

Exploring the bioactivity of pentacyclic triterpenoids as potential antimycobacterial nutraceuticals: Insights through comparative biomolecular modelling

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Abstract

A group of bioactive compounds known as triterpenoids, which are often found in plant materials, have been tested to possess nutritional and pharmaceutical activity. These plant components are referred to as nutraceuticals, and are used as therapeutic agents. In this study, we explore the interactions of betulinic acid (BA), oleanolic acid (OA), ursolic acid (UA), and maslinic acid (MA) against FadA5. Studies have identified FadA5, a trifunctional enzyme-like thiolase, as a target towards Mycobacterium tuberculosis inhibition. The investigation involves molecular dynamics (MD) and hybrid quantum mechanics/molecular mechanics (QM/MM) applications. Analyses of the four pentacyclic triterpenoids binding to FadA5 showed appreciable bioactivity against FadA5. The application of two or more theoretical models to unravel ligand—enzyme binding energies can pave the way for accurate binding affinity prediction and validation.