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**APPLICATIONS OF THE MIXTURES
REPRESENTATION APPROACH IN QSAR
MODELING**

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Various approaches towards mixtures representation for QSAR modeling have been developed and published. Those works mainly dealt with binary mixtures of traditional chemicals (drugs, solvents, etc), most of them limited by additive modeling. Due to the limitations of existing approaches, we developed our own approach based on simplex representation of molecular structure. It is a non-additive scheme that can be applied for QSAR modeling of binary and more complex mixtures.

Earlier we demonstrated application of this approach for modeling of vapor-liquid equilibrium curves of binary mixtures of organic solvents, and antiviral properties of drugs combinations. The mixture representation paradigm and particularly the developed approach of mixture representation was also effectively applied for other QSAR tasks:

- 1) modeling of chemical reactions;
- 2) modeling of ligands binding to artificial receptors;
- 3) modeling of bulk properties of pure chemicals.