Poster/talk Number

Design, Synthesis and Anticolorectal Cancer Activity of 2-Bromoalkoxyanthraquinones

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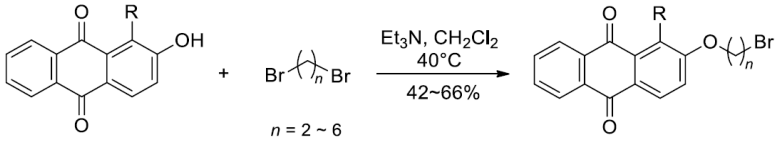
Abstract

The impact of alkoxy chain length and the presence of a 1-hydroxy group in synthesised 2-bromoalkoxyanthraquinones was evaluated against HCT116, HT29, and CCD841 CoN cell lines. Molecular docking was employed to elucidate the interactions between these compounds and potential p53 and KRAS targets. Results indicated that 2-bromoalkoxyanthraquinones with the 1-hydroxy group exhibited greater anticancer activity compared to their counterparts. Specifically, compound **6b** bearing C3 alkoxy chain displayed the most promising antiproliferation activity against HCT116 cells (IC50 = 3.83 ± 0.05 μM) and demonstrated high selectivity for HCT116 over CCD841 CoN cells (SI = 45.47). Molecular docking analysis revealed additional hydrogen bonds between the 1-hydroxy group of 6b and the proteins. Compound **6b** also exhibited adequate lipophilicity (cLogP = 3.27) and ligand efficiency metrics (LE = 0.34; LLE = 2.15) within the acceptable range for an initial hit. This study underscores the potential of the 1-hydroxy group and a short alkoxy chain in enhancing the anti-colorectal cancer activity of 2-bromoalkoxyanthra-quinones. Further optimisation should be possible for compound **6b** as a potential therapeutic agent against colorectal cancer.



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Field of research :1. Organic synthesis, 2. Molecular modelling, 3. Drug design and synthesis