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In vitro cytotoxicity evaluation of thiourea derivatives bearing *Salix sp.* constituent against HK-1 cell lines

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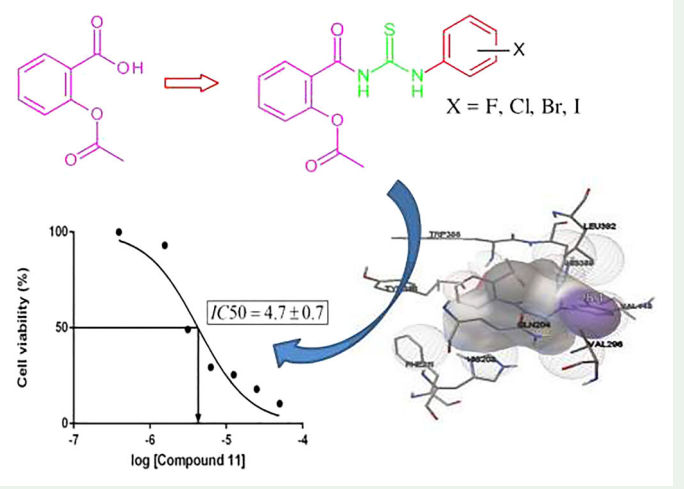
ABSTRACT

In searching for drugs from natural product scaffolds has gained interest among researchers. In this study, a series of twelve halogenated thiourea (**ATX 1-12)** *via* chemical modification of aspirin (a natural product derivative) and evaluated for cytotoxic activity against nasopharyngeal carcinoma (NPC) cell lines, HK-1 via MTS-based colorimetric assay. The cytotoxicity studies demonstrated that halogens at *meta* position of **ATX** showed promising activity against HK-1 cells (IC_{50} value $\leq$15 μM) in comparison to cisplatin, a positive cytotoxic drug (IC_{50} value $=8.9 \pm 1.9$ μM). **ATX 11**, bearing iodine at *meta* position, showed robust cytotoxicity against HK-1 cells with an IC_{50} value of 4.7 ± 0.7 μM. Molecular docking interactions between **ATX 11** and cyclooxygenase-2 demonstrated a robust binding affinity value of −8.1 kcal/mol as compared to aspirin's binding affinity value of −6.4 kcal/mol. The findings represent a promising lead molecule from natural product with excellent cytotoxic activity against NPC cell lines.



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