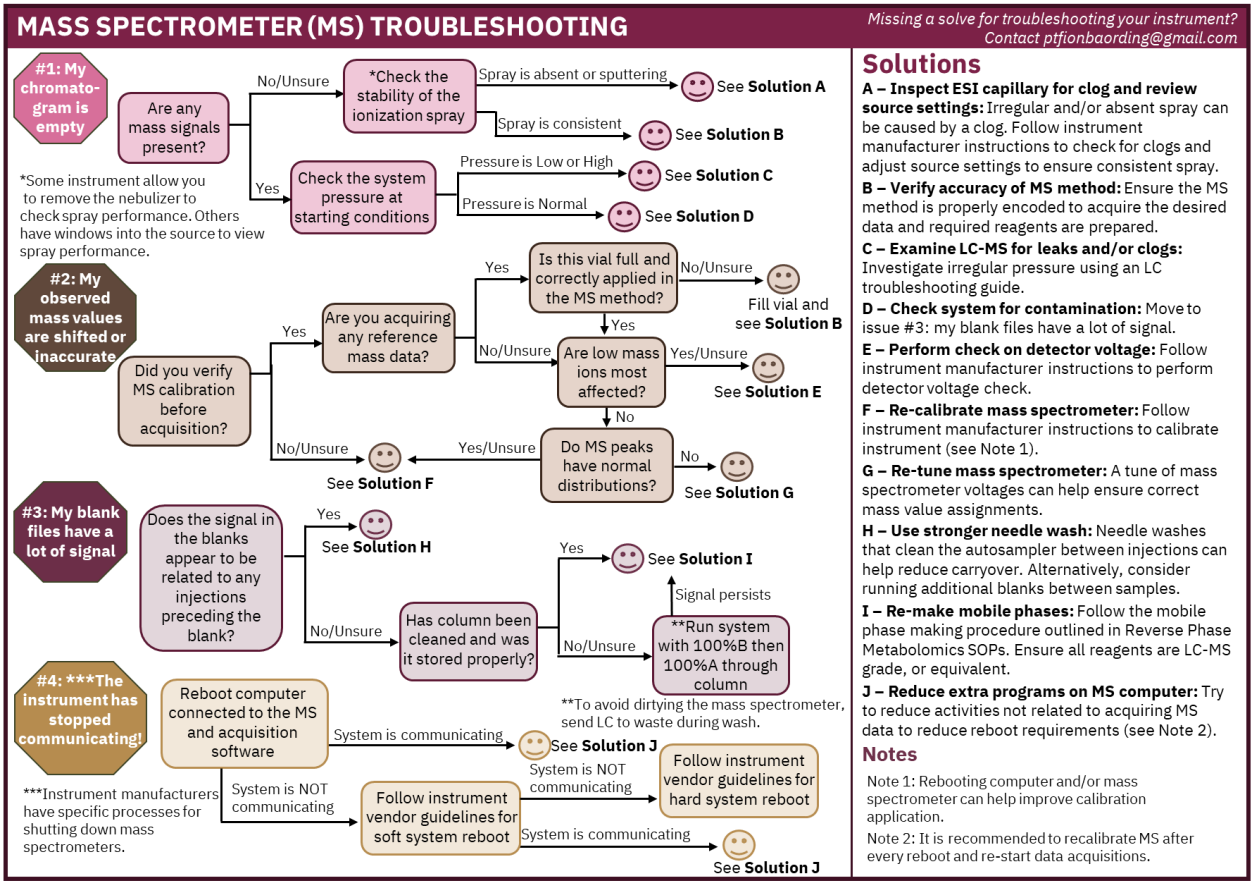
Mass Spectrometer (MS) Troubleshooting Guide

There are four separate flow charts for troubleshooting data review and data upload challenges. The starting point for each flow chart is a challenge you might observe. Each flow chart has end points at each of 8 possible solutions. If there is a missing solve for your problem, you should send an email to: ptfionboarding@gmail.com



Each flow chart is described in detail below. From the following list, select the in-document link corresponding to the problem you're troubleshooting to navigate to the relevant flow chart.

Mass spectrometer problems to troubleshoot

Problem 1: My chromatogram is empty

Problem 2: My observed mass values are shifted or inaccurate

Problem 3: My blank files have a lot of signal

Problem 4: The instrument has stopped communicating

Flow chart 1: Empty chromatogram

1.1: Are any mass signals present?

- No or unsure: Go to item 1.2
- Yes: Go to item 1.3

1.2: Check the stability of the ionization spray.

Some instrument allow you to remove the nebulizer to check spray performance. Others have windows into the source to view spray performance.

- Spray is absent or sputtering: See solution A
- Spray is consistent: See solution B

1.3: Check the system pressure at starting conditions.

- Pressure is Low or High: See solution C
- Pressure is Normal: See solution D

Return to the start of flow chart 1
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Flow chart 2: Mass accuracy errors

2.1: Did you verify MS calibration before acquisition?

- Yes: Go to item 2.2
- No or unsure: See solution F

2.2: Are you acquiring any reference mass data?

- Yes: Go to item 2.3
- No or unsure: Go to item 2.4

2.3: Is this vial full and correctly applied in the MS method?

- No or unsure: Fill vial and see solution B
- Yes: Go to item 2.4

2.4: Are low mass ions most affected?

- Yes or unsure: See solution E
- No: Go to item 2.5

2.5: Do MS peaks have normal distributions?

- Yes or unsure: See solution F
- No: See solution G

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Flow chart 3: High signal in blank

3.1: Does the signal in the blanks appear to be related to any injections preceding the blank?

- Yes: See solution H
- No or unsure: See item 3.2

3.2: Has column been cleaned and was it stored properly?

- Yes: See solution I
- No or unsure: Go to item 3.3

3.3: Run system with 100%B then 100%A through column.

To avoid dirtying the mass spectrometer, send LC to waste during wash.

- Signal persists: See Solution I

Return to the start of flow chart 3
Return to the list of problems

Flow chart 4: Instrument Communication Issues

Instrument manufacturers have specific processes for shutting down mass spectrometers.

4.1: Reboot computer connected to the MS and acquisition software.

- System is communicating: See Solution J
- System is not communicating: Go to item 4.2

4.2: Follow instrument vendor guidelines for soft system reboot.

- System is communicating: See Solution J
- System is not communicating: Go to item 4.3

4.3: Follow instrument vendor guidelines for hard system reboot.

Return to the start of flow chart 4
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Solutions

Solution A: Inspect ESI capillary for clog and review source settings

Irregular and/or absent spray can be caused by a clog. Follow instrument manufacturer instructions to check for clogs and adjust source settings to ensure consistent spray.

Return to the list of problems

Solution B: Verify accuracy of MS method

Ensure the MS method is properly encoded to acquire the desired data and required reagents are prepared.

Return to the list of problems

Solution C: Examine LC-MS for leaks and/or clogs

Investigate irregular pressure using an LC troubleshooting guide.

Return to the list of problems

Solution D: Check system for contamination

Move to issue #3: my blank files have a lot of signal.

Return to the list of problems

Solution E: Perform check on detector voltage

Follow instrument manufacturer instructions to perform detector voltage check.

Return to the list of problems

Solution F: Re-calibrate mass spectrometer

Follow instrument manufacturer instructions to calibrate instrument (see Note 1).

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Solution G: Re-tune mass spectrometer

A tune of mass spectrometer voltages can help ensure correct mass value assignments.

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Solution H: Use stronger needle wash

Needle washes that clean the autosampler between injections can help reduce carryover. Alternatively, consider running additional blanks between samples.

Return to the list of problems

Solution I: Re-make mobile phases

Follow the mobile phase making procedure outlined in Reverse Phase Metabolomics SOPs. Ensure all reagents are LC-MS grade, or equivalent.

Return to the list of problems

Solution J: Reduce extra programs on MS computer

Try to reduce activities not related to acquiring MS data to reduce reboot requirements (see Note 2).

Return to the list of problems

Notes

Note 1

Rebooting computer and/or mass spectrometer can help improve calibration application.

Return to solution F

Note 2

It is recommended to recalibrate MS after every reboot and re-start data acquisitions.

Return to solution J