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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:**

**I. 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.
2. **Wave-number range:** 8000 to 350  $\text{cm}^{-1}$ .
3. **Wave-number accuracy:** Better than 0.005 $\text{cm}^{-1}$
4. **Resolution:** Better than 0.4 $\text{cm}^{-1}$
5. **S/N Ratio:** 1 Min: >55,000:1 peak-to-peak, 0.4  $\text{cm}^{-1}$  resolution, 1 min scan
6. **Interferometer:** Should be permanently aligned and should have frictionless design to ensure unlimited lifetime. We prefer cube corner design. Interferometer should be capable of acquiring data in both scanning directions.
7. **Detector:** Digital Technology high sensitivity Liquid N<sub>2</sub> cooled MCT detector. DTGS also should be part of spectrometer and switching of detector should be software controlled.
8. **Aperture Wheel:** 11 positions, fixed diameters, ranging from 250  $\mu\text{m}$  to 6 mm for optimization of light throughput.
9. **Validation Unit:** FTIR should incorporate internal validation unit.
10. **PC interface:** Suitable interface like Ethernet, **USB 2.0/USB 3.0, CD R/W drive**
11. System should have 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 future.
12. **Sample compartment:** Must be large enough accommodate various sampling accessories like for performing protein analysis as described above.

**II. Sampling accessory:**

1. 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 following specification.
2. Flow-through type transmission cell with CaF<sub>2</sub> windows.
3. Cell must be sealed and not a demountable type.
4. Path length optimized for aqueous solutions should be in the range of 6  $\mu\text{m}$  to 12  $\mu\text{m}$
5. Temperature controlled cell with range from 4 to 50Deg C with suitable thermostat

6. Sample volume: 10 $\mu$ l.
7. Protein concentrations: down to 0.1 $\mu$ g/ $\mu$ l
8. Tubing of cell must be Biocompatible material
9. Suitable Inline filter should be integrated to avoid any possible precipitation of protein that may contaminate cell during filling process.

### **III. 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 vapor compensation** without the need for measuring reference spectra.
6. Software must have quantification software with advanced PLS algorithms for evaluation of protein data generated from FTIR spectrometer. It should include calibration files for protein SS analysis and protein determination.
7. System must be supplied with protein library of basis proteins.

### **IV. Essential Accessories:**

1. System must be supplied with essential spares like syringes, tubing, protein cleaning solutions, filters, water circulating unit, and branded PC.
2. Warranty - 1 Year Mandatory.

### **V. Accessories:**

1. Additional 2 years (After mandatory warranty) of comprehensive warranty must be included with application support and help in studying the protein structural analysis using FTIR.
2. Power back-up for additional 30 mins with 3 KVA UPS.