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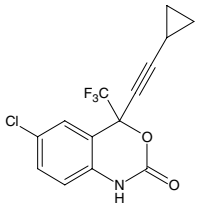
Bioorganic &
Medicinal
Chemistry

Bioorganic & Medicinal Chemistry Vol. 14, No. 17, 2006

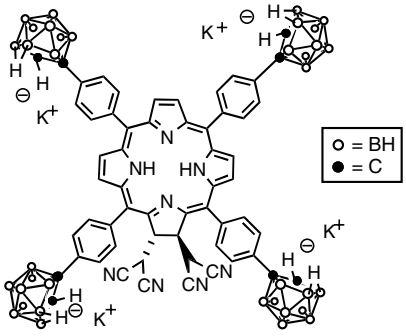
Contents

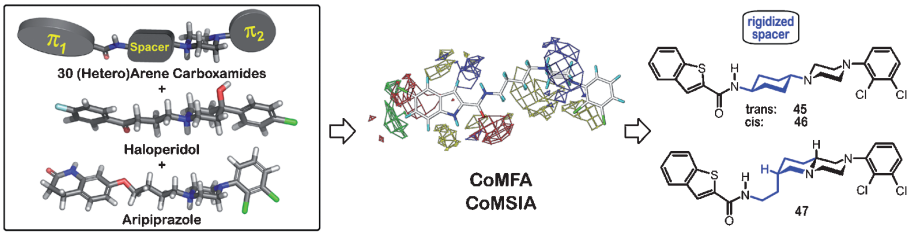
ARTICLES

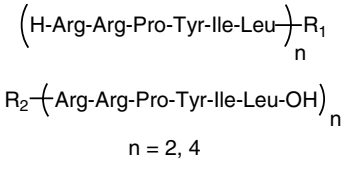


QSAR modeling the inhibitory potency pIC_{90} [mM] of 154 NNRTI of wild-type HIV-1 RT and 56 NNRTI of K-103N mutant form, using forward stepwise regression, the replacement method, and genetic algorithms. Different parallelisms are argued between the activities and the optimal molecular descriptors. Inhibition = function (molecular structural descriptors).

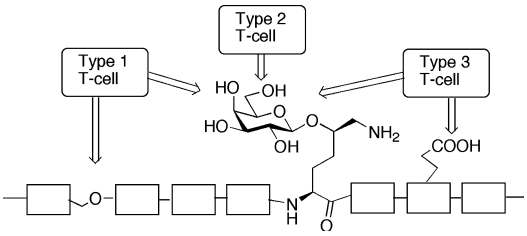
The syntheses of a water-soluble carboranylchlorin are described. This compound has low dark cytotoxicity but is toxic in the presence of light. The new carboranylchlorin is efficiently taken up by T98G cells and it localizes intracellularly preferentially within the lysosomes.



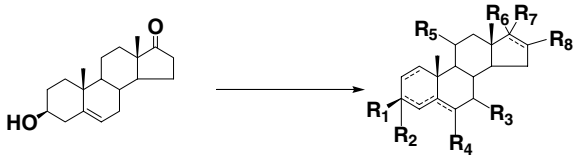




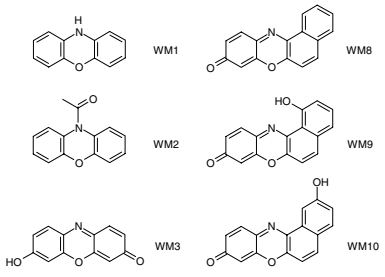
Different dimeric and tetrameric neurotensin(8–13) derivatives containing a lysine (R_1) or a glutamic acid (R_2) core unit were synthesized and evaluated concerning their binding affinity toward the neurotensin receptor.

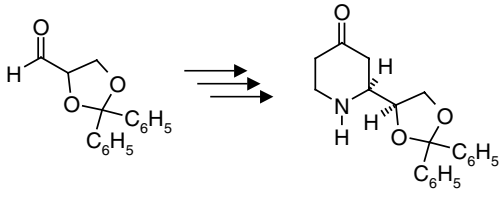


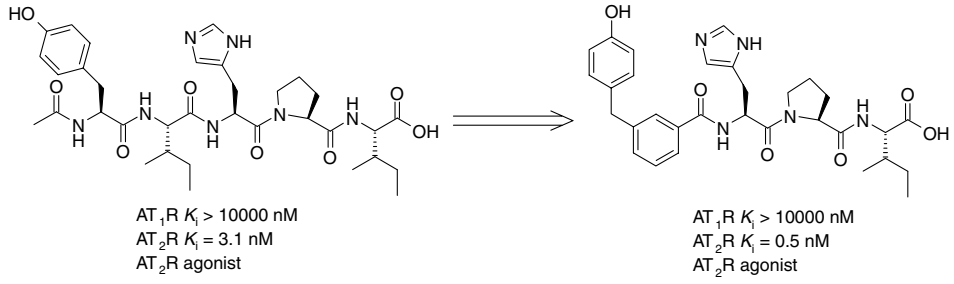
Alanine substituted glycopeptide based on the immunodominant type II collagen epitope, and a methylene ether amide bond isomer was used to probe the T-cell contact points needed for T-cell stimulation.

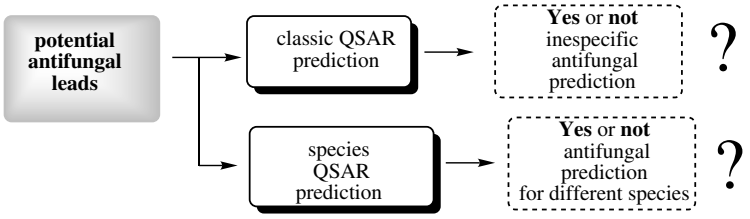


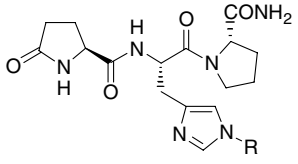
Synthesis and evaluation of a variety of C_{19}-steroids in prostate cancer cell lines. Three steroids were identified that antagonized the effects of DHT and Adiol on the androgen receptor transactivation.

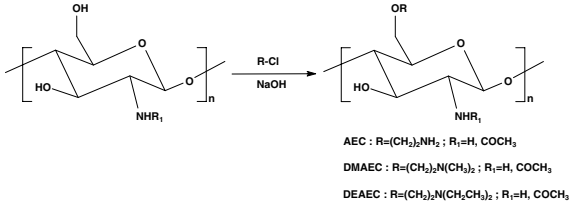


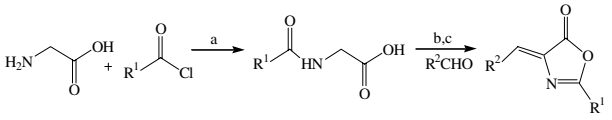






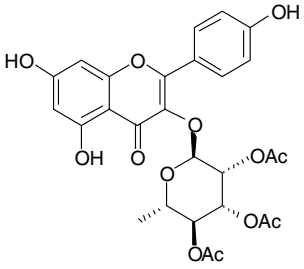




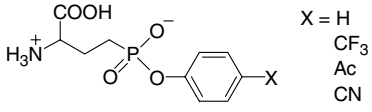


a) Ac_2O or BzCl, 10% NaOH, H_2O; b) Ac_2O, NaOAc, reflux, c) PPA, 80-90 °C

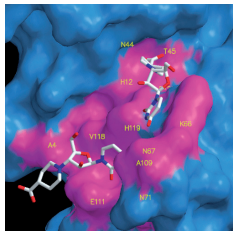
Seventeen oxazolone derivatives were synthesized, characterized, and screened for tyrosinase inhibition.



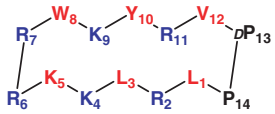
3Ac-SL0101, a specific inhibitor of RSK activity, selectively reduces the growth of human breast cancer cells.



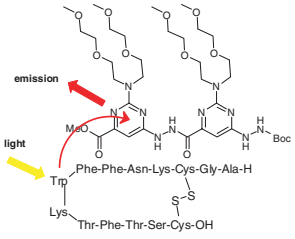
A series of hydrolytically stable monophenyl phosphonoates has been synthesized and found to serve as irreversible and mechanism-based inhibitors of *Escherichia coli* and human γ-glutamyl transpeptidase.

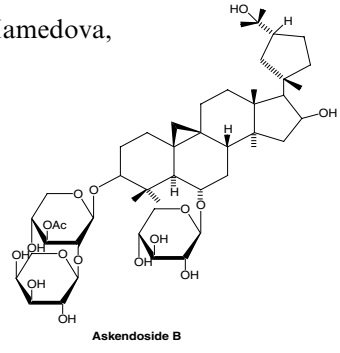


The binding of 3′-*N*-piperidine-4-carboxyl-3′-deoxy-*ara*-uridine to ribonuclease A, a member of a novel class of ribonucleolytic inhibitors, has been studied by X-ray crystallography at 1.7 Å resolution.



In this paper, we quantitatively analyse antimicrobial and haemolytic activities of porcine protegrin-1 mimetics—cyclic cationic peptides with β-hairpin fold synthesised by Robinson et al. [*Bioorg. Med. Chem.* **2005**, *13*, 2055] The presented QSAR models, which use molecular properties related to possible mechanisms of cell membrane disruption that can be easily calculated from readily available data on amino acids, rationalize the relationships between sequences and antimicrobial and haemolytic potencies of the peptides.





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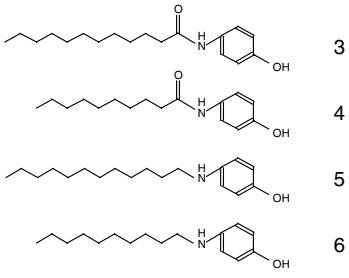
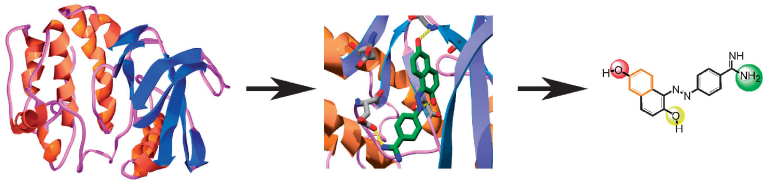
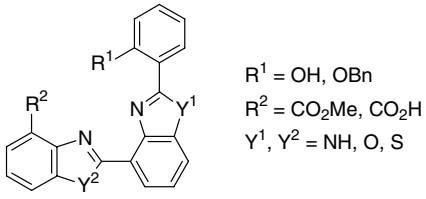
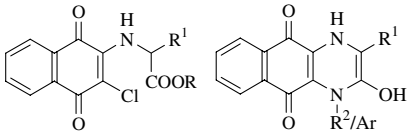






The syntheses of nineteen bis(benzimidazoles), bis(benzoxazoles), benzothiazoles, and their derivatives are described, and their in vitro antitumor activities (Against A-549, BFTC-905, RD, MES-SA, and HeLa cell lines) are evaluated.



The synthesis, antifungal, and antibacterial activities of **3**–**23** are described.

OTHER CONTENTS

*Corresponding author
Supplementary data available via ScienceDirect

COVER

Collagen induced arthritis is a common mouse model for rheumatoid arthritis. Presentation of a glycopeptide fragment from type II collagen by MHC molecules on antigen presenting cells (APCs) for recognition by T cell receptors (TCRs) is a key step in induction of disease. The roles of individual glycopeptide side-chains, in particular galactosylated hydroxylysine 264 and glutamic acid 266, as well as one of the amide bonds for T cell recognition has now been established. [Holm, L.; Bockermann, R.; Wellner, E.; Bäcklund, J.; Holmdahl, R. and Kihlberg, J. *Bioorg. Med. Chem.* **2006,** *15,* 5921.]

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ISSN 0968-0896