Supporting Information

Insighting the Inhibitory Potential of Metal Complexes Supported by (*E*)-2-Morpholino-*N*-(thiophen-2-ylmethylene)ethanamine: Synthesis, Structural Properties, Biological Evaluation and Docking Studies

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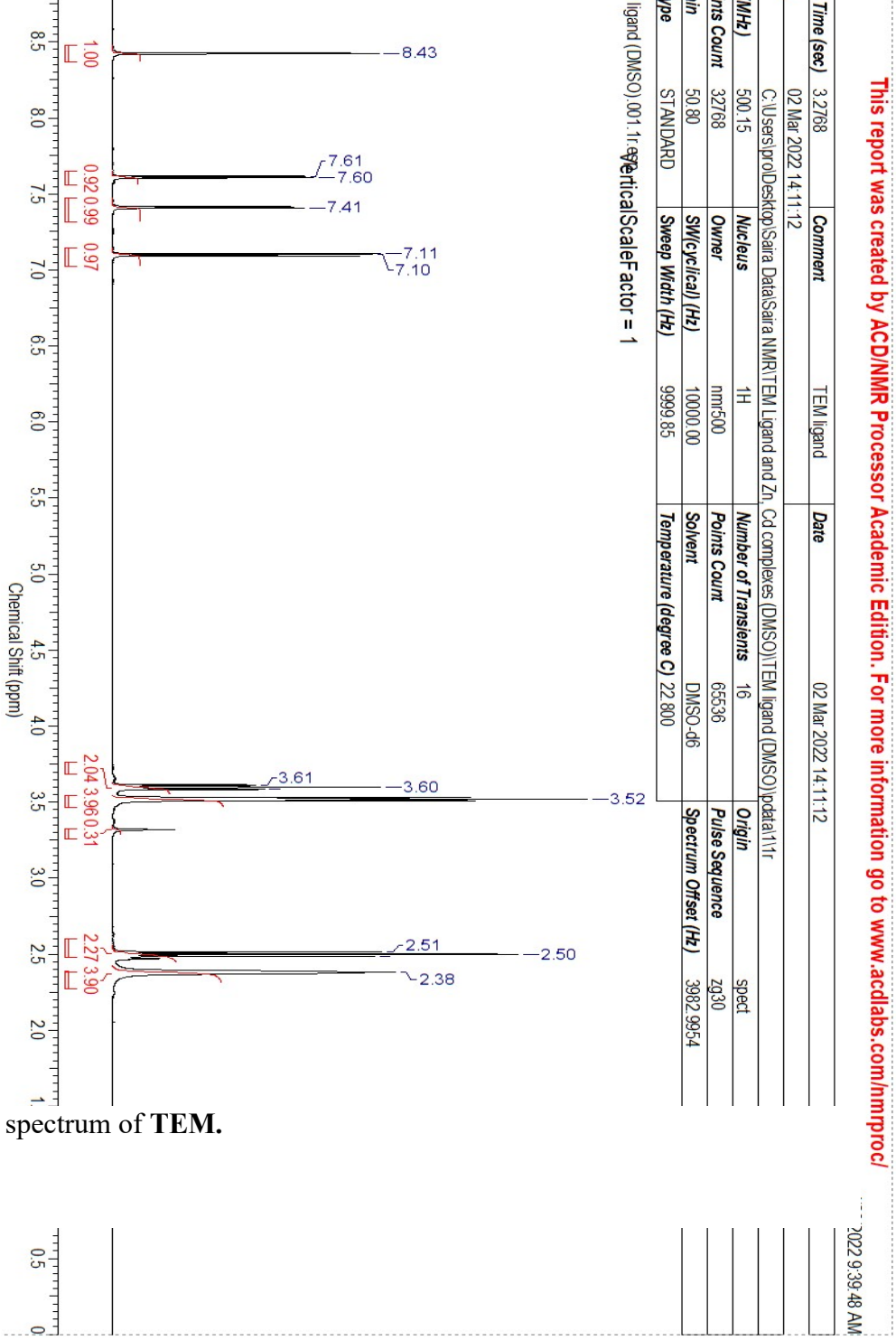

FIGURE S1. ^{1}H NMR spectrum of **TEM.**

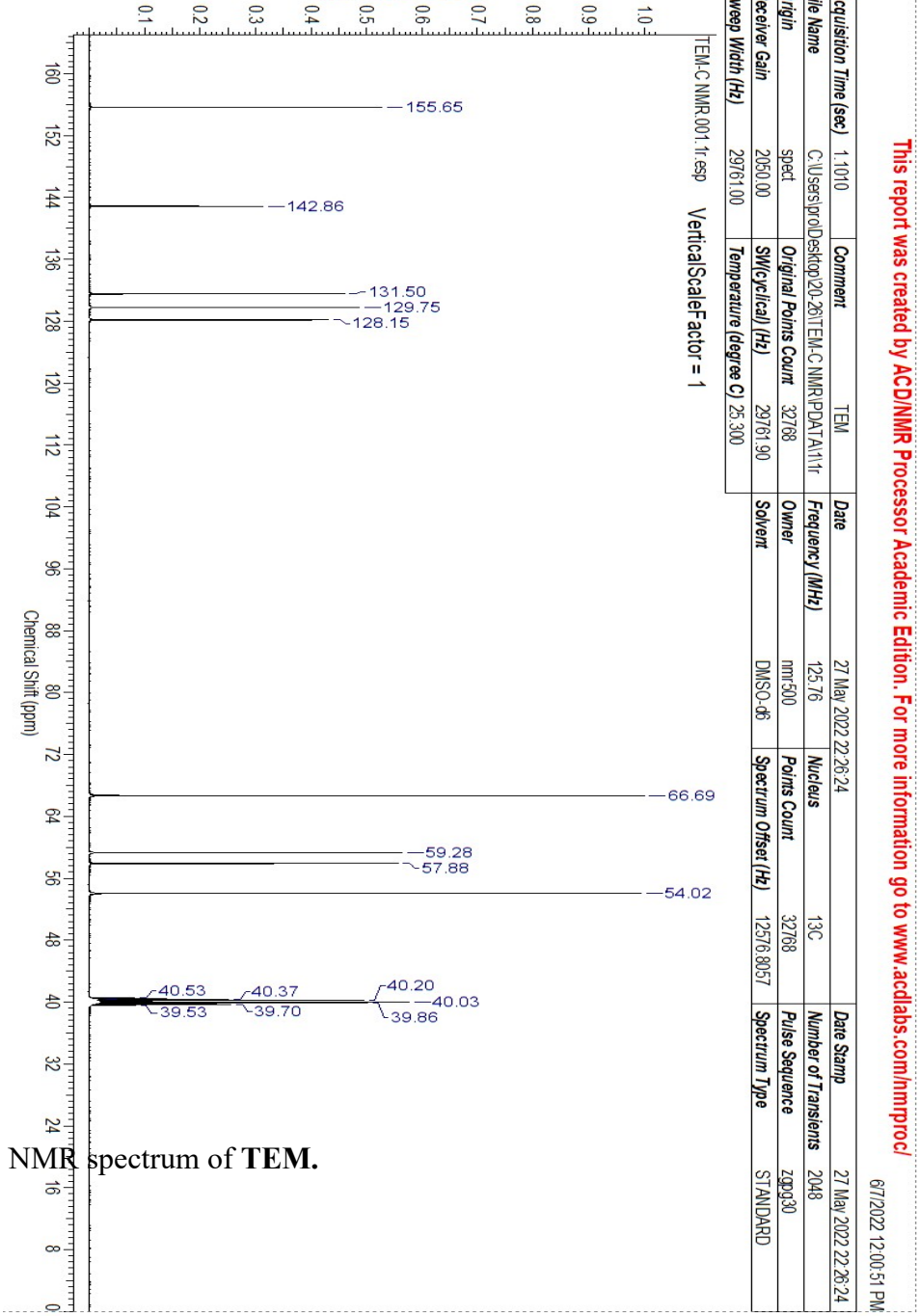

FIGURE S2. ^{13}C NMR spectrum of **TEM.**

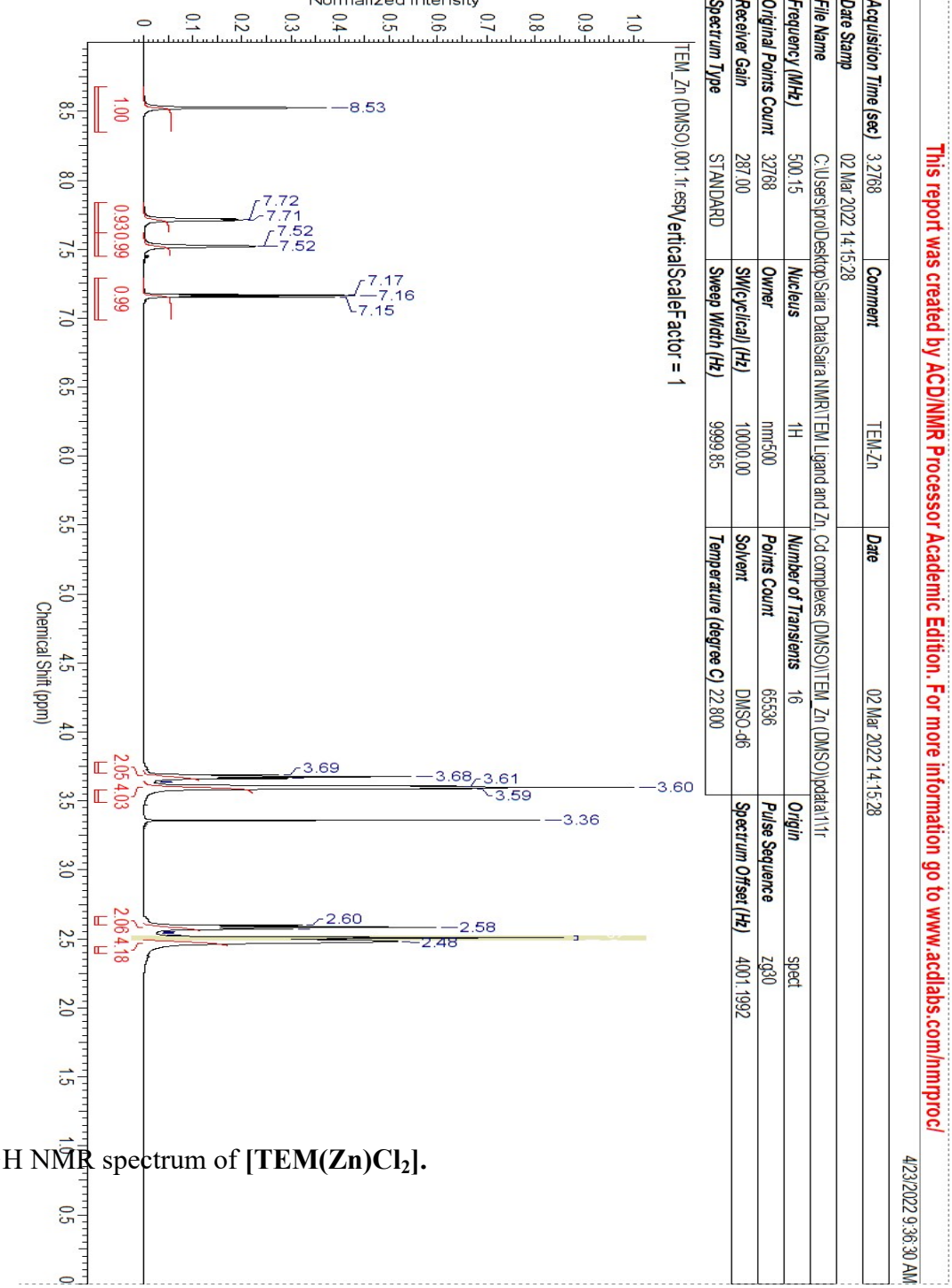

FIGURE S3. ^{1}H NMR spectrum of **[TEM(Zn)Cl_2].**

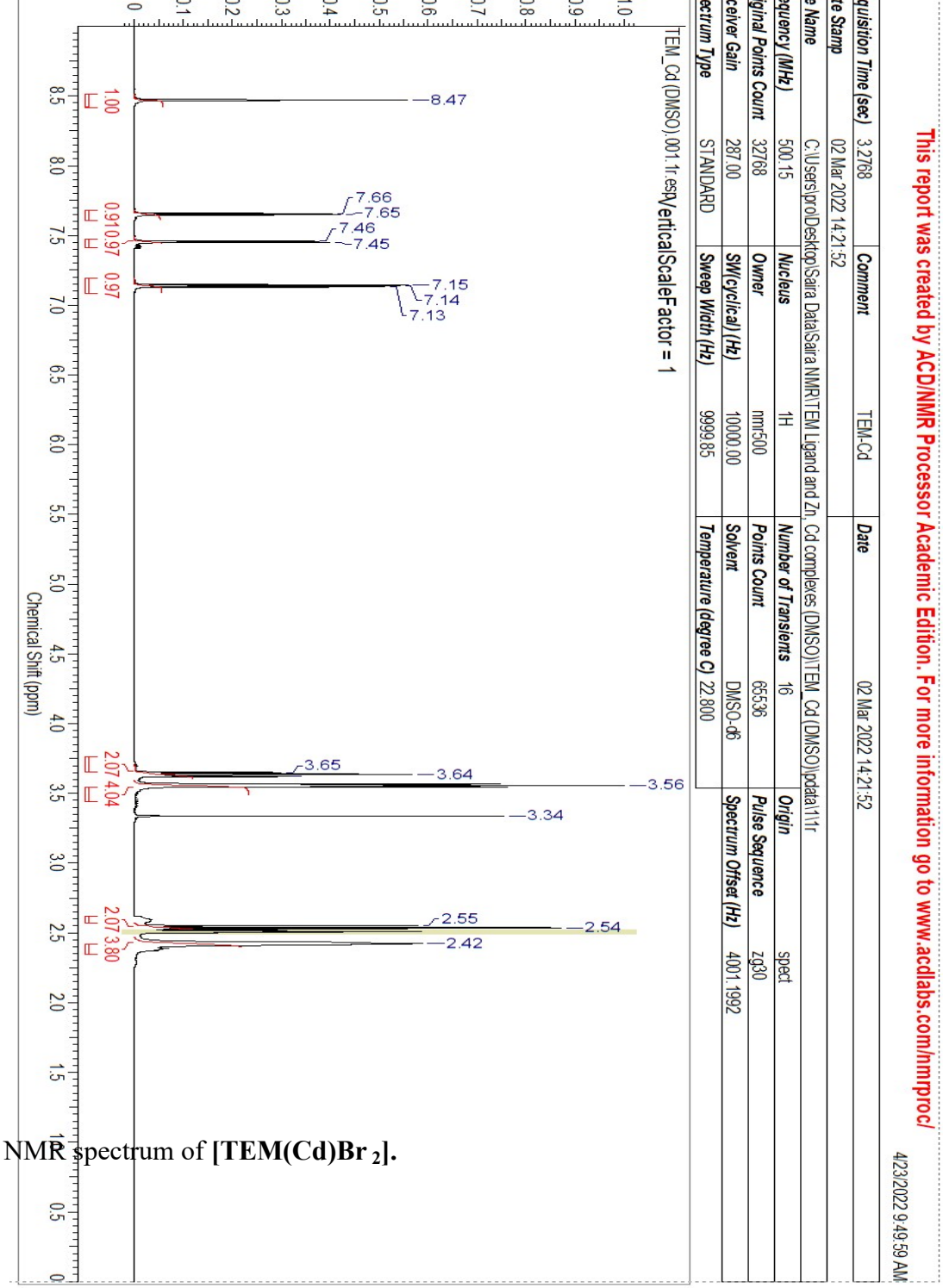

FIGURE S4. ^{1}H NMR spectrum of **[TEM(Cd)Br $_2$].**

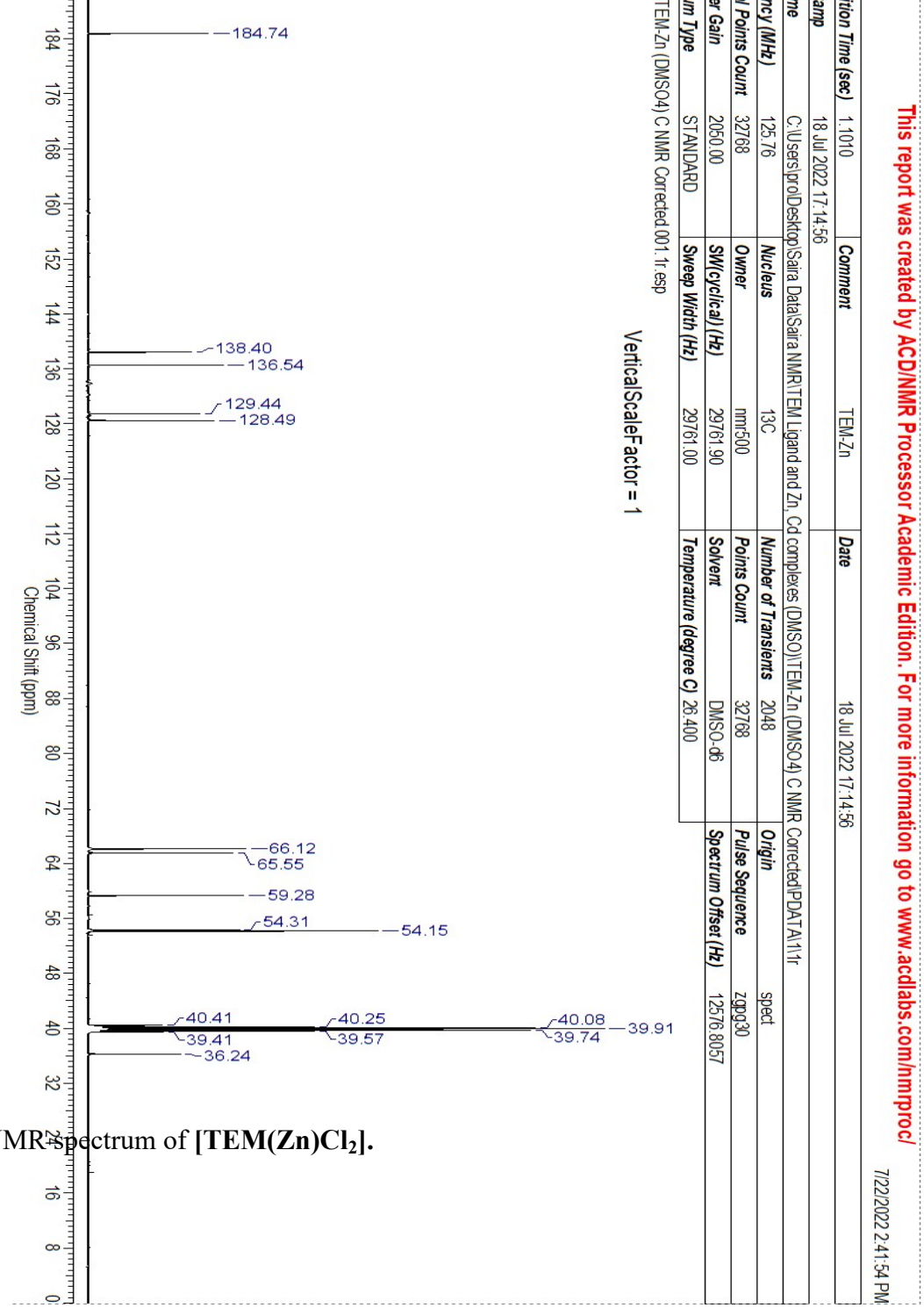

FIGURE S5. ^{13}C NMR spectrum of **[TEM(Zn)Cl_2].**

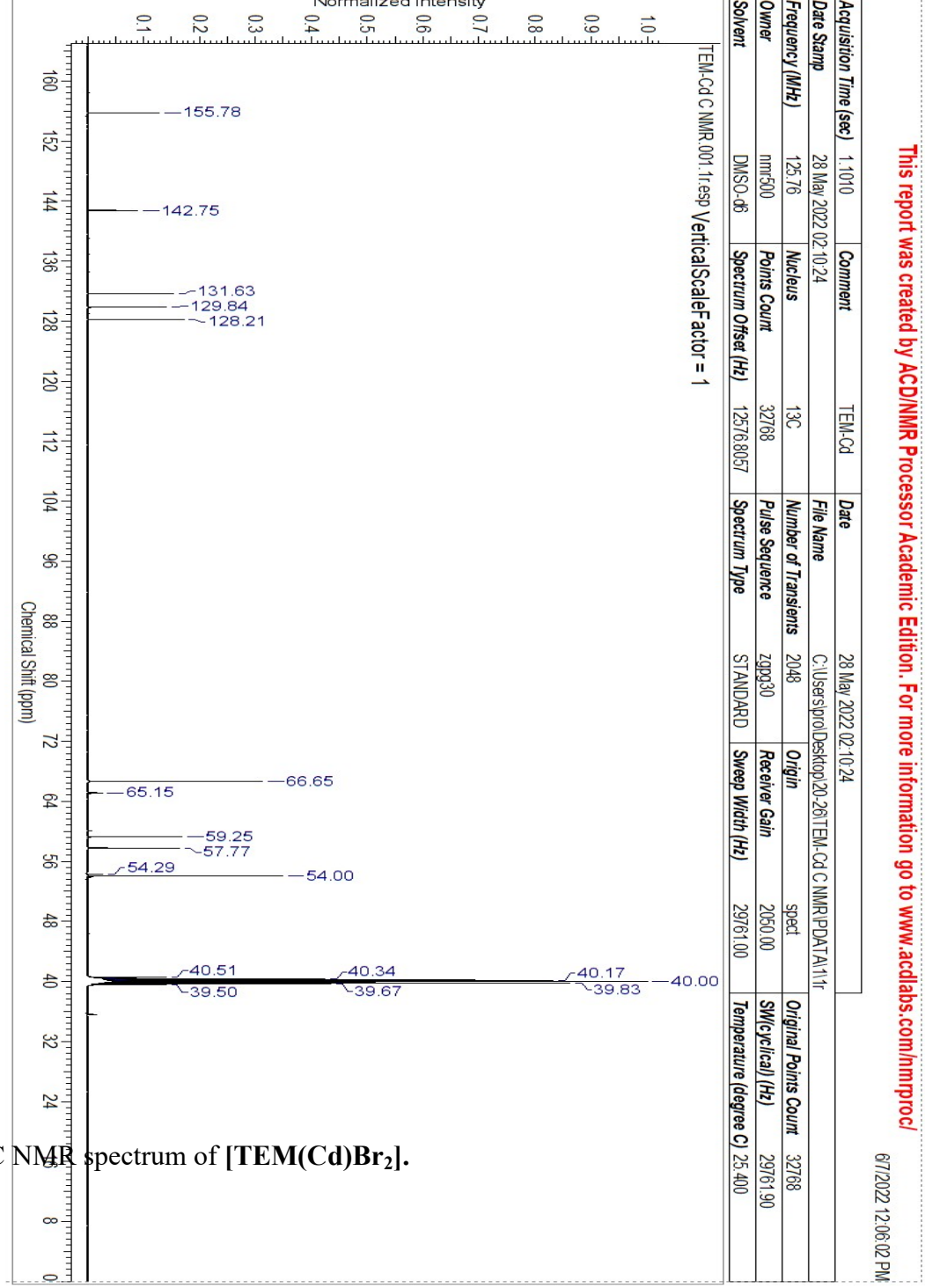

FIGURE S6. ^{13}C NMR spectrum of **[TEM(Cd)Br$_2$].**

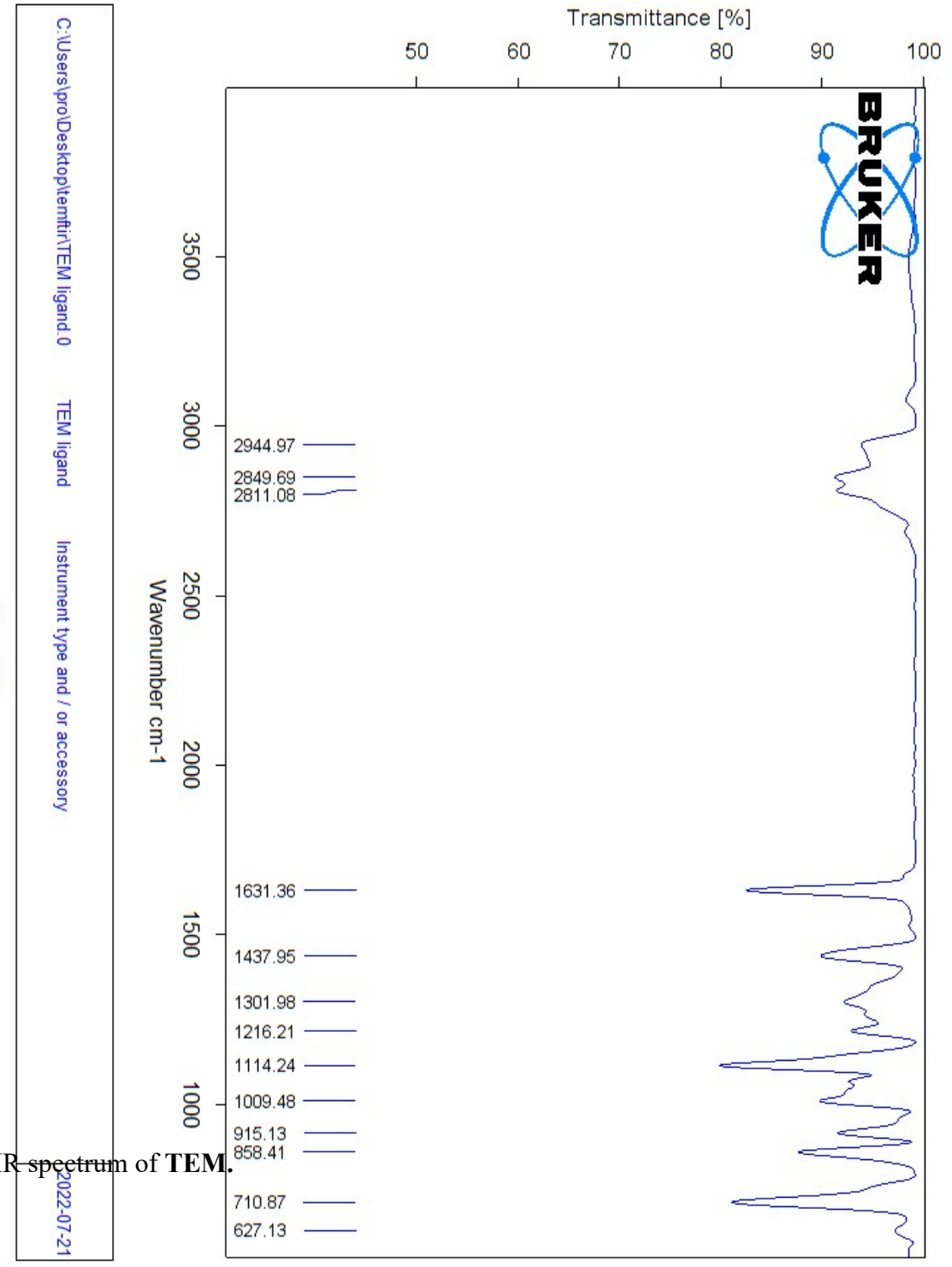

FIGURE S7. FTIR spectrum of **TEM.**

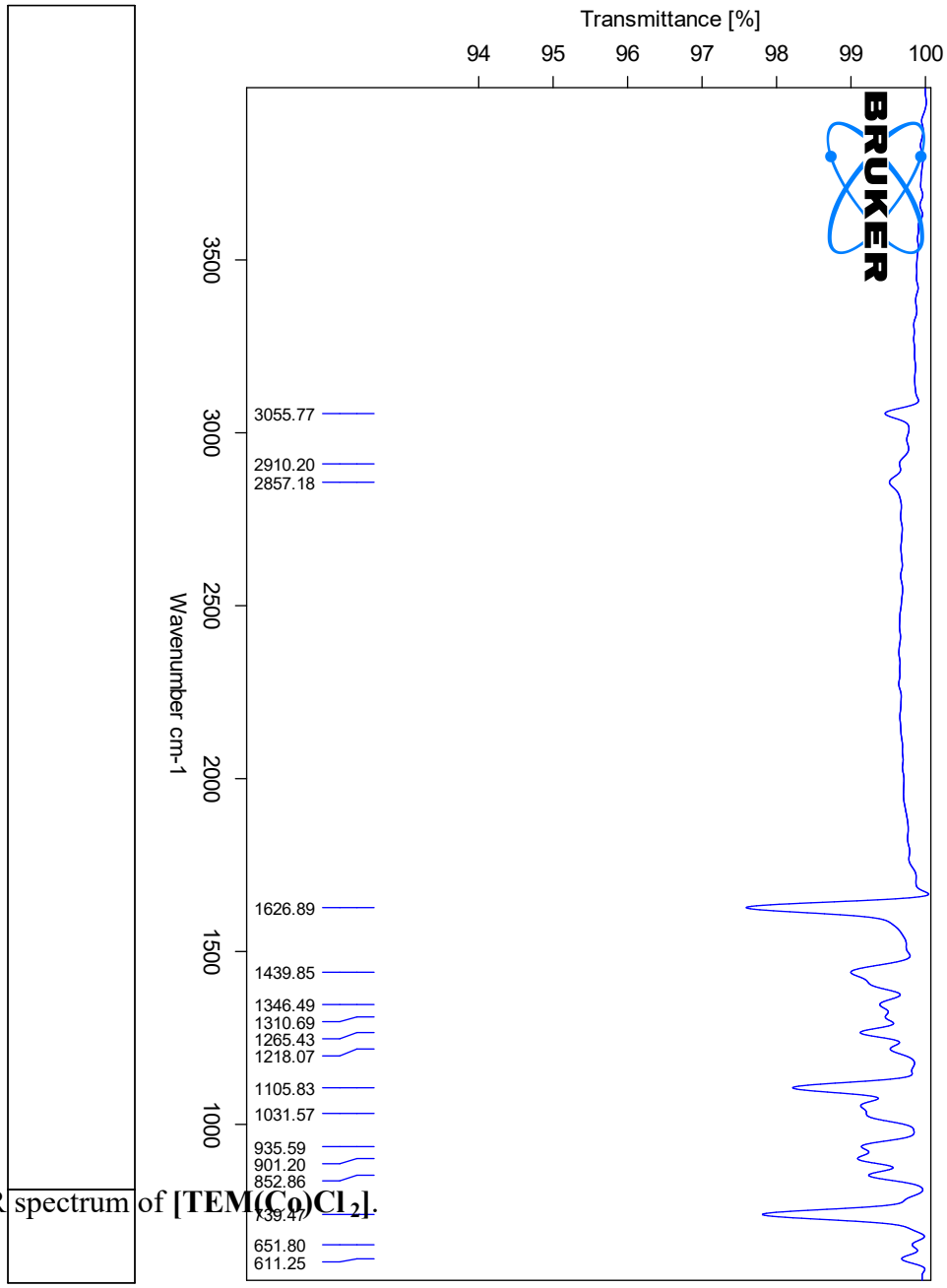

FIGURE S8. FTIR spectrum of **[TEM(Co)Cl$_2$]**.

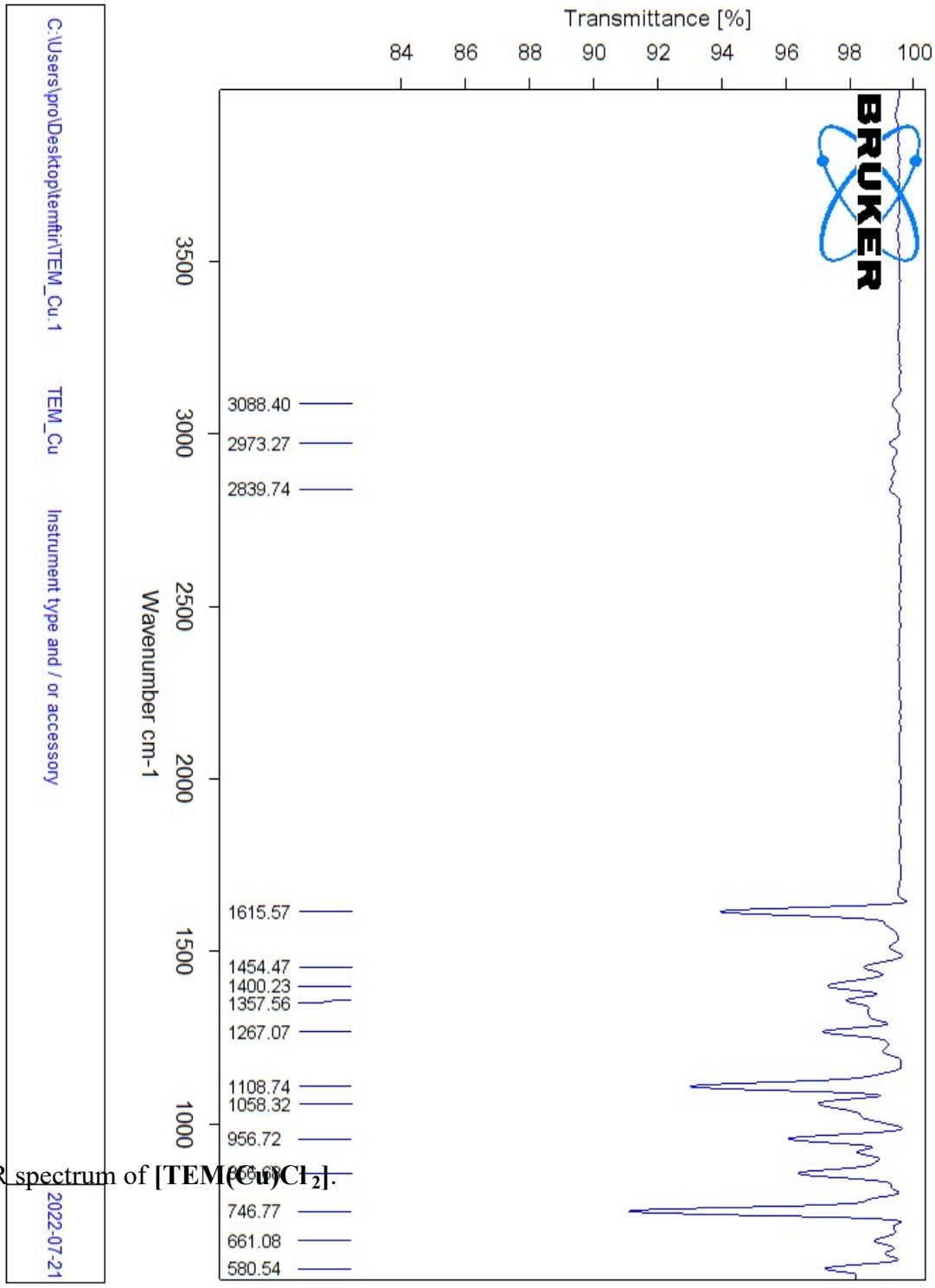

FIGURE S9. FTIR spectrum of **[TEM(Cu)Cl$_2$]**.

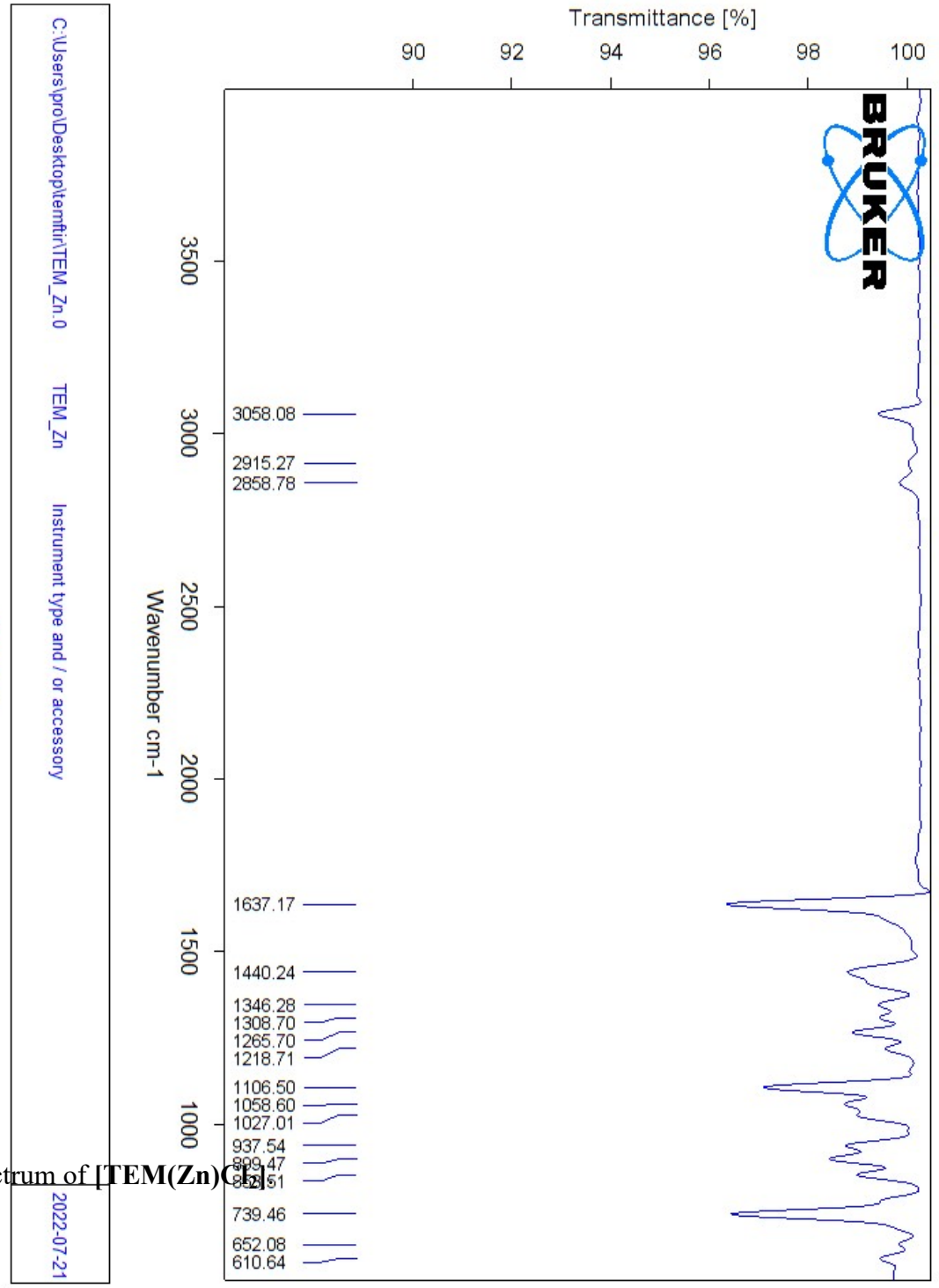

FIGURE S10. FTIR spectrum of **[TEM(Zn)Cl$_2$]**

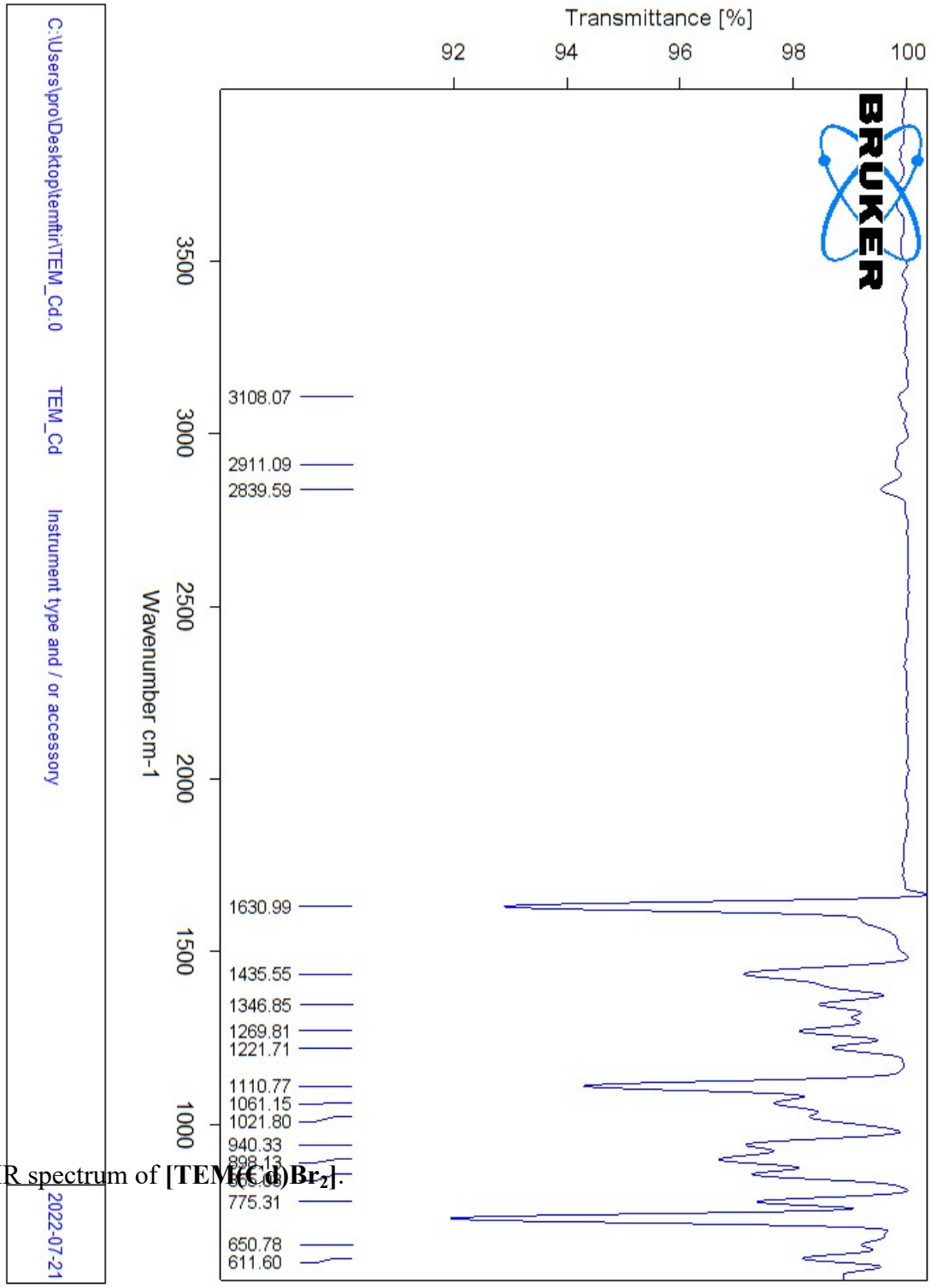

FIGURE S11. FTIR spectrum of **[TEM(Cd)Br_2]**.

EagerSmart Summarize Results

Date : 2022-03-10 at 10:01:48
Method Name : NCHS
Method Filename : EA-C_20220308.mth

Group No : 2 Sample Name	Element % Nitrogen	Carbon	Hydrogen	Sulphur
TEM-Cd	6.04276228	26.9035244	3.344803095	0
TEM-Cd	6.038705349	26.88916397	3.335220575	0

2 Sample(s) in Group No : 2

Component Name	Average
Nitrogen	6.040733814
Carbon	26.89634418
Hydrogen	3.340011835
Sulphur	0

Group No : 5 Sample Name	Element % Nitrogen	Carbon	Hydrogen	Sulphur
TEM-Zn	7.812420845	36.42247009	4.451468468	0
TEM-Zn	7.8266325	36.56750488	4.446727276	0

2 Sample(s) in Group No : 5

Component Name	Average
Nitrogen	7.819526672
Carbon	36.49498749
Hydrogen	4.449097872
Sulphur	0

Group No : 2 Sample Name	Element % Nitrogen	Carbon	Hydrogen	Sulphur
TEM-Cu	8.198022842	36.31325531	4.618414402	0
TEM-Cu	8.262527466	36.41964722	4.642665863	0

2 Sample(s) in Group No : 2

Component Name	Average
Nitrogen	8.230275154
Carbon	36.36645126
Hydrogen	4.630540133
Sulphur	0

Group No : 5 Sample Name	Element % Nitrogen%	Carbon%	Hydrogen%	Sulphur%
TEM-Co(EtOH)	7.748516083	36.93906403	4.580291271	0
TEM-Co(EtOH)	7.747725964	36.99332428	4.601635456	0

2 Sample(s) in Group No : 5

Component Name	Average
Nitrogen%	7.748121023
Carbon%	36.96619415
Hydrogen%	4.590963364
Sulphur%	0

FIGURE S12. Summary of elemental analysis of synthesized complexes.

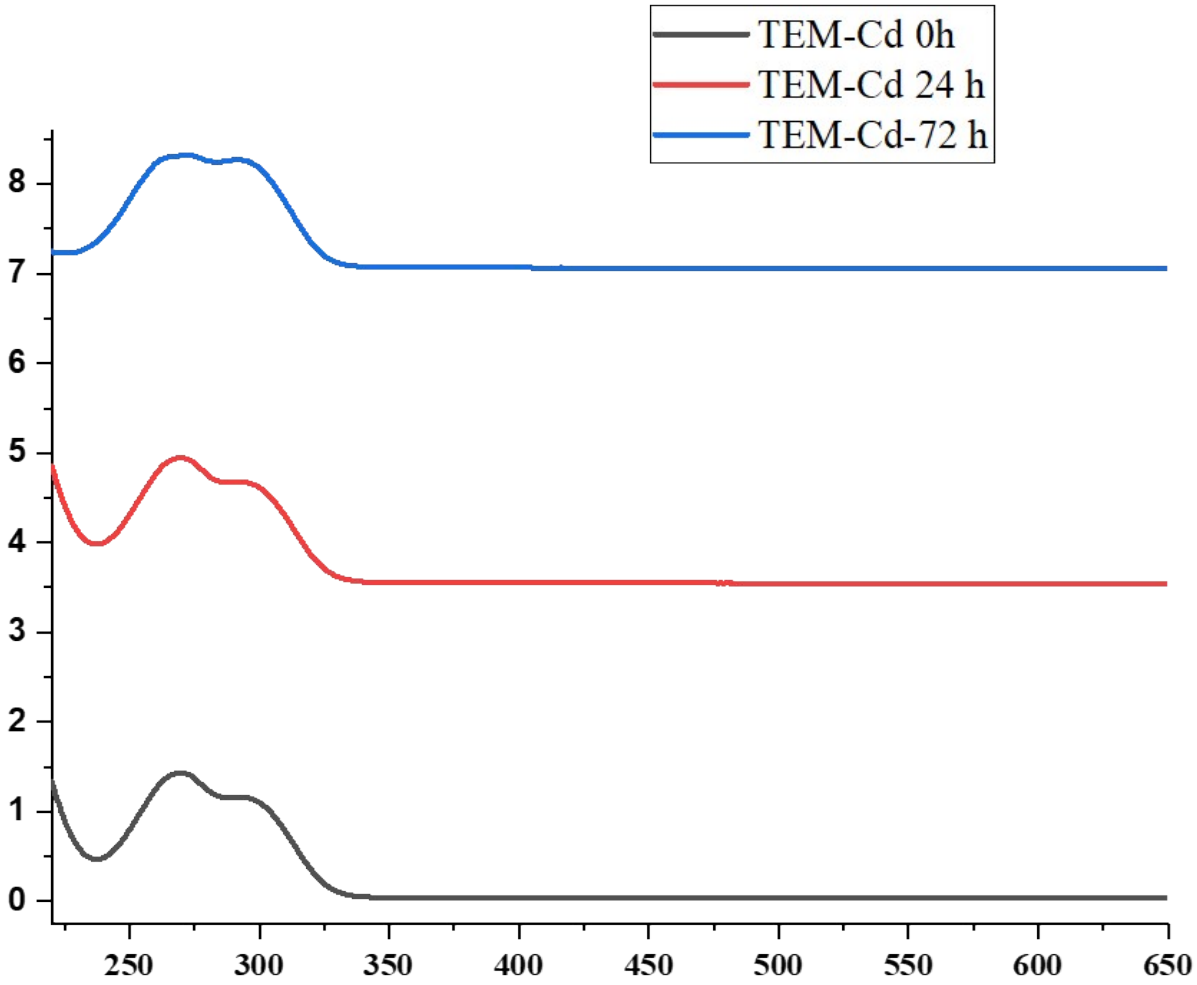

FIGURE S13. Time stability of complex **[TEM(Cd)Br_2]** followed by UV-Vis spectrophotometry at room temperature in acetonitrile.

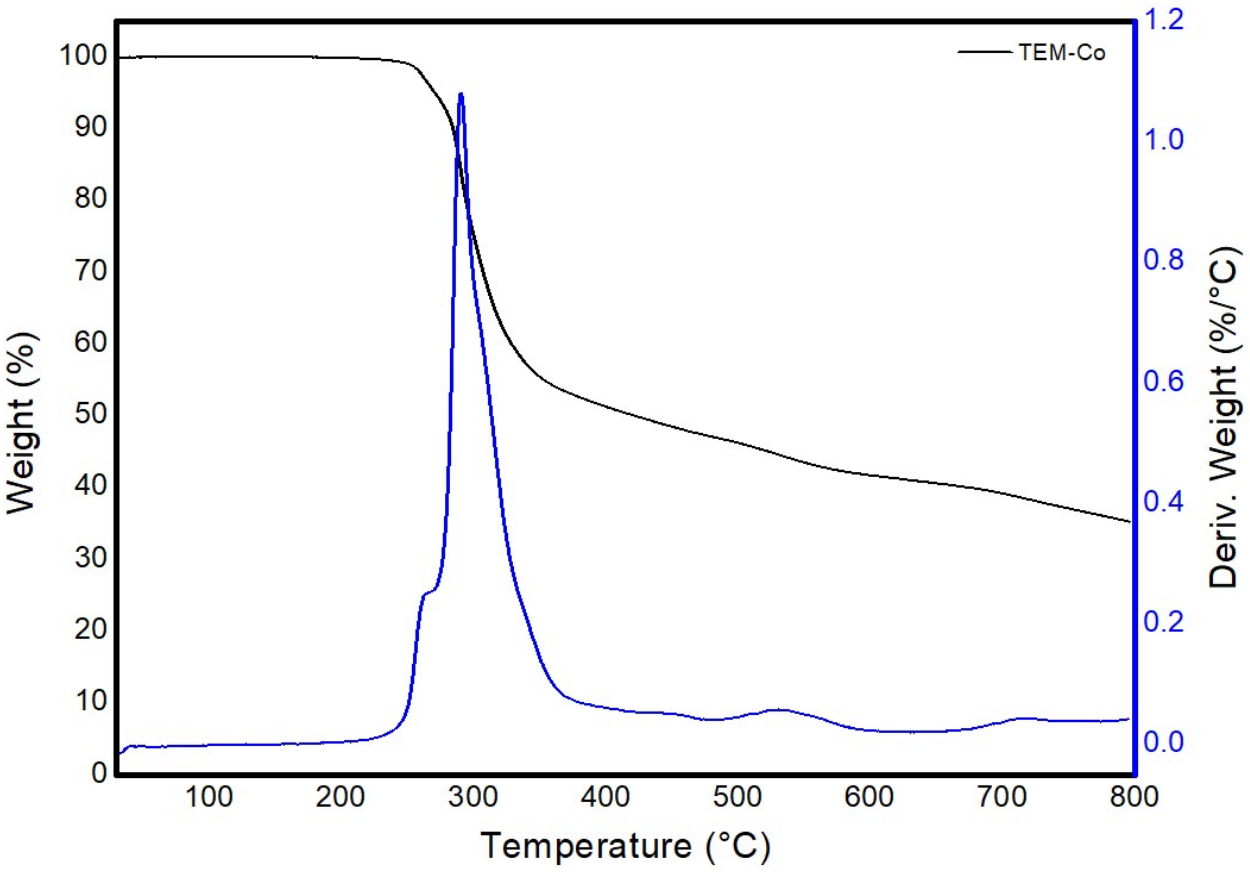

FIGURE S14. TGA thermogram of **[TEM(Co)Cl_2]**.

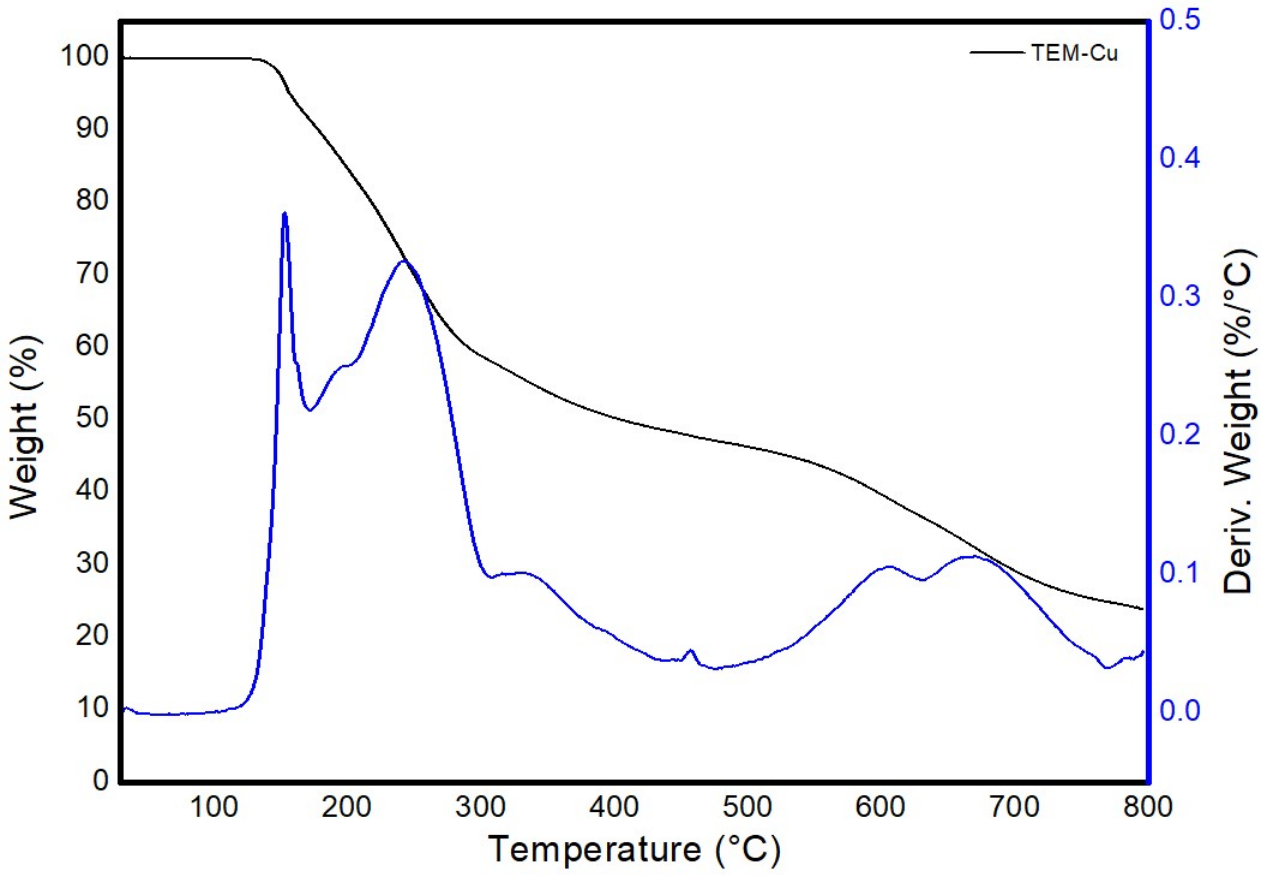

FIGURE S15. TGA thermogram of **[TEM(Cu)Cl_2]**.

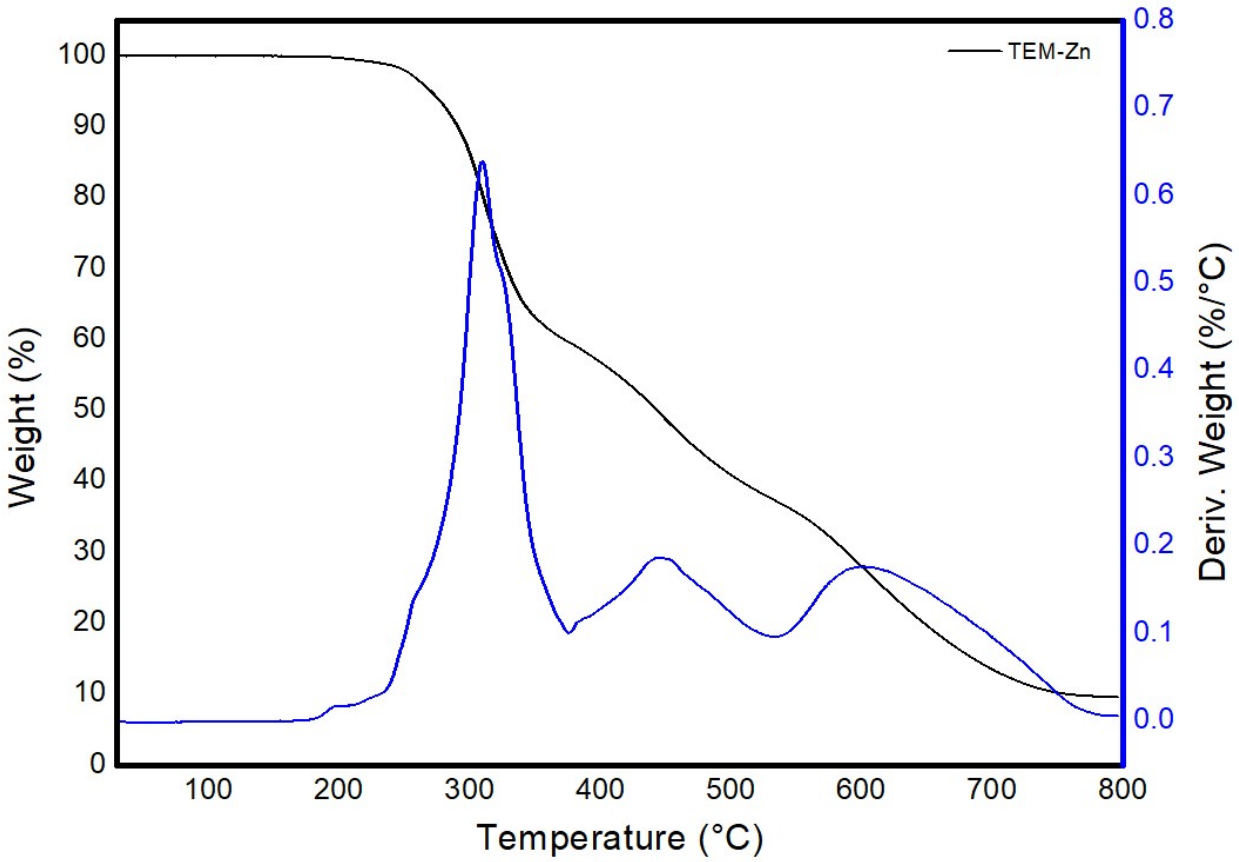

FIGURE S16. TGA thermogram of **[TEM(Zn)Cl_2]**.

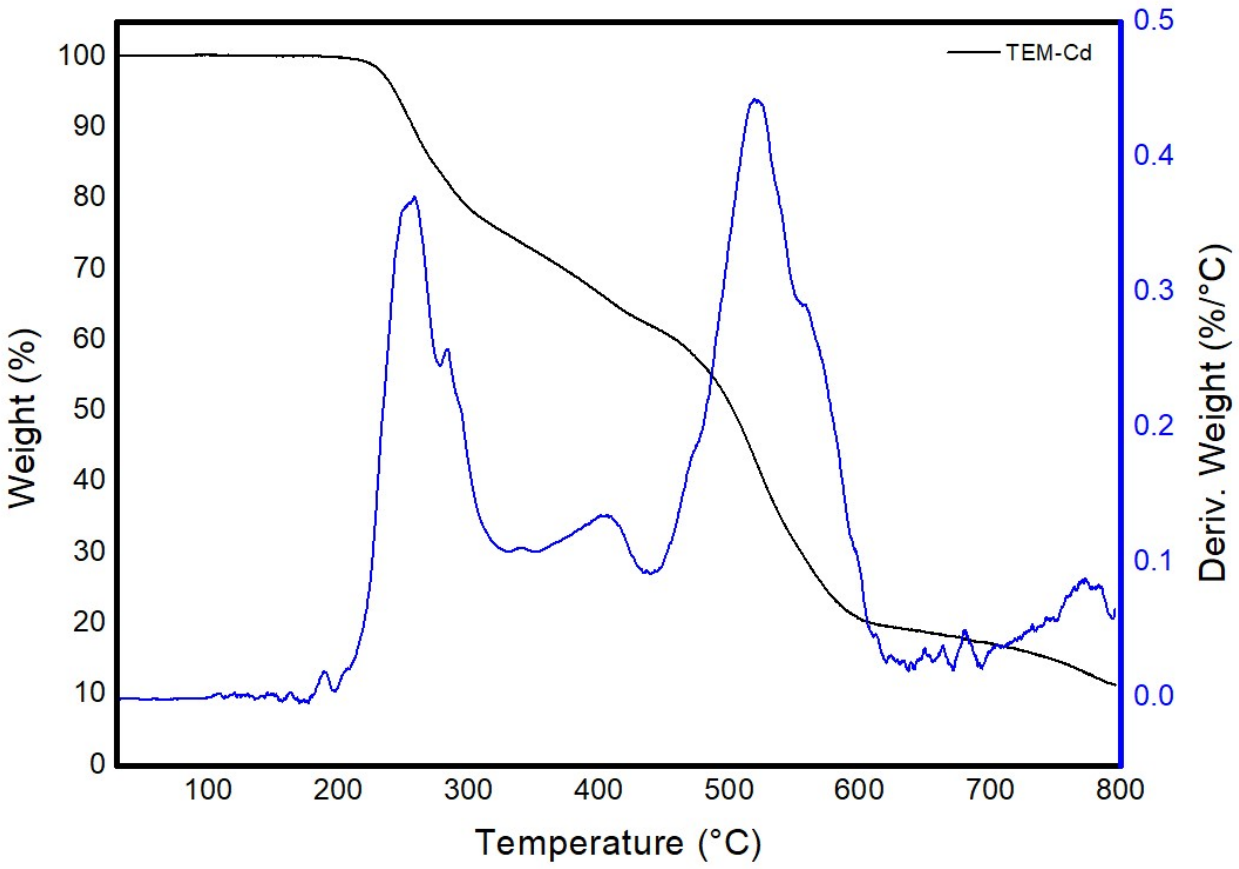

FIGURE S17. TGA thermogram of **[TEM(Cd)Br_2]**.

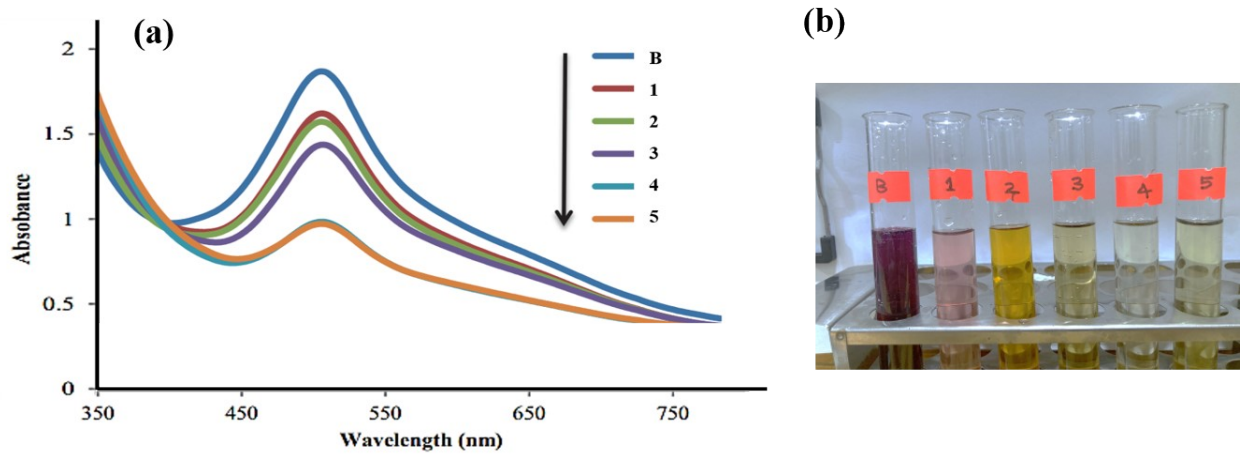

FIGURE S18. (a) Representative absorption spectra of DPPH in the presence and absence of **[TEM(Cd)Br_2]**. **(b)** The arrow represents the decrease in absorption with increasing concentration; the change in the solution colour is also shown.

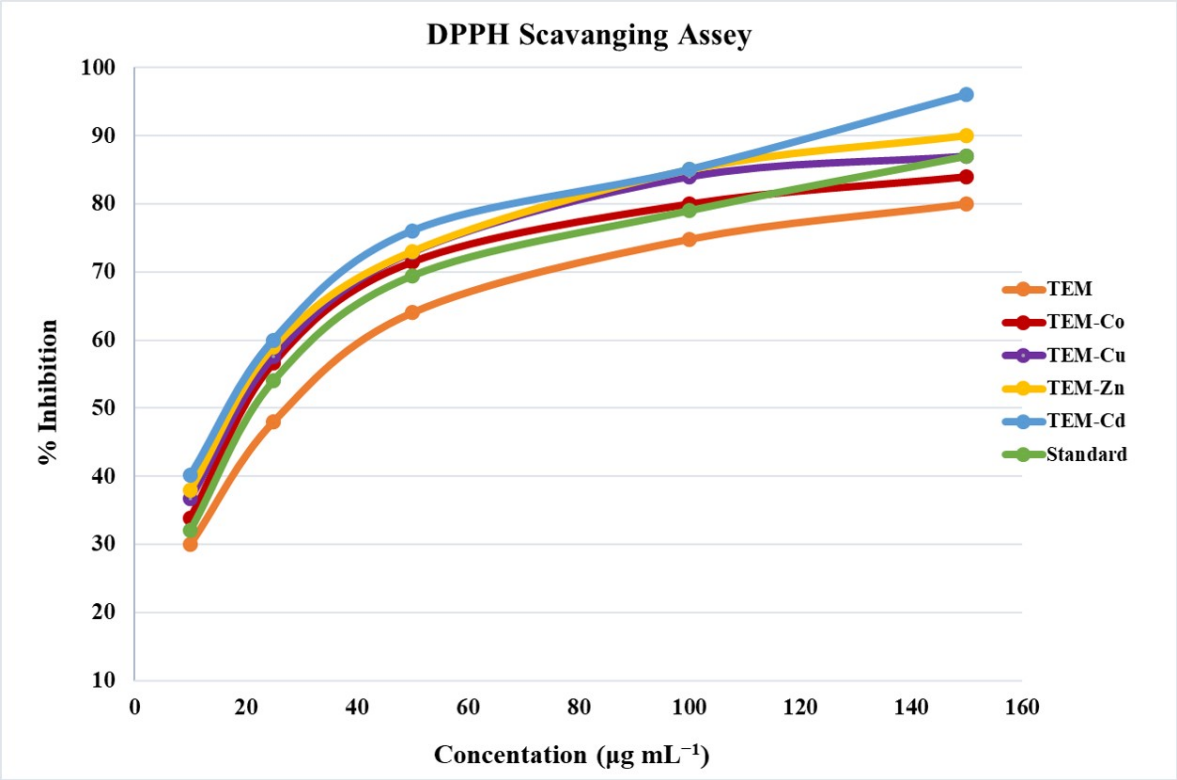

FIGURE S19. Antioxidant activity of TEM and corresponding M(II) complexes.

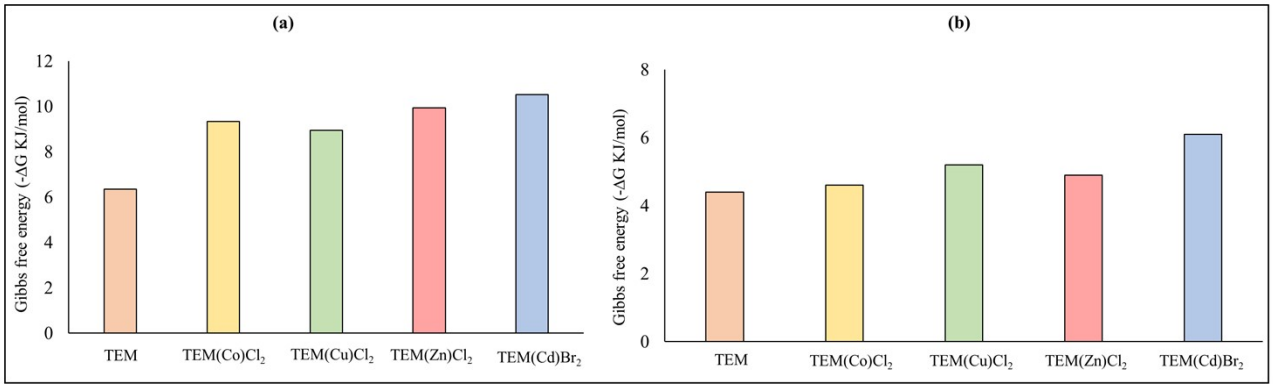

FIGURE S20. Calculated Gibbs free energy of TEM and their metal complexes with **(a)** 2JK6 and (**b**) 2UBP from molecular docking results.

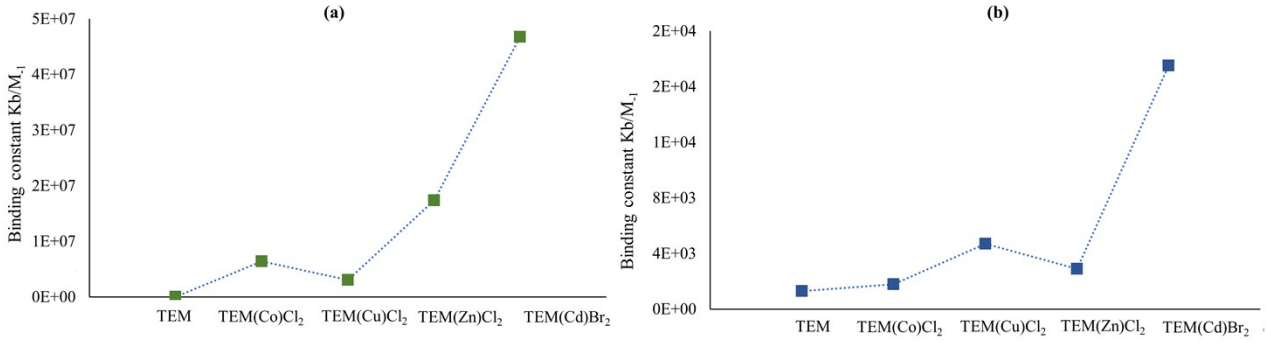

FIGURE S21. Calculated binding constant of **TEM** and their metal complexes with (a) 2JK6 and (b) 2UBP from molecular docking results.

TABLE S1. Structure refinement and crystallographic data of **[TEM(M)X_2]**, (M = Co, Zn; X = Cl; M = Cd, X = Br) complexes.

	[TEM(Co)Cl_2]	**[TEM(Zn)Cl_2]**	**[TEM(Cd)Br_2].CH_2Cl_2**
Empirical formula	$C_{11}H_{16}Cl_2CoN_2OS$	$C_{11}H_{16}Cl_2N_2OSZn$	$C_{11}H_{16}Br_2CdN_2OS.\ CH_2Cl_2$
Formula weight	354.14	360.59	581.46
Temperature (K)	293(2)	293(2)	293(2)
Wavelength (Å)	0.71073	0.71073	0.71073
Crystal system	Triclinic	Triclinic	Monoclinic
Space group	P-1	P-1	$P2_1/c$
Unit cell dimensions			
a (Å)	8.4030(4)	8.4460(4)	8.6766(3)
b (Å)	9.2421(3)	9.2335(4)	15.4523(6)
c (Å)	9.9135(6)	9.9636(5)	14.4470(4)
α (°)	90.781(4)	90.682(4)	90
β (°)	108.380(5)	108.394(4)°	97.237(3)
γ (°)	90.619(3)	90.304(4)°	90
Volume ($Å^3$)	730.46(6)	737.24(6)	1921.53(11)

Z	2	2	4
Density (calculated) (Mg/m^3)	1.610	1.624	2.010
Absorption coefficient (mm^{-1})	1.659	2.158	5.668
F(000)	362	368	1120
Crystal size (mm^3)	0.143 × 0.121 × 0.089	0.125 × 0.058 × 0.010	0.125 × 0.105 × 0.075
θ range for data collection (°)	2.165 to 30.661	2.154 to 26.366	1.938 to 26.371
Index ranges	-11<=h<=11, -13<=k<=13, -13<=l<=13	-10<=h<=10, -11<=k<=11, -12<=l<=12	-10<=h<=10, -19<=k<=19, -17<=l<=18
Reflections collected	12637	9294	14902
Independent reflections	4212 [R(int) = 0.0440]	2981 [R(int) = 0.0318]	3927 [R(int) = 0.0362]
Completeness to θ = 25.242°	99.4	99.2	100.0
Absorption correction	Semi-empirical from equivalents	Semi-empirical from equivalents	Semi-empirical from equivalents
Refinement method	Full-matrix least-squares on F^2	Full-matrix least-squares on F^2	Full-matrix least-squares on F^2
Data/restraints/parameters	4212 / 0 / 163	2987 / 0 / 163	3927 / 0 / 190
Goodness-of-fit on F^2	1.097	1.073	1.122

Final R indices [$I>2\sigma(I)$]	$R_1 = 0.0452$, $wR_2 = 0.1223$	$R_1 = 0.0356$, $wR_2 = 0.0873$	$R_1 = 0.0395$, $wR_2 = 0.0938$
R indices (all data)	$R_1 = 0.0667$, $wR_2 = 0.1404$	$R_1 = 0.0463$, $wR_2 = 0.0916$	$R_1 = 0.0549$, $wR_2 = 0.1064$
Largest diff. peak and hole (e.Å^{-3})	0.657 and -0.979	0.442 and -0.549	0.581 and -0.966

TABLE S2. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($Å^2$ $\times 10^3$) for **[TEM(Co)Cl_2]**. U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
Co(1)	5047(1)	3420(1)	2592(1)	34(1)
Cl(1)	6096(1)	3099(1)	4921(1)	53(1)
S(1)	8139(1)	5958(1)	3330(1)	66(1)
O(1)	2101(3)	-355(2)	1654(3)	62(1)
N(1)	4137(3)	5413(2)	1945(2)	37(1)
C(1)	4768(3)	6693(3)	2064(3)	40(1)
Cl(2)	6627(1)	2447(1)	1400(1)	58(1)
N(2)	2490(3)	2742(2)	2065(2)	35(1)
C(2)	6502(3)	7115(3)	2648(3)	43(1)
C(3)	7084(4)	8543(3)	2773(3)	52(1)
C(4)	8781(5)	8661(4)	3393(4)	73(1)
C(5)	9526(4)	7360(5)	3750(4)	74(1)
C(6)	2293(3)	5297(3)	1331(3)	45(1)
C(7)	1670(3)	4146(3)	2124(3)	42(1)
C(8)	1758(4)	2043(3)	635(3)	45(1)
C(9)	2435(4)	533(3)	606(3)	55(1)
C(10)	2125(4)	1760(3)	3114(3)	45(1)
C(11)	2825(4)	288(3)	3026(4)	57(1)

TABLE S3. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$ × 10^3) for **[TEM(Zn)Cl_2]**. U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
Zn(1)	4941(1)	6611(1)	7403(1)	34(1)
Cl(1)	3928(1)	6911(1)	5086(1)	51(1)
S(1)	1842(1)	4057(1)	6640(1)	64(1)
O(1)	7915(4)	10355(3)	8347(3)	62(1)
N(1)	5834(3)	4577(3)	8045(3)	36(1)
C(1)	5204(4)	3306(3)	7916(3)	38(1)
Cl(2)	3409(1)	7559(1)	8628(1)	56(1)
N(2)	7523(3)	7253(3)	7948(3)	34(1)
C(2)	3480(4)	2896(4)	7335(3)	41(1)
C(3)	2906(5)	1467(4)	7214(4)	47(1)
C(4)	1175(6)	1362(5)	6589(5)	68(1)
C(5)	452(5)	2656(5)	6231(5)	73(1)
C(6)	7673(4)	4690(4)	8664(4)	44(1)
C(7)	8299(4)	5830(3)	7884(4)	42(1)
C(8)	8255(4)	7949(4)	9368(3)	44(1)
C(9)	7589(5)	9465(4)	9402(4)	54(1)
C(10)	7206(5)	9715(4)	6993(4)	55(1)
C(11)	7889(4)	8228(4)	6904(4)	44(1)

TABLE S4. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$ × 10^3) for **[TEM(Cd)Br_2]·CH_2Cl_2**. U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
Cd(1)	3909(1)	6906(1)	6223(1)	38(1)
Br(1)	1390(1)	7368(1)	6788(1)	51(1)
Cl(1)	-742(1)	4643(1)	8074(1)	65(1)
S(1)	2622(2)	4834(1)	6302(1)	60(1)
O(1)	6428(4)	9303(2)	6298(2)	61(1)
N(1)	4536(3)	8018(2)	5235(2)	34(1)
C(1)	2902(4)	5503(3)	4527(3)	45(1)
Br(2)	6150(1)	6364(1)	7340(1)	63(1)
Cl(2)	-281(2)	6134(1)	9292(1)	89(1)
N(2)	3543(4)	6215(2)	4807(2)	40(1)
C(2)	2338(5)	4844(3)	5103(3)	46(1)
C(3)	1465(5)	4142(3)	4760(3)	52(1)
C(4)	1042(5)	3618(3)	5476(4)	59(1)
C(5)	1581(6)	3903(3)	6332(3)	62(1)
C(6)	4039(5)	6809(3)	4100(3)	48(1)
C(7)	3701(5)	7735(3)	4324(2)	43(1)
C(8)	3929(5)	8871(2)	5492(3)	44(1)
C(9)	4814(5)	9208(3)	6379(3)	58(1)
C(10)	7038(5)	8494(3)	6068(3)	58(1)
C(11)	6223(4)	8130(3)	5176(3)	50(1)
C(12)	202(6)	5628(3)	8307(4)	73(1)