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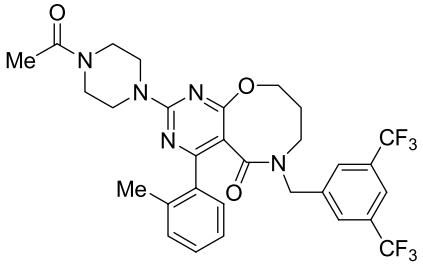
Bioorganic &
Medicinal
Chemistry

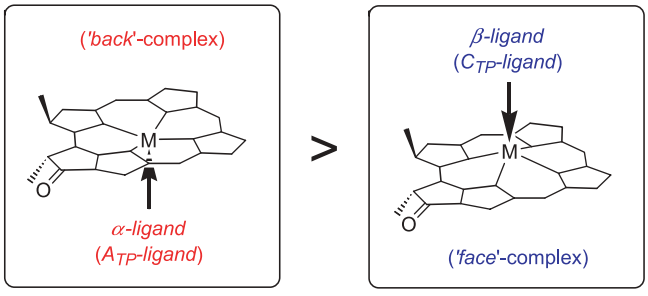
Bioorganic & Medicinal Chemistry Vol. 13, No. 20, 2005

Contents

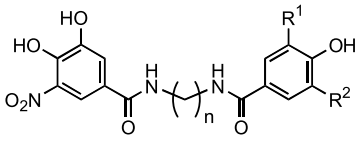
ARTICLES



It was confirmed that in photosynthetic proteins (bacterio)chlorophylls prefer the fifth ligand-binding on the one side of the π-macrocycle.

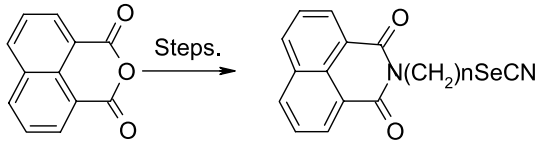


A series of bifunctional compounds were tested in vitro as potential inhibitors of pig liver catechol-*O*-methyltransferase (COMT). The bifunctional compounds were a composite of either two nitrocatechols or one nitrocatechol and one phenol, linked by amide bonds to a spacer unit comprising two to five methylene groups. The unsymmetrical compounds demonstrated strong inhibitory action against COMT with K_i values in the 100 nM range. In comparison, the monofunctional nitrocatechol analogues of these compounds had K_i values that were significantly higher.

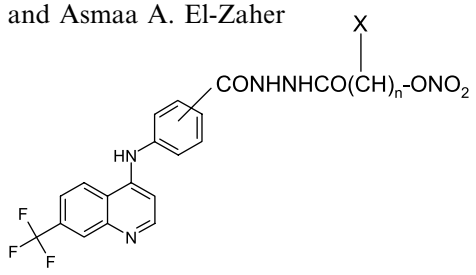


n = 2 - 5
R^1, R^2 = NO_2, OH and H, H

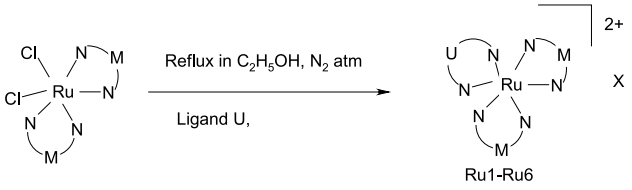
A series of novel organoselenium compounds **4a–d** were synthesized and these compounds were evaluated for their antioxidative activities against DMBA–PMA-induced oxidative stress in Swiss albino mice. The levels of lipid-peroxidation and phase II detoxifying enzymes were measured 15 days after the first DMBA application. Compound **4d** was found to be the most active.



4a, n=2
4b, n=3
4c, n=4
4d, n=5

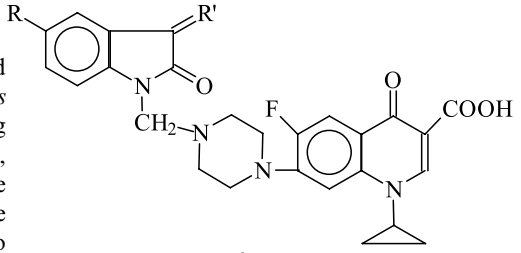


substitution only on position 2 and 4 of the anilino ring
n =1, X = H; n =2, X= CH3; n= 2, X= H



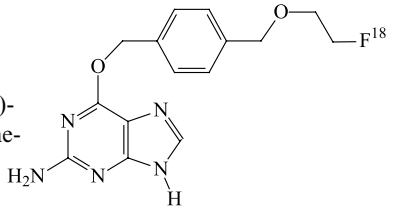
Ru1-Ru6

Where U=tpl, 4-Cl-tpl, 4-MeO-tpl, 4-Me-tpl, 4-NO_2-tpl, pai
M=1,10-phen/2,2'-bpy and X=$(ClO_4)_2$ Ru1-Ru5; X=Cl_2 Ru6



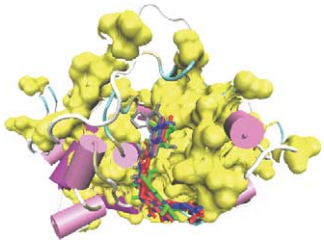
3a-l

Various 7-substituted ciprofloxacin derivatives were synthesized and evaluated for antimycobacterial in vitro and in vivo against *Mycobacterium tuberculosis* and tested the ability of representative compounds to inhibit the supercoiling activity of DNA gyrase from *Mycobacterium smegmatis*. Five compounds (**3a**, **g**–**i**, and **k**) showed most promising activity with MIC_{90} of 0.78 μg/mL and were more potent than parent compound ciprofloxacin. Compound **3h** decreased the bacterial load in spleen tissue with 0.76-log_{10} protections and was considered to be moderately active in reducing bacterial count in spleen.



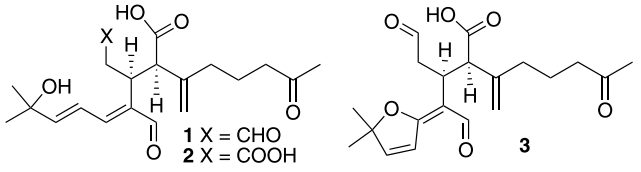
O^6-[^{18}F]FEMBG, [^{18}F]**1**

The synthesis and preliminary biological evaluation of O^6-[4-(2-[^{18}F]fluoroethoxymethyl)-benzyl]guanine, as a novel potential PET probe for the DNA repair protein O^6-alkylguanine-DNA alkyltransferase in cancer chemotherapy, are reported.

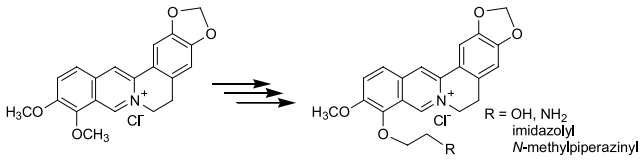


The structure–activity relationship (SAR) and binding mechanism of three biflavones amentoflavone (AMF1), 4‴-methylamentoflavone (AMF2) and 7′,4‴-dimethylamentoflavone (AMF3) were elucidated by density functional theory (DFT) method as well as FlexX methods.

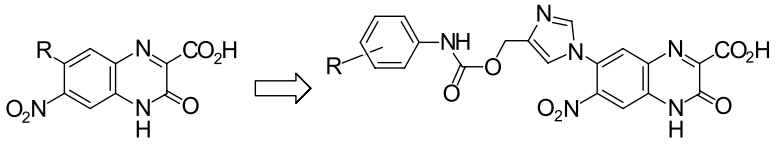
A thermochemical method, a rather simple experimental technique, is used to determine the enthalpy of the formation of 3,6-dibutanoic-1,2,4,5-tetroxane. The study is complemented with suitable theoretical calculations at the semiempirical and ab initio levels. A particular satisfactory agreement between both ways is found for the ab initio calculation at the 6-311G basis set level. Some possible extensions of the present procedure are pointed out.



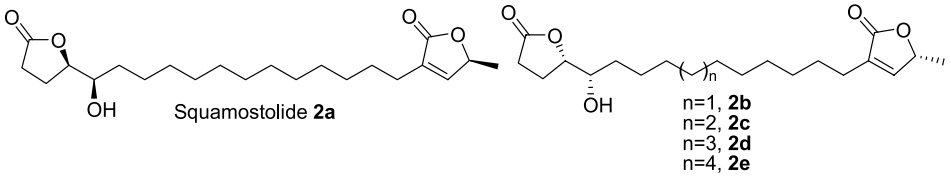
New diterpenoids from a sea anemone of the order Actiara are active against Cdc25B phosphate.



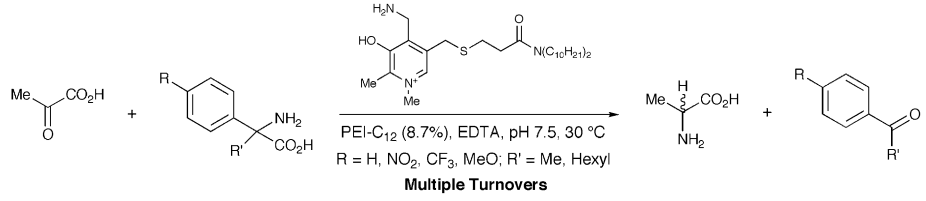
Four new monomodified berberine derivatives have been synthesized in moderate to good yields and have been shown to bind strongly to calf-thymus DNA, presumably via an intercalation mechanism.



We describe the design, synthesis, and biological properties of a novel series of 6-nitro-3-oxoquinoxaline-2-carboxylic acids which bear a substituted phenyl group through a urethane linkage at the 7 position.



Squamostolide and its related analogs were designed and synthesized for biological evaluation. All these compounds were tested for growth inhibition activities against human tumor cell lines, in which one of the compounds showed the most potent cytotoxicity among these derivatives against a full panel of 60 human cancer cell lines. The same compound also showed G2/M phase arrest and a slightly apoptotic effect during flow cytometric analysis.



OTHER CONTENTS

*Corresponding author
ⓘ+ Supplementary data available via ScienceDirect

COVER

2005: Human liver glycogen phosphorylase A (HLGPa) is an attractive target enzyme for discovering anti-type 2 diabetes drugs. This picture shows the interaction model for a series of indole-2-carboxamides to HLGPa derived from molecular docking simulations [Liu, G.; Zhang, Z.; Luo, X.; Shen, J.; Liu, H.; Shen, X.; Chen, K.; Jiang, H. *Bioorg. Med. Chem.* **2004**, *12*, 4147–4157].

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ISSN 0968-0896