

Release Notes

Open Access DIMSpec PFAS Library
High Resolution Accurate Mass Libraries

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Features

The Open Access DIMSpec PFAS library is an open-source, portable mass spectrometry database that was created by the U.S. National Institute of Standards and Technology (NIST) as part of the Database Infrastructure for Mass Spectrometry (DIMSpec) project. The Open Access DIMSpec PFAS library supports nontargeted analysis (NTA) workflows that use high-resolution mass spectrometry (HRMS) to detect, identify, and characterize per- and polyfluoroalkyl substances (PFAS).

The Open Access DIMSpec PFAS library is available to download at sciex.com/products/spectral-library as a nonencrypted SDF format library that includes 132 PFAS compounds.

The library can be installed on computers that have the SCIEX OS software 4.0 and LibraryView software 1.8 installed. The library is compatible with data that was acquired from these systems:

- TripleTOF systems, X500 QTOF systems, and ZenoTOF systems
- QTRAP systems

Use the libraries in the LibraryView software and SCIEX OS software to do these tasks:

- Do rapid compound searches for targeted and nontargeted screening.
- Use the accurate mass, isotopic ratio, and peak area filtering functions in the SCIEX OS software for compound identification.
- Compare a sample to a control for qualitative review with the comparative profiling option that is available in the SCIEX OS software.

Requirements

SCIEX OS Software
An English (US) version of Windows 11 LTSC 2024 is installed on one of these computers: <ul style="list-style-type: none">• SCIEX Workstation – 5860• SCIEX Workstation Plus – 5860
Note: An upgrade service is available to upgrade computers that have Windows 10 installed.

SCIEX OS Software

These applications are installed:

- | |
|--|
| <ul style="list-style-type: none">• A licensed version of the SCIEX OS software 4.0 or later• A licensed version of the LibraryView software 1.8 or later |
|--|

Internet access is available to download the Open Access DIMSpec PFAS library.
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The user is logged on to the computer as a user with Administrator privileges.
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Supported Equipment

- ZenoTOF 7600 systems
- ZenoTOF 7600+ systems
- ZenoTOF 8600 systems
- X500 QTOF systems
- QTRAP systems
- TripleTOF systems

For the best results, when the data processing settings are configured, refer to the section: [Recommended Library Search Settings](#).

Known Issues

Refer to the section: *Known Issues and Limitations* in the document: *LibraryView Software 1.8 Release Notes*

Install the SCIEX OS Software 4.0

- To open the *Software Installation Guide*, click **Start > SCIEX OS > SCIEX OS Documentation > sciex-os-software-installation-guide-en**.

Install the LibraryView Software 1.8

1. If the LibraryView software contains other libraries, then to make a back-up copy of all of the libraries, click **Export > LibraryView Database Snapshot Package (*.lbp)**.
2. To open the *Software Installation Guide*, click **Start > SCIEX > LibraryView Software Installation Guide**.

Install the Open Access DIMSpec PFAS Library

Note: Internet access is required to download the library.

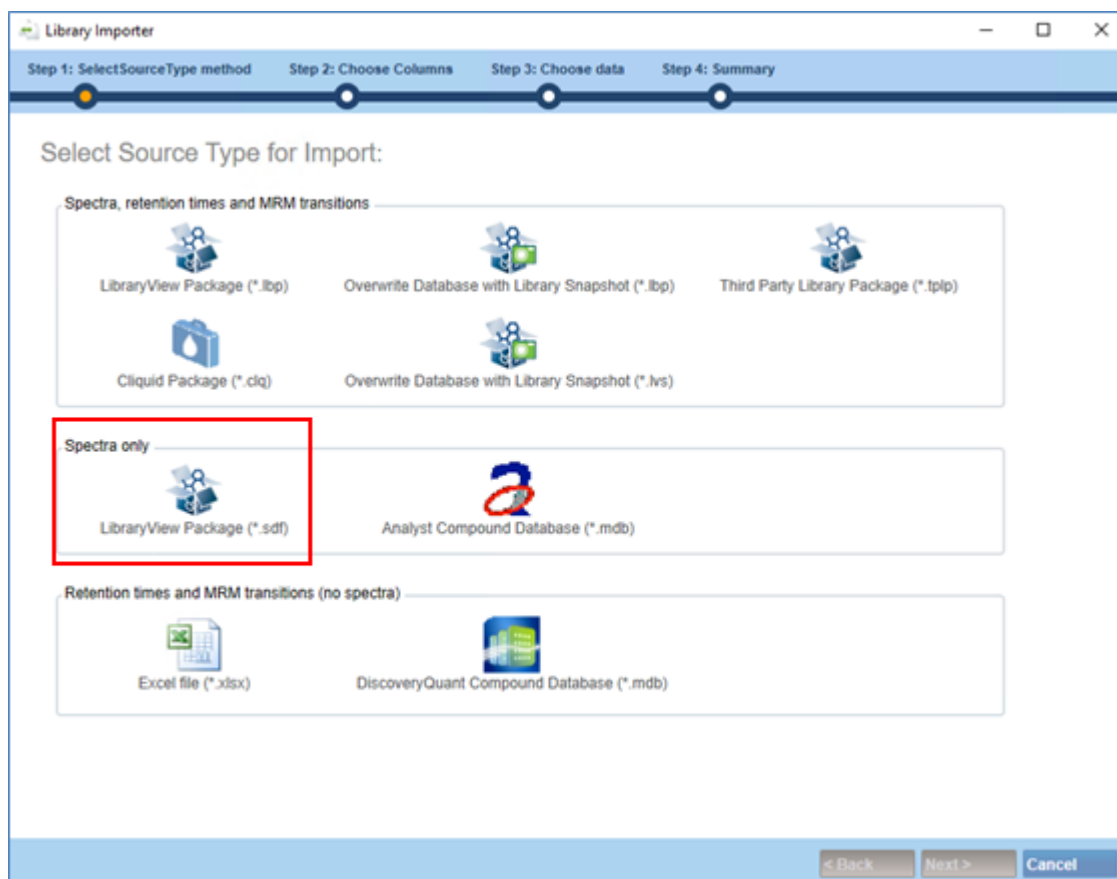
1. Log on to the computer as a Windows user with Administrator privileges.
 2. Go to sciex.com/software-downloads, and then download the required zip file.
-

Tip! To prevent installation issues, save the file to the local computer, in a different location than the desktop.

3. When the download is completed, right-click the downloaded file, and then click **Extract All**.
4. Select a destination folder, and then click **Extract**.
5. In the Spectra only section of the Library Importer dialog, click **LibraryView Package (*.sdf)**.

Installation

Figure 3-1 Library Importer Dialog: Spectra only Section



6. Browse to the files that were extracted, and then click the DIMSpec (Sep 2024) .sdf file.

Figure 3-2 Library Importer Dialog: Import 132 Compounds

The screenshot shows the 'Library Importer' dialog box with a table of compounds. The 'DimSpec (Sep 2024)' library is selected. The 'Compound' column is highlighted, and the 'All' option is selected. The table shows the following data:

Library Name	Compound	Formula	CAS
DimSpec (Sep 2024)	(Perfluorooctyl)ethylphosphonic acid (DimSpec)	C10H6F17O3P	
	(BE)-1,1,2,2,3,3,4,4,5,5,6,7,8,8,8-pentadecafluor...	C8H4F15O3S	
	(BE)-1,1,2,2,3,3,4,4,5,6,7,8,8,8-tetradecafluoro...	C8H2F14O3S	
	(Heptafluorobutano)(pivaloyl)methane (DimSpec)	C10H11F7O2	
	(Perfluorobutyl)-2-phenylmethane (DimSpec)	C10H6F7O2S	
	1-(Perfluorooctyl)propane-2,3-diol (DimSpec)	C11H7F17O2	
	1,1,2,2,3,3,4,4-Octafluorobutane-1-sulphonic aci...	C8H2F8O3S	
	10,2-Fluorotelomer thia propanoamido dimethyl...	C19H18F21NO4S2	
	10,2-Hydrogen-substituted fluorotelomer betaine...	C18H14F20NO2	
	11,1-Fluorotelomer alcohol (DimSpec)	C12H3F23O	
	1H,1H,5H-Perfluoropentanol (DimSpec)	C5H4F8O	
	1H,1H,6H,6H-Perfluorohexane-1,6-diol diacrylat...	C12H10F8O4	
	1H,1H,7H-Dodecafluoro-1-heptanol (DimSpec)	C7H4F12O	

132 from 132 compounds selected.

7. Above the **Compound** column, click **All**.

- Click **Next**.
- Click **Finish**.

Recommended Library Search Settings

The figure that follows shows the recommended library search settings for the SCIEX OS software 4.0.

Figure 3-3 Recommended Library Search Settings for the Open Access DIMSpec PFAS Library

Configure the library search parameters

Perform Library Search

Filtering Options

Library Search Algorithm: Candidate Search

Libraries To Search: Search All Libraries, DimSpec (Sep 2024)

Retention Time +/- 0.5 min

Precursor Mass Tolerance +/- 0.05 Da Use Polarity

Collision Energy +/- 5 eV Use Collision Energy Spread

[Advanced](#)

Scoring Parameters

Fragment Mass Tolerance +/- 0.05 Da Intensity Factor: 10

Ignore Isotopes In Unknown Intensity Threshold: 0.02

Scoring Criteria

Results Sorted By: Purity

Minimal Purity: 10.0 % Use Compound Specific Purity Threshold

Maximal Number Of Hits: 5

- If required, then to increase the processing time, in the **Precursor Mass Tolerance** field, type 0.05.
- To include instrumental differences in the relative intensity, in the **Intensity Factor** field, type 10.
- If required, then to improve the library search results for lower fragment signals, in the **Intensity Threshold** field, type 0.02.

Installation

Figure 3-4 Recommended Flagging Rules for the Open Access DIMSpec PFAS Library

Workflow [← Accept changes and return to Flagging Rules](#)

Components Configure the confidence levels for the qualitative rules, as applicable

Integration Rule name

Library Search

Calculated Columns

Flagging Rules

Advanced

Formula Finder

Non-targeted Peaks

Apply	Qualitative Rule	Acceptable Difference	Marginal Difference	Unacceptable Difference	Combined Score Weight (%)	
<input checked="" type="checkbox"/>	Mass Error (ppm)	< <input type="text" value="5"/>	< <input type="text" value="10"/>	>= <input type="text" value="10"/>	<input type="text" value="20"/>	● Error %
<input type="checkbox"/>	Fragment Mass Error (ppm)	< <input type="text" value="5"/>	< <input type="text" value="10"/>	>= <input type="text" value="10"/>	<input type="text" value="0"/>	○ Absolute
<input type="checkbox"/>	Error in Retention Time	< <input type="text" value="2.5"/>	< <input type="text" value="40"/>	>= <input type="text" value="40"/>	<input type="text" value="20"/>	
<input checked="" type="checkbox"/>	% Difference Isotope Ratio	< <input type="text" value="30"/>	< <input type="text" value="50"/>	>= <input type="text" value="50"/>	<input type="text" value="20"/>	
<input checked="" type="checkbox"/>	Library Hit Score	> <input type="text" value="70"/>	> <input type="text" value="50"/>	<= <input type="text" value="50"/>	<input type="text" value="60"/>	
<input type="checkbox"/>	Formula Finder Score	> <input type="text" value="50"/>	> <input type="text" value="20"/>	<= <input type="text" value="20"/>	<input type="text" value="20"/>	

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