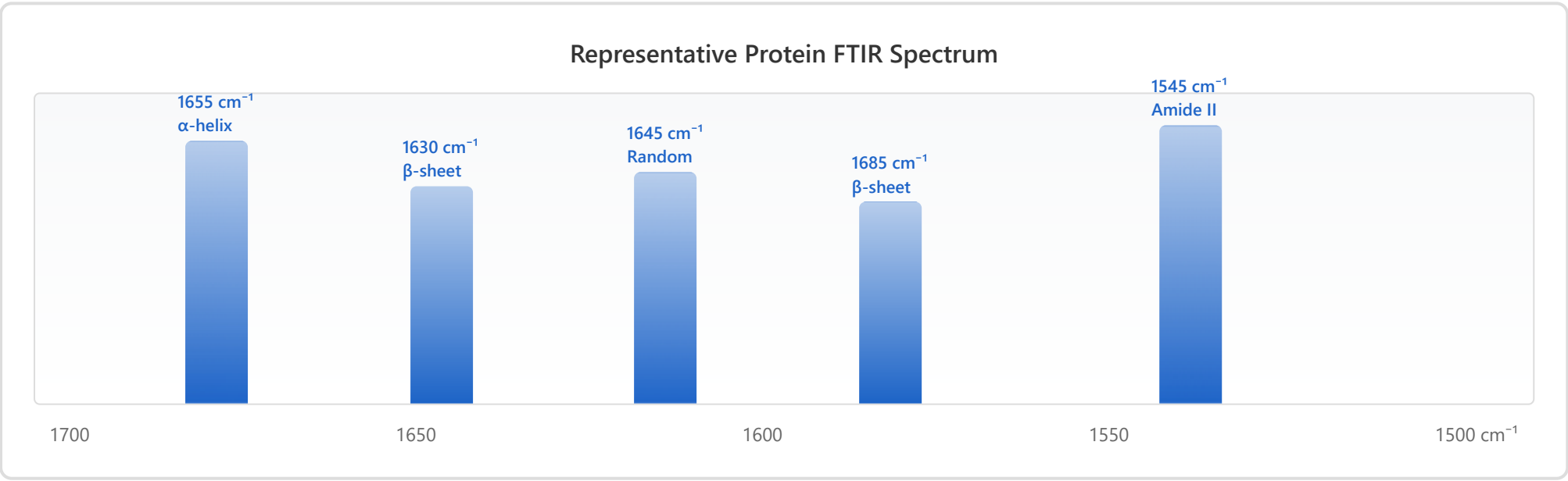
FTIR for Biomolecules

Amide Bands

- Amide I (1600-1700 cm^{-1}): C=O stretch, secondary structure sensitive
- Amide II (1510-1580 cm^{-1}): N-H bend, C-N stretch
- α-helix: 1650-1658 | β-sheet: 1620-1640, 1680-1690 | Random: 1640-1650



Secondary Structure Characteristics

α-helix

1650-1658 cm^{-1}

β-sheet

1620-1640, 1680-1690 cm^{-1}

Random coil

1640-1650 cm^{-1}

α-helix: Forms regular hydrogen bonding patterns due to helical structure, showing strong absorption at 1650-1658 cm^{-1} from C=O stretching vibration.

β-sheet: Shows two characteristic peaks depending on parallel or antiparallel structure. Absorbed at 1620-1640 cm^{-1} (strong peak) and 1680-1690 cm^{-1} (weak peak).

Random coil: Exhibits broad absorption band at 1640-1650 cm^{-1} due to irregular structure.

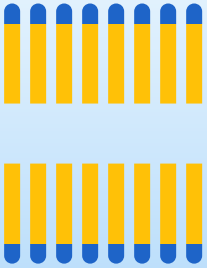
Lipid Analysis

C-H stretch 2800-3000 cm^{-1}. Membrane fluidity studies.

Spectral Deconvolution

Fourier self-deconvolution resolves overlapping bands.

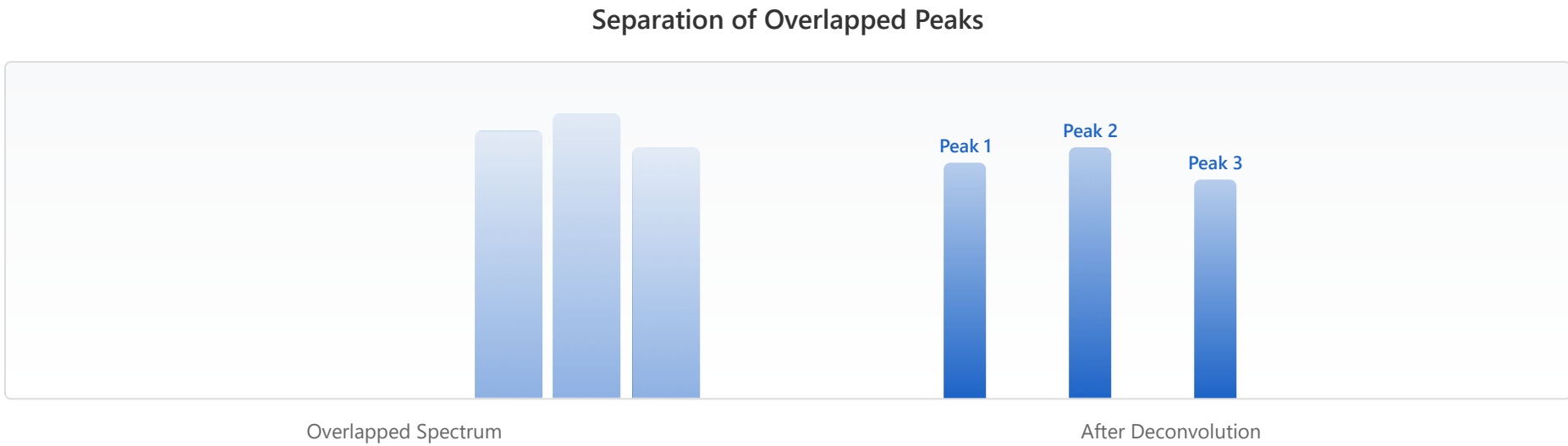
Lipid Analysis



C-H Stretching Vibration (2800-3000 cm^{-1}):

- 2920 cm^{-1}: Asymmetric CH_2 stretch
- 2850 cm^{-1}: Symmetric CH_2 stretch
- Changes in position and intensity of these peaks can be used to analyze fluidity and phase transitions of lipid bilayers.
- Peak shift to higher wavenumbers with increasing temperature indicates increased membrane fluidity.
- Applied in biological membrane studies, drug-membrane interactions, and lipid oxidation research.

Spectral Deconvolution



Fourier Self-Deconvolution:

- Separates overlapped peaks into individual components using mathematical algorithms.
- Enables quantification of various secondary structure components in the complex Amide I region spectrum.
- Used in conjunction with second derivative to enhance resolution.
- Essential technique for protein aggregation, structural changes, and ligand binding studies.
- Caution: Excessive deconvolution can generate artificial peaks, so appropriate parameter selection is important.

Major Applications of Biomolecular FTIR

Protein Structure Analysis

Monitoring protein folding, denaturation, and aggregation states. Studying protein-ligand interactions in drug development.

Pharmaceutical Research

Drug crystalline forms, polymer formulations, stability assessment and quality control of protein therapeutics.

Cell Membrane Research

Phase transitions of lipid bilayers, membrane fluidity, and drug-membrane interaction analysis.

Biosensors

Label-free sensing for biomolecular recognition, immunoassays, and disease marker detection.

Experimental Tips & Precautions

Sample Preparation:

- Use D_2O solution or measure in dry film form to minimize water interference
- Appropriate concentration: Protein 10-50 mg/mL, Lipid 5-20 mg/mL

Spectrum Acquisition:

- Resolution: 2-4 cm^{-1} (general), 1 cm^{-1} (high-resolution analysis)
- Number of scans: Minimum 64 or more (improves signal-to-noise ratio)
- Acquire fresh background spectrum before each measurement

Data Processing:

- Baseline correction
- Atmospheric water vapor/CO_2 correction
- Appropriate smoothing (Savitzky-Golay filter recommended)