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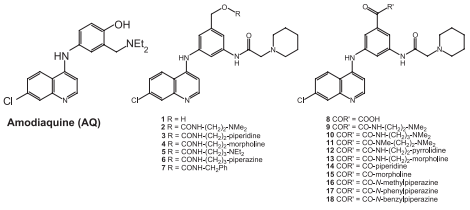
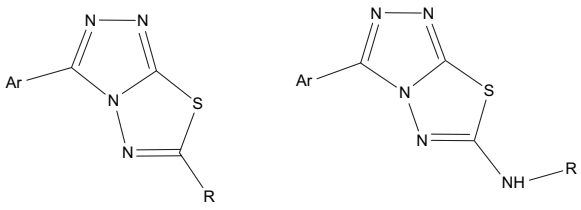
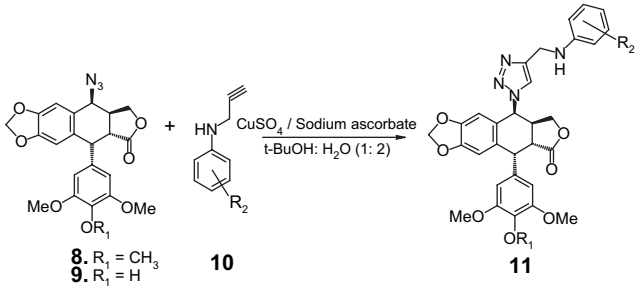
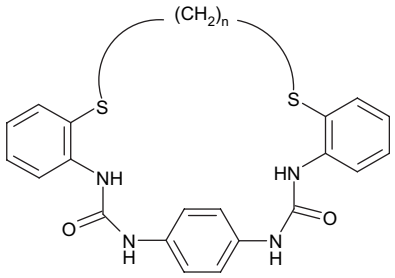
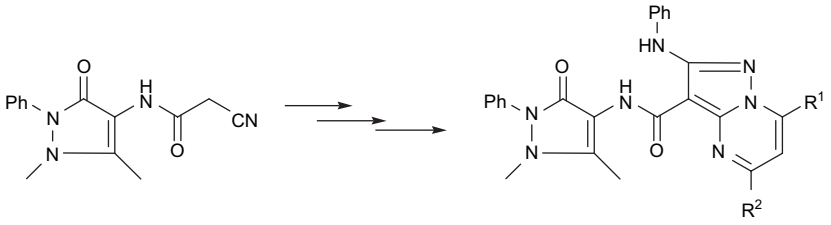
ORIGINAL ARTICLES



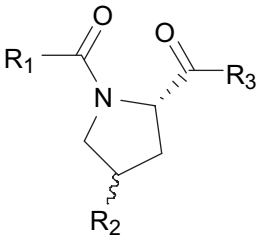


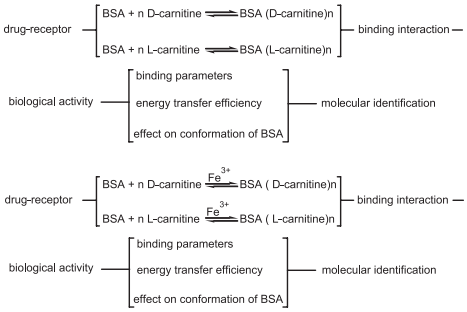


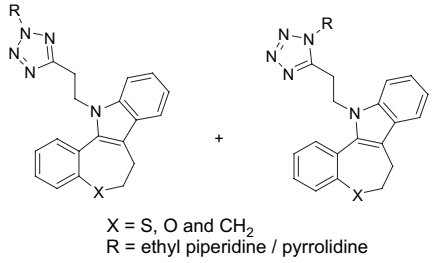


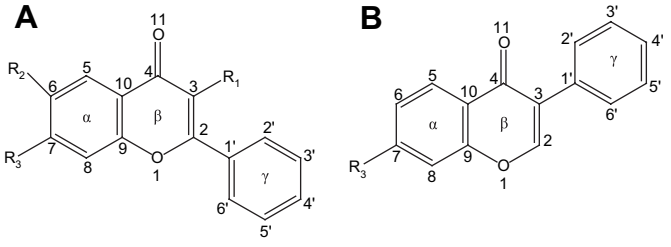


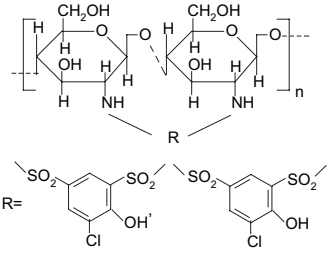
A series of novel pyrrolidine derivatives were designed, synthesized and assayed for their inhibitory activities on matrix metalloproteinase 2 (MMP-2) and aminopeptidase N (AP-N). The results showed that these pyrrolidine derivatives exhibited highly selective inhibition against MMP-2 as compared with AP-N. The hydroxamates **8a–c** were equally or more potent MMP-2 inhibitors than the positive control LY52. The binding mode of the most potent compound **8a** withMMP-2 was proposed. Structure–activity relationships were also briefly discussed.

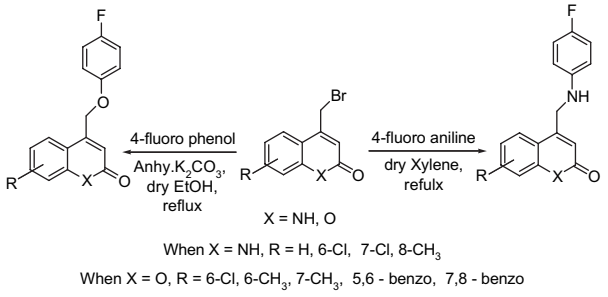


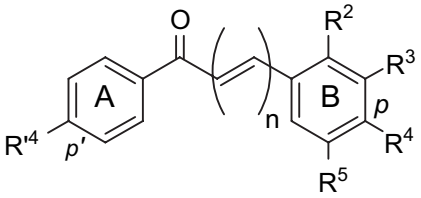




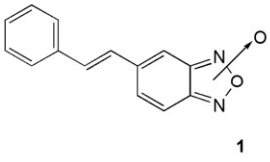


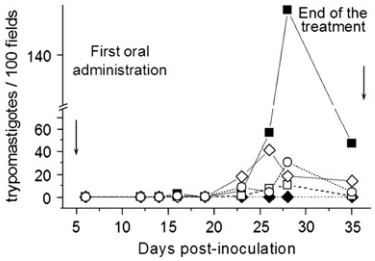




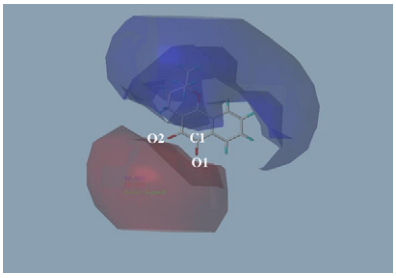


5-Arylethenylbenzofuroxans were studied *in vivo* using acute murine models of Chagas' disease. Compound **1** was the best for treating infection against the four studied strains.



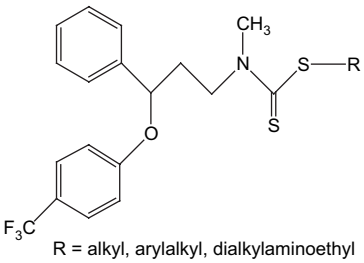


QSAR-2D and -3D treatments were made with a set of trypanocidal *ortho*- and *para*-naphthoquinones. The results indicate that the inhibitory activity of the tripanosonatids's growth is related to the semiquinone electronic state. The inhibitory activity increases as a function of the following factors: (i) a more negative value of the EHOMO; (ii) an increase of the negative charge of atoms O1 and O2 (red field) and of the positive charge QC1 (blue field) and (iii) with an increase in the electronegativity (χ).



SHORT COMMUNICATIONS

Carbodithioic acid esters of fluoxetine prepared by replacing the methylamino function in aminopropane chain with carbodithioic acid group and by adding various *S*-2-hydroxypropyl ester of dialkylamino carbodithioic acid at 3-methylamino group have shown good spermicidal, antifungal and anti-*Trichomonas* activities.



R = alkyl, arylalkyl, dialkylaminoethyl

ERRATUM

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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