

Vion IMS QToF driver 3.1 Guide: System and Method Setup

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BENEFITS

This document describes the new features of the Vion IMS QToF driver pack 3.1. Instrument setup and some MS analysis method features have been updated with the driver pack 3.1. The following topics are discussed:

- Automated IMS pressure lock
- Instrument setup which includes:
 - Detector check
 - Resolution check
 - Lockmass check
 - Mass Calibration
 - CCS calibration
 - High mass calibration
- Setting transmission mode
- Tune page features
- New features of MS Method settings

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KEYWORDS

Vion IMS QToF, Vion Driver pack 3.1

INTRODUCTION

This document provides information on features/updates of Vion IMS QToF driver pack 3.1. There are updates on instrument setup procedures and MS method settings as result of driver pack 3.1 upgrade, in comparison to previous driver packs. For information on earlier driver packs and general system startup refer to document 715005426. There are no changes to the solution required for the system startup and there is no requirement to recreate currently used analysis methods. Ensure the following solutions are available and for information on preparation of these solutions, refer to document 715005426.

CHECKLIST

For system setup and mass/CCS calibration up to 2000 Da:

- Confirm that the Vion wash reservoir contains 50:50 ACN/H₂O
- Confirm that the 50 pg/μL leucine enkephalin lockmass solution is on fluidics position B
- Confirm that the Major Mix calibration solution is on fluidics position C

For high mass calibration (up to 8000 Da):

- Confirm system setup and calibration for both positive and negative sensitivity modes are performed.
- Confirm that the 50 pg/μL leucine enkephalin with 100 fmol/μL [Glu1]-Fibrinopeptide B lockmass solution is on fluidics position B
- Confirm that the 2μg/μL Sodium Iodide calibration solution is on fluidics position C

STANDARDS

MS Leucine Enkephalin Kit ([700002456](#))

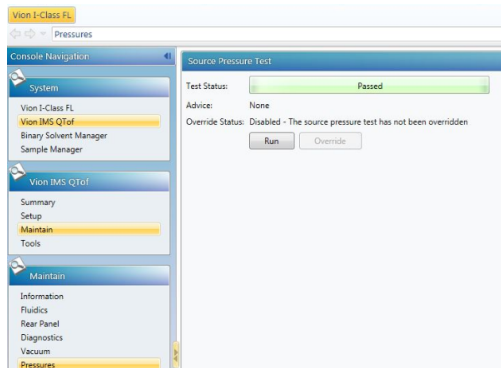
Major Mix IMS/Tof Calibration Kit ([186008113](#))

MS Calibration Solution (Sodium Iodide kit) ([700001593](#))

[Glu1]-Fibrinopeptide B Standard ([700004729](#))

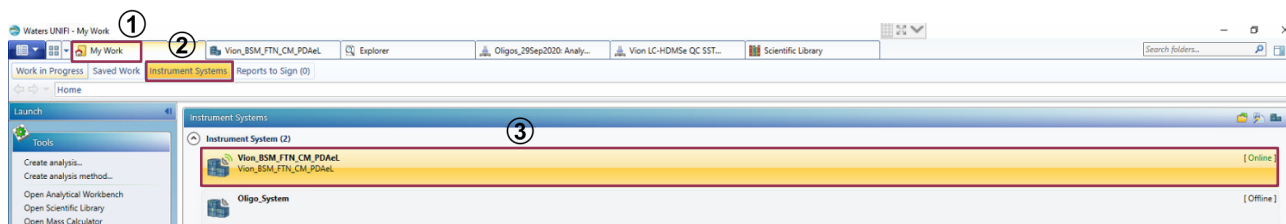
AUTOMATED IMS PRESSURE LOCK

The IMS pressure lock setup procedure now runs and locks automatically during the Instrument Setup process. In Vion IMS QToF drivers lower than 3.1, the IMS pressure lock had to be done manually prior to system setup via MS console. In Vion IMS QToF systems on driver 3.1 and higher, this option is automated and therefore no longer exists on MS console page (see image below).

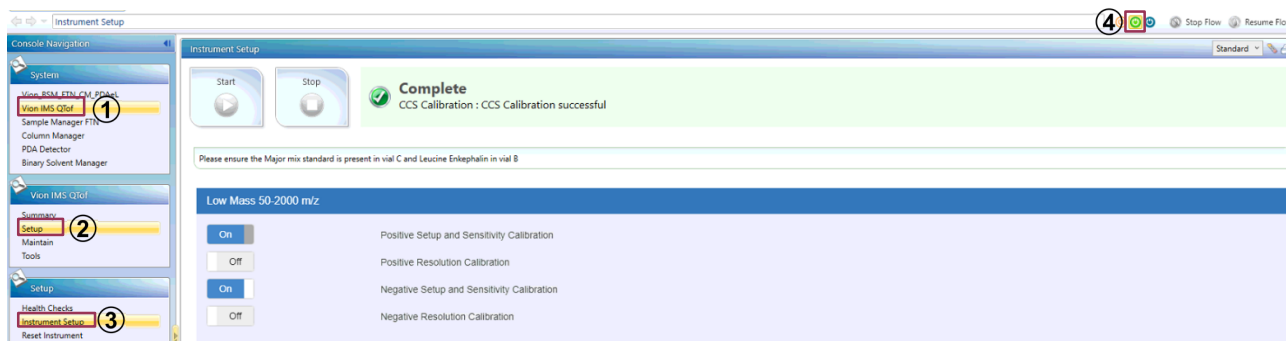


INSTRUMENT SETUP

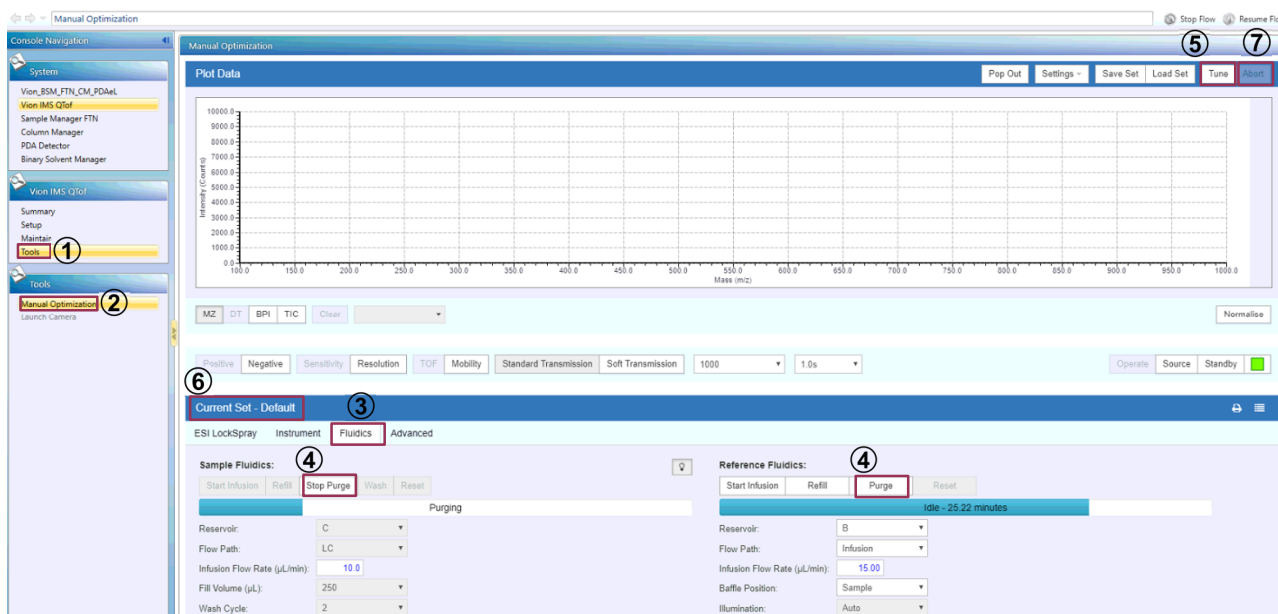
Log in to UNIFI portal, select My Work tab (1) and then Instrument System tab (2). Double-click on your online system (3) to open the Instrument System page.



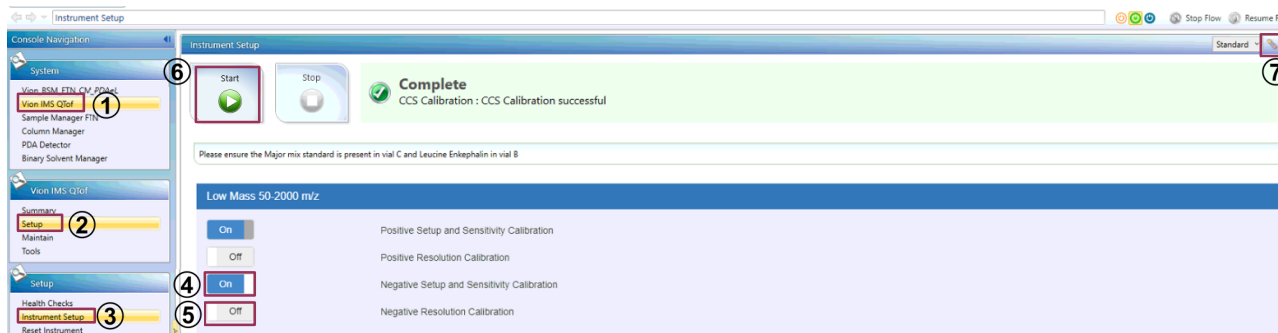
From your instrument system page, select Vion IMS QToF (1), Setup (2) and then Instrument Setup (3), from the Console Navigation systems pane on the left-hand side. Place the MS into operate mode via the green button in the top right-hand corner of the screen (4). After putting the system into Operate mode, allow 30 minutes for the electronics to stabilize before you perform the Vion instrument setup.



In order to prepare the fluidics system prior to instrument setup, select Tools (1) and then Manual Optimization (2) from the Console Navigation pane. Select the Fluidics tab (3) and purge the Sample Fluidics (reservoir C, with Major Mix) and Reference Fluidics (Reservoir B, Leucine Enkephalin) from the appropriate reservoir (4). Once purging is completed, start infusion for both Sample and Reference fluidics and select Tune (5). Ensure Default tune set is loaded (6) and Major Mix and Leucine Enkephalin peaks are visible with good sensitivity and stability. Upon confirmation, press Abort (7).



From your instrument system page, select Vion IMS QToF (1), Setup (2) and then Instrument Setup (3), from the Console Navigation systems pane on the left-hand side. It is now possible to run setup specifically for a desired polarity/analyzer mode. Leave slider to “On” to perform setup (4) or set it to “Off” to skip the instrument setup (5). Please note that the “Positive Setup and Sensitivity calibration” must be performed at all time and cannot be deactivated.

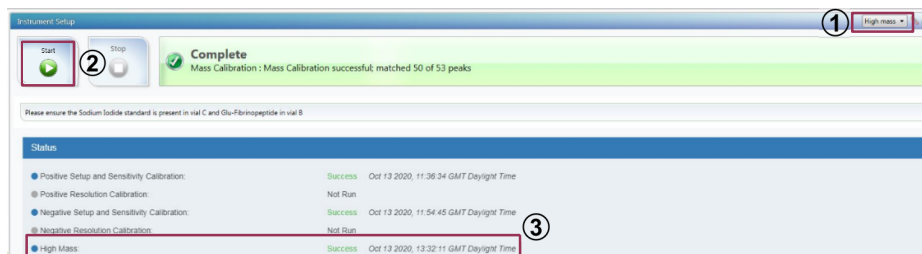


Once desired modes have been selected, press Start (6) to initiate the system setup. Once Instrument Setup is successfully completed, you can print the setup report by pressing the icon or remove all instrument setups by pressing the icon (7).

High mass calibration

The Vion IMS QToF can be calibrated for both Positive and Negative Sensitivity 4000 and 8000 mass ranges. The “Positive Setup and Sensitivity Calibration” and “Negative Setup and Sensitivity Calibration” must be completed successfully prior to High mass calibration. Ensure that the appropriate reference (50 pg/μL leucine enkephalin with 100 fmol/μL [Glu1]-Fibrinopeptide B on reservoir B) and calibration (2 μg/μL Sodium Iodide on reservoir C) solutions are placed in the fluidics. Purge the fluidics as described previously and check the quality of calibrant and lock mass signals.

In instrument setup window, select High mass from the dropdown menu (1), and press start (2). Upon successful completion of the calibration, the status changes to “success”.



What does instrument setup include?

The “Standard” Instrument setup includes four different options and the following actions will be performed in each of those:

1. Positive Setup and Sensitivity Calibration
 - i. Automatic IMS pressure lock
 - ii. ADC Setup for positive polarity
 - iii. Detector setup for positive polarity
 - iv. Resolution optimization for positive sensitivity mode
 - v. Mass calibration in positive sensitivity mode for mass range 1000 Da and 2000 Da
 - vi. CCS calibration in positive sensitivity mode for mass range 1000 Da and 2000 Da for standard transmission*
 - vii. CCS calibration in positive sensitivity mode for mass range 1000 Da and 2000 Da for soft transmission⁺
2. Positive Resolution Calibration
 - i. Resolution optimization for positive resolution mode
 - ii. Mass calibration in positive resolution mode for mass range 1000 Da and 2000 Da
3. Negative Setup and Sensitivity Calibration
 - i. ADC Setup for negative polarity
 - ii. Detector setup for negative polarity
 - iii. Resolution optimization for negative sensitivity mode
 - iv. Mass calibration in negative sensitivity mode for mass range 1000 Da and 2000 Da
 - v. CCS calibration in negative sensitivity mode for mass range 1000 Da and 2000 Da for standard transmission*
 - vi. CCS calibration in negative sensitivity mode for mass range 1000 Da and 2000 Da for soft transmission⁺
4. Negative Resolution Calibration
 - i. Resolution optimization for negative resolution mode
 - ii. Mass calibration in negative resolution mode for mass range 1000 Da and 2000 Da

* *Standard transmission is recommended to be used for non-labile compounds.*

⁺ *Soft transmission is recommended to be used for labile compounds.*

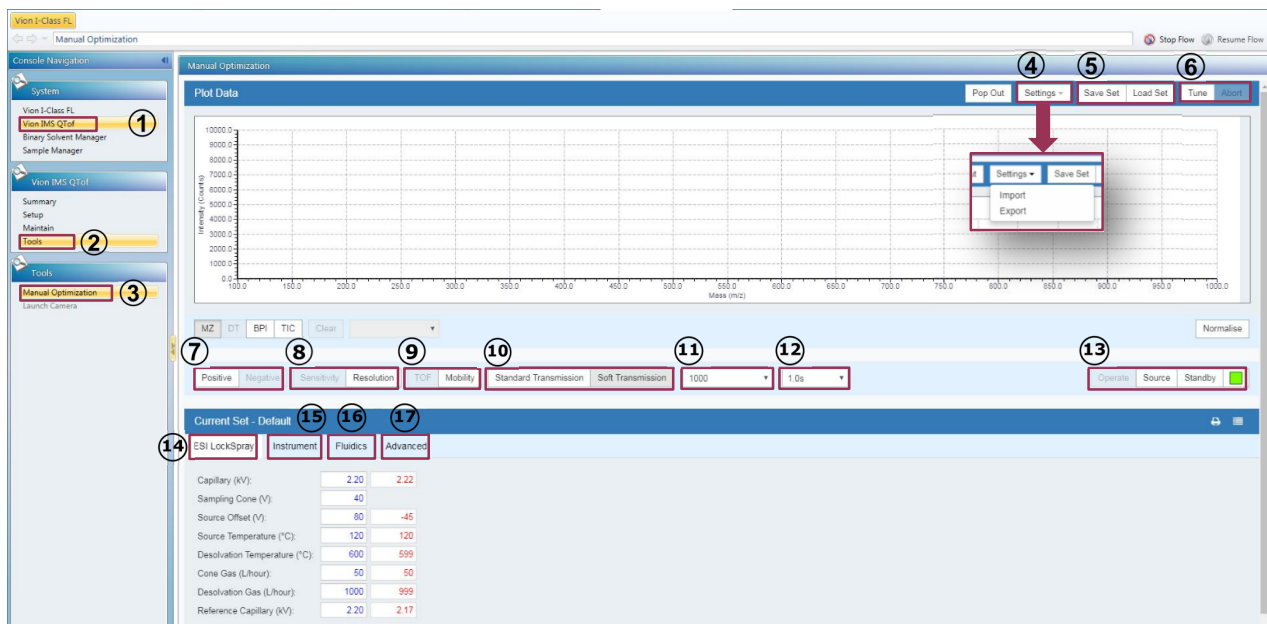
Note: Default and Waters recommended analyzer mode of operation for Vion IMS QTof is Sensitivity.

Note: Positive and Negative Resolution modes are only selectable with Positive and Negative Sensitivity modes respectively.

TUNE PAGE FEATURES

From your instrument system page, select Vion IMS QTof (1), Tools (2) and then Manual Optimization (3), from the Console Navigation systems pane on the left-hand side. Advanced users with access to the Manual Optimization may use the tune page to optimize settings for compounds of interest by direct infusion of the sample. The optimized settings can be exported from the tune page and then imported into Analysis Method or vice versa. Some of the tune page functionalities are illustrated in the figure below.

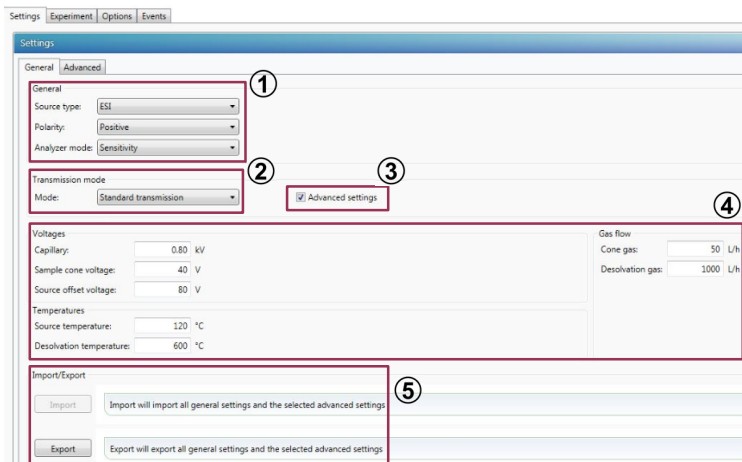
New users are advised to use the default settings. Advanced options may be used to optimize results for specific applications and users are encouraged to consult the Waters Application Teams for additional advice. Optimization of the settings is outside of the scope of this document. For more information contact your local application support team.



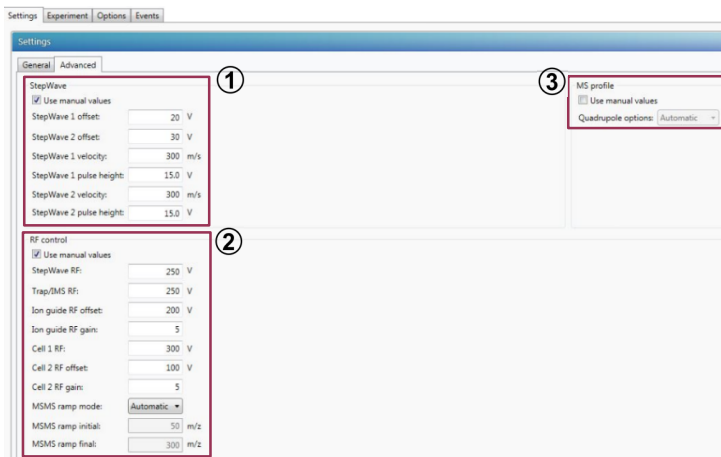
- ①②③ Access path for tune page.
- ④ Import/export of ESI LockSpray, Instrument and Advanced settings between MS Analysis Method and tune page
- ⑤ Save/Load Tune Set.
- ⑥ Press Tune to activate the tune page or Abort to exit the live update.
- ⑦ Selecting polarity mode (Note grayed out option is currently selected).
- ⑧ Selecting analyzer mode.
- ⑨ Selecting TOF or Mobility mode.
- ⑩ Selecting Standard/Soft Transmission operation mode.
- ⑪ Setting mass range.
- ⑫ Scan time.
- ⑬ Put instrument in Operate, Source standby or full Standby.
- ⑭ Source and ionization related parameters
- ⑮ Access to Collision Energy, Quad and DRE parameters.
- ⑯ Access to operation of fluidics for Sample and Reference sprayers.
- ⑰ Access to StepWave, RF and IDC settings.

NEW FEATURES OF MS ANALYSIS METHOD

All the source and ionization parameters, stepWave, RF and Quadrupole parameters are part of the MS Analysis Method for Vion IMS QToF systems on driver pack 3.1 and above. It is also possible to define Standard Transmission (recommended to be used for non-labile compounds) or Soft Transmission (recommended to be used for labile compounds) within the Analysis Method.



- ① Source type, polarity and analyzer mode settings.
- ② Transmission mode; for labile and small molecule applications use Soft transmission mode.
- ③ Select the box to access advanced settings otherwise leave it unticked to use default settings. By selecting the box, the Advanced tab will appear next to General tab.
- ④ These parameters influence ionization efficiency in the source. Adjust capillary and cone voltages, source and gas temperatures to achieve maximum
- ⑤ sensitivity. Use Import/Export buttons to import settings from tune page or export Analysis Methods settings into tune page.



- ① To activate the StepWave settings, select “Use manual values” and enter desired voltages for StepWave.
- ② To activate the RF control settings, select “Use manual values” and enter desired voltages to be applied on various ion optic devices.
- ③ To select between Automatic, Manual or Fixed quadruple options, select “Use manual values” and select desired option from the drop-down menu. The Automatic MS profile is suitable for analysis within 2000 Da mass range for most applications.

For most small molecule applications, it is recommended to use the following Source, StepWave and RF settings in conjunction with Soft Transmission mode to improve low mass transmission of low mass ions and reduce undesirable in-source fragmentations.

In General tab: *Sampling Cone (V) = 30, Source Offset (V) = 50,*

In Advanced tab: *SW1 Offset (V) = 5, SW1 Pulse Height (V) = 5, SW2 Velocity (m/s) = 200, MS Profile = Automatic, Ion Guide RF Gain = 2, Cell2 RF Gain = 2*

For additional information on MS Analysis Method parameter optimization see document 73000745 and for additional information on Vion driver 3.1 see document 715006864.