Abstract of doctoral dissertation, P. Urbaszek MSc., entitled: **"Predicting the adsorption of brominated and/or chlorinated persistent organic pollutants (POPs) on the C_{60} fullerene surface"**

In the last decades, nanotechnology has been developing very dynamically. New materials with high potential of applicability in many fields of industry include carbon nanoparticles, and fullerenes. Some of the applications of these structures are based on their surface interactions potential. However, it should be noted that increasing the production of carbon nanoparticles, including C_{60} fullerene, will also increase the chance of its uncontrolled emission to the environment where substances that can be adsorbed on the surface of these nanoparticles are present. That may increase the toxicological potential of fullerene itself, as well as these substances.

Persistent Organic Pollutants (POPs) are a large group of organic compounds, the common features of which are: persistence in the natural environment, ability to travel long distances in its various components, the toxicological hazard they pose, and the fact that they are most often a by-product of anthropogenic activity. This extremely numerous group includes structures with a very diverse structures: from single-ring benzene derivatives to polycyclic structures. An equally characteristic feature of POPs is the frequent presence of halogenated derivatives of these compounds, such as polychlorinated dibenzo-*p*-dioxins, polybrominated diphenylethers and many others.

Due to the number of POPs structures in the environment, it is impossible to determine the strength of adsorption interactions of these compounds on the C_{60} fullerene surface by experimental methods.

This dissertation presents the results of research based on theoretical chemistry and cheminformatical methods to study the energy of adsorption of 23 congeneric families on the surface of C_{60} fullerene. Studied POPs congeners were substituted by bromine and/or chlorine. The determination of the toxicological potential of such interactions was also studied.

The obtained results are divided into the following stages: 1) cheminformatic analysis of similarity of a 1,840,951 halogenated POPs library in the space of twenty-six structural descriptors determined by theoretical chemistry methods, 2) development of a nano-QSPR model predicting sorption interactions for 1,701 polyhalogenated dibenzo-*p*-dioxin congeners. Studying the relationship between the type and number of halogen substituents on the adsorption energy values. 3) calibration and development of the nano-QSPR model for 20 congeneric families and studying the influence of the basic carbon structure on the adsorption potential of the congeners.