



Bioisosteres in Medicinal Chemistry, Volume 54

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Written with the practicing medicinal chemist in mind, this is the first modern handbook to systematically address the topic of bioisosterism.

As such, it provides a ready reference on the principles and methods of bioisosteric replacement as a key tool in preclinical drug development.

The first part provides an overview of bioisosterism, classical bioisosteres and typical molecular interactions that need to be considered, while the second part describes a number of molecular databases as sources of bioisosteric identification and rationalization. The third part covers the four key methodologies for bioisostere identification and replacement: physicochemical properties, topology, shape, and overlays of protein-ligand crystal structures. In the final part, several real-world examples of bioisosterism in drug discovery projects are discussed.

With its detailed descriptions of databases, methods and real-life case studies, this is tailor-made for busy industrial researchers with little time for reading, while remaining easily accessible to novice drug developers due to its systematic structure and introductory section.

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Editorial Review

Review

“In all, I believe this book is a musthave handbook on bioisosteres. It is highly valuable both as a text book for graduate students and as a book of reference for the medicinal chemist working in the industry as well as in an academic setting.” (*ChemMedChem*, 1 July 2013)

From the Back Cover

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About the Author

Nathan Brown is the Head of the In Silico Medicinal Chemistry group in the Cancer Therapeutics Unit at The Institute of Cancer Research in London (UK). At the ICR, Nathan and his group support our entire drug discovery portfolio together with developing new computational methodologies to enhance our drug design work.

Nathan conducted his doctoral research in Sheffield with Professor Peter Willett focusing on evolutionary algorithms and graph theory. After a two-year Marie Curie fellowship in Amsterdam in collaboration with Professor Johann Gasteiger in Erlangen, he joined the Novartis Institutes for BioMedical Research in Basel for a three-year Presidential fellowship in Basel working with Professors Peter Willett and Karl-Heinz Altmann.

Nathan’s work has led to the pioneering work on multiojective de novo design in addition to a variety of discoveries and method development in bioisosteric identification and replacement, scaffold hopping, molecular descriptors and statistical modelling. Nathan continues to pursue his research in all aspects of in silico medicinal chemistry.

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