## Three-dimensional RNA structures from the NMR chemical shift values

RNA synthesis, regulation and metabolism form one of the key topics in biochemistry and structural biology. The deceptively simple Central Dogma of Life: DNA→RNA→protein, in fact involves thousands of complex biochemical pathways that use RNA molecules of diverse sizes and shapes. These essential molecules of Life carry many intricate functions and their atomic structures are rich in variety.

The first step towards understanding how things work in Nature is to visualize molecular processes in space and time. Nuclear magnetic resonance (NMR) spectroscopy is a powerful method of 3D-imaging of living matter at the molecular level with high spatial resolution. NMR is used for studying molecules and processes noninvasively in their natural environment. The quest for 3D structure in NMR spectroscopy starts from assigning individual resonances – chemical shifts in the NMR spectrum to the specific nuclei in the macromolecule. Subsequently, multidimensional correlation experiments are performed, which yield distance constraints for solving and refining the 3D structure *in silico*. These experiments often take weeks and months. For proteins, methods have been developed to bypass these experiments by directly using chemical shift values for structure determination. For RNA, however, these methods are yet to be developed.

The goal of the project is to perform the first steps in this direction. The project will involve computational analyses of the database of the RNA chemical shift values, which are stored in the Biologic Magnetic Resonance Bank (BMRB). The aim will be (i) to classify and subdivide the RNA sequences / structures on common, structurally-independent blocks and (ii) to analyze similarities between the chemical shift values of these blocks and their dependence on the local structure of the ribose ring, hydrogen bonding of the nucleobase moiety and the RNA helix parameters.

The project will involve learning, using, and achieving proficiency in:

- CcpNMR, a graphics-based interactive NMR assignment and project management program

- Igor Pro, an extraordinarily powerful and extensible scientific graphing, data analysis, image processing and programming software tool for scientists and engineers

- PyMOL & MolMol, impressive software tools for viewing, editing and rendering of 3D molecular structures

- basic programming in the full-featured structured programming language within the Igor Pro interface

- local fitting with general functions and basic knowledge of mathematical statistics

- deep knowledge of RNA structure and function