

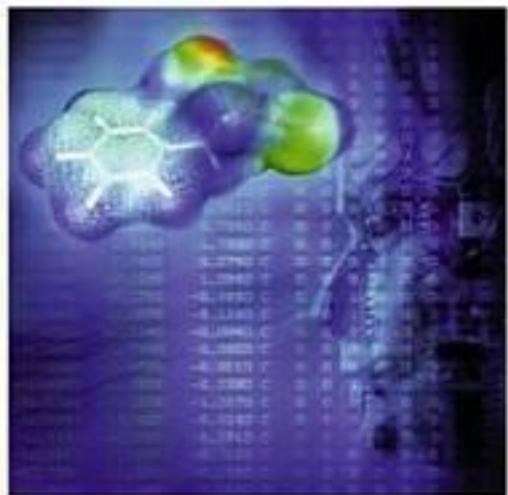
Chemoinformatics

Edited by
Johann Gasteiger and Thomas Engel

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Chemoinformatics

A Textbook



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著者:Johann Gasteiger

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This first work to be devoted entirely to this increasingly important field, the

"Textbook" provides both an in-depth and comprehensive overview of this exciting new area. Edited by Johann Gasteiger and Thomas Engel, the book provides an introduction to the representation of molecular structures and reactions, data types and databases/data sources, search methods, methods for data analysis as well as such applications as structure elucidation, reaction simulation, synthesis planning and drug design. A "hands-on" approach with step-by-step tutorials and detailed descriptions of software tools and Internet resources allows easy access for newcomers, advanced users and lecturers alike.

For a more detailed presentation, users are referred to the "Handbook of Chemoinformatics", which will be published separately. Johann Gasteiger is the recipient of the 1991 Gmelin-Beilstein Medal of the German Chemical Society for Achievements in Computer Chemistry, and the Herman Skolnik Award of the Division of Chemical Information of the American Chemical Society (ACS) in 1997.

Thomas Engel joined the research group headed by Johann Gasteiger at the University of Erlangen-Nuremberg and is a specialist in chemoinformatics.

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