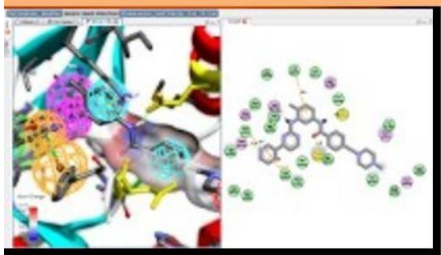
Centurion University
Shaping Lives...
Empowering Communities...

Drug Design Using Biovia



Pre-requisites: Nil
Course Type : Audit (Workshop)
Duration : 30 Hours

Course Objectives:

- To understand the Molecular Modeling Process used in Drug Discovery.
- The concept of Structure and Ligand-based Drug Designing.
- The Molecular Docking processes and their use in drug discovery.
- The Drug-likeness properties of various chemical entities.
- The application of Pharmacophore Modeling in drug discovery.
- To identify potential drug candidates through Virtual Screening of biological compounds.

Learning Outcomes:

- Students will understand the Biovia Tools and their application in drug discovery processes.
- Identify potential biological molecules from synthetic and natural sources by using Biovia.
- Recognize and comprehend various disease targets and select an ideal target for drug discovery.
- Design novel drug candidates for various diseases by using Biovia Discovery Studio.
- Repurpose the already existing drugs for safe and effective medication for various diseases.

Module	Contents	Duration
Module1	• Ligand Structure Handling in Discovery Studio • Introduction to Drug Discovery Processes. Introduction to Biovia Discovery Studio. Ligand sketching using Biovia Discovery Studio. Ligand importing and Handling with Biovia Discovery Studio. Study of Various Chemical and Ligand databases and structure search in the databases. Structure importing from chemical databases and Handling of Large chemical databases. • Practice 1: Create your own Ligand Database using at least 10 natural product molecules and 10 synthetic compounds from published literature with appropriate references enlisted in a word document file. • Protein Structure Handling in Discovery Studio • Practice 2: Identify a disease protein from plant or animal origin and prepare the suitable protein using biovia.	10 hours
Module2	• Drug Receptor Interaction study in Discovery Studio • Theory of Receptor-Ligand Interaction and Molecular Docking. Molecular Docking using Discovery Studio. Lead Identification through Virtual screening. Structure based virtual screening using Discovery Studio.	10 hours
Module3	• Prediction of Ligand properties and Pharmacophore in Discovery Studio • ADMET Descriptors and their theories. Prediction of ADMET properties of Ligands using Discovery Studio. Introduction to pharmacophore model and their use in drug discovery. Pharmacophore modeling using Discovery Studio (Auto Pharmacophore Generation). Pharmacophore modeling using Discovery Studio (Common Feature Pharmacophore Generation). Pharmacophore modeling using Discovery Studio (3D QSAR Pharmacophore Generation). Virtual screening using Pharmacophore model using Discovery Studio.	10 hours
	TOTAL	**30 hours**

Anita Patra

Dr. Anita Patra, Registrar, CUTM

Convenor

Name of the event:

Drug Discovery using BIOVIA

Total number of

participants: 50

Date : 19/05/2018

In drug discovery, scientists now explore chemical space by “learning” from real experiments. The enumeration of all molecules that could be drugs is not currently possible with reasonable resources. However, chemists can use AI and machine learning to explore a large area of chemical space through an iterative generative design process with a fitness function that represents the target product profile. The discovery cycle combines virtual and real (V+R) activities in which the results of virtual generation and evaluation combine with real world synthesis and testing to allow active learning.

Participants during the programme on 19.05.2018

Novel molecules advanced by the virtual ‘generate-test-score ’pruning process move to the lab for synthesis and screening. Real world screening results allow the update of predictive models for subsequent cycles. Optimization of all objectives continues until the target therapeutic profile is met. This iterative V+R cycle accelerates lead candidate design with

improved quality, significantly reducing costs of experimentation and advancing only the most promising candidates to clinical trials.

The followings were the objectives of the programme:

- To learn the tools of BIOVIA in detail,
- To learn about Drug Designing,
- To learn about detailed Protein structure, pharmacophore, basics of Docking and Discovery studio and application in Agriculture, Fisheries and others Sciences
- To learn about the fundamental of Nano Materials and its application in Agriculture, Fisheries and others Sciences

The followings were the learning outcomes of the programme:

- Products/ Patents/ Publications
- To be able to design a drug molecule and identify its applications
- To be able to analyze nanomaterials and use it as Bio-Pesticides and Biofertilizers,
- To be able to design a drug molecule and identify its applications.
- To be able to illustrate the structure of Protein, Pharmacophores and also able to handle Discovery Studio completelyThe following modules were discussed in the event :

Identification of pharmacophore (Automatic/Manually)

Functionalisation of a molecule and study its potential as a drug

Anita Patra

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Convener

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List of Participants
Name of Event: Drug Design Using Biovia
Organized by: Centurion University of Technology and Management Date: 9 April 2018 (Drug Design Using Biovia) and 19 May 2018 (DrugDiscovery using Biovia)

Event Description: Drug Design Using Biovia, webinar was organized in the year of 2017-18. By Centurion University of Technology and Management.

List of Participants:

S. No.	Name	Reg. No.	Presence
1	DIGVIJAY BEHERA	170101120001	Present
2	YEDLA DEEPIKA	170101120002	Present
3	DEBASIS PADHY	170101120003	Present
4	ANKADALA KARUNAKAR	170101120004	Present
5	VALLA PRIYANKA	170101120005	Present
6	REVALLA VIDYA SRI	170101120006	Present
7	DIBYA SAMBIT SAHU	170101120007	Present
8	SEPHALI PANDA	170101120011	Present
9	SOUMYA DEEPTO DASH	170101120012	Present
10	YALALA SANDEEP KUMAR	170101120013	Present
11	M. SAI SPANDANA	170101120014	Present
12	SIRIPURAM LAKSHMI PRASANNA	170101120015	Present
13	CHIKATI DIVYA TEJA	170101120016	Present
14	T. GREESHMA	170101120017	Present
15	VOONA SRIJA	170101120019	Present
16	P. HARSHAVARDHAN	170101120020	Present
17	PRANAY RAJ	170101120021	Present
18	BADAL CHOUDHURY	170101120022	Present
19	G. PAVAN KALYAN	170101120023	Present
20	MONALISA PRADHAN	170101120024	Present
21	SAASWAT PANIGRAHI	170101120025	Present
22	KOTTURU SAI	170101120026	Present
23	ROUTHU DIVYA	170101120028	Present
24	POREDDI PRIYANKA	170101120029	Present
25	METTA DEVENDRA PRASAD	170101120030	Absent
26	ALIBILLI MAHESH	170101120032	Present

27	AYUSHI MISHRA	170101120034	Present
28	DEVARACHETTY SRIYA	170101120035	Present
29	POTNURU MANIKANTA	170101120036	Present
30	KILLAMSETTY PRAVEENA	170101120038	Present
31	TULUGU RAHUL	170101120039	Present
32	DARAPU ABHISHEK	170101120040	Present
33	HRUDANAND NIAL	170101120041	Present
34	DAYA SHANKAR ROUT	170101120043	Present
35	VYSYA RAJU SAI SIRISHA	170101120044	Present
36	ROUTH KARTHIK	170101120045	Present
37	AMOSH KHURA	170101120046	Present
38	ROSHAN KAJUR	170101120047	Present
39	MAJJI REENA	170101120048	Present
40	B.NAGA SATISH KUMAR REDDY	170101120049	Present
41	LAKSHMI NARAYANA MANUKONDA	170101120050	Present
42	ANDHAVARAPU ANUSHA	170101120051	Present
43	PINTU KARJEE	170101120052	Present
44	DHARAM NISHAN MISHAL	170101120053	Present
45	AYUBA BHUYAN	170101120054	Present
46	GONDRU KIRAN KUMAR	170101120055	Present
47	SANJANA SINGH	170101120056	Present
48	PREETI PADMA PATRO	170101120057	Present
49	PADALA VENKATESH	170101120058	Present
50	SAROJ KUMAR NAYAK	170101120059	Present
28	DEVARACHETTY SRIYA	170101120035	Present

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Convener