

Biomolecular Nuclear Magnetic Resonance Spectroscopy

BASIC CONCEPTS OF NMR

- **How does NMR work?**
- **Pulse FT NMR**
- **Resonance assignment**

**NMR text: Chapter 22 in *Protein and Peptide Drug Analysis*
“Solution Structure Determination of Proteins by NMR”**

NMR in Medicine and Biology

- **MRI- Magnetic Resonance Imaging (water)**
- **In-vivo spectroscopy (metabolites)**
- **Solid-state NMR (large structures)**
- ***Solution NMR***
 - **Bioanalytical, primary structure**
 - **Three-dimensional structure**
 - **Molecular motions**
 - **Molecular interactions- binding, reactions**
Ligand screening (Pharma)

Nuclear Spin

- Nuclear spin angular momentum is a quantized property of the nucleus in each atom, which arises from the sub-atomic properties of neutrons and protons
- The nuclear spin angular momentum of each atom is represented by a nuclear spin quantum number (I)
- All nuclei with odd mass numbers have $I=1/2, 3/2, \dots$
- Nuclei with even mass numbers and an even number of protons have $I=0$
- Nuclei with even mass numbers and an odd number of protons have $I=1, 2, 3, \dots$

Biomolecular NMR: primarily spin 1/2 nuclei (^1H , ^{13}C , ^{15}N , ^{31}P)