EDUCATIONAL APPROACHES TO HIGHLIGHT THE ROLES OF COMPUTATIONAL CHEMISTRY FOR GREEN CHEMISTRY AND SUSTAINABILITY

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The key objectives of green chemistry entail the design of environmentally benign substances and of cleaner and safer industrial processes. In modern chemistry, the design of new substances with desired properties largely relies on the knowledge of the properties of their molecules, obtainable from computational chemistry investigations. Consequently, cross-disciplinarity between the two areas is important both in chemistry practice and for the educational level.[1]

The presentation outlines options aimed at familiarising students with the challenges and fundamental roles of molecular design and with the contributions brought by computational chemistry. The main objective is that of promoting a cross-disciplinary outlook between applied and theoretical chemists since the undergraduate chemistry courses. A number of concrete examples are utilised to provide adequate illustration.

References
1. Mammino, L. Current Opinion in Green and Sustainable Chemistry 2018, 13, 76.