Article 12

Sustainable Chemistry in Synthesis of Heterocyclic Systems: [Atom Economy, Yield Economy and Reaction Mass Efficiency As Metrics of Synthetic Reaction Efficiency]

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Abstract:
The abstract should not exceed 250 words and should be presented as a single paragraph, following the style of structured abstracts. However, it should not include specific headings. Here is the suggested structure for the abstract: (A) Background: Provide a broad context for the research question and emphasize the study's purpose. (B) Methods: Briefly describe the main methods or treatments used, including any relevant preregistration numbers. Specify the species and strains of animals, if applicable. (C) Results: Summarize the main findings of the article. (D) Conclusion: State the main conclusions or interpretations derived from the study. It is important to ensure that the abstract is an unbiased representation of the article. It should not include any results that are not presented and supported in the main text, and it should not overstate the main conclusions. Focus on highlighting novel aspects of the study and its key observations. Avoid using non-standard or uncommon abbreviations, b There are many advances in the synthesis of organic compounds like multi-component syntheses. Mechano-synthesis, green synthesis, combinatorial synthesis, and bio-organic synthesis. Solvent-free Mechano synthesis is a significant strategy for the synthesis of the target heterocyclic compounds due to its "green chemistry" aspects; reactions are run solvent-free, atom economy with reduced energy requirements, and easier work-up method. The concept of green chemistry has become a tool for promoting sustainable development in laboratories and industry.

Conventionally, attaining the highest yield and product selectivity were the governing factors of chemical synthetic reactions. Chemists need to measure the efficiency of chemical reactions to assess the alternative routes to target products and their associated economic and environmental costs. The chemical yield (%) of a reaction is measured by comparing how much of the desired product was obtained to how much could theoretically have been obtained given the reaction stoichiometry and the amounts of reactants used. The concept of atom economy (AE) was introduced by Trost (1998). AE looks at the chemical reaction from the perspective of how many input atoms are incorporated into the desired product versus how many are discarded as waste. Although it has improved over time, AE ignores at least two important factors: reaction time and the amount of product actually obtained (yield%). It does not help in comparing two alternative synthetic reactions taking place under different conditions to yield the same target compounds because AE remains the same for these reactions. Therefore, we introduced yield economy (YE = Yield% / time (Min.)) as a new metric to provide a decisive assessment of the yields obtained under mechanochemical and conventional conditions. Assessing a chemical reaction based solely on yield% can be misleading.

On the other hand, Reaction Mass Efficiency (RME) measures the mass of the product divided by the total mass of the reactants. AE gives the theoretical maximum efficiency of

reactant utilization, while RME provides the observed efficiency. These metrics are related to each other and are known as mass-based metrics, which can also be related to the time of reaction. These metrics were applied in different efficient synthetic reactions of a wide range of heterocyclic systems (Fahmy et al., 2016; Fahmy, El-Sayed, & Hemdan, 2016; Fahmy, Rizk, Hemdan, El-Sayed, & Hassaballah, 2018; Fahmy, Rizk, Hemdan, El-Sayed, & Hassaballah, 2020).

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