

# INTRODUCTION

Docking is one of the most common methods used in the virtual screening method based on the structure. The molecular docking method is used to model the interaction between small molecules and proteins at the atomic level, which can be used to describe the behavior of small molecules in the binding site of target proteins. AutoDock is a software for predicting optimal binding conformations of ligands to proteins using different algorithms. This software is the most widely used among researchers who work in the field of computerized drug design, and it has been successfully used in several virtual screenings and the discovery of the Raltegravir drug, an inhibitor of the HIV integrase enzyme.

In this regard, Smart University of Medical Sciences has designed and organized a computational drug design course to teach the basics of docking theory, and introduction to ligand (drug) and protein databases.

## Computational Drug Design Molecular Docking

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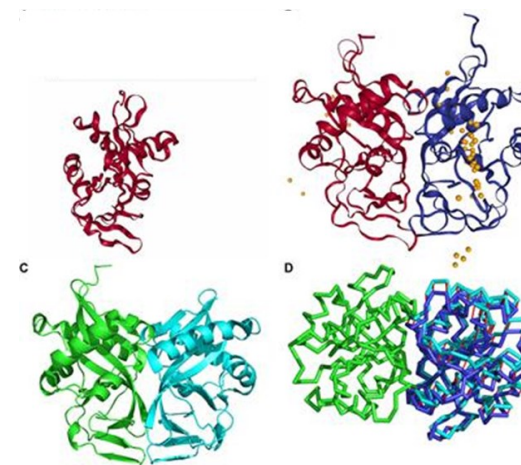


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## COMPUTATIONAL DRUG DESIGN MOLECULAR DOCKING



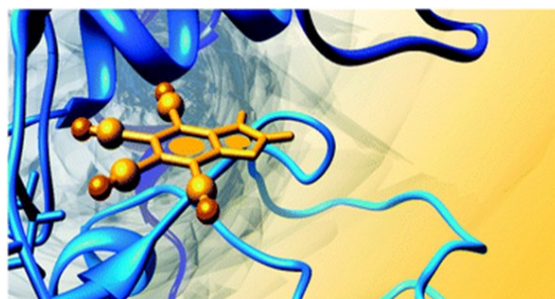
# OBJECTIVES

# COURSE TITLES

# MORE INFO

1

Designing and applying the docking method to discover and design new drugs and using docking in virtual screening to repurpose existing drugs



- Principles of Docking
- Preparation of Macromolecule (protein) Input File
- Preparation of Ligand Structural File
- Autodock and Vina Tutorial
- Extracting and analyzing the results

## Approach:

Offline - At the end of the course, the Q&A session will be held online.

## Language:

Persian

## Certification:

Upon successful completion of the course, students will be issued a certificate jointly signed by Smart University of Medical Sciences

# TARGET GROUP

Graduate students, faculty members, and researchers involved in pharmaceutical research



# SUB.TOPICS

- The ability to screen drugs for the anticipated target in a cost-effective manner
- Investigation and analysis of inhibitor (drug) interaction with the target

