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Bioorganic &
Medicinal
Chemistry

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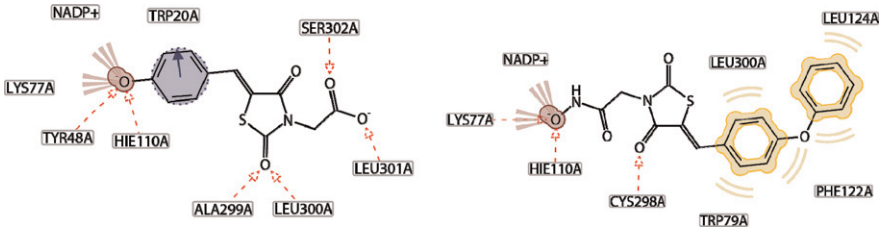
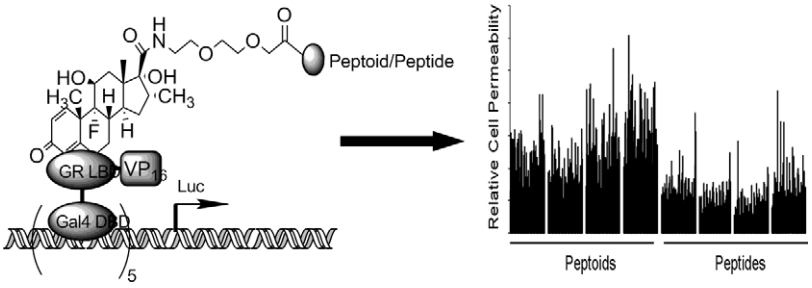
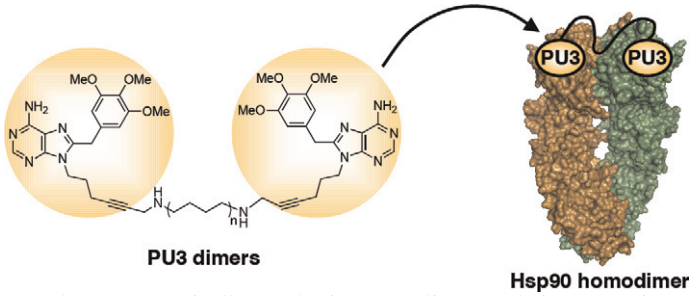
Contents

ARTICLES

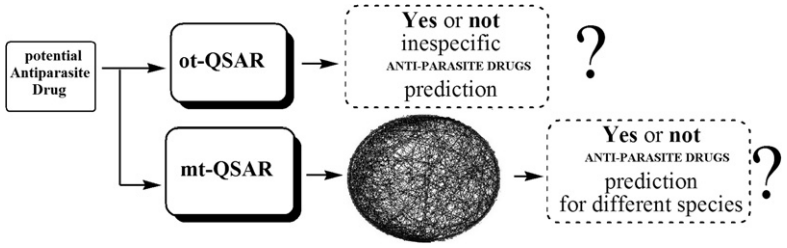


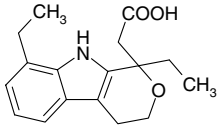


Physicochemical properties evaluation of peptoids and peptides to investigate the higher relative cell permeability of peptoids observed in high-throughput permeability assay.

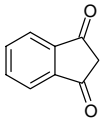


Structure-based drug design was used to systematically synthesize PU3-dimers. Their cytotoxic potency increased as the length of the bridging linker increased.



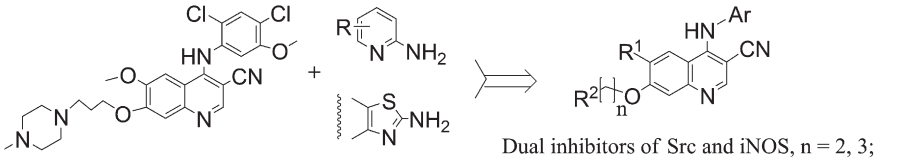


IC_{50} = 17 μM



IC_{50} = 66 μM

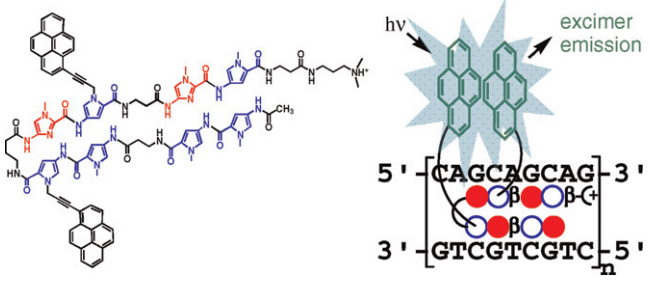
A series of compounds were screened on trihydroxynaphthalene reductase from *Curvularia lunata*, a known plant pathogen and an opportunistic human pathogen, and several structurally diverse hits were obtained. Homology model of the enzyme was built to enable further structure-based design of new and improved inhibitors.

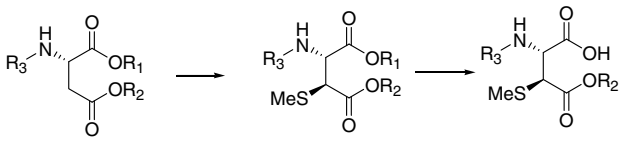


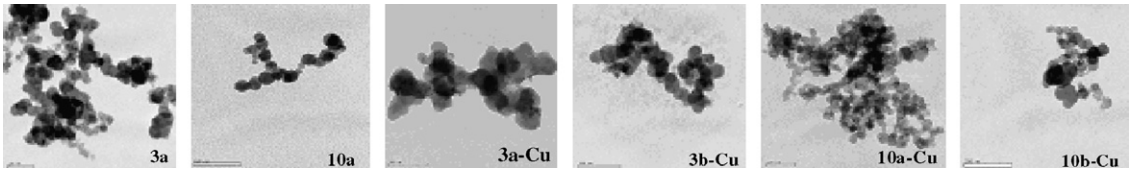
Bosutinib (SKI-606), Src inhibitor

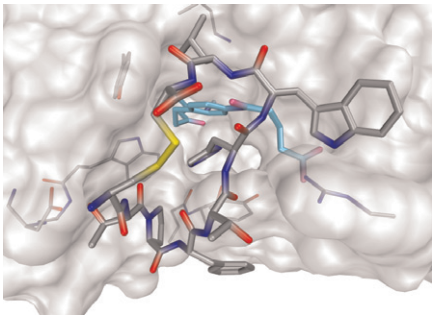
Selective iNOS inhibitors, R = alkyl groups, etc

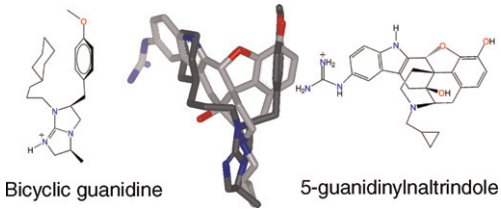
Dual inhibitors of Src and iNOS, n = 2, 3; Ar = 2-(pyridine-yl), 2-(benzothiazole-yl), etc; R^1 = CH_3O, CH_3; R^2 = piperidine, etc.

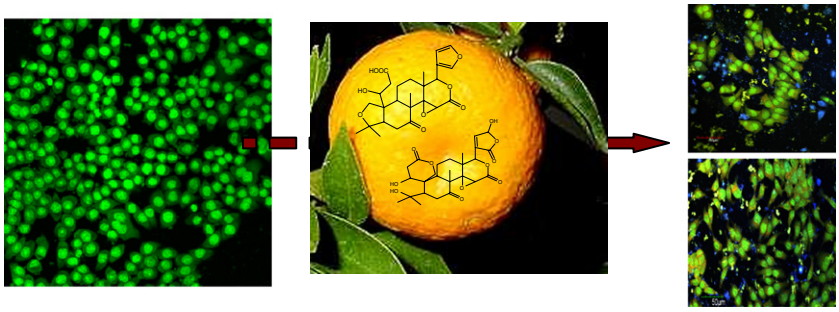


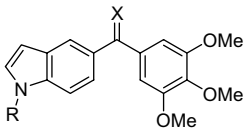






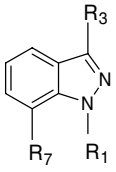






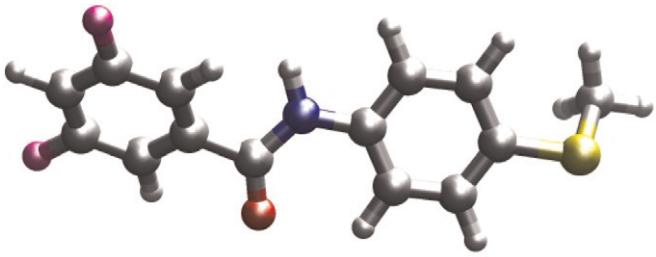
R = Me, Et
X = H/OH, H/OAc, O, NHOH NHOAc, NHNH2, NHNHMe, NHNHAc

The synthesis and biological evaluation of indolylphenstatins, modified on the bridge, are described.

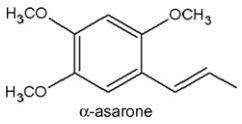


R_1 = H or CH_3
R_3 = H or Br
R_7 = NO_2, CN, CO_2H

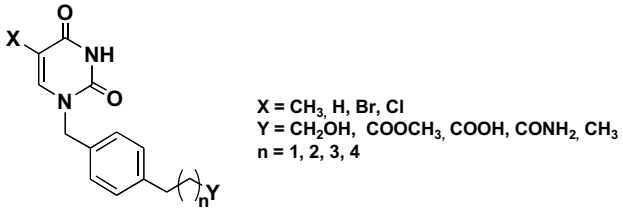
A series of new 7-monosubstituted and 3,7-disubstituted indazoles have been synthesized and tested as inhibitors of nitric oxide synthases.



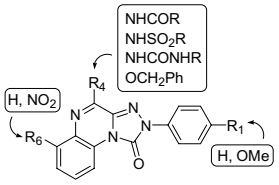
IC_{50} 3.25 μM

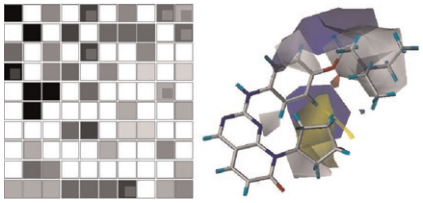


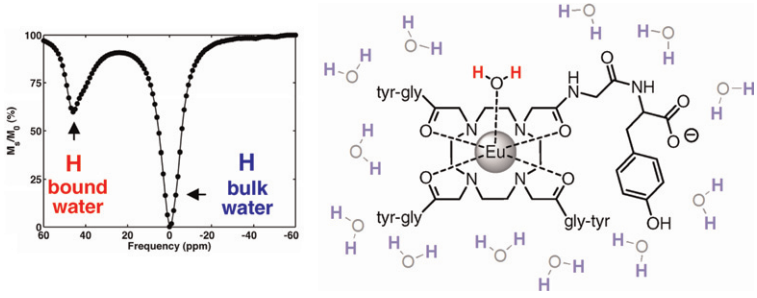
α-Asarone isolated from plants express hypolipidemic activity. In the present paper, we evaluated mutagenic and genotoxic activity of four α-asarone isomers based on the reference Ames test and micronucleus test.

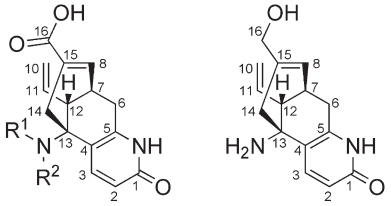


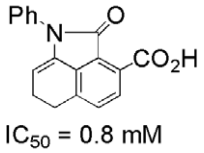
A series of N^1-(4-substituted-benzyl)-pyrimidines as potential inhibitors of thymidine monophosphate kinase of *Mycobacterium tuberculosis* were synthesized and evaluated for their ability to inhibit recombinant enzyme and mycobacterial growth in vitro.



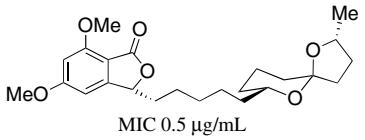


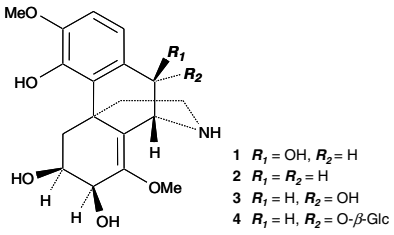


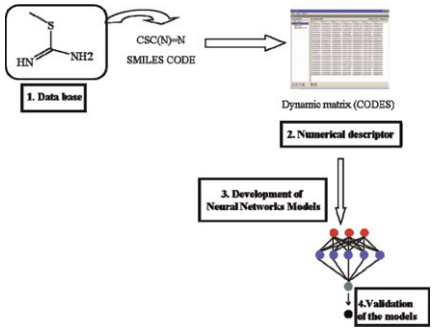


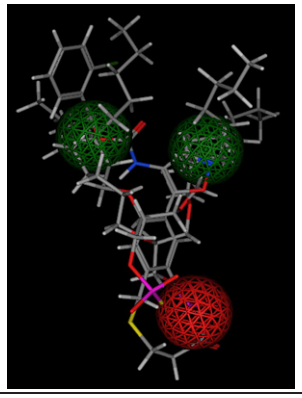


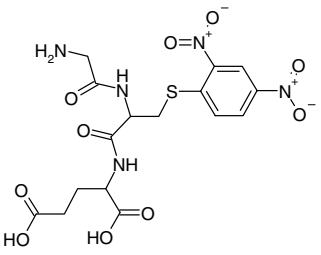
A series of Hyphodermin derivatives were evaluated as potential inhibitors of Glycogen Phosphorylase a, with IC_{50}'s of 0.8–11 mM being observed.

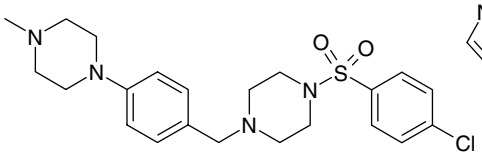




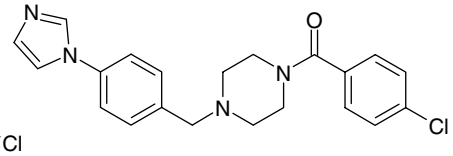




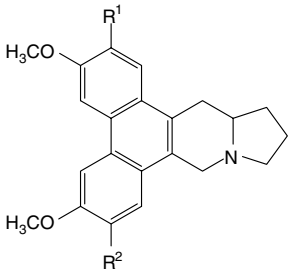




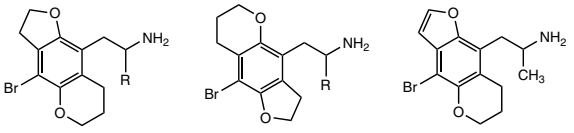
21 EC_{50} = 6nM



22 EC_{50} = 32nM



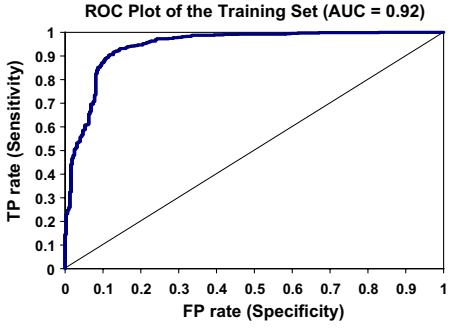
Antofine(1a) $R^1=OCH_3, R^2=H$
Deoxypergularinine(1b) $R^1=H, R^2=OCH_3$

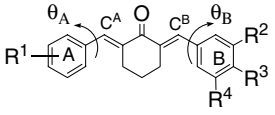


R = H, CH_3 R = H, CH_3

The synthesis and pharmacological characterization of a set of rigidified heterocyclic phenylalkylamine derivatives that have agonist activity at serotonin 5-HT_{2A} receptors is reported. Affinity and functional potency were measured, and drug discrimination in rats was assessed for two of the most potent compounds.

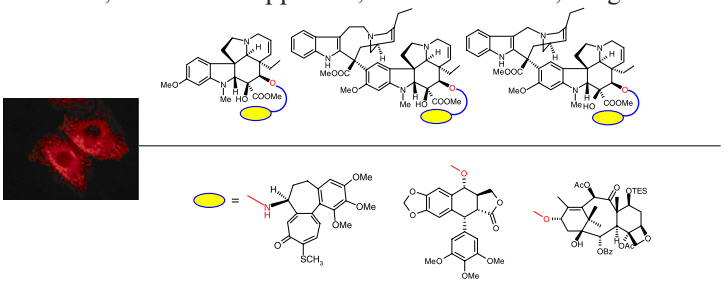
The receiver operating characteristic (ROC) curve of the SVM model built on the basis of the whole training set. Area under curve (AUC) of 0.92 indicates that the model is excellent.

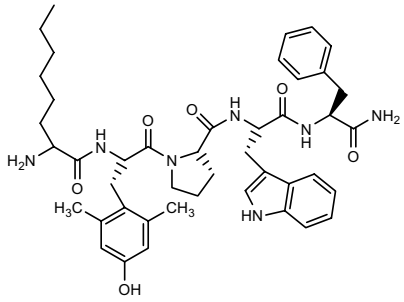


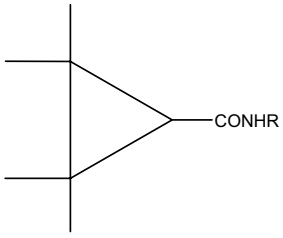


1: R^1= 2-NO_2
2: R^2= 3-NO_2
3: R^3= 4-NO_2

Three series of nitro compounds **1**–**3** were evaluated for cytotoxicity. The variation in potencies was explored by measuring the atomic charges on carbon atoms C^A and C^B, the torsion angle θ_A and θ_B, log *P* values and respiration in rat liver mitochondria.







A series of aromatic tetramethylcyclopropanecarboxamide derivatives were synthesized and some found to be active as anticonvulsants in the murine maximal electroshock and subcutaneous pentylenetetrazole seizure tests.

OTHER CONTENTS

*Corresponding author
Supplementary data available via ScienceDirect

COVER

An insight into biologically relevant chemical space showing the scaffolds of potential natural-product based inhibitors orbiting their target, the protein structure of protein 11-beta steroid dehydrogenase (PDB code 1xu7). Graphic produced using Pymol (http://www.pymol.org). [M. A. Koch, A. Schuffenhauer, M. Scheck, S. Wetzel, M. Casaulta, A. Odermatt, P. Ertl, H. Waldmann, Charting biologically relevant chemical space: A structural classification of natural products (SCONP), *PNAS* **2005**, *102*, 17272–17277 and S. Wetzel, H. Waldmann, Cheminformatic analysis of natural products and their chemical space, *Chimia* **2007**, *61*(6), 355–360].

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