

**Challenges in mechanistic investigation of a flexible aminocatalyst as demonstrated through enamine formation**  
**Osadchuk, Irina; Kanger, Tõnis** ChemistryOpen 2025 / art. 2500116 <https://doi.org/10.1002/open.202500116> <https://chemistry-europe.onlinelibrary.wiley.com/doi/10.1002/open.202500116>

**Computational chemistry approaches for understanding how structure determines properties**

Katritzky, Alan R.; Slavov, Svetoslav H.; Radzivilovits, Maksim; Stoyanova-Slavova, Iva B.; **Karelson, Mati** Zeitschrift für Naturforschung B - a journal of chemical sciences 2009 / 6, p. 773-777

**Computational study of cyclohexylhemicucurbiturils = Tsüklolheksüülhemikukurbituriilide arvutuskeemiline modelleerimine**

Ören, Mario 2015 [https://www.esther.ee/record=b4522693\\*est](https://www.esther.ee/record=b4522693*est)

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Metsala, Andrus; Kriis, Kadri; Kanger, Tõnis Journal of computational chemistry 2025 / art. e70159 <https://doi.org/10.1002/jcc.70159>

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**Reproducibility of QSAR/QSPR models in the scientific literature - perspective for regulatory use**

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