Supplementary Information

Investigating the antibacterial, antioxidant, cytotoxic, and computational studies of Co(II) and Zn(II) compounds of heteroatom-based dicarboxylic acids

Jyoti[a], Priya Bhardwaj[b], Mulaka Maruthi[b*], Sumit Mittal[c*], Anee Mohanty[d*], Sadhika Khullar[a*]

[a]Department of Chemistry, Dr. B R Ambedkar National Institute of Technology Jalandhar, Punjab, 144008, India
[b]Department of Biochemistry, Central University of Haryana, Mehendergarh, Haryana, 123031, India.
[c] School of Advanced Science and Languages, VIT Bhopal University, Sehore, Madhya Pradesh, 466114, India
[d]Department of Biotechnology, Dr. B R Ambedkar National Institute of Technology, Jalandhar, Punjab,144008, India
Corresponding author email: mohantya@nitj.ac.in, Sumit.mittal@vitbhopal.ac.in, khullars@nitj.ac.in

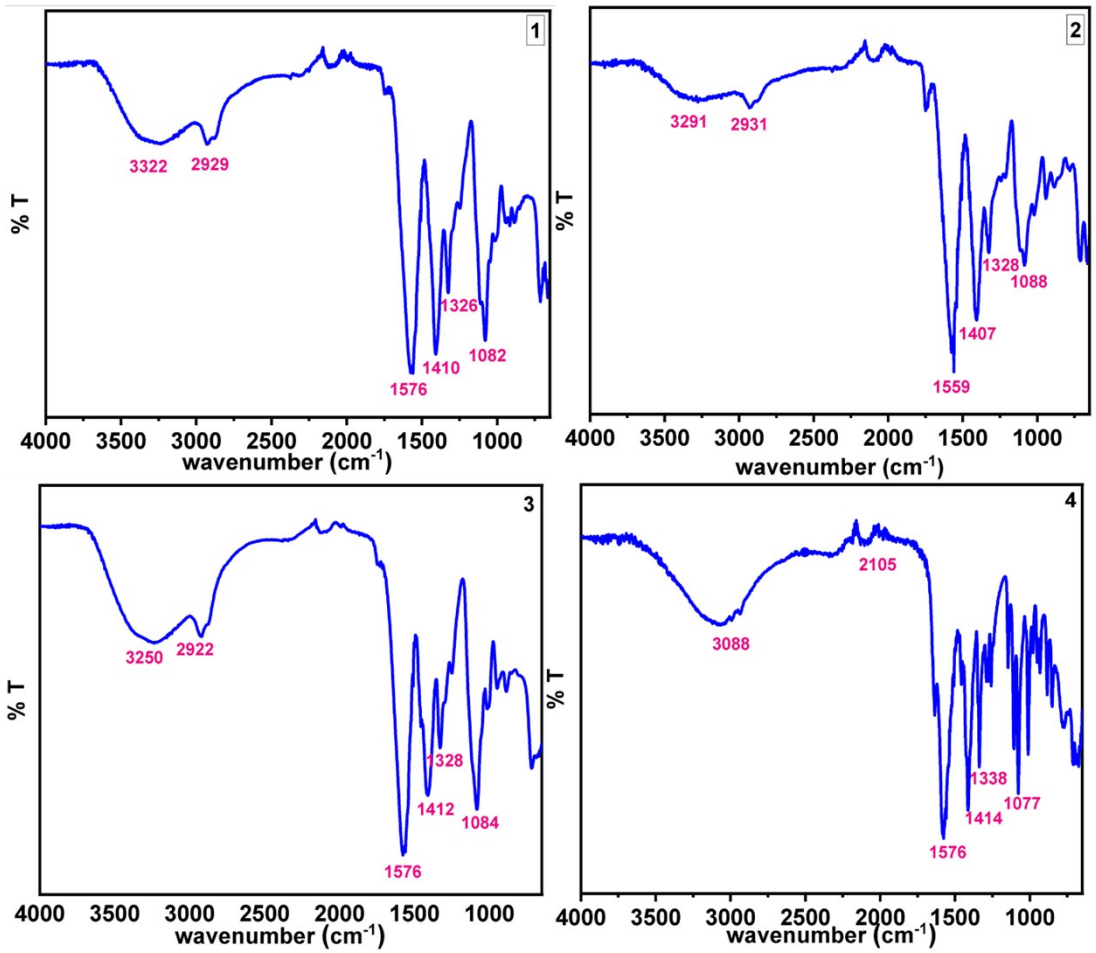
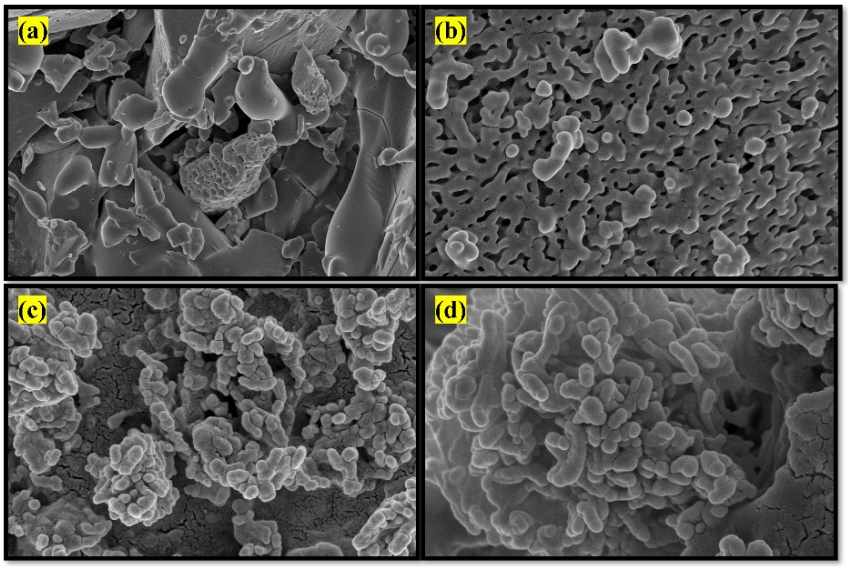
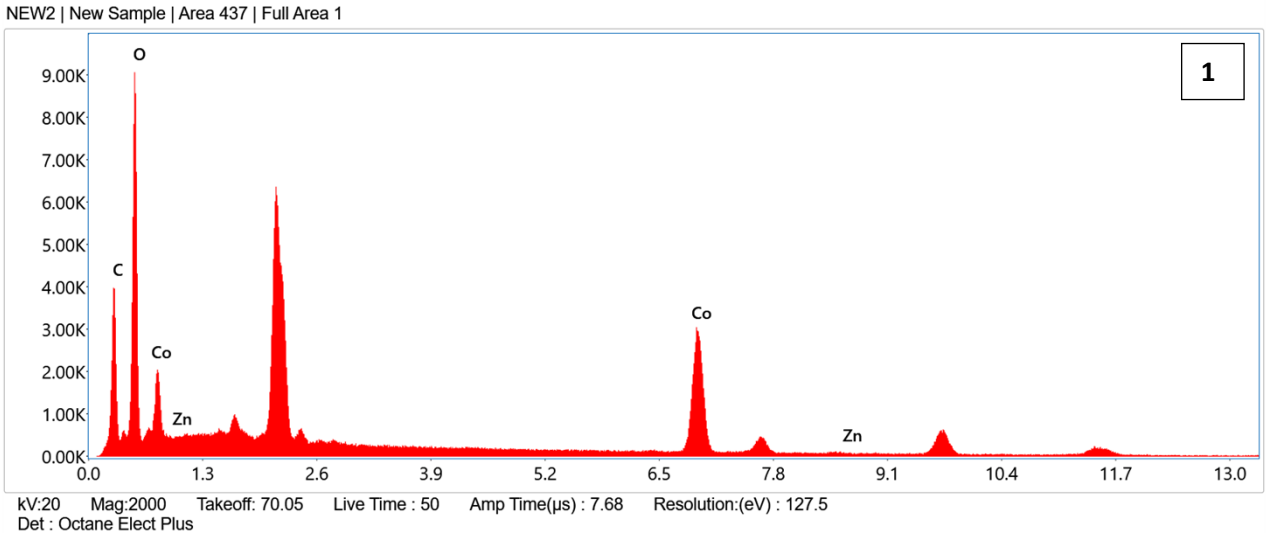
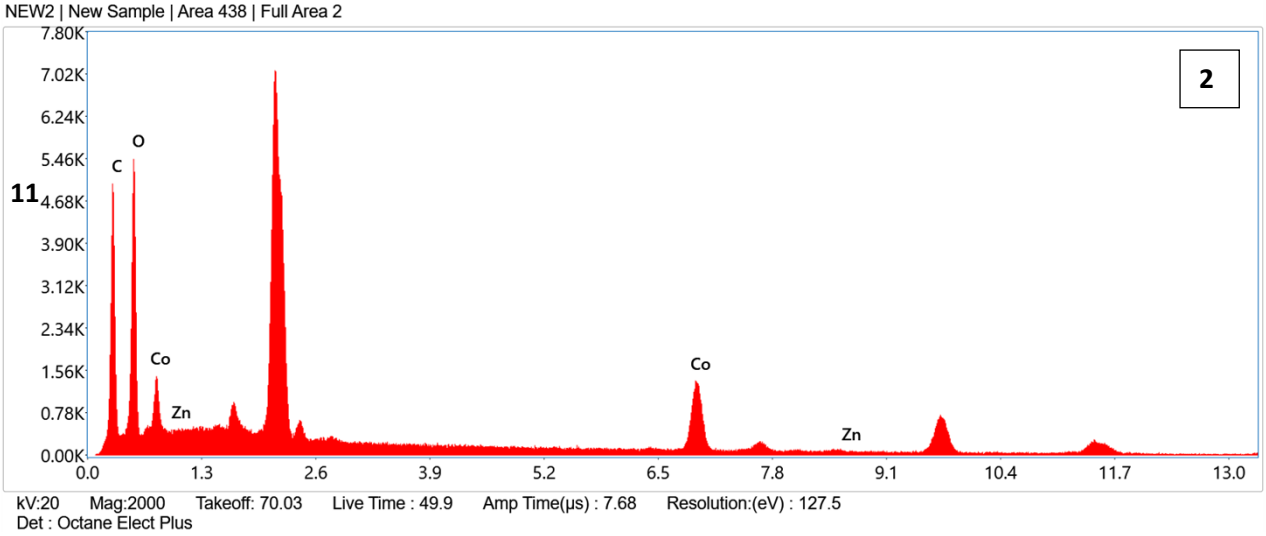
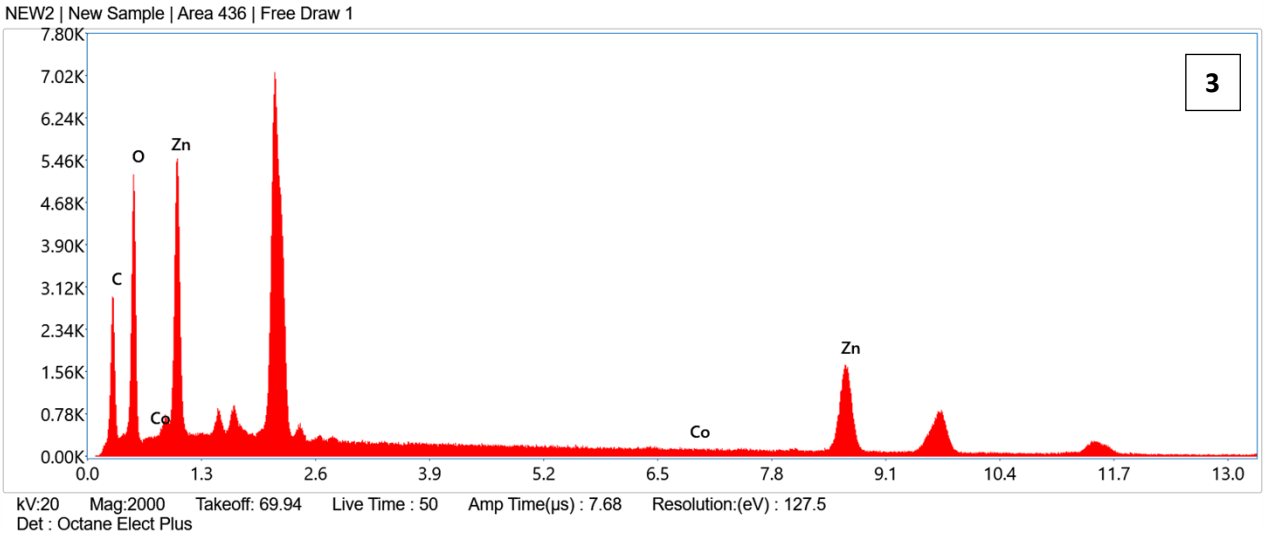


Fig. S1. FTIR spectra of **1-4**.


(a)
(b)
(c)
(d)


NEW2 | New Sample | Area 437 | Full Area 1
1
O
C
Co
Zn
Co
Zn
9.00K
8.00K
7.00K
6.00K
5.00K
4.00K
3.00K
2.00K
1.00K
0.00K
0.0
1.3
2.6
3.9
5.2
6.5
7.8
9.1
10.4
11.7
13.0
kV:20 Mag:2000 Takeoff: 70.05 Live Time : 50 Amp Time(µs) : 7.68 Resolution:(eV) : 127.5
Det : Octane Elect Plus


NEW2 | New Sample | Area 438 | Full Area 2
2
O
C
Co
Zn
Co
Zn
7.80K
7.02K
6.24K
5.46K
4.68K
3.90K
3.12K
2.34K
1.56K
0.78K
0.00K
0.0
1.3
2.6
3.9
5.2
6.5
7.8
9.1
10.4
11.7
13.0
kV:20 Mag:2000 Takeoff: 70.03 Live Time : 49.9 Amp Time(µs) : 7.68 Resolution:(eV) : 127.5
Det : Octane Elect Plus



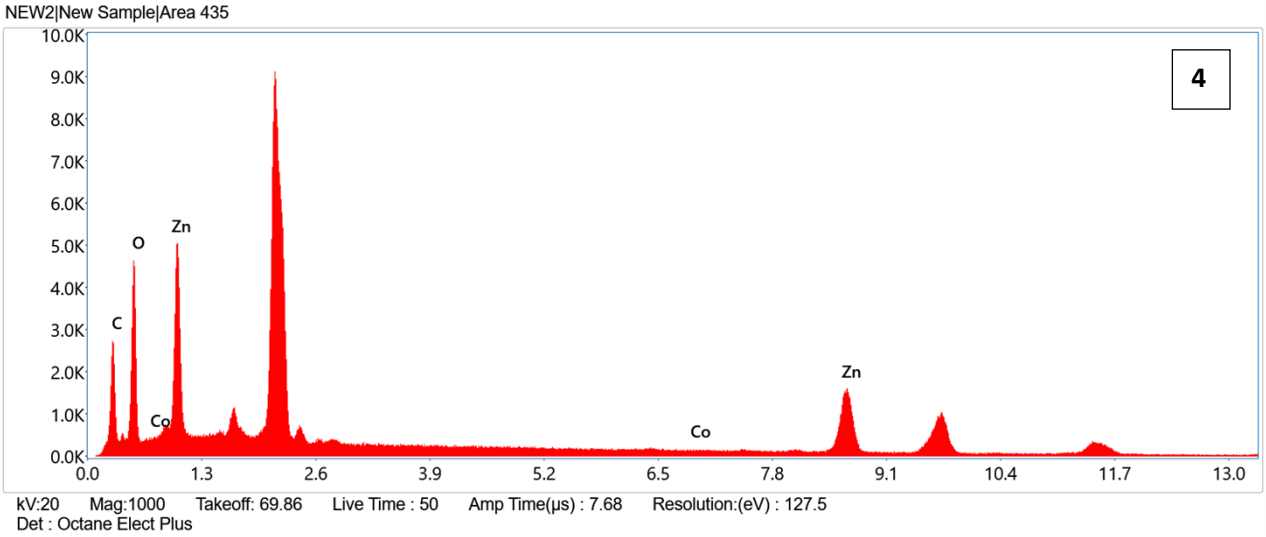


Fig. S2. FE-SEM images of **1-4** and EDX spectra of **1-4.**

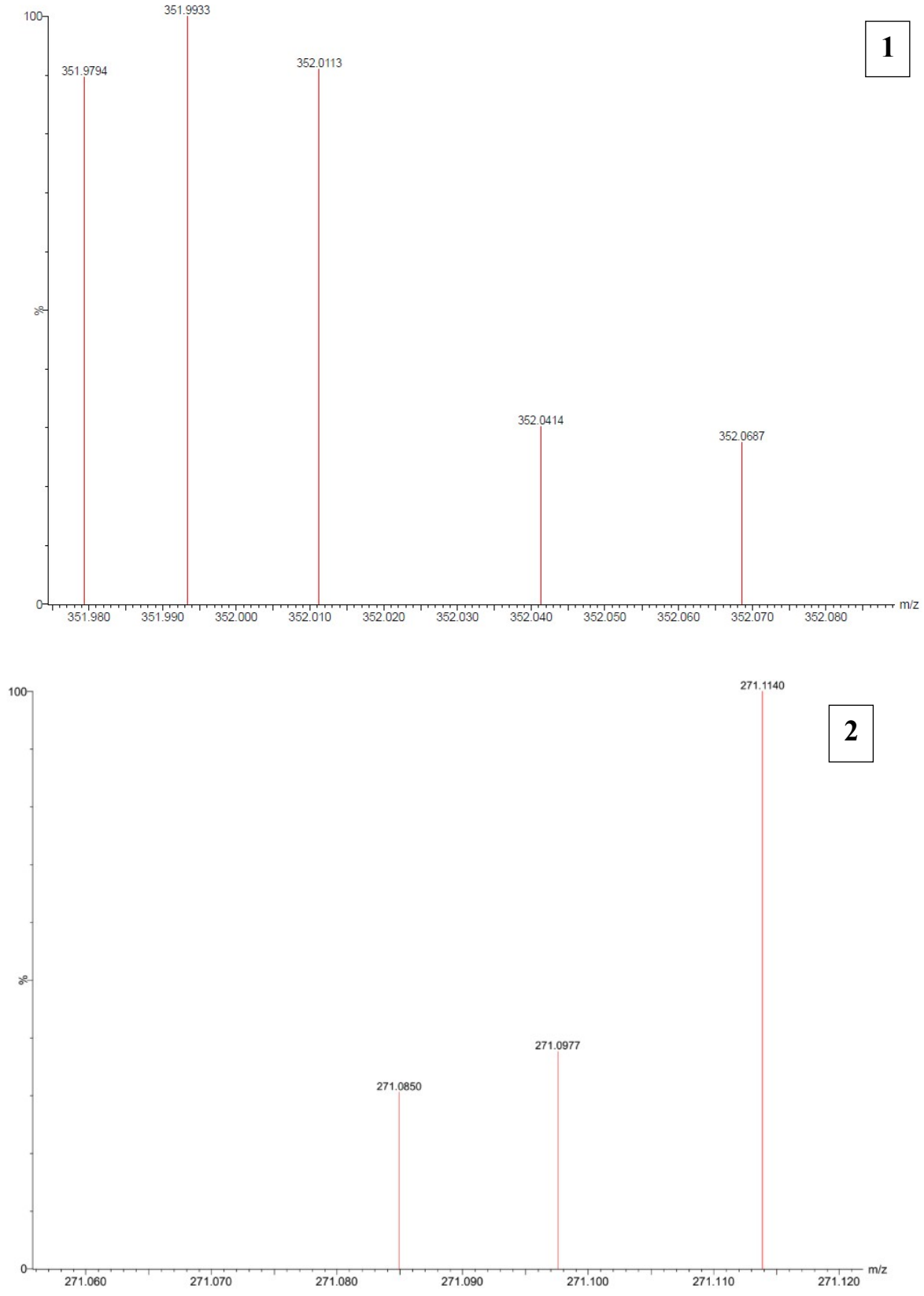


Fig. S3. Mass spectra of **1-2.**

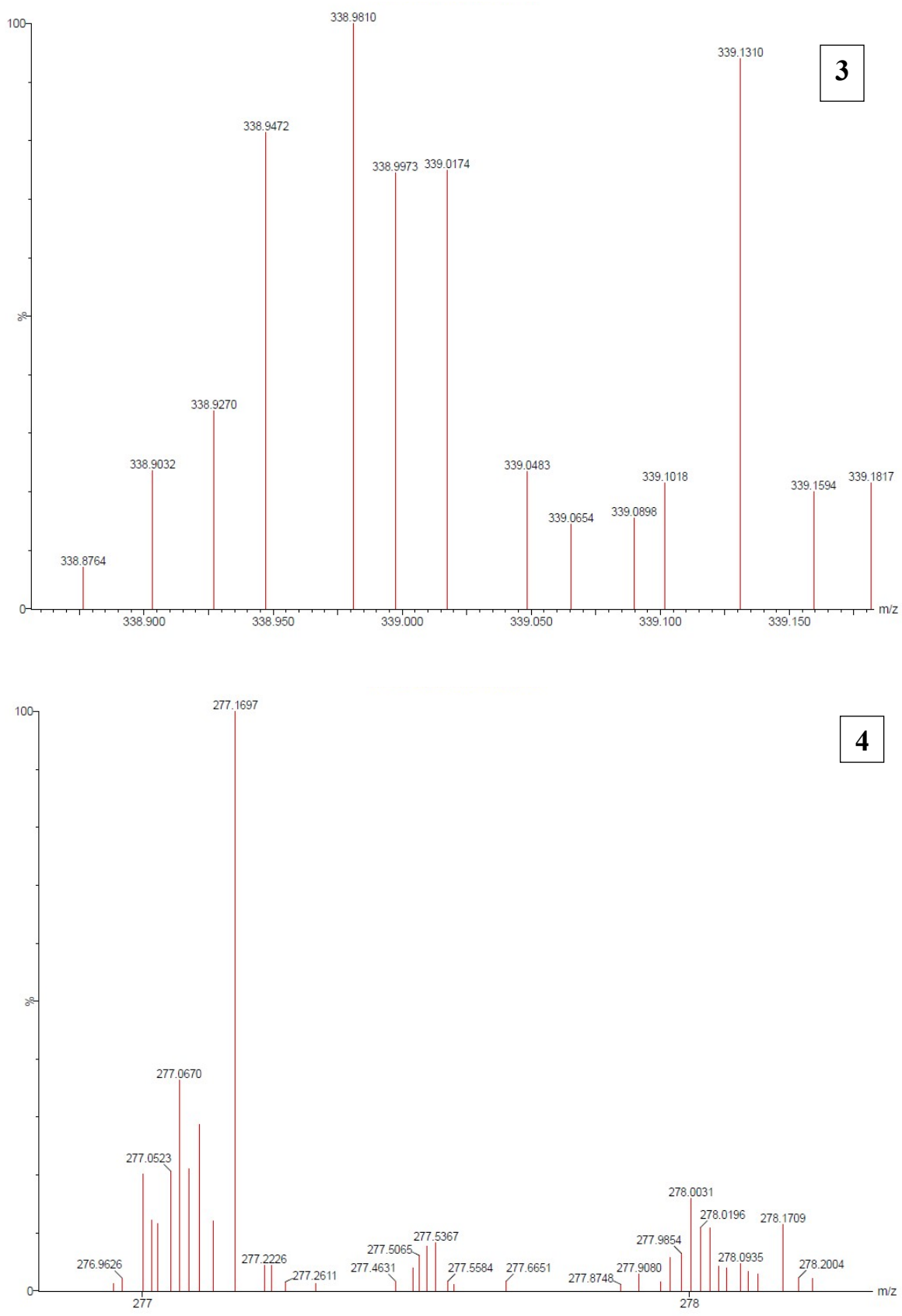


Fig. S4. Mass spectra of **3-4.**

XPS Spectroscopy

In compound **2,** the Co 2p peaks appeared at 781.9 eV ($2p_{3/2}$) and 797.8 eV ($2p_{1/2}$), with a $\Delta E_{3/2\text{-}1/2}$ binding energy gap of two peaks of 15.1 eV, confirming the presence of cobalt is in the Co^{2+} oxidation state as shown in **Fig. S6** along with their corresponding peaks (785.9 and 802.4 eV). The O 1s peak at 532.58 eV also corresponded to the hydroxyl group, **Fig. S6**. Three significant peaks of the C 1s spectrum showed at 285.0 eV (C-C), 286.4 eV (C-O-C), and 288.5 eV (O=C-OH), consistent with the carboxyl group,[S1] as shown in **Fig. S6** . Similarly, compound **3** contains Zn 2p, C 1s, and O 1s peaks. The Zn 2p peaks appeared at 1022.8 eV ($2p_{3/2}$) and 1045.28 eV ($2p_{1/2}$), with a binding energy difference $\Delta E_{3/2\text{-}1/2}$ of 23.2 eV, confirming that zinc exists in Zn^{2+} oxidation state, as shown in **Fig. S7.** The O 1s peak around 532.28 eV corresponded to the hydroxyl group in **Fig. S7**. C 1s peaks at 284.6 eV (C-C), 286.38 eV (C-O), and 288.78 eV (C=O), indicating the presence of the carboxyl group in **Fig. S7.** Similarly, for compound **4**, peaks corresponding to Zn 2p, C 1s, and O 1s were identified. The Zn 2p spectrum exhibited two peaks at 1022.28 eV ($2p_{3/2}$) and 1045.38 eV ($2p_{1/2}$), with a $\Delta E_{3/2\text{-}1/2}$ of 23.1 eV, indicating that the zinc is in the Zn^{2+} oxidation state, as shown in **Fig. S8**. The O1s spectrum, with a peak at 532.18 eV, corresponds to the oxygen atom in the hydroxyl group, as shown in **Fig. S8**. The C 1s spectrum displayed three peaks at 284.78 eV (C-C), 286.48 eV (C-O), and 288.88 eV (C=O), confirming the presence of the carboxyl group as shown in **Fig. S8**.

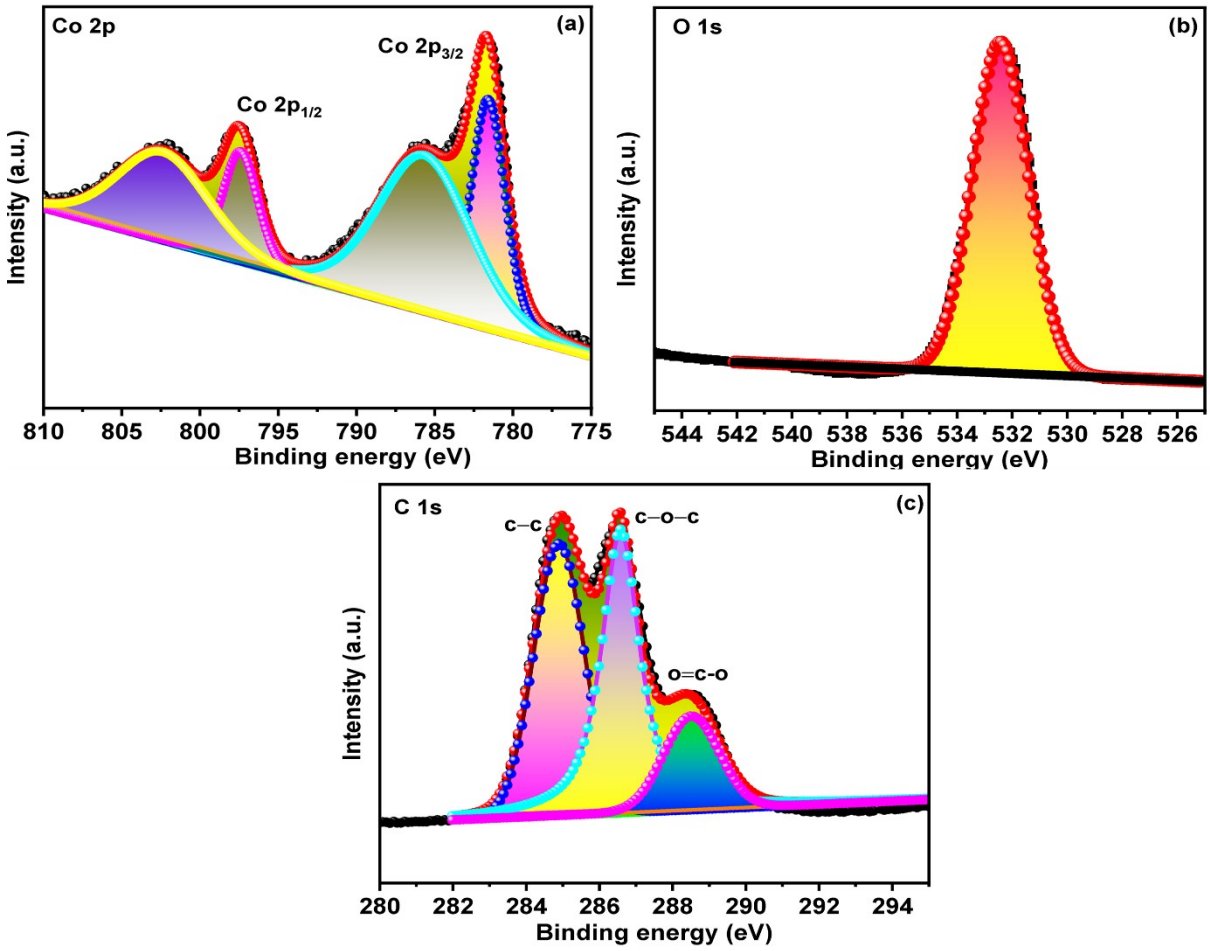


Fig. S5. XPS survey spectra of **1**: Co 2p, O1s and C1s

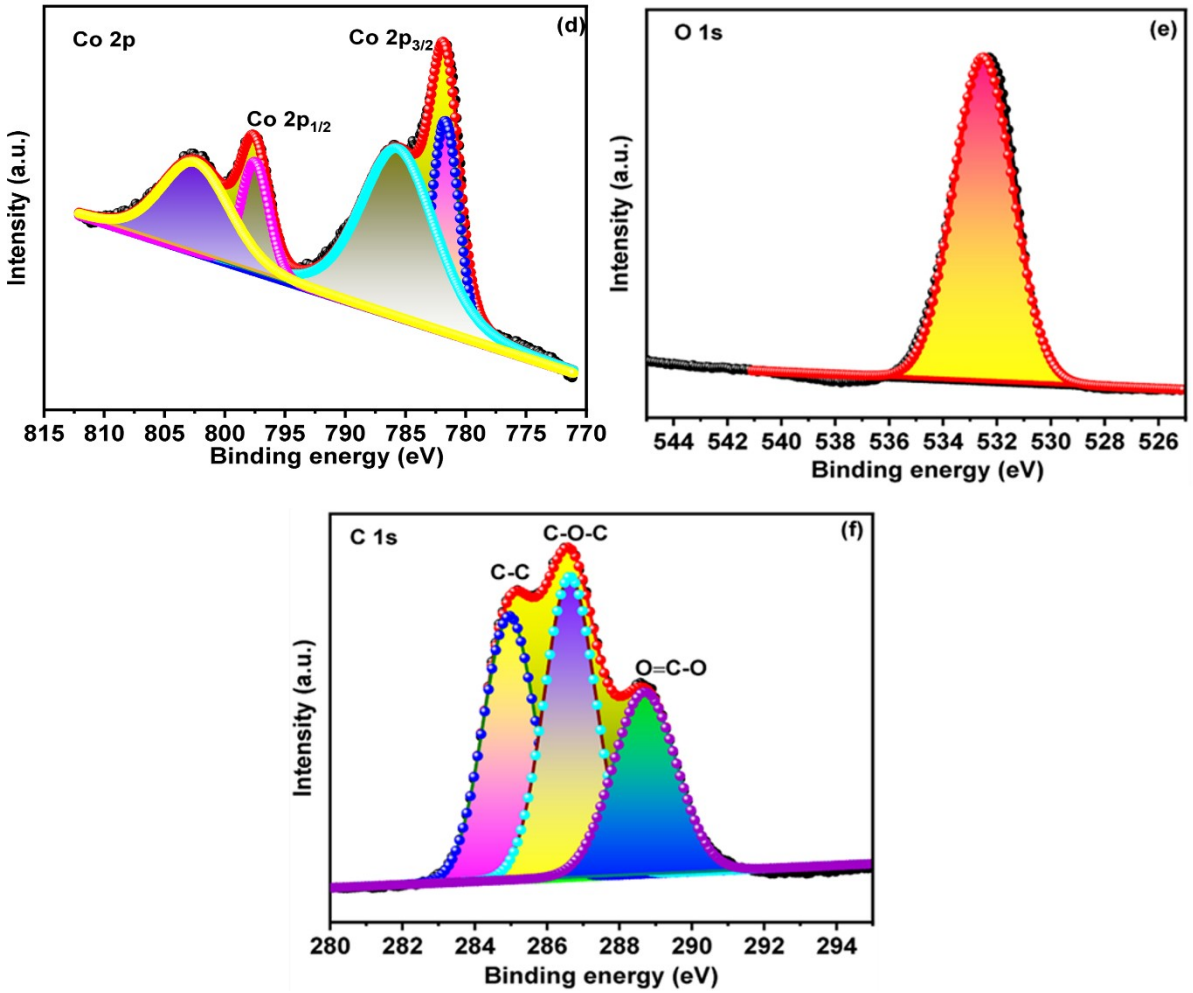


Fig. S6. XPS survey spectra of **2**: Co 2p, O1s and C1s

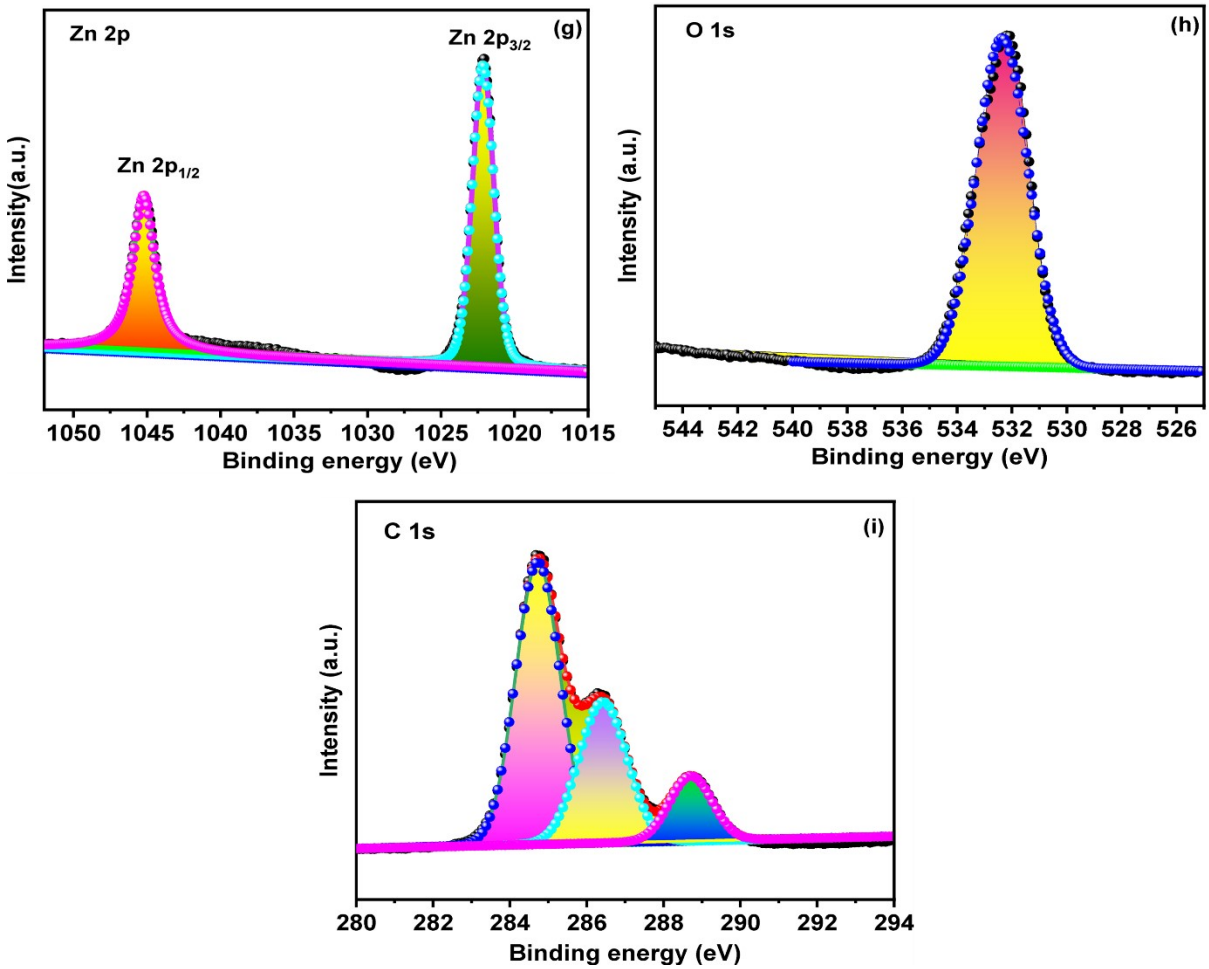


Fig. S7. XPS survey spectra of **3**: Co 2p, O1s and C1s

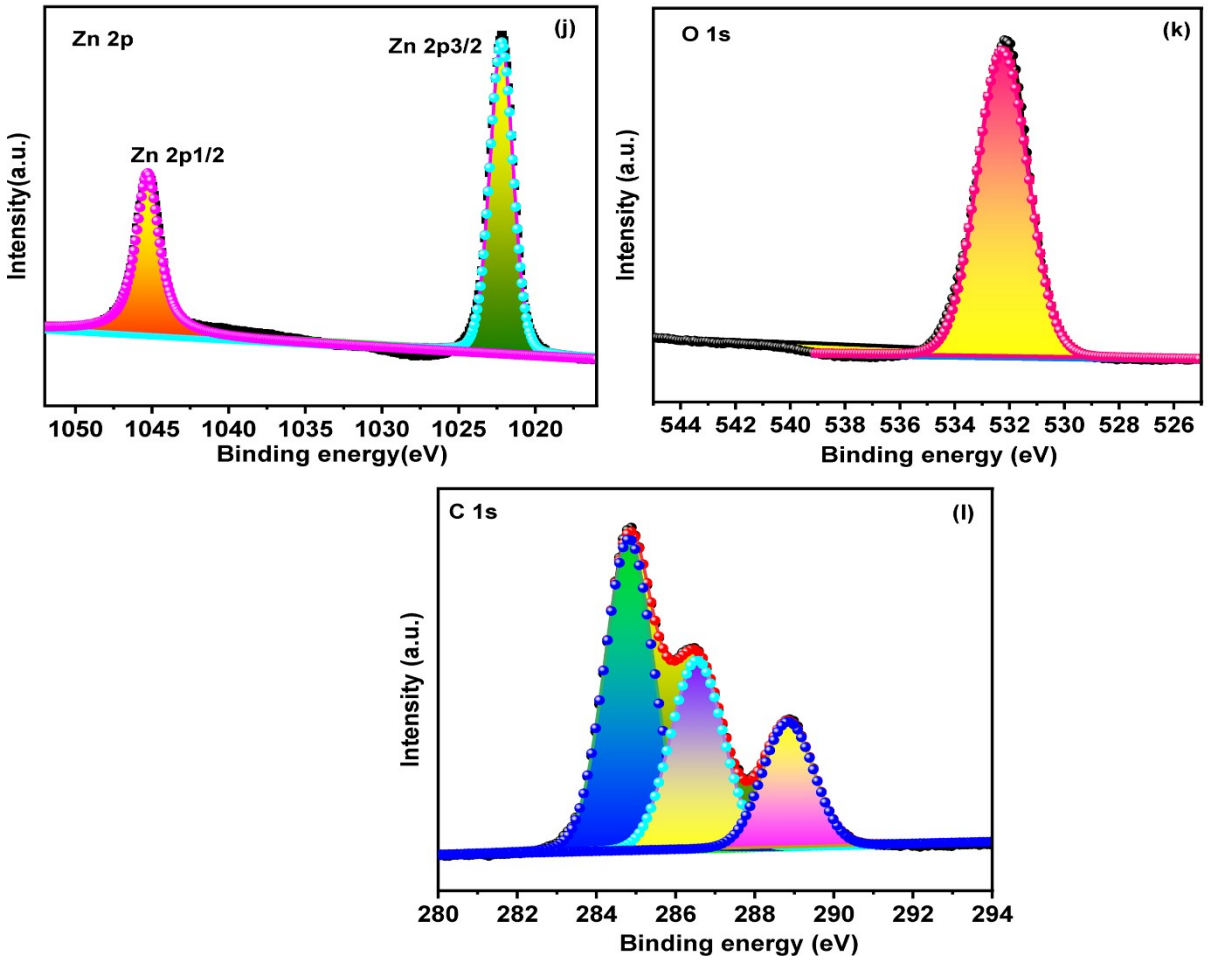


Fig. S8. 4: Zn 2p, O1s and C1s.

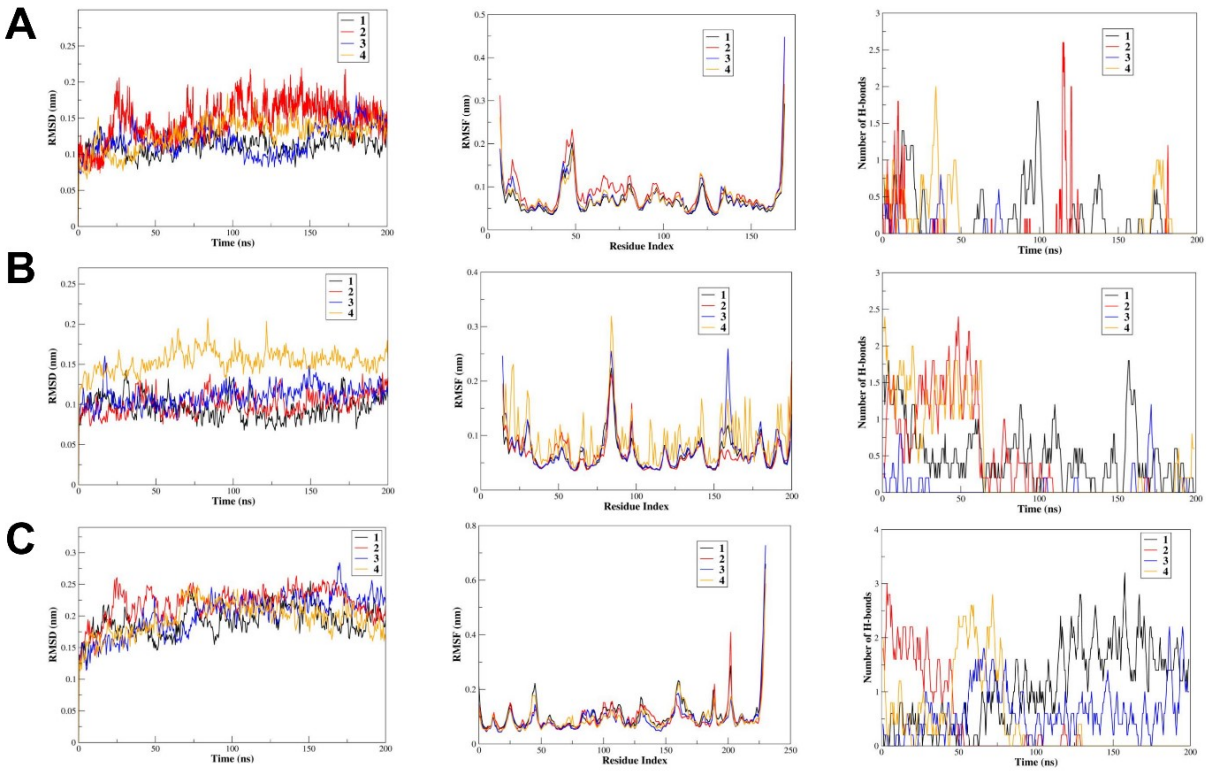


Fig. S9: The root mean square deviation (RMSD), root mean square fluctuation (RMSF), and the number of hydrogen bonds (H-bonds) values for complexes of compounds **1, 2, 3**, and **4** against LasR protein receptor of *Pseudomonas aeruginosa* **(B)**, *Escherichia coli* gyrase B **(A)**, and LcpA ligase from *Bacillus subtilis* **(C)** as calculated from 200 ns all-atom molecular dynamics simulations.

Table S5. Inhibitory percentages of metal salt($Co(OAc)_2.4H_2O$) at various concentrations against the three strains.

Concentration (µg/mL)	*E. coli*	*P. aeruginosa*	*B. subtilis*
125	12.0±0.13	15.1±0.009	12.6±0.05
250	16.6±0.05	23.1±0.04	18.9±0.01
500	23.2±0.01	28.2±0.04	22.9±0.05
600	49.6±0.02	48.0±0.03	43.0±0.01
800	64.1±0.05	57.7±0.008	50.3±0.02
1000	65.30±0.02	63.1±0.01	52.4±0.05

Table S6. Inhibitory percentages of metal salt($Zn(OAc)_2.2H_2O$) at various concentrations against the three strains.

Concentrations (µg/mL)	*E. coli*	*P. aeruginosa*	*B. subtilis*
125	8.45±0.006	6.69±0.005	4.0±0.05
250	14.7±0.03	13.7±0.039	8.93±0.001
500	17.9±0.002	16.7±0.027	18.2±0.05
600	24.7±0.005	20.6±0.01	23.9±0.01
800	40.7±0.001	32.6±0.007	27.0±0.03
1000	53.0±0.01	50.1±0.01	44.6±0.1

Table S7. Inhibitory percentages of parent ligand (H_2toua) at various concentrations against the three strains.

Concentrations (µg/mL)	*E. coli*	*P. aeruginosa*	*B. subtilis*
125	22.2±0.009	7.72±0.01	4.05±0.13
250	24.9±0.004	13.7±0.09	10.3±0.01
500	31.6±0.01	22.1±0.05	11.2±0.010
600	31.4±0.007	34.4±0.03	16.1±.004
800	51.9±0.05	43.2±0.08	22.5±0.04
1000	57.9±0.04	45.8±0.07	30.3±0.005

Table S8. Inhibitory percentages of parent ligand(H_2eoba) at various concentrations against the three strains.

Concentrations (µg/mL)	*E. coli*	*P. aeruginosa*	*B. subtilis*
125	17.1±0.04	8.79±0.05	1.17±0.007
250	21.9±0.004	5.38±0.01	10.9±0.01
500	26.8±0.01	42.5±0.005	10.4±0.03
600	43.8±0.03	55.5±0.01	15.9±0.001
800	49.7±0.01	56.5±0.2	23.7±0.006
1000	57.42±0.09	48.5± 0.01	36.9±0.2

References

S1. N. Joshi, L. F. da Silva, F. M. Shimizu, V. R. Mastelaro, J.-C. M'Peko, L. Lin and O. N. Oliveira Jr, *Microchim. Acta*, 2019, 186, 418.