Bioorganic & Medicinal Chemistry 18 (2010) 7701–7714

Contents lists available at ScienceDirect

Bioorganic & Medicinal Chemistry

journal homepage: www.elsevier.com/locate/bmc

Bioorganic & Medicinal Chemistry Volume 18, Issue 22, 2010

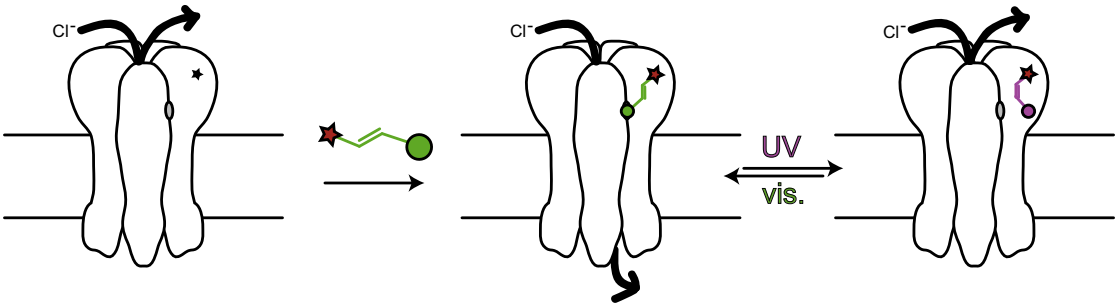
Symposium-in-Print

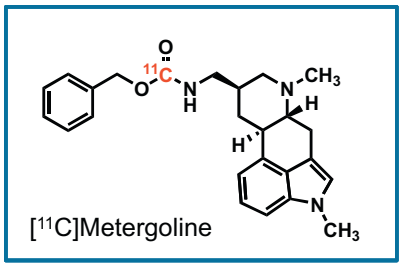
Chemical Neurobiology

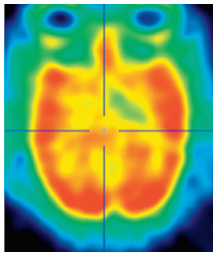
Edited by: Prof. Dirk Trauner

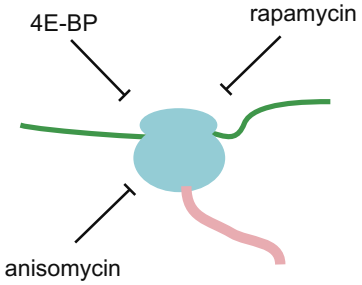
University of Munich, Department of Chemistry, Butenandtstr. 5-13, 81377 Munich, Germany

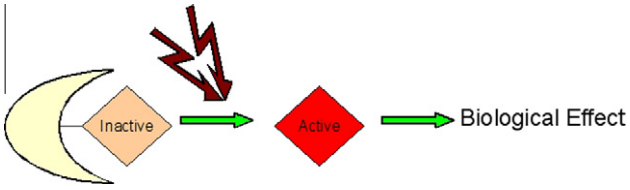
Contents

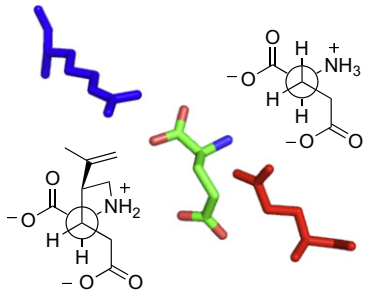




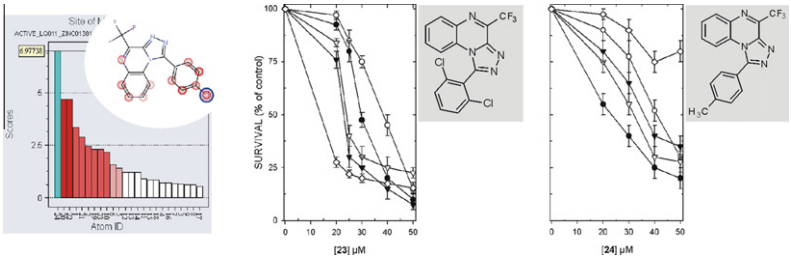


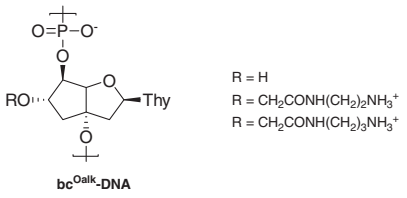


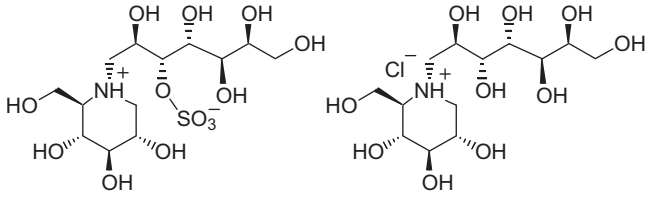


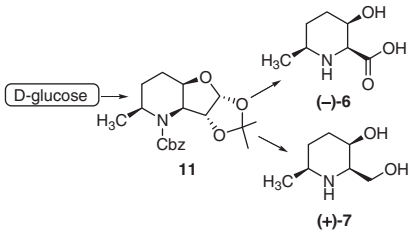


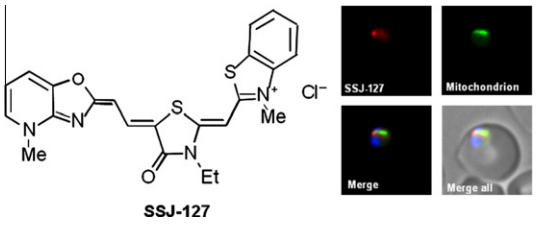
REGULAR ARTICLES



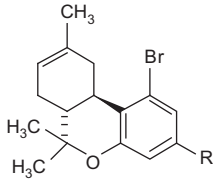




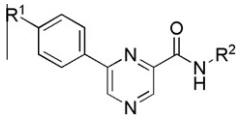


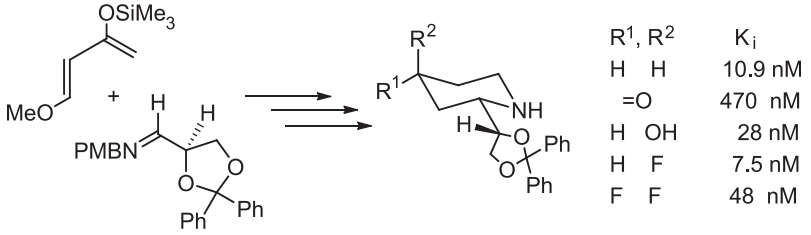


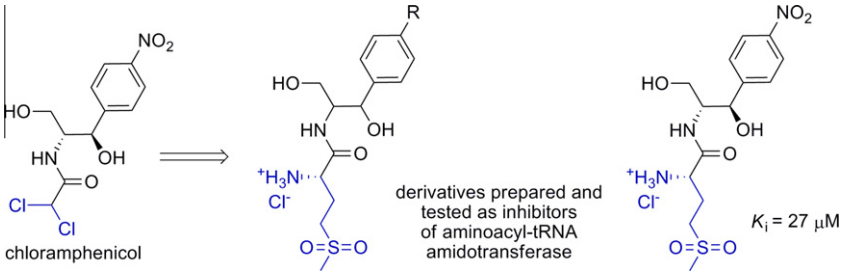
A novel antimalarial rhodacyanine derivative, SSJ-127, is detected in mouse malaria parasites using fluorescence imaging. The SSJ-127-accumulating organelle is clearly different from the mitochondrion and the nucleus in terms of morphology.



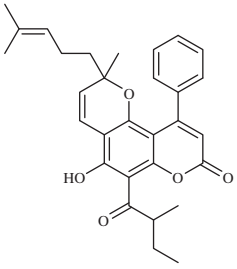
The synthesis and pharmacology of a series of 1-bromo-1-deoxy-3-(1′,1′-dimethylalkyl)-Δ^8-THCs is described. One of these compounds (R = dimethylhexyl) is 52-fold selective for the CB_2 receptor with good (28 nM) affinity for this receptor.



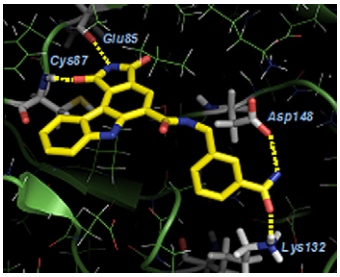




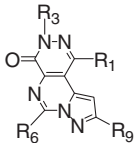
Nine 4-phenylcoumarins have been isolated from *Mesua elegans*, in which three are new; mesuagenin A, mesuagenin C, mesuagenin D, and one is a newly reported natural product; mesuagenin B. Chemical structures were elucidated using spectroscopic techniques, notably 1D and 2D NMR spectroscopy. Four compounds showed significant inhibitory activity against acetylcholinesterase, with mesuagenin B being the most potent (IC_{50} = 0.7 μM).



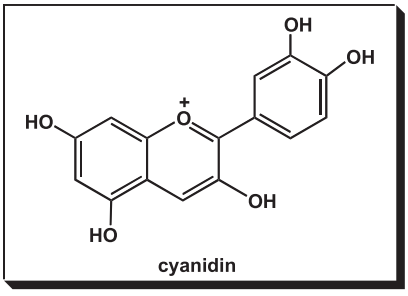
Mesuagenin B

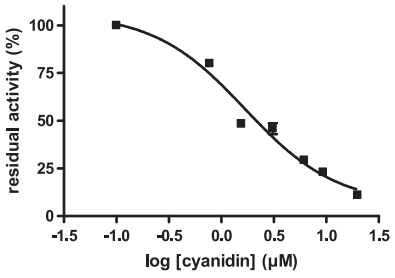


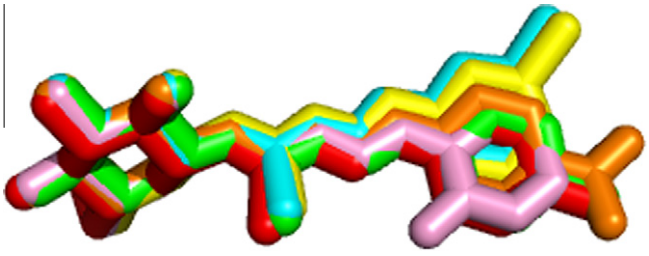
Potent inhibitors of Check point kinase 1 have been developed by a structure-based drug design.



R_1 = CH_3, Ph, Cl, 3-Pyridine, 4-Pyridine3-F-Ph, 4-F-Ph
R_3 = $PhCH_2$, C_4H_9, $Ph(CH)CH_3$
R_6 = Ph, 3-thienyl, 4-OCH_3-Ph
R_9 = CH_3, C_2H_5, iC_3H_7, nC_3H_7, CF_3

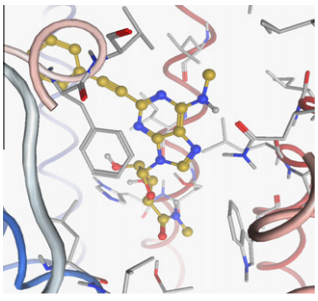


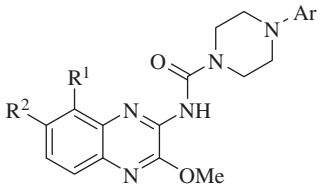




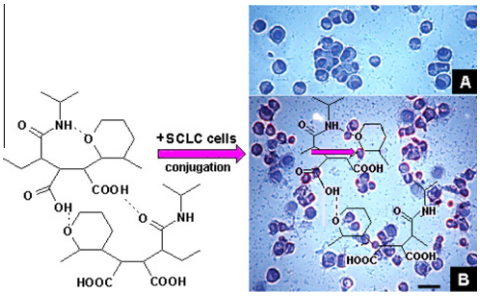
The catalytic site of muscle glycogen phosphorylase b (GPb) has been probed with a group of fifteen aromatic aldehyde 4-(β-D-glucopyranosyl)thiosemicarbazones. The best of these inhibitors displays a IC_{50} value of 5.7 μM.

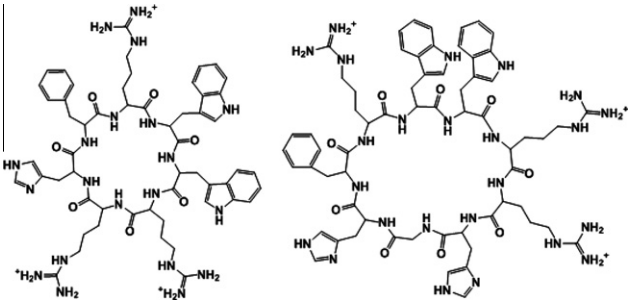
Adenosine A_3 receptor is involved in a variety of key physio-pathological processes and its agonists represent interesting tools for the development of new drugs. In this molecular modeling study, high adenosine A_3 receptor affinities and selectivities of recently reported MECA derivatives were analyzed by using adenosine receptor structural models based on the adenosine A_{2A} receptor crystal structure and molecular docking analysis.

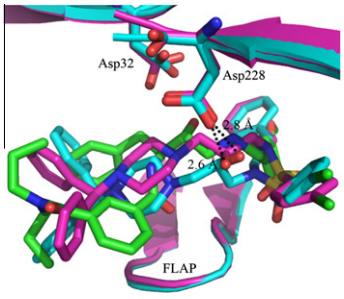


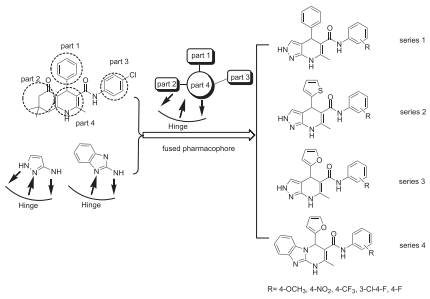


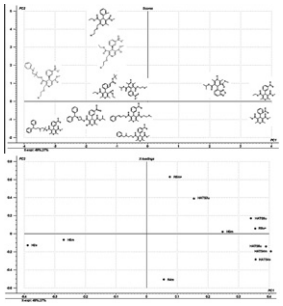
Compound 25: $R^1 = H$
$R^2 = F$
Ar = 3,5-dimethoxyphenyl
IC_{50} = 11 ~ 21 nM

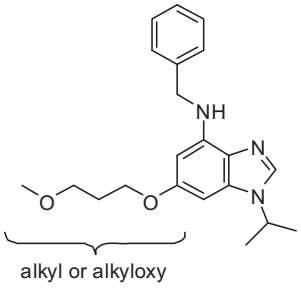


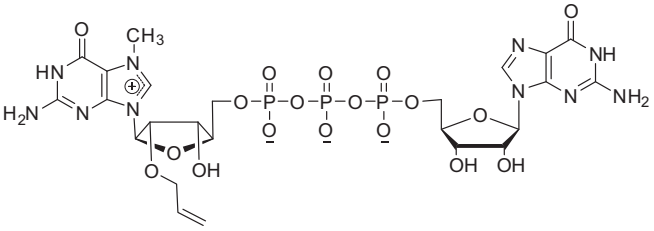




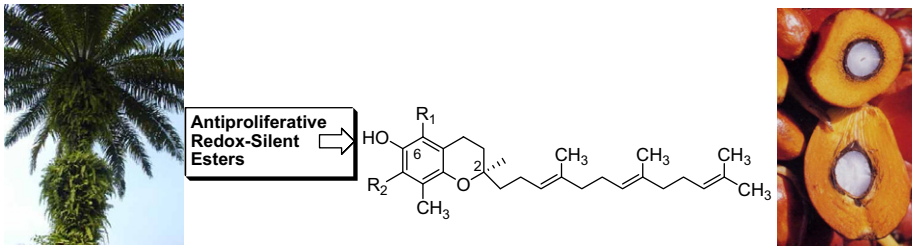


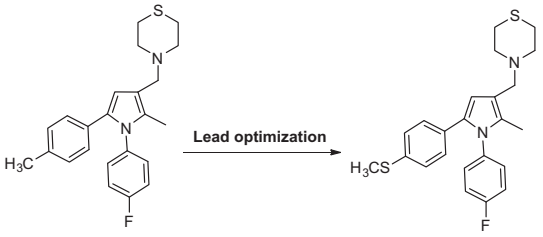


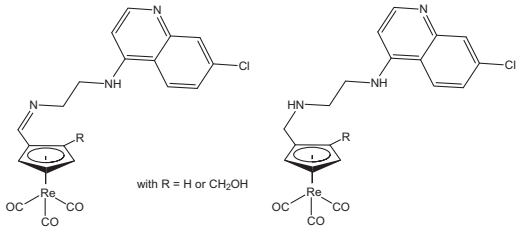




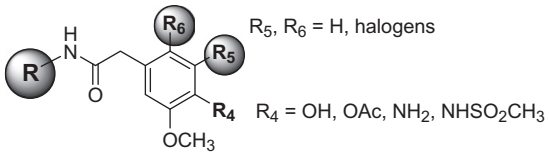
Design, synthesis and substrate properties of 2′-*O*-allyl substituted dinucleotide cap analog, that is, $m^{7,2'\text{-}O\text{-}Allyl}GpppG$ is reported.

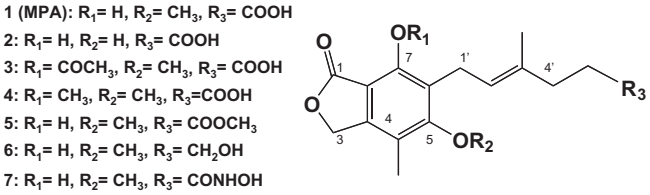


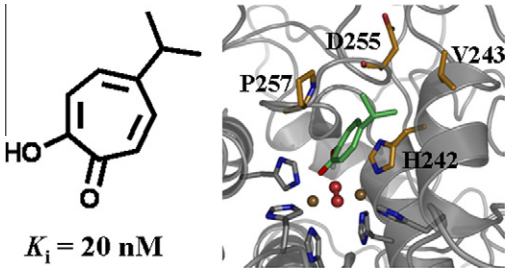


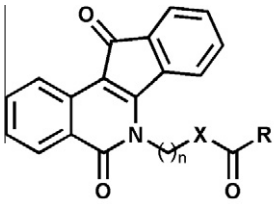


A series of new 4-aminoquinoline-cyrhetrene derivatives have been synthesized and tested for efficacy against both chloroquine-susceptible and chloroquine-resistant strains of *Plasmodium falciparum*. To establish the role of the cyrhethrenyl moiety in the antimalarial activity of this series, purely organic parent compounds were also synthesized and tested.









32 : n = 2, X = NH, COR = Arg

topoisomerase II inhibitor

*Corresponding author

Supplementary data available via ScienceDirect

COVER

The cover shows the crystal structure of an AMPA receptor, as elucidated by Eric Gouaux and colleagues, surrounded by various agonists and antagonists of ionotropic glumatate receptors. It was designed by Dirk Trauner.

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. Also covered in the abstract and citation database SCOPUS®. Full text available on ScienceDirect®

ELSEVIER

ISSN 0968-0896