Auto-Resolution/Calibration Adjust Instructions

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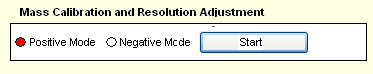
Preamble

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.) Determine the Series of the instrument (check contents of Config Table header for model number).

3.) Select the appropriate pair of default Methods for the Series: Q1 PPG POS, Q2 PPG POS, Q1 PPG NEG, Q2 PPG NEG. The default Methods will already contain mass ranges appropriate for the series, dwell times, step size, etc.

4.) 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).

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

6.) Poll to determine how many ESI source probes are present. If only one ESI probe is present, automatically use that source. If the system is dual source with two ESI probes, pop up a dialog box asking the user to select which source they wish to use.

7.) If necessary, edit the source parameters for the appropriate pair of default Methods. The default Methods assume Source 1 is to be used. If the user selected Source 2, edit the default Methods to set ISV1 (Ch. 203) and NG1 (Ch. 27) to 0. Set NG2 (Ch. 28) to 90.

8.) Refer to the file C:\USERS\PUBLIC\Molana\Instrument\Configuration\Current setting\Parameter\activeParameterTable.xml. Certain lens voltages/settings in the supplied default Methods are to be updated to match the values in this file, as per instructions provided separately. Change either ISV1 or ISV2, to match the active source.

9.) If it is simper, it is acceptable to only revise the Methods which are required for the polarity currently selected.

10.) Revise 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.

11.) Determine the correct detector run bias by running a “plateau curve”. Start with the run bias (DV) at 2000 and check the counts per second (ss-cps) signal level for 10 scans summed for the Q1 PPG POS “flagship” peak for the current instrument series. Verify whether a reasonable peak is present (see Appendix B – Criteria for Peak Validation). Increase the set detector bias by 200 V and check the new ss-cps signal level for the flagship peak, again verifying whether a reasonable peak is present (Appendix B). If reasonable peaks have been present for at least two sequential detector bias values, and the signal increase is less than 30%, you have reached the correct run bias. If no reasonable peak was found up to a bias of 3200V, abort and inform the user. Include an option to CONTINUE once the user has addressed an issue (e.g. refilled a syringe). Once found, write the new detector bias to all default calibration methods.

|  |  |  |
| --- | --- | --- |
| FLAGSHIP PEAKS | |  |
|  | PPG POS | PPG NEG |
| S-100 | 906.67 | 933.64 |
| S-200 | 906.67 | 933.64 |
| S-300 | 732.59 | 759.51 |

12.) 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.

13.) 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 tag line is 5, the search window should span ±5 amu from the expected mass.

14.) If recognizable peaks are present, adjust the DAC settings of the medium Resolution Tables to bring all 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.

15.) 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.

16.) Repeat for Q2 PPG POS/NEG as appropriate. Use the detector bias determined previously.

17.) Upload the new tables to the cRIO.

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

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

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

21.) 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 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 default activeParameterTable.xml files for Series 100, 200, 300. Note Series 300 is provided for reference only. For current purposes Series 200 activeParameterTable.xml is functionally equivalent.

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

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

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

6.) Method Updating Instructions.

7.) Report Contents Sample file.

8.) PPG “Flagship” peak list for each Series

9.) 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).

10.) Sample MassCalibrationReference.cal for each Series

11.) 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).