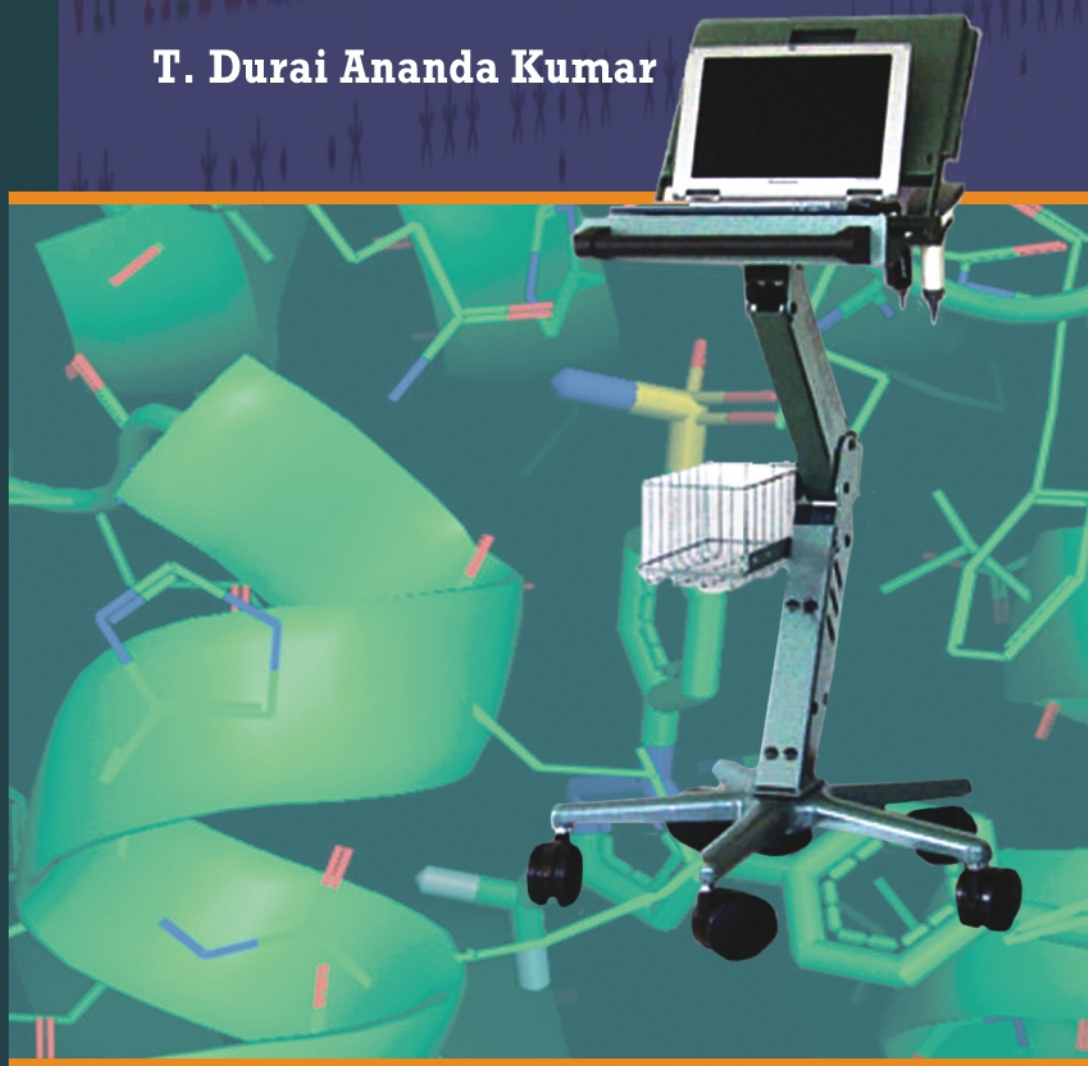




# Elementary Pharmacoinformatics

**T. Durai Ananda Kumar**



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*T. Durai Ananda Kumar*

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Pharmacoinformatics is an informatics based discipline, concerned with the information, design, discovery and development of drugs using high performance computing and graphic tools. This material covers principles and applications of health informatics, cheminformatics and bioinformatics. It comprehensively covers the current advances and in silico strategies used in drug information and drug design. Each of 29 chapters reviews the concepts of pharmacy automation, mechanistic drug design and bioinformatics. The book avoids the use of high level descriptions to convert the subject interesting. This concise source of information will be of immense benefit to the learning community of pharmacy, biotechnology, biomedical engineering and other interdisciplinary fields.

## Distinct features of this book

- Explanations for the entry level student are the important feature of this material
- Neat and self explanatory diagrams are incorporated wherever possible to bring user-friendly material
- Four major parts with 29 chapters proceeds in very systematic and with lucid language
- Each chapter is provided with practical application part, which ensures the better understanding
- Comprehensive overview on in silico methods of drug information and drug design
- Emphasis on molecular level approach of drug design strategies
- The application section of this material provides opportunity to have hands-on-experience

## Contents

1. Databases 2. Data Mining 3. Search Machines 4. Drug Information 5. Pharmacy Automation 6. Drug Discovery 7. Drug Development 8. Drug Design 9. Quantitative Structure Activity Relationship (Qsar) 10. Virtual Screening, 11. Target Identification 12. Molecular Modeling 13. Docking 14. Arguslab 15. Biological Databases, 16. Biophysical Techniques 17. Molecular Biology 18. Homology Modeling 19. Sequence Similarity 20. Dot Matrix 21. Dynamic Programming 22. Heuristic Method 23. Sequence Comparison Methods 24. Phylogenetic Analysis 25. Gene Prediction 26. Scoring System 27. 3D Structure Prediction Using Swiss Model 28. Molecular Visualization, 29. Receptors

## About the Author

**T. Durai Ananda Kumar**, M Pharm, is working as a senior Assistant Professor, in the Department of Pharmaceutical Chemistry, Gokaraju Rangaraju College of Pharmacy, Bachupally, Hyderabad. He is handling Pharmaceutical Organic Chemistry, Medicinal Chemistry and Pharmacoinformatics subjects for B. Pharmacy and M. Pharmacy students. His research activities focus on the synthesis of small molecules, generalization of phase transfer catalysts using DoE and molecular modeling studies on nitrogen heterocycles. He is guiding research projects for M. Pharmacy (Pharmaceutical Chemistry) students. The author is life member of Association of Pharmaceutical Teachers of India and has several research publications in reputed national and international journals.

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