AUTOMATED SEARCH ALGORITHMS FOR STRUCTURAL ISOMERISM: THE PROS AND CONS

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Although automated search algorithms are highly powerful tools to find out various structural isomers for a given elemental composition, human chemical intuition still delivers more geometries than automated searches once we know the initial geometries. This indirectly emphasizes the fact that creating an unbiased algorithm for structural isomerism is simply difficult. Moreover, it also outlines that an integrated approach is necessary between search algorithms and chemical intuition to further our knowledge of chemical space for any given elemental composition.