

Molecular modeling study of leflunomide and its active metabolite analogues.

Autorzy

Jarosław Panek

Aneta Jezierska

Krzysztof Mierzwicki

Zdzisław Latajka

Aleksander Koll

Rok wydania

2005

Czasopismo

Journal of Chemical
Information and Modeling

Numer woluminu

45

Strony

39-48

DOI

10.1021/ci049754d

Kolekcja

Naukowa

Język

Angielski

Typ publikacji

Artykuł

Streszczenie

Leflunomide is known as a compound with various sorts of biological activity, which found a practical application in medicine. Search of current literature revealed an active metabolite of Leflunomide together with its eight analogues synthesized as protein tyrosine kinase inhibitors with potential anticancer activity. Accurate description of the molecular structure of these compounds is valuable. The detailed geometrical parameters description was performed using DFT theory. The conformational analysis and intramolecular proton transfer were considered. Using the most stable conformation the detailed electronic structure description was obtained by analysis of electron density and electrostatic potential distribution in the first step. Next, the topological analysis of the electron density by AIM method and electron localization function (ELF) theories supplemented this study. The AIM and ELF theories were applied to study the topology of the molecules, atomic charges distribution, and details of bonding. The theoretical investigations were performed in the gas phase and by using SCRF/PCM solvent reaction field. In this study the molecular modeling results for Leflunomide and the analogues of its active metabolite are presented.

Adres publiczny

<http://dx.doi.org/10.1021/ci049754d>

Strona internetowa wydawcy

<https://www.acs.org/content/acs/en.html>