Attachment II - Specifications

Performance Specification for a High-Resolution Accurate-Mass Liquid Chromatography Mass Spectrometry (LC-MS) System

A Liquid Chromatography-High Resolution Accurate Mass Spectrometry (LC-HRAM) system is required for the comprehensive chemical characterization of complex biological and aquaculture samples. The primary research application involves the untargeted and targeted analysis of small molecules, including lipids and metabolites, in aquaculture feed ingredients and fish tissues to assess nutritional quality, palatability, and overall metabolic impact of husbandry practices.

Essential Performance Characteristics

The proposed LC-MS system must meet or exceed the following performance specifications to be considered technically acceptable.

1. **Mass Spectrometer**

- Mass Analyzer: The mass spectrometer must be a high-resolution, accurate-mass (HRAM) instrument capable of performing both full-scan analysis and fragmentation (MS/MS) for structural elucidation.
- Mass Resolution: Must be capable of achieving a resolving power of at least 100,000 (FWHM) at m/z 200. Higher resolution is desirable for confident identification of unknown compounds in complex matrices.
- Mass Accuracy: Must demonstrate mass accuracy of ≤ 1 ppm RMS over a 12-hour period using an external calibration standard.
- Scan Rate: Must be capable of scan rates sufficient for compatibility with modern fast chromatography, with a minimum scan rate of ≥ 10 Hz while maintaining a resolution of at least 60,000 FWHM.
- Fragmentation: The system must be capable of performing controlled collision-induced dissociation (e.g., HCD or equivalent) for structural confirmation. The ability to perform in-source fragmentation is also required.
- Ionization Source: Must include an electrospray ionization (ESI) source capable of operating in both positive and negative ion modes without manual reconfiguration.

2. **Liquid Chromatography System**

- System Type: Must be a binary or quaternary Ultra-High Performance Liquid Chromatography (UHPLC) system.
- Pressure: The system pumps and flow path must be capable of operating at pressures up to at least 1,000 bar (approx. 14,500 psi).
- Autosampler: Must include a temperature-controlled autosampler capable of holding sample vials with 96-well plates optional.

3. **System Control and Data Analysis Software**

- A single software platform for integrated control of both the UHPLC and the mass spectrometer is required.
- The software package must include dedicated, advanced workflows for untargeted metabolomics and lipidomics. Required capabilities include:
- Automated peak detection, deconvolution, and integration.
- Retention time alignment across large sample batches.
- Multivariate statistical analysis tools (e.g., PCA, PLS-DA, volcano plots).
- Compound identification through accurate mass, isotopic pattern, and fragmentation library searching.
- Support for creating and searching custom compound libraries.

4. Installation and Training

- Installation: On-site installation and verification of all performance specifications by a factory-certified engineer are required.
- Training: A minimum of 3-5 days of on-site user training covering instrument operation, maintenance, and data analysis software workflows is required.