



## Atropisomers and a copper(II) complex derived from 1,3-dimethyl-5-(8'-quinolinylazo)-6-aminouracil: structures, magnetism and biological properties

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An uracil-azo derivative of quinoline, 1,3-dimethyl-5-(8'-quinolinylnyl-azo)-6-aminouracil ( $H_2L$ , **1**), was synthesized and then converted into its atropisomers, 1,3-dimethyl-8-(8'-quinolinylnyl)azaxanthine ( $\alpha$ -atropisomer (**2**) and  $\beta$ -atropisomer (**3**)). It is indeed a notable accomplishment that the atropisomers were synthesized selectively under dissimilar reaction conditions. Additionally, an axially elongated 5-coordinated distorted square pyramidal copper(II)-complex,  $[Cu^{II}(HL)(H_2O)_2]NO_3$  (**4**), was synthesized from  $H_2L$ , where it acts as a tridentate ligand. Single crystals of compounds **2–4** were analyzed for their stereochemical characterization. The compounds (**2** and **3**) belong to the same space group  $P2_1$  with  $Z = 2$ . Based on a torsional angle about  $N3-N2-C1-C9$ , which is  $48.7(2)^\circ$  for the  $\alpha$ -atropisomer (**2**) and  $-48.7(2)^\circ$  for the  $\beta$ -atropisomer (**3**), respectively, they are revealed to be atropisomers. According to TD-DFT analysis, the  $\alpha$ -atropisomer (**2**) is  $0.05 \text{ kcal mol}^{-1}$  more energetically stable than the  $\beta$ -atropisomer (**3**). The 5-coordinated  $Cu^{II}$  centre adopts a distorted square pyramidal geometry (space group  $P2_1/n$ ,  $Z = 4$ ), wherein the coordination sites were occupied by three-N and two O-donor atoms from the  $HL^-$  moiety and the two  $H_2O$  molecules, respectively. The polycrystalline sample of **4** was subjected to direct current (dc) variable-temperature magnetic susceptibility studies over the temperature range of 1.8–300 K. The magnetic study suggests that copper(II) ions in the crystal lattice have a weak antiferromagnetic interaction, demonstrating the complex to be a mononuclear species. According to the EPR study, the distorted square-pyramidal copper(II) complex may have a  $d_{x^2-y^2}$  orbital as a ground state. All the compounds have shown significant efficacy against the bacterial plant pathogen, *Ralstonia solanacearum* Smith. and the fungal plant pathogen, *Rhizoctonia solani* Kuhn., which cause bacterial wilting of solanaceous crops and sheath blight of rice, respectively. Besides, the atropisomers have demonstrated effectiveness against another bacterial plant pathogen, *Xanthomonas oryzae* pv. *oryzae*, that causes bacterial blight of rice. The atropisomers thus differ with respect to biological efficacy towards both bacterial and fungal diseases.

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