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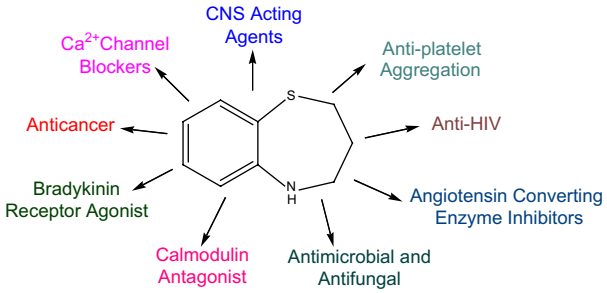

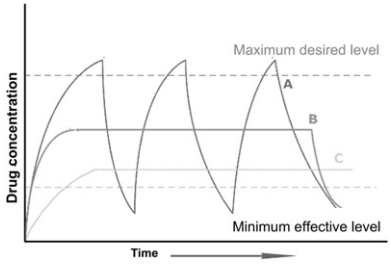

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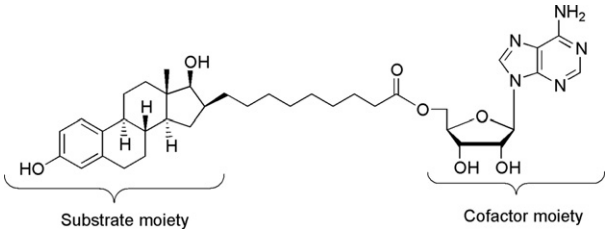
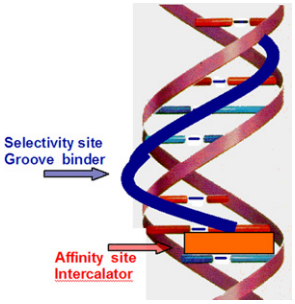
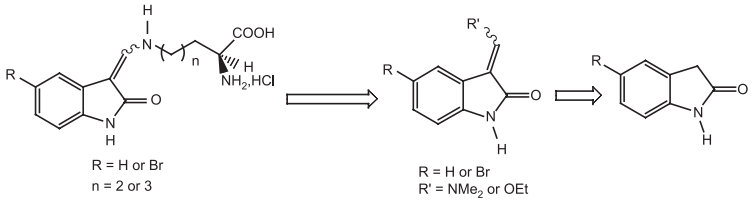
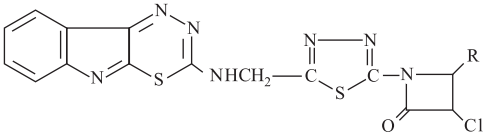
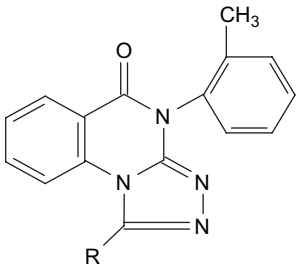


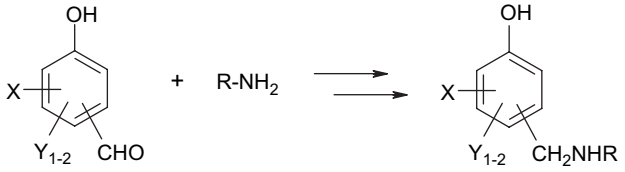


ORIGINAL ARTICLES

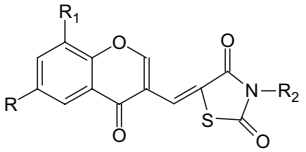




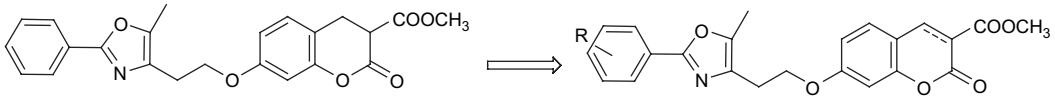


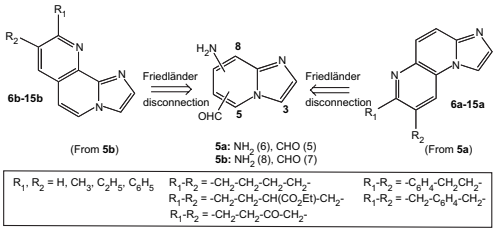


X,Y: H, F, OMe R:($n$$C_{12}H_{25}$), (4-$MeOC_6H_4$)$_3$$COCH_2CH_2$, ($C_6H_5$)$_2$$CHCH_2CH_2$, ($C_6H_5$)$_2$$CCHCH_2CH_2$

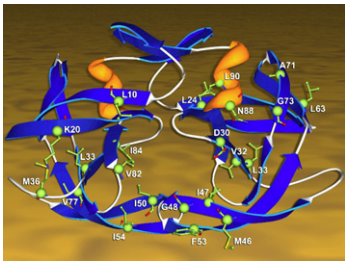


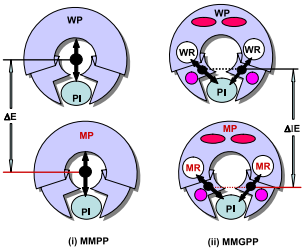
R=H, CH_3, $CH(CH_3)_2$, NO_2 R_2=H, $CH_2COOCH_2CH_3$, CH_2COOH
R_1=H, CH_3

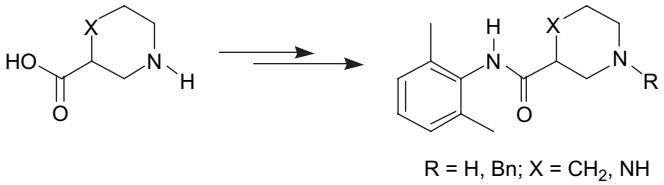


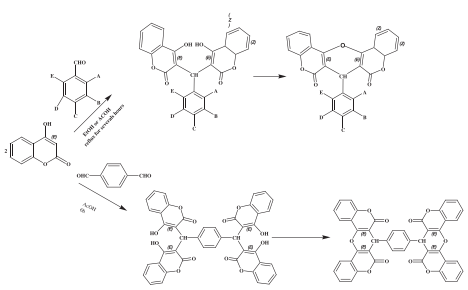


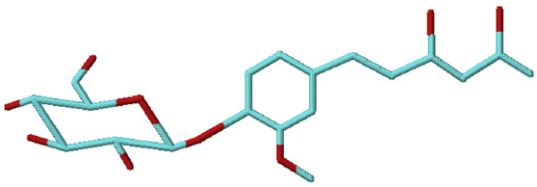
GenMol™ software is used for predicting HIV-1 Protease Inhibitor (PI) resistance. (i) The Molecular Modeling Phenotype Protocol (MMPP) considers the difference ΔE between (PI + wild protease WP) and (PI + mutated protease MP) binding energies. (ii) The Molecular Modeling Genotype–Phenotype Protocol (MMGPP) considers the difference ΔIE between (PI + wild residue WR) and (PI + mutated residue MR) interaction energies.

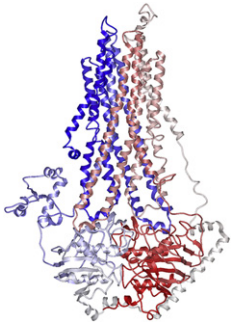




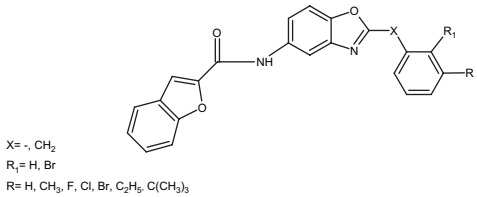


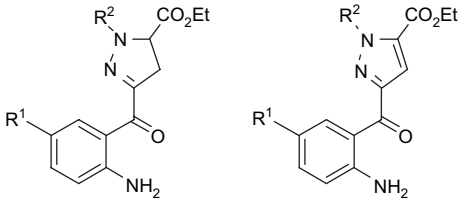


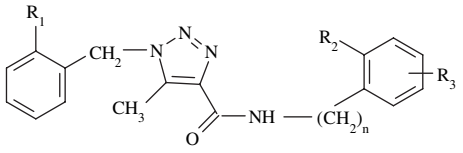




SHORT COMMUNICATIONS







n = 0 : Triazolcarbxanilides ; n = 1 : Triazol-N-benzylamide

COVER

Overlay of the experimental and docked conformations of the ligand fluorescein in complex with an antifluorescein 4-4-20 Fab fragment (PDB code 1flr, 1.85 Å). The top-scoring conformation (purple) selected by the HINT force field, among the 255 poses generated by AutoDock, nearly overlays the crystallographic structure (yellow), while the conformation selected by the AutoDock scoring function (green) reverses the positions of the carbonyl and hydroxyl groups.
Image provided by Francesca Spyrakis, Alessio Amadasi, Micaela Fornabaio, Donald J. Abraham, Andrea Mozzarelli, Glen E. Kellogg, Pietro Cozzini.

* Corresponding authors.

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