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# Development of "structure-property" models in nucleophilic substitution reactions involving azides

Nugmanov R., Madzhidov T., Khaliullina G., Baskin I., Antipin I., Varnek A.
*Kazan Federal University, 420008, Kremlevskaya 18, Kazan, Russia*

## Abstract

© 2014 Pleiades Publishing, Ltd. This paper reports a predictive model for the rate constant of the bimolecular nucleophilic substitution involving the azide moiety. It predicts reaction rate constants in different solvents, including organic mixtures, and with different organic and inorganic azides as reactants. The optimal descriptors describing solvent effects and a cation type in the azide salt were suggested. A reasonably good predictive performance of the model in cross-validation has been demonstrated. The model was applied to predict the rates of the reactions between sodium azide with two conformers of calixarenes as well as 3-bromopropyl phenyl ester. For sterically non-hindered molecules, a good agreement between predicted and experimental reaction rates was observed. On the other hand, the model poorly reproduces the results for sterically hindered molecules.

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## Keywords

chemoinformatics, condensed graph of reaction, molecular modeling, nucleophilic substitution, rate constant