

Bioisosteres and Scaffold Hopping in Medicinal Chemistry

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The twin concepts of bioisosteric replacement and scaffold hopping are increasingly becoming important in modern drug design. The concepts of isosterism stretch back over a century, but only recently have systematic and dataintensive methods been used to explore appropriate replacements. Here, a summary of the history of bioisosterism is presented to provide context to the methods applied. Molecular similarity and data mining methods are introduced as approaches to introduce these replacements to rationalise the space of synthetic targets to consider in a medicinal chemistry project. Lastly, an outlook of the field is given of potential future improvements and areas of focus that should be considered to anyone interested in the field.