

1 Binary copper(II) complex having stepped polymeric structure: synthesis,
2 characterization, DNA-binding and anti-fungal studies.

3 Supplementary material

4 **Single crystal XRD study**

5 Single crystal XRD data was obtained using an Oxford Diffraction Gemini Ultra S CCD
6 diffractometer equipped with graphite monochromated Mo-K α radiation source. The data was
7 solved using CrysAlisPro and structure solved using direct methods with SHELXS-86 and refined
8 with SHELXL-97¹ within the WinGX package.² The drawings were produced using mercury.

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

12 **Electrochemistry**

13 Electrochemical solution experiments were done using an SP-300 potentiostat, serial number
14 0134, BioLogic Scientific Instruments, France. The solvent system was water:DMS (1:4), 0.01 M
15 in KCl purged with N₂. A three electrode cell was employed having saturated Ag/AgCl as
16 reference, glassy carbon electrode as working and platinum as counter electrode. Measurements
17 were made at room temperature. Voltammograms of the complex solution (3 mM) were taken at
18 various scan rates ranging from 25 mVs⁻¹ to 1400 mVs⁻¹ in order to calculate various voltammetric
19 parameters.

20 For DNA binding study through cyclic voltammetry, DNA solution was prepared in water and its
21 concentration was determined using Beer-Lambert's law using molar absorptivity of DNA = 6600
22 M⁻¹.cm⁻¹. Voltammograms of pure complex solution (3 mM) and after the addition of 2, 8, 17, 23,
23 26, 30, 35, 44, 47 and 56 μ M DNA. In order to compare certain voltammetric parameters before
24 and after DNA addition, voltammograms were also taken in range from 25 mVs⁻¹ to 1400 mVs⁻¹
25 after DNA addition.

26 **Absorption spectroscopy**

Solution of the complex at 6 mM was prepared in DMS: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 μ M DNA. Spectra were taken at room temperature in a cell of 1cm 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 which were provided with the instrument. The set 6BF contained the reference materials Anthracene/naphthalene, Ovalene, p-terphenyl, Tetraphenylbutadiene, E11, Rhodamine. The emission wavelength used was 690 nm 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 stop watch was used to measure the flow time of solution. Data were shown as relative viscosity $(\eta/\eta_0)^{1/3}$ vs. binding ratio $([\text{complex}]/[\text{SSDNA}])$ 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 antifungal potential against three fungal strains (*Mucor piriformis*, *Helminthosporium solani* and *Aspergillus niger*) 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

1. Sheldrick, G. M. SHELXL-97, Program for the refinement of crystal structure; University of Göttingen. 1997, Germany.
2. Farrugia, L. J. J. Appl. Crystallogr. 1999, 32, 837.
(<http://dx.doi.org/10.1107/S0021889899006020>)

3. Rehman, A.; Choudhary, M. I.; Thomsen, W. J. Bioassay techniques for drug development, Harwood Academic Press, Amsterdam, The Netherlands. 2001, pp. 14–20. ISBN 9789058230515 - CAT# TF3261

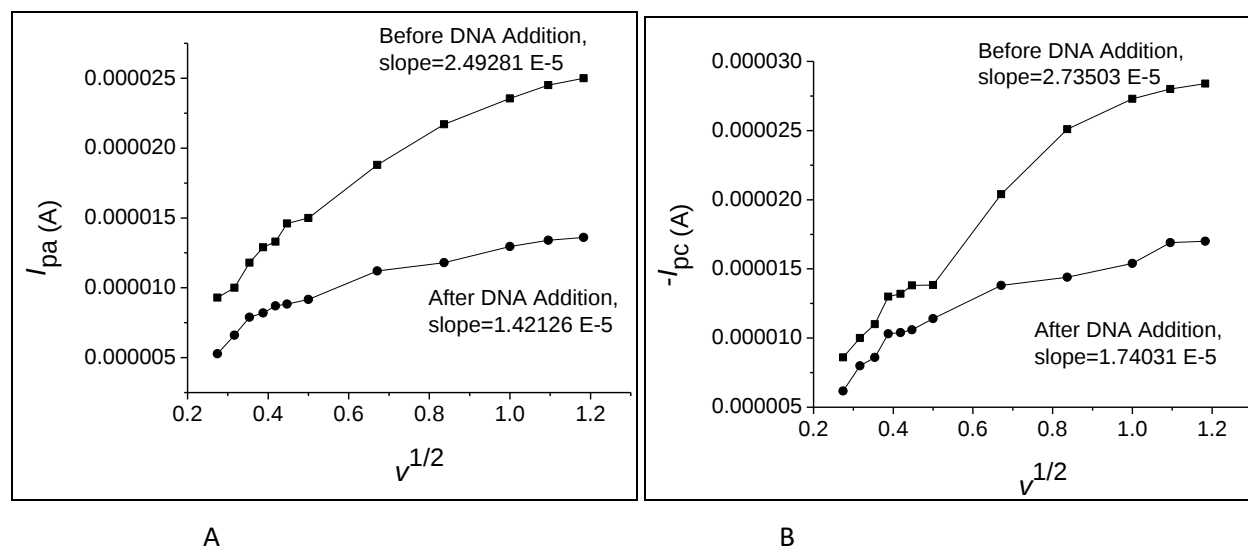


Figure S1: plots of anodic (A) and cathodic (B) peak currents and square root of scan rates. The slope values have been reduced on addition of DNA indicating complex-DNA interaction.

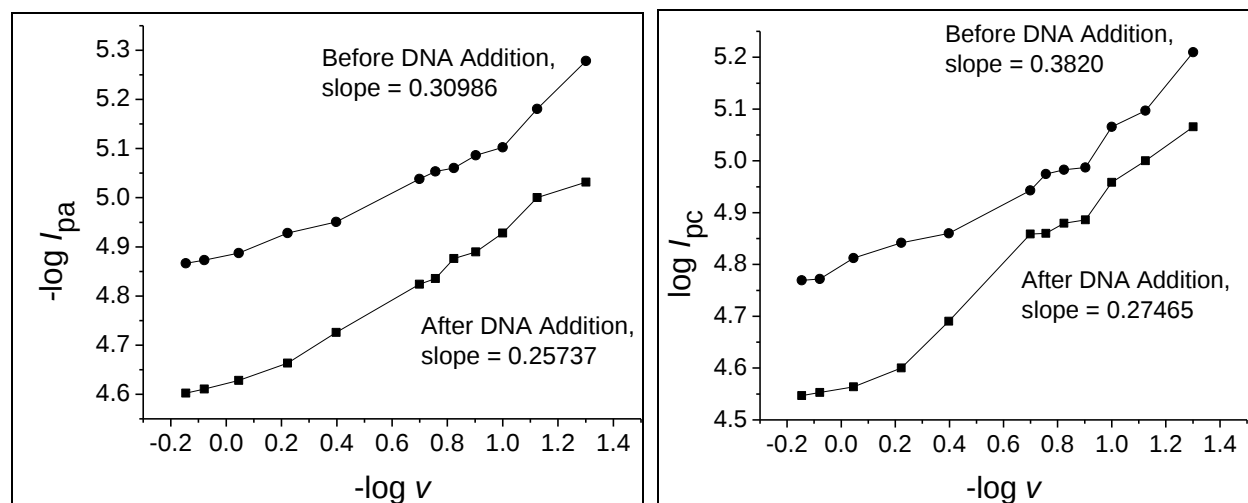


Figure S2: plots of the logarithmic values of scan rate vs. anodic (A) and cathodic (B) peaks currents. The slope values are reduced on addition of DNA indicating interaction of complex with DNA.

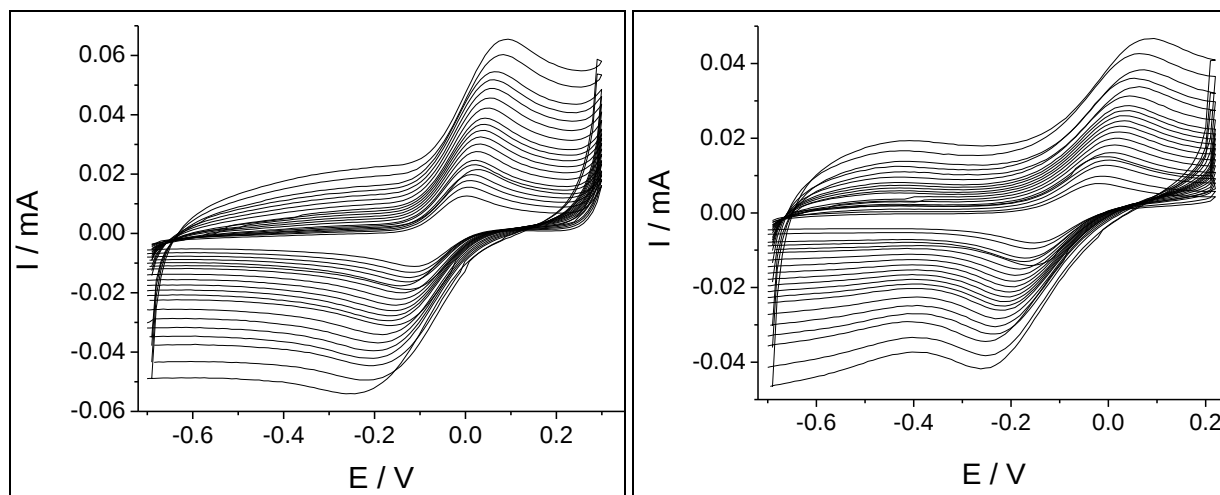


Figure S3: voltammogram of the complex at various scan rates ranging from 25 to 1400 mV/s before (A) and after (B) DNA addition. The shrinking of the current window from $\pm 0.6 \text{ mA}$ to $\pm 0.4 \text{ mA}$ on addition of DNA indicated interaction of complex with DNA.