Integrative Modeling of Macromolecular RNA Structures

Dates: 27-29 August 2018. **Venue:** Center for Ecological Sciences (CES) Seminar Room, 3rd Floor, Biological Sciences Building, IISc-Bangalore
Lecturers: Dhananjay Bhattacharya (DB), Anand Srivastava (AS), Samuela Pasquali (SP), Mahavir Singh (MS)

August 27, 2018 (Monday)

9:00 AM-9:15 AM: Kickoff

9:15 AM-10:45 AM: Lecture 1 (MS)
Fundamentals of RNA structure (primary, secondary, tertiary, structure of various simple and complex motifs, building blocks of macromolecular RNA structure) Structure of long NC-RNA

10:45 AM-11:15 AM: Coffee break

11:15 AM-1:00 PM: Lecture 2 (DB)
Base pairing interactions (Watson-Crick and non-canonical) in RNA, how to detect these, how stable are these, how to understand their structural variations

1:00 PM-2:15 PM: Lunch Break

2:15 PM-4:00 PM: Lecture 3 + Ground work for Hands On 2 (DB)
Geometric parameters based modeling of NTs with canonical and non-canonical base pairs (generally atomistic models, which can be used for all-atom MD simulations.) (~2.0 hours)

4:00 PM-4:30 PM: Coffee break

4:30 PM-6:30 PM: Hands On 1
Usage of tools such as X3DNA, BPFIND, NUPARM. Also, teach numerical characterization of parameters for canonical and non-canonical BPs

---

August 28, 2018 (Tuesday)

9:15 AM-11:00 AM: Lecture 4 (SP)
Investigating RNA 3D structures (predictions and dynamical behavior) and general review on RNA atomistic and coarse-grained force fields.

11:00 AM-11:30 AM: Coffee break

11:45 AM-12:45 PM: Open Research Seminar(DB) CES/Main Auditorium
Title: Computer Simulation of Nucleic Acid Structures: Oligomer or Polymer

1:00 PM-2:15 PM: Lunch Break

2:15 PM-3:45 PM: Lecture 5 + Groundwork for Hands On 2 (AS)
General concepts in Coarse-Graining (CG) and advance sampling techniques in molecular simulation. Application on RNA systems

3:45 PM-4:15 PM: Coffee break

4:30 PM-6:30 PM: Hands On 2
AA and CG simulation of RNA structure and analysis details/protocols. Conformational variability in RNA by advance sampling techniques

---

August 29, 2018 (Wednesday)

9:15 AM-10:45 AM: Lecture 6 (MS)
Biophysical experiments in structural biology of RNA. Details of experimental methods to study RNA secondary structures and spectroscopy methods used in 3D-RNA structure determination (including NMR, CD, UV/VIS and fluorescence spectroscopy methods)

10:45 AM-11:15 AM: Coffee break

11:15 AM-1:00 PM: Lecture 7 (SP/AS) Groundwork for Hands On 3
Discussion on electrostatics (ions and pH) in RNA modeling. Lecture on HiRE-RNA model with focus on how include experimental constraints (SHAPE/ SAXS/ NMR/ FRET etc)

1:00 PM-2:15 PM: Lunch Break

2:30 PM-3:30 PM. Open Research Seminar (SP) in Main Auditorium
Title: Multifunctional energy landscape for an RNA G-quadruplex: an innate molecular switch

3:45 PM-4:15 PM: Coffee break

4:15 PM-6:30 PM: Hands On 3
Experiment-guided Molecular Simulations of RNA structures