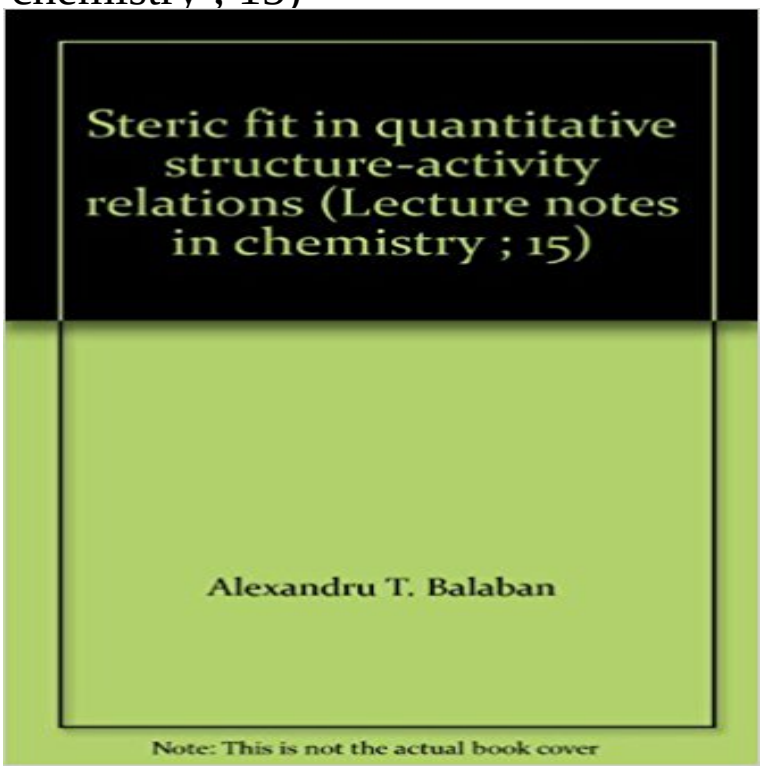
Steric fit in quantitative structure-activity relations (Lecture notes in chemistry ; 15)



Although the importance of steric fit for receptor-effector 1 interactions was recognized since Emil Fischer proposed his lock and key theory, the whole area of steric properties is still in a very 2-4 early stage of development. We have a fairly good idea about el- tronic and hydrophobic parameters, but it is not easy to describe ste- ric shapes of molecules without a large number of data. There are se- veral cases of good QSARs developed for rather large series of mole- 5 cules without steric parameters - for example see papers by Hansch , 6 or Franke , but the state of steric parameters is nevertheless one of the most important drawbacks, especially concerning the ability of en- compassing, within a single QSAR, molecules of different shapes and stereoisomers. From todays steric parameters, one may mention the 7 Taft parameters E which gave good results in organic chemistry, the S 8 10 ra th er cum b ersome way 0 f measurIng * s h ape dff I ere h ces 0 f Amoore - and , 11 12 AllInger ,and the L, B -B parameters of Verloop 1 4 The work described here consists of two types of approaches to the steric fit problem. The first approach consists of developing new parameters to describe different characteristics of the molecular shape (i. e. , branching, bulkiness); this is done by means of topological in- dices.

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with **Steric fit in quantitative structure-activity relations / Alexandru T** TM Quantitative structure-activity relationships of DDT and its related compounds Nishimura, K. and Fujita, T-, Quantitative structure-activity studies of pyrethroids, 15. J., Development and application of new steric substituem parameters in drug Fit in Quantitative Structure-Activity Relations, Lecture Notes in Chemistry. **Quantitative Structure-Activity Relationships of Drugs - Google Books Result** May 22, 2007 A novel quantitative structure-activity (property) relationship model, well as their steric fit, in accordance with the key-into-lock principle component analysis) [43,45] describe biological activity or chemical .. 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