EDUCATION IN GREEN CHEMISTRY SUPPORTED BY COMPUTATIONAL CHEMISTRY - A BRIEF REVIEW

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RESUMO

Green Chemistry (GC) is a multidisciplinary area that aims to reduce or eliminate the use or generation of hazardous substances. In recent years, novel approaches have been developed on the design of chemical products and processes that are benign for the environment and for people. In this context, Computational Chemistry (CC) can also be defined as a multidisciplinary area, which develops and implements software to study the properties of molecules. The use of modeling software developed by CC opens up a range of possibilities with GC. This work aims to investigate the potentials of computational chemistry for teaching Green Chemistry (GC). Our method was based on a systematic review, which mapped scientific articles in Web of Science, during 2002-2022. We applied descriptors and Boolean operators, such as "Green Chemistry" AND "Computational Chemistry", promoting more focused and productive results. In total, three scientific articles were selected, which covered relations between CC and Education in GC. The first selected article, entitled "Introduction to Cheminformatics for Green Chemistry Education" and published in 2019, highlights the use of software to describe chemical structures and to obtain an analysis of the structure and molecular properties and relating how computational chemistry provides these tools focusing on their value in teaching GC. The second article, entitled "Computational Chemistry for Green Design in Chemistry and Pharmacy: Building Awareness in the Classroom", focuses on presenting common and relevant characteristics between GC and CC in education. It offered an overview of the role of CC in making chemical production greener, making an important interrelationship with great potential for both areas. It also highlights the importance of students being familiar with the use of software, as well as the theoretical framework. The third publication, entitled "Computational Chemistry and Green Chemistry: Familiarizing Chemistry Students with the Modes and Benefits of Promising Synergies", combines information from the literature, interactions with specialists and the author's own experience to approach the use of constructive chemistry interfaces computational with the teaching of GC. For this, it is necessary to inform students that there is the possibility of research in GC and CC. These two last papers, published in 2020 and 2022, belong to the same author. We concluded that more research could be done. There is a lack of reports evolving CC and Education in GC. For future chemists, the synergy between these areas (GC and CC) are needed, because it is critical to better creation of benign chemical substances and process design.

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