Title:	In vitro anticancer activity of 4(3H)-quinazolinone derived Schiff base and its Cu(II), Zn(II) and Cd(II) complexes: Preparation, X-ray structural, spectral characterization and theoretical investigations
Authors:	Markad, D. (/jspui/browse?type=author&value=Markad%2C+D.)
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Abstract:	This work reports the synthesis of a novel quinolin-4(3H)-one based Schiff base ligand 3-[(E)-(2,5-dimethoxyphenyl)methylidene]amino-2-methylquinazolin-4(3H)-one (DMPAQ) and its coordination complexes of the type [M(DMPAQ)(phen)]X (1a-1c), where M = Cu(II), Zn(II) and Cd(II) ions, respectively, phen = 1,10-phenanthroline. All the synthesized compounds were characterized using UV–Visible, elemental analysis, FT-IR, 1H NMR, Mass spectroscopy and TGA techniques. The triclinic structure of the DMPAQ is determined by employing single crystal X-ray crystallographic analysis. The characterization results suggested that the ligand, DMPAQ is bidentate and coordinate to the metal center through the lactum oxygen and the azomethine nitrogen. The synthesized DMPAQ ligand and complexes (1a-1c) were screened for their in vitro anticancer activity against the human breast adenocarcinoma cell line, MCF-7. The complexes 1a and 1b displayed significant anticancer activity against MCF-7 cells even at lower GI50 value (GI50 = 0.016 μM) than the standard drug doxorubicin (GI50 = 0.018 μM). Further, we have performed computational DFT studies on the chemical reactivity of the ligand and the three complexes by means of Conceptual Density Functional Theory (CDFT) through the “Koopmans in DFT” (KID) approximation to support the experimentally obtained results.
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