

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

From Medina Franco Jose

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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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Editorial Review

About the Author

Dr. José Medina-Franco received a Bachelor of Science degree in chemistry from the National Autonomous University of Mexico (UNAM) in 1998. That same year, he joined Procter & Gamble in Mexico City, working in the research and development department. He received a Master of Science degree in 2002 and a Ph.D. degree in 2005, both from the UNAM. In 2005, he joined the University of Arizona as a postdoctoral fellow. Dr. Medina-Franco was named Assistant Member at the Torrey Pines Institute for Molecular Studies in Florida in August 2007. Since then, he has conducted research and academic activities at the Institute of Chemistry, UNAM and Mayo Clinic in Scottsdale. In 2014, he was named Full Time Research Professor of the Pharmacy Department, UNAM where he leads a computational group focused on the discovery and development of epi-drugs. He also serves as an Adjunct Professor at the Florida Atlantic University. Dr. Medina-Franco has more than 8 years of experience working on molecular modeling of DNMT inhibitors. He has lead one of the first research groups applying computational tools for drug discovery of epi-hits. His research group has published several research papers, reviews and book chapters focused on the development of DNMT inhibitors using computational methods. One of the major contributions of his group has been the identification of a distinct DNMT inhibitor with a novel molecular scaffold. The hit compound has been used as a starting point for optimization programs and has served as reference for virtual screening campaigns. Dr. Medina-Franco's group has also initiated a novel computer-guided drug repurposing project.

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Helen McCormick:

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