Electronic Supplementary Information

for

Mechanistic studies of in vitro anti-proliferative and anti-inflammatory activities of Zn(II)-NSAID complexes of 1,10-phenanthroline-5,6-dione in MDA-MB-231 cells

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Table S1 *Calculated bond parameters for complex* ***1***.

Distances/ Angles (Å)/(°)	**[(phendione)Zn^{II} $(NPR)_2$]**(uB3LYP/LanL2DZ) *S*=1	**[(phendione)$Zn^{II}(NPR)_2$ (H_2O)]** (uB3LYP/LanL2DZ) *S*=1	**[(phendione)$Zn^{II}(NPR)_2$ $(H_2O)_2$]** (uB3LYP/LanL2DZ) *S*=1
Zn1-N1	2.16694	2.22425	2.24091
Zn1-N2	2.19130	2.18747	2.23378
Zn1-O1	2.38534	-	-
Zn1-O2	2.04800	1.97596	2.11871
Zn1-O3	1.96073	2.02377	2.10618
Zn1-O5	-	2.12977	2.09425
Zn1-O6	-	-	2.09685
C1-O1	1.29040	1.27050	1.29844
C1-O2	1.31975	1.32373	1.29837
C2-O3	1.32548	1.30941	1.30029
C2-O4	1.27400	1.28943	1.29663
N1-Zn1-N2	76.51474	75.38380	74.23851
N1-Zn1-O1	83.22922	-	-
N1-Zn1-O2	109.39755	102.95942	88.31118
N1-Zn1-O3	116.29566	92.96100	92.84043
N1-Zn1-O5	-	163.01920	164.61915
N1-Zn1-O6	-	-	90.39890
N2-Zn1-O1	148.48231	-	-
N2-Zn1-O2	104.12818	127.88643	89.18720
N2-Zn1-O3	105.99976	105.03099	92.57759
N2-Zn1-O5	-	87.63814	90.42103
N2-Zn1-O6	-	-	164.17810
O1-Zn1-O3	104.55093	-	-
O2-Zn1-O3	129.61688	126.92425	178.10148
Energy (kJ/mol)	-6091.802×10^3	-6292.780×10^3	-6545.774×10^3

Table S2 *Calculated bond parameters for complex* ***2***.

Distances /Angles (Å)/(°)	**[(phendione)$Zn^{II}(MFN)_2$]** (uB3LYP/LanL2DZ) *S*=1
Zn1-N1	2.20393
Zn1-N2	2.20389
Zn1-O1	2.17990
Zn1-O3	2.15212
Zn1-O2	2.15208
Zn1-O4	2.17993
C1-O2	1.30569
C2-O3	1.30568
C2-O4	1.32737
N1-Zn1-N2	75.51244
N1-Zn1-O1	90.47603
N1-Zn1-O2	98.09571
N1-Zn1-O3	96.36871
N1-Zn1-O4	152.85140
N2-Zn1-O1	152.86096
N2-Zn1-O2	96.38246
N2-Zn1-O3	98.07909
N2-Zn1-O4	90.47429
O4-Zn1-O3	62.17800
O1-Zn1-O3	106.61288
O2-Zn1-O3	161.67947
O1-Zn1-O4	110.77742
O1-Zn1-O2	62.17884
Energy(kJ/mol)	-6187.654×10^3

Table S3 *Cytotoxic activity data (IC_{50}) for the complexes and phendione against human breast cancer cell line (MDA-MB-231) at different time.*

	1D	**2D**	**3D**
Complex **1**	1.5 μM	0.6 μM	0.5 μM
Complex **2**	0.7 μM	0.4 μM	0.4 μM
Phendione	0.3 μM	0.4 μM	0.3 μM
Phendione + naproxen	0.7 μM	0.6 μM	0.4 μM
Phendione + mefenamic acid	0.7 μM	0.5 μM	0.4 μM

Table S4 *Production of prostagladin in PGE_2 assay experiment on breast cancer MDA-MB-231 cell line. The amount of PGE_2 in control was considered as 100%. Zn^{2+} stands for zinc(II) pechlorate hydrate salt. Standard deviation values are shown in parentheses.*

Well	**Amount of PGE_2 produced (%)**
Control	100
Zn^{2+}	79.75 (±4.27)
Phendione	69.35 (±3.68)
Complex **1**	10.45 (±0.55)
Naproxen	13.08 (±1.28)
Complex **2**	17.79 (±0.46)
Mefenamic acid	11.22 (±0.96)

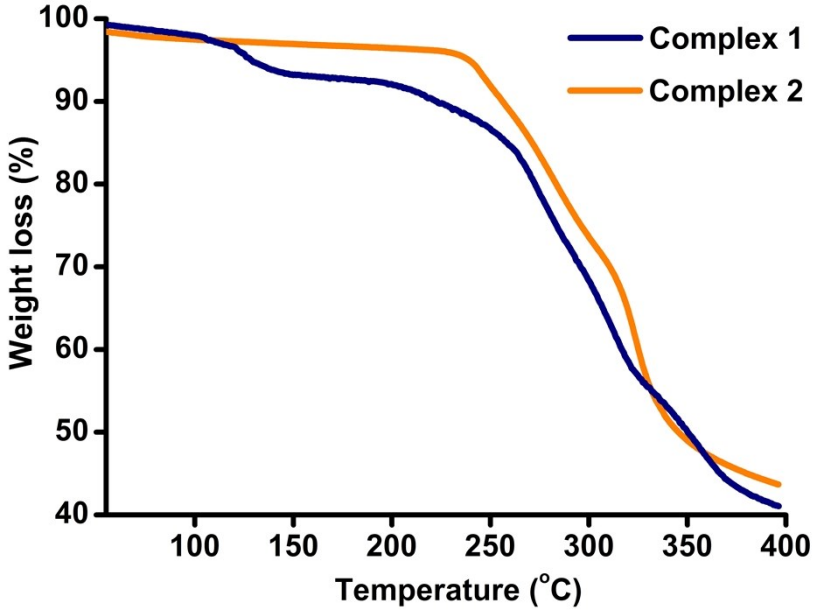

Fig. S1 *TGA curves for complexes **1** and **2**.*

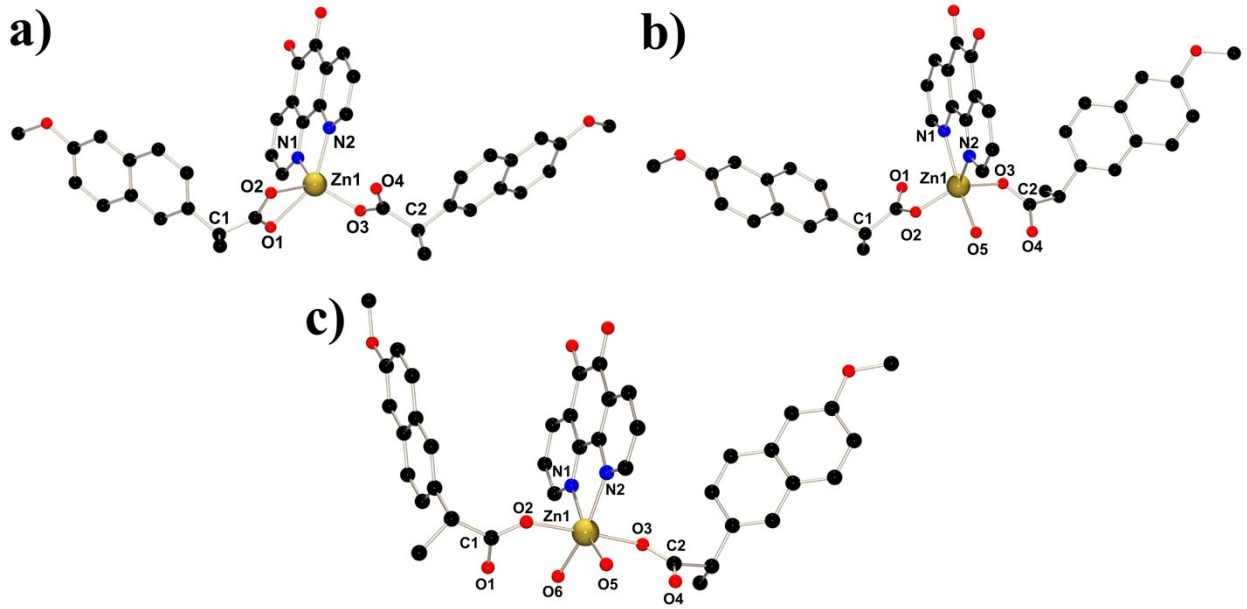

Fig. S2 *DFT optimized geometries of (a) [(phendione)$Zn^{II}(NPR)_2$], (b)[(phendione)$Zn^{II}(NPR)_2(H_2O)$], and (c) [(phendione)$Zn^{II}(NPR)_2(H_2O)_2$] (**1**). For **1**, the O1 and O6 (also O5 and O4 in c) are in hydrogen bonding interaction with the O··O distance of 2.46Å.*

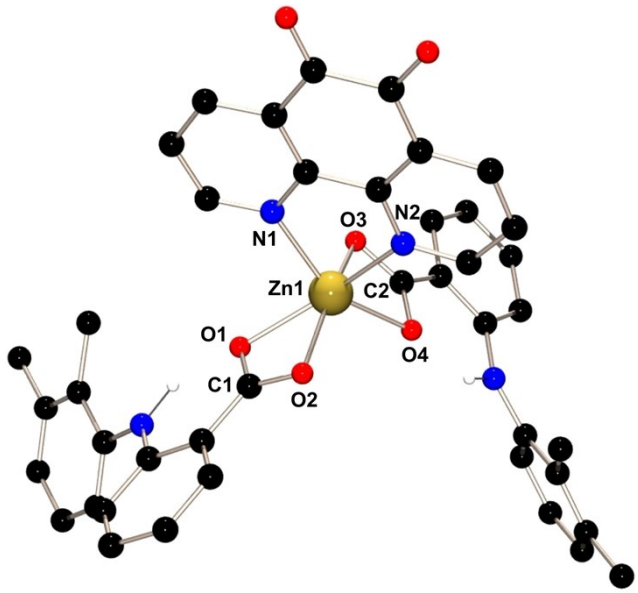

Fig. S3 *DFT optimized geometry of [(phendione)Zn^{II}(MFN)$_2$] (**2**).*

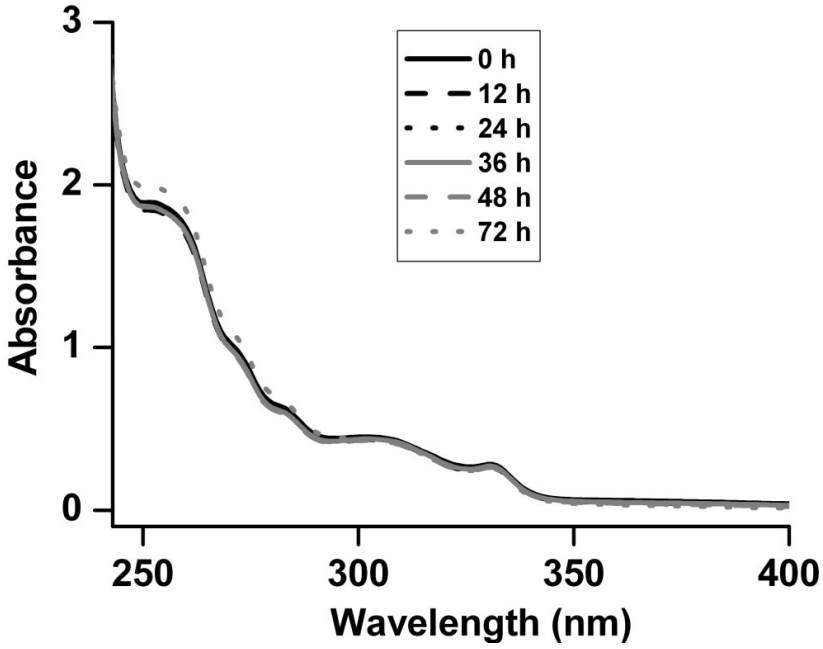

Fig. S4 *UV-vis spectra of **1** in 2% DMSO-PBS buffer recorded at regular time interval for over 72 h of incubation at 310 K.*

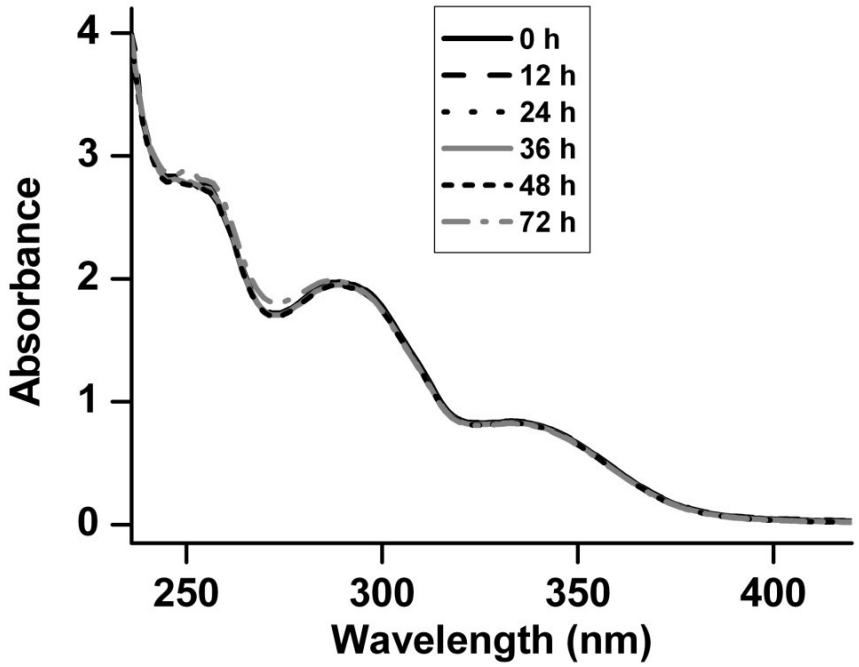

Fig. S5 *UV-vis spectra of* ***2*** *in 2% DMSO-PBS buffer recorded at regular time interval for over 72 h of incubation at 310 K.*

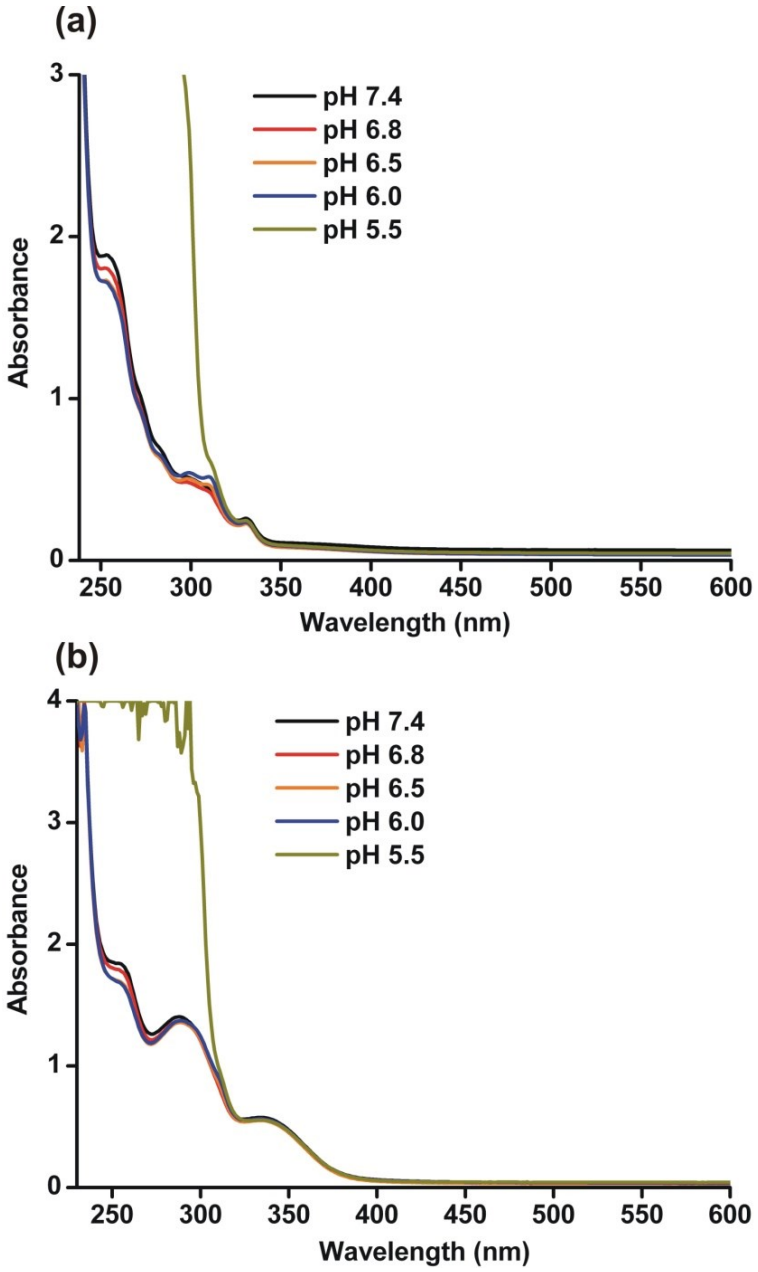

Fig. S6 *Stability of (a) complex* ***1*** *and (b) complex* ***2*** *at different pH in 2% DMSO-PBS or phthalate buffer at 310 K.*

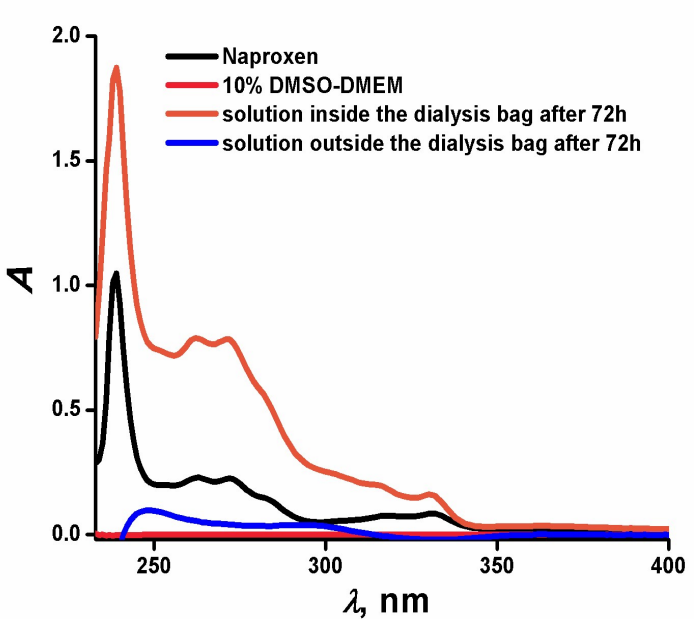

Fig. S7 *UV-Vis spectra of* ***1*** *in medium after 72h of in vitro dialysis.*

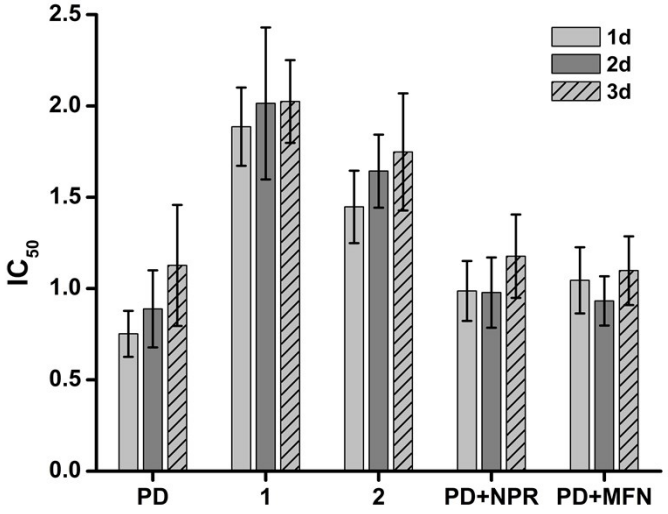

Fig. S8 *IC_{50} values of phendione, physical mixture of phendione and naproxen, and phendione and mefenamic acid, and complexes* ***1*** *and* ***2*** *on mouse macrophage RAW 264.7 cells. PD, NPR and MFN stand for phendione, naproxen, and mefenamic acid, respectively.*

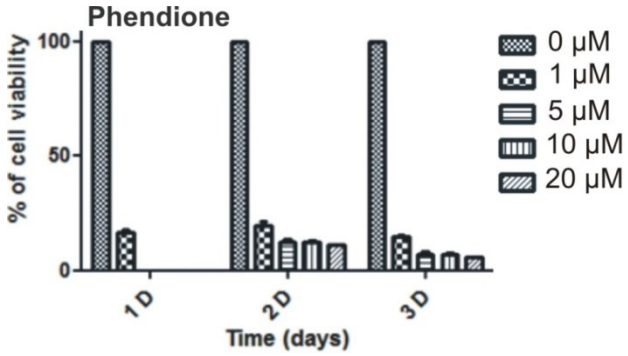

Fig. S9 *MTT assay of phendione on the MDA-MB-231 cell line; 1D, 2D, and 3D stand for 24, 48, and 72 h, respectively.*

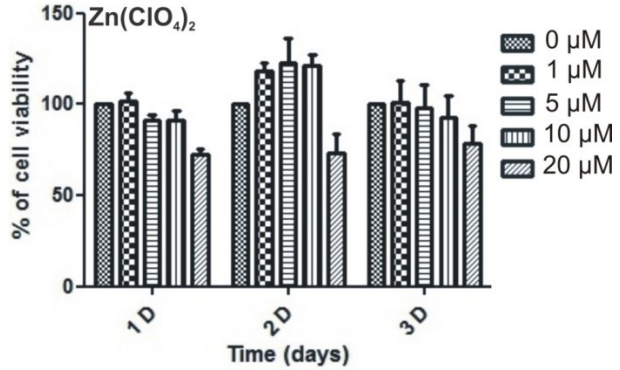

Fig. S10 *MTT assay of $Zn(ClO_4)_2,6H_2O$ on the MDA-MB-231 cell line; 1D, 2D, and 3D stand for 24, 48, and 72 h, respectively.*

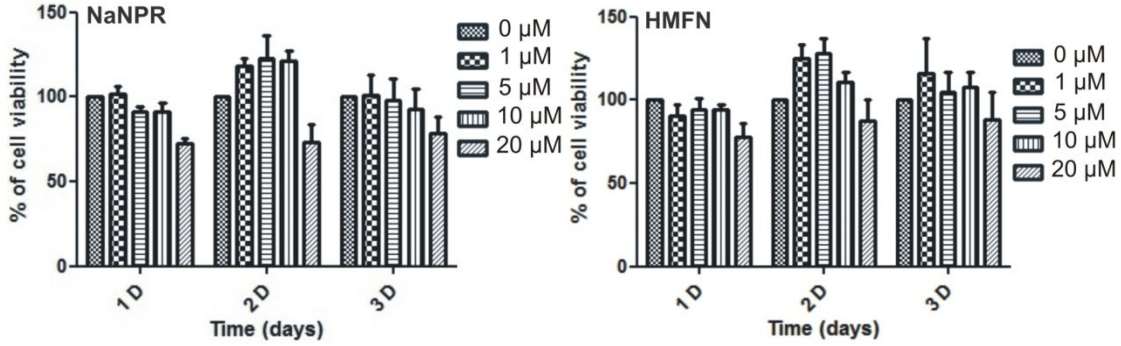

Fig. S11 *MTT assay of NaNPR, HMFN on the MDA-MB-231 cell line; 1D, 2D, and 3D stand for 24, 48, and 72 h, respectively.*

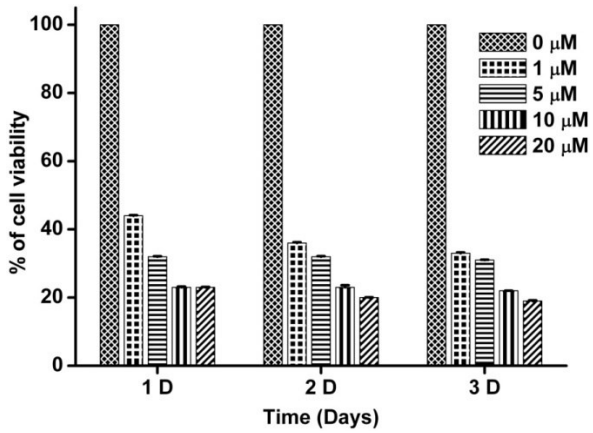

Fig. S12 *MTT assay of phendione + NaNPR (1:2 ratio) on the MDA-MB-231 cell line; 1D, 2D, and 3D stand for 24, 48, and 72 h, respectively.*

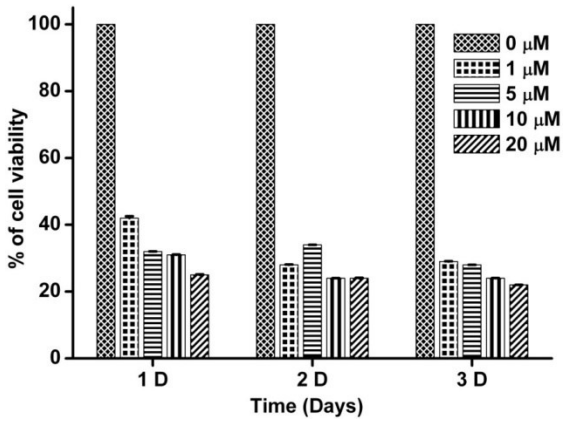

Fig. S13 *MTT assay of phendione + HMFN (1:2 ratio) on the MDA-MB-231 cell line; 1D, 2D, and 3D stand for 24, 48, and 72 h, respectively.*

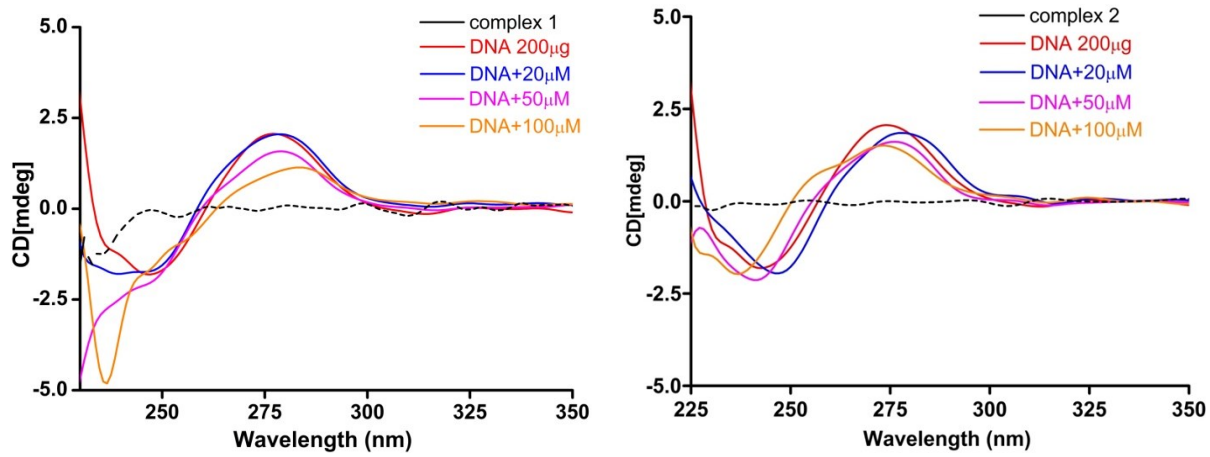

Fig. S14 *CD of CT DNA after addition of* ***1*** *and* ***2*** *in DMSO-water at 298 K.*

Cartesian coordinates for the optimised structures

Cartesian coordinates for the optimized structure of [(phendione)$Zn^{II}(NPR)_2$]:

Atom	Coordinates (Angstroms)		
	X	Y	Z
Zn	-0.04180300	-1.06419400	-0.08205600
O	-1.65893800	-1.93040200	0.82835700
O	1.64077500	-1.87561200	-0.67786300
N	-0.68092200	0.71178600	-1.14650500
N	0.51960000	0.56943500	1.26623000
C	-0.47719000	1.88645900	-0.49618300
C	0.04625900	4.31456100	1.07908600
C	0.43382200	2.96977500	1.58555600

C	0.17656600	1.80812800	0.82749000
C	-1.29356100	0.70668400	-2.35493100
H	-1.46050500	-0.27355300	-2.78862200
C	1.06895500	2.82323900	2.83958600
H	1.27027500	3.71005300	3.43317900
C	-0.87323200	3.12276300	-1.04849700
C	-0.63982200	4.39624700	-0.31253900
C	1.42863400	1.54241800	3.27897600
H	1.92756200	1.39286200	4.23000500
C	-1.49734500	3.12175400	-2.31581700
H	-1.80517200	4.06818400	-2.75036500
C	1.14404300	0.42747000	2.46124500
H	1.43582400	-0.58815600	2.71180600
C	-1.71024900	1.90291000	-2.97489100
H	-2.19516100	1.86374500	-3.94388700
C	-2.26220400	-2.36116800	-0.26354500
C	2.46309600	-2.31445900	0.26453200
O	0.25218200	5.35778400	1.72988600
O	-0.97303800	5.50388200	-0.77704600
O	2.21104200	-2.18803300	1.50693000
O	-1.71927600	-2.12009400	-1.40908200

C	3.75215500	-2.99175000	-0.23053100
C	3.93551500	-4.36110000	0.47437500
H	3.08607800	-5.02241200	0.26099000
H	4.85342100	-4.84796900	0.12312200
H	3.99754100	-4.23267700	1.55995200
C	4.95996800	-2.07640900	-0.01907800
C	5.32006000	-1.63783400	1.30055600
C	5.74336900	-1.67401000	-1.09383800
C	6.43009600	-0.83585100	1.50909400
H	4.69201500	-1.93674600	2.13529400
C	6.89698600	-0.84582400	-0.91374600
H	5.48204900	-1.99197900	-2.10225600
C	7.25547200	-0.41580400	0.41482500
H	6.69087400	-0.51323600	2.51538300
H	3.62336500	-3.15302100	-1.30547700
C	7.71417800	-0.42783700	-2.00567600
C	8.40364900	0.40524600	0.59978900
C	8.83288800	0.37428600	-1.81036200
H	9.43526500	0.67525800	-2.66163200
C	9.17919400	0.79366600	-0.48888200
H	7.45214000	-0.74785300	-3.01232000

H	8.69046700	0.73778100	1.59361700
O	10.28738600	1.60072600	-0.19956200
C	11.15109600	2.02992800	-1.28913600
H	10.60511700	2.64793100	-2.01595300
H	11.93255300	2.62844400	-0.81609100
H	11.60643200	1.17164700	-1.80309500
C	-3.58661500	-3.11401500	-0.14944200
H	-3.74543100	-3.59536300	-1.12076400
C	-3.50662700	-4.20072900	0.95337300
H	-2.71009100	-4.92154300	0.72997600
H	-3.28819900	-3.75028600	1.92651600
H	-4.45860900	-4.74125500	1.01831400
C	-4.73599900	-2.13134500	0.09411000
C	-5.80086700	-2.05235000	-0.79465000
C	-4.74143200	-1.29089000	1.25865100
C	-6.90044900	-1.16388000	-0.57026900
H	-5.81031900	-2.67885200	-1.68556600
C	-5.78994000	-0.41942300	1.50387300
H	-3.89699500	-1.34066300	1.94083800
C	-6.90204400	-0.32701700	0.60372400
H	-5.78079200	0.20991300	2.39173800

C	-8.00438500	-1.07428300	-1.46912600
C	-7.99397200	0.55707300	0.83258200
C	-9.05585800	0.61836200	-0.06564800
C	-9.06433900	-0.20638500	-1.23278900
H	-9.89088800	-0.16278600	-1.93493400
H	-8.01342500	-1.70295600	-2.35743500
H	-8.01428500	1.19375800	1.71270000
O	-10.07944600	1.51964600	0.25083300
C	-11.23526000	1.61356300	-0.62875200
H	-11.88400100	2.36225600	-0.16938400
H	-10.94801000	1.94561000	-1.63641500
H	-11.76891100	0.65495200	-0.69382500

Cartesian coordinates for the optimized structure of [(phendione)Zn^{II}(NPR)$_2$(H$_2$O)]:

Atom	Coordinates (Angstroms)		
	X	Y	Z
Zn	0.18309700	-1.14235500	-0.64976500
O	-1.52142000	-1.95738600	0.07548700
O	1.99052600	-1.93990600	-0.61061000
N	-0.44327100	0.71898500	-1.61314500
N	0.27651500	0.38445000	0.96498700

C	-0.59569900	1.79063400	-0.79315300
C	-0.86453500	3.98400700	1.14777600
C	-0.33500200	2.65526500	1.55559300
C	-0.20898700	1.60479500	0.62134800
C	-0.77938900	0.82099800	-2.92141300
H	-0.64154200	-0.08544100	-3.50193700
C	0.05603500	2.41242700	2.89192500
H	-0.03918100	3.21179500	3.62084400
C	-1.09524100	3.02396000	-1.26335900
C	-1.25446000	4.18326600	-0.34216400
C	0.56143500	1.15277000	3.23656200
H	0.88148500	0.93206800	4.24892300
C	-1.44246800	3.13255000	-2.62790700
H	-1.82974200	4.07739200	-2.99749300
C	0.66570100	0.15329900	2.24386000
H	1.09638700	-0.82994100	2.42572600
C	-1.28262600	2.02039700	-3.46613200
H	-1.54353700	2.06523000	-4.51771300
C	-2.36184600	-2.76849900	-0.51639700
C	2.72420300	-2.31773300	0.42438900
O	-1.00116900	4.92580300	1.95376600
O	-1.68265000	5.28747300	-0.73122000
O	2.35419600	-2.20760400	1.63481800
O	-2.21772300	-3.17953200	-1.73003100
O	-0.10416500	-2.10725600	-2.52656300

H	0.66884000	-2.64284700	-2.78381900
H	-0.98485700	-2.65313000	-2.37126900
C	4.10348500	-2.91373500	0.07281000
C	4.35794500	-4.20386400	0.89311400
H	3.59403800	-4.96065000	0.67250400
H	5.34311300	-4.62102900	0.65078000
H	4.31800800	-3.99228300	1.96644100
C	5.20469100	-1.87430600	0.29372300
C	5.41413400	-1.30078400	1.59398100
C	6.03508700	-1.48458500	-0.74982400
C	6.42746200	-0.38243000	1.81490400
H	4.74919600	-1.59156100	2.40286000
C	7.09203300	-0.53887300	-0.55610900
H	5.88704800	-1.90411600	-1.74411000
C	7.29953300	0.02723100	0.75340100
H	6.57391900	0.04256500	2.80612800
H	4.07500900	-3.16093100	-0.99369500
C	7.95625000	-0.13266100	-1.61563900
C	8.35049900	0.96693700	0.95208400
C	8.97906400	0.78577400	-1.40718500
H	9.62111100	1.07424600	-2.23341100
C	9.17530300	1.34066000	-0.10503200
H	7.80796200	-0.55506500	-2.60764600
H	8.52313900	1.40332300	1.93203400
O	10.17865100	2.27186800	0.19474300

C	11.08244800	2.69896600	-0.86254600
H	10.54006900	3.19798300	-1.67814000
H	11.76239100	3.40984700	-0.38822500
H	11.65764200	1.85341400	-1.26550900
C	-3.58678000	-3.24473600	0.27919300
H	-4.03028200	-4.04744900	-0.31917000
C	-3.15763800	-3.81301900	1.65541800
H	-2.46539700	-4.65497000	1.52807200
H	-2.64963300	-3.05017100	2.25356800
H	-4.03680900	-4.16661700	2.20746700
C	-4.61442900	-2.11725100	0.40567400
C	-5.85346300	-2.21826500	-0.21529300
C	-4.32340900	-0.94136100	1.17672600
C	-6.83907800	-1.18721400	-0.09781300
H	-6.08920400	-3.09924600	-0.81049000
C	-5.25628800	0.07385100	1.31309000
H	-3.34791900	-0.85632200	1.64679900
C	-6.54188600	-0.01346400	0.68463900
H	-5.02359400	0.95591600	1.90696700
C	-8.11566300	-1.27800300	-0.72775400
C	-7.52030400	1.01317700	0.80774200
C	-8.75662700	0.89138800	0.17936800
C	-9.06153400	-0.26745500	-0.59968100
H	-10.02447800	-0.36574900	-1.09064500
H	-8.34897600	-2.16018800	-1.32062700

H	-7.31616000	1.90434400	1.39482700
O	-9.64810500	1.95539000	0.36186400
C	-10.96287900	1.88928300	-0.25909400
H	-11.46183100	2.81707400	0.02841500
H	-10.88746500	1.83684300	-1.35436200
H	-11.53996400	1.03109500	0.11301200

Cartesian coordinates for the optimized structure of [(phendione)$Zn^{II}(NPR)_2(H_2O)_2$]:

Atom	Coordinates (Angstroms)		
	X	Y	Z
Zn	0.14862168	-1.03865140	-0.01606900
O	-1.61194250	-1.57922470	0.48332279
O	1.81152821	-1.70579025	-0.65264785
N	-0.18093552	0.49557579	-1.19481488
N	0.56353329	0.40967710	1.25627196
C	-0.14029912	1.67645058	-0.62221469
C	0.05641629	4.13361122	0.97649284
C	0.42500098	2.76629843	1.59292524
C	0.29829614	1.63026955	0.81567170
C	-0.43675046	0.36929691	-2.50402489
H	-0.40185799	-0.59455898	-2.96760067
C	0.89169488	2.61972472	2.89923986
H	0.98836992	3.46778480	3.54437509

C	-0.44822306	2.85264052	-1.28634263
C	-0.39575158	4.17641313	-0.50353090
C	1.23742321	1.32545409	3.34632984
H	1.62612809	1.18260559	4.33235250
C	-0.78428692	2.77599272	-2.64195365
H	-1.05179435	3.65372605	-3.19371809
C	1.06823508	0.21769118	2.48604395
H	1.33700360	-0.76448617	2.81600998
C	-0.75559099	1.51388332	-3.26495767
H	-0.97954210	1.41962119	-4.30549757
C	-2.33452002	-2.34261366	-0.28248595
C	2.57812393	-2.29661891	0.21222808
O	0.12597710	5.18512037	1.65835268
O	-0.70512341	5.26355847	-1.05287166
O	2.18496318	-2.41348826	1.40185876
O	-2.02662000	-2.49314299	-1.53866503
O	-0.80942516	-1.87550373	-1.43900000
H	-0.66339541	-2.82114432	-1.40299667
H	-1.74904678	-1.69542305	-1.34582245
C	3.94593943	-2.86465326	-0.18995245
C	4.21472289	-4.13623738	0.64125979
H	3.45418521	-4.86006542	0.43790483
H	5.16989596	-4.53859412	0.37615400
H	4.20687492	-3.89360963	1.68247842
C	5.06151540	-1.83439101	0.08744754

C	5.65638009	-1.79844671	1.35737950
C	5.49209768	-0.94895284	-0.91167190
C	6.68671805	-0.95068917	1.61589248
H	5.29514470	-2.44896396	2.12743034
C	6.57368977	-0.09934030	-0.65672623
H	5.00605264	-0.92926827	-1.86433829
C	7.18434162	-0.11239105	0.60458531
H	7.12239426	-0.92634743	2.59349585
H	3.93805504	-3.11179039	-1.23154656
C	7.05014027	0.75607394	-1.66075246
C	8.29499346	0.70949179	0.85115371
C	8.16463097	1.56501394	-1.41780439
H	8.53986006	2.20754730	-2.18809721
C	8.79409312	1.53416335	-0.17129097
H	6.56482277	0.78848070	-2.61288195
H	8.76375071	0.70395402	1.81277097
O	9.94748467	2.34877376	0.04758675
C	10.67999285	2.45363400	-1.17961890
H	10.05272063	2.87658989	-1.93583852
H	11.53367545	3.08004229	-1.03344327
H	11.00090792	1.48046080	-1.48731247
C	-3.56749556	-3.05880712	0.30671346
H	-3.82373283	-3.89869704	-0.30928026
C	-3.24298482	-3.56111667	1.72373420
H	-2.42292488	-4.24565821	1.67617176

H	-2.98178899	-2.73481572	2.34915632
H	-4.09936218	-4.05816524	2.12968396
C	-4.74965985	-2.06743344	0.39033416
C	-5.67928310	-1.92261340	-0.65160632
C	-4.87907627	-1.29364016	1.55398527
C	-6.74089917	-1.01283510	-0.50151906
H	-5.58416692	-2.49970691	-1.54756183
C	-5.89803210	-0.40934247	1.69265538
H	-4.16298893	-1.40489740	2.34083908
C	-6.84440133	-0.25455485	0.67302424
H	-5.98055033	0.17471138	2.58709567
C	-7.69870157	-0.85887473	-1.51618245
C	-7.89510506	0.65826775	0.83325701
C	-8.85518285	0.80933314	-0.17516061
C	-8.75884082	0.04879229	-1.35015924
H	-9.49275130	0.16243202	-2.12042139
H	-7.62149190	-1.43305424	-2.41598573
H	-7.96122482	1.24174525	1.72959124
O	-9.93316101	1.73853512	-0.00177543
C	-11.10212645	1.27055997	-0.68457971
H	-11.90037725	1.97029308	-0.54682467
H	-10.89108737	1.17232827	-1.72686346
H	-11.39085362	0.32052713	-0.28773003
O	0.11170929	-2.21353011	1.48529881
H	0.99188721	-2.57326981	1.63226537

H	-0.17070606	-1.72959526	2.26337701

Cartesian coordinates for the optimized structure of [(phendione)$Zn^{II}(MFN)_2$]:

Atom	Coordinates (Angstroms)		
	X	Y	Z
Zn	0.00037300	1.03758200	0.00052900
O	0.80253500	0.69513700	-1.96692500
O	-0.80190600	0.69481300	1.96784300
C	-2.76651400	-0.33689300	3.72788100
H	-2.00048400	0.35635900	4.06224800
N	1.23771600	2.77954300	0.54062300
C	-4.41961800	-3.03685000	-0.13417100
N	-1.23569600	2.78054800	-0.53938800
C	-4.84800300	-2.84976800	-1.48029800
C	2.76650100	-0.33715400	-3.72733500
H	2.00110200	0.35694400	-4.06138500
C	0.67801300	3.99115800	0.29864000
C	-0.70618800	6.51484100	-0.31734700
C	-4.62665300	-1.50087500	-2.14528500
H	-4.89441500	-0.68558500	-1.46057200
H	-5.22214300	-1.39336200	-3.05550100
H	-3.57151600	-1.35574900	-2.42444900
C	-1.34350500	5.19853900	-0.59720900
C	-0.67482800	3.99171100	-0.29779600

C	2.47495400	2.70864400	1.08169600
H	2.86491700	1.70787700	1.23438000
C	-2.63363900	5.12629100	-1.16771500
H	-3.15674100	6.04828300	-1.40339000
C	1.34786200	5.19744200	0.59765600
C	0.71183300	6.51429900	0.31727900
C	-3.20534700	3.86976200	-1.41236100
H	-4.19460300	3.77590000	-1.84650800
C	2.63792600	5.12412900	1.16822200
H	3.16190800	6.04570300	1.40358000
C	-2.47301100	2.71067300	-1.08041100
H	-2.86393200	1.71024300	-1.23281600
C	3.20839900	3.86712500	1.41330800
H	4.19754500	3.77244000	1.84751600
C	-3.74447600	-1.61815900	1.85337400
C	1.75865900	-0.05375400	-1.48757500
C	-2.76886900	-0.68658400	2.35527700
C	-1.75860300	-0.05317200	1.48819100
C	-4.71337400	-2.11883600	2.77119000
H	-5.49332700	-2.78064300	2.41293400
C	2.76847100	-0.68755600	-2.35491300
C	3.74324100	-1.62024400	-1.85343600
C	5.45635700	-3.93418300	2.16942400
C	4.62572900	-1.50580600	2.14524600
H	4.89434400	-0.69044900	1.46094300

H	5.22132600	-1.39937100	3.05552500
H	3.57073800	-1.35970800	2.42447600
C	-3.71108800	-0.85672300	4.61644600
H	-3.69810000	-0.57912500	5.66643400
C	4.41699900	-3.04058100	0.13338200
C	4.84566300	-2.85459300	1.47957300
C	-5.64972300	-5.16173800	-1.51042200
H	-6.12303400	-5.98427400	-2.04181700
C	-5.45972900	-3.92838100	-2.17072600
C	4.71172000	-2.12133100	-2.77147000
H	5.49105400	-2.78402800	-2.41351800
C	-4.69432800	-1.74267500	4.11695400
H	-5.45672300	-2.13819400	4.78526200
C	4.59550600	-4.29035200	-0.50328500
H	4.21645200	-4.44427100	-1.50811900
C	-4.59942800	-4.28676200	0.50186900
H	-4.22059200	-4.44157700	1.50665000
C	3.71065700	-0.85736300	-4.61611500
H	3.69797500	-0.57920700	-5.66595600
C	-5.22154000	-5.33897100	-0.18337800
H	-5.35218100	-6.29992300	0.30888000
C	5.64504100	-5.16740900	1.50848600
H	6.11754200	-5.99068900	2.03945000
C	5.92024500	-3.79291400	3.61122700
H	6.33072000	-4.73990900	3.97828500

H	5.09699400	-3.50503600	4.27887900
H	6.70470000	-3.03005100	3.71612300
C	4.69306700	-1.74446000	-4.11704000
H	5.45513000	-2.14033100	-4.78551600
C	5.21658200	-5.34353300	0.18138700
H	5.34619500	-6.30436900	-0.31136200
C	-5.92336100	-3.78592400	-3.61249000
H	-6.70705500	-3.02224000	-3.71706800
H	-6.33473900	-4.73232700	-3.98006100
H	-5.09977800	-3.49852000	-4.27993200
O	-1.27015600	7.59646600	-0.57412800
O	1.27685700	7.59546600	0.57363100
N	-3.74161900	-1.96453400	0.50664600
H	-3.07423600	-1.41463700	-0.04785800
N	3.74002800	-1.96728900	-0.50687800
H	3.07315200	-1.41703500	0.04788600
O	-1.78618500	-0.20003100	0.16927100
O	1.78610900	-0.20121400	-0.16870700

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