[P16] Assessment of Optimal Reaction Conditions: Deprotection in Catalytic Hydrogenation Conditions

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Synthesis of complex structures became a central problem of organic chemistry. The complexity of structures prevents rapid synthesis of given structures due to the fact that the choice of synthetic strategy and adjustment of reaction conditions becomes more and more challenging. Recently it became clear that computational technologies could come to the scene and assist chemists in prediction of optimal solvents, catalysts and other conditions. However, only first steps were done in this direction. Recently, Struebing et al.[1] published a mixed quantum mechanics – linear free energy relationship based approach for prediction of optimal solvent for bimolecular reactions. Marcou et al.[2] built classification model to predict optimal type of solvent and type of catalyst for Michael reaction using machine learning methods. Brief review of these works will be presented.

New approach that extracts expert knowledge on optimal conditions of deprotection reactions from large amount of raw and "big" reaction data in a fully automatic workflow will be presented. The approach is based on Condensed Graph of Reaction [3] approach. It was applied to approx. 142000 hydrogenation reactions taken from Reaxys database. The approach allows to build in a fully automatic way Green's Reactivity Charts[4] that could be updated as new reaction appears in database. Unlike ordinary Charts published in the book[4], our tables are based on analysis of all the information existing in the database with explicitly stated rules. Moreover, advanced analysis could be performed and more detailed information could be extracted. The approach also could provide information on selectivity of group deprotection.

The tool for prediction of optimal conditions for these reactions based on similarity principle was developed. The hypothesis was that similar reactions proceed in similar conditions. The approach allows assessing optimal conditions for desired deprotection reaction. Clear advantage of the approach over expert knowledge acquired from the "manual" analysis of the literature will be demonstrated.

Bibliography:

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