

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

**One Day Series: Module –I**

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

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

**Number of students: 25-30**

**Charges: Rs. 500/ per student**

**Note 1: Does not include accommodation and food**

**Note2: Hands on training with their laptop**

**One Week: Module –III**

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

**Number of students: 25 - 30**

**Charges: Rs. 2000/ per student**

**Note 1: Does not include accommodation and food**

**Note2: Hands on training with their laptop**

**One Month: Module -IV**

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

**Number of students: Limited to 10-15 students**

**Charges: Rs. 9,000/ per student**

**Note 1: Does not include accommodation and food**