

Supplementary Material

Phenanthroline complexation enhances the cytotoxic activity of the VO-chrysin system

Agustin Actis Dato¹, Luciana G. Naso¹, Marilin Rey², Pablo J. Gonzalez², Evelina G. Ferrer¹, Patricia A.M. Williams^{1,*}.

¹Centro de Química Inorgánica (CEQUINOR, UNLP, CONICET), Departamento de Química, Facultad de Ciencias Exactas, Universidad Nacional de La Plata, Bv. 120 N° 1465, CP 1900, La Plata, Buenos Aires, Argentina.

² Departamento de Física, Facultad de Bioquímica y Ciencias Biológicas, Universidad Nacional del Litoral and CONICET, S3000ZAA Santa Fe, Argentina.

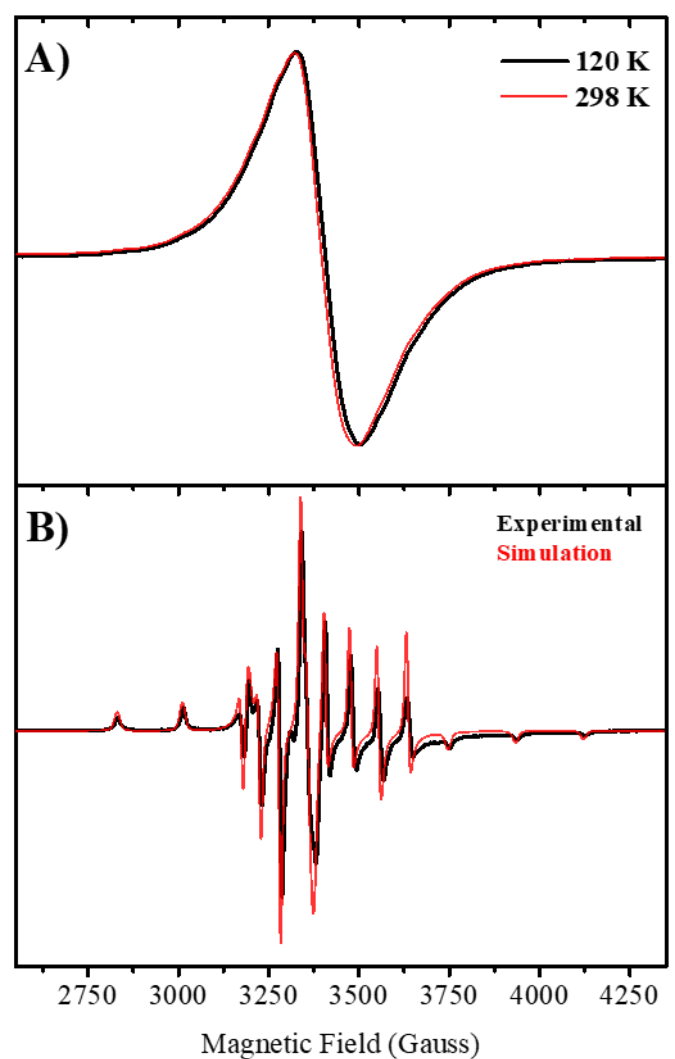


Figure S1. EPR spectrum of [VO(chrys)phenCl]. A) Powder sample at 120 K (black) and 298 K (red). B) Frozen DMSO solution EPR spectrum recorded at 120 K (black) together with simulation (red). EPR spectra of both powder and DMSO solution were recorded in a Bruker EMX-Plus spectrometer, equipped with a rectangular cavity. Experimental conditions: 100 kHz modulation field, 4 Gpp modulation amplitude and 2 mW microwave power. The spectra were baseline corrected using WinEPR Processing software (Bruker, Inc) and simulations were performed with the Easy Spin 5.2.3. toolbox based on MATLAB assuming an axial spin-Hamiltonian. The spin Hamiltonian parameters obtained were $g_{||} = 1.941$; $A_{||} = 162.2 \times 10^{-4} \text{ cm}^{-1}$; $g_{\perp} = 1.977$; $A_{\perp} = 59.5 \times 10^{-4} \text{ cm}^{-1}$.

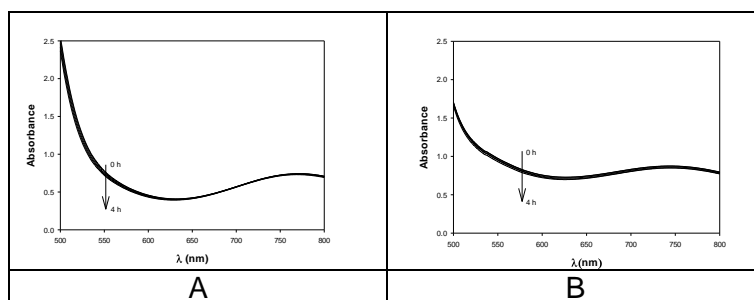


Figure S2. Spectral variation of a dissolution of [VO(chrys)phenCl] in A) DMSO, B) DMSO/H₂O 1/99 (1×10^{-2} M), during 4h.

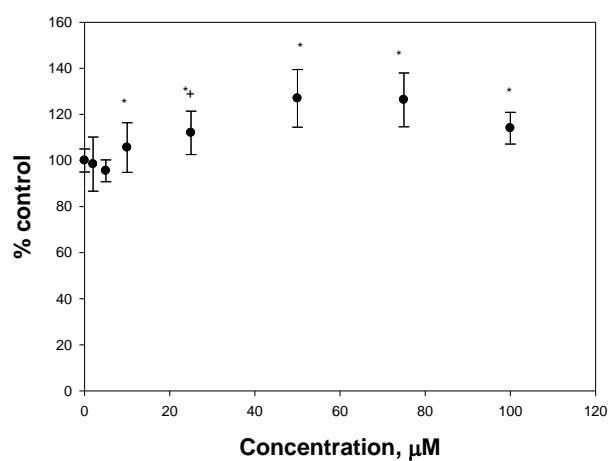


Figure S3. Cell viability assay at different of [VO(chrys)phenCl] concentrations after treatment for 24 h on HEK293 cells. The results are expressed as a percentage of the control level and represent the mean \pm the standard error of the mean (SEM) from three separate experiments. * indicates significant values in comparison with the control level ($p < 0.05$).

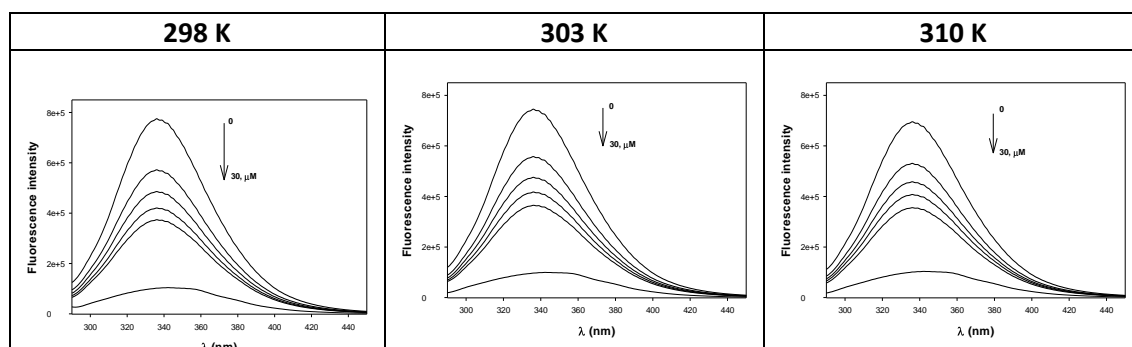


Figure S4. The fluorescence spectra of BSA at various temperatures for VOchrysen (0, 4, 6, 8, 10, 30 μM). $\lambda_{\text{ex}} = 280 \text{ nm}$, $[\text{BSA}] = 6 \mu\text{M}$.

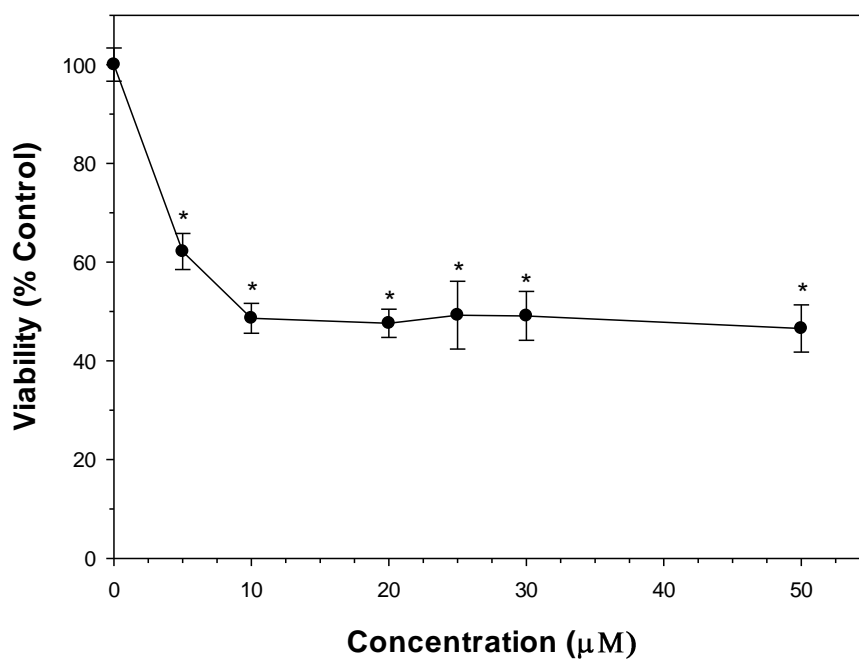


Figure S5. Cell viability assay of a mixture of sodium metavanadate, chrysin and phen (1:1:1), physiological pH at different concentrations after treatment for 24 h on A549 cells. The results are expressed as a percentage of the control level and represent the mean \pm the standard error of the mean (SEM) from three separate experiments. * indicates significant values in comparison with the control level ($p < 0.05$).

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Not active	Set Capillary	4000 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	950 m/z	Set Collision Cell RF	150.0 Vpp	Set Divert Valve	Source

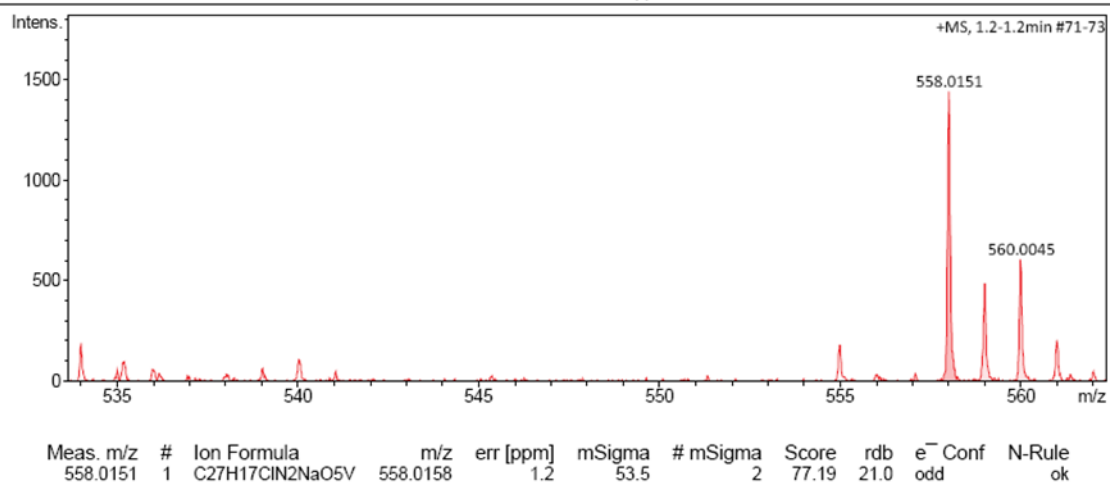


Figure S6. Electrospray ionization–mass spectrometry (ESI-MS) spectrum of [VO(chrys)phenCl]