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Computational modelling, green synthesis and biological activity of arylsulfonilamides as NNRTIs against HIV-1

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Background

The development of new and potent anti-HIV compounds has become almost obligatory for the scientific community due to rapid emergence of drug resistant mutations. In pursuance of developing new anti-HIV molecules, we herein report the design, synthesis and anti-HIV properties of a series of potent arylsulfonilamide derivatives as NNRTIs.

Methods

Development of arylsulfonilamides as NNRTIs involved both the computational and synthetic methods. On the basis of extensive docking experiments, ten promising compounds out of **55** initially taken were synthesized using green protocols and their *in vitro* anti-HIV activity assessed in TZM bl cells by luciferase assay and reverse transcriptase (RT) inhibition assay against wild type HIV-1 RT.

Results

The compounds showed very promising *in silico* results as reflected by their lower ΔG values-high binding affinity, significant scoring functions high RT- ligand stabilization energy and close interatomic contacts through strong H-bonds with Lys103, His235, Tyr318, Lys101 and Val179; pi-pi interaction with Tyr181 and pi-cation interaction through Lys101, which all together predicted high EC_{50} values. However, the molecules showed unimpressive inhibitory action against HIV-1 under *in vitro* conditions. The encouraging part of this study was that these compounds behaved as NNRTIs as per our expectations, on the basis of results obtained during HIV-RT assay.

Conclusions

In the present study, it has been observed that promising *in silico* results are not always corroborated by the desired *in vitro* results. Nevertheless, it is a part and parcel of drug discovery process, where successful drug development is nearly a hard nut to crack.

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