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Computational study on 3D structure of L-aspartic acid and L-glutamic acid: molecular descriptors and properties

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Abstract. The aim of this work is to provide a comprehensive and complex analysis of molecular descriptors and properties of two similar amino acids, L-Aspartic acid and L-Glutamic acid, using a software tool for calculations and properties predictions. As amino acids are model compounds for predicting the physical-chemical properties and behavior of biological, larger molecules as peptides or proteins, researches were focused on providing accurate mechanical calculations using: molecular/mechanical methods. Our study aims to initiate a linear scaling approach, by dividing a large system into small subsystems and performing the calculations for each, individually, then, embedding and correcting the information globally. The calculations were performed on the 3D structure of the studied amino acids that were first generated, as CPK model, and optimized by energy minimization. A comparative assay on their topological, molecular descriptors and properties was conducted, in vacuum and in water, using the Hartree-Fock model and second-order Møller–Plesset perturbation theory MP2 for predicting structure, energy and property calculations with Spartan'14 software. Values of molecular properties such as area, volume, polar surface area, polarizability, ovality, logP, dipole moment, HOMO-LUMO gap, distances and angles between atoms, were obtained. The results have been interpreted in terms of electronic effects of side chain groups, molecular deformability, steric factors and reactivity. This approach can be extended to other amino acids in order to predict protein-ligand interactions, important aspects in drug design studies and protein engineering.

Keywords: amino acids, computational molecular descriptors

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