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Bioorganic &
Medicinal
Chemistry

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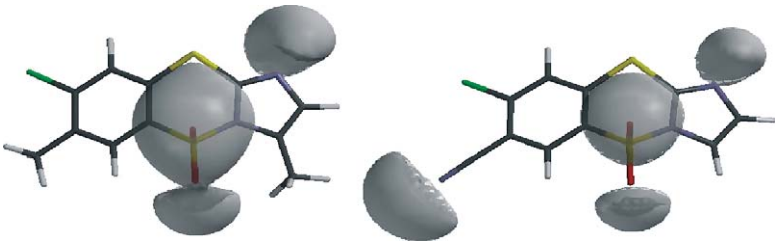
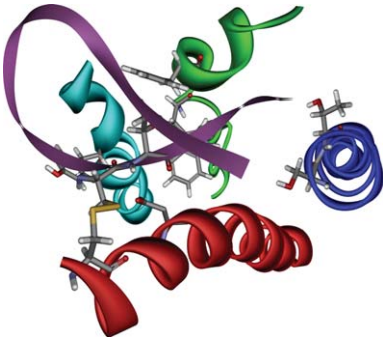
Contents

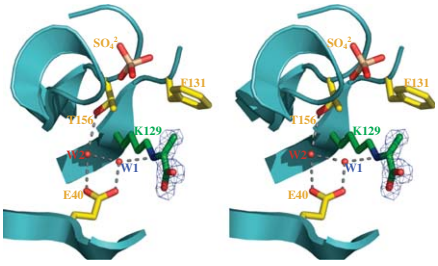
ARTICLES

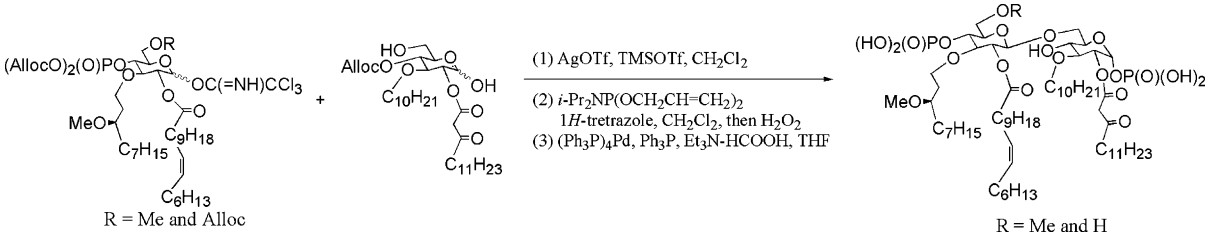


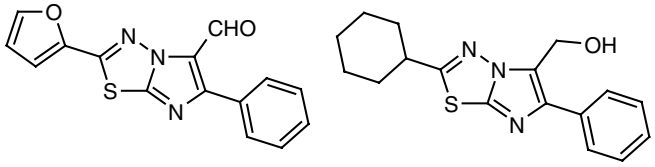
A flexible docking of a series of arylpiperazine derivatives with structurally different aryl part to the binding site of a model of human 5-HT_{1A} receptor was exercised. The influence of structure and hydrophobic properties of aryl moiety on binding affinities was discussed and a model for ligand binding in the hydrophobic part of the binding site was proposed.



A mechanism for catalysis by the Class I aldolase 2-keto-3-deoxy-6-phosphogluconate aldolase is reported based on crystallographic studies of native and mutant variants of both the *Thermotoga maritima* and *Escherichia coli* KDPG aldolase.

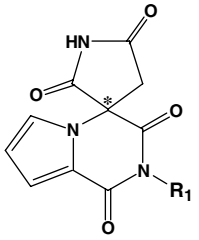




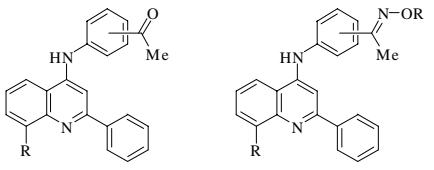


The synthesis of the powerful antitubercular agents with 100% inhibitory activity (MIC > 6.25 μg/ml), antibacterial and antifungal agents is reported.

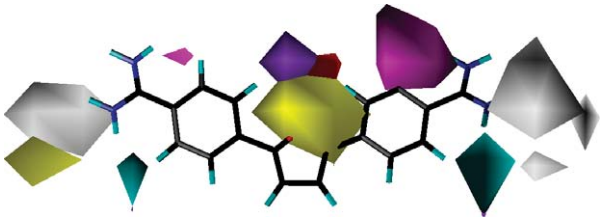
Previous reports have demonstrated that new Cre recombinase specificities can be developed for symmetrically designed *lox* mutants through directed evolution. The development of Cre variants that allow the recombination of true asymmetric *lox* mutant sites has not yet been addressed, however. In the present study, we demonstrate that a mixture of two different site-specific Cre recombinase molecules (wt Cre and a mutant Cre) catalyzes efficient recombination between two asymmetric *lox* sites in vitro, presumably via formation of a functionally active heterotetrameric complex. The results may broaden the application of site-specific recombination in basic and applied research, including the custom-design of recombinases for natural, asymmetric, *lox*-related target sequences present in the genome. Future applications may potentially include genomic manipulations, for example, site-specific integrations, deletions or substitutions within precise regions of the genomes of mammalians and other organisms.

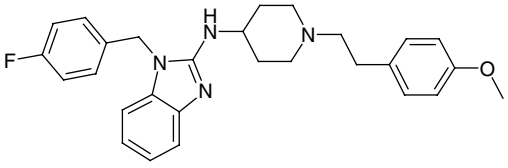


Quantitative structure–activity relationship of spirosuccinimide type aldose reductase inhibitors and the in vivo inhibitory activity of sorbitol accumulation is investigated with racemate physicochemical descriptors.

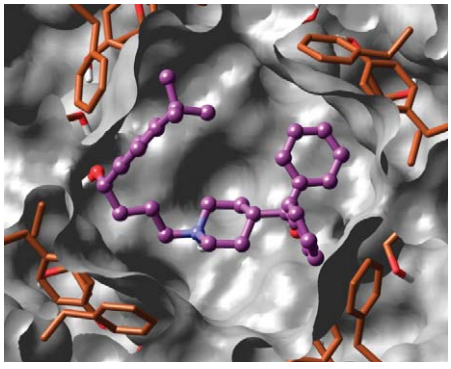


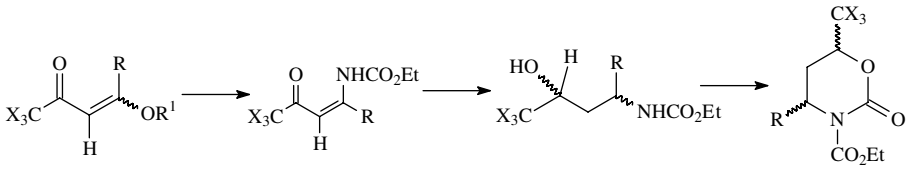
A number of 4-anilino-2-phenylquinoline derivatives were synthesized and evaluated for antiproliferative activity.



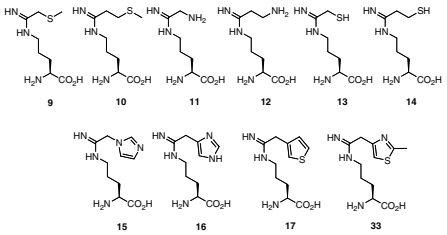


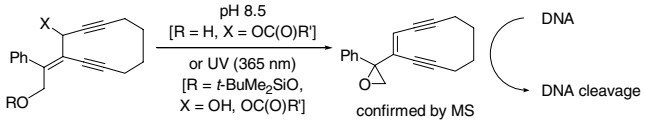
Astemizole, withdrawn from the market due to QT prolongation concerns. CODESSA program is exploited to propose a method for the prediction of torsadogenic cardiotoxicity of drugs due to hERG channel blockade.

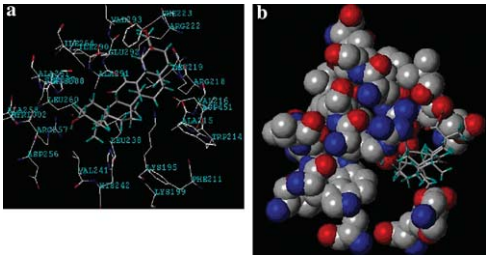




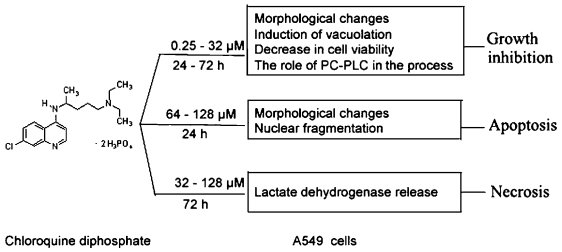
X = F, Cl; R = H, Me, Ph, 4-Me-Ph



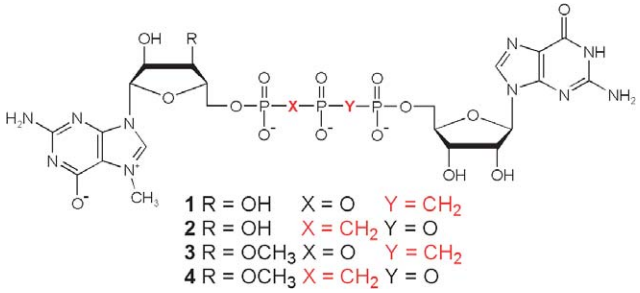


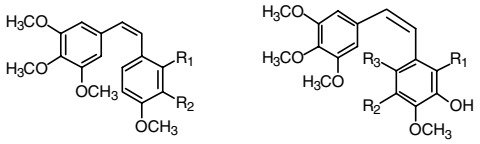


The interaction model between glycyrrhetinic acid (GEA) and HSA. (a) Only residues around 6.5 Å of GEA are displayed. The residues of HSA are represented using lines and the GEA structure is represented using a stick model. (b) GEA–HSA spacefill conformation. Protein atoms are shown in CPK representation and the GEA structure is represented using a stick model. The model shown GEA can bind to subdomain IIA of HSA, namely, site I. This result indicated that hydrophobic interaction played an important role.



Chloroquine diphosphate (CQ) could inhibit cell growth, elicit cell apoptosis, and induce necrosis in A549 cells at different concentrations. Moreover, the results suggested the involvement of PC-PLC in cell growth inhibition by CQ at lower concentrations.





7, R_1=NH_2, R_2=H **29**, R_1=NH_2, R_2= R_3=H

OTHER CONTENTS

*Corresponding author
ⓘ+ Supplementary data available via ScienceDirect

COVER

2006: The cover figure shows a synthetic multifunctional pore that is composed of rigid-rod staves (para-octiphenyls, tan) and beta-sheet hoops (arrows) and can be activated with external ligands (fullerenes, golden spheres) and closed with internal blockers (alpha-helix, red ribbon) [Gorteau, V.; Bollot, G.; Mareda, J.; Pasini, D.; Tran, D.-H.; Lazar, A. N.; Coleman, A. W.; Sakai, N.; Matile, S. *Bioorg. Med. Chem.* **2005**, *13*, 5171–5180].

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