Bachelor/master project

Master thesis project in organic chemistry/ synthesis and evaluation of azetidinium salts (15/30 hp)

Welcome with your application

Organic chemistry, Chemistry and Chemical Engineering, CHALMERS.
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ABSTRACT: In Organic chemistry there is a large variety of chemical transformation that can be performed by a tool-box of reagents. Reagents that are selective, robust and has high reproducibility and makes a chemical transformation that not many other reagents can promote successfully often becomes the standard reagents in many labs. Furthermore, if the have a fairly low price, don't need extreme temperatures and can be reused in an efficient way they may find their way into industrial organic chemistry.

One new class of reagents are the azetidinium salts. Azetidinium salts (AZ's) are prepared from epichlorohydrin and an amine. Either the AZ's can be produced in one pot or through a two-step sequence wherein an azetidine is first produced, then subsequently reacted to give AZ's.

For AZ's to become a standard reagent there are some challenges that has to be overcome.
Firstly, process methods that makes it possible to synthesize a plethora of different types of Az's has to be developed. Secondly, their use and excellence compared to other reagents has to be proven. These two challenges have reached a proof-of-concept level but needs further development and be advocated with realizable and evidence-based arguments.

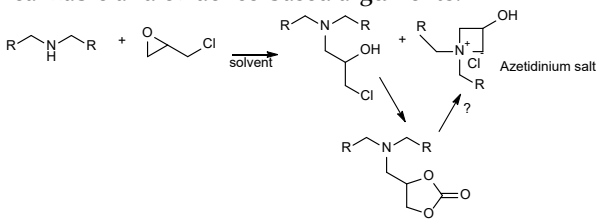

Figure 1 Schematic presentation of synthetic routes for azetidinium salts and a carbonate derivative

For AZ's it is general accepted that the azetidinium group can be in two different conformations with the -OH group in equatorial or axial direction, this have never been spectroscopically been proved, nor has their assumed different reactivity been discussed.

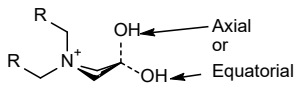

Figure 2 3-D presentation of AZ's

The thesis project

A project outline could be to first make a set of AZ's with the aim to get an understanding on how functional groups in the alkylamine scaffold affects the AZ's yield, then there are several routes forward,
i) An industrial perspective; investigate the scalability of AZ's,
ii) make them into "standard reagents" by showing their excellence in a specific chemical transformation,
iii) a medicinal perspective by creating chiral AZ's and show how they can be adapted in the synthesis of pharmaceuticals.
iv) investigate their reactivity and their ability to form enantiomeric enriched products when reacting with chiral molecules.

There are also, as for almost all projects, the need for a literature study, report writing, communicate the results and your curiosity and skills to relate chemical details with molecular properties and envisage applications. Assignment of NMR and FTIR spectra and detailed documentation are other important parts of the project.