



## ADVION EXPRESSION CMS

Clarity Control Module

ENG

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To facilitate the orientation in the **Advion Expression CMS** manual and **Clarity** chromatography station, different fonts are used throughout the manual. Meanings of these fonts are:

*Open File* (italics) describes the commands and names of fields in **Clarity**, parameters that can be entered into them or a window or dialog name.

WORK1 (capitals) indicates the name of the file and/or directory.

ACTIVE (capital italics) marks the state of the station or its part.

Chromatogram (blue underlined) marks clickable links referring to related chapters.

The bold text is sometimes also used for important parts of the text and the name of the **Clarity** station. Moreover, some sections are written in format other than normal text. These sections are formatted as follows:

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**Note:**           Notifies the reader of relevant information.

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**Caution:**       Warns the user of possibly dangerous or very important information.

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**Marks the problem statement or trouble question.**

**Description:**   Presents more detailed information on the problem, describes its causes, etc.

**Solution:**       Marks the response to the question, presents a procedure how to remove it.

# 1 Advion Expression CMS Control Module

This manual describes the setting of the **Advion Expression CMS** detector. The control module enables direct control of the instrument over USB line.



*Fig. 1: Advion Expression CMS detector*

Direct control means that the MS detector can be completely controlled from the **Clarity** environment. Instrument method controlling the analysis conditions will be saved in the measured chromatograms.

## 2 Requirements

- **Clarity** installation with LC Control module (p/n A24) and MS Extension (p/n A38).
- USB A-B cable (p/n SK06).

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*Note:* Cables are not part of **Clarity** Control Module. It is strongly recommended to order required cables together with the Control Module.

# 3 Installation Procedure

## 3.1 Hardware - Wiring

The **Advion Expression CMS** detector is controlled by USB communication. It uses standard USB A-B cable.

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*Note:* In some cases, the **Advion Expression CMS** detector loses the communication with the control software. In such case it is necessary to unplug the communication cable from the computer and plug it back.

### 3.2 Clarity Configuration

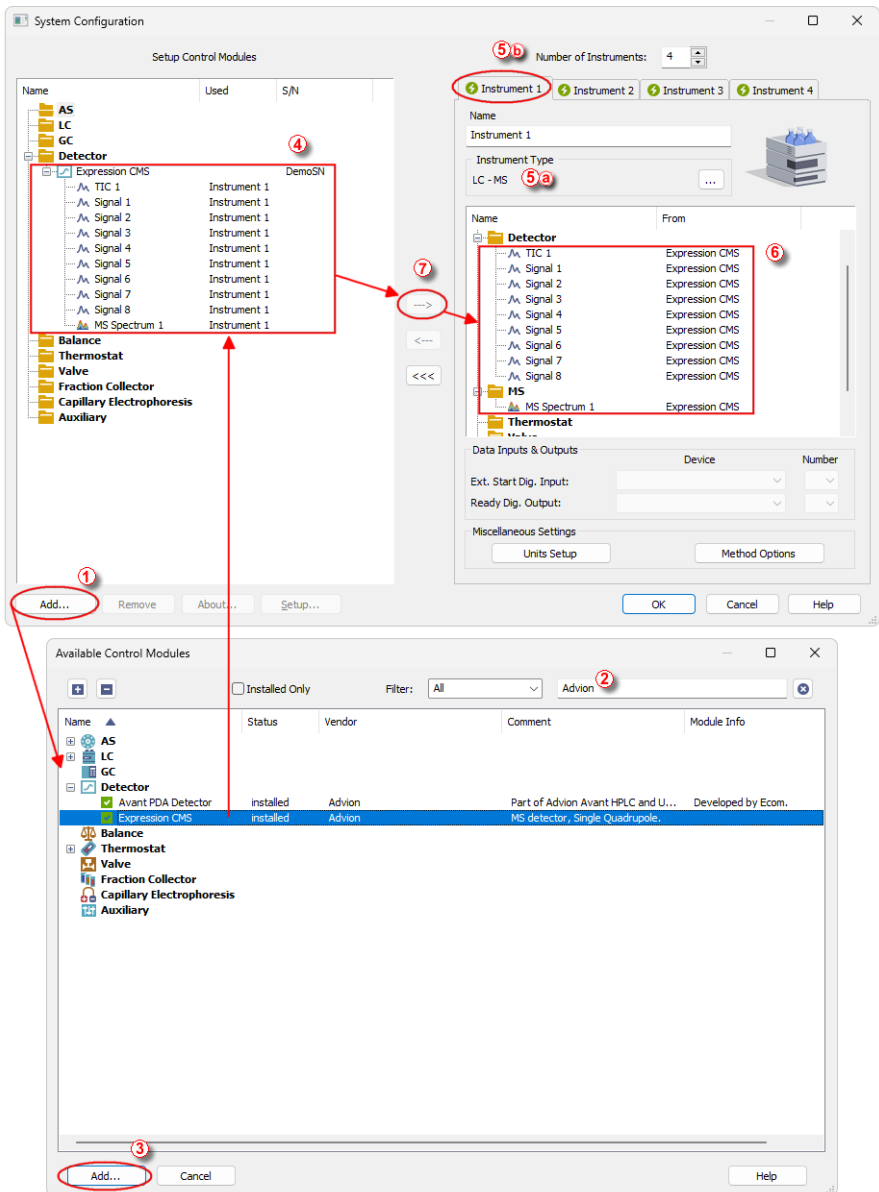



Fig. 2: How to add Advion Expression CMS



- Start the **Clarity** station by clicking on the  icon on the desktop.
- Invoke the *System Configuration* dialog accessible from the *Clarity* window using the *System - Configuration...* command.
- Press the *Add* button ① (see Fig. 2 on pg. 4.) to invoke the *Available Control Modules* dialog.
- You can specify the searching filter ② to simplify the finding of the driver.
- Select the **Expression CMS** and press the *Add* ③ button.

The [Expression CMS Setup](#) dialog will appear (see Fig. 3 on pg. 5.).

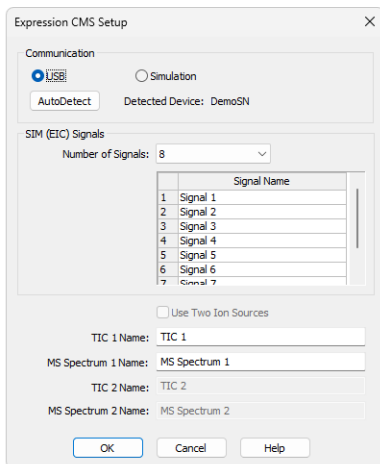



Fig. 3: Expression CMS Setup

- Select the correct *Communication* mode and press the *AutoDetect* button to check the presence of the detector.

**Note:** Other fields from this dialog are described later in the description of the [Expression CMS Setup](#) dialog.

- Press the *OK* button.

The **Expression CMS** will appear in the *Setup Control Modules* list ④ of the *System Configuration* dialog.

- Change the *Instrument Type* ⑤ ⑥ on the desired *Instrument* tab ⑤ ⑥ to LC - MS and drag the appropriate item from the *Setup Control Modules* list on the left to the *Instrument* tab on the right ⑥ , or use the  button ⑦ .

**Note:** The configuration dialog of the **Advion Expression CMS** detector ([Expression CMS Setup](#)) can be displayed any time by double-clicking on its icon or using the *Setup* button.

## 4 Using the control module

New [MS](#) tab is created in the *Method Setup* dialog. It can be accessed by using the *Method - MS Control...* command from the *Instrument* window.

### 4.1 Method Setup - MS - General

The *Method Setup - MS* tab for the **Advion Expression CMS** detector has three sub-tabs: *General*, where all information on the acquisition of the signal is set, [Contact Closures](#) settings for the detector's digital inputs and outputs are set and the [Analog I/O](#) sub-tab containing the settings for the external signals processed by the **Advion Expression CMS** and analog output signal settings.

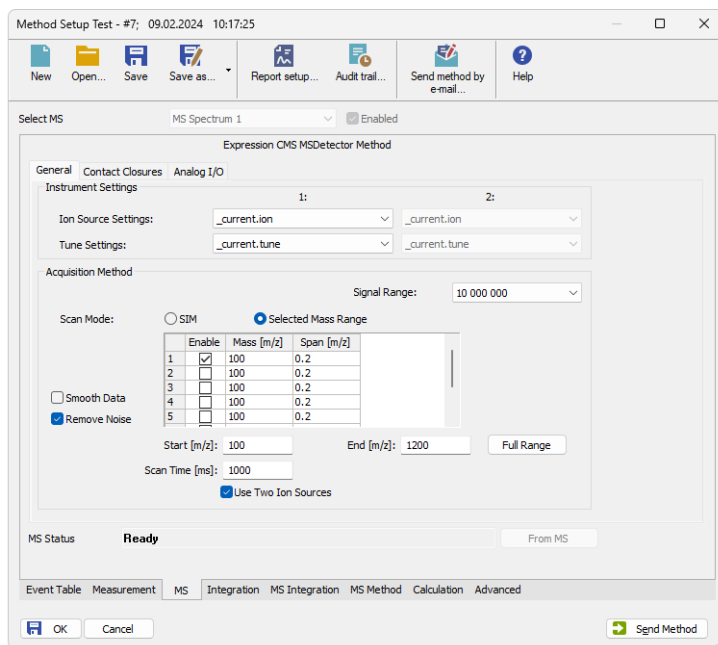


Fig. 4: Method Setup - MS - General

### Instrument Settings

This section allows to set the *Ion Source Settings* file and *Tune Settings* file. Both of these files are saved in Mass Express-compatible format and saved in the ADVIONMS subdirectory of the **Clarity** installation directory (C:\CLARITY\BIN by default). The preparation of your own *Ion Source Settings* and *Tune Settings* files can be performed in the [Tuning / Ion Source](#) dialog.

#### Ion Source Settings

Defines the particular *Ion Source Settings* file used for the given method. In case of two ion sources, a setting for each ion source is present.

**Tune Settings**

Defines the particular *Tune Settings* file used for the given method. In case of two ion sources, a setting for each ion source is present.

**Acquisition Method**

Some fields in this section change depending on whether the method is used for *Single Ion Monitoring (SIM)* or *Scan* acquisition.

**Signal Range**

Parameter specifying how intense single ion signals are expected from the **Advion Expression CMS**. The higher the setting is, the higher signals can be acquired, but the precision of data on intensity axis becomes lower. Signal of a single ion exceeding the set value will be trimmed to the set value. Maximum TIC signal intensity in **Clarity** is 10000 times higher than *Signal Range* set.

**Scan Mode**

Allows to select between *SIM* mode and *Selected Mass Range (Scan)* mode:

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**Scan Mode - Selected Mass Range**

In the Selected Mass Range mode, the data being acquired are whole spectral scans defined using *Start*, *End* and *Scan Time* parameters. Moreover, some of the  $m/z$  ion signals may be extracted from the gathered spectra, which is important for some devices (e.g. coupling of the fraction collector to the **Advion Expression CMS** detector). The maximum number of extracted signals to be set here is dependent on the maximum signals set in the [Expression CMS Setup](#) dialog. Particular signals are enabled by using the checkbox in the *Enable* column on a particular row.

**Mass [m/z]**

Defines the central mass of the ion being acquired. The value must lay in the range of  $m/z$  10-1200 including the *Span [m/z]* of the ion window.

**Span [m/z]**

Sets the span of the given ion being acquired. This span is symmetrically divided around the *Mass [m/z]* and must be larger than 0. Default value is 0.2.

**Start [m/z]**

Sets the lowest  $m/z$  value being scanned. This parameter must be lower than *End [m/z]* value, but cannot go below 10.

**End [m/z]**

Sets the highest  $m/z$  value being scanned. This parameter must be higher than *Start [m/z]* value, but cannot go above 1200.

**Scan Time**

Defines the time during which the detector takes one complete scan from *Start [m/z]* to *End [m/z]*. The data resolution is 0.05  $m/z$ .

**Note:**

The maximum scanning speed of the **Advion Expression CMS** detector varies according to its subtype, for basic CMS it is 5000 AMU/s, which means the lowest possible value of *Scan Time* is dependent on the range selected. The lower the scan time is, the better results will be obtained from the chromatographic point of view (more data points on a peak), but the higher the scan time is, the better sensitivity the detector will have (obtaining each  $m/z$  value over longer time).

**Full Range**

Sets the values in the *Start [m/z]* and *End [m/z]* to their maximum values according to the subtype of the **Advion Expression CMS** detector.

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## Scan Mode - SIM

Acquisition Method

Signal Range: 10 000 000

Scan Mode:  SIM  Selected Mass Range

	Enable	Mass [m/z]	Span [m/z]	Dwell Time [ms]
1	<input checked="" type="checkbox"/>	100	0.2	50
2	<input type="checkbox"/>	100	0.2	50
3	<input type="checkbox"/>	100	0.2	50
4	<input type="checkbox"/>	100	0.2	50
5	<input type="checkbox"/>	100	0.2	50

Smooth Data

Remove Noise

Fig. 5: Scan Mode - SIM

In the SIM mode, the section is reduced to just the table allowing to set the SIM signals numbers and their m/z values. The table has one additional column, *Dwell Time*.

### Dwell Time [ms]

Sets the time for which the detector will gather the data for a given SIM ion. The value must be at least 1 ms, the default value is 50 ms.

### Smooth Data

Defines whether spectral data will be smoothed by using Savitzky-Golay filter. While checked, the spectral data are smoother, but might be less precise.

### Remove Noise

Defines whether the noise will be deducted from the measured data. Before the acquisition, the **Advion Expression CMS** detector calculates the average electronic signal noise and then sets all the data with intensity of less then the average noise plus three times it's standard deviation to zero.

### Use Two Ion Sources

Accesses the second ion source setting and second tune setting for the **Advion Expression CMS** detectors which have two ion sources. The *Use Two Ion Sources* checkbox must be also checked in the [Expression CMS Setup](#) dialog.

### 4.1.1 Method Setup - MS - Contact Closures

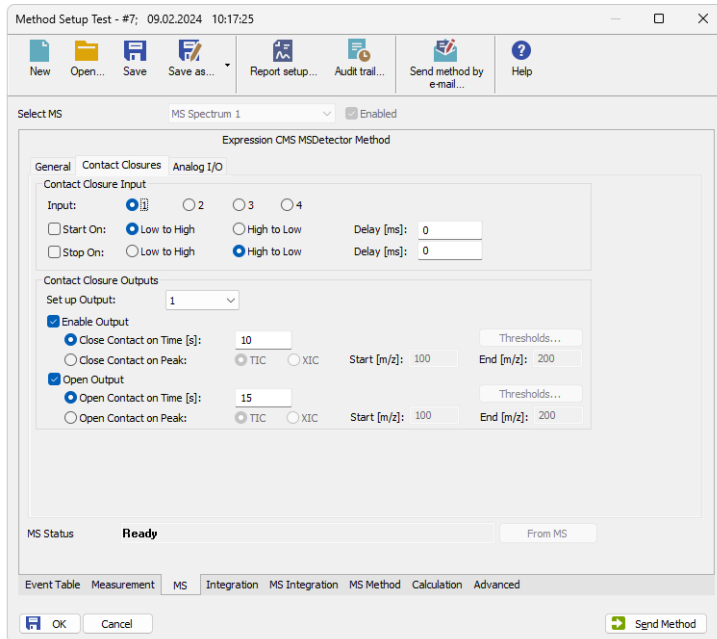


Fig. 6: Method Setup - Acquisition - Output

This sub-tab contains means to control the digital inputs and outputs of the **Advion Expression CMS**.

#### Contact Closure Input

Section defining the options to start and stop the analysis of **Advion Expression CMS**. If the analysis should be started based on digital input, select the particular *Input* in the first line, check the *Start On* checkbox, select the expected input level change (*Low to High* or *High to Low*) and the *Delay [ms]* which should precede the stating of the analysis after the contact closure input is invoked. Same behavior can be set for stopping the analysis based on an input, just using the *Stop On* checkbox and appropriate row.

*Note:* Under standard conditions, **Clarity** does not use digital inputs organized this way to start and stop analyses. **Clarity** is usually started by an autosampler (whose inject marker may, however, be connected to a selected contact closure input and used this way if the autosampler is not controlled by **Clarity**), and ended by elapsing the *End Time* as set on the *Method Setup - Measurement* tab.

#### Contact Closure Outputs

Section defining the behavior of the contact closure outputs of the **Advion Expression CMS**. To use the functionality, select the output to be triggered in the

Set up *Output* row, select the event which will produce the triggering of the output in the *Enable Output* section (either *Close Contact on Time [s]* or *Close Contact on Peak*) and particular parameters for the triggering (time in case of the first option, *TIC* signal or extracted ion (*XIC*) with it's *Start [m/z]* and *End [m/z]* values. The parameters for the detection of a peak can be set in the *Set up Contact Closure Output Thresholds* dialog invoked by using the *Thresholds...* button:

Sets up the conditions when the *Close Contact on Peak* parameter is triggered. Basic setting contains setting just the signal threshold - signal value which is satisfied when the signal is *Above* or *Below* the value set in the *Intensity* field. It is possible to define the time for which the signal has to be above or below the mentioned value before the contact closure is triggered in the *Past Threshold Time [s]* field.

Additionally, further condition may be defined using the *Gradient* checkbox - this row also specifies whether the signal must be concurrently to the given threshold rising or falling by defining the signal *Slope*.

Once the conditions are met, the contact closure output is triggered after the time defined in the *Delay [s]* field.

**Note:** Each of the four contact closure outputs may be triggered only once during the course of the analysis.

## 4.1.2 Method Setup - MS - Analog I/O

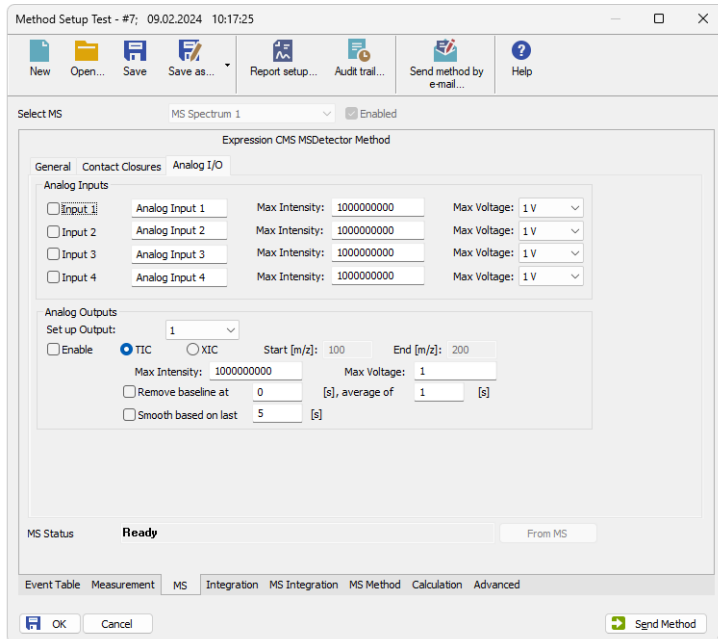


Fig. 7: Method Setup - MS - Analog I/O

The *Analog I/O* tab allows to set parameters for analog inputs and outputs. **Advion Expression CMS** detector can receive up to four analog signals and process them in the same manner as the native signals are processed, and can put voltages on up to four analog outputs to provide the analog signal to other devices.

### Analog Inputs

This section allows to set the behavior of up to four analog inputs. Each analog input is enabled by checking the appropriate checkbox (*Input 1..4*), which consecutively allows to add the name of the input in **Clarity** and map the input voltages (as set in the *Max Voltage* field) to signal intensity in **Clarity** (as set in the *Max Intensity* field). The value set in the *Max Intensity* will always correspond to the input voltage set in the *Max Voltage* field, higher voltage will be trimmed. Values allowed in the *Max Voltage* field are *100 mV*, *1 V* or *10 V*.

*Note:* Analog signals received in this way are stored in **Clarity** as Auxiliary signals, which means no Integration is possible on them. They are, however, sufficient for monitoring other device's flow, pressure, temperature etc.

### Analog Outputs

Section allowing to set the behavior of up to four analog outputs. To set the behavior of the particular output, it is necessary to select it in the *Set up Output*



field. By checking the *Enable* checkbox, the output will be provided based on either *TIC* signal or *XIC* signal (as created with a range from *Start [m/z]* to *End [m/z]*). The mapping of the signal intensity from **Advion Expression CMS** detector to output voltage is provided by *Max Intensity* and *Max Voltage* fields - the two values set correspond to each other, where *Max Voltage* may be set between 1 V and 10 V.


Additionally, the signal being sent to analog output connector may be further processed in **Advion Expression CMS** by applying baseline removal and/or signal smoothing. If *Remove Baseline* checkbox is checked, the output signal will be zero until the time specified in the first field on the row (in seconds) is reached. Before that time, the average baseline signal is calculated in a time window as long as defined in the second field on the row (again set in seconds). For this reason, the second field value must always be smaller or equal to the value in the first field.

The smoothing of the analog signal is defined by checking the *Smooth* checkbox, the time parameter of the smoothing is set in the field on the row. It governs the time for which the signal will be smoothed, delaying the analog output by several seconds. It is recommended, if the smoothing is to be used, to set the interval long enough so that at least 5 data points can be gathered in the interval (thus when the scan time is 500 ms, the time set should be at least 2.5 seconds).

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*Note:* The baseline removal and smoothing must be set for each output signal independently.

## 4.2 Device Monitor

The window with the detector status can be invoked by the *Monitor - Device Monitor* command from the *Instrument* window or using the  *LC Monitor* icon. It displays the actual values for most detector parameters, allows to set the detector to *OPERATE* and *STANDBY* state, work with the detector vacuum and also enter the [Tuning / Ion Source](#) dialog for setting it up.

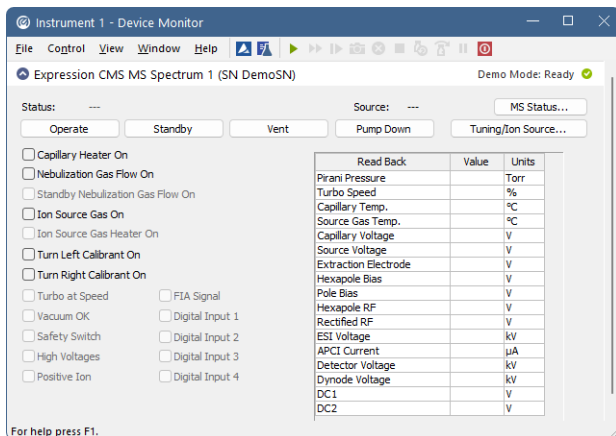


Fig. 8: Device Monitor

### Status

Shows the general status of the **Advion Expression CMS** detector. Upon starting **Clarity**, the detector is *VENTED* and needs to be first switched to *STANDBY* state by using the *Pump Down* button, then to the *OPERATE* state to be able to gather data.

**Caution:** Please head the instructions by **Advion** company on working with the **Advion Expression CMS** detector to prevent possible damage done to the detector.

### MS Status

Button allowing to display the *Hardware Configuration* dialog displaying the status of the detector including it's *Firmware* version and the version of the control libraries (SDK) used to operate it.

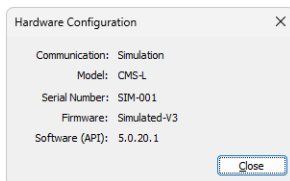


Fig. 9: Hardware Configuration

**Operate**

Switches the **Advion Expression CMS** detector to *OPERATE* state. The command is only available when the detector is in the *STANDBY* state.

**Standby**

Button switching the detector to *STANDBY* state when it is in the *OPERATE* state. It is recommended to keep the detector in the *STANDBY* state instead of switching it down completely, unless the powering down should be for a long period of time.

**Vent**

Button allowing to vent the detector, when it is in the *STANDBY* state. A confirmation message is issued upon using the *Vent* button.

**Pump Down**

Press the *Pump Down* button when the detector is *VENTED* and you want to shift it to the *STANDBY* state. The vacuum will be built in the **Advion Expression CMS** detector, but the detector itself will not be switched to the *STANDBY* state unless 30-minutes timer in the *VENTED* state is elapsed. The timer can be seen in the *Status* field.

**Tuning/Ion Source**

Opens the [Tuning / Ion Source](#) dialog serving for maintenance and calibration of the **Advion Expression CMS** detector.

**Capillary Heater On**

Monitors (and allows to control) the status of the ion source capillary heater. The heater is automatically switched on when the detector is put into *OPERATE* mode, but is not switched off when it is then put to *STANDBY* mode. You can switch the heater on and off manually. The actual temperature of the capillary heater can be seen in the *Capillary Temp.* field of the **Readback Table**.

**Nebulization Gas Flow On**

Monitors (and allows to control) the status of the nebulization gas flow. The flow is automatically switched on when the detector is put into *OPERATE* mode, and is switched off when it is then put to *STANDBY* mode. You can switch the flow on and off manually.

**Standby Nebulization Gas Flow On**

Monitors the status of the nebulization gas flow when the **Advion Expression CMS** detector is in *STANDBY* state. Compared to the *OPERATE* state, the nebulization gas flow is greatly reduced during the *STANDBY*.

**Ion Source Gas On**

Monitors (and allows to control) the status of the ion source heated gas flow. The flow is automatically switched on when the detector is put into *OPERATE* mode, and is switched off when it is then put to *STANDBY* mode. You can switch the flow on and off manually.

**Ion Source Gas Heater On**

Monitors the status of the ion source gas heater, which should be automatically switched on when the when the *Ion Source Gas Flow* is started.

### Turn Left Calibrant On

Switches the valve to the left calibrant vial. When the checkbox is checked, the calibrant from the left vial flows into the detector.

### Turn Right Calibrant On

Switches the valve to the right calibrant vial. When the checkbox is checked, the calibrant from the right vial flows into the detector.

Other parameters status may be monitored in the *Device Monitor* window, including the *Turbo At Speed*, *Vacuum OK*, *Safety Switch*, *High Voltages*, *Positive Ion*, *FIA Signal* and the states of *Digital Inputs*. These serve mostly for diagnostic reasons when the Ad does not work and cannot be changed from the Device Monitor window.

### Readback Table

Table showing the readbacks from the **Advion Expression CMS** detector.

## 4.2.1 Tuning / Ion Source

The dialog for performing maintenance operations on the **Advion Expression CMS** detector, like performing manual and automatic tunes, m/z calibration and performance tests. The dialog consists of several tabs, each of which is described in it's own section.

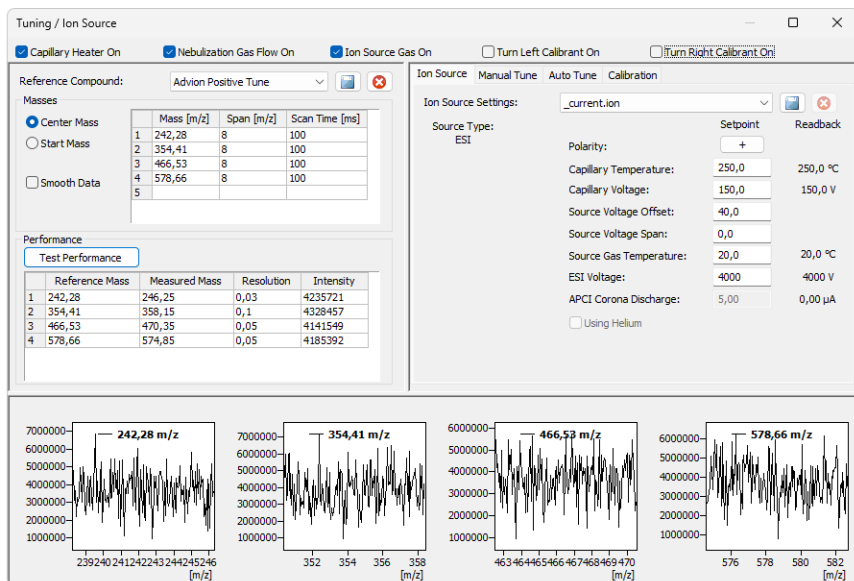



Fig. 10: Tuning / Ion Source

### Reference Compound

Selects and loads the preset parameters for the calibration compound. It is possible to save your own *Reference Compound* sets by using the  button, where you

will be prompted to enter the desired file name. Loading a fresh *Reference Compound* tune set loads the values into the *Masses* section.

### Masses

Section showing the values as set in the *Reference Compound* tune file. You can display the section in two modes - either showing the *Center Mass* and the *Span* (symetrically divided around it) or *Start Mass* mode showing the *Start Mass* and the *End Mass* in the *Masses Table*.

#### Masses Table

A table showing the parameters of the *Reference Compound*, namely their *Mass [m/z]* and *Scan Time [ms]*.

#### Smooth Data

When checked, smoothes the *Tune Graphs* for the display.

### Performance

Section showing the results of the **Advion Expression CMS** detector overall performance under the given ion source settings, tune settings and on the given calibration reference compound.

#### Test Performance

When pressed, performs the **Performance** test. It's results are then shown in the *Performance Table*.

#### Performance Table

Table showing the results of the **Performance** test. The table contains a row for each mass defined in the *Masses Table*, showing *Reference* and *Measured* mass, peak *Resolution* (peak width at half height) and peak *Intensity*. The expected and measured mass should not differ by more than  $0.1$  m/z, while the *Resolution* should be in  $0.5 - 0.7$  m/z range.

### Tune Graphs

Lower section of the *Tuning / Ion Source* dialog is filled with **Tune Graphs** - one graph for each mass as set in the *Masses Table*. The X axis displays the m/z values as defined in the *Span [m/z]* column, the vertical axis shows the peak intensity. The graphs can be zoomed independently of each other.

### Ion Source

Section showing (and allowing to change) various parameters of the Ion Source settings. The values can be changed, the changes can be then saved using the



button. Changes may also be cancelled by using the



### Ion Source Settings

Allows to select the particular ion source settings file to be displayed and changed.

## Manual Tune

Tab for performing manual tune.

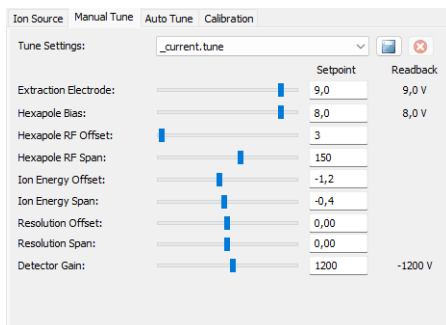




Fig. 11: Manual Tune

This tabs allows the user to manually change the parameters set automatically during the *Auto Tune* program and also few others. The changes are made to the tune file selected in the *Tune Settings* field and must be saved after the change is done using the  button. Changes may also be cancelled by using the  button.

**Caution:** Changing any of the parameters on the *Manual Tune* tab is strongly recommended only to people with deep understanding of how the **Advion Expression CMS** detector and **MS Detectors** in general work and may lead to damage done to the hardware.

## Auto Tune

Tab for performing automatic tune.

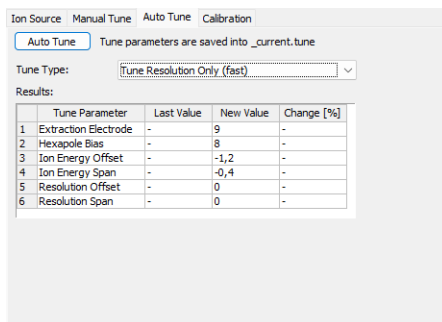


Fig. 12: Auto Tune

### Auto Tune

Button allowing to perform the tune adjustment. The received tune settings are saved into the `_CURRENT.TUNE` file, which can be then saved under another name. The tune program expect for the particular calibrant to be switched and correct ion source settings loaded.

### Tune Type

Allows to select between various tune types. Three types of the auto tune take differing amount of time to perform and adjust differing number of parameters.

*Tune Resolution Only (fast)* is the default choice of tune. It only adjusts the *Resolution* parameters and can only be performed when peaks are visible in the tune graphs for all masses that are to be tuned.

*Tune All Parameters (regular)* is tune program which will first adjust the *Extraction Electrode* and *Hexapole Bias* parameters and later tune *Ion Energy* and *Resolution* settings. It also requires peaks be present in all tuning graphs.

*Find Peaks and Tune All Parameters (extreme)* is the most extreme tune program, which first performs the peak search and then the *Tune All Parameters* program.

### Results

The table showing the results of the automatic tune in respect to values previously contained in the tune file and values of the same parameters after the tune was performed.

## Calibration

Tab for performing the m/z calibration.

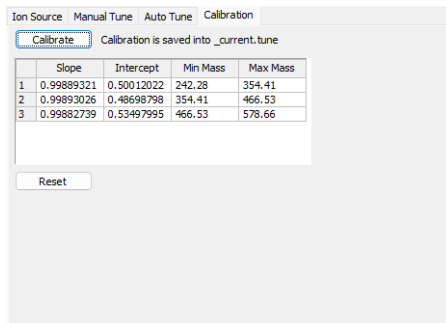


Fig. 13: Calibration

### Calibrate

Using the button performs the m/z calibration on a set of masses as defined in the *Masses Table* in the left side of the *Tuning / Ion Source* dialog. It is necessary to have the peaks visible in all tune graphs for the successful finish of the m/z calibration.

### Calibration Table

Shows the resulting correlation factors on different mass ranges.

### Reset

Button allowing to return to current settings rather than using the newly calibrated results.



### 4.3 Expression CMS Setup

The *Expression CMS Setup* dialog serves for the correct setting of the communication between **Clarity** and the **Advion Expression CMS** detector.

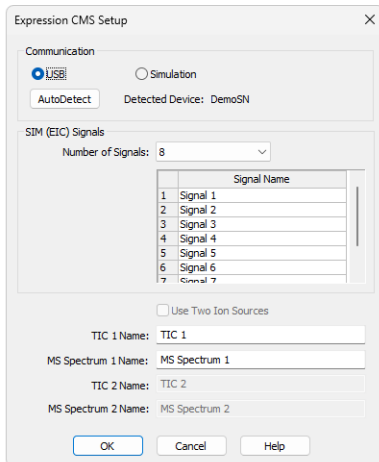


Fig. 14: Expression CMS Setup

#### Communication

Section allowing to set the communication with the **Advion Expression CMS** detector. Two communication modes are available - *USB* (for connecting to the live detector) and *Simulation* (for DEMO regime without the detector).

#### AutoDetect

Serves for detecting the **Advion Expression CMS** detector. If the communication attempt is successful, the serial number of the detector is displayed next to the button.

#### SIM (EIC) Signals

Section allowing to set the behavior of the **Advion Expression CMS** detector while in the SIM (Single Ion Monitoring) mode.

#### Number of Signals

Sets the maximum number of EIC (Extracted Ion Chromatograms) signals usable in the SIM mode.

*Note:* **Clarity** allows to work with the signals in SIM mode in the same way as with standard chromatographic signals. The number of signals set in this field is reserved for SIM signals and cannot be used while working in the Scan mode - therefore if you will only be working in the Scan mode, it might be useful to set the number of SIM signals used to 0 not to block other functions of the **MS Evaluation** extension (like extracting additional signals from the acquired spectra on request).

#### SIM Name

Allows to set custom names to the EIC signals in the SIM mode.

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*Note:* The actual values of m/z used for particular signals are defined later in the [Method Setup - MS - General](#) dialog.

**Use Two Ion Sources**

Allows to use two ion sources in the same analysis. The particular usage of both ion sources (or either of them) is later set per method in the [Method Setup - MS](#) dialog. Availability of the *Use Two Ion Sources* option depends on the autodetected model of the detector.

**TIC 1(2) Name**

Allows to set a custom name for TIC (Total Ion Current) signal.

**MS Spectrum 1(2) Name**

Allows to set a custom name for the acquired spectrum. Spectra (if there are more of them in a single chromatogram) will be referenced based on this name.

# 5 Report Setup

All of the detector settings accessible on the [Method Setup - MS](#) tab for the **Advion Expression CMS** detector are reported. To do so, the *Instrument Control* parameter on the *Method* tab of the *Report Setup* dialog must be checked.

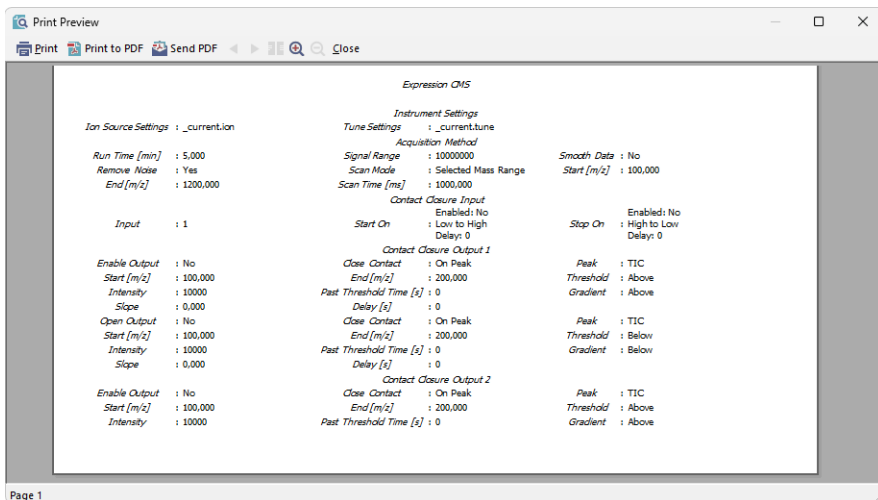


Fig. 15: Report Setup