

Title: Synthesis and molecular docking of new quinoline derivatives as VEGFR-2 inhibitors

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The quinoline ring system has long been known as a versatile nucleus in the design and synthesis of biologically active compounds as several quinoline derivatives exhibit a broad spectrum of pharmacological activities from antibacterial, antifungal, antimalarial, anthelmintic, antipsychotic, and anticancer. Several compounds containing the quinoline scaffold are currently in the clinical use as anticancer agents. Vascular endothelial growth factor receptor-2 (VEGFR-2) plays a vital role in cancer angiogenesis. In this study, based on the structure activity relationships and common pharmacophoric features shared by various VEGFR-2 inhibitors such as: sorafenib and tivozanib, as well as analysis of their binding modes; a series of novel quinoline derivatives were designed and synthesized as chemotherapeutic agents targeting cancer through the inhibition of VEGFR-2 activity. Docking simulation of the newly synthesized compounds into the active site of VEGFR-2 was performed to explore the probable binding interactions. All synthesized compounds were fit in the active pocket of VEGFR-2 (PDB ID 4ASE); with docking score ranges from -9.6791 to -9.1496 kcal/mole. Compound number VIb showed the best docking score while compound VId showed the least docking score. Our target compounds may serve as model molecules for the development of quinoline based anticancer agents.

Biography

Zeinab Sayed Fathy Ismail Elfakharany; completed Bachelor's degree in Pharmacy from Cairo University; working as a teaching assistant in October University for Modern Sciences and Arts located in Cairo, Egypt. My scope of interset is drug design and how to synthesize various organic molecules as a medicinal chemist.Currently studying quinoline based derivatives in the aim to fullfil my Master degree in pharmaceutical sciences, Cairo university,Egypt.

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