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Review

Green Chemistry Metrics, A Review

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Abstract: Attending both, The United Nations Decade of Education for Sustainable Development (2005-2014) and the United Nations 2030 Agenda for Sustainable Development, this review is presented, bearing in mind that Green Chemistry is essential to contribute to sustainability. In this work is compiled all the information related to green chemistry metrics, so that the stakeholders could appropriately select a model, under the green chemistry protocol, to evaluate how much green is a process; the review was organized considering the following convenient sections: the mass valuation, the recognition of the human health and environmental impact, metrics using computational programs (software, and spreadsheets), and finally global metrics. To develop this review were consulted the principal databases, since 1998 the appearance of the first green chemistry textbook, to date; a massive number of references were attained involving the keywords below proposed, also six languages were observed, highlighting the English language. It is important to highlight that the twelve principles of green chemistry are conceptual and offer little quantitative information, in addition, almost all the reported metric green propositions do not consider the twelve principles, and only few paper offer how to obtain an appropriate evaluation about the greenness of a research. In this sense, it is convenient to note that only in the Spanish literature exist two metrics that consider all the principles. Finally, to our knowledge, and after a deep search in the literature, it is the first review that covers the different features of green chemistry: mass, environment/ human health., and in some cases the use of computational programs.

Keywords: Review; green chemistry; metrics; sustainable development; 2030 agenda

Table S1. The twelve green engineering principles. Data from Ref [1].

Principle	Meaning
1	Designers need to strive to ensure that all material and energy inputs and outputs are as inherently nonhazardous as possible
2	It is better to prevent waste than to treat or clean up waste after it is formed
3	Separation and purification operations should be designed to minimize energy consumption and materials use
4	Products, processes, and systems should be designed to maximize mass, energy, space, and time efficiency
5	Products, processes, and systems should be output pulled rather than input pushed through the use of energy and materials
6	Embedded entropy and complexity must be viewed as an investment when making design choices on recycle, reuse, or beneficial disposition
7	Targeted durability, not immortality, should be a design goal
8	Design for unnecessary capacity or capability (e.g., one size fits all) solutions should be considered a design flaw
9	Material diversity in multicomponent products should be minimized to promote disassembly and value retention
10	Design of products, processes, and systems must include integration and interconnectivity with available energy and materials flows
11	Products, processes, and systems should be designed for performance in a commercial afterlife
12	Material and energy inputs should be renewable rather than depleting

Table S2. The twelve green analytical principles. Data from Ref [2].

Principle	Meaning
1	Direct analytical techniques should be applied to avoid sample treatment
2	Minimal samples size and minimal number of samples are goals
3	*In situ* measurements should be performed
4	Integration of analytical processes and operations saves energy and reduces the use of reagents
5	Automated and miniaturized methods should be selected
6	Derivatization should be avoided
7	Generation of a large volume of analytical waste should be avoided and proper management of analytical waste should be provided
8	Multianalyte or multiparameter methods are preferred *versus* methods using one analyte at a time
9	The use of energy should be minimized
10	Reagents obtained from renewable sources should be preferred
11	Toxic reagents should be eliminated or replaced
12	The safety of the operator should be increased

Table S3. The ten green principles for the sample preparation. Data from Ref [3,4].

Principle	Meaning
1	Sample preparation carried-out *in situ*
2	Alternative safer solvents and reagents
3	Materials are sustainable, reusable and renewable
4	Prevent or minimize waste generation
5	Low size
6	Enhance sample throughput
7	Promote integration of steps and automation
8	Reduce energy consumption
9	Ensure green post-sample preparation analysis
10	Protect the operator

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