



An Introduction to Chemoinformatics

Andrew R. Leach, V.J. Gillet

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This book aims to provide an introduction to the major techniques of chemoinformatics. It is the first text written specifically for this field. The first part of the book deals with the representation of 2D and 3D molecular structures, the calculation of molecular descriptors and the construction of mathematical models. The second part describes other important topics including molecular similarity and diversity, the analysis of large data sets, virtual screening, and library design. Simple illustrative examples are used throughout to illustrate key concepts, supplemented with case studies from the literature.

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