NMR based structure calculations

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The course outline is the following:

- Molecular Structure: Conformation, Supramolecular structure
- Structure and dynamics: Strategies of NMR structure calculations
- Basics of Molecular Mechanics
- Force fields
- Energy minimisation for geometry optimisation
- Molecular Dynamics and simulated annealing
- Restrained MD
- NMR parameters used in structure calculation: NOE, 1H/2D exchange rates, Vicinal Scalar Coupling, Chemical Shift, RDC, PRE
- Practical aspects of NOEs
- Structure determination with NMR data
- Simulation protocols
- Validation