

Xevo® TQ-S Performance Maintenance Technical Reference

This procedure describes how to perform the performance maintenance tasks required to complete the [Xevo TQ-S Performance Maintenance Protocol](#) (p/n 715002463).

Parts required

CAUTION: *The 176- PM kit part numbers can only be ordered by customers. Field service engineers must order the relevant 201- PM kit part number and the Xevo TQ-S sample kits ([Table 2](#)) separately.*

Table 1: Parts available for customers to order

Part number	Description	Qty
176002745	Xevo TQ-S PM Kit (Rotary Pump) w/chem	1
176002744	Xevo TQ-S PM Kit (Scroll Pump) w/chem	1

Table 2: Parts available for field service engineers to order

Part number	Description	Qty
201000236	Xevo TQ-S PM Kit (Rotary Pump)	1
700004729	[Glu ¹]-fibrinopeptide B	1
186006846	MS cleaning solution	1
700005331	Xevo TQ-S Setup Solution	1
700005471	Xevo TQ-S IntelliStart Resolution and Calibration Sample Kit	1
201000235	Xevo TQ-S PM Kit (Scroll Pump)	1
700004729	[Glu ¹]-fibrinopeptide B	1
186006846	MS cleaning solution	1
700005331	Xevo TQ-S Setup Solution	1
700005471	Xevo TQ-S IntelliStart Resolution and Calibration Sample Kit	1

CAUTION: *For systems with the tool-free probe, order the relevant probe capillary assembly, as described in the [Probe Capillary Assemblies Technical Reference Sheet](#) (p/n 715004774).*

Table 3: Optional parts

Part number	Description	Qty
700004842	APGC Service Kit	1
700009464	HT Diverter Rotor/Stator Kit ***	1
700005744	IonSABRE II Probe Service Kit	1
700004677	NanoLockSpray Reference Probe Service Kit **	1
700004670	Outer API Source Service Kit *	1
700004730	Outer APPI Source Service Kit	1

NOTE: * Certain items within the 700004670 Outer API Source Service Kit can also be used for the UniSpray source.

NOTE: ** Certain items within the 700004677 NanoLockSpray Reference Probe Service Kit can also be used for the NanoFlow source.

NOTE: *** On sites where the customer is experiencing high failure rates of the diverter valve, use the kit to replace the valve during the PM visit.

Tools/materials required

Waters sample kits

The following additional Waters chemical kit(s) may be required:

- Xevo TQ-S Setup Solution 700005331
- Xevo TQ-S IntelliStart Resolution and Calibration Sample Kit 700005471
- [Glu¹]-fibrinopeptide B 700004729
- MS cleaning solution 186006846

Chemicals

- LCMS grade water
- LCMS grade methanol
- Formic acid (minimum 95%)

Labware

- Paper towels, lint-free
- Ultrasonic bath
- 1000-mL beaker
- 500-mL graduated cylinder
- Waste container for roughing pump oil (2.5 L capacity, minimum)

Tools

- 2-mm Allen wrench
- 2.5-mm Allen wrench
- 3-mm Allen wrench
- 8-mm Allen wrench
- 12-mm Allen wrench (rotary pump)
- 7-mm open end wrench
- 8-mm open end wrench
- Flatblade (jeweler's) screwdrivers
- Pin spanner (if replacing turbo pump oil cartridges)
- Phillips #2 screwdriver
- Needlenose pliers or forceps
- O-ring removal kit (supplied with instrument)
- Fiberglass pencil (recommended, p/n 0901018)
- Lapping paper
- Nitrile gloves

Procedure

The procedure to complete the performance maintenance consists of four sections:

Perform the sections, confirm the steps listed for each procedure, and record the results in the [Xevo TQ-S Performance Maintenance Protocol](#) (p/n 715002463).

1. [Removing the calibration](#)
2. [Performing pre-performance maintenance checks](#)
3. [Performing maintenance tasks](#)
4. [Performing post-performance maintenance checks](#)

Software

1. Record the following software in the [Xevo TQ-S Performance Maintenance Protocol](#) (p/n 715002463):
 - Software version installed on the host PC
 - Service Pack or SCN installed
 - Application Managers installed

Removing the calibration

Calibration

CAUTION: *The instrument must be uncalibrated throughout the PM protocol.*

1. Record the current calibration file name and conditions in the [Xevo TQ-S Performance Maintenance Protocol](#) (p/n 715002463).
2. Load the Uncal.cal or Default.cal file to remove all calibrations from the system.

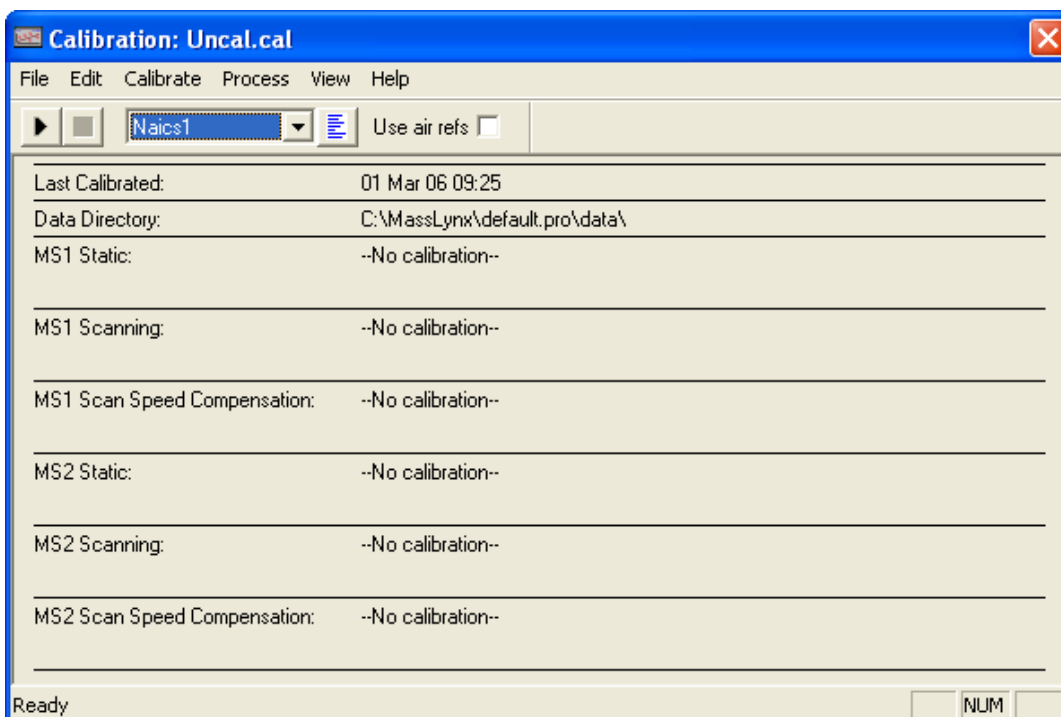


Figure 1 - Calibration file

Performing pre-performance maintenance checks

If the instrument fails to perform adequately during initial checks, it may need service work beyond the scope of the performance maintenance protocol; in such cases extra service work may incur additional parts and labor charges.

Perform the steps listed for each procedure, and record the results in the [Xevo TQ-S Performance Maintenance Protocol](#) (p/n 715002463).

Vacuum

Check the instrument vacuum:

1. Ensure the collision gas is turned off.
2. Check the analyzer MS2 Penning and the collision cell Pirani vacuum gauge readings.
3. Record the results in the [Xevo TQ-S Performance Maintenance Protocol](#) (p/n 715002463).

Heaters

Check the source and desolvation heaters.

1. Set the source heater to **150 °C** and confirm that it stabilizes at 150 ± 3 °C.
2. Set the desolvation heater to **650 °C**, the API gas to **1200 L/hour**, and confirm that the heater stabilizes at 650 ± 10 °C.
3. Record the results in the [Xevo TQ-S Performance Maintenance Protocol](#) (p/n 715002463).

Interlocks

WARNING: It is critical that the source interlocks are in an operational state to protect users.

1. Check that the source interlock activates as required when the source enclosure is opened.

Mass scale and resolution

Assess the mass scale setup and resolution across the mass range in MS1 and MS modes.

NOTE: *The Advanced MS Tune page parameters and Interscan parameters must be set to automatic during the PM.*

1. Open four Tune page MS1 mass windows at 59.05, 455.27, 1080.80, and 2034.64 Da.
2. Infuse Waters Xevo TQ-S setup solution at a flow rate of 10 μ L/minute using the integrated fluidics.
3. Optimize the source parameters and probe position to give the most intense signal.
4. Complete the following steps for MS1 scan (MS1):
 - a. Ensure the collision gas is off.
 - b. Set the LM resolution 1 and LM resolution 2 values to **3**.
 - c. Set the HM resolution 1 and HM resolution 2 values to **15**.
5. Acquire **2.3 minutes** of MCA data for MS1 (scan function MS1 scan) from 15 to 2048 Da in 10 second scan; use a suitable filename, for example "DDMMYY_MS1_PRE_PM".
6. Ensure that the resolution is consistent across the range scanned and that the measured masses are within ± 1 Da of the actual masses.

NOTE: *If the measured mass is outside ± 1 Da or the FWHM resolution is not within 0.4 to 0.6 Da, adjustments are required by a qualified Waters engineer.*

7. Record the results in the [Xevo TQ-S Performance Maintenance Protocol](#) (p/n 715002463).
8. Switch on the collision gas for MS scan (MS2).
9. Acquire **2.3 minutes** of MCA data for MS (scan function MS2 scan) from 15 Da to 2048 Da in 10 second scan; use a suitable filename, for example "DDMMYY_MS2_PRE_PM".
10. Check that the resolution is consistent across the range scanned and that the measured masses are within ± 1 Da of the actual masses.

NOTE: *If the measured mass is outside ± 1 Da or the FWHM resolution is not within 0.4 to 0.6 Da, adjustments are required by a qualified Waters engineer.*

11. Record the results in the [Xevo TQ-S Performance Maintenance Protocol](#) (p/n 715002463).
12. Switch to the Negative Ion mode and perform the following steps:
 - a. Open two mass windows to display MS mode masses of 255.3 and 554.3 and ensure a signal is present.
 - b. Switch off the collision gas.
 - c. Open two mass windows to display MS1 mode masses of 255.3 and 554.3 and ensure a signal is present.
13. Record the high mass DC balance for MS1 and MS2 observed on the Resolution tab of the Tune page in the [Xevo TQ-S Performance Maintenance Protocol](#) (p/n 715002463).

PMT voltage

1. Check that the detector gain is set to **1.0**.
2. Check the positive ion multiplier voltage on the MS Tune page Diagnostics tab.
3. Record the results in the [Xevo TQ-S Performance Maintenance Protocol](#) (p/n 715002463).
4. Repeat these steps for Negative Ion mode.

Firmware version

1. Run the MS SWAT software to see the version of the PCB firmware.
2. Consult [Service Notes](#) database to ensure the correct firmware version is installed.

Performing maintenance tasks

For more information on these procedures, refer to the relevant [operator's guide](#) and the [Xevo TQ-S Installation Manual](#) (p/n 715002461).

Perform the steps listed for each procedure in the [Xevo TQ-S Performance Maintenance Protocol](#) (p/n 715002463).

WARNING: *The following procedures may expose the performer to toxic substances representing a biohazard. Wear nitrile gloves when necessary.*

Use of a fume cupboard for mixing or cleaning is recommended.

Vent, power-off, inspect

1. Vent the instrument through MassLynx and confirm the following:
 - The turbo pump spins down to approximately 50% before the vent valve opens
 - The rotary pump switches off at approximately 45%
2. Check that the instrument cooling fans (located in the electronics box and at the rear of the chassis) are working.
3. Power-off the instrument and unplug the instrument and rotary/scroll pump cables.
4. Inspect the fluidics system and all liquid waste tubing for any signs of solvent leakage or damage.
5. Inspect the source exhaust line and trap bottle; drain any condensed solvent.

Source door latch mechanism

NOTE: *If the source door handle is broken or the source door is difficult to open and close, perform the following step.*

1. Perform the procedure as described in [Testing the Source Door Latch Mechanism/Universal Sources](#) (p/n 715005533).

Source

1. Disassemble the ion source and ion support block.
2. Remove the cone gas cone, sample cone and sample cone O-ring.
3. Wipe the cover plate with methanol.
4. Sonicate the ion block:

WARNING: *Formic acid is hazardous. Wear nitrile gloves when using it.*

- a. In 50:50 methanol/water plus 10% formic acid for 20 to 30 minutes.
 - b. In 100% water for 10 minutes.
 - c. In 99:1 methanol/water for 10 minutes.
 - d. Blow dry the ion block using nitrogen.
5. Remove the StepWave assembly.
 6. Disassemble the StepWave (remove the ion guide from the differential apertures).

NOTE: *Click the links to play animations showing how to perform the following procedures:*

- [Removing the StepWave assembly](#)
 - [Disassembling the StepWave assembly](#)
7. Refer to the [StepWave Ion Guide Cleaning Instructions Addendum](#) (p/n 715003880) for a detailed description of how to remove and clean the StepWave assembly.
 8. Reassemble the StepWave ion guide assembly and insert into the instrument.
 9. Replace the source cartridge heater.
 10. Install the new sample cone.
 11. Reassemble the ion source, using all of the relevant parts contained in the PM kit.
 12. Replace all source enclosure O-rings, including:
 - Source enclosure door O-ring
 - Source enclosure glass O-ring
 - Probe adjuster O-ring
 - Gas seal O-rings (x 3)
 - Source LED O-ring

NOTE: *In some cases more aggressive cleaning may be required; refer to the relevant [operator's guide](#) for details.*

ESI probe

1. Replace the probe capillary assembly as described in [Probe Capillary Assemblies Technical Reference Sheet](#) (p/n 715004774).
2. Dismantle and rebuild the ESI probe using the relevant parts from the PM kit; the following parts must be replaced:
 - Capillary
 - Liner tube
 - Ferrule
 - PEEK union
 - Conductive sleeve
 - Viton probe gasket
 - Probe tip
 - Probe tip gasket

NOTE: *Position the new capillary inside the new PEEK union in such a way that there is no dead volume.*

Click the links to play animations showing how to perform the following procedures:

- [Removing the ESI probe](#)
- [Disassembling the ESI probe](#)

Vacuum system

Systems using rotary pumps

1. Replace the Penning gauge body.
2. Inspect the backing vacuum hoses for evidence of damage, collapse, or back streaming.
3. Check the security of joints and clamps.
4. Replace the exhaust oil mist filter element in the rotary pump; wear the gloves supplied in the kit.
5. Change the oil in the rotary pump.
6. Check inlet anti-suckback valve.

NOTE: *Refer to the [Rotary Pump Technical Reference Sheet](#) (p/n 715002808) for details.*

Systems using scroll pumps

1. Replace the Penning gauge body.
2. Inspect the backing vacuum hoses for evidence of damage or collapse.
3. Check the security of joints and clamps.
4. Replace the exhaust spring and valve pad.

5. Replace the tip seal in the scroll pump.

NOTE: *XDS35i pumps and XDS100B pumps use identical tip seals. XDS46i pump tip seals are 210 mm longer.*

The Xevo TQ-S PM Kit (p/n 201000235) contains two tip seal kits; tip seal kit XDS35i / XDS100B (p/n 6061146-S) and tip seal kit XDS46i (p/n 700005663). For instruments equipped with an XDS35i pump and an XDS100B pump, tip seal kit XDS46i (p/n 700005663) can be cut down to length to fit either pump.

Internal turbo pumps

The turbo pump oil cartridges need to be replaced every two years, during performance maintenance.

1. Consult [Replacing Oil Cartridges and Bearings / nEXT Turbo Pumps](#) (p/n 715003655) to assess the condition of the turbo pumps.

NOTE: *A red flag indicates the pumps have been operating for more than two years using the current cartridge.*

Fan filters

1. Replace the fan filters on the front and side panels with the new filters supplied in the PM kit.

Power-up

1. Plug in all power leads and switch on the system power.
2. Click **Vacuum > Pump..** in MassLynx, and confirm that the pumps start.

Gas supplies and exhausts

1. Empty the source exhaust bottle.
2. Check the source exhaust outlet tubing is connected to a suitable gas extraction system (separate from the roughing pump exhaust).
3. Check the security and integrity of all external gas supply lines.
4. Check that the nitrogen supply is at the correct pressure (6 to 7 bar).
5. Check that the collision gas supply is at the correct pressure (0.5 bar).

Source and probe options (if applicable)

CAUTION: *PM parts for source options are not supplied in the instrument PM kit and must be ordered separately.*

APCI IonSABRE II probe

1. Dismantle and rebuild the APCI probe using the relevant parts; the following parts must be replaced:
 - Capillary
 - Ferrule
 - Filter
2. Replace the APCI corona pin.

APPI

1. Replace all source enclosure O-rings, including:
 - Source enclosure door O-ring
 - Source enclosure glass O-ring
 - Probe adjuster O-ring
 - Gas seal O-rings (x 3)
 - Source LED O-ring
 - Lamp shaft seals
2. Replace the APPI corona pin.
3. Replace the APPI lamp shaft O-rings.

NanoFlow

1. Replace all source enclosure O-rings, including:
 - Source enclosure door O-ring
 - Source enclosure glass O-ring
 - Probe adjuster O-ring
 - Gas seal O-rings (x 3)
 - Source LED O-ring
2. Replace the fused silica adaptor, PEEK fittings, and union.

TRIZAIC

1. Replace all source enclosure O-rings, including:
 - Source enclosure door O-ring
 - Source enclosure glass O-ring
 - Probe adjuster O-ring
 - Gas seal O-rings
 - Source LED O-ring
2. Replace the following parts on the analyte sprayer:
 - TRIZAIC tile
 - PEEK fittings
 - Fused silica line to emitter

3. Dismantle and rebuild the reference probe using the relevant parts from the PM kit. Replace the following parts on the reference probe:
 - Taper tip emitter
 - PEEK fittings
 - Union
 - Fused silica line to emitter

APGC

1. Replace all source enclosure O-rings, including:
 - Source enclosure door O-ring
 - Source enclosure viewing window O-ring
 - Gas seal O-rings (x 2)
2. Replace the heated transfer line components contained within the PM kit.
3. Replace the APMC corona pin.

UniSpray

1. Replace the following source enclosure O-rings as described in [UniSpray Source Enclosure Assembly Technical Reference Sheet](#) (p/n 715005294).
 - Source enclosure door O-ring
 - Source enclosure glass O-ring
 - Gas seal O-rings (x 2)
 - Source LED O-ring

ionKey

1. Replace all source enclosure O-rings, including:
 - Source enclosure door O-ring
 - Source enclosure glass O-ring
 - Probe adjuster O-ring
 - Gas seal O-rings
 - Source LED O-ring

Performing post-performance maintenance checks

Pump the instrument down and repeat the pre-performance maintenance checks to verify that the instrument performance is satisfactory.

Perform the steps listed for each procedure, and record the results in the [Xevo TQ-S Performance Maintenance Protocol](#) (p/n 715002463).

Vacuum

1. Check the instrument vacuum.
2. Record the results in the [Xevo TQ-S Performance Maintenance Protocol](#) (p/n 715002463).

Heaters

1. Check the source and desolvation heaters.
2. Record the results in the [Xevo TQ-S Performance Maintenance Protocol](#) (p/n 715002463).

Mass scale and resolution

Assess the mass scale and resolution setup, including ion energy and DC balance.

1. Optimize the ion energy in MS1 Positive Ion mode:
 - a. In Positive Ion mode, open a single MS1 Scan window to display mass 59.05 Da with a span of 3.
 - b. Set the MS1 DC balance to **0** on the Resolution tab.
 - c. Set the collision energy to **5** on the Source tab.
 - d. Optimize the MS1 ion energy to maximize the intensity of the m/z 59.05 ion.
 - e. Tune the ion energy so that the intensity of the m/z 59.05 ion drops to 5 to 10% of the maximum intensity obtained in the previous step.
 - f. Add **0.5 V** to the current ion energy value; this is the optimal low mass ion energy for MS1.
2. Optimize the DC balance in MS1 mode:
 - a. In Positive Ion mode, open a single MS1 Scan window to display mass 2034.64 Da with a span of 3.
 - b. Adjust the DC balance to maximize the intensity of the 2034.64 Da signal.

NOTE: Do not adjust beyond ± 3 V.

- c. Adjust the DC balance so that intensity of the m/z 2034.64 ion drops to 5 to 10% of the maximum intensity.
 - d. Adjust the DC balance value by **± 0.5 V** so that the intensity of the m/z 2034.64 signal increases; this is the optimum DC balance.
3. Acquire **2.3 minutes** of MCA data for MS1 (scan function MS1 scan) from 15 to 2048 Da in 10 second scan; use a suitable filename, for example, "DDMMYY_MS1_POST_PM".
 4. Record the results in the [Xevo TQ-S Performance Maintenance Protocol](#) (p/n 715002463).

5. Ensure that the resolution is consistent across the range scanned and that the measured masses are within ± 1 Da of the actual masses.

NOTE: *If the measured mass is outside ± 1 Da or the FWHM resolution is not within 0.4 to 0.6 Da, adjustments will have to be made to the instrument by a qualified Waters engineer.*

6. Switch on the collision gas for MS scan (MS2).
7. Optimize the ion energy in MS2 Positive Ion mode:
 - a. In Positive Ion mode, open a single MS Scan window to display mass 59.05 Da with a span of 3.
 - b. Set the MS2 DC balance to **0** on the Resolution tab.
 - c. Set the collision energy to **5** on the Source tab.
 - d. Optimize the MS2 ion energy to maximize the intensity of the m/z 59.05 ion.
 - e. Tune the ion energy so that the intensity of the m/z 59.05 ion drops to 10% of the maximum intensity obtained in step 1e.
 - f. Add **1.0 V** to the current ion energy value; this is the optimal low mass ion energy for MS2.
8. Optimize the DC balance in MS2 mode:
 - a. In Positive Ion mode, open a single MS Scan window to display mass 2034.64 Da with a span of 3.
 - b. Adjust the DC balance to maximize the intensity of the 2034.64 Da signal.

NOTE: *Do not adjust beyond ± 3 V.*

- c. Adjust the DC balance so that intensity of the m/z 2034.64 ion drops to 10 to 15% of the maximum intensity.
 - d. Adjust the DC balance value by **± 1.0 V** so that the intensity of the m/z signal increases; this is the optimum DC balance.
9. Acquire **2.3 minutes** of MCA data for MS (scan function MS2 scan) from 15 Da to 2048 Da in 10 second scan; use a suitable filename, for example, "DDMMYY_MS2_POST_PM".
10. Record the results in the [Xevo TQ-S Performance Maintenance Protocol](#) (p/n 715002463).
11. Check that the resolution is consistent across the range scanned and that the measured masses are within ± 1 Da of the actual masses.

NOTE: *If the measured mass is outside ± 1 Da or the FWHM resolution is not within 0.4 to 0.6 Da, adjustments will have to be made to the instrument by a qualified Waters engineer.*

12. Switch to Negative Ion mode and perform the following steps:
 - a. Open two mass windows to display MS mode masses of 255.3 and 554.3 and ensure a signal is present.
 - b. Switch off the collision gas.
 - c. Open two mass windows to display MS mode masses of 255.3 and 554.3 and ensure a signal is present.
13. Record the results in the [Xevo TQ-S Performance Maintenance Protocol](#) (p/n 715002463).

Charging test

CAUTION: *If the charging test fails, inspect the quadrupole for ion burns and clean as described in the [Quadrupole Assembly Technical Reference Sheet](#) (p/n 715002661), and then clean the collision cell as described in the [ScanWave Collision Cell Technical Reference Sheet](#) (p/n 715002816).*

Ensure that the instrument has been pumping for at least 2 hours before running the charging test.

Positive ion beam test

Switch on the API gas, place the instrument into Operate, and then infuse the Xevo TQ-S leucine enkephalin set-up solution at 10 µL/min.

1. Set the Desolvation temperature and gas flow rate to the same values in the ESI positive and the ESI negative tunes pages (550 L/hr, 200 °C).
2. On the Tune page, set the following parameters:

Table 4: Tune page parameters

Function	Set	Mass	Span	Gain
MS1 Scan	n/a	59.05	5	10
MS1 Scan	n/a	455.27	5	10
MS1 Scan	n/a	1080.8	5	10
MS1 Scan	n/a	2034.62	5	15

3. Optimize the capillary voltage.
4. Set the following parameters:
 - Sample cone voltage **80 V**
 - Ion block offset voltage **60 V**
 - MS1 LM resolution **3**
 - HM resolution **15**
5. Set the ion energy to the optimum for the instrument.

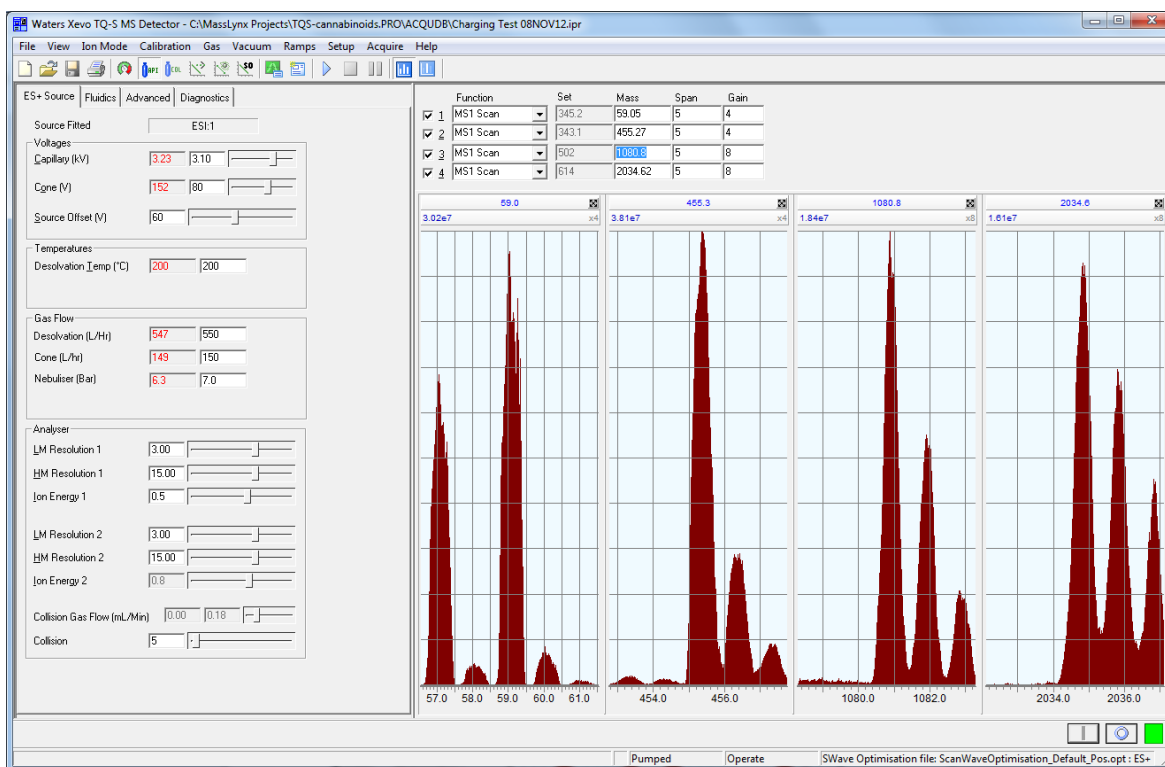


Figure 2 - Example of a positive Ion beam

6. Click **Ion mode > ESI –ve ion** and check for a beam in negative ion.
7. Set the following masses:
 - Window 1 **59 Da**
 - Window 2 **255.3 Da**
 - Window 3 **554.3 Da**
8. Optimize the capillary voltage.
9. Set the following parameters:
 - Sample cone voltage **40 V**
 - Ion block offset voltage **60 V**
 - MS1 LM resolution **3**
 - HM resolution **15**

10. Set the ion energy to the optimum for the instrument.

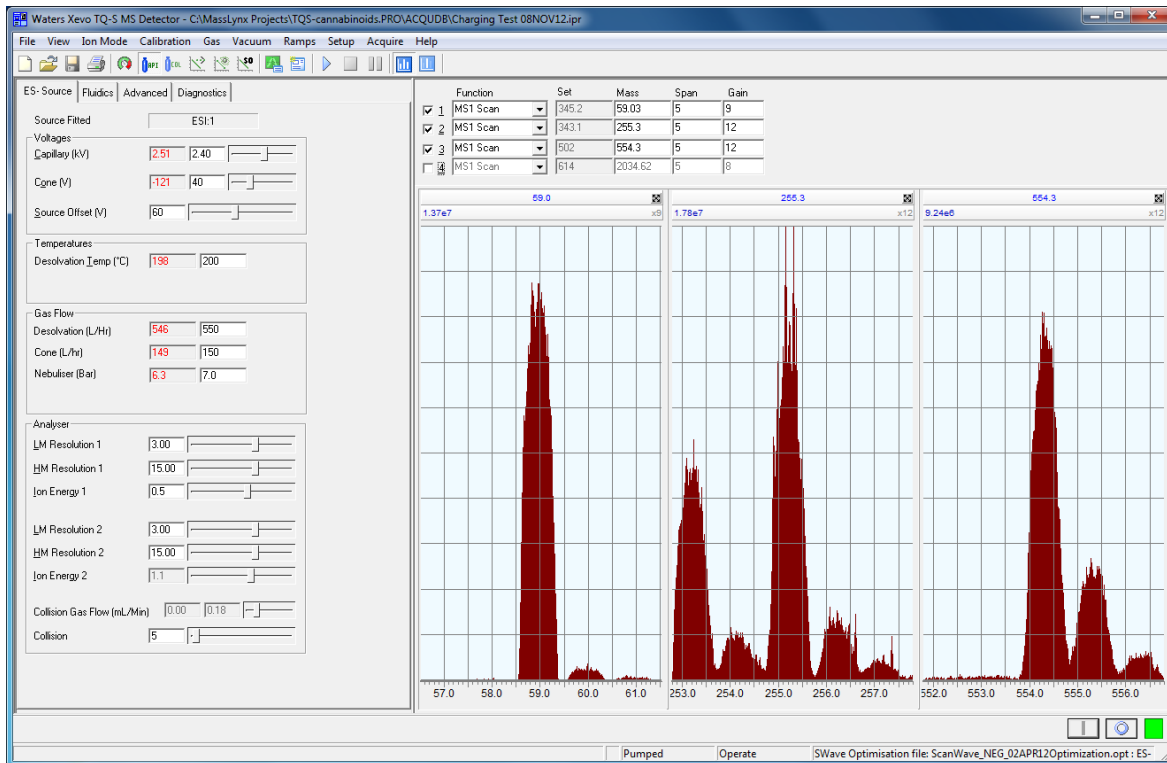


Figure 3 - Example of a Negative Ion beam

Preparation

1. Create the following MS method experiment file or download the file from the [Xevo TQ-S Reference Information](#) area of the Waters Portal ([Figure 4](#)).

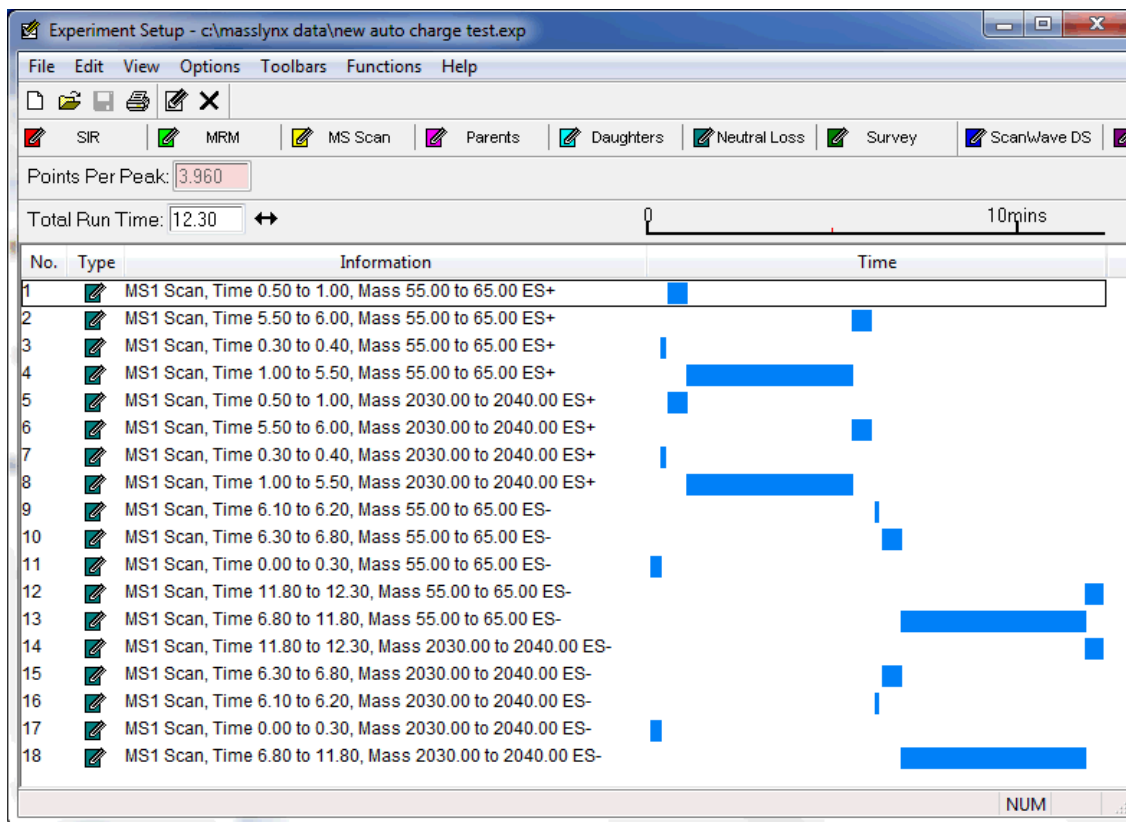


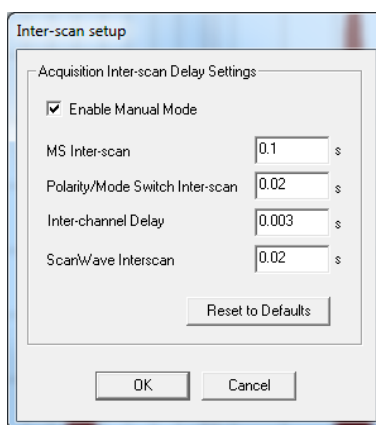
Figure 4 - MS method experiment

NOTE: Each Function has the parameters MS1 mode, Continuum, scan time of 0.5 seconds.

Table 5: Function settings

Function	ES mode	Start time	End time	Start mass	End mass
1	Positive	0.50	1.00	55.00	65.00
2		5.50	6.00	55.00	65.00
3		0.30	0.40	55.00	65.00
4		1.00	5.50	55.00	65.00
5		0.50	1.00	2030.00	2040.00
6		5.50	6.00	2030.00	2040.00
7		0.30	0.40	2030.00	2040.00
8		1.00	5.50	2030.00	2040.00
9	Negative	6.10	6.20	55.00	65.00
10		6.30	6.80	55.00	65.00
11		0.00	0.30	55.00	65.00
12		11.80	12.30	55.00	65.00
13		6.80	11.80	55.00	65.00
14		11.80	12.30	2030.00	2040.00
15		6.30	6.80	2030.00	2040.00
16		6.10	6.20	2030.00	2040.00
17		0.00	0.30	2030.00	2040.00
18		6.80	11.80	2030.00	2040.00

2. Change the inter-scan delay to duplicate the Tune page.

*Figure 5 - Inter-scan setup dialog*

CAUTION: Once the charging test is complete, the inter-scan delay must be reset to the state (automatic or manual) used by the customer.

3. Use this experiment file in the sample list page.
4. Ensure that the file name represents the serial number of the Xevo TQ-S.
5. Save the sample list.

Acquisition

1. Set fluidics to Infusion.
2. Set a flow rate of 10 $\mu\text{L}/\text{min}$ and start the infusion.
3. Start the acquisition.

NOTE: The run takes 12 minutes to complete.

Processing

1. Open the chromatogram TIC functions shown in [Table 6](#):

Table 6: Chromatogram TIC functions

Function number	ESI mode	Description
1	Positive	Low mass intensity at start of run
2	Positive	Low mass intensity at end of run
5	Positive	High mass intensity at start of run
6	Positive	High mass intensity at end of run
10	Negative	Low mass intensity at start of run
12	Negative	Low mass intensity at end of run

2. Use Global / Replace and Smooth all the chromatograms using the settings in [Figure 6](#):

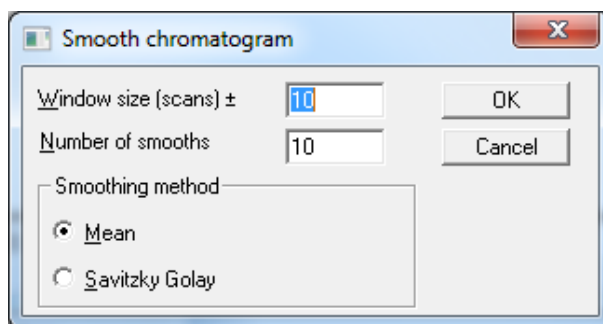


Figure 6 - Smooth chromatogram settings

3. Calculate the % difference between the following functions, using the equation in [Figure 7](#):

- Functions 1 and 2 (Low mass Positive Ion mode)
- Functions 5 and 6 (High mass Positive Ion mode)
- Functions 10 and 12 (Low mass Negative Ion mode)

$$\% \text{ Difference} = 100 \times \left(\left(\frac{\text{End of run smoothed TIC Intensity}}{\text{Start of run smoothed TIC Intensity}} \right) - 1 \right)$$

Figure 7 - % difference equation

NOTE: *Negative % results = loss of intensity over time.
Positive % results = a gain of intensity over time.*

Specification

If any of the traces are outside the following tolerances, then charging is present.

- Functions 1 and 2 must not exceed -18% to +13%
 - Functions 5 and 6 must not exceed -23% to +27%
 - Functions 10 and 12 must not exceed -19% to +15%
1. If the charging test fails, clean the collision cell, check the quadrupole for ion burn, and clean if necessary.
 2. Repeat the charging test as described above.

Report and printout

1. Label the chromatogram functions 2, 6, and 12 with their respective % Difference values.
2. Screen capture and print the chromatogram in portrait configuration and label with the instrument serial number.

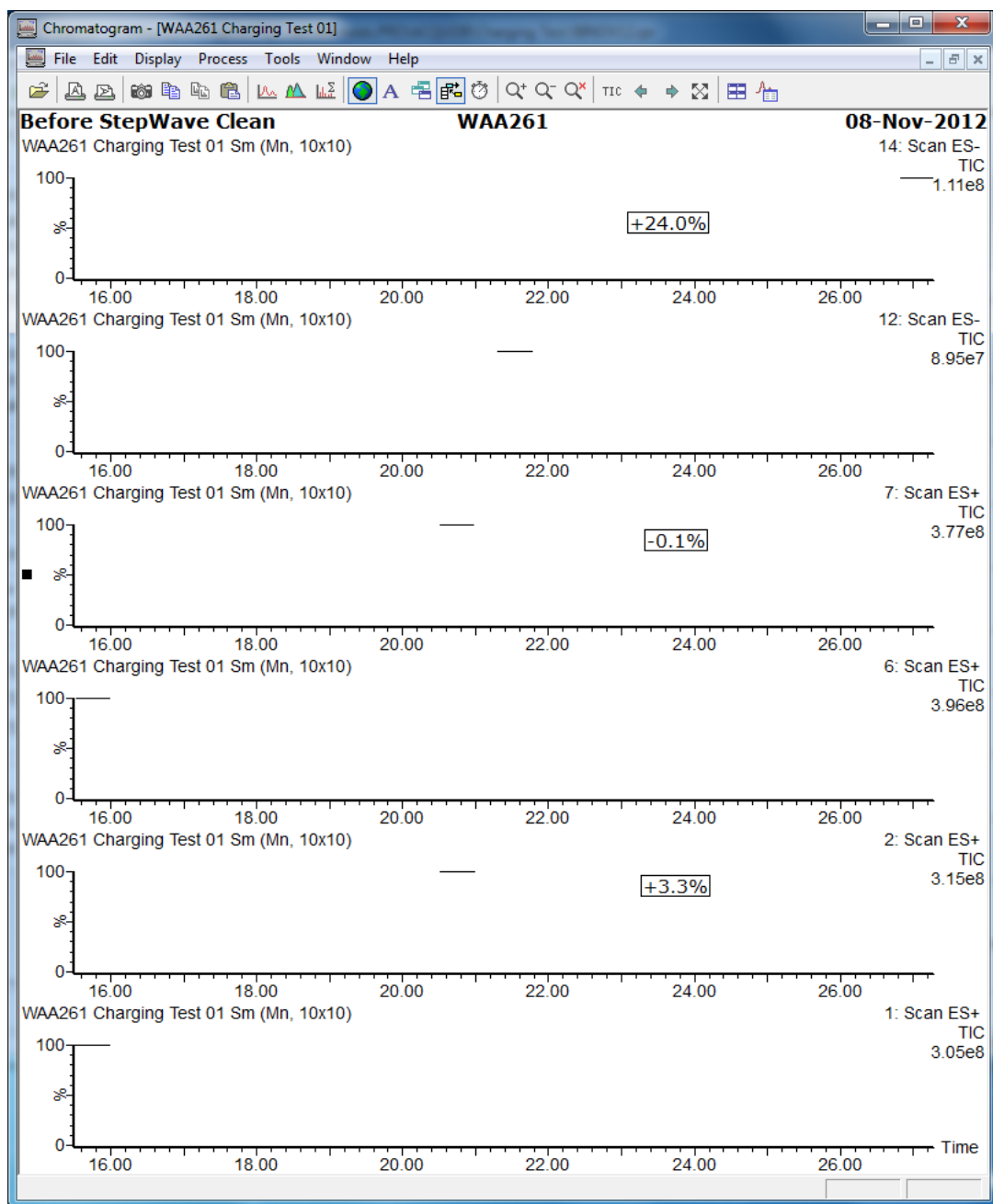


Figure 8 - Example of charging test chromatogram showing a failure

CAUTION: Once the charging test is complete, the inter-scan delay (Figure 5) must be reset to the state (automatic or manual) used by the customer.

Calibration

Use IntelliStart™ to perform an instrument resolution setup and calibration for each of the resolution modes used by the customer; refer to the [Xevo TQ-S Installation Manual](#) (p/n 715002461) for details of the calibration procedure.

ScanWave™ enhancement

Perform the following steps to verify the current ScanWave optimization in Positive Ion mode:

1. Load the saved positive optimization file and ensure that **Optimization Enabled** is selected.
2. Infuse 100 fmol/μL [Glu¹]-fibrinopeptide B at 10 μL/min using the integrated fluidics.
3. Open one MS1 Tune page at 786 Da.
4. Adjust the source parameters so that the intensity of the precursor ion is <10% when the Tune page is set to 1.
5. Leave the LM resolution on 3 and HM resolution on 15 and record this position. Use this method in the Method Editor Daughters of field ([Figure 9](#)).
6. Open the collision gas and set the collision gas pressure to **3E-3 mbar**.
7. Create two experimental methods, one with a single daughter scan and the other with a single ScanWave DS; use the parameters shown in [Figure 9](#).

NOTE: *It is recommended that the collision cell pressure is set at 3E-3 mbar.*

Figure 9 - Daughter scan (left) and ScanWave DS (right) parameters

8. Create two runs on the sample list, one for the daughter scan experiment and one for the ScanWave DS experiment.

9. Ensure that the sample text clearly indicates which experiment is being run, then acquire both runs.
10. Open the resulting chromatograms on a single page and smooth both with the settings shown in [Figure 10](#).

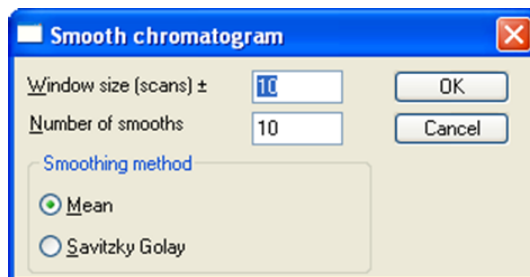


Figure 10 - Smoothing the chromatogram

11. Compare the smoothed chromatograms; ensure the ratio of the maximum TIC values is $> \times 7$.
12. If the required enhancement is not observed, perform a ScanWave optimization.

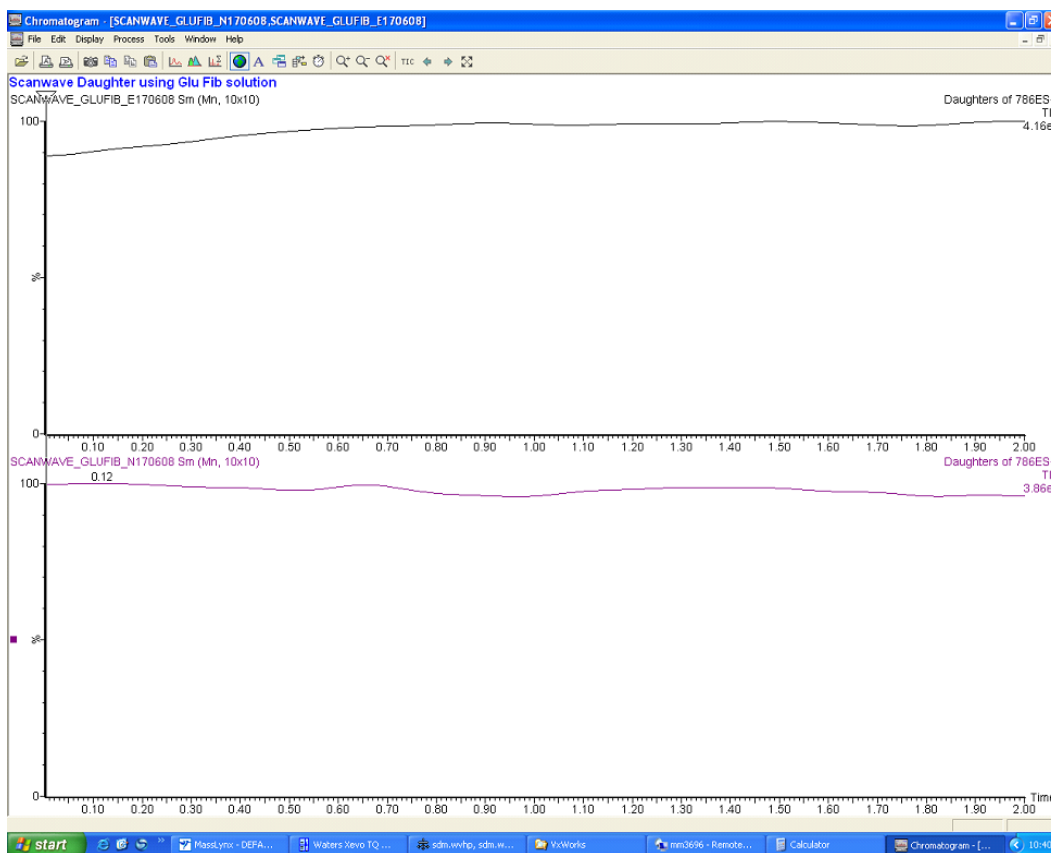


Figure 11 - Comparing the chromatograms

13. Record the results in the [Xevo TQ-S Performance Maintenance Protocol](#) (p/n 715002463).

14. Verify the current ScanWave optimization in Negative Ion mode:

- Load the saved negative optimization file and ensure that **Optimization Enabled** is selected.
- Infuse 300 fmol/ μ L [Glu¹]-fibrinopeptide B at 10 μ L/min using the integrated fluidics and optimize the intensity of this ion; the intensity of the precursor ion must be <10% when the gain of the Tune page is set to 1.
- Create two experimental methods, one with a single daughter scan and the other with a single ScanWave DS; use the parameters shown in Figure 12.

NOTE: It is recommended that the collision cell pressure is set at $3E-3$ mbar.



Figure 12 - Daughter scan (left) and ScanWave DS (right) parameters

- Create two runs on the sample list, one for the daughter scan experiment and one for the ScanWave DS experiment.
- Ensure that the sample text clearly indicates which experiment is being run. Acquire both runs.
- Open the resulting chromatograms on a single page and smooth both with the following settings.

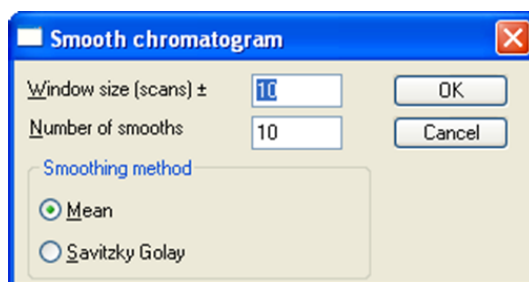


Figure 13 - Smoothing the chromatogram

18. Compare the smoothed chromatograms; ensure the ratio of the maximum TIC values is $>x7$.
19. If necessary, perform a ScanWave optimization in Negative Ion mode.

NOTE: See the [Xevo TQ-S ScanWave Collision Cell Assembly Technical Reference Sheet](#) (p/n 715002816) for full details of the ScanWave optimization procedure.

20. Record the results in the [Xevo TQ-S Performance Maintenance Protocol](#) (p/n 715002463).

Target Registry back-up

It is advisable to backup the information on the instrument flash memory to the host PC in case of accidental loss of settings.

1. Click the **Advanced** tab of the MS Tune page, and deselect **Manual Control**.
2. Place the instrument into Standby.
3. Exit MassLynx.
4. Browse to and double-click the **C:\MassLynx\Vulcan\TargetRegistryEditor.exe** file.
5. Type **1147** as the password.

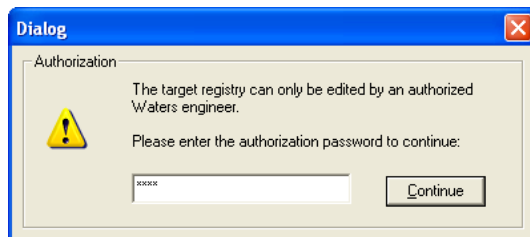


Figure 14 - Opening the Target Registry Editor

CAUTION: Do not alter any of the settings contained in the registry view.

6. Right-click in the view and select **Export All**.
7. Export the settings to an appropriate folder on the host PC.
8. When complete, close the Target Registry Editor and re-open MassLynx.
9. Record the results in the [Xevo TQ-S Performance Maintenance Protocol](#) (p/n 715002463).

Appendix: Replacing the turbo pump oil cartridges

CAUTION: *Replace the oil cartridges on all three pumps to minimize disruption to the customer.*

Tools/materials required

- Pin-spanner
- 3 x replacement oil cartridges (p/n 700009084)

NOTE: *A pin-spanner can be ordered from Farnell (p/n 1379081).*

WARNING: *Wear chemical-resistant, powder-free gloves while performing this procedure to avoid direct contact with pump oil.*

Procedure

The procedure to replace the oil cartridges consists of the following sections:

1. Replacing the oil cartridges
2. Resetting the service flags
3. Checking the counters

Replacing the oil cartridges

1. Remove the right-hand panel.
2. Note the initial configuration of the vacuum system.

NOTE: *At the end of the procedure, ensure that the configuration has been replaced correctly.*



Figure 15 - Vacuum system initial configuration

3. Disconnect or remove all flexible piping from the turbo pump ports.
4. On the left-hand turbo pump, loosen the locking screw on the fan cowling assembly.
5. Rotate the assembly to the left to unlock it.
6. Lower the fan cowling assembly (with the turbo fan attached), and carefully lift away from the pump.



Figure 16 - Location of screws on fan cowling strip

7. Unscrew the oil cartridge in the base of the turbo pump using the pin-spanner (Figure 17).



Figure 17 - Turbo pump showing location of oil cartridge

8. Screw in a new oil cartridge.
9. Tighten the cartridge using the pin-spanner.
10. Replace the fan cowling assembly and turbo fan, and rotate the assembly to the right to lock it.
11. Tighten the locking screw to secure the assembly.
12. Remove and retain the two screws from the bracket holding the pressure gauge beneath the central turbo pump (Figure 18).
13. Move the gauge aside gently, ensuring no tubing connections are damaged.



Figure 18 - Location of pressure gauge bracket screws

14. Rotate the solenoid valve beneath the central turbo pump to the right to allow enough room to access the central turbo pump with the pin-spanner (Figure 19).
15. Remove the KF25 to KF16 reducer.

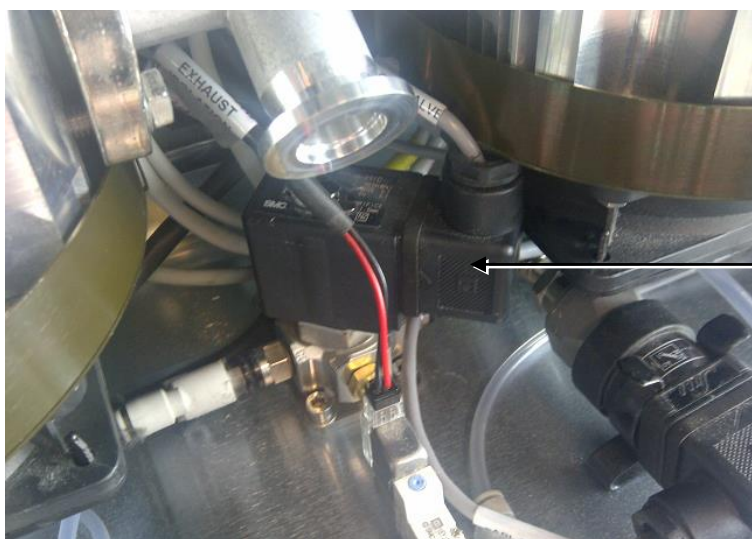


Figure 19 - Solenoid valve rotated to the right

16. On the central turbo pump, repeat steps 4 to 11 to replace the cartridge.
17. Replace the bracket holding the pressure gauge beneath the central turbo pump, securing it using the the two screws retained.
18. Rotate the solenoid valve beneath the central turbo pump to the left to allow enough room to access the right-hand turbo pump with the pin-spanner.
19. On the right-hand turbo pump, repeat steps 4 to 11 to replace the cartridge.
20. Return the solenoid valve to its initial position.
21. Reconnect all vacuum connections and piping to their initial configurations, as shown in [Figure 15](#).
22. Replace and secure the right-hand panel.

Resetting the service flag

After replacing the oil cartridge, the service flag for the pump ([Figure 20](#)) must be reset within the software. This is achieved by sending a command to the pump, using the following procedure.

CAUTION: *The command must be sent to each pump where the oil cartridge has been replaced.*

1. Open the MassLynx MS Tune page.
2. Click **View > Advanced**.
3. Click **View > System and View > System Diagnostics** to access the advanced MS Tune page tabs.

NOTE: *This page is not for customer use and is password protected. The password is 1147.*

4. Click the **Turbo Diagnostics** tab ([Figure 20](#)).
5. Click the Request drop-down list, and Select **No change**.
6. Enter the string to send to the pump, in the Command field, in the format #dd:98!C886 1.

NOTE: *dd is the address of the pump to be reset. Addresses start from 01 and count upwards; on the Xevo TQ-S the values are 01, 02, and 03.*

CAUTION: *There is a space between 886 and 1.*

7. Click the Request drop-down list, and select **Send arbitrary RS485 command once only**.
8. Click **Send**, to reset the turbo pump.

- Click the Request drop-down list, and Select **No change**.

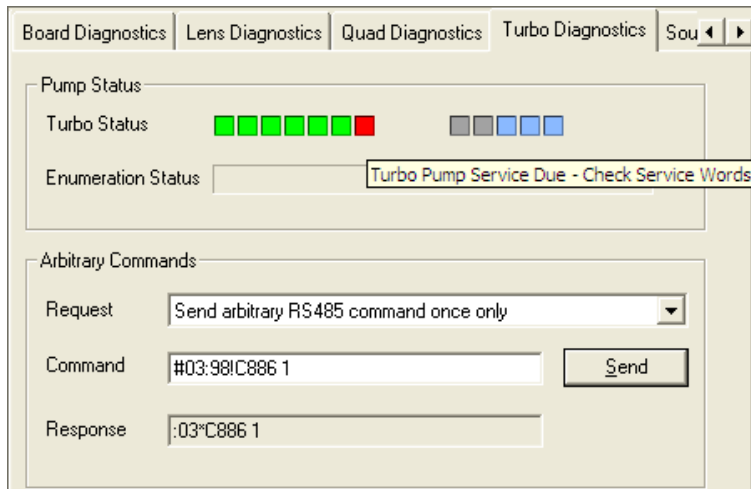


Figure 20 - Sending the service flag commands

- Check the response received (which scrolls across the Response field) is in the format #98:dd*C886 1.

NOTE: The response received is similar to command sent. The address at the start of the response string and the asterisk mark (originally an exclamation mark) have changed.

Checking the counters

Once the flag has been reset, check that the counter on each pump has returned to the expected value. The counter records the number of hours run by the oil cartridge to date, and the number of hours until the next change is required.

CAUTION: The counter check must be performed for each pump where the oil cartridge has been replaced.

- Click the **Turbo Diagnostics** tab (Figure 21).
- Select **No change** from the drop-down Request list.
- Enter the string to send to the pump in the Command field, in the format #dd:98?V886.

NOTE: dd is the address of the pump to be reset. Addresses start from 01 and count upwards; on the Xevo TQ-S the values are 01, 02, and 03.

4. Click the Request drop-down list, and select **Send arbitrary RS485 command once only**.
5. Click **Send**, to reset the turbo pump.
6. Click the Request drop-down list, and Select **No change**.

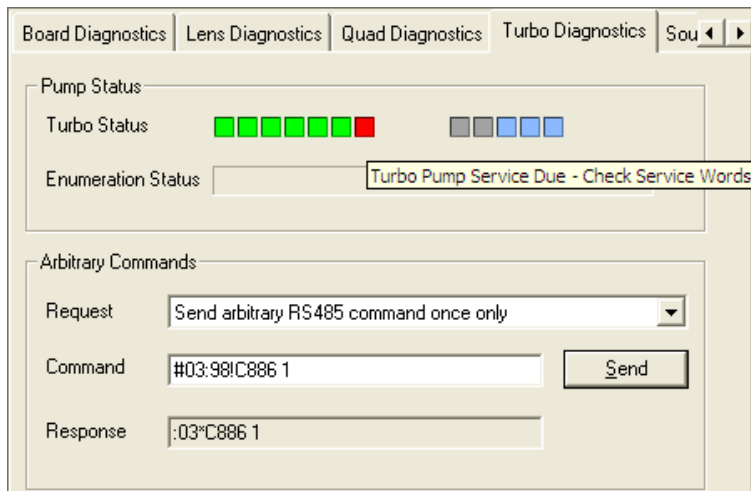


Figure 21 - Sending the service flag commands

7. Check the response received (which scrolls across the Response field) is in the format #98:dd*V886 x;yyyyy.

NOTE: *X represents the number of hours run by the oil cartridge to date, yyyyyy represents the number of hours until the next oil cartridge change is required. For example #98:dd*V886 5;17519 means the oil cartridge has been in use for five hours, and a replacement is required in 17,519 hours (approximately two years).*