Maintaining lab operations in extraordinary times

Dealing with operating impacts from the COVID-19 Coronavirus

LC/QQQ & LC/QToF  Thursday, April 23rd
Important general information for managing lab operations
Follow your SOP’s – but here are some additional things to consider

• How has operational changes affected your SOP’s? Are there impacts to instrument maintenance, qualifications, etc? Has instrument usage changed as this may affect service/consumable replacement intervals? Document these and prepare a plan to bring them online once you resume normal operations.

• Develop a new schedule/routine for working in the lab. This is a challenging time for everyone and routine helps everyone acclimate to these impacts.

• Prioritize time in the lab - Can any tasks be shifted remote or online (training, remote monitoring, data analysis)? Is your IT department aware of these and is bandwidth/VPN/remote access capable of handling this.

• Are service providers allowed on-site? Or is there remote work they can do? Discuss this before any scheduled visit. Our service teams are currently offering free live video conferences to support labs around the world – more info at the end of the presentation.

• Proactively replace lab consumables before you see performance issues. If ordering supplies, check if shipping/receiving/logistics for your company has been affected.

• When you return to normal operations, have a detailed restart plan that outlines priorities and timelines. Agilent will provide additional information on returning/restarting your lab in a few weeks.
Maintaining Lab Operations in Extraordinary Times
Multishift 24/7 Operations to Normal Load with Limited Lab Access

We are in unique times, full of uncertainty, stress and concerns. The goal of this webinar is to provide you the necessary knowledge (Tips/Tricks) to keep your laboratory’s LC’s, LC/TQ, and LC/Q-TOF’s fully operational no matter the workload and varying laboratory access conditions.

- **Peek a Boo**: Using Remote Access Tools to Keep Systems up and Healthy
- **A Clean LC is a Healthy LC**: From Mobile Phase to Sample Preparation
- **A Clean MS is a Healthy MS**: Key Activities to Keep LC/TQ and LC/Q-TOF Operational
- **Limited Access**: Prioritizing Key Activities to Keep Operational with Limited Lab Access
- **Running 24/7 Operations**: Keeping Systems Operational Under High Load Conditions
- **Be Prepared**: Key Consumables and MS Parts for Routine DIY Maintenance
- **My Systems Down 😞 We got you Covered 😊** New Field Service Remote Access Capability

*Remember… Agilent is Open, We are Working and Ready to Help You in Many Ways*
Remote Access of LC/TQ and LC/Q-TOF Systems

Enabling Desktop Remote Access on LCMS PC

- Launch “Control Panel”, Click on “System and Security tab”
- In Systems Area click on “Allow remote access” line to launch the System Properties Window and Select “Remote” tab
- Check “Allow remote access connection to this computer” and then click on Advanced Tab
- Check box “Allow this computer to be controlled remotely”

Next, try logging into LCMS PC from a different PC. Remember you need to have the **IP address** or **PC name**; User name and Password for the LCMS PC.

- Launch “Remote Desktop Connection” and select “Show Options”
- Type in the Computer name or IP address
- Type in User Name
- When Prompted Type in Password
Remote Access of MassHunter LCMS Systems Possible with ChemLaunch Software

Data Analysis Clients

Reprocess Anywhere

Laboratory  Dorm  Anywhere  Library  Coffee Shop

ChemLaunch

Laboratories

Workstations in lab
ChemLaunch for MassHunter
Takes MassHunter Data Analysis and provides it outside the lab

- Thin client
  - Web Access to MassHunter DA
  - No software loading at clients
  - No validation needed

- GCMS
- LCMS
- Quant
- Qual
- ICPMS
- HPLC
- GC
- MPP and BioConfirm
Hygiene – Do you want the hands that washed these bottles to touch your instrument? I don’t think so
Tips and Trick to Keeping your LC System Up and Running

A **Clean** LC is a **HAPPY** LC/MS…

- Keep Glassware and Mobile Phase Bottles CLEAN
- Avoid SOAP and Detergents and Dishwashers!
- To Avoid growth of Bacteria and Algae
  - Make-Up Fresh Mobile Phase Solvents Weekly
  - Use 99% Water 1% Organic in Bottle A
  - 1% Water to Organic mobile phase
- Prevent High Pressure Issues:
  - Filter Samples Prior to Placing into AutoSampler
  - Guard Column before Analytical Column
  - Install an Inline Filter after Autosampler

Previously Recorded Tips and Tricks LC and LCMSD Webinar April 17th
Mobile Phase Hygiene: Glassware Cleaning, Filters and Caps

Improper cleaning of solvent bottles can cause contamination of mobile phases and resulting in major chemical background and poor MS performance

- Wash solvent bottles with hot water, deionized water, and organic solvent (IPA or acetonitrile).
- Leave glassware inverted on paper towels on bench or on clean pegboard dowels to dry.
- Avoid using detergents If it is necessary to use detergents to get glassware clean, re-wash with plenty of hot water and cold water so that all detergent residues are removed.
- Clean Bottles, Mobile Phase Bottle Caps, Solvent Filters, UltraPure LCMS Grade Solvents

Dirty Solvent Bottles
Replace Glass Filters with Stainless Steel
Use Mobile Phase Caps not AL Foil or Parafilm

Agilent Infinitylab UltraPure
5191–4496 Acetonitrile
5191–4497 Methanol
5191–4498 Water
Keep HPLC Healthy: Don’t Forget the Seal Wash and Needle Wash

Using pump seal wash will prevent buffer salt from building up on pump seals.

- Seal wash solvent – Water with 10% Isopropanol (IPA)
- Seal wash should be set to run periodically regardless of instrument is acquiring data or not.
- Seal wash is set to run automatically for 1290 pumps
- Make sure seal wash solvent bottle is not empty

Using needle wash option will reduce carryover

- Keep needle wash solution bottles filled with fresh solvent
Do I have Enough Mobile Phase to Keep LC Running?
Real Time Monitoring Mobile Phase and Waste Levels

- Right Click in LC Icon
- Click on “Bottle Fillings..”
- Brings up new window
- Fill in Actual Volume and Total Volume for all bottles

To prevent pump for going dry
- Check both boxes here
- Set solvent level to 0.05 L
- Position solvent filter at the bottom of the mobile phase bottle

Remember Waste Bottle also
- Fill in Total Volume of Waste
Carry-Over Reduction is Key for Trace-Level Quantitation using LCMS/MS

Newer, UHPLC methods may have lower injection volumes

‘Sticky samples or more sensitive detectors may require aggressive cleaning

Composition and order of Rinse Solvent is key to good performance…

**e.g.**  S1: 2% Organic/water   S2: 90/10 ACN/Water   S3: 50/50 MeOH/ACN

Always Remember to go back to Initial Mobile Phase S1 Bottle to ensure best Chromatography
Early Maintenance Feedback Limits (Lab Advisor and MassHunter)
Back Home in Chicago…No Sunbathing We Have Snow in April..
A Clean Mass Spectrometer is a Healthy Mass Spectrometer

Top Ten Activities to Complete Each Week no Matter Access

1. Make up *new mobile phase solvents* and check solvent waste
2. Clean *LCMS source, spray shield and the cap* on glass capillary
3. Visually *check spray nebulizer* ensure not blocked or damaged and has a good spray
4. Refill if needed *calibration/tuning solution* from stock solution
5. For LC/Q-TOF refill if needed *reference solution* bottle A from stock solution
6. For LC/Q-TOF do a *mass calibration* to ensure good mass accuracy
7. For LC/TQ always a good idea to run *new calibration curves*
8. Make up new samples
9. *Backup data* make sure hard drive is not full
10. Check for any *software service patches* on Agilent.com website
Quick ESI/Jet Stream Cleaning Procedure:

Clean spray chamber with 100% Water followed by 100% Organic

Do not Use Chemwipes Use Lint free Clothes

Don’t spray solvent directly into the ion transfer capillary as that may affect vacuum.
LC/MS Source Maintenance

Clean the spray shield, capillary cap and end plate with 4000 grit paper
Quick ESI/Jet Stream Source Cleaning Procedure:

‘Dilute & Shoot’ Application

4000 Grit Paper

8660-0827

After Cleaning Spray Shield and Cap
Recommend to Sonicate in 50/50 Water/ACN for at least 20 minutes

**Always Wear Gloves** When Handling MS Parts
Checking Performance of LC/TQ and LC/Q-TOF Systems

Proper Spray is required for good signal

Check Nebulizer with Magnifier

Adjust / Clean / Service Nebulizer as needed

Check CDS tubing/fluidic
Why Checking the LCMS Nebulizer is so Critical

Indications the spray needle may be blocked or damaged include:

- Loss of signal
- Inconsistent or sputtering signal
- Increased LC back pressure
- Off-axis spraying
- Dripping from the nebulizer
Checking Performance of Nebulizer
New Nebulizer Needle Adjustment Tool

40x Magnifier

Vertical #2 Position

Vertical #1 Position

LED Flashlight

Nebulizer Needle
Examples of Bad Nebulizers.. Good Spray Critical for Good LCMS!

1. Needle is too far out of the nozzle
2. Needle too far in
3. Needle is clogged with salt
4. Needle is partially blocked
5. Needle is touching the nozzle
6. Needle is not concentric in nozzle
7. Nozzle body is damaged
8. Needle is damaged
9. Needle is damaged
10. Nozzle is dirty

Maintaining Lab Operations in Extraordinary Times: LC/TQ LC/Q-TOF Slides Will Be Sent to Everyone DE.5422685185
LC/TOF & LC/Q-TOF AJS Tuning/Calibration Mix 10:1 Dilution

Add components in order to a clean glass CDS bottle

- 10 mL ESI-L Low Concentration Tuning Mix
- 85.5 mL LC/MS-grade acetonitrile
- 4.5 mL Water, 18 MΩ-cm resistivity or better
- 3 µL HP-0321 solution from G1969-85003 Biopolymer Reference Mass Kit

When Placing on LC/MS System Always Check to Make Sure you have “Good/Tight Seal”
If one sees waves when tuning/calibrating that indicates a poor seal that may cause problem with tune: Best replace bottle with new bottle.
Add components in order to a clean 1L Nalgene bottle, mix, & transfer 100mL to clean CDS bottle.

- 950 mL Acetonitrile
- 50 mL 18MΩ DI water
- ES-TOF Reference Mass Kit G1969-85001*
  - 0.4 mL purine (121)
  - 1.0 mL HP-921(922)

Actual concentrations of reference masses varies by LC/Q-TOF model and parameters. **Abundances should be < 150,000 counts at scan rate 1 spectrum/sec, If higher then dilute.**
Additional Resources for Maintenance and Troubleshooting for LC/TQ

PC Based LC/TQ Resources

Self-Paced Course Online At Agilent University

7) Troubleshooting - LC/MS
Need guidance on how to plan and execute an investigation of your LC/MS? Are you aware of how important the vacuum system is to the performance of your LC/MS? The modules in this series address some of the most common issues and provide in-depth solutions.

8) Maintenance - LC/MS
Are you responsible for taking care of the LC/MS in your lab? Do you know the recommended Best Practices and Maintenance Schedules for your Agilent 6400 Series Triple Quadrupole LC/MS? The modules in this series will answer these questions.

7) Maintenance - LC/MS
Are you responsible for taking care of the LC/MS in your lab? Do you know the recommended Best Practices and Maintenance Schedules for your Agilent Ultivo Triple Quadrupole LC/MS? The modules in this series will answer these questions.

- MassHunter Data Acquisition
- Mass Spectrometer
  - Maintenance Guide (animated)
  - Safety Guide
- eFamiliarization
- Installation Guide

LCMS-MULTI-2270s - Troubleshooting Series for Agilent LC/MS Instruments
LCMS-6400-1201s - Essential Housekeeping Tasks and Best Practices for Agilent 6400 Series QQQ LC/MS
LCMS-ULTV-1200s - Essential Housekeeping Tasks and Best Practices for Agilent Ultivo LC/TQ
Additional Resources for Maintenance, Troubleshooting for LC/Q-TOF

Time of Flight and Quadrupole Time of Flight LC/MS Resource App

Resources
This version supports MassHunter Data Acquisition:
- 8.09.00 for all 6200 Series LC/TOF and 6500 Series LC/Q-TOF (except 6546 LC/Q-TOF)
- 10.0 for 6546 LC/Q-TOF
- 10.1 for all 6200 Series LC/TOF and 6500 Series LC/Q-TOF (except 6560 Ion Mobility LC/Q-TOF)

› MassHunter Data Acquisition Manuals
› Mass Spectrometer
  Maintenance Guide (animated).pdf
  Safety Guide
  Drift Gas Setup Guide (for IM-QTOF)
  G2582A Drift Gas Upgrade Kit Quick Start Guide

› eFamiliarization
› Installation Guides

Self-Paced Course Online At Agilent University

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LCMS-6400-1201s - Essential Housekeeping Tasks and Best Practices for Agilent 6400 Series QQQ LC/MS
Using Scripts in Worklists.
Reduce Mobile Phase Solvent Consumption

From Worklist…

Right click in upper left box..
Select “Add Script” which brings up
Select Script Box contains pull downs for all
the various scripts available in worklist

To Reduce Mobile Phase Consumption Use the following Scripts
SCP_InstrumentStandby Puts the instrument on standby
SCP_LoadIdleMethod Loads an idle method which may have LC at low flow
SCP_PumpsAllOff Turns off any LC Pumps
SCP_PumpsAllandMSRefOff Turns off any LC Pumps and Turns off Ref Bottle A


# Be Prepared.. Key Consumables and LCMS Parts to Always Have

<table>
<thead>
<tr>
<th>Agilent Part Number</th>
<th>Part Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>G1958-67098</td>
<td>LCMS ESI, MMI, AJS Nebulizer</td>
</tr>
<tr>
<td>G1946-67037</td>
<td>LCMS APCI and APPI Nebulizer</td>
</tr>
<tr>
<td>G1958-60137</td>
<td>ESI, MMI, AJS Needle Replacement Kit</td>
</tr>
<tr>
<td>G1946-68704</td>
<td>APCI APPI Needle Replacement Kit</td>
</tr>
<tr>
<td>G1947-20029</td>
<td>Corona Needle for APCI</td>
</tr>
</tbody>
</table>

**Replacement Capillaries**

<table>
<thead>
<tr>
<th>Agilent Part Number</th>
<th>Part Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>G7604-60000</td>
<td>0.6mm x 180mm Dielectric Ion injector</td>
</tr>
<tr>
<td>G1960-80060</td>
<td>0.6 mm ID Fast Polarity Switching</td>
</tr>
<tr>
<td>G6301-80004</td>
<td>Ultivo Ion Injector</td>
</tr>
<tr>
<td>G1964-80659</td>
<td>0.61mm x 90mm Hexabore for 6550B, 6490, &amp; 6495 iFunnel</td>
</tr>
<tr>
<td>G1969-85000</td>
<td>ESI-L Low Concentration Tuning Mix</td>
</tr>
<tr>
<td>G1969-85001</td>
<td>ES-TOF Reference Mass Kit</td>
</tr>
<tr>
<td>G1969-85003</td>
<td>ESI Biopolymer Reference Kit</td>
</tr>
<tr>
<td>5043-1222</td>
<td>InfinityLab Stay Safe cap starter kit</td>
</tr>
</tbody>
</table>

Don’t Forget to Order Sample Vials, Sample Caps, Needle Seat Capillaries and LC Parts!!
DIY Trouble Shooting Mass Spectrometer Hardware Issues
Check the Dash Board and Instrument Logbook for Errors

Always Check for Errors in the System Logbook Viewer

Common Errors are Leaks and Overpressure!
Simple Trouble Shooting Procedures for LC/TQ and LC/Q-TOF
That don’t require venting system!

• **Is LC operating correctly?** Check Pressure Trace, Ripple, Air Bubbles, Purge, Leak

• **Inspect/Replace nebulizer needle**
  - New needle (G1960-20031); or use the kit with the needle, ferrule, and needle holder (G1958-60137)

• **Clean Source:**
  - Wipe with no lint cloth (05980-60051) and water followed by organic solvent
  - Clean Capillary Cap and Spray Shield – remove residue with 4000 grit mesh (8660-0827), sonicate in water then organic solvent

• **For gate valve/vac shield enabled** systems (Ultivo, 6495B/C, 6545XT, 6546) can remove capillary
  - For transmission loss across all the tune masses, clean the capillary using procedure document.

• **For only for low m/z ions transmission loss**, replace with new capillary
  - 180 mm single bore dielectric capillary ("Ion injector", not for polarity switching): G7604-60000
  - 180 mm single bore resistive capillary (fast polarity switching): G1960-80060
  - 90 mm hexabore capillary for QQQ (1 GigOhm resistance): G1964-80659
  - 90 mm hexabore capillary for QTOF (120 MegOhm resistance): G1964-80661

• **Retest and Retune system! Run System Suitability Standard Mixture!**
# Check Vacuum

<table>
<thead>
<tr>
<th>Instrument Model</th>
<th>Rough Vacuum</th>
<th>High Vacuum (CC Gas ON)</th>
<th>High Vacuum* (CC Gas OFF)</th>
<th>TOF vacuum, (QTOF only) With CC gas ON</th>
</tr>
</thead>
<tbody>
<tr>
<td>Ultivo</td>
<td>~1.5 Torr</td>
<td>~2.5*10⁻⁵ Torr</td>
<td></td>
<td></td>
</tr>
<tr>
<td>G6470</td>
<td>≤ 2.5 Torr</td>
<td>2– 3.5 * 10⁻⁵ Torr</td>
<td>3 – 6 * 10⁻⁶ Torr</td>
<td></td>
</tr>
<tr>
<td>G6495B</td>
<td>≤ 3.3 Torr</td>
<td>3.0 – 4.5 * 10⁻⁵ Torr</td>
<td>2 – 5 * 10⁻⁶ Torr</td>
<td></td>
</tr>
<tr>
<td>G6495C</td>
<td>&lt;2 Torr</td>
<td>3.0 – 4.0 * 10⁻⁵ Torr</td>
<td>1 – 5 * 10⁻⁶ Torr</td>
<td></td>
</tr>
<tr>
<td>G6530</td>
<td>1.5-2.5 Torr</td>
<td>~2 * 10⁻⁵ Torr</td>
<td>~3 * 10⁻⁶ Torr</td>
<td>~2 * 10⁻⁷ Torr</td>
</tr>
<tr>
<td>G6540, G6545</td>
<td>1.5-2.5 Torr</td>
<td>~5*10⁻⁵ Torr</td>
<td>~3 * 10⁻⁶ Torr</td>
<td>~2 * 10⁻⁷ Torr</td>
</tr>
<tr>
<td>G6545XT</td>
<td>1.5-2.5 Torr</td>
<td>~2– 3.5 * 10⁻⁵ Torr</td>
<td>~2– 3.5 * 10⁻⁵ Torr</td>
<td>~8 * 10⁻⁸ Torr</td>
</tr>
<tr>
<td>G6546</td>
<td>1.5-2.5 Torr</td>
<td>~5*10⁻⁵ Torr</td>
<td>~3 * 10⁻⁶ Torr</td>
<td>~2 * 10⁻⁷ Torr</td>
</tr>
<tr>
<td>G6550</td>
<td>2.5-3.5 Torr</td>
<td>~5*10⁻⁵ Torr</td>
<td>~3 * 10⁻⁶ Torr</td>
<td>~2 * 10⁻⁷ Torr</td>
</tr>
</tbody>
</table>

*Please note that turning “off” CC gas does not immediately show the ultimate HV pressure. The CC gas tubing has very small conductance and it takes ~20-30 minutes for complete evacuation.*
## Common Problems Associated with Pressure Problems

<table>
<thead>
<tr>
<th>Rough Vacuum</th>
<th>Vacuum Level “too good” possible causes</th>
<th>Vacuum Level “not good enough” possible causes</th>
</tr>
</thead>
<tbody>
<tr>
<td>Rough Vacuum</td>
<td>Plugged Capillary</td>
<td>• Gross Vacuum Leak</td>
</tr>
<tr>
<td></td>
<td></td>
<td>• Low Oil Level</td>
</tr>
<tr>
<td></td>
<td></td>
<td>• Insufficient Drying Gas Flow</td>
</tr>
<tr>
<td></td>
<td></td>
<td>• Insufficient Drying Gas Temperature</td>
</tr>
<tr>
<td></td>
<td></td>
<td>• Defective Rough Pump</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>High Vacuum</th>
<th>Insufficient Collision Cell Gas Flow</th>
<th>• Too much Collision Cell Gas Flow</th>
</tr>
</thead>
<tbody>
<tr>
<td>High Vacuum</td>
<td></td>
<td>• Vacuum Leak</td>
</tr>
<tr>
<td></td>
<td></td>
<td>• Failing Turbo Pump</td>
</tr>
</tbody>
</table>

More Details can be found in the online Agilent University Troubleshooting Course
Wishing you all Good Memories of Past Vacations..
Till we are back to traveling

Webinar on restarting your LC/TQ and LC/Q-TOF systems will take place in Early May
Resources for Support

https://community.agilent.com/

- Agilent support resources: https://community.agilent.com/community/resources
- Collection of support material https://community.agilent.com/docs/DOC-1856
- Agilent chemistries and supplies information: http://www.agilent.com/chem/agilentresources
- Agilent University http://www.agilent.com/crosslab/university
- Youtube – Agilent Channel
Additional online e-seminars and educational material

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Register here

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Agilent offers over 400 online, self-paced courses of which over half are free. Find training for specific instruments using [Agilent University Learning Paths](https://www.agilent.com/en/training-events/events/agilent-university).

Running Start
Train beginners using comprehensive Running Start courses at a value price. These five- to eleven-hour courses have no pre-requisites and are designed to make you productive quickly.

Cloud Lab Online Courses
For the ultimate in online, self-paced training with real hands on software labs, try [Agilent quant courses](https://www.agilent.com/en/training-events/events/agilent-university) with cloud laboratory. An Agilent exclusive offering that delivers better retention of complex learning.

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Remote Custom Training

Agilent offers customized live Instructor-led Training delivered remotely to a single customer site at a time of your choosing. For additional information, please reach out to your Regional Customer Education Coordinator team.

Virtual Instructor Led Training

Agilent has now introduced Live Instructor-led Training; delivered remotely to a group of customers covering standardized contents (https://inter.viewcentral.com/events/cust/catalog2.aspx?cid=agilent&pid=1&lid=1&app_id=3). This live e-Learning offers many of the benefits of classroom training without the need to travel.
Contact Agilent Technical Support

1-800-227-9770 Option 3, Option 3:
Option 1 for GC/GCMS Columns and Supplies
Option 2 for LC/LCMS Columns and Supplies
Option 3 for Sample Preparation, Filtration and QuEChERS
Option 4 for Spectroscopy Supplies
Option 5 for Chemical Standards

800 Phone lines available 8-5 in all US time zones

gc-column-support@Agilent.com
lc-column-support@agilent.com
spp-support@agilent.com
spectro-supplies-support@agilent.com
chem-standards-support@agilent.com
Additional support – Live one-on-one video conference with our service team

• Agilent Service Engineers are currently running live video conferences to remotely support labs around the world.

• To request a one-on-one video conference with one of our service engineers, please send your request through the polling survey and indicate the following:

  Name, Company, and instrumentation requiring support or questions

• We will get back to you shortly to schedule a video conference
In Summary

We at Agilent understand the restrictions and hardship many of you are going through because we’re experiencing them as well.

Given all that we are going through, Agilent remains a stable and continuing resource to meet and exceed your analytical measurement needs.

We are open for business and here to help.

Any questions?

All unanswered chat questions will be followed up post-event. Slides will be distributed to the email address you registered with.