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## Optimisation of the polymer support properties of an aminated aldol reaction catalyst

### Aim

Explorative experimental study of potential structures of an aldol reaction catalyst, focusing on the support properties. Following the synthesis and characterisation of a well-selected set of catalyst candidates, their performance will be assessed and compared using the model aldol reaction of 4-nitrobenzaldehyde with acetone in an aqueous environment.

### Justification

The aldol reaction is an organic reaction in which two carbonyl compounds are coupled via the creation of new carbon-carbon bonds, yielding heavier and more complex molecules. As such, it has applications in the pharmaceutical industry and fine chemicals production. Additionally, the reaction could also play an important role in the valorisation of biomass-derived molecules.

Currently, aldol reactions are industrially mainly performed using homogeneous strong base catalysts. Out of safety and sustainability considerations, heterogeneous catalysts are preferred over homogeneous catalysts. Therefore, over the past two decades, several heterogeneous alternatives have been explored: zeolites, hydrotalcites and mixed oxides, aminated silicas and polymers... The latter amine-based catalysts are interesting because of their exceptional properties. After thorough experimental and computational research, an amine catalyst, consisting of amine active sites grafted on a polymer resin support containing promoting hydroxyl groups, turned out to offer a satisfactory combination of reasonable activity, high selectivity and stability over longer time when used in water.

Detailed information is currently available about the effect of amine structure, the presence of promoting groups, the role of certain solvents and the support material on the catalytic activity and stability. However, there still remains room for optimisation of the support structure and the reaction environment (solvent-support effects). The structure of the poly(ethylene glycol) methacrylate support and its interactions with different solvents, should be the first focus for further investigations. An important property in this perspective, is the swellability of the polymer, since this substantially determines the accessibility of the amine active centres. Therefore, in this thesis, we want to explore how the current state-of-the-art aminated polymer resin catalyst can be improved by tuning the support properties and the reaction solvent.

### Program

Explorative study of different poly(ethylene glycol) methacrylate polymers or derived materials as support material for amine-based aldol reaction catalysts. For the proposed materials, a synthesis route should be developed and executed. The synthesised materials will then be tested in the model aldol reaction of 4-nitrobenzaldehyde with acetone. Furthermore, different reaction solvents will be explored, in order to investigate the solvent-support interactions. These experiments will be performed in both a batch-type reactor, for assessing the catalytic activity, as well as a continuous flow reactor, for assessing the stability.