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Detailed Technical Specifications for Fourier Transform Infrared (FTIR) Spectroscopy for PROTEIN QUANTITATIVE STRUCTURAL ANALYSIS:

FTIR SPECTROMETER for Protein analysis in aqueous and solid-state measurement using accessories to perform secondary structure analysis and Protein/DNA interaction study. Following are the brief specifications of each module:

Basic FTIR Spectrometer System:

FTIR must be research-grade and incorporate a high throughput interferometer and Gold Coated optics for maximum light throughput. Entire FTIR optics should be sealed and desiccated. A humidity indicator LED must be located on the instrument and viewable from outside the spectrometer.

1. **Optics:** Sealed Optics with purging facility, may be maybe coated to have highest performance in mid IR regime.
2. **Light Source :**High-intensity light source for mid IR range suitable to analyze protein structure
3. **Wave number range:** 7500 or higher to 350 cm⁻¹.
4. **Wave number accuracy:** Better than 0.005cm⁻¹
5. **Wavelength Resolution:** 0.5 cm⁻¹ or better
6. **S/N Ratio:** 1 Min: >55,000:1 peak-to-peak, 4 cm⁻¹ resolution, 1 min scan
7. **Interferometer:** Should be permanently aligned and should have a frictionless design to ensure an unlimited lifetime. We prefer a cube corner design. The interferometer should be capable of acquiring data in both scanning directions.
8. **Detector: 1.** Digital Technology high sensitivity Liquid N₂ cooled MCT detector.
9. **Detector: 2.** DTGS also should be part of the spectrometer, and switching of the detector should be software controlled.
10. **Aperture Wheel:** 11 positions, fixed diameters, ranging from 250 μm to 6 mm for optimization of light throughput.
11. **Validation Unit:** FTIR should incorporate an internal validation unit.
12. **PC interface: High-performance PC** Suitable interface like Ethernet
13. The system should have the facility to take a beam out of the spectrometer for external experiments like TGA/Microscope and Raman module. We intend to use this feature in the future.

Sample compartment: Must be large enough to accommodate various sampling accessories for performing protein analysis in liquid and solid mode, as described above.

Sampling accessories:

- (A) Accessory to perform protein conformation in solution, very accurate protein concentration determination, quick prediction of the secondary structure (Alpha Helix, Beta Sheet), etc., using a highly precise liquid cell with the following specification.

1. Flow-through type transmission cell with CaF₂ windows.
2. The cell must be sealed and not a demountable type.
3. Path length optimized for aqueous solutions must be 7µm.
4. Temperature-controlled cell with a range from 4 to 50Deg C with a suitable thermostat.
5. Sample volume: 10µl or better
6. Protein concentrations: < 0.1µg/µl
7. The tubing of the cell must be Biocompatible material.
8. A suitable Inline filter should be integrated to avoid any possible precipitation of protein that may contaminate the cell during the filling process

B. Accessory for detection of temperature-induced conformational changes (protein dynamics), Study of aggregation and fibrillation processes, Protein-ligand binding process, etc. using a bio-compatible ATR with the following specification.

1. Sample Volume: minimum 10 µl
2. Path length: 6 µm or better
3. Automated Temperature ramps from 4 Deg C – 95 Deg C with a suitable thermostat
4. Temperature sensor adaptable at sample chamber
5. Teflon Inert sample interface (Teflon and stainless steel)
6. A suitable Chiller must be supplied with temperature accuracy =/-0.1 Deg.

Software:

1. **Easy to use and powerful for routine as well as research experiments.**
2. The spectrometer software should provide **wizards for routine applications.**
3. All **spectral data** resulting from one measurement must be stored **within one single file.** Additionally, the results of manipulations (e.g., calculation of derivatives) and evaluations (e.g. peak picking, quantification) performed on this data shall be stored in the same spectrum file for easy data handling and well-arranged filing.
4. **Software must have real-time diagnostic features of critical components of FTIR like laser, source, detector, and interferometer.**
5. The spectrometer software should include functions for **automated water vapour compensation** without the need for measuring reference spectra.
6. Software must have quantification software with deconvolution and % quantification of protein secondary structure. It should include calibration files for protein Secondary Structure analysis and protein determination.
7. The system must be supplied with a protein library of a large number of proteins.

Essential Accessories:

The system must be supplied with essential spares like syringes, tubing, protein cleaning solutions, filters, chiller units, etc.

1. All accessories for N₂ gas purging
2. Minimum 3 cells for liquid sample analysis
3. KBr Pellet accessories.
4. **Computers accessories:** One Branded state-of-art Desktop PC from a reputed make (with a latest processor at least i5or i7, LED monitor at least 21” size, 8 GB RAM and 1 TB hard disk and preloaded with latest Operating System software. Power Backup: Online UPS 3kVA with Minimum 30 minutes of backup.

5. 5 years of comprehensive warranty must be included with application support and help in studying the protein structural analysis using FTIR.
6. Provide a list of 5 installations in Institutes of national importance and a list of engineers and application specialists with the organization.