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SUPPLEMENTARY MATERIAL TO

A binary copper(II) complex having a stepped polymeric structure: Synthesis, characterization, DNA-binding and anti-fungal studies

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Single crystal XRD study

Single crystal XRD data was obtained using an Oxford Diffraction Gemini Ultra S CCD diffractometer equipped with a graphite monochromated Mo-K_α radiation source. The data was solved using CrysAlisPro and structure solved using direct methods with SHELXS-86 and refined with SHELXL-97[1] within the WinGX package.[2] The drawings were produced using Mercury.

Crystallographic information about the crystal presented in this paper has been submitted to the Cambridge Crystallographic Data Centre with CCDC #951569. For free acquisition of the data: Fax: +44-1223-336-033; E-Mail: deposit@ccdc.cam.ac.uk, http://www.ccdc.cam.ac.uk.

Electrochemistry

Electrochemical solution experiments were realized using an SP-300 potentiostat, BioLogic Scientific Instruments, France. The solvent system was water:DMSO (1:4), 0.01 M in KCl purged with N_2. A three electrode cell was employed having saturated Ag/AgCl as the reference, a glassy carbon electrode as the working and platinum as the counter electrode. All potentials are referred to Ag/AgCl electrode. Measurements were made at room temperature. Voltammograms of the complex solution (3 mM) were taken at various scan rates rang-

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ing from 25 to 1400 mV s^{-1} in order to calculate various voltammetric parameters.

For the DNA binding study through cyclic voltammetry, a DNA solution was prepared in water and its concentration was determined using the Beer–Lambert law using a molar absorption of DNA of 6600 M^{-1} cm^{-1}. Voltammograms of pure complex solution (3 mM) and after the addition of 2, 8, 17, 23, 26, 30, 35, 44, 47 and 56 μM DNA were recorded. In order to compare certain voltammetric parameters before and after DNA addition, voltammograms were also taken in range from 25 to 1400 mV s^{-1} after DNA addition.

Absorption spectroscopy

Solution of the complex at 6 mM was prepared in DMSO:water (4:1) and its spectra were taken in pure form as well as in the presence of 10, 20, 30, 40, 50, 60, 70 and 80 μM DNA. Spectra were taken at room temperature in a cell of 1 cm path length.

Fluorescence spectroscopy

A PerkinElmer LS 45 fluorescence spectrometer was used for fluorescence measurements. Instrument was calibrated against the set 6BF, the certified reference materials that were provided with the instrument. The set 6BF contained the reference materials anthracene/naphthalene, ovalene, *p*-terphenyl, tetraphenylbutadiene, E11, rhodamine. The emission and excitation wavelengths used were 690 and 417 nm, respectively and the slit width was 10 nm.

Viscosity measurement

Complex solutions were prepared in aqueous DMSO (1:4) and their viscosities were measured with Ubbelohde viscometer at room temperature. Digital stopwatch was used to measure the flow time of solution. Data were shown as relative viscosity $(\eta/\eta_0)^{1/3}$ *vs*. binding ratio ([complex]/[ssDNA]) where η shows viscosity of ssDNA with complex and η_0 is the viscosity of DNA alone. The values of viscosities were also calculated from the observed flow time of ssDNA-containing solution (t_0) where $\eta = t - t_0$.

Antifungal studies

The synthesized complex was screened for its antifungal potential against three fungal strains (*Mucor piriformis*, *Helminthosporium solani* and *Aspergillus niger*, isolated from soil) using the agar tube dilution method and the resulting activity was compared with that of terbinafine acting as standard drug. According to the standard procedure if the percent growth inhibition is more than 70 %, the result is termed significant, 60–70 % good, 50–60 % moderate and below 50 % non-significant activity.[3]

Table S-I. Crystal data and structure refinement parameters for the complex

Empirical formula	$C_{36}H_{36}Cu_2O_8$
Formula weight, g mol^{-1}	723.72
Temperature, K	296(2)
Wavelength, Å	0.71073
Crystal system	Monoclinic
Space group	$P2_1/n$
Unit cell dimensions	
a / Å	17.2182(19)
b /Å	5.2503(4)
c / Å	17.8257(18)
α / °	90
β / °	98.101(4)
γ / °	90
Volume, Å^3	1595.4(3)
Z	4
Density (calculated), Mg/m^3	1.507
Absorption coefficient, mm^{-1}	1.386
F(000)	748
Crystal size, mm^3	0.24 × 0.16 × 0.15
θ range for data collection, °	1.539 to 27.985
Index ranges	$-22 \le h \le 22$; $-4 \le k \le 6$; $-23 \le l \le 23$
Reflections collected	3839
Independent reflections	2118
Completeness to θ, %	99.8 %
Refinement method	Full-matrix LS on F^2
Data / restraints / parameters	2118 / 0 / 204
Goodness-of-fit on F^2	0.960
Final R indices [I>2sigma(I)]	$R1$ = 0.1111, $wR2$ = 0.0483
R indices (all data)	$R1$ = 0.1184, $wR2$ = 0.0907

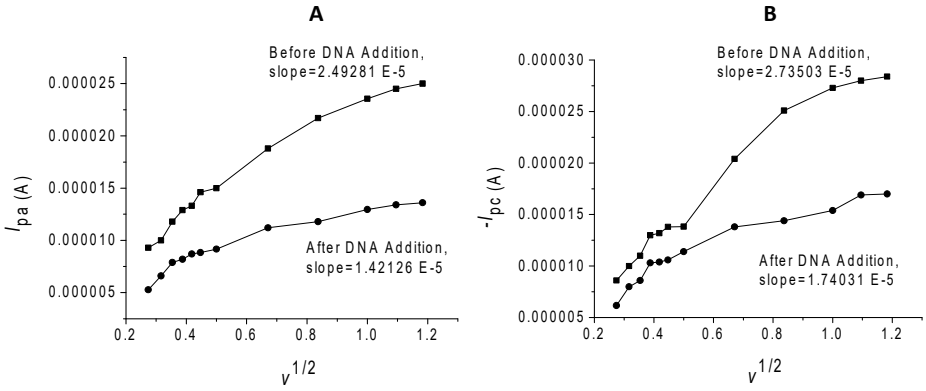

Fig. S-1. Plots of anodic (A) and cathodic (B) peak currents and square root of scan rates. The slope values were reduced on addition of DNA, indicating complex–DNA interaction.

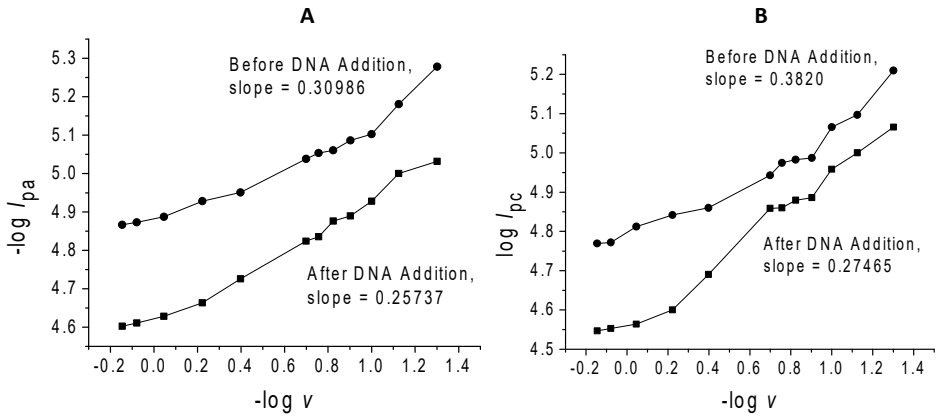

Fig. S-2. Plots of the logarithmic values of scan rate *vs*. anodic (A) and cathodic (B) peaks currents. The slope values were reduced on addition of DNA, indicating interaction of the complex with DNA.

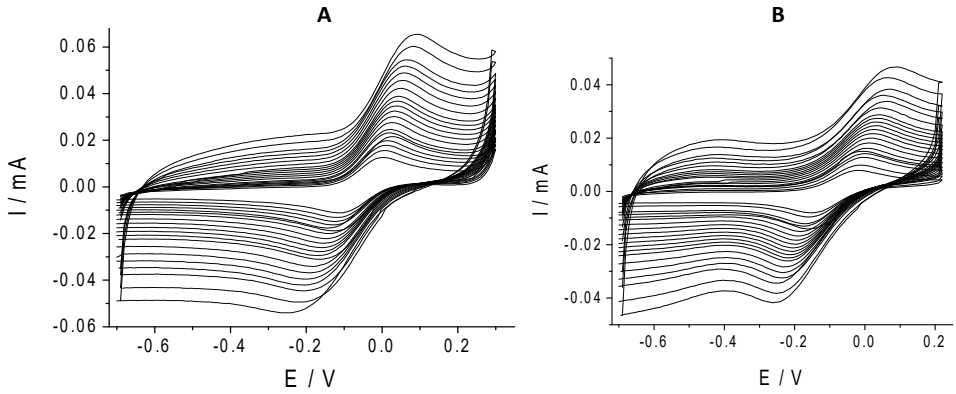

Fig. S-3. Voltammograms of the complex (3 mM) at various scan rates ranging from 25 to 1400 mV s^{-1} before (A) and after (B) 26 μM DNA addition. The shrinking of the current window from ± 0.6 mA to ± 0.4 mA on addition of DNA indicated interaction of the complex with DNA.

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