Expert Systems in Chemistry Research

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Expert systems allow scientists to access, manage, and apply data and specialized knowledge from various disciplines to their own research. **Expert Systems in Chemistry Research** explains the general scientific basis and computational principles behind expert systems and demonstrates how they can improve the efficiency of scientific workflows and support decision-making processes.

Focused initially on clarifying the fundamental concepts, limits, and drawbacks of using computer software to approach human decision making, the author also underscores the importance of putting theory into practice. The book highlights current capabilities for planning and monitoring experiments, scientific data management and interpretation, chemical characterization, problem solving, and methods for encoding chemical data. It also examines the challenges as well as requirements, strategies, and considerations for implementing expert systems effectively in an existing laboratory software environment.

Expert Systems in Chemistry Research covers various artificial intelligence technologies used to support expert systems, including nonlinear statistics, wavelet transforms, artificial neural networks, genetic algorithms, and fuzzy logic. This definitive text provides researchers, scientists, and engineers with a cornerstone resource for developing new applications in chemoinformatics, systems design, and other emerging fields.

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