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# CORAL: predictive models for cytotoxicity of functionalized nanozeolites based on quasi-SMILES

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**Abstract**

Unlike the well-known simplified molecular input-line entry system (SMILES), the so-called quasi-SMILES contains information related to physicochemical and biochemical conditions by a special additional symbols (codes), each standing for different conditions (time exposure, concentration, type of cell, etc.). Thus, quasi-SMILES can be used to build up models for cytotoxicity of functionalized nanozeolites using a mathematical function of eclectic information. These calculations were done with the Monte Carlo CORAL software. The statistical quality of models based on quasi-SMILES was usually considerably better than the statistical quality of models based on traditional SMILES.

Keywords: Cytotoxicity, functionalized nanozeolites, quasi-SMILES, CORAL software