Abstract

Four new complexes derived from adamantly containing hydrazone (**APH**) ligand with Cu(II) (**1**), Co(II) (**2**), Ni(II) (**3**) and Zn(II) (**4**), have been synthesized and characterized using different physicochemical methods. The structure of the ligand **APH** and its copper complex **1** have been established by single-crystal X-ray diffraction direct methods, which reveal that complex **1** has distorted square-pyramidal geometry. Complexes **1**-**4** are screened against seven human cancer cell lines namely, breast cancer cell lines (MCF7, T47D, MDA-MB-231), prostate cancer cell lines (PC3, DU145) and the colorectal cancer cell line Coco-2, for their antiproliferative activities. Complex **1** has shown a promising anticancer activity compared to the other ones. The structural and spectroscopic analysis of **APH** and its complexes are confirmed by DFT calculations.