Drug Designing Winter Training

NTHRYS provides Drug Designing Winter Training for interested candidates at its Hyderabad facility, Telangana. Please refer below for more details including Fee strctures, Eligibility, Protocols and Modules etc.,. Please do call / message / whatsapp for more details on 9014935156 [India - +91]

Eligibility: BSc / BTech / MSc / MTech / MPhil / PhD in any Life Sciences studying or completed students

Protocols / Techniques Covered

Module - I - Molecular Modeling

1. Homology Modeling
2. Threading and fold recognition
3. Ab-initio prediction
1. Homology Modeling
    1. Template detection (Tools: BLAST,FASTA,PDB-Blast)
    2. Target –Template Alignment (Clustalw, Smith-Waterman)
    3. Backbone generation
    4. Modeling of side chains and loops (Modeller, CPH-Modeller, Swiss-Model)
    5. Model validation and optimization (WHATCHECK,VERIFY-3D, ERRAT)
2. Threading of Fold Recognition:
    1. 2D Threading [Tools: CASP, Gene Threader, 3DPSSM]
    2. 3D Threading
3. Ab-initio prediction - Theory

Module - II - Drug Designing

1. Structure Based Drug Design (SBDD)
2. Ligand Based Drug Design (LBDD)

1. Structure Based Drug Design

1. Collection of Structure
    1. Known structure (PDB)
    2. Unknown Structure (Homology Modeling)
2. Structure Validation
    1. Profiles 3D
    2. Ramachandran Plot
    3. Disorder Analysis
3. Defining Binding sites
4. Small molecules search from databases (ZIN,C TCM, Drug bank,KEGG,PubChem)
5. ADMET Check
6. Docking
    1. Candidates from docking result
    2. Candidate from bioactivity prediction
7. Protein – Ligand complex formation
8. Molecular Dynamic simulation (MD simulation)
9. Thermodynamics Study:
    1. state of system
    2. changing state of system
    3. Conversation of energy
    4. Applied first law
    5. study flow energy equation
10. Molecular Mechanics
    1. Derivatives of molecular mechanics energy function
11. Force field calculation:
    1. Bond angle
    2. Bond Bending
    3. Bond stretching
    4. Angle bending
    5. Torsion terms
    6. Non-bonded interactions
    7. Electrostatic interactions
    8. Modeling Van der Waals interactions
    9. Hydrogen bonding in molecular mechanics
    10. Monte Carlo simulations (Algorithm)
12. Energy minimization & Optimization:
    1. Root Mean Square Deviation calculation (RMSD)
    2. Radius of Gyration
    3. Root Mean Square Function Calculation
    4. Dictionary of protein secondary structure analysis
    5. Energy calculation of system
    6. Mean square displacement
    7. Distance analysis of molecular interactions
    8. Torsion angle calculation
    9. Principle component analysis
    10. Estimation of molecular pathways

11. Disorder analysis
12. Clustering analysis

13. Potential Lead compound

Module - III

1. Ligand Based Drug Design
    1. Small molecule with bioactivity
        1. Docking
            1. Evaluating Co-relation
            2. Obtained Co-efficients
            3. Weighted score models
        2. Molecular properties check
        3. Descriptors selection by genetic algorithm
            1. Multiple linear regression models
            2. Support vector machine (SVM)
            3. Bayesian Networks Models
        4. QSAR(Quantitative Structure Activity Relationship)
            1. Comparative molecular field analysis (COMFA)
            2. Comparative molecular similarity index analysis (COMSIA)
            3. 3D QSAR Pharmacophor model
    2. Bioactivity prediction
    3. Protein –Ligand complex
    4. Molecular Dynamic Simulation,energy minimization and optimization
        1. Root mean square deviation (RMSD)
        2. Radius of Gyration
        3. Root Mean Square Function Calculation
        4. Dictionary of protein secondary structure analysis
        5. Energy calculation of system
        6. Mean square displacement
        7. Distance analysis of molecular interactions
        8. Torsion angle calculation
        9. Principle component analysis
        10. Estimation of molecular pathways
        11. Disorder analysis
        12. Clustering analysis
    5. Potential Lead compound

5 Days - Module - I, 6 Hours Work a day
10 Days - Module - I + Docking, 6 Hours Work a day
20 Days - Module - I & II, 4 Hours work a day
1 Month - Module - I,II & 1.1 of Module III, 4 Hours work a day
45 Days - Modules - I, II & III, 4 Hours work a day
Note: International Institution Students [Even Indian Nationals studying or studied at abroad] will be charged 20% extra to the fee given below.

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Fee details in Rs per student					
Fee	5 Days	10 Days	20 days	1 Month	45 Days
Individual	30700	32400	42000	52700	63100
Group 2 - 4	29000	29000	39800	50200	60100
Group 5 - 7	28700	28700	39300	49700	59400
Group 8 - 10	28400	28400	38900	49200	58800