

[P5] Predicting reaction conditions for Michael reactions

G. Marcou¹, A. De Luca¹, D. Horvath¹, J. Aires de Susa², D. Latino², A. Varnek¹

¹Laboratory of Chemoinformatics, University of Strasbourg, 1 rue Blaise Pascal, 67000 Strasbourg (France)

²Departamento de Química, Faculdade de Ciências e Tecnologia, Universidade Nova de Lisboa 2829-516 Caparica, (Portugal)

In order to identify the structural reaction patterns describing different sub-types of reactions, partial derivative QSPR technology ³ and Condensed Graph of Reaction approach have been applied.

One can distinguish different types of Michael β -addition reactions, which proceed under different combinations of solvent (e.g., hydrophobic, aprotic polar, protic) and catalyst (e.g., Brønsted acid, Lewis acid, Lewis base, "no catalyst"). The question arises: which reaction conditions – particular solvent and catalyst – are the most favorable to carry out a given reaction? To answer this question, a number of 2-classes classification models have been built on a set of 198 Michael reactions retrieved from literature. Different machine-learning methods (SVM, Naïve Bayes and Random Forest) in combination with different types of descriptors (ISIDA fragments¹ issued from Condensed Graphs of Reactions², MOLMAP³, EED, CDK⁴) have been used. Obtained models have a reasonable predictive performance in 3 times 3-fold cross-validation: Balance Accuracy varies from 0.7 to 1.

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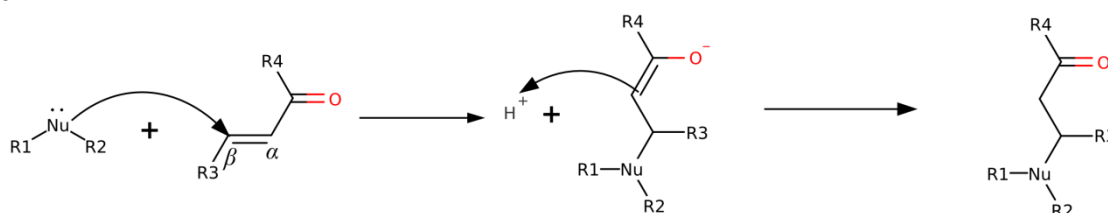


Figure 1. Michael β -addition reaction: optimal reaction conditions (solvent, catalyst) depend on nucleophile type (N or S) and the substituents R1, R2, R3 and R4.

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