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Bioorganic & Medicinal Chemistry Vol. 12, No. 2, 2004

Bioorganic & Medicinal Chemistry

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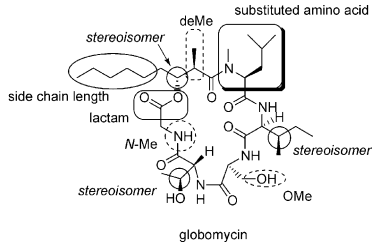
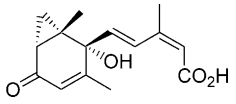
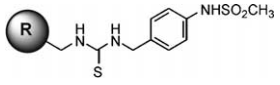
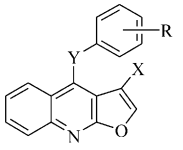




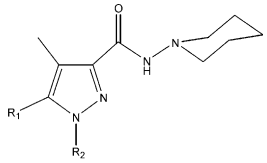
The highly potent and long-lasting activity of 5′α,8′-cycloabscisic acid is caused by resistance to abscisic acid 8′-hydroxylase, and it is partially metabolized to the glucose conjugate.



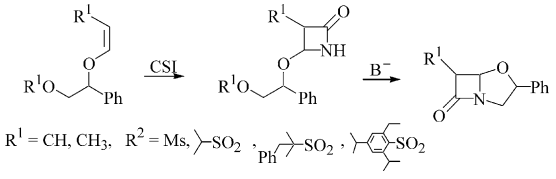
Analysis of structure–activity relationships in the 'C-Region' of *N*-[4-(methylsulfonylamino)benzyl]thiourea analogues is described as vanilloid receptor antagonists.



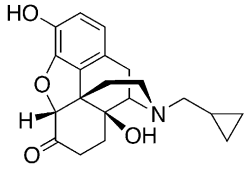
X = H, Cl
Y = O, NH
R = CHO, COMe, C(=NOH)Me, C(=NOMe)Me, CH=CHCOMe, CH_2CH_2COMe, $CH_2CH_2CH(OH)Me$



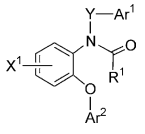
R_1 = 4-chlorophenyl, R_2 = cyclopentyl
R_1 = 4-chlorophenyl, R_2 = cyclohexyl
R_1 = 4-chlorophenyl, R_2 = cycloheptyl
R_1 = 4-chlorophenyl, R_2 =3-methylcyclohexyl
R_1 = 4-chlorophenyl, R_2 = 4-methylcyclohexyl
R_1 = 4-chlorophenyl, R_2 = 4-methylphenyl
R_1 = cyclohexyl, R_2 = 4-chlorophenyl
R_1 = cycloheptyl, R_2 = 4-chlorophenyl
R_1 = cyclohexyl, R_2 = cyclohexyl



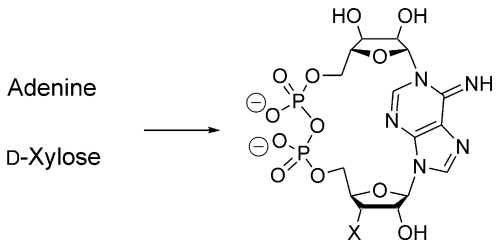
R^1 = CH, CH_3, R^2 = Ms,

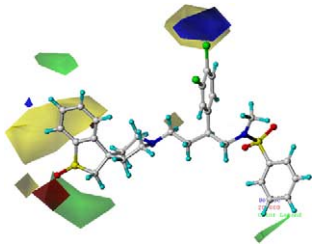


Naltrexone

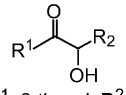


The design, synthesis and structure–affinity relationships of aryloxyanilide derivatives as novel peripheral benzodiazepine receptor ligands are described.





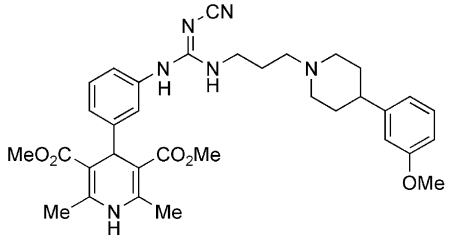
3D-QSAR models have been built for a series of piperidine-based CCR5 antagonists using CoMFA and CoMSIA approaches. The derived 3D-QSAR models showed predictive capabilities and a high level of internal consistency. The resulting contour maps can be used to identify structural features relevant to binding affinity, and can aid in the future development of potential anti-HIV agents.



1: R^1=2-thenyl, R^2=2-thenyl
2: R^1=2-furyl, R^2=2-furyl
3: R^1=C_6H_5, R^2=H
4: R^1=CH_3, R^2=H

A variety of hydroxyketones and diketones were evaluated for their effect on the jack bean urease. 2,2-Thenoin (**1**), furoin (**2**), 2-hydroxy-1-phenylethanone (**3**) and acetol (**4**) showed potent inhibitory activity against the enzyme, comparable with hydroxyurea. However, the corresponding-diketones exhibited little or no ability to inhibit the urease.

Structure–activity studies around the urea linkage in BMS-193885 identified the cyanoguanidine moiety (as represented by **20**) as an effective urea replacement in a series of dihydropyridine NPY Y_1 receptor antagonists.



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*Corresponding author

COVER

2004: Overlaps of the eight known aldolase alpha-beta barrels in 2-Deoxyribose-5-phosphate aldolase (DERA). Ribbon model for DERA is shown in green, with key Lys residues capable of Schiff base formation highlighted in stick figure. Reactive Lys167 is shown in yellow. DeSantis, G.; Liu, J.; Clark, D. P.; Heine, A.; Wilson, I. A.; and Wong, C.-H. *Bioorganic & Medical Chemistry* **2003**, *11*, 43–52.

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