Mitochondria-localizing dicarbohydrazide Ln complexes and their mechanism of in vitro anticancer activity

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Table S1 Crystal data and structure refinement details for complex **1**.

Empirical formula	$C_{73}H_{61}Dy_5N_{16}O_{24}$
Formula weight	2358.87
Temperature/K	150.01
Crystal system	triclinic
Space group	*P*-1
a/Å	15.3966(8)
b/Å	17.1849(9)
c/Å	20.4428(10)
α/°	111.135(2)
β/°	90.178(2)
γ/°	101.146(2)
Volume/Å^3	4934.2(4)
Z	2
ρ_{calc}mg/mm^3	1.588
m/mm^{-1}	3.809
F(000)	2266.0
Crystal size/mm^3	0.29 × 0.21 × 0.14
Radiation	MoKα (λ = 0.71073)
2θ range /°	4.286 to 52.948
Index ranges	-19 ≤ h ≤ 19, -21 ≤ k ≤ 21, -25 ≤ l ≤ 25
Reflections collected	97397
Independent reflections	20341 [R_{int} = 0.0831, R_{sigma} = 0.0645]
Data/restraints/parameters	20341/64/1077
Goodness-of-fit on F^2	1.085
Final R indexes [I>=2σ (I)]	R_1 = 0.0668, wR_2 = 0.1562
Largest diff. peak/hole / e Å^{-3}	4.58/-2.64

[a] $R_1 = \Sigma ||F_o| - |F_c|| / \Sigma |F_o|$; [b] $wR_2 = [\Sigma w(F_o^2 - F_c^2)^2 / \Sigma w(F_o^2)^2]^{1/2}$.

Table S2 Selected bond lengths (Å) for complex **1**.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
Dy1	Dy3	3.7882(8)	Dy1	O19	2.425(7)
Dy1	O16	2.633(9)	Dy1	O6	2.427(8)
Dy1	O21	2.252(8)	Dy1	O15	2.638(8)
Dy1	O7	2.423(8)	Dy1	O22	2.397(10)
Dy1	N12	2.595(10)	Dy1	N9	2.613(10)
Dy2	Dy3	3.7463(8)	Dy2	Dy4	3.9355(8)
Dy2	O19	2.394(8)	Dy2	O20	2.398(8)
Dy2	O3	2.328(8)	Dy2	O2	2.331(8)
Dy2	O14	2.451(8)	Dy2	O10	2.222(8)
Dy2	N6	2.539(9)	Dy2	N3	2.563(10)
Dy3	O19	2.388(8)	Dy3	O21	2.237(8)
Dy3	O2	2.335(8)	Dy3	O1	2.226(8)
Dy3	O12	2.317(8)	Dy3	O13	2.334(9)
Dy3	N1	2.528(10)	Dy4	O16	2.398(8)
Dy4	O3	2.381(8)	Dy4	O14	2.498(8)
Dy4	O7	2.415(8)	Dy4	O4	2.184(9)
Dy4	O8	2.252(8)	Dy4	N14	2.508(10)
Dy4	N16	2.539(11)	Dy5	O6	2.417(8)
Dy5	O15	2.382(8)	Dy5	O9	2.364(8)
Dy5	O11	2.351(9)	Dy5	O5	2.198(9)
Dy5	O17	2.429(9)	Dy5	O18	2.436(10)
Dy5	N7	2.499(10)			

Table S3 Selected bond angles (°) for complex **1**.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
O19	Dy1	Dy3	37.74(18)	Dy4	O16	Dy1	111.6(3)
O19	Dy1	O16	71.4(3)	O19	Dy1	O6	86.0(3)
O19	Dy1	O15	72.1(3)	Dy5	O6	Dy1	117.8(3)
O19	Dy1	N12	133.7(3)	O19	Dy1	N9	130.6(3)
O16	Dy1	Dy3	106.0(2)	Dy3	O21	Dy1	115.1(3)
O16	Dy1	O15	48.2(3)	Dy5	O15	Dy1	111.3(3)
O6	Dy1	Dy3	88.7(2)	O6	Dy1	O16	108.9(3)
O6	Dy1	O15	60.8(3)	O6	Dy1	N9	62.4(3)
O6	Dy1	N12	123.7(3)	Dy2	O3	Dy4	113.4(3)
O21	Dy1	Dy3	32.3(2)	O21	Dy1	O16	134.2(3)
O21	Dy1	O19	70.1(3)	Dy2	O2	Dy3	106.8(3)

O21	Dy1	O6	92.2(3)	O21	Dy1	O7	98.2(3)
O21	Dy1	O15	134.6(3)	Dy2	O14	Dy4	105.3(3)
O21	Dy1	O22	144.2(3)	O21	Dy1	N9	74.0(3)
O21	Dy1	N12	73.8(3)	Dy4	O7	Dy1	118.8(3)
O15	Dy1	Dy3	106.17(19)	O7	Dy1	Dy3	98.1(2)
O7	Dy1	O19	93.9(3)	O7	Dy1	O16	60.8(3)
O7	Dy1	O6	168.9(3)	O7	Dy1	O15	108.6(3)
O7	Dy1	N12	63.5(3)	O7	Dy1	N9	124.3(3)
O22	Dy1	Dy3	174.8(2)	O22	Dy1	O19	145.4(3)
O22	Dy1	O16	78.7(3)	O22	Dy1	O6	87.7(3)
O22	Dy1	O15	75.2(3)	O22	Dy1	O7	86.1(3)
O22	Dy1	N12	76.6(3)	O22	Dy1	N9	74.3(3)
N12	Dy1	Dy3	102.4(2)	N12	Dy1	O16	119.9(3)
N12	Dy1	O15	151.2(3)	N12	Dy1	N9	61.3(3)
N9	Dy1	Dy3	100.8(2)	N9	Dy1	O15	115.4(3)
N9	Dy1	O16	151.8(3)	O19	Dy2	O20	130.6(3)
O19	Dy2	O14	73.9(3)	O19	Dy2	N6	150.9(3)
O19	Dy2	N3	122.4(3)	O20	Dy2	O14	70.5(3)
O20	Dy2	N6	78.2(3)	O20	Dy2	N3	74.7(3)
O3	Dy2	O19	106.9(3)	O3	Dy2	O20	88.6(3)
O3	Dy2	O2	165.2(3)	O3	Dy2	O14	66.0(3)
O3	Dy2	N6	63.9(3)	O3	Dy2	N3	126.8(3)
O2	Dy2	O19	70.0(3)	O2	Dy2	O20	83.3(3)
O2	Dy2	O14	99.6(3)	O2	Dy2	N6	125.8(3)
O2	Dy2	N3	62.7(3)	O14	Dy2	N6	120.5(3)
O14	Dy2	N3	142.7(3)	O10	Dy2	O19	77.7(3)
O10	Dy2	O20	150.6(3)	O10	Dy2	O3	89.9(3)
O10	Dy2	O2	103.2(3)	O10	Dy2	O14	134.5(3)
O10	Dy2	N6	74.9(3)	N6	Dy2	N3	63.3(3)
O10	Dy2	N3	82.8(3)	O19	Dy3	N1	128.5(3)
O21	Dy3	O19	71.0(3)	O21	Dy3	O2	140.1(3)
O21	Dy3	O12	96.0(3)	O21	Dy3	O13	87.7(3)
O21	Dy3	N1	156.3(3)	O2	Dy3	O19	70.0(3)
O2	Dy3	N1	62.7(3)	O1	Dy3	O19	157.7(3)
O1	Dy3	O21	86.9(3)	O1	Dy3	O12	97.5(3)
O1	Dy3	O13	101.6(3)	O1	Dy3	N1	72.5(3)
O12	Dy3	O19	82.8(3)	O12	Dy3	O2	87.5(3)
O12	Dy3	O13	160.7(3)				

Table S4 Crystal data and structure refinement details for complex **2**.

Empirical formula	$C_{74}H_{65}N_{16}O_{25}Tb_5$
Formula weight	2373.02
Temperature/K	150.01
Crystal system	triclinic
Space group	*P*-1
a/Å	15.4410(9)
b/Å	17.2204(10)
c/Å	20.4129(11)
α/°	111.301(2)
β/°	90.017(2)
γ/°	101.333(2)
Volume/Å^3	4943.1(5)
Z	2
ρ_{calc}mg/mm^3	1.594
m/mm^{-1}	3.602
F(000)	2292.0
Crystal size/mm^3	0.26 × 0.21 × 0.14
Radiation	MoKα (λ = 0.71073)
2θ range for data collection/°	4.296 to 52.986
Index ranges	-19 ≤ h ≤ 19, -21 ≤ k ≤ 21, -25 ≤ l ≤ 25
Reflections collected	105653
Independent reflections	20401 [Rint = 0.0770, Rsigma = 0.0535]
Data/restraints/parameters	20401/13/1097
Goodness-of-fit on F^2	1.036
Final R indexes [I>=2σ (I)]	R_1 = 0.0458, wR_2 = 0.1098
Largest diff. peak/hole / e Å^{-3}	2.30/-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 S5 Selected bond lengths (Å) for complex **2**.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
Tb4	Tb3	3.7640(5)	Tb4	O15	2.641(5)
Tb4	O22	2.237(5)	Tb4	O6	2.428(5)
Tb4	O16	2.634(5)	Tb4	O21	2.410(4)
Tb4	O7	2.421(5)	Tb4	O20	2.369(5)
Tb4	N14	2.579(6)	Tb4	N11	2.600(6)
Tb2	O2	2.307(5)	Tb2	O21	2.381(4)
Tb2	O3	2.318(5)	Tb2	O12	2.222(5)
Tb2	O19	2.377(5)	Tb2	O13	2.434(5)
Tb2	N3	2.524(6)	Tb2	N6	2.552(6)

Tb3	O22	2.227(5)	Tb3	O21	2.391(5)
Tb3	O3	2.321(4)	Tb3	O14	2.328(5)
Tb3	O10	2.293(5)	Tb3	O4	2.220(5)
Tb3	N8	2.517(6)	Tb5	O6	2.400(5)
Tb5	O16	2.365(5)	Tb5	O11	2.354(5)
Tb5	O9	2.320(5)	Tb5	O5	2.182(5)
Tb5	O17	2.427(5)	Tb5	O18	2.437(5)
Tb5	N9	2.477(6)	Tb1	O15	2.374(5)
Tb1	O2	2.374(5)	Tb1	O7	2.397(5)
Tb1	O1	2.183(5)	Tb1	O13	2.482(5)
Tb1	O8	2.239(5)	Tb1	N16	2.482(6)
Tb1	N1	2.528(7)			

Table S6 Selected bond angles (°) for complex **2**.

Atom	**Atom**	**Atom**	**Angle/°**	**Atom**	**Atom**	**Atom**	**Angle/°**
O22	Tb4	O15	134.50(17)	O22	Tb4	O16	134.89(17)
O22	Tb4	O6	92.65(18)	O22	Tb4	O21	70.60(16)
O22	Tb4	O7	98.11(18)	O22	Tb4	N14	73.47(18)
O22	Tb4	O20	144.57(19)	Tb2	O2	Tb1	113.67(19)
O22	Tb4	N11	74.21(18)	O6	Tb4	N11	62.46(17)
O6	Tb4	O15	109.00(16)	Tb2	O21	Tb3	102.84(17)
O6	Tb4	O16	60.54(16)	Tb3	O21	Tb4	103.27(17)
O6	Tb4	N14	124.20(17)	Tb1	O7	Tb4	119.1(2)
O16	Tb4	O15	48.52(15)	Tb2	O3	Tb3	107.07(18)
O21	Tb4	O15	71.37(16)	O21	Tb4	O7	93.03(16)
O21	Tb4	O6	86.47(16)	O21	Tb4	N14	133.34(18)
O21	Tb4	O16	72.07(16)	O21	Tb4	N11	131.27(17)
O7	Tb4	O15	60.09(16)	Tb2	O13	Tb1	105.70(19)
O7	Tb4	O6	168.41(17)	O7	Tb4	O16	108.30(16)
O7	Tb4	N14	63.65(17)	O20	Tb4	O15	77.68(18)
O7	Tb4	N11	124.75(17)	O20	Tb4	O6	87.79(18)
O20	Tb4	O16	74.75(19)	O20	Tb4	N14	77.1(2)
O20	Tb4	O21	144.63(19)	O20	Tb4	N11	74.7(2)
O20	Tb4	O7	85.94(18)	N11	Tb4	O16	115.12(18)
N14	Tb4	O15	119.14(17)	N14	Tb4	N11	61.75(18)
N14	Tb4	O16	151.27(18)	N11	Tb4	O15	151.29(18)
O2	Tb2	O21	105.93(17)	O2	Tb2	O19	89.42(18)
O2	Tb2	O3	165.14(17)	O2	Tb2	O13	65.88(16)
O2	Tb2	N3	64.22(17)	O21	Tb2	N3	150.83(18)
O2	Tb2	N6	127.18(17)	O21	Tb2	N6	122.88(17)

O21	Tb2	O13	73.79(16)	O3	Tb2	O21	70.30(16)
O3	Tb2	O19	82.97(18)	O3	Tb2	N6	62.95(17)
O3	Tb2	O13	99.45(17)	O12	Tb2	O2	89.70(19)
O3	Tb2	N3	125.99(17)	O12	Tb2	O21	77.74(18)
O12	Tb2	O3	103.16(19)	N10	N9	Tb5	117.1(4)
O12	Tb2	O19	150.81(18)	O19	Tb2	N3	78.46(18)
O12	Tb2	O13	134.74(19)	O19	Tb2	N6	74.78(18)
O12	Tb2	N3	74.93(19)	O13	Tb2	N6	142.57(18)
O12	Tb2	N6	82.65(19)	N3	Tb2	N6	63.32(18)
O19	Tb2	O21	130.28(16)	O22	Tb3	O21	71.13(17)
O19	Tb2	O13	70.21(17)	O22	Tb3	O3	140.31(18)
O22	Tb3	O10	95.61(18)	O22	Tb3	O14	88.05(18)
O22	Tb3	N8	155.85(18)	O3	Tb3	O21	70.07(16)
O21	Tb3	N8	128.91(17)	O3	Tb3	O14	77.74(18)
O10	Tb3	O3	87.43(18)	O10	Tb3	O21	82.56(17)
O10	Tb3	O14	160.49(18)	O14	Tb3	N8	107.09(18)
O10	Tb3	N8	76.48(19)	O14	Tb3	O21	80.52(17)

Table S7 Crystal data and structure refinement details for complex **3**.

Empirical formula	$C_{74}H_{65}Gd_5N_{16}O_{25}$
Formula weight	2364.67
Temperature/K	150.15
Crystal system	triclinic
Space group	*P*-1
a/Å	15.3903(11)
b/Å	17.2122(14)
c/Å	20.4239(16)
α/°	111.207(3)
β/°	90.116(4)
γ/°	101.204(3)
Volume/Å^3	4932.3(7)
Z	2
ρ_{calc}mg/mm^3	1.592
m/mm^{-1}	3.387
F(000)	2282.0
Crystal size/mm^3	0.26 × 0.21 × 0.14
Radiation	MoKα (λ = 0.71073)
2θ range for data collection/°	4.35 to 52.044
Index ranges	-18 ≤ h ≤ 18, -21 ≤ k ≤ 21, -25 ≤ l ≤ 25
Reflections collected	81851

Independent reflections	19104 [R_{int} = 0.1003, R_{sigma} = 0.0810]
Data/restraints/parameters	19104/37/1097
Goodness-of-fit on F^2	0.999
Final R indexes [I>=2σ (I)]	R_1 = 0.0531, wR_2 = 0.1289
Largest diff. peak/hole / e $Å^{-3}$	2.47/-1.87

Table S8 Selected bond lengths (Å) for complex **3.**

Atom	Atom	Length/Å	Atom	Atom	Length/Å
Gd2	O19	2.383(6)	Gd2	O15	2.466(5)
Gd2	N6	2.545(7)	Gd2	O12	2.236(6)
Gd2	O3	2.329(6)	Gd2	O2	2.338(5)
Gd2	N3	2.559(7)	Gd2	O20	2.395(5)
Gd1	O18	2.310(6)	Gd1	O1	2.231(6)
Gd1	O21	2.238(6)	Gd1	O16	2.321(6)
Gd1	N1	2.528(7)	Gd1	O2	2.328(5)
Gd1	O20	2.404(5)	Gd3	O9	2.440(6)
Gd3	O11	2.366(6)	Gd3	O8	2.187(6)
Gd3	O13	2.381(6)	Gd3	O7	2.415(5)
Gd3	O17	2.339(6)	Gd3	O10	2.433(6)
Gd3	C62	2.789(10)	Gd3	N16	2.496(8)
Gd4	O21	2.260(6)	Gd4	O14	2.644(6)
Gd4	O6	2.440(6)	Gd4	N14	2.600(7)
Gd4	O13	2.642(6)	Gd4	N11	2.576(7)
Gd4	O7	2.429(6)	Gd5	N8	2.539(8)
Gd4	O20	2.417(5)	Gd4	O22	2.396(6)
Gd5	O15	2.492(6)	Gd5	O14	2.390(6)
Gd5	O6	2.406(6)	Gd5	O4	2.213(7)
Gd5	O3	2.390(6)	Gd5	O5	2.259(6)
Gd5	N9	2.489(8)			

Table S9 Selected bond angles (°) for complex **3.**

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
O19	Gd2	O15	70.3(2)	O19	Gd2	O20	130.13(18)
O19	Gd2	N6	78.3(2)	O15	Gd2	N3	142.8(2)
O19	Gd2	N3	74.8(2)	N6	Gd2	N3	62.7(2)
O15	Gd2	N6	120.4(2)	Gd2	O15	Gd5	105.3(2)
O12	Gd2	O19	150.8(2)	Gd5	O14	Gd4	111.7(2)
O12	Gd2	O15	134.9(2)	O12	Gd2	O3	89.9(2)

O12	Gd2	N6	75.1(2)	O12	Gd2	N3	82.3(2)
O12	Gd2	O2	102.6(2)	Gd5	O6	Gd4	118.7(2)
O12	Gd2	O20	77.8(2)	O20	Gd2	N3	122.8(2)
O3	Gd2	O19	89.3(2)	O18	Gd1	O16	159.5(2)
O3	Gd2	O15	66.16(19)	O18	Gd1	N1	75.7(2)
O3	Gd2	N6	64.1(2)	O18	Gd1	O2	86.8(2)
O3	Gd2	O2	165.78(19)	O18	Gd1	O20	82.2(2)
O3	Gd2	N3	126.5(2)	O1	Gd1	O18	97.7(2)
O3	Gd2	O20	106.6(2)	O1	Gd1	O21	86.8(2)
O2	Gd2	O19	83.1(2)	O1	Gd1	O16	102.6(2)
O2	Gd2	O15	99.87(19)	O1	Gd1	N1	72.3(2)
O2	Gd2	N6	125.3(2)	O1	Gd1	O2	132.3(2)
O2	Gd2	N3	62.9(2)	O1	Gd1	O20	157.6(2)
O2	Gd2	O20	70.14(19)	O21	Gd1	O18	96.4(2)
O20	Gd2	O15	73.8(2)	O21	Gd1	O16	87.6(2)
O20	Gd2	N6	151.3(2)	O21	Gd1	N1	156.1(2)
O21	Gd1	O20	70.98(19)	O21	Gd1	O2	140.1(2)
O16	Gd1	N1	107.7(2)	O13	C66	C65	120.5(8)
O16	Gd1	O2	77.5(2)	O8	Gd3	O7	134.6(2)
O16	Gd1	O20	80.1(2)	O2	Gd1	N1	62.9(2)
O2	Gd1	O20	70.13(18)	O11	Gd3	O13	79.3(2)
O20	Gd1	Gd2	38.60(13)	O11	Gd3	O7	132.6(2)
O20	Gd1	N1	128.60(19)	O11	Gd3	O10	128.3(2)
O9	Gd3	C62	26.5(2)	O11	Gd3	C62	101.4(3)
O9	Gd3	N16	117.0(2)	O11	Gd3	N16	149.1(2)
O8	Gd3	O13	160.0(2)	O8	Gd3	O9	88.1(2)
O8	Gd3	O17	88.6(2)	O8	Gd3	O11	81.8(2)
O8	Gd3	O10	106.9(2)	Gd2	O20	Gd1	102.6(2)
O8	Gd3	N16	71.6(2)	Gd1	O20	Gd4	103.69(19)
O13	Gd3	O9	81.2(2)	O13	Gd3	N16	128.4(2)
O13	Gd3	O7	64.8(2)	O13	Gd3	O10	80.2(2)
O17	Gd3	O11	77.5(2)	O17	Gd3	O9	154.0(2)
O17	Gd3	O7	75.0(2)	O17	Gd3	O13	93.7(2)
O17	Gd3	O10	150.8(2)	O17	Gd3	N16	86.2(2)
O7	Gd3	O10	76.5(2)	O7	Gd3	O9	123.8(2)
O7	Gd3	N16	65.4(2)	O10	Gd3	O9	53.6(2)
O21	Gd4	Gd1	32.37(14)	O10	Gd3	N16	75.9(2)

Atom	**Atom**	**Atom**	**Angle/°**	**Atom**	**Atom**	**Atom**	**Angle/°**
Dy2	Dy1	Dy4	73.714(9)	O7	Dy5	N12	64.72(18)
O20	Dy1	N1	128.46(16)	O22	Dy5	N12	76.0(2)

O19	Dy1	O20	70.87(16)	Dy2	O20	Dy1	102.85(18)
O19	Dy1	O1	87.50(17)	Dy2	O20	Dy4	140.7(2)
O19	Dy1	O2	139.74(17)	Dy1	O19	Dy4	114.6(2)
O19	Dy1	O9	87.14(18)	O19	Dy1	N1	156.91(17)
O19	Dy1	O11	95.40(19)	O1	Dy1	O20	158.36(16)
O1	Dy1	O2	131.38(17)	O1	Dy1	O11	101.02(18)
O1	Dy1	O9	97.77(18)	O1	Dy1	N1	72.73(16)
O3	Dy2	O20	105.03(16)	O2	Dy1	O20	69.83(15)
O3	Dy2	O2	165.88(17)	O2	Dy1	O9	78.58(17)
O3	Dy2	O21	92.32(17)	O2	Dy1	N1	62.63(16)
O3	Dy2	O10	65.50(16)	O9	Dy1	O20	81.10(17)
O3	Dy2	N3	127.96(17)	O9	Dy1	N1	106.86(18)
O2	Dy2	O20	69.81(16)	O11	Dy1	O20	82.09(17)
O2	Dy2	O21	81.60(18)	O11	Dy1	O2	87.63(18)
O2	Dy2	O10	100.40(15)	O11	Dy1	O9	161.13(16)
O2	Dy2	N3	62.74(15)	O11	Dy1	N1	77.36(19)
O2	Dy2	N4	126.77(17)	O20	Dy2	O10	72.98(16)
O21	Dy2	O20	128.13(16)	O20	Dy2	N3	122.91(17)
O21	Dy2	O10	70.83(16)	O20	Dy2	N4	150.62(18)
O21	Dy2	N3	74.46(18)	O15	Dy2	N3	81.96(19)
O21	Dy2	N4	80.82(18)	O15	Dy2	N4	74.84(19)
O15	Dy2	O20	78.10(17)	O10	Dy2	N3	143.36(18)
O15	Dy2	O3	89.93(18)	O10	Dy2	N4	119.97(17)
O15	Dy2	O2	101.49(18)	N4	Dy2	N3	64.19(18)
O15	Dy2	O21	151.67(17)	O20	Dy4	O13	72.29(15)
O15	Dy2	O10	134.61(18)	O20	Dy4	O14	72.05(16)
O20	Dy4	O7	84.62(17)	O20	Dy4	O6	93.35(16)
O20	Dy4	N9	136.31(18)	O20	Dy4	N10	130.31(16)
O17	Dy4	O14	73.82(18)	O17	Dy4	N9	75.0(2)
O17	Dy4	O6	86.99(19)	O17	Dy4	N10	75.94(19)
O17	Dy4	O7	89.1(2)	O6	Dy4	O13	61.27(16)
O6	Dy4	O14	110.11(16)	O6	Dy4	N10	124.42(17)
O7	Dy4	O13	109.21(16)	O6	Dy4	N9	62.88(17)
O7	Dy4	O6	170.35(17)	O7	Dy4	O14	60.29(15)

Table S10 Crystal data and structure refinement details for complex **4**.

Empirical formula	$C_{67}H_{61}Dy_5N_{12}O_{25}$
Formula weight	2246.77
Temperature/K	293(2)
Crystal system	triclinic

Space group	*P*-1
a/Å	15.4027(2)
b/Å	15.9505(3)
c/Å	19.8366(4)
α/°	108.286(2)
β/°	90.116(4)
γ/°	102.3810(10)
Volume/Å^3	4456.31(15)
Z	2
ρ_{calc}mg/mm^3	1.674
m/mm^{-1}	2.630
F(000)	2154.0
Crystal size/mm^3	0.3 × 0.2 × 0.1
Radiation	CuKα (λ = 1.54178)
2θ range for data collection/°	4.758 to 153.166
Index ranges	-19 ≤ h ≤ 19, -20 ≤ k ≤ 19, -24 ≤ l ≤ 24
Reflections collected	54969
Independent reflections	18000 [R_{int} = 0.0510, R_{sigma} = 0.0464]
Data/restraints/parameters	18000/18/1007
Goodness-of-fit on F^2	1.108
Final R indexes [I>=2σ (I)]	R_1 = 0.0481, wR_2 = 0.1243
Largest diff. peak/hole / e Å^{-3}	1.92/-1.75

Table S11 Selected bond lengths (Å) for complex **4.**

Atom	**Atom**	**Length/Å**	**Atom**	**Atom**	**Length/Å**
Dy2	O2	2.444(5)	Dy2	O21	2.388(5)
Dy2	O3	2.438(5)	Dy2	O13	2.647(5)
Dy2	O14	2.578(5)	Dy2	O19	2.369(5)
Dy2	N3	2.595(6)	Dy2	N4	2.606(6)
Dy4	O7	2.310(5)	Dy4	O6	2.335(5)
Dy4	O21	2.409(4)	Dy4	O22	2.368(5)
Dy4	O16	2.249(5)	Dy4	O17	2.415(5)
Dy4	N9	2.517(5)	Dy4	N10	2.509(6)
Dy3	O6	2.363(5)	Dy3	O3	2.383(4)
Dy3	O14	2.351(4)	Dy3	O17	2.409(5)
Dy3	O5	2.244(5)	Dy3	O4	2.236(5)
Dy3	N6	2.484(6)	Dy3	N7	2.507(6)
Dy1	O2	2.408(5)	Dy1	O1	2.198(5)
Dy1	O13	2.361(4)	Dy1	O15	2.331(5)
Dy1	O11	2.459(5)	Dy1	O9	2.291(5)

Dy1	O12	2.482(5)	Dy1	N1	2.450(6)
Dy5	O7	2.353(5)	Dy5	O21	2.404(4)
Dy5	O8	2.234(5)	Dy5	O20	2.271(5)
Dy5	O18	2.370(5)	Dy5	O10	2.367(6)
Dy5	N12	2.523(6)	Dy5	O23	2.454(7)

Table S12 Selected bond angles (°) for complex **4.**

Atom	**Atom**	**Atom**	**Angle/°**	**Atom**	**Atom**	**Atom**	**Angle/°**
O2	Dy2	O13	59.37(14)	O18	Dy5	O23	144.2(3)
O2	Dy2	O14	108.63(15)	O10	Dy5	Dy2	96.12(15)
O2	Dy2	N3	62.34(16)	O10	Dy5	Dy4	87.99(15)
O2	Dy2	N4	124.00(17)	O10	Dy5	O21	80.92(18)
O21	Dy2	O2	84.58(15)	O10	Dy5	O23	67.7(3)
O21	Dy2	O3	96.14(15)	N12	Dy5	Dy2	166.62(13)
O21	Dy2	O13	72.73(14)	N12	Dy5	Dy4	97.45(13)
O21	Dy2	O14	74.21(15)	O23	Dy5	Dy2	89.7(2)
O21	Dy2	N3	128.44(17)	O23	Dy5	Dy4	148.1(2)
O21	Dy2	N4	137.11(17)	O23	Dy5	N12	95.6(2)
O3	Dy2	O2	168.84(15)	O20	Dy2	O2	97.67(19)
O3	Dy2	O13	110.15(14)	O20	Dy2	O21	69.52(16)
O3	Dy2	O14	61.17(14)	O20	Dy2	O3	92.99(19)
O3	Dy2	N3	123.92(16)	O20	Dy2	O13	137.39(17)
O3	Dy2	N4	62.12(16)	O20	Dy2	O14	132.39(17)
O20	Dy2	N3	76.70(18)	O20	Dy2	O19	146.26(18)
O20	Dy2	N4	74.97(19)	Dy2	O20	Dy5	115.2(2)
O14	Dy2	O13	49.29(14)	O19	Dy2	N4	74.12(18)
O14	Dy2	N3	150.79(16)	N3	Dy2	O13	114.14(16)
O14	Dy2	N4	116.79(17)	N3	Dy2	N4	61.96(18)
O19	Dy2	O2	88.59(16)	N4	Dy2	O13	147.41(17)
O19	Dy2	O21	144.22(16)	O7	Dy4	O6	164.56(17)
O19	Dy2	O3	84.34(17)	O7	Dy4	O21	70.74(16)
O19	Dy2	O13	73.60(16)	O7	Dy4	O22	84.14(17)
O19	Dy2	O14	74.88(16)	O7	Dy4	O17	98.22(17)
O19	Dy2	N3	77.10(18)	O7	Dy4	N9	126.91(18)
O22	Dy4	O21	132.41(16)	O6	Dy4	O21	105.56(16)
O22	Dy4	O17	71.49(17)	O6	Dy4	O22	88.13(17)
O22	Dy4	N9	78.65(17)	O6	Dy4	O17	66.59(16)
O22	Dy4	N10	75.20(18)	O6	Dy4	N9	64.02(17)
O16	Dy4	O7	103.46(19)	O6	Dy4	N10	127.03(17)
O16	Dy4	O6	90.02(18)	O21	Dy4	O17	72.96(16)

O16	Dy4	O21	77.72(16)	O21	Dy4	N9	148.41(16)
O16	Dy4	O22	148.97(18)	O21	Dy4	N10	122.91(17)
O16	Dy4	O17	134.99(18)	O16	Dy4	N10	81.37(19)
O17	Dy4	N9	122.15(17)	O6	Dy3	O17	66.25(16)
O17	Dy4	N10	143.52(17)	N10	Dy4	N9	63.51(18)
O6	Dy3	N6	150.19(19)	O6	Dy3	O3	123.80(16)
O6	Dy3	N7	62.98(17)	O3	Dy3	N6	64.95(18)
O3	Dy3	O17	73.43(16)	O3	Dy3	N7	151.58(18)
O14	Dy3	O6	75.16(17)	O14	Dy3	N6	127.68(19)
O14	Dy3	O3	65.32(16)	O14	Dy3	N7	93.63(18)
O14	Dy3	O17	87.41(17)	O17	Dy3	Dy4	36.43(11)
O17	Dy3	N7	126.98(17)	O17	Dy3	N6	93.36(19)

Table S13 Crystal data and structure refinement details for complex **5**.

Empirical formula	$C_{72}H_{66}Dy_5N_{12}O_{25}$
Formula weight	2311.86
Temperature/K	293(2)
Crystal system	triclinic
Space group	*P*-1
a/Å	15.3856(2)
b/Å	16.2878(2)
c/Å	19.7277(2)
α/°	78.4020(10)
β/°	74.5510(10)
γ/°	78.4430(10)
Volume/Å^3	4611.04(10)
Z	2
ρ_{calc}mg/mm^3	1.665
m/mm^{-1}	2.189
F(000)	2224.0
Crystal size/mm^3	0.38 × 0.26 × 0.22
Radiation	CuKα (λ = 1.54178)
2θ range for data collection/°	4.704 to 153.38
Index ranges	-19 ≤ h ≤ 19, -20 ≤ k ≤ 20, -24 ≤ l ≤ 18
Reflections collected	57142
Independent reflections	18701 [R_{int} = 0.0457, R_{sigma} = 0.0425]
Data/restraints/parameters	18701/11/1051
Goodness-of-fit on F^2	1.130
Final R indexes [I>=2σ (I)]	R_1 = 0.0432, wR_2 = 0.1088
Largest diff. peak/hole / e Å^{-3}	1.71/-1.97

Table S14 Selected bond lengths (Å) for complex **5.**

Atom	Atom	Length/Å	Atom	Atom	Length/Å
Dy4	O25	2.386(4)	Dy4	O6	2.392(4)
Dy4	O7	2.426(4)	Dy4	O16	2.560(4)
Dy4	O23	2.354(4)	Dy4	O10	2.308(4)
Dy4	O15	2.621(4)	Dy4	N9	2.599(5)
Dy4	N10	2.594(5)	Dy1	O2	2.328(4)
Dy1	O25	2.364(4)	Dy1	O11	2.367(4)
Dy1	O20	2.332(4)	Dy1	O1	2.213(4)
Dy1	O10	2.407(4)	Dy1	O22	2.450(5)
Dy1	N1	2.512(5)	Dy2	O2	2.314(4)
Dy2	O12	2.410(4)	Dy2	O3	2.302(4)
Dy2	O25	2.429(4)	Dy2	O14	2.258(4)
Dy2	N3	2.550(5)	Dy2	N4	2.531(5)
Dy2	O21	2.393(4)	Dy3	O12	2.481(4)
Dy3	O6	2.400(4)	Dy3	O4	2.208(4)
Dy3	O3	2.369(4)	Dy3	O16	2.389(4)
Dy3	O5	2.197(4)	Dy5	O7	2.414(4)
Dy3	N7	2.491(5)	Dy5	O15	2.350(4)
Dy3	N6	2.522(5)	Dy5	O18	2.429(5)
Dy5	O8	2.197(5)	Dy5	O17	2.450(5)
Dy5	O13	2.332(5)	Dy5	O19	2.309(5)
Dy5	N12	2.468(6)			

Table S15 Selected bond angles (°) for complex **5**.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
O25	Dy4	O6	98.81(13)	O13	Dy5	C66	103.2(2)
O25	Dy4	O7	79.66(14)	O19	Dy5	O7	76.21(16)
O25	Dy4	O16	74.45(13)	O19	Dy5	O15	94.80(15)
O25	Dy4	O15	72.76(13)	O19	Dy5	O18	151.37(17)
O25	Dy4	N9	140.75(14)	O19	Dy5	O17	153.97(18)
O25	Dy4	N10	125.36(15)	O19	Dy5	O13	76.62(18)
O6	Dy4	O7	171.09(14)	N12	Dy5	C66	101.2(2)
O6	Dy4	O16	61.74(13)	Dy2	O2	Dy1	108.53(15)
O6	Dy4	O15	110.63(13)	Dy1	O25	Dy4	107.48(15)
O6	Dy4	N9	62.69(14)	Dy1	O25	Dy2	103.64(14)
O6	Dy4	N10	124.31(15)	Dy2	O12	Dy3	106.13(15)
O7	Dy4	O16	109.54(14)	Dy4	O25	Dy2	134.40(17)
O7	Dy4	O15	60.49(14)	O7	Dy4	N9	123.67(15)
O7	Dy4	N10	62.30(16)	Dy4	O6	Dy3	116.81(15)

O16	Dy4	O15	49.47(12)	O16	Dy4	N10	152.50(15)
O16	Dy4	N9	117.30(14)	O23	Dy4	O25	144.80(15)
O23	Dy4	O16	77.88(14)	O23	Dy4	O6	86.64(14)
O23	Dy4	O15	72.80(15)	Dy3	O16	Dy4	111.09(15)
O23	Dy4	N9	72.19(16)	O10	Dy4	O23	144.20(15)
O23	Dy4	N10	75.92(16)	O10	Dy4	O15	141.20(14)
O10	Dy4	O25	70.97(14)	O10	Dy4	N9	74.01(15)
O10	Dy4	O6	88.24(15)	O10	Dy4	N10	77.97(16)
O10	Dy4	O7	99.45(16)	N9	Dy4	O15	144.67(15)
O10	Dy4	O16	129.31(14)	N10	Dy4	O15	113.52(15)
Dy5	O7	Dy4	118.24(18)	N10	Dy4	N9	61.63(16)
Dy2	O3	Dy3	113.62(16)	O2	Dy1	O25	70.84(14)
O2	Dy1	O11	72.44(14)	O25	Dy1	O22	102.23(17)
O2	Dy1	O20	75.97(16)	O25	Dy1	N1	131.17(14)
O2	Dy1	O10	132.12(14)	O11	Dy1	O10	74.56(15)
O2	Dy1	O22	146.45(16)	O11	Dy1	O22	140.00(16)
O2	Dy1	N1	62.84(15)	O11	Dy1	N1	99.96(15)
O25	Dy1	O11	79.27(13)	O20	Dy1	O25	81.76(14)
O25	Dy1	O10	69.68(13)	O20	Dy1	O11	147.04(15)
O1	Dy1	O2	122.64(16)	O20	Dy1	O10	122.92(16)
O1	Dy1	O25	153.24(14)	O20	Dy1	O22	70.52(17)
O1	Dy1	O11	83.36(15)	O1	Dy1	O20	122.49(16)
O1	Dy1	N1	71.79(16)	O1	Dy1	O10	86.20(15)
O10	Dy1	O22	68.94(18)	O1	Dy1	O22	78.55(18)
O10	Dy1	N1	157.86(15)	O2	Dy2	O25	69.92(13)
O22	Dy1	N1	107.60(19)	O2	Dy2	N3	62.85(14)
O2	Dy2	O12	97.78(14)	O2	Dy2	O21	82.57(15)
O12	Dy2	O25	72.70(13)	O2	Dy2	N4	125.72(15)
O12	Dy2	N4	122.39(15)	O12	Dy2	N3	143.76(15)
O25	Dy2	N4	150.79(14)	O25	Dy2	N3	121.32(14)

Table S16 Crystal data and structure refinement details for complex **6**.

Empirical formula	$C_{66}H_{57}Dy_5N_{12}O_{23}$
Formula weight	2198.73
Temperature/K	293(2)
Crystal system	triclinic
Space group	*P*-1
a/Å	15.6215(3)
b/Å	16.9622(3)
c/Å	20.0435(4)

α/°	74.828(2)
β/°	73.689(2)
γ/°	62.780(2)
Volume/Å^3	4477.19(17)
Z	2
ρ_{calc}mg/mm^3	1.432
m/mm^{-1}	4.918
F(000)	2102.0
Crystal size/mm^3	0.36 × 0.29 × 0.24
Radiation	MoKα (λ = 0.71073)
2θ range for data collection/°	3.332 to 60.456
Index ranges	-18 ≤ h ≤ 21, -22 ≤ k ≤ 20, -26 ≤ l ≤ 25
Reflections collected	51813
Independent reflections	20688 [R_{int} = 0.0428, R_{sigma} = 0.0550]
Data/restraints/parameters	20688/16/976
Goodness-of-fit on F^2	1.022
Final R indexes [I>=2σ (I)]	R_1 = 0.0468, wR_2 = 0.1176
Largest diff. peak/hole / e Å^{-3}	3.31/-1.71

Table S17 Selected bond lengths (Å) for complex **6.**

Atom	Atom	Length/Å	Atom	Atom	Length/Å
Dy1	O20	2.387(4)	Dy1	O9	2.322(5)
Dy1	O19	2.224(4)	Dy1	O11	2.276(5)
Dy1	O1	2.224(4)	Dy1	N1	2.536(5)
Dy1	O2	2.316(4)	Dy2	O20	2.373(4)
Dy2	O3	2.312(4)	Dy2	O10	2.455(5)
Dy2	O2	2.332(4)	Dy2	N3	2.527(6)
Dy2	O21	2.368(5)	Dy2	N4	2.509(5)
Dy2	O15	2.250(5)	Dy4	O20	2.391(4)
Dy4	O19	2.241(5)	Dy4	O6	2.430(5)
Dy4	O13	2.597(5)	Dy4	O7	2.423(5)
Dy4	O17	2.368(6)	Dy4	N10	2.587(6)
Dy4	O14	2.659(5)	Dy4	N9	2.605(5)
Dy3	O3	2.354(5)	Dy3	O10	2.462(4)
Dy3	O4	2.207(5)	Dy3	O5	2.249(6)
Dy3	O13	2.406(5)	Dy3	N7	2.486(7)
Dy3	O6	2.391(5)	Dy3	N6	2.509(6)
Dy5	O12	2.310(6)	Dy5	O7	2.407(5)
Dy5	O16	2.360(5)	Dy5	O22	2.384(7)
Dy5	O14	2.372(5)	Dy5	O23	2.418(6)

Dy5	N12	2.478(6)	Dy5	O8	2.221(5)

Table S18 Selected bond angles (°) for complex **6**.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
O20	Dy1	N1	128.46(16)	O22	Dy5	N12	76.0(2)
O19	Dy1	O20	70.87(16)	Dy2	O20	Dy1	102.85(18)
O19	Dy1	O1	87.50(17)	Dy2	O20	Dy4	140.7(2)
O19	Dy1	O2	139.74(17)	Dy1	O19	Dy4	114.6(2)
O19	Dy1	O9	87.14(18)	O19	Dy1	N1	156.91(17)
O19	Dy1	O11	95.40(19)	Dy2	O3	Dy3	113.84(19)
O1	Dy1	O2	131.38(17)	O1	Dy1	O20	158.36(16)
O1	Dy1	O9	97.77(18)	O1	Dy1	O11	101.02(18)
O2	Dy1	O20	69.83(15)	O1	Dy1	N1	72.73(16)
O2	Dy1	O9	78.58(17)	O2	Dy1	N1	62.63(16)
O9	Dy1	O20	81.10(17)	O9	Dy1	N1	106.86(18)
O11	Dy1	O9	161.13(16)	O2	Dy2	O20	69.81(16)
O11	Dy1	N1	77.36(19)	O2	Dy2	O21	81.60(18)
O20	Dy2	O10	72.98(16)	O2	Dy2	O10	100.40(15)
O20	Dy2	N3	122.91(17)	O2	Dy2	N3	62.74(15)
O20	Dy2	N4	150.62(18)	O2	Dy2	N4	126.77(17)
O3	Dy2	O20	105.03(16)	O21	Dy2	O20	128.13(16)
O3	Dy2	O2	165.88(17)	O21	Dy2	O10	70.83(16)
O3	Dy2	O21	92.32(17)	O21	Dy2	N3	74.46(18)
O3	Dy2	O10	65.50(16)	O21	Dy2	N4	80.82(18)
O3	Dy2	N3	127.96(17)	O15	Dy2	O20	78.10(17)
O3	Dy2	N4	64.06(18)	O15	Dy2	O3	89.93(18)
O11	Dy1	O2	87.63(18)	O15	Dy2	O2	101.49(18)
O15	Dy2	O10	134.61(18)	O15	Dy2	N3	81.96(19)
O15	Dy2	O21	151.67(17)	O15	Dy2	N4	74.84(19)
O10	Dy2	N3	143.36(18)	O20	Dy4	O7	84.62(17)
O10	Dy2	N4	119.97(17)	O20	Dy4	N10	130.31(16)
N4	Dy2	N3	64.19(18)	O20	Dy4	N9	136.31(18)
O20	Dy4	Dy1	38.14(10)	O19	Dy4	O20	70.52(15)
O20	Dy4	O13	72.29(15)	O19	Dy4	O13	133.84(17)
O20	Dy4	O14	72.05(16)	O19	Dy4	O17	145.68(18)
O20	Dy4	O6	93.35(16)	O19	Dy4	O14	135.87(16)
O19	Dy4	N10	74.97(18)	O19	Dy4	O6	94.66(18)
O19	Dy4	N9	75.34(17)	O19	Dy4	O7	93.55(18)
O13	Dy4	O14	49.02(15)	O17	Dy4	O13	76.25(18)
O13	Dy4	N9	117.48(16)	O17	Dy4	O14	73.82(18)

O17	Dy4	O20	143.71(18)	O17	Dy4	O6	86.99(19)
O17	Dy4	O7	89.1(2)	O6	Dy4	O13	61.27(16)
O17	Dy4	N10	75.94(19)	O6	Dy4	O14	110.11(16)
O17	Dy4	N9	75.0(2)	O6	Dy4	N10	124.42(17)
O7	Dy4	O14	60.29(15)	O6	Dy4	N9	62.88(17)
O7	Dy4	O6	170.35(17)	O7	Dy4	O13	109.21(16)

Table S19 Inhibitory rates (%) of Ln(III) complexes **1-6**, L, L^1 and cisplatin against A549, HeLa, SK-OV-3, and HL-7702 cells for 48 h.

Compounds	HeLa	A549	SK-OV-3/DDP	HL-7702
L	20.12±0.19	38.96±1.49	15.66±1.01	25.69±2.69
L^1	23.19±0.14	18.06±1.34	15.09±1.57	20.36±2.23
1	54.69±1.10	58.01±0.42	70.25±1.37	40.56±1.58
2	28.06±1.23	38.07±0.49	45.09±0.75	38.48±1.16
3	35.69±0.60	41.03±1.50	53.62±0.32	35.22±0.73
4	42.01±0.29	21.09±1.03	69.02±0.45	25.36±0.79
5	43.69±1.00	24.55±1.36	52.03±1.26	41.58±1.42
6	52.63±0.77	28.74±1.42	59.06±1.10	38.99±0.52
Cisplatin	68.96±0.81	60.53±0.58	35.06±0.27	58.36±1.09

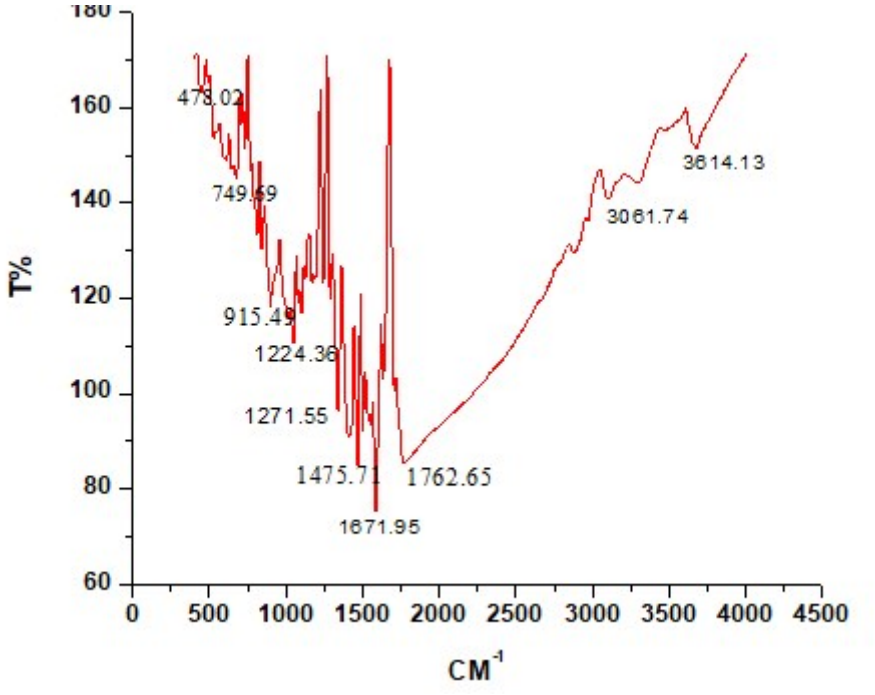

Fig. S1 IR (KBr) spectra of complex **1.**

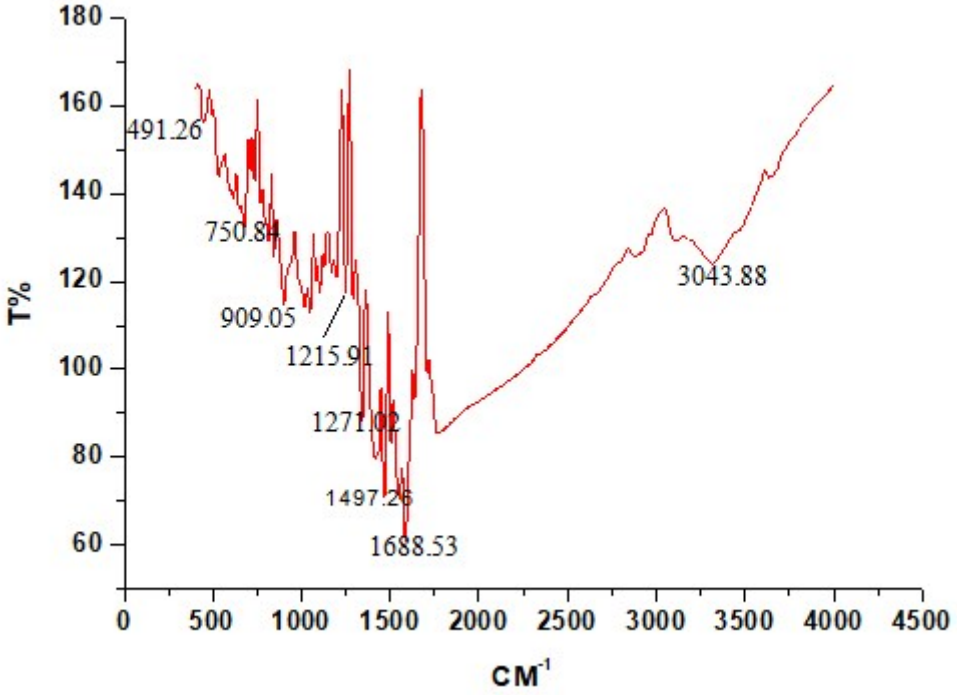

Fig. S2 IR (KBr) spectra of complex **2.**

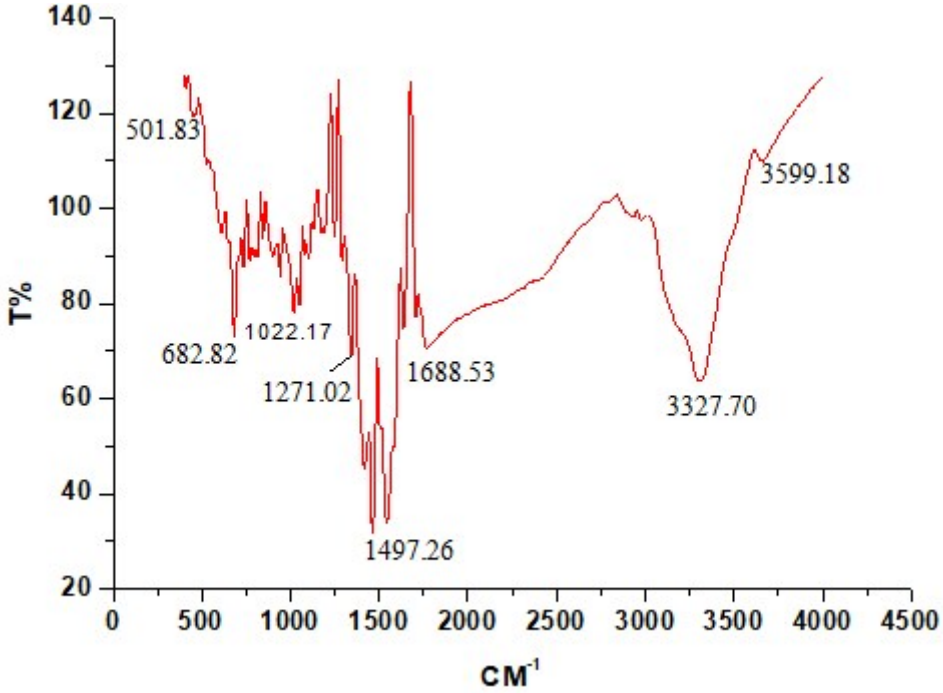

Fig. S3 IR (KBr) spectra of complex **3.**

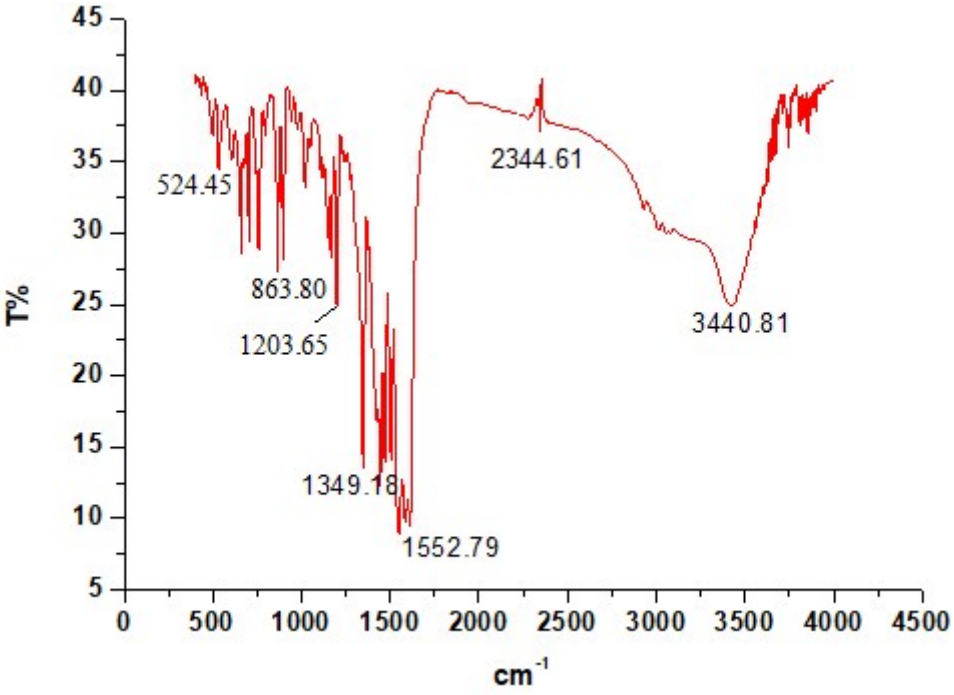

Fig. S4 IR (KBr) spectra of complex **4.**

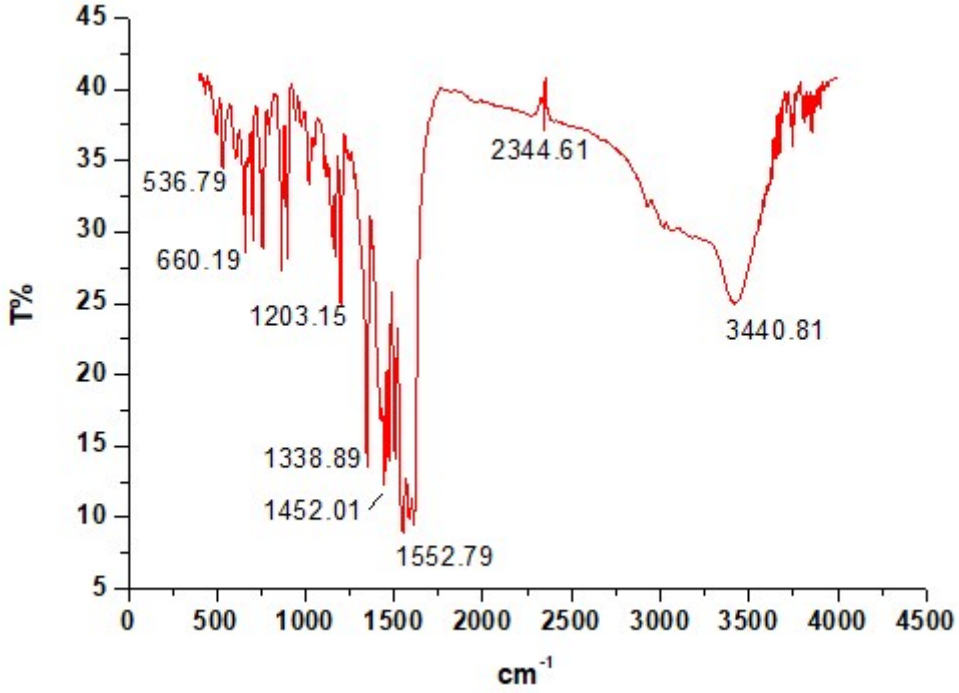

Fig. S5 IR (KBr) spectra of complex **5.**

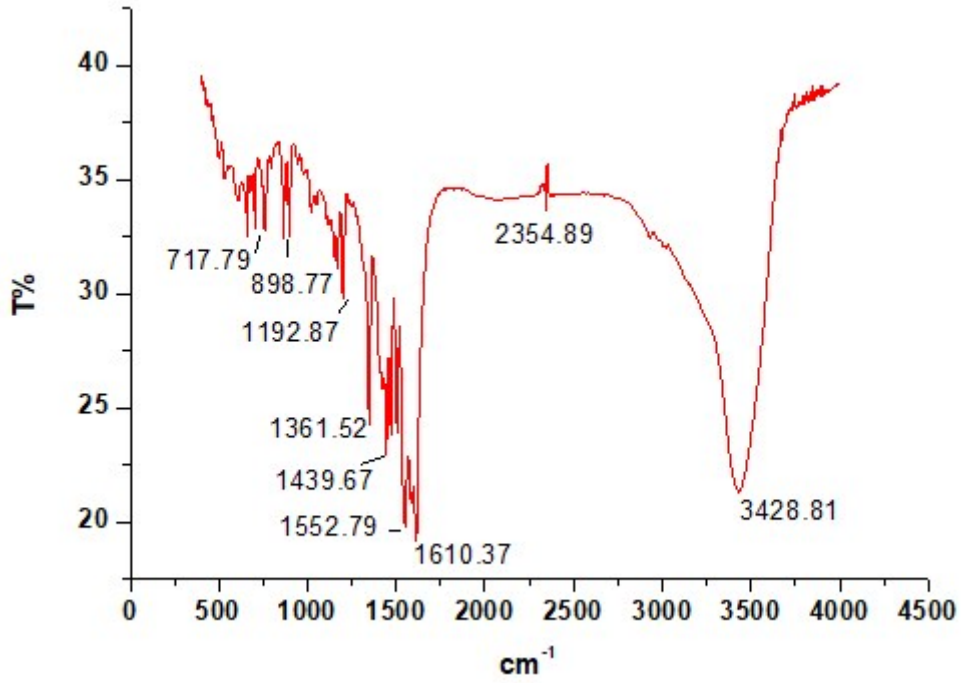

Fig. S6 IR (KBr) spectra of complex **6.**

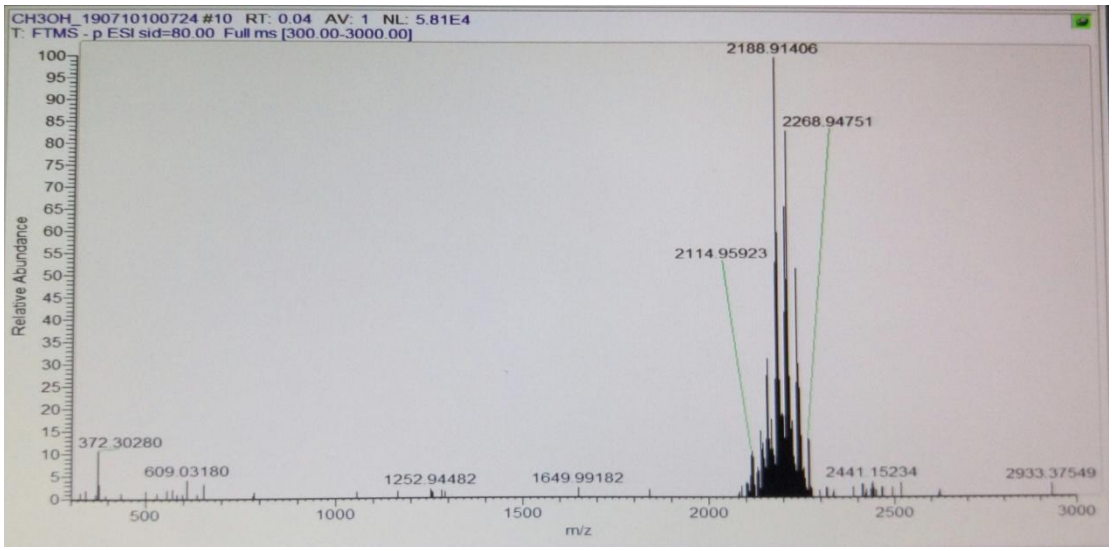

Fig. S7 ESI-MS spectra of complex **1**.

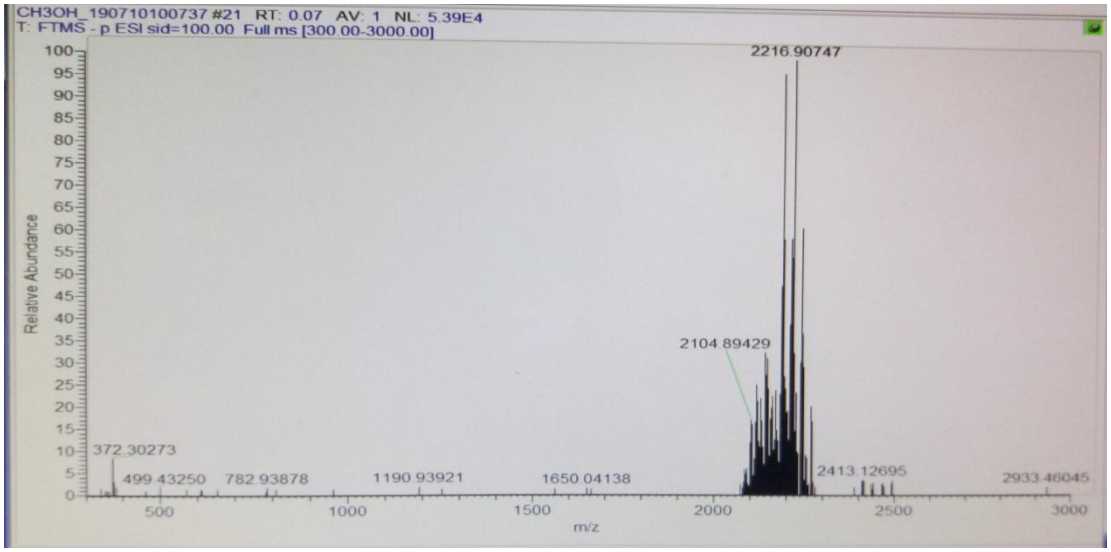

Fig. S8 ESI-MS spectra of complex **2**.

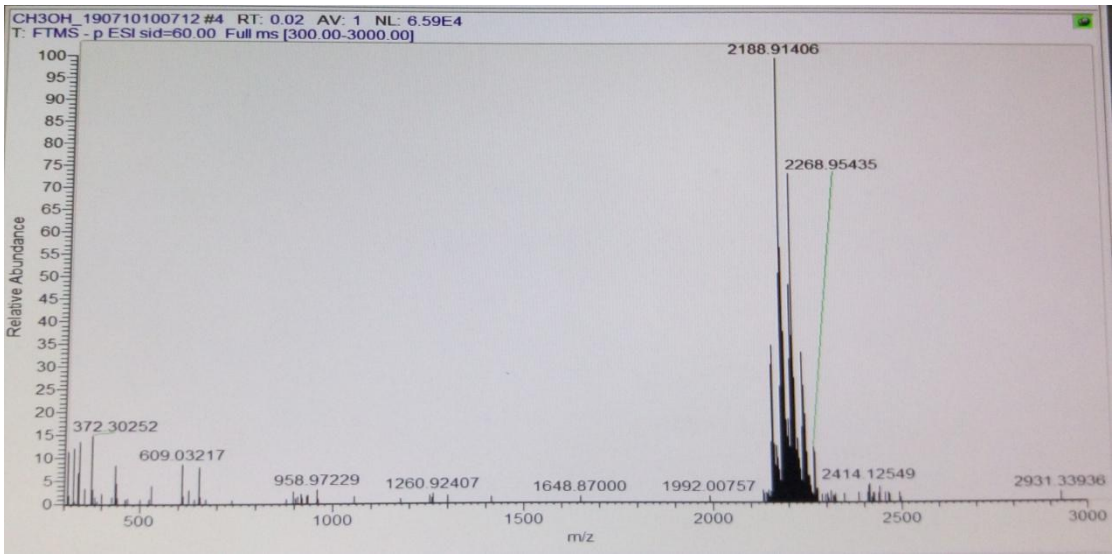

Fig. S9 ESI-MS spectra of complex **3**.

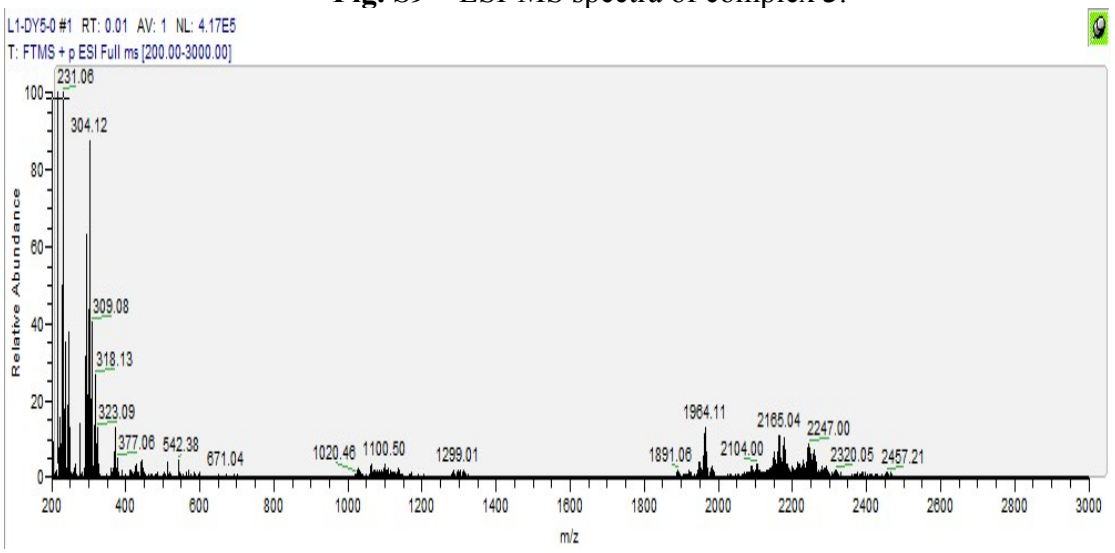

Fig. S10 ESI-MS spectra of complex **4**.

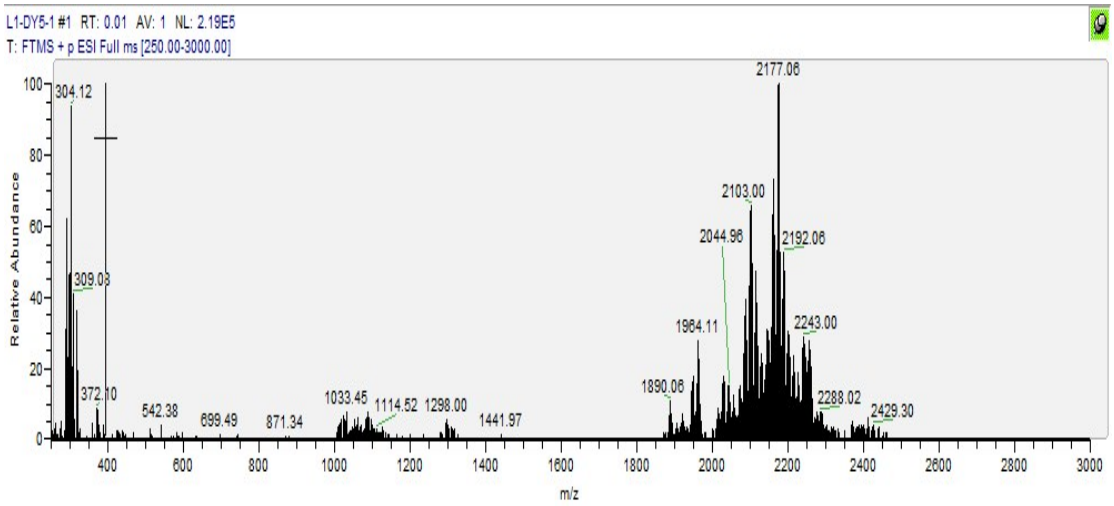

Fig. S11 ESI-MS spectra of complex **5**.

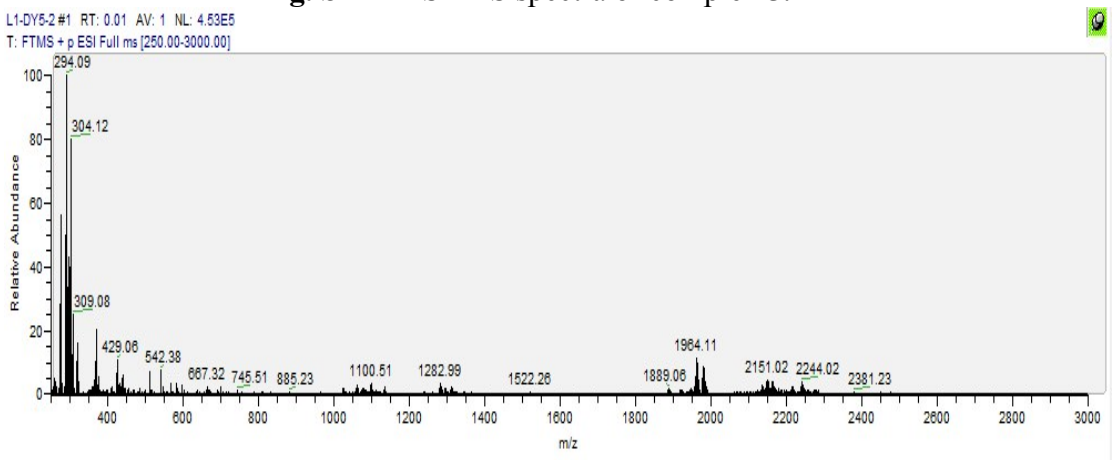

Fig. S12 ESI-MS spectra of complex **6**.

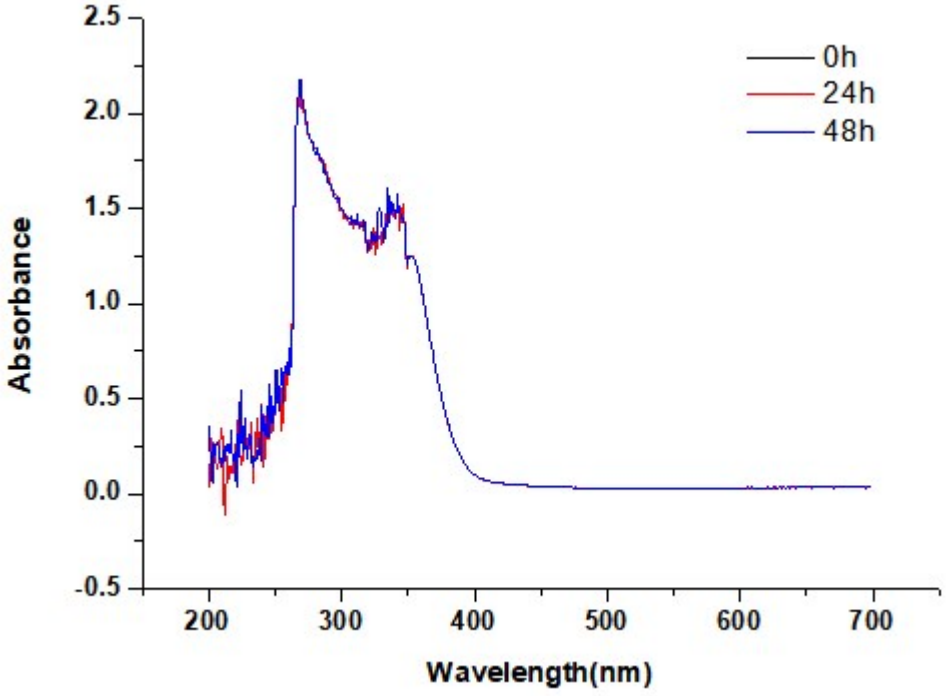

Fig. S13 UV-vis spectra of **L.**

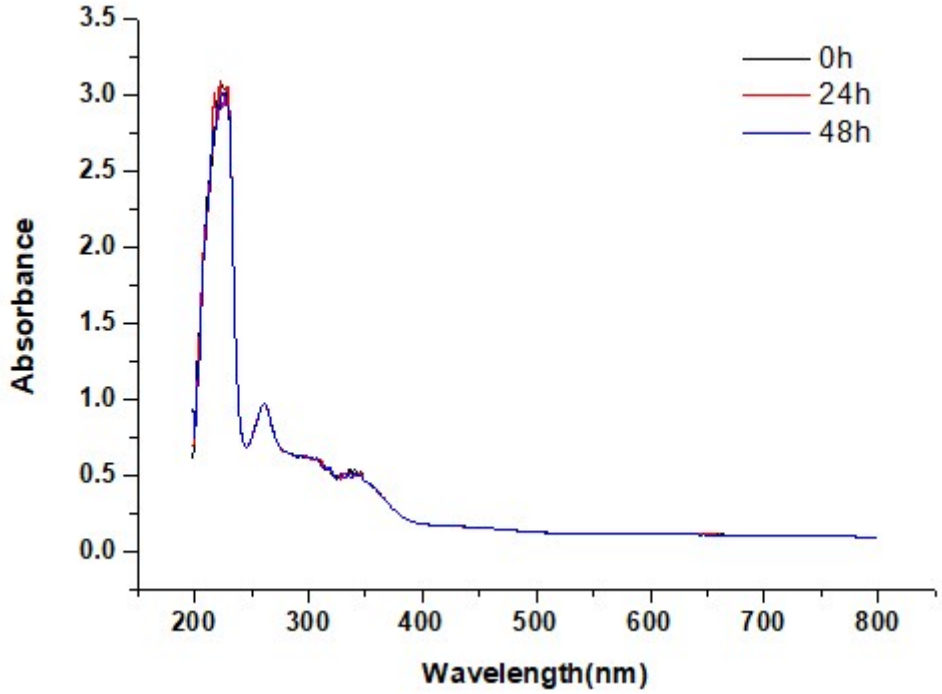

Fig. S14 UV-vis spectra of **L[1].**

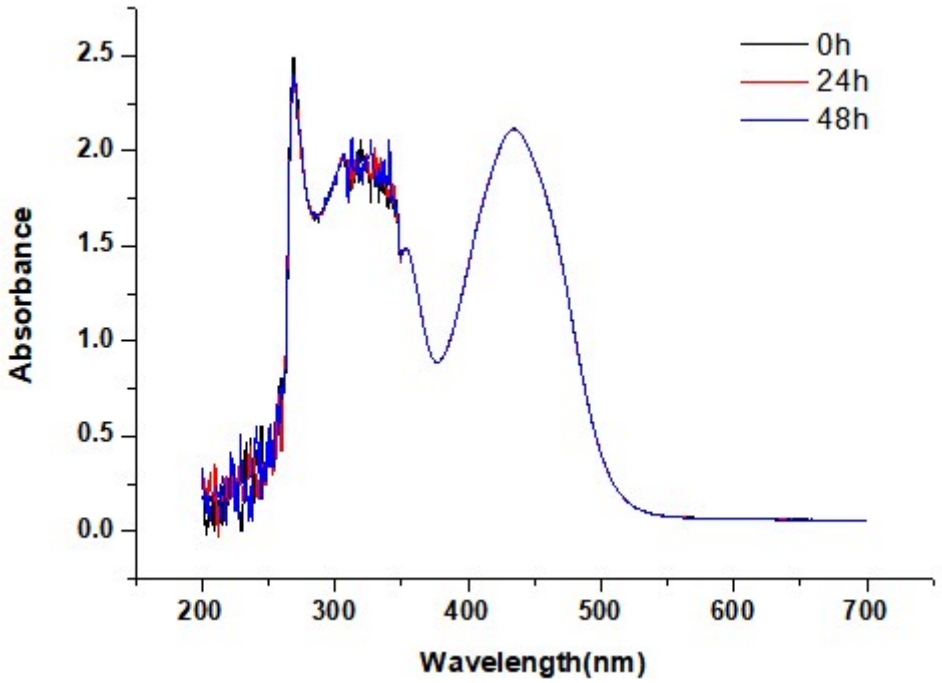

Fig. S15 UV-vis spectra of complex **1**.

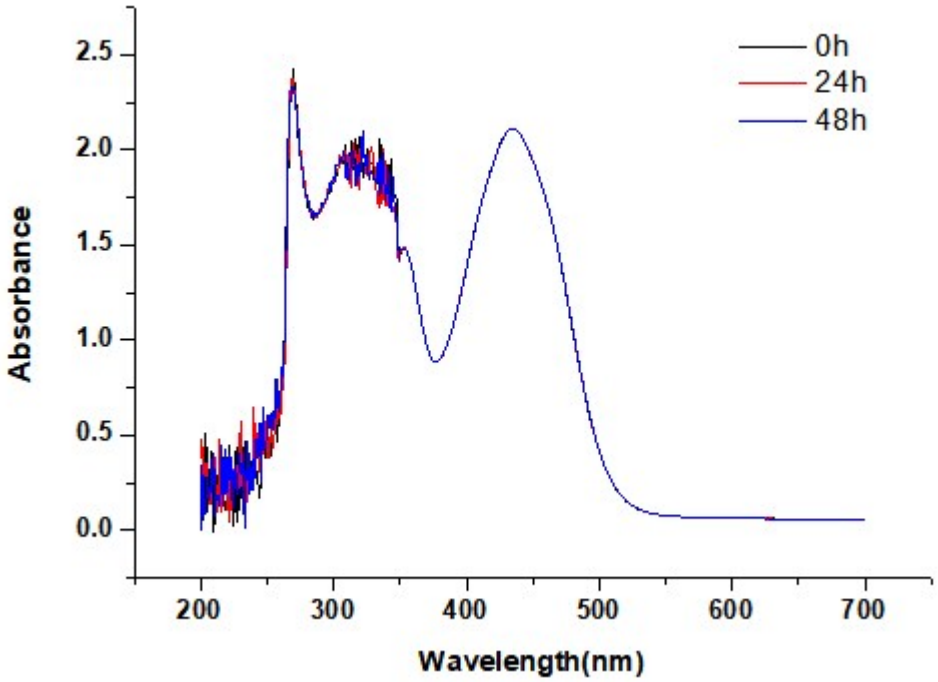

Fig. S16 UV-vis spectra of complex **2**.

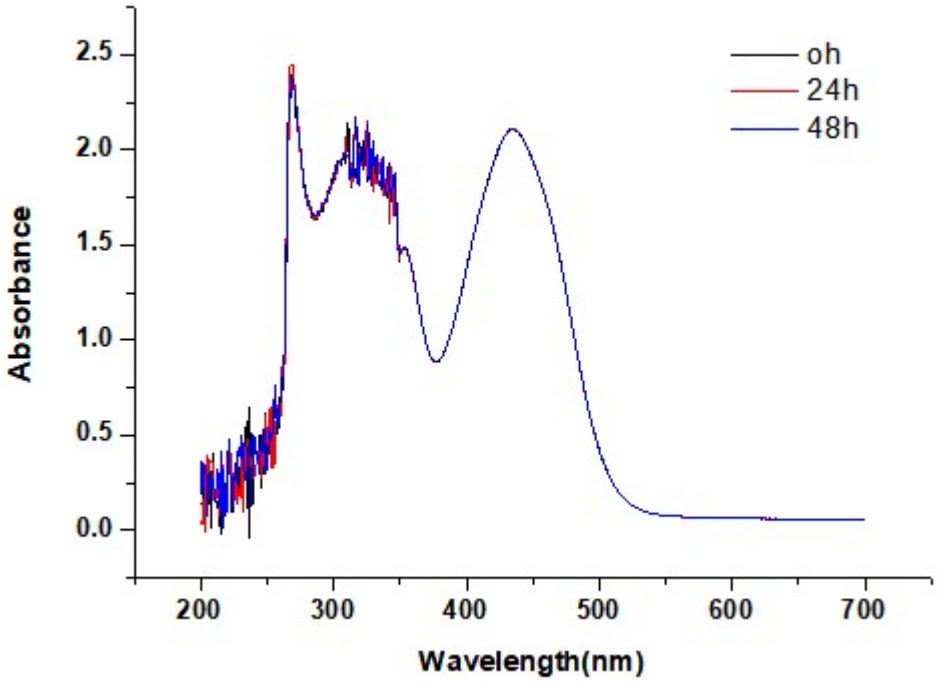

Fig. S17 UV-vis spectra of complex **3**.

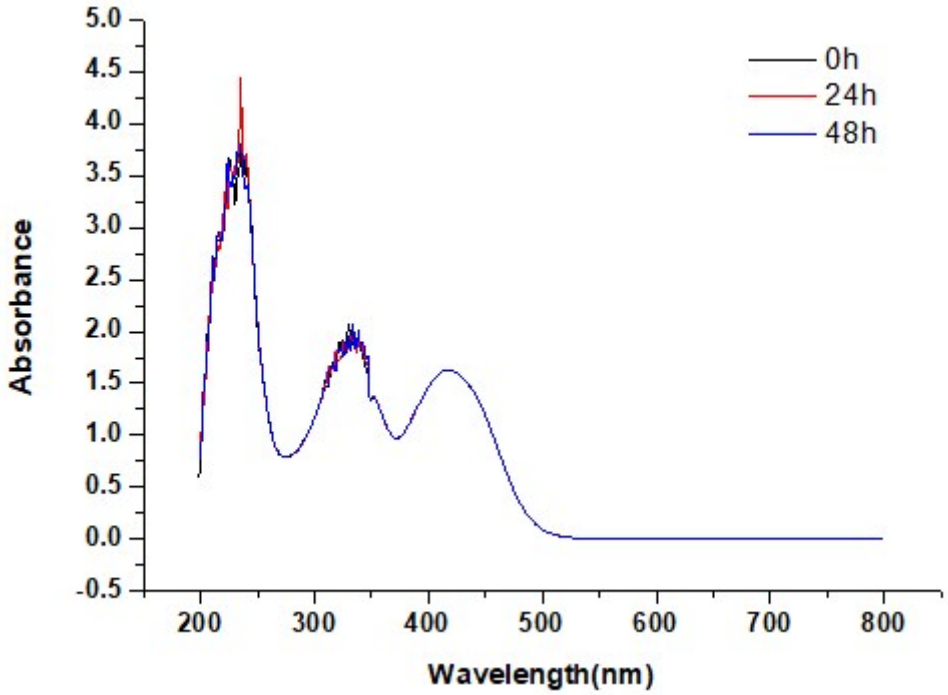

Fig. S18 UV-vis spectra of complex **4.**

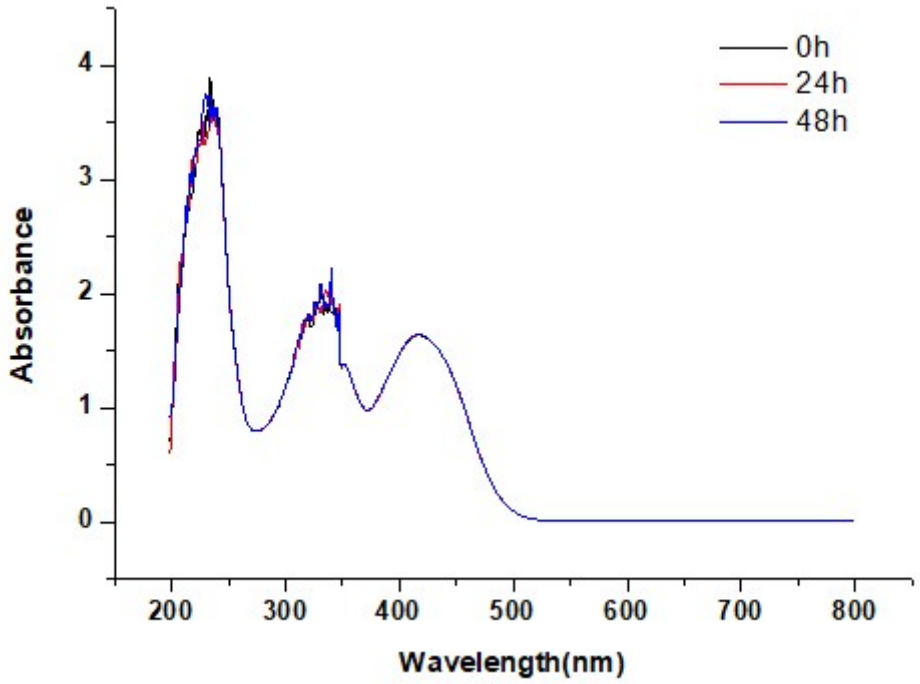

Fig. S19 UV-vis spectra of complex **5.**

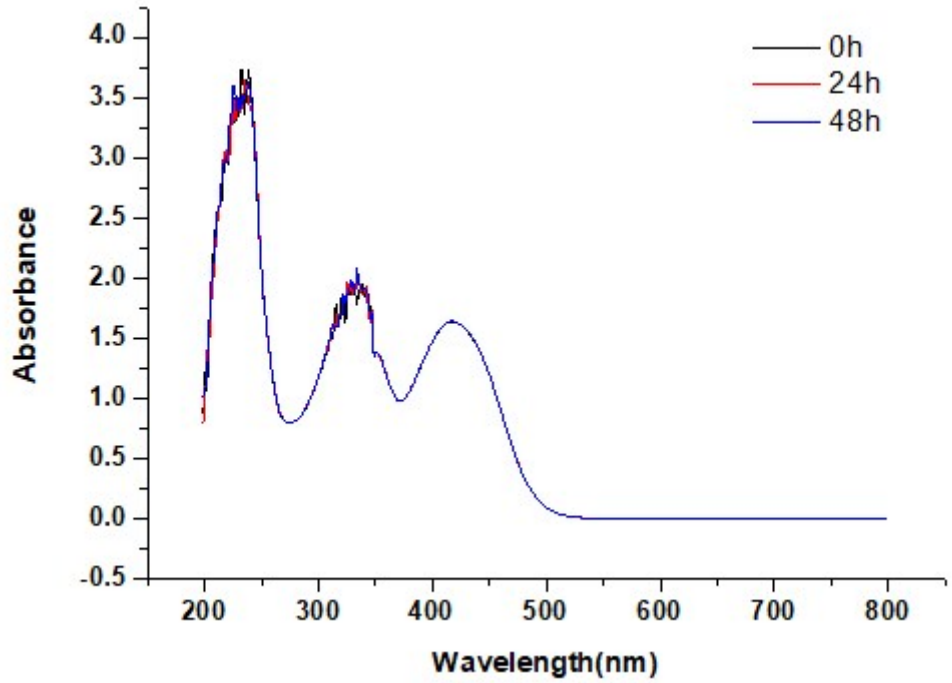

Fig. S20 UV-vis spectra of complex **6.**

Materials and Instrumentatio

All reagents including acetate salts and solvents were obtained from commercial sources,they were used without further purification. Elemental analyses for C, H, and N were performed using a Vario Micro Cube analyzer. UVevisible spectra and fluorescence spectra were performed on a Shimadzu UV-1800 spectrophotometer and a Hitachi RF-4500 fluorescence spectrometer, respectively. Infrared spectra were recorded in the range of 4000-400 cm^{-1} on Perkin-Elmer Spectrum Two FT/IR spectrometer using a KBr pellet.

X-ray crystallography

The orange block-shaped crystals crystal of complex 1,2,3 (0.27 ,0.16, 0.10 mm) were measured on a Bruker Smart Apex II. The anisotropic thermal parameters and positions of all nonhydrogen atoms were refined on F2 by full-matrix least squares techniques with the SHELX-97 program package .

In vitro cytotoxicity

The HeLa, A549, SK-OV-3/DDP, HL-7702cancer cell lines and the normal liver cell HL-7702 were obtained from the Shanghai Institute for Biological Science (China). Cytotoxicity was determined using the MTT assay (MTT = 3-(4,5-dimethyl-2-thiazolyl)-2,5-diphenyl-2Htetrazolium bromide). Taking cells into the logarithmic growth phase, 180 μL (about 4500-5000 cells) of cell containing medium were inoculated on a 96-well culture plate. The cells were cultured for 24 h at 37 ^{o}C in a humidification containing 5% CO_2 . After the cells are attached, add into the sample in an amount of 20 μL, per sample were seted 6 replicate holes, set the corresponding

blank control at the same time. Continue to train for 48 h, add 10 μL MTT reagent (concentration 5 mg/mL) to each well. After continuing to incubate for 4 h, the supernatant was aspirated. Add 150μL of DMSO to each well, slightly oscillate for 5-8 min to fully dissolve the crystalline particles. The blank control group is zeroed, The absorbance value (Å value) after removing the background light absorption value was measured by a microplate reader at a wavelength of 490 nm. Then calculate cell proliferation inhibition rate and IC_{50} value.

Assay of antimetastatic effect

1. Seeding cells: digest and count the cells, adjust the cell density to $1x10^5$ cells/mL, take 100 μL of cell suspension and add into the Transwell chamber, then add 500 μL of medium containing 20% FBS to the lower chamber;
2. Culture cells: 24-well cell culture plates are placed at 37 ^oC in a 5% CO_2 incubator for 24 h;
3. Cell count: wipe the cells in the upper chamber with a cotton swab, remove Transwell, invert, air-dry, add 500 μL of 0.1% crystal violet to a 24-well plate, place cells in it, immerse the membrane in the dye, remove after 30 min at 37 ^oC, wash with PBS, take 3 fields of view on the diameter, and take a photo (magnification 200 ×) , count finally.

Drug-DNA interaction study

Prepare 1% agarose gel with PBS buffer (0.08 mol/L PBS, pH = 8.5, 0.08 mol/L boric acid, 0.0024 mol/L EDTA), the PBS buffer was used as electrode buffer solution, then added 0.5 μL Pbr322 plasmid DNA(5 mg/μL) into a sterilized microplastic centrifuge tube, Subsequently added different concentrations of compound and buffer with PBS solution constanted volume to 10 μL. After reacting at a constant temperature of 37 ^oC for 1 hour, added 2 μL of LoadingBuffer solution as an electrophoresis process, the indicator is evenly mixed and the sample is loaded into the agarose gel tank. Electrophoresis at 80 V/cm for 2 h, stop electrophoresis when bromophenol blue walks to the edge of the rubber sheet. The entire agarose gel was stained in EB solution for 30 min, then imaging with the 2020 D-type gel imaging split system.

Cell cycle analysis

SK-OV-3/DDP cells were seeded in 6-well plates and incubated in the presence or absence of 1 (8μM) and 3 (18μM) for 24 h. Collecting cells, store with 70% ice ethanol at 20 ^oC for 12 h. Then discard 70% ice ethanol, wash with pre-cooled D-Hanks for 2-3 times. After suspending cells with 0.5 mL of 50μg/mL RNase, set at 37 ^oC for 30 min, followed by incubated with the DNA staining solution propidium iodide (PI) (Keygen Biotech, China) at 4° C for 30 min. The cells were detected by flow cytometry (BECKMAN-COULTER) at 488 nm. Using EXPO32 ADC analysis software to analyze the data.

Apoptosis analysis

SK-OV-3/DDP cells were seeded in 6-well plates (3×105 cells/well) and incubated in the presence or absence of **1** (8 μM) and **3** (18 μM) for 24 h to induce cancer cell apoptosis. After incubation, the cancer cells were harvested and incubated with 5.0 μL of Annexin-V/FITC (Keygen Biotech, China) in binding buffer (10 mM HEPES, 140 mM NaCl, and 2.5 mM $CaCl_2$ at pH 7.4) at room temperature for 30.0 min. PI solution was then added to the medium for another 5.0 min of incubation. Almost 10,000 events were collected for each sample and analyzed by flow cytometry (BECKMAN-COULTER). The percentage of apoptotic cells was calculated with EXPO32 ADC Analysis software.

Intracellular localization

1. SK-OV-3/DDP cells were firstly incubated with **1** (8 μM) and **3** (18 μM), then dilute the mitochondrial staining solution with serum-free culture solution to a final concentration of 50 nM according to 1: 1000. After removing the cell culture solution, add an appropriate volume of diluted mitochondrial staining solution. Incubate cells in a 37 ^{o}C for 20 min.
2. Wash the cells 3 times with serum-free cell culture solution to fully remove mitochondrial stains that have not entered the cells.
3. Nuclei were counterstained with DAPI for 10 min, and the cells were washed 3 times with serum-free cell culture solution, observe the mitochondria in the cells.