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Co-crystal synthesis of betulinic and oleanolic acids with isoniazid

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Statement of the Problem: There are several major problems associated with the treatment and management of TB, one of them is the treatment of the co-infection of TB and HIV. 8.8 million patients are newly diagnosed with active TB, with 1.6 million patients of this figure die of TB. The spread of the human immunodeficiency virus (HIV) have been reported to fuel the TB epidemic, especially in sub-Saharan Africa, where over 28% of TB patients are HIV positive. Combine treatment of TB and HIV in the past involves a high pill count, this invariably pave way for adherence problems and overlapping toxicity profiles of the anti-TB and antiretroviral drugs.

Aim: The purpose of this study is to develop new sets of anti-TB agents with multi-target activities against HIV and TB. It is expected that such compounds or agents will therefore and probably a promising approach to address this problem. Such agents will remove the problem of drug interaction and overlapping of toxic profile that are common when two or more drugs are administered for the treatment of the two diseases separately.

Methodology & Theoretical Orientation: The co-crystal synthesis of betulinic acid (BA) and oleanolic acid (OA) with the foremost first line anti-tubercular drug isoniazid (INH) were carried out for the first time in ratio (1:1) under different condition of moisture following the procedure reported by Vijayaraji et al. The synthesized compounds were characterized by P-XRD, TGA and SEM then evaluated for anti-mycobacterial activity MABA test, against H37RV [ATCC27294] strain, cytotoxicity activity MTT test using human embryonic kidney [HEK293] and human hepatocellular carcinoma [HepG2] cell lines.

Results: The co-crystallization of BA, OA with INH, increased the anti-TB MIC values in the range of 0.45 uM to 1.06 Um. The cytotoxicity of the test compound to the two human cell line (HEK293 and HepG2) was in the range of IC50 ≥300 mg, indicating low toxicity level.

Conclusion & Significance: Co-crystal compound of BA and OA with INH is probable which may further be explored as template for the synthesis of potent anti-TB drug hit/lead. Recommendation is that, this can further be explored for better treatment of TB/HIV co-infection.

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Novel PtNi (111) catalyst: DFT study of C5H9COOH adsorption

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Novel bimetallic surfaces present unique geometries and electronic properties for catalysis. In this work, the density functional theory (DFT) is used to study bimetallic surface compounds of a monolayer of Pt on Ni (111) and their interaction with an organic acid molecule, the cis-3-hexenoic acid (C5H9COOH). We have found significant major properties for the PtNi (111) than Ni (111) catalyst. The PtNi (111) surface is more active on the preservation of the double carbon–carbon bond of the original organic acid. The hydrogenolysis is not being promoted suggesting that the catalyst could be adequate for the industrial oils hydrogenation. The remarkable property of PtNi (111) is that it is active to the conversion from the unsaturated acid to alcohol.

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