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Bioorganic &
Medicinal
Chemistry

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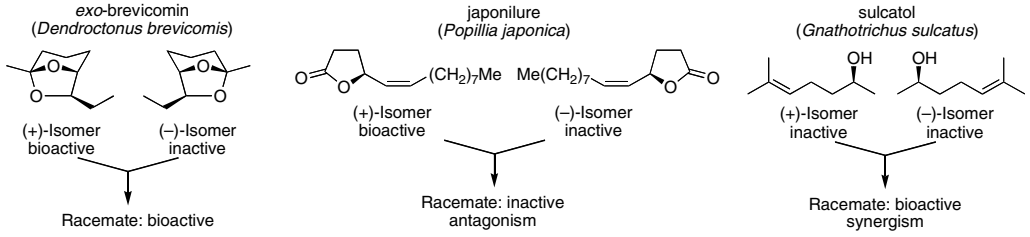
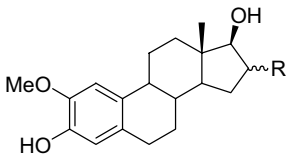
Contents

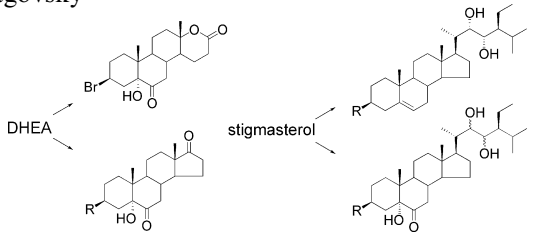
REVIEW



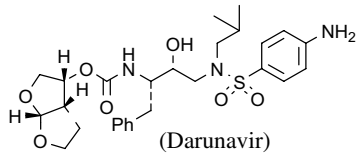
ARTICLES



A series of 16-substituted 2-methoxyestradiol analogs were synthesized and evaluated for antiproliferative activity, estrogenicity, and the ability to form glucuronide and sulfonate conjugates.

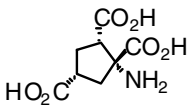


Several synthetic stigmastanes and androstane were able to inhibit the TNF-β production. Some of them were shown to be more potent inhibitors than DHEA.

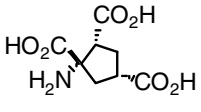


(Darunavir)

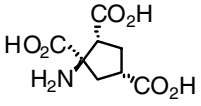
This perspective article describes our structure-based design efforts targeting the protein-backbone of HIV-1 protease to combat drug- resistance. Darunavir has been recently approved for the treatment of drug- resistant HIV.



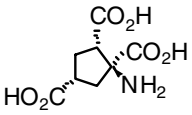
(1*R*,2*S*,4*R*)-**1**



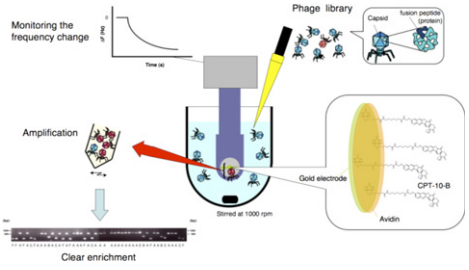
(1*S*,2*R*,4*S*)-**1'**

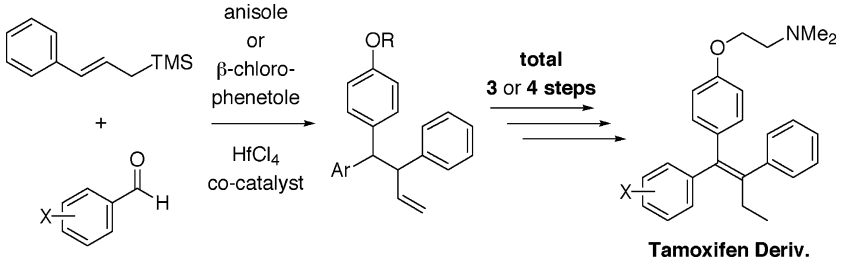


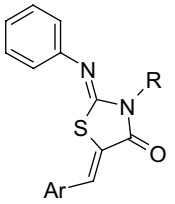
(1*R*,2*R*,4*S*)-**2**

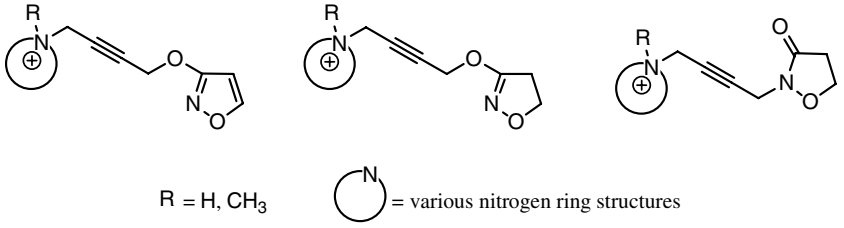


(1*S*,2*S*,4*R*)-**2'**

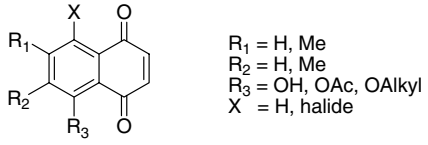


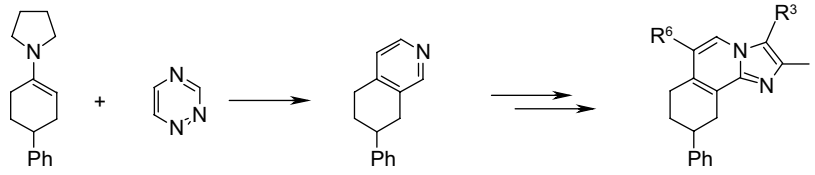




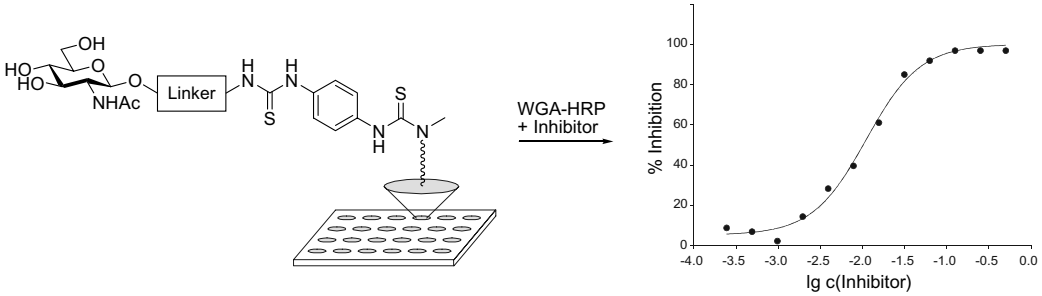


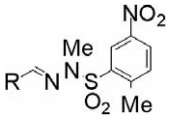
A series of nonquaternized and quaternized butynyl derivatives related to Oxotremorine was synthesized, and tested at muscarinic receptor subtypes (mAChRs).



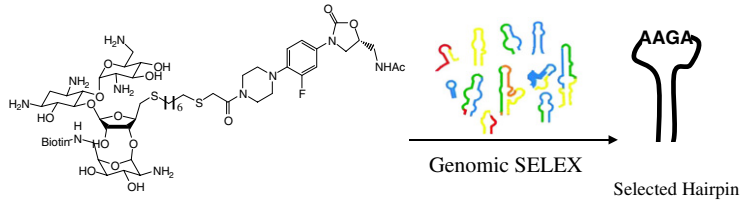


A series of novel tetrahydroimidazo[2,1-*a*]isoquinolines were prepared based on a hetero Diels–Alder reaction between an enamine and 1,2,4-triazine as key step and their inhibiting effect on the gastric proton pump enzyme was assessed.

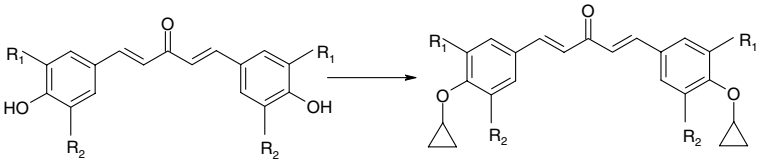




A novel series of sulfonohydrazides were synthesised and evaluated for inhibition of isoforms of PI3K, and inhibition of cell proliferation. Molecular modelling helps to rationalise the observed SAR.

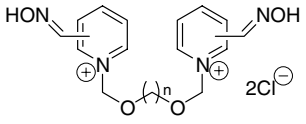


In the present study, four novel dienone cyclopropoxy curcumin analogs **1a**–**4a** were synthesized by nucleophillic substitution reaction with cyclopropyl bromide. The tumor inhibitory and anti-angiogenic effects of the synthetic compounds were studied on mouse Ehrlich ascites tumor (EAT) in vivo. The compounds **1a**–**4a** increased the life span (% ILS) of EAT bearing mice with corresponding significant reduction in ascites volume and cell number and induced apoptotic bodies in EAT cells. Anti-angiogenic studies of the compounds demonstrated significant reduction of microvessel density (MVD) in the peritoneum wall sections of mice and induced avascular zone in CAM model.



1. $R_1 = OCH_3$, $R_2 = OCH_3$
2. $R_1 = OCH_3$, $R_2 = H$
3. $R_1 = H$, $R_2 = H$
4. $R_1 = CH_3$, $R_2 = CH_3$

1a. $R_1 = OCH_3$, $R_2 = OCH_3$
2a. $R_1 = OCH_3$, $R_2 = H$
3a. $R_1 = H$, $R_2 = H$
4a. $R_1 = CH_3$, $R_2 = CH_3$



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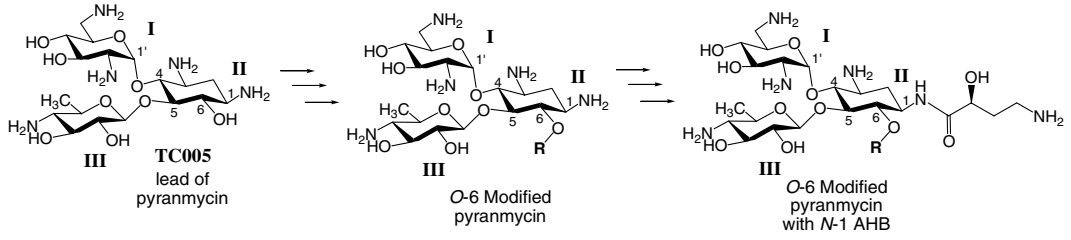
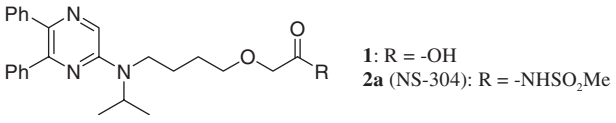
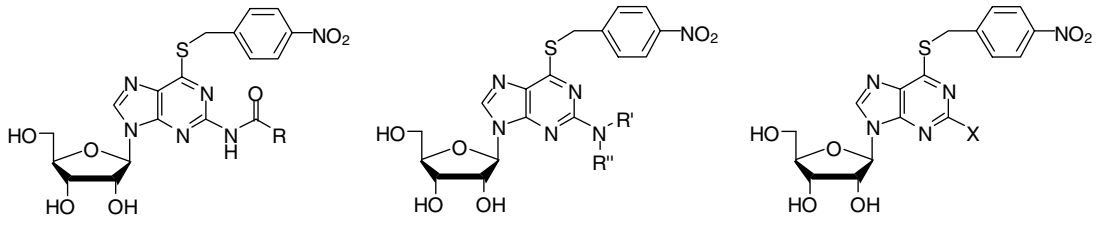
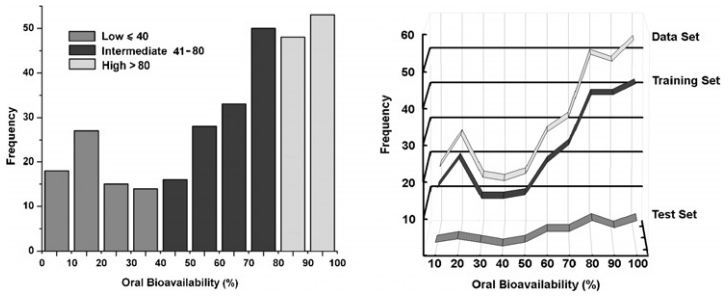




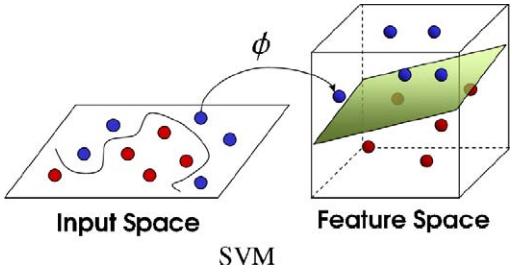
N-Acylsulfonamide and *N*-acylsulfonylurea derivatives of prostacyclin receptor agonist **1** were evaluated as prodrugs of **1** in vitro and in vivo. These types of analogues, including NS-304 (**2a**), were found to have potential as new prostacyclin receptor agonist prodrugs with long-lasting activity.

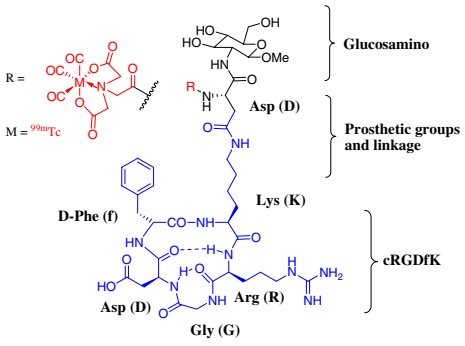


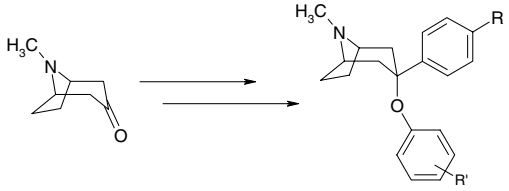
The synthesis and flow cytometric investigation of structure–activity relationship of new C^2-purine position substituted analogs of NBMPR as inhibitors of the human equilibrative nucleoside transporter (hENT1) is reported.

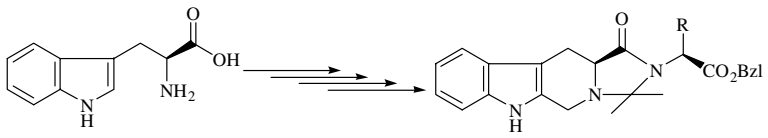


Support vector machine (SVM) as a new nonlinear feature mapping method was applied together with genetic algorithm as a variable subset selection techniques for modeling of the induction of apoptosis by 4-aryl-4-H-chromenes with the descriptors calculated from the molecular structure alone using a quantitative structure–activity relationship technique.

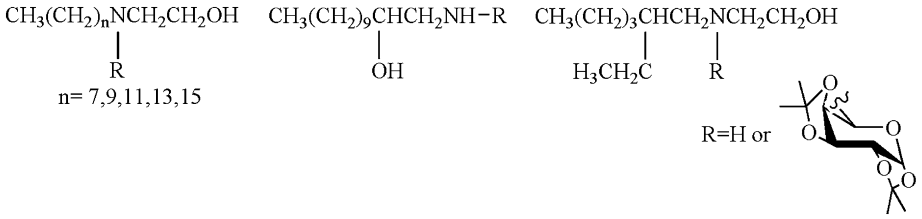






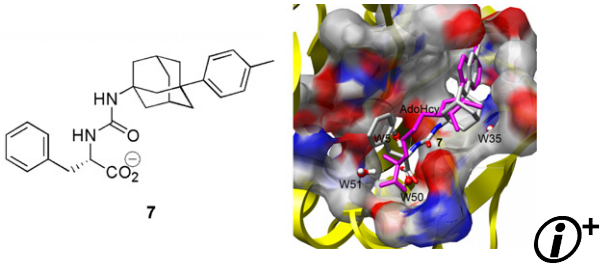


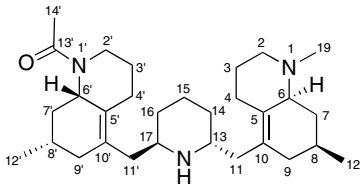
Wherein R represents the side chain of L-amino acids.

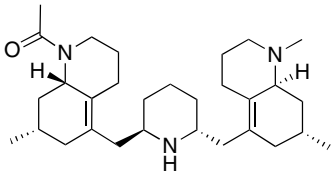


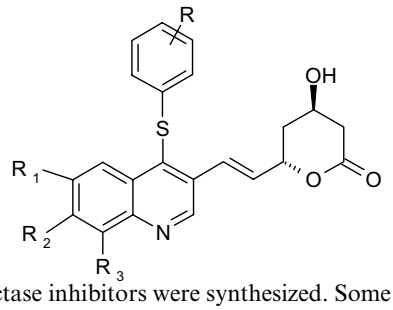
N- and C-alkylated amino alcohols and their glycosylated analogues were prepared and evaluated for their antitubercular activity.

Using a combination of virtual screening and bioassay activity testing, a novel inhibitor of a flavivirus mRNA capping methyltransferase has been identified.

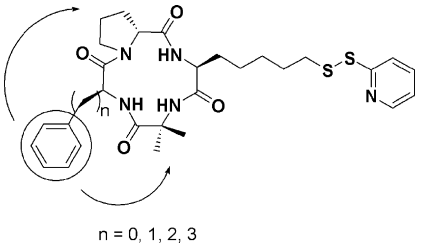






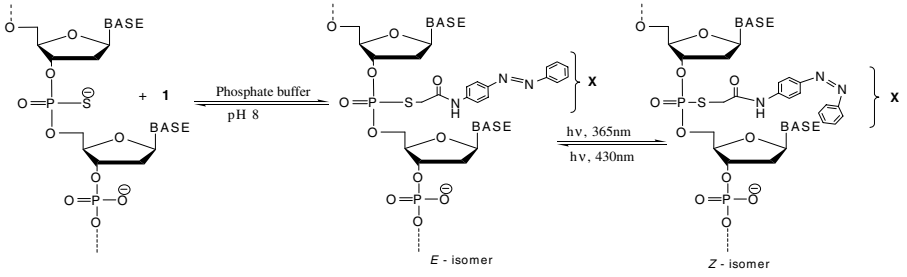


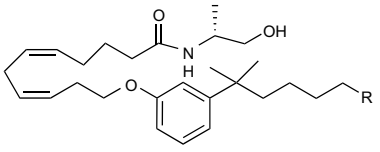
Novel 4-thiophenyl quinoline-based HMG CoA reductase inhibitors were synthesized. Some compounds showed great potency in vitro.

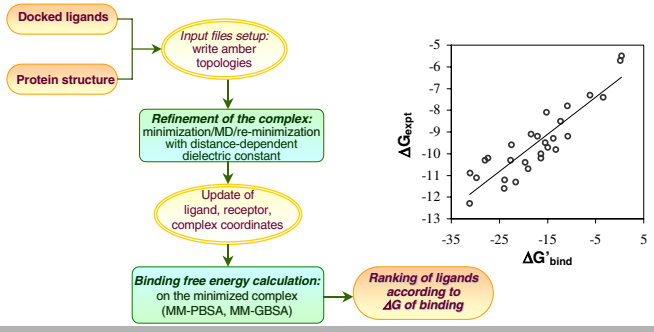


n = 0, 1, 2, 3

A new protocol has been developed for incorporation of photoisomerizable azobenzene substituent into synthetic PS-oligonucleotides.







OTHER CONTENTS

*Corresponding author
ⓘ+ Supplementary data available via ScienceDirect

COVER

Computational procedure for the prediction of relative free energies of binding. The structure of aldose reductase, the test-case enzyme used for validating the procedure, is shown as ribbon diagrams in the upper-left (holoenzyme) and lower (complex with a ligand) side of the figure. The procedure is able to screen automatically and iteratively molecules contained in databases (exemplified by the ensemble of 3D chemical structures in the upper-right corner) of compounds. Ranking and compound selection is based on binding free energy computation with molecular mechanics Poisson-Boltzmann surface area method (central part of the figure) [Ferrari, A. M.; Degliesposti, G.; Sgobba, M.; Rastelli, G. *Bioorg. Med. Chem.* **2007**, *15*, 7865–7877].

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