Supplementary Information

New mixed-ligand Zn(II)-based MOF as a nanocarrier platform for improved antibacterial activity of clinically approved drug Levofloxacin.

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Experimental

Single crystals of $[C_{60}H_{48}N_6O_{15}Zn_3]_n$ **[Zn-nMOF]** were colorless block-shaped. A suitable crystal was selected and mounted on a Bruker APEX-II CCD diffractometer. The crystal was kept at 100(2) K during data collection. Using Olex2[1], the structure was solved with olex2.solve[2] structure solution program using Charge Flipping and refined with the olex2.refine[3] refinement package using Gauss-Newton minimization.

Crystal structure determination of [Zn-nMOF)

Crystal Data for $C_{60}H_{48}N_6O_{15}Zn_3$ (M =1290.276 g/mol): orthorhombic, space group $Pna2_1$ (no. 33), a = 16.372(3) Å, b = 21.997(4) Å, c = 15.285(3) Å, V = 5504.5(18) Å^3, Z = 4, T = 100(2) K, μ(Mo Kα) = 1.374 mm^{-1}, *Dcalc* = 1.557 g/cm^3, 74321 reflections measured ($4.46° \leq 2\Theta \leq 56.62°$), 13648 unique ($R_{int}$ = 0.1034, R_{sigma} = 0.0802) which were used in all calculations. The final R_1 was 0.0976 (I>=2u(I)) and wR_2 was 0.2212 (all data).

Computational details

The dispersion corrected density functional theory (DFT-D3) employing the hybrid of Becke's three-parameter exchange and correlation functional with the Lee-Yang-Parr functional (B3LYP) implemented in Gaussian 09 software[4] was used for geometry optimization calculations of the Zn-nMOF in the ground state. For atoms of the given MOF, mixed basis sets, 6-31G(d,p) + LANL2DZ, were specified. For Zinc atom, effective core potential basis i.e. LANL2DZ was employed while double zeta basis set involving polarization functions i.e. 6-31G(d,p) was utilized to define C, H, N, O atoms. The coordinates for the input geometry were taken from the crystal information file of Zinc-based metal organic framework. The molecular electrostatic potentials (MESP) map and some related theoretical parameters were investigated at same level of theory.

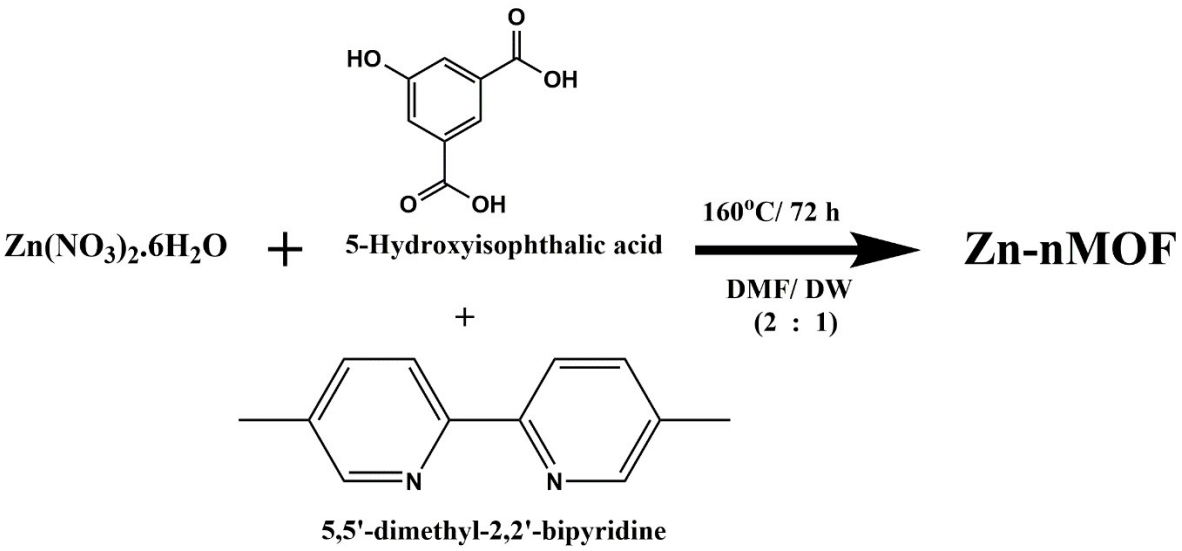

Figure S1: Reaction scheme for the synthesis of Zn-nMOF

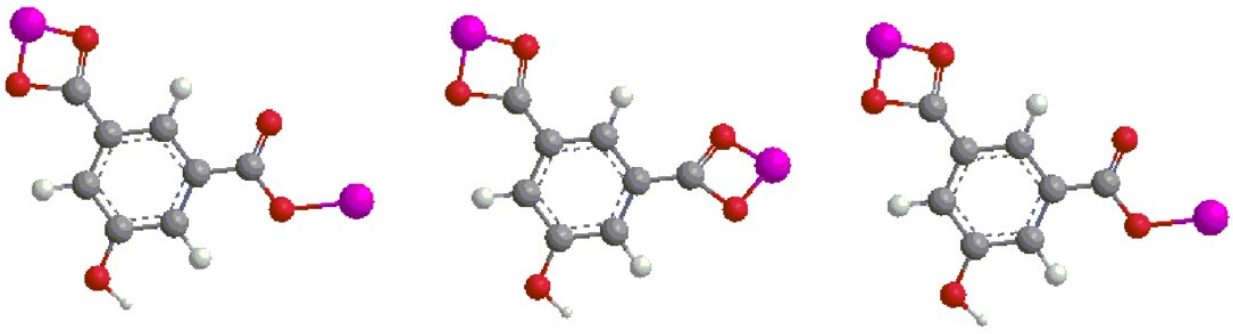

Figure S2. Different binding modes of linker 5-hydroxyisophthalic acid in Zn-nMOF.

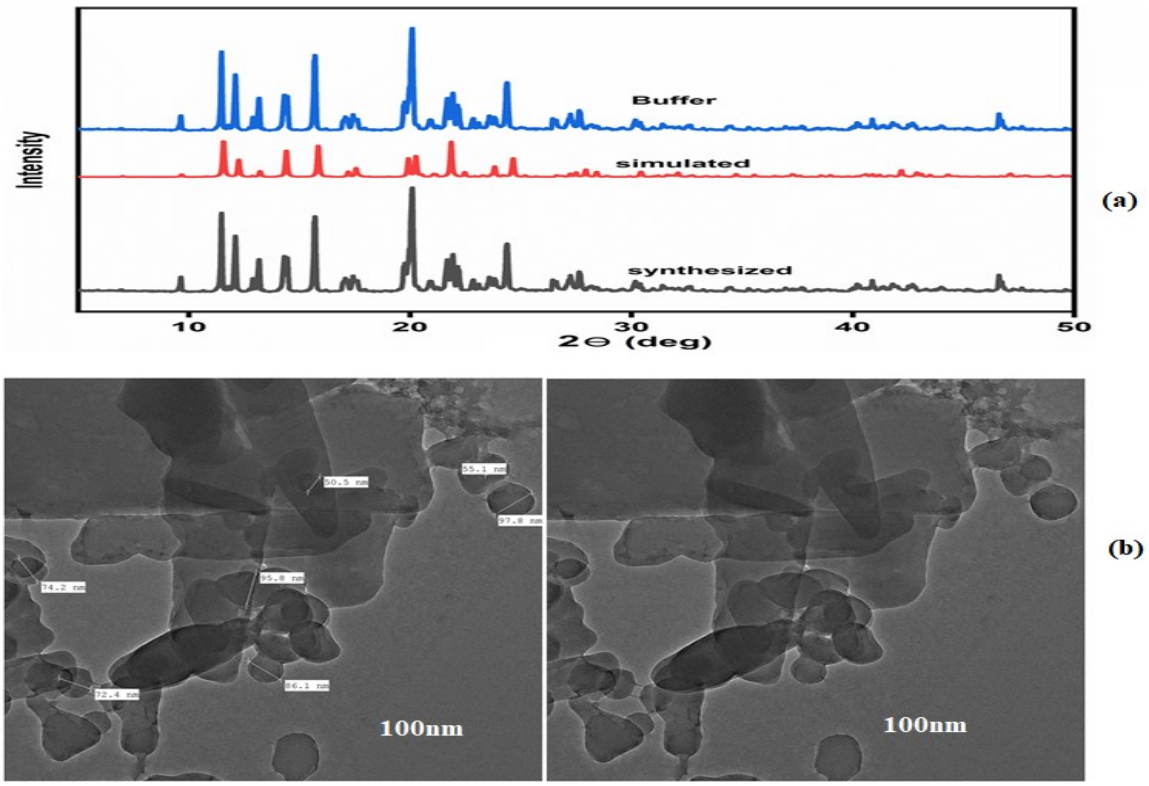

Figure S3: (**a**) PXRD pattern of synthesized, simulated, and after buffer treatment, and (**b**) TEM images of Zn-nMOF.

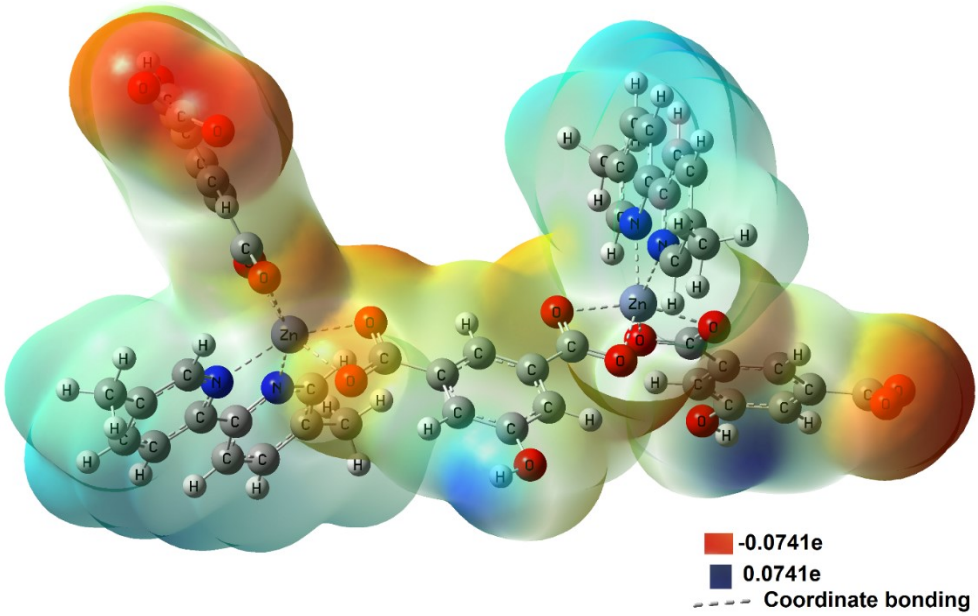

Figure S4. MESP map of the Zn-nMOF.

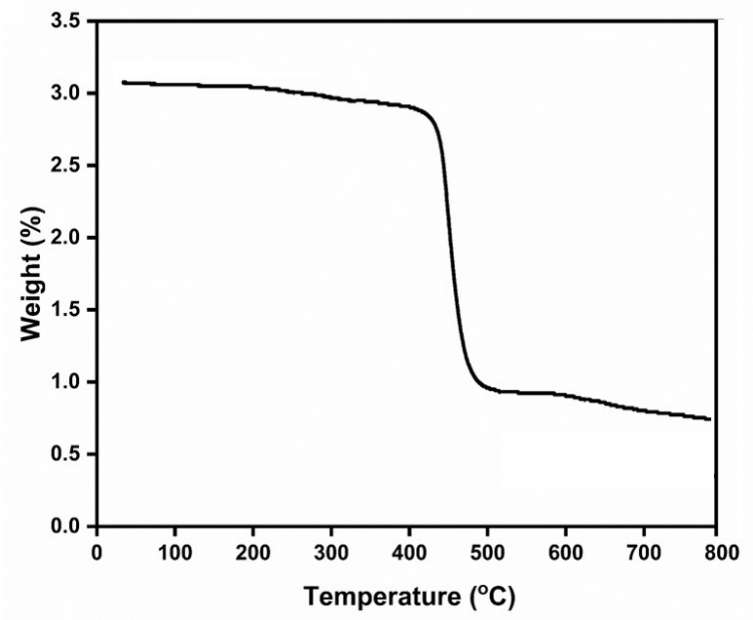

Figure S5: Thermogravimetric analysis (TGA) curve of Zn-nMOF.

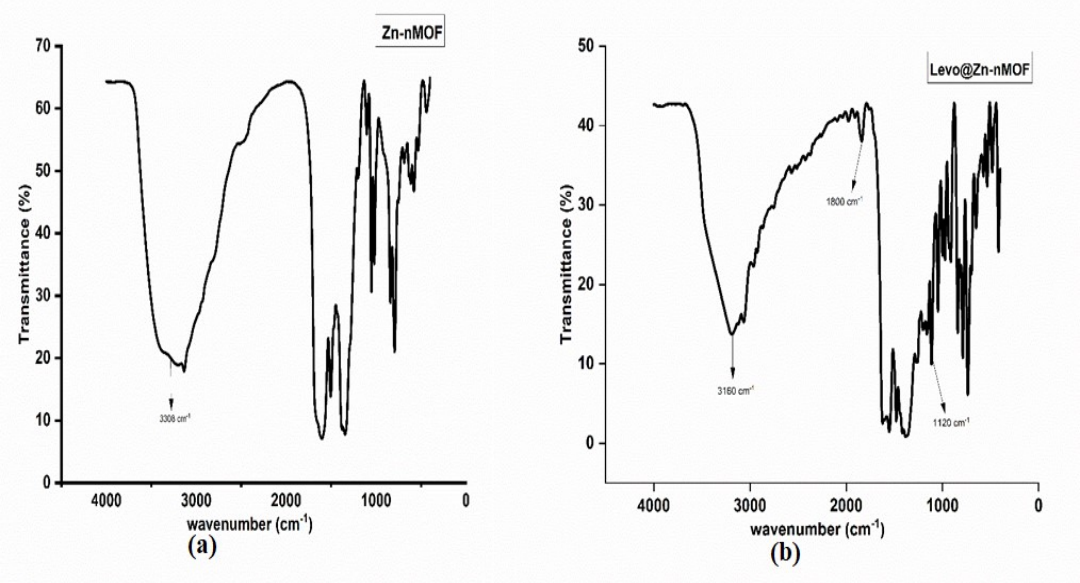

Figure S6. (**a**) IR spectrum of Zn-nMOF and (**b**)Levo@Zn-nMOF.

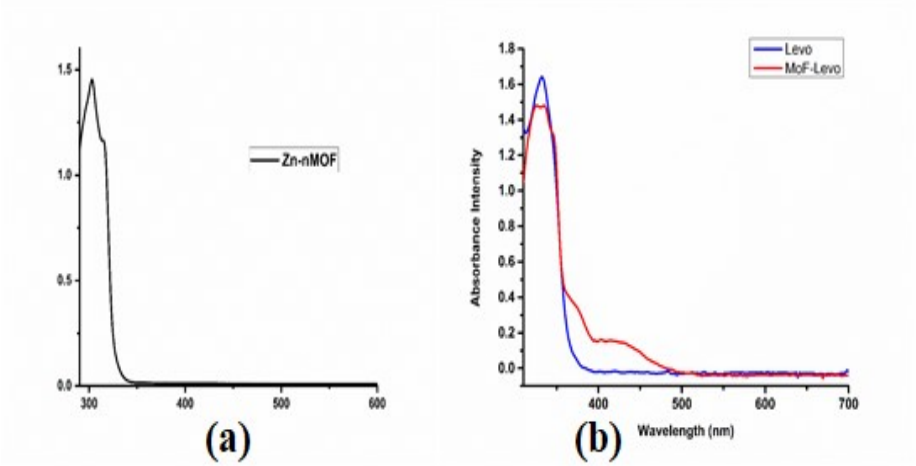

Figure S7. (**a**) UV-visible spectra of pure Zn-nMOF and (**b**).pure Levofloxacin and Levo@Zn-nMOF

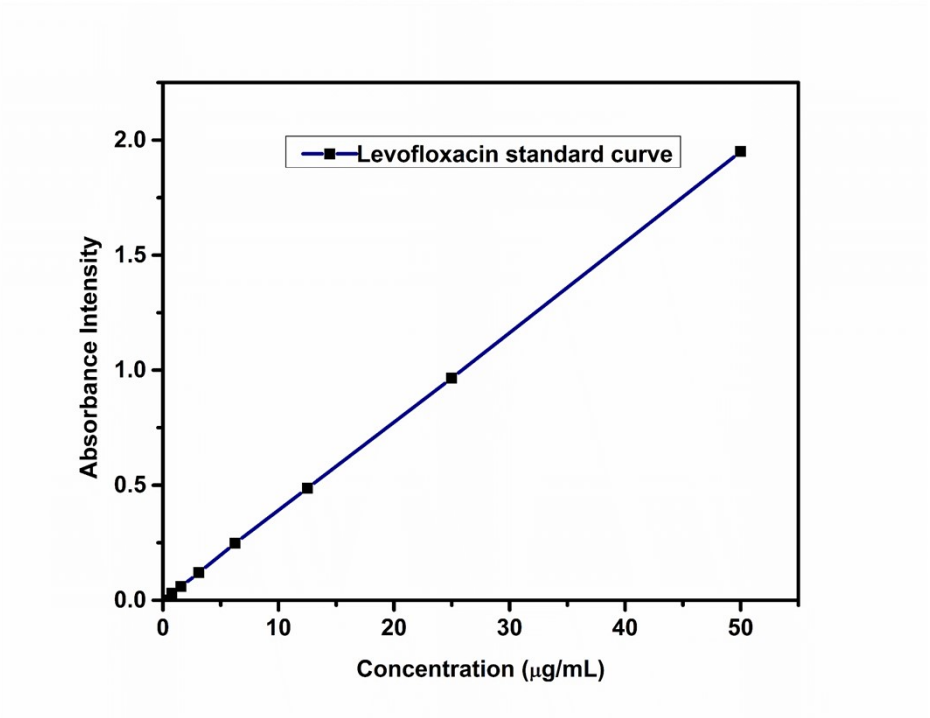

Figure S8. Standard curve of pure drug levofloxacin plotted at 290 nm.

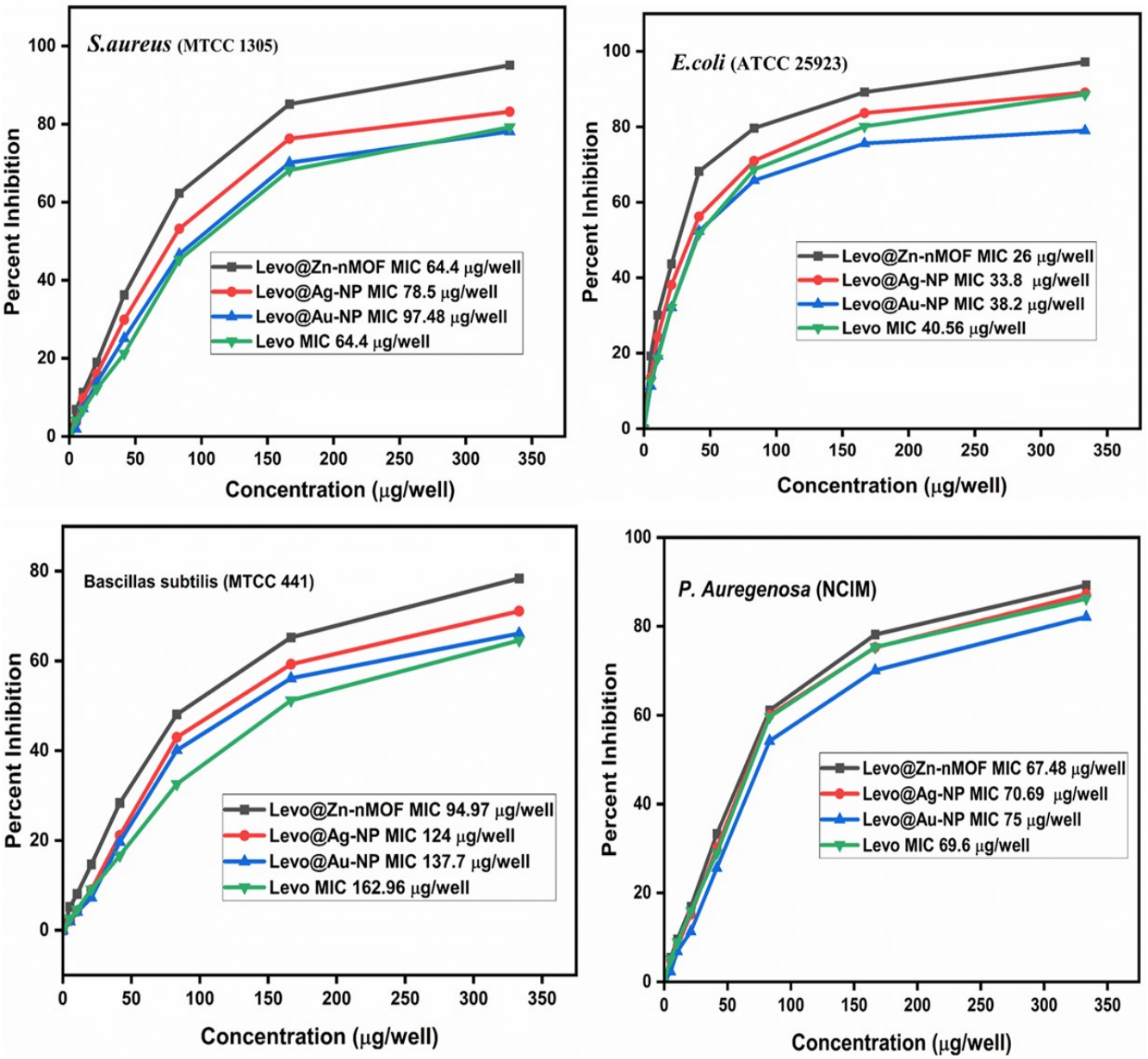

Figure S9: Comparative analysis of antibacterial activity of Levo@Zn-nMOF, Levo@Ag-NP, Levo@Au-NP, and pure levofloxacin (levo) drug against the gram-positive and gram-negative bacteria.

Table S1

Table Crystal data and structure refinement for Zn-nMOF (CCDC 2119311).

Identification code	Zn-nMOF
Empirical formula	$C_{60}H_{48}N_6O_{15}Zn_3$
Formula weight	1290.276
Temperature/K	100(2)
Crystal system	Orthorhombic
Space group	$Pna2_1$
a/Å	16.372(3)
b/Å	21.997(4)
c/Å	15.285(3)
α/°	89.71(3)
β/°	89.99(3)
γ/°	89.98(3)
Volume/Å^3	5504.5(18)
Z	4
ρ_{calc}g/cm^3	1.557
μ/mm^{-1}	1.374
F(000)	2649.3
Crystal size/mm^3	0.39 × 0.23 × 0.15
Radiation	Mo Kα (λ = 0.71073)
2Θ range for data collection/°	4.46 to 56.62
Index ranges	$-21 \le h \le 21$, $-29 \le k \le 29$, $-20 \le l \le 20$
Reflections collected	74321
Independent reflections	13648 [R_{int} = 0.1034, R_{sigma} = 0.0802]
Data/restraints/parameters	13648/1/767
Goodness-of-fit on F^2	1.068
Final R indexes [I>=2σ (I)]	R_1 = 0.0976, wR_2 = 0.1873
Final R indexes [all data]	R_1 = 0.1410, wR_2 = 0.2212
Largest diff. peak/hole / e Å^{-3}	3.76/-5.84

Table S2 Bond Lengths for Zn-nMOF

Atom	Atom	Length/Å	Atom	Atom	Length/Å
Zn3	O14[1]	2.322(7)	O7	C33	1.303(14)
Zn3	O15[1]	2.075(6)	O10	C37	1.237(15)
Zn3	O12	1.917(7)	O8	C39	1.382(10)
Zn3	N5	2.088(7)	O5	C20	1.326(11)
Zn3	N6	2.060(9)	O3	C16	1.385(13)
Zn3	C60[1]	2.548(10)	N4	C27	1.337(13)
O11	C54	1.210(12)	N4	C32	1.350(12)
O14	C60	1.308(9)	N3	C26	1.381(13)
O13	C57	1.397(11)	N3	C21	1.341(13)
O15	C60	1.254(11)	N2	C12	1.305(17)
O12	C54	1.308(10)	N2	C7	1.414(14)
N5	C48	1.379(12)	N1	C6	1.296(17)
N5	C53	1.347(10)	N1	C1	1.34(2)
N6	C47	1.325(12)	C38	C36	1.386(13)
N6	C42	1.365(11)	C38	C39	1.393(13)
C54	C55	1.490(11)	C36	C35	1.372(13)
C58	C59	1.394(12)	C36	C37	1.529(13)
C58	C57	1.374(13)	C25	C26	1.393(12)
C60	C59	1.507(13)	C25	C24	1.390(13)
C61	C59	1.399(13)	C26	C27	1.502(13)
C61	C55	1.385(13)	C39	C40	1.386(14)
C48	C47	1.473(11)	C30	C31	1.509(16)
C48	C49	1.369(13)	C30	C32	1.389(14)
C47	C46	1.398(12)	C30	C29	1.348(17)
C53	C51	1.379(14)	C5	C4	1.346(17)
C51	C50	1.436(17)	C5	C6	1.446(17)
C51	C52	1.525(14)	C27	C28	1.393(17)
C46	C45	1.400(12)	C35	C34	1.395(13)
C42	C43	1.421(14)	C40	C34	1.429(13)
C57	C56	1.368(13)	C20	C18	1.504(16)
C56	C55	1.418(11)	C24	C22	1.391(15)
C50	C49	1.405(15)	C18	C17	1.370(14)
C44	C43	1.484(16)	C18	C19	1.428(14)
C43	C45	1.364(14)	C12	C10	1.399(19)
Zn2	O6	1.991(8)	C17	C16	1.39(2)
Zn2	O5	1.932(7)	C4	C2	1.32(2)
Zn2	N4	2.090(9)	C22	C23	1.504(14)
Zn2	N3	2.041(9)	C22	C21	1.389(16)

Table S2 Bond Lengths for Zn-nMOF

Atom	Atom	Length/Å	Atom	Atom	Length/Å
Zn2	C33	2.575(9)	C6	C7	1.450(18)
Zn1	O2	1.962(8)	C14	C19	1.411(14)
Zn1	O9[2]	2.074(9)	C14	C13	1.496(14)
Zn1	O10[2]	2.283(10)	C14	C15	1.404(13)
Zn1	N2	2.002(10)	C28	C29	1.378(18)
Zn1	N1	2.169(14)	C33	C34	1.480(11)
Zn1	C13	2.574(10)	C7	C8	1.405(15)
Zn1	C37[2]	2.491(10)	C2	C3	1.50(2)
O2	C13	1.286(11)	C2	C1	1.45(2)
O4	C20	1.234(12)	C9	C8	1.381(17)
O1	C13	1.248(10)	C9	C10	1.355(19)
O6	C33	1.281(14)	C15	C16	1.39(2)
O9	C37	1.279(14)	C10	C11	1.535(18)

[1]1-X,1-Y,-1/2+Z; [2]+X,+Y,-1+Z

Table S3 Bond Angles for Zn-nMOF.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
O15[1]	Zn3	O14[1]	59.9(2)	C37	O9	Zn1[4]	92.9(8)
O12	Zn3	O14[1]	111.4(3)	C37	O10	Zn1[4]	84.6(7)
O12	Zn3	O15[1]	111.6(3)	C20	O5	Zn2	113.0(6)
N5	Zn3	O14[1]	140.0(3)	C27	N4	Zn2	114.9(7)
N5	Zn3	O15[1]	95.5(3)	C32	N4	Zn2	127.8(7)
N5	Zn3	O12	106.8(3)	C32	N4	C27	117.3(9)
N6	Zn3	O14[1]	94.5(3)	C26	N3	Zn2	116.0(6)
N6	Zn3	O15[1]	132.8(3)	C21	N3	Zn2	125.4(8)
N6	Zn3	O12	114.7(3)	C21	N3	C26	118.5(9)
N6	Zn3	N5	79.5(3)	C12	N2	Zn1	122.8(9)
C60[1]	Zn3	O14[1]	30.7(2)	C7	N2	Zn1	114.3(8)
C60[1]	Zn3	O15[1]	29.3(2)	C7	N2	C12	122.3(11)
C60[1]	Zn3	O12	116.1(3)	C6	N1	Zn1	114.3(11)
C60[1]	Zn3	N5	118.7(3)	C1	N1	Zn1	126.7(11)
C60[1]	Zn3	N6	115.7(3)	C1	N1	C6	118.9(14)
C60	O14	Zn3[2]	84.2(6)	C39	C38	C36	118.0(8)
C60	O15	Zn3[2]	96.8(5)	C35	C36	C38	122.0(9)
C54	O12	Zn3	112.9(6)	C37	C36	C38	119.0(9)
C48	N5	Zn3	113.1(5)	C37	C36	C35	119.0(9)
C53	N5	Zn3	126.1(6)	C24	C25	C26	119.0(9)

Table S3 Bond Angles for Zn-nMOF.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
C53	N5	C48	120.7(7)	C25	C26	N3	121.1(8)
C47	N6	Zn3	115.3(6)	C27	C26	N3	113.7(9)
C42	N6	Zn3	124.0(6)	C27	C26	C25	125.0(10)
C42	N6	C47	120.2(8)	C38	C39	O8	121.2(8)
O12	C54	O11	124.1(8)	C40	C39	O8	116.8(8)
C55	C54	O11	121.1(8)	C40	C39	C38	122.0(8)
C55	C54	O12	114.8(8)	C32	C30	C31	121.0(10)
C57	C58	C59	118.9(9)	C29	C30	C31	123.5(11)
O14	C60	Zn3[2]	65.0(5)	C29	C30	C32	115.5(11)
O15	C60	Zn3[2]	53.9(4)	C6	C5	C4	113.4(11)
O15	C60	O14	118.9(8)	C26	C27	N4	115.9(10)
C59	C60	Zn3[2]	174.7(6)	C28	C27	N4	120.0(10)
C59	C60	O14	119.9(8)	C28	C27	C26	123.9(10)
C59	C60	O15	121.1(7)	C34	C35	C36	120.3(8)
C55	C61	C59	116.7(8)	C34	C40	C39	118.6(8)
C60	C59	C58	116.2(8)	O5	C20	O4	123.4(10)
C61	C59	C58	122.7(9)	C18	C20	O4	121.2(9)
C61	C59	C60	121.0(8)	C18	C20	O5	115.4(8)
C47	C48	N5	115.0(7)	C22	C24	C25	119.7(9)
C49	C48	N5	120.5(8)	C17	C18	C20	122.5(10)
C49	C48	C47	124.3(9)	C19	C18	C20	117.7(9)
C48	C47	N6	116.3(8)	C19	C18	C17	119.8(11)
C46	C47	N6	120.3(8)	C10	C12	N2	122.7(12)
C46	C47	C48	123.4(8)	C16	C17	C18	120.6(12)
C51	C53	N5	121.9(9)	C2	C4	C5	128.9(14)
C50	C51	C53	118.1(9)	C23	C22	C24	121.6(10)
C52	C51	C53	121.6(10)	C21	C22	C24	118.4(10)
C52	C51	C50	120.3(9)	C21	C22	C23	120.0(11)
C45	C46	C47	119.6(9)	C5	C6	N1	122.7(12)
C43	C42	N6	122.4(8)	C7	C6	N1	115.2(12)
C58	C57	O13	115.6(8)	C7	C6	C5	122.0(10)
C56	C57	O13	123.7(8)	C13	C14	C19	121.1(8)
C56	C57	C58	120.6(9)	C15	C14	C19	119.4(10)
C55	C56	C57	119.9(9)	C15	C14	C13	119.5(9)
C49	C50	C51	118.8(10)	C29	C28	C27	120.3(11)
C50	C49	C48	119.9(11)	O6	C33	Zn2	49.2(5)
C44	C43	C42	118.2(10)	O7	C33	Zn2	73.1(5)
C45	C43	C42	116.4(9)	O7	C33	O6	122.2(9)
C45	C43	C44	125.4(11)	C34	C33	Zn2	166.8(8)
C43	C45	C46	121.0(10)	C34	C33	O6	118.0(10)

Table S3 Bond Angles for Zn-nMOF.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
C61	C55	C54	119.9(8)	C34	C33	O7	119.7(10)
C56	C55	C54	119.0(9)	C6	C7	N2	116.8(9)
C56	C55	C61	121.1(9)	C8	C7	N2	116.5(12)
O5	Zn2	O6	119.9(3)	C8	C7	C6	126.7(10)
N4	Zn2	O6	124.3(3)	C3	C2	C4	127.8(17)
N4	Zn2	O5	107.6(3)	C1	C2	C4	112.0(14)
N3	Zn2	O6	104.8(4)	C1	C2	C3	119.8(16)
N3	Zn2	O5	113.1(3)	C2	C1	N1	123.7(14)
N3	Zn2	N4	79.5(3)	C30	C32	N4	125.6(10)
C33	Zn2	O6	29.2(4)	C22	C21	N3	122.9(11)
C33	Zn2	O5	115.3(3)	C14	C19	C18	119.5(10)
C33	Zn2	N4	105.3(3)	C40	C34	C35	119.0(8)
C33	Zn2	N3	126.7(4)	C33	C34	C35	121.6(9)
O9[3]	Zn1	O2	106.7(3)	C33	C34	C40	119.4(9)
O10[3]	Zn1	O2	134.2(3)	O2	C13	Zn1	48.0(5)
O10[3]	Zn1	O9[3]	60.3(3)	O1	C13	Zn1	72.7(6)
N2	Zn1	O2	116.4(3)	O1	C13	O2	120.7(10)
N2	Zn1	O9[3]	136.9(4)	C14	C13	Zn1	164.6(6)
N2	Zn1	O10[3]	88.7(4)	C14	C13	O2	117.0(8)
N1	Zn1	O2	95.6(5)	C14	C13	O1	122.2(8)
N1	Zn1	O9[3]	96.6(4)	C28	C29	C30	120.9(12)
N1	Zn1	O10[3]	127.9(5)	C10	C9	C8	124.7(12)
N1	Zn1	N2	78.7(5)	C16	C15	C14	119.8(12)
C13	Zn1	O2	29.2(3)	O9	C37	Zn1[4]	56.3(6)
C13	Zn1	O9[3]	110.7(4)	O10	C37	Zn1[4]	65.8(6)
C13	Zn1	O10[3]	109.6(3)	O10	C37	O9	121.5(10)
C13	Zn1	N2	107.5(4)	C36	C37	Zn1[4]	168.2(7)
C13	Zn1	N1	122.5(4)	C36	C37	O9	118.4(11)
C37[3]	Zn1	O2	127.2(3)	C36	C37	O10	120.1(11)
C37[3]	Zn1	O9[3]	30.9(4)	C17	C16	O3	118.0(13)
C37[3]	Zn1	O10[3]	29.6(4)	C15	C16	O3	121.2(13)
C37[3]	Zn1	N2	112.2(4)	C15	C16	C17	120.8(11)
C37[3]	Zn1	N1	113.2(4)	C9	C8	C7	118.2(11)
C37[3]	Zn1	C13	116.0(3)	C9	C10	C12	115.3(12)
C13	O2	Zn1	102.8(6)	C11	C10	C12	120.3(14)
C33	O6	Zn2	101.6(7)	C11	C10	C9	124.3(14)

[1]1-X,1-Y,-1/2+Z; [2]1-X,1-Y,1/2+Z; [3]+X,+Y,-1+Z; [4]+X,+Y,1+Z

Table S4

S.No	MOF	Loading Efficiency	Reference
1	Zn_8 $(Ad)_4$ $(BPDC)_6$ O_2 $(NH_2$ $(CH_3)_2)$	30.48 wt%	[5]
2	Zn_3 $(curcumin)_{27}(DMA)_3$ (ethanol)	0.24 *g*/*g*	[6]
3	[Zn_2 $(1,4\text{-bdc})_2$ (dabco)n]	15 wt%	[7]
4	[Zn $(tbda)]_n$	12.59%	[8]

References

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