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Synthesis, characterization, *in silico* anti-ovarian cancer activity and quantum chemical calculations of 3-β-(2-(6-methoxynaphthalene-2yl)propionoxy)-stigmast-5-en

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The current research work incorporates the synthesis, spectroscopic analysis, and *in silico* studies to evaluate anti-ovarian cancer potential and theoretical studies of 3-β-(2-(6 methoxynaphthalene-2yl)propionoxy)-stigmast-5-en (**2**). Synthesis of compound **2** was carried out by conjugating β-sitosterol (**1**) with Naproxen through highly efficient Steglich esterification. The structure elucidation of the synthesised compound has been done using ^{1}H NMR, IR and UV as well as mass spectrometry. Arti-ovarian cancer potential of the compound **2** has been evaluated using its interaction with the ovarian cancer protein 2UZR (binding energy (ΔG) of –6.0 Kcal/mole) with the help of molecular docking studies. Topological parameters have been analyzed by "Atom in molecule" AIM theory. High value of first hyper polarizability (β_o =6.071 × 10^{-30}esu) of compound **2** indicates that it can be utilized as an ideal material for NLO applications.

Keywords: β-Sitosterol, Anti-ovarian cancer activity, Molecular docking, NLO, AIM