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Medicinal
Chemistry

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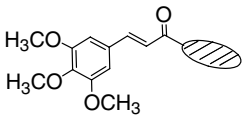
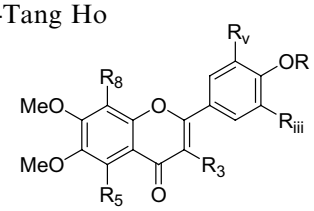
Contents

ARTICLES



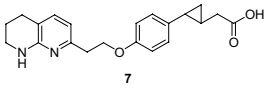
The mounting of the 3-(3,4,5-trimethoxyphenyl)-1-oxo-2-propenyl group onto different molecular scaffolds resulted in compounds displaying potent MDR-reversal properties and the ability to display selective cytotoxicity for malignant cells.

Herein we describe the isolation, syntheses and evaluation of (hydroxylated) polymethoxyflavones in HL-60 cancer cell proliferation and apoptosis induction assays. Two 5-hydroxylated polymethoxyflavones showed strong inhibition activities and apoptosis.



R_3: H, OH, OMe; **R_5**: OH, OMe
R_8: H, OMe; **R_{iii}**: H, OH, OMe
R_v: H, OMe; **R**: H, Me

The tripeptide RGD a common binding motif in several ligands that bind to $\alpha_v\beta_3$, has been depeptidized and optimized in our efforts toward discovering a small molecule inhibitor. The cyclopropyl containing new lead compound was optimized for potency, selectivity, and for its ADME properties.



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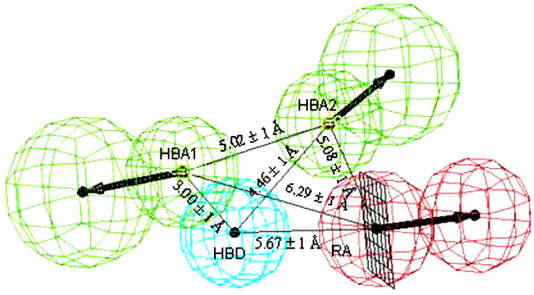
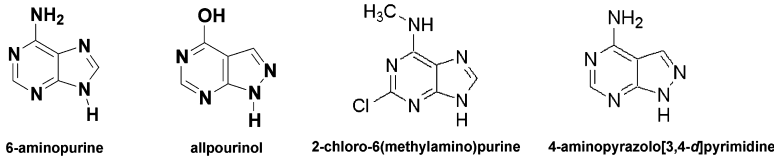
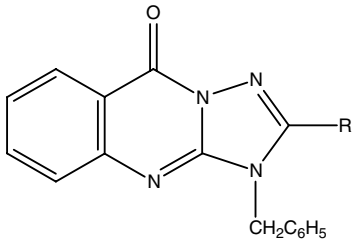
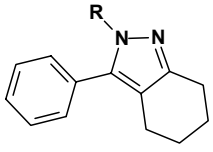




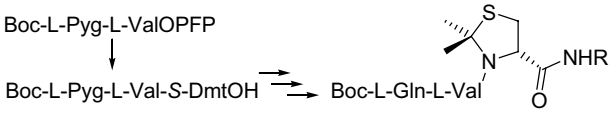
The 6-aminopurine and its analogues were evaluated as xanthine oxidase inhibitors. These inhibitors are likely to be adopted as candidates to treat gout.

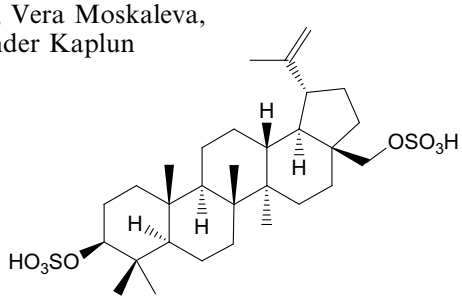


In the present study, a new series of 3-benzyl-2-substituted-3*H*-[1,2,4]triazolo[5,1-*b*]quinazolin-9-ones were synthesized and pharmacological screening of their antihypertensive activity is described.

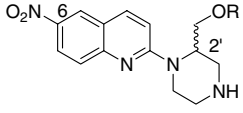


Molecular docking calculations followed by a number of in vivo biological assays were used to identify novel anti-inflammatory agents among the class of 2,3-diaryl-4,5,6,7-tetrahydro-2*H*-indazoles.

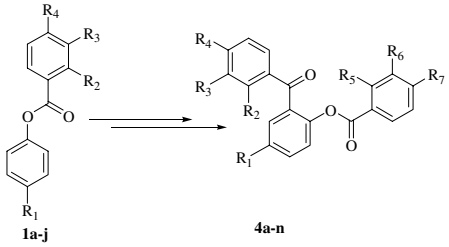




Betulin disulfate



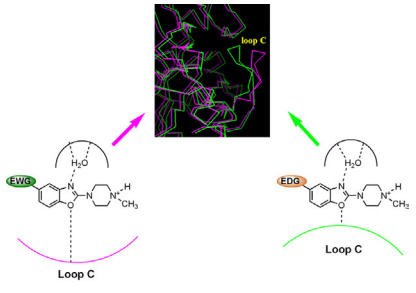
R = H, Me, Et, *n*-Pr, *n*-Bu

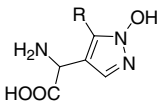


1a-j **4a-n**

The newly synthesized compounds benzoyloxy benzophenones **4a–n** were screened for their anti-inflammatory activity and compared with standard drugs.

Substituted benzoxazoles uniquely modify the function of the 5-HT$_3$ receptor ion channel gating system. SAR and computational study explained structure and function of the 5-HT$_3$ receptor (EWG:electron withdrawing group, EDG: electron donating group).

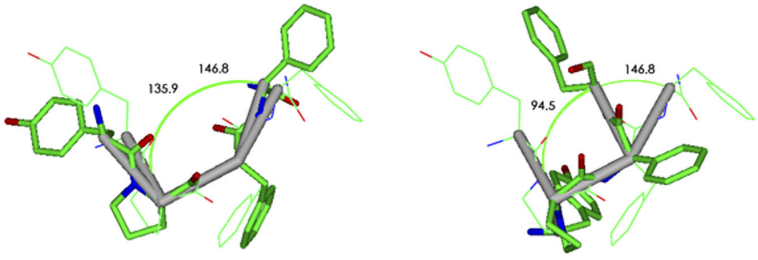




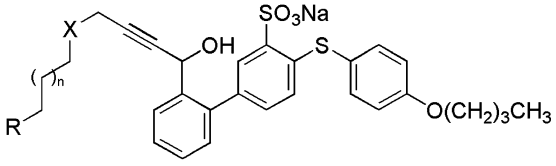
5b R = CH_2CH_3
5c R = $CH_2CH_2CH_3$
5d R = $CH_2CH_2CH_2CH_3$
5e R = $CH_2CH_2CH_2CH_2CH_3$
5f R = CH_2-cyclo-Pr
5g R = CH_2-cyclo-Hex

5a R = Br
5h R = Ph
5i R = CH_2Ph
5j R = CH_2CH_2Ph
5k R = $CH_2CH_2CH_2Ph$
5l R = $CHPh_2$

5-Substituted 1-pyrazolol analogues of ibotenic acid have been synthesized and pharmacologically characterized. The compounds represent glutamate receptor ligands with highly variable pharmacological profiles and include subtype-selective compounds.

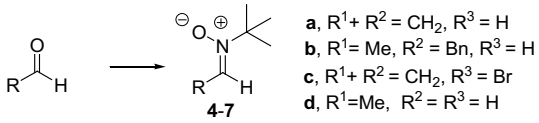


The conformations of EM-2 analogs varied from extended to folded structure as bioactivity decreases.

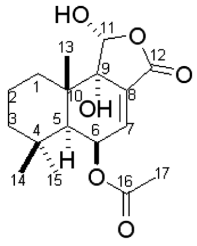


R = OH, X = O, n = 5
$S1P_1$ IC_{50} = 0.031 μM

A QSAR study was developed, employing the 2D-autocorrelation descriptors and a set of 37 naphthoquinone ester derivatives, in order to model the cytotoxicity of these compounds against oral human epidermoid carcinoma. A comparison with other approaches was carried out. Mathematical models were obtained by means of the MRA and the variables were selected using the genetic algorithm. The model relative to the 2D-autocorrelation descriptors was considered the best, based on the statistical results.



Protective effects against microvascular damages in ischemia/reperfusion in the 'hamster cheek pouch' assay.



11α-Hydroxycinnamosmolide (**1**) is a novel anti-mycobacterial drimane sesquiterpenoid lactone from *Warburgia salutaris* an endangered South African tree of medicinal importance.

OTHER CONTENTS

*Corresponding author
ⓘ+ Supplementary data available via ScienceDirect

COVER

Terfenadine (an antihistamine pulled from the market in 1997) bound to a model of an open form of the homo-tetrameric pore domain of hERG, produced using Schrödinger's "Induced Fit Docking" technology [Farid, R.; Day, T.; Friesner, R. A.; Pearlstein, R. A. *Bioorg. Med. Chem.* **2006,** *14*, 3160–3173].

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