

## STRESZCZENIE W JĘZYKU ANGIELSKIM

Ecotoxicology is a dynamically developing field of science that allows to determine the toxicity of tested compounds towards organisms living in the environment, and thus the impact of these substances on the natural environment. Examples of organisms that are used in ecotoxicity tests are bioluminescent bacteria *Aliivibrio fischeri*, which allow to determine toxicity of xenobiotics based on the measurable effect of inhibition of bioluminescence.

The main purpose of this doctoral dissertation was to determine the ecotoxicity of unexplored ionic xenobiotics (ammonium ionic liquids) and non-ionic ones (pharmaceutical active substances (API) and auxiliary substances), using the above-mentioned bacteria, and to derive the QSAR (*Quantitative Structure-Activity Relationship*) equations allowing to link the structural features of the studied groups of compounds with their activity against *A. fischeri*.

As a result of the conducted research, the EC<sub>50</sub> values (*A. fischeri*) of ionic xenobiotics with herbicidal properties from the group of chiral and achiral ammonium haloacetates, 2,2'-thiodiacetates as well as phenoxyacetates and phenylthioacetates were determined. The QSAR equation was developed for quantitative correlation of ecotoxicity to *A. fischeri* with quantum-chemical descriptors of the tested ammonium compounds. As a result, the developed QSAR model will enable the design of ionic herbicidal compounds with low ecotoxicity to aquatic organisms, and therefore safer for the environment.

Ecotoxicological studies in the field of non-ionic xenobiotics were based on the poorly water-soluble drugs from the group of angiotensin II receptor blockers (ARBs), their pharmaceutical formulations, as well as individual excipients used in these formulations. The ecotoxicity of various API-API, API-excipient and excipient-excipient mixtures was tested and compared to ecotoxicity predicted using common CA and IA models. A QSAR model has also been developed for the group of ARBs and biphenyls, which will allow an early assessment of the environmental risk related to the presence of these compounds and their derivatives/metabolites in the ecosystem. It is worth emphasizing that in the case of poorly water soluble active substances from the ARBs group, these tests were possible only thanks to the development of a special modification of the commercial Microtox<sup>®</sup> test as a part of this work.

The obtained results constitute an original contribution to the state of the art in the field of ecotoxicity of active substances from the ARBs group, towards *A. fischeri* bacteria, which so far was unknown. The modification of the Microtox<sup>®</sup> test, developed and described in this doctoral dissertation, allows ecotoxicity testing of poorly soluble compounds, including pharmaceuticals for which the application of a standard protocol using aqueous solutions was impossible. Moreover, ecotoxicological studies carried out on the group of new ammonium ionic liquids may be useful in designing other, structurally similar, ionic herbicidal compounds.

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