Auto-Resolution/Calibration Adjust Instructions

Oct. 25, 2013

Heather Gamble

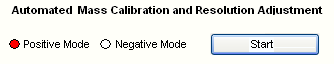
Preamble

This utility is intended to be used by customers. It assumes the current calibration settings are close (e.g. ±5amu of correct).

Service and especially Commissioning are likely to encounter situations where a significantly larger correction is required. The current proposal is to handle this via Service Tool.

User Interface

Add a Quadrupole Calibration button to Ionica Server. Ionica Server is being redesigned, with the exact layout yet to be determined, but the Auto Cal/Res section could be as illustrated below.



Implementation

Clicking on the button should activate an automated routine.

1.) Verify that the Mass Spec is “Ready” (check “System Status”) and that no Method is currently running/Ionica Server is not busy (check “Get Status”). If Ionica Server is busy or the Mass Spec is in an error state, inform the user and abort the routine.

2.) A set of default Molana format PPG Methods appropriate for the specific model and instrument at the current time can be found in C:\USERS\PUBLIC\Molana\Instrument\Project\MS Methods\Automated Calibration Methods. They will be named Q1 PPG POS Default.xml, Q2 PPG POS Default.xml, Q1 PPG NEG Default.xml, and Q2 PPG NEG Default.xml. Note only one pair (POS or NEG) will be required at a time. Verify that the required default files are present and in the correct location. If they are not, abort and inform the user “Default calibration method not found”.

3.) The following information should be read from the Molana format Method files:

Source ID (could be 1 or 2)

Source type (if not ESI for active source, abort and inform user that Default Method is incorrect).

Scan type (should match the filename)

Source/Ion path voltages (Experiment/Mass level) - M1RF, EV, ED (Series 100 only), M1, L1, M2, L2, PF, Q1, CCL1, CCL2, CE, CCAF, CCL3, CCL4, Q2, ID, DISC, DV, CC P, ISV (1 or 2, as appropriate), CAP.

Any mass dependent parameter information should be preserved and used.

Source/Ion path voltages (Method Level) - . Set inactive ISV to 0. Set CD to 0. Set HORN, DG, NG1, HG1, NG2, HG2, SX, HSID T, P1 T, P2 T.

Number of Mass windows. NOTE not all peaks will necessarily be used when adjusting Cal/Res. Which mass windows (peaks) will be used should be read from the Molana format file MassCalibrationReference.cal.

Start/Stop masses or Centre/Width information for each mass window.

Step Size

Dwell Time

Resolution (Should be Unit/Unit)

4.) The following information in the Molana format Method files should be disregarded:

Number of Scans (use what you need to get the job done).

NOTE not all peaks will necessarily be used when adjusting Cal/Res. Which mass windows (peaks) will be used should be read from the Molana format file MassCalibrationReference.cal. Additional peaks listed in the Default Methods may still be scanned, but the information should be disregarded.

5.) For each mode/polarity, keep the pole orientation as saved in the current Config Table (i.e. do not read/overwrite when loading a Method).

6.) Save the current tables as My Tables-YYMMDD-old.tbl.

7.) Determine the mass ranges to be measured based on information contained in the Molana file C:\USERS\PUBLIC\Molana\Instrument\Configuration\Current setting\Calibration\MassCalibrationReference.cal. If the <Use> tag line for a given mass indicates “True”, use that mass range. If it indicates “False”, delete that mass range from the revised method, or simply ignore the data from that mass range.

8.) Run the revised Q1 PPG POS Method. Confirm that there is a recognizable peak in every active mass window (see Appendix B). If not, abort and inform the user. Include an option to CONTINUE once the user has addressed an issue (e.g. refilled a syringe), or QUIT otherwise.

9.) When searching for peaks, use the peak search window and counts threshold from the <SearchRange> tag line in the file C:\USERS\PUBLIC\Molana\Instrument\Configuration\Current setting\Parameter\peakSearchParameters.xml. If the value in the peak search window tag line is 5, the search window should span ±5 amu from the expected mass.

10.) If recognizable peaks are present, adjust the DAC settings of the medium Resolution Tables to bring all active peak widths within the appropriate range for the resolution selected by the user. Calculate the peak width at the % height found in the Molana file peakSearchParameters.xml.

Resolution FWHM Peak Width Range (amu)

Unit 0.65 – 0.8

Display the results of each scan using RealTimeDataViewer. NOTE: This will require that information on scan type, mass ranges, etc. be provided to RealTimeDataViewer in the correct format.

11.) Adjust mass calibration DAC settings as necessary to bring all peaks within ±0.1 amu of the expected mass. Display the results of each scan using RealTimeDataViewer.

12.) Repeat for Q2 PPG POS/NEG as appropriate.

13.) Upload the new tables to the cRIO.

14.) Save My Tables-YYMMDD.tbl to C:\USERS\Public\Molana\Sim.

15.) Copy the file C:\USERS\PUBLIC\Molana\Instrument\Configuration\Current setting\Calibration\targetResolution.res to [same path]\targetResolution-YYMMDD-old.res.

16.) Edit the targetResolution.res file. Write the new calibration and resolution DAC settings into the calibration and unit resolution tables for the current polarity.

17.) Edit the resolution DAC settings in targetResolution.res for the appropriate polarity high and low resolution tables as per current Production defaults. Currently for High resolution, add 200 to all Resolution DAC values. For Low resolution, subtract 200 (relative to unit).

Reporting

A report template will be provided.

APPENDIX A: Supporting Files and Documentation

1.) Initial Ion Sniffer format Default Method Files for Q1 PPG POS (Series 100, 200, 300), Q2 PPG POS (Series 100, 200, 300), Q1 PPG NEG (Series 100, 200, 300), Q2 PPG NEG (Series 100, 200, 300).

2.) Initial targetResolution.res files for Series 100, 200, 300.

3.) Service Tool format initial default My Tables.tbl files for Series 100, 200, 300.

4.) Lists of standard PPG masses for each series.

5.) Report Contents Sample file.

6.) Initial default Molana format Method files for Q1 PPG POS (Series 100, 200, 300), Q2 PPG POS (Series 100, 200, 300), Q1 PPG NEG (Series 100, 200, 300), Q2 PPG NEG (Series 100, 200, 300).

7.) Sample MassCalibrationReference.cal for each Series

8.) Sample peakSearchParameters.xml file.

APPENDIX B: Peak Validation Criteria

1.) Maximum counts must be less than 7e6 single scan counts per second.

2.) Minimum counts at the peak maximum must be above the peak threshold (single scan counts per second) read from the Molana text file peakSearchParameters.xml.

3.) There must be a peak (recognizable maximum).