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Synthesis, antimicrobial, anticancer evaluation and molecular docking with Bax and MDM2 of dibromosterculic acid

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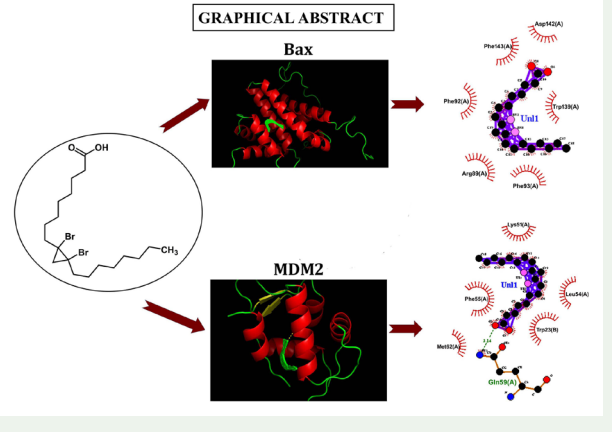
ABSTRACT

Dibromosterculic acid [8-(1,2-dibromo-2-octylcyclopropyl)-octanoic acid], a new synthetic derivative was prepared by bromination of sterculic acid. This synthetic derivative showed strong fungicidal activity against two pathogenic fungal species namely *Penicillium chrysogenum* and *Aspergillus niger* with minimum inhibitory concentration (MIC) value of 0.007 mg/ml and good bactericidal activity against *Bacillus subtilis* and *Xanthomonas sp.* with MIC value of 0.015 mg/ml. Cytotoxic activity on both normal (MCF-10A) and cancerous (MDA-MB-468) cell lines revealed that the survivability percentage of normal cells was unaffected, whereas cancerous cells were decreased greatly by dibromosterculic acid with 50% survivability at 9 µg/ml concentration. Molecular-docking using AutoDock 4.2 with Bax exhibited strong pi-sigma interaction with PHE-93, pi-alkyl and alkyl interaction with TRP-139, ARG-89 and PHE-92 whereas MDM2 revealed strong hydrogen bond interaction with GLN-59 and pi-alkyl interaction with PHE-55. All experimental parameters suggested that this synthetic derivative would be valuable for target-specific drug development with nominal side effects.



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