drinking water [1]. The conventional wastewater treatment equipment is not designed to remove the residual pharmaceutical pollutants [2]. Heterogeneous photocatalysis is considered to be one of the promising methods to remove the pharmaceuticals from water [1, 2]. However, the performance of the existing heterogeneous photocata-lysts is not sufficient. Therefore they are not applicable for industrial-scale implementation.

The aim of this study was to find the appropriate substance to simulate the pharmaceuitical waste in experiments on photocatalytic degradation with the help of ZnO-based photocatalysts. Several drags were chosen as a potential model substance. As the photocatalitic activity of catalysts is evaluated by measuring the concentration of a drag, the UV-Vis spectra of potential model substances were investigated (Fig. 1).

As it is clearly seen in Figure 1, caffeine has a well-pronounced peak at around 270 nm. Caffeine was chosen as a model substance in further experiments. Figure 2 shows the calibration curve of caffeine. The linear range of the absorbance-concentration relationship was found to be between 50.0 mg/l and 400 mg/l.

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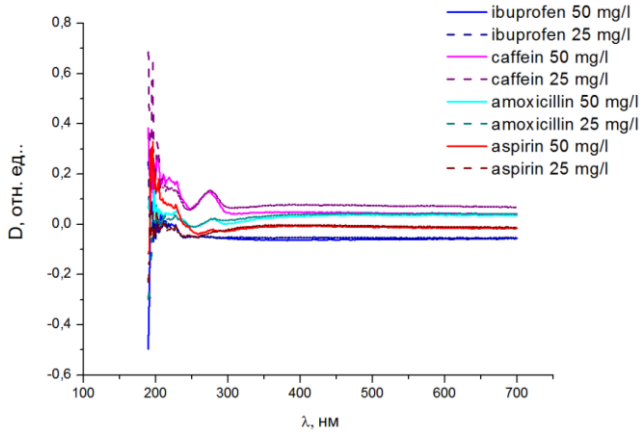

Fig. 1. – UV-VIS spectra of caffeine, ibuprofen, aspirin, amoxicillin

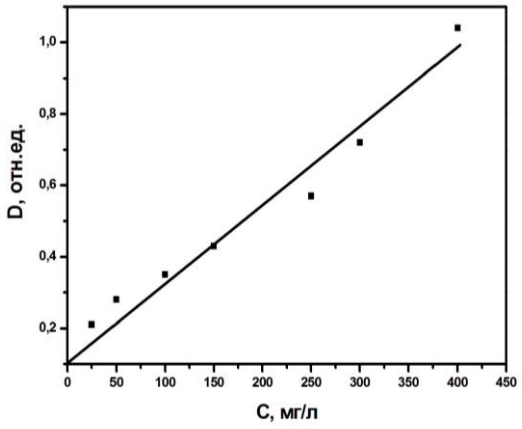

Fig. 2. – Calibration curve of caffeine

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QUANTUM-CHEMICAL CALCULATION OF ANTIOXIDANT PROPERTIES OF SULFORAPHANE

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In the present study geometry optimization and electronic structure of the molecule sulforaphane have been carried out using the Density Functional Theory (DFT) in the solvent water for the first time.

Keywords: antioxidant activity, sulforaphane, electronic spectrum.

The method of molecular mechanics (MM+) of HyperChem 08 software package was chosen to calculate the starting geometry of the sulforaphane molecule. The starting geometry of the molecule was further optimized in the solvent (water) by the semi-empirical PM7 method of the Gaussian 09W software package until the global min-imum of the total energy of the studied systems was reached. To determine the global energy

minimum and the most stable conformers, all stationary points on the surface of the potential energy of molecules were found and analyzed. The PM7 method is used to find optimized geometric configurations, total energy of molecules, electronic properties and enthalpy of substance formation [1]. Gauss View 06 and ChemCraft 1.7 were used to visualize the results.

Complete quantum-chemical modeling of equilibrium geometry and electronic structure of sulforaphane molecule

Full optimization and calculation of the electronic structure were carried out by the nonempirical method of density functional theory (DFT/B3LYP) in the basis 6-31G*. This method is used to calculate optimized geometries, electron absorption spectra, values of total energy and heat of formation and is used by us to calculate the electron absorption spectrum of a sulforaphane molecule [2]. The electron spectrum of the sulforaphane molecule is calcu-lated for 20 single-electron excitations in the region of 118–204 nm.

The theoretical absorption spectrum of an optimized sulforaphane molecule in a solvent is calculated using the Gaussian 16 software package, using the theory level TDB3LYP/6-311G*. The averaged scaling factor of the program in the calculation of UV spectra is 0.99. A solvaton model was used to account for water, which does not take into account the microscopic structure of the solvent in order to save machine time in calculations.

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REDEVELOPMENT AND THE ENVIRONMENTAL COMPONENT OF SECURITY

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The main problems and limitations of redevelopment are design solutions, efficiency, economic and environmental component.

The main problems and limitations that arise during redevelopment include:

– difficulties in combining design decisions with urban development plans for the development of adjacent areas;

– difficulties in transporting the territory the unsuitability of retained buildings and structures for new functions or technologies;

– dilapidation of fixed assets; the possibility or impossibility of increasing the load on existing communications, networks and infrastructure;

– economic issues of the concept (investment efficiency); environmental problems of the site and the impact of the facility on adjacent territories.

The environmental criteria of building structures, decoration materials, household and industrial appliances include three main groups: safety for human health of materials, their resistance to external factors, their ability to neutralize the side effects of operation, as well as, of course, the safety of their operation.

Finally, it is important to remember that not only the materials from which the products are made must be safe, but also the process of its operation. Today, modern safety standards imply not only protection against harmful emissions or electromagnetic fields, but also the silent operation of household appliances, because the so-called noise pollution is a common cause of hearing loss and nervous disorders in residents of large cities. Sounds whose intensity does not exceed 35 dBA are considered to be absolutely harmless from this point of view, i.e. the volume of the human voice. At night, extraneous noise should not be louder than 27-28 dBA, otherwise they can disturb sleep. This characteristic is especially relevant for air conditioners, which in hot weather do not turn off around the