

## Ecotoxicity prediction of the new imidazole liquids with a phosphorus containing anion using QSAR

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*Motivation and Aim:* The ionic liquids are broadly used in various fields of science and technology. In A.E. Favorsky Irkutsk Institute of Chemistry, Siberian Branch of the Russian Academy of Sciences the approaches to directed synthesis of new functional organophosphorous compounds from elemental phosphorus (using Trofimov-Gusarova reaction) [1] are developed. These approaches successfully develop including using the phenomenon of defect formation in a solid structure of this chemical element [2–4]. Recently, previously unknown hypophosphites were received. These hypophosphites are 1-*n*-, 1-alkyl- and 1-vinyl-3*n*-imidazolium, which are ionic liquids at room temperature. The aim of our work was to calculate the forecast of ecotoxicity of these new phosphorus-containing ionic liquids.

*Methods and Algorithms:* The calculations were carried out using quantitative structure-activity relationships (QSARs) and quantitative structure-property relationships (QSPRs) to estimate the physics-chemical and ecotoxic properties of new ionic liquid.

*Results:* The model shows a group contribution method that considers three main groups of descriptors in the ionic liquid structure: the anion, the cation and the substitutions (carbon chains linked to the cation). Based on these descriptors, their contribution to the ecotoxicity of the ionic liquid has been evaluated by means of a multilinear regression model.

*Conclusion:* The received results using quantitative structure–activity relationships approach (QSAR) for estimating the ecotoxicity correlate with the literature data for similar compounds [5].

### References

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