



TopSpec - 829157

WP1 – Omnitrap and IMS Development and Testing

Deliverable: D1.2 – Modified Omnitrap with updated software

Author: Dimitris Papanastasiou, Fasmatech Science & Technology

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D1.2 Modified Omnitrap with updated software

The Omnitrap software platform for driving the instrument is being developed in C# language using the .NET framework. The original code used for operating the prototype instrument is currently being restructured and a significant part of the code has been completed. Both Omnitrap platforms developed for partners Karolinska Institutet (KI) and Institut Pasteur (IP) are now operating using the new platform, while future updates will be generated and both instruments will be upgraded to enhance functionality and ease of operation. The new code is carefully organized and has resulted into a scalable software platform where different electronics components can be added and/or removed with minimum effort, allowing the same software platform to support all the different hardware extensions that are currently available for the Omnitrap technology. These include the ion mobility spectrometer, the VUV diffuse light source, a thermal version of the hydrogen atom source and new extensions currently being developed, for example coupling the Omnitrap technology to a TOF mass analyzer, a RF transfer line etc. The architecture of the code is presented in Figure 1. The main electronics units including (i) the electron source, (ii) the plasma ion source, (iii) the FPGA, (iv) the UartHub, (v) the vacuum control system, (vi) the multilevel DC switch and (vii) the ion mobility spectrometer have been organized into the new architecture. The completion of this task allows the TRL5 Omnitrap platforms to be fully operational with the new code architecture. Future updates will include changes in “Automated Procedures”, the method of creating “Sequence” files, the generation of a “log file” to support trouble shooting and other “MS Communication” related functionality to improve integration with the Orbitrap mass spectrometer further.

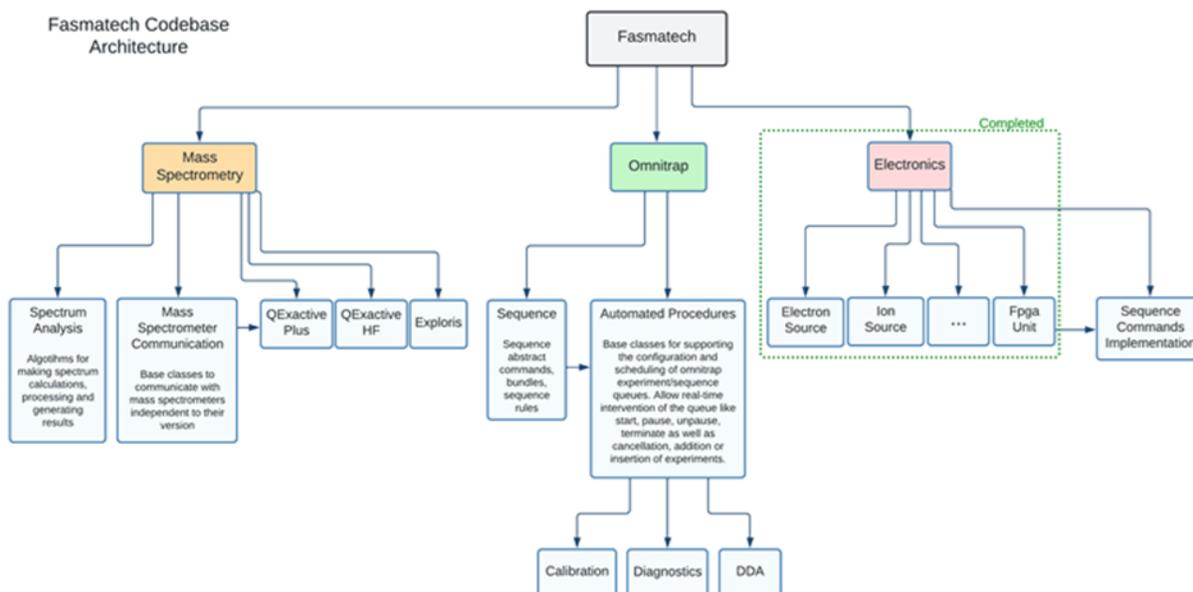


Figure 1. Omnitrap software platform architecture highlighting the part of the code that has been restructured.

The original .NET framework graphical user-interface (GUI) approach that was based on Windows Forms Applications (WinForms) is now been transferred to Windows Presentation Foundation (WPF). Although this was extremely time consuming, the GUI is now extremely more appealing and with many additional features that improve the experience of Omnitrap users considerably.

Figure 2 shows the new GUI where the operating environment is divided into three main regions. The menu on the left hand-side is used for mostly controlling the static parameters of the instrument, such as the “Electron Source”, the plasma “Ion Source” and the rectangular “RF Generator”. A “Vacuum” monitor tab has been introduced to visualize the “vacuum-state-machine” algorithm developed for controlling the different vacuum states of the instrument and also allowing synchronization with the Orbitrap MS vacuum system. An additional tab for the “Ion Mobility” spectrometer has been included in the software platform developed for partner KI. An additional “Diagnostics” tab has also been developed allowing users and service engineers to test the different trapping regions of the Omnitrap platform and evaluate performance.

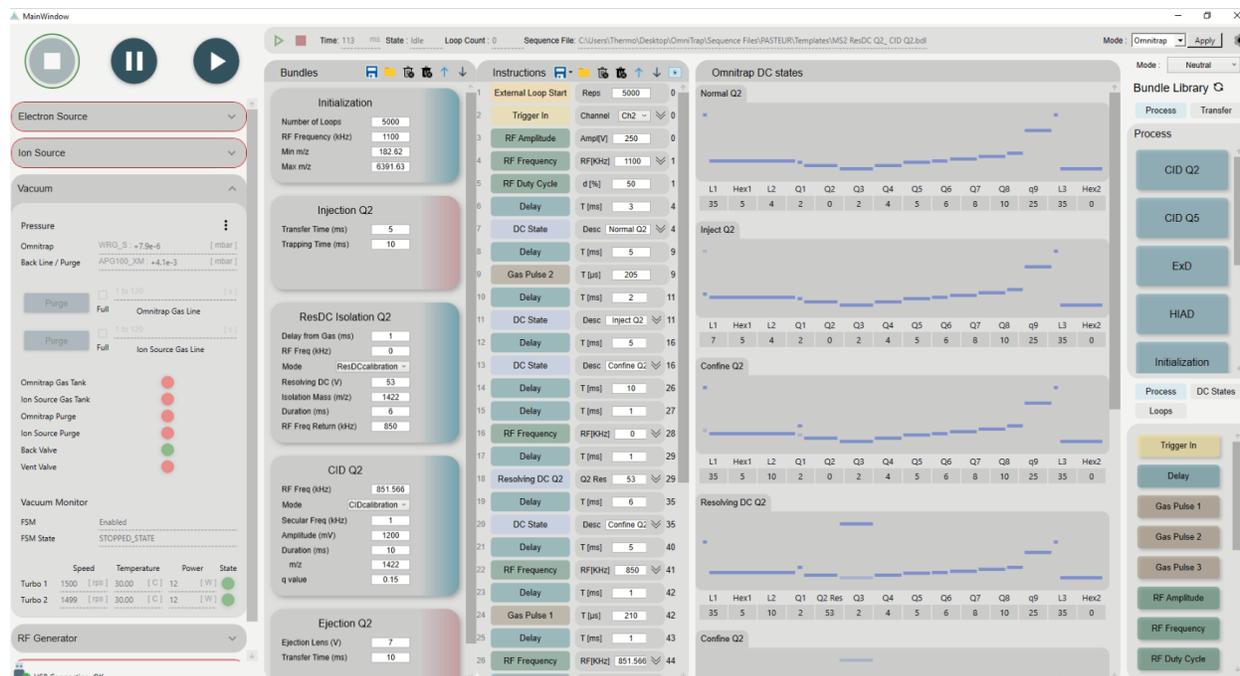


Figure 2. Omnitrap platform GUI allowing the user to operate the instrument, monitor parameters and design new experiments.

The central part of the user-interface is devoted to visualizing the experimental workflow, in other words, the sequence files developed that enable the extreme versatility of the Omnitrap platform to be harnessed with ease. To improve the experience of Omnitrap users, two separate modes have been developed. In “Expert” mode, the user has access to all the instructions necessary to run an experiment. All parameters are accessible and provide ultimate flexibility to control and optimize a particular experimental workflow. The user can group instructions into “Bundles” and select only a fraction of the parameters to remain accessible. This is an important mode for non-expert users, providing reduced complexity and access to just a few important parameters to tune the instrument. Figure 2 shows the “Neutral” mode, where both “Bundles” and the fully developed sequence file including all instructions are visible. A series of chematic diagrams highlighting the DC profile established along the ion optical axis of the Omnitrap platform is also available, allowing the user to visualize the position of the ions during the course of an experiment.

A library containing instructions and an extended set of DC profiles is available in the library on the right hand-side menu of the GUI. The user can drag and drop instructions into the sequence list and develop new experiments or re-organize existing experimental workflows. Instructions can be added or deleted, moved up and down, grouped, replaced and saved into bundles or as fully developed sequence files. A library of “Bundles” is also made available.

Figure 3 shows the different control menus available on the right hand side tabs, while Figure 4 shows the libraries available for developing experimental workflows. The “Bundle” library is developed by grouping instructions from the “Instruction” library to describe a “Process” or a “Transfer”. Processes refer to ion manipulation functionalities that involve activation, dissociation, isolation or accumulation of the ion population. Transfer events are used to define the movement of the ions between the different trapping regions available in the Omnitrap platform.

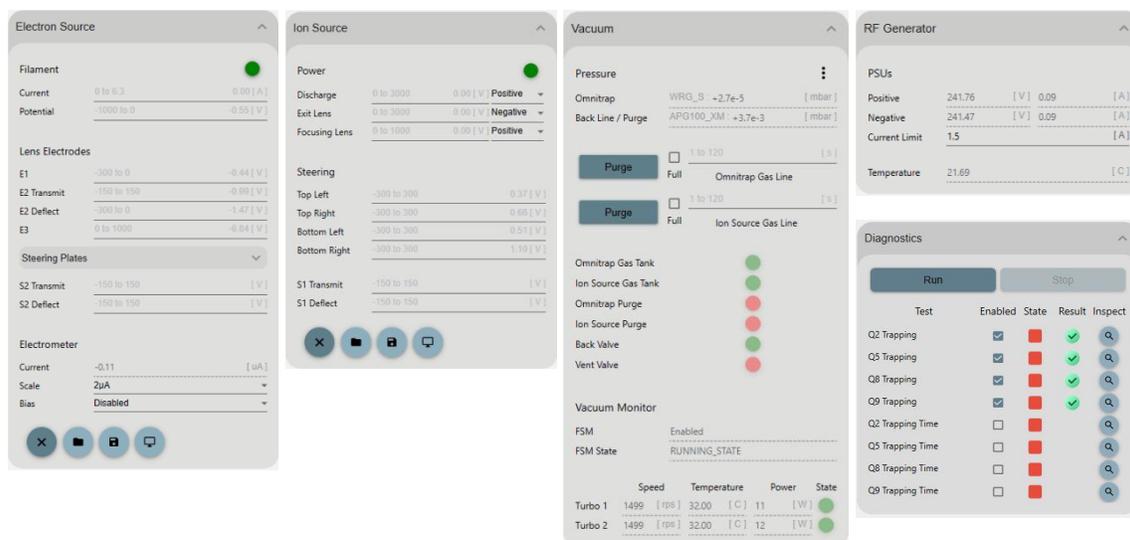


Figure 3. Control menus available in the Omnitrap platform GUI for operating the “Electron Source”, the plasma “Ion Source”, the rectangular “RF Generator”, for monitoring the vacuum state of the instrument and for running “Diagnostics” tests to evaluate the performance of the instrument.

A significant number of parameters are available through the “vacuum-state-machine” algorithm developed to monitor and control the vacuum state of the instrument. Additional test software has been developed that is accessible to engineers to set pressure thresholds and timing values while also monitoring the turbomolecular pumps, shown in Figure 5. The vacuum state machine can be bypassed using the test software and manual control of the vacuum system becomes available. The test software is also used to test all other electronics units available in the Omnitrap platform. The latest version of the vacuum state machine is described using the block diagram of Figure 6.

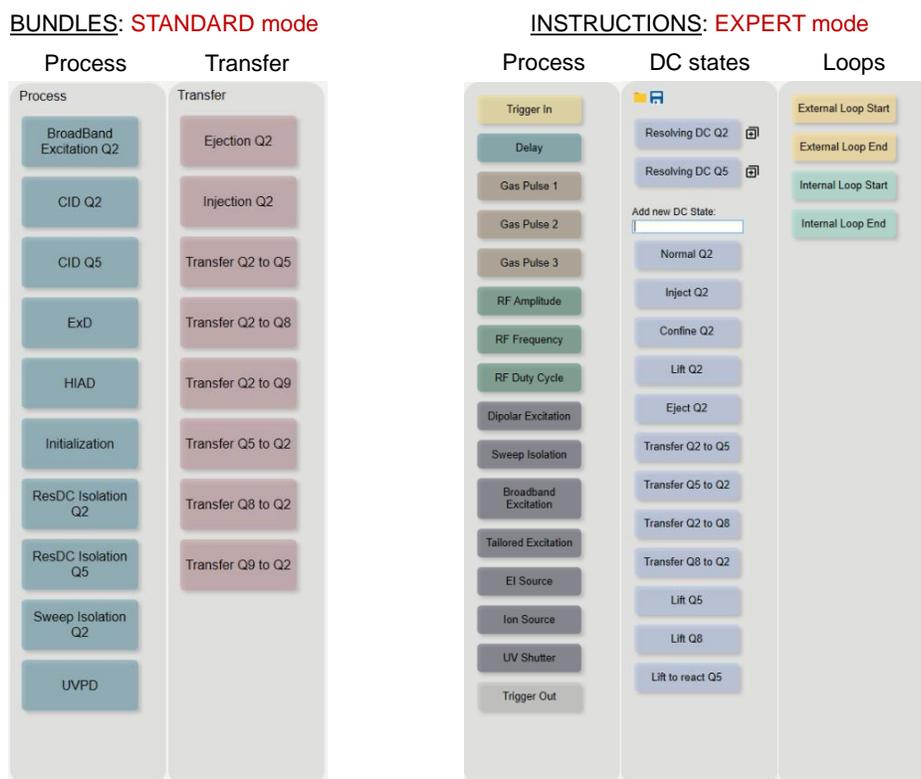


Figure 4. Bundle and Instruction libraries available for developing experimental workflows.

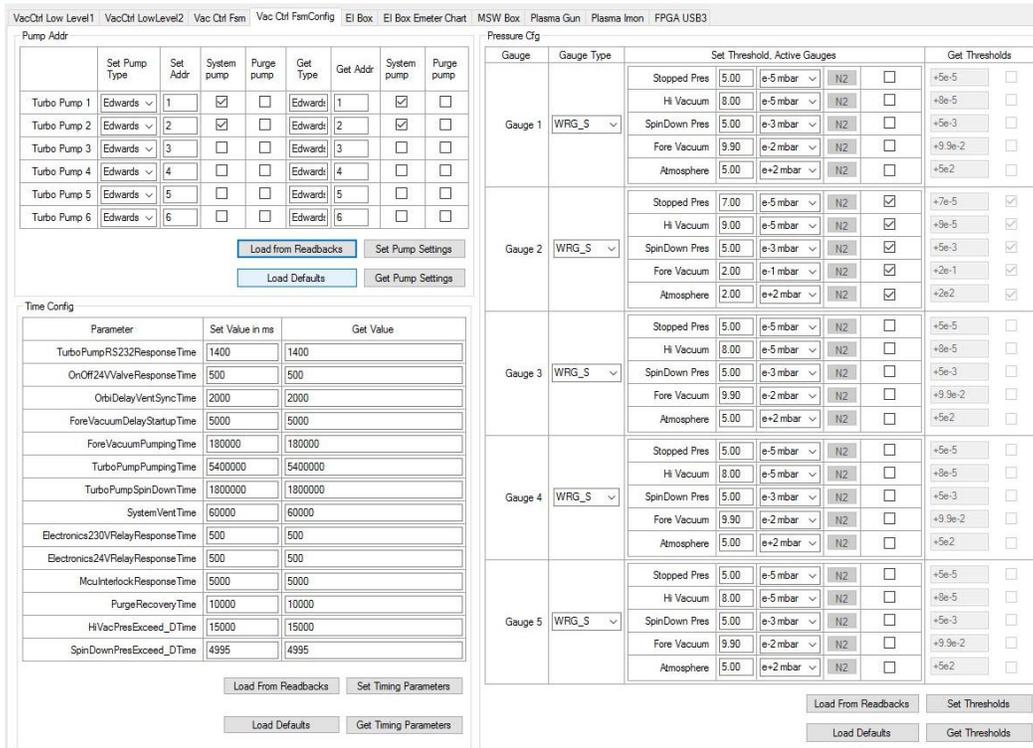


Figure 5. Test software for defining parameters of the vacuum state machine and testing all electronics units.

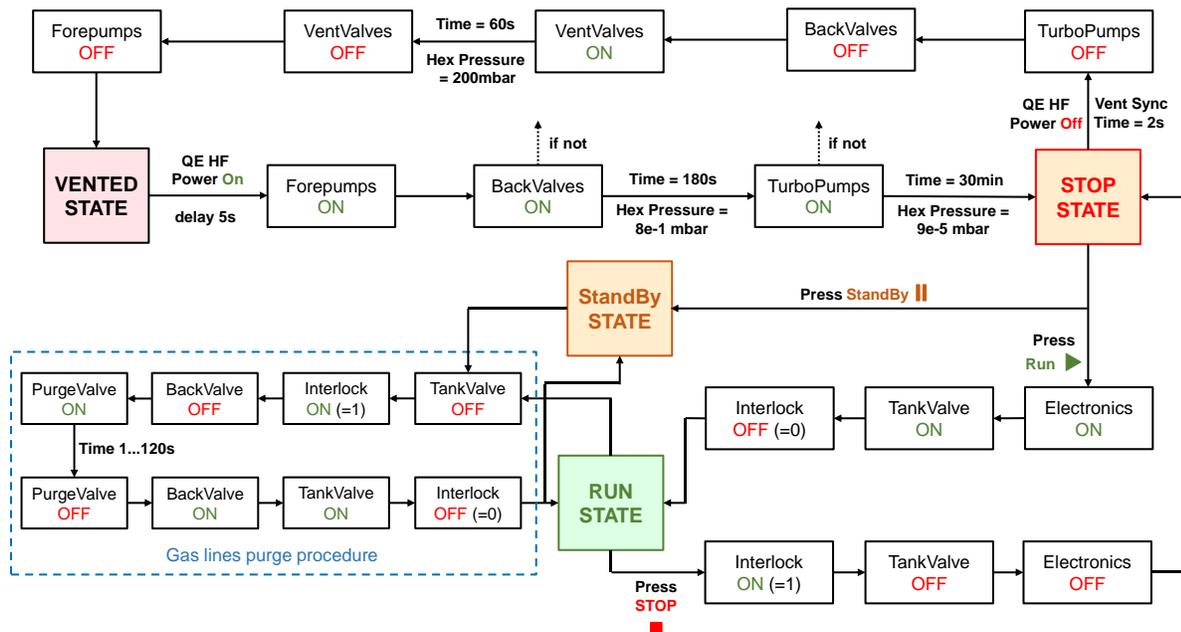


Figure 6. Block diagram of the latest version of the vacuum state machine developed for operating the Omnitrap platform coupled to Orbitrap mass spectrometers.

The Omnitrap software platform offers a wide range of options available through the main icon shown in Figure 7. The updated version of the software described above is specific to the GUI developed for driving the Omnitrap platform . All other GUIs of the Omnitrap platform software suite will continue to develop until the end of the TopSpec project and beyond.

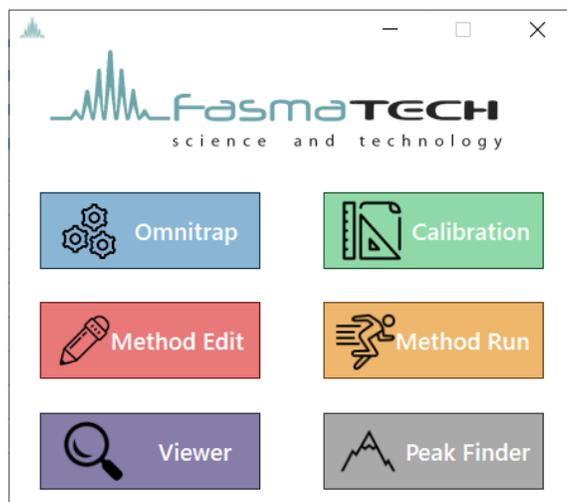


Figure 7. Omnitrap platform software suite.

In addition to the Omnitrap platform software, updated versions of the Tune software of the Orbitrap MS systems (Q Exactive & Exploris 480) have been produced. Figure 8 shows the finalized version used for installing the Omnitrap platform at partner IP in March 2022. A description of the critical parameters is also provided.

Instrument		System ...
Current Scan		
Control		
Settings		
Define Scan		
Ion transfer		
HCD event		
HCD Time * (ms)	3.0	
Purge Time * (ms)	5.0	
HCD Field Gradient --- Purge * (V)	30.0	
HCD External Instrument Mode		
External Instrument Mode *	Off	
HCD External Instrument - Clean HCD*	Off	
HCD External Instrument - Clean C-Trap*	Off	
HCD RF Off Time * (ms)	10	
Offset to External Instrument * (V)	13	
Gradient to External Instrument * (V)	-55	
Transfer Time to External Instrument * (ms)	20	
Offset from External Instrument * (V)	3	
Gradient from External Instrument * (V)	25	
Transfer Time from External Instrument * (ms)	100	
C-Trap Exit Lens Close * (V)	35	
HCD Exit Lens Mode	Trigger	
HCD Exit Lens to External Instrument * (V)	10	
HCD Exit Lens from External Instrument * (V)	-10	
Trigger Voltage High * (V)	-35	
Trigger Voltage Low * (V)	35	
Intact Protein mode	Off	
HMR mode	Off	
Trapping gas pressure setting *	1.0	
Spectrum data type	Profile	
C-Trap Charge Detector Support *	On	
Mass Calibration Data		

External Instrument Mode: This mode is used for transferring ions out of the back of the HCD-cell to the Omnitrap, which is connected instead of the electrometer. When in MS2 scan mode, turning this feature "On" sends ions to the HCD-cell and initiates the external instrument HCD-cell sequence (offset to/from, gradient to/from, transfer time to/from etc.). The *NCE* or *Direct eV* setting (found under the "Define Scan" menu) defines the injection energy into the HCD-cell. For minimum fragmentation during transportation set "*HCD Energy (NCE)*" to 1 and "*HCD Direct eV Setting*" to 3.

Define Scan	
Misc.	
First mass * (m/z)	150
Last mass * (m/z)	2000.0
Isolation Range Low * (m/z)	150
Isolation Range High * (m/z)	2000.0
Resolution *	60000
HCD Energy * (NCE)	1
HCD Direct eV Setting	3
Send full profile data	0

Offset to/from External Instrument (V): Sets the voltage of the front the HCD-cell DC gradient when ions are transported/returned to/from the omnitrap.

Gradient to/from External Instrument (V): Determines the gradient applied across the HCD-cell. This number, when added to the value of "*Offset to External Instrument (V)*", is the voltage applied to the back of the HCD-cell DC gradient when ions are transported/returned to/from the omnitrap.

Transfer Time to/from External Instrument (V): The time that the HCD-cell voltages are held to transport ions from/to the HCD-cell to/from the omnitrap.

Omnitrap / Orbitrap Synchronization Rule:

$$Transfer\ Time\ to\ Ext.\ Instrument \geq Omnitrap\ Injection\ Q2\ Time$$

$$Transfer\ Time\ to\ Ext.\ Instrument + Transfer\ Time\ from\ Ext.\ Instrument \geq Omnitrap\ Total\ Sequence\ Time$$

11	DC State	Desc	Inject Q2	11
12	Delay	T [ms]	5	16
13	DC State	Desc	Confine Q2	16
14	Delay	T [ms]	10	26

← Omnitrap Injection Q2 Time

Figure 8. Updated version of the Tune software developed for operating the Orbitrap MS systems coupled to the Omnitrap technology.