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Bridging the gap between cheminformatics and bioinformatics for the first time, Computational Approaches in Cheminformatics and Bioinformatics provides insight on how to blend these two sciences for progressive research benefits. It describes the development and evolution of these fields, how chemical information may be used for biological relations and vice versa, the implications of these new connections, and foreseeable developments in the future.

Using algorithms and domains as workflow tools, this revolutionary text drives bioinformaticians to consider chemical structure, and similarly, encourages cheminformaticians to consider large biological systems such as protein targets and networks.

Computational Approaches in Cheminformatics and Bioinformatics covers:

- Data sources available for modelling and prediction purposes
- Developments of conventional Quantitative Structure-Activity Relationships (QSAR)
- Computational tools for manipulating chemical and biological data
- Novel ways of probing the interactions between small molecules and proteins

Also including insight from public (NIH), academic, and industrial sources (Novartis, Pfizer), this book offers expert knowledge to aid scientists through industry and academic study. The invaluable applications for drug discovery, cellular and molecular biology, enzymology, and metabolism make Computational Approaches in Cheminformatics and Bioinformatics the essential guidebook for evolving drug discovery research and alleviating the issue of chemical control and manipulation of various systems.

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Computational Approaches in Cheminformatics and Bioinformatics From Wiley Bibliography

- Sales Rank: #3645826 in Books
- Published on: 2012-01-04
- Original language: English
- Number of items: 1
- Dimensions: 9.55" h x .95" w x 6.30" l, 1.40 pounds
- Binding: Hardcover
- 292 pages

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Editorial Review

About the Author

RAJARSHI GUHA, PhD, is a Research Scientist at the NIH Center for Translational Therapeutics in Rockville, Maryland. His research covers a variety of topics in cheminformatics and chemical data mining, addressing software and methodology development as well as applications in areas such as high throughput screening and high content imaging of small molecules and siRNA's. Prior to working at the NIH, he was a visiting assistant professor in the School of Informatics and Computing, Indiana University.

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