Conformational Dynamics in Biomolecular Recognition
& Optimization of NMR Experiments for Ultrahigh Magnetic Fields

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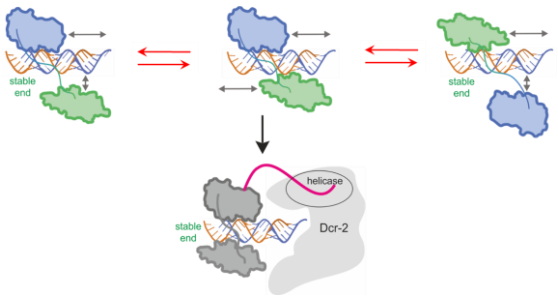
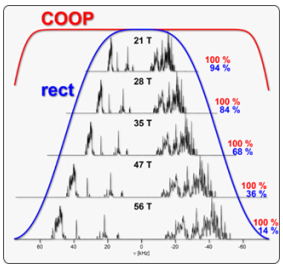
Protein-RNA interactions play essential roles in virtually all aspects of gene regulation, where single- or doublestranded RNAs are recognized by RNA binding proteins (RBPs). Most eukaryotic RBPs are multi-domain proteins that comprise multiple structural domains to mediate protein-RNA or protein-protein recognition often employing avidity, cooperativity and dynamic interactions [1-5].



We employ integrative structural biology to unravel the molecular mechanisms involving these regulatory RNP (ribonucleoprotein) complexes. For these studies, solution NMR-spectroscopy and SAXS/SANS provide unique information on functionally important dynamics and are combined with X-ray crystallography and electron microscopy to elucidate the structural mechanisms and dynamics of regulatory RNPs.

Recent progress will be presented that highlight the role of conformational dynamics and population shifts in molecular recognition of single- and double-stranded RNA by RBPs involved in splicing regulation and microRNA biogenesis.

Current progress will also be presented on the development of radiofrequency pulses and pulse elements using optimal control methods to enable NMR spectroscopy at ultrahigh magnetic fields (>1 GHz) which we pursue in collaboration with the Glaser lab at TUM. We have previously developed an ultrabroadband decoupling scheme with minimal decoupling artifacts at modest *rf* power [6]. We are now implementing cooperative pulses to achieve broadband excitation and chemical shift evolution in common biomolecular NMR pulse sequences with improved performance at current and future available magnetic fields.



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