Indian Journal of Heterocyclic Chemistry
Vol. 36 - Number 02 (Apr-Jun 2026) 199-210
https://connectjournals.com/01951.2026.36.199
https://doi.org/10.59467/IJHC.2026.36.199

ISSN (Print) : 0971-1627
ISSN (Online) : 2456-4311

Green synthesis, anti-ovarian cancer, molecular docking, and distribution, metabolism, excretion, and toxicity study of indole chalcone hybrid derivatives

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ABSTRACT The indolyl analogs of chalcones, namely *E*-1-aryl-3-(1-methyl-1*H*-indol-3-yl)prop-2-en-1-ones (**1a-g**) were synthesized involving Claisen Schmidt reaction between 1-methylindole-3-carboxaldehyde and acetophenones by three **Methods (A-C).** The green approaches using ultrasound irradiations **(Method B)** and microwave irradiations **(Method C)** provided a significant improvement over the conventional approach (**Method A**), which afforded yields of only 62–78%. The anticancer effects of seven indole derivatives were evaluated on a SKOV-3 ovarian cancer cell line, with results between 1.061 ± 0.17 and 43.34 ± 0.36 μM, with compound **1c** being the most effective (IC_{50}) and compound **1g** was the least, with 290.8 ± 9.325. Molecular docking of these compounds was conducted to study their interactions with epidermal growth factor receptor, estimated glomerular filtration rate (PDB ID 4HJO), and binding strength. Absorption, distribution, metabolism, excretion, and toxicity have identified indole derivatives as having beneficial qualities by examining the relationships between their structures, physical and chemical properties.

KEY WORDS Indole, Chalcone, Estimated glomerular filtration rate, Ultrasound, Microwave, Green chemistry.

How to cite this article: Shebeeb, S.A. and Alsalim, T.A. Green synthesis, anti-ovarian cancer, molecular docking, and distribution, metabolism, excretion, and toxicity study of indole chalcone hybrid derivatives, *Indian J. Heterocycl. Chem.*, **2026**, *36*, 199–210. *https://doi.org/10.59467/IJHC.2026.36.199*