ANALYSIS OF MOLECULAR INTERACTIONS OF THE ENERGY STRUCTURE OF LIPOIC ACID

Jumabaev F.R.
Abdulloeva M.G.
Sharipov A.T.
Tashkent Pharmaceutical Institute, Uzbekistan
E-mail: farhodjumaboyev1@gmail.com. Tel . +998998938750
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Relevance: Lipoic acid (LA) is a sulfur-containing organic compound with powerful antioxidant properties, neutralizing free radicals and reducing oxidative stress. This helps prevent diseases such as skin aging, neurodegenerative disorders, cancer, and cardiovascular diseases. Lipoic acid also activates liver enzymes, which helps in detoxification, removal of toxins and heavy metals, and maintaining liver health. Due to the improvement of the body's metabolism, LA is used in medicine as a drug for the treatment of diabetes and cancer. Its antioxidant activity also helps protect cells from damage caused by oxidative stress, slowing down the aging process, improving tissue regeneration, and maintaining cellular health at the molecular level. Lipoic acid, therefore, becomes not only an important element in the therapeutic approach, but also a promising means for the prevention of many diseases associated with metabolic disorders and aging of the body.

The purpose of the study is to analyze molecular energy, which helps to understand how molecules interact in a structure, what forces influence their behavior, and how these interactions affect their physicochemical properties.

Materials and methods: *CrystalExplorer* 17.5 software was used to analyze the energy structure.

Results: In this work, the molecular structure of lipoic acid was studied using CrystalExplorer 17.5. Energy structure analysis is used to investigate the interaction pattern and pairwise intermolecular bonds. The total energy calculations take into account parameters such as electrostatic, polarization, dispersion, and exchange-repulsion energies. Using the B3LYP/6-31G(d,p) basis set, the total interaction energy is determined by creating a cluster with a radius of 3.8 Å around the selected molecule using CrystalExplorer 17.5. The total interaction energy is calculated from the interactions of molecular pairs, which are divided into four energy components: electrostatic (E_{ele}), polarization (E_{pol}), dispersion (E_{dis}), and exchange-repulsion (E_{er}). Each of these components is multiplied by the corresponding scaling factor: 1.057 for electrostatics, 0.740 for polarization, 0.871 for dispersion, and 0.618 for exchange-repulsion. In this analytical structure, the cylindrical shape represents the intensity of interaction energies such as the Coulomb energy (red), dispersion energy (green), and total energy (blue). Analysis of the energy structure shows that the total energy (-139.4 kJ/mol) is the major component, accounting for the majority of the dispersion energy (-133.9 kJ/mol). Other energy components calculated include electrostatic energy (-46.1 kJ/mol), polarization energy (-20.8 kJ/mol), and exchange-repulsion energy (66.7 kJ/mol).

Conclusions: Energy structure analysis shows that the total interaction energy of molecules is mainly determined by dispersion energy. Electrostatic and polarization energies have a smaller contribution, and the exchange-repulsion energy, with a positive value, reflects the repulsive forces between molecules. These data are useful for understanding molecular interactions and their influence on the physicochemical properties of materials.