



ExDControl Software

for the e-MSion ExD Series



User Guide

Revision A.3 • December 2020

Notices

Patents

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Customer Feedback

e-MSion welcomes your feedback, questions, and suggestions for improvement on this guide.

You can reach us at Support@e-MSion.com. We deeply appreciate your assistance in our efforts to continuously improve the quality of our documentation.

Contact Us

For technical questions regarding the ExD Cell, contact e-MSion via the following:

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About this Guide

The purpose of this document is to:

- Explain the main features of the ExDControl software.
- Provide practical guidelines for routine use of the ExD Cell.

The intended primary audience is end-users.

Related Documentation

- *e-MSion ExD Option User Guide*
- *e-MSion ExD Controller User Guide*

Terms Used

- MS1 stands for “Total Ion,” “MS,” or “Full MS” mode.
- MS2 stands for “Isolation,” “MS/MS,” or “All-Ion Fragmentation” mode.

Safety Information

Symbols

WARNING

A Warning indicates a hazard. If the contents of the message are not observed, the health and/or safety of personnel may suffer.

CAUTION

A Caution indicates a hazard. If the contents of the message are not observed, equipment may be damaged and/or data may be lost.

NOTE

A Note contains helpful information and tips.

Contents

What is e-MSion ExD?	4
Essential concepts	4
Getting Started	5
Before you begin...	5
To open the ExDControl software	5
To connect to the ExD Controller/instrument	5
To open an ExD tune file	6
To create a new ExD profile	6
ExDControl Software Features	7
Main Window	7
Manual Tune Tab	8
Auto Tune Tab	9
Menu Bar	10
Filament Parameters Window	14
Profiles Table	15
Automatic Profile Switching	16
Spectrum Graph Window	16
ExDControl Software Installation	17
To uninstall the ExDControl software	17
To reinstall or update the ExDControl software	17

What is e-MSion ExD?

The e-MSion ExD Series is a group of hardware/software packages that equip mass spectrometers with the ability to perform electron-based fragmentation (ExD).

- The *ExD Cell* confines electrons to the path of the instrument ion beam using a compact arrangement of permanent magnets and electrostatic (DC) lenses around an electron-emitting *filament*.
- The *ExD Controller* supplies a voltage to each of the lenses and current to heat the filament according to input from the *ExDControl* software.

NOTE

For a more in-depth description of ExD Cell function, see your *ExD Option User Guide*.

Essential concepts

The effect of the ExD Cell on passing ions is controlled by two factors: the *filament heating current* and the voltage *profile* of the eight lens elements (L1, L2, LM3, L4, FB, L4, LM5, L6, and L7).

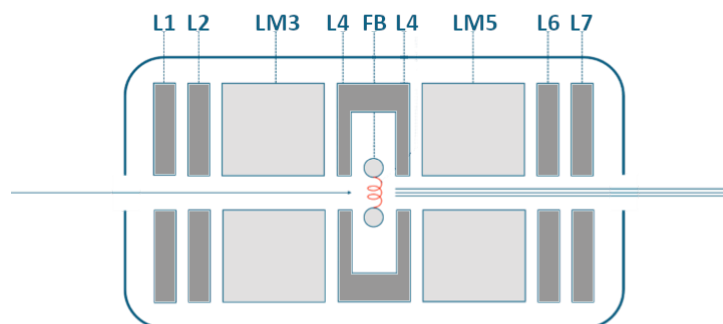


Figure 1. A cross-sectional diagram of the ExD Cell. The filament is the red coil, lenses are dark grey, and lens magnets are light grey.

The ExD Cell can be tuned for either ion transmission or ECD by adjusting the lens profile and filament heating current in the ExDControl software.

For best performance, the ExD Cell should be tuned with the instrument in the scan and operating mode that will be used to record data, since these settings affect ion energy and beam geometry. Optimal lens profiles will differ between:

- MS1 vs. MS2
- ToF vs. IM mode
- Positive vs. Negative mode

On certain instrument platforms only, the ExDControl software will automatically switch between profiles designated for MS1 and MS2 as the instrument changes scan type. See [Automatic Profile Switching](#).

NOTE

For the instrument to transmit ions, the ExD Cell must be operational and properly tuned.

Getting Started

Before you begin...

1. All product component parts must be installed and configured by trained personnel prior to their use.
2. Make sure you have read the safety guidelines in the *ExD User Guide*.

To open the ExDControl software

1. Double-click the desktop shortcut icon or open the Windows Start Menu of your instrument PC and click **E-MSION > ExDControl**.



Or, go to **C:\Program Files\E-MSION** (or alternate installation location) and double-click the **ExDControl.exe** application file.

Figure 2. ExDControl.exe icon.

To connect to the ExD Controller/instrument

NOTE

To operate the ExD Cell, the ExDControl software must be connected to the ExD Controller.

1. If the ExD Controller does not automatically connect after the ExDControl software launches, click **Connect > Connect**.

If connection is successful, the **Connect** option will be replaced by a **Disconnect** option in the menu.

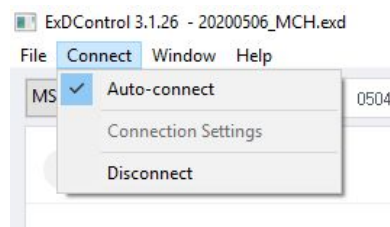


Figure 3. The appearance of the **Connect** menu when the ExD Controller is connected.

If the connection attempt is unsuccessful, see [Connection Settings](#).

CAUTION

In order to establish ExDControl software connection, the ExD Controller must be installed and powered ON. See the *ExD Controller User Guide* for guidance.

CAUTION

If a “New Controller version available” prompt appears after connection asking to update the ExD Controller firmware, **FIRST** disconnect the ethernet cable **AND** connect the USB cable from the ExD Controller to the instrument control PC **BEFORE** clicking “Yes” to begin the update.

Initiating the firmware update with both USB and Ethernet cables connected to the ExD Controller may disrupt the firmware update and cause the Controller to malfunction.

To open an ExD tune file

NOTE

From day-to-day, ExD profiles can be reused as long as the instrument tune settings have not changed significantly from the settings used when the profiles were developed.

At the start of each day,

1. Click **File > Open** and load the ExD tune file (*.exd) used the previous day.
2. Check the performance of any profiles in the drop-down profiles menu that you want to reuse. *At minimum, you should always maintain working MS1 and MS2 profiles for ion transmission with the filament in **Standby**.*

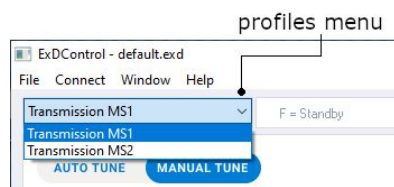


Figure 4. Use the drop-down menu to select the active ExD Cell profile.

Use a standard sample to compare performance day-to-day. If signal intensity and/or resolution declines significantly, try optimizing the profile using the tune procedures in your *ExD Option User Guide*. If this fails, check the instrument condition.

3. To save changes to the ExD tune file, click **File > Save**. To save the tune file as a new file, click **File > Save As**.

To create a new ExD profile

To create an ExD profile for a new sample or method,

1. Click **Window > Profiles Table** to open the **Profiles Table**.

MS1	MS2	Tuned For	Profile	Description	L1	L2	LM3	L4	FB	LM5	L6	L7
<input checked="" type="checkbox"/>	<input type="checkbox"/>	MS1			0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
<input type="checkbox"/>	<input checked="" type="checkbox"/>	MS2			0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0

Figure 5. The **Profiles Table**, showing a pair of profiles not yet tuned for transmission in MS1 and MS2.

2. Click the **Add** button in the **Profiles Table** to add a new profile to the list.
 - a. Enter a name in the profile column.
 - b. Fill in the description column. Record the filament current amperage, scan mode, and sample used to tune the profile here.
3. Follow the instructions in your *ExD Option User Guide* to tune the lens profile and, if necessary, to optimize the filament heating current.

ExDControl Software Features

Main Window

When you first start the ExDControl software, the main window appears.

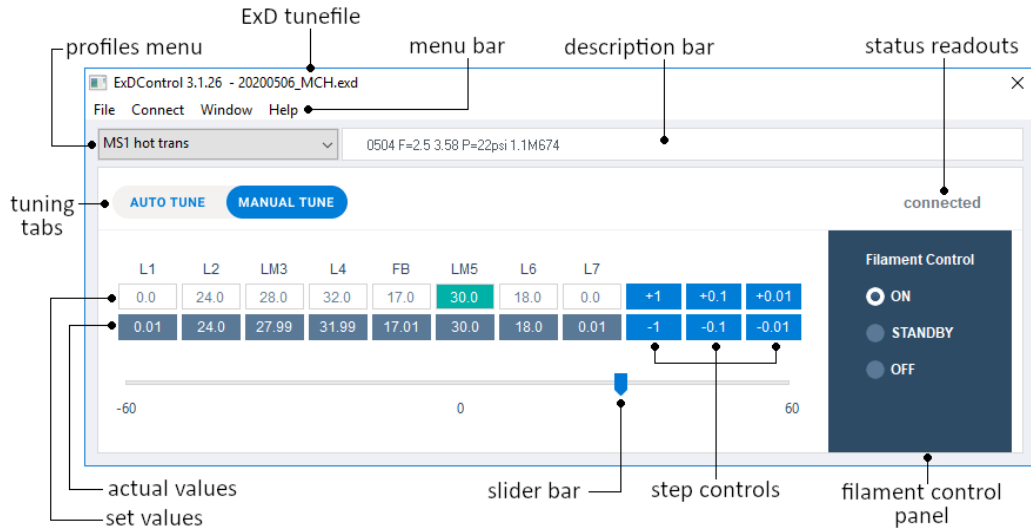


Figure 6. ExDControl Main Window and Manual Tune Tab.

NOTE

“L” = Lens. “LM” = Lens/Magnet. “FB” = Filament Bias. See Essential Concepts.

ExD tune file The name of the loaded ExD tune file. The ExD tune file (*.exd) file type stores a saved list of lens profiles.

Menu bar Holds the essential tools for the ExDControl software. See [Menu Bar](#).

Status readouts Displays the software connection status.

- If in standalone mode ([Figure 11](#)), then the ExDControl software window will display “Connected to Controller.”
- If in instrument-aware mode ([Figure 11](#)), then the ExDControl software window will display readouts of the instrument state.



Figure 7. Instrument state readouts.

- If no network connection exists, then the ExDControl software window will display “Not connected.”

Profiles menu	Displays the name of the active lens profile. Use to select which profile in the ExD tune file is active.
Description bar	Displays the description for the active lens profile.
Tuning tabs	Use the Manual Tune tab to make changes to the active lens profile in real time. The Auto Tune tab is currently under development.

Manual Tune Tab

Actual values	Voltages measured by the ExD Controller for each lens.
Set values	Voltages set by the user or the ExDControl software for each lens. Adjust the set value for a selected lens using the step controls, the slider bar, or by manually entering a value into the field and pressing Enter .
Step controls	Click the +/- 1.0, 0.1, and 0.01 V step buttons to change the set value for a selected lens.
Slider bar	Use the slider bar to adjust the set value for a selected lens.
Filament control	Use this panel to set the filament to On , Standby , or Off .

CAUTION

A consistent difference of > 5% between set and actual values for a lens indicates a fault with either the ExD Controller or ExD Cell wiring.

Auto Tune Tab

NOTE

Not currently available for Waters instruments.

Use the **Auto Tune** tab to automatically tune the ExD Cell. Autotuning aims to develop a viable profile for either transmission or ECD, as specified by the user.

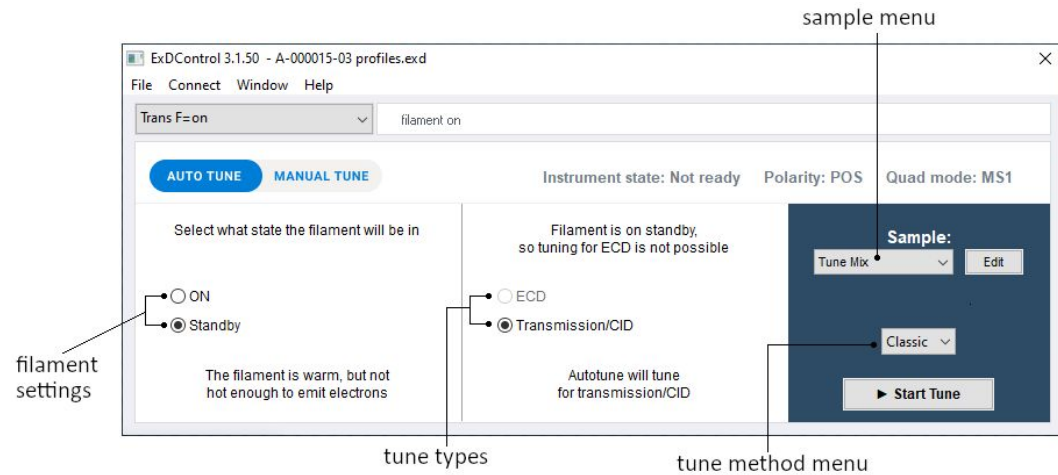
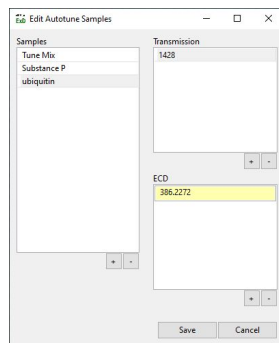


Figure 8. ExDControl Auto Tune tab.

- | | |
|-------------------|--|
| Filament settings | Select a filament setting: On or Standby . You can only autotune for ECD if the filament setting is On . |
| Tune types | Select what to tune for: ECD or Transmission/CID . |
| Tune method menu | Choose the autotune method. <ul style="list-style-type: none"> ● Classic Starting from scratch, this setting tunes for transmission or ECD by individually adjusting each element of the cell. ● Refine Starting from a previously tuned profile. Refine the tune to increase transmission or ECD fragmentation. This is a fine tune to be used for small adjustments. |
| Sample menu | Choose the sample to tune with. |
| Edit | Click to add/remove samples from the sample menu. |

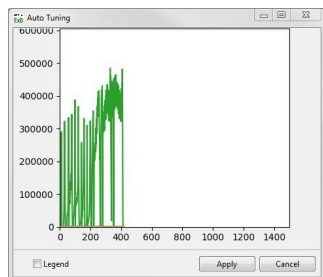


- Click the **+/-** button below the **Samples** panel to add/remove samples from the list.
- For a new transmission tuning standard, add ion(s) to the **Transmission** panel.
- For a new ECD tuning standard, add the precursor ion to the **Transmission** panel and the ECD fragment ion(s) to the **ECD** panel in the Edit window.

Figure 9. ExDControl Edit Autotune Samples window. To open, click the **Edit** button in the **Auto Tune** tab.

Start Tune

Click to begin the autotune.



Once the tune is complete (5-10 minutes), click **Apply** to accept the profile generated. Click **Cancel** to revert all lens voltages to their original values.

Figure 10. After clicking **Start Tune**, the **Auto Tuning** pop-up window appears to illustrate the tune progress by graphing signal intensity vs. scans.

CAUTION

Make sure the sample is flowing before starting the tune. If autotuning fails, check the intensity of the precursor. The concentration of the tuning standard may need to be adjusted.

Menu Bar

The menu bar contains important tools and features.

File

Load Loads an ExD tune file.

Save Saves the contents of the Profiles Table to an ExD tune file.

Save as Saves the contents of the Profiles Table to a new ExD tune file, named by the user.

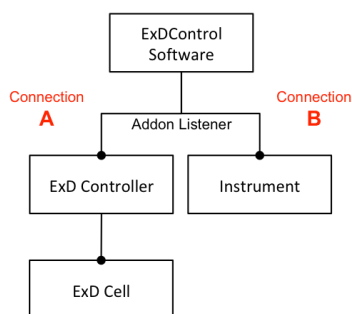
Connect

Auto-connect If checked, the ExDControl software will automatically connect to the ExD Controller/instrument after launch.

Connection Settings Advanced settings for configuring the ExDControl software network.

Depending on the instrument, the ExDControl software can operate in either instrument-aware or standalone mode:

Instrument-aware mode:



Standalone mode:

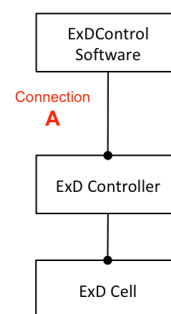


Figure 11. ExDControl software to ExD Controller/instrument network diagrams.

- In instrument-aware mode, the ExDControl software detects both the instrument and the ExD Controller, and will automatically switch between designated ExD profiles in unison with changes in the instrument scan type. See **Automatic Profile Switching**.

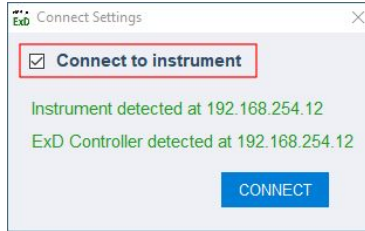


Figure 12. Instrument-aware Connection Settings window for the ExD AQ-250 Option.

Checking “*Connect to instrument*” enables instrument-aware mode.

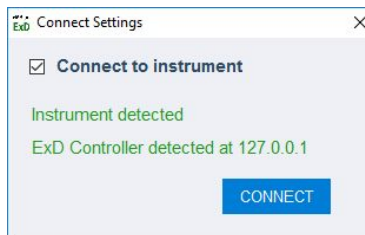


Figure 13. Instrument-aware Connection Settings window for the ExD TQ-160 Option.

Holding **Shift** and clicking **Connect** in the **Connect Settings** window (**Figure 12**) will allow you to directly enter the instrument IP address and the ExD Controller IP address to operate in instrument-aware mode.

Table 1. Instrument-aware IP address for each ExD Option.

ExD Option	Instrument-Aware IP Address
ExD AQ-250	192.168.254.12
ExD TQ-160	127.0.0.1

- In standalone mode, the ExDControl software only connects to the ExD Controller. Automatic profile switching is disabled, as the software is unaware of changes in instrument scan type.

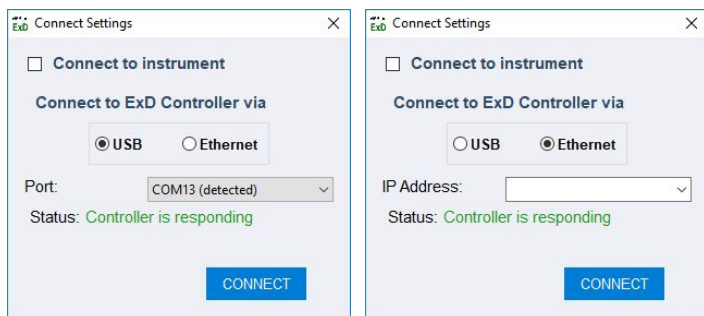


Figure 14. In standalone mode, select the connection type used to connect the ExDControl software to the ExD Controller.

Table 2. Standalone connection type(s) for each ExD Option.

ExD Option	Standalone Connection Type
ExD AQ-250	USB or Ethernet (IP: 192.168.254.50)
ExD TQ-160	Ethernet (IP: 127.0.0.1)
ExD WS-250	USB
ExD WK-150	Ethernet (IP: 192.168.1.50)

Connect Connects the ExDControl software to the ExD Controller and/or the instrument using the last used connection settings.

Disconnect Disconnects the ExDControl software from the ExD Controller and/or the instrument.

Window

Always on Top If checked, enables ExDControl software windows to always be visible in front of other application windows.

Versions Shows a history of saved changes to the ExD tune file. Changes can be reverted by double-clicking a save state from the list.

Profiles Table Shows the **Profiles Table**, which contains a list of all the profiles saved in the open ExD tune file. See **Profiles Table**.

Voltage Graph Shows a Voltage Graph of the ExD Cell lens profile.

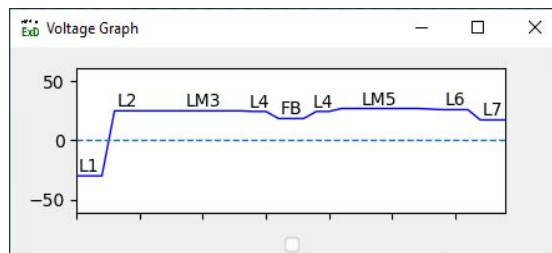
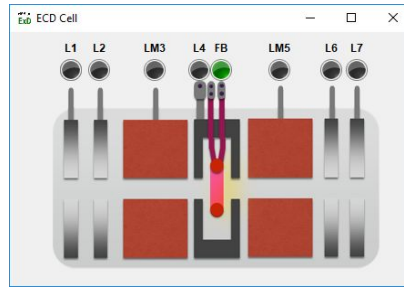


Figure 15. ExDControl Voltage Graph window.

Filament Parameters Shows the **Filament Parameters** window, where the filament **On** current can be adjusted. The window also contains diagnostic readouts of the filament circuit. See **Filament Parameters Window**.

Cell

Shows a diagram of the ExD Cell.



- Lens buttons turn green when the user selects the lens in the manual tune tab.
- The filament in the center of the cell turns red with a yellow “electron cloud” when the user turns the filament **On**.

Figure 16. ExDControl Cell display window.

Console

Shows a developer console for advanced operation.

Collision Cell Gas Pressure

ExD AQ-250 Option only.

Allows the user to adjust the collision cell gas pressure. This parameter cannot be adjusted in some versions of Agilent MassHunter Data Acquisition (e.g. B.08 and B.09).



Figure 17. ExDControl Collision Cell Gas Pressure window.

Offset Voltage

Shows a window for setting the offset voltage in the ExD Controller that adds to every lens voltage. This value is set during installation of the ExD Cell and should not be altered.

Spectrum Graph

Shows a live mass spectrum with the ability to record small time-segments of data. See [Spectrum Graph Window](#).

Verification

ExD AQ-250 Option only. Shows a window containing automated functions for system verification and troubleshooting.

Help

About

Shows ExDControl software application and addon version numbers and developer contact information.

Filament Parameters Window

Use the **Filament Parameters** window to control the filament, adjust the filament **On** current, and view readouts of filament circuit physical quantities.

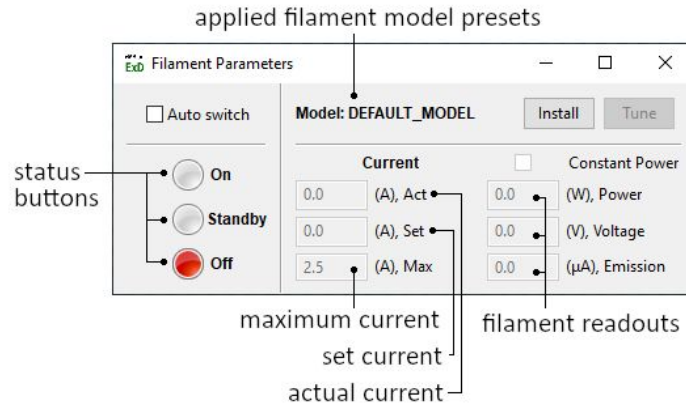


Figure 18. ExDControl **Filament Parameters** window.

Auto switch	If checked, the filament state will automatically change to match the instrument state (Standby or On).
Status buttons	Click to change the filament state in real time. Settings include Off (0.0 A), Standby (0.5 A), and On .
Set current	The set filament current. If the filament is On , alter the set current by typing a value in the Set box and pressing Enter .
Actual current	The actual filament current measured by the ExD Controller. If the voltage difference between the set and actual current is greater than 5%, then the text turns red.
Maximum current	The upper limit for the filament heating current.
Constant power	Checking this box enables automatic adjustment of the filament On current to keep the power level constant. This compensates for changes in the circuit, such as thinning of the wire over time.

NOTE

Operating the filament in constant power mode will extend its lifespan.

Filament readouts	Power, voltage, and electron emission of the filament circuit, as measured by the ExD Controller.
Tune	Automatically determines the optimum filament heating current for thermal emission. Using a preset profile and starting at 0 A, this method ramps the current while checking the emission current reading until a predetermined threshold is passed.

Profiles Table

Use the **Profiles Table** to view the list of all profiles in the loaded ExD tune file and to add or remove profiles from the list.

MS1	MS2	Tuned For	Profile	Description	L1	L2	LM3	L4	FB	LM5	L6	L7
<input checked="" type="checkbox"/>	<input type="checkbox"/>	MS1	MS1 hot trans	0623 F=2.0Ax2.26V 22psi tunemix 1.3M922 2GHz	-30.0	19.0	24.0	26.0	20.5	24.0	18.0	0.0
<input type="checkbox"/>	<input type="checkbox"/>	MS2	MS2 standby	0504 F=2.5Ax3.61V 22psi tunemix 320K922	0.0	24.0	25.0	25.0	20.5	24.5	12.0	0.0
<input type="checkbox"/>	<input type="checkbox"/>	MS2	MS2 hot trans	0626 F=2.07Ax2.65V 22psi subP 3.3M674 2GHz	0.0	24.0	25.5	25.5	21.0	25.0	14.0	0.0
<input type="checkbox"/>	<input type="checkbox"/>	MS2	MS2 ECD	0626 F=2.07Ax2.63V 22 psi subP 32K624	0.0	27.5	31.5	36.4	25.2	29.5	25.5	0.0
<input type="checkbox"/>	<input type="checkbox"/>	MS1	MS1 ECD	0623 ECD CE0 1.95A peptide	-40.0	21.0	26.0	31.0	22.0	26.0	21.0	0.0
<input type="checkbox"/>	<input checked="" type="checkbox"/>	MS2	MS2 ECD	0623 ECD CE0 1.95A peptide	-30.0	26.7	30.2	34.7	23.9	28.2	21.2	0.0

Figure 19. The **Profiles Table**, showing an example of a set of profiles developed for transmission and for ECD on an Agilent 6545XT LC/Q-TOF.

Add Click to add a new profile to the table. All voltages for a new profile will initially be set to 0 V.

Remove Click to remove a highlighted profile from the table. The profile currently in use by the ExD Cell cannot be removed.

MS1/MS2 *Only available if the ExDControl software connection is instrument-aware (see [Connection Settings](#)).*

Check the MS1 or MS2 box next to a profile to designate it for use while the instrument is scanning in MS1 or MS2. A profile may only be designated for a particular scan type if it was last tuned for that scan type.

NOTE

Use the profiles menu in the main window to apply any profile, regardless of which scan type the profile was last tuned for.

Tuned for Indicates whether the last change made to a profile occurred while the instrument was in MS1 or MS2.

Profile Enter the profile name here.

Description Enter the profile description here.

e-MSion *highly recommends* that you record at minimum the instrument operating mode and scan mode, sample identity, and filament current used with each profile here.

Lens profile The set values for the lenses. To change a value, select the box, type the new value, and press **Enter**.

Automatic Profile Switching

NOTE

Only active when ExDControl software connection is instrument-aware (see [Connection Settings](#)). Check with e-MSion to determine whether ExDControl profile switching on your instrument is fast enough for LC/MS/MS or DDA.

As the instrument changes scan types, the ExDControl software will automatically switch to the profile designated for the active scan type. This feature exists for two reasons:

- Mass isolation affects ion energy and beam geometry. Because the ExD Cell does not have a focusing multipole, it needs to be tuned differently in MS1 versus MS2 to optimize ion transmission.
- One profile can be dedicated to maximizing ion transmission in MS1 while a second profile is dedicated to maximizing ECD efficiency in MS2. Other experimental schemes are possible with user customization.

Spectrum Graph Window

NOTE

Only usable if the ExDControl software is instrument-aware (see [Connection Settings](#)) and the instrument is On.

Use the spectrum graph window to record spectra independently from the instrument control software. Spectra are processed and saved in .mzml format by ExDConvert, an e-MSion software tool for ExD data processing.

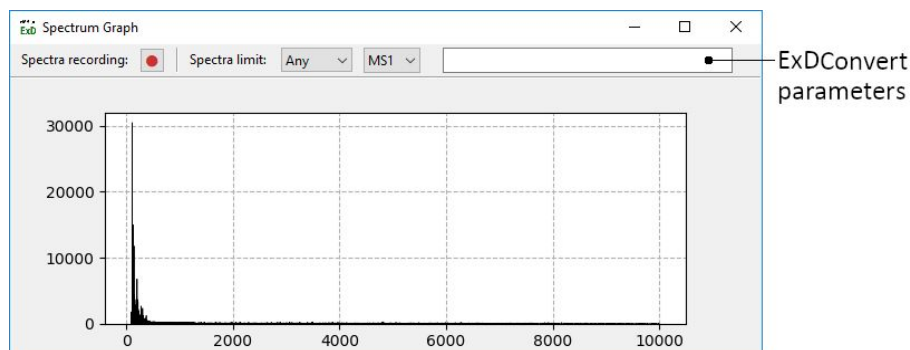


Figure 20. ExDControl Spectrum Graph window.

Spectra Recording	Click the icon to start and stop recording.
Spectra Limit	Select the number of spectra to record.
MS1/MS2	Select which scan type is assigned to the recorded spectra in the .mzml file metadata. This option allows for greater downstream analysis flexibility.
ExDConvert parameters	Enter parameters for ExDConvert here. Contact e-MSion for guidance.

ExDControl Software Installation

To uninstall the ExDControl software

1. Go to **C: > Program Files > E-MSION** and run the `uninstall.exe` application.

Uninstalling the ExDControl software will not delete the **E-MSION** folder in **C:\Users\“username”** where saved information such as collected data, tune files, and configuration files is stored.

To reinstall or update the ExDControl software

1. Go to <https://e-msion.com/downloads> and click the **Download** button.
2. Unzip/extract the installer file.
3. Run the installer file “**ExDControl_<version number>_setup.exe**” and follow directions in the installation wizard.

NOTE

You may need to grant access permission for Windows Defender and antivirus software in order to run the installer.

4. To verify software installation, confirm that the following file directories have been created:

```
C:\
|----Program Files
      |----ExDControl
|----Users
      |----“username”
            |----E-MSION
                  |----ExDControl
```

5. Click ExDControl software menu item **Connect > Connection Settings** to complete the installation process. If the connection attempt is unsuccessful, see [Connection Settings](#).

CAUTION

In order to establish ExDControl software connection, the ExD Controller must be installed and powered ON. See the *ExD Controller User Guide* for guidance.



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MAN-Gen-002-A2

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Until its next release, this guide is valid for the 3.1.0 version or higher of the ExDControl software.