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Titolo	Cheminformatics and its Applications // edited by Amalia Stefaniu, Azhar Rasul, Ghulam Hussain
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Descrizione fisica	1 online resource (xiii, 175 pages)
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Sommario/riassunto	Cheminformatics has emerged as an applied branch of Chemistry that involves multidisciplinary knowledge, connecting related fields such as chemistry, computer science, biology, pharmacology, physics, and mathematical statistics. The book is organized in two sections, including multiple aspects related to advances in the development of informatic tools and their specific use in compound structure databases with various applications in life sciences, mainly in medicinal chemistry, for identification and development of new therapeutically active molecules. The book covers aspects related to genomic analysis, semantic similarity, chemometrics, pattern recognition techniques, chemical reactivity prediction, drug-likeness assessment, bioavailability, biological target recognition, machine-based drug discovery and design. Results from various computational tools and methods are discussed in the context of new compound design and development, sharing promising opportunities, and perspectives.