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In vitro cytotoxicity evaluation of thiourea derivatives bearing \textit{Salix sp.} constituent against HK-1 cell lines

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\textbf{ABSTRACT}

In searching for drugs from natural product scaffolds has gained interest among researchers. In this study, a series of twelve halogenated thiourea (\textbf{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 \textbf{ATX} showed promising activity against HK-1 cells (IC\textsubscript{50} value \leq 15 \textmu M) in comparison to cisplatin, a positive cytotoxic drug (IC\textsubscript{50} value = 8.9 \pm 1.9 \textmu M). \textbf{ATX 11}, bearing iodine at meta position, showed robust cytotoxicity against HK-1 cells with an IC\textsubscript{50} value of 4.7 \pm 0.7 \textmu M. Molecular docking interactions between \textbf{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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Aspirin; thiourea; cytotoxicity; molecular docking; cyclooxygenase-2

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Supplemental data for this article can be accessed \texttt{https://doi.org/10.1080/14786419.2018.1517120}.

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