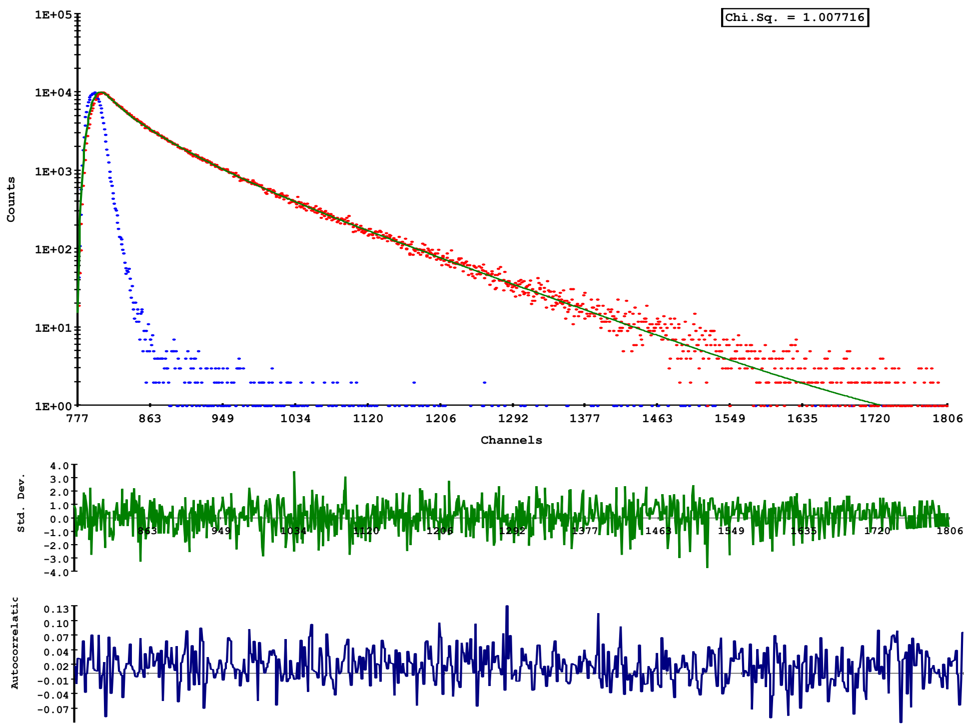
DAS6 v6.6. - HORIBA Jobin Yvon   EGTQ-Cd3eq.das; EGTQ-Cd3eq [XSQ=1.008947]   28/11/2017




```
Calculated using 3 exponentials

Prompt data : Prompt
Decay data : Decay

The initial paramters are:

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

 T1 Estimate = 7.586029 ch;          4.16243E-10    sec
 T2 Estimate = 15.17206 ch;          8.32486E-10    sec
 T3 Estimate = 30.34412 ch;          1.664972E-09   sec

 A Free
 B1 Free
 B2 Free
 B3 Free

 Prompt and decay LO = 777    ch;    4.263374E-08   sec
 Prompt and decay HI = 1359   ch;    7.45679E-08    sec

 Background on prompt = 44
 Time calibration = 5.486969E-11 sec/ch

The fitted parameters are:
   Chi-squared Probability =   43.40381 percent
 H Durbin-Watson Parameter =   2.053351
   Negative residuals      =   39.22652 percent
 S Residuals < 1 s.dev     =    67.9558 percent ev = 1.846938E-12  sec
 T Residuals < 2 s.dev     =   97.05341 percent ev = 1.748121E-11  sec
 T Residuals < 3 s.dev     =   99.63168 percent ev = 1.031822E-11  sec
 T                                             ev = 6.18669E-11   sec
 A Residuals < 4 s.dev     =   99.81584 percent ev = 9.419094E-02
 B1    = 0.1266575     [ 31.52 Rel.Ampl][ 0.67 Alpha] S.Dev = 1.130463E-03
 B2    = 6.077619E-02  [ 59.97 Rel.Ampl][ 0.32 Alpha] S.Dev = 3.14106E-04
 B3    = 2.068207E-03  [ 8.51 Rel.Ampl][ 0.01 Alpha] S.Dev = 2.423551E-05
 Average Life Time = 5.053373E-10  sec
 CHISQ = 1.008947            [ 535 degrees of freedom ]
```

Fig. S15. Fluorescent lifetime measurement of 34 μM EGTQ in the presence of 3 equiv. of Cd^{2+} in methanol-HEPES buffer (9:1, 50 mM HEPES, 0.1 M KCl, pH = 7.5) at 370 nm at 25 °C (λ_{ex} = 331 nm).

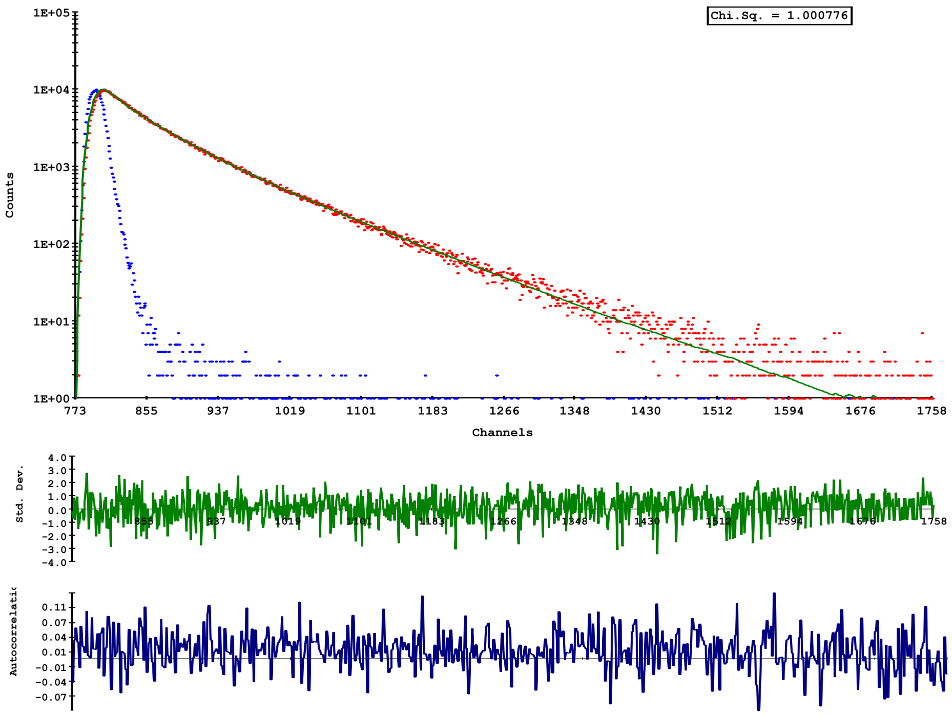
DAS6 v6.6. - HORIBA Jobin Yvon 6-MeOEGTQ-Zn3eq.das; 6-MeOEGTQ-Zn3eq [XSQ=1.007716] 28/11/2017




```
Calculated using 3 exponentials

Prompt data : Prompt
Decay data : Decay

The initial paramters are:

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

 T1 Estimate = 35.466   ch;          1.946008E-09   sec
 T2 Estimate = 70.93201 ch;          3.892017E-09   sec
 T3 Estimate = 141.864  ch;          7.784034E-09   sec

 A Free
 B1 Free
 B2 Free
 B3 Free

 Prompt and decay LO = 777    ch;    4.263374E-08   sec
 Prompt and decay HI = 1846   ch;    1.012894E-07   sec

 Background on prompt = 44
 Time calibration = 5.486969E-11 sec/ch

The fitted parameters are:

 Hi reduced to: 1806 ch

 SHIFT = -1.515205     ch;   -8.313881E-11 sec     S.Dev = 1.755233E-12   sec
 T1    = 48.7605       ch;   2.675473E-09  sec     S.Dev = 1.080716E-10   sec
 T2    = 14.46415      ch;   7.936435E-10  sec     S.Dev = 3.000368E-11   sec
 T3    = 111.7488      ch;   6.13162E-09   sec     S.Dev = 3.134438E-11   sec
 A     = 0.2916461                                 S.Dev = 7.474625E-02
 B1    = 3.381996E-02  [ 43.14 Rel.Ampl][ 0.41 Alpha] S.Dev = 2.351569E-04
 B2    = 3.403675E-02  [ 12.88 Rel.Ampl][ 0.41 Alpha] S.Dev = 4.316361E-04
 B3    = 1.504482E-02  [ 43.98 Rel.Ampl][ 0.18 Alpha] S.Dev = 6.597432E-05
 Average Life Time = 2.530069E-09  sec
 CHISQ = 1.007716            [ 1022 degrees of freedom ]

 Chi-squared Probability =     42.516 percent
 Durbin-Watson Parameter =    1.972445
 Negative residuals      =    41.16505 percent
 Residuals < 1 s.dev     =    69.51456 percent
 Residuals < 2 s.dev     =    95.04855 percent
 Residuals < 3 s.dev     =    99.51456 percent
 Residuals < 4 s.dev     =         100 percent
```

Fig. S16. Fluorescent lifetime measurement of 34 μM 6-MeOEGTQ in the presence of 3 equiv. of Zn^{2+} in methanol-HEPES buffer (9:1, 50 mM HEPES, 0.1 M KCl, pH = 7.5) at 400 nm at 25 °C (λ_{ex} = 331 nm).

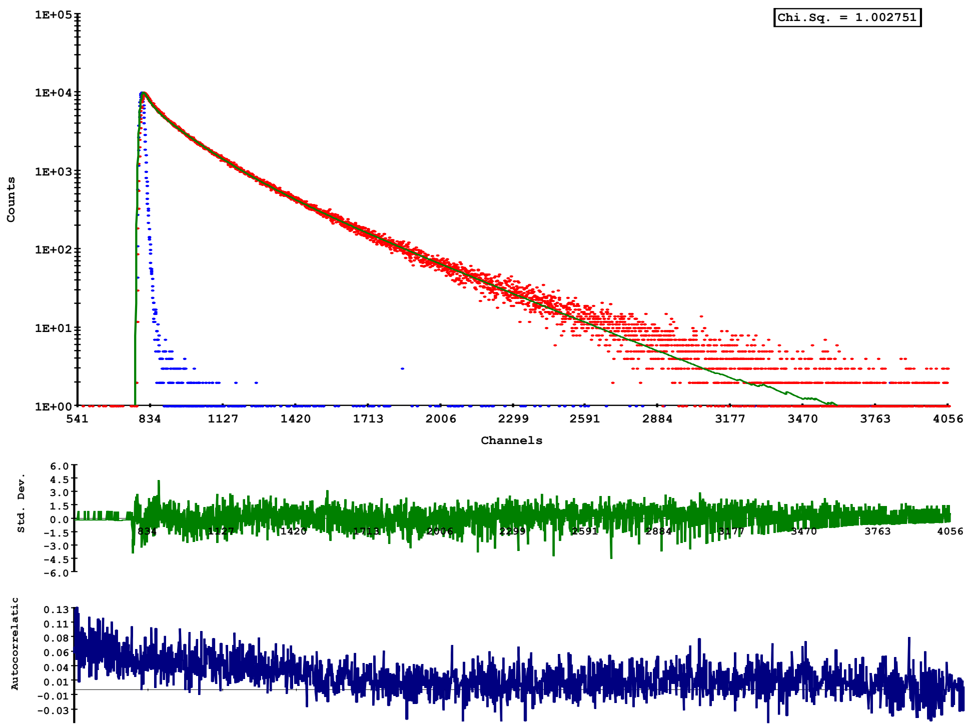
DAS6 v6.6. - HORIBA Jobin Yvon   6-MeOEGTQ-Cd3eq.das; 6-MeOEGTQ-Cd3eq [XSQ=1.000776]   28/11/2017




```
Calculated using 3 exponentials

Prompt data : Prompt
Decay data : Decay

The initial paramters are:

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

 T1 Estimate = 34.15521 ch;          1.874086E-09   sec
 T2 Estimate = 68.31042 ch;          3.748172E-09   sec
 T3 Estimate = 136.6208 ch;          7.496343E-09   sec

 A Free
 B1 Free
 B2 Free
 B3 Free

 Prompt and decay LO = 773    ch;    4.241427E-08   sec
 Prompt and decay HI = 1798   ch;    9.86557E-08    sec

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

The fitted parameters are:

 Hi reduced to: 1758 ch

 SHIFT = -1.535257     ch;   -8.423909E-11 sec     S.Dev = 1.91863E-12   sec
 T1    = 12.31128      ch;    6.755162E-10  sec     S.Dev = 8.275124E-11  sec
 T2    = 46.84394      ch;    2.570312E-09  sec     S.Dev = 5.669799E-11  sec
 T3    = 101.0398      ch;    5.544023E-09  sec     S.Dev = 2.748387E-11  sec
 A     = 0.1115768                                  S.Dev = 7.576162E-02
 B1    = 2.374297E-02  [ 7.48 Rel.Ampl][ 0.30 Alpha] S.Dev = 4.676534E-04
 B2    = 3.720786E-02  [ 44.60 Rel.Ampl][ 0.47 Alpha] S.Dev = 2.526488E-04
 B3    = 1.853837E-02  [ 47.93 Rel.Ampl][ 0.23 Alpha] S.Dev = 8.037989E-05
 Average Life Time = 2.697873E-09  sec
 CHISQ = 1.000776               [ 978 degrees of freedom ]
  Chi-squared Probability =    48.71476 percent
  Durbin-Watson Parameter =    2.095582
  Negative residuals      =    42.39351 percent
  Residuals < 1 s.dev     =    67.13996 percent
  Residuals < 2 s.dev     =    95.53753 percent
  Residuals < 3 s.dev     =    99.69574 percent
  Residuals < 4 s.dev     =         100 percent
```

Fig. S17. Fluorescent lifetime measurement of 34 μM 6-MeOEGTQ in the presence of 3 equiv. of Cd^{2+} in methanol-HEPES buffer (9:1, 50 mM HEPES, 0.1 M KCl, pH = 7.5) at 400 nm at 25 °C (λ_{ex} = 331 nm).

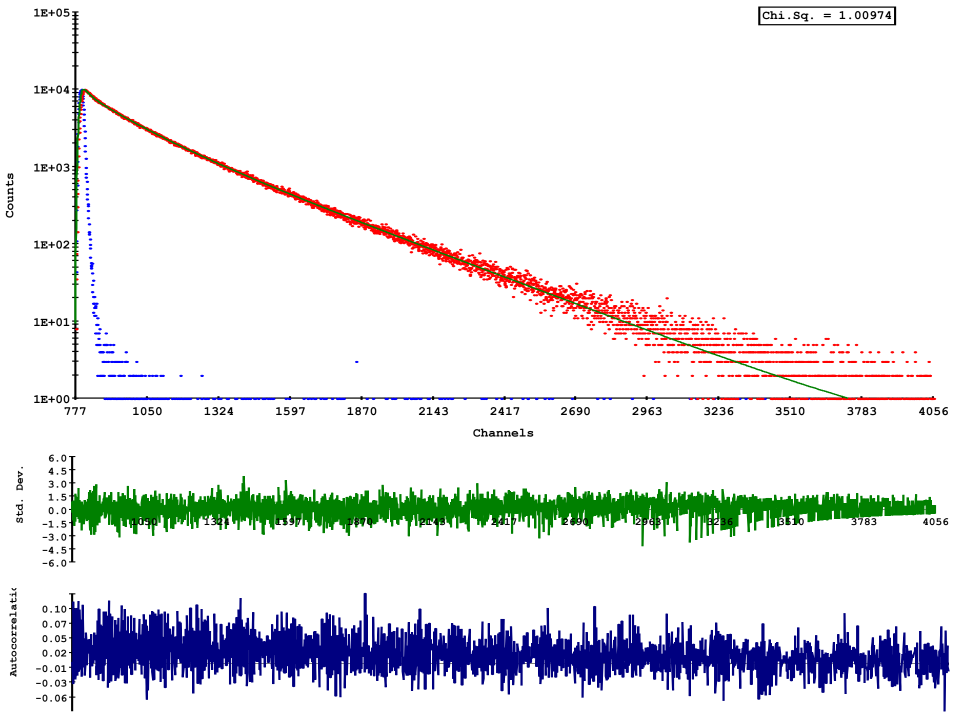
DAS6 v6.6. - HORIBA Jobin Yvon TriMeOEGTQ-Zn3eq.das; TriMeOEGTQ-Zn3eq [XSQ=1.002751] 28/11/2017




```
Calculated using 3 exponentials

Prompt data : Prompt
Decay data : Decay

The initial paramters are:

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

 T1 Estimate = 109.9688 ch;           6.033956E-09    sec
 T2 Estimate = 219.9377 ch;           1.206791E-08    sec
 T3 Estimate = 439.8754 ch;           2.413582E-08    sec

 A Free
 B1 Free
 B2 Free
 B3 Free

 Prompt and decay LO = 541     ch;    2.96845E-08     sec
 Prompt and decay HI = 4096    ch;    2.247462E-07    sec

 Background on prompt = 4.291845E-03
 Time calibration = 5.486969E-11 sec/ch

The fitted parameters are:

 Hi reduced to: 4056 ch

 SHIFT = -1.513461      ch;   -8.30431E-11  sec     S.Dev = 1.670556E-12  sec
 T1    = 141.1131       ch;   7.74283E-09   sec     S.Dev = 1.155756E-10  sec
 T2    = 25.15203       ch;   1.380084E-09  sec     S.Dev = 3.189612E-11  sec
 T3    = 336.0152       ch;   1.843705E-08  sec     S.Dev = 5.264494E-11  sec
 A     = 0.200263                                   S.Dev = 3.158575E-02
 B1    = 2.882735E-02  [ 47.64 Rel.Ampl][ 0.43 Alpha] S.Dev = 9.239081E-05
 B2    = 2.644205E-02  [ 7.79 Rel.Ampl][ 0.40 Alpha] S.Dev = 2.275948E-04
 B3    = 1.132664E-02  [ 44.57 Rel.Ampl][ 0.17 Alpha] S.Dev = 2.955703E-05
 Average Life Time = 7.035364E-09   sec
 CHISQ = 1.002751             [ 3508 degrees of freedom ]
 Chi-squared Probability =    45.1028 percent
 Durbin-Watson Parameter =   1.883291
 Negative residuals      =   45.05119 percent
 Residuals < 1 s.dev     =   69.14107 percent
 Residuals < 2 s.dev     =    95.6769 percent
 Residuals < 3 s.dev     =   99.54494 percent
 Residuals < 4 s.dev     =   99.91467 percent
```

Fig. S18. Fluorescent lifetime measurement of 34 μM TriMeOEGTQ in the presence of 3 equiv. of Zn^{2+} in methanol-HEPES buffer (9:1, 50 mM HEPES, 0.1 M KCl, pH = 7.5) at 460 nm at 25 °C (λ_{ex} = 331 nm).

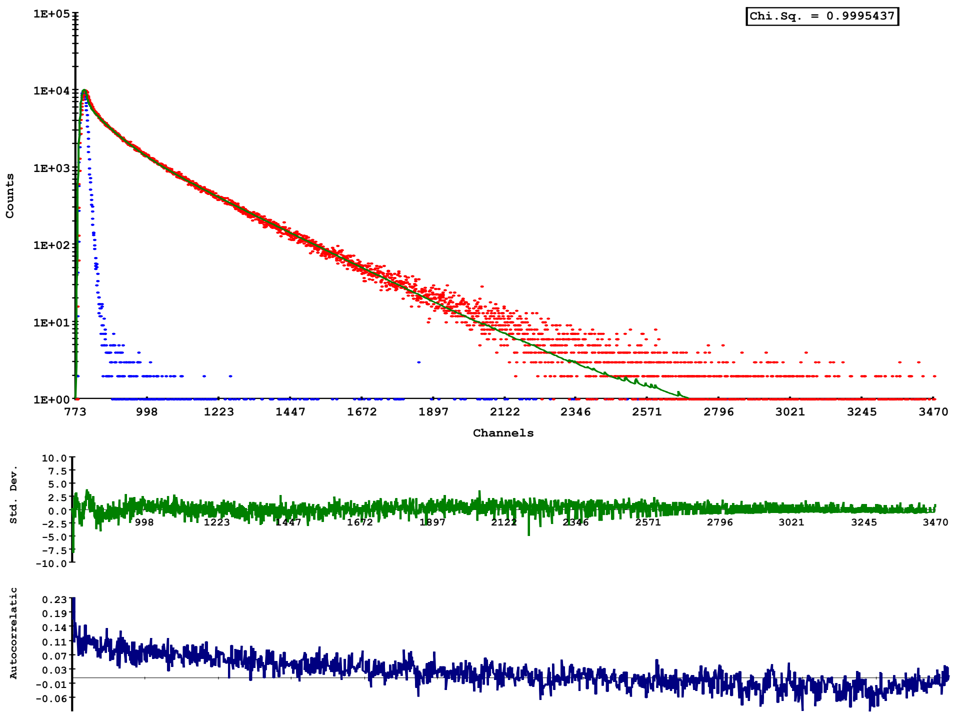
DAS6 v6.6. - HORIBA Jobin Yvon TriMeOEGTQ-Cd3eq.das; TriMeOEGTQ-Cd3eq [XSQ=1.00974] 28/11/2017




```
Calculated using 3 exponentials

Prompt data : Prompt
Decay data : Decay

The initial paramters are:

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

 T1 Estimate = 134.0705 ch;         7.356406E-09   sec
 T2 Estimate = 268.141  ch;         1.471281E-08   sec
 T3 Estimate = 536.282  ch;         2.942562E-08   sec

 A Free
 B1 Free
 B2 Free
 B3 Free

 Prompt and decay LO = 777    ch;   4.263374E-08   sec
 Prompt and decay HI = 4096   ch;   2.247462E-07   sec

 Background on prompt = 44
 Time calibration = 5.486969E-11 sec/ch

The fitted parameters are:

 Hi reduced to: 4056 ch

 SHIFT = -1.341346     ch;   -7.359924E-11 sec     S.Dev = 1.719459E-12  sec
 T1    = 157.6339      ch;    8.649319E-09  sec     S.Dev = 1.553869E-10  sec
 T2    = 25.02599      ch;    1.373168E-09  sec     S.Dev = 5.579243E-11  sec
 T3    = 340.4107      ch;    1.867823E-08  sec     S.Dev = 4.057563E-11  sec
 A     = 0.2240426                                  S.Dev = 4.043933E-02
 B1    = 0.0255833     [ 34.07 Rel.Ampl][ 0.41 Alpha] S.Dev = 1.085194E-04
 B2    = 1.535933E-02  [ 3.25 Rel.Ampl][ 0.24 Alpha] S.Dev = 2.34627E-04
 B3    = 2.179616E-02  [ 62.68 Rel.Ampl][ 0.35 Alpha] S.Dev = 4.269542E-05
 Average Life Time = 1.035217E-08  sec
  Chi-squared Probability =    34.42407 percent edom ]
  Durbin-Watson Parameter =    1.994152
  Negative residuals      =    41.82927 percent
  Residuals < 1 s.dev     =    67.92683 percent
  Residuals < 2 s.dev     =    95.79269 percent
  Residuals < 3 s.dev     =    99.51219 percent
  Residuals < 4 s.dev     =    99.96951 percent
```

Fig. S19. Fluorescent lifetime measurement of 34 μM TriMeOEGTQ in the presence of 3 equiv. of Cd^{2+} in methanol-HEPES buffer (9:1, 50 mM HEPES, 0.1 M KCl, pH = 7.5) at 460 nm at 25 °C (λ_{ex} = 331 nm).

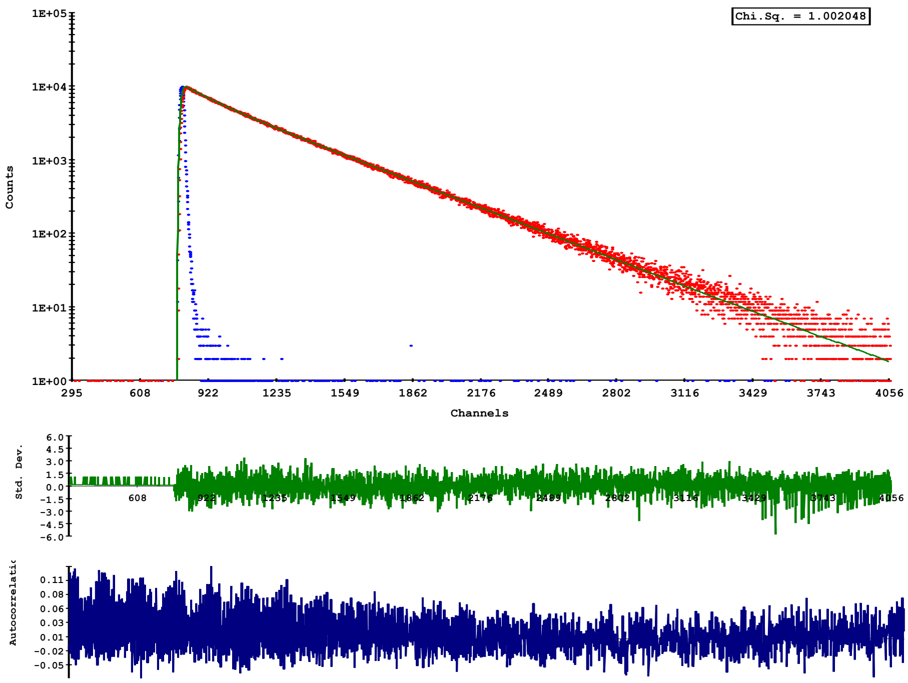
DAS6 v6.6. - HORIBA Jobin Yvon TriMeOBAPTQ-Zn3eq.das; TriMeOBAPTQ-Zn3eq [XSQ=0.9995437] 28/11/2017




```
Calculated using 3 exponentials

Prompt data : Prompt
Decay data : Decay

The initial paramters are:

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

 T1 Estimate = 71.71756 ch;        3.93512E-09    sec
 T2 Estimate = 143.4351 ch;        7.87024E-09    sec
 T3 Estimate = 286.8702 ch;        1.574048E-08   sec

 A Free
 B1 Free
 B2 Free
 B3 Free

 Prompt and decay LO = 773    ch;   4.241427E-08   sec
 Prompt and decay HI = 3510   ch;   1.925926E-07   sec

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

The fitted parameters are:

 Hi reduced to: 3470 ch

 SHIFT = -0.9710709    ch;   -5.328235E-11 sec     S.Dev = 1.371561E-12  sec
 T1    = 67.90377      ch;   3.725858E-09  sec     S.Dev = 5.769091E-11  sec
 T2    = 215.0958      ch;   1.180224E-08  sec     S.Dev = 2.830314E-11  sec
 T3    = 4.178766      ch;   2.292876E-10  sec     S.Dev = 6.037716E-12  sec
 A     = 0.4475275                                 S.Dev = 3.266365E-02
 B1    = 2.263113E-02  [ 29.04 Rel.Ampl][ 0.12 Alpha] S.Dev = 1.097853E-04
 B2    = 1.437266E-02  [ 58.41 Rel.Ampl][ 0.07 Alpha] S.Dev = 3.151938E-05
 B3    = 0.1589292     [ 12.55 Rel.Ampl][ 0.81 Alpha] S.Dev = 8.637102E-04
 Average Life Time = 1.48209E-09   sec
 CHISQ = 0.9995437           [ 2690 degrees of freedom ]
  Chi-squared Probability =      50.305 percent
  Durbin-Watson Parameter =    1.666534
  Negative residuals      =     42.6983 percent
  Residuals < 1 s.dev     =    71.42328 percent
  Residuals < 2 s.dev     =     95.9229 percent
  Residuals < 3 s.dev     =    99.44403 percent
  Residuals < 4 s.dev     =    99.88881 percent
```

Fig. S20. Fluorescent lifetime measurement of 34 μM TriMeOBAPTQ in the presence of 3 equiv. of Zn^{2+} in methanol-HEPES buffer (9:1, 50 mM HEPES, 0.1 M KCl, pH = 7.5) at 460 nm at 25 °C (λ_{ex} = 331 nm).

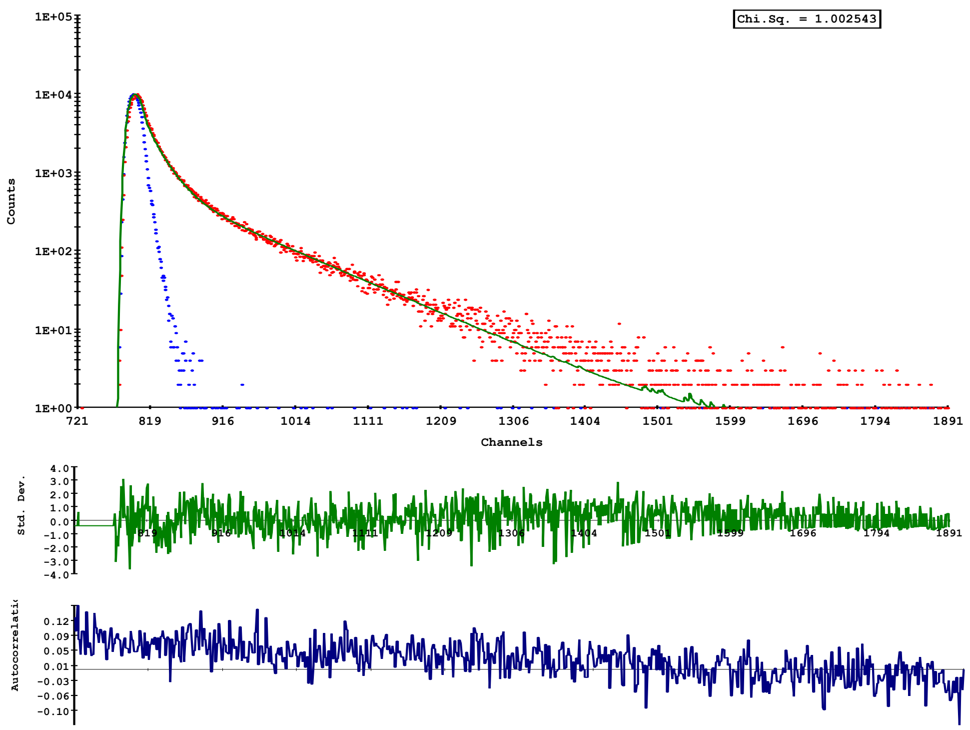
DAS6 v6.6. - HORIBA Jobin Yvon   TriMeOBAPTQ-Cd3eq.das; TriMeOBAPTQ-Cd3eq2Fitting [XSQ=1.002048]   29/11/2017




```
Calculated using 2 exponentials

Prompt data : Prompt
Decay data : Decay

The initial paramters are:

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

 T1 Estimate = 177.505  ch;         9.739646E-09  sec
 T2 Estimate = 710.0201 ch;         3.895858E-08  sec

 A Free
 B1 Free
 B2 Free

 Prompt and decay LO = 295    ch;   1.618656E-08  sec
 Prompt and decay HI = 4096   ch;   2.247462E-07  sec

 Background on prompt = 4.175365E-03
 Time calibration = 5.486969E-11 sec/ch

The fitted parameters are:

 Hi reduced to: 4056 ch

 SHIFT = 1.085647      ch;   5.956912E-11  sec     S.Dev = 1.690789E-12  sec
 T1    = 131.0415      ch;   7.190204E-09  sec     S.Dev = 1.43216E-10   sec
 T2    = 381.0735      ch;   2.090939E-08  sec     S.Dev = 2.059914E-11  sec
 A     = -0.1317284                                S.Dev = 3.733724E-02
 B1    = 1.255781E-02  [ 9.55 Rel.Ampl][ 0.23 Alpha] S.Dev = 9.513563E-05
 B2    = 4.091037E-02  [ 90.45 Rel.Ampl][ 0.77 Alpha] S.Dev = 3.930576E-05
 Average Life Time = 1.768723E-08  sec
 CHISQ = 1.002048               [ 3756 degrees of freedom ]

 Chi-squared Probability =   46.16037 percent
 Durbin-Watson Parameter =    2.03966
 Negative residuals      =     38.437 percent
 Residuals < 1 s.dev     =   69.08559 percent

 Residuals < 2 s.dev     =   95.16215 percent
 Residuals < 3 s.dev     =   99.52153 percent
 Residuals < 4 s.dev     =   99.84051 percent
```

Fig. S21. Fluorescent lifetime measurement of 34 μM TriMeOBAPTQ in the presence of 3 equiv. of Cd^{2+} in methanol-HEPES buffer (9:1, 50 mM HEPES, 0.1 M KCl, pH = 7.5) at 460 nm at 25 °C (λ_{ex} = 331 nm).

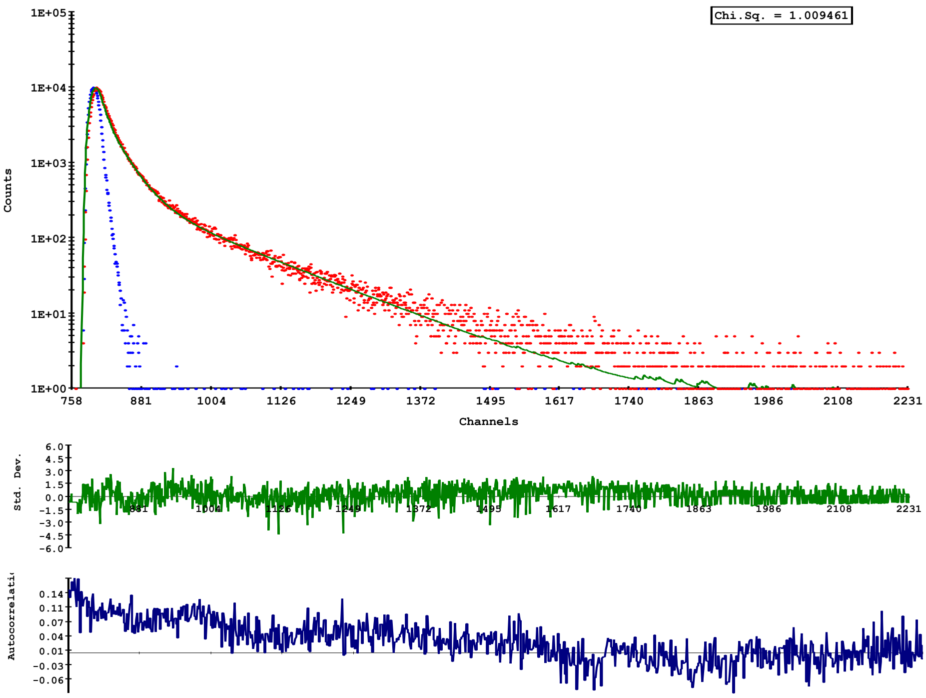
DAS6 v6.6. - HORIBA Jobin Yvon TQTACN-Zn(400).das; TQTACN-Zn [XSQ=1.002543] 13/11/2018




```
Calculated using 3 exponentials

Prompt data : Prompt
Decay data : Decay

The initial paramters are:

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

 T1 Estimate = 17.08746 ch;            9.375838E-10   sec
 T2 Estimate = 34.17493 ch;            1.875168E-09   sec
 T3 Estimate = 68.34985 ch;            3.750335E-09   sec

 A Free
 B1 Free
 B2 Free
 B3 Free

 Prompt and decay LO = 721    ch;      3.956104E-08   sec
 Prompt and decay HI = 1931   ch;      1.059534E-07   sec

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

The fitted parameters are:

 Hi reduced to: 1891 ch

 SHIFT = -0.6023685    ch;   -3.305177E-11 sec     S.Dev = 1.543106E-12  sec
 T1    = 21.45963      ch;    1.177483E-09  sec     S.Dev = 2.105889E-11  sec
 T2    = 2.673482      ch;    1.466931E-10  sec     S.Dev = 7.561361E-12  sec
 T3    = 106.3772      ch;    5.836883E-09  sec     S.Dev = 3.693903E-11  sec
 A     = 0.3993898                                 S.Dev = 4.788223E-02
 B1    = 0.033521      [ 37.34 Rel.Ampl][ 0.10 Alpha] S.Dev = 1.980716E-04
 B2    = 0.3015539     [ 41.84 Rel.Ampl][ 0.89 Alpha] S.Dev = 1.562831E-03
 B3    = 3.771347E-03  [ 20.82 Rel.Ampl][ 0.01 Alpha] S.Dev = 2.072202E-05
 Average Life Time = 3.119976E-10   sec
 CHISQ = 1.002543              [ 1163 degrees of freedom ]
 Chi-squared Probability =    47.00817 percent
 Durbin-Watson Parameter =    1.745352
 Negative residuals      =     44.1503 percent
 Residuals < 1 s.dev     =    70.70879 percent
 Residuals < 2 s.dev     =    95.13236 percent
 Residuals < 3 s.dev     =    99.40222 percent
 Residuals < 4 s.dev     =         100 percent
```

Fig. S22. Fluorescent lifetime measurement of 34 μM TQTACN in the presence of 2 equiv. of Zn^{2+} in methanol-HEPES buffer (9:1, 50 mM HEPES, 0.1 M KCl, pH = 7.5) at 400 nm at 25 °C (λ_{ex} = 331 nm).

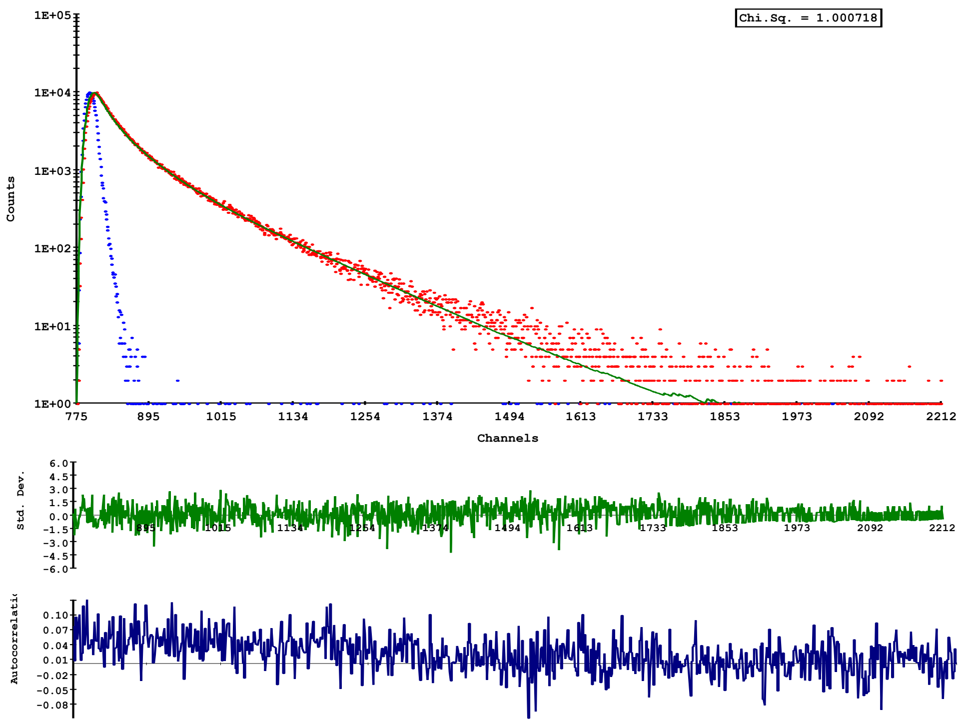
DAS6 v6.6. - HORIBA Jobin Yvon   TQTACN-Cd(430).das; TQTACN-Cd [XSQ=1.009461]   13/11/2018




```
Calculated using 3 exponentials

Prompt data : Prompt
Decay data : Decay

The initial paramters are:

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

 T1 Estimate = 21.06766 ch;           1.155976E-09   sec
 T2 Estimate = 42.13531 ch;           2.311952E-09   sec
 T3 Estimate = 84.27063 ch;           4.623903E-09   sec

 A Free
 B1 Free
 B2 Free
 B3 Free

 Prompt and decay LO = 758    ch;     4.159122E-08   sec
 Prompt and decay HI = 2271   ch;     1.246091E-07   sec

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

The fitted parameters are:

 Hi reduced to: 2231 ch

 SHIFT = -1.186267     ch;    -6.509011E-11 sec      S.Dev = 1.415209E-12  sec
 T1    = 29.80781      ch;    1.635545E-09  sec      S.Dev = 3.155645E-11  sec
 T2    = 7.228899      ch;    3.966474E-10  sec      S.Dev = 7.705444E-12  sec
 T3    = 144.596       ch;    7.933936E-09  sec      S.Dev = 6.252031E-11  sec
 A     = 0.6769493                                   S.Dev = 4.491195E-02
 B1    = 0.032822       [ 47.49 Rel.Ampl][ 0.24 Alpha] S.Dev = 1.641378E-04
 B2    = 0.1044377      [ 36.64 Rel.Ampl][ 0.75 Alpha] S.Dev = 5.99373E-04
 B3    = 2.261286E-03   [ 15.87 Rel.Ampl][ 0.02 Alpha] S.Dev = 1.444804E-05
 Average Life Time = 8.10256E-10    sec
 CHISQ = 1.009461              [ 1466 degrees of freedom ]

  Chi-squared Probability =   39.44881 percent
  Durbin-Watson Parameter =   1.712493
  Negative residuals      =   39.75577 percent
  Residuals < 1 s.dev     =   68.65672 percent
  Residuals < 2 s.dev     =   96.94708 percent
  Residuals < 3 s.dev     =    99.5251 percent
  Residuals < 4 s.dev     =   99.86431 percent
```

Fig. S23. Fluorescent lifetime measurement of 34 μM TQTACN in the presence of 2 equiv. of Cd^{2+} in methanol-HEPES buffer (9:1, 50 mM HEPES, 0.1 M KCl, pH = 7.5) at 430 nm at 25 °C (λ_{ex} = 331 nm).

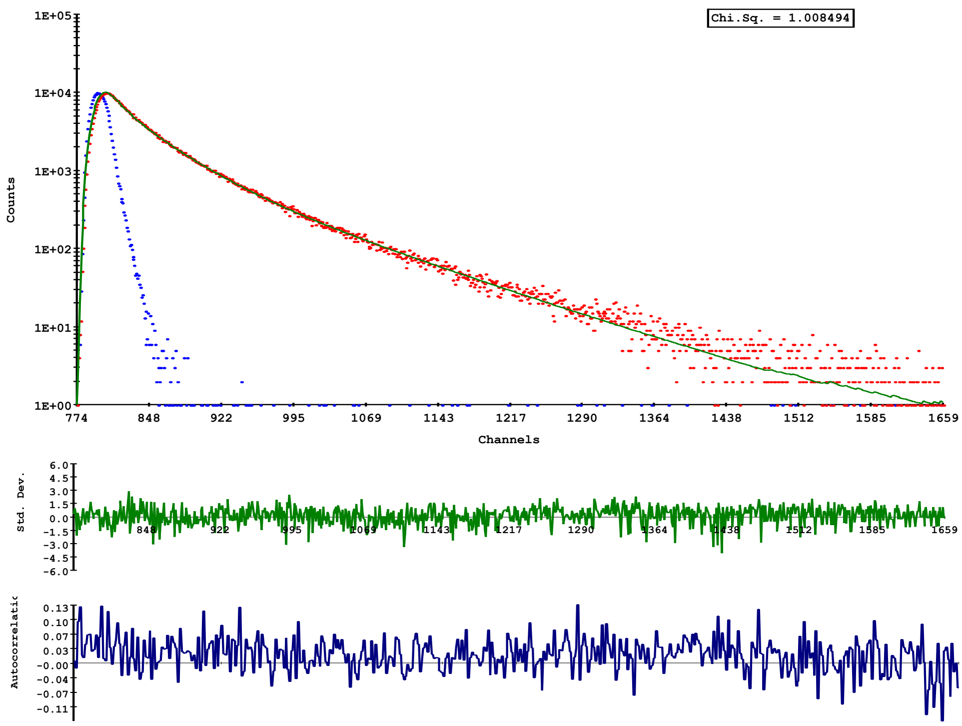
DAS6 v6.6. - HORIBA Jobin Yvon   6-MeOTQTACN-Zn(430).das; 6-MeOTQTACN-Zn [XSQ=1.000718]   13/11/2018




```
Calculated using 3 exponentials

Prompt data : Prompt
Decay data : Decay

The initial paramters are:

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

 T1 Estimate = 32.99875 ch;          1.810631E-09   sec
 T2 Estimate = 65.9975  ch;          3.621262E-09   sec
 T3 Estimate = 131.995  ch;          7.242524E-09   sec

 A Free
 B1 Free
 B2 Free
 B3 Free

 Prompt and decay LO = 775    ch;    4.252401E-08   sec
 Prompt and decay HI = 2252   ch;    1.235665E-07   sec

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

The fitted parameters are:

 Hi reduced to: 2212 ch

 SHIFT = -0.9908015    ch;   -5.436497E-11 sec      S.Dev = 1.511775E-12  sec
 T1    = 46.5347       ch;   2.553344E-09  sec      S.Dev = 1.03436E-10   sec
 T2    = 15.67823      ch;   8.602596E-10  sec      S.Dev = 1.686203E-11  sec
 T3    = 125.3808      ch;   6.879606E-09  sec      S.Dev = 3.646886E-11  sec
 A     = 0.3617765                                  S.Dev = 0.0455973
 B1    = 2.860537E-02  [ 42.03 Rel.Ampl][ 0.33 Alpha] S.Dev = 2.005311E-04
 B2    = 4.895177E-02  [ 24.23 Rel.Ampl][ 0.57 Alpha] S.Dev = 3.972751E-04
 B3    = 8.52488E-03   [ 33.74 Rel.Ampl][ 0.10 Alpha] S.Dev = 4.077398E-05
 Average Life Time = 2.018986E-09  sec
 CHISQ = 1.000718               [ 1430 degrees of freedom ]

 Chi-squared Probability =   48.73662 percent
 Durbin-Watson Parameter =   1.857808
 Negative residuals      =    43.0459 percent
 Residuals < 1 s.dev     =   69.19332 percent
 Residuals < 2 s.dev     =   96.17525 percent
 Residuals < 3 s.dev     =    99.6523 percent
 Residuals < 4 s.dev     =   99.93046 percent
```

Fig. S24. Fluorescent lifetime measurement of 34 μM 6-MeOTQTACN in the presence of 2 equiv. of Zn^{2+} in methanol-HEPES buffer (9:1, 50 mM HEPES, 0.1 M KCl, pH = 7.5) at 430 nm at 25 °C (λ_{ex} = 331 nm).

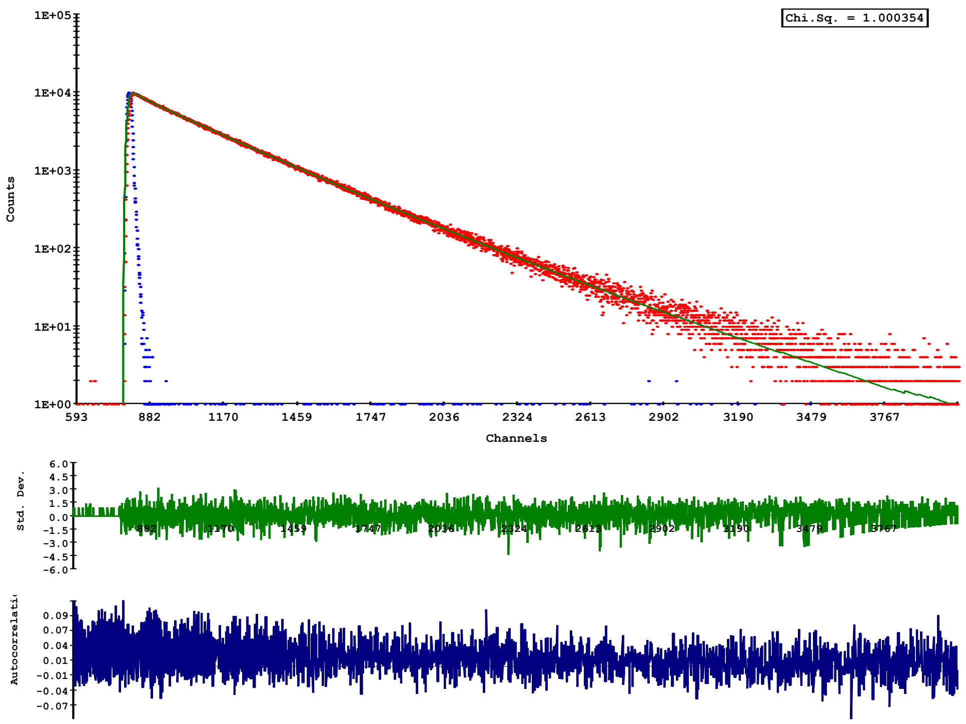
DAS6 v6.6. - HORIBA Jobin Yvon 6-MeOTQTACN-Cd(400).das; 6-MeOTQTACN-Cd [XSQ=1.008494] 13/11/2018




```
Calculated using 3 exponentials

Prompt data : Prompt
Decay data : Decay

The initial paramters are:

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

 T1 Estimate = 25.93744 ch;          1.423179E-09   sec
 T2 Estimate = 51.87488 ch;          2.846358E-09   sec
 T3 Estimate = 103.7498 ch;          5.692717E-09   sec

 A Free
 B1 Free
 B2 Free
 B3 Free

 Prompt and decay LO = 774    ch;    4.246914E-08   sec
 Prompt and decay HI = 1699   ch;    9.32236E-08    sec

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

The fitted parameters are:

 Hi reduced to: 1659 ch

 SHIFT = -1.406008     ch;   -7.714724E-11 sec     S.Dev = 1.693751E-12  sec
 T1    = 11.04103      ch;   6.058176E-10  sec     S.Dev = 3.549986E-11  sec
 T2    = 40.80308      ch;   2.238852E-09  sec     S.Dev = 3.357549E-11  sec
 T3    = 103.8871      ch;   5.700252E-09  sec     S.Dev = 4.176666E-11  sec
 A     = 0.4336076                                 S.Dev = 0.0861363
 B1    = 4.649272E-02  [ 17.12 Rel.Ampl][ 0.49 Alpha] S.Dev = 4.796895E-04
 B2    = 4.038089E-02  [ 54.96 Rel.Ampl][ 0.43 Alpha] S.Dev = 2.100912E-04
 B3    = 8.056391E-03  [ 27.92 Rel.Ampl][ 0.08 Alpha] S.Dev = 4.795345E-05
 Average Life Time = 1.732818E-09  sec
 CHISQ = 1.008494              [ 878 degrees of freedom ]

 Chi-squared Probability =   42.33385 percent
 Durbin-Watson Parameter =   1.989746
 Negative residuals      =   40.97065 percent
 Residuals < 1 s.dev     =   69.75169 percent
 Residuals < 2 s.dev     =   95.82393 percent
 Residuals < 3 s.dev     =    99.3228 percent
 Residuals < 4 s.dev     =   99.88713 percent
```

Fig. S25. Fluorescent lifetime measurement of 34 μM 6-MeOTQTACN in the presence of 2 equiv. of Cd^{2+} in methanol-HEPES buffer (9:1, 50 mM HEPES, 0.1 M KCl, pH = 7.5) at 400 nm at 25 °C (λ_{ex} = 331 nm).

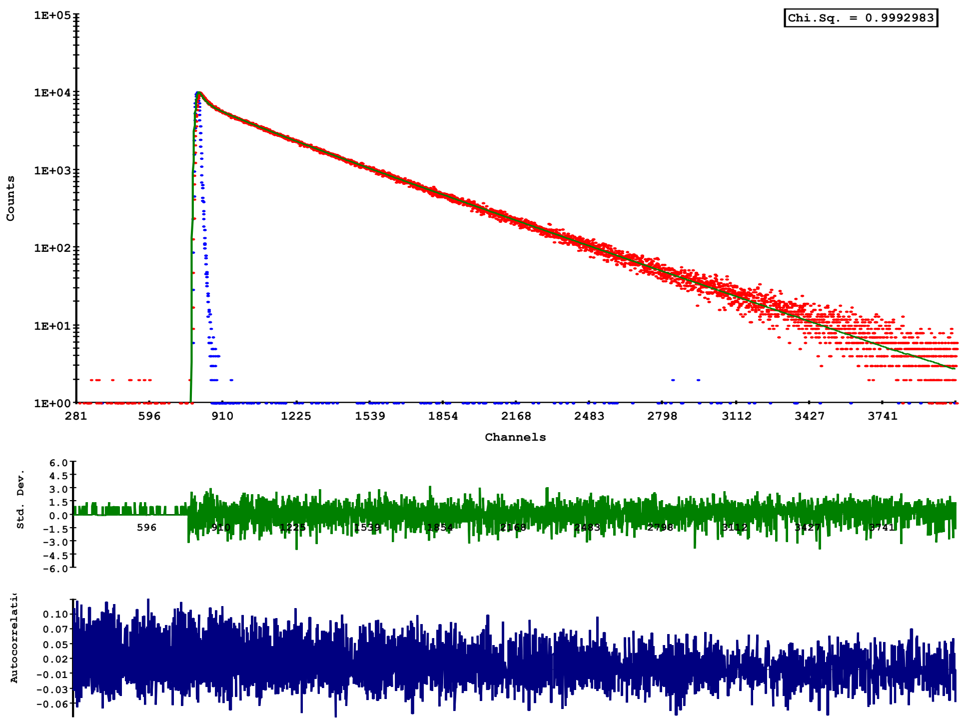
DAS6 v6.6. - HORIBA Jobin Yvon   TriMeOTQTACN-Zn(490).das; TriMeOTQTACN-Zn [XSQ=1.000354]   13/11/2018




```
Calculated using 3 exponentials

Prompt data : Prompt
Decay data : Decay

The initial paramters are:

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

 T1 Estimate = 148.943   ch;          8.172456E-09    sec
 T2 Estimate = 297.886   ch;          1.634491E-08    sec
 T3 Estimate = 595.7721  ch;          3.268983E-08    sec

 A Free
 B1 Free
 B2 Free
 B3 Free

 Prompt and decay LO = 593    ch;     3.253772E-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 = -1.606446     ch;   -8.814519E-11 sec      S.Dev = 1.868659E-12  sec
 T1    = 33.47426      ch;   1.836722E-09  sec      S.Dev = 2.101768E-10  sec
 T2    = 262.092       ch;   1.43809E-08   sec      S.Dev = 2.093338E-10  sec
 T3    = 389.0543      ch;   2.134728E-08  sec      S.Dev = 1.200582E-10  sec
 A     = 7.716215E-02                               S.Dev = 4.246895E-02
 B1    = 5.068578E-03  [ 1.14 Rel.Ampl][ 0.09 Alpha] S.Dev = 1.818532E-04
 B2    = 3.668423E-02  [ 64.56 Rel.Ampl][ 0.67 Alpha] S.Dev = 1.115349E-04
 B3    = 1.313167E-02  [ 34.30 Rel.Ampl][ 0.24 Alpha] S.Dev = 6.582256E-05
 Average Life Time = 1.488923E-08  sec
 CHISQ = 1.000354             [ 3456 degrees of freedom ]

  Chi-squared Probability =   49.09356 percent
  Durbin-Watson Parameter =   2.028572
  Negative residuals      =   44.97691 percent
  Residuals < 1 s.dev     =   67.20554 percent
  Residuals < 2 s.dev     =   95.95843 percent
  Residuals < 3 s.dev     =   99.62471 percent
  Residuals < 4 s.dev     =   99.94226 percent
```

Fig. S26. Fluorescent lifetime measurement of 34 μM TriMeOTQTACN in the presence of 1 equiv. of Zn^{2+} in methanol-HEPES buffer (9:1, 50 mM HEPES, 0.1 M KCl, pH = 7.5) at 490 nm at 25 °C (λ_{ex} = 331 nm).

DAS6 v6.6. - HORIBA Jobin Yvon   TriMeOTQTACN-Cd(490).das; TriMeOTQTACN-Cd [XSQ=0.9992983]   13/11/2018




```
Calculated using 3 exponentials

Prompt data : Prompt
Decay data : Decay

The initial paramters are:

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

 T1 Estimate = 185.0465 ch;          1.015344E-08   sec
 T2 Estimate = 370.093  ch;          2.030689E-08   sec
 T3 Estimate = 740.186  ch;          4.061377E-08   sec

 A Free
 B1 Free
 B2 Free
 B3 Free

 Prompt and decay LO = 281    ch;    1.541838E-08   sec
 Prompt and decay HI = 4096   ch;    2.247462E-07   sec

 Background on prompt = 2.024292E-03
 Time calibration = 5.486969E-11 sec/ch

The fitted parameters are:

 Hi reduced to: 4056 ch

 SHIFT = -2.160237     ch;    -1.185315E-10 sec     S.Dev = 1.586205E-12  sec
 T1    = 201.0937      ch;    1.103395E-08  sec     S.Dev = 4.531502E-10  sec
 T2    = 416.4765      ch;    2.285193E-08  sec     S.Dev = 3.739936E-11  sec
 T3    = 22.18578      ch;    1.217327E-09  sec     S.Dev = 2.362652E-11  sec
 A     = 8.421974E-02                               S.Dev = 3.938364E-02
 B1    = 8.697198E-03  [ 12.05 Rel.Ampl][ 0.13 Alpha] S.Dev = 9.170287E-05
 B2    = 2.913807E-02  [ 83.58 Rel.Ampl][ 0.44 Alpha] S.Dev = 4.240498E-05
 B3    = 2.864082E-02  [ 4.38 Rel.Ampl][ 0.43 Alpha] S.Dev = 2.284693E-04
 Average Life Time = 1.198462E-08  sec
 CHISQ = 0.9992983             [ 3768 degrees of freedom ]

  Chi-squared Probability =    50.9089 percent
  Durbin-Watson Parameter =   2.066888
  Negative residuals      =   48.99364 percent
  Residuals < 1 s.dev     =   70.23305 percent
  Residuals < 2 s.dev     =   94.86229 percent
  Residuals < 3 s.dev     =   99.44386 percent
  Residuals < 4 s.dev     =   99.97352 percent
```

Fig. S27. Fluorescent lifetime measurement of 34 μM TriMeOTQTACN in the presence of 1 equiv. of Cd^{2+} in methanol-HEPES buffer (9:1, 50 mM HEPES, 0.1 M KCl, pH = 7.5) at 490 nm at 25 °C (λ_{ex} = 331 nm).

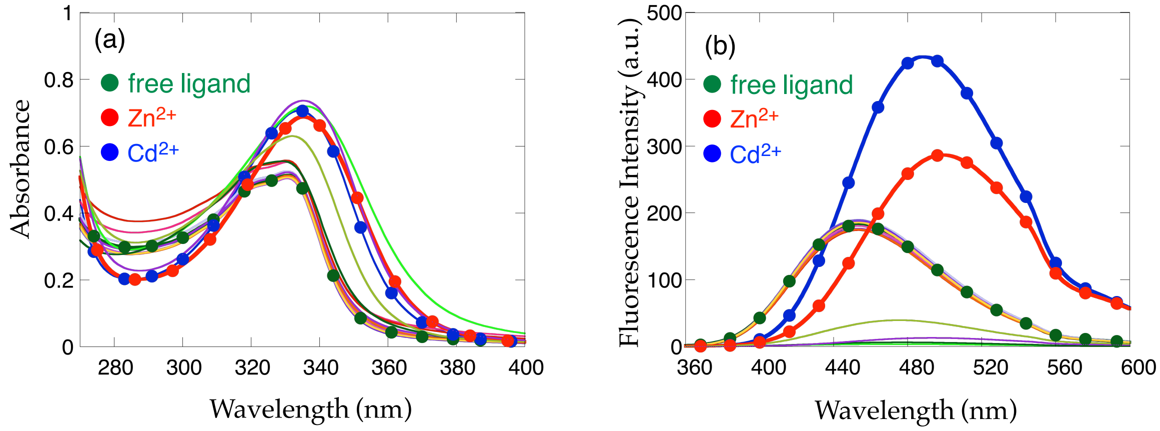
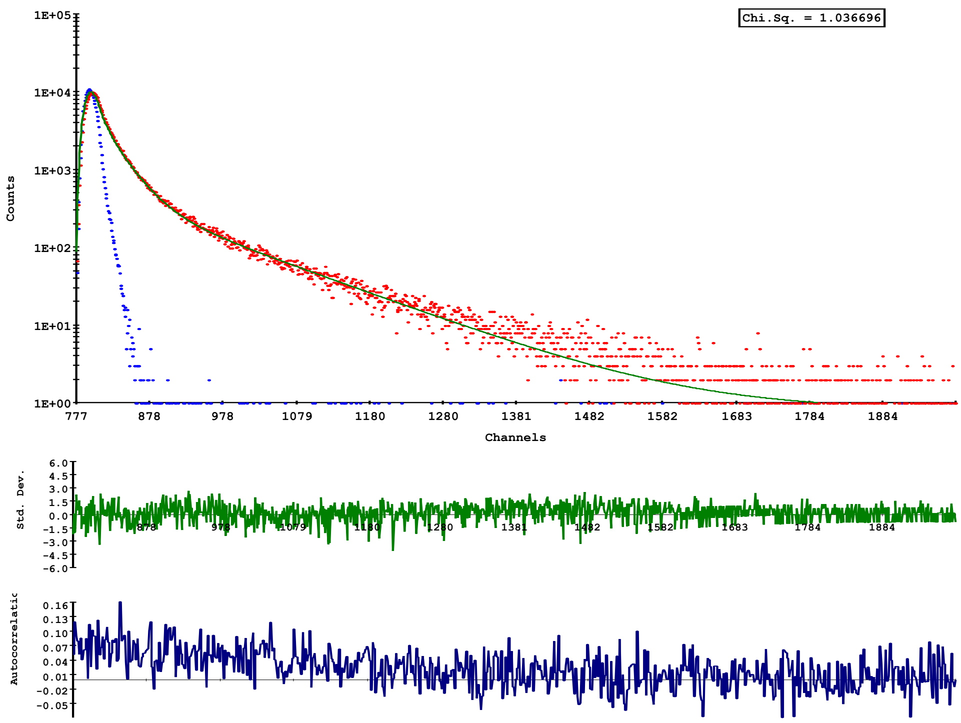


Fig. S28. (a) UV-vis absorption and (b) fluorescence spectra of 34 μM TriMeOTQTACN in DMF-H_2O (1:1) at 25 °C in the presence of 2 equiv. of various metal ions (λ_{ex} = 343 nm).

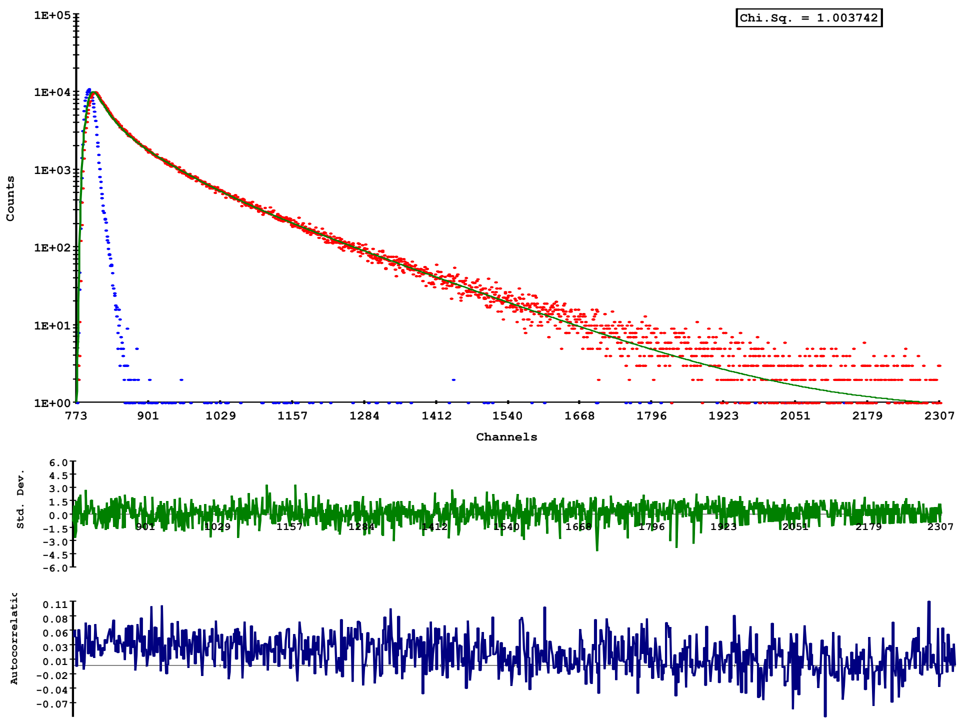
DAS6 v6.6. - HORIBA Jobin Yvon   TQTACN-Zn.das; TQTACN-Zn [XSQ=1.036696]   13/11/2018




```
Calculated using 3 exponentials

Prompt data : Prompt
Decay data : Decay

The initial paramters are:

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

 T1 Estimate = 18.46088 ch;          1.012943E-09   sec
 T2 Estimate = 36.92175 ch;          2.025885E-09   sec
 T3 Estimate = 73.84351 ch;          4.05177E-09    sec

 A Free
 B1 Free
 B2 Free
 B3 Free

 Prompt and decay LO = 777    ch;    4.263374E-08   sec
 Prompt and decay HI = 2025   ch;    1.111111E-07   sec

 Background on prompt = 48
 Time calibration = 5.486969E-11 sec/ch

The fitted parameters are:

 Hi reduced to: 1985 ch

 SHIFT = -2.18724       ch;   -1.200132E-10 sec     S.Dev = 1.426215E-12  sec
 T1    = 26.57634       ch;   1.458235E-09  sec     S.Dev = 2.352696E-11  sec
 T2    = 5.033764       ch;   2.76201E-10   sec     S.Dev = 6.762096E-12  sec
 T3    = 126.4596       ch;   6.9388E-09    sec     S.Dev = 5.450828E-11  sec
 A     = 0.8070258                                  S.Dev = 5.229276E-02
 B1    = 0.0352206      [ 47.65 Rel.Ampl][ 0.20 Alpha] S.Dev = 1.704312E-04
 B2    = 0.1381522      [ 35.40 Rel.Ampl][ 0.78 Alpha] S.Dev = 7.937829E-04
 B3    = 2.633994E-03   [ 16.96 Rel.Ampl][ 0.01 Alpha] S.Dev = 1.664899E-05
 Average Life Time = 6.124449E-10  sec
 CHISQ = 1.036696             [ 1201 degrees of freedom ]

 Chi-squared Probability =    18.36174 percent
 Durbin-Watson Parameter =    1.890074
 Negative residuals       =   39.04053 percent
 Residuals < 1 s.dev      =   67.24566 percent
 Residuals < 2 s.dev      =   95.86435 percent
 Residuals < 3 s.dev      =   99.50372 percent
 Residuals < 4 s.dev      =   99.91729 percent
```

Fig. S29. Fluorescent lifetime measurement of 34 μM TQTACN in the presence of 2 equiv. of Zn^{2+} in DMF-H_2O (1:1) at 400 nm at 25 °C (λ_{ex} = 331 nm).

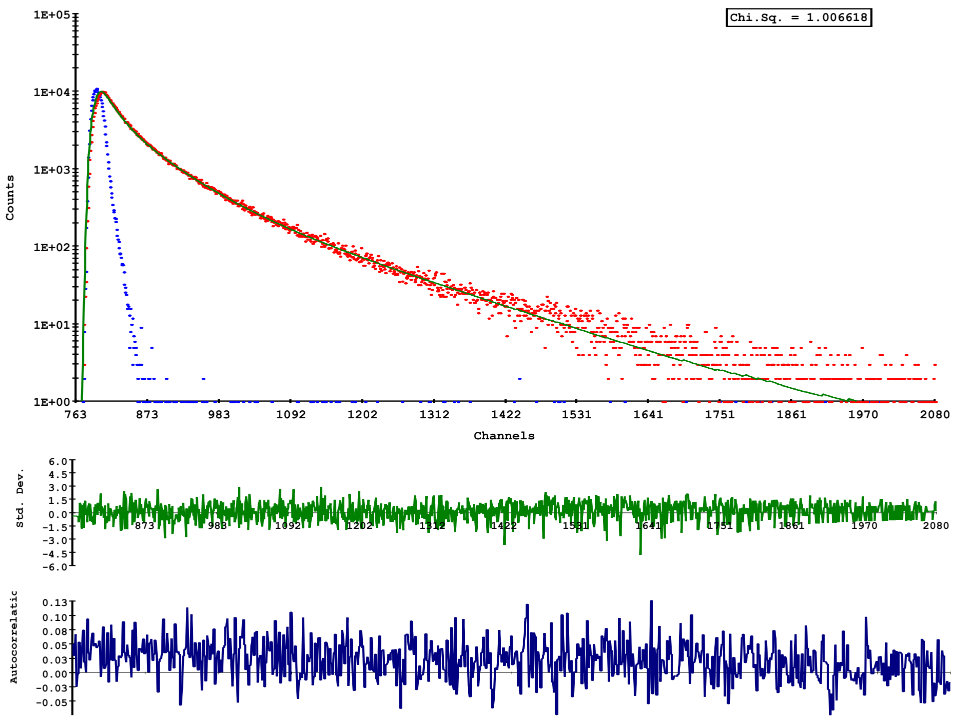
DAS6 v6.6. - HORIBA Jobin Yvon 6-MeOTQTACN-Zn.das; 6-MeOTQTACN-Zn [XSQ=1.003742] 13/11/2018




```
Calculated using 3 exponentials

Prompt data : Prompt
Decay data : Decay

The initial paramters are:

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

 T1 Estimate = 44.74927 ch;          2.455378E-09   sec
 T2 Estimate = 89.49854 ch;          4.910756E-09   sec
 T3 Estimate = 178.9971 ch;          9.821512E-09   sec

 A Free
 B1 Free
 B2 Free
 B3 Free

 Prompt and decay LO = 773    ch;    4.241427E-08   sec
 Prompt and decay HI = 2347   ch;    1.287791E-07   sec

 Background on prompt = 1
 Time calibration = 5.486969E-11 sec/ch

The fitted parameters are:

 Hi reduced to: 2307 ch

 SHIFT = -0.9687317    ch;   -5.3154E-11   sec     S.Dev = 1.541391E-12  sec
 T1    = 67.13506      ch;   3.683679E-09  sec     S.Dev = 1.307127E-10  sec
 T2    = 18.65355      ch;   1.023514E-09  sec     S.Dev = 1.473535E-11  sec
 T3    = 167.3204      ch;   9.180815E-09  sec     S.Dev = 4.925808E-11  sec
 A     = 0.7743567                                 S.Dev = 5.854542E-02
 B1    = 2.064888E-02  [ 37.89 Rel.Ampl][ 0.26 Alpha] S.Dev = 1.362912E-04
 B2    = 5.236536E-02  [ 26.70 Rel.Ampl][ 0.65 Alpha] S.Dev = 3.005992E-04
 B3    = 7.742947E-03  [ 35.41 Rel.Ampl][ 0.10 Alpha] S.Dev = 3.483262E-05
 Average Life Time = 2.485811E-09  sec
 CHISQ = 1.003742             [ 1527 degrees of freedom ]

 Chi-squared Probability =    45.4105 percent
 Durbin-Watson Parameter =   1.898707
 Negative residuals      =   42.73616 percent
 Residuals < 1 s.dev     =   65.99348 percent
 Residuals < 2 s.dev     =   96.93811 percent
 Residuals < 3 s.dev     =   99.54398 percent
 Residuals < 4 s.dev     =   99.93485 percent
```

Fig. S30. Fluorescent lifetime measurement of 34 μM 6-MeOTQTACN in the presence of 2 equiv. of Zn^{2+} in DMF-H_2O (1:1) at 430 nm at 25 °C (λ_{ex} = 331 nm).

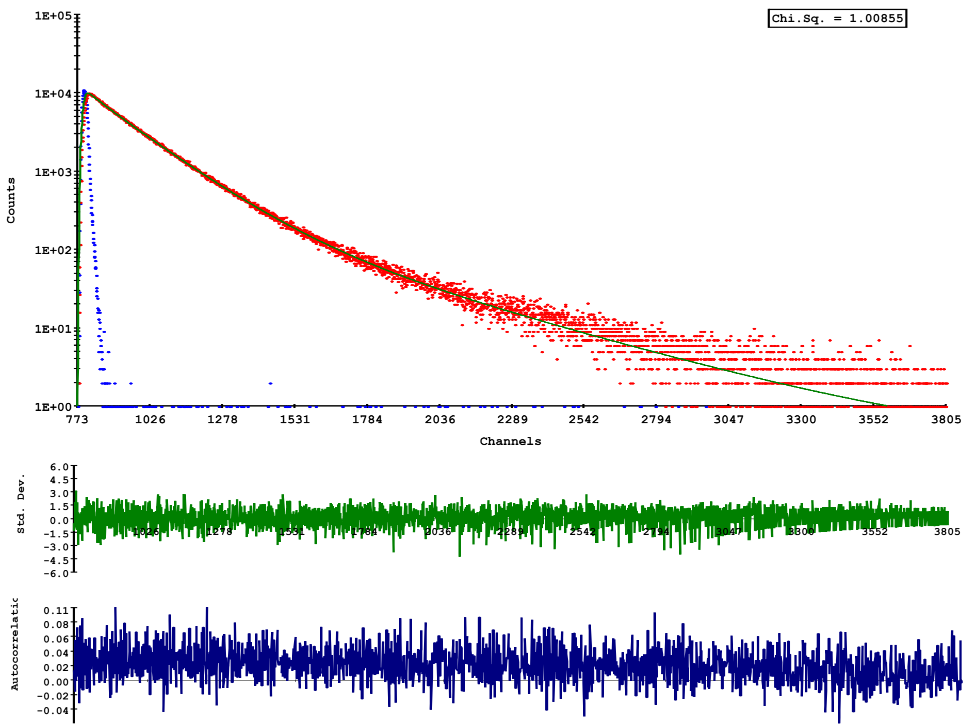
DAS6 v6.6. - HORIBA Jobin Yvon 6-MeOTQTACN-Cd.das; 6-MeOTQTACN-Cd [XSQ=1.006618] 13/11/2018




```
Calculated using 3 exponentials

Prompt data : Prompt
Decay data : Decay

The initial paramters are:

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

 T1 Estimate = 32.94073 ch;          1.807448E-09    sec
 T2 Estimate = 65.88147 ch;          3.614895E-09    sec
 T3 Estimate = 131.7629 ch;          7.229791E-09    sec

 A Free
 B1 Free
 B2 Free
 B3 Free

 Prompt and decay LO = 763    ch;    4.186557E-08    sec
 Prompt and decay HI = 2120   ch;    1.163237E-07    sec

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

The fitted parameters are:

 Hi reduced to: 2080 ch

 SHIFT = -1.83422      ch;   -1.00643E-10  sec     S.Dev = 1.643072E-12  sec
 T1    = 18.10037      ch;    9.931614E-10  sec     S.Dev = 2.803743E-11  sec
 T2    = 58.64867      ch;    3.218034E-09  sec     S.Dev = 4.649888E-11  sec
 T3    = 157.0865      ch;    8.619288E-09  sec     S.Dev = 6.918845E-11  sec
 A     = 0.3782228                                  S.Dev = 6.093455E-02
 B1    = 5.189956E-02  [ 29.89 Rel.Ampl][ 0.63 Alpha] S.Dev = 3.121735E-04
 B2    = 2.608861E-02  [ 48.68 Rel.Ampl][ 0.32 Alpha] S.Dev = 1.380178E-04
 B3    = 4.288055E-03  [ 21.43 Rel.Ampl][ 0.05 Alpha] S.Dev = 2.752335E-05
 Average Life Time = 2.096094E-09  sec
 CHISQ = 1.006618             [ 1310 degrees of freedom ]
  Chi-squared Probability =   42.77866 percent
  Durbin-Watson Parameter =   1.896776
  Negative residuals      =   39.90895 percent
  Residuals < 1 s.dev     =   67.98179 percent
  Residuals < 2 s.dev     =   96.43399 percent
  Residuals < 3 s.dev     =   99.77238 percent
  Residuals < 4 s.dev     =   99.92413 percent
```

Fig. S31. Fluorescent lifetime measurement of 34 μM 6-MeOTQTACN in the presence of 2 equiv. of Cd^{2+} in DMF-H_2O (1:1) at 430 nm at 25 °C (λ_{ex} = 331 nm).

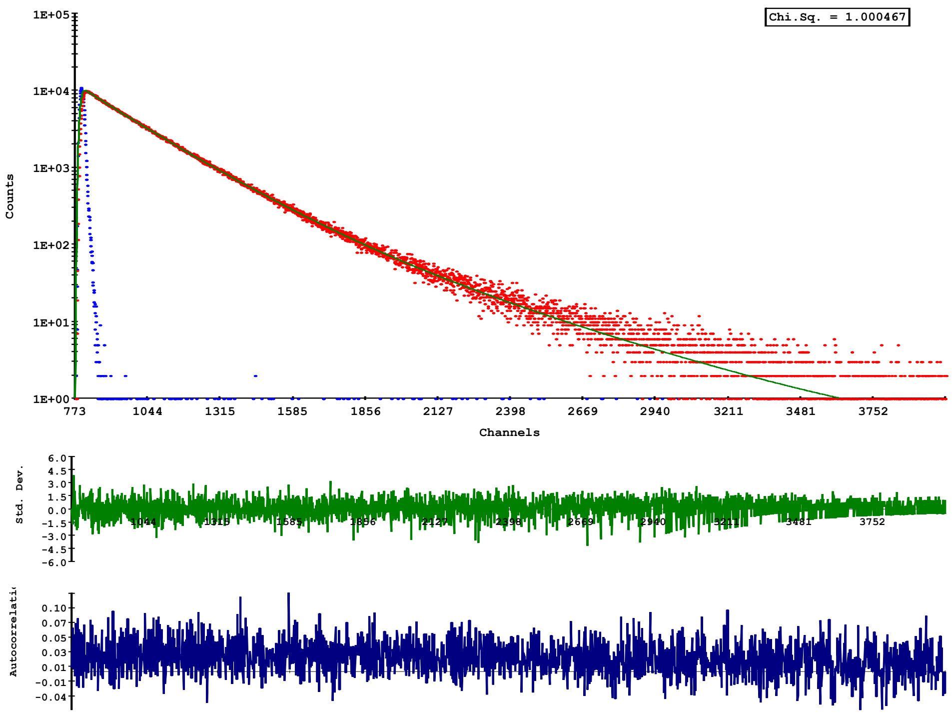
DAS6 v6.6. - HORIBA Jobin Yvon   TriMeOTQTACN-Zn.das; TriMeOTQTACN-Zn [XSQ=1.00855]   13/11/2018




```
Calculated using 3 exponentials

Prompt data : Prompt
Decay data : Decay

The initial paramters are:

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

 T1 Estimate = 93.56949 ch;          5.134128E-09   sec
 T2 Estimate = 187.139  ch;          1.026826E-08   sec
 T3 Estimate = 374.278  ch;          2.053651E-08   sec

 A Free
 B1 Free
 B2 Free
 B3 Free

 Prompt and decay LO = 773    ch;    4.241427E-08   sec
 Prompt and decay HI = 3845   ch;    2.109739E-07   sec

 Background on prompt = 1
 Time calibration = 5.486969E-11 sec/ch

The fitted parameters are:

 Hi reduced to: 3805 ch

 SHIFT = -1.365857     ch;    -7.494416E-11 sec     S.Dev = 1.647471E-12  sec
 T1    = 55.9687       ch;    3.070985E-09  sec     S.Dev = 4.330906E-10  sec
 T2    = 159.5689      ch;    8.755494E-09  sec     S.Dev = 4.140631E-11  sec
 T3    = 425.2911      ch;    2.333559E-08  sec     S.Dev = 2.041509E-10  sec
 A     = 0.3334286                                  S.Dev = 4.385593E-02
 B1    = 4.010295E-03  [ 2.48 Rel.Ampl][ 0.07 Alpha] S.Dev = 1.72742E-04
 B2    = 4.895742E-02  [ 86.36 Rel.Ampl][ 0.88 Alpha] S.Dev = 9.211167E-05
 B3    = 2.374089E-03  [ 11.16 Rel.Ampl][ 0.04 Alpha] S.Dev = 1.539178E-05
 Average Life Time = 8.969039E-09  sec
 CHISQ = 1.00855              [ 3025 degrees of freedom ]

 Chi-squared Probability =    36.6891 percent
 Durbin-Watson Parameter =   1.969958
 Negative residuals      =   40.68579 percent
 Residuals < 1 s.dev     =    67.5239 percent
 Residuals < 2 s.dev     =    95.8457 percent
 Residuals < 3 s.dev     =   99.60435 percent
 Residuals < 4 s.dev     =   99.93406 percent
```

Fig. S32. Fluorescent lifetime measurement of 34 μM TriMeOTQTACN in the presence of 2 equiv. of Zn^{2+} in DMF-H_2O (1:1) at 490 nm at 25 °C (λ_{ex} = 331 nm).

DAS6 v6.6. - HORIBA Jobin Yvon   TriMeOTQTACN-Cd.das; TriMeOTQTACN-Cd [XSQ=1.000467]   13/11/2018




```
Calculated using 3 exponentials

Prompt data : Prompt
Decay data : Decay

The initial paramters are:

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

 T1 Estimate = 109.2261 ch;           5.993204E-09   sec
 T2 Estimate = 218.4523 ch;           1.198641E-08   sec
 T3 Estimate = 436.9045 ch;           2.397281E-08   sec

 A Free
 B1 Free
 B2 Free
 B3 Free

 Prompt and decay LO = 773     ch;    4.241427E-08   sec
 Prompt and decay HI = 4063    ch;    2.229355E-07   sec

 Background on prompt = 1
 Time calibration = 5.486969E-11 sec/ch

The fitted parameters are:

 Hi reduced to: 4023 ch

 SHIFT = -1.231932     ch;    -6.759574E-11 sec     S.Dev = 1.632807E-12  sec
 T1    = 49.63755      ch;    2.723597E-09  sec     S.Dev = 4.271196E-10  sec
 T2    = 196.9528      ch;    1.080674E-08  sec     S.Dev = 5.55515E-11   sec
 T3    = 415.0886      ch;    2.277578E-08  sec     S.Dev = 2.003468E-10  sec
 A     = 0.2605065                                  S.Dev = 3.940901E-02
 B1    = 2.603263E-03  [ 1.17 Rel.Ampl][ 0.05 Alpha] S.Dev = 1.639226E-04
 B2    = 4.849254E-02  [ 86.51 Rel.Ampl][ 0.89 Alpha] S.Dev = 8.275859E-05
 B3    = 3.27789E-03   [ 12.32 Rel.Ampl][ 0.06 Alpha] S.Dev = 2.339116E-05
 Average Life Time = 1.114129E-08   sec
 CHISQ = 1.000467               [ 3243 degrees of freedom ]

 Chi-squared Probability =   48.92025 percent
 Durbin-Watson Parameter =    1.98911
 Negative residuals      =   41.31037 percent
 Residuals < 1 s.dev     =   68.93263 percent
 Residuals < 2 s.dev     =   95.69363 percent
 Residuals < 3 s.dev     =    99.5386 percent
 Residuals < 4 s.dev     =   99.96924 percent
```

Fig. S33. Fluorescent lifetime measurement of 34 μM TriMeOTQTACN in the presence of 2 equiv. of Cd^{2+} in DMF-H_2O (1:1) at 490 nm at 25 °C (λ_{ex} = 331 nm).

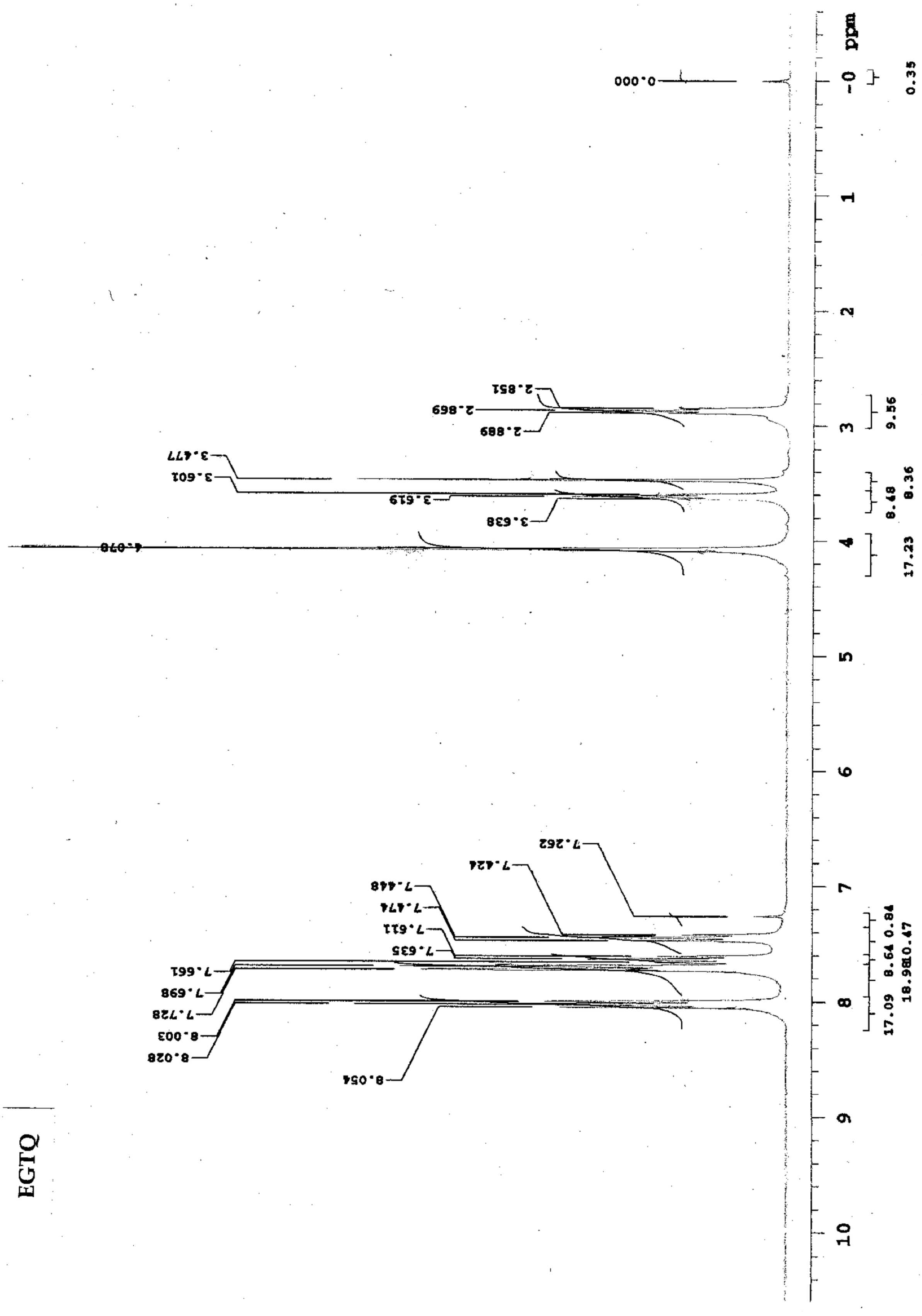


Fig. S34. [1]H NMR spectrum for EGTQ in $CDCl_3$.

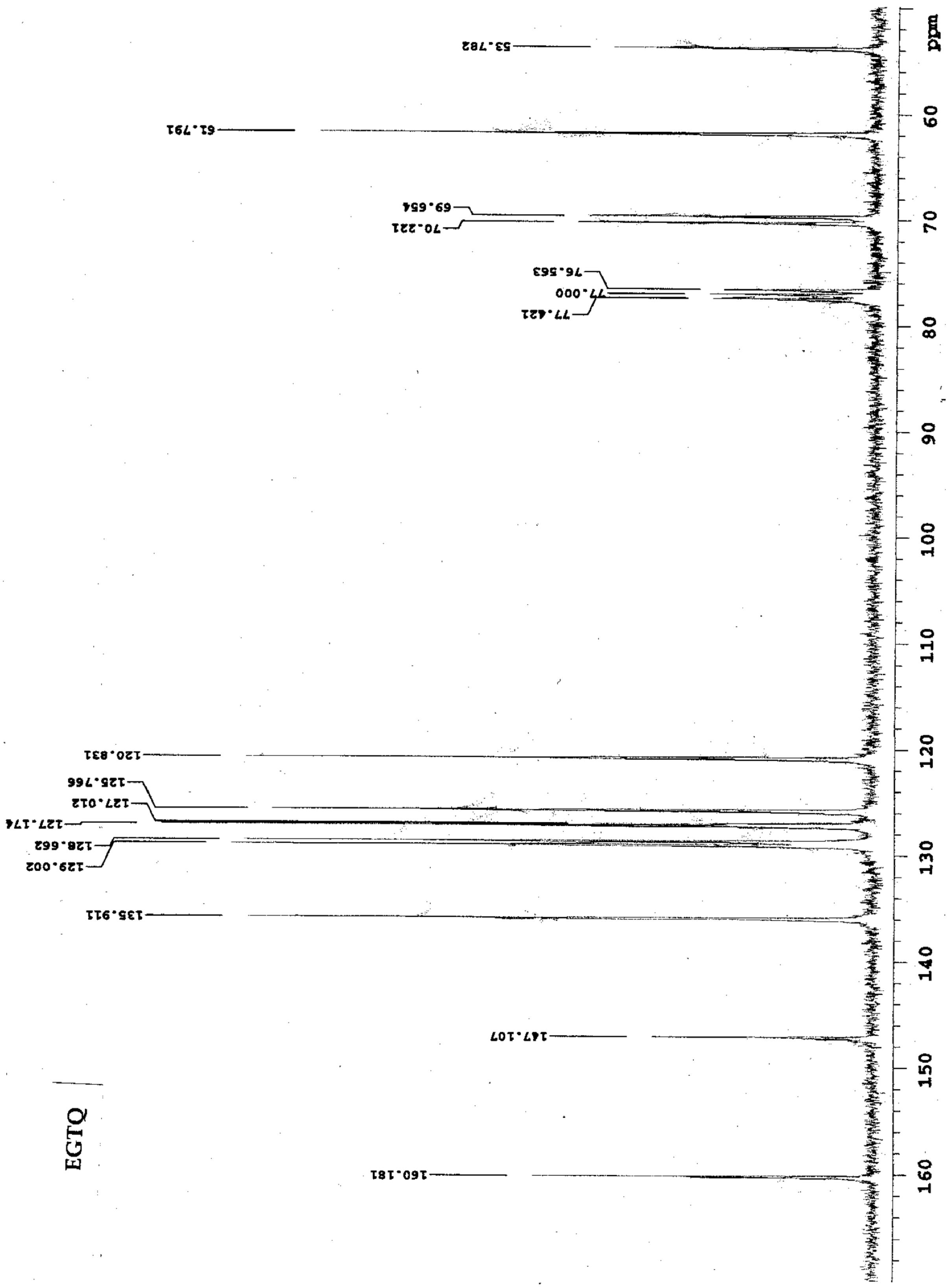


Fig. S35. ^{13}C NMR spectrum for EGTQ in $CDCl_3$.

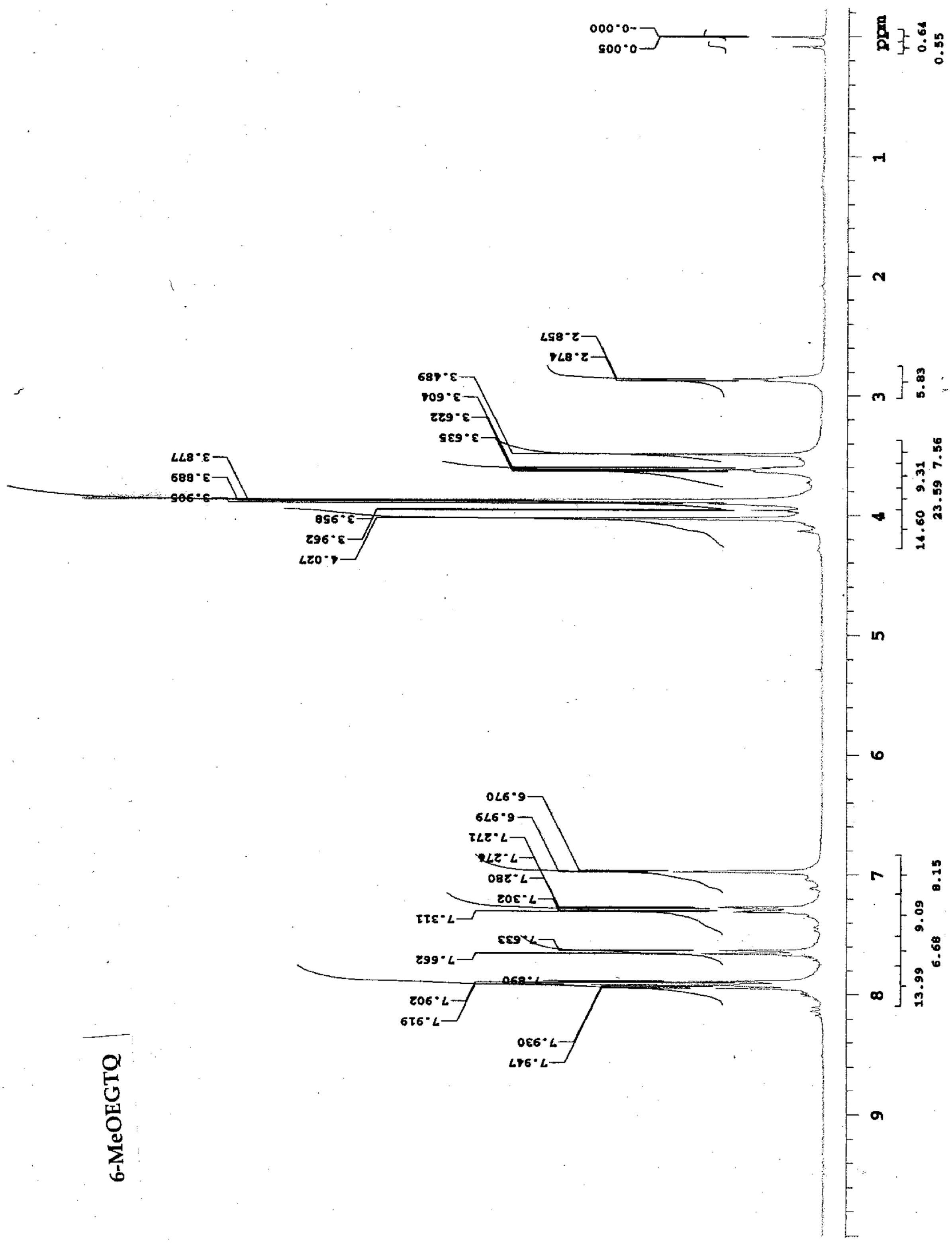


Fig. S36. ^{1}H NMR spectrum for 6-MeOEGTQ in $CDCl_3$.

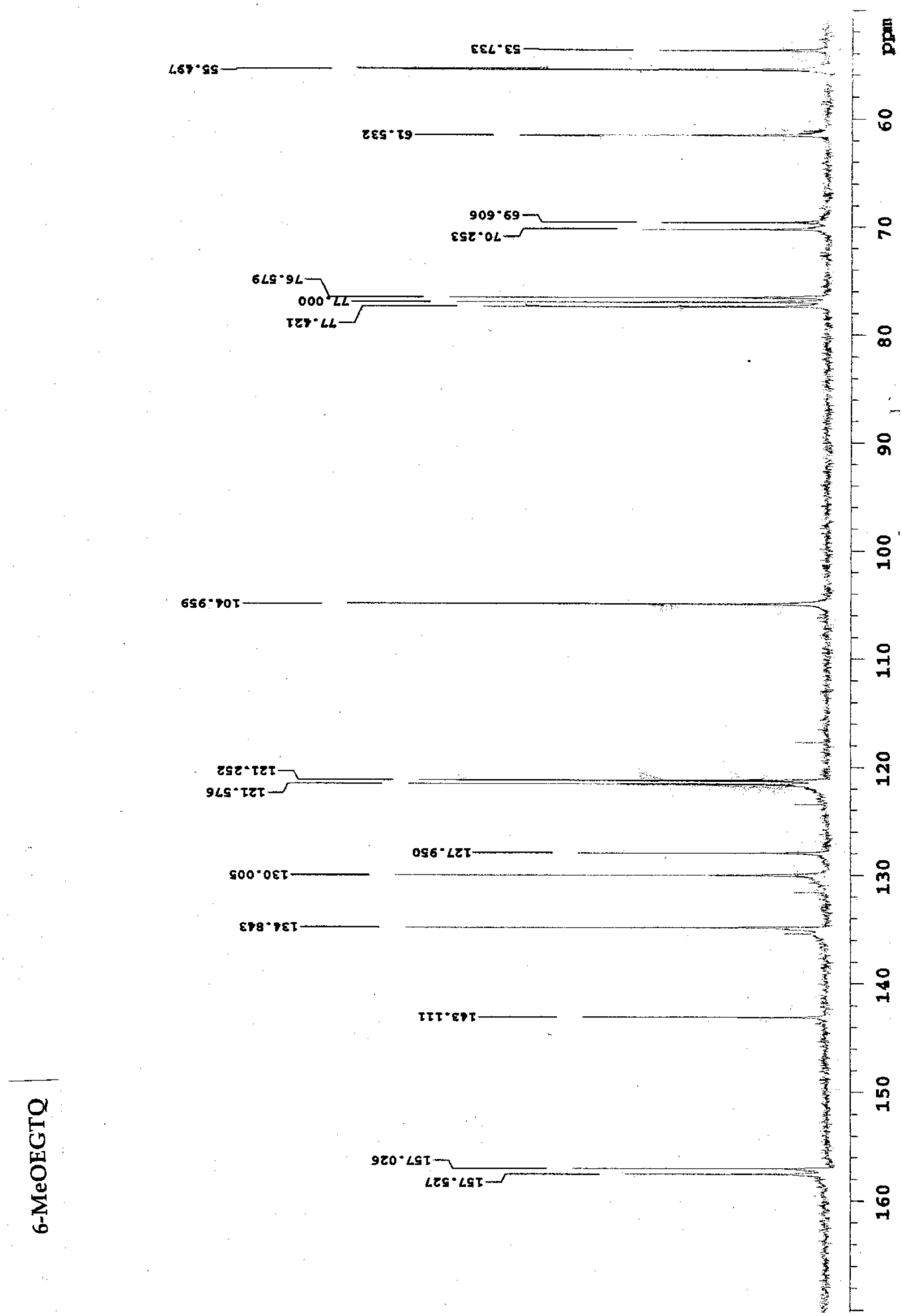


Fig. S37. ^{13}C NMR spectrum for 6-MeOEGTQ in $CDCl_3$.

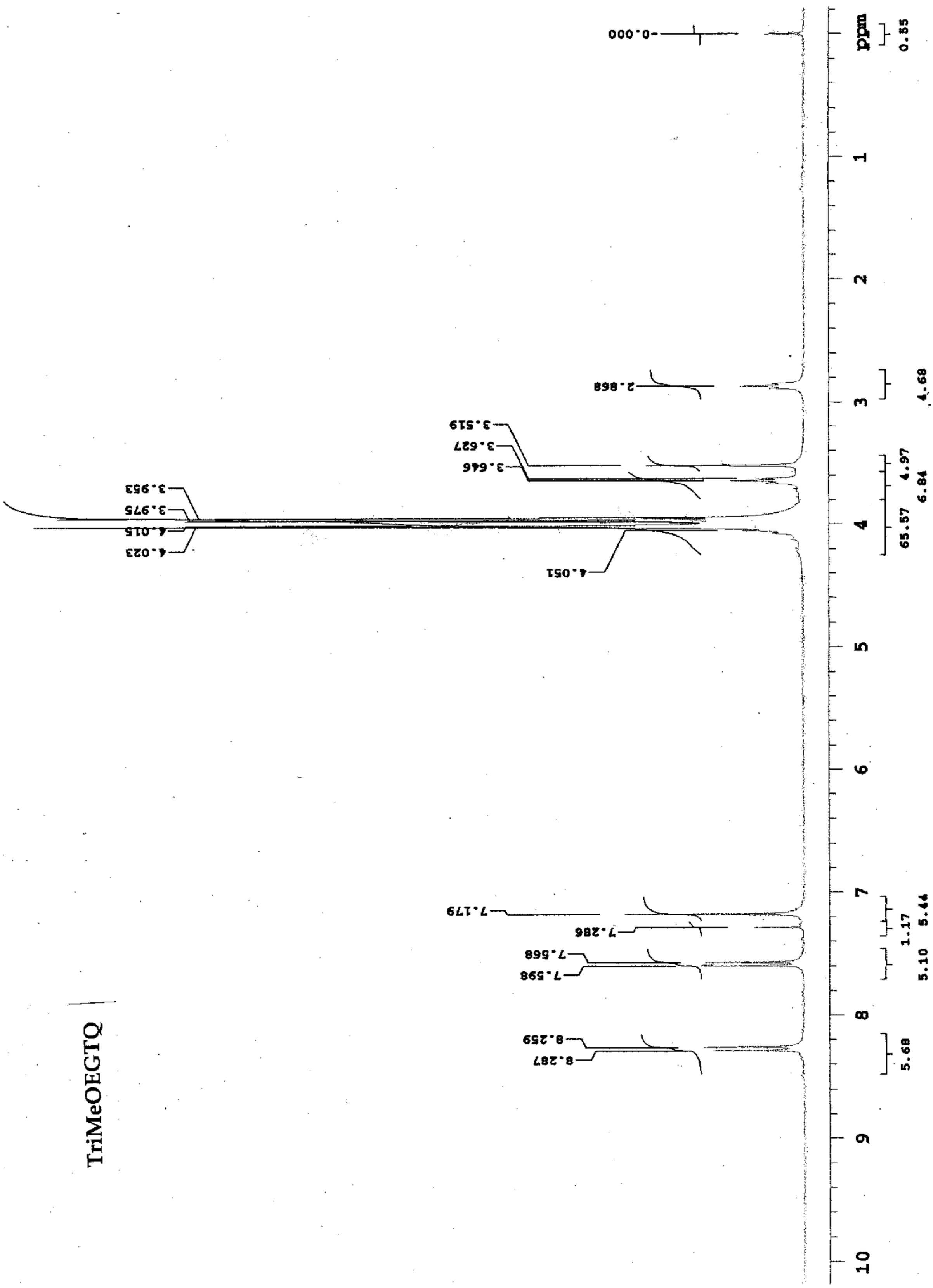


Fig. S38. ^{1}H NMR spectrum for TriMeOEGTQ in $CDCl_3$.

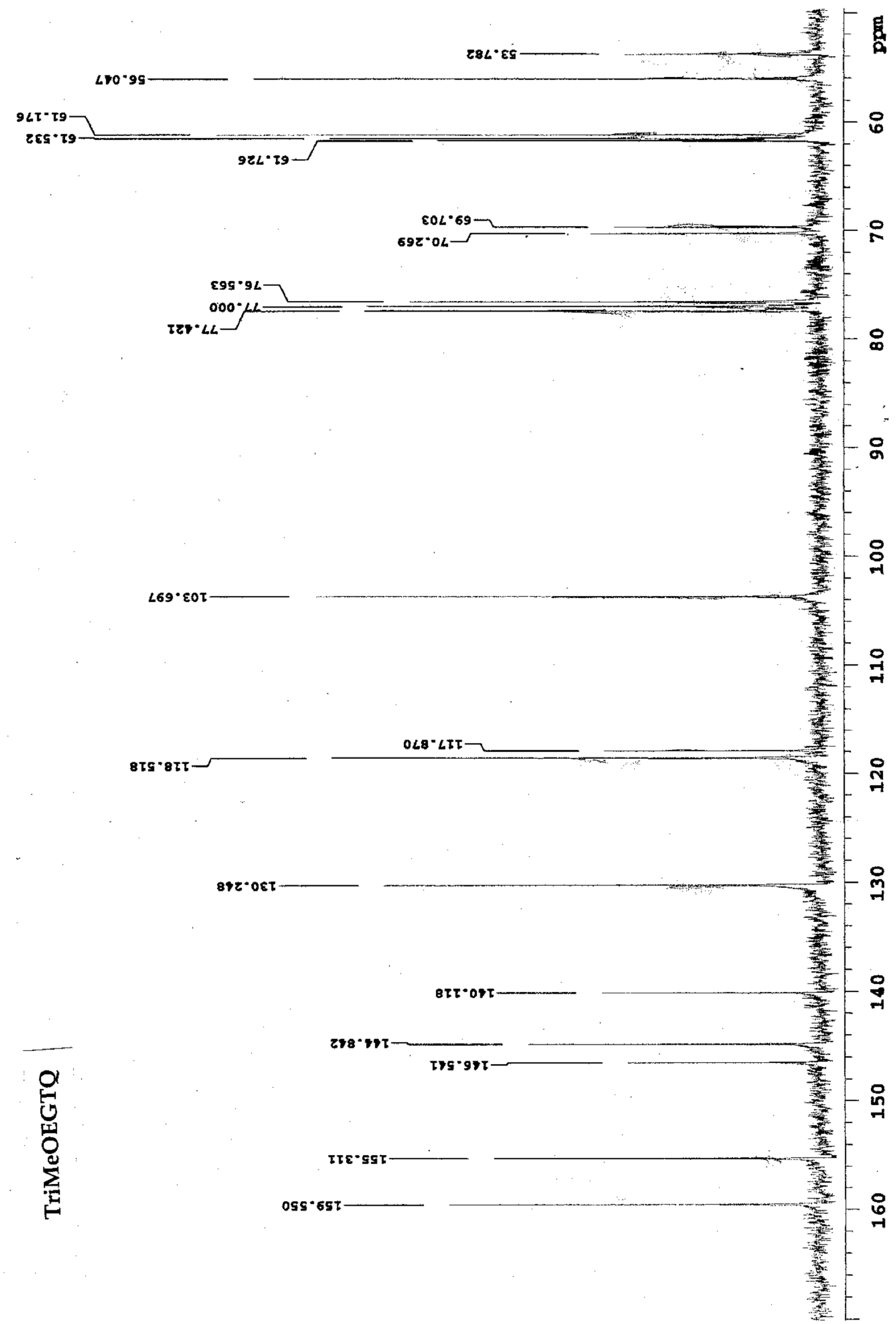


Fig. S39. ^{13}C NMR spectrum for TriMeOEGTQ in $CDCl_3$.

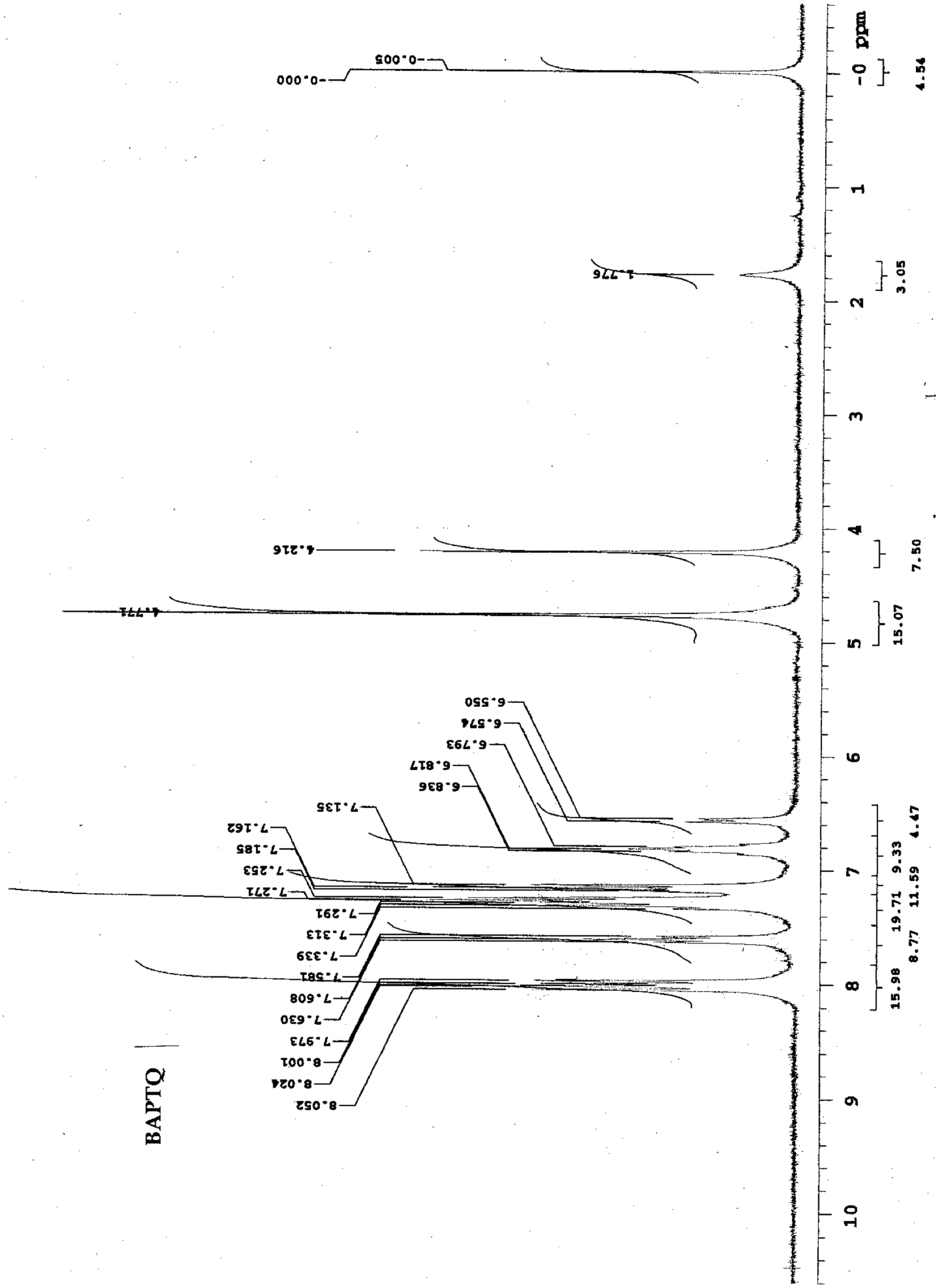


Fig. S40. ^{1}H NMR spectrum for BAPTQ in $CDCl_3$.

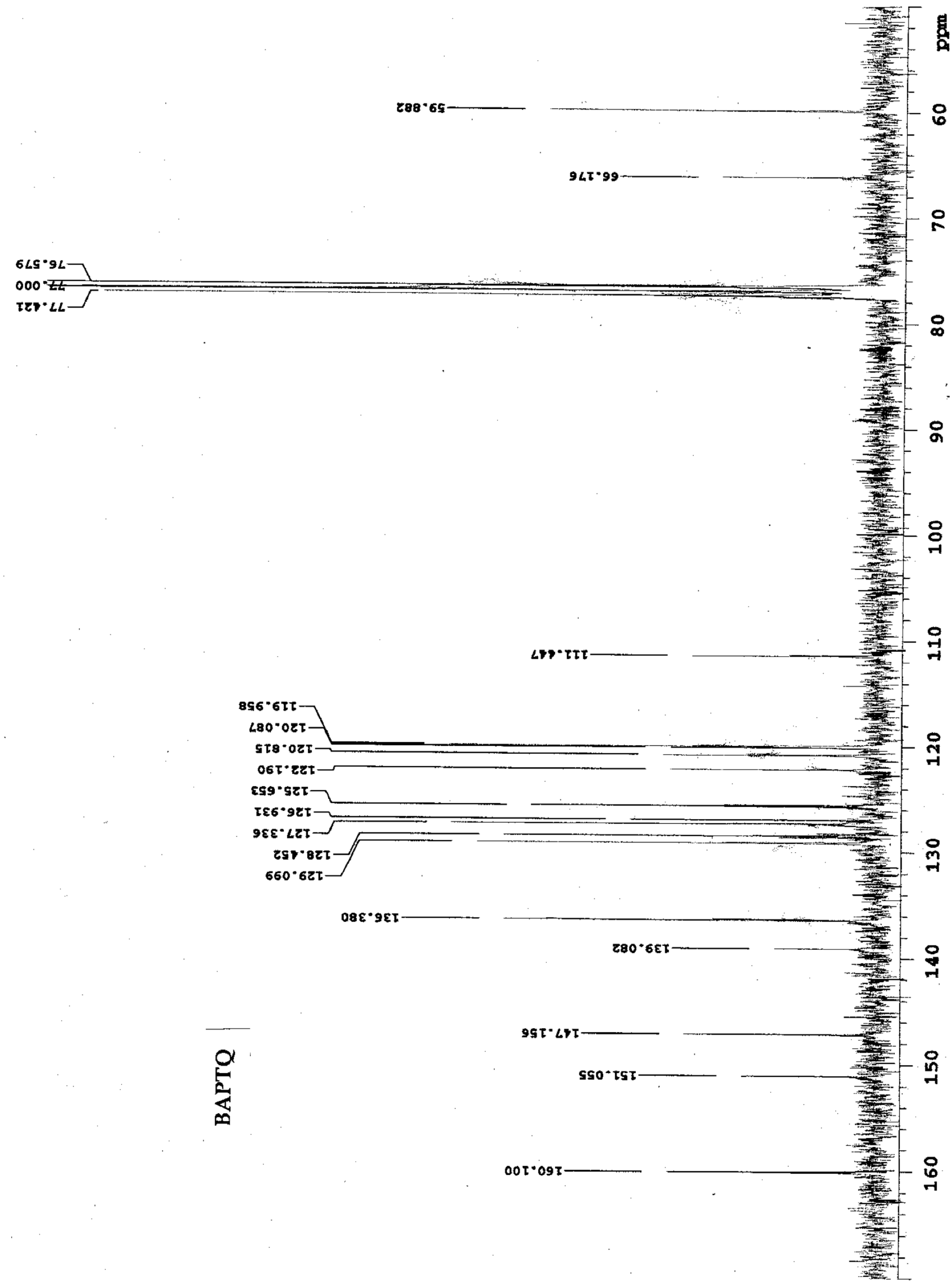


Fig. S41. ^{13}C NMR spectrum for BAPTQ in $CDCl_3$.

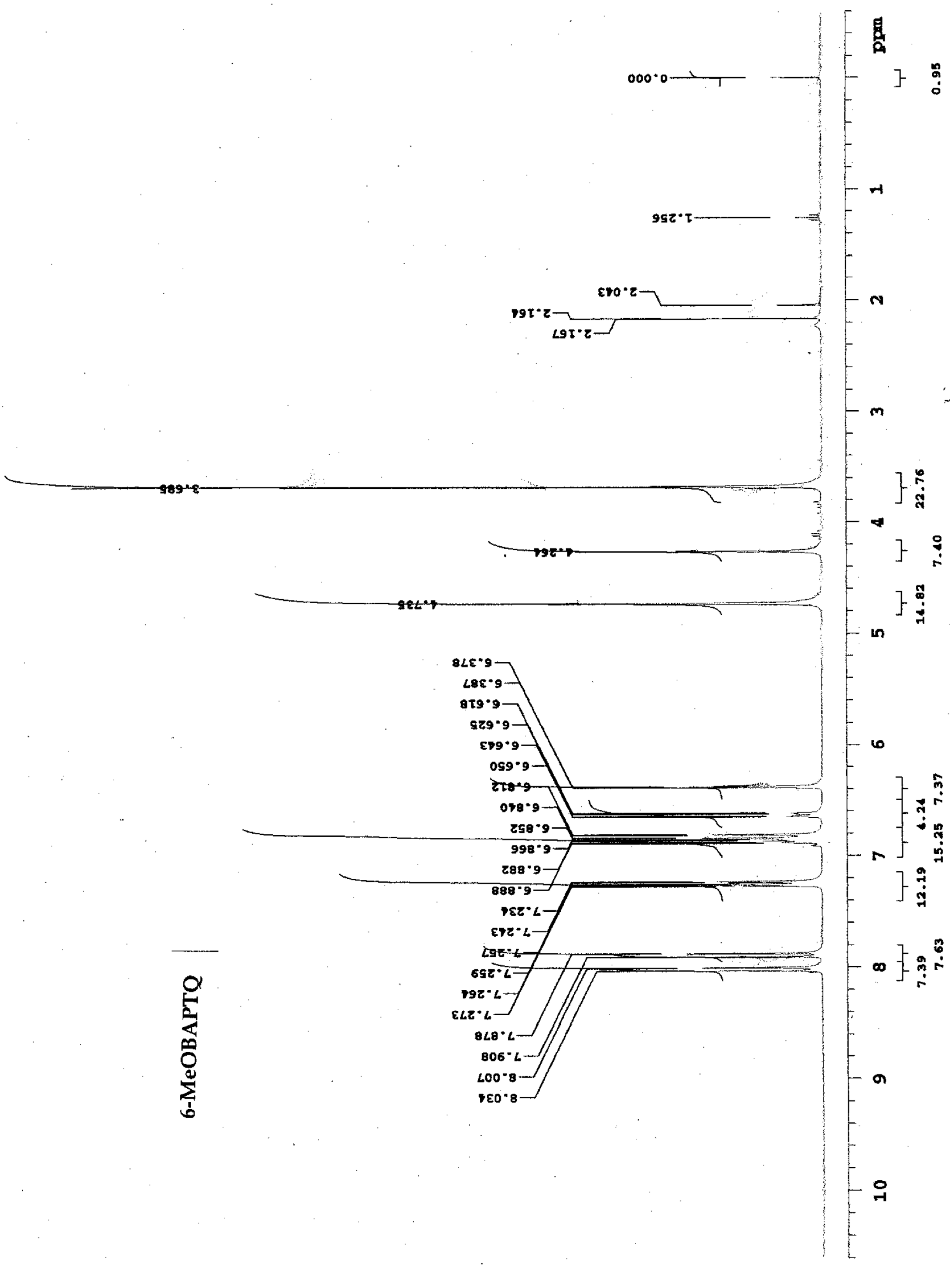


Fig. S42. ^{1}H NMR spectrum for 6-MeOBAPTQ in $CDCl_3$.

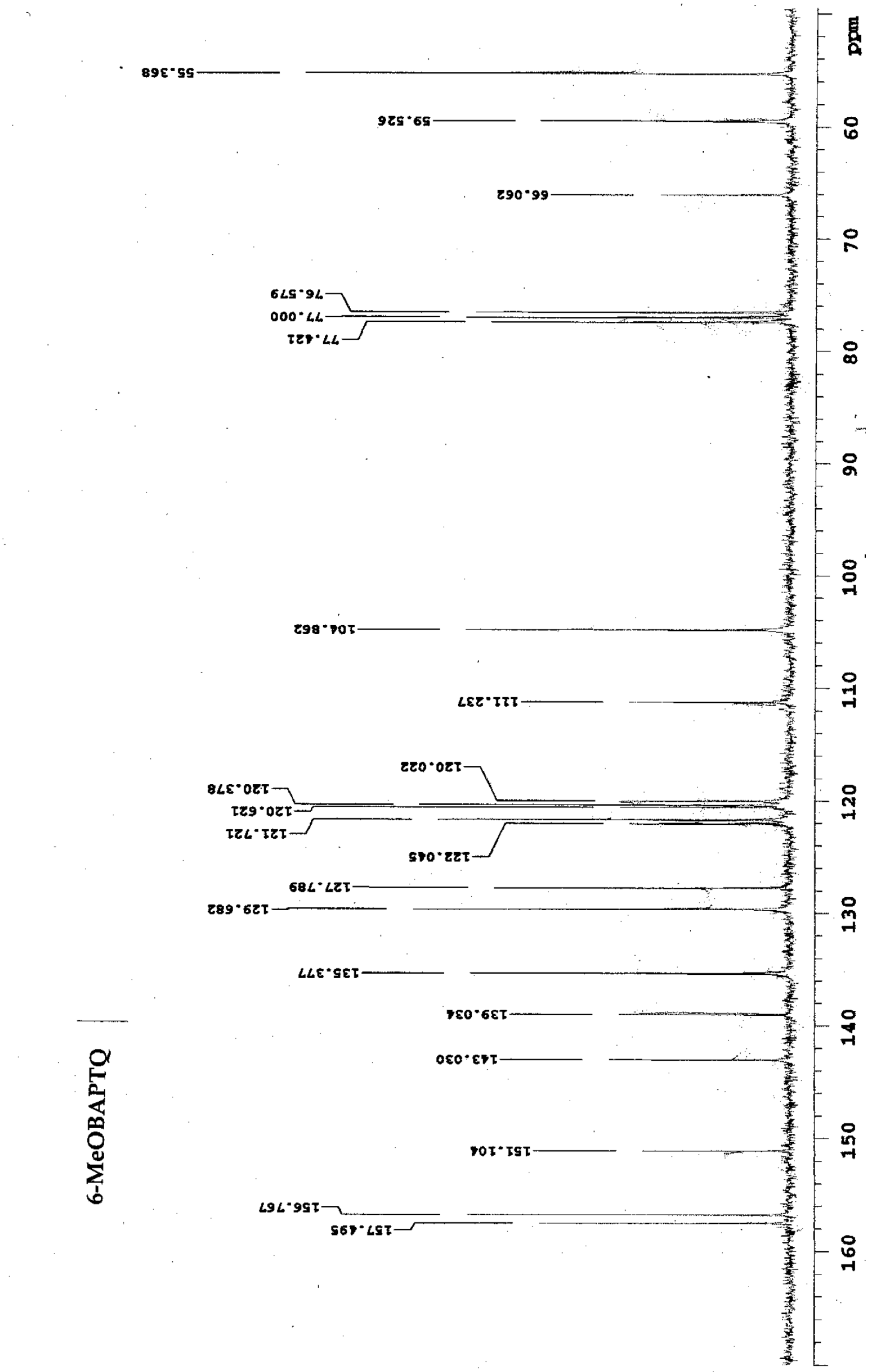


Fig. S43. ^{13}C NMR spectrum for 6-MeOBAPTQ in $CDCl_3$.

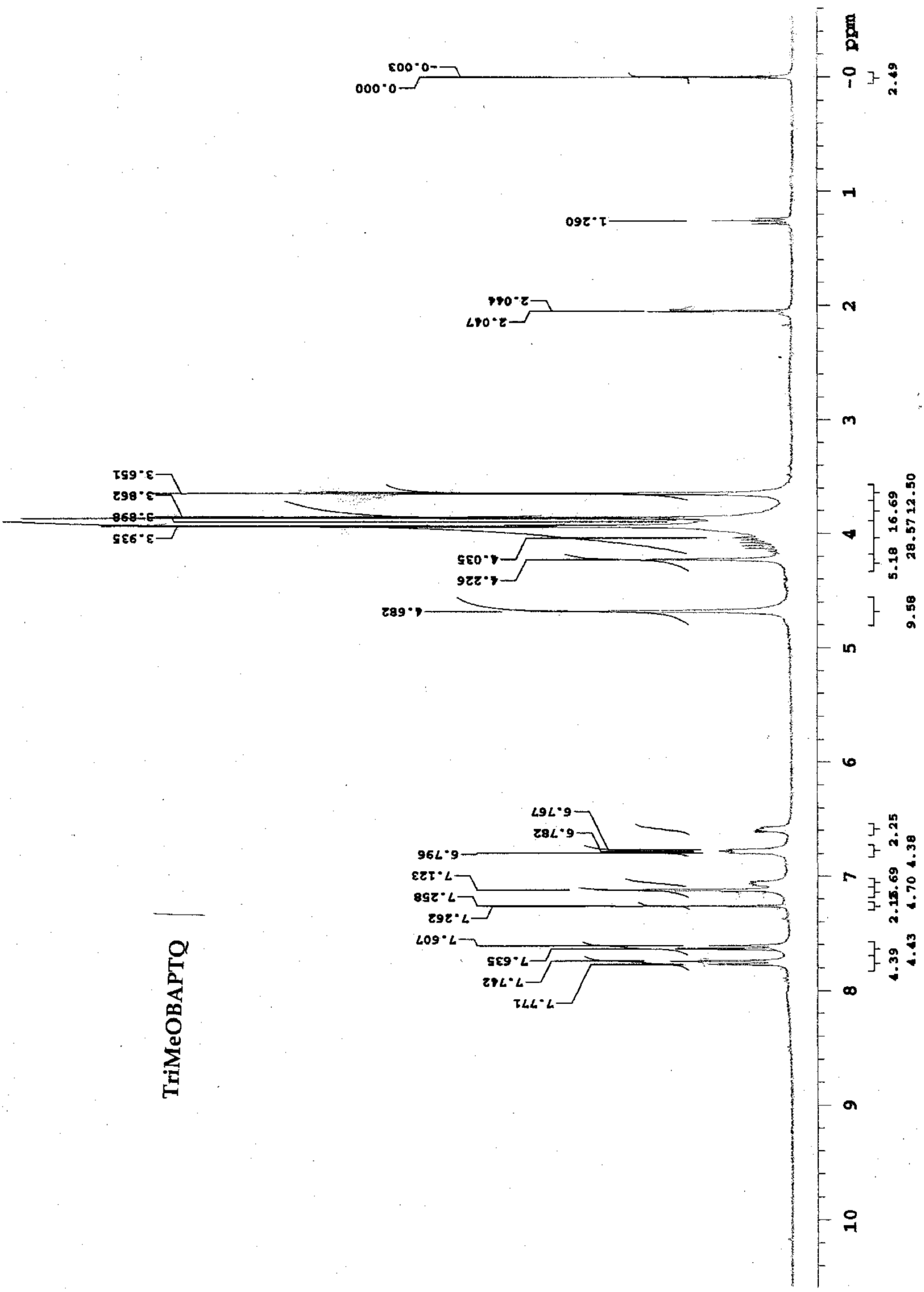


Fig. S44. [1]H NMR spectrum for TriMeOBAPTQ in $CDCl_3$.

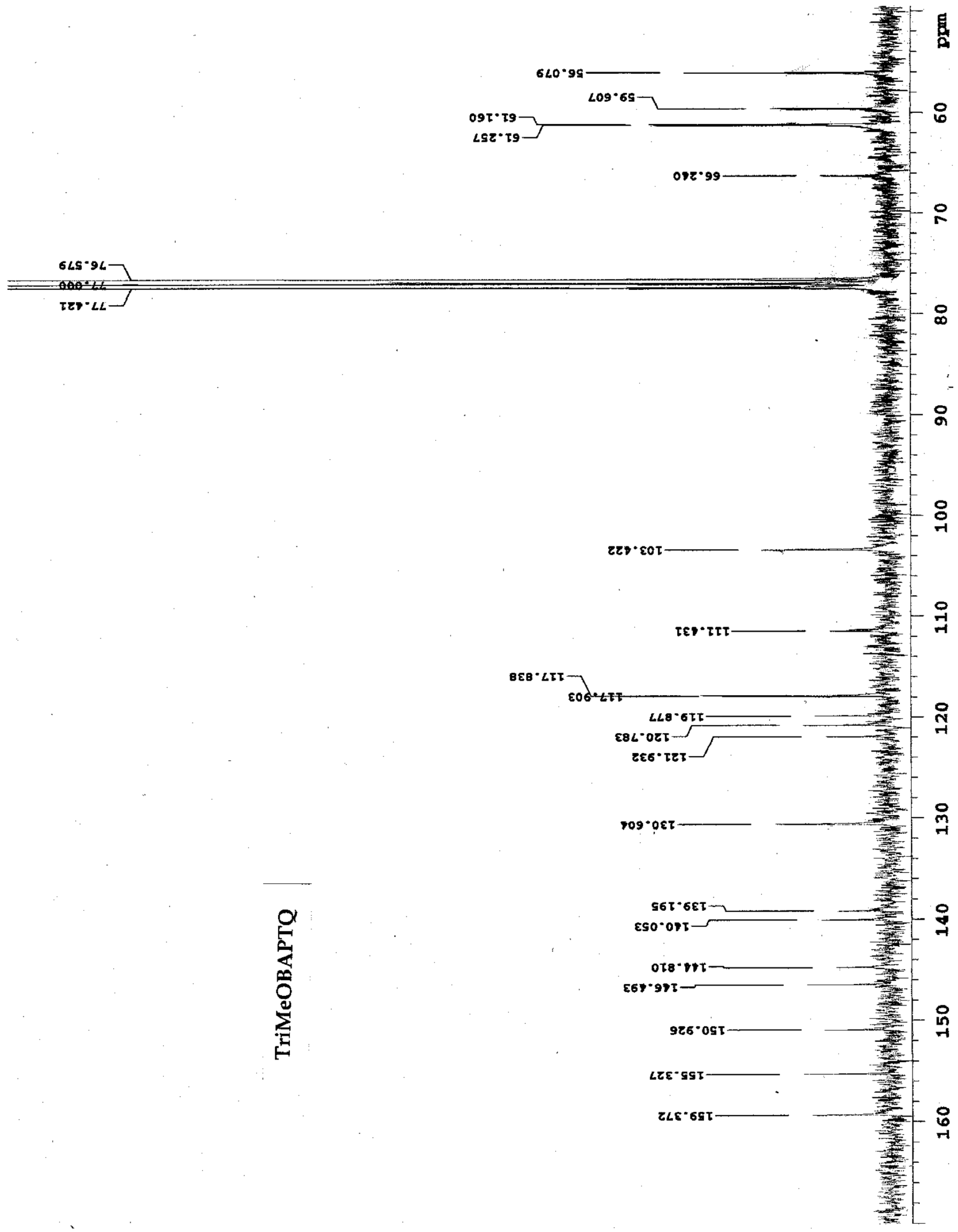


Fig. S45. ^{13}C NMR spectrum for TriMeOBAPTQ in $CDCl_3$.

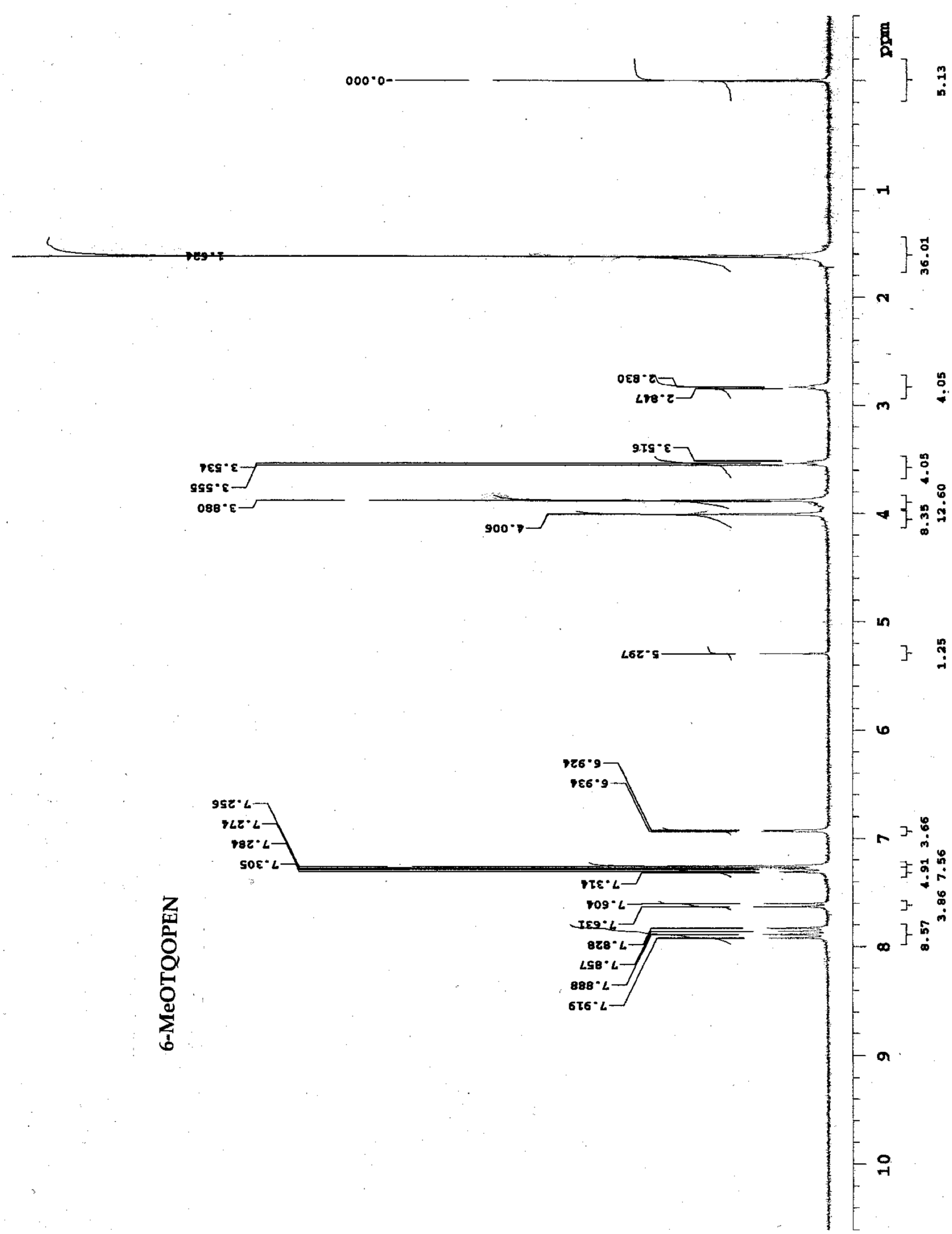


Fig. S46. ^{1}H NMR spectrum for 6-MeOTQOPEN in $CDCl_3$.

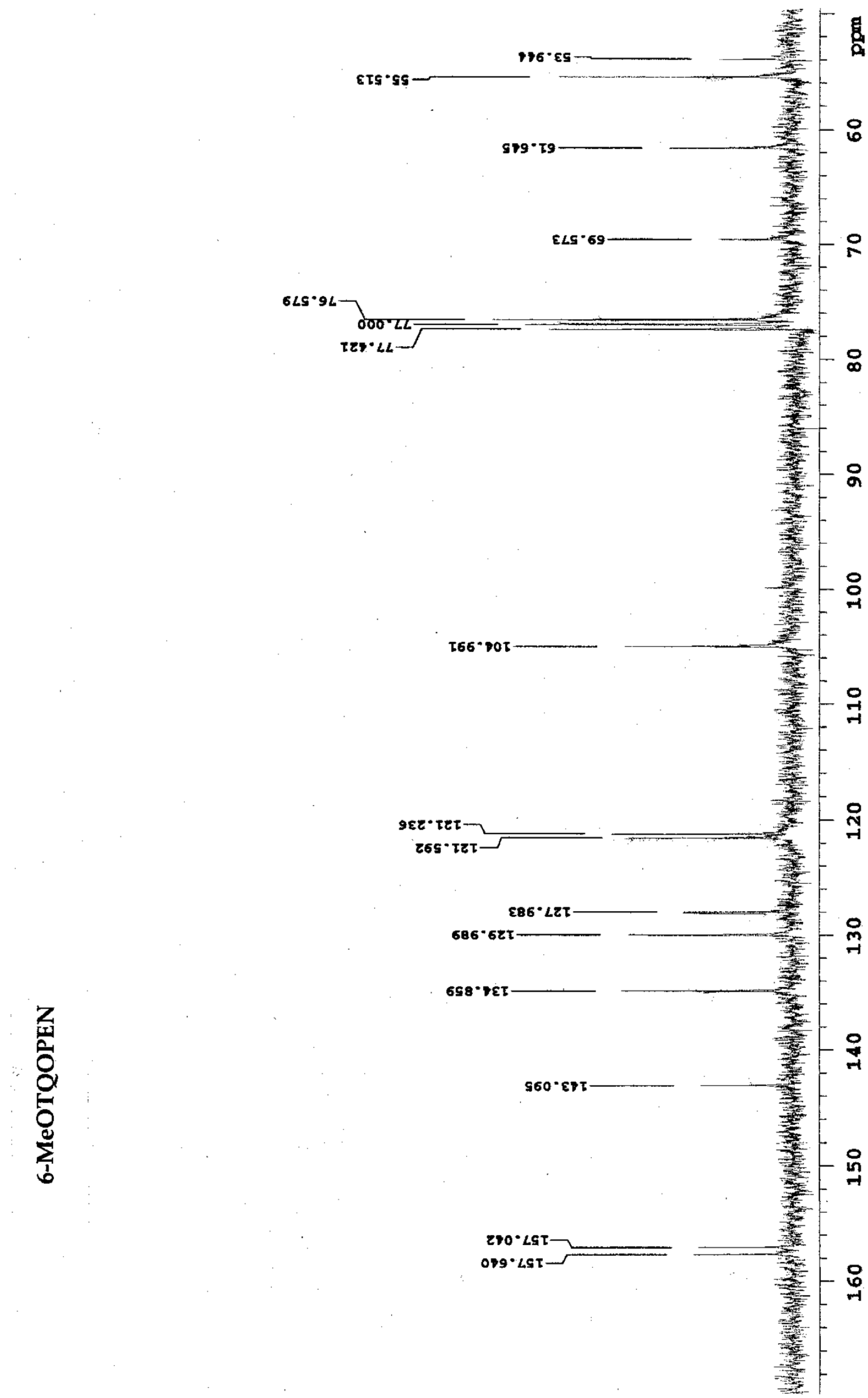


Fig. S47. ^{13}C NMR spectrum for 6-MeOTQOPEN in $CDCl_3$.

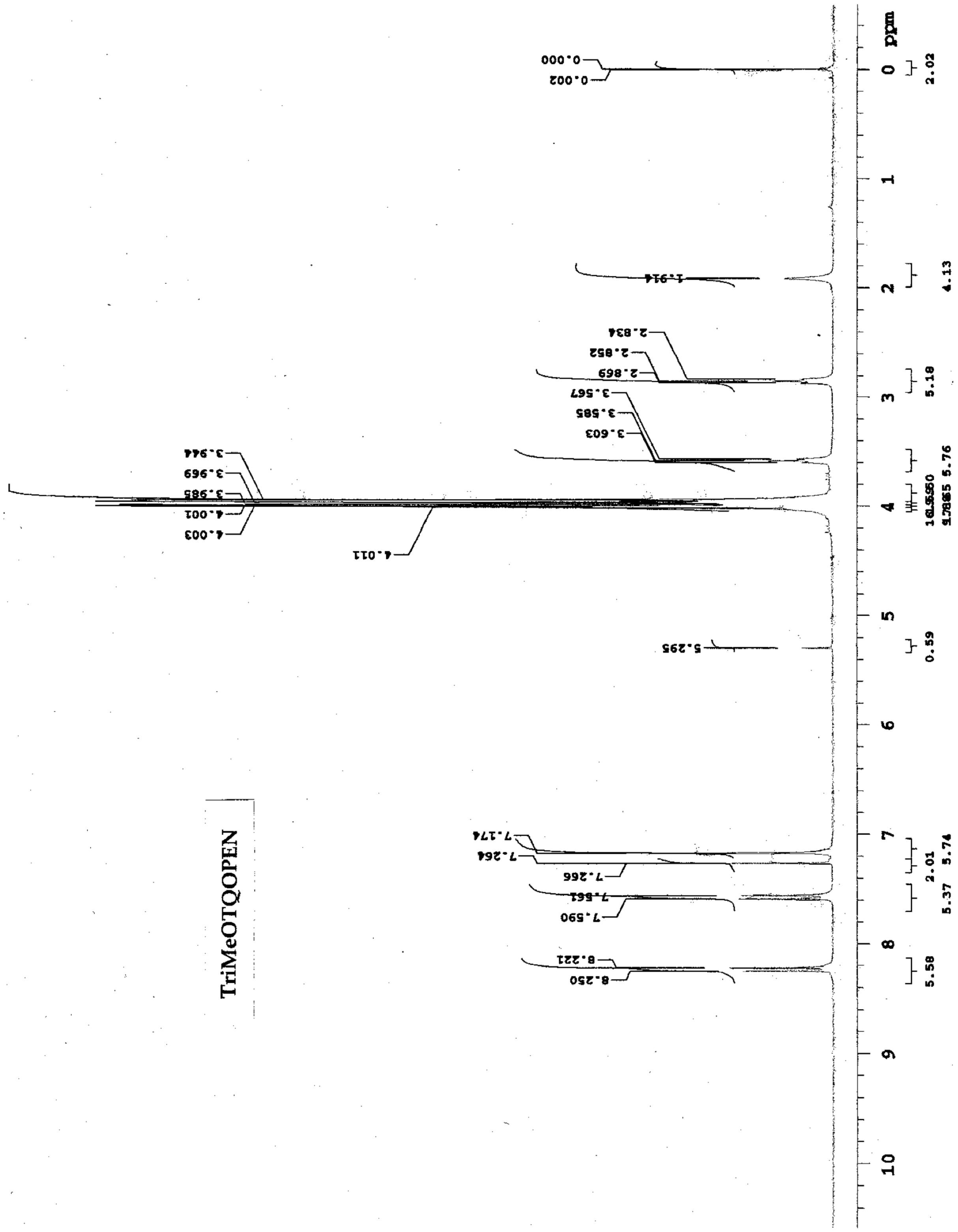


Fig. S48. ^{1}H NMR spectrum for TriMeOTQOPEN in $CDCl_3$.

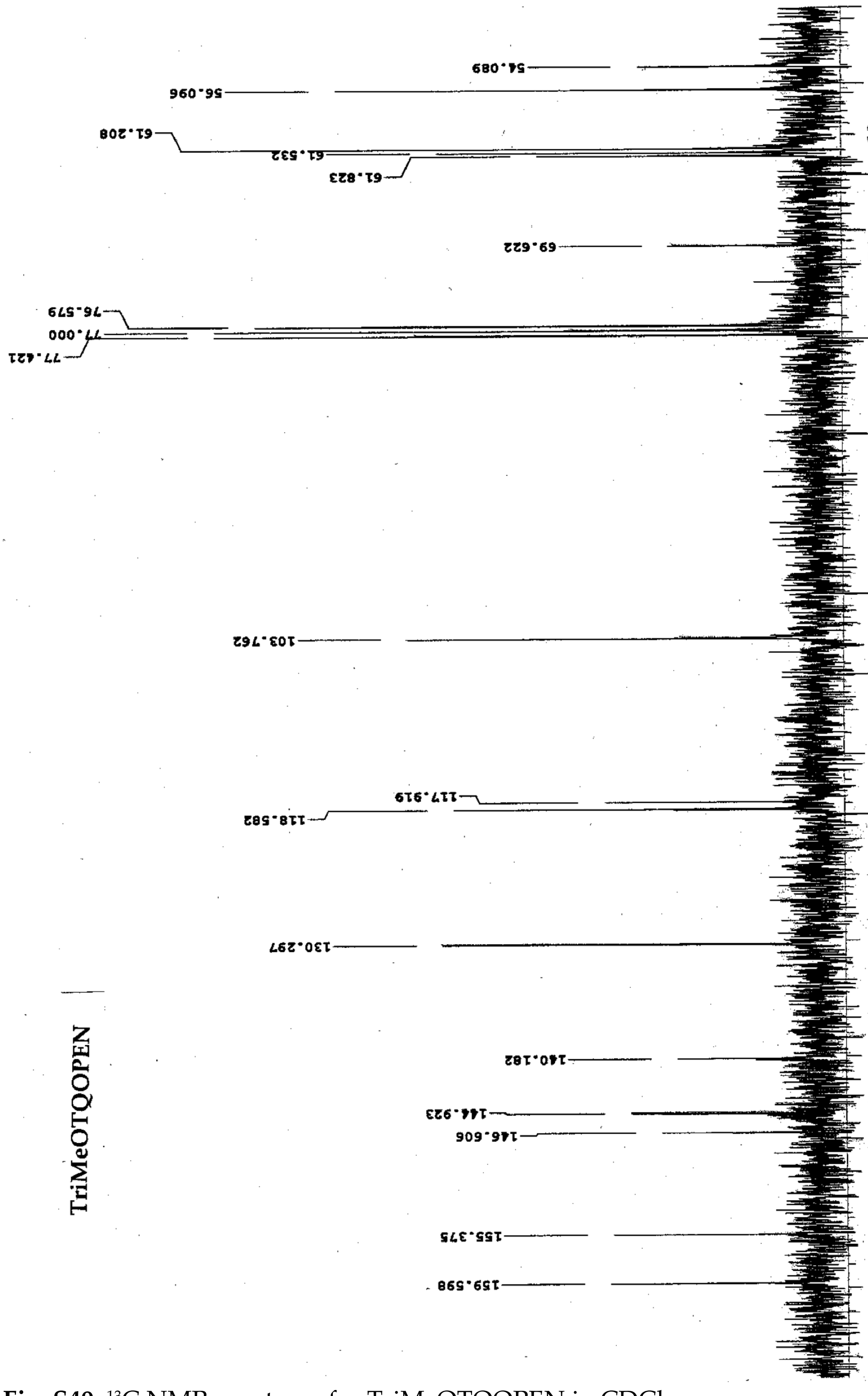


Fig. S49. ^{13}C NMR spectrum for TriMeOTQOPEN in $CDCl_3$.

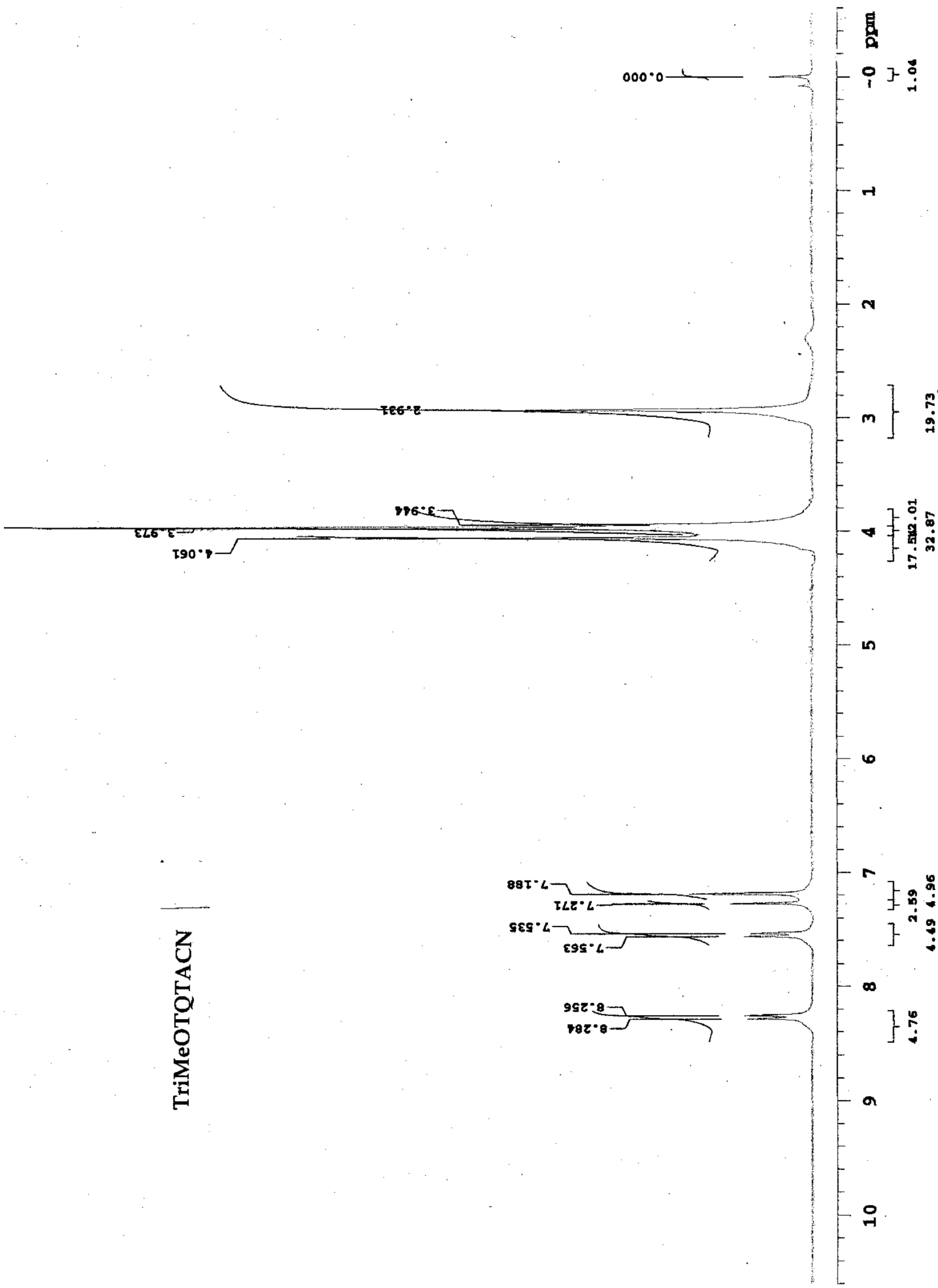


Fig. S50. ^{1}H NMR spectrum for TriMeOTQTACN in $CDCl_3$.

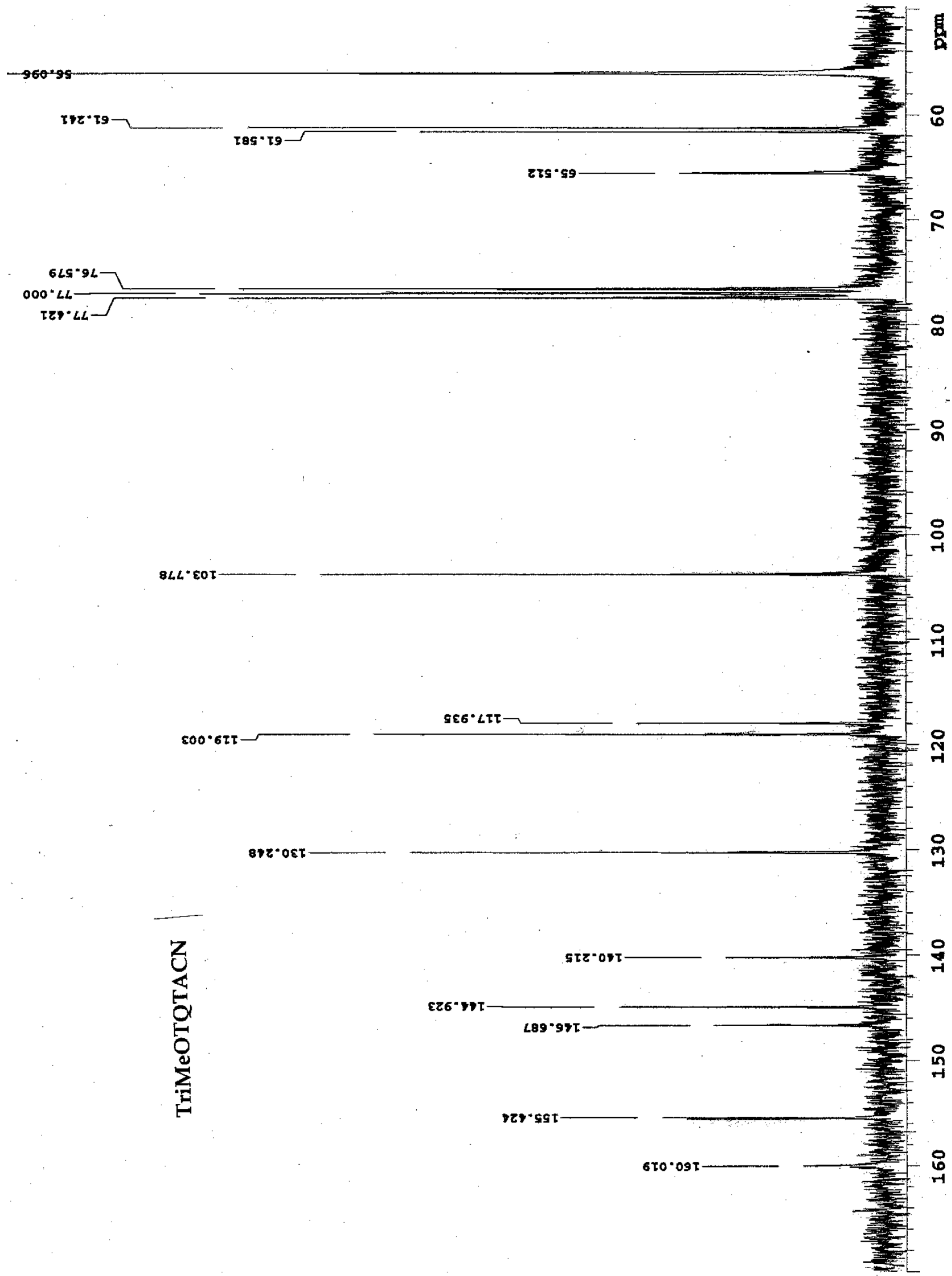


Fig. S51. ^{13}C NMR spectrum for TriMeOTQTACN in $CDCl_3$.

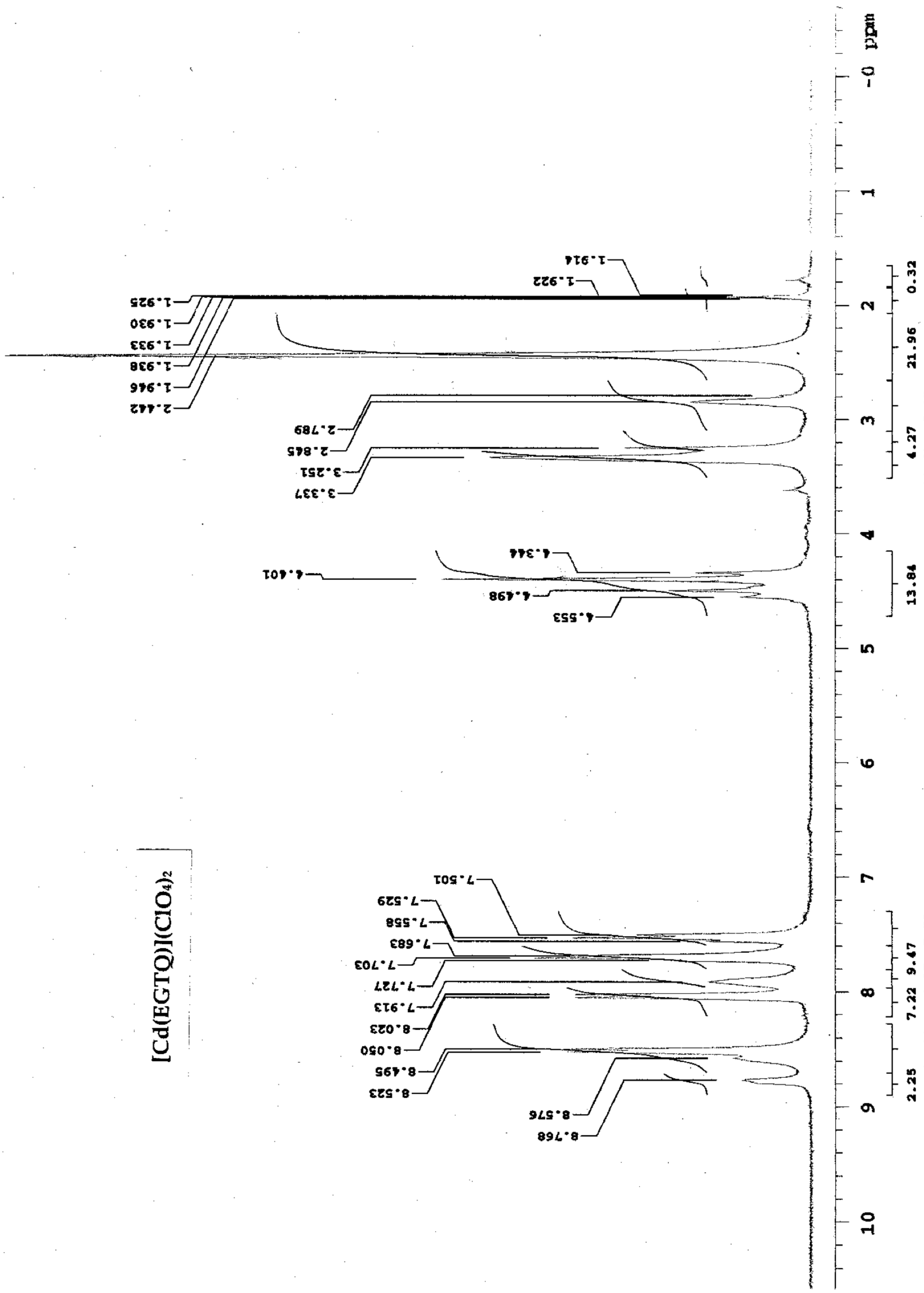


Fig. S52. [1]H NMR spectrum for $[Cd(EGTQ)](ClO_4)_2$ in CD_3CN.

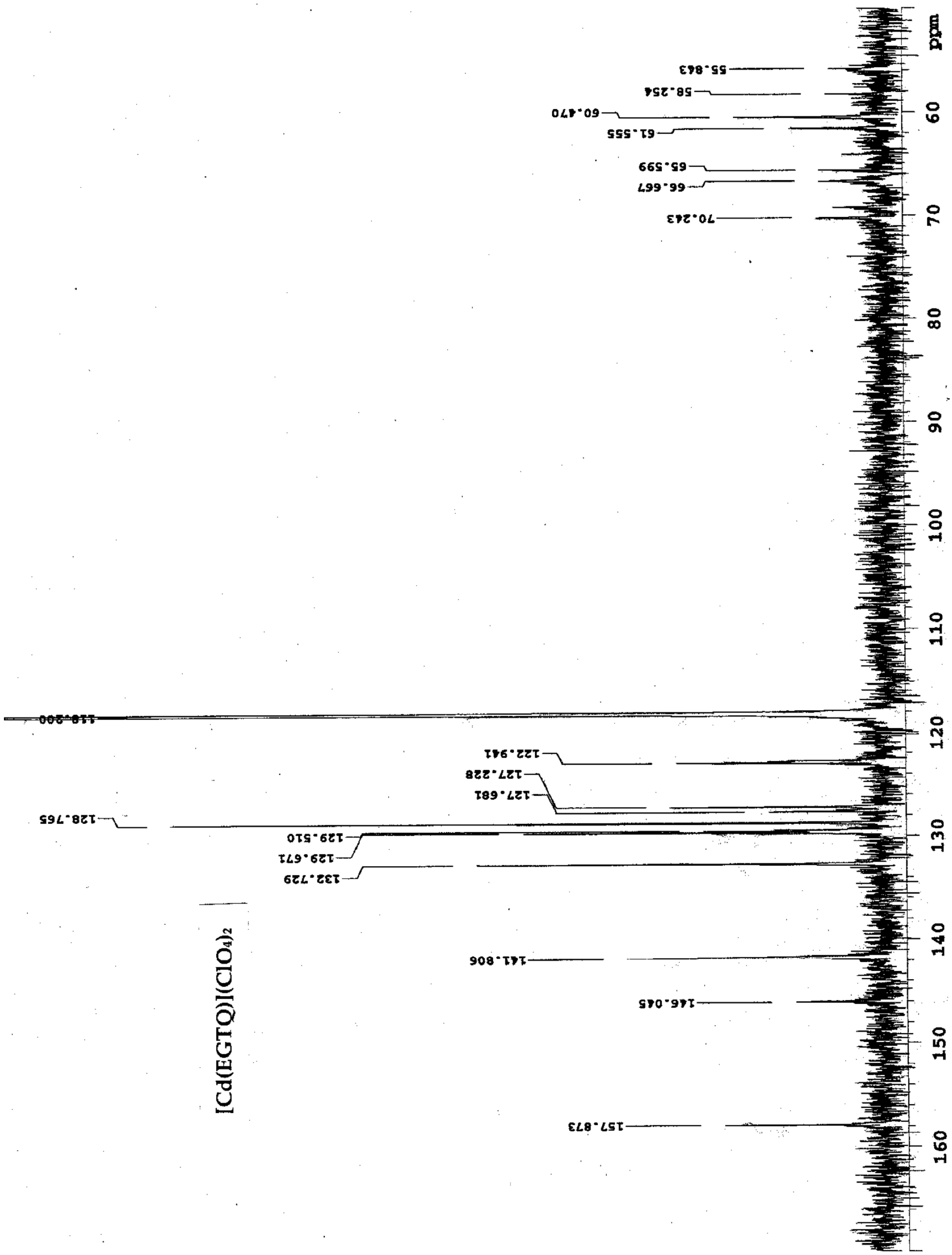


Fig. S53. ^{13}C NMR spectrum for $[Cd(EGTQ)](ClO_4)_2$ in CD_3CN.

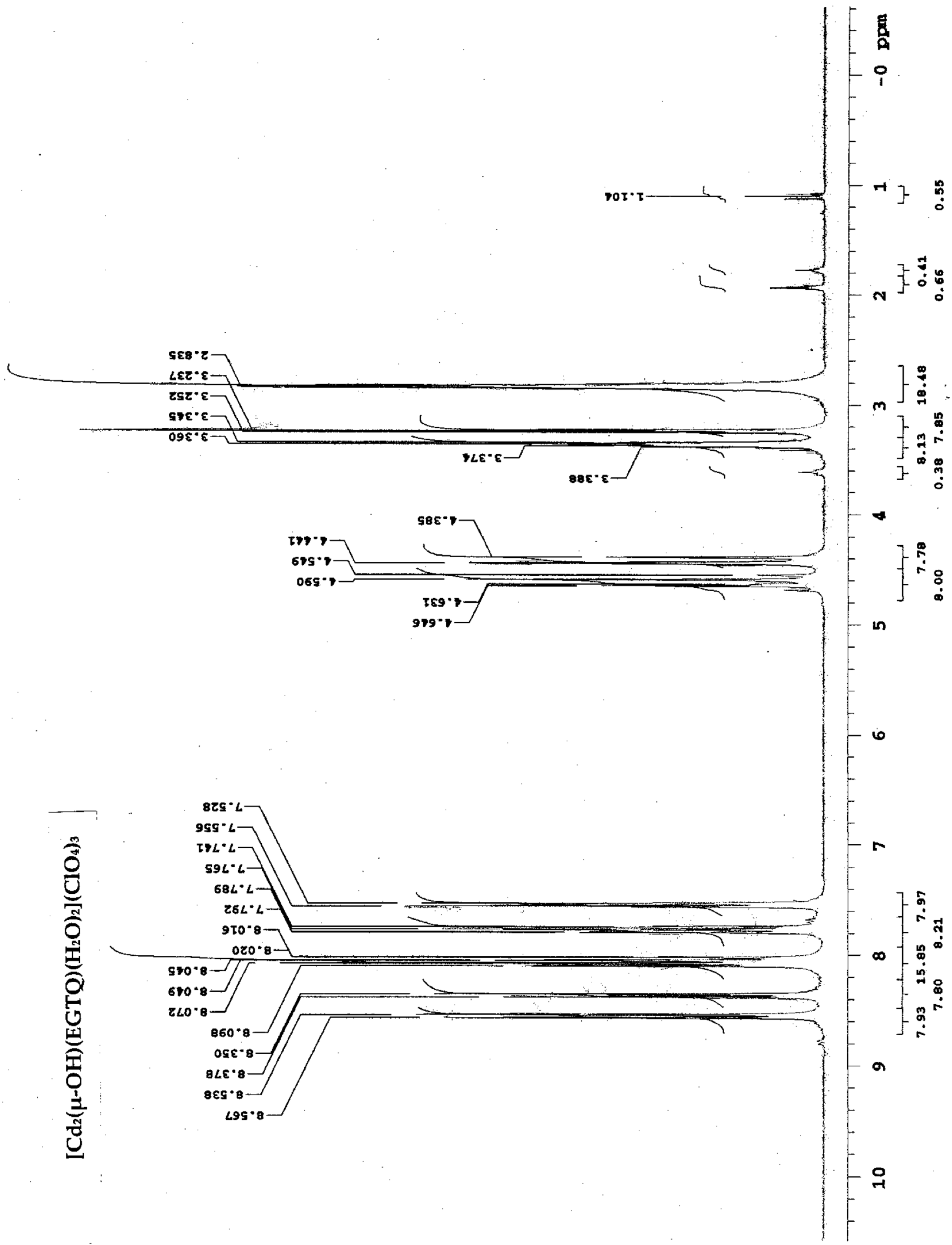


Fig. S54. ^{1}H NMR spectrum for $[Cd_2(\mu\text{-}OH)(EGTQ)(H_2O)_2](ClO_4)_3$ in CD_3CN.

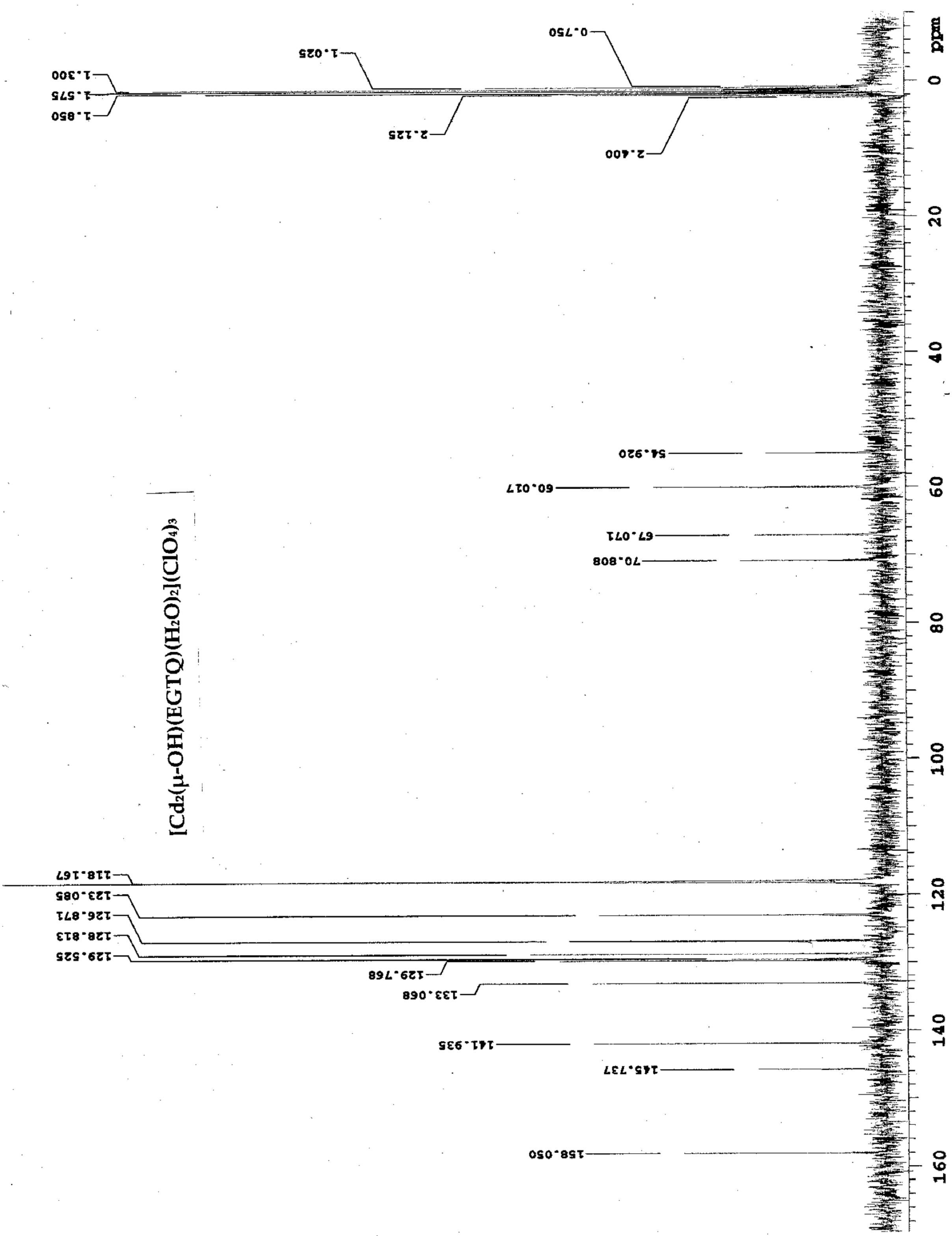


Fig. S55. [13]C NMR spectrum for $[Cd_2(\mu\text{-}OH)(EGTQ)(H_2O)_2](ClO_4)_3$ in CD_3CN.

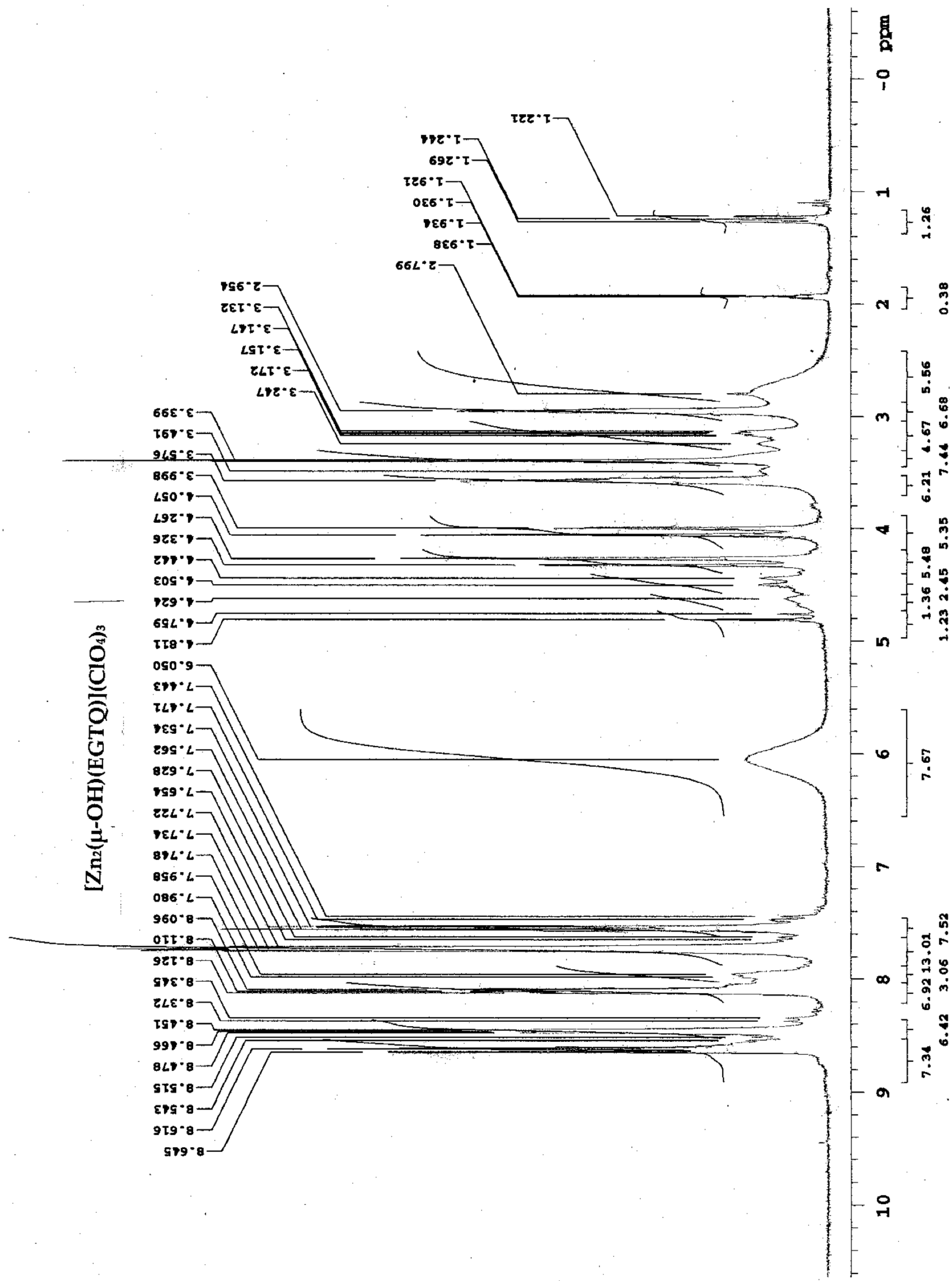


Fig. S56. ^{1}H NMR spectrum for $[Zn_2(\mu\text{-}OH)(EGTQ)](ClO_4)_3$ in CD_3CN.

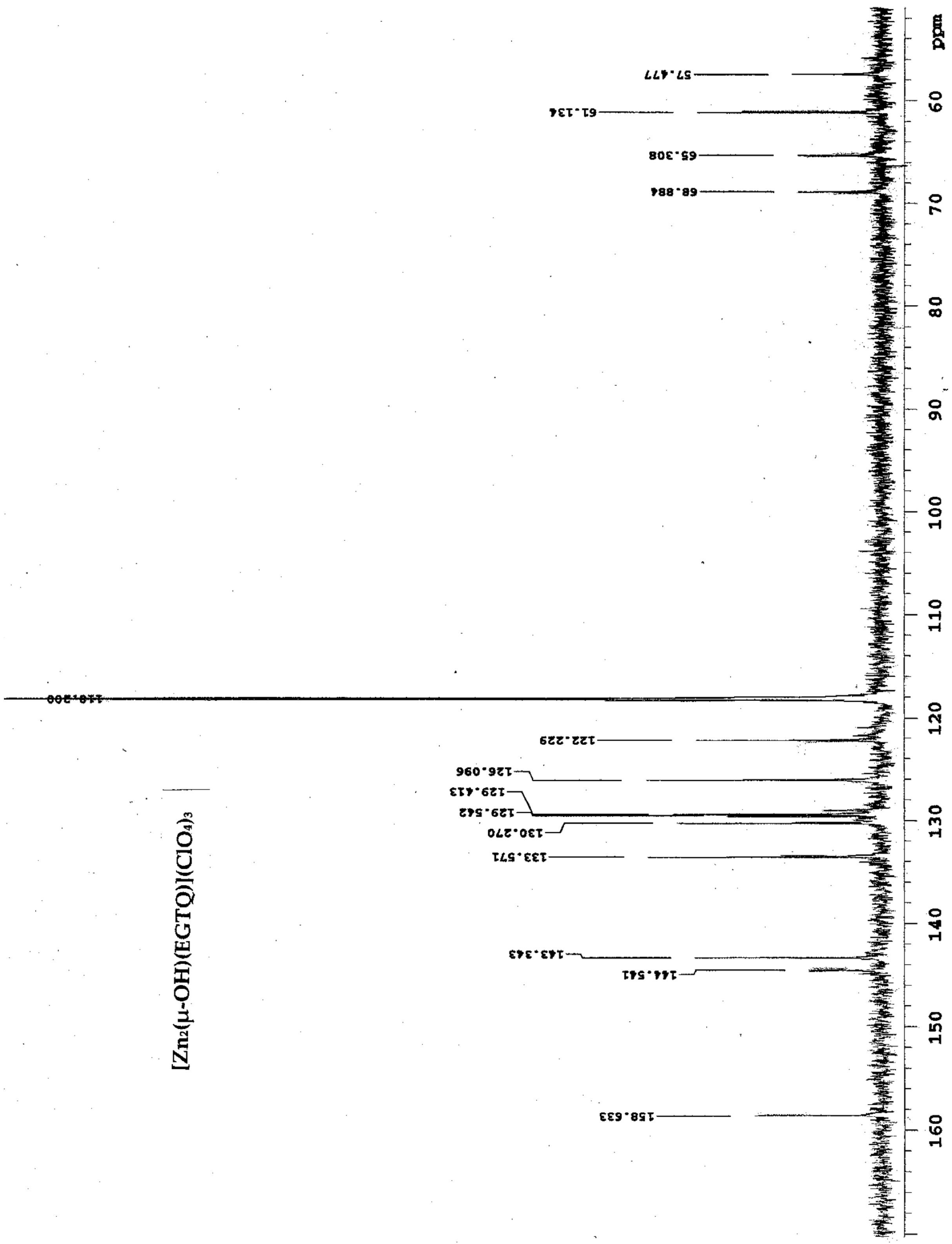


Fig. S57. ^{13}C NMR spectrum for $[Zn_2(\mu\text{-}OH)(EGTQ)](ClO_4)_3$ in CD_3CN.

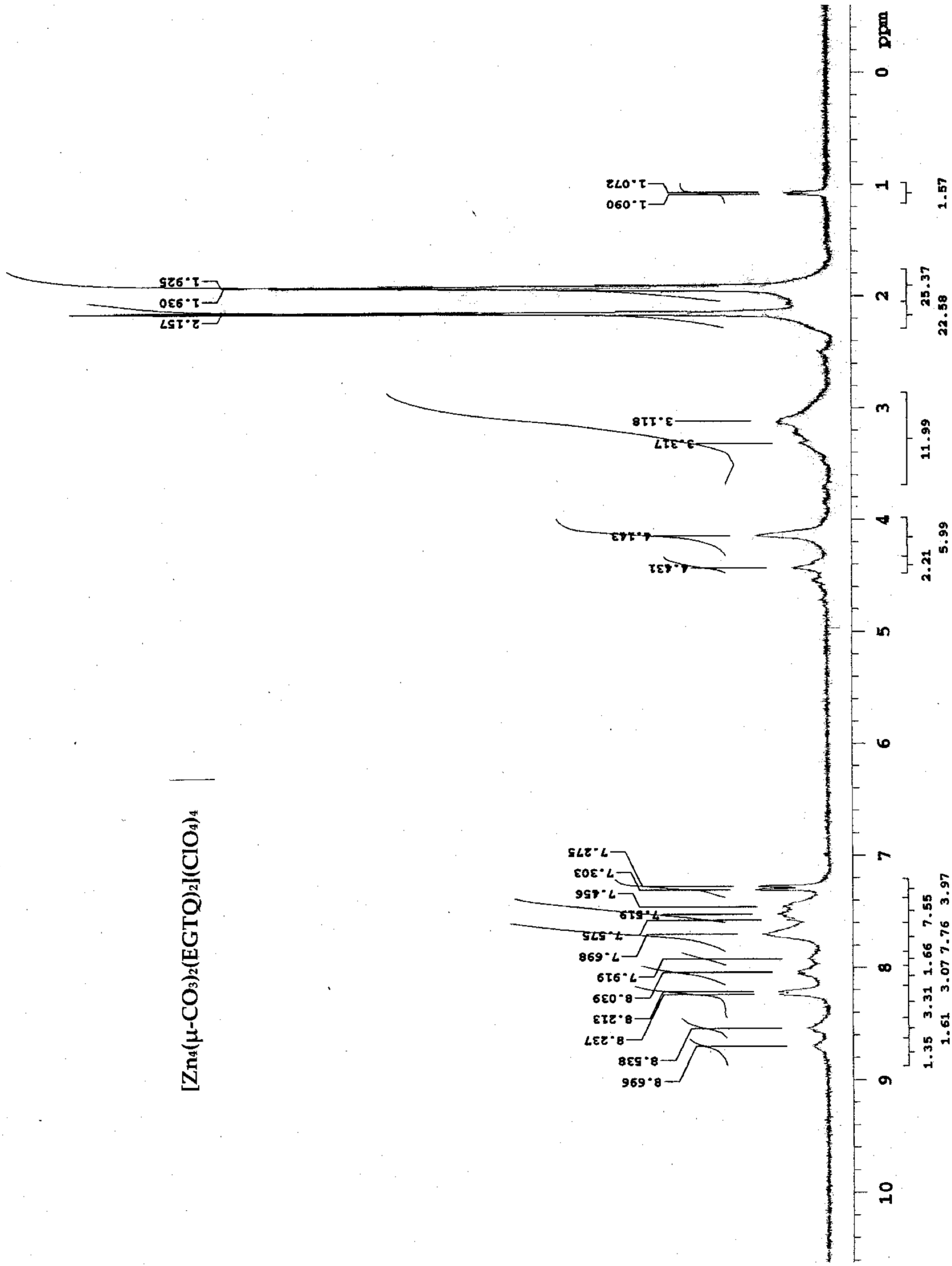


Fig. S58. [1]H NMR spectrum for $[Zn_4(\mu\text{-}CO_3)_2(EGTQ)_2](ClO_4)_4$ in CD_3CN.

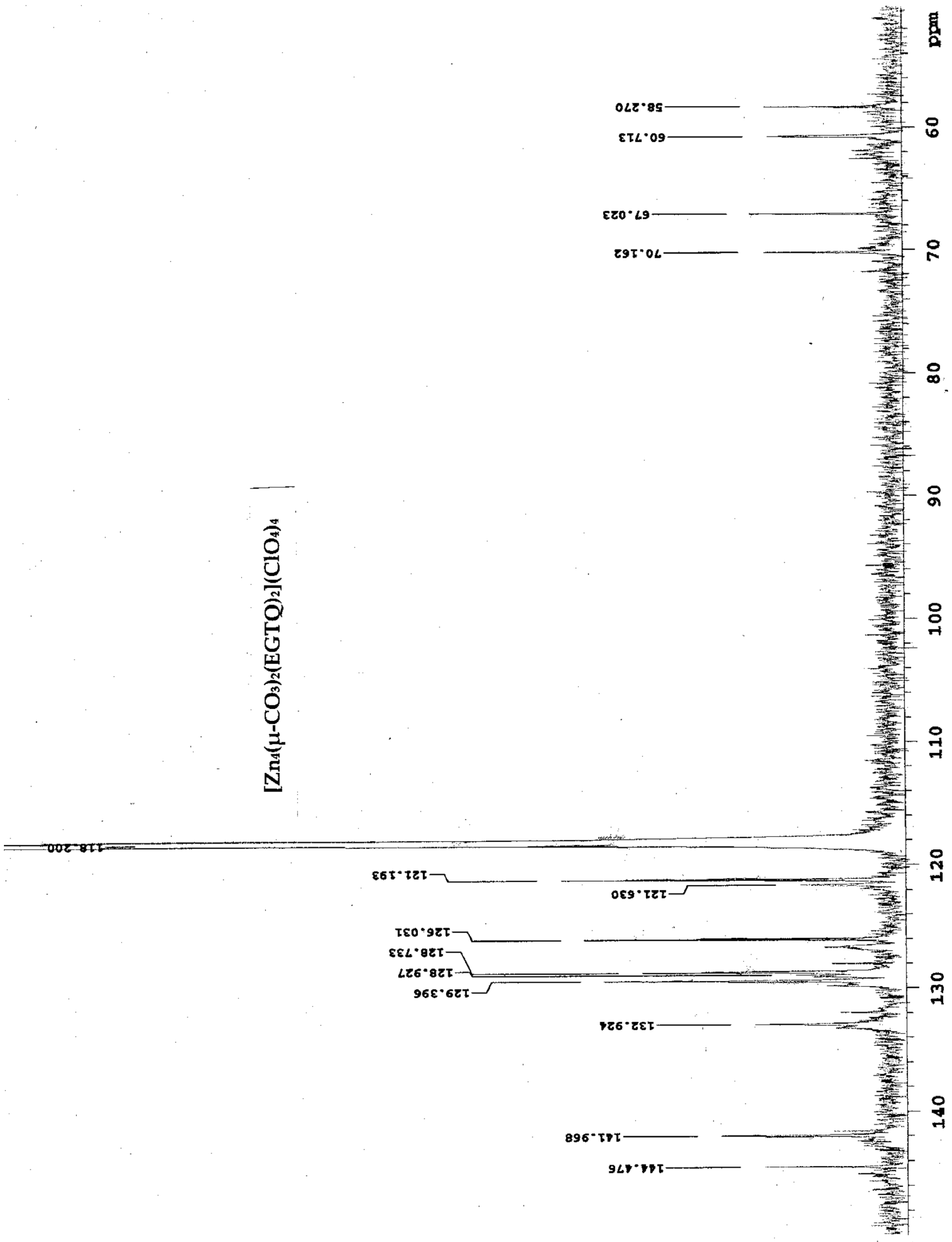


Fig. S59. ^{13}C NMR spectrum for $[Zn_4(\mu\text{-}CO_3)_2(EGTQ)_2](ClO_4)_4$ in CD_3CN.

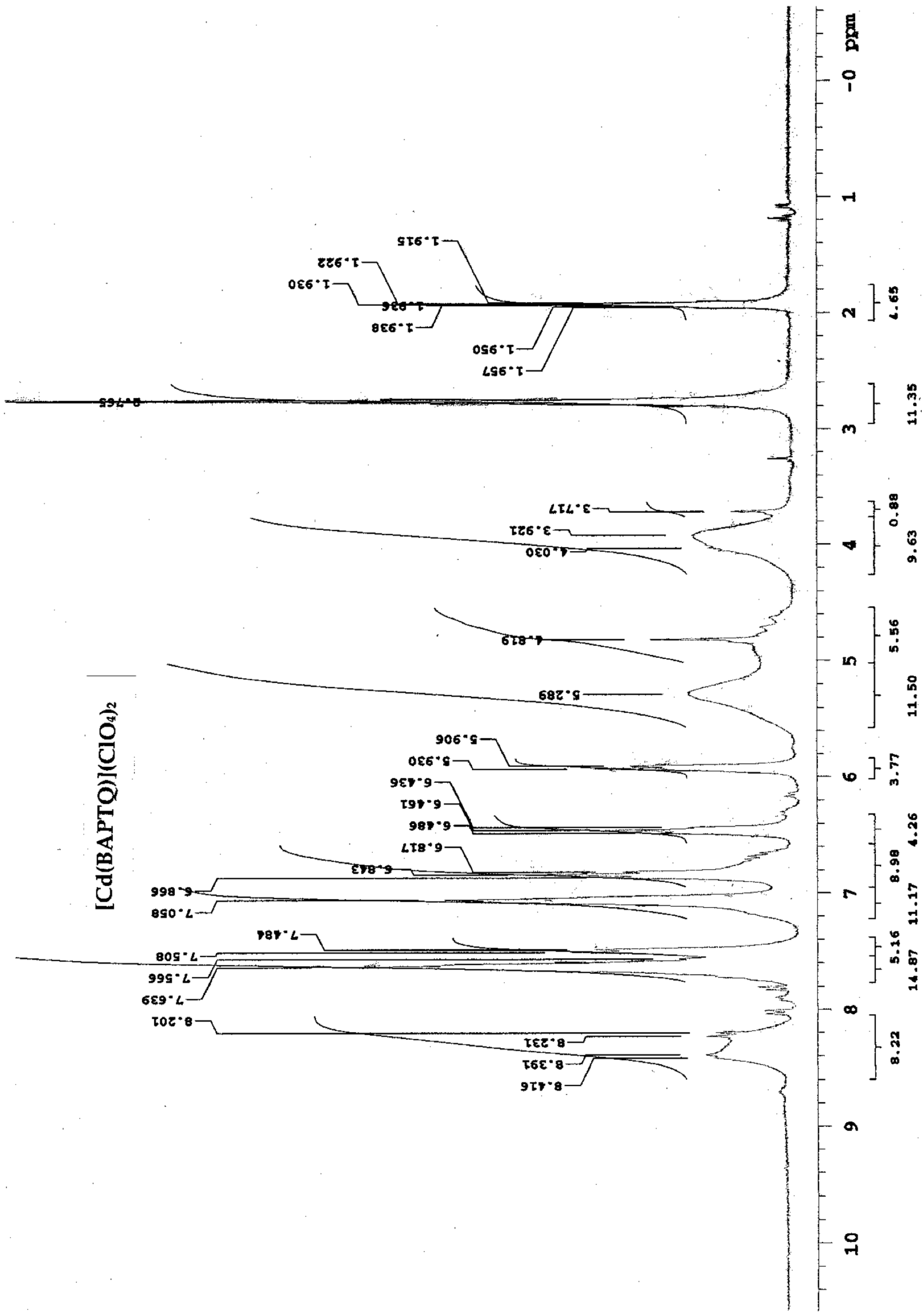


Fig. S60. ^{1}H NMR spectrum for $[Cd(BAPTQ)](ClO_4)_2$ in CD_3CN.

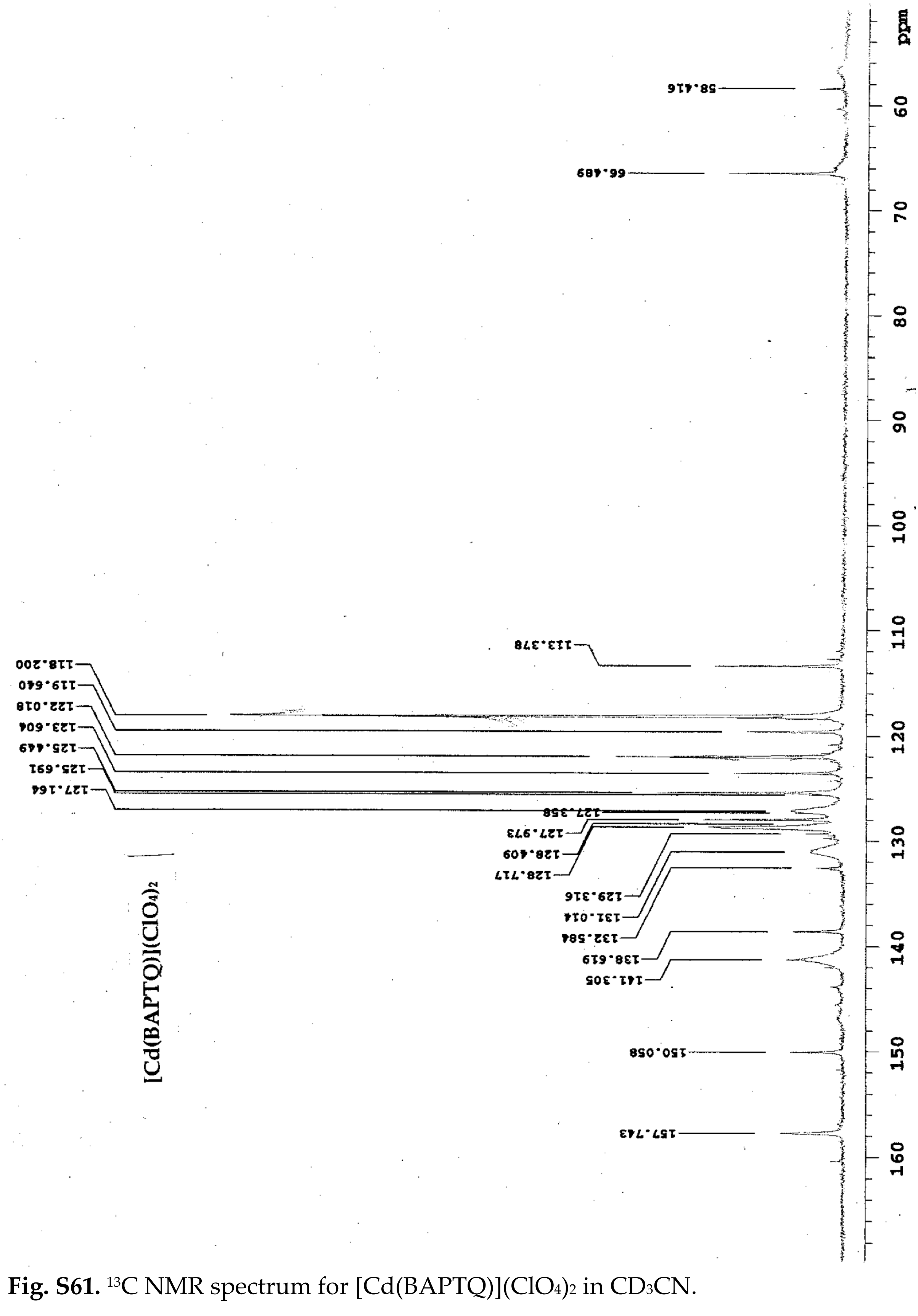


Fig. S61. [13]C NMR spectrum for $[Cd(BAPTQ)](ClO_4)_2$ in CD_3CN.

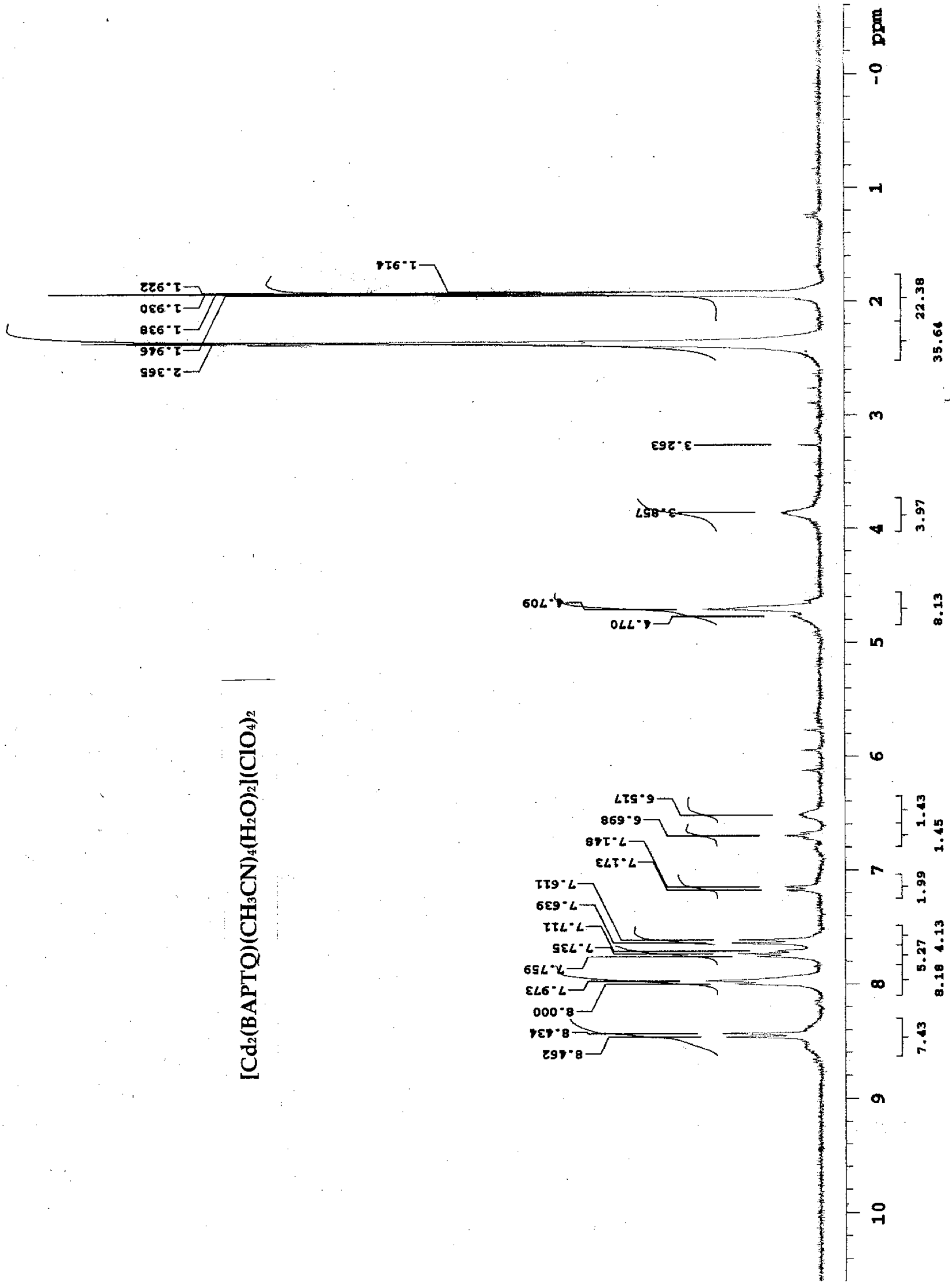


Fig. S62. [1]H NMR spectrum for $[Cd_2(BAPTQ)(CH_3CN)_4(H_2O)_2](ClO_4)_2$ in CD_3CN.

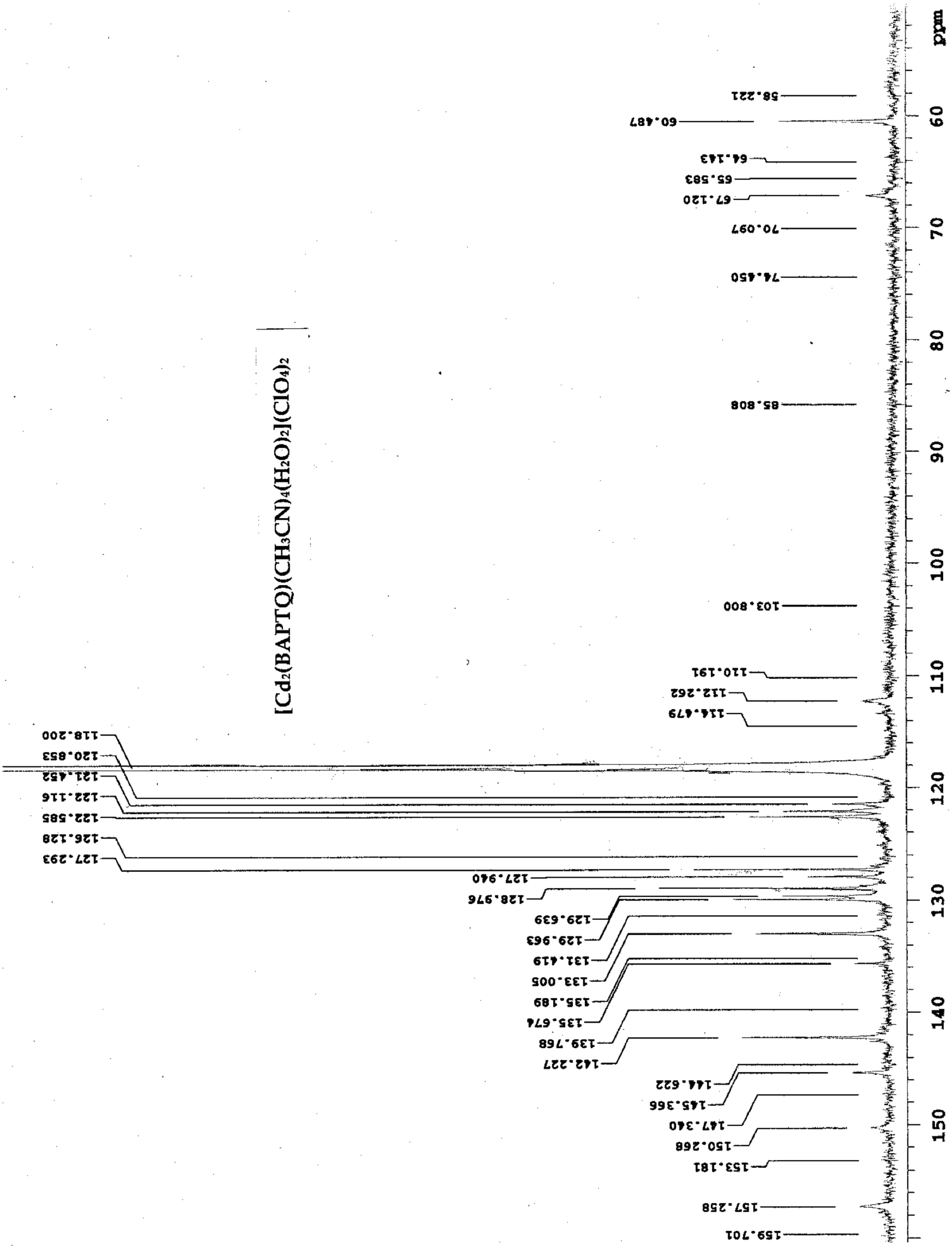


Fig. S63. ^{13}C NMR spectrum for $[Cd_2(BAPTQ)(CH_3CN)_4(H_2O)_2](ClO_4)_2$ in CD_3CN.

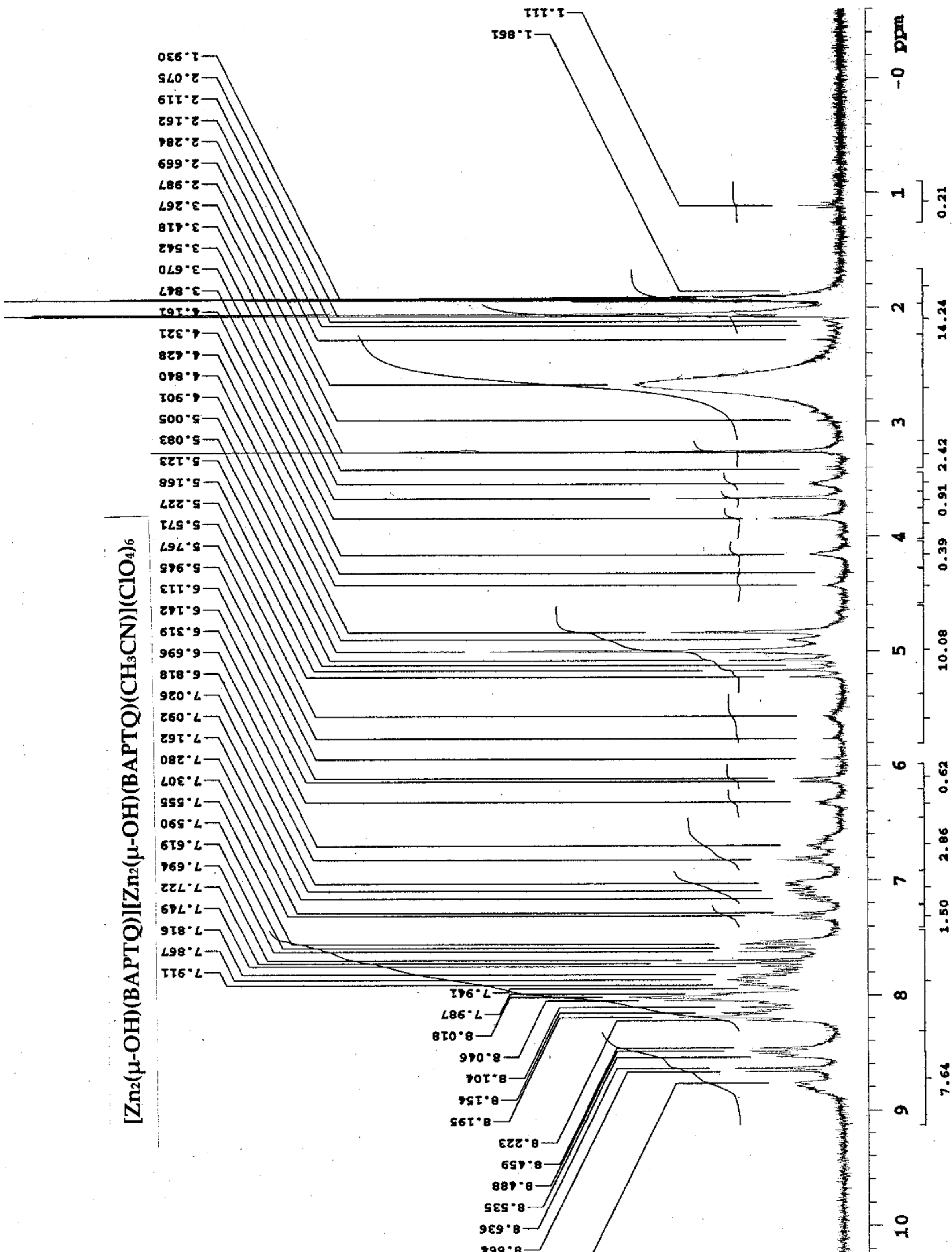


Fig. S64. ^{1}H NMR spectrum for $[Zn_2(\mu\text{-}OH)(BAPTQ)][Zn_2(\mu\text{-}OH)(BAPTQ)(CH_3CN)](ClO_4)_6$ in CD_3CN.

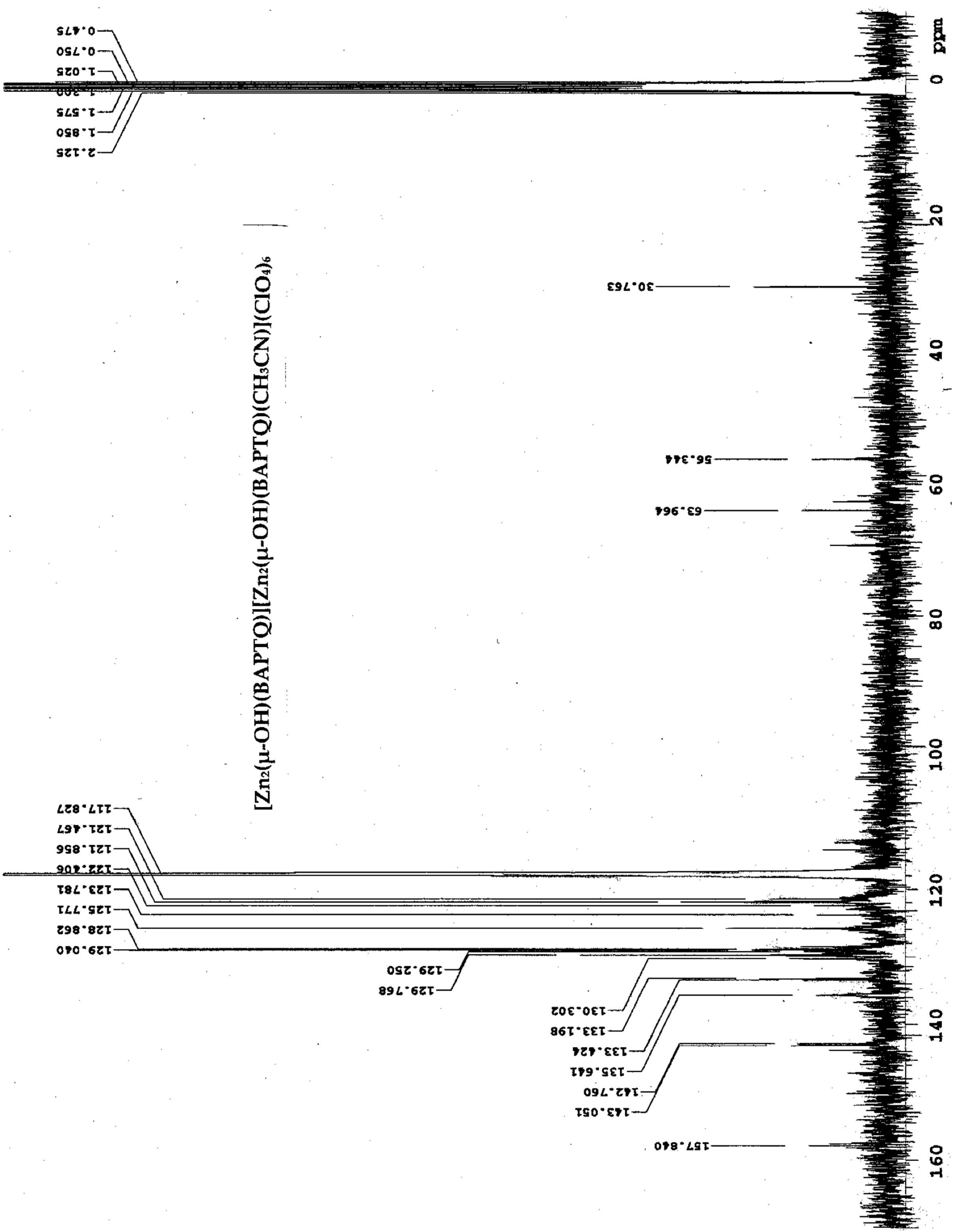


Fig. S65. ^{13}C NMR spectrum for $[Zn_2(\mu\text{-}OH)(BAPTQ)][Zn_2(\mu\text{-}OH)(BAPTQ)(CH_3CN)](ClO_4)_6$ in CD_3CN.