Bioorganic & Medicinal Chemistry 16 (2008) 9083–9092

Contents lists available at ScienceDirect

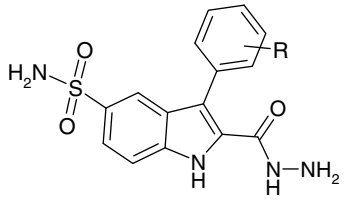
Bioorganic & Medicinal Chemistry

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

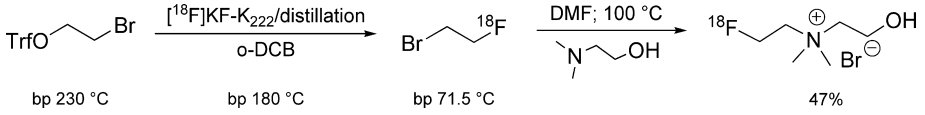
Bioorganic & Medicinal Chemistry Vol. 16, No. 20, 2008

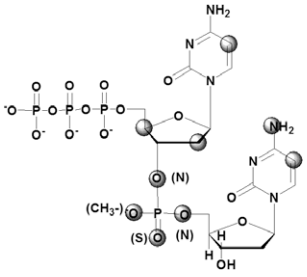
Contents

ARTICLES

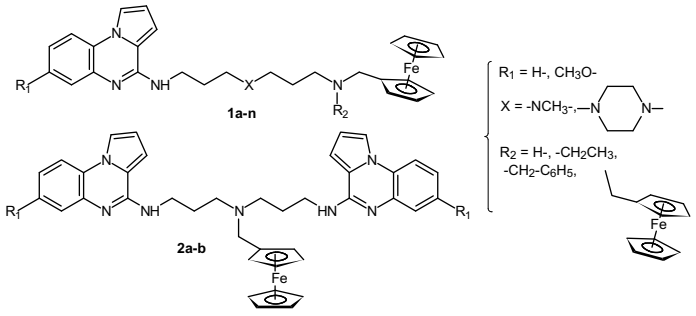


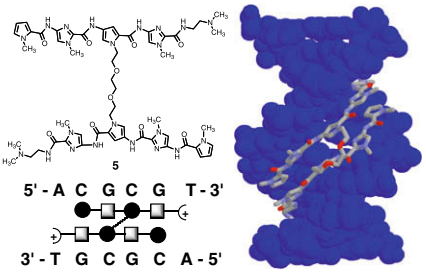
R = H, Me, F, Cl, Br, OMe, etc.

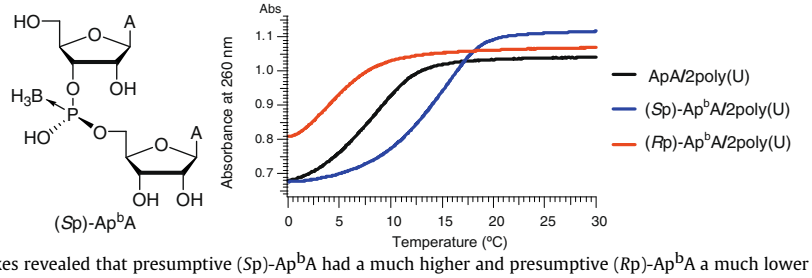




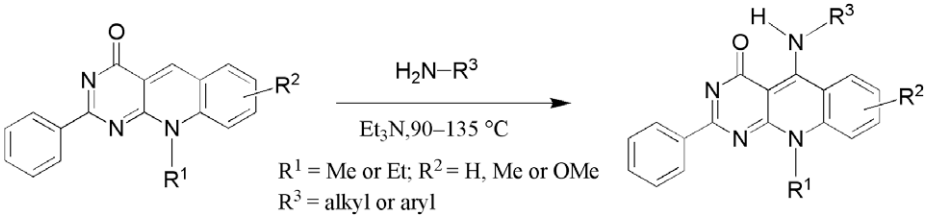
5'-Triphosphocytidilyl(3'-phospho-5')cytidine. The possible sites of ribose-phosphate backbone and heterocyclic base modifications are indicated

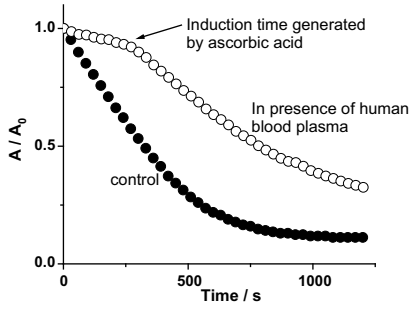




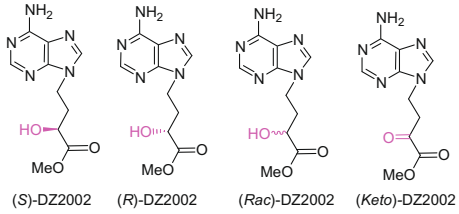


T_m values of dimer/2poly(U) complexes revealed that presumptive (*Sp*)-Ap^{b}A had a much higher and presumptive (*Rp*)-Ap^{b}A a much lower affinity for poly(U) than the natural dimer did, ApA. In contrast, the T_m values of the dimer/2poly(dT) complexes were all similar.

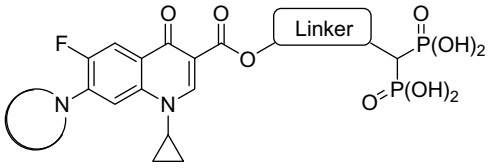




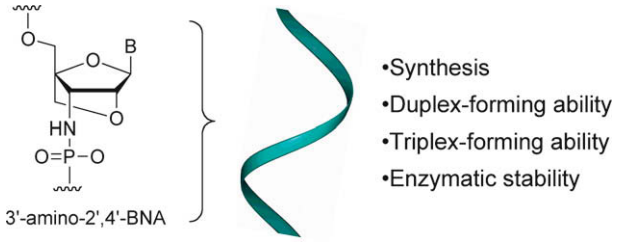
The ORAC methodology using pyrogallol red as probe has been employed to estimate the antioxidant capacity and simultaneously, the concentration of ascorbic acid in human blood plasma and human urine.

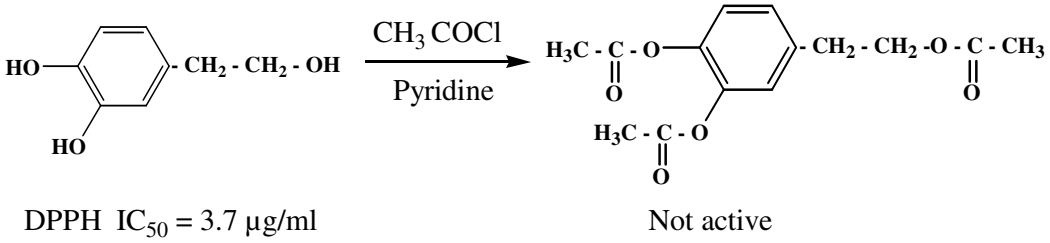


DZ2002 and its stereoisomers were efficiently prepared and evaluated on their potency against SAHase and mixed lymphocyte reaction (MLR). In accordance with respective inhibitory potency of SAHase, the immunosuppressive potency order was demonstrated as (*S*)-DZ2002 > (*Rac*)-DZ2002 > (*R*)-DZ2002 > (*Keto*)-DZ2002. These results indicate that the 2′-chiral center of DZ2002 plays a critical role for their function. Therefore, quality control to prepare optical (*S*)-DZ2002 is necessary for further biological studies.

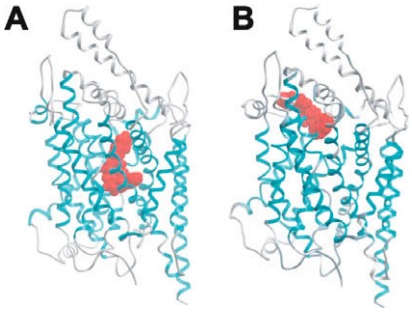


Bisphosphonated fluoroquinolone esters were synthesized and evaluated in vitro. These compounds were found to display strong affinity for bone and their ability to regenerate the parent drug was tailored. The efficacy of a representative class of these prodrugs as prophylactic treatments in a rat model of osteomyelitis is presented.

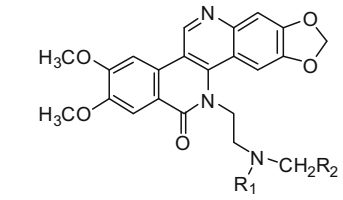




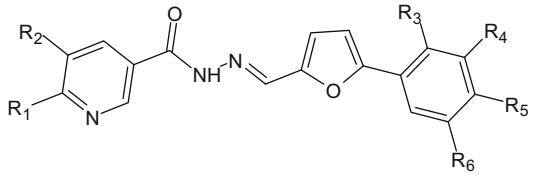
Hydroxytyrosol recovered from Meski cultivar table-olive wastewater processing and its synthesized acetyl analogue, triacetylhydroxytyrosol, were tested for their biological activities.



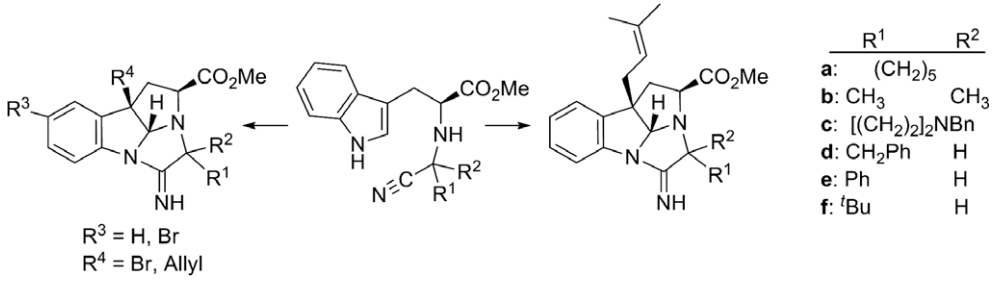
Ligand-binding sites of buspirone analogues (indicated in red) in the 3D model of SERT based on the $LeuT_{Aa}$ X-ray crystal structure. (A) A putative high-affinity binding site. (B) A putative low-affinity binding site.



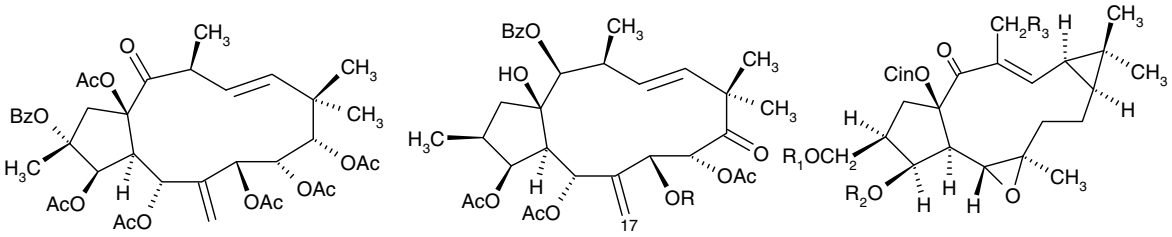
R1 = methyl, ethyl, isopropyl
R2 = cyano, trifluoromethyl, ethynyl, aminocarbonyl

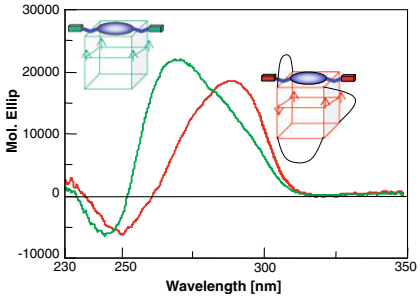


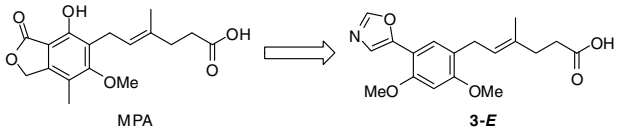
SAR analysis of 86 arylcarboxylic acid hydrazides using atom pair descriptors defines key molecular features important for these compounds to induce macrophage TNF-α production.



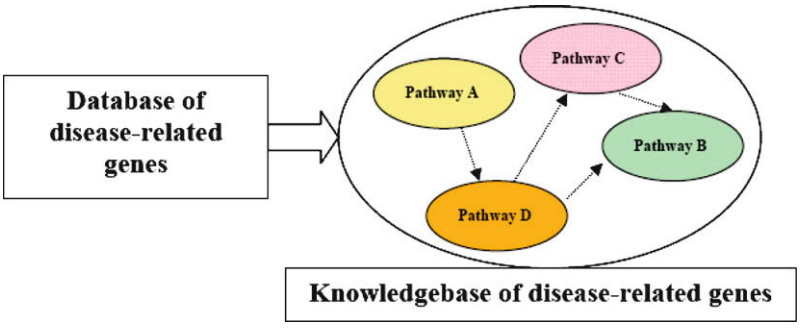
R^3 = H, Br
R^4 = Br, Allyl

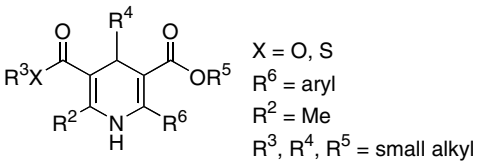


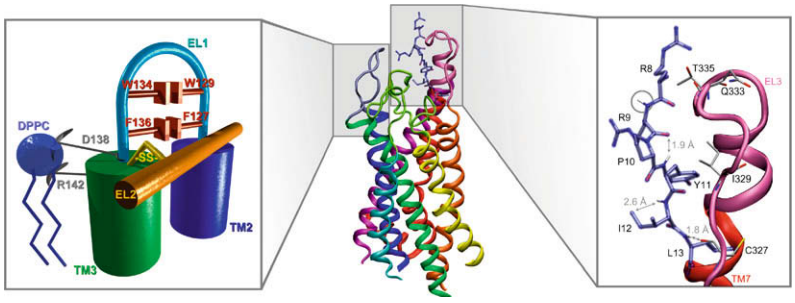


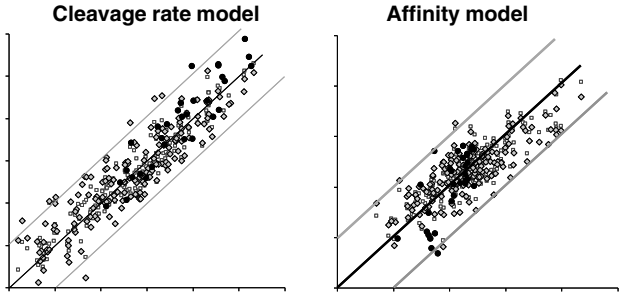


Aiming to circumvent the metabolic liability imposed by mycophenolic acid (MPA), a series of MPA analogs have been designed by combining the structural elements of MPA and known IMPDH inhibitors.

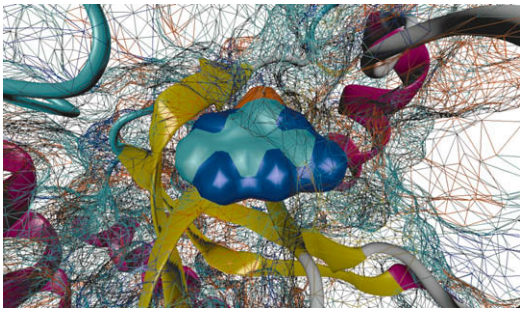


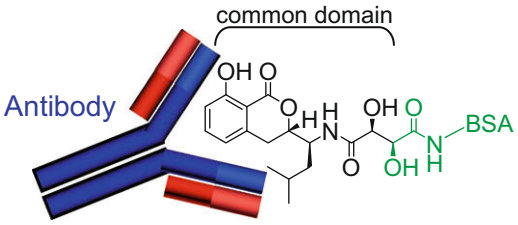






We describe here the use of a new set of empirical scoring functions to assess ligand-binding affinities. This figure illustrates one of the complex used in the test set.





Specific recognition of the common domain of the Amicoumacin family.

*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].

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