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Pyrazoline-based chalcone derivatives and their Cu(II) complexes: Synthesis, molecular docking study, and anti-cancer evaluation against MCF-7 and A549 cancer cells

Sabah M. Mazal, Raed A. Alharis, Zainab A. M. Al-Shuhaib*, Kawkab A. Hussein and Sadiq M. H. Ismael
Department of Chemistry, College of Education for Pure Sciences, University of Basrah, Basrah, Iraq

ABSTRACT Pyrazoline derivatives (**3a-f**) and their copper(II) complexes were synthesized and characterized using spectroscopic methods. The *in vitro* cytotoxic activities of selected compounds against the human cancer cell lines (MCF-7) and (A549) were evaluated by MTT assay. 1-(3-(2,4-Dimethoxyphenyl)-5-(p-tolyl)-4,5-dihydro-1*H*-pyrazol-1-yl)ethan-1-one (**3f**) displayed a significant cytotoxic activity with IC_{50} values of 30.39 and 31.34 µg/mL, against MCF-7 and A549, respectively. Copper(II)-pyrazoline complex (**3eCu**) exhibited a significant cytotoxic activity, with IC_{50} values of 5.77 and 4.10 µg/mL against MCF-7 and A549, respectively. Molecular docking study showed the best binding poses of **3f** and copper(II)-pyrazoline complex (**3eCu**) with the proteins 5T92 and 4JPS, respectively. The absorption, distribution, metabolism, and excretion profile and pharmacokinetic predictions revealed that complex **3eCu** met all parameters within acceptable ranges.

KEY WORDS Anticancer activity, Copper(II) complexes, Chalcone, Molecular docking, Pyrazoline.

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