Supporting Information

Important cytotoxic and cytostatic effects of new Copper(I)-phosphane compounds with NN, NO and NS bidentate ligands

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Supplementary Figures S1 – S3

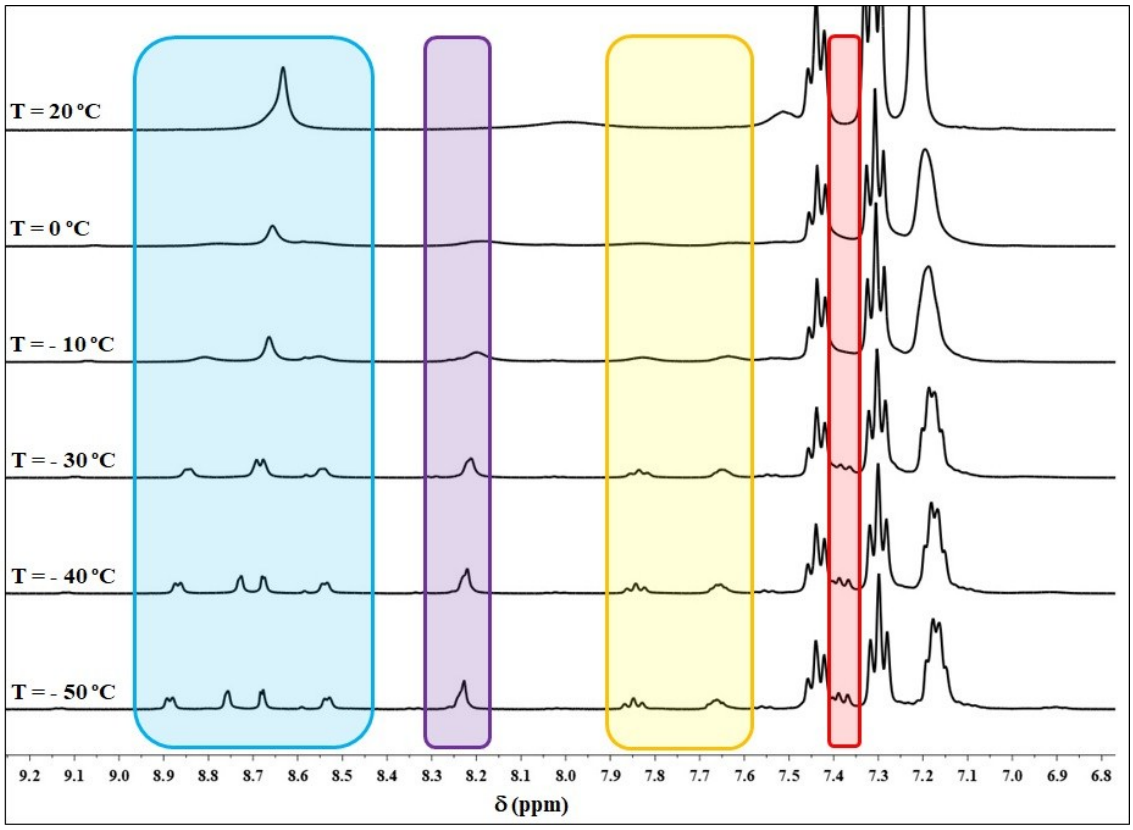

Figure S1 *^{1}H NMR spectra of compound **4** at different temperatures*

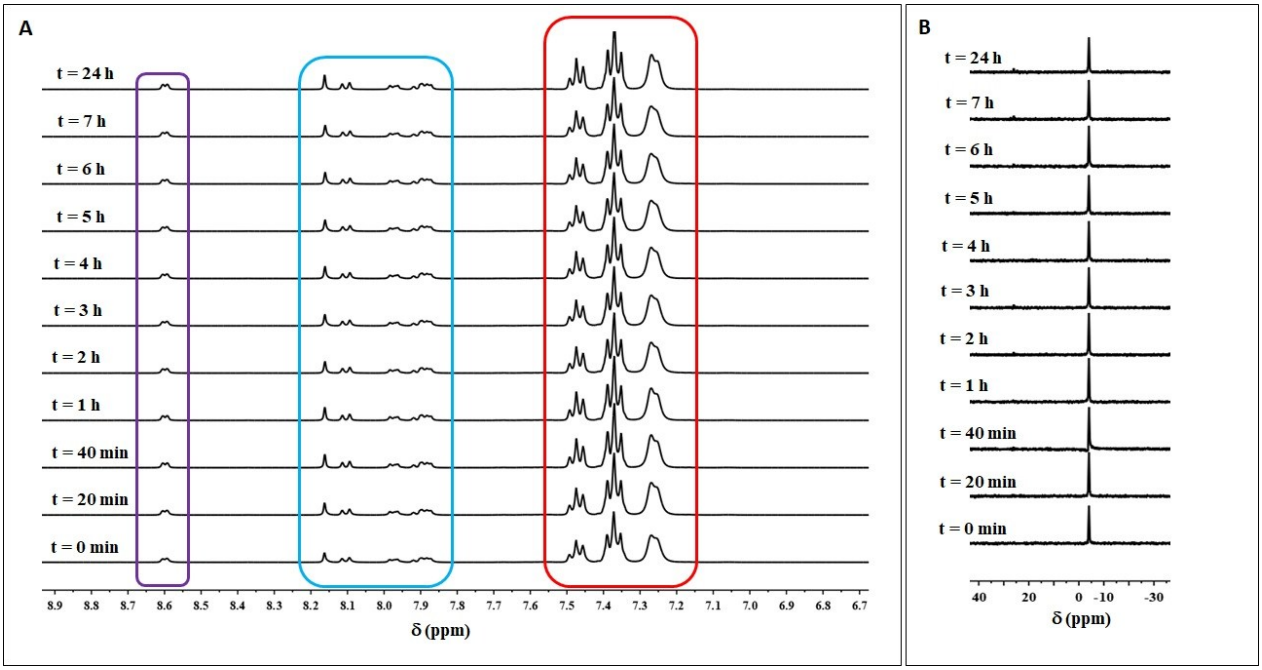

Figure S2 *Evaluation of complex **1** stability by ^{1}H- (**A**) and ^{31}P-NMR (**B**) over 24 h.*

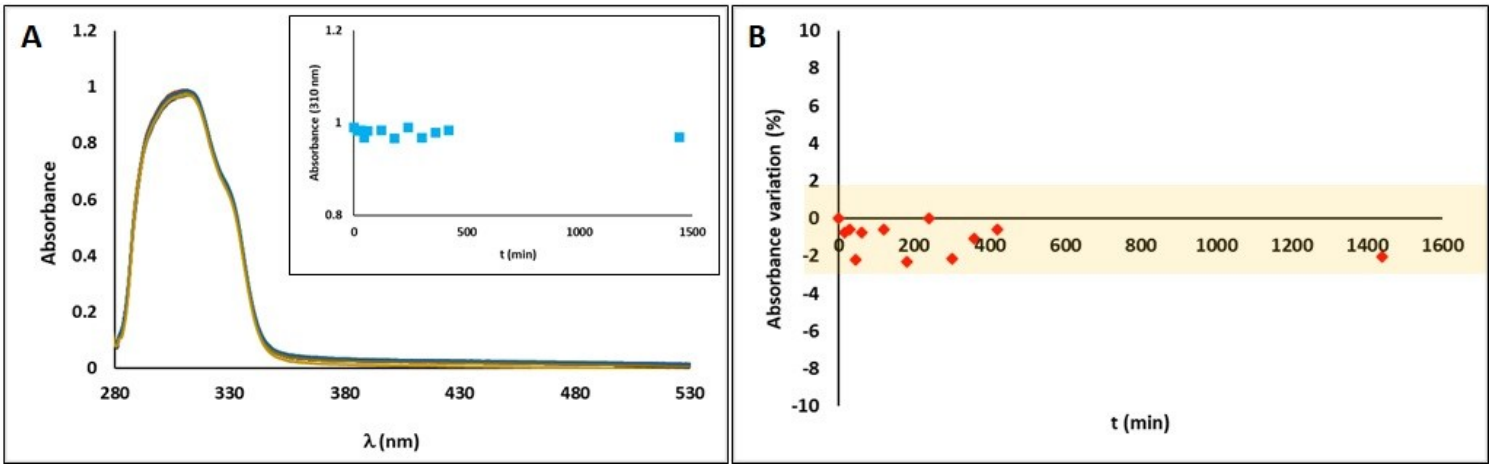

Figure S3 *Evaluation of the stability of complex* ***1*** *by UV-vis spectroscopy over 24 hours in 1%DMSO/ DMEM+GlutaMAX-I™ solution. (**A**) UV–visible spectra recorded over time, from 0 min up to 1440 min=24 h, for a 36.1 µM solution; inset: changes in absorbance observed at 310 nm (■); (**B**) absorbance variation percentage along time (0 min to 1440 min) (♦).*

Compound	1	2	3	4	5
Bond lengths (Å)					
Cu(1) – N(1)	2.0303(17)	2.050(3)	2.076(3)	2.078(4)	2.099(2)
Cu(1) – X	2.6902(6)	2.211(2)	2.099(3)	2.104(4)	2.055(2)
Cu(1) – P(1)	2.2507(6)	2.2423(11)	2.2796(9)	2.2474(14)	2.2569(8)
Cu(1) – P(2)	2.2509(6)	2.2442(11)	2.2836(9)	2.2459(14)	2.2593(7)
N(1) – C(1)	1.343(3)	1.331(4)	1.341(4)	1.348(6)	1.346(4)
N(1) – C(5)	1.359(3)	1.353(4)	1.343(4)	1.334(6)	1.351(4)
X – C(6)	1.754(2)	1.222(3)	1.218(4)	1.350(6)	1.351(4)
X – C(7)	–	–	1.346(4)		
X – C(9)	1.744(2)	–	–	1.339(6)	-
X – C(10)	–	–	–		1.344(4)
X – C(11)	–	–	1.341(4)		
Angles (°)					
X – Cu(1) – N(1)	77.76(5)	76.55(9)	92.17(11)	79.18(15)	79.64(9)
P(2) – Cu(1) – P(1)	129.37(2)	125.96(4)	123.14(3)	123.76(5)	124.91(3)
N(1) – Cu(1) – P(1)	116.39(5)	116.53(8)	115.06(8)	117.33(12)	113.19(6)
N(1) – Cu(1) – P(2)	113.17(5)	112.17(8)	103.38(8)	109.34(12)	107.90(6)
P(1) – Cu(1) – X	106.55(2)	105.06(7)	105.53(8)	104.33(11)	109.64(7)
P(2) – Cu(1) – X	93.08(2)	107.66(6)	113.43(8)	113.93(11)	112.53(6)
C(6) – Cu(1) – X	–	113.51(19)	–	–	–
C(9) – Cu(1) – X	–	–	–	–	–
C(1) – N(1) – Cu(1)	118.86(15)	125.2(2)	115.5(2)	125.8(4)	127.5(2)
C(5) – N(1) – Cu(1)	122.46(14)	116.4(2)	126.5(2)	113.7(3)	113.27(19)
C(1) – N(1) – C(5)	118.52(18)	118.0(3)	117.1(3)	118.1(4)	117.8(3)
C(6) – X– Cu(1)	87.80(8)	113.51(19)	–	111.8(3)	114.73(18)

C(9) – X– Cu(1)	142.85(7)	–	–	127.2(3)	–
C(9) – X– C(6)	91.56(11)	–	–	–	–
C(10) – X– Cu(1)	–	–	–	–	126.1(2)
C(10) – X– C(6)	–	–	–	–	118.4(2)
C(7) – X– Cu(1)	–	–	125.5(2)	–	–
C(11) – X– Cu(1)	–	–	117.7(2)	–	–
C(11) – X– C(7)	–	–	116.3(3)	–	–
N(1) – C(1) – C(2)	122.6(2)	124.0(3)	124.2(4)	122.6(5)	122.7(3)
N(1) – C(5) – C(4)	121.1(2)	121.1(3)	121.9(3)	122.4(4)	121.9(3)
N(1) – C(5) – C(6)	117.17(18)	114.3(3)	121.6(3)	114.9(4)	115.4(2)
X – C(6) – C(5)	111.85(18)	118.7(3)	–	113.9(4)	115.3(2)
X – C(6) – C(7)	111.72(16)	118.8(3)	–	120.3(4)	121.8(3)
X – C(7) – C(6)	–	121.2(3)	–	–	–
X – C(7) – C(8)	–		122.4(3)	–	–
X – C(9) – C(8)	110.56(18)	–	–	120.9(4)	–
X – C(10) – C(9)	126.91(16)	–	–	–	122.7(3)
X – C(11) – C(10)	–	–	124.2(4)	–	–

Table S3 *Selected Bonds (Å) and Bonds Angles (°) of the cations $[Cu(PPh_3)_2(L)]^+$ (L= pbt, **1**; bopy, **2**; dpk, **3**; dpp, **4**; 2,2'bipy, **5**).*

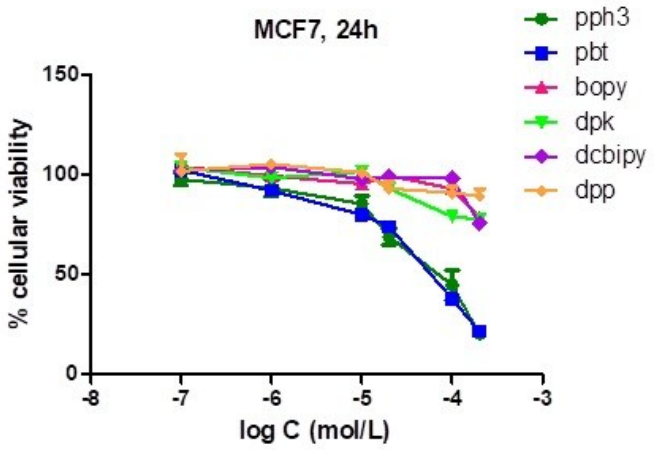

Figure S4 *Determination of the IC_{50} values for free heteroaromatic and phosphane ligands by the MTT assay. Dose-response curves obtained with the MCF7 cells after incubation of the compounds for 24h, 37ºC.*