Objective of the Workshop

1. To familiarize basic concepts of computational chemistry/biology for drug design
2. Hands on training in various computational chemistry/biology packages
3. Case studies on drug discovery projects using CADD methods

The workshop is so designed that the participants would spend about 50% of their time in learning from lectures covering basic concepts of computational chemistry with emphasis on drug design and drug discovery. The other 50% of the time will be spent on hands-on experience on useful computational chemistry tools applied to drug design and drug discovery through elucidation of some case studies.

Selection of Participants

Eligibility criteria:

1. Candidates with background relevant to the workshop at graduate level with a minimum of 50% marks in their final year of the last degree or a minimum of 70% in the GATE/UGC-NET/NET/SET.
2. Candidates with research interests in simulation and modelling of complex systems.

Submission of application:

Application forms can be downloaded from the CMSD website in pdf format and must be accompanied by the relevant degree certificates in hard copy and must be sent to the CMSD, UoH, Hyderabad.

Registration:

1. Payment of the full registration fee is mandatory (Rs. 2500).
2. Registration form should be accompanied by a recent photograph and signature of the candidate.
3. Selection of participants will be based on the merit list of the applicants and on the content of their CV.

Registration Form

Name:
Designation:
Institution:
Address:
Contact Phone(s):
E-mail:

TECHNICAL PROGRAM

Day 1: Quantum Mechanics

Aug 2: Quantum Mechanics
1. M. Dorgra (IITM), G. N. Satyam (IITM), R. Shankar (IITM) & S. Sanjay (IITM)
2. Workshop: Hands on training
3. Practice: 6.30 PM - 8.00 PM

Day 2: Molecular Mechanics and Dynamics

Aug 3: Molecular Mechanics and Dynamics
1. Abhishek Mita (IITM), R. N. Nagaiah (IITM), B. Jaya Prakash (IITM) & S. Sanjay (IITM)
2. Workshop: Hands on training
3. Practice: 6.30 PM - 8.00 PM

Day 3: Sequence Analysis, Structure Prediction and Docking

Aug 4: Sequence Analysis, Structure Prediction and Docking
1. Lalitha Gopinath (IITM), SreeHarsha Vedeti (IITM)
2. Workshop: Hands on training
3. Practice: 6.30 PM - 8.00 PM

Day 4: QSAR

Aug 5: QSAR
1. Anand Kondapu (IITM), SreeHarsha Vedeti (IITM)
2. Workshop: Hands on training
3. Practice: 6.30 PM - 8.00 PM

Day 5: Free Energy Calculation Methods

Aug 6: Free Energy Calculation Methods
1. K. N. M. Prathyushchandara (IITM), B. Jaya Prakash (IITM) & S. Sanjay (IITM)
2. Workshop: Hands on training
3. Practice: 6.30 PM - 8.00 PM

Day 6: Drug Design

Aug 7: Drug Design
1. Rami Reddy (IITM), A. S. Sanjay (IITM)
2. Workshop: Hands on training
3. Practice: 6.30 PM - 8.00 PM