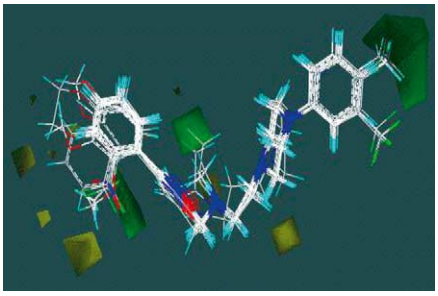
ELSEVIER

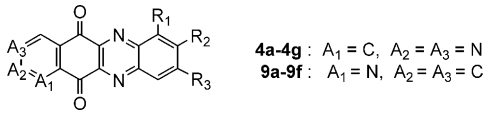
Bioorganic & Medicinal Chemistry Vol. 12, No. 7, 2004

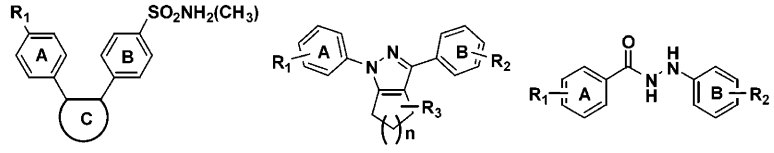
Bioorganic & Medicinal Chemistry

Contents

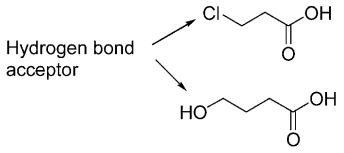


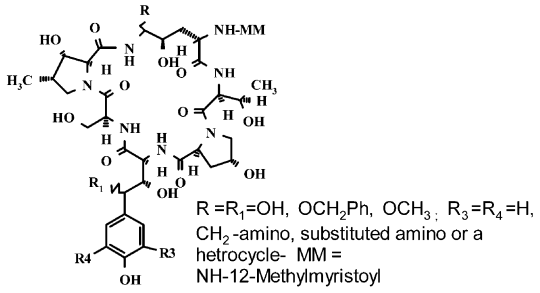
Comparative molecular field analysis (CoMFA) and comparative molecular similarity indices analysis (CoMSIA) were performed on a series of isoxazolyl compounds as a potent T-type calcium channel blockers.



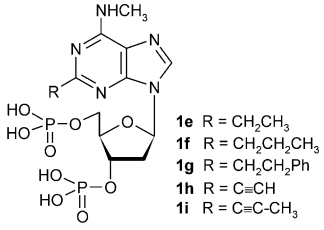


Energetic and structural differences in the interactions between the three chemical classes of selective COX-2 inhibitors and the COX-2 enzyme were investigated by the 3D-QSAR andflexible docking studies.

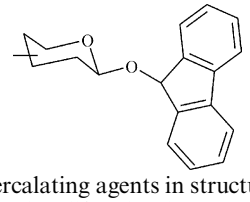




Mannich bases of Mulundocandin as antifungals are synthesized.

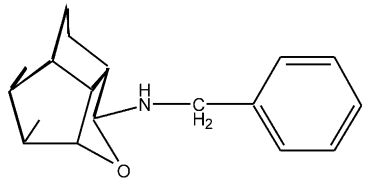


2-Alkylated deoxyadenosine nucleotides **1e**–**i** were synthesized and tested as $P2Y_1$ receptor antagonists and inhibitors of platelet functions.



Novel 9-fluoren-β-*O*-glycosides, designed as DNA-intercalating agents in structural correlation with antiviral tilorone and anticancer anthracyclines, have been prepared, then screened for antiproliferative, immunostimulating and antiviral properties against HSV-1 and HSV-2 viruses. Compounds displaying significant antiviral activity against HSV-2 are acetylated **1** and deprotected **6** 9-fluorenyl-*O*-D-arabinopyranoses, whereas 9-fluorenyl-*O*-D-glucopyranose **3** is the most effective on HSV-1 replication, followed by **1** and **6**. The conformational properties of these compounds have been evaluated by molecular modelling techniques.

QSAR calculations of ^{13}C NMR chemical shifts (ppm, TMS = 0) on carbinol carbon atoms have been attempted using a large set of distance based topological indices: Wiener (W)-, Szeged (Sz)-, PI (Padmakar-Ivan) and Connectivity ($^m\chi$, $^m\chi^v$) indices. The regression analysis has shown that excellent results are obtained in multiparametric regression. The predictive power of the proposed models are discussed using cross-validated parameters.



NGP1-01

OTHER CONTENTS

*Corresponding author

Supplementary data available via ScienceDirect

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.

Indexed/Abstracted in: Indexed/Abstracted in: Beilstein, Biochemistry & Biophysics Citation Index, CANCERLIT, Chemical Abstracts, Chemistry Citation Index, Current Awareness in Biological Sciences/BIOBASE, Current Contents: Life Sciences, EMBASE/Excerpta Medica, MEDLINE, PASCAL, Research Alert, Science Citation Index, SciSearch, TOXFILE

ELSEVIER

ISSN 0968-0896