

Oral Session IV

Respiratory and Hepatitis Infections

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The Development of an Antirhinovirus Model based on Small Molecule Conformations. G.D. Diana, D.J. Aldous, A.M. Treasurywala, E.P. Jaeger and D.C. Pevear Sterling Winthrop Pharmaceuticals Research Division, Collegeville, PA. 19426, USA

The use of rational drug design for the discovery of broad spectrum antirhinovirus agents is stifled by the structural diversity of the >100 serotypes comprising this group of viruses.

We have previously presented a model based on X-ray crystallography of compounds bound to HRV-14, which qualitatively describes properties of molecules contributing to activity against this serotype. We have now explored the possibility of designing a model based on a conformational analysis of the isolated small molecules, coupled with an algorithmic superimposition method, exclusive of X-ray crystallography. A comparison is made of the results of this approach for HRV-14 and -1A, with the corresponding model based on X-ray data.