NMR User Training for Industry

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Global Research & Development

Focus Areas

- Basic Concepts
- Sample Preparation
- Experiments
- Interpretation

Basic Concepts (B.S./M.S.)

- Superconducting magnets; field strengths
- Basic one-pulse expt
  - RF pulse, excitation, relaxation, FID, FT
- Most common NMR active nuclei
- General block diagram of a spectrometer
- Understand tune, lock and shim
- When to use NMR
  - structural elucidations; used w/ MS, IR, etc.

Sample Preparation (All)

- Sensitivity compared to other techniques
- Purity requirements
- Quantity vs. solubility (for liquids)
- Effect of residual solids or salts (for liquids)
- Sample volume
  - effect on sensitivity
  - effect on shimming
- Ph.D. only: SSNMR sample requirements

Experiments (B.S./M.S.)

- Required:
  - Set parameters, acquire & process 1D proton and carbon data
  - Set parameters, acquire & process 2D homonuclear proton data
  - Archive and retrieve data
- Recommended:
  - Set parameters, acquire & process 2D heteronuclear data (inverse detection)
  - Lock and shim manually

Experiments (Ph.D.)

- Required:
  - Set parameters, acquire & process 2D gradient heteronuclear inverse expts
  - Understand symmetrization, digital filtering, linear prediction, apodization
  - Familiarity w/ other nuclei (^{19}F, ^{15}N, ^{31}P)
- Recommended:
  - Perform linear prediction, apodization & baseline correction
  - Perform spectral simulations

Interpretation (B.S./M.S.)

- Required:
  - Proton chemical shifts, multiplicity, scalar couplings, integration
  - nOe & homonuclear decoupling
  - Carbon chemical shifts, coupling to other nuclei (^{1}H, ^{19}F), relative peak intensities
  - DEPT, APT, quantitative carbon
  - 2D homonuclear correlations
- Recommended:
  - T_1 relaxation

Interpretation (Ph.D.)

- Required:
  - 2D short-range and long-range heteronuclear correlations
  - Appropriate selection of experiments to address specific questions
- Recommended:
  - Chemical exchange
  - T_1 relaxation