

**MODULES FOR SUMMER/WINTER TRAINING IN COMPUTATIONAL APPROACHES AND WORKING IN
MEDICINAL/ORGANIC CHEMISTRY RESEARCH LABS**

One Day Series: Module –I

Name of the Modules	Molecular Docking: Computational approaches in Drug Design
Techniques covers	Lecture-I: Introduction to docking and its importance Demonstration of Sybyl software: <ul style="list-style-type: none">• Drawing and energy minimization of ligand• Editing of protein structure• Ligand-protein docking• Result analysis and understanding bio-molecular interactions• Scope for further structural modification Lecture-II: Case studies

Number of students: 60-70

Charges: Rs. 250/ per student

Note 1: Does not include accommodation and food

Two Days Series: Module –II

Name of the Modules	Molecular Docking: Computational approaches in Drug Design
Techniques covers	Day -1 Lecture-I: Introduction to docking and its importance. Demonstration of Sybyl software: <ul style="list-style-type: none">• Drawing and energy minimization of ligand• Editing of protein structure• Ligand-protein docking• Result analysis and understanding bio-molecular interactions• Scope for further structural modification Lecture-II: Case studies
	Day -2 Hands on Training only for molecular docking

Number of students: 10

Charges: Rs. 500/ per student

Note 1: Does not include accommodation and food

One Week: Module –III

Name of the Modules	Molecular Docking: Computational approaches in Drug Design and 3D-QSAR
Techniques covers	<p>Day-1</p> <p>Lecture-I: Introduction to docking and its importance.</p> <p>Demonstration of Sybyl software:</p> <ul style="list-style-type: none"> • Drawing and energy minimization of ligand • Editing of protein structure • Ligand-protein docking • Result analysis and understanding bio-molecular interactions • Scope for further structural modification <p>Lecture-II: Case studies</p> <p>Day -2</p> <p>Hands on training</p>
	3D-QSAR in Drug Design and Development
	<p>Day -3</p> <p>Lecture-III :</p> <ul style="list-style-type: none"> • Introduction on SAR and QSAR • 3D-QSAR Modeling,; • COMFA and COMSIA studies <p>Demonstration of Sybyl software:</p> <ul style="list-style-type: none"> • Execution of QSAR study using the software • Analysis of the result • Lead optimization <p>Day -4</p> <p>Hands on training</p> <p>Day -5</p> <p>Lecture IV:</p> <p>Application of Molecular Docking and QSAR in Drug Discovery</p>

Number of students: 10

Charges: Rs. 2000/ per student

Note 1: Does not include accommodation and food

One Month: Module -IV

Name of the module	Working in Organic / Medicinal Chemistry Research Labs
Techniques covers	1.Lecture: <ul style="list-style-type: none">• Set up of organic lab• Proper placement and precautions for chemicals & solvents• Basic requirements to work in organic chemistry lab• Writing of experimental details and recording of the results.• Protocol: From Setting up a reaction to purification• Safety aspects and preventive measures 2.Training: <ul style="list-style-type: none">• Setting up, monitoring and work-up of a reaction• Purification of the desired product (chromatography techniques)• Use of different instruments and equipment during reactions. 3.Identification of the product- <ul style="list-style-type: none">• Determination of Melting point• Recording of IR spectra and its interpretation• Recording of Mass spectra and its interpretation

Number of students: Limited to 10-15 students

Charges: Rs. 9,000/ per student

Note 1: Does not include accommodation and food