

Template for abstract preparation

INTRODUCTION TO COMPUTER AIDED DRUG DESIGN

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A large sum of money is spent in the research field to get effective drug for a disease, but till date there is no new drug discovered in India because of many reasons. To overcome this, many technologies are now developed like site directed mutagenesis, virtual drug screening, docking study, receptor surface mapping and many more. In early 90's there were a great deal of optimism that computers will play a major role in the improvement of drug design. At present a large sum of money is spent in the research field to get effective drug for a disease, but till date there is no new drug discovered in India because of many reasons. To overcome this, many computational technologies are now developed like Site directed mutagenesis, Virtual drug screening, Docking study, Receptor surface mapping and many more. Such designing of drug is generally computer assisted molecular modeling and does not include dosage analysis, pharmacokinetics. But still they are very useful and suitable today. Now-a-days many computer software packages are available which can help in determining physiochemical property and biological activity of new chemical entities prior to their real synthesis. This will decrease time, money and labor spent on research and making research more target oriented and efficient. The theme is if we are not getting new leads for future then why not to optimize the existing drugs for the benefit of the society.