



Epi-Informatics: Discovery and Development of Small Molecule Epigenetic Drugs and Probes

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Epi-Informatics: Discovery and Development of Small Molecule Epigenetic Drugs and Probes features multidisciplinary strategies with strong computational approaches that have led to the successful discovery and/or optimization of compounds that act as modulators of epigenetic targets. This book is intended for all those using or wanting to learn more about computational methodologies in epigenetic drug discovery, including molecular modelers, informaticians, pharmaceutical scientists, and medicinal chemists.

With a better understanding of different molecular modeling and cheminformatic approaches, readers can incorporate these techniques into their own drug discovery projects that may involve chemical synthesis and medium- or high-throughput screening. In addition, this book highlights the significance of epigenetic targets to the public health for molecular modelers and chemoinformaticians. The goal of this reference is to stimulate ongoing multidisciplinary research and to further improve current computational methodologies and workflows in order to accelerate the discovery and development of epi-drugs and epi-probes.

- Focuses on the discovery of epi-drugs as candidates to be used in therapy including combined therapies
- Describes new computational methodologies and screening assays utilizing recent and emerging novel structural data
- Highlights the discovery, development and optimization of epi-probes, which are molecular probes that elucidate epigenetic mechanisms
- Includes important topics such as computational-guided optimization of epi-hits, virtual screening to identify novel compounds for epigenetic targets, development and mining of epigenetic molecular databases, SAR modeling of screening data and much more

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