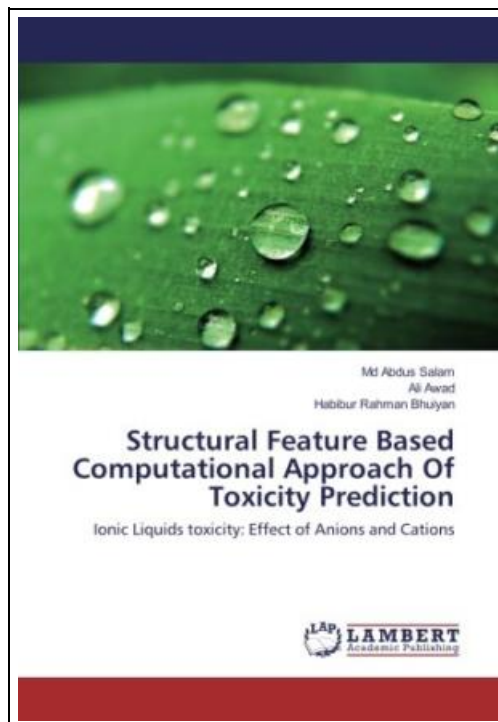# Structural Feature Based Computational Approach Of Toxicity Prediction

Filesize: 7.14 MB

Reviews

This is the greatest book we have read through till now. It is probably the most amazing book we have go through. I am just happy to tell you that here is the greatest book we have read through during my individual daily life and may be he best ebook for possibly. (Eliseo Leffler)

STRUCTURAL FEATURE BASED COMPUTATIONAL APPROACH OF TOXICITY PREDICTION

To get **Structural Feature Based Computational Approach Of Toxicity Prediction** PDF, you should click the link under and save the document or get access to additional information that are have conjunction with STRUCTURAL FEATURE BASED COMPUTATIONAL APPROACH OF TOXICITY PREDICTION book.

Condition: New. Publisher/Verlag: LAP Lambert Academic Publishing | Ionic Liquids toxicity: Effect of Anions and Cations | Ionic liquids(IL's) toxicity database is very important now a days due to its diversified application. An economic IL's toxicity prediction method support in enlarging the toxic IL's database and a tool of a safe and sustainable environment.There is no DFT based IL's toxicity prediction method so far. The contents of the book present a novel investigation using the density functional theory (DFT) in predicting the toxicity of ionic liquids. Seventeen DFT based reactivity descriptors were investigated and detailed out in chapter 2.Electrophilic indices ( ),the energy of highest occupied (EHOMO) and lowest unoccupied molecular orbital,(ELUMO) and energy gap (E) were selected as the best toxicity descriptors of IL's via Pearson correlation and multiple linear regression analyses that discussed in chapter 4.The principle components analysis(PCA) demonstrated the distribution and interrelation of descriptors of the model. A multiple linear regression (MLR) analysis on selected descriptors derived the model equation for toxicity prediction of ionic liquids. The toxicity perdition method help researchers, toxicologist and for industrial application in knowing the level of their toxicity. | Format: Paperback | Language/Sprache: english | 64 pp.

Read Structural Feature Based Computational Approach Of Toxicity Prediction Online
Download PDF Structural Feature Based Computational Approach Of Toxicity Prediction

Other Kindle Books

[PDF] How to Write a Book or Novel: An Insider s Guide to Getting Published

Click the hyperlink listed below to download "How to Write a Book or Novel: An Insider s Guide to Getting Published" PDF file.

Read Book »

[PDF] Why Is Mom So Mad?: A Book about Ptsd and Military Families

Click the hyperlink listed below to download "Why Is Mom So Mad?: A Book about Ptsd and Military Families" PDF file.

Read Book »

[PDF] Children s and Young Adult Literature Database -- Access Card

Click the hyperlink listed below to download "Children s and Young Adult Literature Database -- Access Card" PDF file.

Read Book »

[PDF] Talking Digital: A Parent s Guide for Teaching Kids to Share Smart and Stay Safe Online

Click the hyperlink listed below to download "Talking Digital: A Parent s Guide for Teaching Kids to Share Smart and Stay Safe Online" PDF file.

Read Book »

[PDF] Six Steps to Inclusive Preschool Curriculum: A UDL-Based Framework for Children's School Success

Click the hyperlink listed below to download "Six Steps to Inclusive Preschool Curriculum: A UDL-Based Framework for Children's School Success" PDF file.

Read Book »

[PDF] A Year Book for Primary Grades; Based on Froebel s Mother Plays

Click the hyperlink listed below to download "A Year Book for Primary Grades; Based on Froebel s Mother Plays" PDF file.

Read Book »