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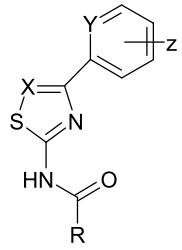
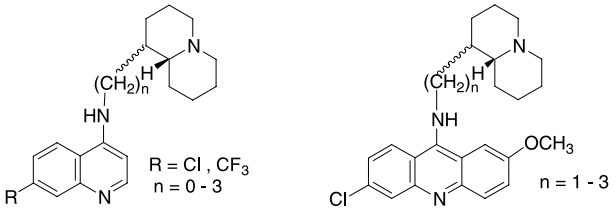
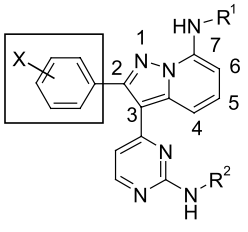
Contents

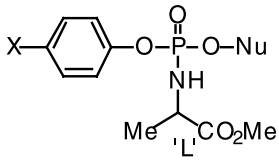
ARTICLES



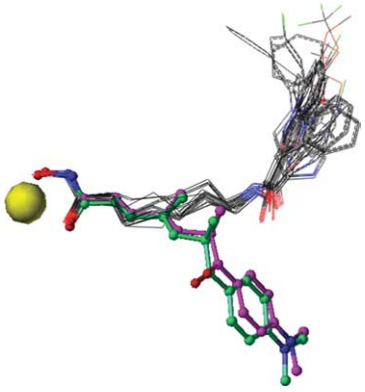
A QSAR study was carried out on thiazole and thiadiazole analogues on adenosine A_1 and A_3 receptors.



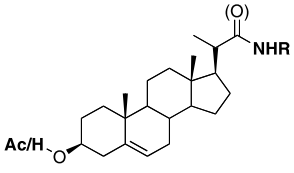


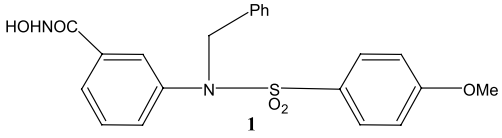


Changing the nucleoside group of a series of phosphoramidate derivatives affects the enzyme mediated hydrolysis rate of the compounds. d4T and AZT-substituted analogs were activated by enzymes such as lipases, esterases, and proteases. On the other hand, 3dT-substituted derivatives were comparatively less prone to hydrolysis under similar experimental conditions. Also, we show that d4T derivatives were more active compared to the AZT and 3dT derivatives.



Docking simulations and 3D-QSAR analyses were conducted on a series of indole amide analogues as potent HDAC inhibitors. Based on the docking results, a novel binding mode in the human HDAC1 catalytic core is presented, and enzyme/inhibitor interactions and discussed. Based on the binding mode, predictive 3D-QSAR models were established.





1

A QSAR study has been made on four different series of anthranilic acid-based matrix metalloproteinase inhibitors as represented by **1** to find that the sulfonamide group plays a very important role in the inhibition activity of these inhibitors.

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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