Lecturers: Dhananjay Bhattacharya (DB), Anand Srivastava (AS), Samuela Pasquali (SP), Mahavir Singh (MS)

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 (~ 1.5 hours)

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, etc (~1.5 hours)

Lecture 3 (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)

Lecture 4 (SP): A general review on RNA atomistic force fields, which should follow DB's second lecture. This can also contain a session on importance of electrostatics for DNA and RNA and different strategies for dealing with the ions in simulation framework. (~2 hours)

Lecture 5/6 (AS+SP): Discuss the general concepts in Coarse-Graining (CG) by AS. SP will follow this lecture with RNA specific discussions on CG with focus on HiRE-RNA model from her lab. (~2-3 hours)

Lecture 7 (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) (~2 hours)

Lecture 8 (SP): Discuss the various 3D prediction methods (general overview of the strategies of the ones that are mainly used) (~1-2 hours)

Lecture 9 (AS): Detail discussion on advance sampling techniques in molecular simulation (with focus on metadynamics and replica exchange) and go into details of how to use that in RNA structure determination. Concept of CV-driven advance sampling, extended Hamiltonian and free-energy minimization) (~3 hours)

Lecture 10 (SP): Discuss how to include local constraints and SHAPE (which is still very much up for debate as per SP) and describe SAXS and discuss how to use SAXS data both with Svergund's tools and with CG. AS lab is preparing hands-on modules (details below) (~2-3 hours)

Hands On (Mostly to be done by AS with help of student volunteers)

Hands On 1: Usage of tools such as X3DNA, BPFIND, NUPARM. Also, teach numerical characterization of parameters for canonical and non-canonical BPs. (2 hours)

Hands On 2: CG simulation of RNA structure and analysis details/protocols. SHAPE data incorporation (if possible – nontrivial exercise – should do on simple motifs) (3 hours)

Hands On 3: NMR guided CGMD simulation of RNA systems. (3 hours)

Hands On 4: SAXS driven molecular simulation on RNA structure. AS lab will coordinate/modulate all the hands on modules. (3 hours)