NLM AIDSLINE

4-hydroxy-5,6-dihydro-2H-pyran-2-ones.3. Bicyclic and hetero-aromatic ring systems as 3-position scaffolds to bind to S1' and S2' of the HIV-1 protease enzyme.

Ellsworth EL; Domagala J; Prasad JV; Hagen S; Ferguson D; Holler T; Hupe

December 30, 1999

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5,6-Dihydro-2H-pyran-2-ones are potent inhibitors of HIV-1 protease, which bind to the S1, S2, S1', and S2' pockets and have a unique binding mode with the catalytic aspartyl groups and the flap region of the enzyme. Efforts to explore 3-position heterocyclic scaffolds that bind to the S1' and S2' pockets have provided a number of selected analogs that display high HIV-1 protease inhibitory activity. reserved.

JOURNAL ARTICLE Binding Sites Computer Simulation Drug Design Hydrocarbons, Aromatic/CHEMISTRY Hydrogen-Ion Concentration HIV Protease/CHEMISTRY/*METABOLISM HIV Protease Inhibitors/*CHEMISTRY/*METABOLISM/PHARMACOLOGY Inhibitory Concentration 50 Models, Molecular Molecular Structure Pyrones/*CHEMICAL SYNTHESIS/METABOLISM/*PHARMACOLOGY Software Structure-Activity Relationship Sugar Alcohols/METABOLISM Valine/ANALOGS & DERIVATIVES/METABOLISM

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