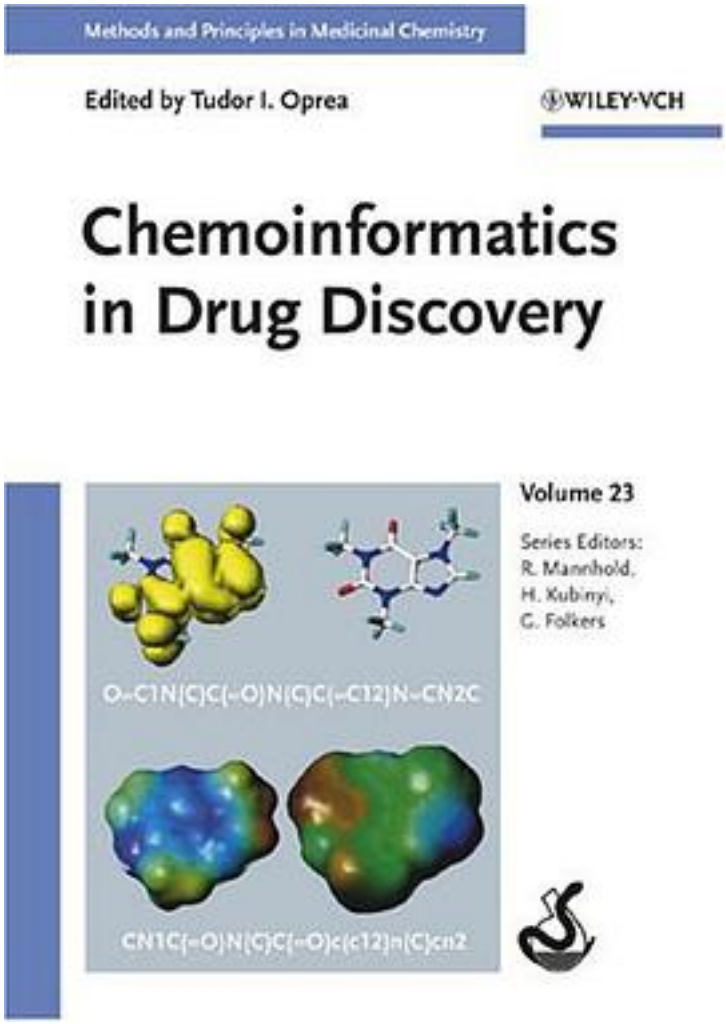
Chemoinformatics in Drug Discovery



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This handbook provides the first-ever inside view of today's integrated approach to

rational drug design. Chemoinformatics experts from large pharmaceutical companies, as well as from chemoinformatics service providers and from academia demonstrate what can be achieved today by harnessing the power of computational methods for the drug discovery process. With the user rather than the developer of chemoinformatics software in mind, this book describes the successful application of computational tools to real-life problems and presents solution strategies to commonly encountered problems. It shows how almost every step of the drug discovery pipeline can be optimized and accelerated by using chemoinformatics tools—from the management of compound databases to targeted combinatorial synthesis, virtual screening and efficient hit-to-lead transition. An invaluable resource for drug developers and medicinal chemists in academia and industry.

作者介绍:

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标签

评论

as a 2005 edtion of chemoinformatics textbook for drug discovery, it seems a little bit out of date from a 2011 reader's point of view, since things change very fast in CADD aera.

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书评

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