Synthetic Route Design of Low Molecular Weight Alcohols, Acids, Esters

Retrosynthetic Analysis

Fig.1 The synthesis route to a target molecule

- Retrosynthetic analysis (RTSA) is a technique for solving problems in the planning of organic syntheses. This is achieved by imaginary breaking of bonds (disconnections) and by the conversion of one functional group into another (functional group interconversions). This means retrosynthesis is a process starting with the end products you want to make and working backwards to the starting materials through multiple reactions (see Fig.1).
- The RTSA method is a computational, data-driven approach designed to identify potential synthetic routes for a structure of interest. The operation of RTSA has two distinct phases. The training phase, RTSA-Train, consumes all available reaction data and produces a collection of chemical structure decomposition rules and information required for synthetic route design. RTSA-Design receives the hypothesis structure(s) and designs possible synthetic routes using the collection of decomposition rules obtained during training.

Design Principle

- Short route
- High yield
- Mild reaction condition
- High purity
- Simple separation procedure
- Convenient for raw materials availability

Service Areas

Based upon the concept of transferring academic knowledge into valuable industrial applications, Alfa Chemistry assists in designing and optimizing new synthetic routes, our service area include but not limited to:

- Small molecules synthetic route design
- Small molecules synthetic route optimization
- Building blocks and complex intermediates
- Innovative routes and compounds
- Reference compounds etc.

Reference: https://carboxyl.alfa-chemistry.com/synthetic-route-design.html