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In silico evaluation of quinoline-piperazine hybrids targeting breast cancer pathways

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ABSTRACT Cancer remains a major global health challenge and a leading cause of mortality among women, with breast cancer (BC) accounting for a substantial proportion of cancer-related deaths worldwide. Ongoing research mainly focused on developing new chemotherapeutic agents that offer improved selectivity and therapeutic effectiveness. The quinoline and piperazine derivatives have been reported to possess notable anticancer activities. The objective of the present study was to develop some quinoline clubbed piperazine hybrids as potential BC agents through acting on different pathways. The designed derivatives were docked using PyRx, Autodock software against the four PDB IDs: 3ERT, 3PP0, 2W96, and 4FA6. Moreover, their absorption, distribution, metabolism, and excretion (ADMET) properties were also predicted using the pkCSM tool. The *in-silico* study highlights the therapeutic potential of quinoline–piperazine hybrid molecules for the treatment of BC. Out of the 23 designed derivatives, all compounds showed good to moderate binding affinities, but compound QP12 exhibited the highest binding affinity toward against all three targets, while QP18 showed the best affinity with 2W96, indicating their strong binding interactions. These QP12 and QP18 displayed favorable ADMET characteristics, reinforcing their suitability for further drug development. The results offer a compelling rationale for subsequent *in vitro* and *in vivo* evaluations to confirm their anticancer efficacy and elucidate their mechanisms of action. The combination of quinoline and piperazine scaffolds represents a strategic direction for developing novel BC therapeutics.

KEY WORDS *In silico*, Piperazine, Quinoline, Breast cancer, Absorption, distribution, metabolism, and excretion.

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INTRODUCTION