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Self-assembled renewable nano-sized pentacyclic triterpenoid maslinic acids in aqueous medium for anti-leukemic, antibacterial and biocompatibility studies: An insight into targeted proteins-compound interactions based mechanistic pathway prediction through molecular docking

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Abstract

Maslinic acid is a naturally occurring dihydroxy, mono-carboxy bioactive triterpenoid. Its bulky structure was the main hindrance in the path of biological activity. Sodium and potassium salts of nano-sized triterpenoid maslinic acid were prepared from maslinic acid and its self-assembly property was studied in aqueous and aqueous-organic binary liquid mixtures. Morphology of the compounds studied by Field Emission Scanning Electron Microscopy (FESEM), Atomic Force Microscopy (AFM), High Resolution Transmission Electron Microscopy (HRTEM), Optical Microscopy, Fourier Transform Infrared Spectroscopy (FTIR) and X-ray diffraction (XRD) revealed vesicular morphology of the self-assemblies. Selective cytotoxicity was performed in leukemic (K-562 and KG-1a) and PBMC cells. Among the three self-assemblies (maslinic acid **1**, sodium maslinate **2** and potassium maslinate **3**), sodium maslinate **2** showed better antileukemic efficacy. Sodium maslinate **2** induced apoptosis in leukemic cells by elevating ROS levels and disrupting the cellular antioxidant system. From the *in-silico* studies, it was confirmed that **2** interacted with extrinsic and intrinsic apoptotic proteins of leukemic cells and killed those cells by inducing apoptotic pathways. The compounds **1**, **2** and **3** showed significant antibacterial efficacy against *E.coli* strain through binding with several periplasmic membrane fusion protein (MFP) and limiting the efflux system leading to arrestation of antimicrobial resistance.

Keywords

Self-assembly, Maslinic acid, Sodium maslinate, Potassium maslinate, Leukemia, Protein targeting