Research in Pharmaceutical Sciences, 2012;7(5)
School of Pharmacy and Pharmaceutical Sciences
Isfahan University of Medical Sciences

Conformational analysis of novel anti HIV 1,2,3,4-tetrahydropyrimidones

A. Fassihi, L. Saghaie, S. Rafi'i pur alavi*, M. Mohammadpour

Department of Medicinal Chemistry, Faculty of Pharmacy, Isfahan University of Medical Sciences, Isfahan, Iran

Background and Aims: Despite the success of highly active antiretroviral therapy, AIDS still remains as one of the most important world health problems. Also, toxicity of current available drugs and multidrug resistant strains is a problem. In a recent study some novel Biginelli derivatives of 1,2,3,4-tetrahydropyrimidine-2-one were evaluated as potential anti-HIV(human immunodeficiency virus). It was proved that 1,2,3,4-tetrahydropyrimidine-2-ones contained substituted phenyl group at C-4, and arylamide group at C-5 of pyrimidine ring posses more anti-HIV-1 effects. Presented study was designed to conformational analysis about some 1,2,3,4-tetrahydropyrimidine-2-ones which were Synthesized and evaluated as potential anti-HIV agants.
Methods: 39 tetrahydropyrimidinone compounds were optimized by using of the molecular mechanics MM+ and semi empirical PM3 method in Hyperchem7.0 software and DFT (Density Functional Theory, B3LYP) calculations with 6-31G* basis set by using Gaussian98 program.
Results: The Hyperchem program and the GaussView 5.0.8 program are used to analysis the structural characteristics included bond lengths, angles and dihedrals. Results based on DFT were somewhat similar to those obtained using PM3 and MM+ optimization methods.
Conclusion: Analysis of the optimized structures of Tetrahydropyrimidines was shown that the six-memberd ring adopts a Twisted Boat conformation. Analyze of optimum values of the proposed dihedrals reflect the orientations of the C-4 aryl ring and C-5 carbonyl groups respect to the heterocyclic ring, shown that the aryl and Tetrahydropyrimidine rings are not Perpendicular to each other. Also, analysis of dihedrals was shown that in all cases the C-5 carbonyl group forms the coplanar conformation with respect to the Tetrahydropyrimidines boat plane.

Keywords: Conformational Analysis; Tetrahydropyrimidinones; Semiempirical; DFT