



Design and Use of Relational Databases in Chemistry

TJ O'Donnell

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Optimize Your Chemical Database

Design and Use of Relational Databases in Chemistry helps programmers and users improve their ability to search and manipulate chemical structures and information, especially when using chemical database "cartridges". It illustrates how the organizational, data integrity, and extensibility properties of relational databases are best utilized when working with chemical information.

The author facilitates an understanding of existing relational database schemas and shows how to design new schemas that contain tables of data and chemical structures. By using database extension cartridges, he provides methods to properly store and search chemical structures. He explains how to download and install a fully functioning database using free, open-source chemical extension cartridges within PostgreSQL. The author also discusses how to access a database on a computer network using both new and existing applications.

Through examples of good database design, this book shows you that relational databases are the best way to store, search, and operate on chemical information.

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