Dear Thomas,

related to the above feature suggest is a second one, this time to extend working via chemistry -> enumerate combinatorial library.

So far, reactants either are to be sketched again .or. load from a file about either one of the reactants. Would it be possible to extend the «add» function so that one may refer back to the currently open file to define the starting material by column? With the above test file reactions.dwar, this would be to point to column «amines» for one, and «chlorides» for the second line when «enumerate combinatorial library» asks for the reagents to permutate with each other.

At present «merge by reaction» constraints the set of products generated to reactions line-by-line.

Norwid

File Attachments
1) suggest_02.gif, downloaded 1310 times