

Cellular and Computational Studies of Proteasome Inhibition and Apoptosis Induction in Human Cancer Cells by Amino Acid Schiff Base-Copper Complexes

Jian Zuo ^{a,b}, Caifeng Bi ^a, Yuhua Fan ^{a,*}, Daniela Buac ^b, Chiara Nardon ^{b,c}, Kenyon G. Daniel ^{d,e},
Q. Ping Dou ^{b,*}

^a College of Chemistry and Chemical Engineering, Ocean University of China, Qingdao, Shandong 266100, People's Republic of China

^b Molecular Therapeutics Program, Barbara Ann Karmanos Cancer Institute, Departments of Oncology, Pharmacology and Pathology, School of Medicine, Wayne State University, Detroit, Michigan 48201, United States

^c Department of Chemical Sciences, University of Padova, Via Marzolo 1, 35131 Padova, Italy

^d Virtual Screening and Molecular Modeling Core, Moffitt Cancer Center and Research Institute, Tampa, Florida 33612, United States

^e Department of Cell Biology, Microbiology, and Molecular Biology, University of South Florida, Tampa, Florida 33620, United States

* Corresponding authors. Fax: 0532-66781932. E-mail: fanyuhua301@163.com (Yuhua Fan)

Fax: 313-576-8307. E-mail: doup@karmanos.org (Q. Ping Dou)

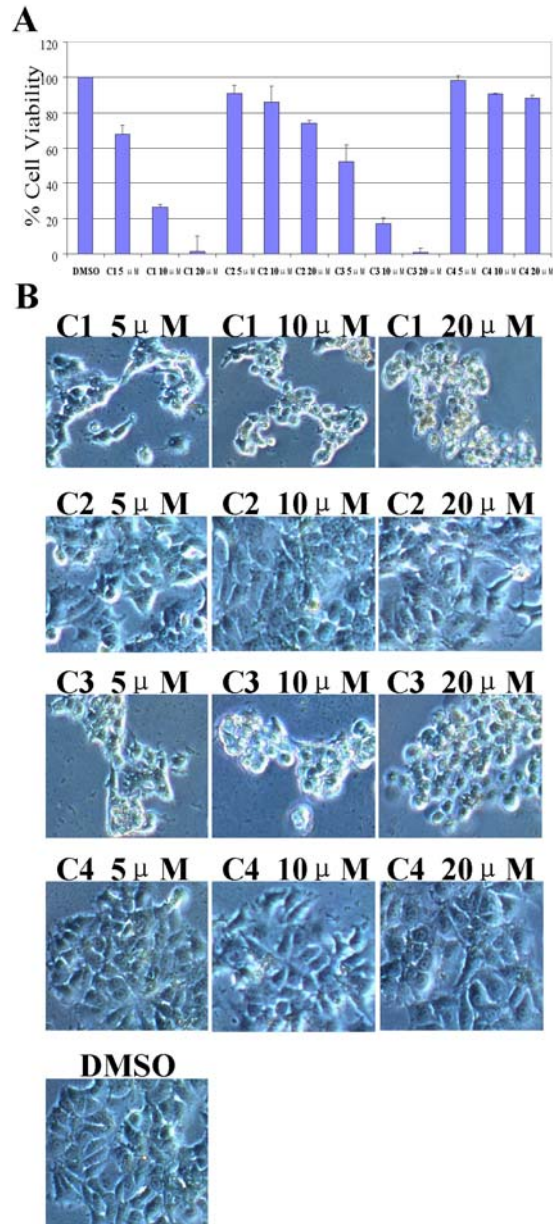


Figure S1. Dose response experiment using C1, C2, C3 and C4 in human breast cancer MCF-7 cells. MCF-7 cells were treated with either solvent DMSO or indicated concentrations of C1-C4 for 24 h. (A) MTT assay. (B) Morphological changes.

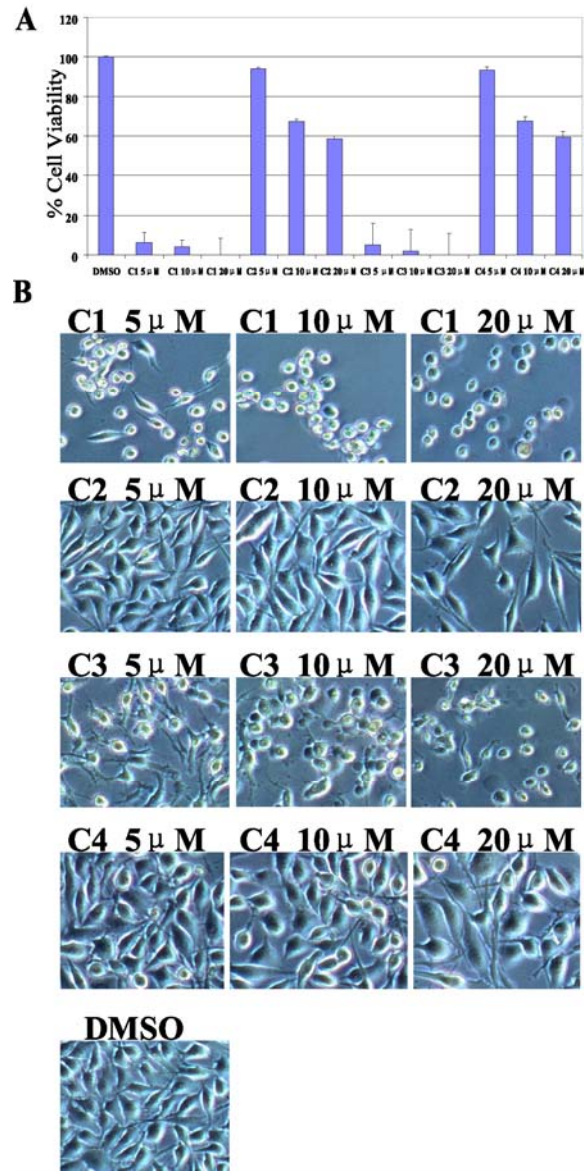


Figure S2. Dose response experiment using C1, C2, C3 and C4 in human prostate cancer PC-3 cells. PC-3 cells were treated with either solvent DMSO or indicated concentrations of C1-C4 for 24 h. (A) MTT assay. (B) Morphological changes.

Table S1. Crystal data and structure refinement for complexes 1 and 2

	C 1	C 2
Empirical formula	C ₂₅ H ₄₁ CuN ₃ O ₁₃ S	C ₂₃ H ₂₉ CuN ₃ O ₇ S
Formula weight	687.21	555.09
Crystal system	Monoclinic	Monoclinic
Space group	<i>C2/c</i>	<i>P2₁/c</i>
<i>a</i> (Å)	22.510(2)	11.0970(11)
<i>b</i> (Å)	21.479(2)	19.101(2)
<i>c</i> (Å)	14.8300(17)	13.2031(12)
α (°)	90	90
β (°)	92.7460(10)	114.1490(10)
γ (°)	90	90
<i>V</i> (Å ³)	7162.0(13)	2553.7(4)
<i>Z</i>	8	4
ρ_{calc} (Mg/m ³)	1.275	1.444
μ (mm ⁻¹)	0.727	0.984
<i>F</i> (000)	2888	1156
Theta range (°)	2.34-25.02	2.00-25.02
Temperature (K)	298(2)	298(2)
Wavelength (Å)	0.71073	0.71073
Crystal size (mm ³)	0.45 x 0.26 x 0.25	0.49 x 0.45 x 0.40
No. of data collected	14700	12559
No. of data used	6031	4505
<i>R</i> ₁ [<i>I</i> > 2σ(<i>I</i>)]	0.0784	0.0333
<i>wR</i> ₂ [<i>I</i> > 2σ(<i>I</i>)]	0.1798	0.0772
<i>R</i> ₁ [all data]	0.1710	0.0545
<i>wR</i> ₂ [all data]	0.1967	0.0902
GOF	1.003	1.041