Supporting Information for

Ni(II) Curcumin Complexes for Cellular Imaging and Photo-triggered *in vitro* Anticancer Activity

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Table S1. Selected Crystallographic Data for the complex [Ni(acac)(phen)₂(ClO₄)]

Empirical formula	C ₂₉ H ₂₃ Cl N ₄ Ni O ₆
Fw, g M ⁻¹	617.67
Crystal system	monoclinic
Space group	<i>C</i> 2/c
<i>a</i> , Å	32.2598(15)
<i>b</i> , Å	10.2015(4)
<i>c</i> , Å	17.2389(7)
α , °	90
β , °	107.362(3)
γ , °	90
<i>V</i> , Å ³	5414.8(4)
<i>Z</i>	8
<i>T</i> , K	296(2)
ρ_{calcd} , g cm ⁻³	1.515
λ , Å (Mo-K α)	0.71073
μ , cm ⁻¹	0.867
Data / restraints / parameters	6560 / 0/ 373
<i>F</i> (000)	2544
Goodness-of-fit	1.029
<i>R</i> (<i>F</i> _o) ^a , I>2 σ (I) [<i>wR</i> (<i>F</i> _o) ^b]	0.0443 [0.1212]
<i>R</i> (all data) [<i>wR</i> (all data)]	0.0701 [0.1384]
Largest diff. peak and hole (e Å ⁻³)	0.397, -0.521

^a $R = \sum ||F_o| - |F_c|| / \sum |F_o|$, ^b $wR = \{ \sum [w(F_o^2 - F_c^2)^2] / \sum [w(F_o^2)] \}^{1/2}$; $w = [\sigma^2(F_o)^2 + (AP)^2 + BP]^{-1}$, where $P = (F_o^2 + 2F_c^2)/3$, A = 0.0758; B = 3.1016

Table S2. Selected bond distances (Å) and bond angles (°) of [Ni(acac)(phen)₂(ClO₄)] (**4**)

Ni1-N1	2.113(2)	N3-Ni1-N2	172.94(8)
Ni1-N2	2.087(2)	O1-Ni1-N4	88.81(7)
Ni1-N3	2.080(2)	O2-Ni1-N4	171.78(8)
Ni1-N4	2.097(2)	N3-Ni1-N4	79.66(8)
Ni1-O1	2.0234(17)	N2-Ni1-N4	96.58(8)
Ni1-O2	2.0310(16)	O1-Ni1-N1	171.20(8)
O1-Ni1-O2	90.28(7)	O2-Ni1-N1	89.16(7)
O1-Ni1-N3	93.73(8)	N3-Ni1-N1	95.06(8)
O2-Ni1-N3	92.25(8)	N2-Ni1-N1	79.09(9)
O1-Ni1-N2	92.15(8)	N4-Ni1-N1	92.97(8)
O2-Ni1-N2	91.61(7)		

Table S3: DNA and protein binding constants for the Complexes [Ni(cur)(L)₂](OAc) (**1-3**) and [Ni(acac)(L)₂](OAc) (**4-6**) (L = phen, **1, 4**; dpq, **2, 5**; dppz, **3, 6**)

Complex No.	Binding constant (M ⁻¹)		
	<i>ct</i> -DNA		HSA
	K _b	K _{app}	
1	7.38 (±0.79) × 10 ⁵	1.02 × 10 ⁶	1.47 (±0.02) × 10 ⁵
2	7.60 (±0.54) × 10 ⁵	2.52 × 10 ⁶	5.23 (±0.03) × 10 ⁵
3	8.30 (±0.38) × 10 ⁵	5.24 × 10 ⁶	7.38 (±0.07) × 10 ⁵
4	7.74 (±0.48) × 10 ⁵	5.74 × 10 ⁴	1.65 (±0.02) × 10 ⁵
5	8.80 (±0.44) × 10 ⁵	1.60 × 10 ⁵	4.56 (±0.07) × 10 ⁵
6	9.64 (±0.56) × 10 ⁵	3.60 × 10 ⁵	4.73 (±0.09) × 10 ⁵

Table S4: The content of nickel (ng per 10⁶ cells) in A549 cells after incubation with the complexes **3** and **6** (10 μM) for 4 h.

Complex	Nickel (ng per 10 ⁶ cells)
3	510 ± 10.8
6	44 ± 1.2

Table S5: The content of nickel (ng per 10⁶ cells) in the nuclei and mitochondria of A549 cells after incubation with the complexes **3** and **6** (10 μM) for 4 h.

Complex	Nickel (ng per 10 ⁶ cells)	
	Nuclei	Mitochondria
3	10.6 ± 0.4	24.1 ± 0.7
6	4.8 ± 0.2	13.5 ± 0.6

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Scheme S3. Synthetic scheme for the complexes 4-6.

Figure S1. ^1H NMR spectra of the ligands dpq and dppz.

Figure S2. ESI-MS spectrum of complex **1** in methanol showing the $[M-(OAc)]^+$ peak at $m/z = 785.2062$.

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Figure S4. ESI-MS spectrum of complex **3** in methanol showing the $[M-(OAc)]^+$ peak at $m/z = 989.2551$.

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