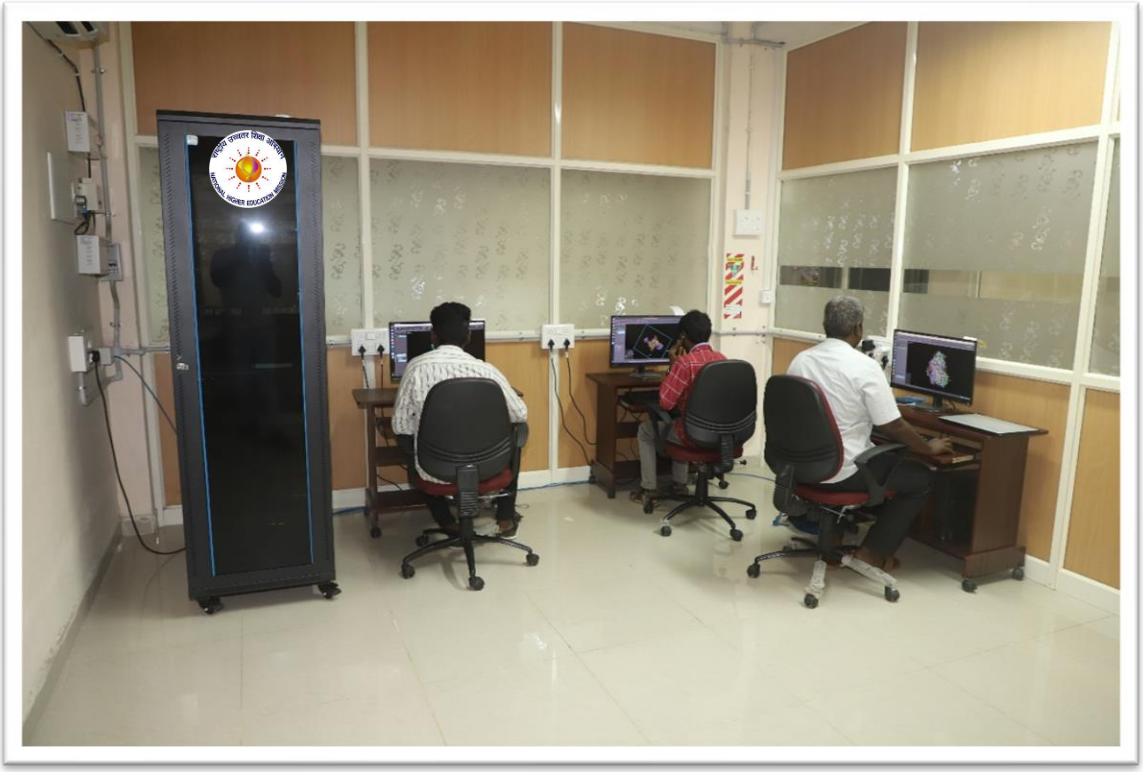
Molecular Modelling Facility

Molecular Modelling Facility is a comprehensive software package developed by Schrödinger, Inc. It is designed for molecular modelling, simulations, and computational chemistry research. This facility provides a wide range of tools and algorithms for studying molecular structures, properties, and interactions.



Key Features and Capabilities:

1. **Molecular Visualization:** Advanced molecular visualization tools allow users to visualize and interact with molecular structures in 3D. This helps in analyzing molecular geometry, conformational changes, and molecular interactions.
2. **Quantum Mechanics Simulations:** Schrödinger's provides powerful quantum mechanics simulation capabilities for studying molecular electronic structure and properties.
3. **Molecular Dynamics Simulations:** The software supports molecular dynamics simulations for studying the dynamic behavior of molecules and molecular systems over time. This includes simulations of protein-ligand interactions, protein folding, and molecular diffusion.

4. **Structure-Based Drug Design:** This facility includes tools for structure-based drug design, allowing researchers to predict and optimize the binding affinity of small molecules to target proteins. This is useful in drug discovery and development.
5. **Quantitative Structure-Activity Relationship (QSAR) Modeling:** The software provides tools for QSAR modeling, which is used to predict the biological activity of chemical compounds based on their molecular structure. This is important in rational drug design and toxicity prediction.
6. **High-Throughput Screening:** It supports high-throughput virtual screening of chemical libraries against target proteins, enabling the rapid identification of potential drug candidates.
7. **Integration and Workflow Automation:** The facility integrates seamlessly with other computational chemistry tools and databases, allowing users to streamline their workflows and automate repetitive tasks.

Overall, this facility is a powerful platform for molecular modeling and computational chemistry research, widely used by academic researchers, pharmaceutical companies, and biotechnology firms.

Details of MMF

<table>
<tr><th>Hardware Specifications</th><th>Software Specifications</th></tr>
<tr><td rowspan="2"><u>Lenovo SR650 Rack Server- 1 No</u>
Intel Xenon Silver 4214 12C 85W 2.2GHz Processor
32GB TRUDDR4 2933MHz RDIMM
2*2.5’ 1.2 TB10k SAS 12GB Hotswap 512n Hard Disk
2*2.5’ 480GB 6GB Hotswap SSD Harddisk
Nvidia Quadro RTX5000 16GB Graphic card</td><td><u>SCHRODINGER Inc.</u>
Tokens for interchangeable library including ConfGen, Epik, Glide, Impact, LigPrep, MacroModel, Prime, QikProp, SiteMap</td></tr>
<tr><td>KNIME Access Licence</td></tr>
<tr><td>Lenovo Thinkcentre- Client system – 3 No
Intel Core i5 10th Gen, Intel B460 Motherboard
8GB DDR4 memory; 1 TB SATA Hard disk
Nvidia 2 GB Graphic card</td><td>Maestro Access Licence</td></tr>
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