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An insight into the potent antioxidant activity of a dithiocarbohydrazone appended *cis*-dioxidomolybdenum (VI) complexes

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In search of antioxidants with enriched potency, the present study focus on the design and synthesis of a dithiocarbohydrazone, H_3TCL derived from thiocarbohydrazide and 3-ethoxysalicylaldehyde and its coordination complexes with molybdenum, *viz*, $[MoO_2(HTCL)D]$ (**1**–**2**) (where D = methanol (**1**), DMSO (**2**)) and $[MoO_2(HTCL)D]\cdot DMF$ (where D = H_2O (**3**)). The synthesized compounds were characterised by elemental analysis, spectroscopic techniques (FT-IR, UV–vis and ^{1}H-NMR), conductivity measurements and cyclic voltammetry. Moreover the solid state structures of all the three complexes were established by single crystal X-ray diffraction analysis as mononuclear neutral species in which the molybdenum centre assumes a distorted octahedral geometry. The dithiocarbohydrazone binds to the molybdenum centre through its phenolate oxygen, O(1), azomethine nitrogen, N(1) and thioenolate sulfur, S(1) in a dianionic tridentate mode. The assessment of intermolecular contacts in the crystal arrangement was quantified using Hirshfeld surface analysis. Further the antioxidant potential of the dithiocarbohydrazone, H_3TCL and its molybdenum complexes **1**–**3** were evaluated using 1,1-diphenyl-2-picrylhydrazyl(DPPH), 2,2′-azinobis-3-ethylbenzothiazoline-6-sulfonic acid (ABTS) and total antioxidant assays. The antioxidant activities were then compared with standard antioxidant, *L*-ascorbic acid. The antioxidant potential of the synthesized compounds were then validated by molecular docking studies. Molecular modelling study was achieved to evaluate the recognition of target compound at the binding pocket of the human antioxidant enzyme, 3MNG. The docking results showed that the complexes selectively bond to the vital amino acids present in the binding pocket of the target enzyme, 3MNG.

KEYWORDS

antioxidant assay-, dithiocarbohydrazone; Hirshfeld surface analysis, *L* -ascorbic acid, molecular docking, X-ray diffraction analysis

