Electronic Supplementary Information

for

Are the metal identity and stoichiometry of metal complexes important for colchicine site binding and inhibition of tubulin polymerization?

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1. NMR Data



Chart S1. Atom numbering of ligands for the assignment of NMR resonances.



 $R_1 = H, R_2 = H$ (HL^{3'})

Chart S2. Line drawings of oxidized TSCs and their atom numbering for the assignment of NMR resonances.



Figure S1A. ¹H NMR spectrum of HL¹.



Figure S1B. ¹³C NMR spectrum of HL¹.



Figure S2B. ¹³C NMR spectrum of HL².

Figure S3A. ¹H NMR spectrum of HL³.

Figure S3B. ¹³C NMR spectrum of HL³.

Figure S5B. ¹³C NMR spectrum of HL³'.

		HL ¹ (E-)	HL1'	HL ² (<i>E</i> -)	HL ³ (E-)	HL ³ '
H ₃	CH _{py}	8.32 (d, 1H)	8.16 (d, 1H)	8.42 (d, 1H)	8.34 (s, 1H)	8.02 (d, 1H)
H ₄	CH _{py}	7.80 (t, 1H)	8.08 (d, 1H)	7.77 (t, 1H)	7.82 (s, 1H)	7.95 (d, 1H)
H ₅	CH _{py}	7.42 (d, 1H)	7.58 (d, 1H)	7.44 (d, 1H)	7.54 (s, 1H)	7.53 (d, 1H)
H ₇	CH=N	8.11 (s, 1H)	-	-	8.15 (s, 1H)	-
H ₇ .	$CH_3(C=N)$	-	-	2.45 (s, 3H)	-	-
H ₉	NH (closer to py)	11.86 (s, 1H)	-	10.43 (s, 1H)	12.04 (s, 1H)	-
H ₁₁	NH (closer to ph)	9.98 (s, 1H)	10.26 (s, 1H)	9.93 (s, 1H)	10.24 (s, 1H)	10.65 (s, 1H)
H ₁₃₊₁₇	CH _{ph}	7.01 (s, 2H)	7.16 (s, 2H)	7.01 (s, 2H)	7.44 (d, 2H)	7.67 (d, 2H)
H ₁₄₊₁₆	CH _{ph}	-	-	-	7.39 (t, 2H)	7.38 (t, 2H)
H ₁₅	CH _{ph}	-	-	-	7.23 (t, 1H)	7.04 (s, 1H)
H ₁₈	OH _{ph}	8.21 (s, 1H)	8.12 (s, 1H)	8.23 (s, 1H)	-	-
H ₁₉₊₂₀	CH ₃	2.17 (s, 6H)	2.18 (s, 6H)	2.17 (s, 6H)	-	-
H_{22} (H_{19} for	NH _(morph)	-	10.14 (s, 1H	-	11.38 (s, 1H)	-
HL° and HL°)	CH N					
H_{21} (H_{18} lor H_{13} and H_{13})	$CH_2 - N_{(morph)}$		4.59 (s, 2H)	3.64 (s, 2H)		3.66 (s, 2H)
H (H	СН	3 50 (s. 6H)			3 50 (s. 6H)	
for HI 3 and	(closer to O)	5.57 (3, 011)	4.00 (s, 2H)	3 60 (s. 4H)	5.57 (8, 011)	3.61 (m,
$HI^{3'}$			3.72 (s, 2H)	5.00 (3, 411)		4H)
	CH					
for HI 3 and	$C_{12} (morph)$	242(s 4H)	3.50 (s, 2H)	2 43 (s 4H)	2 42 (s 4H)	2 47 (s 4H)
$HL^{3'}$		2.72 (3, 711)	3.29 (s, 2H)	2.73 (3, 111)	2.72 (3, 711)	2.77 (3, 111)

Assignment of proton resonances in ¹H NMR spectra of the morp-TSCs (solvent: DMSO- d_6).

		HL ¹ (<i>E</i> -)	HL1'	HL ² (<i>E</i> -)	HL ³ (E-)	HL ³ '
C ₂	Сру	153.23	149.67	153.92	149.17*	148.41
C ₃	CH_{py}/C_{py}	119.40	119.89	119.50	121.19	117.75
C ₄	CH _{py}	137.33	139.38	136.74	138.10	137.94
C ₅	CH _{py}	123.63	125.79	122.82	125.57	123.64
C ₆	CH _{py}	158.16*	149.70	156.90	153.76	158.70
C ₇	C=N	143.00	-	138.86	139.38	-
C ₇	thiadiazole	-	157.91	-	-	159.67
C _{7'}	$CH_3(C=N)$	-	-	12.26	-	-
C ₁₀	C=S	176.98	-	177.28	176.99	-
<i>C</i> ₁₀	S-C-N	-	167.84	-	-	165.57
C ₁₂	$C_{\rm ph}$	130.65	132.89	130.33	142.47	140.43
C ₁₃₊₁₇	CH _{ph}	126.75	119.48	126.27	126.65	117.65
C ₁₄₊₁₆	C(CH ₃) _{ph}	124.30	125.61	123.79	128.61	129.13
C ₁₅	C(OH) _{ph}	151.57	150.77	151.07	126.10	122.18
C ₁₉₊₂₀	$C(CH_3)_{ph}$	17.10	17.33	16.60	-	-
C_{21} (C_{18} for HL ³ and	CH ₂ -N _(morph)	64.39	59.42	66.20	60.23	63.53
$HL^{3'}$						
C ₂₄₊₂₅	CH _{2 (morph)}	66.65	63.77	64.13	63.59	66.22
$(C_{21+22} \text{ for } HL^3 \text{ and }$	(closer to O)					
HL ^{3'})						
C ₂₃₊₂₆	CH _{2 (morph)}	53.79	52.35	53.24	51.86	53.24
$(C_{20+23} \text{ for } HL^3 \text{ and }$	(closer to N)					
$ HL^{3'})$						

Assignment of ¹³ C resonances in ¹³ C NMR spectra of the morp-TSCs (solvent: DMSO-d ₆)).
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*Resonances were assigned by using ¹H–¹³C HSQC, ¹H–¹³C HMBC and ¹H–¹H COSY NMR spectra.

Figure S7A. ¹H NMR spectrum of 2.

Figure S7B. ¹³C NMR spectrum of 2.

Figure S8B. ¹³C NMR spectrum of **3**.

Figure S9B. ¹³C NMR spectrum of 7.

Figure S10A. ¹H NMR spectrum of 8.

Figure S10B. ¹³C NMR spectrum of 8.

		HL ¹ (E-)	1	7	8*
H ₃	CH _{py}	8.32 (d, 1H)	8.01 (d, 1H)	7.66 (d, 1H)	7.91 (d, <i>I</i> H)
H ₄	CH _{py}	7.80 (t, 1H)	8.17 (t, 1H)	8.13 (t, 1H)	8.26 (t, 1H)
H ₅	CH _{py}	7.42 (d, 1H)	7.64 (d, 1H)	7.54 (d, 1H)	7.87 (d, <i>I</i> H)
H ₇	CH=N	8.11 (s, 1H)	9.02 (s, 1H)	8.36 (s, 1H)	not detected
H ₉	NH (closer to py)	11.86 (s, 1H)	-	-	-
H ₁₁	NH (closer to ph)	9.98 (s, 1H)	10.20 (s, 1H)	9.52 (s, 1H)	not detected
H ₁₃₊₁₇	CH _{ph}	7.01 (s, 2H)	7.04 (b, 2H)	7.23 (s, 2H	7.08 (s, 2H)
H ₁₈	OH _{ph}	8.21 (s, 1H)	8.56 – 8.19 (b, 1H)	8.01 (s, 1H)	not detected
H ₁₉₊₂₀	CH _{3ph}	2.17 (s, 6H)	2.13 (s, 6H)	2.15 (s, 6H)	2.14 (s, 6H)
H ₂₂	NH _(morph)	-	-	-	-
H ₂₁	CH ₂ -N _(morph)		3.69 (s, 4H)* +	3.91 (s, 2H)	5.09 (s, 2H)
		3 50 (s. 6H)	(H _{24/25})		
H ₂₄₊₂₅	CH _{2 morph}	5.59 (8, 011)	3.49 (s, 2H)	3.81 (s, 4H)	3.98 (m, 1H)
	(closer to O)		3.41 (s, 2H)		3.74 (m, 1H)
H ₂₃₊₂₆	CH _{2 morph}	2 42 (s 4H)	2.37 (s, 2H)	2.77 (s, 4H)	3.37 (m, 1H)
	(closer to N)	2.72 (3, 11)	2.19 (s, 2H)		3.33 (m, 1H)

Assignment of proton resonances in ¹H NMR spectra of **1**, **7** and **8** (solvent: DMSO- d_6).

*Measured in DMSO- d_6 + 10% MeOD- d_4 .

		HL ¹ (<i>E</i> -)	1	7	8*
C ₂	C _{py}	153.23	158.70	148.09	158.80
C ₃	CH _{py} /C _{py}	119.40	126.51	122.53	127.21
C ₄	CH _{py}	137.33	140.74	141.86	141.87
C ₅	CH _{py}	123.63	127.31	123.13	130.38
C ₆	CH _{py}	158.16	not detected	153.63	152.41
C ₇	C=N	143.00	not detected	137.28	not detected
C ₁₀	C=S	176.98	-	-	-
<i>C</i> ₁₀	S-C-N	-	not detected	not detected	not detected
C ₁₂	C _{ph}	130.65	not detected	131.94	not detected
C ₁₃₊₁₇	CH _{ph}	126.75	not detected	122.08	124.84
C ₁₄₊₁₆	C(CH ₃) _{ph}	124.30	125.09	124.01	not detected
C ₁₅	C(OH) _{ph}	151.57	151.04*	149.16	not detected
C ₁₉₊₂₀	C(CH ₃) _{ph}	17.10	17.28	16.84	16.97
C ₂₁	CH ₂ -N _(morph)	64.39	60.06*	60.77	63.55
C ₂₄₊₂₅	CH _{2 (morph)} (closer	66.65	65.62	64.91	58.14
	to O)				
C ₂₃₊₂₆	CH _{2 (morph)} (closer to N)	53.79	53.29	53.38	51.41

Assignment of ¹³C resonances in ¹³C NMR spectra of 1, 7 and 8 (solvent: DMSO- d_6).

*Resonances were assigned by using ¹H–¹³C HSQC, ¹H–¹³C HMBC and ¹H–¹H COSY NMR spectra.

2.	Crystallographic data collection
	Table S1. Crystal Data and Details of Data Collection and Refinement for [Co ^{III} (HL ¹)(L ¹)](NO ₃) ₂ ·H ₂ O (1), [Co ^{III} (HL ³)(L ³)](NO ₃) ₂ (3) ₂ ·H ₂ O (1), [Co ^{III} (HL ³)(L ³)](NO ₃) ₂ (3) ₂ ·H ₂ O (1), [Co ^{III} (HL ³)(L ³)](NO ₃) ₂ (3) ₂ ·H ₂ O (1), [Co ^{III} (HL ³)(L ³)](NO ₃) ₂ (3) ₂ ·H ₂ O (1), [Co ^{III} (HL ³)(L ³)](NO ₃) ₂ (3) ₂ ·H ₂ O (1), [Co ^{III} (HL ³)(L ³)](NO ₃) ₂ (3) ₂ ·H ₂ O (1), [Co ^{III} (HL ³)(L ³)](NO ₃) ₂ (3) ₂ ·H ₂ O (1), [Co ^{III} (HL ³)(L ³)](NO ₃) ₂ (3) ₂ ·H ₂ O (1), [Co ^{III} (HL ³)(L ³)](NO ₃) ₂ (3) ₂ ·H ₂ O (1), [Co ^{III} (HL ³)(L ³)](NO ₃) ₂ ·H ₂ O (1), [Co ^{III} (HL ³)(L ³)](NO ₃) ₂ (3) ₂ ·H ₂ O (1), [Co ^{III} (HL ³)(L ³)](NO ₃) ₂ (3) ₂ ·H ₂ O (1), [Co ^{III} (HL ³)(L ³)](NO ₃) ₂ (3) ₂ ·H ₂ O (1), [Co ^{III} (HL ³)(L ³)](NO ₃) ₂ (3) ₂ ·H ₂ O (1), [Co ^{III} (HL ³)(L ³)](NO ₃) ₂ (3) ₂ ·H ₂ O (1), [Co ^{III} (HL ³)(L ³)](NO ₃) ₂ ·H ₂ O (1), [Co ^{III} (HL ³)(L ³)](NO ₃) ₂ (3) ₂ ·H ₂ O (1), [Co ^{III} (HL ³)(L ³)](NO ₃) ₂ ·H ₂ O (1), [Co ^{III} (HL ³)(L ³)](NO ₃) ₂ (3) ₂ ·H ₂ O (1), [Co ^{III} (HL ³)(L ³)](NO ₃) ₂ ·H ₂ O (1), [Co ^{III} (HL ³)(L ³)](NO ₃) ₂ ·H ₂ O (1), [Co ^{III} (HL ³)(L ³)](NO ₃) ₂ ·H ₂ O (1), [Co ^{III} (HL ³)(L ³)](NO ₃) ₂ ·H ₂ O (1), [Co ^{III} (HL ³)(L ³)](NO ₃) ₂ ·H ₂ O (1), [Co ^{III} (HL ³)(L ³)](NO ₃) ₂ ·H ₂ O (1), [Co ^{III} (HL ³)(L ³)](NO ₃) ₂ ·H ₂ O (1), [Co ^{III} (HL ³)(L ³)](NO ₃) ₂ ·H ₂ O (1), [Co ^{III} (HL ³)(L ³)](NO ₃) ₂ ·H ₂ O (1), [Co ^{III} (HL ³)(L ³)](NO ₃) ₂ ·H ₂ O (1), [Co ^{III} (HL ³)(L ³)](NO ₃) ₂ ·H ₂ O (1), [Co ^{III} (HL ³)(L ³)](NO ₃) ₂ ·H ₂ O (1), [Co ^{III} (HL ³)(L ³)](NO ₃) ₂ ·H ₂ O (1), [Co ^{III} (HL ³)(L ³)](NO ₃) ₂ ·H ₂ O (1), [Co ^{III} (HL ³)(L ³)](NO ₃) ₂ ·H ₂ O (1), [Co ^{III} (HL ³)(L ³)](NO ₃) ₂ ·H ₂ O (1), [Co ^{III} (HL ³)(L ³)](NO ₃) ₂ ·H ₂ O (1), [Co ^{III} (HL ³)(L ³)](NO ₃) ₂ ·H ₂ O (1), [Co ^{III} (HL ³)(L ³)](NO ₃) ₂ ·H ₂ O (1), [Co ^{III} (HL ³)(L ³)(L ³)](NO ₃) ₂ ·H ₂ O (1), [Co ^{III} (HL ³)(L ³)
	$[Fe^{III}(L^2)_2]NO_3(4), [Fe^{III}(HL^3)(L^3)](NO_3)_2(6).$

compound	$[Co^{III}(HL^1)(L^1)](NO_3)_2 \cdot H_2O$	$[Co^{III}(HL^3)(L^3)](NO_3)_2$	$[Fe^{III}(L^2)_2]NO_3$	$[Fe^{III}(HL^3)(L^3)](NO_3)_2$
empirical formula	$C_{40}H_{51}CoN_{12}O_{11}S_2$	$C_{38}H_{49}CoN_{12}O_{10}S_2$	C _{42.65} H _{54.60} FeN ₁₁ O _{7.65} S ₂	$C_{36}H_{41}FeN_{12}O_8S_2$
fw	998.97	956.94	963.74	889.78
space group	$P2_1/c$	$P2_1/n$	$P2_1/n$	$P2_1/n$
<i>a</i> , Å	19.607(3)	17.659(4)	16.8583(16)	17.7730(5)
<i>b</i> , Å	17.3104(15)	9.9034(13)	13.8926(7)	9.9333(2)
<i>c</i> , Å	15.5505(15)	24.975(7)	21.7744(17)	24.8488(7)
α, \circ				
β, \circ	109.389(10)	95.42(2)	107.706(7)	95.264(2)
γ, °				
<i>V</i> [Å ³]	4978.7(11)	4348.1(17)	4858.1(7)	4368.4(2)
Ζ	4	4	4	4
λ [Å]	0.71073	0.71073	0.71073	0.71073
$ ho_{ m calcd}, { m g~cm^{-3}}$	1.333	1.462	1.318	1.353
cryst size, mm ³	$0.17 \times 0.11 \times 0.04$	$0.25 \times 0.12 \times 0.03$	$0.20 \times 0.12 \times 0.01$	$0.30 \times 0.14 \times 0.02$
<i>T</i> [K]	100(2)	100(2)	100(2)	100(2)
μ , mm ⁻¹	0.495	0.561	0.456	0.503
R_1^a	0.0526	0.0416	0.0851	0.0325
WR_2^b	0.1289	0.1053	0.2308	0.0762
GOF ^c	0.918	0.929	0.953	0.945
CCDC no.	2354137	2354138	2354139	2354140

 ${}^{a}R_{1} = \Sigma ||F_{o}| - |F_{c}||/\Sigma |F_{o}|. \ {}^{b}wR_{2} = \{\Sigma [w(F_{o}^{2} - F_{c}^{2})^{2}]/\Sigma [w(F_{o}^{2})^{2}]\}^{1/2}. \ {}^{c}GOF = \{\Sigma [w(F_{o}^{2} - F_{c}^{2})^{2}]/(n-p)\}^{1/2}, \text{ where n is the number of reflections and p is the total number of parameters refined.}$

Table S2. Crystal Data and Details of Data Collection and Refinement for [Ni^{II}(L¹)]Cl·CH₃OH, [Zn^{II}(L¹)Cl]·CH₃OH and [Pd^{II}(HL¹)Cl]Cl

compound	[Ni ^{II} (L ¹)]Cl·CH ₃ OH	$[Zn^{II}(L^1)Cl] \cdot CH_3OH$	[Pd ^{II} (HL ¹)Cl]Cl	$[H_2L^1]NO_3$
empirical formula	C ₂₁ H ₂₈ ClN ₅ NiO ₃ S	C ₂₀ H ₂₄ ClN ₅ O ₂ SZn	C ₂₀ H ₂₇ Cl ₂ N ₅ O ₃ PdS	C ₂₀ H ₂₄ N ₆ O ₅ S
fw	524.70	499.32	576.81	460.51
space group	Pnn2	PĪ	I2/c	$P2_1/n$
<i>a</i> , Å	20.022(3)	9.5512(16)	13.9557(12)	13.9111(13)
<i>b</i> , Å	8.8256(10)	9.8642(17)	15.1993(13)	8.5430(6)
<i>c</i> , Å	17.135(2)	12.120(2)	24.0558(18)	18.0419(18)
α , °		87.313(14)		
β , °		80.712(13)	102.430(5)	92.547(8)
γ, °		70.063(12)		
V[Å ³]	3027.9(7)	1059.3(3)	4983.0(7)	2142.0(3)
Ζ	4	2	8	4
λ [Å]	0.71073	0.71073	0.71073	1.54178
$ ho_{ m calcd}$, g cm ⁻³	1.151	1.565	1.538	1.428
cryst size, mm ³	$0.70 \times 0.075 \times 0.075$	$0.20 \times 0.08 \times 0.035$	$0.13 \times 0.08 \times 0.02$	$0.30 \times 0.14 \times 0.02$
<i>T</i> [K]	296(2)	100(2)	100(2)	100(2)
μ , mm ⁻¹	0.824	1.412	1.069	1.744
R_1^a	0.0301	0.0565	0.0369	0.0700
wR_2^b	0.0603	0.1678	0.0687	0.2007
GOF ^c	1.022	1.088	0.854	0.985
CCDC no.	2354141	2354142	2354143	2354144

^a $R_1 = \Sigma ||F_o| - |F_c|| / \Sigma |F_o|$. ^b $wR_2 = \{\Sigma [w(F_o^2 - F_c^2)^2] / \Sigma [w(F_o^2)^2] \}^{1/2}$. ^c GOF = $\{\Sigma [w(F_o^2 - F_c^2)^2] / (n-p) \}^{1/2}$, where *n* is the number of reflections and *p* is the total number of parameters refined.

Figure S11. ORTEP view of $[H_2L^1]NO_3$

3. Solution Stability Studies

Figure S12. Changes of absorbance values measured for (a) HL^1 , (b) HL^2 and (c) HL^3 in DMSO (**•**), at pH 2 (**•**), at pH 7.4 (**•**), at pH 11.7 in glove box (**•**) and in a normal cuvette (**•**) over time at the absorbance maximum; { $c_{ligand} = 50 \ \mu M$; $\ell = 1 \ cm$; $t = 25.0 \ ^{\circ}C$ }. S20

Figure S13. UV–vis absorption spectra recorded for HL² at (a) pH 2 and (b) pH 11.7, and for HL³ at (c) pH 2 and (d) pH 11.7 over time; { $c_{\text{ligand}} = 50 \ \mu\text{M}$; $\ell = 1 \text{ cm}$; $t = 25.0 \ ^{\circ}\text{C}$ }.

Figure S14. pH-potentiometric titration curves of the studied proligands HL^1-HL^3 in 30% (v/v) DMSO/H₂O. Base equivalent: $(n_{KOH} - n_{HCl}) / n_{ligand}$; { $\ell = 1 \text{ cm}$; I = 0.1 M (KCl); t = 25.0 °C}.

Figure S15. UV–vis absorption spectra recorded for (a) complex **2** at pH 2 and for complex **5** (b) at pH 2, (c) complex **2** in DMSO, and (d) complex **2** at pH 7.4 over time; $\{c_{complex} = 21 \ \mu M \ (2) \text{ or } 23 \ \mu M \ (5); \ell = 1 \text{ cm}; t = 25.0 \ ^{\circ}\text{C}\}.$

Figure S16. UV–vis absorption spectra recorded for complex **4** (green lines) and **HL**² (black lines) at pH 11.7 over time in the glove box; { $c = 23 \mu$ M; $\ell = 1 \text{ cm}$; t = 25.0 °C}.

4. Spectroelectrochemistry

Figure S17. Cyclic voltammograms of the nickel complex **6** (a) in the cathodic and (b) in the anodic part, as well as of the zinc(II) complex 7 (c) in the cathodic and (d) in the anodic part in DMSO/ nBu_4NPF_6 (Pt working electrode, scan rate: 100 mV s⁻¹). Asterisk indicates the follow up products formed upon reduction and oxidation, respectively.

Figure S18. Cyclic voltammograms of palladium(II) complex **8** (a) in the cathodic part and (b) in both the anodic and cathodic parts in the presence of ferrocene in DMSO/ nBu_4NPF_6 (Pt working electrode, scan rate: 100 mV s⁻¹).

Figure S19. (a) Difference UV–vis–NIR spectra detected simultaneously during the *in situ* reduction of **3** in $nBu_4NPF_6/DMSO$ in the region of the first cathodic peak (forward scan). Inset: respective cyclic voltammogram (Pt-microstructured honeycomb working electrode, scan rate $v = 10 \text{ mV s}^{-1}$). (b) Difference UV–vis–NIR spectra taken during cyclic voltametric scan of **3** shown in 3D mode.

Figure S20. (a) UV–vis–NIR spectra detected simultaneously upon the *in situ* reduction of **1** in $nBu_4NPF_6/DMSO$ in the region of the first cathodic peak; inset: respective cyclic voltammogram (Pt-microstructured honeycomb working electrode, scan rate $v = 10 \text{ mV s}^{-1}$); (b) Difference UV–vis–NIR spectra taken upon cyclic voltametric scan of **1** shown in 3D mode.

Figure S21. (a) UV–vis–NIR spectra of **4** in DMSO; (b) Spectroelectrochemistry of **4** in $nBu_4NPF_6/DMSO$ in the region of the first cathodic peak - evolution of difference UV–vis–NIR spectra measured simultaneously upon forward scan (Pt-microstructured honeycomb working electrode, scan rate $v = 10 \text{ mV s}^{-1}$).

Figure S22. UV–vis–NIR spectra measured simultaneously upon the *in situ* reduction of **5** in $nBu_4NPF_6/DMSO$ in the region of the first cathodic peak (forward scan); inset: respective cyclic voltammogram (Pt-microstructured honeycomb working electrode, scan rate $v = 10 \text{ mV s}^{-1}$).

5. NCI-60 One-Dose Screen

Figure S23. One dose mean graph for HL¹.

Panel/Cell Line	Growth Percent	Mean Growth Percent - Growth Percent
Leukemia		
CCRF-CEM	9.88	
HL-60(1B)	9.95	
MOLT-4	20.25	
RPMI-8226	19.90	
Non-Small Cell Lung Cancer	1. Sec. 19.	
A549/ATCC	32.99	
EKVX	11.57	
HOP-62	35.42	
NCI-H228	3.87	
NCI-H23	39.11	
NCI-H460	16.84	
NCI-H522	41.07	
Colon Cancer		
LCC 2009	42.66	
HCT-116	23.27	
HCT-15	21.66	
HT29	46.63	
KM12	19.29	
SW-620	24.42	
CNS Cancer	20.02	
SE-205	27 12	
SF-539	-3.39	
SNB-19	29.94	
U251	19.67	
Melanoma	44.50	
LOX IMVI	11.58	
MDA-MB-435	46.08	
SK-MEL-2	30.88	
SK-MEL-28	43.48	
SK-MEL-5	17.84	
UACC-257	70.40	
UACC-82	22.88	
OVCAR-3	19.42	
OVCAR-4	34.07	
OVCAR-5	53.27	
OVCAR-8	28.12	
NCI/ADR-RES	11.28	
SK-OV-3	45.55	
796-0	40.28	
A498	84.67	
ACHN	13.35	
CAKI-1	20.76	
RXF 393	58.80	
SN12C	30.72	
Prostate Cancer	53.62	
PC-3	39.54	
DU-145	41.09	
Breast Cancer		
MCF7	12.73	
MDA-MB-231/ATCC	47.22	
BT-549	40.82	
T-47D	31.19	
MDA-MB-468	-15.72	
Mean	30.54	
Delta	46.26	
Range	100.39	
	450	100 50 0 50 100 150
	100	C TTT)

Figure S24. One dose mean graph for HL².

Panel/Cell Line	Growth Percent	Mean Growth Percent - Growth Percent
Leukemia	2000	
CCRF-CEM	88.42	
HL-60(TB)	106.42	
K-562	106.98	
DDML 9228	02.70	
SR	106.50	
Non-Small Cell Lung Cancer		
A549/ATCC	101.08	
EKVX	98.00	
HOP-62	100.04	
NCLH228	102.03	
NCI-H23	96.35	
NCI-H460	99.40	
NCI-H522	99.80	
Colon Cancer		
COLO 205	88.37	
HCC-2998	01.55	
HCT-15	98.34	
HT29	114.55	
KM12	101.52	
SW-620	101.99	
CNS Cancer	100.55	
SE-205	100.00	
SE-539	82.69	
SNB-19	89.61	
U251	96.16	
Melanoma		
LOX IMVI	92.21	
MDA_MR_425	93.00	
SK-MEL-2	100.22	
SK-MEL-28	96.69	
SK-MEL-5	95.53	
UACC-257	96.01	
UACC-82	90.17	
OVCAR-2	117 11	
OVCAR-4	99.41	
OVCAR-5	91.25	
OVCAR-8	103.34	
NCI/ADR-RES	104.51	
SK-OV-3	98.07	
786-0	95.73	
A498	109.22	
ACHN	98.80	
CAKI-1	81.82	
RXF 393	115.85	
SN12C	99.03	
Prostate Cancer	85.05	
PC-3	84.03	
DU-145	110.89	
Breast Cancer		
MCF7	88.22	
MDA-MB-231/ATCC	92.80	
BT-549	73.42	
T-47D	95.62	
MDA-MB-468	42.10	
	05.70	
Mean	85.79	
Rance	75.01	
i van ge	10.01	
	150	100 50 0 -50 -100 -150

Figure S25. One dose mean graph for 3.

Figure S26. One dose mean graph for 6.

Figure S27. One dose mean graph for 7.

Panel/Cell Line	Growth Percent	Mean Growth Percent - Growth Percent
Leukemia		
CCRF-CEM	6.14	
HL-60(TB)	24.85	
K-562	26.90	
MOLT-4	23.58	
RPMI-8226	37.50	
SR	30.54	
Non-Small Cell Lung Cancer		
A549/ATCC	52.02	
EKVX	72.38	
HOP-62	50.38	
HOP-92	82.78	
NCI-H226	58.82	
NCI-H23	74.34	
NCI-H460	53.44	
Colon Concer	-01.07	
COLO 205	51 50	
HCC-2998	81.90	
HCT-116	18.05	
HCT-15	36.09	
HT29	78.34	
KM12	62.48	
SW-620	26.51	
CNS Cancer		
SF-268	66.41	
SF-295	80.54	
SF-539	69.45	
SNB-19	69.20	
U251	49.23	
Melanoma		
LOX IMVI	37.91	
M14	20.18	
MDA-MB-435	9.85	
SK-MEL 20	05.70	
SK-MEL-20	31.25	
UACC-257	66.88	
UACC-62	64.43	
Ovarian Cancer	04.45	
OVCAR-3	6.66	
OVCAR-4	57.10	
OVCAR-5	82.86	
OVCAR-8	61.54	
NCI/ADR-RES	71.20	
SK-OV-3	67.05	
Renal Cancer		
786-0	32.80	
A498	(4.5/	
CAKLA	12.60	
BYE 303	43.00	
SN12C	78.02	
TK-10	87.32	
Prostate Cancer	07.02	
PC-3	52.10	
DU-145	62.80	
Breast Cancer	100 M 100 M	
MCF7	19.92	
MDA-MB-231/ATCC	57.40	
HS 578T	74.15	
BT-549	30.11	
T-47D	24.66	
MDA-MB-468	-1.96	
	10.44	
Mean	48.11	
Dena	129.98	
Range	109.19	

Figure S28. One dose mean graph for 8.

6. NCI-60 5-Dose Screen

Figure

1.

Figure S30. Dose response curves for 2.

S35

Figure S31. Dose response curves for 4.

S36

7. Molecular docking

Figure S33. (a) The docked pose of **8** (ball-and-stick) in the colchicine site of tubulin. The cocrystalized ligand (LOC) is shown in line format (green), its hydrogen atoms are not shown for clarity. The protein surface is rendered with blue color depicting regions with a partial positive charge on the surface, red color depicting regions with a partial negative charge and grey showing neutral areas. (b) The predicted binding of complex **8**, amino acids within 5 Å are shown in line format. Complex formation of the amide side chain of β Asn258 with the Pd(II) could occur as shown in this docking image (black solid line, 3.7 Å).