Electronic Supporting Information Materials

Complexes of Lanthanides(III) with mixed 2,2'-bipyridyl and 5,7-dibromo-8-quinolinoline chelating ligands as a new class of promising anti-cancer agents

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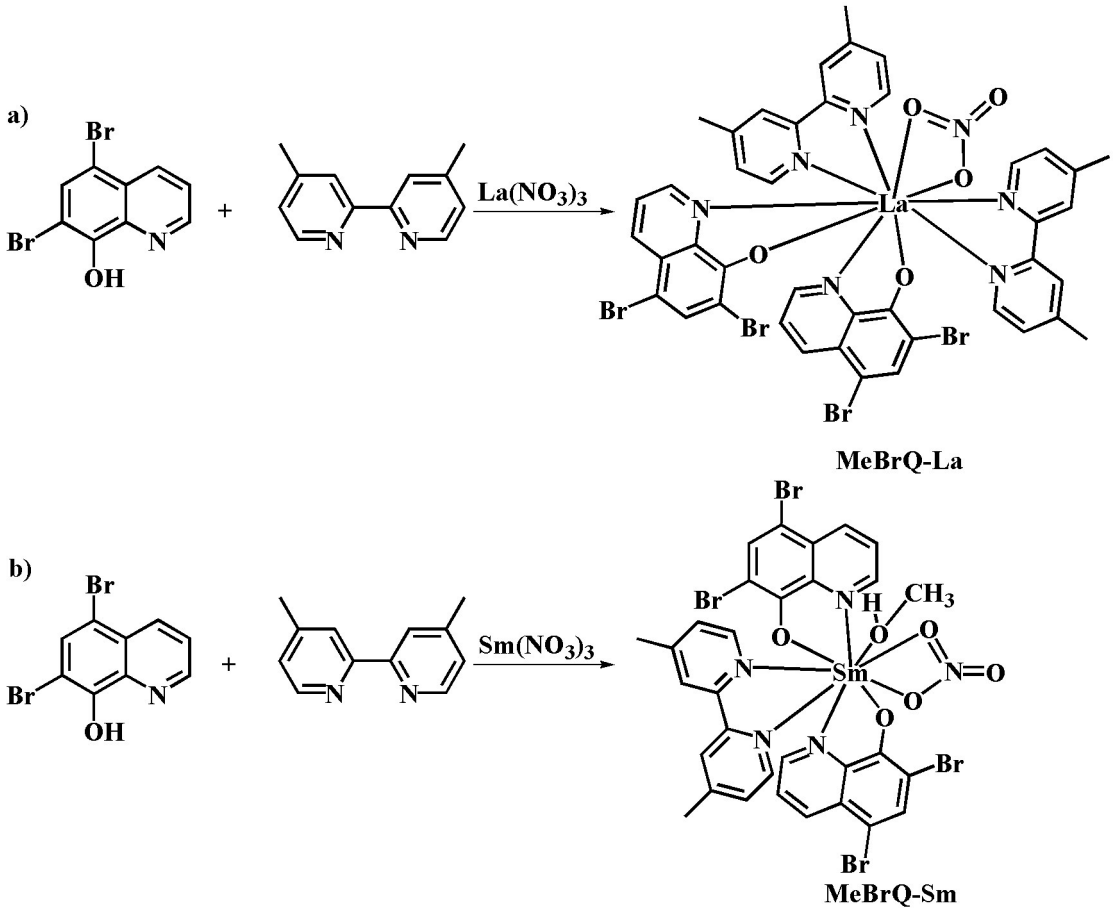

Scheme S1. Synthetic route for **MeBrQ-La** (a) and **MeBrQ-Sm** (b) complexes. Reagents are the following: $La(NO_3)_3 \cdot 6H_2O$ or $Sm(NO_3)_3 \cdot 6H_2O$, CH_3OH/CH_2Cl_2 (10:1), 65 °C, 12 h.

Table S1. Crystal data and structure refinement details for **MeBrQ-La**.

Empirical formula	$C_{42}H_{32}Br_4LaN_7O_5$
Formula weight	1173.29
Temperature/K	293(2)
Crystal system	monoclinic
Space group	C2/c
a/Å	26.0817(16)
b/Å	20.6620(12)
c/Å	19.7728(11)
α/°	90
β/°	125.502(2)
γ/°	90
Volume/Å^3	8674.6(9)
Z	8
ρ_{calc}mg/mm^3	1.797
m/mm^{-1}	4.722
F(000)	4560.0
Crystal size/mm^3	0.346 × 0.297 × 0.149
2Θ range for data collection	5.774 to 55.112°
Index ranges	$-33 \le h \le 33$, $-26 \le k \le 26$, $-25 \le l \le 25$
Reflections collected	68847
Independent reflections	10005[R(int) = 0.0505]
Data/restraints/parameters	10005/0/536
Goodness-of-fit on F^2	1.023
Final R indexes [I>=2σ (I)]	R_1 = 0.0405, wR_2 = 0.0784
Final R indexes [all data]	R_1 = 0.0703, wR_2 = 0.0889
Largest diff. peak/hole / e Å^{-3}	1.81/-1.68

[a] $R_1 = \Sigma \, ||F_o| - |F_c|| / \Sigma |F_o|$; [b] $wR_2 = [\Sigma w(F_o^2 - F_c^2)^2 / \Sigma w(F_o^2)^2]^{½}$.

Table S2. Selected bond lengths (Å) for **MeBrQ-La**.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
La1	O1	2.642(4)	C5	C6	1.397(7)
La1	O2	2.747(3)	C5	C9	1.421(6)
La1	O4	2.401(2)	C6	C7	1.359(7)
La1	O5	2.400(3)	C7	C8	1.388(7)
La1	N1	2.781(3)	C10	C11	1.377(6)
La1	N2	2.779(3)	C11	C12	1.365(7)
La1	N3	2.790(3)	C12	C13	1.514(7)
La1	N4	2.744(3)	C12	C14	1.377(7)
La1	N6	2.808(3)	C14	C15	1.383(6)
La1	N7	2.779(3)	C15	C16	1.486(6)
Br1	C25	1.901(4)	C16	C17	1.384(6)

Br2	C23	1.898(4)	C17	C18	1.381(6)
Br3	C4	1.891(5)	C18	C19	1.513(7)
Br4	C2	1.883(4)	C18	C20	1.362(7)
O1	N5	1.262(6)	C20	C21	1.371(7)
O2	N5	1.256(5)	C22	C23	1.388(5)
O3	N5	1.221(5)	C22	C30	1.433(5)
O4	C22	1.293(5)	C23	C24	1.402(6)
O5	C1	1.295(5)	C24	C25	1.356(6)
N1	C10	1.323(5)	C25	C26	1.412(6)
N1	C15	1.337(5)	C26	C27	1.408(6)
N2	C16	1.341(5)	C26	C30	1.422(5)
N2	C21	1.345(5)	C27	C28	1.351(6)
N3	C8	1.330(5)	C28	C29	1.400(6)
N3	C9	1.361(5)	C31	C32	1.376(6)
N4	C29	1.318(5)	C32	C33	1.383(6)
N4	C30	1.361(5)	C33	C34	1.513(7)
N6	C37	1.342(5)	C33	C35	1.380(7)
N6	C42	1.336(6)	C35	C36	1.380(6)
N7	C31	1.331(5)	C36	C37	1.480(6)
N7	C36	1.351(5)	C37	C38	1.393(6)
C1	C2	1.398(6)	C38	C39	1.376(7)
C1	C9	1.444(6)	C39	C40	1.515(7)
C2	C3	1.387(7)	C39	C41	1.364(7)
C3	C4	1.362(7)	C41	C42	1.383(6)
C4	C5	1.409(6)			

Table S3. Selected bond angles (°) for **MeBrQ-La**.

Atom	**Atom**	**Atom**	**Angle/°**	**Atom**	**Atom**	**Atom**	**Angle/°**
O1	La1	O2	46.75(12)	C2	C1	C9	114.9(4)
O1	La1	N1	90.79(12)	C1	C2	Br4	118.1(4)
O1	La1	N2	72.32(12)	C3	C2	Br4	118.4(3)
O1	La1	N3	147.05(11)	C3	C2	C1	123.3(4)
O1	La1	N4	137.09(12)	C4	C3	C2	120.6(4)
O1	La1	N6	65.17(13)	C3	C4	Br3	118.2(4)
O1	La1	N7	77.99(11)	C3	C4	C5	121.0(5)
O2	La1	N1	64.35(10)	C5	C4	Br3	120.6(4)
O2	La1	N2	90.62(11)	C4	C5	C9	117.8(4)
O2	La1	N3	136.24(10)	C6	C5	C4	125.3(5)
O2	La1	N6	98.48(11)	C6	C5	C9	116.8(4)
O2	La1	N7	67.98(10)	C7	C6	C5	120.1(5)
O4	La1	O1	131.32(11)	C6	C7	C8	119.5(5)
O4	La1	O2	85.16(11)	N3	C8	C7	123.4(4)

O4	La1	N1	70.04(9)	N3	C9	C1	115.0(4)
O4	La1	N2	123.59(10)	N3	C9	C5	122.7(4)
O4	La1	N3	70.62(9)	C5	C9	C1	122.2(4)
O4	La1	N4	62.29(9)	N1	C10	C11	123.6(4)
O4	La1	N6	128.20(10)	C12	C11	C10	119.5(4)
O4	La1	N7	76.60(9)	C11	C12	C13	121.5(5)
O5	La1	O1	104.45(12)	C11	C12	C14	117.2(4)
O5	La1	O2	150.25(11)	C14	C12	C13	121.3(5)
O5	La1	O4	124.18(9)	C12	C14	C15	120.5(4)
O5	La1	N1	117.50(9)	N1	C15	C14	121.5(4)
O5	La1	N2	69.86(10)	N1	C15	C16	116.7(3)
O5	La1	N3	61.52(9)	C14	C15	C16	121.8(4)
O5	La1	N4	76.42(9)	N2	C16	C15	116.7(3)
O5	La1	N6	68.46(10)	N2	C16	C17	121.7(4)
O5	La1	N7	119.51(9)	C17	C16	C15	121.7(4)
N1	La1	N3	73.15(10)	C18	C17	C16	120.6(4)
N1	La1	N6	155.68(11)	C17	C18	C19	120.2(5)
N2	La1	N1	57.91(10)	C20	C18	C17	117.6(4)
N2	La1	N3	74.79(10)	C20	C18	C19	122.1(5)
N2	La1	N6	108.08(10)	C18	C20	C21	119.4(4)
N2	La1	N7	150.30(10)	N2	C21	C20	124.0(4)
N3	La1	N6	125.20(10)	O4	C22	C23	124.4(4)
N4	La1	O2	127.97(11)	O4	C22	C30	119.9(3)
N4	La1	N1	127.66(10)	C23	C22	C30	115.7(4)
N4	La1	N2	140.79(10)	C22	C23	Br2	118.9(3)
N4	La1	N3	71.86(10)	C22	C23	C24	122.9(4)
N4	La1	N6	76.21(10)	C24	C23	Br2	118.1(3)
N4	La1	N7	65.75(9)	C25	C24	C23	119.8(4)
N7	La1	N1	122.93(10)	C24	C25	Br1	118.3(3)
N7	La1	N3	134.91(10)	C24	C25	C26	122.1(4)
N7	La1	N6	58.10(10)	C26	C25	Br1	119.6(3)
N5	O1	La1	100.8(3)	C25	C26	C30	116.7(4)
N5	O2	La1	95.8(3)	C27	C26	C25	126.2(4)
C22	O4	La1	126.1(2)	C27	C26	C30	117.1(4)
C1	O5	La1	128.5(2)	C28	C27	C26	120.0(4)
C10	N1	La1	118.5(3)	C27	C28	C29	119.4(4)
C10	N1	C15	117.6(3)	N4	C29	C28	122.8(4)
C15	N1	La1	123.1(2)	N4	C30	C22	115.8(3)
C16	N2	La1	123.6(3)	N4	C30	C26	121.5(4)
C16	N2	C21	116.8(4)	C26	C30	C22	122.6(3)
C21	N2	La1	119.3(3)	N7	C31	C32	124.3(4)
C8	N3	La1	128.1(3)	C31	C32	C33	119.5(4)
C8	N3	C9	117.4(4)	C32	C33	C34	121.8(5)
C9	N3	La1	114.5(3)	C35	C33	C32	116.0(4)
C29	N4	La1	127.1(3)	C35	C33	C34	122.2(5)

C29	N4	C30	119.0(3)	C36	C35	C33	122.0(4)
C30	N4	La1	113.8(2)	N7	C36	C35	121.1(4)
O2	N5	O1	116.4(4)	N7	C36	C37	116.5(4)
O3	N5	O1	121.8(5)	C35	C36	C37	122.4(4)
O3	N5	O2	121.7(5)	N6	C37	C36	117.2(3)
C37	N6	La1	122.4(3)	N6	C37	C38	121.2(4)
C42	N6	La1	118.3(3)	C38	C37	C36	121.7(4)
C42	N6	C37	117.5(4)	C39	C38	C37	120.9(5)
C31	N7	La1	118.8(3)	C38	C39	C40	120.5(5)
C31	N7	C36	116.9(3)	C41	C39	C38	117.4(4)
C36	N7	La1	124.0(3)	C41	C39	C40	122.1(5)
O5	C1	C2	124.9(4)	C39	C41	C42	119.6(5)
O5	C1	C9	120.1(3)	N6	C42	C41	123.4(5)

Table S4. Crystal data and structure refinement details for **MeBrQ-Sm**.

Empirical formula	$C_{124}H_{96}Br_{16}N_{20}O_{24}Sm_4$
Formula weight	4130.16
Temperature/K	293(2)
Crystal system	triclinic
Space group	P-1
a/Å	9.7421(4)
b/Å	16.9016(6)
c/Å	25.0742(9)
α/°	72.9580(10)
β/°	85.7190(10)
γ/°	74.7950(10)
Volume/Å^3	3809.2(2)
Z	1
ρ_{calc}g/cm^3	1.800
μ/mm^{-1}	5.782
F(000)	1980.0
Crystal size/mm^3	0.24 × 0.21 × 0.12
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	5.878 to 55.068
Index ranges	$-12 \le h \le 12$, $-21 \le k \le 21$, $-32 \le l \le 32$
Reflections collected	81304
Independent reflections	17513 [R_{int} = 0.0704, R_{sigma} = 0.0749]
Data/restraints/parameters	17513/6/859
Goodness-of-fit on F^2	1.022
Final R indexes [I>=2σ (I)]	R_1 = 0.0479, wR_2 = 0.0897

Final R indexes [all data]	$R_1 = 0.1039$, $wR_2 = 0.1048$
Largest diff. peak/hole / e Å^{-3}	1.18/-0.85

Table S5. Selected bond lengths (Å) for **MeBrQ-Sm**.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
Sm1	O2	2.296(3)	C45	C49	1.428(9)
Sm1	O1	2.285(3)	N1	C6	1.364(7)
Sm1	O3	2.547(4)	N1	C7	1.319(7)
Sm1	N3	2.653(4)	N7	C46	1.359(7)
Sm1	N2	2.658(4)	N7	C47	1.329(7)
Sm1	O4	2.623(4)	C44	C43	1.352(9)
Sm1	O6	2.495(4)	C44	Br8	1.898(6)
Sm1	N4	2.598(4)	N10	O11	1.213(6)
Sm1	N1	2.586(4)	C23	C22	1.381(7)
Sm2	O7	2.291(3)	C8	C7	1.405(8)
Sm2	O8	2.298(3)	C8	C9	1.353(9)
Sm2	O10	2.571(3)	C39	C38	1.401(8)
Sm2	N6	2.644(4)	C39	C40	1.345(8)
Sm2	N9	2.591(4)	C55	C54	1.490(7)
Sm2	O9	2.528(4)	C55	C56	1.382(7)
Sm2	O12	2.515(4)	C21	C22	1.377(7)
Sm2	N8	2.661(4)	C21	C30	1.520(7)
Sm2	N7	2.583(5)	C21	C20	1.375(8)
Sm2	N10	2.967(5)	C15	C10	1.429(8)
Br5	C33	1.905(5)	C15	C14	1.421(7)
Br1	C2	1.888(6)	C6	C5	1.427(7)
O2	C10	1.300(6)	C6	C1	1.432(7)
O7	C32	1.306(6)	C5	C4	1.378(8)
O1	C1	1.299(6)	C5	C9	1.402(8)
O8	C41	1.283(6)	C37	C36	1.416(7)
O3	N5	1.254(6)	C37	C32	1.440(7)
O5	N5	1.223(6)	C46	C41	1.432(7)
N3	C19	1.341(7)	C54	C53	1.385(7)
N3	C23	1.346(6)	C58	C57	1.378(8)
O10	N10	1.269(6)	C58	C59	1.371(7)
N2	C15	1.360(7)	C25	C26	1.377(8)
N2	C16	1.309(7)	C27	C26	1.365(7)
O4	N5	1.264(5)	C27	C28	1.374(7)
N6	C37	1.349(6)	C4	C3	1.369(9)
N6	C38	1.325(7)	C4	Br2	1.904(6)

O6	C31	1.416(7)	C36	C40	1.406(8)
N4	C24	1.346(6)	C49	C48	1.331(10)
N4	C28	1.337(6)	C10	C11	1.382(8)
N9	C55	1.336(6)	C18	C14	1.389(9)
N9	C59	1.332(7)	C18	C17	1.345(9)
O9	N10	1.254(6)	C42	C41	1.383(8)
C35	C34	1.360(8)	C42	C43	1.413(8)
C35	C36	1.396(8)	C42	Br7	1.887(6)
C35	Br6	1.895(5)	C26	C29	1.518(7)
C33	C34	1.396(7)	C16	C17	1.407(8)
C33	C32	1.374(7)	C2	C3	1.386(8)
C19	C20	1.370(7)	C2	C1	1.391(7)
O12	C62	1.393(8)	C53	C52	1.385(8)
N8	C54	1.345(6)	C47	C48	1.384(9)
N8	C50	1.349(7)	C50	C51	1.375(8)
C24	C23	1.480(7)	C57	C61	1.526(7)
C24	C25	1.383(7)	C57	C56	1.353(8)
C13	C14	1.399(9)	C51	C52	1.368(9)
C13	C12	1.354(9)	C52	C60	1.520(8)
C13	Br4	1.907(6)	C12	C11	1.413(8)
C45	C44	1.403(9)	C11	Br3	1.892(6)
C45	C46	1.428(8)			

Table S6. Selected bond angles (°) for **MeBrQ-Sm**.

Atom	**Atom**	**Atom**	**Angle/°**	**Atom**	**Atom**	**Atom**	**Angle/°**
O2	Sm1	O3	102.55(13)	C50	N8	Sm2	121.3(3)
O2	Sm1	N3	74.00(13)	N4	C24	C23	116.8(4)
O2	Sm1	N2	64.28(13)	N4	C24	C25	121.4(5)
O2	Sm1	O4	139.19(12)	C25	C24	C23	121.8(4)
O2	Sm1	O6	77.96(13)	C14	C13	Br4	119.7(6)
O2	Sm1	N4	135.82(12)	C12	C13	C14	122.3(6)
O2	Sm1	N1	87.30(14)	C12	C13	Br4	118.0(5)
O1	Sm1	O2	133.02(12)	C44	C45	C46	117.9(6)
O1	Sm1	O3	76.94(13)	C44	C45	C49	127.0(6)
O1	Sm1	N3	129.40(12)	C49	C45	C46	115.1(6)
O1	Sm1	N2	73.05(13)	C6	N1	Sm1	114.0(3)
O1	Sm1	O4	75.29(12)	C7	N1	Sm1	128.0(4)
O1	Sm1	O6	141.82(13)	C7	N1	C6	118.0(5)
O1	Sm1	N4	78.48(12)	C46	N7	Sm2	113.8(3)

O1	Sm1	N1	66.01(13)	C47	N7	Sm2	126.9(4)
O3	Sm1	N3	147.68(13)	C47	N7	C46	119.2(5)
O3	Sm1	N2	67.29(13)	C45	C44	Br8	119.1(5)
O3	Sm1	O4	48.99(11)	C43	C44	C45	121.7(6)
O3	Sm1	N4	116.27(13)	C43	C44	Br8	119.1(6)
O3	Sm1	N1	136.16(13)	O10	N10	Sm2	59.7(3)
N3	Sm1	N2	132.33(14)	O9	N10	Sm2	57.6(3)
O4	Sm1	N3	113.25(12)	O9	N10	O10	117.3(5)
O4	Sm1	N2	113.25(12)	O11	N10	Sm2	179.1(5)
O6	Sm1	O3	74.09(14)	O11	N10	O10	120.2(6)
O6	Sm1	N3	73.78(14)	O11	N10	O9	122.4(5)
O6	Sm1	N2	116.36(14)	N3	C23	C24	116.7(4)
O6	Sm1	O4	67.01(11)	N3	C23	C22	122.3(5)
O6	Sm1	N4	92.57(13)	C22	C23	C24	121.1(4)
O6	Sm1	N1	149.14(14)	C9	C8	C7	118.9(6)
N4	Sm1	N3	61.98(13)	C40	C39	C38	119.2(6)
N4	Sm1	N2	149.65(13)	N9	C55	C54	116.4(4)
N4	Sm1	O4	68.16(12)	N9	C55	C56	121.9(5)
N1	Sm1	N3	76.16(13)	C56	C55	C54	121.7(5)
N1	Sm1	N2	79.76(13)	C22	C21	C30	121.5(5)
N1	Sm1	O4	133.41(12)	C20	C21	C22	116.6(5)
N1	Sm1	N4	79.26(13)	C20	C21	C30	121.9(5)
O7	Sm2	O8	134.90(12)	N2	C15	C10	115.2(4)
O7	Sm2	O10	135.28(13)	N2	C15	C14	122.3(5)
O7	Sm2	N6	64.68(12)	C14	C15	C10	122.5(5)
O7	Sm2	N9	137.15(13)	N1	C6	C5	122.8(5)
O7	Sm2	O9	91.70(14)	N1	C6	C1	115.1(5)
O7	Sm2	O12	80.32(13)	C5	C6	C1	122.2(5)
O7	Sm2	N8	75.01(13)	C4	C5	C6	117.4(6)
O7	Sm2	N7	87.58(14)	C4	C5	C9	126.5(6)
O7	Sm2	N10	113.74(15)	C9	C5	C6	116.0(6)
O8	Sm2	O10	73.54(12)	N6	C37	C36	123.1(5)
O8	Sm2	N6	73.88(13)	N6	C37	C32	115.1(4)
O8	Sm2	N9	76.96(13)	C36	C37	C32	121.7(5)
O8	Sm2	O9	87.46(15)	C21	C22	C23	120.6(5)
O8	Sm2	O12	140.56(13)	C45	C46	C41	121.8(6)
O8	Sm2	N8	127.58(13)	N7	C46	C45	122.5(5)
O8	Sm2	N7	65.90(14)	N7	C46	C41	115.6(5)
O8	Sm2	N10	79.98(14)	N6	C38	C39	122.7(6)
O10	Sm2	N6	108.24(12)	N8	C54	C55	116.6(4)
O10	Sm2	N9	72.21(13)	N8	C54	C53	121.8(5)
O10	Sm2	N8	118.37(13)	C53	C54	C55	121.5(5)
O10	Sm2	N7	135.80(14)	C35	C34	C33	119.8(5)
O10	Sm2	N10	25.22(13)	C59	C58	C57	119.6(6)
N6	Sm2	N8	132.28(13)	C26	C25	C24	120.7(5)

N6	Sm2	N10	87.32(14)	C26	C27	C28	120.4(5)
N9	Sm2	N6	149.15(14)	C5	C4	Br2	120.6(5)
N9	Sm2	N8	62.14(14)	C3	C4	C5	121.7(6)
N9	Sm2	N10	97.41(15)	C3	C4	Br2	117.8(5)
O9	Sm2	O10	49.99(13)	C35	C36	C37	118.3(5)
O9	Sm2	N6	66.56(13)	C35	C36	C40	125.6(5)
O9	Sm2	N9	122.17(14)	C40	C36	C37	116.1(5)
O9	Sm2	N8	141.37(15)	C48	C49	C45	120.4(7)
O9	Sm2	N7	139.89(14)	O7	C32	C33	125.1(5)
O9	Sm2	N10	24.77(13)	O7	C32	C37	119.4(5)
O12	Sm2	O10	67.40(12)	C33	C32	C37	115.4(5)
O12	Sm2	N6	123.37(14)	O2	C10	C15	119.6(5)
O12	Sm2	N9	86.03(14)	O2	C10	C11	124.1(6)
O12	Sm2	O9	71.87(15)	C11	C10	C15	116.2(5)
O12	Sm2	N8	70.21(15)	C17	C18	C14	120.4(6)
O12	Sm2	N7	146.69(15)	C41	C42	C43	123.5(6)
O12	Sm2	N10	67.12(14)	C41	C42	Br7	118.7(5)
N8	Sm2	N10	133.69(13)	C43	C42	Br7	117.8(5)
N7	Sm2	N6	77.13(13)	C25	C26	C29	121.6(5)
N7	Sm2	N9	82.02(14)	C27	C26	C25	117.1(5)
N7	Sm2	N8	76.72(14)	C27	C26	C29	121.3(6)
N7	Sm2	N10	145.19(15)	O8	C41	C46	120.1(5)
C10	O2	Sm1	126.8(3)	O8	C41	C42	124.3(5)
C32	O7	Sm2	126.2(3)	C42	C41	C46	115.7(5)
C1	O1	Sm1	124.4(3)	N4	C28	C27	122.8(5)
C41	O8	Sm2	124.5(3)	C13	C14	C15	116.9(6)
N5	O3	Sm1	99.1(3)	C18	C14	C13	126.5(6)
C19	N3	Sm1	121.5(3)	C18	C14	C15	116.5(6)
C19	N3	C23	116.8(4)	N2	C16	C17	121.6(6)
C23	N3	Sm1	119.5(3)	C3	C2	Br1	119.9(5)
N10	O10	Sm2	95.1(3)	C3	C2	C1	122.3(6)
C15	N2	Sm1	113.6(3)	C1	C2	Br1	117.8(4)
C16	N2	Sm1	127.0(4)	C4	C3	C2	120.5(6)
C16	N2	C15	119.0(5)	C52	C53	C54	120.5(5)
N5	O4	Sm1	95.1(3)	N7	C47	C48	121.3(7)
C37	N6	Sm2	114.1(3)	C19	C20	C21	120.5(5)
C38	N6	Sm2	127.3(4)	N1	C7	C8	123.2(6)
C38	N6	C37	118.2(5)	N8	C50	C51	122.7(6)
O3	N5	O4	116.8(5)	C58	C57	C61	121.4(6)
O5	N5	O3	121.8(5)	C56	C57	C58	117.1(5)
O5	N5	O4	121.4(5)	C56	C57	C61	121.4(6)
C31	O6	Sm1	134.7(4)	O1	C1	C6	120.1(5)
C24	N4	Sm1	122.4(3)	O1	C1	C2	124.3(5)
C28	N4	Sm1	119.9(3)	C2	C1	C6	115.6(5)
C28	N4	C24	117.6(4)	C8	C9	C5	121.1(6)

C55	N9	Sm2	122.9(3)	C52	C51	C50	120.5(6)
C59	N9	Sm2	119.9(3)	C53	C52	C60	121.6(6)
C59	N9	C55	117.2(4)	C51	C52	C53	117.0(5)
N10	O9	Sm2	97.6(3)	C51	C52	C60	121.4(7)
C34	C35	C36	121.1(5)	C13	C12	C11	119.7(6)
C34	C35	Br6	118.2(5)	C10	C11	C12	122.3(6)
C36	C35	Br6	120.6(5)	C10	C11	Br3	118.5(5)
C34	C33	Br5	118.4(4)	C12	C11	Br3	119.2(5)
C32	C33	Br5	117.7(4)	C44	C43	C42	119.4(6)
C32	C33	C34	123.7(5)	C18	C17	C16	120.1(6)
N3	C19	C20	123.2(5)	C57	C56	C55	121.0(5)
C62	O12	Sm2	134.5(4)	N9	C59	C58	123.2(5)
C54	N8	Sm2	118.7(3)	C39	C40	C36	120.7(5)
C54	N8	C50	117.4(5)	C49	C48	C47	121.5(7)

Table S7. Crystal data and structure refinement details for **MeMBrQ-Ho**.

Empirical formula	$C_{32}H_{24}Br_4HoN_5O_5$
Formula weight	1043.13
Temperature/K	293(2)
Crystal system	orthorhombic
Space group	Pccn
a/Å	29.5503(11)
b/Å	29.9584(12)
c/Å	16.0497(6)
α/°	90
β/°	90
γ/°	90
Volume/Å^3	14208.5(9)
Z	16
ρ_{calc}g/cm^3	1.951
μ/mm^{-1}	6.773
F(000)	7968.0
Crystal size/mm^3	0.21 × 0.15 × 0.11
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	5.922 to 55.112
Index ranges	-38 ≤ h ≤ 38, -38 ≤ k ≤ 38, -20 ≤ l ≤ 20
Reflections collected	219785
Independent reflections	16361 [R_{int} = 0.1437, R_{sigma} = 0.0811]
Data/restraints/parameters	16361/0/855
Goodness-of-fit on F^2	1.037
Final R indexes [I>=2σ (I)]	R_1 = 0.0546, wR_2 = 0.0767
Final R indexes [all data]	R_1 = 0.1372, wR_2 = 0.0951

Largest diff. peak/hole / e Å^{-3}	0.79/-0.63

Table S8. Selected bond lengths (Å) for **MeMBrQ-Ho**.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
Ho2	O6	2.195(4)	C52	C51	1.357(9)
Ho2	O7	2.183(4)	N9	C59	1.353(7)
Ho2	N6	2.601(4)	N9	C63	1.339(7)
Ho2	O8	2.481(5)	C50	C51	1.396(8)
Ho2	N7	2.594(5)	O3	N5	1.247(8)
Ho2	O9	2.419(5)	C28	C29	1.368(9)
Ho2	N8	2.513(4)	C28	C31	1.509(9)
Ho2	N9	2.521(5)	C28	C27	1.371(9)
Ho2	N10	2.873(7)	C59	C60	1.387(7)
Ho1	O2	2.158(4)	C43	C44	1.495(9)
Ho1	N2	2.608(5)	C38	C33	1.440(8)
Ho1	O4	2.473(5)	C38	C37	1.407(8)
Ho1	O1	2.196(4)	C45	C44	1.417(8)
Ho1	N1	2.594(5)	C45	C46	1.352(9)
Ho1	N4	2.507(5)	C33	C34	1.377(8)
Ho1	O3	2.446(5)	C60	C61	1.378(8)
Ho1	N3	2.492(5)	C6	C1	1.431(8)
Ho1	N5	2.890(8)	C6	C5	1.422(8)
Br5	C50	1.891(6)	C47	C46	1.391(8)
Br6	C52	1.909(6)	C16	C15	1.422(9)
Br8	C34	1.895(7)	C16	C11	1.433(9)
Br4	C12	1.883(7)	C15	C14	1.415(11)
Br7	C36	1.899(7)	C15	C19	1.411(11)
Br1	C2	1.885(7)	C1	C2	1.377(9)
O6	C49	1.301(6)	C37	C36	1.410(9)
O7	C33	1.298(7)	C37	C41	1.413(10)
O10	N10	1.213(7)	C11	C12	1.375(9)
N6	C48	1.373(7)	C61	C62	1.365(9)
N6	C44	1.330(7)	C61	C64	1.499(8)
O2	C11	1.311(7)	N3	C21	1.343(8)
C48	C49	1.428(8)	C5	C4	1.401(10)
C48	C47	1.423(7)	C5	C9	1.404(10)
N2	C16	1.374(8)	C2	C3	1.390(9)
N2	C17	1.336(8)	C36	C35	1.357(9)
C49	C50	1.381(8)	C14	C13	1.349(10)
O4	N5	1.270(8)	C14	Br3	1.899(7)
O5	N5	1.216(8)	C12	C13	1.395(9)
O1	C1	1.308(7)	C34	C35	1.392(9)

N1	C6	1.374(8)	C26	C27	1.386(8)
N1	C7	1.338(8)	C30	C29	1.377(9)
C25	N3	1.355(7)	C39	C40	1.403(9)
C25	C26	1.484(9)	C39	C42	1.505(9)
C25	C24	1.384(8)	C4	Br2	1.896(6)
O8	N10	1.256(7)	C4	C3	1.361(10)
N7	C38	1.386(8)	C17	C18	1.402(11)
N7	C39	1.330(8)	C17	C20	1.497(10)
O9	N10	1.264(7)	C63	C62	1.375(9)
N8	C56	1.350(7)	C23	C22	1.359(9)
N8	C57	1.336(7)	C23	C32	1.517(9)
N4	C26	1.345(7)	C23	C24	1.375(9)
N4	C30	1.332(8)	C7	C8	1.406(9)
C56	C59	1.469(8)	C7	C10	1.475(9)
C56	C55	1.386(7)	C41	C40	1.339(10)
C54	C55	1.375(8)	C22	C21	1.375(9)
C54	C58	1.376(8)	C9	C8	1.341(10)
C54	C53	1.508(8)	C58	C57	1.379(8)
C52	C47	1.415(9)	C18	C19	1.321(11)

Table S9. Selected bond angles (°) for **MeMBrQ-Ho**.

Atom	**Atom**	**Atom**	**Angle/°**	**Atom**	**Atom**	**Atom**	**Angle/°**
O6	Ho2	N6	67.48(14)	C49	C50	Br5	118.1(4)
O6	Ho2	O8	81.18(17)	C49	C50	C51	123.1(6)
O6	Ho2	N7	81.55(15)	C51	C50	Br5	118.8(5)
O6	Ho2	O9	131.62(17)	N5	O3	Ho1	97.7(5)
O6	Ho2	N8	78.00(14)	C29	C28	C31	121.7(7)
O6	Ho2	N9	136.81(14)	C29	C28	C27	117.5(6)
O6	Ho2	N10	106.20(19)	C27	C28	C31	120.8(7)
O7	Ho2	O6	127.66(15)	N9	C59	C56	116.3(5)
O7	Ho2	N6	81.02(14)	N9	C59	C60	120.7(5)
O7	Ho2	O8	129.14(16)	C60	C59	C56	123.0(5)
O7	Ho2	N7	67.57(16)	O10	N10	Ho2	176.9(5)
O7	Ho2	O9	84.40(17)	O10	N10	O8	121.8(7)
O7	Ho2	N8	141.35(15)	O10	N10	O9	122.4(8)
O7	Ho2	N9	79.61(15)	O8	N10	Ho2	59.4(3)
O7	Ho2	N10	106.64(18)	O8	N10	O9	115.8(6)
N6	Ho2	N10	77.96(14)	O9	N10	Ho2	56.6(3)
O8	Ho2	N6	73.43(14)	N7	C38	C33	115.4(6)

O8	Ho2	N7	161.59(17)	N7	C38	C37	123.5(6)
O8	Ho2	N8	77.49(15)	C37	C38	C33	121.1(6)
O8	Ho2	N9	108.24(16)	C46	C45	C44	121.7(6)
O8	Ho2	N10	25.83(16)	N6	C44	C43	120.2(5)
N7	Ho2	N6	105.52(14)	N6	C44	C45	120.3(6)
N7	Ho2	N10	172.25(19)	C45	C44	C43	119.4(6)
O9	Ho2	N6	87.00(15)	O7	C33	C38	119.5(6)
O9	Ho2	O8	51.64(17)	O7	C33	C34	124.0(6)
O9	Ho2	N7	146.46(18)	C34	C33	C38	116.5(6)
O9	Ho2	N8	98.67(16)	C61	C60	C59	121.4(6)
O9	Ho2	N9	76.48(17)	N1	C6	C1	116.3(5)
O9	Ho2	N10	25.87(16)	N1	C6	C5	122.4(6)
N8	Ho2	N6	137.45(15)	C5	C6	C1	121.3(6)
N8	Ho2	N7	92.72(15)	C52	C47	C48	116.9(6)
N8	Ho2	N9	64.04(15)	C46	C47	C48	117.7(6)
N8	Ho2	N10	89.05(15)	C46	C47	C52	125.4(6)
N9	Ho2	N6	155.59(15)	N2	C16	C15	123.2(6)
N9	Ho2	N7	80.51(15)	N2	C16	C11	115.9(6)
N9	Ho2	N10	93.52(17)	C15	C16	C11	120.8(7)
O2	Ho1	N2	67.80(16)	C14	C15	C16	117.1(7)
O2	Ho1	O4	133.55(19)	C19	C15	C16	115.9(8)
O2	Ho1	O1	121.53(16)	C19	C15	C14	127.0(8)
O2	Ho1	N1	79.39(16)	O1	C1	C6	119.3(6)
O2	Ho1	N4	80.35(16)	O1	C1	C2	124.1(6)
O2	Ho1	O3	87.72(19)	C2	C1	C6	116.5(6)
O2	Ho1	N3	139.67(17)	C38	C37	C36	118.1(6)
O2	Ho1	N5	111.1(2)	C38	C37	C41	116.2(7)
N2	Ho1	N5	169.84(18)	C36	C37	C41	125.7(7)
O4	Ho1	N2	158.3(2)	O2	C11	C16	119.6(6)
O4	Ho1	N1	76.70(16)	O2	C11	C12	123.1(6)
O4	Ho1	N4	101.94(18)	C12	C11	C16	117.3(6)
O4	Ho1	N3	75.10(18)	C60	C61	C64	120.4(6)
O4	Ho1	N5	25.92(19)	C62	C61	C60	116.9(6)
O1	Ho1	N2	78.80(17)	C62	C61	C64	122.7(7)
O1	Ho1	O4	84.4(2)	C54	C55	C56	121.2(5)
O1	Ho1	N1	67.51(16)	C25	N3	Ho1	122.0(4)
O1	Ho1	N4	142.83(15)	C21	N3	Ho1	120.4(4)
O1	Ho1	O3	132.79(19)	C21	N3	C25	117.5(6)
O1	Ho1	N3	82.98(17)	C4	C5	C6	117.7(6)
O1	Ho1	N5	109.3(2)	C4	C5	C9	125.8(6)
N1	Ho1	N2	108.71(16)	C9	C5	C6	116.5(7)
N1	Ho1	N5	80.57(16)	C1	C2	Br1	118.7(5)
N4	Ho1	N2	83.91(16)	C1	C2	C3	123.0(7)
N4	Ho1	N1	149.66(17)	C3	C2	Br1	118.3(6)
N4	Ho1	N5	85.95(19)	C37	C36	Br7	119.6(6)

O3	Ho1	N2	148.15(19)	C35	C36	Br7	118.9(6)
O3	Ho1	O4	51.2(2)	C35	C36	C37	121.6(6)
O3	Ho1	N1	85.15(18)	C15	C14	Br3	118.8(7)
O3	Ho1	N4	71.69(18)	C13	C14	C15	122.5(7)
O3	Ho1	N3	97.75(19)	C13	C14	Br3	118.6(7)
O3	Ho1	N5	25.33(19)	C11	C12	Br4	118.6(5)
N3	Ho1	N2	89.24(18)	C11	C12	C13	122.9(7)
N3	Ho1	N1	140.74(17)	C13	C12	Br4	118.5(6)
N3	Ho1	N4	64.01(17)	C33	C34	Br8	118.4(5)
N3	Ho1	N5	85.73(18)	C33	C34	C35	123.1(6)
C49	O6	Ho2	125.8(4)	C35	C34	Br8	118.5(5)
C33	O7	Ho2	126.6(4)	N4	C26	C25	115.4(5)
C48	N6	Ho2	110.5(3)	N4	C26	C27	121.9(6)
C44	N6	Ho2	130.3(4)	C27	C26	C25	122.6(6)
C44	N6	C48	119.0(5)	N4	C30	C29	124.0(6)
C11	O2	Ho1	126.2(4)	N7	C39	C40	122.0(7)
N6	C48	C49	116.3(5)	N7	C39	C42	118.6(6)
N6	C48	C47	122.0(5)	C40	C39	C42	119.3(7)
C47	C48	C49	121.7(6)	C5	C4	Br2	120.4(6)
C16	N2	Ho1	109.9(4)	C3	C4	C5	121.6(6)
C17	N2	Ho1	132.8(5)	C3	C4	Br2	118.0(6)
C17	N2	C16	117.2(6)	N2	C17	C18	122.0(8)
O6	C49	C48	119.9(5)	N2	C17	C20	118.3(7)
O6	C49	C50	123.4(5)	C18	C17	C20	119.7(8)
C50	C49	C48	116.7(5)	N9	C63	C62	123.3(6)
N5	O4	Ho1	95.7(5)	C36	C35	C34	119.5(7)
C1	O1	Ho1	125.9(4)	C22	C23	C32	121.7(7)
C6	N1	Ho1	110.9(4)	C22	C23	C24	117.3(6)
C7	N1	Ho1	130.1(5)	C24	C23	C32	121.0(6)
C7	N1	C6	119.0(5)	N1	C7	C8	120.2(7)
N3	C25	C26	115.7(5)	N1	C7	C10	119.7(6)
N3	C25	C24	120.6(6)	C8	C7	C10	120.1(7)
C24	C25	C26	123.6(6)	C40	C41	C37	120.1(7)
N10	O8	Ho2	94.8(4)	C23	C22	C21	120.1(7)
C38	N7	Ho2	110.7(4)	C41	C40	C39	121.0(7)
C39	N7	Ho2	131.9(5)	O4	N5	Ho1	58.4(4)
C39	N7	C38	117.1(6)	O5	N5	Ho1	179.6(7)
N10	O9	Ho2	97.6(4)	O5	N5	O4	121.7(9)
C56	N8	Ho2	121.8(4)	O5	N5	O3	122.9(9)
C57	N8	Ho2	120.8(4)	O3	N5	Ho1	57.0(4)
C57	N8	C56	117.3(5)	O3	N5	O4	115.4(7)
C26	N4	Ho1	122.0(4)	C8	C9	C5	120.0(7)
C30	N4	Ho1	121.3(4)	C54	C58	C57	119.5(6)
C30	N4	C26	116.7(5)	N3	C21	C22	123.1(7)
N8	C56	C59	116.0(5)	C45	C46	C47	119.1(6)

N8	C56	C55	121.2(6)	C52	C51	C50	119.3(6)
C55	C56	C59	122.7(5)	C28	C29	C30	119.3(7)
C55	C54	C58	117.1(5)	C14	C13	C12	119.3(7)
C55	C54	C53	121.0(6)	N8	C57	C58	123.7(6)
C58	C54	C53	121.9(6)	C9	C8	C7	121.9(7)
C47	C52	Br6	119.4(5)	C19	C18	C17	121.2(8)
C51	C52	Br6	118.3(5)	C61	C62	C63	120.1(7)
C51	C52	C47	122.3(6)	C28	C27	C26	120.5(6)
C59	N9	Ho2	120.8(4)	C23	C24	C25	121.4(6)
C63	N9	Ho2	121.1(4)	C4	C3	C2	119.7(7)
C63	N9	C59	117.5(5)	C18	C19	C15	120.5(8)

Table S10. Crystal data and structure refinement details for **MeMBrQ-Lu**.

Empirical formula	$C_{32}H_{24}Br_4LuN_5O_5$
Formula weight	1053.17
Temperature/K	293(2)
Crystal system	orthorhombic
Space group	Pccn
a/Å	29.587(3)
b/Å	29.910(3)
c/Å	15.9860(18)
α/°	90
β/°	90
γ/°	90
Volume/Å^3	14147(3)
Z	16
ρ_{calc}g/cm^3	1.978
μ/mm^{-1}	7.356
F(000)	8032.0
Crystal size/mm^3	0.26 × 0.21 × 0.14
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	5.78 to 55.146
Index ranges	$-38 \leq h \leq 38$, $-38 \leq k \leq 36$, $-20 \leq l \leq 20$
Reflections collected	216179
Independent reflections	16325 [R_{int} = 0.1341, R_{sigma} = 0.0726]
Data/restraints/parameters	16325/0/855
Goodness-of-fit on F^2	1.082
Final R indexes [I>=2σ (I)]	R_1 = 0.0731, wR_2 = 0.1615
Final R indexes [all data]	R_1 = 0.1374, wR_2 = 0.1922
Largest diff. peak/hole / e Å^{-3}	2.71/-1.15

Table S11. Selected bond lengths (Å) for **MeMBrQ-Lu**.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
Lu1	O1	2.157(7)	N8	C57	1.347(13)
Lu1	O2	2.139(7)	N8	C53	1.335(15)
Lu1	N1	2.581(7)	O8	N10	1.253(15)
Lu1	N4	2.485(7)	C5	C10	1.406(16)
Lu1	O4	2.448(8)	C5	C6	1.419(12)
Lu1	N3	2.468(8)	C5	C4	1.410(15)
Lu1	N5	2.833(11)	N5	O3	1.265(13)
Lu1	N2	2.550(9)	N9	C58	1.340(12)
Lu1	O3	2.367(8)	N9	C62	1.341(15)
Lu2	O7	2.120(7)	O9	N10	1.257(15)
Lu2	O6	2.167(8)	C9	C10	1.366(16)
Lu2	N6	2.579(8)	C9	C8	1.393(15)
Lu2	N7	2.565(9)	C15	C16	1.420(15)
Lu2	N8	2.443(9)	C15	C20	1.410(17)
Lu2	O8	2.443(10)	C15	C14	1.381(17)
Lu2	N9	2.467(9)	C60	C64	1.519(17)
Lu2	O9	2.388(9)	C60	C59	1.393(18)
Lu2	N10	2.835(11)	C60	C61	1.353(18)
Br2	C8	1.902(10)	C28	C29	1.372(16)
Br1	C10	1.904(9)	C28	C32	1.495(16)
Br8	C52	1.899(11)	C23	C22	1.370(15)
Br6	C42	1.900(10)	C23	C31	1.527(14)
Br7	C50	1.905(12)	C16	N2	1.392(14)
Br3	C18	1.898(12)	C16	C17	1.426(14)
Br4	C20	1.893(12)	C49	C50	1.370(15)
Br5	C40	1.876(12)	C49	C48	1.415(15)
O1	C7	1.292(11)	C42	C41	1.366(19)
O2	C17	1.310(12)	C42	C37	1.405(18)
O7	C49	1.313(12)	C36	C37	1.379(17)
N1	C6	1.366(12)	C36	C35	1.35(2)
N1	C2	1.331(12)	N2	C12	1.342(14)
O6	C39	1.297(12)	C12	C13	1.431(18)
C24	C25	1.392(13)	C12	C11	1.486(17)
C24	C23	1.368(15)	C34	C35	1.416(17)
O5	N5	1.207(12)	C34	C33	1.480(18)
O10	N10	1.224(14)	C41	C40	1.408(16)
N6	C34	1.343(13)	C37	C38	1.418(14)
N6	C38	1.362(14)	C50	C51	1.378(16)
C27	C26	1.401(13)	C18	C17	1.372(15)
C27	C28	1.376(16)	C18	C19	1.395(16)
N7	C48	1.367(15)	C48	C47	1.424(15)
N7	C44	1.345(14)	C2	C1	1.496(15)
C55	C54	1.382(16)	C59	C58	1.393(15)
C55	C63	1.508(15)	C58	C57	1.483(16)

C55	C56	1.371(16)	C13	C14	1.348(19)
N4	C26	1.353(12)	C44	C45	1.407(19)
N4	C30	1.338(14)	C44	C43	1.516(19)
O4	N5	1.268(13)	C39	C40	1.381(16)
C7	C6	1.443(14)	C39	C38	1.452(14)
C7	C8	1.389(14)	C20	C19	1.359(17)
C3	C4	1.341(16)	C57	C56	1.396(14)
C3	C2	1.417(13)	C22	C21	1.364(15)
C52	C51	1.371(19)	C30	C29	1.374(16)
C52	C47	1.408(19)	C53	C54	1.362(16)
N3	C25	1.353(11)	C46	C47	1.408(19)
N3	C21	1.335(13)	C46	C45	1.32(2)
C25	C26	1.470(15)	C62	C61	1.357(17)

Table S12. Selected bond angles (°) for **MeMBrQ-Lu**.

Atom	**Atom**	**Atom**	**Angle/°**	**Atom**	**Atom**	**Atom**	**Angle/°**
O1	Lu1	N1	68.4(2)	O5	N5	O4	122.7(12)
O1	Lu1	N4	137.3(2)	O5	N5	O3	122.1(13)
O1	Lu1	O4	80.6(3)	O4	N5	Lu1	59.6(5)
O1	Lu1	N3	78.3(2)	O3	N5	Lu1	55.9(5)
O1	Lu1	N5	106.2(3)	O3	N5	O4	115.1(9)
O1	Lu1	N2	80.8(3)	C58	N9	Lu2	120.8(7)
O1	Lu1	O3	132.1(3)	C58	N9	C62	117.0(9)
O2	Lu1	O1	127.1(3)	C62	N9	Lu2	122.2(7)
O2	Lu1	N1	79.9(3)	N10	O9	Lu2	97.2(8)
O2	Lu1	N4	79.6(3)	C10	C9	C8	119.0(10)
O2	Lu1	O4	129.4(3)	C20	C15	C16	117.1(11)
O2	Lu1	N3	142.7(3)	C14	C15	C16	116.9(12)
O2	Lu1	N5	106.5(3)	C14	C15	C20	126.0(12)
O2	Lu1	N2	68.7(3)	C59	C60	C64	119.9(13)
O2	Lu1	O3	84.3(3)	C61	C60	C64	124.3(13)
N1	Lu1	N5	77.0(2)	C61	C60	C59	115.8(11)
N4	Lu1	N1	154.2(3)	C27	C28	C32	120.2(11)
N4	Lu1	N5	94.0(3)	C29	C28	C27	117.1(10)
N4	Lu1	N2	80.3(3)	C29	C28	C32	122.7(12)
O4	Lu1	N1	72.9(2)	C24	C23	C22	117.9(9)
O4	Lu1	N4	109.2(3)	C24	C23	C31	120.6(10)
O4	Lu1	N3	76.1(3)	C22	C23	C31	121.5(11)
O4	Lu1	N5	26.5(3)	C15	C16	C17	121.6(10)
O4	Lu1	N2	160.0(3)	N2	C16	C15	122.4(10)
N3	Lu1	N1	137.4(3)	N2	C16	C17	116.0(10)
N3	Lu1	N4	65.0(3)	C5	C10	Br1	119.9(8)

N3	Lu1	N5	88.1(3)	C9	C10	Br1	118.1(9)
N3	Lu1	N2	93.0(3)	C9	C10	C5	122.0(9)
N2	Lu1	N1	106.5(2)	N1	C6	C7	115.3(8)
N2	Lu1	N5	173.0(3)	N1	C6	C5	123.0(9)
O3	Lu1	N1	86.4(3)	C5	C6	C7	121.7(9)
O3	Lu1	N4	76.0(3)	O7	C49	C50	123.7(10)
O3	Lu1	O4	52.7(3)	O7	C49	C48	118.9(10)
O3	Lu1	N3	97.5(3)	C50	C49	C48	117.4(10)
O3	Lu1	N5	26.3(3)	C41	C42	Br6	117.7(10)
O3	Lu1	N2	146.8(3)	C41	C42	C37	121.9(10)
O7	Lu2	O6	120.7(3)	C37	C42	Br6	120.4(10)
O7	Lu2	N6	77.9(3)	C35	C36	C37	119.5(11)
O7	Lu2	N7	68.7(3)	C16	N2	Lu1	110.0(6)
O7	Lu2	N8	141.3(3)	C12	N2	Lu1	131.5(8)
O7	Lu2	O8	133.4(3)	C12	N2	C16	118.3(10)
O7	Lu2	N9	80.4(3)	N2	C12	C13	120.7(12)
O7	Lu2	O9	88.0(3)	N2	C12	C11	119.9(11)
O7	Lu2	N10	111.3(4)	C13	C12	C11	119.4(11)
O6	Lu2	N6	68.5(3)	N6	C34	C35	119.3(12)
O6	Lu2	N7	78.6(3)	N6	C34	C33	120.3(10)
O6	Lu2	N8	83.1(3)	C35	C34	C33	120.4(11)
O6	Lu2	O8	83.2(4)	C42	C41	C40	120.3(12)
O6	Lu2	N9	143.1(3)	C3	C4	C5	119.5(9)
O6	Lu2	O9	133.1(3)	C42	C37	C38	117.1(11)
O6	Lu2	N10	108.4(4)	C36	C37	C42	125.4(11)
N6	Lu2	N10	79.0(3)	C36	C37	C38	117.5(12)
N7	Lu2	N6	109.7(3)	C49	C50	Br7	117.8(8)
N7	Lu2	N10	170.7(3)	C49	C50	C51	124.4(12)
N8	Lu2	N6	140.7(3)	C51	C50	Br7	117.7(10)
N8	Lu2	N7	89.6(3)	C7	C8	Br2	117.2(7)
N8	Lu2	N9	65.0(3)	C7	C8	C9	124.1(10)
N8	Lu2	N10	85.2(3)	C9	C8	Br2	118.7(8)
O8	Lu2	N6	75.5(3)	N5	O3	Lu1	97.9(7)
O8	Lu2	N7	157.2(4)	C17	C18	Br3	117.9(8)
O8	Lu2	N8	74.6(3)	C17	C18	C19	123.6(11)
O8	Lu2	N9	104.2(3)	C19	C18	Br3	118.5(9)
O8	Lu2	N10	26.1(3)	N7	C48	C49	116.9(10)
N9	Lu2	N6	148.3(3)	N7	C48	C47	122.7(11)
N9	Lu2	N7	82.9(3)	C49	C48	C47	120.4(12)
N9	Lu2	N10	87.8(3)	N1	C2	C3	119.8(10)
O9	Lu2	N6	84.8(3)	N1	C2	C1	120.9(9)
O9	Lu2	N7	148.2(3)	C3	C2	C1	119.3(9)
O9	Lu2	N8	96.5(3)	C58	C59	C60	120.5(11)
O9	Lu2	O8	52.2(4)	N9	C58	C59	121.7(11)
O9	Lu2	N9	71.7(3)	N9	C58	C57	116.4(9)

O9	Lu2	N10	26.1(4)	C59	C58	C57	121.9(10)
C7	O1	Lu1	125.4(6)	C14	C13	C12	120.1(12)
C17	O2	Lu1	126.4(6)	N7	C44	C45	121.6(13)
C49	O7	Lu2	126.1(6)	N7	C44	C43	118.0(11)
C6	N1	Lu1	110.4(6)	C45	C44	C43	120.4(12)
C2	N1	Lu1	130.3(7)	O6	C39	C40	123.2(10)
C2	N1	C6	119.2(8)	O6	C39	C38	120.5(10)
C39	O6	Lu2	124.8(7)	C40	C39	C38	116.3(9)
C23	C24	C25	119.9(9)	C41	C40	Br5	118.4(10)
C34	N6	Lu2	130.0(8)	C39	C40	Br5	119.4(8)
C34	N6	C38	119.2(9)	C39	C40	C41	122.1(11)
C38	N6	Lu2	110.9(6)	N6	C38	C37	122.6(10)
C28	C27	C26	120.7(10)	N6	C38	C39	115.1(9)
C48	N7	Lu2	109.3(6)	C37	C38	C39	122.2(11)
C44	N7	Lu2	133.5(8)	O2	C17	C16	118.7(9)
C44	N7	C48	117.2(10)	O2	C17	C18	124.9(10)
C54	C55	C63	122.0(12)	C18	C17	C16	116.4(10)
C56	C55	C54	116.3(10)	C15	C20	Br4	119.5(9)
C56	C55	C63	121.7(11)	C19	C20	Br4	118.4(9)
C26	N4	Lu1	120.0(6)	C19	C20	C15	122.1(11)
C30	N4	Lu1	121.5(7)	N8	C57	C58	114.6(9)
C30	N4	C26	117.8(8)	N8	C57	C56	122.2(11)
N5	O4	Lu1	93.9(6)	C56	C57	C58	123.0(10)
O1	C7	C6	120.5(9)	O10	N10	Lu2	178.0(13)
O1	C7	C8	124.1(9)	O10	N10	O8	122.7(15)
C8	C7	C6	115.4(8)	O10	N10	O9	121.4(16)
C4	C3	C2	122.1(10)	O8	N10	Lu2	59.2(6)
C51	C52	Br8	117.8(11)	O8	N10	O9	115.9(11)
C51	C52	C47	122.4(11)	O9	N10	Lu2	56.7(6)
C47	C52	Br8	119.8(11)	C21	C22	C23	119.7(11)
C25	N3	Lu1	121.9(6)	N4	C30	C29	122.9(11)
C21	N3	Lu1	121.6(6)	N8	C53	C54	122.5(11)
C21	N3	C25	116.5(8)	C53	C54	C55	121.5(12)
C24	C25	C26	122.6(8)	C28	C29	C30	120.5(11)
N3	C25	C24	122.0(9)	C36	C35	C34	122.0(12)
N3	C25	C26	115.2(8)	N3	C21	C22	124.0(10)
C57	N8	Lu2	122.2(7)	C52	C51	C50	117.7(12)
C53	N8	Lu2	120.3(7)	C45	C46	C47	119.1(13)
C53	N8	C57	117.3(9)	N9	C62	C61	122.9(11)
N10	O8	Lu2	94.7(8)	C60	C61	C62	122.1(13)
C27	C26	C25	122.4(9)	C55	C56	C57	120.2(10)
N4	C26	C27	120.9(9)	C20	C19	C18	118.9(12)
N4	C26	C25	116.7(8)	C52	C47	C48	117.6(12)
C10	C5	C6	117.9(10)	C52	C47	C46	125.0(12)
C10	C5	C4	125.8(9)	C46	C47	C48	117.3(13)

C4	C5	C6	116.4(10)	C46	C45	C44	122.1(14)
O5	N5	Lu1	176.4(8)	C13	C14	C15	121.6(13)

Table S13. Crystal data and structure refinement details for **MeOMBrQ-Ho**.

Empirical formula	$C_{32}H_{24}Br_4HoN_5O_7$
Formula weight	1075.09
Temperature/K	293(2)
Crystal system	monoclinic
Space group	$P2_1/c$
a/Å	13.5152(7)
b/Å	17.1668(8)
c/Å	16.0298(8)
α/°	90
β/°	105.757(2)
γ/°	90
Volume/Å^3	3579.4(3)
Z	4
ρ_{calc}mg/mm^3	1.995
m/mm^{-1}	6.728
F(000)	2056.0
Crystal size/mm^3	0.42 × 0.089 × 0.031
2Θ range for data collection	5.282 to 52.744°
Index ranges	$-16 \le h \le 16$, $-21 \le k \le 21$, $-17 \le l \le 17$
Reflections collected	49472
Independent reflections	6823[R(int) = 0.0959]
Data/restraints/parameters	6823/1344/446
Goodness-of-fit on F^2	1.150
Final R indexes [I>=2σ (I)]	R_1 = 0.0809, wR_2 = 0.2148
Final R indexes [all data]	R_1 = 0.1234, wR_2 = 0.2324
Largest diff. peak/hole / e Å^{-3}	3.04/-1.54

Table S14. Selected bond lengths (Å) for **MeOMBrQ-Ho**.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
Ho1	O2	2.726(13)	C1	C2	1.37(2)
Ho1	O3	2.100(11)	C1	C10	1.55(2)
Ho1	O6	2.032(11)	C2	C3	1.485(16)
Ho1	O7	2.270(11)	C3	C4	1.41(2)
Ho1	N1	2.745(15)	C4	C5	1.38(2)
Ho1	N2	2.522(15)	C5	C6	1.48(2)
Ho1	N3	2.750(15)	C5	C10	1.492(16)

Ho1	N5	2.751(15)	C6	C7	1.33(2)
Br1	C18	1.868(18)	C7	C8	1.489(16)
Br2	C16	2.073(19)	C8	C9	1.49(2)
Br3	C4	2.219(19)	C11	C12	1.48(2)
Br4	C2	2.003(17)	C12	C13	1.50(3)
O1	O2	1.839(16)	C13	C14	1.39(2)
O1	N5	1.138(18)	C14	C15	1.38(2)
O2	N5	1.171(17)	C15	C16	1.47(2)
O3	N5	1.360(19)	C15	C20	1.467(16)
O4	C29	1.55(2)	C16	C17	1.27(2)
O4	C32	1.48(3)	C17	C18	1.53(3)
O5	C21	1.38(3)	C18	C19	1.42(2)
O5	C22	1.35(2)	C19	C20	1.42(2)
O6	C1	1.49(2)	C22	C23	1.47(3)
O7	C19	1.41(2)	C22	C25	1.50(3)
N1	C27	1.41(2)	C23	C24	1.38(3)
N1	C31	1.43(2)	C25	C26	1.38(2)
N2	C24	1.45(2)	C26	C27	1.493(16)
N2	C26	1.49(2)	C27	C28	1.486(16)
N3	C12	1.34(2)	C28	C29	1.49(3)
N3	C20	1.42(2)	C29	C30	1.43(3)
N4	C8	1.41(2)	C30	C31	1.56(3)
N4	C10	1.37(2)			

Table S15. Selected bond angles (°) for **MeOMBrQ-Ho**.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
O2	Ho1	N1	117.7(4)	C1	C2	C3	128.0(16)
O2	Ho1	N3	167.5(4)	C3	C2	Br4	130.3(12)
O2	Ho1	N5	24.7(4)	C4	C3	C2	131.7(15)
O3	Ho1	O2	53.4(4)	C3	C4	Br3	130.7(12)
O3	Ho1	O7	82.7(4)	C5	C4	Br3	123.2(13)
O3	Ho1	N1	88.9(5)	C5	C4	C3	106.1(16)
O3	Ho1	N2	102.0(5)	C4	C5	C6	111.4(15)
O3	Ho1	N3	134.3(4)	C4	C5	C10	122.3(16)
O3	Ho1	N5	28.8(4)	C6	C5	C10	126.3(15)
O6	Ho1	O2	76.4(4)	C7	C6	C5	103.6(16)
O6	Ho1	O3	127.5(5)	C6	C7	C8	128.0(17)
O6	Ho1	O7	128.7(4)	N4	C8	C7	131.0(15)
O6	Ho1	N1	132.1(4)	N4	C8	C9	103.4(14)
O6	Ho1	N2	77.5(5)	C7	C8	C9	125.5(16)
O6	Ho1	N3	97.9(4)	N4	C10	C1	98.9(13)

O6	Ho1	N5	100.3(5)	N4	C10	C5	128.9(15)
O7	Ho1	O2	129.8(4)	C5	C10	C1	132.1(14)
O7	Ho1	N1	79.5(4)	N3	C12	C11	112.8(16)
O7	Ho1	N2	142.8(5)	N3	C12	C13	120.4(16)
O7	Ho1	N3	62.4(4)	C11	C12	C13	126.8(15)
O7	Ho1	N5	108.7(4)	C14	C13	C12	126.8(17)
N1	Ho1	N3	58.0(4)	C15	C14	C13	112.9(17)
N1	Ho1	N5	105.2(4)	C14	C15	C16	117.6(16)
N2	Ho1	O2	76.8(5)	C14	C15	C20	119.4(16)
N2	Ho1	N1	63.9(5)	C20	C15	C16	123.1(15)
N2	Ho1	N3	91.2(5)	C15	C16	Br2	124.4(13)
N2	Ho1	N5	87.9(5)	C17	C16	Br2	120.8(15)
N3	Ho1	N5	161.1(4)	C17	C16	C15	114.8(17)
N5	O1	O2	37.8(9)	C16	C17	C18	122.2(17)
O1	O2	Ho1	115.4(7)	C17	C18	Br1	120.4(12)
N5	O2	Ho1	78.9(10)	C19	C18	Br1	112.7(14)
N5	O2	O1	36.6(9)	C19	C18	C17	126.9(16)
N5	O3	Ho1	103.3(8)	O7	C19	C18	128.0(15)
C32	O4	C29	117.3(15)	O7	C19	C20	122.6(15)
C22	O5	C21	117.9(18)	C20	C19	C18	109.4(16)
C1	O6	Ho1	127.7(9)	N3	C20	C15	127.8(15)
C19	O7	Ho1	128.6(9)	C19	C20	N3	108.5(14)
C27	N1	Ho1	122.8(10)	C19	C20	C15	123.7(16)
C27	N1	C31	111.9(14)	O5	C22	C23	120.5(18)
C31	N1	Ho1	125.0(11)	O5	C22	C25	113.8(17)
C24	N2	Ho1	115.5(12)	C23	C22	C25	125.7(17)
C24	N2	C26	124.5(14)	C24	C23	C22	112.7(19)
C26	N2	Ho1	119.6(10)	C23	C24	N2	122.9(19)
C12	N3	Ho1	129.5(12)	C26	C25	C22	120.0(18)
C12	N3	C20	112.5(15)	N2	C26	C27	124.1(15)
C20	N3	Ho1	117.9(10)	C25	C26	N2	114.3(15)
C10	N4	C8	102.2(14)	C25	C26	C27	121.5(17)
O1	N5	Ho1	176.9(13)	N1	C27	C26	108.9(14)
O1	N5	O2	105.6(16)	N1	C27	C28	120.6(14)
O1	N5	O3	130.0(14)	C28	C27	C26	130.6(16)
O2	N5	Ho1	76.5(10)	C27	C28	C29	130.1(16)
O2	N5	O3	124.4(14)	C28	C29	O4	134.0(16)
O3	N5	Ho1	48.0(7)	C30	C29	O4	117.2(16)
O6	C1	C10	131.4(13)	C30	C29	C28	108.8(17)
C2	C1	O6	128.8(15)	C29	C30	C31	120.3(17)
C2	C1	C10	99.7(15)	N1	C31	C30	128.3(16)
C1	C2	Br4	101.7(12)				

Table S16. Inhibitory rates (%) of **MeMBrQ-Lu**, **MeOMBrQ-Ho**, **MeMBrQ-Ho**, **MeBrQ-La**, **MeBrQ-Sm**, $Ho(NO_3)_3 \cdot 6H_2O$, $Lu(NO_3)_3 \cdot 6H_2O$, $La(NO_3)_3 \cdot 6H_2O$, $Sm(NO_3)_3 \cdot 6H_2O$, MBrQ-H, BrQ-H, cisplatin, 4,4'-dimethyl-2,2'-bipyridyl (Me), 4,4'-dimethoxy-2,2'-bipyridine (MeO) against SK-OV-3/DDP, NCI-H460 and HeLa cancer cells for 48 h.

Compounds	SK-OV-3/DDP	NCI-H460	HeLa	HL-7702
MBrQ-H	25.16 ± 0.19	38.19 ± 1.15	28.06 ± 0.47	30.11 ± 1.18
4,4'-dimethyl-2,2'-bipyridyl (Me)	19.15 ± 0.63	25.58 ± 1.87	20.51 ± 0.37	30.15 ± 2.01
4,4'-dimethoxy-2,2'-bipyridine (MeO)	25.84 ± 0.75	30.85 ± 0.28	21.33 ± 0.79	28.19 ± 1.06
MeMBrQ-Lu	73.26 ± 0.32	87.02 ± 0.97	90.51 ± 0.29	40.49 ± 2.06
MeOMBrQ-Ho	85.01 ± 1.31	93.54 ± 0.20	95.63 ± 0.36	45.21 ± 0.93
MeMBrQ-Ho	79.02 ± 0.41	91.19 ± 0.15	91.12 ± 1.06	42.87 ± 1.88
BrQ-H	35.29 ± 0.77	51.74 ± 1.09	40.88 ± 0.35	39.98 ± 1.53
MeBrQ-La	69.33 ± 1.22	82.17 ± 0.62	88.71 ± 1.62	38.66 ± 0.69

MeBrQ-Sm	62.11 ± 0.37	75.11 ± 1.64	80.23 ± 1.79	41.28 ± 1.45
$Ho(NO_3)_3 \cdot 6H_2O$	18.25 ± 0.96	21.09 ± 1.84	15.28 ± 2.01	28.55 ± 1.06
$Lu(NO_3)_3 \cdot 6H_2O$	20.77 ± 1.25	16.54 ± 2.15	20.11 ± 1.14	20.89 ± 1.47
$La(NO_3)_3 \cdot 6H_2O$	21.33 ± 0.36	18.46 ± 0.46	16.96 ± 0.42	24.33 ± 1.09
$Sm(NO_3)_3 \cdot 6H_2O$	15.26 ± 0.85	20.17 ± 0.98	20.41 ± 0.55	25.64 ± 0.64
cisplatin	40.25 ± 2.02	65.23 ± 0.41	69.54 ± 0.94	64.58 ± 1.11

Table S17. Cellular distribution of **MeOMBrQ-Ho** (5.0 nM), cisplatin (12.6 μM) and **MeMBrQ-Ho** (125.0 nM) in HeLa cells after 24 h of incubation.

	total	nuclear fraction	mitochondrial fraction
MeOMBrQ-Ho	(12.32±0.11 nmol of Pt)/10^6 cells	(3.84±0. 05 nmol of Ho)/10^6 cells	(6.01±0.09 nmol of Ho)/10^6 cells
MeMBrQ-Ho	(7.51±0.09 nmol of Ho)/10^6 cells	(2.35±0.19 nmol of Ho)/10^6 cells	(4.10±0.05 nmol of Ho)/10^6 cells
cisplatin	(4.85±0.05 nmol of Pt)/10^6 cells	(0.99±0.10 nmol of Pt)/10^6 cells	(2.68±0.07 nmol of Pt)/10^6 cells

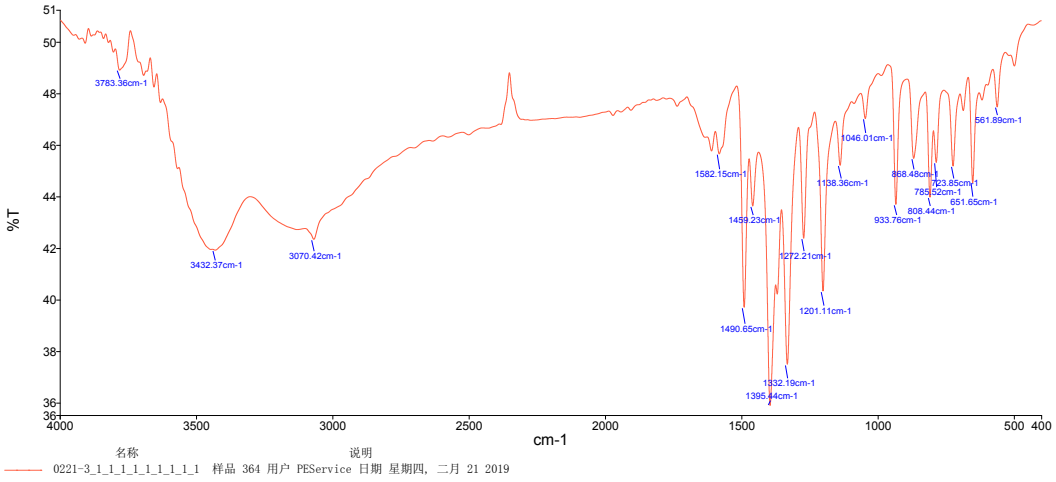

Figure S1. IR (KBr) spectra of **MeBrQ-Sm**.

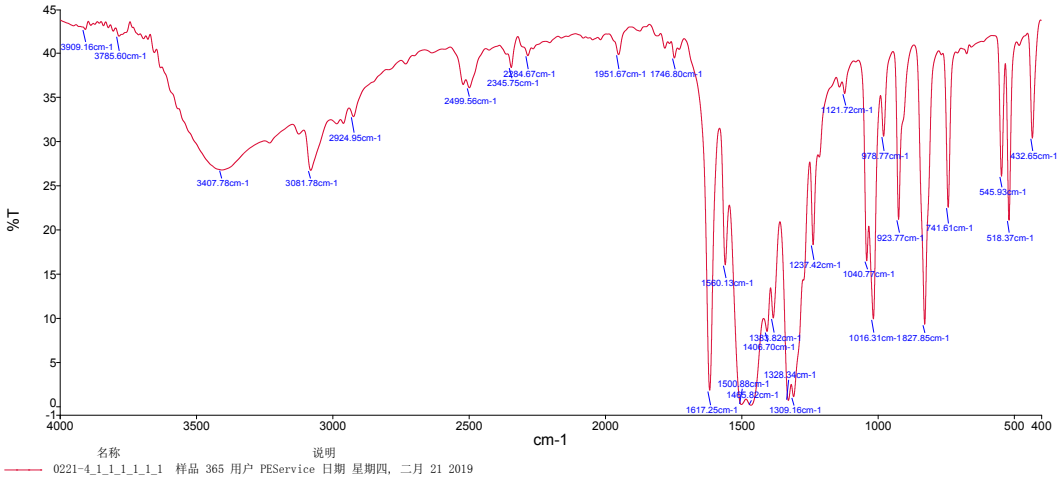

Figure S2. IR (KBr) spectra of **MeMBrQ-Ho**.

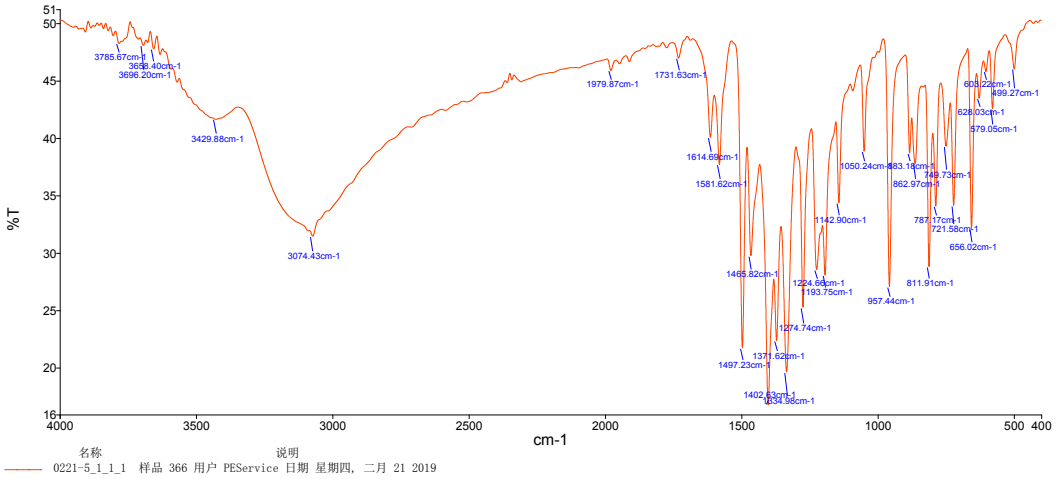

Figure S3. IR (KBr) spectra of **MeBrQ-La**.

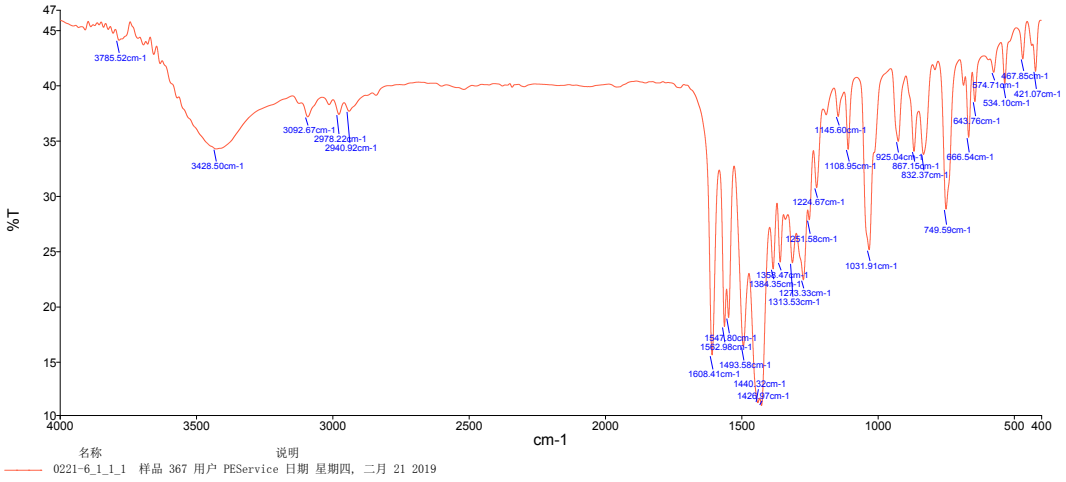

Figure S4. IR (KBr) spectra of **MeOMBrQ-Ho**.

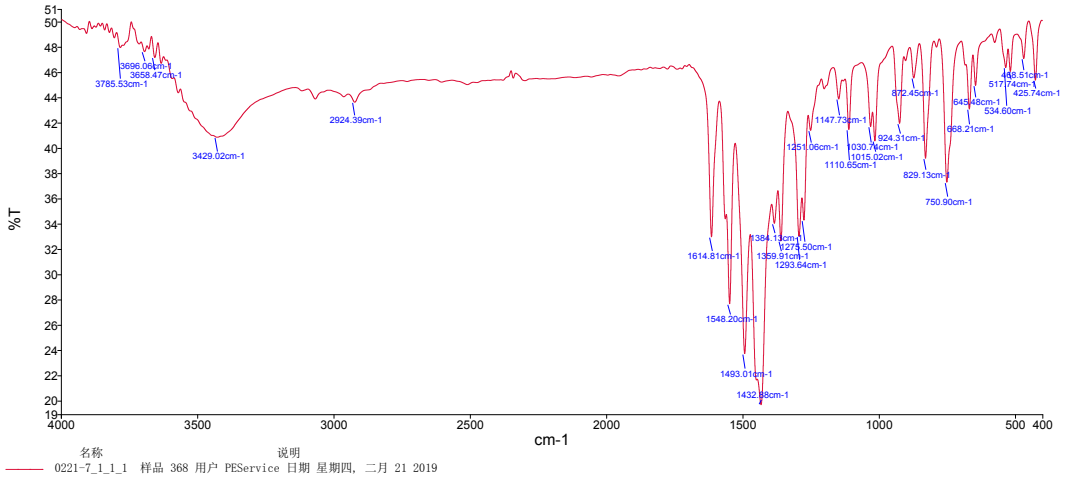

Figure S5. IR (KBr) spectra of **MeMBrQ-Lu**.

Table S18. ROS generation assay (OD value) in HeLa cells after treatment with **MeMBrQ-Ho** and **MeOMBrQ-Ho** for 24 h, respectively.

	OD1	OD2	OD3	mean value of OD	SD
Control	22.642	25.884	27.348	25.291	2.408
MeOMBrQ-Ho	40.567	42.325	44.936	42.609	2.198
MeMBrQ-Ho	43.278	41.455	39.121	41.285	2.084

Table S19. The tumor volume in treated and non-treated mice from the date of surgery to the study end point in the Hela xenograft model.

Group	Tumor Volume (mm^3) (start)	Tumor Volume (mm^3) (end)	T/C (%)
Control	82.4±27.0	1127.8±180.7	-
MeOMBrQ-Ho (5.0 mg/kg)	82.0±26.5	490.0±150.9	42.9[a]

a mean $p<0.05$, *p vs* vehicle control

Table S20. Average body weight in treated and non-treated mice from the date of surgery to the study end point in the Hela xenogfart model.

Group	Body Weight (g) (start)	Body Weight (g) (end)	RBW (%) (end)
Control	18.7±1.2	20.7±1.4	110.7
MeOMBrQ-Ho (5.0 mg/kg)	18.5±0.8	20.1±0.6	108.6

Table S21. In Vivo Anticancer Activity of **MeOMBrQ-Ho** (5.0 mg/kg) toward Hela Tumor Xenograft.

Group	average tumor weight(mean ± SD g)	inhibition of tumor growth(%)
Control	1.562±0.148	-
MeOMBrQ-Ho (5.0 mg/kg)	0.769±0.096	50.8

[a] mean $p<0.05$, *pvs* control.

Experimental methods

MTT assay for cell viability

The cells were incubated in the presence of different concentrations of **MeMBrQ-Lu**, **MeOMBrQ-Ho**, **MeMBrQ-Ho**, **MeBrQ-La**, **MeBrQ-Sm**, $Ho(NO_3)_3 \cdot 6H_2O$, $Lu(NO_3)_3 \cdot 6H_2O$, $La(NO_3)_3 \cdot 6H_2O$, $Sm(NO_3)_3 \cdot 6H_2O$, MBrQ-H, BrQ-H, cisplatin, 4,4'-dimethyl-2,2'-bipyridyl (Me), 4,4'-dimethoxy-2,2'-bipyridine (MeO) for 48 h, before they were then reacted with MTT (2.0 mg/mL) (3-[4,5-dimethylthiazol-2-yl]-2,5-diphenyl tetrazolium bromide) at 37 °C for 4 h. The reaction product, formazan, was extracted with dimethyl sulphoxide (DMSO) and the absorbance was read at 540 nm as previously described. The assays were performed in triplicate, and results are expressed as the percent reduction in cell viability compared to untreated control cultures for at least five independent experiments. IC_{50} values refer to the concentration needed to inhibit 50% of cell viability in the presence of the **MeMBrQ-Lu**, **MeOMBrQ-Ho**, **MeMBrQ-Ho**, **MeBrQ-La**, **MeBrQ-Sm**, $Ho(NO_3)_3 \cdot 6H_2O$, $Lu(NO_3)_3 \cdot 6H_2O$, $La(NO_3)_3 \cdot 6H_2O$, $Sm(NO_3)_3 \cdot 6H_2O$, MBrQ-H, BrQ-H, cisplatin, 4,4'-dimethyl-2,2'-bipyridyl (Me), 4,4'-dimethoxy-2,2'-bipyridine (MeO).

Cellular uptake of MeOMBrQ-Ho and MeMBrQ-Ho in HeLa cancer cells. The HeLa cancer cells (~10 million cells) were treated with **MeOMBrQ-Ho** (1.0 nM), cisplatin (12.62 μM) and **MeMBrQ-Ho** (125.0 nM) for 24 h at 37 °C in a humidified 5% CO_2 incubator. The spent media was removed, and the cells were washed with 5 mL of PBS, scraped, and collected in 5 mL of PBS. The scrapped cells were spun down, by centrifuging at 2500 rpm for 10 min. The cell pellet obtained was dissolved in 1 M NaOH (1 mL) and diluted with 2% (v/v) HNO_3 (5 mL) for determining whole

cell Pt or Ho content. Another set was treated similarly, nuclear fraction, and mitochondria fraction were isolated as described by Schreiber and Liang et al [1,2], and the final solution was made up to 5 mL using 2% (v/v) HNO_3. The amount of Pt or Ho taken up by the cells was determined by ICP-MS. The instrument was calibrated for Pt complexes using standard solutions containing 10, 50, 100, 500 and 1000 ppb Pt or Ho metal.

TRAP-silver staining assay

Telomerase extract was prepared from HeLa cells. A modified version of the TRAP assay was used. PCR was performed in a final 50 μL reaction volume composed of reaction mix (45 μL) containing Tris-HCl (20 mM, pH 8.0), deoxynucleotide triphosphates (50 mM), $MgCl_2$ (1.5 mM), KCl (63 mM), EGTA (1 mM), Tween-20 (0.005%), BSA (20.0 μg/mL), primer HTG21 (3.5 pmol; 5'-G_3ACHTUNGTRENUNG[T_2AG_3]3-3'), primer TS (18 pmol; 5'-AATCCG TCGAGCAGAGTT-3'), primer CXext (22.5 pmol; 5'-GTGCCCTTACCCTT ACCCTTACCCTAA-3'), primer NT (7.5 pmol; 5'-ATCGCTTCTCGGCCTTTT-3'), TSNT internal control (0.01 amol; 5'-ATTCCGTCGAGCAGAGTTAAAAGG CCGAGAAGCGAT-3'), Taq DNA polymerase (2.5 U), and telomerase (100 ng). **MeOMBrQ-Ho** (1.0 nM) and **MeMBrQ-Ho** (125.0 nM) or distilled water were added (5 μL). PCR was performed in an Eppendorf Master cycler equipped with a hot lid and incubated for 30 min at 30 °C, followed by 92 °C 30 s, 52 °C 30 s, and 72 °C 30 s for 30 cycles. After amplification, loading buffer (8 μL; 5×TBE buffer, 0.2% bromophenol blue, and 0.2% xylene cyanol) was added to the reaction. An aliquot (15.0 μL) was loaded onto a nondenaturing acrylamide gel (16%; 19:1) in 1×TBE buffer and resolved at 200.0 V for 1.0 h. The Gels were fixed and then stained with $AgNO_3$.

Flow Cytometric Analysis

In cell cycle analysis, the HeLa cancer cells were maintained with 10% fetal calf serum in 5% CO_2 at 37°C. After treatment with **MeOMBrQ-Ho** (1.0 nM) and **MeMBrQ-Ho** (125.0 nM), the cells were harvested by trypsinization and rinsed with PBS. After centrifugation, the pellet (10^5−10^6 cells) was suspended in 1.0 mL of PBS and then fixed by dropwise addition of 9 mL of precooled (4 °C) 70% ethanol under violent shaking. After treatment, cells were collected and fixed with ice-cold 70% ethanol at −20 °C overnight. Fixed cells were resuspended in 0.5 mL of PBS containing 50 μg/mL propidium iodide and 100 μg/mL RNase A. The cell cycle distribution was analyzed by FACS Calibur flow cytometer (BD) and calculated using ModFIT LT software (BD).

Cell apoptosis analysis

The cell apoptosis was detected by flow cytometric analysis of annexin V staining. Briefly, adherent HeLa cells were harvested and suspended in the annexin-binding buffer (5×10^5 cells/mL). Then cells were incubated with annexin V-FITC and PI for 1.5 h at room temperature in the dark and immediately analyzed by flow cytometry. The data are presented as biparametric dot plots showing PI red fluorescence vs annexin V-FITC green fluorescence.

Immunofluorescence

HeLa cells (10^5−10^6 cells) were grown on polylysine-coated coverslips, rinsed in phosphate-buffered saline, fixed in cold methanol for 20 min, permeabilized for 10 min in 0.5% Triton X-100 on ice, and blocked in 5% BSA for 30 min at room temperature. The coverslips were incubated with rabbit monoclonal anti-H2A.X (Abcam) primary antibodies for 3.0 h at 25 °C. The coverslips were washed and incubated with fluorescein conjugated Alexa Fluor® 488 Goat Anti-Rabbit IgG (H+L)

(1:1000) secondary antibodies. Finally, the cells stained with 0.1 mg/mL DAPI. Fluorescence images were captured using LeicaTCS-SP5 confocal microscope, (Germany, magnification 400×).

Flow cytometry analysis of ΔΨm

JC-1 Assay Kit was used to detect the changes of ΔΨm. HelA cells (5×10^5 cells/mL) were inoculated in 6-well plate for 24 h and then treated with **MeOMBrQ-Ho** (1.0 nM) and **MeMBrQ-Ho** (125.0 nM) for 24 h. After incubation, the HeLa cells were washed and resuspended with PBS. For analysis, 0.5 mL PBS buffer solution (lincluding 10 μg/mL JC-1 staining) was added into the suspension in darkness for 30.0 min at 37 ° C. The green fluorescence percentage from JC-1 monomers was detected by flow cytometry, which demonstrated the decrease of ΔΨm.

Assessment of intracellular ROS levels in HeLa cells

The ROS Assay Kit (Beyotime) with fluorescent probe 2,7-dichloro fluorescein diacetate (DCFH-DA) was used to detect the intracellular ROS levels. Firstly, HeLa cells were treated with DCFH-DA (1: 250) in cell culture medium and kept in dark place for 30 min at 37 ° C, and then the HeLa cells were washed with 1 mL PBS. Subsequently, the cells were treated with **MeOMBrQ-Ho** (1.0 nM) and **MeMBrQ-Ho** (125.0 nM) for 24 h, and immediately measured the cellular fluorescence using a fluorescence photometer (GC126N, China) with excitation and emission wavelengths of 488 and 525 nm, respectively.

In vitro transwell migration assay

The inhibition of tumor cell migration was assessed by the Boyden chamber (Corning Falcon) migration assay in 24-well cell culture plate with 8.0 μm pore. Briefly, HeLa cancer cells were collected, centrifuged, and re-suspended with serum-free medium. The top chambers were seeded with 5×10^5 cells in 200 μL of serum-free

1640 medium containing different dose of **MeOMBrQ-Ho** (1.0 nM) and **MeMBrQ-Ho** (125.0 nM). The bottom chambers were filled with 600 μL of complete medium supplemented with different dose of **MeOMBrQ-Ho** (1.0 nM) and **MeMBrQ-Ho** (125.0 nM). After 24 h incubation, non-migrated cells were removed with cotton swabs, and migrated cells were fixed with cold 4% paraformaldehyde and stained with 0.2% crystal violet for 1 min. Then the chambers were washed using water, and the membrane was left to dry. Images were taken with an inverted microscope (Olympus) and cells from three random areas per filter were counted.

Anticancer Activity toward HeLa *in Vivo*

HeLa cells were harvested and injected subcutaneously into the right flank of nude mice with 5×10^6 cells in 200 μL of serum-free medium. When the xenograft tumor growth to the volume about 1000 mm^3, the mice were killed and the tumor tissue were cut into about 1.5 mm^3 small pieces, and then transplanted into the right flank of female nude mice, When tumors reach a volume of 80-190 mm^3 on all mice, the mice were randomized into vehicle control and treatment groups (n=6/group), received the following treatments: (a) control, 5.0% v/v DMSO/saline vehicle, (b) **MeOMBrQ-Ho** at dose 5.0 mg/kg every two day (5.0% v/v DMSO/saline). The tumor volumes were determined every three days by measuring length (*l*) and width (*w*) and calculating volume, tumor volume and inhibition of tumor growth were calculated using formulas 1−3:[3−6]

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

The tumor relative increment rate: $T/C\ (\%) = T_{RTV}/C_{RTV}\times100\%$ (2)

inhibition of tumor growth: $IR(\%) = (W_c - W_t)/W_c\times100\%$ (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 controlled group respectively.

In addition, HeLa xenograft mouse models were purchased from Beijing HFK Bioscience Co., Ltd (Beijing, China, approval No. SCXK 2014-004). The animal procedures were approved by the Institute of Radiation Medicine Chinese Academy of Medical Sciences (Tian Jin, China, approval No. SYXK 2014-0002). And all of the experimental procedures were carried out in accordance with the NIH Guidelines for the Care and Use of Laboratory Animals. Animal experiments were approved by the Animal Care and Use Committee of Institute of Radiation Medicine Chinese Academy of Medical Sciences.

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 assesses by using Student's *t* test for unpaired data, and p values of <0.05 were considered significant.

Abbreviations

SD, standard deviation; TBS, Tris-HCl buffer; MTT, 3-(4,5-dimethylthiazol-2-yl)-2,5-diphenyltetrazolium bromide; TGI, tumor growth inhibition; PI, propidium iodide; MMP, mitochondrial membrane potential; JC-1, 5,5′,6,6′-tetrachloro-1,1′,3,3′-tetraethylbenzimidazolylcarbocyanine; IR, tumor growth inhibition rate.

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