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Bioorganic & Medicinal Chemistry

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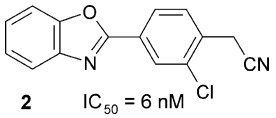
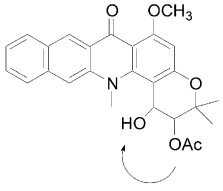
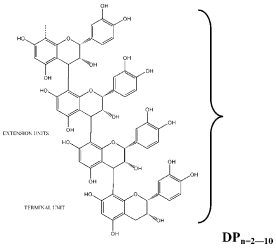
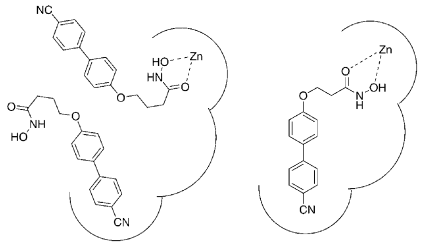


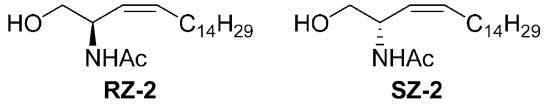
2 IC_{50} = 6 nM





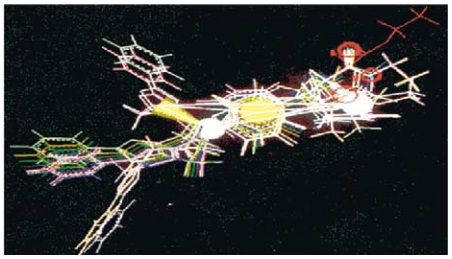
Antioxidant and radical scavenging oligomeric proanthocyanidins are isolated and identified with the help of spectral data and chemical degradation, from the methanol extract of the buds of *Mammea longifolia*.



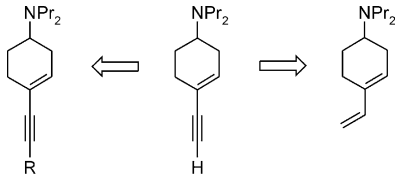


(*2R,3Z*)- and (*2S,3Z*)-2-Acetylamino-3-octadecen-1-ol were prepared and their antileukemic activities were examined against HL-60 cells.

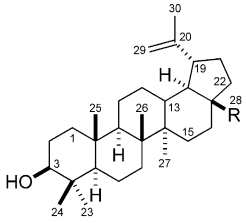
Three peptide amides, $HPRK(Py)_4HPRK\text{-}NH_2$ (PyH-12), $HPRK(Py)_3HPRK\text{-}NH_2$ (PyH-11) and $HPRK(Py)_2HPRK\text{-}NH_2$ (PyH-10), were synthesized. On a 5′-^{32}P-labeled 158-mer Watson strand, the most distinctive DNase I footprinting blockages seen with all three peptides occur around sequences 5′-GAGAAAAT-3′ and 5′-CGGT-3′. On the complementary 5′-^{32}P-labeled Crick strand, only PyH-12 strongly discriminates the 5′-TTT-3′ site. Possible interactions of the amino acid side chains of these peptides with DNA bases are discussed.



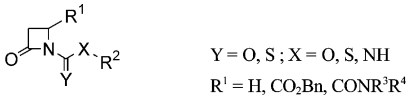
The identification of pharmacophore and three dimensional quantitative structure–activity studies have been performed on a set of N-(2-benzoylphenyl)-L-tyrosine for tbeir PPARγ agonist activity by using the logico-structural based method which describe the properties and distribution of primary and secondary biophore sites in the three dimensional space

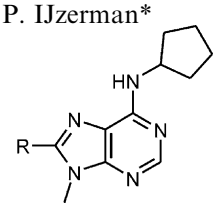


Employing the D3 agonist FAUC 73 as a lead compound, novel nonaromatic bioisosteres were synthesized via palladium-catalyzed cross-coupling and investigated for their binding properties.

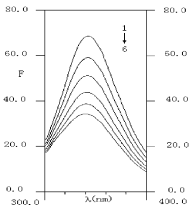


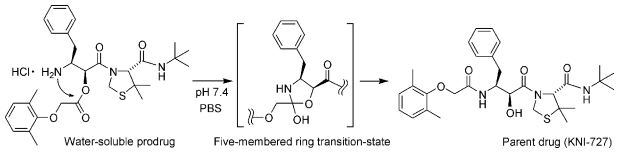
Several betulinic acid analogues were synthesized and shown to modify erythrocyte membrane according to their hydrogen bonding properties; the presence of the compounds in the erythrocyte membrane inhibited invasion and growth of malaria parasites.



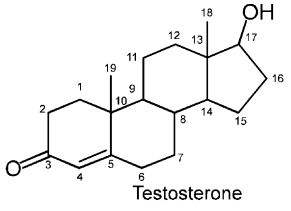


Derivatives of the above general structure were synthesized and tested as ligands for adenosine A_1 receptors. Several compounds showed nanomolar affinity, some of them behaving as neutral antagonists, whereas others proved to be inverse agonists with varying degrees of (negative) intrinsic activity.

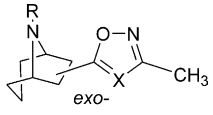




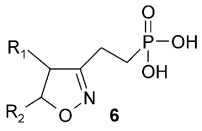
Based on the *O*→*N* acyl migration strategy, water-soluble prodrugs of small-sized dipeptide HIV protease inhibitors were designed and synthesized.

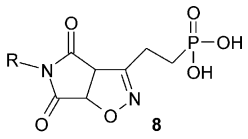


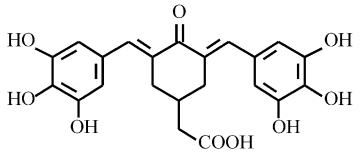
Testosterone is primarily male sex hormone. The Density Functional Theory (DFT)-based QSAR study of 75 derivatives of Testosterone is presented with PM3 calculations on WinMopac 7.21 software.

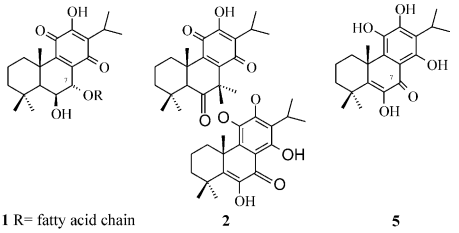


Homoepiboxidine (R−H, X = CH), its *N*-methyl and *N*-benzyl derivatives, as well as two oxadiazole (R = H, CH_3, X = N) analogues were prepared. In vitro binding and functional activities at several nicotinic acetylcholine receptor subtypes were evaluated as well as in vivo analgesia and toxicities.





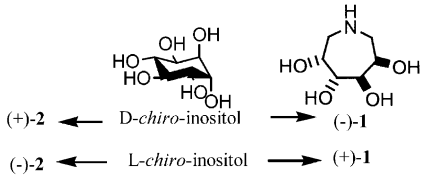




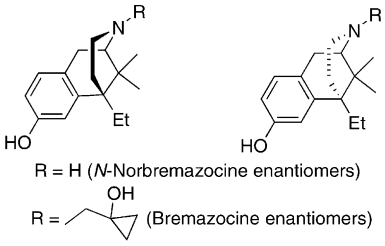
1 R= fatty acid chain
3 R= Ac
4 R= H

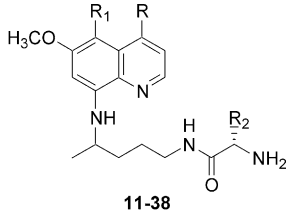
2 **5**

The effect of natural abietane diterpenes of the royleanone and coleon type on the proliferation of human lymphocytes and mouse splenocytes proliferation induced by different mitogens is described. Their effect on the CD69 expression and apoptosis is also reported.

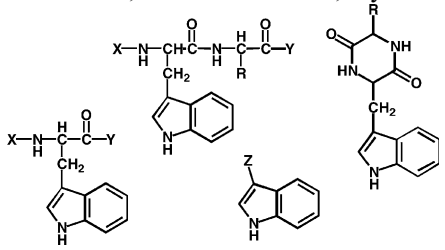


Synthesis and enzyme inhibition properties of four C_2 symmetric tetrahydroxyazepanes.

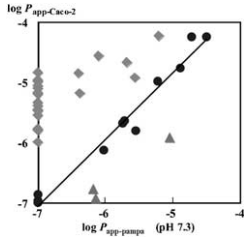




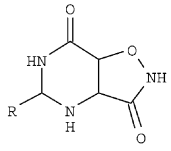
Synthesis and potent in vivo antimalarial activities of a series of L-amino acid conjugates of N^8-(4-amino-1-methylbutyl)-5-alkoxy-4-ethyl-6-methoxy-8-quinolinamines and primaquine against drug-sensitive and multi-drug resistant strain of *Plasmodium* are described.



The permeability of dipeptide derivatives containing tryptophans and indole derivatives through Caco-2 cells was used as an in vitro intestinal absorption model in order to clarify structural factors which influence their intestinal epithelial permeation and metabolism.

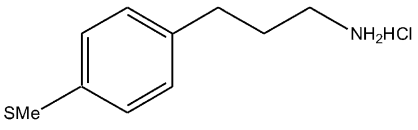


To evaluate absorption of compounds across the membrane via a transcellular route, the permeability of peptide derivatives and related compounds was measured by the parallel artificial membrane permeation assay (PAMPA). The relationship between Caco-2 cell permeability and artificial lipid membrane permeability was then determined.

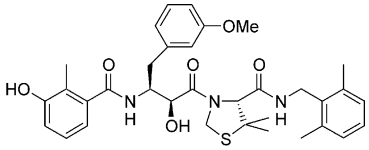


A series of new 5-alkyl and 5-arylisoxazolo[4,5-*d*]pyrimidinones were prepared from 4-amino-3-oxo-isoxazolidine-5-carboxylic acid amide. Some of the aryl derivatives of isoxazolo[4,5-*d*]pyrimidine were tested.

A new molecule, the 4-methyl-thio-phenyl-propylamine, was synthesized and its biological interaction with different amine oxidases such as semicarbazide sensitive amine oxidase (SSAO) [E.C.1.4.3.6], and Monoamine Oxidase [E.C.1.4.3.4] under its two isoforms, MAO A and MAO B, has been assesed. The substrate specifities of MAO and SSAO overlap to some extent. In this context the search for new molecules, able to discriminate between these different amine oxidases is very important as it will allow greater elucidation of the role of SSAO in physiological and pathological conditions. We report for the first time, the synthesis and evaluation of a new molecule which has a high affinity towards the SSAO family of enzymes, more so than previously described and furthermore an ability to discriminate between the different amine oxidases.

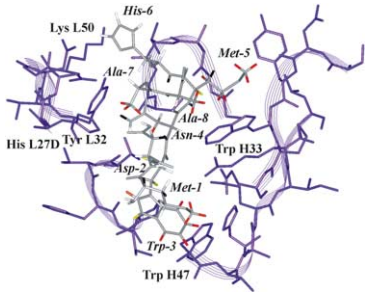


4-Methyl-thio-phenyl-propylamine



12n

SM-322377 (**12n**) had potent antiviral activity against not only wild type HIV-1but also the multi-drug-resistant HIV-1.



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*Corresponding author

COVER

2004: Overlaps of the eight known aldolase alpha-beta barrels in 2-Deoxyribose-5-phosphate aldolase (DERA). Ribbon model for DERA is shown in green, with key Lys residues capable of Schiff base formation highlighted in stick figure. Reactive Lys167 is shown in yellow. DeSantis, G.; Liu, J.; Clark, D. P.; Heine, A.; Wilson, I. A.; and Wong, C.-H. *Bioorganic & Medical Chemistry* **2003**, *11*, 43–52.

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