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ORIGINAL ARTICLE

An efficient synthesis towards the core of Crinipellin: TD-DFT and docking studies

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Abstract In this present report, we are describing a novel route for the synthesis of the tetracyclic ring systems, a common core of crinipellin, via oxidative dearomatization, cycloaddition and oxa-di-pi-methane rearrangement. We are also concerned to explore a route to tetracyclic core (**1e**) of Crinipellin and tricyclic core (**1g**) of Allicaol B through intermolecular diels alder reaction and photochemically 1,2 acyl shift. Moreover, docking study of compound 13 and 16 is investigated against AcrB multidrug efflux pump of *Escherichia coli* (PDB ID: 1T9U), main protease of SARS COV-2 (PDB ID: 6W63), DNA gyrase of *Streptococcus pneumonia* (PDB ID: 4Z2C), human estrogen receptor alpha (PDB ID: 3ERT), human lanosterol 14-alpha-demethylase (CYP51)(PDB ID: 3JUS) and cyclooxygenase-2 (Prostaglandin Synthase-2) (PDB ID: 1CX2). The obtained results are important for the exploitation of the therapeutic potential of these derivatives as antimicrobial,

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