

Application Builder

MS Sensor Application Builder

File Application Help

Search NIST: _____

Library: Mainlib

Compound Name
 CAS Registry Number
 Chemical Formula

Benzen

Search

Mass Spectrum | Peak Table | Compound Information

Normalized Abundance

Benzen

M/Z

Add Delete

Display Compound: Ethane

Combined Peaks | Combined Spectrum

Compound	Amount%	Selected M/Z	1	2	12	13	14	15	16	17
Ethane	2	30		0.002	0.004	0.009	0.028	0.040	0.001	
Ethylene	3			0.001	0.006	0.012	0.027	0.004		
Propane	1				0.001	0.002	0.007	0.022	0.001	
Propene	1	42	0.008	0.001	0.002	0.004	0.009	0.014	0.001	
Methane	20	15			0.338	0.942	1.813	7.884	8.880	0.14

Sync mass range of spectra
 Display detailed results

C:\Users\Public\Documents\Diablo MS Sensor 4.0\Application Builder\Syngas_Mix.mssapp

Diablo MS Sensor 4.0
Application Builder

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Manual Revision 20181031-0947

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Getting Started

Introduction

The MS Sensor Application Builder software is a tool to help users develop direct sampling mass spectrometry applications where spectral interference must be considered (like applications for the Diablo 5000A Real-Time Gas Analyzer). The Application Builder software uses the NIST Mass Spectral Library of 267,376 chemical compounds and the user's estimate of compound concentration to generate a combined sample spectrum and a table of sample m/z values with estimates of potential interference.

Note: You should expect some instrument-to-instrument variation in the actual mass spectra produced for a particular compound when compared with the NIST Library spectra used by Application Builder. Consequently, you should consider the Application Builder results to be estimates to help you with your evaluation of an application, rather than a rigorous and quantitative determination of the actual interferences.

Software Requirements

The MS Sensor Application Builder software is compatible with Windows 7 SP1, Windows 8/8.1, and Windows 10.

The .NET Framework 4.5.2 must be installed before trying to run Application Builder. The .NET Framework will be installed automatically, if necessary, when you install the software from the distribution media, or if you use the single-file installer. If you use the web-based installer the .NET Framework 4.5.2 will be downloaded automatically if necessary. You can also download and install the .NET Framework 4.5.2 from Microsoft using the following link:

<https://www.microsoft.com/en-us/download/details.aspx?id=42642>

Note: The .NET Framework 4.5.2 is included with all versions of the Windows 10 operating system.

NIST Mass Spectral Library

This software requires the NIST Mass Spectral Library to be licensed and installed on the computer. You can purchase a special, discounted license of the NIST 17 library at the time you purchase the Application Builder license.

For more information on the NIST Mass Spectral Library, visit the following link:

<http://chemdata.nist.gov/>

DEMO Library and Application

If you choose the “Complete Setup” when installing the Application Builder software, then a small “demo” library and corresponding application file will be installed to help you evaluate the software.

The demo library is installed to the folder: “C:\NIST DEMO\MSSEARCH\mssensor_demo”

The demo application is: C:\Users\Public\Documents\Diablo MS Sensor 4.0\Application Builder\air_demo.mssapp

IMPORTANT: The spectra included in the demo library are “synthetic” and were not derived experimentally or copied from an experimentally derived source like the NIST library. Although they should resemble the actual spectra of those library compounds, you should only use them for demonstration and evaluation purposes.

Installation

Note: We recommended installing the NIST Mass Spectral Library before installing the Application Builder software. Refer to the NIST Mass Spectral Library User’s Guide for information on installing the library.

The Application Builder software is installed by running the setup program on the distribution flash drive/CD, or the installation program downloaded from our web site.

Important: You must be logged on with Administrator privileges when you install the software (but you can run the software thereafter as a standard user)

There are two different versions of the installation program that can be downloaded from our web site:

1. A web-based installer that should be used to update an existing installation of the software or to install the software on a computer that has Internet access. This version of the installer will download the required .NET Framework 4.5.2 files automatically over the Internet if required.
2. A single-file installer that should be used to install the software on a computer with no access to the Internet. This version of the installer includes the .NET Framework 4.5.2 and is consequently much larger in size.

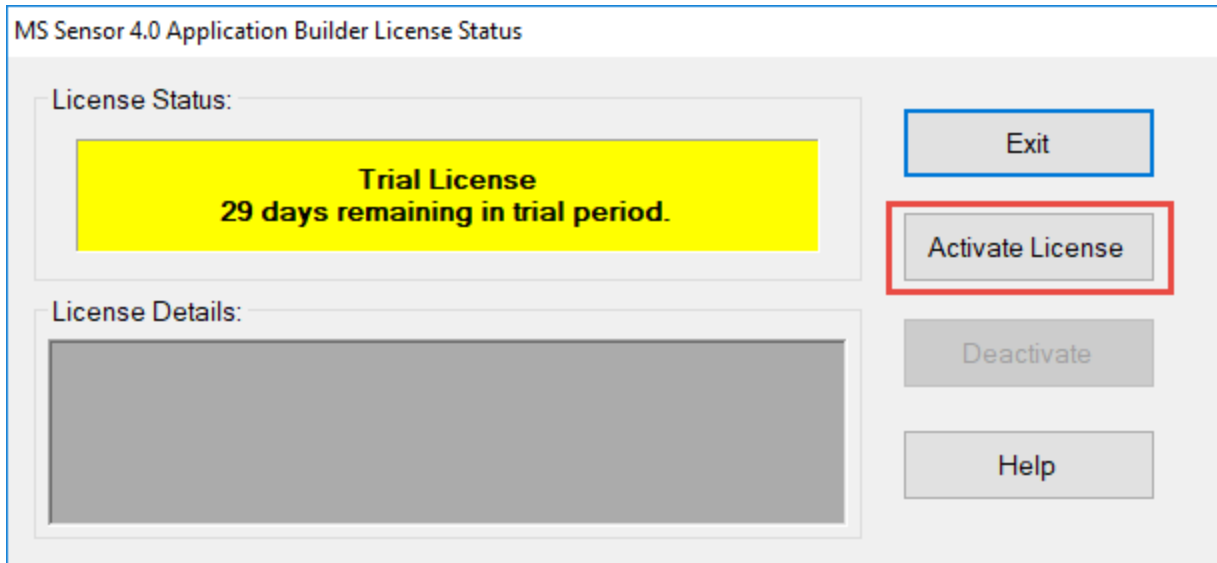
Note: The .NET Framework 4.5.2 is included with all versions of the Windows 10 operating system. Consequently, you should use the web-based installer to install Application Builder onto a computer running Windows 10.

Software Licensing and Activation

When you run the software for the first time, you will have a trial license that allows you to use and evaluate the program for up to 30 days. The program is fully-functional during the trial period. In order to continue using the software after the 30-day trial period, you must purchase a license and then activate the software.

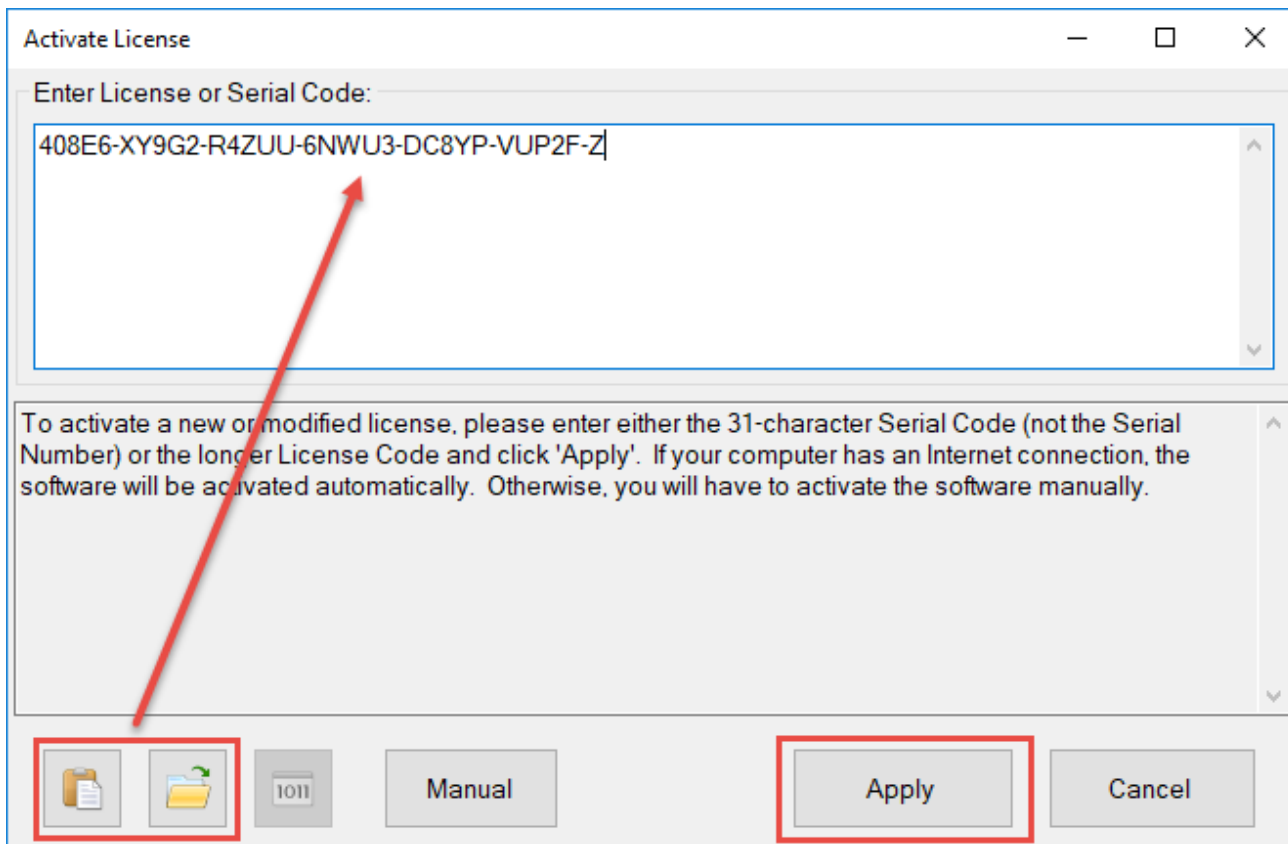
Note: The Application Builder software is included with the MS Sensor 4.0 software. After activating the MS Sensor 4.0 software running on the same computer, the Application Builder software will also reflect the MS Sensor 4.0 license status. However, if you want to run the Application Builder software on a different computer, you will need to activate the software.

To activate your license, click the “Activate License” button on the License Status window that is displayed when you start the software or when you click the menu option, “Help > License Status...”.



When you purchase your software license, you will receive a 31-character Serial License Code (this is different than the shorter Serial Number). To activate the software, you must enter that License Code into the text box on the “Activate License” window. If you copy the Serial License Code to the Windows Clipboard from an email message, you can paste into the text box using the “Paste” button. Alternatively, if you received a text file containing the Serial License Code, you can load it using the “File Open” button.

Note: If you received a distribution USB flash drive, a text file containing your serial license code may be saved on the flash drive.

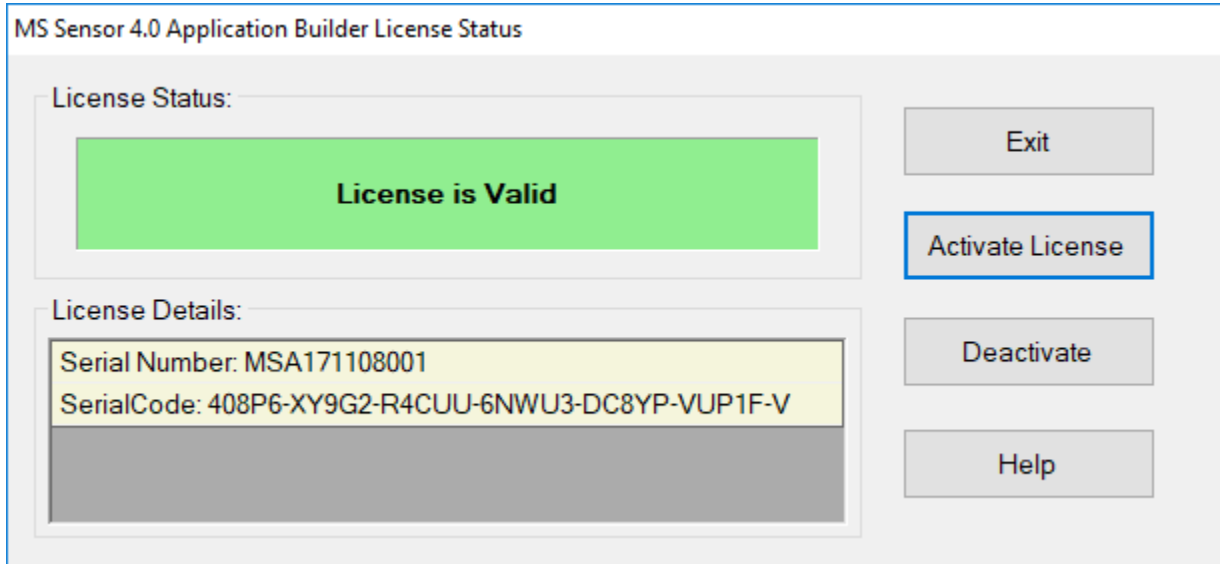


After entering the Serial License Code, click the “Apply” button. If your computer is connected to the Internet, the software will contact the License Server and automatically activate the software.

If your computer is not connected to the Internet, or if there is a problem contacting the License Server, then you will need to activate the software manually by clicking the “Manual” button and following the instructions.

Refer to the Software License Guide for more information about licensing and activation.

Note: An Internet connection is only required when applying an activation code or deactivating the software. No Internet connection is required during normal operation of the software.



Guide to Application Builder

Overview

All of the functionality of the Application Builder software is accessed through the menus and panels of the main user interface. Each of these elements is described in more detail below.

MS Sensor Application Builder

File Application Help

Search NIST: _____

Library: Mainlib

Compound Name
 CAS Registry Number
 Chemical Formula

Benzene

Search

Benzen-d5-amine
Benzene
benzene, 1,1'-(1,10-decanediylbis(oxy))b
Benzene, 1,1'-(1,1,10,10-tetramethyl-1,1
Benzene, 1,1'-(1,1,10,10-tetramethyl-1,1
Benzene, 1,1',1'',1''',1''''-(1,2
Benzene, 1,1',1'',1''',1''''-(1,3-cyclop
Benzene, 1,1',1'',1''',1''''-[bi-
Benzene, 1,1',1'',1''',1''''-(1,2,3,4-butanete
Benzene, 1,1',1'',1''',1''''-(1,2,3,4-cyclobut
Benzene, 1,1',1'',1''',1''''-(1,2,3-butatriene
Benzene, 1,1',1'',1''',1''''-(1,2-cyclopropane
Benzene, 1,1',1'',1''',1''''-(1,2-diisocyno-1
Benzene, 1,1',1'',1''',1''''-(1,2-ethanediylid
Benzene, 1,1',1'',1''',1''''-(1,2-ethanediylid

Mass Spectrum | Peak Table | Compound Information

Benzene

Normalized Abundance

M/Z

45
40
35
30
25
20
15
10
5
0

5 10 15 20 25 30 35 40 45 50 55 60 65 70 75 80

39 55 52 77 78

Add Delete

Display Compound: Ethane

Combined Peaks | Combined Spectrum

Compound	Amount%	Selected M/Z	1	2	12	13	14	15	16	17
Ethane	2	30		0.002	0.004	0.009	0.028	0.040	0.001	
Ethylene	3			0.001	0.006	0.012	0.027	0.004		
Propane	1				0.001	0.002	0.007	0.022	0.001	
Propene	1	42	0.008	0.001	0.002	0.004	0.009	0.014	0.001	
Methane	20	15			0.338	0.942	1.813	7.884	8.880	0.14

Sync mass range of spectra Display detailed results

C:\Users\Public\Documents\Diablo MS Sensor 4.0\Application Builder\Syngas_Mix.msssapp

The Main Menu

File Menu

New Application: Click this option to clear the current application and create a new application. Make sure to save the current application if you want to load it at a later time.

Open Application: Click this option to load an existing application from disk. Application files have a file extension of “.mssapp”, and are stored by default in the folder:

C:\Users\Public\Documents\Diablo MS Sensor 4.0\Application Builder

Save Application: Click this option to save any changes you have made to the current application. If you haven't yet saved the application, then the “Save Application As” dialog will be displayed.

Save Application As: Click this option to save the current application to a new application file.

Export Application to MS Sensor: If the MS Sensor 4.0 software is installed on the current computer, you can click this menu option to export the current application to MS Sensor. See the MS Sensor 4.0 reference manual for more information on how using the Application Data Import Wizard to create a new method from the application data.

Print Report: Click this option to print a report for the current application.

Save Report As: Click this option to save the report for the current application to an Adobe Acrobat “PDF” file.

Set NIST Library Folder: Use this option to change the NIST library folder used by Application Builder. You would need to do this if you have multiple versions of the NIST Library installed on your system, or if you are using the Application Builder Demo Library and want to switch to the actual NIST Library. NIST Libraries are typically installed in the folder, “C:\NISTXX\mssearch”, where “XX” is the release year. Currently this folder is “C:\NIST17\mssearch”. You can select either the C:\NIST17 folder or the actual “mssearch” folder.

Update NIST Numbers: This is an advanced option that should only be used at the direction of Diablo Analytical Support when upgrading applications from older versions of Application Builder.

Application Menu

Edit Settings

The “Edit Settings” menu option allows you to customize the behavior of the current application. See the description of each setting below.

The screenshot shows a dialog box titled "Edit Application Settings". It has a close button (X) in the top right corner. The dialog is divided into two main sections. The first section is labeled "Application Description:" and contains a large, empty text area. The second section is labeled "Application Settings:" and contains four input fields, each with a numerical value: "Interference Warning Level" is 2, "Interference Failure Level" is 25, "Abundance Threshold" is 5, and "Peak Label Threshold" is 10. To the right of these input fields is a button labeled "<- Reset". At the bottom of the dialog are two buttons: "OK" and "Cancel".

Application Description: The Application Description is displayed in the printed or saved report.

Interference Warning Level: If the total interference from other compounds at a particular m/z is greater than this setting as a relative % of a compound's corrected abundance at the same m/z, then an interference warning will be generated (the m/z will be shown in a yellow cell in the combined peaks table).

Interference Failure Level: If the total interference from other compounds at a particular m/z is greater than this setting as a relative % of a compound's corrected abundance at the same m/z, then an interference failure will be generated (the m/z will be shown in a red cell in the combined peaks table).

Abundance Threshold: If the corrected abundance of a peak as a relative % of the base peak abundance is less than this setting, then this peak will be considered too low in intensity to use in the application (the m/z will be shown in a gray cell in the combined peaks table)

Peak Label Threshold: This sets the size of the peak in mass spectrum plots that will have the m/z label displayed at the top of the peak. The setting is the % of the base peak abundance. The purpose is to prevent peak labels on small peaks from complicating the display of the spectrum.

Help Menu

View Help: Displays this help file.

License Status: Display the license status for the Application Builder software. See "[Software Licensing and Activation](#)" on page 2 for information on activating the software.

View Release Notes: Opens the release notes (readme.txt) for the current software release in Windows Notepad. You should always review the release notes when you install a new version of the software to see if there are any important changes that didn't make it into the manual.

About MS Sensor Application Builder: Displays a window with information about the Application Builder software, including the version, and the current NIST Library folder being used.

The Search Panel

The Search Panel is the interface to the NIST Mass Spectral Library (or the small "demo" library if you have not installed the NIST library).

The Library List: This list box will contain all of the libraries that are present in the current library folder. In a typical NIST Mass Spectral Library installation, the only option will be "Mainlib". However, if you have created additional custom libraries in the same library folder, they will also be listed here.

Library Search Options: You can search the selected library by entering a Compound Name, a CAS Registry Number, or a Chemical Formula.

Search Results: After selecting the desired search options and entering the corresponding search term, click the "Search" button. The names of any compounds in the selected library that match your search options will be displayed in the search results list (including compound aliases/synonyms). If you select one of the search results, the mass spectrum and compound information will be displayed in the Spectrum Panel for review.

Search NIST: _____

Library: _____

Mainlib

Compound Name
 CAS Registry Number
 Chemical Formula

Benzene

Search

Benzen-d5-amine
Benzen
 benzene, 1,1'-[1,10-decanediylbis(oxy)]b
 Benzene, 1,1'-(1,1,10,10-tetramethyl-1,1
 Benzene, 1,1'-(1,1,10,10-tetramethyl-1,1
 Benzene, 1,1',1'',1''',1''''-(1,2
 Benzene, 1,1',1'',1''',1''''-(1,3-cyclop
 Benzene, 1,1',1'',1''',1''''-[bi-
 Benzene, 1,1',1'',1''''-(1,2,3,4-butanete
 Benzene, 1,1',1'',1''''-(1,2,3,4-cyclobut
 Benzene, 1,1',1'',1''''-(1,2,3-butatriene
 Benzene, 1,1',1'',1''''-(1,2-cyclopropane
 Benzene, 1,1',1'',1''''-(1,2-diisocyano-1
 Benzene, 1,1',1'',1''''-(1,2-ethanediylid
 Benzene, 1,1',1'',1''''-(1,2-ethanediylid

The Spectrum Panel

The Spectrum Panel is used to display the spectrum, peak table, and compound information of either a library search result, or of one of the compounds you have added to the combined peaks table.

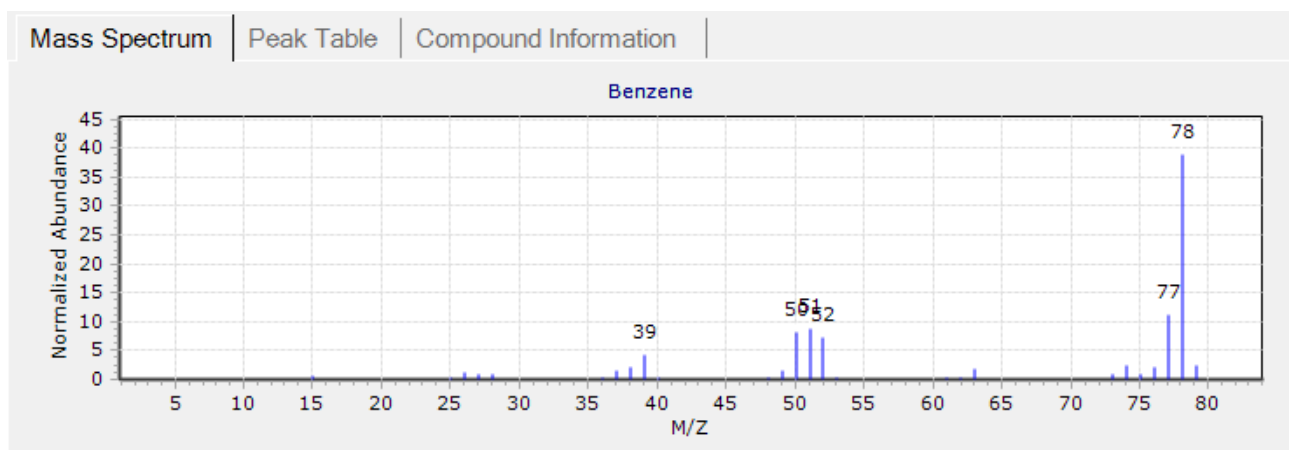
Mass Spectrum Tab

The Mass Spectrum plot displays the spectrum of either the selected library search result or the selected compound in the combined peaks table.

Zooming: You can zoom into the spectrum by *left* clicking the *upper left* of the desired zoom range, and then dragging the zoom rectangle to the *lower right* of the desired region. You can un-zoom by double clicking anywhere in the plot window.

Panning: You can drag the spectrum to a new location by *right* clicking anywhere in the plot window and then dragging the entire spectrum to the desired location.

Copying to the Clipboard: You can copy the spectrum to the Windows Clipboard by right clicking anywhere on the spectrum and selecting "Copy Spectrum to Clipboard" from the pop-up menu.



Peak Table Tab

The Peak Table displays the spectrum of either the selected library search result or the selected compound in the combined peaks table in tabular form.

Copy to clipboard: You can select a region from the Peak Table and then copy it to the Windows Clipboard by right clicking the table and selecting, "Copy Selection to Clipboard" from the pop-up menu.

Mass Spectrum | **Peak Table** | Compound Information

M/Z	Abundance	Normalized Abundance
15	12	0.467
25	7	0.272
26	34	1.322
27	26	1.011
28	21	0.816
36	6	0.233
37	42	1.633
38	56	2.177
39	111	4.316

Compound Information Tab

The Compound Information table displays information about either the selected library search result or selected compound in the combined peaks table. The information included in the table depends on the version of the NIST Library (or demo library) you have selected, but can include the CAS Number, Molecular Weight, and any synonyms that have been defined.

Copy to clipboard: You can select a region from the Compound Information table and then copy it to the Windows Clipboard by right clicking the table and selecting, "Copy Selection to Clipboard" from the pop-up menu.

Mass Spectrum	Peak Table	Compound Information
Compound Name	Benzene	
CAS Number	71432	
Formula	C6H6	
Molecular Weight	78	
	[6]Annulene Benzol Benzole Coal naphtha Cyclohexatriene Phenyl hydride Pyrobenzol	

The Combined Peaks Panel

The Combined Peaks Panel is where the compounds you have added to your application are saved and displayed.

Adding, Deleting, and Viewing Spectra

Click the “Add” button to add the compound/spectrum currently displayed in the Spectrum Panel to your application. You will be prompted to enter an estimated amount.

Click the “Delete” button to delete the compound currently selected in the Combined Peaks Table from the application.

You can display the mass spectrum, peak table, and compound information for any compound in your application either by selecting that compound in the “Display Compound” list, or by clicking the compound’s row in the Combined Peaks table.

Add	Delete	Display Compound: <input type="text" value="Ethane"/>
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Combined Peaks Table

The Combined Peaks table displays all of the m/z values present in the spectra of all of the compounds in your application. In the default mode the table displays the corrected abundance for each m/z value in each compounds spectrum, allowing you to evaluate where there will be potential spectral interferences.

Note: Corrected Abundance = Normalized Abundance * Amount% / 100

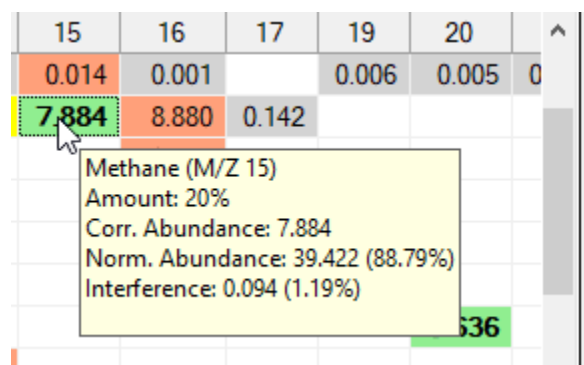
Combined Peaks		Combined Spectrum									
Compound	Amount%	Selected M/Z	1	2	12	13	14	15	16	17	19
Ethane	2	30		0.002	0.004	0.009	0.028	0.040	0.001		
Ethylene	3			0.001	0.006	0.012	0.027	0.004			
Propane	1				0.001	0.002	0.007	0.022	0.001		0.002
Propene	1	42	0.008	0.001	0.002	0.004	0.009	0.014	0.001		0.006
Methane	20	15			0.338	0.942	1.813	7.884	8.880	0.142	

Sync mass range of spectra
 Display detailed results

Spectral interferences are calculated for each peak in a compound's spectrum by adding the corrected abundance for all other compounds at a particular m/z, and then comparing that "interference" with the corrected abundance of the compound. The cells in the table are then color coded as follows:

Green:	The total interference from other compounds at that same m/z is less than the "Interference Warning Level" in the Application Settings (less than 2% of the compound's corrected abundance at this m/z by default)
Yellow	The total interference from other compounds at that same m/z is greater than the "Interference Warning Level" and less than the "Interference Failure Level" in the Application Settings (less than 25% of the compound's corrected abundance at this m/z by default)
Red	The total interference from other compounds at that same m/z is greater than the "Interference Failure Level" in the Application Settings (greater than 25% of the compound's corrected abundance at this m/z by default)
Gray:	The corrected abundance is less than the "Abundance Threshold" in the Application Settings (5% of the abundance of the base peak in this compound's spectrum)

You can review the detailed interference results for a particular peak by placing the cursor over the desired cell in the table – a "tool tip" will pop up displaying the detail. You can also check the "Display detailed results" checkbox" (see ["Display detailed results"](#) on page 12).



Copy to clipboard: You can select a region from the Combined Peaks table and then copy it to the Windows Clipboard by right clicking the table and selecting, "Copy Selection to Clipboard as Text" from the pop-up menu. You can also copy the entire table to the clipboard by selecting "Copy Table to Clipboard as Image".

Changing Estimated Amounts

You can change the estimated amount of any of the compounds in your application by double clicking the amount you want to change in the Combined Peaks table. You can enter a new amount (in %) into the "Compound Amount" window. After clicking "OK" your application will be updated to reflect the new amount.

Compound Amount

Enter estimated % Amount in your sample for: Methane

OK

Cancel

20

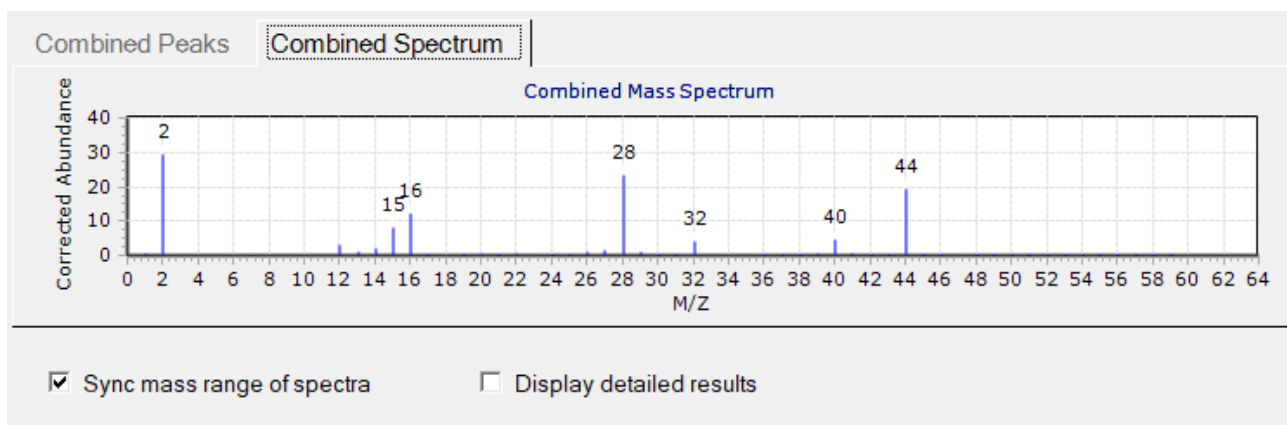
Combined Spectrum

The Combined Spectrum plot is a spectrum that combines all of the individual corrected peak abundances at each m/z to produce an overall spectrum of the sample.

Zooming: You can zoom into the spectrum by *left* clicking the *upper left* of the desired zoom range, and then dragging the zoom rectangle to the *lower right* of the desired region. You can un-zoom by double clicking anywhere in the plot window.

Panning: You can drag the spectrum to a new location by *right* clicking anywhere in the plot window and then dragging the entire spectrum to the desired location.

Copying to the Clipboard: You can copy the spectrum to the Windows Clipboard by right clicking anywhere on the spectrum and selecting “Copy Spectrum to Clipboard” from the pop-up menu.



Sync mass range of spectra

If you check the “Sync mass range of spectra” option, then each of the individual spectra displayed in the Mass Spectrum tab will have the full mass range of the combined spectrum. If this option is unchecked, then the individual spectra in the Mass Spectrum tab will be displayed over the mass range of peaks present in that compound’s spectrum.

Display detailed results

If you check this option, then the combined peak table will be expanded to include the following detail:

Methane	1.813 9.067 (20.42%) 0.108 (5.94%)	7.884 39.422 (88.79%) 0.094 (1.19%)	8.880 44.400 (100.00%) 3.039 (34.22%)	0.142 0.711 (1.60%) 0.000 (0.00%)
---------	--	---	---	---

Line 1: The corrected abundance (normalized peak abundance x concentration estimate / 100)

Line 2: The normalized abundance of the peak in the spectrum (with the % of the base peak in parenthesis). The base peak is the peak with the highest abundance in the spectrum.

Line 3: The total interference from other compounds at that m/z (and the relative % this interference represents of the compound's corrected abundance).

Note: The relative% of the interference is the value used to set interference and failure warnings.

Building an Application

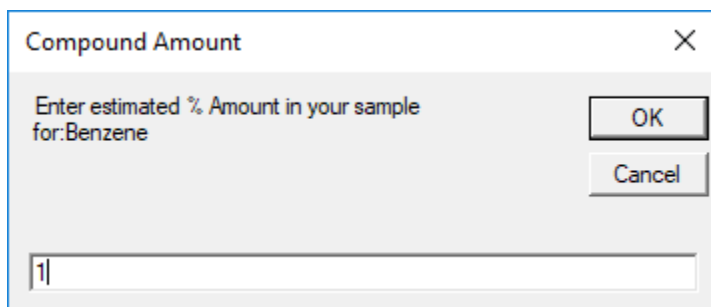
The following approach is typically used to build and evaluate an application using Application Builder:

Define Your Sample

In order to make the application evaluation meaningful, you should first identify all of the compounds that could potentially be present in your sample and estimate the maximum concentration you expect for them. Make sure to include any diluent/makeup gas, and any other components that might be present like water vapor or atmospheric nitrogen and oxygen.

Create the Application

Once you have defined your sample, you can create a new application by searching the library for each compound in your sample and adding it to the application by clicking the "Add" button. You will be prompted to enter the estimated concentration (in %) for that compound:



After adding a compound to the application, the Combined Peaks table and spectrum will be updated to reflect the impact the new compound has on the application.

Evaluate the Results

When you have added all of the compounds in your sample to the application, you can evaluate the interference levels as indicated by the color-coding of the cells for each m/z in the Combined Peaks table (see "[Combined Peaks Table](#)" on page 10 for details).

Application Builder will select the "best" m/z value to monitor for each compound in the application and display that in the "Selected m/z" column of the Combined Peaks table:

Compound	Amount%	Selected M/Z
Ethane	2	30
Ethylene	3	
Propane	1	
Propene	1	42
Methane	20	15
Oxygen	5	32

Note: If there are no m/z values for a particular compound that have interference values fall below the Interference Failure Level set for your application, then the "Selected M/Z" will be left blank, and the compound name will be displayed in red to indicate there are potentially significant issues with the compound in the current application.

You can override the “Selected M/Z” for a particular compound by right clicking on the cell in the Combined Peaks table for the desired m/z, and select “Manually Select this M/Z for Compound” from the pop-up menu. Manually selected m/z values are displayed in italics in the “Selected M/Z” column.

Refine the Results

Once you have done your initial evaluation it is often helpful to refine the results by adjusting the estimated compound amounts to see the impact on the interference analysis. You can also add/remove compounds from the application depending on the experimental flexibility you have. For example you can assess different diluent/make up gases to see how they impact the application.

Save the Application

You can save your application so that it can be recalled at a later time by clicking the “File > Save...” or “File > Save As...” menu options. Application files have a file extension of “.mssapp”, and are stored by default in the folder:

C:\Users\Public\Documents\Diablo MS Sensor 4.0\Application Builder

Save and Print the Report

Finally, you can save or print an Application Builder Report using the “File > Print Report...” or “File > Save Report As...” menu options.

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