Electronic Supporting Information Materials

Synthesis and anticancer mechanisms of zinc(II)-8-hydroxyquinoline complexes with 1,10-phenanthroline ancillary ligands

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Table S1. Crystal data and structure refinement for DQ1.

Empirical formula	$C_{30}H_{20}I_4N_4O_4Zn$
Formula weight	1073.47
Temperature/K	150.0
Crystal system	monoclinic
Space group	$P2_1/n$
a/Å	13.3296(7)
b/Å	16.3132(8)
c/Å	16.2439(9)
α/°	90
β/°	113.9813(19)
γ/°	90
Volume/Å^3	3227.3(3)
Z	4
ρ_{calc}mg/mm^3	2.209
m/mm^{-1}	4.629
F(000)	2008.0
Crystal size/mm^3	0.36 × 0.25 × 0.19
2Θ range for data collection	3.71 to 52.79°
Index ranges	-16 ≤ h ≤ 16, -20 ≤ k ≤ 20, -20 ≤ l ≤ 20
Reflections collected	56637
Independent reflections	6634[R(int) = 0.0815]
Data/restraints/parameters	6634/0/390
Goodness-of-fit on F^2	1.010
Final R indexes [I>=2σ (I)]	R_1 = 0.0353, wR_2 = 0.0677
Final R indexes [all data]	R_1 = 0.0693, wR_2 = 0.0797

Largest diff. peak/hole / e Å^{-3}	0.91/-0.88

Table S2. Bond Lengths for DQ1.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
I1	C2	2.087(6)	C2	C1	1.394(8)
I3	C11	2.094(5)	C2	C3	1.403(8)
I4	C13	2.110(5)	C4	C5	1.416(8)
I2	C4	2.096(5)	C4	C3	1.371(8)
Zn1	O2	2.110(4)	C26	C25	1.390(8)
Zn1	O1	2.084(4)	C26	C27	1.395(8)
Zn1	N3	2.150(4)	C13	C14	1.409(8)
Zn1	N1	2.145(4)	C13	C12	1.373(8)
Zn1	N4	2.168(4)	C24	C23	1.505(8)
Zn1	N2	2.137(4)	C24	C25	1.376(7)
O2	C10	1.291(6)	C1	C6	1.449(7)
O1	C1	1.288(6)	C14	C15	1.424(8)
O4	C21	1.342(6)	C14	C18	1.397(8)
O4	C29	1.434(7)	C5	C6	1.426(7)
O3	C26	1.348(6)	C5	C9	1.413(8)
O3	C30	1.444(7)	C11	C12	1.392(8)
N3	C23	1.341(7)	C28	C27	1.386(8)
N3	C19	1.333(7)	C23	C22	1.386(7)
N1	C6	1.362(7)	C21	C22	1.394(8)
N1	C7	1.327(7)	C21	C20	1.383(7)
N4	C24	1.354(7)	C16	C17	1.405(8)
N4	C28	1.333(7)	C20	C19	1.389(8)
N2	C16	1.313(7)	C8	C9	1.354(8)
N2	C15	1.363(7)	C8	C7	1.397(8)
C10	C11	1.397(8)	C17	C18	1.356(8)
C10	C15	1.456(7)			

Table S3. Bond Angles for DQ1.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
O2	Zn1	N3	96.19(15)	C12	C13	I4	118.0(4)
O2	Zn1	N1	90.21(16)	C12	C13	C14	120.6(5)

O2	Zn1	N4	95.33(15)	N4	C24	C23	115.4(5)
O2	Zn1	N2	78.56(15)	N4	C24	C25	122.4(5)
O1	Zn1	O2	166.50(14)	C25	C24	C23	122.2(5)
O1	Zn1	N3	96.12(15)	O1	C1	C2	125.9(5)
O1	Zn1	N1	78.47(15)	O1	C1	C6	120.1(5)
O1	Zn1	N4	92.99(15)	C2	C1	C6	114.0(5)
O1	Zn1	N2	95.35(16)	C13	C14	C15	117.5(5)
N3	Zn1	N4	76.05(17)	C18	C14	C13	126.4(5)
N1	Zn1	N3	169.34(17)	C18	C14	C15	116.1(5)
N1	Zn1	N4	94.92(17)	C4	C5	C6	117.0(5)
N2	Zn1	N3	92.72(17)	C9	C5	C4	126.0(5)
N2	Zn1	N1	96.91(17)	C9	C5	C6	117.0(5)
N2	Zn1	N4	166.69(17)	C10	C11	I3	119.1(4)
C10	O2	Zn1	113.2(3)	C12	C11	I3	117.8(4)
C1	O1	Zn1	113.5(3)	C12	C11	C10	123.1(5)
C21	O4	C29	118.9(4)	C4	C3	C2	121.2(5)
C26	O3	C30	117.9(5)	N4	C28	C27	124.8(5)
C23	N3	Zn1	117.2(4)	N3	C23	C24	115.4(5)
C19	N3	Zn1	125.5(4)	N3	C23	C22	123.4(5)
C19	N3	C23	117.4(5)	C22	C23	C24	121.3(5)
C6	N1	Zn1	111.5(3)	O4	C21	C22	124.6(5)
C7	N1	Zn1	128.1(4)	O4	C21	C20	116.2(5)
C7	N1	C6	119.9(5)	C20	C21	C22	119.1(5)
C24	N4	Zn1	116.0(4)	C24	C25	C26	119.3(5)
C28	N4	Zn1	126.7(4)	C23	C22	C21	118.2(5)
C28	N4	C24	117.3(5)	N2	C16	C17	122.4(5)
C16	N2	Zn1	128.2(4)	N1	C6	C1	115.1(5)
C16	N2	C15	119.1(5)	N1	C6	C5	120.9(5)
C15	N2	Zn1	112.7(3)	C5	C6	C1	124.0(5)
O2	C10	C11	124.9(5)	C28	C27	C26	117.0(5)
O2	C10	C15	120.6(5)	C21	C20	C19	118.1(5)
C11	C10	C15	114.5(5)	C9	C8	C7	119.3(5)
C1	C2	I1	118.7(4)	N3	C19	C20	123.8(5)
C1	C2	C3	123.4(5)	C8	C9	C5	120.6(6)
C3	C2	I1	117.8(4)	C13	C12	C11	121.2(5)
C5	C4	I2	120.4(4)	N2	C15	C10	114.9(5)
C3	C4	I2	119.1(4)	N2	C15	C14	122.2(5)
C3	C4	C5	120.4(5)	C14	C15	C10	123.0(5)
O3	C26	C25	115.5(5)	C18	C17	C16	119.0(5)
O3	C26	C27	125.3(5)	C17	C18	C14	121.2(5)

C25	C26	C27	119.2(5)	N1	C7	C8	122.2(5)
C14	C13	I4	121.4(4)				

Table S4. Crystal data and structure refinement for DQ2.

Empirical formula	$C_{33}H_{28}N_4O_3Zn$
Formula weight	593.96
Temperature/K	150.0
Crystal system	triclinic
Space group	P-1
a/Å	10.4644(5)
b/Å	10.8189(5)
c/Å	13.1161(7)
α/°	91.618(2)
β/°	104.1950(10)
γ/°	104.5620(10)
Volume/Å^3	1386.92(12)
Z	2
ρ_{calc}mg/mm^3	1.422
m/mm^{-1}	1.025
F(000)	616.0
Crystal size/mm^3	0.36 × 0.25 × 0.13
2Θ range for data collection	6.08 to 114.18°
Index ranges	$-12 \le h \le 13$, $-13 \le k \le 13$, $-16 \le l \le 16$
Reflections collected	14990
Independent reflections	5583[R(int) = 0.0274]
Data/restraints/parameters	5583/0/374
Goodness-of-fit on F^2	1.000
Final R indexes [I>=2σ (I)]	R_1 = 0.0315, wR_2 = 0.0814
Final R indexes [all data]	R_1 = 0.0323, wR_2 = 0.0819
Largest diff. peak/hole / e Å^{-3}	0.35/-0.56

Table S5. Bond Lengths for DQ2.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
Zn1	O1	2.0202(10)	C25	C24	1.414(2)
Zn1	O2	2.0102(10)	C2	C1	1.499(2)

Zn1	N2	2.2474(12)	C2	C3	1.419(2)
Zn1	N3	2.2041(12)	C9	C8	1.411(2)
Zn1	N4	2.2269(12)	C9	C10	1.369(2)
Zn1	N1	2.2924(12)	C8	C7	1.393(2)
O1	C7	1.3133(17)	C20	C15	1.416(2)
O2	C17	1.3036(18)	C20	C19	1.373(2)
O3	C33	1.399(3)	C15	C14	1.413(2)
N2	C16	1.3762(18)	C29	C28	1.346(3)
N2	C12	1.3328(18)	C29	C24	1.435(2)
N3	C25	1.3573(19)	C17	C18	1.398(2)
N3	C21	1.3284(19)	C23	C24	1.403(2)
N4	C26	1.3595(19)	C23	C22	1.368(3)
N4	C32	1.326(2)	C18	C19	1.400(2)
N1	C6	1.3710(18)	C30	C31	1.371(3)
N1	C2	1.3291(19)	C11	C12	1.497(2)
C6	C7	1.4410(19)	C4	C5	1.414(2)
C6	C5	1.4221(19)	C4	C3	1.357(2)
C26	C27	1.411(2)	C10	C5	1.412(2)
C26	C25	1.441(2)	C12	C13	1.418(2)
C27	C30	1.401(3)	C31	C32	1.403(2)
C27	C28	1.440(2)	C13	C14	1.364(2)
C16	C15	1.416(2)	C21	C22	1.405(2)
C16	C17	1.4438(19)			

Table S6. Bond Angles for DQ2.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
O1	Zn1	N2	102.33(4)	N3	C25	C24	122.43(14)
O1	Zn1	N3	87.47(4)	C24	C25	C26	119.49(13)
O1	Zn1	N4	95.73(4)	N1	C2	C1	119.26(13)
O1	Zn1	N1	77.73(4)	N1	C2	C3	121.33(14)
O2	Zn1	O1	176.57(4)	C3	C2	C1	119.41(14)
O2	Zn1	N2	79.03(4)	C10	C9	C8	121.31(14)
O2	Zn1	N3	95.58(4)	C7	C8	C9	121.62(14)
O2	Zn1	N4	83.53(4)	C19	C20	C15	118.84(14)
O2	Zn1	N1	98.95(4)	O1	C7	C6	119.34(12)
N2	Zn1	N1	100.76(4)	O1	C7	C8	123.13(13)
N3	Zn1	N2	94.68(4)	C8	C7	C6	117.53(12)

N3	Zn1	N4	75.65(5)	C16	C15	C20	120.23(14)
N3	Zn1	N1	160.52(5)	C14	C15	C16	116.67(14)
N4	Zn1	N2	159.16(4)	C14	C15	C20	123.10(14)
N4	Zn1	N1	93.11(4)	C28	C29	C24	120.88(15)
C7	O1	Zn1	117.74(9)	O2	C17	C16	120.09(12)
C17	O2	Zn1	115.86(8)	O2	C17	C18	123.13(13)
C16	N2	Zn1	107.47(9)	C18	C17	C16	116.77(13)
C12	N2	Zn1	133.62(10)	C22	C23	C24	119.92(14)
C12	N2	C16	118.78(13)	C17	C18	C19	121.94(14)
C25	N3	Zn1	114.17(9)	C31	C30	C27	119.73(15)
C21	N3	Zn1	127.34(10)	C3	C4	C5	120.00(14)
C21	N3	C25	118.37(13)	C9	C10	C5	119.34(13)
C26	N4	Zn1	113.23(9)	C20	C19	C18	121.71(14)
C32	N4	Zn1	127.65(10)	N2	C12	C11	119.51(14)
C32	N4	C26	118.22(13)	N2	C12	C13	121.11(14)
C6	N1	Zn1	107.76(8)	C13	C12	C11	119.36(13)
C2	N1	Zn1	133.38(10)	C4	C5	C6	116.51(14)
C2	N1	C6	118.86(12)	C10	C5	C6	120.26(13)
N1	C6	C7	117.30(12)	C10	C5	C4	123.23(13)
N1	C6	C5	122.80(12)	C30	C31	C32	119.07(15)
C5	C6	C7	119.90(13)	C29	C28	C27	121.35(15)
N4	C26	C27	122.65(14)	N4	C32	C31	122.89(15)
N4	C26	C25	117.91(12)	C14	C13	C12	120.60(14)
C27	C26	C25	119.44(14)	N3	C21	C22	122.91(15)
C26	C27	C28	119.26(15)	C4	C3	C2	120.48(14)
C30	C27	C26	117.41(15)	C25	C24	C29	119.48(15)
C30	C27	C28	123.31(15)	C23	C24	C25	117.39(14)
N2	C16	C15	122.96(13)	C23	C24	C29	123.10(15)
N2	C16	C17	116.57(12)	C13	C14	C15	119.80(14)
C15	C16	C17	120.46(13)	C23	C22	C21	118.91(15)
N3	C25	C26	118.07(12)				

Table S7. Crystal data and structure refinement for DQ3.

Empirical formula	$C_{36}H_{32}I_4N_4O_2Zn$
Formula weight	1125.62
Temperature/K	150.00
Crystal system	triclinic
Space group	P-1

a/Å	15.8190(7)
b/Å	15.9473(8)
c/Å	17.2056(8)
α/°	115.116(2)
β/°	104.391(2)
γ/°	95.426(2)
Volume/Å^3	3706.4(3)
Z	4
ρ_{calc}mg/mm^3	2.017
m/mm^{-1}	18.791
F(000)	2136.0
Crystal size/mm^3	0.12 × 0.1 × 0.08
2Θ range for data collection	5.21 to 114.612°
Index ranges	-19 ≤ h ≤ 19, -19 ≤ k ≤ 19, -21 ≤ l ≤ 21
Reflections collected	45815
Independent reflections	15199[R(int) = 0.0504]
Data/restraints/parameters	15199/0/859
Goodness-of-fit on F^2	1.043
Final R indexes [I>=2σ (I)]	R_1 = 0.0401, wR_2 = 0.0960
Final R indexes [all data]	R_1 = 0.0566, wR_2 = 0.1031
Largest diff. peak/hole / e Å^{-3}	1.14/-1.94

Table S8. Bond Lengths for DQ3.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
I1	C4	2.103(5)	I5	C66	2.095(5)
I2	C2	2.102(5)	I6	C68	2.106(5)
I3	C18	2.106(5)	I7	C57	2.098(5)
I4	C16	2.099(5)	I8	C59	2.106(5)
Zn1	O1	2.083(3)	Zn2	O3	2.051(4)
Zn1	O2	2.084(4)	Zn2	O4	2.047(4)
Zn1	N1	2.162(4)	Zn2	N5	2.236(4)
Zn1	N2	2.140(4)	Zn2	N6	2.235(4)
Zn1	N3	2.159(4)	Zn2	N7	2.151(4)
Zn1	N4	2.174(4)	Zn2	N8	2.136(4)
O1	C1	1.285(6)	O3	C65	1.282(6)
O2	C15	1.288(6)	O4	C56	1.281(6)
N1	C10	1.327(7)	N5	C70	1.361(7)

N1	C14	1.355(7)	N5	C71	1.321(7)
N2	C6	1.363(6)	N6	C61	1.373(6)
N2	C9	1.320(6)	N6	C62	1.328(6)
N3	C24	1.341(6)	N7	C47	1.340(6)
N3	C28	1.343(6)	N7	C51	1.336(6)
N4	C19	1.338(6)	N8	C37	1.340(7)
N4	C23	1.348(6)	N8	C42	1.353(6)
C1	C2	1.388(7)	C37	C38	1.379(7)
C1	C6	1.450(7)	C38	C39	1.390(8)
C2	C3	1.414(7)	C39	C41	1.393(7)
C3	C4	1.367(8)	C39	C43	1.535(7)
C4	C5	1.410(7)	C41	C42	1.376(7)
C5	C6	1.427(6)	C42	C47	1.505(7)
C5	C7	1.419(8)	C43	C44	1.533(7)
C7	C8	1.357(7)	C43	C45	1.519(9)
C8	C9	1.413(7)	C43	C46	1.537(8)
C10	C11	1.418(8)	C47	C48	1.388(7)
C11	C12	1.353(8)	C48	C49	1.412(7)
C12	C13	1.417(8)	C49	C50	1.396(7)
C13	C14	1.426(7)	C49	C52	1.525(7)
C13	C18	1.408(8)	C50	C51	1.390(8)
C14	C15	1.453(7)	C52	C53	1.545(7)
C15	C16	1.392(7)	C52	C54	1.536(7)
C16	C17	1.403(8)	C52	C55	1.541(8)
C17	C18	1.375(8)	C56	C57	1.411(7)
C19	C20	1.386(7)	C56	C61	1.457(7)
C20	C21	1.390(7)	C57	C58	1.388(8)
C21	C22	1.404(7)	C58	C59	1.387(7)
C21	C33	1.535(7)	C59	C60	1.412(7)
C22	C23	1.389(7)	C60	C61	1.408(8)
C23	C24	1.497(7)	C60	C64	1.420(7)
C24	C25	1.396(7)	C62	C63	1.388(8)
C25	C26	1.398(7)	C63	C64	1.371(8)
C26	C27	1.407(7)	C65	C66	1.403(7)
C26	C29	1.518(7)	C65	C70	1.460(8)
C27	C28	1.376(7)	C66	C67	1.404(7)
C29	C30	1.540(7)	C67	C68	1.362(8)
C29	C31	1.530(8)	C68	C69	1.426(8)
C29	C32	1.533(8)	C69	C70	1.428(7)
C33	C34	1.508(8)	C69	C73	1.423(8)

C33	C35	1.510(9)	C71	C72	1.399(8)
C33	C36	1.530(8)	C72	C73	1.361(8)

Table S9. Bond Angles for DQ3.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
O1	Zn1	O2	161.76(13)	O3	Zn2	N5	77.75(15)
O1	Zn1	N1	89.89(15)	O3	Zn2	N6	93.76(16)
O1	Zn1	N2	78.38(14)	O3	Zn2	N7	160.18(16)
O1	Zn1	N3	104.52(15)	O3	Zn2	N8	94.42(15)
O1	Zn1	N4	91.28(14)	O4	Zn2	O3	98.93(15)
O2	Zn1	N1	78.21(15)	O4	Zn2	N5	93.46(15)
O2	Zn1	N2	89.71(15)	O4	Zn2	N6	77.53(15)
O2	Zn1	N3	90.17(15)	O4	Zn2	N7	95.31(16)
O2	Zn1	N4	103.13(14)	O4	Zn2	N8	160.96(15)
N1	Zn1	N4	93.75(15)	N6	Zn2	N5	166.64(15)
N2	Zn1	N1	98.79(15)	N7	Zn2	N5	87.74(16)
N2	Zn1	N3	95.31(15)	N7	Zn2	N6	102.75(16)
N2	Zn1	N4	163.67(17)	N8	Zn2	N5	102.64(16)
N3	Zn1	N1	161.61(15)	N8	Zn2	N6	88.15(15)
N3	Zn1	N4	74.88(15)	N8	Zn2	N7	75.48(16)
C1	O1	Zn1	114.4(3)	C65	O3	Zn2	114.4(3)
C15	O2	Zn1	114.4(3)	C56	O4	Zn2	113.8(3)
C10	N1	Zn1	127.7(4)	C70	N5	Zn2	108.3(3)
C10	N1	C14	120.4(5)	C71	N5	Zn2	132.3(4)
C14	N1	Zn1	111.4(3)	C71	N5	C70	118.9(5)
C6	N2	Zn1	112.3(3)	C61	N6	Zn2	109.1(3)
C9	N2	Zn1	127.5(3)	C62	N6	Zn2	132.4(4)
C9	N2	C6	120.2(4)	C62	N6	C61	117.9(5)
C24	N3	Zn1	117.9(3)	C47	N7	Zn2	117.3(3)
C24	N3	C28	117.6(4)	C51	N7	Zn2	123.3(3)
C28	N3	Zn1	124.5(3)	C51	N7	C47	119.2(5)
C19	N4	Zn1	125.1(3)	C37	N8	Zn2	123.6(4)
C19	N4	C23	117.7(4)	C37	N8	C42	118.1(4)
C23	N4	Zn1	117.1(3)	C42	N8	Zn2	118.1(3)
O1	C1	C2	125.6(5)	N8	C37	C38	122.8(5)
O1	C1	C6	120.0(4)	C37	C38	C39	120.0(5)
C2	C1	C6	114.4(4)	C38	C39	C41	116.6(5)

C1	C2	I2	117.6(4)	C38	C39	C43	122.6(5)
C1	C2	C3	123.0(5)	C41	C39	C43	120.7(5)
C3	C2	I2	119.4(4)	C42	C41	C39	121.1(5)
C4	C3	C2	121.0(5)	N8	C42	C41	121.4(5)
C3	C4	I1	118.6(4)	N8	C42	C47	113.8(4)
C3	C4	C5	120.4(4)	C41	C42	C47	124.8(5)
C5	C4	I1	120.9(4)	C39	C43	C46	111.3(5)
C4	C5	C6	117.6(5)	C44	C43	C39	110.8(4)
C4	C5	C7	126.3(4)	C44	C43	C46	108.7(4)
C7	C5	C6	116.0(4)	C45	C43	C39	107.0(4)
N2	C6	C1	114.9(4)	C45	C43	C44	110.0(5)
N2	C6	C5	121.8(4)	C45	C43	C46	109.1(5)
C5	C6	C1	123.3(4)	N7	C47	C42	115.2(4)
C8	C7	C5	121.0(5)	N7	C47	C48	121.6(4)
C7	C8	C9	119.3(5)	C48	C47	C42	123.2(4)
N2	C9	C8	121.7(5)	C47	C48	C49	120.6(4)
N1	C10	C11	121.0(5)	C48	C49	C52	120.9(4)
C12	C11	C10	119.3(5)	C50	C49	C48	116.1(5)
C11	C12	C13	121.5(5)	C50	C49	C52	122.9(5)
C12	C13	C14	115.6(5)	C51	C50	C49	120.1(5)
C18	C13	C12	126.6(5)	N7	C51	C50	122.4(5)
C18	C13	C14	117.7(5)	C49	C52	C53	111.4(4)
N1	C14	C13	122.1(5)	C49	C52	C54	107.9(5)
N1	C14	C15	115.4(4)	C49	C52	C55	110.7(4)
C13	C14	C15	122.5(5)	C54	C52	C53	108.9(5)
O2	C15	C14	119.8(5)	C54	C52	C55	109.2(4)
O2	C15	C16	125.2(5)	C55	C52	C53	108.7(5)
C16	C15	C14	115.0(5)	O4	C56	C57	124.4(5)
C15	C16	I4	118.1(4)	O4	C56	C61	121.9(4)
C15	C16	C17	122.8(5)	C57	C56	C61	113.6(5)
C17	C16	I4	119.0(4)	C56	C57	I7	118.1(4)
C18	C17	C16	120.9(5)	C58	C57	I7	118.4(4)
C13	C18	I3	120.5(4)	C58	C57	C56	123.4(5)
C17	C18	I3	118.7(4)	C59	C58	C57	121.1(5)
C17	C18	C13	120.5(5)	C58	C59	I8	118.0(4)
N4	C19	C20	123.5(5)	C58	C59	C60	119.8(5)
C19	C20	C21	119.6(5)	C60	C59	I8	122.1(4)
C20	C21	C22	116.7(4)	C59	C60	C64	125.1(5)
C20	C21	C33	120.6(4)	C61	C60	C59	118.1(5)
C22	C21	C33	122.7(4)	C61	C60	C64	116.8(5)

C23	C22	C21	120.3(5)	N6	C61	C56	113.4(5)
N4	C23	C22	122.0(4)	N6	C61	C60	122.8(4)
N4	C23	C24	115.0(4)	C60	C61	C56	123.7(4)
C22	C23	C24	123.0(4)	N6	C62	C63	123.1(5)
N3	C24	C23	114.9(4)	C64	C63	C62	119.7(5)
N3	C24	C25	122.1(4)	C63	C64	C60	119.5(5)
C25	C24	C23	122.9(4)	O3	C65	C66	125.4(5)
C24	C25	C26	120.9(4)	O3	C65	C70	120.4(5)
C25	C26	C27	115.5(5)	C66	C65	C70	114.1(4)
C25	C26	C29	124.2(4)	C65	C66	I5	118.0(4)
C27	C26	C29	120.3(5)	C65	C66	C67	123.5(5)
C28	C27	C26	120.3(5)	C67	C66	I5	118.4(4)
N3	C28	C27	123.4(5)	C68	C67	C66	121.4(5)
C26	C29	C30	109.1(4)	C67	C68	I6	119.2(4)
C26	C29	C31	109.0(5)	C67	C68	C69	119.8(5)
C26	C29	C32	111.6(4)	C69	C68	I6	121.0(4)
C31	C29	C30	108.9(5)	C68	C69	C70	118.2(5)
C31	C29	C32	109.8(5)	C73	C69	C68	125.4(5)
C32	C29	C30	108.5(5)	C73	C69	C70	116.4(5)
C34	C33	C21	111.6(4)	N5	C70	C65	115.4(4)
C34	C33	C35	111.0(6)	N5	C70	C69	122.0(5)
C34	C33	C36	107.7(5)	C69	C70	C65	122.6(5)
C35	C33	C21	108.8(4)	N5	C71	C72	123.3(5)
C35	C33	C36	108.4(5)	C73	C72	C71	119.0(5)
C36	C33	C21	109.4(4)	C72	C73	C69	120.3(5)

Table S10. Crystal data and structure refinement for DQ4.

Empirical formula	$C_{42}H_{24}I_4N_4O_2Zn$
Formula weight	1189.62
Temperature/K	150.0
Crystal system	monoclinic
Space group	$P2_1/c$
a/Å	10.8579(4)
b/Å	23.2132(8)
c/Å	15.9267(5)
α/°	90
β/°	108.1264(12)
γ/°	90

Volume/Å^3	3815.1(2)
Z	4
ρ_{calc}mg/mm^3	2.071
m/mm^{-1}	3.924
F(000)	2248.0
Crystal size/mm^3	0.38 × 0.21 × 0.15
2Θ range for data collection	3.948 to 52.784°
Index ranges	-13 ≤ h ≤ 13, -29 ≤ k ≤ 29, -19 ≤ l ≤ 19
Reflections collected	89463
Independent reflections	7804[R(int) = 0.0674]
Data/restraints/parameters	7804/0/478
Goodness-of-fit on F^2	1.065
Final R indexes [I>=2σ (I)]	R_1 = 0.0484, wR_2 = 0.1240
Final R indexes [all data]	R_1 = 0.0565, wR_2 = 0.1331
Largest diff. peak/hole / e Å^{-3}	1.78/-1.90

Table S11. Bond Lengths for DQ4.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
I3	C11	2.097(6)	C3	C2	1.405(8)
I2	C4	2.095(6)	C21	C31	1.486(9)
I4	C13	2.094(6)	C21	C22	1.424(8)
I1	C2	2.098(6)	C21	C20	1.385(8)
Zn1	O1	2.093(4)	C31	C36	1.390(9)
Zn1	O2	2.095(4)	C31	C32	1.408(9)
Zn1	N3	2.173(5)	C27	C22	1.431(8)
Zn1	N4	2.168(5)	C27	C26	1.357(9)
Zn1	N1	2.162(5)	C16	C17	1.385(9)
Zn1	N2	2.139(5)	C28	C25	1.427(8)
O1	C1	1.299(7)	C28	C37	1.485(9)
O2	C10	1.280(7)	C24	C23	1.436(8)
N3	C23	1.357(8)	C24	C25	1.395(8)
N3	C19	1.324(8)	C8	C9	1.352(10)
C11	C10	1.398(9)	C5	C6	1.428(8)
C11	C12	1.392(9)	C5	C9	1.423(9)
C10	C15	1.457(8)	C23	C22	1.418(8)
N4	C24	1.374(8)	C42	C41	1.396(9)
N4	C30	1.318(8)	C42	C37	1.387(9)

C7	N1	1.319(8)	C25	C26	1.440(8)
C7	C8	1.411(9)	C2	C1	1.381(9)
N1	C6	1.346(8)	C6	C1	1.446(9)
N2	C15	1.368(8)	C17	C18	1.365(9)
N2	C16	1.318(8)	C41	C40	1.366(11)
C4	C3	1.372(9)	C20	C19	1.398(9)
C4	C5	1.409(9)	C36	C35	1.385(10)
C13	C14	1.419(8)	C40	C39	1.395(11)
C13	C12	1.373(9)	C32	C33	1.394(10)
C15	C14	1.419(8)	C35	C34	1.378(11)
C14	C18	1.415(8)	C37	C38	1.400(10)
C29	C28	1.387(9)	C33	C34	1.384(12)
C29	C30	1.389(9)	C38	C39	1.390(10)

Table S12. Bond Angles for DQ4.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
O1	Zn1	O2	164.20(16)	C36	C31	C21	122.2(6)
O1	Zn1	N3	104.75(18)	C36	C31	C32	118.9(6)
O1	Zn1	N4	87.91(18)	C32	C31	C21	118.8(6)
O1	Zn1	N1	77.54(17)	C26	C27	C22	121.8(6)
O1	Zn1	N2	91.17(18)	N2	C16	C17	123.1(6)
O2	Zn1	N3	87.56(17)	C29	C28	C25	117.8(6)
O2	Zn1	N4	104.94(18)	C29	C28	C37	118.5(6)
O2	Zn1	N1	91.21(18)	C25	C28	C37	123.6(6)
O2	Zn1	N2	78.69(17)	N4	C24	C23	116.7(5)
N4	Zn1	N3	75.91(19)	N4	C24	C25	122.2(5)
N1	Zn1	N3	97.70(19)	C25	C24	C23	121.0(5)
N1	Zn1	N4	162.17(19)	C9	C8	C7	119.6(6)
N2	Zn1	N3	161.32(19)	C4	C5	C6	117.8(5)
N2	Zn1	N4	95.33(19)	C4	C5	C9	126.1(5)
N2	Zn1	N1	95.20(19)	C9	C5	C6	116.1(6)
C1	O1	Zn1	114.7(4)	N3	C23	C24	117.0(5)
C10	O2	Zn1	112.8(4)	N3	C23	C22	123.5(5)
C23	N3	Zn1	115.3(4)	C22	C23	C24	119.5(5)
C19	N3	Zn1	127.3(4)	C37	C42	C41	120.2(7)
C19	N3	C23	117.3(5)	C28	C25	C26	123.4(5)
C10	C11	I3	116.8(5)	C24	C25	C28	118.3(6)

C12	C11	I3	119.4(5)	C24	C25	C26	118.1(5)
C12	C11	C10	123.8(6)	N4	C30	C29	123.4(6)
O2	C10	C11	125.9(6)	C3	C2	I1	116.7(5)
O2	C10	C15	120.0(5)	C1	C2	I1	120.1(4)
C11	C10	C15	114.1(5)	C1	C2	C3	122.9(6)
C24	N4	Zn1	115.0(4)	N1	C6	C5	122.1(6)
C30	N4	Zn1	126.6(4)	N1	C6	C1	115.5(5)
C30	N4	C24	118.4(5)	C5	C6	C1	122.3(6)
N1	C7	C8	121.7(6)	C21	C22	C27	124.2(6)
C7	N1	Zn1	127.0(4)	C23	C22	C21	117.7(5)
C7	N1	C6	120.1(5)	C23	C22	C27	118.0(5)
C6	N1	Zn1	112.8(4)	C18	C17	C16	118.8(6)
C15	N2	Zn1	111.0(4)	C40	C41	C42	120.5(7)
C16	N2	Zn1	129.2(4)	C8	C9	C5	120.4(6)
C16	N2	C15	119.1(5)	C21	C20	C19	120.4(6)
C3	C4	I2	117.5(5)	C35	C36	C31	120.3(7)
C3	C4	C5	120.5(5)	N3	C19	C20	123.6(6)
C5	C4	I2	121.8(4)	C17	C18	C14	120.9(6)
C14	C13	I4	121.0(4)	C27	C26	C25	121.0(5)
C12	C13	I4	119.1(5)	C41	C40	C39	120.1(6)
C12	C13	C14	119.8(6)	O1	C1	C2	124.9(6)
N2	C15	C10	115.2(5)	O1	C1	C6	119.4(5)
N2	C15	C14	121.8(5)	C2	C1	C6	115.6(5)
C14	C15	C10	122.9(5)	C33	C32	C31	120.4(7)
C13	C14	C15	118.1(5)	C34	C35	C36	120.2(7)
C18	C14	C13	125.7(6)	C42	C37	C28	120.4(6)
C18	C14	C15	116.1(5)	C42	C37	C38	119.1(6)
C28	C29	C30	119.8(6)	C38	C37	C28	120.3(6)
C4	C3	C2	120.8(6)	C34	C33	C32	119.2(7)
C22	C21	C31	122.7(5)	C35	C34	C33	120.9(7)
C20	C21	C31	120.0(5)	C39	C38	C37	120.1(7)
C20	C21	C22	117.3(6)	C38	C39	C40	119.8(7)
C13	C12	C11	121.2(6)				

Table S13. Crystal data and structure refinement for DQ5.

Empirical formula	$C_{30}H_{20}Cl_4N_4O_2Zn$
Formula weight	675.67
Temperature/K	150.0

Crystal system	monoclinic
Space group	C2/c
a/Å	7.8637(2)
b/Å	26.8187(7)
c/Å	13.3443(4)
α/°	90
β/°	91.9651(10)
γ/°	90
Volume/Å^3	2812.58(13)
Z	4
ρ_{calc}mg/mm^3	1.596
m/mm^{-1}	1.290
F(000)	1368.0
Crystal size/mm^3	0.38 × 0.24 × 0.13
2Θ range for data collection	4.308 to 52.756°
Index ranges	-9 ≤ h ≤ 9, -33 ≤ k ≤ 33, -16 ≤ l ≤ 16
Reflections collected	22511
Independent reflections	2888[R(int) = 0.0281]
Data/restraints/parameters	2888/0/187
Goodness-of-fit on F^2	1.022
Final R indexes [I>=2σ (I)]	R_1 = 0.0240, wR_2 = 0.0639
Final R indexes [all data]	R_1 = 0.0284, wR_2 = 0.0663
Largest diff. peak/hole / e Å^{-3}	0.29/-0.19

Table S14. Bond Lengths for DQ5.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
Zn1	O1	2.0969(12)	C6	C5	1.421(2)
Zn1	O1^1	2.0969(12)	C6	N1	1.356(2)
Zn1	N2	2.1534(14)	C1	C2	1.396(2)
Zn1	N2^1	2.1534(14)	C5	C4	1.410(2)
Zn1	N1^1	2.1500(14)	C5	C9	1.411(2)
Zn1	N1	2.1499(14)	C4	C3	1.372(2)
Cl1	C2	1.7445(17)	C9	C8	1.366(3)
Cl2	C4	1.7465(17)	C2	C3	1.401(2)
O1	C1	1.290(2)	C13	C12	1.383(2)
N2	C14	1.341(2)	C12	C11	1.390(3)
N2	C10	1.339(2)	C7	C8	1.404(2)

C14	C14[1]	1.495(3)	C7	N1	1.321(2)
C14	C13	1.388(2)	C11	C10	1.385(2)
C6	C1	1.455(2)	C11	C15	1.504(2)

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

Table S15. Bond Angles for DQ5.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
O1[1]	Zn1	O1	163.22(7)	O1	C1	C6	120.24(15)
O1[1]	Zn1	N2	100.42(5)	O1	C1	C2	125.44(15)
O1	Zn1	N2	92.80(5)	C2	C1	C6	114.31(15)
O1[1]	Zn1	N2[1]	92.80(5)	C4	C5	C6	117.62(15)
O1	Zn1	N2[1]	100.42(5)	C4	C5	C9	125.33(16)
O1	Zn1	N1[1]	90.22(5)	C9	C5	C6	117.02(15)
O1	Zn1	N1	78.45(5)	C5	C4	Cl2	118.97(13)
O1[1]	Zn1	N1[1]	78.45(5)	C3	C4	Cl2	120.05(13)
O1[1]	Zn1	N1	90.22(5)	C3	C4	C5	120.97(16)
N2	Zn1	N2[1]	76.18(7)	C8	C9	C5	120.21(16)
N1	Zn1	N2	166.40(5)	C1	C2	Cl1	118.21(13)
N1	Zn1	N2[1]	95.00(5)	C1	C2	C3	123.67(15)
N1[1]	Zn1	N2[1]	166.40(5)	C3	C2	Cl1	118.11(13)
N1[1]	Zn1	N2	95.00(5)	C12	C13	C14	119.45(16)
N1	Zn1	N1[1]	95.42(7)	C13	C12	C11	120.18(16)
C1	O1	Zn1	113.76(10)	N1	C7	C8	122.49(16)
C14	N2	Zn1	116.22(11)	C12	C11	C15	122.61(16)
C10	N2	Zn1	124.87(11)	C10	C11	C12	116.41(15)
C10	N2	C14	118.86(14)	C10	C11	C15	120.99(16)
N2	C14	C14[1]	115.67(9)	N2	C10	C11	124.13(16)
N2	C14	C13	120.97(14)	C9	C8	C7	118.96(16)
C13	C14	C14[1]	123.36(10)	C4	C3	C2	120.32(16)
C5	C6	C1	123.01(15)	C6	N1	Zn1	112.24(11)
N1	C6	C1	115.27(15)	C7	N1	Zn1	128.09(12)
N1	C6	C5	121.69(15)	C7	N1	C6	119.61(15)

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

Table S16. Crystal data and structure refinement for DQ6.	
Empirical formula	$C_{42}H_{24}Cl_4N_4O_2Zn$
Formula weight	823.82
Temperature/K	150.0
Crystal system	monoclinic
Space group	$P2_1/c$
a/Å	10.6616(6)
b/Å	22.4031(13)
c/Å	15.5392(9)
α/°	90
β/°	107.604(2)
γ/°	90
Volume/Å^3	3537.8(4)
Z	4
ρ_{calc}mg/mm^3	1.547
m/mm^{-1}	2.647
F(000)	1672.0
Crystal size/mm^3	0.36 × 0.25 × 0.21
2Θ range for data collection	6.224 to 114.044°
Index ranges	$-13 \leq h \leq 13$, $-28 \leq k \leq 25$, $-19 \leq l \leq 19$
Reflections collected	31840
Independent reflections	7204[R(int) = 0.0370]
Data/restraints/parameters	7204/0/478
Goodness-of-fit on F^2	1.045
Final R indexes [I>=2σ (I)]	R_1 = 0.0302, wR_2 = 0.0811
Final R indexes [all data]	R_1 = 0.0322, wR_2 = 0.0823
Largest diff. peak/hole / e Å^{-3}	0.35/-0.46

Table S17. Bond Lengths for DQ6.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
Zn1	O1	2.0743(11)	C36	C37	1.486(2)
Zn1	O2	2.0840(11)	C36	C35	1.384(2)
Zn1	N4	2.1747(13)	C36	C32	1.429(2)
Zn1	N3	2.1886(13)	C29	C30	1.435(2)
Zn1	N1	2.1763(13)	C29	C28	1.412(2)
Zn1	N2	2.1532(13)	C29	C25	1.423(2)
Cl2	C4	1.7492(16)	C6	C1	1.449(2)

Cl1	C2	1.7388(16)	C8	C9	1.365(3)
Cl4	C13	1.7488(17)	C13	C12	1.368(3)
Cl3	C11	1.7429(17)	C28	C33	1.450(2)
O1	C1	1.2898(19)	C26	C25	1.373(2)
O2	C10	1.289(2)	C26	C27	1.396(2)
N4	C33	1.361(2)	C25	C24	1.495(2)
N4	C34	1.328(2)	C42	C37	1.397(2)
N3	C28	1.356(2)	C42	C41	1.393(3)
N3	C27	1.327(2)	C33	C32	1.410(2)
N1	C7	1.325(2)	C24	C23	1.394(2)
N1	C6	1.363(2)	C24	C19	1.386(2)
N2	C15	1.363(2)	C18	C17	1.367(3)
N2	C16	1.322(2)	C4	C3	1.365(2)
C11	C10	1.402(2)	C23	C22	1.389(2)
C11	C12	1.400(3)	C37	C38	1.395(2)
C15	C14	1.417(2)	C35	C34	1.395(2)
C15	C10	1.451(2)	C40	C41	1.378(3)
C14	C13	1.418(2)	C40	C39	1.385(3)
C14	C18	1.412(2)	C2	C1	1.394(2)
C31	C30	1.358(2)	C2	C3	1.403(2)
C31	C32	1.441(2)	C16	C17	1.402(2)
C7	C8	1.409(2)	C22	C21	1.382(3)
C5	C6	1.422(2)	C39	C38	1.388(2)
C5	C4	1.416(2)	C19	C20	1.391(3)
C5	C9	1.414(2)	C21	C20	1.381(3)

Table S18. Bond Angles for DQ6.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
O1	Zn1	O2	163.36(4)	C5	C6	C1	123.11(14)
O1	Zn1	N4	103.54(5)	C9	C8	C7	119.04(15)
O1	Zn1	N3	86.79(5)	C14	C13	Cl4	119.39(13)
O1	Zn1	N1	77.76(5)	C12	C13	Cl4	119.81(13)
O1	Zn1	N2	91.66(5)	C12	C13	C14	120.78(15)
O2	Zn1	N4	89.11(5)	C31	C30	C29	121.62(14)
O2	Zn1	N3	107.11(5)	N3	C28	C29	123.37(14)
O2	Zn1	N1	89.83(5)	N3	C28	C33	116.77(13)
O2	Zn1	N2	78.64(5)	C29	C28	C33	119.84(14)

N4	Zn1	N3	75.39(5)	C25	C26	C27	120.43(15)
N4	Zn1	N1	98.57(5)	C29	C25	C24	123.00(14)
N1	Zn1	N3	161.70(5)	C26	C25	C29	118.02(14)
N2	Zn1	N4	160.52(5)	C26	C25	C24	118.96(14)
N2	Zn1	N3	93.66(5)	C41	C42	C37	120.59(17)
N2	Zn1	N1	96.50(5)	N4	C33	C28	116.50(13)
C1	O1	Zn1	115.36(10)	N4	C33	C32	123.68(14)
C10	O2	Zn1	112.86(10)	C32	C33	C28	119.82(13)
C33	N4	Zn1	115.82(10)	C23	C24	C25	120.17(15)
C34	N4	Zn1	126.62(11)	C19	C24	C25	120.37(15)
C34	N4	C33	117.47(14)	C19	C24	C23	119.22(15)
C28	N3	Zn1	115.41(10)	C17	C18	C14	120.20(16)
C27	N3	Zn1	126.85(11)	C5	C4	Cl2	119.95(13)
C27	N3	C28	117.67(13)	C3	C4	Cl2	118.92(13)
C7	N1	Zn1	128.65(11)	C3	C4	C5	121.05(15)
C7	N1	C6	119.11(14)	C22	C23	C24	119.71(16)
C6	N1	Zn1	112.03(10)	C42	C37	C36	119.91(15)
C15	N2	Zn1	111.31(10)	C38	C37	C36	121.62(14)
C16	N2	Zn1	129.07(11)	C38	C37	C42	118.44(15)
C16	N2	C15	119.41(14)	C36	C35	C34	120.57(15)
C10	C11	Cl3	117.87(13)	C8	C9	C5	120.31(15)
C12	C11	Cl3	118.55(13)	C41	C40	C39	119.71(17)
C12	C11	C10	123.56(16)	C1	C2	Cl1	118.90(12)
N2	C15	C14	121.69(14)	C1	C2	C3	123.02(15)
N2	C15	C10	114.84(14)	C3	C2	Cl1	118.05(13)
C14	C15	C10	123.46(14)	C36	C32	C31	123.92(14)
C15	C14	C13	117.41(15)	C33	C32	C31	118.64(13)
C18	C14	C15	117.03(15)	C33	C32	C36	117.43(14)
C18	C14	C13	125.54(15)	N2	C16	C17	122.49(16)
O2	C10	C11	125.34(15)	O1	C1	C6	120.05(14)
O2	C10	C15	120.63(14)	O1	C1	C2	125.14(15)
C11	C10	C15	114.02(14)	C2	C1	C6	114.81(14)
C30	C31	C32	121.08(14)	C21	C22	C23	120.73(16)
N1	C7	C8	122.60(16)	C40	C41	C42	120.28(17)
C4	C5	C6	117.15(14)	N4	C34	C35	123.18(15)
C9	C5	C6	116.87(15)	C4	C3	C2	120.75(15)
C9	C5	C4	125.96(15)	N3	C27	C26	123.05(15)
C35	C36	C37	119.98(14)	C40	C39	C38	120.41(17)
C35	C36	C32	117.51(14)	C18	C17	C16	119.02(16)
C32	C36	C37	122.50(14)	C13	C12	C11	120.63(15)

C28	C29	C30	118.46(14)	C24	C19	C20	120.66(16)
C28	C29	C25	117.40(14)	C20	C21	C22	119.71(16)
C25	C29	C30	124.10(14)	C21	C20	C19	119.92(17)
N1	C6	C5	122.05(14)	C39	C38	C37	120.54(16)
N1	C6	C1	114.77(13)				

Table S19. Crystal data and structure refinement for DQ7.

Identification code	
Empirical formula	$C_{31}H_{24}Cl_2I_2N_4O_3Zn$
Formula weight	890.61
Temperature/K	150.0
Crystal system	monoclinic
Space group	$P2_1/c$
a/Å	10.7899(3)
b/Å	22.2877(7)
c/Å	14.1425(5)
α/°	90
β/°	108.9750(10)
γ/°	90
Volume/Å^3	3216.21(18)
Z	4
ρ_{calc}mg/mm^3	1.839
m/mm^{-1}	12.291
F(000)	1728.0
Crystal size/mm^3	0.36 × 0.25 × 0.16
2Θ range for data collection	6.706 to 104.996°
Index ranges	$-12 \leq h \leq 12$, $-26 \leq k \leq 25$, $-16 \leq l \leq 7$
Reflections collected	28658
Independent reflections	5585[R(int) = 0.0784]
Data/restraints/parameters	5585/0/392
Goodness-of-fit on F^2	1.026
Final R indexes [I>=2σ (I)]	R_1 = 0.0540, wR_2 = 0.1356
Final R indexes [all data]	R_1 = 0.0567, wR_2 = 0.1381
Largest diff. peak/hole / e Å^{-3}	1.81/-1.07

Table S20. Bond Lengths for DQ7.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
I1	C2	2.108(6)	C1	C2	1.401(7)
I2	C11	2.091(5)	C14	C15	1.434(8)
Zn1	O1	2.064(3)	C14	C13	1.411(8)
Zn1	O2	2.084(3)	C14	C18	1.407(9)
Zn1	N2	2.198(4)	C7	C8	1.402(8)
Zn1	N1	2.133(4)	C2	C3	1.397(8)
Zn1	N4	2.202(4)	C9	C5	1.413(8)
Zn1	N3	2.151(4)	C9	C8	1.375(8)
Cl2	C13	1.748(5)	C5	C4	1.420(8)
Cl1	C4	1.746(6)	C24	C25	1.399(8)
O1	C1	1.292(6)	C24	C23	1.482(8)
O2	C10	1.301(6)	C25	C26	1.376(9)
O3	C31	1.408(7)	C13	C12	1.353(9)
N2	C15	1.354(7)	C19	C20	1.408(8)
N2	C16	1.325(7)	C23	C22	1.386(8)
N1	C6	1.365(6)	C11	C12	1.411(8)
N1	C7	1.334(7)	C20	C21	1.392(9)
N4	C24	1.355(7)	C20	C29	1.492(9)
N4	C28	1.336(7)	C28	C27	1.404(8)
N3	C19	1.327(7)	C17	C16	1.391(9)
N3	C23	1.354(7)	C17	C18	1.366(9)
C6	C1	1.443(8)	C22	C21	1.380(9)
C6	C5	1.421(8)	C4	C3	1.363(9)
C10	C15	1.444(8)	C27	C26	1.383(9)
C10	C11	1.395(7)	C27	C30	1.504(9)

Table S21. Bond Angles for DQ7.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
O1	Zn1	O2	104.79(14)	N2	C15	C14	121.7(5)
O1	Zn1	N2	97.62(15)	C14	C15	C10	122.1(5)
O1	Zn1	N1	79.72(15)	C1	C2	I1	117.9(4)
O1	Zn1	N4	165.46(15)	C1	C2	C3	123.2(5)
O1	Zn1	N3	92.01(15)	C3	C2	I1	118.9(4)
O2	Zn1	N2	78.03(15)	C8	C9	C5	119.8(5)
O2	Zn1	N1	87.92(14)	C6	C5	C9	117.8(5)

O2	Zn1	N4	89.02(15)	C6	C5	C4	117.1(5)
O2	Zn1	N3	161.23(15)	C9	C5	C4	125.0(5)
N2	Zn1	N4	89.59(16)	C9	C8	C7	119.3(5)
N1	Zn1	N2	164.59(16)	N4	C24	C25	120.9(5)
N1	Zn1	N4	96.54(16)	N4	C24	C23	115.3(5)
N1	Zn1	N3	103.52(16)	C25	C24	C23	123.8(5)
N3	Zn1	N2	91.70(16)	C26	C25	C24	119.1(5)
N3	Zn1	N4	75.09(17)	C14	C13	Cl2	119.4(5)
C1	O1	Zn1	112.9(3)	C12	C13	Cl2	118.5(4)
C10	O2	Zn1	114.1(3)	C12	C13	C14	122.0(5)
C15	N2	Zn1	110.7(3)	N3	C19	C20	123.6(5)
C16	N2	Zn1	129.7(4)	N3	C23	C24	115.7(5)
C16	N2	C15	119.4(5)	N3	C23	C22	121.0(5)
C6	N1	Zn1	110.5(3)	C22	C23	C24	123.3(5)
C7	N1	Zn1	128.7(3)	C10	C11	I2	118.1(4)
C7	N1	C6	120.0(4)	C10	C11	C12	122.8(5)
C24	N4	Zn1	115.5(3)	C12	C11	I2	119.1(4)
C28	N4	Zn1	124.5(4)	C19	C20	C29	121.5(6)
C28	N4	C24	118.8(5)	C21	C20	C19	115.5(5)
C19	N3	Zn1	123.0(4)	C21	C20	C29	123.0(5)
C19	N3	C23	119.6(5)	N4	C28	C27	123.7(5)
C23	N3	Zn1	117.4(4)	C13	C12	C11	120.1(5)
N1	C6	C1	115.5(4)	C18	C17	C16	119.8(5)
N1	C6	C5	121.0(5)	C21	C22	C23	118.7(5)
C5	C6	C1	123.5(5)	N2	C16	C17	122.5(5)
O2	C10	C15	120.1(4)	C5	C4	Cl1	118.4(5)
O2	C10	C11	124.4(5)	C3	C4	Cl1	120.9(4)
C11	C10	C15	115.5(4)	C3	C4	C5	120.7(5)
O1	C1	C6	120.6(4)	C22	C21	C20	121.6(5)
O1	C1	C2	125.0(5)	C28	C27	C30	119.8(5)
C2	C1	C6	114.4(5)	C26	C27	C28	116.5(5)
C13	C14	C15	117.1(5)	C26	C27	C30	123.6(5)
C18	C14	C15	116.7(5)	C25	C26	C27	121.0(5)
C18	C14	C13	126.1(5)	C4	C3	C2	121.0(5)
N1	C7	C8	122.0(5)	C17	C18	C14	119.9(5)
N2	C15	C10	116.2(4)				

Table S22. Crystal data and structure refinement for DQ8.

Empirical formula	$C_{28}H_{16}Cl_2I_2N_4O_2Zn$
Formula weight	830.52
Temperature/K	150.0
Crystal system	orthorhombic
Space group	Pbca
a/Å	15.2339(4)
b/Å	16.1890(4)
c/Å	22.6467(5)
α/°	90
β/°	90
γ/°	90
Volume/Å^3	5585.2(2)
Z	8
ρ_{calc}mg/mm^3	1.975
m/mm^{-1}	13.730
F(000)	3184.0
Crystal size/mm^3	0.36 × 0.26 × 0.13
2Θ range for data collection	6.792 to 114.032°
Index ranges	-19 ≤ h ≤ 16, -13 ≤ k ≤ 20, -28 ≤ l ≤ 27
Reflections collected	51197
Independent reflections	5711[R(int) = 0.0871]
Data/restraints/parameters	5711/6/352
Goodness-of-fit on F^2	1.058
Final R indexes [I>=2σ (I)]	R_1 = 0.0422, wR_2 = 0.1121
Final R indexes [all data]	R_1 = 0.0457, wR_2 = 0.1149
Largest diff. peak/hole / e Å^{-3}	1.19/-2.08

Table S23. Bond Lengths for DQ8.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
I2	C11	2.092(4)	C23	C22	1.393(6)
I1	C2	2.092(4)	C23	C24	1.481(6)
Zn1	O2	2.052(3)	C11	C10	1.387(5)
Zn1	O1	2.044(3)	C11	C12	1.416(6)
Zn1	N4	2.173(3)	C14	C13	1.410(6)
Zn1	N3	2.176(3)	C14	C15	1.421(5)
Zn1	N2	2.163(4)	C20	C21	1.383(7)
Zn1	N1	2.180(3)	C3	C2	1.414(5)

Cl1	C4	1.742(4)	C3	C4	1.375(7)
Cl2	C13	1.742(4)	C10	C15	1.449(6)
O2	C10	1.307(5)	C2	C1	1.395(5)
O1	C1	1.291(5)	C1	C6	1.453(6)
N4	C24	1.349(6)	C26	C27	1.383(7)
N4	C28	1.338(6)	C26	C25	1.381(7)
N3	C19	1.342(6)	C5	C4	1.413(6)
N3	C23	1.344(5)	C5	C6	1.422(5)
N2	C16	1.317(6)	C5	C9	1.400(6)
N2	C15	1.360(5)	C12	C13	1.357(7)
N1	C7	1.321(6)	C22	C21	1.381(7)
N1	C6	1.362(5)	C8	C7	1.407(6)
C19	C20	1.375(6)	C8	C9	1.372(6)
C18	C17	1.367(7)	C24	C25	1.395(6)
C18	C14	1.408(7)	C28	C27	1.384(6)
C17	C16	1.408(6)			

Table S24. Bond Angles for DQ8.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
O2	Zn1	N4	90.52(12)	C19	C20	C21	119.1(5)
O2	Zn1	N3	163.77(12)	C4	C3	C2	120.7(4)
O2	Zn1	N2	79.51(12)	O2	C10	C11	124.6(4)
O2	Zn1	N1	100.88(12)	O2	C10	C15	120.6(3)
O1	Zn1	O2	98.33(12)	C11	C10	C15	114.8(3)
O1	Zn1	N4	169.11(12)	C3	C2	I1	119.5(3)
O1	Zn1	N3	96.72(12)	C1	C2	I1	117.9(3)
O1	Zn1	N2	96.46(12)	C1	C2	C3	122.6(4)
O1	Zn1	N1	78.87(12)	O1	C1	C2	124.5(4)
N4	Zn1	N3	75.27(13)	O1	C1	C6	120.4(3)
N4	Zn1	N1	93.29(12)	C2	C1	C6	115.1(3)
N3	Zn1	N1	87.93(12)	C25	C26	C27	119.7(4)
N2	Zn1	N4	91.36(12)	C4	C5	C6	117.3(4)
N2	Zn1	N3	92.83(12)	C9	C5	C4	125.4(4)
N2	Zn1	N1	175.33(13)	C9	C5	C6	117.3(4)
C10	O2	Zn1	113.5(3)	C13	C12	C11	120.3(4)
C1	O1	Zn1	115.0(3)	C21	C22	C23	118.7(4)
C24	N4	Zn1	116.2(3)	C9	C8	C7	119.0(4)

C28	N4	Zn1	124.5(3)	C14	C13	Cl2	119.9(4)
C28	N4	C24	118.8(4)	C12	C13	Cl2	118.9(3)
C19	N3	Zn1	124.0(3)	C12	C13	C14	121.2(4)
C19	N3	C23	119.2(4)	N4	C24	C23	115.9(4)
C23	N3	Zn1	116.4(3)	N4	C24	C25	121.2(4)
C16	N2	Zn1	129.7(3)	C25	C24	C23	122.9(4)
C16	N2	C15	119.5(4)	N4	C28	C27	123.2(4)
C15	N2	Zn1	110.6(3)	C22	C21	C20	119.3(4)
C7	N1	Zn1	129.8(3)	N2	C16	C17	122.8(4)
C7	N1	C6	119.2(3)	C3	C4	Cl1	119.5(3)
C6	N1	Zn1	110.6(3)	C3	C4	C5	121.1(4)
N3	C19	C20	122.1(4)	C5	C4	Cl1	119.4(3)
C17	C18	C14	120.5(4)	N1	C7	C8	122.6(4)
C18	C17	C16	118.6(4)	N1	C6	C1	115.0(3)
N3	C23	C22	121.6(4)	N1	C6	C5	121.7(4)
N3	C23	C24	115.5(4)	C5	C6	C1	123.3(3)
C22	C23	C24	122.9(4)	C26	C27	C28	117.9(4)
C10	C11	I2	118.0(3)	C26	C25	C24	119.1(4)
C10	C11	C12	123.2(4)	C8	C9	C5	120.2(4)
C12	C11	I2	118.7(3)	N2	C15	C14	121.7(4)
C18	C14	C13	125.6(4)	N2	C15	C10	115.3(3)
C18	C14	C15	116.9(4)	C14	C15	C10	123.0(4)
C13	C14	C15	117.5(4)				

Table S25. Crystal data and structure refinement for DQ9.

Empirical formula	$C_{37}H_{36}Cl_2I_2N_4O_3Zn$
Formula weight	974.77
Temperature/K	150.0
Crystal system	monoclinic
Space group	$P2_1/n$
a/Å	12.1978(5)
b/Å	25.8911(11)
c/Å	12.7977(5)
α/°	90
β/°	107.537(2)
γ/°	90
Volume/Å^3	3853.8(3)
Z	4

ρ_{calc}mg/mm^3	1.680
m/mm^{-1}	10.024
F(000)	1920.0
Crystal size/mm^3	0.36 × 0.26 × 0.21
2Θ range for data collection	5.94 to 114.218°
Index ranges	-15 ≤ h ≤ 15, -32 ≤ k ≤ 27, -15 ≤ l ≤ 15
Reflections collected	30666
Independent reflections	7872[R(int) = 0.0543]
Data/restraints/parameters	7872/18/450
Goodness-of-fit on F^2	1.070
Final R indexes [I>=2σ (I)]	R_1 = 0.0485, wR_2 = 0.1243
Final R indexes [all data]	R_1 = 0.0598, wR_2 = 0.1300
Largest diff. peak/hole / e Å^{-3}	1.61/-1.35

Table S26. Bond Lengths for DQ9.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
I2	C11	2.099(5)	C15	C14	1.421(7)
I1	C2	2.102(5)	C4	C3	1.369(8)
Zn1	O2	2.095(4)	C4	C5	1.415(8)
Zn1	O1	2.066(4)	C16	C17	1.409(8)
Zn1	N1	2.144(4)	C20	C21	1.385(8)
Zn1	N2	2.160(4)	C20	C19	1.381(7)
Zn1	N3	2.187(4)	C23	C24	1.491(7)
Zn1	N4	2.184(4)	C23	C22	1.381(7)
Cl1	C4	1.738(5)	C24	C25	1.386(7)
Cl2	C13	1.737(5)	C6	C5	1.415(7)
O2	C10	1.300(6)	C25	C26	1.391(8)
O1	C1	1.291(6)	C22	C21	1.394(7)
N1	C7	1.326(7)	C21	C29	1.515(8)
N1	C6	1.354(7)	C5	C9	1.422(8)
N2	C15	1.363(7)	C27	C26	1.384(8)
N2	C16	1.304(7)	C27	C28	1.384(8)
C11	C10	1.390(7)	C26	C33	1.537(8)
C11	C12	1.410(7)	C14	C13	1.422(8)
N3	C23	1.355(6)	C14	C18	1.411(8)
N3	C19	1.328(6)	C17	C18	1.372(8)
C2	C1	1.395(7)	C33	C35	1.534(9)

C2	C3	1.408(8)	C33	C36	1.530(9)
N4	C24	1.340(6)	C33	C34	1.515(10)
N4	C28	1.331(6)	C8	C9	1.350(9)
C1	C6	1.455(7)	C29	C32	1.412(12)
C10	C15	1.443(7)	C29	C31	1.476(11)
C12	C13	1.360(8)	C29	C30	1.669(13)
C7	C8	1.399(8)	O3	C37	1.432(14)

Table S27. Bond Angles for DQ9.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
O2	Zn1	N1	92.58(15)	N2	C16	C17	123.1(5)
O2	Zn1	N2	78.38(15)	C4	C3	C2	120.3(5)
O2	Zn1	N3	90.41(15)	C19	C20	C21	120.1(5)
O2	Zn1	N4	162.35(15)	N3	C23	C24	115.1(4)
O1	Zn1	O2	103.48(15)	N3	C23	C22	121.8(5)
O1	Zn1	N1	78.87(15)	C22	C23	C24	123.1(4)
O1	Zn1	N2	95.97(14)	N4	C24	C23	115.7(4)
O1	Zn1	N3	164.27(15)	N4	C24	C25	121.6(5)
O1	Zn1	N4	92.59(15)	C25	C24	C23	122.7(4)
N1	Zn1	N2	168.36(17)	N1	C6	C1	114.8(4)
N1	Zn1	N3	93.34(16)	N1	C6	C5	122.4(5)
N1	Zn1	N4	97.72(16)	C5	C6	C1	122.8(5)
N2	Zn1	N3	94.04(15)	C24	C25	C26	121.0(5)
N2	Zn1	N4	92.91(16)	C23	C22	C21	121.1(5)
N4	Zn1	N3	74.78(16)	C20	C21	C22	116.0(5)
C10	O2	Zn1	114.1(3)	C20	C21	C29	122.5(5)
C1	O1	Zn1	114.0(3)	C22	C21	C29	121.5(5)
C7	N1	Zn1	129.0(4)	C4	C5	C6	118.2(5)
C7	N1	C6	119.0(5)	C4	C5	C9	125.5(5)
C6	N1	Zn1	112.0(3)	C6	C5	C9	116.4(5)
C15	N2	Zn1	111.7(3)	C28	C27	C26	119.8(5)
C16	N2	Zn1	128.6(4)	C25	C26	C33	120.1(5)
C16	N2	C15	119.7(4)	C27	C26	C25	116.3(5)
C10	C11	I2	119.0(4)	C27	C26	C33	123.7(5)
C10	C11	C12	122.9(5)	N4	C28	C27	123.3(5)
C12	C11	I2	118.0(4)	C15	C14	C13	117.4(5)
C23	N3	Zn1	116.7(3)	C18	C14	C15	117.4(5)

C19	N3	Zn1	125.7(3)	C18	C14	C13	125.2(5)
C19	N3	C23	117.2(4)	C18	C17	C16	118.6(5)
C1	C2	I1	118.0(4)	N3	C19	C20	123.7(5)
C1	C2	C3	123.7(5)	C35	C33	C26	110.4(6)
C3	C2	I1	118.3(4)	C36	C33	C26	110.2(5)
C24	N4	Zn1	117.0(3)	C36	C33	C35	108.8(6)
C28	N4	Zn1	124.6(4)	C34	C33	C26	109.0(5)
C28	N4	C24	117.9(4)	C34	C33	C35	109.4(5)
O1	C1	C2	125.4(5)	C34	C33	C36	109.0(7)
O1	C1	C6	120.2(5)	C12	C13	Cl2	119.7(5)
C2	C1	C6	114.4(4)	C12	C13	C14	121.0(5)
O2	C10	C11	124.7(5)	C14	C13	Cl2	119.3(4)
O2	C10	C15	119.9(5)	C17	C18	C14	119.8(5)
C11	C10	C15	115.4(5)	C9	C8	C7	119.4(5)
C13	C12	C11	120.5(5)	C8	C9	C5	120.3(5)
N1	C7	C8	122.5(5)	C21	C29	C30	105.2(6)
N2	C15	C10	115.9(4)	C32	C29	C21	115.6(7)
N2	C15	C14	121.3(5)	C32	C29	C31	121.4(8)
C14	C15	C10	122.8(5)	C32	C29	C30	100.4(9)
C3	C4	Cl1	119.2(4)	C31	C29	C21	112.1(6)
C3	C4	C5	120.7(5)	C31	C29	C30	98.0(8)
C5	C4	Cl1	120.1(4)				

Table S28. Crystal data and structure refinement for DQ10.

Empirical formula	$C_{120}H_{82}Cl_8I_8N_{16}O_{17}Zn_4$
Formula weight	3580.38
Temperature/K	150.0
Crystal system	monoclinic
Space group	$P2_1/c$
a/Å	18.6601(6)
b/Å	16.0154(6)
c/Å	10.7225(4)
α/°	90.00
β/°	104.4049(12)
γ/°	90.00
Volume/Å^3	3103.67(19)
Z	1
ρ_{calc}mg/mm^3	1.916

m/mm^{-1}	2.996
F(000)	1720.0
Crystal size/mm^3	0.45 × 0.37 × 0.29
2Θ range for data collection	4.5 to 50.02°
Index ranges	-22 ≤ h ≤ 22, -19 ≤ k ≤ 19, -12 ≤ l ≤ 12
Reflections collected	43747
Independent reflections	5459[R(int) = 0.0666]
Data/restraints/parameters	5459/6/396
Goodness-of-fit on F^2	0.997
Final R indexes [I>=2σ (I)]	R_1 = 0.0387, wR_2 = 0.0995
Final R indexes [all data]	R_1 = 0.0519, wR_2 = 0.1155
Largest diff. peak/hole / e Å^{-3}	0.63/-1.17

Table S29. Bond Lengths for DQ10.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
I1	C2	2.086(5)	N4	C24	1.370(6)
I2	C11	2.090(5)	C3	C4	1.356(8)
Zn1	O2	2.104(3)	C12	C13	1.365(8)
Zn1	N1	2.138(4)	C20	C21	1.389(9)
Zn1	O1	2.123(3)	C20	C19	1.377(8)
Zn1	N3	2.179(4)	N2	C15	1.359(6)
Zn1	N4	2.135(4)	N2	C16	1.314(7)
Zn1	N2	2.116(4)	C6	C1	1.457(7)
Cl1	C4	1.749(5)	C6	C5	1.425(7)
Cl2	C13	1.755(6)	C14	C15	1.421(8)
O2	C10	1.282(6)	C14	C13	1.416(8)
N1	C6	1.370(6)	C14	C18	1.404(8)
N1	C7	1.323(7)	C8	C7	1.396(8)
O3	C21	1.340(6)	C8	C9	1.370(8)
O3	C29	1.442(8)	C4	C5	1.395(8)
O1	C1	1.287(6)	C28	C27	1.377(8)
N3	C23	1.341(7)	C24	C25	1.370(7)
N3	C19	1.339(7)	C24	C23	1.491(7)
C11	C10	1.392(7)	C25	C26	1.398(8)
C11	C12	1.411(8)	C21	C22	1.395(8)
C2	C3	1.414(8)	C27	C26	1.387(8)
C2	C1	1.397(7)	C23	C22	1.392(7)

O4	C30	1.412(7)	C16	C17	1.395(8)
O4	C26	1.343(7)	C9	C5	1.410(8)
C10	C15	1.467(7)	C18	C17	1.361(8)
N4	C28	1.335(7)			

Table S30. Bond Angles for DQ10.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
O2	Zn1	N1	95.79(15)	N1	C6	C5	121.5(5)
O2	Zn1	O1	169.13(14)	C5	C6	C1	123.5(4)
O2	Zn1	N3	94.71(15)	C13	C14	C15	116.9(5)
O2	Zn1	N4	97.29(14)	C18	C14	C15	116.9(5)
O2	Zn1	N2	78.76(15)	C18	C14	C13	126.1(5)
N1	Zn1	N3	166.12(16)	N2	C15	C10	115.0(5)
O1	Zn1	N1	77.81(15)	N2	C15	C14	121.5(5)
O1	Zn1	N3	93.11(15)	C14	C15	C10	123.5(5)
O1	Zn1	N4	91.91(14)	C9	C8	C7	119.6(5)
N4	Zn1	N1	93.57(16)	C3	C4	Cl1	118.8(4)
N4	Zn1	N3	76.08(16)	C3	C4	C5	121.7(5)
N2	Zn1	N1	97.59(16)	C5	C4	Cl1	119.5(4)
N2	Zn1	O1	93.26(15)	O1	C1	C2	126.1(5)
N2	Zn1	N3	93.35(16)	O1	C1	C6	119.6(4)
N2	Zn1	N4	168.48(16)	C2	C1	C6	114.2(4)
C10	O2	Zn1	113.6(3)	N4	C28	C27	125.8(5)
C6	N1	Zn1	112.3(3)	N4	C24	C23	115.3(5)
C7	N1	Zn1	127.9(4)	C25	C24	N4	121.7(5)
C7	N1	C6	119.4(4)	C25	C24	C23	123.0(5)
C21	O3	C29	117.6(5)	C24	C25	C26	120.3(5)
C1	O1	Zn1	113.5(3)	O3	C21	C20	116.8(5)
C23	N3	Zn1	115.7(3)	O3	C21	C22	124.8(5)
C19	N3	Zn1	127.0(4)	C20	C21	C22	118.3(5)
C19	N3	C23	117.3(5)	C28	C27	C26	117.2(5)
C10	C11	I2	117.8(4)	N1	C7	C8	122.4(5)
C10	C11	C12	123.0(5)	N3	C23	C24	115.6(4)
C12	C11	I2	119.2(4)	N3	C23	C22	123.4(5)
C3	C2	I1	118.7(4)	C22	C23	C24	121.0(5)
C1	C2	I1	118.8(4)	N3	C19	C20	123.6(6)
C1	C2	C3	122.4(5)	N2	C16	C17	122.6(5)

C26	O4	C30	117.4(5)	C12	C13	Cl2	119.4(4)
O2	C10	C11	126.1(5)	C12	C13	C14	121.2(5)
O2	C10	C15	119.6(4)	C14	C13	Cl2	119.4(5)
C11	C10	C15	114.4(5)	C8	C9	C5	119.9(5)
C28	N4	Zn1	127.0(3)	C4	C5	C6	117.0(5)
C28	N4	C24	116.4(4)	C4	C5	C9	125.8(5)
C24	N4	Zn1	115.6(3)	C9	C5	C6	117.1(5)
C4	C3	C2	121.1(5)	C17	C18	C14	120.2(5)
C13	C12	C11	121.0(5)	C18	C17	C16	119.2(5)
C19	C20	C21	119.1(5)	C23	C22	C21	118.3(5)
C15	N2	Zn1	112.7(3)	O4	C26	C25	115.3(5)
C16	N2	Zn1	127.8(4)	O4	C26	C27	126.2(5)
C16	N2	C15	119.4(5)	C27	C26	C25	118.5(5)
N1	C6	C1	115.0(4)				

Table S31. Crystal data and structure refinement for DQ11.

Empirical formula	$C_{42}H_{24}Br_4N_4O_2Zn$
Formula weight	1001.66
Temperature/K	200.0
Crystal system	monoclinic
Space group	$P2_1/c$
a/Å	10.7702(4)
b/Å	22.6651(9)
c/Å	15.6764(6)
α/°	90.00
β/°	108.0150(10)
γ/°	90.00
Volume/Å^3	3639.1(2)
Z	4
ρ_{calc}mg/mm^3	1.828
m/mm^{-1}	4.263
F(000)	1960.0
Crystal size/mm^3	0.38 × 0.21 × 0.13
2Θ range for data collection	6.18 to 121.32°
Index ranges	$-13 \le h \le 11$, $-29 \le k \le 29$, $-20 \le l \le 20$
Reflections collected	47211
Independent reflections	8309[R(int) = 0.0499]
Data/restraints/parameters	8309/0/482

Goodness-of-fit on F^2	1.007
Final R indexes [I>=2σ (I)]	R_1 = 0.0346, wR_2 = 0.0824
Final R indexes [all data]	R_1 = 0.0357, wR_2 = 0.0831
Largest diff. peak/hole / e $Å^{-3}$	0.98/-1.04

Table S32. Bond Lengths for DQ11.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
Br1	C2	1.900(3)	C14	C13	1.419(3)
Br1'	C2	1.837(6)	C14	C18	1.414(3)
Br2	C4	1.906(2)	C32	C36	1.426(3)
Br3	C11	1.896(2)	C32	C31	1.439(3)
Zn1	O1	2.0815(16)	C32	C33	1.412(3)
Zn1	O2	2.0878(16)	C28	C29	1.409(3)
Zn1	N3	2.1850(19)	C28	C33	1.446(3)
Zn1	N2	2.150(2)	C13	C12	1.366(4)
Zn1	N4	2.1765(19)	C29	C30	1.434(3)
Zn1	N1	2.1696(19)	C34	C35	1.395(3)
O1	C1	1.291(3)	C36	C35	1.383(3)
O2	C10	1.283(3)	C36	C37	1.487(3)
N3	C34	1.325(3)	C31	C30	1.360(3)
N3	C33	1.357(3)	C18	C17	1.362(4)
N2	C15	1.359(3)	C11	C12	1.398(4)
N2	C16	1.327(3)	C26	C27	1.393(3)
Br4	C13	1.908(2)	C9	C8	1.358(4)
N4	C28	1.356(3)	C9	C5	1.422(3)
N4	C27	1.325(3)	C23	C22	1.391(3)
N1	C7	1.319(3)	C23	C24	1.385(4)
N1	C6	1.361(3)	C6	C5	1.420(3)
C2	C1	1.399(3)	C16	C17	1.399(4)
C2	C3	1.401(3)	C21	C22	1.386(4)
C10	C15	1.451(3)	C21	C20	1.375(4)
C10	C11	1.404(3)	C38	C37	1.391(3)
C1	C6	1.451(3)	C38	C39	1.393(4)
C25	C29	1.427(3)	C20	C19	1.374(4)
C25	C26	1.378(3)	C41	C42	1.392(4)
C25	C23	1.490(3)	C41	C40	1.379(5)
C7	C8	1.411(4)	C42	C37	1.395(3)

C15	C14	1.417(3)	C19	C24	1.390(4)
C4	C5	1.413(3)	C39	C40	1.376(5)
C4	C3	1.365(4)			

Table S33. Bond Angles for DQ11.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
O1	Zn1	O2	163.63(6)	C33	C32	C36	117.5(2)
O1	Zn1	N3	103.94(7)	C33	C32	C31	118.4(2)
O1	Zn1	N2	91.56(7)	N4	C28	C29	123.3(2)
O1	Zn1	N4	87.06(7)	N4	C28	C33	116.74(19)
O1	Zn1	N1	77.89(7)	C29	C28	C33	119.91(19)
O2	Zn1	N3	88.66(7)	C14	C13	Br4	119.57(19)
O2	Zn1	N2	78.48(7)	C12	C13	Br4	119.33(18)
O2	Zn1	N4	106.47(7)	C12	C13	C14	121.1(2)
O2	Zn1	N1	90.15(7)	C25	C29	C30	123.8(2)
N2	Zn1	N3	160.82(7)	C28	C29	C25	117.4(2)
N2	Zn1	N4	94.45(7)	C28	C29	C30	118.7(2)
N2	Zn1	N1	96.02(7)	N3	C34	C35	122.8(2)
N4	Zn1	N3	75.46(7)	C32	C36	C37	122.9(2)
N1	Zn1	N3	98.20(7)	C35	C36	C32	117.5(2)
N1	Zn1	N4	161.85(7)	C35	C36	C37	119.6(2)
C1	O1	Zn1	114.93(14)	C30	C31	C32	121.3(2)
C10	O2	Zn1	112.84(14)	C17	C18	C14	120.3(2)
C34	N3	Zn1	126.68(16)	C10	C11	Br3	117.50(18)
C34	N3	C33	118.0(2)	C12	C11	Br3	118.67(17)
C33	N3	Zn1	115.24(14)	C12	C11	C10	123.8(2)
C15	N2	Zn1	111.40(15)	N3	C33	C32	123.3(2)
C16	N2	Zn1	128.68(16)	N3	C33	C28	116.82(19)
C16	N2	C15	119.6(2)	C32	C33	C28	119.83(19)
C28	N4	Zn1	115.63(14)	C36	C35	C34	120.7(2)
C27	N4	Zn1	126.52(16)	C25	C26	C27	120.4(2)
C27	N4	C28	117.8(2)	C8	C9	C5	120.4(2)
C7	N1	Zn1	128.33(17)	C22	C23	C25	120.4(2)
C7	N1	C6	119.3(2)	C24	C23	C25	120.3(2)
C6	N1	Zn1	112.23(14)	C24	C23	C22	119.0(2)
Br1'	C2	Br1	13.1(5)	N1	C6	C1	114.79(19)
C1	C2	Br1	119.15(18)	N1	C6	C5	122.0(2)

C1	C2	Br1'	117.2(3)	C5	C6	C1	123.1(2)
C1	C2	C3	123.1(2)	N2	C16	C17	122.1(2)
C3	C2	Br1	117.69(18)	C9	C8	C7	119.0(2)
C3	C2	Br1'	118.8(3)	C18	C17	C16	119.3(2)
O2	C10	C15	120.64(19)	C20	C21	C22	120.4(3)
O2	C10	C11	125.5(2)	C21	C22	C23	120.0(3)
C11	C10	C15	113.9(2)	C31	C30	C29	121.2(2)
O1	C1	C2	125.2(2)	C4	C5	C9	126.1(2)
O1	C1	C6	120.1(2)	C4	C5	C6	117.2(2)
C2	C1	C6	114.6(2)	C6	C5	C9	116.6(2)
C29	C25	C23	123.4(2)	C37	C38	C39	120.6(3)
C26	C25	C29	117.8(2)	C19	C20	C21	120.0(2)
C26	C25	C23	118.8(2)	C13	C12	C11	120.4(2)
N1	C7	C8	122.7(2)	C4	C3	C2	120.6(2)
N2	C15	C10	114.85(19)	C40	C41	C42	120.2(3)
N2	C15	C14	121.6(2)	C41	C42	C37	120.5(3)
C14	C15	C10	123.5(2)	C20	C19	C24	120.0(3)
C5	C4	Br2	120.58(18)	C38	C37	C36	120.0(2)
C3	C4	Br2	118.01(18)	C38	C37	C42	118.5(2)
C3	C4	C5	121.3(2)	C42	C37	C36	121.4(2)
C15	C14	C13	117.2(2)	C40	C39	C38	120.2(3)
C18	C14	C15	116.9(2)	N4	C27	C26	123.1(2)
C18	C14	C13	125.9(2)	C39	C40	C41	120.0(3)
C36	C32	C31	124.1(2)	C23	C24	C19	120.4(3)

Table S34. Crystal data and structure refinement for DQ12.

Empirical formula	$C_{30}H_{26}Cl_2N_4O_4Zn$
Formula weight	642.82
Temperature/K	150.0
Crystal system	orthorhombic
Space group	Pcan
a/Å	9.2856(4)
b/Å	15.9893(6)
c/Å	18.7952(7)
α/°	90.00
β/°	90.00
γ/°	90.00
Volume/Å^3	2790.53(19)

Z	4
ρ_{calc}mg/mm^3	1.530
m/mm^{-1}	2.215
F(000)	1320.0
Crystal size/mm^3	0.36 × 0.26 × 0.19
2Θ range for data collection	9.5 to 114.28°
Index ranges	-11 ≤ h ≤ 10, -16 ≤ k ≤ 20, -23 ≤ l ≤ 15
Reflections collected	24343
Independent reflections	2856[R(int) = 0.0612]
Data/restraints/parameters	2856/6/189
Goodness-of-fit on F^2	1.005
Final R indexes [I>=2σ (I)]	R_1 = 0.0657, wR_2 = 0.2108
Final R indexes [all data]	R_1 = 0.0776, wR_2 = 0.2222
Largest diff. peak/hole / e Å^{-3}	1.07/-0.69

Table S35 Bond Lengths for DQ12.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
Zn1	O1[1]	2.052(3)	C6	C5	1.415(6)
Zn1	O1	2.052(3)	C14	C14[1]	1.494(8)
Zn1	N1	2.157(3)	C14	C13	1.388(6)
Zn1	N1[1]	2.157(3)	C1	C2	1.383(6)
Zn1	N2[1]	2.182(4)	C12	C11	1.378(7)
Zn1	N2	2.182(4)	C12	C13	1.391(6)
Cl1	C4	1.736(5)	C5	C9	1.396(7)
O1	C1	1.314(5)	C5	C4	1.424(7)
N1	C6	1.365(6)	C2	C3	1.390(7)
N1	C7	1.314(6)	C10	C11	1.383(6)
N2	C14	1.344(6)	C9	C8	1.375(8)
N2	C10	1.342(5)	C3	C4	1.382(8)
O2	C15	1.310(8)	C7	C8	1.404(7)
C6	C1	1.450(6)			

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

Table S36. Bond Angles for DQ12.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
O1[1]	Zn1	O1	100.06(19)	N1	C6	C5	121.4(4)
O1	Zn1	N1	79.64(12)	C5	C6	C1	122.5(4)
O1	Zn1	N1[1]	97.26(12)	N2	C14	C14[1]	115.4(2)
O1[1]	Zn1	N1	97.26(12)	N2	C14	C13	121.5(4)
O1[1]	Zn1	N1[1]	79.64(12)	C13	C14	C14[1]	123.1(3)
O1	Zn1	N2	164.42(13)	O1	C1	C6	119.3(4)
O1	Zn1	N2[1]	93.28(13)	O1	C1	C2	124.2(4)
O1[1]	Zn1	N2[1]	164.42(13)	C2	C1	C6	116.4(4)
O1[1]	Zn1	N2	93.28(13)	C11	C12	C13	119.8(5)
N1	Zn1	N1[1]	175.2(2)	C6	C5	C4	117.3(4)
N1[1]	Zn1	N2[1]	90.79(13)	C9	C5	C6	117.7(4)
N1[1]	Zn1	N2	93.01(13)	C9	C5	C4	125.0(4)
N1	Zn1	N2	90.79(13)	C1	C2	C3	122.0(5)
N1	Zn1	N2[1]	93.01(13)	N2	C10	C11	122.3(5)
N2[1]	Zn1	N2	74.81(19)	C8	C9	C5	120.2(4)
C1	O1	Zn1	114.3(3)	C4	C3	C2	121.6(4)
C6	N1	Zn1	110.6(3)	C10	C11	C12	118.4(4)
C7	N1	Zn1	130.1(3)	C14	C13	C12	118.6(5)
C7	N1	C6	119.3(4)	N1	C7	C8	123.0(5)
C14	N2	Zn1	117.0(3)	C9	C8	C7	118.4(5)
C10	N2	Zn1	123.5(3)	C5	C4	Cl1	118.6(4)
C10	N2	C14	119.4(4)	C3	C4	Cl1	121.2(4)
N1	C6	C1	116.1(4)	C3	C4	C5	120.2(4)

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

Table S37. Crystal data and structure refinement for DQ13.

Empirical formula	$C_{65}H_{54}Br_8N_8O_{10}Zn_2$
Formula weight	1877.18
Temperature/K	150.15
Crystal system	monoclinic
Space group	$P2_1/c$
a/Å	15.6954(8)
b/Å	20.7335(10)
c/Å	21.0048(10)
α/°	90
β/°	90.004(2)

γ/°	90
Volume/Å^3	6835.4(6)
Z	4
ρ_{calc}mg/mm^3	1.824
m/mm^{-1}	4.544
F(000)	3680.0
Crystal size/mm^3	0.35 × 0.29 × 0.16
2Θ range for data collection	3.66 to 114.23°
Index ranges	-19 ≤ h ≤ 15, -25 ≤ k ≤ 22, -26 ≤ l ≤ 25
Reflections collected	74326
Independent reflections	13975[R(int) = 0.0708]
Data/restraints/parameters	13975/37/850
Goodness-of-fit on F^2	1.082
Final R indexes [I>=2σ (I)]	R_1 = 0.0658, wR_2 = 0.1763
Final R indexes [all data]	R_1 = 0.0815, wR_2 = 0.1884
Largest diff. peak/hole / e Å^{-3}	2.62/-1.42

Table S38. Bond Lengths for DQ13.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
Br1	C19	1.883(8)	C14	C15	1.338(15)
Zn1	O1	2.102(5)	C15	C16	1.408(12)
Zn1	N1	2.199(7)	C16	C17	1.417(13)
Zn1	O2	2.110(5)	C16	C21	1.424(12)
Zn1	N2	2.134(7)	C17	C18	1.375(12)
Zn1	N3	2.130(7)	C18	C19	1.408(12)
Zn1	N4	2.122(7)	C19	C20	1.368(12)
O1	C20	1.299(10)	C20	C21	1.450(11)
N1	C1	1.308(12)	C22	C23	1.406(13)
N1	C12	1.365(11)	C23	C24	1.398(13)
C1	C2	1.443(13)	C24	C25	1.403(11)
Br2	C17	1.883(9)	C25	C26	1.424(13)
O2	C29	1.306(9)	C25	C30	1.404(12)
N2	C10	1.336(12)	C26	C27	1.323(12)
N2	C11	1.365(12)	C27	C28	1.422(13)
C2	C3	1.367(15)	C28	C29	1.413(11)
Zn2	O3	2.106(5)	C29	C30	1.432(10)
Zn2	O4	2.097(5)	C31	C32	1.394(14)

Zn2	N5	2.157(7)	C32	C33	1.365(17)
Zn2	N6	2.197(7)	C33	C34	1.425(14)
Zn2	N7	2.172(7)	C34	C35	1.430(15)
Zn2	N8	2.140(7)	C34	C42	1.394(12)
Br3	C28	1.888(8)	C35	C36	1.366(16)
N3	C13	1.321(11)	C36	C37	1.434(13)
N3	C21	1.358(11)	C37	C38	1.432(14)
C3	C4	1.401(15)	C37	C41	1.405(12)
O3	C50	1.286(9)	C38	C39	1.363(14)
Br4	C26	1.912(9)	C39	C40	1.382(13)
N4	C22	1.332(11)	C41	C42	1.448(12)
N4	C30	1.386(11)	C43	C44	1.404(13)
C4	C5	1.378(15)	C44	C45	1.353(13)
C4	C12	1.436(13)	C45	C46	1.414(13)
O4	C59	1.291(9)	C46	C47	1.416(11)
C5	C6	1.411(18)	C46	C51	1.434(11)
Br5	C47	1.929(8)	C47	C48	1.345(13)
N5	C31	1.325(13)	C48	C49	1.409(12)
N5	C42	1.346(11)	C49	C50	1.392(11)
C6	C7	1.438(15)	C50	C51	1.433(12)
Br6	C49	1.887(9)	C52	C53	1.369(12)
N6	C40	1.325(11)	C53	C54	1.401(12)
N6	C41	1.343(10)	C54	C55	1.388(11)
C7	C8	1.408(16)	C55	C56	1.423(11)
C7	C11	1.391(12)	C55	C60	1.410(11)
Br7	C56	1.892(8)	C56	C57	1.361(12)
N7	C43	1.321(11)	C57	C58	1.401(12)
N7	C51	1.384(10)	C58	C59	1.398(11)
C8	C9	1.384(16)	C59	C60	1.455(11)
Br8	C58	1.888(9)	O5	C61	1.353(15)
N8	C52	1.332(11)	O6	C62	1.456(17)
N8	C60	1.363(10)	O7	C63	1.303(17)
C9	C10	1.395(14)	O8	C64	1.32(2)
C11	C12	1.416(13)	O9	C65	1.416(9)
C13	C14	1.409(14)			

Table S39. Bond Angles for DQ13.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
O1	Zn1	N1	99.6(2)	C17	C18	C19	121.3(8)
O1	Zn1	O2	163.4(2)	C18	C19	Br1	117.3(6)
O1	Zn1	N2	95.1(2)	C20	C19	Br1	120.0(6)
O1	Zn1	N3	78.6(2)	C20	C19	C18	122.7(8)
O1	Zn1	N4	91.9(2)	O1	C20	C19	125.2(8)
O2	Zn1	N1	94.3(2)	O1	C20	C21	119.0(7)
O2	Zn1	N2	96.7(2)	C19	C20	C21	115.8(8)
O2	Zn1	N3	88.8(2)	N3	C21	C16	121.0(8)
O2	Zn1	N4	78.8(2)	N3	C21	C20	116.3(7)
N2	Zn1	N1	77.3(3)	C16	C21	C20	122.7(8)
N3	Zn1	N1	172.1(3)	N4	C22	C23	122.5(8)
N3	Zn1	N2	95.1(3)	C24	C23	C22	118.0(8)
N4	Zn1	N1	90.8(3)	C23	C24	C25	120.8(8)
N4	Zn1	N2	167.0(3)	C24	C25	C26	125.1(8)
N4	Zn1	N3	96.9(3)	C24	C25	C30	117.5(8)
C20	O1	Zn1	113.9(5)	C30	C25	C26	117.5(7)
C1	N1	Zn1	128.6(6)	C25	C26	Br4	119.8(6)
C1	N1	C12	119.6(8)	C27	C26	Br4	118.9(7)
C12	N1	Zn1	111.3(6)	C27	C26	C25	121.3(8)
N1	C1	C2	123.8(9)	C26	C27	C28	120.9(8)
C29	O2	Zn1	112.5(4)	C27	C28	Br3	118.4(6)
C10	N2	Zn1	128.3(6)	C29	C28	Br3	119.1(6)
C10	N2	C11	117.0(8)	C29	C28	C27	122.5(7)
C11	N2	Zn1	114.7(6)	O2	C29	C28	124.6(7)
C3	C2	C1	116.2(9)	O2	C29	C30	121.3(7)
O3	Zn2	N5	98.3(2)	C28	C29	C30	114.0(7)
O3	Zn2	N6	91.3(2)	N4	C30	C25	121.8(7)
O3	Zn2	N7	78.7(2)	N4	C30	C29	114.2(7)
O3	Zn2	N8	94.0(2)	C25	C30	C29	123.9(7)
O4	Zn2	O3	164.3(2)	N5	C31	C32	121.6(10)
O4	Zn2	N5	92.1(2)	C33	C32	C31	120.1(11)
O4	Zn2	N6	102.5(2)	C32	C33	C34	119.1(9)
O4	Zn2	N7	88.8(2)	C33	C34	C35	123.2(9)
O4	Zn2	N8	77.7(2)	C42	C34	C33	116.7(9)
N5	Zn2	N6	76.5(3)	C42	C34	C35	120.1(9)
N5	Zn2	N7	95.3(3)	C36	C35	C34	121.7(8)
N7	Zn2	N6	166.1(2)	C35	C36	C37	119.0(8)
N8	Zn2	N5	165.0(3)	C38	C37	C36	121.1(8)
N8	Zn2	N6	94.7(3)	C41	C37	C36	120.8(9)

N8	Zn2	N7	95.6(3)	C41	C37	C38	118.1(8)
C13	N3	Zn1	128.0(7)	C39	C38	C37	117.0(8)
C13	N3	C21	119.8(8)	C38	C39	C40	120.3(9)
C21	N3	Zn1	112.2(5)	N6	C40	C39	124.4(8)
C2	C3	C4	122.2(9)	N6	C41	C37	123.3(8)
C50	O3	Zn2	113.6(5)	N6	C41	C42	117.4(7)
C22	N4	Zn1	127.8(6)	C37	C41	C42	119.3(8)
C22	N4	C30	119.3(7)	N5	C42	C34	123.0(8)
C30	N4	Zn1	112.9(5)	N5	C42	C41	117.9(7)
C3	C4	C12	117.1(9)	C34	C42	C41	119.1(8)
C5	C4	C3	122.9(9)	N7	C43	C44	124.1(8)
C5	C4	C12	120.0(9)	C45	C44	C43	118.2(9)
C59	O4	Zn2	113.9(5)	C44	C45	C46	120.8(8)
C4	C5	C6	120.5(9)	C45	C46	C47	126.8(8)
C31	N5	Zn2	126.1(6)	C45	C46	C51	118.0(7)
C31	N5	C42	119.4(8)	C47	C46	C51	115.2(8)
C42	N5	Zn2	114.5(6)	C46	C47	Br5	118.2(6)
C5	C6	C7	119.9(10)	C48	C47	Br5	119.3(6)
C40	N6	Zn2	129.5(6)	C48	C47	C46	122.5(8)
C40	N6	C41	116.8(7)	C47	C48	C49	120.7(8)
C41	N6	Zn2	113.5(6)	C48	C49	Br6	117.9(6)
C8	C7	C6	121.8(9)	C50	C49	Br6	119.7(6)
C11	C7	C6	119.6(10)	C50	C49	C48	122.4(8)
C11	C7	C8	118.6(9)	O3	C50	C49	123.8(8)
C43	N7	Zn2	130.5(6)	O3	C50	C51	121.2(7)
C43	N7	C51	119.0(7)	C49	C50	C51	115.0(7)
C51	N7	Zn2	110.5(5)	N7	C51	C46	119.9(7)
C9	C8	C7	119.0(9)	N7	C51	C50	116.1(7)
C52	N8	Zn2	128.7(6)	C50	C51	C46	124.1(7)
C52	N8	C60	117.7(7)	N8	C52	C53	123.9(8)
C60	N8	Zn2	113.3(5)	C52	C53	C54	118.7(8)
C8	C9	C10	118.1(9)	C55	C54	C53	119.6(8)
N2	C10	C9	124.5(9)	C54	C55	C56	124.5(7)
N2	C11	C7	122.8(9)	C54	C55	C60	117.4(7)
N2	C11	C12	117.1(8)	C60	C55	C56	118.1(7)
C7	C11	C12	120.2(9)	C55	C56	Br7	119.8(6)
N1	C12	C4	121.0(8)	C57	C56	Br7	120.2(6)
N1	C12	C11	119.2(8)	C57	C56	C55	119.9(7)
C11	C12	C4	119.7(8)	C56	C57	C58	121.2(8)
N3	C13	C14	122.1(9)	C57	C58	Br8	117.4(6)

C15	C14	C13	119.3(9)	C59	C58	Br8	118.9(6)
C14	C15	C16	120.8(9)	C59	C58	C57	123.6(8)
C15	C16	C17	125.4(9)	O4	C59	C58	126.1(8)
C15	C16	C21	117.1(8)	O4	C59	C60	120.1(7)
C17	C16	C21	117.5(8)	C58	C59	C60	113.8(7)
C16	C17	Br2	119.7(7)	N8	C60	C55	122.7(7)
C18	C17	Br2	120.3(7)	N8	C60	C59	113.9(7)
C18	C17	C16	120.0(8)	C55	C60	C59	123.3(7)

Table S40. Crystal data and structure refinement for DQ14.

Empirical formula	$C_{31}H_{18}Br_4Cl_2N_4O_3Zn$
Formula weight	950.38
Temperature/K	150.0
Crystal system	monoclinic
Space group	C2/c
a/Å	15.449(2)
b/Å	17.284(2)
c/Å	23.770(3)
α/°	90.00
β/°	93.610(4)
γ/°	90.00
Volume/Å^3	6334.4(14)
Z	8
ρ_{calc}mg/mm^3	1.993
m/mm^{-1}	5.895
F(000)	3680.0
Crystal size/mm^3	0.36 × 0.25 × 0.13
2Θ range for data collection	6.48 to 113.94°
Index ranges	$-18 \leq h \leq 19$, $-16 \leq k \leq 21$, $-29 \leq l \leq 28$
Reflections collected	26887
Independent reflections	6445[R(int) = 0.0424]
Data/restraints/parameters	6445/7/413
Goodness-of-fit on F^2	1.007
Final R indexes [I>=2σ (I)]	R_1 = 0.0660, wR_2 = 0.1938
Final R indexes [all data]	R_1 = 0.0688, wR_2 = 0.1973
Largest diff. peak/hole / e Å^{-3}	2.13/-1.38

Table S41. Bond Lengths for DQ14.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
Br3	C11	1.891(5)	N1	C6	1.360(7)
Br4	C13	1.898(5)	C1	C2	1.392(8)
Br1	C2	1.894(6)	C1	C6	1.452(8)
Br2	C4	1.904(6)	C5	C4	1.406(8)
Zn1	O2	2.068(4)	C5	C6	1.436(8)
Zn1	O1	2.081(4)	C5	C9	1.418(9)
Zn1	N2	2.174(5)	C4	C3	1.371(10)
Zn1	N3	2.167(5)	C7	C8	1.419(9)
Zn1	N4	2.163(5)	C23	C24	1.436(8)
Zn1	N1	2.179(5)	C23	C22	1.400(8)
Cl2	C28	1.744(6)	C27	C26	1.356(10)
O2	C10	1.292(7)	C27	C22	1.434(9)
O1	C1	1.297(7)	C28	C25	1.420(9)
N2	C15	1.358(7)	C28	C29	1.366(9)
N2	C16	1.334(7)	C2	C3	1.406(9)
O3	C31	1.390(8)	C12	C11	1.404(8)
N3	C23	1.362(7)	C16	C17	1.407(9)
N3	C19	1.323(8)	C24	C25	1.422(7)
C13	C14	1.430(8)	C25	C26	1.429(8)
C13	C12	1.367(8)	C9	C8	1.364(9)
C14	C15	1.427(7)	C18	C17	1.367(9)
C14	C18	1.403(8)	C30	C29	1.418(8)
N4	C24	1.360(7)	C22	C21	1.438(9)
N4	C30	1.315(7)	C19	C20	1.407(9)
C10	C15	1.451(7)	C21	C20	1.342(10)
C10	C11	1.401(7)	C21	Cl1	1.621(8)
N1	C7	1.308(7)	C21	Cl1'	1.746(18)

Table S42. Bond Angles for DQ14.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°

O2	Zn1	O1	169.75(16)	C5	C4	Br2	119.5(5)
O2	Zn1	N2	78.62(16)	C3	C4	Br2	119.4(4)
O2	Zn1	N3	93.17(15)	C3	C4	C5	121.0(6)
O2	Zn1	N4	93.42(16)	N1	C7	C8	122.8(5)
O2	Zn1	N1	93.57(17)	N3	C23	C24	116.9(5)
O1	Zn1	N2	94.57(17)	N3	C23	C22	123.6(5)
O1	Zn1	N3	93.85(16)	C22	C23	C24	119.5(5)
O1	Zn1	N4	95.44(16)	C26	C27	C22	122.2(5)
O1	Zn1	N1	78.42(16)	C25	C28	Cl2	120.3(4)
N2	Zn1	N1	87.95(18)	C29	C28	Cl2	118.3(5)
N3	Zn1	N2	171.53(17)	C29	C28	C25	121.5(5)
N3	Zn1	N1	94.70(18)	C1	C2	Br1	118.7(5)
N4	Zn1	N2	101.38(17)	C1	C2	C3	123.3(6)
N4	Zn1	N3	76.82(17)	C3	C2	Br1	118.0(4)
N4	Zn1	N1	169.29(17)	C13	C12	C11	120.6(5)
C10	O2	Zn1	113.3(3)	N1	C6	C1	115.7(5)
C1	O1	Zn1	114.5(3)	N1	C6	C5	121.3(5)
C15	N2	Zn1	109.5(3)	C5	C6	C1	123.0(5)
C16	N2	Zn1	128.7(4)	N2	C16	C17	121.5(5)
C16	N2	C15	119.5(5)	N4	C24	C23	118.0(5)
C23	N3	Zn1	114.3(4)	N4	C24	C25	122.1(5)
C19	N3	Zn1	128.3(4)	C25	C24	C23	119.8(5)
C19	N3	C23	117.4(5)	C10	C11	Br3	118.3(4)
C14	C13	Br4	120.8(4)	C10	C11	C12	123.3(5)
C12	C13	Br4	118.5(4)	C12	C11	Br3	118.3(4)
C12	C13	C14	120.7(5)	C28	C25	C24	116.3(5)
C15	C14	C13	117.5(5)	C28	C25	C26	124.2(5)
C18	C14	C13	125.3(5)	C24	C25	C26	119.4(5)
C18	C14	C15	117.1(5)	C8	C9	C5	120.3(5)
C24	N4	Zn1	113.9(4)	C17	C18	C14	120.1(5)
C30	N4	Zn1	127.1(4)	C18	C17	C16	119.8(5)
C30	N4	C24	118.9(5)	N4	C30	C29	124.1(5)
O2	C10	C15	120.1(4)	C27	C26	C25	119.9(5)
O2	C10	C11	124.9(5)	C23	C22	C27	119.1(5)
C11	C10	C15	115.0(5)	C23	C22	C21	116.2(5)
C7	N1	Zn1	128.6(4)	C27	C22	C21	124.6(5)
C7	N1	C6	119.9(5)	C9	C8	C7	118.7(6)
C6	N1	Zn1	111.2(4)	C28	C29	C30	117.0(5)
N2	C15	C14	121.9(5)	C4	C3	C2	120.7(5)
N2	C15	C10	115.5(5)	N3	C19	C20	123.7(6)

C14	C15	C10	122.6(5)	C22	C21	Cl1	120.8(8)
O1	C1	C2	125.3(5)	C22	C21	Cl1'	140.0(13)
O1	C1	C6	120.1(5)	C20	C21	C22	120.0(5)
C2	C1	C6	114.6(5)	C20	C21	Cl1	119.2(8)
C4	C5	C6	117.3(5)	C20	C21	Cl1'	100.0(13)
C4	C5	C9	125.9(6)	Cl1	C21	Cl1'	19.6(7)
C9	C5	C6	116.8(5)	C21	C20	C19	119.1(6)

Table S43. Crystal data and structure refinement for DQ15.

Empirical formula	$C_{64.5}H_{41}Br_8ClN_8O_4Zn_2$
Formula weight	1797.52
Temperature/K	150.00
Crystal system	monoclinic
Space group	C2/c
a/Å	24.006(2)
b/Å	22.7289(17)
c/Å	23.4966(19)
α/°	90
β/°	103.614(4)
γ/°	90
Volume/Å^3	12460.4(18)
Z	8
ρ_{calc}g/cm^3	1.916
μ/mm^{-1}	5.176
F(000)	6984.0
Crystal size/mm^3	0.16 × 0.12 × 0.04
Radiation	GaKα (λ = 1.34139)
2Θ range for data collection/°	4.722 to 114.456
Index ranges	$-30 \le h \le 24$, $-28 \le k \le 26$, $-29 \le l \le 29$
Reflections collected	51754
Independent reflections	12678 [R_{int} = 0.0535, R_{sigma} = 0.0508]
Data/restraints/parameters	12678/1731/1070
Goodness-of-fit on F^2	1.062
Final R indexes [I>=2σ (I)]	R_1 = 0.0452, wR_2 = 0.1064
Final R indexes [all data]	R_1 = 0.0627, wR_2 = 0.1148
Largest diff. peak/hole / e Å^{-3}	0.61/-0.53

Table S44. Bond Lengths for DQ15.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
Zn1	N1_1	2.132(4)	C8_5	C9_5	1.413(6)
Zn1	O1_1	2.072(3)	C8_5	C10_5	1.412(7)
Zn1	N1_4	2.164(4)	C9_5	N2_5	1.357(6)
Zn1	O1_4	2.061(3)	C10_5	C11_5	1.370(8)
Zn1	N1_5	2.190(4)	C11_5	C12_5	1.394(7)
Zn1	N2_5	2.198(4)	C12_5	N2_5	1.328(6)
Zn2	N1_2	2.154(4)	C1_6	C2_6	1.398(7)
Zn2	O1_2	2.061(3)	C1_6	C9_6	1.452(6)
Zn2	N1_6	2.184(4)	C1_6	N1_6	1.346(6)
Zn2	N2_6	2.256(4)	C2_6	C3_6	1.426(7)
Zn2	N1_8	2.193(5)	C2_6	C6_6	1.445(8)
Zn2	O1_8	2.052(6)	C3_6	C4_6	1.368(8)
Zn2	N1_9	1.99(3)	C4_6	C5_6	1.397(7)
Zn2	O1_9	2.05(5)	C5_6	N1_6	1.328(6)
Zn2	N1_10	2.22(4)	C6_6	C7_6	1.389(8)
Zn2	O1_10	2.27(5)	C6_6	C13_6	1.515(8)
C1_1	C2_1	1.416(6)	C7_6	C8_6	1.439(8)
C1_1	C9_1	1.447(7)	C7_6	C14_6	1.524(8)
C1_1	N1_1	1.363(5)	C8_6	C9_6	1.397(7)
C2_1	C3_1	1.413(7)	C8_6	C10_6	1.425(7)
C2_1	C6_1	1.425(6)	C9_6	N2_6	1.357(6)
C3_1	C4_1	1.369(7)	C10_6	C11_6	1.368(8)
C4_1	C5_1	1.406(7)	C11_6	C12_6	1.383(8)
C5_1	N1_1	1.317(6)	C12_6	N2_6	1.338(6)
C6_1	C7_1	1.356(7)	C1_7	Cl1_7	1.606(19)
C6_1	Br1_1	1.896(5)	C1_7	Cl2_7	1.60(2)
C7_1	C8_1	1.405(7)	C1_8	C2_8	1.424(7)
C8_1	C9_1	1.390(6)	C1_8	C9_8	1.433(8)
C8_1	Br2_1	1.901(5)	C1_8	N1_8	1.372(7)
C9_1	O1_1	1.295(5)	C2_8	C3_8	1.423(9)
C1_2	C2_2	1.419(6)	C2_8	C6_8	1.420(9)
C1_2	C9_2	1.448(6)	C3_8	C4_8	1.357(9)
C1_2	N1_2	1.376(6)	C4_8	C5_8	1.394(9)
C2_2	C3_2	1.409(7)	C5_8	N1_8	1.329(7)
C2_2	C6_2	1.411(7)	C6_8	C7_8	1.370(9)

Table S44. Bond Lengths for DQ15.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
C3_2	C4_2	1.360(7)	C6_8	Br1_8	1.909(5)
C4_2	C5_2	1.393(7)	C7_8	C8_8	1.396(7)
C5_2	N1_2	1.319(6)	C8_8	C9_8	1.400(8)
C6_2	C7_2	1.363(7)	C8_8	Br2_8	1.881(6)
C6_2	Br1_2	1.910(4)	C9_8	O1_8	1.299(6)
C7_2	C8_2	1.396(6)	C1_9	C2_9	1.426(12)
C8_2	C9_2	1.400(6)	C1_9	C9_9	1.433(12)
C8_2	Br2_2	1.896(5)	C1_9	N1_9	1.372(12)
C9_2	O1_2	1.300(5)	C2_9	C3_9	1.422(13)
C1_4	C5_4	1.411(7)	C2_9	C6_9	1.418(13)
C1_4	C6_4	1.445(7)	C3_9	C4_9	1.357(14)
C1_4	N1_4	1.373(6)	C4_9	C5_9	1.394(13)
C2_4	C3_4	1.389(7)	C5_9	N1_9	1.329(12)
C2_4	N1_4	1.314(6)	C6_9	C7_9	1.368(13)
C3_4	C4_4	1.373(7)	C6_9	Br1_9	1.906(11)
C4_4	C5_4	1.404(7)	C7_9	C8_9	1.395(12)
C5_4	C9_4	1.430(7)	C8_9	C9_9	1.400(12)
C6_4	C7_4	1.405(7)	C8_9	Br2_9	1.877(11)
C6_4	O1_4	1.302(6)	C9_9	O1_9	1.299(11)
C7_4	C8_4	1.387(7)	C1_10	C2_10	1.428(12)
C7_4	Br1_4	1.893(6)	C1_10	C9_10	1.433(12)
C8_4	C9_4	1.369(8)	C1_10	N1_10	1.374(12)
C9_4	Br2_4	1.904(5)	C2_10	C3_10	1.422(13)
C1_5	C5_5	1.414(7)	C2_10	C6_10	1.419(13)
C1_5	C9_5	1.437(6)	C3_10	C4_10	1.355(14)
C1_5	N1_5	1.359(6)	C4_10	C5_10	1.393(13)
C2_5	C3_5	1.389(7)	C5_10	N1_10	1.329(12)
C2_5	N1_5	1.314(6)	C6_10	C7_10	1.369(14)
C3_5	C4_5	1.372(7)	C6_10	Br1_10	1.907(11)
C4_5	C5_5	1.407(7)	C7_10	C8_10	1.397(12)
C5_5	C6_5	1.451(7)	C8_10	C9_10	1.401(12)
C6_5	C7_5	1.357(8)	C8_10	Br2_10	1.881(11)
C6_5	C13_5	1.519(8)	C9_10	O1_10	1.298(11)
C7_5	C8_5	1.458(7)	C1_11	Cl1_11	1.61(2)
C7_5	C14_5	1.515(7)	C1_11	Cl2_11	1.64(2)

Table S45. Bond Angles for DQ15.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
N1_1	Zn1	N1_4	163.70(14)	C4_5	C5_5	C1_5	115.8(4)
N1_1	Zn1	N1_5	101.38(14)	C4_5	C5_5	C6_5	124.4(5)
N1_1	Zn1	N2_5	97.46(14)	C5_5	C6_5	C13_5	116.5(5)
O1_1	Zn1	N1_1	79.35(13)	C7_5	C6_5	C5_5	120.7(5)
O1_1	Zn1	N1_4	94.11(13)	C7_5	C6_5	C13_5	122.8(5)
O1_1	Zn1	N1_5	88.78(13)	C6_5	C7_5	C8_5	120.4(4)
O1_1	Zn1	N2_5	162.89(13)	C6_5	C7_5	C14_5	122.0(5)
N1_4	Zn1	N1_5	93.32(14)	C8_5	C7_5	C14_5	117.6(5)
N1_4	Zn1	N2_5	93.02(14)	C9_5	C8_5	C7_5	119.8(4)
O1_4	Zn1	N1_1	87.73(13)	C10_5	C8_5	C7_5	124.1(4)
O1_4	Zn1	O1_1	104.97(13)	C10_5	C8_5	C9_5	116.1(5)
O1_4	Zn1	N1_4	79.50(14)	C8_5	C9_5	C1_5	119.5(4)
O1_4	Zn1	N1_5	164.80(13)	N2_5	C9_5	C1_5	117.3(4)
O1_4	Zn1	N2_5	91.61(14)	N2_5	C9_5	C8_5	123.1(4)
N1_5	Zn1	N2_5	75.28(14)	C11_5	C10_5	C8_5	120.2(5)
N1_2	Zn2	N1_6	96.39(14)	C10_5	C11_5	C12_5	119.5(5)
N1_2	Zn2	N2_6	87.59(14)	N2_5	C12_5	C11_5	122.4(5)
N1_2	Zn2	N1_8	164.68(18)	C1_5	N1_5	Zn1	115.1(3)
N1_2	Zn2	N1_10	104.0(8)	C2_5	N1_5	Zn1	125.9(3)
N1_2	Zn2	O1_10	175.9(15)	C2_5	N1_5	C1_5	118.8(4)
O1_2	Zn2	N1_2	79.92(13)	C9_5	N2_5	Zn1	114.8(3)
O1_2	Zn2	N1_6	87.15(14)	C12_5	N2_5	Zn1	126.4(3)
O1_2	Zn2	N2_6	155.99(14)	C12_5	N2_5	C9_5	118.6(4)
O1_2	Zn2	N1_8	102.5(2)	C2_6	C1_6	C9_6	119.4(5)
O1_2	Zn2	N1_10	122(2)	N1_6	C1_6	C2_6	123.6(4)
O1_2	Zn2	O1_10	104.0(19)	N1_6	C1_6	C9_6	117.0(4)
N1_6	Zn2	N2_6	73.85(14)	C1_6	C2_6	C3_6	116.1(5)
N1_6	Zn2	N1_8	98.83(19)	C1_6	C2_6	C6_6	120.7(4)
N1_6	Zn2	N1_10	146.8(17)	C3_6	C2_6	C6_6	123.2(5)
N1_6	Zn2	O1_10	85.2(13)	C4_6	C3_6	C2_6	119.3(5)
N2_6	Zn2	O1_10	89(2)	C3_6	C4_6	C5_6	120.2(5)
N1_8	Zn2	N2_6	95.0(2)	N1_6	C5_6	C4_6	121.4(5)
O1_8	Zn2	N1_2	86.93(16)	C2_6	C6_6	C13_6	117.9(5)
O1_8	Zn2	O1_2	108.49(19)	C7_6	C6_6	C2_6	119.5(5)
O1_8	Zn2	N1_6	164.36(19)	C7_6	C6_6	C13_6	122.7(5)
O1_8	Zn2	N2_6	91.07(19)	C6_6	C7_6	C8_6	120.0(5)
O1_8	Zn2	N1_8	77.94(18)	C6_6	C7_6	C14_6	121.9(5)
N1_9	Zn2	N1_2	173.4(13)	C8_6	C7_6	C14_6	118.1(5)

Table S45. Bond Angles for DQ15.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
N1_9	Zn2	O1_2	99.9(19)	C9_6	C8_6	C7_6	120.9(4)
N1_9	Zn2	N1_6	90.2(12)	C9_6	C8_6	C10_6	115.4(5)
N1_9	Zn2	N2_6	95(2)	C10_6	C8_6	C7_6	123.8(5)
N1_9	Zn2	O1_9	83.2(12)	C8_6	C9_6	C1_6	119.1(4)
O1_9	Zn2	N1_2	90.4(9)	N2_6	C9_6	C1_6	116.4(4)
O1_9	Zn2	O1_2	101.3(15)	N2_6	C9_6	C8_6	124.5(4)
O1_9	Zn2	N1_6	170.0(11)	C11_6	C10_6	C8_6	119.8(5)
O1_9	Zn2	N2_6	99.2(16)	C10_6	C11_6	C12_6	120.4(5)
N1_10	Zn2	N2_6	81(2)	N2_6	C12_6	C11_6	121.8(5)
N1_10	Zn2	O1_10	72.9(9)	C1_6	N1_6	Zn2	115.5(3)
C2_1	C1_1	C9_1	123.1(4)	C5_6	N1_6	Zn2	124.3(4)
N1_1	C1_1	C2_1	121.8(4)	C5_6	N1_6	C1_6	119.3(4)
N1_1	C1_1	C9_1	115.1(4)	C9_6	N2_6	Zn2	112.9(3)
C1_1	C2_1	C6_1	117.1(4)	C12_6	N2_6	Zn2	127.8(3)
C3_1	C2_1	C1_1	117.1(4)	C12_6	N2_6	C9_6	118.0(4)
C3_1	C2_1	C6_1	125.8(4)	Cl2_7	C1_7	Cl1_7	129(2)
C4_1	C3_1	C2_1	120.4(5)	C2_8	C1_8	C9_8	123.2(5)
C3_1	C4_1	C5_1	118.2(5)	N1_8	C1_8	C2_8	121.9(5)
N1_1	C5_1	C4_1	123.4(4)	N1_8	C1_8	C9_8	114.9(4)
C2_1	C6_1	Br1_1	119.4(4)	C3_8	C2_8	C1_8	116.7(6)
C7_1	C6_1	C2_1	120.9(4)	C6_8	C2_8	C1_8	116.9(5)
C7_1	C6_1	Br1_1	119.6(3)	C6_8	C2_8	C3_8	126.4(5)
C6_1	C7_1	C8_1	120.9(4)	C4_8	C3_8	C2_8	119.8(6)
C7_1	C8_1	Br2_1	119.5(3)	C3_8	C4_8	C5_8	120.3(6)
C9_1	C8_1	C7_1	122.8(4)	N1_8	C5_8	C4_8	122.5(6)
C9_1	C8_1	Br2_1	117.6(4)	C2_8	C6_8	Br1_8	120.0(5)
C8_1	C9_1	C1_1	115.1(4)	C7_8	C6_8	C2_8	121.1(5)
O1_1	C9_1	C1_1	120.5(4)	C7_8	C6_8	Br1_8	118.8(5)
O1_1	C9_1	C8_1	124.5(4)	C6_8	C7_8	C8_8	120.6(6)
C1_1	N1_1	Zn1	111.7(3)	C7_8	C8_8	C9_8	122.8(6)
C5_1	N1_1	Zn1	129.1(3)	C7_8	C8_8	Br2_8	118.9(5)
C5_1	N1_1	C1_1	119.0(4)	C9_8	C8_8	Br2_8	118.3(4)
C9_1	O1_1	Zn1	113.4(3)	C8_8	C9_8	C1_8	115.4(5)
C2_2	C1_2	C9_2	123.2(4)	O1_8	C9_8	C1_8	120.4(5)
N1_2	C1_2	C2_2	121.3(4)	O1_8	C9_8	C8_8	124.2(5)
N1_2	C1_2	C9_2	115.5(4)	C1_8	N1_8	Zn2	108.9(4)
C3_2	C2_2	C1_2	116.9(4)	C5_8	N1_8	Zn2	130.4(4)
C3_2	C2_2	C6_2	126.3(4)	C5_8	N1_8	C1_8	118.8(5)

Table S45. Bond Angles for DQ15.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
C6_2	C2_2	C1_2	116.8(4)	C9_8	O1_8	Zn2	113.5(4)
C4_2	C3_2	C2_2	120.8(4)	C2_9	C1_9	C9_9	121(2)
C3_2	C4_2	C5_2	118.8(5)	N1_9	C1_9	C2_9	122.2(18)
N1_2	C5_2	C4_2	123.2(4)	N1_9	C1_9	C9_9	115.2(16)
C2_2	C6_2	Br1_2	118.7(4)	C3_9	C2_9	C1_9	116.5(17)
C7_2	C6_2	C2_2	122.0(4)	C6_9	C2_9	C1_9	115.3(17)
C7_2	C6_2	Br1_2	119.3(3)	C6_9	C2_9	C3_9	128.0(19)
C6_2	C7_2	C8_2	119.9(4)	C4_9	C3_9	C2_9	119(2)
C7_2	C8_2	C9_2	123.6(4)	C3_9	C4_9	C5_9	121(2)
C7_2	C8_2	Br2_2	117.6(3)	N1_9	C5_9	C4_9	121(2)
C9_2	C8_2	Br2_2	118.7(3)	C2_9	C6_9	Br1_9	120.2(15)
C8_2	C9_2	C1_2	114.3(4)	C7_9	C6_9	C2_9	123.9(16)
O1_2	C9_2	C1_2	120.7(4)	C7_9	C6_9	Br1_9	115.8(15)
O1_2	C9_2	C8_2	124.9(4)	C6_9	C7_9	C8_9	118.5(17)
C1_2	N1_2	Zn2	110.3(3)	C7_9	C8_9	C9_9	122.4(17)
C5_2	N1_2	Zn2	130.6(3)	C7_9	C8_9	Br2_9	118.7(15)
C5_2	N1_2	C1_2	119.0(4)	C9_9	C8_9	Br2_9	118.6(15)
C9_2	O1_2	Zn2	113.3(3)	C8_9	C9_9	C1_9	116.5(17)
C5_4	C1_4	C6_4	123.3(4)	O1_9	C9_9	C1_9	120.3(19)
N1_4	C1_4	C5_4	121.4(4)	O1_9	C9_9	C8_9	123(2)
N1_4	C1_4	C6_4	115.3(4)	C1_9	N1_9	Zn2	107.5(17)
N1_4	C2_4	C3_4	123.1(5)	C5_9	N1_9	Zn2	133(2)
C4_4	C3_4	C2_4	119.1(5)	C5_9	N1_9	C1_9	119(2)
C3_4	C4_4	C5_4	119.8(5)	C9_9	O1_9	Zn2	104(3)
C1_4	C5_4	C9_4	117.3(5)	C2_10	C1_10	C9_10	120(2)
C4_4	C5_4	C1_4	117.5(5)	N1_10	C1_10	C2_10	122(2)
C4_4	C5_4	C9_4	125.2(5)	N1_10	C1_10	C9_10	115.5(19)
C7_4	C6_4	C1_4	114.5(4)	C3_10	C2_10	C1_10	115(2)
O1_4	C6_4	C1_4	120.9(4)	C6_10	C2_10	C1_10	117(2)
O1_4	C6_4	C7_4	124.6(5)	C6_10	C2_10	C3_10	126(2)
C6_4	C7_4	Br1_4	117.8(4)	C4_10	C3_10	C2_10	119(2)
C8_4	C7_4	C6_4	123.7(5)	C3_10	C4_10	C5_10	122(2)
C8_4	C7_4	Br1_4	118.4(4)	N1_10	C5_10	C4_10	120(2)
C9_4	C8_4	C7_4	120.4(5)	C2_10	C6_10	Br1_10	118.6(18)
C5_4	C9_4	Br2_4	120.1(4)	C7_10	C6_10	C2_10	122(2)
C8_4	C9_4	C5_4	120.8(5)	C7_10	C6_10	Br1_10	118.3(19)
C8_4	C9_4	Br2_4	119.1(4)	C6_10	C7_10	C8_10	117.3(19)
C1_4	N1_4	Zn1	110.6(3)	C7_10	C8_10	C9_10	123(2)

Table S45. Bond Angles for DQ15.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
C2_4	N1_4	Zn1	130.4(3)	C7_10	C8_10	Br2_10	117.2(17)
C2_4	N1_4	C1_4	119.0(4)	C9_10	C8_10	Br2_10	118.1(17)
C6_4	O1_4	Zn1	113.6(3)	C8_10	C9_10	C1_10	116.5(18)
C5_5	C1_5	C9_5	119.8(4)	O1_10	C9_10	C1_10	119(2)
N1_5	C1_5	C5_5	123.0(4)	O1_10	C9_10	C8_10	124(2)
N1_5	C1_5	C9_5	117.2(4)	C1_10	N1_10	Zn2	115.6(19)
N1_5	C2_5	C3_5	122.7(4)	C5_10	N1_10	Zn2	124(2)
C4_5	C3_5	C2_5	119.3(5)	C5_10	N1_10	C1_10	119(2)
C3_5	C4_5	C5_5	120.4(5)	C9_10	O1_10	Zn2	115(2)
C1_5	C5_5	C6_5	119.7(4)	Cl1_11	C1_11	Cl2_11	126(2)

Table S46. Crystal data and structure refinement for DQ16.

Empirical formula	$C_{30}H_{20}Br_4N_4O_2Zn$
Formula weight	853.51
Temperature/K	150.0
Crystal system	triclinic
Space group	P-1
a/Å	11.3799(11)
b/Å	16.5376(15)
c/Å	17.8074(16)
α/°	99.938(3)
β/°	108.176(3)
γ/°	104.649(3)
Volume/Å^3	2963.0(5)
Z	4
ρ_{calc}mg/mm^3	1.913
m/mm^{-1}	5.143
F(000)	1656.0
Crystal size/mm^3	0.36 × 0.25 × 0.14
2Θ range for data collection	4.72 to 114.52°
Index ranges	$-14 \le h \le 14$, $-20 \le k \le 20$, $-22 \le l \le 21$
Reflections collected	39567
Independent reflections	12056[R(int) = 0.0520]
Data/restraints/parameters	12056/0/743
Goodness-of-fit on F^2	0.998

Final R indexes [I>=2σ (I)]	R_1 = 0.0383, wR_2 = 0.0981
Final R indexes [all data]	R_1 = 0.0438, wR_2 = 0.1018
Largest diff. peak/hole / e Å^{-3}	0.66/-0.96

Table S47. Bond Lengths for DQ16.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
Br8	C43	1.910(3)	N1	C7	1.330(4)
Br1	C2	1.902(3)	N7	C49	1.335(4)
Br5	C32	1.894(3)	N7	C53	1.350(4)
Br4	C13	1.908(3)	C4	C3	1.371(5)
Br6	C34	1.898(3)	C4	C5	1.413(5)
Br7	C41	1.898(3)	C33	C32	1.402(5)
Br2	C4	1.903(3)	C31	C32	1.391(4)
Br3	C11	1.891(3)	C38	C39	1.363(5)
Zn1	O2	2.065(2)	C8	C9	1.363(5)
Zn1	O1	2.060(2)	C8	C7	1.407(5)
Zn1	N4	2.131(3)	C41	C40	1.398(5)
Zn1	N3	2.159(3)	C41	C42	1.399(5)
Zn1	N2	2.225(3)	C40	C45	1.452(4)
Zn1	N1	2.193(3)	C9	C5	1.415(5)
Zn2	O3	2.086(2)	C24	C25	1.382(5)
Zn2	O4	2.091(2)	C24	C23	1.489(4)
Zn2	N5	2.158(3)	C48	C44	1.417(5)
Zn2	N6	2.202(3)	C48	C47	1.372(5)
Zn2	N8	2.175(3)	C19	C20	1.384(5)
Zn2	N7	2.177(3)	C45	C44	1.429(4)
O3	C31	1.298(4)	C54	C53	1.493(5)
O4	C40	1.293(4)	C54	C55	1.397(5)
O2	C10	1.290(4)	C1	C6	1.453(4)
O1	C1	1.291(4)	C1	C2	1.391(4)
C37	N5	1.329(4)	C35	C39	1.423(5)
C37	C38	1.401(5)	C59	C51	1.504(5)
C14	C13	1.414(5)	C28	C27	1.382(5)
C14	C15	1.423(4)	C12	C11	1.392(5)
C14	C18	1.412(5)	C6	C5	1.422(4)
C43	C44	1.420(5)	C10	C15	1.450(4)
C43	C42	1.365(5)	C10	C11	1.402(5)

N5	C36	1.360(4)	C16	C17	1.400(5)
C30	C26	1.500(5)	C3	C2	1.404(5)
C34	C33	1.370(5)	C25	C26	1.400(5)
C34	C35	1.412(4)	C27	C26	1.392(5)
N6	C45	1.359(4)	C56	C55	1.381(5)
N6	C46	1.322(4)	C56	C57	1.390(5)
N4	C24	1.352(4)	C56	C60	1.507(5)
N4	C28	1.340(4)	C49	C50	1.386(5)
C36	C31	1.453(4)	C53	C52	1.387(4)
C36	C35	1.415(4)	C22	C23	1.388(4)
N3	C19	1.336(4)	C22	C21	1.392(5)
N3	C23	1.354(4)	C52	C51	1.388(5)
N2	C16	1.319(4)	C18	C17	1.371(5)
N2	C15	1.360(4)	C21	C29	1.503(5)
N8	C54	1.348(4)	C21	C20	1.385(5)
N8	C58	1.336(4)	C47	C46	1.408(5)
C13	C12	1.375(5)	C58	C57	1.383(5)
N1	C6	1.362(4)	C51	C50	1.394(5)

Table S48. Bond Angles for DQ16.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
O2	Zn1	N4	100.83(10)	C42	C41	Br7	118.4(3)
O2	Zn1	N3	103.81(9)	O4	C40	C41	125.2(3)
O2	Zn1	N2	77.54(10)	O4	C40	C45	120.4(3)
O2	Zn1	N1	87.29(10)	C41	C40	C45	114.4(3)
O1	Zn1	O2	155.90(9)	C8	C9	C5	120.4(3)
O1	Zn1	N4	96.21(9)	C33	C32	Br5	117.7(2)
O1	Zn1	N3	96.61(9)	C31	C32	Br5	118.4(2)
O1	Zn1	N2	83.64(9)	C31	C32	C33	123.9(3)
O1	Zn1	N1	78.53(9)	N4	C24	C25	121.9(3)
N4	Zn1	N3	76.56(10)	N4	C24	C23	115.5(3)
N4	Zn1	N2	96.89(10)	C25	C24	C23	122.6(3)
N4	Zn1	N1	168.75(10)	C47	C48	C44	119.8(3)
N3	Zn1	N2	173.44(10)	N3	C19	C20	123.3(3)
N3	Zn1	N1	94.04(10)	N6	C45	C40	115.1(3)
N1	Zn1	N2	92.43(10)	N6	C45	C44	122.1(3)
O3	Zn2	O4	159.80(8)	C44	C45	C40	122.8(3)

O3	Zn2	N5	78.45(9)	N8	C54	C53	116.2(3)
O3	Zn2	N6	89.19(10)	N8	C54	C55	121.5(3)
O3	Zn2	N8	90.72(9)	C55	C54	C53	122.3(3)
O3	Zn2	N7	105.07(9)	O1	C1	C6	120.8(3)
O4	Zn2	N5	88.54(9)	O1	C1	C2	124.8(3)
O4	Zn2	N6	77.46(10)	C2	C1	C6	114.4(3)
O4	Zn2	N8	105.44(10)	C34	C35	C36	117.6(3)
O4	Zn2	N7	90.87(9)	C34	C35	C39	125.5(3)
N5	Zn2	N6	98.64(10)	C36	C35	C39	116.9(3)
N5	Zn2	N8	161.99(10)	N4	C28	C27	123.0(3)
N5	Zn2	N7	93.13(10)	C13	C12	C11	120.2(3)
N8	Zn2	N6	95.51(10)	N1	C6	C1	115.0(3)
N8	Zn2	N7	75.68(10)	N1	C6	C5	121.8(3)
N7	Zn2	N6	163.12(10)	C5	C6	C1	123.2(3)
C31	O3	Zn2	113.53(18)	O2	C10	C15	120.7(3)
C40	O4	Zn2	114.81(19)	O2	C10	C11	125.1(3)
C10	O2	Zn1	112.58(19)	C11	C10	C15	114.2(3)
C1	O1	Zn1	113.98(19)	N2	C16	C17	122.6(3)
N5	C37	C38	122.7(3)	C4	C3	C2	120.0(3)
C13	C14	C15	117.2(3)	C14	C15	C10	123.3(3)
C18	C14	C13	125.6(3)	N2	C15	C14	121.6(3)
C18	C14	C15	117.2(3)	N2	C15	C10	115.0(3)
C44	C43	Br8	120.2(2)	C24	C25	C26	120.2(3)
C42	C43	Br8	119.0(2)	C28	C27	C26	119.6(3)
C42	C43	C44	120.8(3)	C4	C5	C9	125.7(3)
C37	N5	Zn2	128.9(2)	C4	C5	C6	117.2(3)
C37	N5	C36	119.1(3)	C9	C5	C6	117.1(3)
C36	N5	Zn2	112.0(2)	C55	C56	C57	117.3(3)
C33	C34	Br6	119.1(2)	C55	C56	C60	121.6(3)
C33	C34	C35	120.7(3)	C57	C56	C60	121.1(4)
C35	C34	Br6	120.2(2)	C38	C39	C35	120.1(3)
C45	N6	Zn2	111.7(2)	C1	C2	Br1	117.5(2)
C46	N6	Zn2	128.9(2)	C1	C2	C3	123.8(3)
C46	N6	C45	119.3(3)	C3	C2	Br1	118.6(2)
C24	N4	Zn1	116.6(2)	N7	C49	C50	123.6(3)
C28	N4	Zn1	125.1(2)	N7	C53	C54	115.5(3)
C28	N4	C24	118.1(3)	N7	C53	C52	122.0(3)
N5	C36	C31	114.8(3)	C52	C53	C54	122.4(3)
N5	C36	C35	121.9(3)	C43	C44	C45	117.5(3)
C35	C36	C31	123.3(3)	C48	C44	C43	125.6(3)

C19	N3	Zn1	126.3(2)	C48	C44	C45	116.9(3)
C19	N3	C23	118.0(3)	C56	C55	C54	120.6(3)
C23	N3	Zn1	115.5(2)	C23	C22	C21	120.2(3)
C16	N2	Zn1	130.1(2)	N3	C23	C24	115.7(3)
C16	N2	C15	119.5(3)	N3	C23	C22	121.6(3)
C15	N2	Zn1	108.6(2)	C22	C23	C24	122.7(3)
C54	N8	Zn2	116.1(2)	C25	C26	C30	120.6(3)
C58	N8	Zn2	125.9(2)	C27	C26	C30	122.2(3)
C58	N8	C54	117.7(3)	C27	C26	C25	117.2(3)
C14	C13	Br4	119.9(2)	N1	C7	C8	123.0(3)
C12	C13	Br4	118.8(3)	C53	C52	C51	120.4(3)
C12	C13	C14	121.2(3)	C17	C18	C14	119.7(3)
C6	N1	Zn1	110.4(2)	C12	C11	Br3	118.4(3)
C7	N1	Zn1	130.6(2)	C12	C11	C10	123.9(3)
C7	N1	C6	118.9(3)	C10	C11	Br3	117.7(2)
C49	N7	Zn2	126.1(2)	C22	C21	C29	121.6(4)
C49	N7	C53	117.6(3)	C20	C21	C22	117.6(3)
C53	N7	Zn2	116.4(2)	C20	C21	C29	120.9(3)
C3	C4	Br2	119.3(3)	C48	C47	C46	119.4(3)
C3	C4	C5	121.3(3)	N6	C46	C47	122.6(3)
C5	C4	Br2	119.4(3)	C43	C42	C41	120.7(3)
C34	C33	C32	120.4(3)	N8	C58	C57	123.6(3)
O3	C31	C36	120.4(3)	C58	C57	C56	119.3(3)
O3	C31	C32	125.6(3)	C19	C20	C21	119.3(3)
C32	C31	C36	114.0(3)	C18	C17	C16	119.3(3)
C39	C38	C37	119.0(3)	C52	C51	C59	121.3(3)
C9	C8	C7	118.7(3)	C52	C51	C50	117.2(3)
C40	C41	Br7	117.9(2)	C50	C51	C59	121.5(3)
C40	C41	C42	123.7(3)	C49	C50	C51	119.2(3)

Table S49. Crystal data and structure refinement for DQ17.

Empirical formula	$C_{30}H_{20}Br_4N_4O_4Zn$
Formula weight	885.51
Temperature/K	150.0
Crystal system	monoclinic
Space group	$P2_1/n$
a/Å	13.0380(6)
b/Å	16.0310(7)

c/Å	15.9974(7)
α/°	90
β/°	113.843(2)
γ/°	90
Volume/Å^3	3058.3(2)
Z	4
ρ_{calc}mg/mm^3	1.923
m/mm^{-1}	5.169
F(000)	1720.0
Crystal size/mm^3	0.36 × 0.25 × 0.16
2Θ range for data collection	6.466 to 114.166°
Index ranges	-16 ≤ h ≤ 16, -19 ≤ k ≤ 20, -19 ≤ l ≤ 20
Reflections collected	28962
Independent reflections	6246[R(int) = 0.0460]
Data/restraints/parameters	6246/0/390
Goodness-of-fit on F^2	1.038
Final R indexes [I>=2σ (I)]	R_1 = 0.0315, wR_2 = 0.0756
Final R indexes [all data]	R_1 = 0.0384, wR_2 = 0.0787
Largest diff. peak/hole / e Å^{-3}	0.67/-0.76

Table S50. Bond Lengths for DQ17.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
Br3	C11	1.899(3)	C14	C18	1.409(4)
Br1	C2	1.895(3)	C2	C1	1.399(4)
Br2	C4	1.907(3)	C2	C3	1.401(4)
Br4	C13	1.902(3)	C13	C12	1.365(4)
Zn1	O2	2.0842(19)	C4	C3	1.368(4)
Zn1	N2	2.147(2)	C4	C5	1.414(4)
Zn1	O1	2.0980(19)	C12	C11	1.410(4)
Zn1	N4	2.178(2)	C1	C6	1.449(4)
Zn1	N3	2.152(2)	C6	C5	1.419(4)
Zn1	N1	2.145(2)	C11	C10	1.398(4)
O2	C10	1.293(3)	C23	C22	1.386(4)
N2	C15	1.363(3)	C23	C24	1.495(4)
N2	C16	1.324(4)	C28	C27	1.381(4)
O1	C1	1.295(3)	C10	C15	1.445(4)
N4	C28	1.341(4)	C26	C25	1.393(4)

N4	C24	1.354(4)	C26	C27	1.391(4)
O3	C21	1.350(3)	C16	C17	1.403(4)
O3	C29	1.431(4)	C7	C8	1.397(4)
N3	C23	1.341(4)	C19	C20	1.368(4)
N3	C19	1.347(4)	C25	C24	1.387(4)
O4	C26	1.349(4)	C21	C22	1.396(4)
O4	C30	1.436(4)	C21	C20	1.390(4)
N1	C6	1.363(4)	C18	C17	1.370(4)
N1	C7	1.323(4)	C5	C9	1.411(4)
C14	C13	1.407(4)	C9	C8	1.367(4)
C14	C15	1.422(4)			

Table S51. Bond Angles for DQ17.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
O2	Zn1	N2	78.70(8)	O1	C1	C2	125.0(3)
O2	Zn1	O1	166.27(8)	O1	C1	C6	120.5(2)
O2	Zn1	N4	93.01(8)	C2	C1	C6	114.5(2)
O2	Zn1	N3	95.69(8)	N1	C6	C1	115.4(2)
O2	Zn1	N1	93.60(8)	N1	C6	C5	121.2(3)
N2	Zn1	N4	93.72(9)	C5	C6	C1	123.4(3)
N2	Zn1	N3	168.01(9)	C12	C11	Br3	117.8(2)
O1	Zn1	N2	90.95(8)	C10	C11	Br3	118.5(2)
O1	Zn1	N4	96.68(8)	C10	C11	C12	123.6(3)
O1	Zn1	N3	96.10(8)	N3	C23	C22	123.0(2)
O1	Zn1	N1	78.84(8)	N3	C23	C24	115.4(2)
N3	Zn1	N4	75.87(9)	C22	C23	C24	121.6(2)
N1	Zn1	N2	98.23(9)	N4	C28	C27	124.2(3)
N1	Zn1	N4	167.28(9)	O2	C10	C11	124.9(3)
N1	Zn1	N3	92.66(9)	O2	C10	C15	120.9(2)
C10	O2	Zn1	112.78(17)	C11	C10	C15	114.2(2)
C15	N2	Zn1	111.52(17)	N2	C15	C14	121.6(2)
C16	N2	Zn1	128.7(2)	N2	C15	C10	114.8(2)
C16	N2	C15	119.2(2)	C14	C15	C10	123.5(2)
C1	O1	Zn1	113.23(17)	C4	C3	C2	120.6(3)
C28	N4	Zn1	127.0(2)	O4	C26	C25	115.4(3)
C28	N4	C24	117.4(2)	O4	C26	C27	125.7(3)
C24	N4	Zn1	115.50(18)	C27	C26	C25	118.9(3)

C21	O3	C29	117.6(2)	N2	C16	C17	122.9(3)
C23	N3	Zn1	117.24(18)	N1	C7	C8	122.9(3)
C23	N3	C19	117.6(2)	N3	C19	C20	123.6(3)
C19	N3	Zn1	125.18(19)	C24	C25	C26	119.2(3)
C26	O4	C30	118.3(3)	O3	C21	C22	124.8(3)
C6	N1	Zn1	111.88(18)	O3	C21	C20	116.3(3)
C7	N1	Zn1	128.6(2)	C20	C21	C22	118.8(3)
C7	N1	C6	119.5(2)	C28	C27	C26	118.0(3)
C13	C14	C15	117.2(3)	C17	C18	C14	120.4(3)
C13	C14	C18	125.6(3)	C18	C17	C16	118.7(3)
C18	C14	C15	117.2(3)	C23	C22	C21	118.3(3)
C1	C2	Br1	118.6(2)	N4	C24	C23	116.0(2)
C1	C2	C3	123.2(3)	N4	C24	C25	122.3(3)
C3	C2	Br1	118.2(2)	C25	C24	C23	121.7(3)
C14	C13	Br4	119.8(2)	C4	C5	C6	117.2(3)
C12	C13	Br4	118.6(2)	C9	C5	C4	125.5(3)
C12	C13	C14	121.6(3)	C9	C5	C6	117.3(3)
C3	C4	Br2	118.3(2)	C19	C20	C21	118.7(3)
C3	C4	C5	121.1(3)	C8	C9	C5	120.3(3)
C5	C4	Br2	120.6(2)	C9	C8	C7	118.8(3)
C13	C12	C11	119.9(3)				

Table S52. Crystal data and structure refinement for DQ18.

Empirical formula	$C_{30}H_{20}Br_4N_4O_2Zn$
Formula weight	853.51
Temperature/K	150.0
Crystal system	orthorhombic
Space group	Pbca
a/Å	14.0723(5)
b/Å	17.9629(6)
c/Å	23.2832(8)
α/°	90.00
β/°	90.00
γ/°	90.00
Volume/Å^3	5885.5(4)
Z	8
ρ_{calc}mg/mm^3	1.926
m/mm^{-1}	5.319

F(000)	3312.0
Crystal size/mm^3	0.36 × 0.25 × 0.14
2Θ range for data collection	6.6 to 114.3°
Index ranges	-17 ≤ h ≤ 16, -22 ≤ k ≤ 22, -29 ≤ l ≤ 29
Reflections collected	63594
Independent reflections	6043[R(int) = 0.0768]
Data/restraints/parameters	6043/0/372
Goodness-of-fit on F^2	1.006
Final R indexes [I>=2σ (I)]	R_1 = 0.0344, wR_2 = 0.0778
Final R indexes [all data]	R_1 = 0.0531, wR_2 = 0.0860
Largest diff. peak/hole / e Å^{-3}	0.47/-0.59

Table S53. Bond Lengths for DQ18.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
Br1	C2	1.894(3)	C2	C3	1.405(5)
Br4	C13	1.907(3)	C23	C24	1.481(5)
Br3	C11	1.893(4)	C23	C22	1.391(4)
Br2	C4	1.898(3)	C18	C14	1.415(5)
Zn1	O1	2.074(2)	C18	C17	1.371(5)
Zn1	O2	2.047(2)	C1	C6	1.445(4)
Zn1	N3	2.175(3)	C6	C5	1.417(5)
Zn1	N4	2.188(3)	C21	C20	1.393(5)
Zn1	N1	2.186(3)	C21	C22	1.387(5)
Zn1	N2	2.183(3)	C15	C10	1.451(5)
O1	C1	1.299(4)	C15	C14	1.418(4)
O2	C10	1.292(4)	C24	C25	1.382(5)
N3	C23	1.350(4)	C4	C3	1.363(5)
N3	C19	1.343(4)	C4	C5	1.420(5)
N4	C24	1.346(4)	C28	C27	1.383(5)
N4	C28	1.342(4)	C5	C9	1.418(5)
N1	C6	1.367(4)	C20	C19	1.391(5)
N1	C7	1.322(4)	C20	C29	1.498(5)
N2	C15	1.368(4)	C16	C17	1.400(5)
N2	C16	1.323(4)	C9	C8	1.361(5)
C13	C12	1.360(5)	C26	C27	1.390(5)
C13	C14	1.416(5)	C26	C25	1.383(5)
C11	C10	1.400(5)	C7	C8	1.394(5)

C11	C12	1.404(5)	C27	C30	1.507(5)
C2	C1	1.398(4)			

Table S54. Bond Angles for DQ18.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
O1	Zn1	N3	161.45(9)	O1	C1	C6	120.3(3)
O1	Zn1	N4	90.19(9)	C2	C1	C6	115.0(3)
O1	Zn1	N1	78.03(9)	N1	C6	C1	115.1(3)
O1	Zn1	N2	89.94(9)	N1	C6	C5	122.3(3)
O2	Zn1	O1	105.45(9)	C5	C6	C1	122.6(3)
O2	Zn1	N3	91.27(10)	C22	C21	C20	119.9(3)
O2	Zn1	N4	161.93(10)	N2	C15	C10	114.8(3)
O2	Zn1	N1	96.65(9)	N2	C15	C14	121.9(3)
O2	Zn1	N2	79.01(9)	C14	C15	C10	123.3(3)
N3	Zn1	N4	74.82(10)	N4	C24	C23	115.7(3)
N3	Zn1	N1	92.33(10)	N4	C24	C25	120.8(3)
N3	Zn1	N2	101.32(10)	C25	C24	C23	123.4(3)
N1	Zn1	N4	95.40(10)	C3	C4	Br2	119.6(3)
N2	Zn1	N4	92.26(10)	C3	C4	C5	120.5(3)
N2	Zn1	N1	165.72(10)	C5	C4	Br2	119.9(3)
C1	O1	Zn1	114.75(19)	O2	C10	C11	124.6(3)
C10	O2	Zn1	114.0(2)	O2	C10	C15	120.9(3)
C23	N3	Zn1	117.0(2)	C11	C10	C15	114.5(3)
C19	N3	Zn1	123.4(2)	C13	C12	C11	120.5(3)
C19	N3	C23	119.4(3)	C4	C3	C2	120.6(3)
C24	N4	Zn1	116.5(2)	C13	C14	C15	117.1(3)
C28	N4	Zn1	124.4(2)	C18	C14	C13	125.7(3)
C28	N4	C24	119.1(3)	C18	C14	C15	117.2(3)
C6	N1	Zn1	111.3(2)	N4	C28	C27	123.7(3)
C7	N1	Zn1	130.1(2)	C6	C5	C4	118.0(3)
C7	N1	C6	118.5(3)	C6	C5	C9	116.9(3)
C15	N2	Zn1	109.8(2)	C9	C5	C4	125.0(3)
C16	N2	Zn1	130.6(2)	C21	C20	C29	121.7(3)
C16	N2	C15	118.7(3)	C19	C20	C21	117.1(3)
C12	C13	Br4	118.9(3)	C19	C20	C29	121.2(3)
C12	C13	C14	121.4(3)	C21	C22	C23	119.5(3)
C14	C13	Br4	119.8(3)	N3	C19	C20	123.2(3)

C10	C11	Br3	118.5(3)	N2	C16	C17	123.4(3)
C10	C11	C12	123.1(3)	C8	C9	C5	119.5(3)
C12	C11	Br3	118.5(3)	C25	C26	C27	120.5(3)
C1	C2	Br1	119.2(2)	N1	C7	C8	122.9(3)
C1	C2	C3	123.1(3)	C28	C27	C26	116.4(3)
C3	C2	Br1	117.6(2)	C28	C27	C30	121.4(3)
N3	C23	C24	115.6(3)	C26	C27	C30	122.2(3)
N3	C23	C22	120.6(3)	C18	C17	C16	118.7(3)
C22	C23	C24	123.7(3)	C9	C8	C7	119.9(3)
C17	C18	C14	120.1(3)	C24	C25	C26	119.3(3)
O1	C1	C2	124.7(3)				

Table S55. Crystal data and structure refinement for DQ19.

Empirical formula	$C_{31}H_{17}Br_4Cl_3N_4O_2Zn$
Formula weight	968.85
Temperature/K	150.0
Crystal system	monoclinic
Space group	$P2_1/n$
a/Å	12.9747(3)
b/Å	17.8849(5)
c/Å	15.6864(4)
α/°	90.00
β/°	113.5075(8)
γ/°	90.00
Volume/Å^3	3337.95(15)
Z	4
ρ_{calc}mg/mm^3	1.928
m/mm^{-1}	5.801
F(000)	1872.0
Crystal size/mm^3	0.37 × 0.26 × 0.18
2Θ range for data collection	4.56 to 52.78°
Index ranges	$-16 \le h \le 15$, $-22 \le k \le 22$, $-19 \le l \le 19$
Reflections collected	59448
Independent reflections	6811[R(int) = 0.0648]
Data/restraints/parameters	6811/6/410
Goodness-of-fit on F^2	1.002
Final R indexes [I>=2σ (I)]	R_1 = 0.0408, wR_2 = 0.1108
Final R indexes [all data]	R_1 = 0.0566, wR_2 = 0.1209

Largest diff. peak/hole / e Å^{-3}	0.81/-0.71

Table S56. Bond Lengths for DQ19.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
Zn1	O2	2.057(3)	C24	C25	1.408(6)
Zn1	O1	2.069(3)	C13	C14	1.419(6)
Zn1	N2	2.148(3)	C13	C12	1.360(6)
Zn1	N4	2.178(3)	C10	C15	1.446(6)
Zn1	N3	2.210(4)	C6	C1	1.441(6)
Zn1	N1	2.166(4)	C6	C5	1.424(6)
Br3	C11	1.892(4)	C15	C14	1.422(5)
Br4	C13	1.897(4)	C14	C18	1.414(6)
Br2	C4	1.900(4)	C19	C20	1.401(6)
Br1	C2	1.898(5)	C9	C5	1.408(6)
Br1'	C2	1.955(6)	C9	C8	1.355(7)
Cl1	C26	1.752(4)	C1	C2	1.395(6)
Cl2	C31	1.727(8)	C4	C5	1.410(6)
O2	C10	1.293(5)	C4	C3	1.355(7)
O1	C1	1.292(5)	C2	C3	1.402(7)
N2	C15	1.363(5)	C26	C25	1.450(6)
N2	C16	1.316(5)	C26	C27	1.338(7)
N4	C24	1.355(5)	C22	C27	1.445(6)
N4	C30	1.322(6)	C22	C21	1.392(6)
N3	C23	1.359(5)	C25	C28	1.396(7)
N3	C19	1.346(5)	C30	C29	1.390(7)
N1	C6	1.374(5)	C18	C17	1.354(7)
N1	C7	1.315(5)	C8	C7	1.408(7)
C11	C10	1.387(6)	C29	C28	1.367(7)
C11	C12	1.408(6)	C16	C17	1.411(6)
C23	C24	1.428(6)	C20	C21	1.383(7)
C23	C22	1.413(6)	Cl3	C31	1.688(9)

Table S57. Bond Angles for DQ19.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
O2	Zn1	O1	164.52(12)	N2	C15	C10	115.4(3)

O2	Zn1	N2	79.56(12)	N2	C15	C14	121.3(4)
O2	Zn1	N4	97.22(12)	C14	C15	C10	123.3(4)
O2	Zn1	N3	92.82(12)	C13	C14	C15	117.0(4)
O2	Zn1	N1	91.39(12)	C18	C14	C13	126.4(4)
O1	Zn1	N2	90.60(13)	C18	C14	C15	116.6(4)
O1	Zn1	N4	95.21(13)	N3	C19	C20	123.5(4)
O1	Zn1	N3	99.23(12)	C8	C9	C5	120.2(4)
O1	Zn1	N1	78.98(12)	O1	C1	C6	121.0(4)
N2	Zn1	N4	165.41(13)	O1	C1	C2	124.6(4)
N2	Zn1	N3	90.51(13)	C2	C1	C6	114.4(4)
N2	Zn1	N1	102.31(13)	C13	C12	C11	120.4(4)
N4	Zn1	N3	75.37(13)	C5	C4	Br2	119.9(3)
N1	Zn1	N4	91.95(13)	C3	C4	Br2	118.4(4)
N1	Zn1	N3	167.04(13)	C3	C4	C5	121.7(4)
C10	O2	Zn1	113.3(2)	Br1	C2	Br1'	22.44(14)
C1	O1	Zn1	113.6(3)	C1	C2	Br1	118.5(4)
C15	N2	Zn1	110.4(2)	C1	C2	Br1'	116.3(4)
C16	N2	Zn1	129.3(3)	C1	C2	C3	123.1(4)
C16	N2	C15	120.0(4)	C3	C2	Br1	118.0(3)
C24	N4	Zn1	115.1(3)	C3	C2	Br1'	118.3(4)
C30	N4	Zn1	126.0(3)	C9	C5	C6	117.3(4)
C30	N4	C24	118.9(4)	C9	C5	C4	126.3(4)
C23	N3	Zn1	114.1(3)	C4	C5	C6	116.4(4)
C19	N3	Zn1	128.3(3)	C25	C26	Cl1	117.4(3)
C19	N3	C23	117.5(4)	C27	C26	Cl1	118.9(4)
C6	N1	Zn1	110.7(3)	C27	C26	C25	123.7(4)
C7	N1	Zn1	129.7(3)	C23	C22	C27	119.1(4)
C7	N1	C6	119.6(4)	C21	C22	C23	118.7(4)
C10	C11	Br3	118.0(3)	C21	C22	C27	122.2(4)
C10	C11	C12	123.3(4)	C24	C25	C26	117.0(4)
C12	C11	Br3	118.6(3)	C28	C25	C24	117.7(4)
N3	C23	C24	117.3(4)	C28	C25	C26	125.3(4)
N3	C23	C22	122.4(4)	N4	C30	C29	122.8(5)
C22	C23	C24	120.3(4)	C17	C18	C14	121.1(4)
N4	C24	C23	117.7(4)	C26	C27	C22	119.5(4)
N4	C24	C25	121.8(4)	C9	C8	C7	119.6(4)
C25	C24	C23	120.5(4)	C28	C29	C30	119.0(4)
C14	C13	Br4	119.7(3)	N2	C16	C17	122.3(4)
C12	C13	Br4	119.2(3)	C18	C17	C16	118.7(4)
C12	C13	C14	121.1(4)	C21	C20	C19	118.7(4)

O2	C10	C11	124.7(4)	C20	C21	C22	119.3(4)
O2	C10	C15	120.6(4)	N1	C7	C8	122.2(4)
C11	C10	C15	114.7(4)	C4	C3	C2	120.6(4)
N1	C6	C1	115.1(4)	C29	C28	C25	119.8(4)
N1	C6	C5	121.1(4)	Cl3	C31	Cl2	114.3(6)
C5	C6	C1	123.7(4)				

Table S58. Crystal data and structure refinement for DQ20.

Empirical formula	$C_{18}H_{16}Br_2N_2OZn_{0.5}$
Formula weight	468.83
Temperature/K	150.0
Crystal system	monoclinic
Space group	C2/c
a/Å	12.6190(6)
b/Å	26.8446(13)
c/Å	11.0084(5)
α/°	90.00
β/°	111.4939(17)
γ/°	90.00
Volume/Å^3	3469.8(3)
Z	8
ρ_{calc}mg/mm^3	1.795
m/mm^{-1}	5.353
F(000)	1848.0
Crystal size/mm^3	0.39 × 0.36 × 0.31
2Θ range for data collection	4.48 to 52.84°
Index ranges	$-15 \leq h \leq 15$, $-33 \leq k \leq 33$, $-13 \leq l \leq 13$
Reflections collected	33167
Independent reflections	3572[R(int) = 0.0624]
Data/restraints/parameters	3572/0/216
Goodness-of-fit on F^2	1.012
Final R indexes [I>=2σ (I)]	R_1 = 0.0289, wR_2 = 0.0709
Final R indexes [all data]	R_1 = 0.0388, wR_2 = 0.0753
Largest diff. peak/hole / e Å^{-3}	0.38/-0.31

Table S59. Bond Lengths for DQ20.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
Br1	C2	1.897(3)	C6	C5	1.425(3)
Br2	C4	1.904(3)	C1	O1	1.283(3)
Zn1	N1[1]	2.168(2)	C4	C5	1.404(4)
Zn1	N1	2.168(2)	C4	C3	1.372(4)
Zn1	N2	2.168(2)	C17	C15	1.544(4)
Zn1	N2[1]	2.168(2)	C5	C9	1.419(4)
Zn1	O1	2.0860(19)	C14	C14[1]	1.504(5)
Zn1	O1[1]	2.0860(19)	C14	C13	1.384(4)
N1	C6	1.359(3)	C10	C11	1.386(4)
N1	C7	1.322(3)	C8	C9	1.357(4)
N2	C14	1.350(3)	C8	C7	1.401(4)
N2	C10	1.329(4)	C13	C12	1.396(4)
C16	C15	1.531(4)	C18	C15	1.525(4)
C2	C1	1.398(4)	C11	C12	1.385(4)
C2	C3	1.402(4)	C12	C15	1.531(4)
C6	C1	1.458(4)			

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

Table S60. Bond Angles for DQ20.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
N1	Zn1	N1[1]	170.71(12)	O1	C1	C2	126.0(2)
N1[1]	Zn1	N2[1]	89.88(8)	O1	C1	C6	120.3(2)
N1	Zn1	N2[1]	97.56(8)	C5	C4	Br2	120.0(2)
N1[1]	Zn1	N2	97.56(8)	C3	C4	Br2	119.0(2)
N1	Zn1	N2	89.88(8)	C3	C4	C5	121.0(2)
N2	Zn1	N2[1]	73.81(12)	C6	C5	C4	117.7(2)
O1	Zn1	N1[1]	95.74(7)	C9	C5	C6	116.7(2)
O1[1]	Zn1	N1	95.74(7)	C9	C5	C4	125.6(2)
O1	Zn1	N1	78.07(8)	N2	C14	C14[1]	114.04(14)
O1[1]	Zn1	N1[1]	78.07(8)	C13	C14	N2	121.5(2)
O1[1]	Zn1	N2	95.54(8)	C13	C14	C14[1]	124.50(16)
O1	Zn1	N2	162.88(8)	N2	C10	C11	123.2(3)
O1	Zn1	N2[1]	95.54(8)	C9	C8	C7	119.3(3)
O1[1]	Zn1	N2[1]	162.88(8)	C14	C13	C12	120.8(3)
O1	Zn1	O1[1]	97.72(11)	C2	C3	C4	120.3(3)

C6	N1	Zn1	111.44(17)	C8	C9	C5	120.2(2)
C7	N1	Zn1	129.30(18)	N1	C7	C8	122.8(3)
C7	N1	C6	119.1(2)	C12	C11	C10	119.8(3)
C14	N2	Zn1	119.05(17)	C13	C12	C15	122.1(3)
C10	N2	Zn1	122.79(19)	C11	C12	C13	116.6(3)
C10	N2	C14	118.1(2)	C11	C12	C15	121.3(2)
C1	C2	Br1	118.55(19)	C16	C15	C18	108.2(3)
C1	C2	C3	124.1(2)	C16	C15	C12	111.6(3)
C3	C2	Br1	117.4(2)	C17	C15	C16	109.1(3)
N1	C6	C1	114.9(2)	C17	C15	C18	109.4(3)
N1	C6	C5	121.9(2)	C17	C15	C12	107.3(2)
C5	C6	C1	123.2(2)	C18	C15	C12	111.2(2)
C2	C1	C6	113.7(2)	C1	O1	Zn1	113.91(16)

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

Table S61. The cell viability against SK-OV-3CR and HL-7702 after incubation for 48 h at different concentrations of each compound by a cell counting Kit-8 (CCK-8) assay.

	SK-OV-3CR	HL-7702
H-Q1	>50	>50
H-Q2	>50	>50
H-Q3	>50	>50
H-Q4	>50	>50
H-Q5	>50	>50
H-Q6	>50	>50
D1	>50	>50
D2	>50	>50
D3	>50	>50
D4	>50	>50
D5	>50	>50
D6	>50	>50
D7	>50	>50
D8	>50	>50
D9	>50	>50
D10	>50	>50
$Zn(NO_3)_2 \cdot 6H_2O$	>50	>50

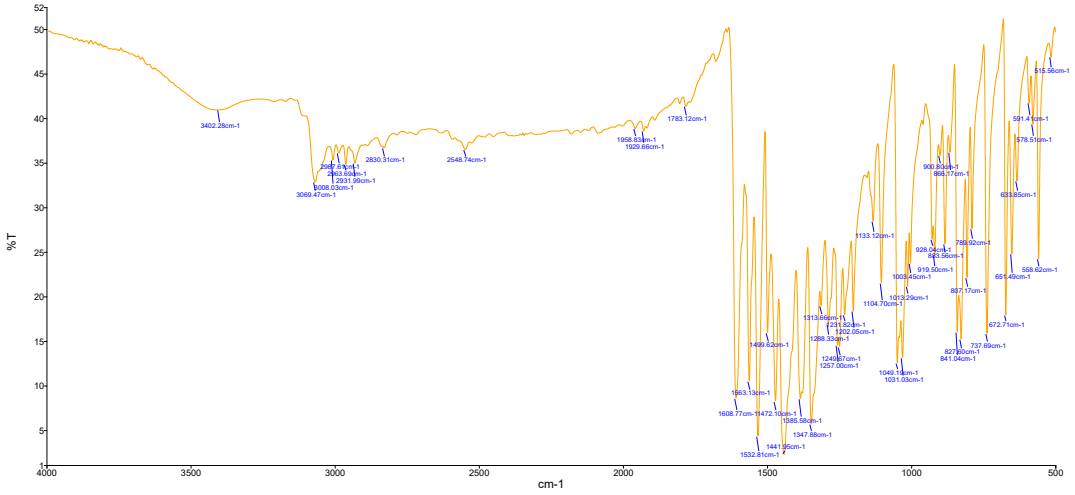


Figure S1. IR (KBr) of **DQ1**.

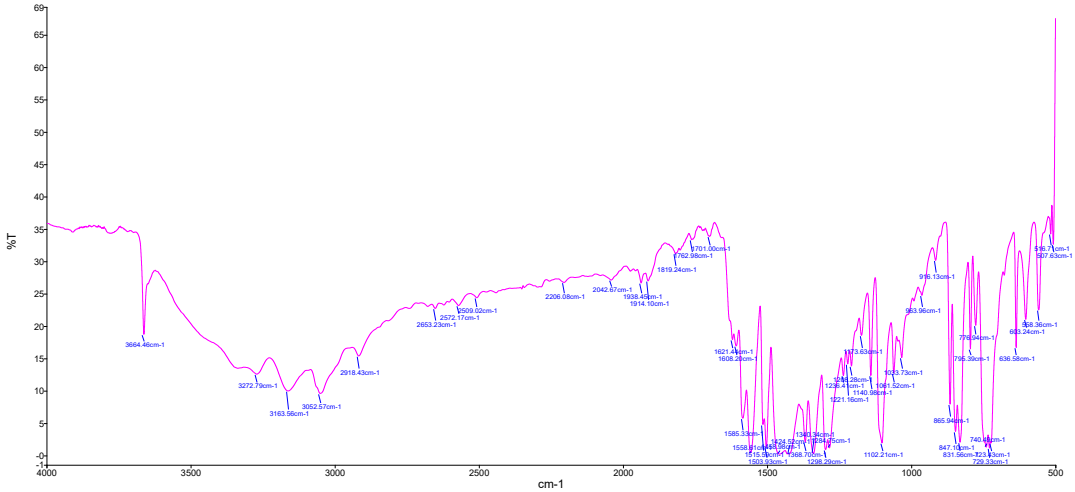


Figure S2. IR (KBr) of **DQ2**.

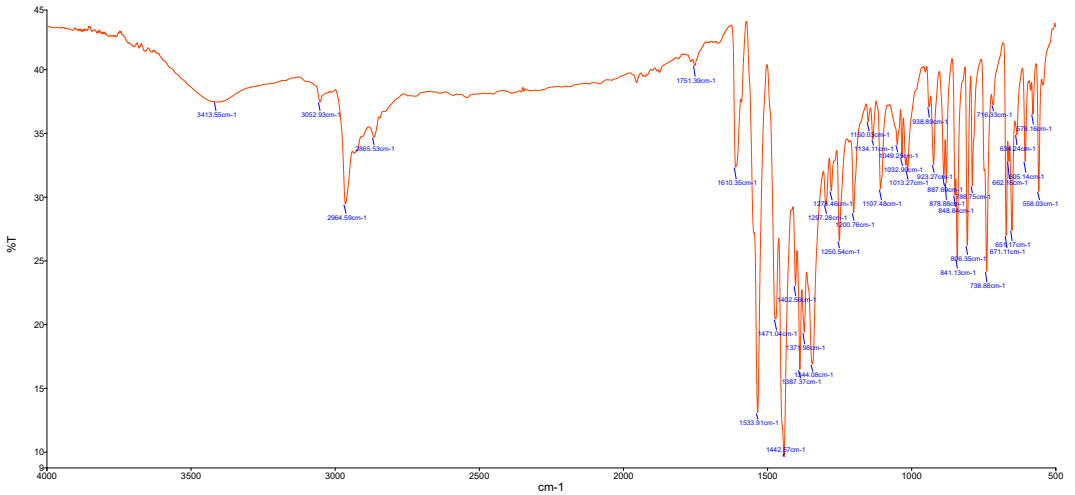


Figure S3. IR (KBr) of **DQ3**.

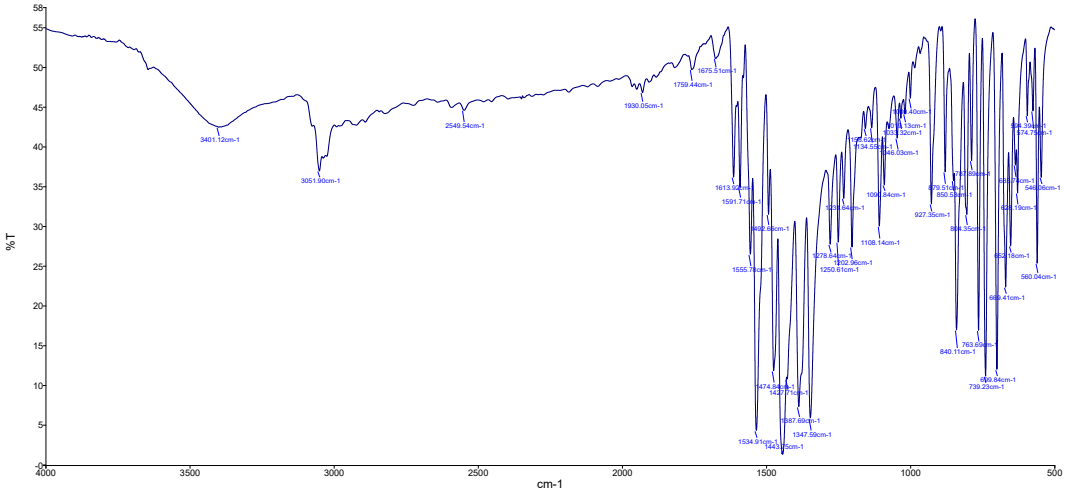


Figure S4. IR (KBr) of **DQ4**.

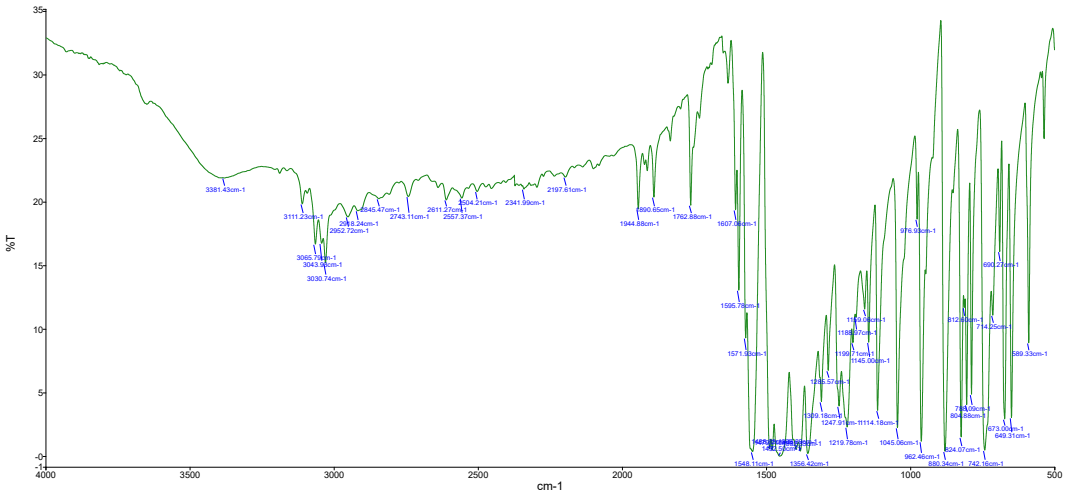


Figure S5. IR (KBr) of **DQ5**.

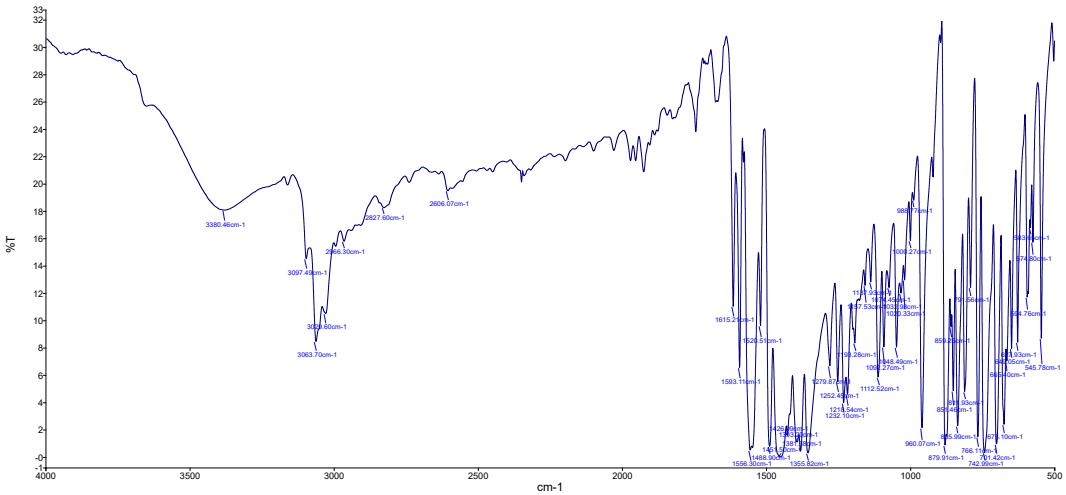


Figure S6. IR (KBr) of **DQ6**.

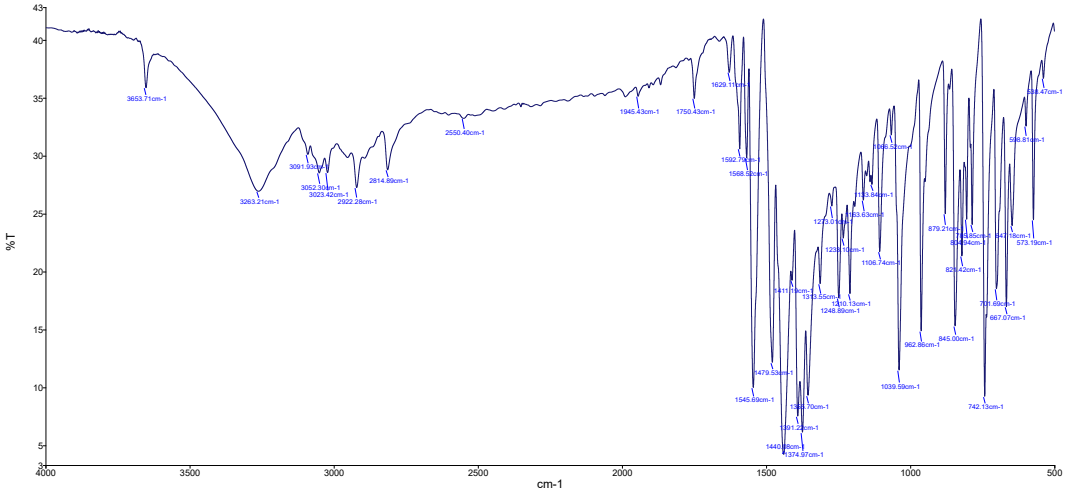


Figure S7. IR (KBr) of **DQ7**.

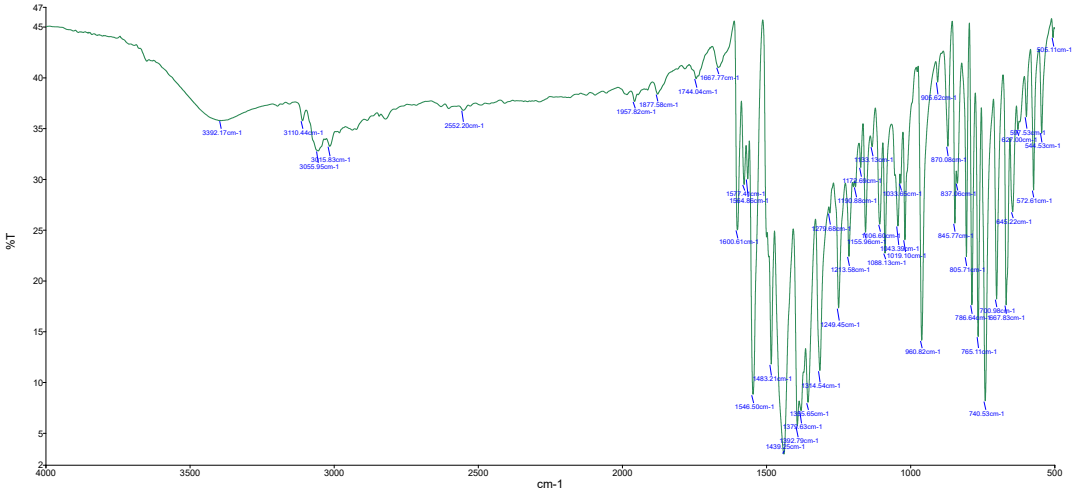


Figure S8. IR (KBr) of **DQ8**.

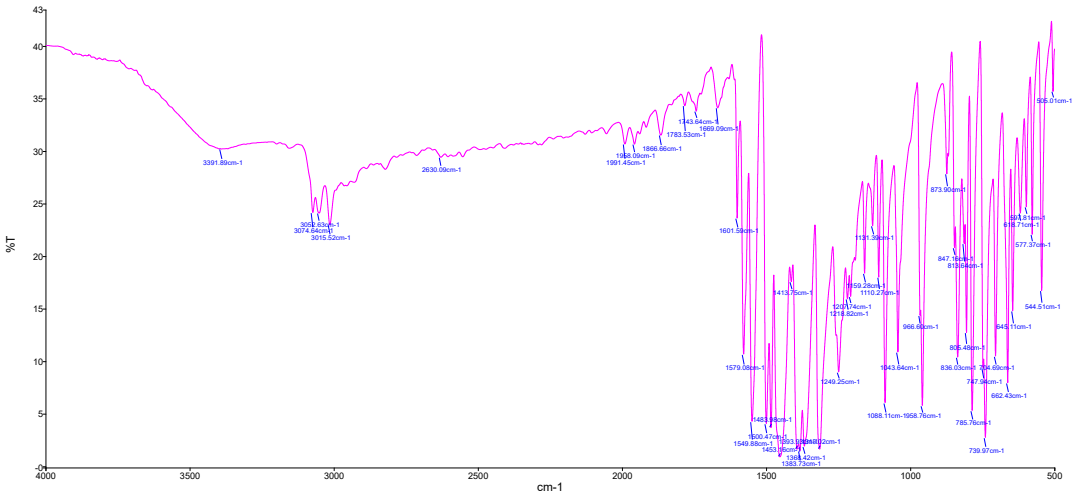


Figure S9. IR (KBr) of **DQ9**.

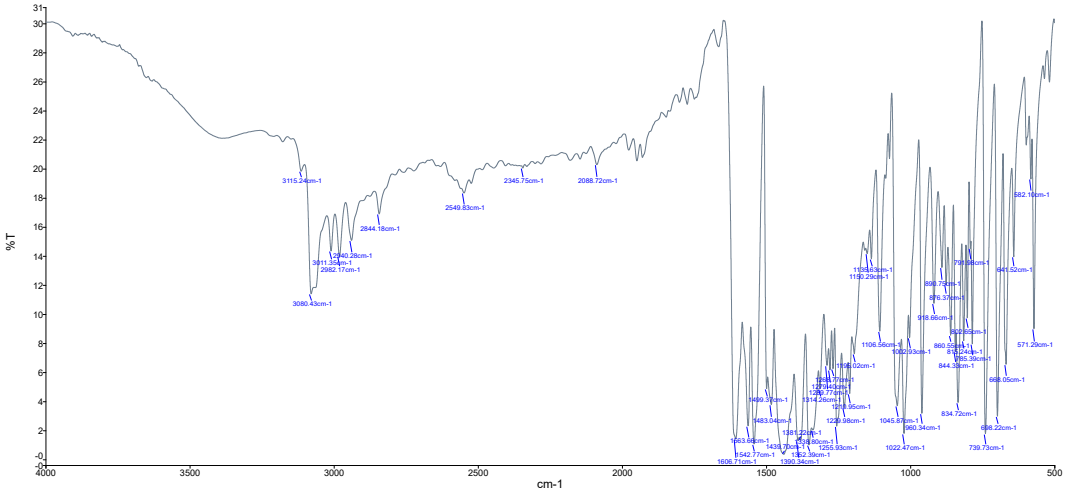


Figure S10. IR (KBr) of **DQ10**.

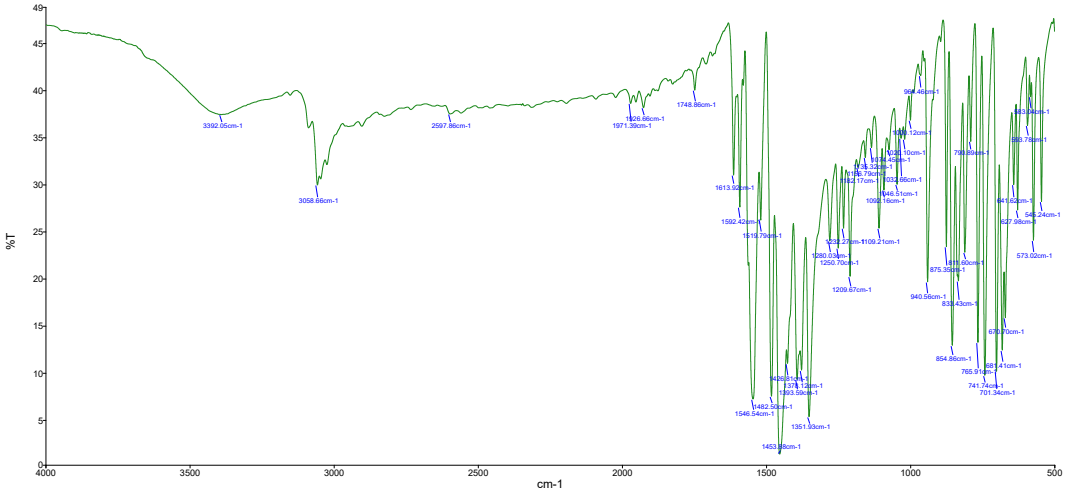


Figure S11. IR (KBr) of **DQ11**.

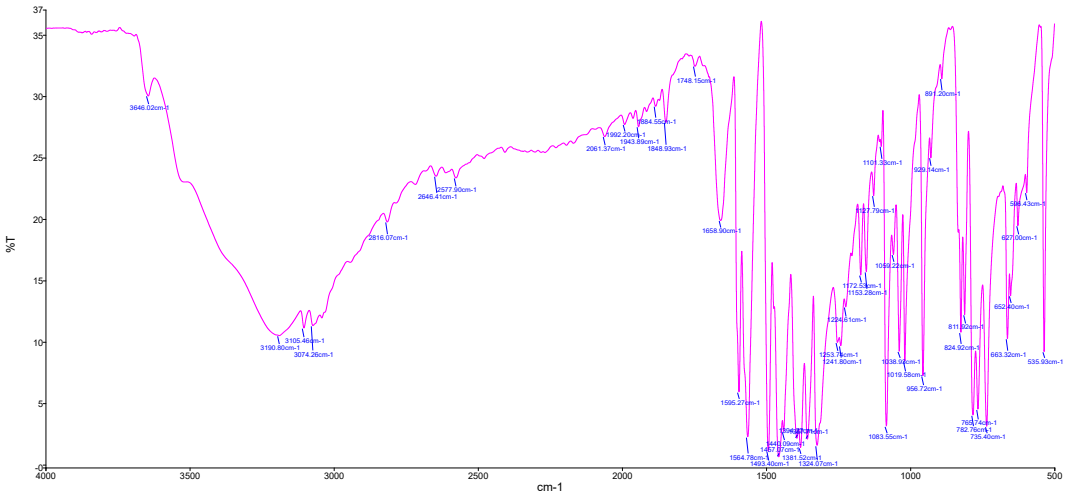


Figure S12. IR (KBr) of **DQ12**.

Figure S13. IR (KBr) of **DQ13**.

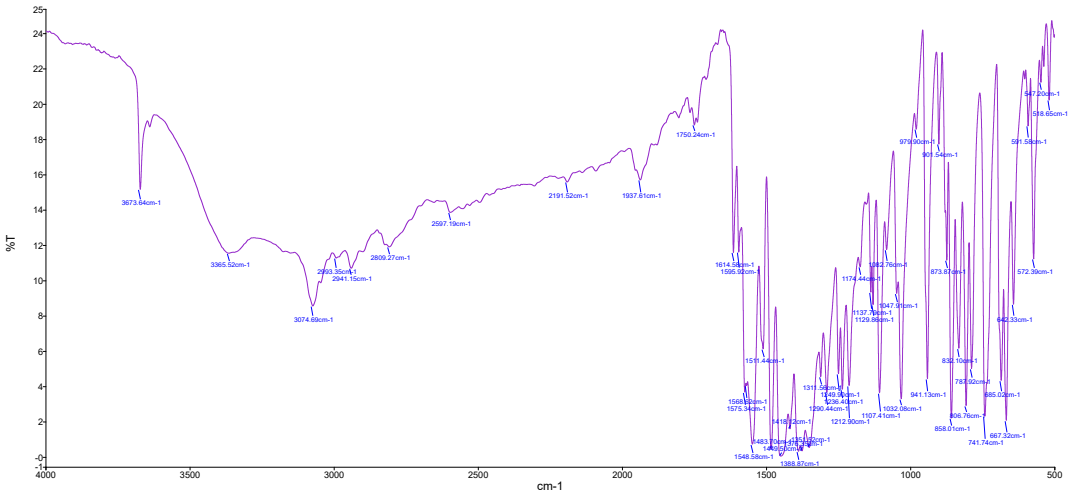


Figure S14. IR (KBr) of **DQ14**.

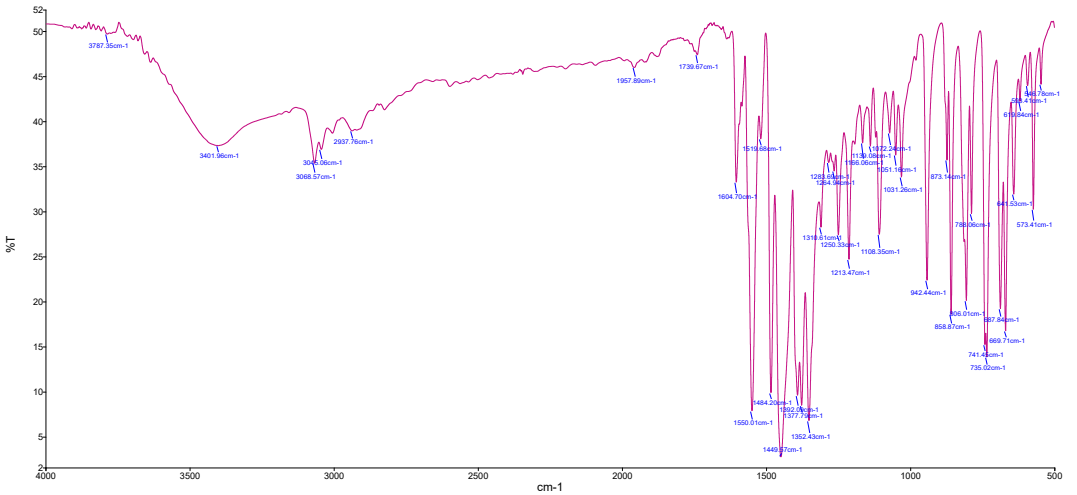


Figure S15. IR (KBr) of **DQ15**.

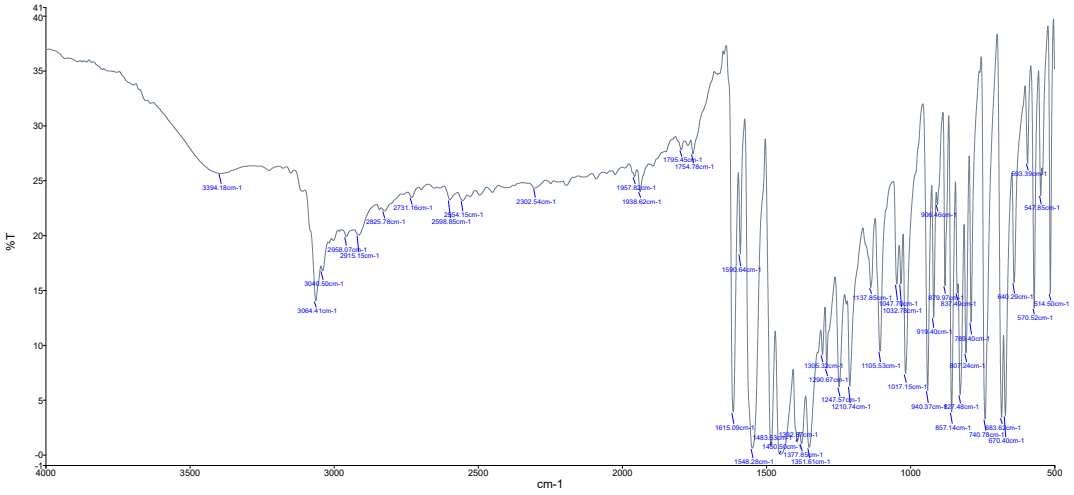


Figure S16. IR (KBr) of **DQ16**.

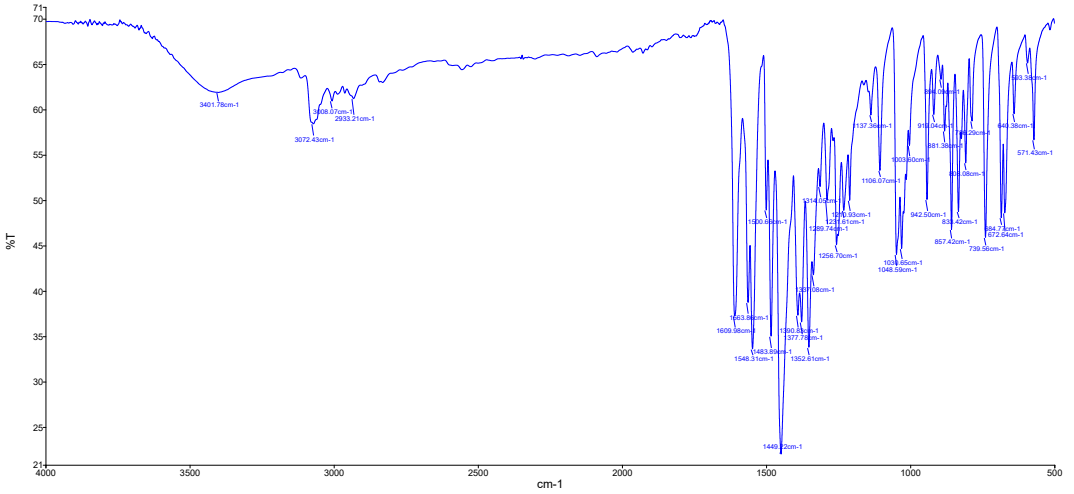


Figure S17. IR (KBr) of **DQ17**.

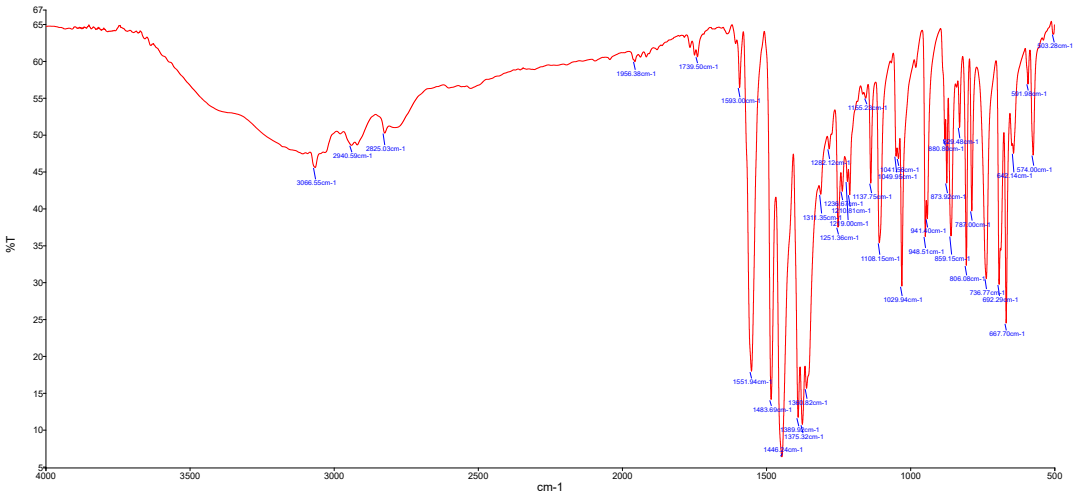


Figure S18. IR (KBr) of **DQ18**.

Figure S19. IR (KBr) of **DQ19**.

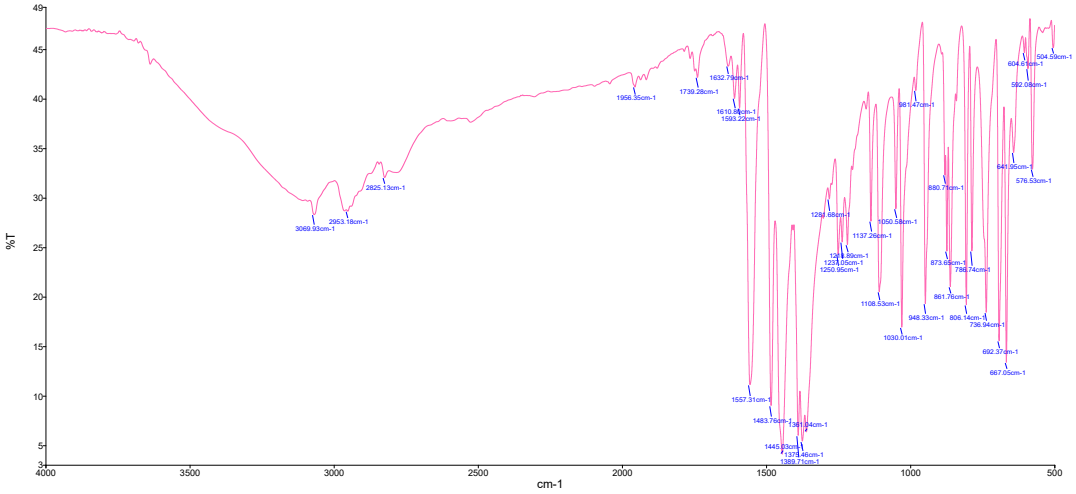


Figure S20. IR (KBr) of **DQ20**.

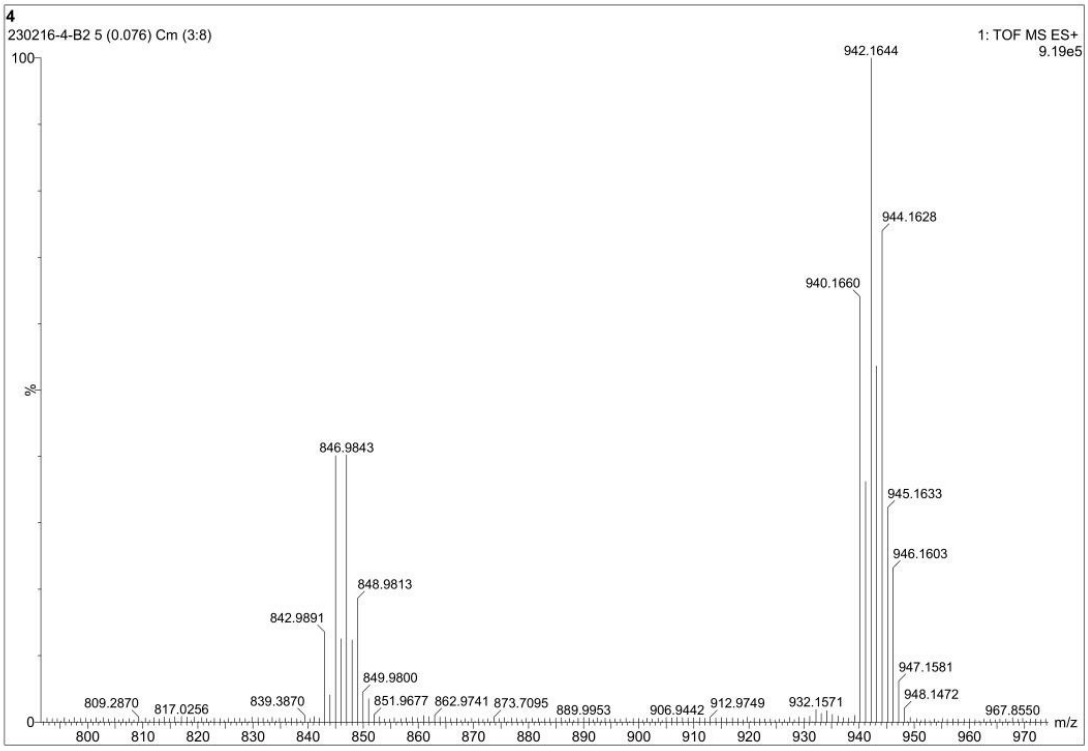


Figure S21. ESI-MS of **DQ6**.

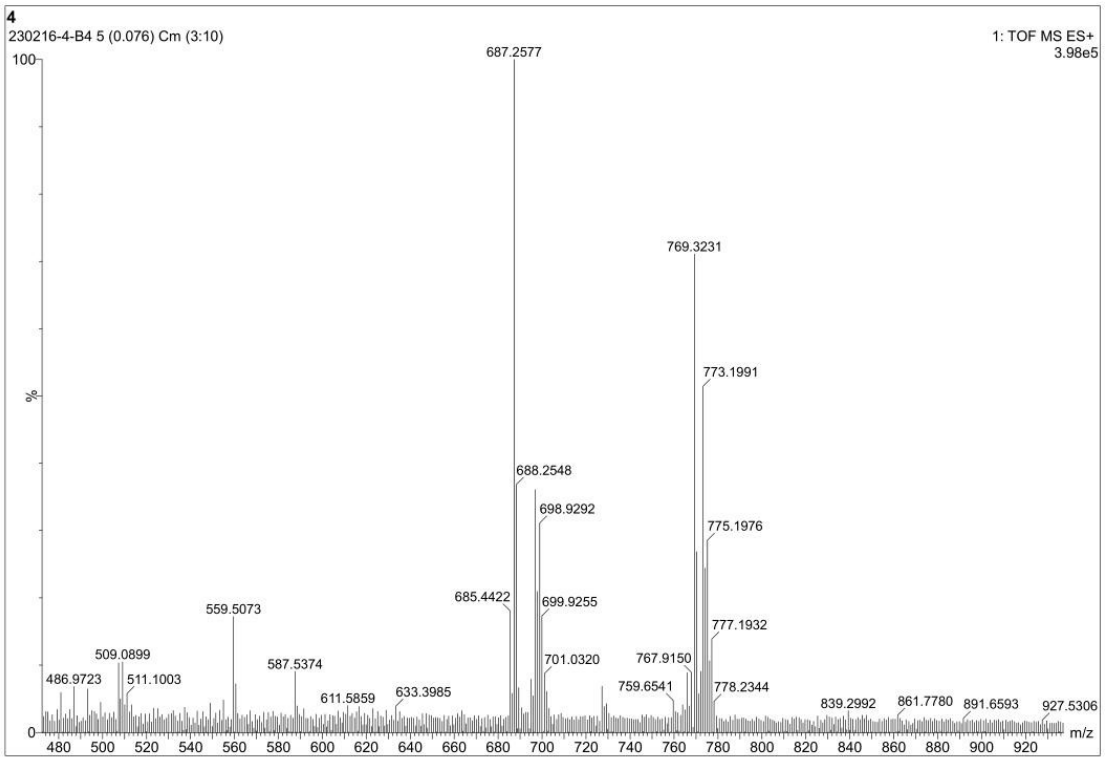


Figure S22. ESI-MS of **DQ11**.

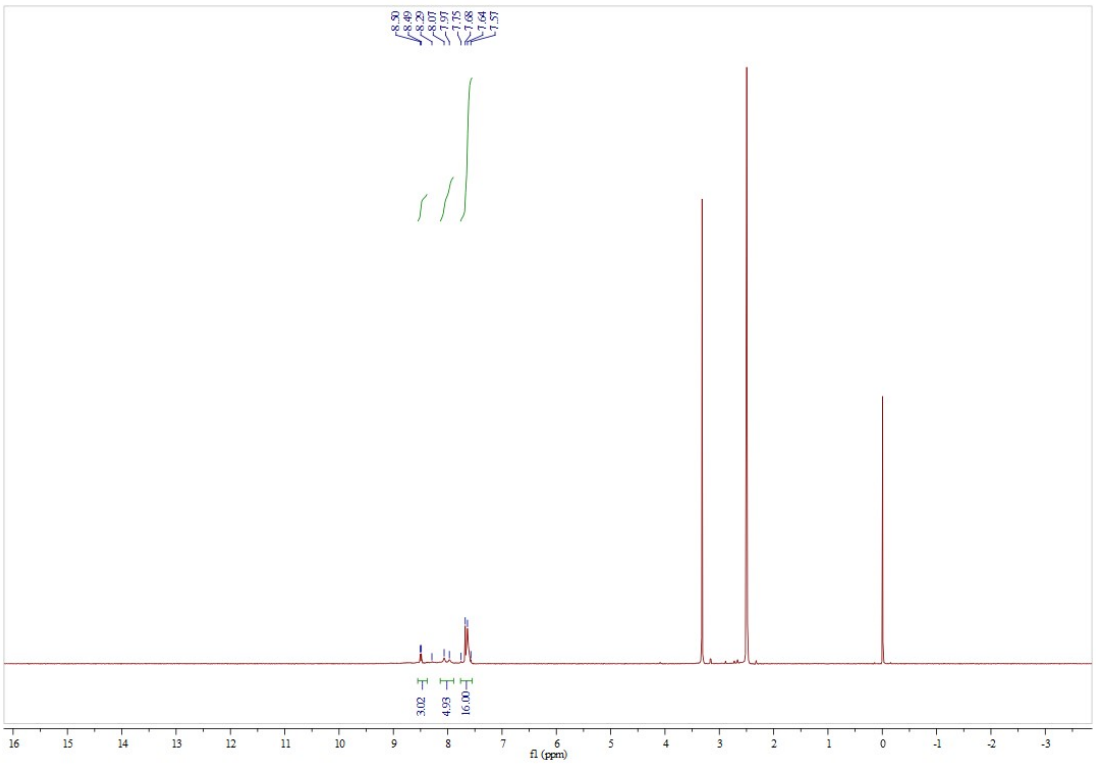


Figure S23. ^{1}H NMR of **DQ6**.

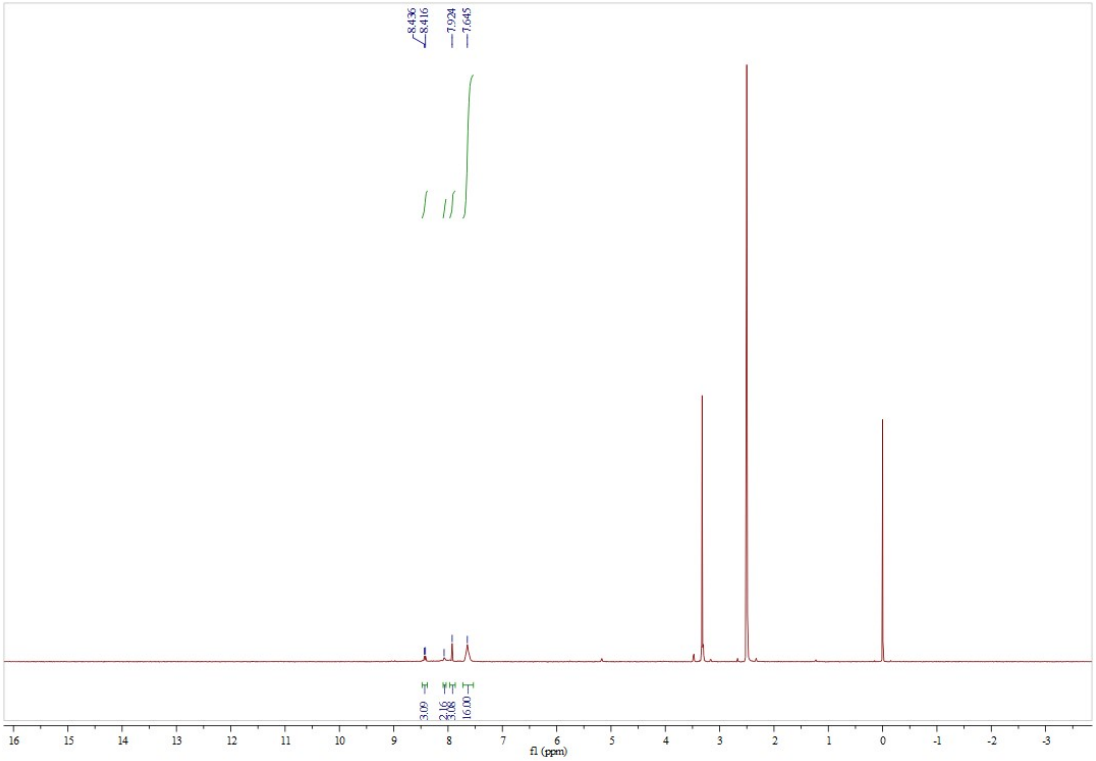


Figure S24. ^{1}H NMR of **DQ11**.

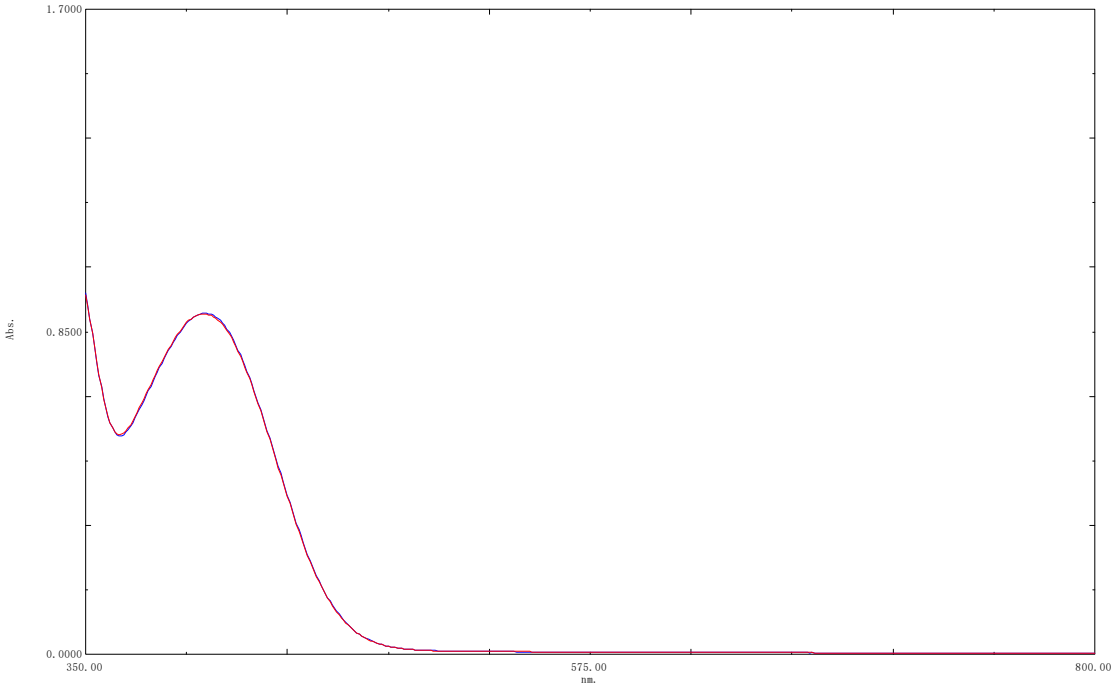


Figure S25. UV-Vis absorption spectra of **DQ6** (3.0×10^{-5} M) in Tris-HCl solution (10mM, pH7.35) in the time course 0 h (blue) and 48 h (red), respectively.

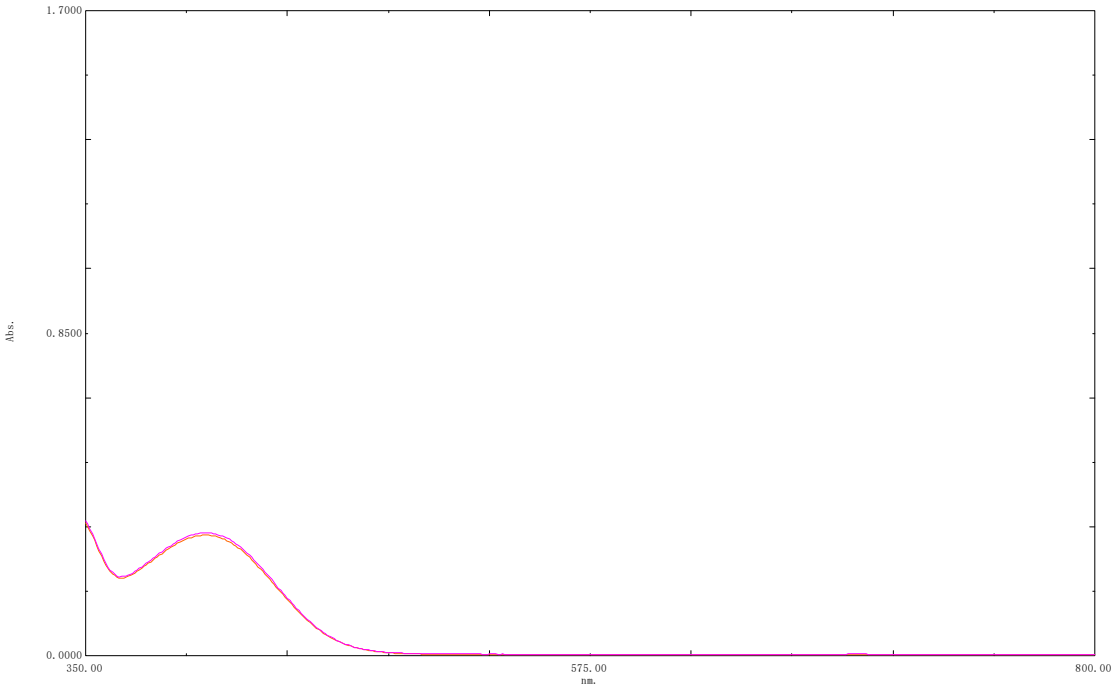


Figure S26. UV-Vis absorption spectra of **DQ11** (3.0×10^{-5} M) in Tris-HCl solution (10mM, pH7.35) in the time course 0 h (fuchsia) and 48 h (orange-yellow), respectively.

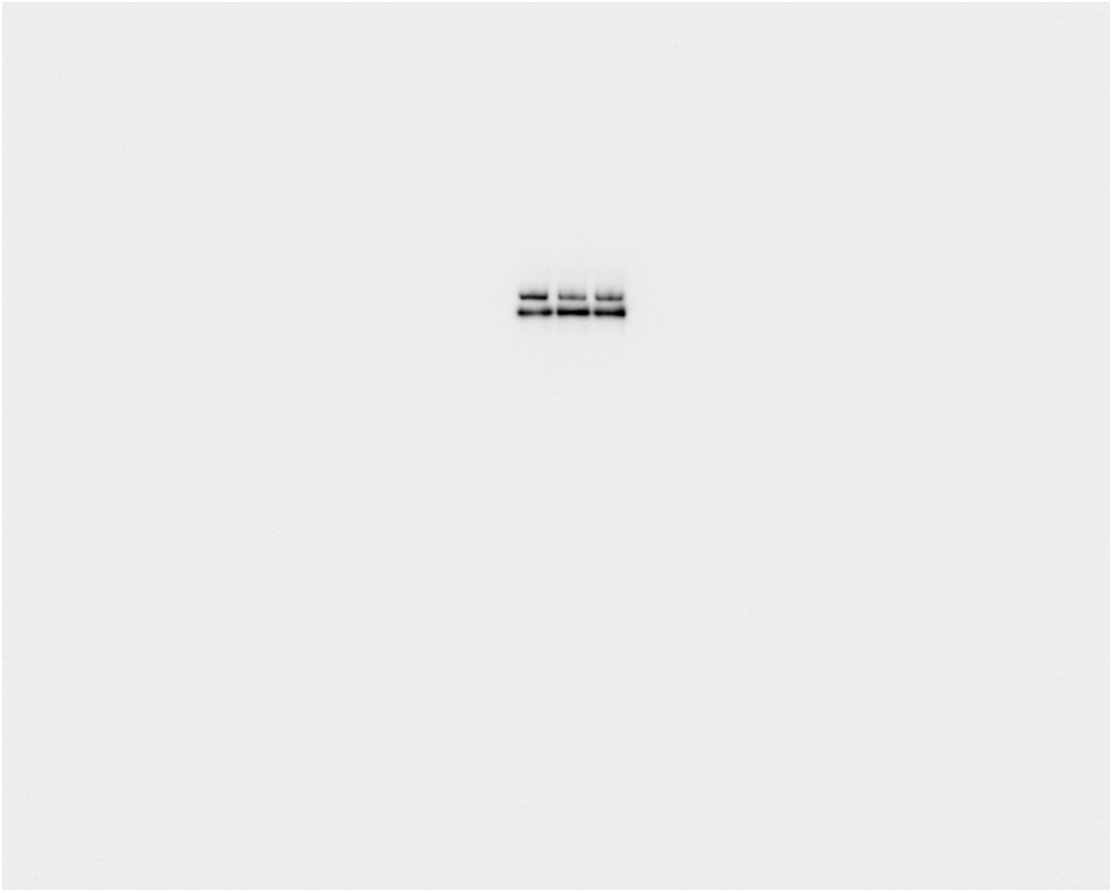
Original picture of Western blot analysis：

Beclin-1

FNUDC1

GAPDH

LC3



P62

Parkin

PINK1

Table S62. The tumor volume (cm^3) in **DQ6** treated and non-treated mice from the date of surgery to the study end point in the SK-OV-3 xenograft model (mean±SD, n=6).

	1d	3d	5d	7d	9d	11d	13d	15d	17d	19d	21d
non-treated group	0.096±0.009	0.141±0.014	0.197±0.015	0.335±0.042	0.473±0.062	0.594±0.060	0.717±0.074	0.820±0.083	0.936±0.093	1.050±0.097	1.207±0.107
DQ6 treated group	0.097±0.004	0.120±0.009	0.149±0.017	0.212±0.032	0.288±0.030	0.338±0.030	0.400±0.030	0.430±0.028	0.466±0.035	0.516±0.047	0.577±0.062

* $p < 0.01$, *p vs* vehicle control.

Table S63. Average body weight (g) in **DQ6** treated and non-treated mice from the date of surgery to the study end point in the SK-OV-3 xenograft model (mean±SD, n=6).

	1d	3d	5d	7d	9d	11d	13d	15d	17d	19d	21d
non-treated group	18.8±0.4	19.1±0.4	19.3±0.5	19.5±0.5	19.8±0.6	20.1±0.6	20.3±0.6	20.6±0.7	20.8±0.7	21.1±0.8	21.4±0.8
DQ6 treated group	18.7±0.6	19±0.6	19.3±0.6	19.6±0.7	19.9±0.7	20.1±0.7	20.4±0.8	20.6±0.8	20.9±0.9	21.1±0.9	21.3±0.9

* $p < 0.01$, *p vs* vehicle control.

Table S64. In vivo anti-cancer activity of **DQ6** (2.0 mg/kg) toward SK-OV-3 tumor xenograft (mean±SD, n=6).

	mg/kg	average tumor weight (mean ± SD, g)	inhibition of tumor growth (%)
non-treated group	-	1.27±0.05	-
DQ6 treated group	2.0	0.64±0.03	49.8

* p <0.01, p *vs* vehicle control.

Table S65. Depletion of the mitochondrial respiration complexes I in SK-OV-3CR cells after incubation with **DQ6** (2.25μM) and **DQ11** (10.39μM), at 37 °C, for 48.0 h (n = 3, p < 0.05).

Group	ΔA	Cpr	complexes I (U/mg prot)	Mean	SD
control	0.045	0.992	72.95803703	72.49	1.45
	0.047	1.066	70.86528676		
	0.042	0.917	73.63827097		
DQ6	0.019	1.040	29.39078196	29.98	1.37
	0.018	0.998	29.00126009		
	0.021	1.071	31.54052605		
DQ11	0.02	0.911	35.30538499	35.64	1.29
	0.023	0.998	37.05716567		
	0.023	1.071	34.54438567		

ΔA: Measured value for each sample; Cpr: The protein concentration of each sample; All assays and calculation process were performed according to the manufacturer's instructions (mitochondrial respiratory chain complexes I and IV, Solarbio Life Sciences, Beijing, China).

Table S66. Depletion of the mitochondrial respiration complexes IV in SK-OV-3CR cells after incubation with **DQ6** (2.25μM) and **DQ11** (10.39μM), at 37 °C, for 48.0 h (n = 3, $p < 0.05$).

Group	ΔA	Cpr	complexes IV (U/mg prot)	Mean	SD
	0.08	1.025	85.77642986		
control	0.067	1.010	72.86999288	78.77	6.52
	0.067	0.948	77.65188905		
	0.03	1.013	32.56151578		
DQ6	0.035	1.081	35.58300438	33.70	1.64
	0.03	1.000	32.96670992		
	0.039	1.073	39.95630452		
DQ11	0.039	1.104	38.83005931	39.84	0.96
	0.034	0.917	40.74223574		

Table S67. Depletion of ATP level in SK-OV-3CR cells after incubation with **DQ6** (2.25μM) and **DQ11** (10.39μM), at 37 °C, for 48.0 h (n = 3, $p < 0.05$).

group	control	**DQ6**	**DQ11**
OD values	60937	34371	37371
	60302	34613	36613
	59740	34220	37220
after correction for the OD values	60921	34355	37355
	60286	34597	36597
	59724	34204	37204
ATP (μM)	4.91748	2.7922	3.0322
	4.86668	2.81156	2.97156
	4.82172	2.78012	3.02012
mean of ATP (μM)	4.87	2.79	3.01
SD	0.05	0.02	0.03

Experimental section

The other methods

The materials, instrumentation, cytotoxicity assay, and the other anticancer mechanism of the zinc(II) coordination complexes **DQ1**–**DQ20** in SK-OV-3CR cancer cells were similar to those illustrated in previous work [1-5].

In vivo assays

When SK-OV-3 tumors reach a volume of 0.096 cm^3 on all the mice, the mice were randomized into vehicle control and treatment groups (n=6/group), received the following treatments: (a) vehicle control, 5.0% v/v DMSO/ saline vehicle, (b) **DQ6** at dose 2.0 mg/kg every two day (5.0% v/v DMSO/saline). The tumor volumes were determined every two days by measuring length (*l*) and width (*w*) and calculating volume, tumor volume and inhibition of tumor growth were calculated using formulas 1−3 [3-7]:

Tumor volume: $V = (w^2 \times l)/2$ (1)

The tumor relative increment rate: $T/C\ (\%) = T_{RTV}/C_{RTV} \times 100\%$ (2)

inhibition of tumor growth: $IR(\%) = (W_c - W_t)/W_c \times 100\%$ (3)

Where w and l mean the shorter and the longer diameter of the tumor respectively; T_{RTV} and C_{RTV} was the RTV of treated group and control group respectively. (RTV: relative tumor volume, $RTV = V_t / V_0$); W_t and W_c mean the average tumor weight of complex-treated and vehicle control group respectively.

In addition, the SK-OV-3 xenograft mouse models were purchased from Shanghai Lingchang Biotechnology Company Limited (Shanghai, China, approval No. SCXK (Hu) 2018-0003. The animal procedures were approved by Nanjing Ramda Pharmaceutical Co., Ltd. (Jiangsu, China, approval No. SYXK(Su) 2022-0038). And all of the experimental procedures were carried out in accordance with the NIH Guidelines for the Care and Use of Laboratory Animals. The animal experiments were approved by Nanjing Ramda Pharmaceutical Co., Ltd. (Jiangsu, China).

Statistical Analysis

The experiments have been repeated from three to five times, and the results obtained are presented as means ± standard deviation (SD). Significant changes were assessed by using Student's t test for unpaired data, and p values of <0.05 or <0.01 were considered significant.

Notes and references

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