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# Green synthesis of some new 4-phenyl-4,5-dihydro-1*H*-benzo[*f*][1,3,5] triazepin-2(3*H*)-ones, *in-silico* molecular docking (PDB ID: 3ERT), ADME, and evaluation of anticancer activity in breast cancer cell lines

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**ABSTRACT** We have synthesized some new 4-phenyl-4,5-dihydro-1*H*-benzo[*f*][1,3,5]triazepin-2(3*H*)-one derivatives by a green, facile approach involving a one-pot three-component condensation involving various aldehydes with *o*-phenylenediamine and urea in ethanol as solvent and sodium tungstate as a catalyst. The reaction provided good to excellent yields in a short time. Molecular docking with breast cancer target protein 3ERT and absorption, distribution, metabolism, and excretion studies indicated good binding energies and drug-like properties. The derivatives also showed notable *in vitro* anticancer activity against MCF-7 cells, highlighting their potential as new anticancer agents. Biological evaluations are ongoing.

**KEY WORDS** Anticancer, Benzotriazepine, Breast cancer, Three-component synthesis.

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