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1-Benzyl-3,5-*bis*[(1,3-diaryl-1*H*-pyrazol-4-yl)methylene]piperidin-4-ones: Synthesis, *in vitro* cytotoxicity evaluation, and *in silico* molecular docking studies

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ABSTRACT Synthesis of an array of new molecular hybrids, 1-benzyl-3,5-*bis*[(1,3-diaryl-1*H*-pyrazol-4-yl)methylene] piperidin-4-ones **(3a-3f)** has been accomplished from pyrazole based carbaldehydes and N-benzylpiperidin-4-one via Claisen-Schmidt reaction. Cytotoxicity evaluation reveals that the *para*-bromo moiety possessing hybrid **3a** displayed the most potent activity (half-maximal inhibitory concentration: ~12 and ~37 μM against SW1990 and AsPC1 pancreatic cancer cells, respectively) among the synthesized ones. Molecular docking examination exposes the potent hybrid **3a** communicates strongly with B-cell lymphoma-2 protein with a binding energy −9.4 kcal.mol^{-1}.

KEY WORDS Piperidin-4-one, Pyrazole, Cancer, B-Cell lymphoma, Cytotoxicity.

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