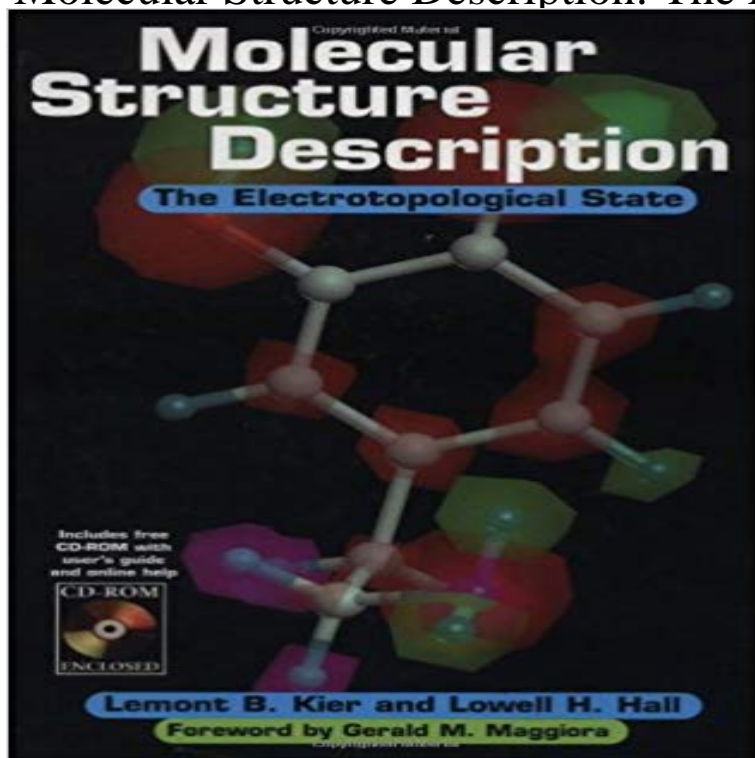


Molecular Structure Description: The Electrotopological State



The entire thrust of industrial drug research is now directed toward the use of predictive methods and strategies to reduce the number of compounds made and tested. Furthermore, these theoretical/computational methods are increasingly part of a general approach to chemical problems. Among non-empirical structure indices, the electrotopological state of atoms in a molecule is a new paradigm, providing a descriptor of intermolecular interactions at submolecular sights that is easy to calculate and information-rich. One of the authors (Hall) has included the E-state in his widely used MOLCONN computer program. Tripos has incorporated this index as an optional module for structure-activity analyses using a new Web-based tool called CHEMenlighten.

Key Features* Reflects the rich experience of the authors as developers of the E-state method* Provides a first-hand account of the origins and use of this new paradigm * Includes E-Calc software on CD-ROM for hands-on experience with the method * Offers strategies for drug design

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Electrotopological State By Lemont B. Kier and Lowell H. Hall. Forward by Gerald M. Maggiora. Academic Press, 1999. **An Electrotopological-State Index for Atoms in Molecules** The electrotopological state (E-state) is presented as a representation of molecular structure useful for definition of a space for chemical structures. This E-state **Topological Indices and Related Descriptors in QSAR and QSPAR - Google Books Result** Molecular Structure Description. The Electrotopological State By Lemont B. Kier and Lowell H. Hall. Forward by Gerald M. Maggiora. Academic Press, 1999. **The E-state as the basis for molecular structure space definition and : Molecular Structure Description: The Electrotopological State: Lemont B. Kier, Lowell H. Hall. Handbook of Molecular Descriptors - Google Books Result** An Electrotopological-State Index for Atoms in Molecules. Pharm. The Molecular Connectivity of Non-Sigma Electrons. Rep. 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(1999) Molecular Structure Description: The Electrotopological State, **Molecular Drug Properties: Measurement and Prediction - Google Books Result** Derivation and significance of valence molecular connectivity. J. Pharm. Sci. Molecular Structure Description: The Electrotopological State. Academic Press **Molecular Structure Description The Electrotopological State** Molecular Structure Description: The Electrotopological State Lemont B. Kier and Lowell H. Hall Academic Press (1999). 2. 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