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Chemistry

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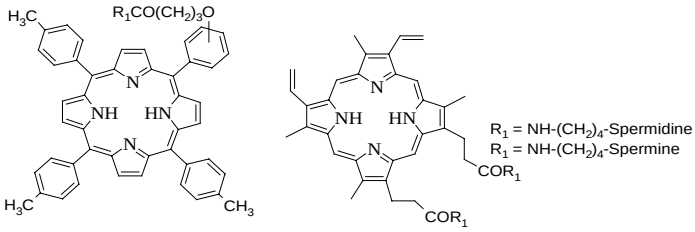
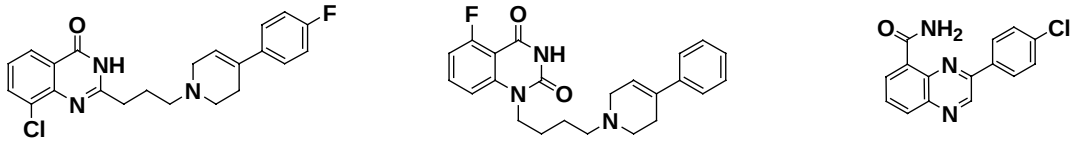
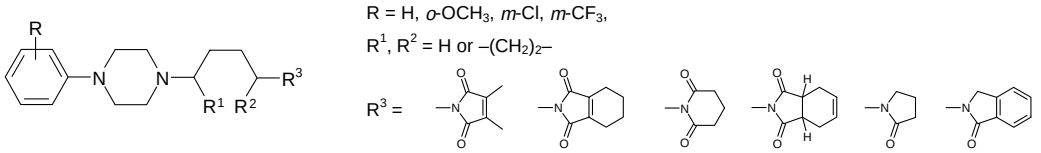
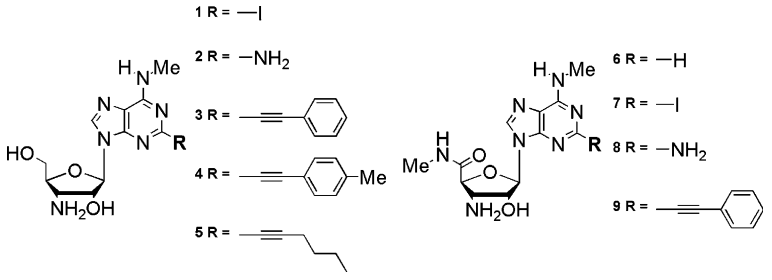
Contents

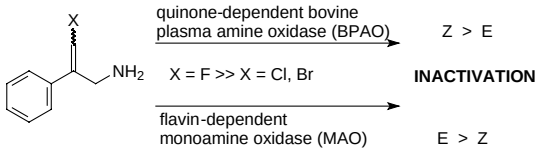
ARTICLES





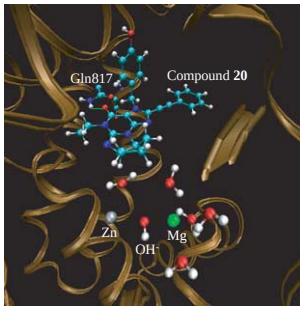




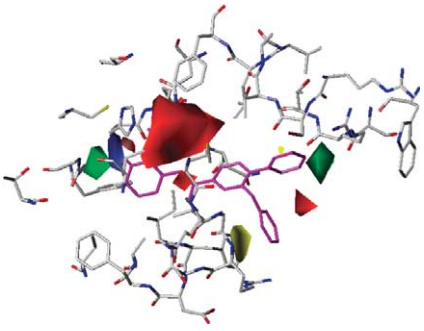


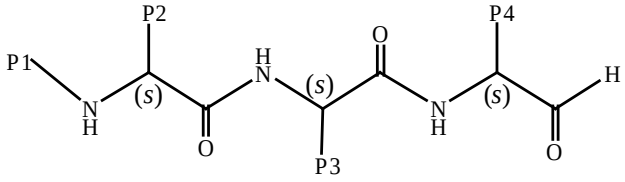
Two-dimensional topological descriptors and three-dimensional pharmacophore hypothesis were used to investigate and compare different classes of dopamine antagonists. Molconn-Z and BCUT topological descriptors were employed to develop a classification model for 1475 dopamine antagonists from MDDR database. The combining both of classification using topological descriptors and functional feature hypotheses could be a useful tool to predict selective antagonists.

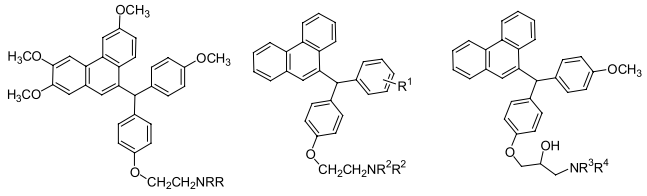
Understanding the structure–activity and structure–selectivity correlation of cyclic guanine derivatives as phosphodiesterase-5 inhibitors by molecular docking, CoMFA and CoMSIA analyses



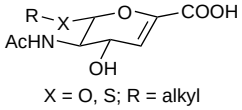
We performed CoMFA and CoMSIA based on the docking conformations of benzoylaminobenzoic acid derivatives into the active site of FabH enzyme. Mapping the 3D QSAR models into the active site of FabH provides a useful perspective for the active site of FabH.







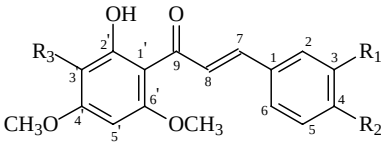
The biosynthesis of [^{13}C]glycogen from [^{13}C]pyruvate via the gluconeogenic pathway is monitored in surgically removed perfused livers by ^{13}C NMR. The rapid breakdown of [^{13}C]glycogen (glycogenolysis) following the addition of 50 pM exogenous glucagon is then monitored in real time using this technique. The concentration-dependent inhibition of glucagon-mediated glycogenolysis is demonstrated for both the peptidyl glucagon antagonist **1** and structurally diverse synthetic glucagon antagonists **2**–**7**. Perfused livers were obtained from a transgenic mouse strain that exclusively expresses the functional human glucagon receptor, conferring human relevance to the activity observed with these antagonists.



X = O, S; R = alkyl

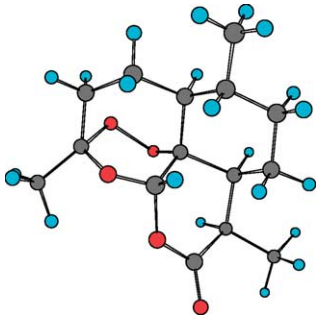
Glucuronide-Based Neu5Ac2en Mimetics

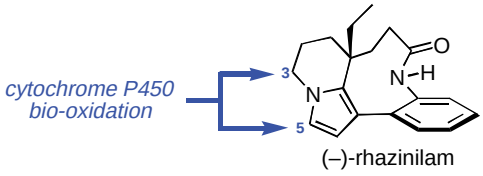
The synthesis and biological evaluation of a series of glucuronide-based Neu5Ac2en mimetics are presented.



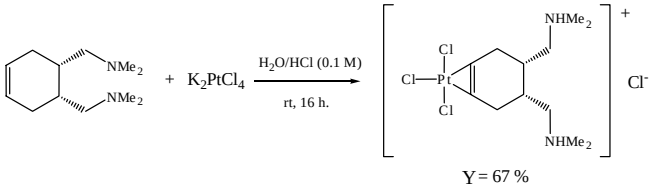
10 R_1= NO_2, R_2= H, R_3= H
12 R_1= H, R_2= F, R_3= H
19 R_1= NO_2, R_2= H, R_3= Br

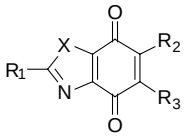
The DFT B3LYP method was employed to calculate the mechanism for the reductive decomposition of artemisinin. A set of radical anions and neutral species supposed to be relevant in the mechanism of action of artemisinin were calculated. Primary and secondary radicals centered on C_4 were found as the most stable species.



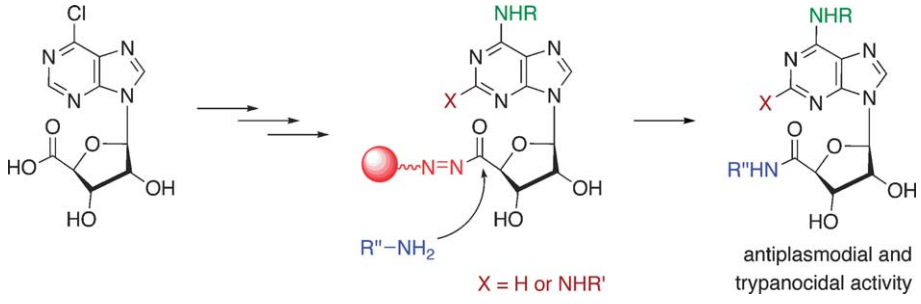


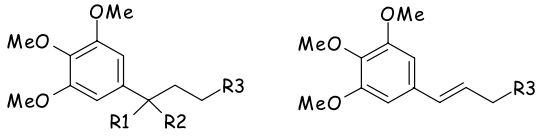
The ability of this new platinum complex to modiufy secondary DNA structure was explored by circular dichroism (CD). Electrophoretic mobility showed changes in tertiary DNA structure, and atomic force microscopy (AFM) revealed morphological changes of plasmid DNA (pBR322). A lower cytotoxicity but also a lower resistant factor was observed for the here described organometallic compound than for cisplatin, against A2780 and A2780cisR ovarian cancer cell lines.



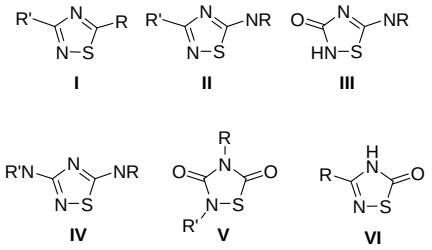


Quantitative structure–activity relationship studies for antifungal 1,4-quinone derivatives using comparative molecular field analysis (CoMFA) and recursive partitioning (RP) analysis are reported.





Several novel hypolipidemic α-asarones have been synthesized and 3D QSAR has been modeled.



OTHER CONTENTS

*Corresponding author
ⓘ+ Supplementary data available via ScienceDirect

COVER

2006: The cover figure shows a synthetic multifunctional pore that is composed of rigid-rod staves (para-octiphenyls, tan) and beta-sheet hoops (arrows) and can be activated with external ligands (fullerenes, golden spheres) and closed with internal blockers (alpha-helix, red ribbon) [Gorteau, V.; Bollot, G.; Mareda, J.; Pasini, D.; Tran, D.-H.; Lazar, A. N.; Coleman, A. W.; Sakai, N.; Matile, S. *Bioorg. Med. Chem.* **2005**, *13*, 5171–5180].

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