



The mass spectrometers are tuned as defined based on the particular platform in use, assay performance requirements, and specimen types tested.

NOTE: Instruments must be tuned at least as frequently as recommended by the manufacturer. Acceptable tolerance limits for tune parameters must be defined, and tuning records retained.

Tandem mass spectrometers require tuning at the time of maintenance that requires shutdown of the vacuum.

Evidence of Compliance:

- ✓ Records of tuning

****NEW** 08/24/2023**

CBG.17150 Validation, Monitoring, and Annual Verification of MS Data Analysis Tools

Phase II



The laboratory validates data analysis tools used for compound identification and quantification when first installed and after any modifications, as applicable, and verifies performance at least annually.

NOTE: Data analysis tools may be used for various processes, such as integration of targeted and untargeted peaks, evaluating acceptability of calibration and control performance, stability of baseline, calculation of ion mass ratios, discrimination of positive and negative results, and assessing risk of carryover. Data analysis tools (eg, software or code-based rules, algorithms, machine learning) used for automated data analysis must be verified using defined acceptability criteria. Version control of custom data analysis tools is required. Reassessment of lower limit of quantification (LLOQ) and other decision points may be used to ensure that a shift has not occurred due to instrument performance or another factor impacting assay performance.

Customized data analysis tools, and modifications to that software, should be appropriately documented and records should allow for tracking to identify persons that have added or modified that software. The purpose of the computer program, the way it functions, and its interaction with other programs must be clearly stated. The level of detail should be adequate to support troubleshooting, system modifications, or additional programming.

Evidence of Compliance:

- ✓ Records of validation and revalidation after modifications **AND**
- ✓ Records of monitoring for changes to software update tools and other change impacting performance

REFERENCES

- 1) Vincente FB, Lin DC, Haymond S. Automation of chromatographic peak review and order to result data transfer in a clinical mass spectrometry laboratory. *Clin Chim Acta*. 2019;498(11):84-9.

CBG.17300 Identification Criteria - Single Stage Mass Spectrometry

Phase II



The identification criteria for single stage mass spectrometry (ie, GC/MS, LC/MS) are in compliance with recommendations.

NOTE: One acceptable criterion for compound identification by GC/MS using ion ratios is that the unknown result must have ion ratios within a predefined tolerance limit. This limit should be supported by either literature references or through experimental means. Such ion ratio tolerance limits may differ based on the technique applied (eg, GC/MS versus LC/MS) as well as the analyte(s) being determined (eg, compounds with mainly ions of low abundance); thus, a defined limit to cover all methods and analytes cannot be given.

Identification using ion ratios typically requires the use of at least two ion ratios. However, one ion ratio of two characteristic ions may be acceptable if there are only a few characteristic ratios AND if there are other identifying characteristics, eg, retention time. The internal standard's identification should be monitored with at least one ion ratio. An acceptable criterion for compound identification using total spectra is that the unknown result must have a "spectral