THE METHOD OF ESTIMATION ANTIOXIDANT ACTIVITY OF THE COMPOUNDS ACCORDING TO QUANTUM-CHEMICAL PARAMETERS

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The evaluation of antioxidant activity (AOA) of substances is an urgent task for chemistry, biology, medicine. The experimental methods used for this purpose are very diverse, however, it is worth noting that the range of results is wide and they are not always comparable. Therefore, the researcher is faced with the task of choosing the method of evaluation of AOA. An alternative to the experiment may be a method based on the results of quantum chemical calculations of the electronic structure of antioxidant molecules. The calculation has been implemented on the example of chemical structures, in which AOA was acknowledged (trolox, Quercitin, Gallic and ascorbic acids, etc.) The energy characteristics of the molecules were determined by method of DFT B3LYP/6-31G(d,p) by program [1] with the full energy optimization and the calculation of normal oscillation frequencies. The calculated energies of the highest the occupied (E_{homo}) and the lowest the vacant (E_{lvmo}) molecular orbitals, electronegativity (χ), "chemical hardness" (η) and electrophilicity (ω) play an important role in the chemical stability of the molecule and allows to make conclusion about the possibility of sending or receiving an electron. The indices of the reaction ability of antioxidants were calculated. The relationship of the reaction ability of antioxidants from energy of the lower vacant molecular orbital is constructed according to these indices. The linear equations with good correlation coefficients describes obtained relationships.

For example, for electronegativity such relationship has the form:

χ = -13.453 Enuma+64.691; (R2=0.8672)

The indicators of antioxidant activity of compounds, which need to estimate, compare with indicators of the selected standard antioxidant (reference), according to the results of quantum-chemical calculations of the value (E_{lvmo}). The graphical comparison has the greatest usability and visibility. The compounds with indices of reaction ability on the graph relationship χ, η, ω from (E_{lvmo}) which can see on the left of the standard show weak antioxidant properties, on the right of the standard are strong antioxidant properties. The difference in indexes can serve as criterion of quantitative estimation of relative activity of antioxidants.

References

1. Granovsky A.A. GAMESS v.7.1. (http: //classic.chem.msu.su /gran/ games /index.html)