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Bioorganic & Medicinal Chemistry

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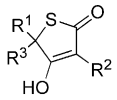
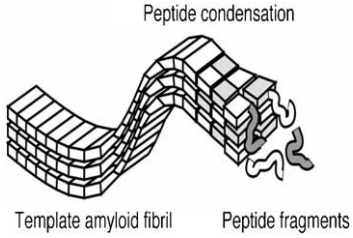
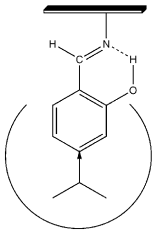
ARTICLES

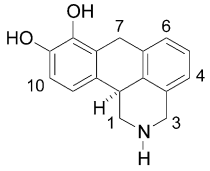




A peptide self-replicating system based on the β-structure of the amyloid-like fibril was designed and constructed.

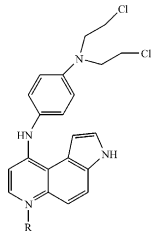
A group of 18 benzaldehyde derivatives was characterized as a family of mixed type inhibitors on the oxidation of L-3, 4-dihydroxyphenylalanine (L-DOPA) catalyzed by *Sacrophaga neobelliaria* phenoloxidase (PO), presumably by forming a Schiff base with a primary amino group of the enzyme. Inhibition constants and IC_{50} were determined. Cuminaldehyde was the most active inhibitor with an IC_{50} of 0.0067 mM. Vanillin was the least active inhibitor with an IC_{50} of 38 mM. It was shown that hydrophobicity of the substituent at the para position of the aldehyde group played major role on inhibition activity: one unit increase in Hansch–Fujita π value of the substituent led to about 4.5 [95% confidence interval is (7.9, 2.6)] -fold increase on IC_{50}. It presumably helps fitting the formed Schiff base to the hydrophobic protein pocket (∪). Electron-donating effect (↑) of the substituent at the *para* position of the aldehyde group was less important than hydrophobicity. Hydroxyl group at the ortho position of the aldehyde group contributed to higher inhibition activity, presumably by forming a quasi-six-membered ring with the unshared pair of electrons on the nitrogen atom of the amino group through intramolecular hydrogen bonding.

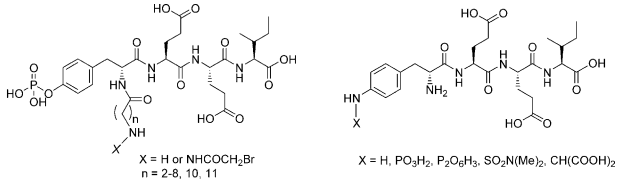


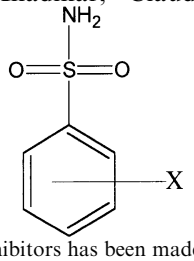


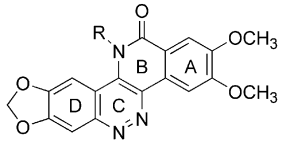
(*S*)-8,9-Dihydroxy-2,3,7,11b-tetrahydro-1H-dibenz[*de,h*]isoquinoline

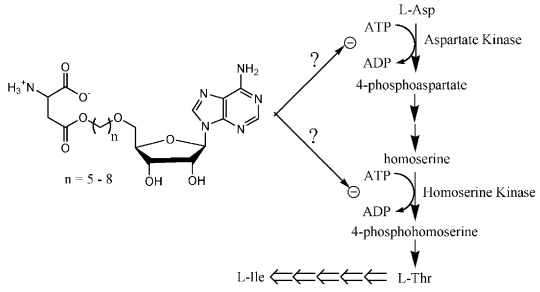
DINAPSOLINE



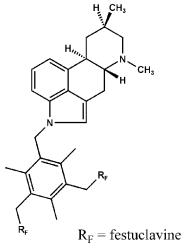


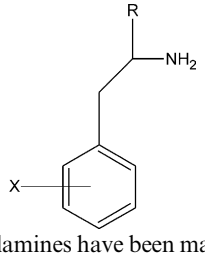






Starting from three monomeric ergolines (terguride, festuclavine, pergolide) *N,N′*-spacer-linked oligomeric derivatives were prepared and evaluated for their in vitro activity against *Plasmodium falciparum*.





QSAR studies on a series of psychotomimetic phenylalkylamines have been made using a combination of MTD method and topological methodology. The topological indices used being a pool of distance-based topological indices. The regression analysis have shown that excellent results are obtained in multiparametric model containing MTD parameters, topological indices in that quantum chemical parameters has to be introduced. The predictive power of the proposed model is discussed on the basis if cross validation parameters.

OTHER CONTENTS

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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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