Table S1 IC_{50} values of **1–49** against cancer and normal cell lines, at different incubation time, mechanism of action, target and cell cycle arrest.

Complex Number	Cell line/IC_{50} (μM) [1,2]			Mechanism of action	Cell Cycle arrest	Target	Ref.
3.1. C, N, P and S Monodentate ligands							
1a	518A2; > 50	DLD-1; > 100	KB-V1; n.d		n.d		160
	HCT-116; n.d	MCF-7; n.d	PANC-1; > 100				
	HT-29; n.d						
1b	518A2; > 100	DLD-1; > 100	KB-V1; n.d				
	HCT-116; n.d	MCF-7; n.d	PANC-1; > 100				
	HT-29; n.d						
2a	HCT-116 (SRB); 84 ± 1	NCI-H460 (SRB); > 100	SiHa (SRB); > 100	Trx-R inhibition	n.d	Trx-R	16
	SW480 (SRB); > 100						
2b	HCT-116; 21 ± 1	NCI-H460; 26 ± 2	SiHa; 30 ± 2				
	SW480; 24 ± 1						
3 [T]	HCT-116 $p53^{+/+}$; 24 ± 2	A2780cisR; 14.9 ± 0.8	PNT2 [(N)]; 33.23 ± 0.06		n.d		162
	A2780; 6.4 ± 0.2	MCF-7; 66 ± 1					
4a	HCT-116 (SRB); 46 ± 8	NCI-H460 (SRB); 43 ± 6	SiHa (SRB); 36 ± 4		n.d		163
	SW480 (SRB); 77 ± 3						
4b	HCT-116; 25 ± 1	NCI-H460; 41 ± 5	SiHa; 26 ± 2				
	SW480; 28 ± 5						
5	HCT-116 (SRB); >100	NCI-H460 (SRB); >100	SiHa (SRB); >100		n.d		164

6a	HT-29; 92.0 ± 1.0		A2780; n.d		A2780cis; n.d		n.d		157
6b *	HCT-116; > 100		MIA-PaCa-2; > 100		ARPE-19/ (N) ; >100	Inactive	n.d		165
6c	A549; 92.3 ± 3.1		Hela; > 100		BEAS-2B (N); n.d		n.d		31
7 *	HCT-116; 37.79 ± 4.89		MIA-PaCa-2; 52.13 ± 12.28		ARPE-19 (N); >100		n.d		165
8a T	HT-29; 4.82 ± 0.85		HCT-116 $p53^{+/+}$; 4.23 ± 0.64		HCT-116 $p53^{-/-}$; 5.17 ± 1.13		n.d		166
	ARPE-19 (N); 7.35 ± 3.42								
8b *	HT-29; > 100		HCT-116 $p53^{+/+}$; > 100		HCT-116 $p53^{-/-}$; > 100				
	ARPE-19 (N); >100								
9a T	A549	39.2 ± 2.2	HeLa	>100	BEAS-2B (N)	65.7 ± 1.3	ROS/NADH	n.d	166
9b T		35.6 ± 1.3		>100		68.3 ± 2.2			
9c T		43.7 ± 1.2		57.4 ± 1.5		66.9 ± 2.1	ROS/NADH		
9d T		36.5 ± 2.4		52.6 ± 1.3		53.8 ± 1.4			
10a T		31.4 ± 1.7		67.7 ± 0.6		77.6 ± 2.2	ROS/NADH	G_2/M	
10b T		26.7 ± 0.9		33.5 ± 1.3		83.2 ± 1.7	**1A**		Mitochondria
10c T		36.8 ± 1.2		85.5 ± 1.6		65.6 ± 2.3		n.d	
10d T		40.5 ± 1.4		42.4 ± 2.4		73.0 ± 0.9			
10e T		72.1 ± 1.2		78.9 ± 1.7		82.6 ± 1.1			

10f [T]		65.6 ± 1.2		67.3 ± 0.7		78.4 ± 1.0				
11	A2780 (bovine cat B)	> 500					Inhibit Cathpesin B.	n.d		167
12		> 500								
13		349 ± 10								
14		> 500								
15a	518A2 (SRB); 0.3 ± 0.1		8505C (SRB); 0.2 ± 0.0		A253 (SRB); 0.2 ± 0.0			n.d		168, 169
	MCF-7 (SRB); 0.2 ± 0.1		SW480 (SRB); 0.6 ± 0.2							
15b	518A2 (SRB); 0.7 ± 0.4		8505C (SRB); 0.6 ± 0.0		A253 (SRB); 0.5 ± 0.1					
	MCF-7 (SRB); 0.3 ± 0.0		SW480 (SRB); 1.0 ± 0.4							
15c	518A2; 4.4 ± 2.5		8505C; 5.8 ± 1.3		A253; 4.9 ± 0.1					
	MCF-7; 6.7 ± 1.4		SW480; 4.5 ± 0.1							
16a	518A2; 1.0 ± 0.6		8505C; 0.5 ± 0.2		A253; 0.4 ± 0.0					
	MCF-7; 0.4 ± 0.1		SW480; 1.0 ± 0.3							
16b	518A2; 0.4 ± 0.2		8505C; 0.3 ± 0.1		A253; 0.3 ± 0.1		ROS/RNS/Apoptosis.			
	MCF-7; 0.1 ± 0.1		SW480; 0.9 ± 0.4							
17	Sk-mel (WST-1; Roche); 510		SH-4 (WST-1; Roche); 300		Colo-829 (WST-1; Roche); 480			n.d		170
	C-32 (WST-1; Roche); 560		MCF-7 (WST-1; Roche); 370		T47D (WST-1; Roche); 450					
	MDA-MB-231 (WST-1; Roche); 7.8 ± 1									
18a [T]	CT26 (24h); n.d		MCF-7 (24h); 65.7 ± 2.8		DU-145 (24h); 11.8 ± 1.1		**2A** DNA damage	G_2/M	Nucleus and cytoplasm	25, 171
	A549 (24h); 68.8 ± 1.7		PANC-1 (24h); 43.0 ± 1.3		HEK-293T [(N)] (24h); 42.1 ± 2.1					
18a [T]	CT26 (24h + 48h); 6.4 ± 0.3		MCF-7 (24h + 48h); 35.0 ± 0.9		DU-145 (24h + 48h); 4.8 ±					

			0.1				
	A549 (24h + 48h); 29.5 ± 0.7	PANC-1 (24h + 48h); 8.7 ± 0.2	HEK-293T [(N)] (24h + 48h); 28.5 ± 1.5				
18b [T]	CT26 (24h); n.d	MCF-7 (24h); 68.8 ± 5.3	DU-145 (24h); 12.9 ± 2.1		n.d		
	A549 (24h); 71.4 ± 1.6	PANC-1 (24h); 42.6 ± 18.1	HEK-293T [(N)] (24h); 41.8 ± 1.7				
18b [T]	CT26 (24h + 48h); 5.6 ± 0.4	MCF-7 (24h + 48h); 29.3 ± 0.2	DU-145 (24h + 48h); 5.5 ± 0.2				
	A549 (24h + 48h); 26.7 ± 1.6	PANC-1 (24h + 48h); 7.8 ± 0.6	HEK-293T [(N)] (24h + 48h); 21.4 ± 1.2				
18c [T]	CT26 (24h); n.d	MCF-7 (24h); 61.8 ± 4.1	DU-145 (24h); 9.1 ± 0.5	**2A** DNA damage	G_2/M		
	A549 (24h); 64.8 ± 2.8	PANC-1 (24h); 40.3 ± 4.1	HEK-293T [(N)] (24h); 44.1 ± 1.2				
18c [T]	CT26 (24h + 48h); 4.1 ± 0.7	MCF-7 (24h + 48h); 29.3 ± 0.2	DU-145 (24h + 48h); 23.0 ± 1.7				
	A549 (24h + 48h); 27.4 ± 1.7	PANC-1 (24h + 48h); 7.8 ± 0.6	HEK-293T [(N)] (24h + 48h); 28.0 ± 1.7				
18d [T]	CT26 (24h); n.d	MCF-7 (24h); 35 ± 0.9	DU-145 (24h); 9.1 ± 0.5	**2A** DNA damage	n.d		
	A549 (24h); 69.7 ± 4.1	PANC-1 (24h); 8.7 ± 0.3	HEK-293T [(N)] (24h); 28.5 ± 1.5				
18d [T]	CT26 (24h + 48h); 5.8 ± 0.2	MCF-7 (24h+48h); 33.7 ± 3.8	DU-145 (24h + 48h); 5.1 ± 0.4				
	A549 (24h + 48h); 27.4 ± 1.7	PANC-1 (24h + 48h); 8.1 ± 1.1	HEK-293T [(N)] (24h + 48h); 28.0 ± 1.7				

19	MCF-7; 85 ± 8	Du-145; 19 ± 3	A549; 12 ± 3		S-phase at low conc. G_0/G_1- at high conc.	Nucleus and cytoplasm	172
	PANC-1; 91 ± 13	HaCaT; 320 ± 19					
20	MCF-7; 56 ± 6	Du-145; 13 ± 2	A549; 16 ± 3		n.d		
	PANC-1; 85 ± 16	HaCaT; 302 ± 22					
3.2.1. Bidentate ligands (C^C ligands)							
21a	HeLa	> 100		NADH	n.d		173, 174
21b		22.6 ± 0.9					
21c		8.3 ± 0.9		**1B**	G_0/G_1	Lysosome	
21d		46.3 ± 1.6		NADH	n.d		
21e		15.3 ± 0.2					
21f		5.8 ± 0.3		NADH/ROS/Apoptosis	disrupt G_1, G_2/M		
21g		18.1 ± 0.1		NADH	n.d		
21h		5.8 ± 0.5					
21i		3.4 ± 0.1		NADH/ROS/Apoptosis	disrupt G_1, G_2/M		
21j		7.7 ± 0.1		NADH	n.d.		
21k		5.2 ± 0.3					
21l		2.9 ± 0.1					
22a		11.8 ± 1.2		NADH	n.d.		175
22b		5.9 ± 0.4		**1A**	Disturb sub-	Mitochondria	

	A549					G_1		
22c		4.6 ± 0.2			**1AB**	S-phase	Lysosome /Mitochondria	
22d		3.9 ± 0.7			NADH	n.d.		
3.2.2. Bidentate ligands (C^O ligands)								
23	A2780 (SRB)	10.8 ± 1.7			DNA Damage	n.d		176
24a		3.28 ± 0.14						177
24b		2.55 ± 0.03						
24c		6.53 ± 0.50						
24d		2.14 ± 0.50						
24e		0.70 ± 0.04						
24f [T]	B16; 2.5 ± 0.2	SW620; 2.6 ± 0.1	C6; 2.4 ± 0.3	MCF-7; 8.6 ± 0.2	**1A or 2A**	n.d	Mitochondria	180
	HCT-116; 8.0 ± 0.2	A2780; 5.5 ± 0.5	MRC-5 [(N)]; 6.7 ± 0.2					
24g [T]	B16; 6.7 ± 0.6	SW620; 10.4 ± 0.4	C6; 4.0 ± 0.3	MCF-7; 12.0 ± 1.3				
	HCT-116; 8.0 ± 0.6	A2780; 7.3 ± 0.6	MRC-5 [(N)]; 3.7 ± 0.2					
24h [T]	B16; 1.2 ± 0.2	SW620; 2.0 ± 0.1	C6; 2.00 ± 0.01	MCF-7; 2.5 ± 0.2	**1A or 2A**		Mitochondria	
	HCT-116; 1.3 ± 0.3	A2780; 1.3 ± 0.1	MRC-5 [(N)]; 2.4 ± 0.3					
25	A549 (SRB); 0.56				NADH/ROS	n.d		21
26a	4.5 ± 0.2	3.7 ± 0.3	9.6 ± 0.4	10.36 ± 0.07	NADH/ROS	n.d	DNA	184
26b	2.7 ± 0.3	6.8 ± 0.1	4.8 ± 0.3	2.1 ± 0.3			DNA/Cytosol	
26c	> 50	n.d	n.d	n.d			DNA	
26d	> 60	n.d	n.d	n.d			DNA/ Cytosol	

26e	A2780 (SRB)	6.9 ± 0.3	HCT-116 (SRB)	21.3 ± 0.7	MCF-7 (SRB)	11.6 ± 0.5	A549 (SRB)	15.8 ± 0.4			DNA	
26f		4.4 ± 0.4		18.8 ± 0.5		6.5 ± 0.3		5.9 ± 0.1				
26g		24.73 ± 2.30		n.d		n.d		n.d				
26h		2.7 ± 0.1		27.5 ± 0.9		11.4 ± 0.4		20.1 ± 0.3				
26i		> 50		n.d		n.d		n.d				
26j		47 ± 0.1		57.3 ± 0.9		47 ± 2		89 ± 1				
26k		47.3 ± 0.1		29.3 ± 0.8		28.6 ± 0.9		56.67 ± 0.04				
26l		13.29 ± 0.88		n.d		n.d		n.d				
26m		1.18 ± 0.08		n.d		n.d		n.d				
26n		3.9 ± 0.2		9.6 ± 0.6		3.7 ± 0.1		8.7 ± 0.3				
26o		1.26 ± 0.01		n.d		n.d		n.d				
27a	A2780	1.0 ± 0.1	A549	3.98 ± 0.06	MCF-7	1.82 ± 0.08			ROS/MMP	No effect	Mitochondria	185
27b		0.80 ± 0.01		4.3 ± 0.2		3 .8 ± 0.1				n.d		
27c		1.26 ±		4.0 ± 0.1		2.4 ± 0.2						

	(SRB)	0.07	(SRB)		(SRB)					
27d		1.42 ± 0.04		4.7 ± 0.9		2.55 ± 0.07				
27e		0.32 ± 0.06		0.62 ± 0.06		0.20 ± 0.04	ROS/MMP	No effect	Mitochondria	
27f		1.4 ± 0.2		6.5 ± 0.8		3.9 ± 0.3		n.d		
27g		1.4 ± 0.3		5.9 ± 0.9		2.7 ± 0.2				
27h		1.6 ± 0.3		15.9 ± 0.3		8.8 ± 0.8				
28a [T]	A2780 (MTS); 0.56 ± 0.04		MDA-MB-231 (MTS); 0.52 ± 0.03		MRC-5 [(N)] (MTS); 2.35 ± 0.09		NADH	n.d		186
	A2780cis (MTS); 1.08 ± 0.05									
28b	A2780 (MTS); n.d		MDA-MB-231 (MTS); n.d		MRC-5 [(N)] (MTS); n.d		NADH			
	A2780cis (MTS); n.d									
29a [T]	A549	3.9 ± 0.1	HeLa	3.3 ± 0.5	HepG2	3.1 ± 0.1	BEAS-2B [(N)]	1.8 ± 0.2	**1B**	G_2/M	Lysosome	30
29b [T]		3.9 ± 0.1		3.6 ± 0.3		2.5 ± 0.1		2.4 ± 0.2	NADH			
29c [T]		12.8 ± 0.6		14.8 ± 2.6		11.9 ± 0.7		5.0 ± 0.1	**1B**	G_2/M	Lysosome	
29d [T]		8.6 ± 0.3		8.1 ± 0.1		11.4 ± 0.7		8.9 ± 1.6	NADH			
30a [T]		2.8 ± 0.8		1.6 ± 0.2		1.9 ± 0.1	**1B** Migration inhibition.		n.d	Lysosome	187
30b [T]		23.0 ± 0.7		7.3 ± 1.6		7.0 ± 1.5					

30c [T]	A549	7.4 ± 0.1	HeLa	2.5 ± 0.1	BEAS-2B [(N)]	1.6 ± 0.5	NADH			
30d [T]		39.5 ± 2.7		40.6 ± 2.8		45.7 ± 1.4				
30e [T]		3.5 ± 0.1		1.3 ± 0.1		1.7 ± 0.2				
30f [T]		13.0 ± 0.5		8.6 ± 0.6		11.8 ± 2.4				
31a [T]	A549; 23.2 ± 3.6			HeLa; 18.7 ± 2.7			ROS/Raise NF-κB activity. **2B** Migration inhibition.	S-phase	Lysosome	188
	HepG2; 19.4 ± 7.5			BEAS-2B [(N)]; 19.96 ± 0.7						
31b [T]	A549; 36.8 ± 1.6			HeLa; 28.2 ± 3.8				n.d		
	HepG2; 28.7 ± 6.9			BEAS-2B [(N)]; 30.12 ± 0.3						
32a [T]	MCF-7 (MTS); 0.11 ± 0.03		HCT-116 (MTS); 0.25 ± 0.01		PANC-1 (MTS); 0.60 ± 0.08		Trx-R inhibition ROS\MMP\apoptosis	n.d	Trx-R inhibition	155
	MDA-MB-231 (MTS); 0.22 ± 0.02		MIA-PaCa-2 (MTS); 0.27 ± 0.01		MRC-5 [(N)] (MTS); 1.16 ± 0.30					
32b [T]	MCF-7 (MTS); 0.06 ± 0.02		HCT-116 (MTS); 0.18 ± 0.07		PANC-1 (MTS); 0.26 ± 0.04					
	MDA-MB-231 (MTS);0.14 ± 0.01		MIA-PaCa-2 (MTS); 0.20 ± 0.01		MRC-5 [(N)] (MTS); 1.33 ± 0.00					
32c [T]	MCF-7 (MTS); 0.05 ± 0.01		HCT-116 (MTS);0.22 ± 0.01		PANC-1 (MTS); 0.45 ± 0.01					
	MDA-MB-231 (MTS); 0.23 ± 0.02		MIA-PaCa-2 (MTS); 0.37 ± 0.03		MRC-5 [(N)] (MTS); 1.90 ± 0.43					
32d [T]	MCF-7 (MTS); 0.05 ± 0.01		HCT-116 (MTS); 0.16 ± 0.00		PANC-1 (MTS); 0.34 ± 0.02					
	MDA-MB-231 (MTS); 0.29 ± 0.03		MIA-PaCa-2 (MTS); 0.29 ± 0.03		MRC-5 [(N)] (MTS); 4.59 ± 1.71					
32e [T]	MCF-7 (MTS); 0.22 ± 0.00		HCT-116 (MTS); 0.44 ± 0.10		PANC-1 (MTS); 0.79 ± 0.07					
	MDA-MB-231 (MTS); 0.44 ± 0.02		MIA-PaCa-2 (MTS); 0.53 ± 0.02		MRC-5 [(N)] (MTS); 1.52 ± 0.17					

32f [T]	MCF-7 (MTS); 0.19 ± 0.02	HCT-116 (MTS); 0.39 ± 0.10	PANC-1 (MTS); 0.63 ± 0.01					
	MDA-MB-231 (MTS); 0.55 ± 0.10	MIA-PaCa-2 (MTS); 0.43 ± 0.01	MRC-5 [(N)] (MTS); 5.50 ± 0.00					
33a [T]	MCF-7 (MTS)	9.30 ± 1.09	MRC-5 [(N)] (MTS)	15.20 ± 0.59				176
33b [T]		3.34 ± 0.70		16.63 ± 0.00				
33c [T]		1.85 ± 1.13		16.18 ± 0.00				
33d [T]		4.42 ± 1.19		5.54 ± 0.00				
33e [T]		5.05 ± 0.35		19.82 ± 0.00				
34 [T]		14.90 ± 3.39		35.74 ± 5.99				
35a [T]	HT-29; 0.98 ± 0.02	A2780 (crystal violet); 1.87 ± 0.04	5637 (crystal violet); 5.56 ± 0.25		Apoptosis /angiogenesis	S-phase		191, 192
	A2780cisR (crystal violet); 1.77 ± 0.04	SISO (crystal violet); 5.49 ± 0.93	EA.hy926 [(N)] (crystal violet); 2.85 ± 0.10					
	T47D (crystal violet); 2.27 ± 0.04	LCLC (crystal violet); 9.86 ± 1.04	A427; 3.78 ± 0.41					
35b	HT-29; 9.16 ± 0.98		T47D (crystal violet); 6.67 ± 0.29			n.d		
	A2780 (crystal violet); 6.09 ± 0.18		A2780cisR (crystal violet); 4.43 ± 0.12					
35c	HT-29; 2.40 ± 0.07		T47D (crystal violet); 2.34 ± 0.22					
	A2780 (crystal violet); 1.82 ± 0.02		A2780cisR (crystal violet); 2.07 ± 0.06					
35d [T]	A2780 (crystal violet); 3.60 ± 0.28	A2780cisR (crystal violet); 5.65 ± 0.78	5637 (crystal violet); 9.37 ± 0.53	A427 (crystal violet); 7.25 ± 0.28	Apoptosis angiogenesis			192
	LCLC (crystal	SISO (crystal violet);	HT-29; 8.68 ± 0.92	EA.hy926 [(N)] (crystal				

	violet); 15.14 ± 0.49	13.87 ± 0.17		violet); >8				
35e [T]	A2780; 2.31 ± 0.39	A2780cisR; 3.37 ± 0.41	5637; 2.95 ± 0.71	A427; 4.28 ± 0.55	Angiogenesis			
	LCLC; 5.58 ± 0.33	SISO; 4.76 ± 0.87	HT-29; 9.50 ± 0.75	EA.hy926 [(N)]; 2.99 ± 0.09				
35f [T]	A2780; 2.70 ± 0.13	A2780cisR; 1.93 ± 0.15	5637; 2.45 ± 0.10	A427; 2.62 ± 0.56	Apoptosis angiogenesis			
	LCLC; 6.63 ± 0.88	SISO; 6.65 ± 0.04	HT-29; 3.77 ± 0.31	EA.hy926 [(N)]; 5.22 ± 0.88				
35g [T]	A2780; 2.78 ± 0.12	A2780cisR; 1.70 ± 0.38	5637; 3.70 ± 0.09	A427; 2.35 ± 0.62	ROS angiogenesis			
	LCLC; 5.10 ± 0.33	SISO; 3.42 ± 0.26	HT-29; 6.27 ± 0.69	EA.hy926 [(N)]; 1.19 ± 0.05				
35h [T]	A2780; 2.29 ± 0.46	A2780cisR; 3.76 ± 0.64	5637; 5.15 ± 0.12	A427; 2.34 ± 0.06				
	LCLC; 3.47 ± 0.13	SISO; 3.61 ± 0.93	HT-29; 5.73 ± 0.43	EA.hy926 [(N)]; 1.98 ± 0.40				
35i [T]	A2780; 1.22 ± 0.41	A2780cisR; 1.21 ± 0.48	5637; 1.48 ± 0.88	A427; 1.59 ± 0.34	Angiogenesis			
	LCLC; 3.61 ± 0.21	SISO; 3.79 ± 0.31	HT-29; 4.01 ± 0.56	EA.hy926 [(N)]; 5.95 ± 0.92				
36a [*]		> 100		> 100		n.d		193
36b [*]		55.7 ± 3.3		> 100				
36c [*]		42.8 ± 2.3		> 100				

36d [T]	A549	19.6 ± 1.3	BEAS-2B [(N)]	35.1 ± 2.1				
36e [T]		51.0 ± 5.2		32.6 ± 1.4				
36f [T]		11.9 ± 0.8		8.6 ± 0.1				
36g [T]		7.9 ± 0.4		5.7 ± 0.5				
36h [T]		6.6 ± 1.7		4.9 ± 0.1	**1AB**		Lysosome /Mitochondria	
37a	A549	> 100			NADH	n.d		137
37b		> 100						
37c		25.86 ± 1.2						
37d		14.05 ± 0.1			**1B**	G_2/M		
37e		9.15 ± 0.2				n.d		
37f		3.04 ± 0.5						
37g		2.21 ± 0.2						
37h		1.99 ± 0.1			**1B**	G_2/M	Lysosome	
37i		3.94 ± 0.3				n.d		
37j		3.64 ± 0.3			NADH			
37k		> 100						
37l		7.44 ± 0.3						
37m [T]	A549	4.21 ± 0.3	BEAS-2B [(N)]	3.58 ± 0.3	NADH/ROS	n.d		194
37n [T]		3.25 ± 0.2		2.03 ± 0.2				
37o [T]		1.84 ± 0.1		0.60 ± 0.3				
37p [T]		4.39 ± 0.1		3.43 ± 0.1				

37 [T]		2.67 ± 0.1		1.21 ± 0.3				
37r [T]		0.85 ± 0.2		4.60 ± 0.5	**1B**	G_0/G_1	Lysosome	
38a	A549	18.2 ± 0.1				n.d		195
38b		15.6 ± 2.0						
38c		12.3 ± 2.3						
38d		8.9 ± 0.1						
38e		6.7 ± 0.7						
38f		5.9 ± 0.2			**1B**	Sub-G_1 and G_2/M	Lysosome	
39a [T]	MDA-MB-231; 3.33 ± 0.09		MDA-MB-468; 0.95 ± 0.03					196, 197
	HCT-116; 3.47 ± 0.11		HEK-293T [(N)]; 23.95 ± 0.28					
39b [T]	MDA-MB-231; 1.19 ± 0.05		MDA-MB-468; 0.52 ± 0.02		**2A** Anti-metastasis	G_2/M	Mitochondria	
	HCT-116; 1.36 ± 0.01		HEK-293T [(N)]; 18.57 ± 0.05					
39c [T]	MDA-MB-231; 2.77 ± 0.06		MDA-MB-468; 0.75 ± 0.06					
	HCT-116; 1.59 ± 0.04		HEK-293T [(N)]; 22.92 ± 0.02					
39d [T]	MDA-MB-231; 1.19 ± 0.05		MDA-MB-468; 0.52 ± 0.02					
	HCT-116; 5.4 ± 0.09		HEK-293T [(N)]; 17.23 ± 0.12					
40a	HeLa	4.17 ± 0.11			NADH/ROS/Apoptosis	n.d		198
40b		4.05 ± 0.47						
40c		3.56 ± 0.68						
40d		3.73 ± 0.99						
40e		4.47 ± 0.29						
40f		5.81 ± 0.61						

40g	3.46 ± 0.29					
40h	3.06 ± 0.38					
40i	3.35 ± 0.24					
40j	3.36 ± 0.57					
41	HeLa; 8.6 ± 1.0	hTERT-RPE1; 11.1 ± 0.7	ER-stress and disrupts Golgi structure	n.d	Mitochondria and Lysosome	199
42 [T]	MT4 (MTS); 32	A549 (MTS); 6	Interacts with the guanosine nucleoside of the DNA.	n.d	DNA interaction	200
	HeLa (MTS); 54	HEK-293 [(N)] (MTS); 15				
43a	NCI-H460 (SRB 72h); 21 ± 6	HCT-116 (SRB 72h); 36 ± 1		n.d	Nuclear DNA is not the target	201
	SiHa (SRB 72h);12 ± 2	SW480 (SRB 72h); 70 ± 19				
43b	NCI-H460; 10 ± 1	HCT-116; 17 ± 2			Cytoplasm	
	SiHa; 13 ± 1	SW480; 26 ± 4				
44a	HeLa	n.d	Apoptosis	n.d		139
44b		n.d				
44c		n.d				
44d		28.52 ± 8.56				
45a		7.33 ± 0.28		G_2-phase		
45b		17.52 ± 0.64		n.d		
45c		45.02 ± 3.07				
45d		n.d				
45e		2.01 ± 0.28		G_2, S-phases		

46a	A549	< 20			ROS/Apoptosis	G_2/M		16
46b		< 30				n.d		
46c		> 30						
47a	K562	1.10				n.d		115
47b		0.73						
47c	K562; 0.26	MCF-7; 5.52	A549; 2.09		**2A**	Sub-G_1	Mitochondria	
	K562/A02; 1.95	MCF-7/ADM; 18.81						
47d	K562	0.95				n.d		
47e		0.67						
47f		1.06						
47g		0.53						
47h		1.00						
47i		0.62						
47j		0.94						
47k		4.77						
47l		1.13						
47m		0.61						
47n		1.20						
47o		0.87						

3.2.3. Bidentate ligands C^N ligands

48a		20.8 ± 2.2		6.7 ± 0.2				n.d		114
48b [T]		16.7 ± 2.2		5.6 ± 0.2	BEAS-2B [(N)]	2.5 ± 0.2	NADH//MMP/Apoptosis	G_0/G_1		

48c	A549	16.5 ± 0.8	HeLa	5.9 ± 0.1				n.d		
48d		13.7 ± 1.3		6.4 ± 0.4			NADH//MMP/Apoptosis			
48e		8.5 ± 0.9		4.0 ± 0.7			NADH//MMP/Apoptosis			
48f [T]		3.9 ± 0.1		3.1 ± 0.1	BEAS-2B [(N)]	3.2 ± 0.1	**1B**		Lysosome	
48g		5.3 ± 0.9		3.5 ± 0.2						
48h		5.4 ± 0.4		3.6 ± 0.4						
48i		3.0 ± 0.2		3.0 ± 0.2						
48j		2.5 ± 0.6		2.6 ± 0.2						
48k		2.6 ± 0.1		2.4 ± 0.1						
48l		3.3 ± 0.5		2.2 ± 0.5			**2A**	G_0/G_1		
49a [T]	A549; 5.0 ± 0.6	CT26; 5.4 ± 0.8	GL261; 9.1 ± 1.5	HCT-116; 6.8 ± 0.3	HeLa; 4.7 ± 0.2			n.d		125
	HepG2; 5.7 ± 0.5	HT-29; 6.3 ± 0.9	16HBE [(N)]; 6.9 ± 0.5	BEAS-2B [(N)]; 7.4 ± 0.8						
49b [T]	A549; 3.7 ± 0.5	CT26; 4.0 ± 0.1	GL261; 7.4 ± 0.7	HCT-116; 5.2 ± 0.5	HeLa; 3.9 ± 0.7		**2B**	G_2/M	Lysosome	
	HepG2; 4.3 ± 0.2	HT-29; 5.0 ± 0.5	16HBE [(N)]; 5.4 ± 0.9	BEAS-2B [(N)]; 5.8 ± 0.2						
49c [T]	A549; 3.8 ± 0.2	CT26; 4.3 ± 0.3	GL261; 8.1 ± 0.4	HCT-116; 5.1 ± 0.9	HeLa; 4.2 ± 0.5			n.d		
	HepG2; 4.7 ± 0.6	HT-29; 5.3 ± 0.3	16HBE [(N)]; 6.3 ± 0.6	BEAS-2B [(N)]; 7.4 ± 0.8						
49d [T]	A549; 4.0 ± 0.7	CT26; 4.6 ± 0.5	GL261; 7.7 ±	HCT-116; 5.9 ±	HeLa; 4.0 ±					

			0.6	0.1	0.8				
	HepG2; 4.4 ± 0.4	HT-29; 4.8 ± 0.7	16HBE [N]; 6.5 ± 0.4	BEAS-2B [N]; 7.9 ± 0.7					

[1] IC_{50} is defined as the concentration of drug required to inhibit cell growth by 50% compared to the control. Each value represents the mean ± standard deviation from two or three independent experiments.

[2] Cell viability was determined by the MTT assay, other than this is mentioned.

[T]: The complex was examined against normal cell line; *: The complex was safe to the tested normal cell with IC_{50} > 100 µM; [N]: Normal cell line; n.d: not determined.

Mechanism of action according to Fig. 3 (within the main text): **1A** pathway: NADH/ROS/MMP/Apoptosis. **1B** pathway: NADH/ROS/LMP/Apoptosis. **1AB** pathway: NADH/ROS/MMP/LMP/Apoptosis. **2A** pathway: ROS/MMP/Apoptosis.

Full names and Abbreviations of Cell lines: 16HBE, human bronchial epithelial cell lines; 518A2, human melanoma cell line; 5637, human bladder cancer cells; 8505C, human thyroid carcinoma; ARPE-19, human retinal epithelial cells; A253, human submandibular gland carcinoma; A2780, human ovarian carcinoma cell lines; A2780R/A2780cisR; Cisplatin resistant human ovarian; A427, human lung carcinoma cells; A549, Human lung carcinoma cell line; A549R, cisplatin resistant human lung carcinoma cell line; BEAS-2B, human non-tumorigenic lung epithelial cell line; BEL-7402, human hepatoma cell line; BHK21, normal healthy kidney cells; Caco-2, human colon carcinoma cell lines; Capan2, pancreatic adenocarcinoma cell line; CH1/PA-1, ovarian teratocarcinoma cell lines; CHO, normal Chinese hamster ovarian cells; CHO-K1, Chinese Hamster Ovary-K1 Cells; CNS cancer, Central nervous system cancer; Colo-829, human, umbilical metastasis, melanoma; CRL-2115, human skin fibroblast adherent; CT26, mouse colon carcinoma; DL, Dalton's ascites lymphoma; DLD-1, human colorectal adenocarcinoma cells; DU-145, human prostatic carcinoma; EA.hy926, human umbilical vein endothelial cell line; HaCaT, human keratinocyte cell line; HCT-116, colon cancer cell line; HCT-116 p53-/-, colon cancer cell line depleted p53; HEK-293T, human embryonic kidney cell lines; HeLa, cervical cancer cell line; HepG2, human liver cancer cell line; HFF-1, human skin cell lines; HL-60, human leukaemia; HT29, human colorectal adenocarcinoma cells; KMST-6, human skin fibroblast cell line; LCLC-103H, human lung carcinoma cells; LoVo, colorectal adenoma; LO2, human normal liver; MCF-7, human breast cancer cell line; MCF-10, human breast cancer cell lines; MDA-MD-435S, human breast cancer cell lines; MDB-MA-231, human breast cancer cell line; MES-OV, ovarian cancer cells; MIA PaCa-2, pancreatic carcinoma cell lines; MRC-5, human fetal lung fibroblast cells; OVCAR-3, ovarian adenocarcinoma cell line; Panc-1, pancreatic ductular adenocarcinoma cell line; PC3, human prostatic carcinoma; PNT2, normal prostate cell line; Saos, osteosarcoma cell line; SiHa, cervical cancer cell line; SISO, human uterine cervical adenocarcinoma cells; SKOV-3, human ovarian cancer cell line; SW620, human colon cell lines; U87, human glioblastoma cell lines; WHCO1, esophageal cancer cell line; WI-38, human fetal lung fibroblast cells.