Optico-physical technologies of diagnostics of the biological activity of gydroxyl-containing aromatic compounds

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System researches of optico-physical properties and the quantum-chemistry analysis of the electronic structure of biologically active organic compounds today are the actual problems of modern Life Sciences.

New types of molecules of phenols class and their analogues, benzaldehydes, and aromatic acids, which show high effect in suppressing viruses of herpes, influenza, HIV-infection, and of some other diseases, are synthesized.

Empirical correlations between the electronic structure, FTIR spectra, luminescent properties, and the pharmacological action of biologically active oxygen-containing molecules are revealed. Specific spectroscopic signs of the biological efficiency of oxygen-containing molecules are found from experiment. Formation of intramolecular hydrogen bonds in molecules under study is accompanied by the enhancement of the antivirus activity.

Quantum-chemistry calculations of the electronic structure of biomolecules have shown that there exists a direct relationship between the growth of the electronic density (-) of oxygen atoms of the hydroxyl O-H group and the intramolecular hydrogen O-H···O=C bonding, and, as a consequence, the enhancement of the antivirus efficiency of investigated molecules.

A high reliability of the system spectroscopic analysis and quantum-chemistry calculations of biomolecules used for testing and forecasting the pharmacological efficiency of new medical products is demonstrated.

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