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QSAR and molecular docking directed synthesis and preliminary evaluation of novel non-nucleoside HCV NS5B polymerase inhibitors

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Purpose: The HCV NS5B RNA-dependent RNA polymerase (RdRp) is a central enzyme in the replication of the viral genome and has since become a target of choice for screening and design of small molecule inhibitors for viral replication interference.

Experimental description: A series of 4-pyridyl-1H-benzimidazole-4-(N-R1-carboxamide) derivatives was synthesised using two step reaction and NS5B RNA dependent RNA polymerase inhibition assay was used for *in vitro* evaluation. For *in silico* screening, the multiple regression analysis based QSAR model and molecular docking studies (FlexX) were used.

Results: From in house compound library screening using NS5B polymerase enzymatic assay, we identified some benzimidazole derivatives. The activities were predicted using the QSAR generated models. Along with QSAR predictions, molecular docking studies were used to evaluate binding of these series of compounds at allosteric pocket (AP-1) of NS5B polymerase.

Conclusions: The QSAR and molecular docking directed study explains effects of substituents at position 2 and 4 of benzimidazole nucleus for HCV NS5B polymerase inhibition. *In vitro* preliminary evaluation results in identification of three compounds (4c, 4e, 4f) as promising NS5B inhibitor leads. Docking analysis of NS5B polymerase (AP-1) provided insight for the rational design of novel HCV inhibitors.

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Terbinafine based nail lacquer for treatment of nail fungal infections

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This study focused on the synthesis and characterization of polyurethanes to prepare a nail lacquer formulation with terbinafine hydrochloride in order to obtain a topical nail release system. The synthesis of polymer was carried out by the reaction of IPDI, PPG and isosorbide with 6:1:5 ratio, under a dry nitrogen atmosphere using 0.5 mL of DABCO as catalyst. The polymer was characterized by FTIR, NMR, DSC PALS and the biocompatibility with keratinocytes cell was studied. The *in vitro* release profile of terbinafine from diferent nail lacquer formulatios was investigated using Franz Cells. The FTIR spectrum showed a band of 1695 cm-1 attributed to the stretching vibration of the C=O carbonyl of urethane. The PU melting temperature was around 60 oC. The presence of protons of -NH- between 5.2 and 7.5 ppm in the 1H NMR spectrum in DMSO confirm the reaction between the isosorbide hydroxyl groups and the pre-polymer isocyanate groups. The PU presents cell viability measured by the MTT reduction. The release profile, demonstrated that the formulation had the ability to release the drug. In this research, new polyurethane was synthesized and characterized. The polyurethane synthesized presented biocompatibility. The results so far obtained are promising for a novel terbinafine based nail lacquer for the treatment of fungal infections

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