Concepts towards a sustainable synthesis design

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A simple quantitative approach to enable chemists to compare alternative chemical syntheses on the lab bench with respect to their resource usage is proposed. This may be useful for the systematic design of more sustainable processes. The computer program EATOS allows to perform the calculation of the mass index S^{-1} and of the environmental factor E.

 $S^{-1} = \sum$ Raw materials [kg] / Product [kg]

$E = \sum$ Waste [kg] / Product [kg]

By this means, mass balances of different syntheses and sequences of syntheses can be compared in a graphical interactive presentation. The stoichiometric equation and the amounts of raw materials are necessary for the determination of mass balances. EATOS can easily be used to discuss and compare chemical reactions with respect to their resource efficiency and waste generation, and to improve them to become more environmentally benign. Examples are given in the literature. Information obtained by EATOS are especially valuable in the early stage of synthesis design.