

Classification Regions: A Tool for Streamlining the Interpretation of Complex GCxGC Data

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NOTE: This document is intended to provide an introduction to the Classifications feature of LECO's ChromaTOF® software for GCxGC. All examples shown utilized ChromaTOF version 4.22. Some features and the software layout may be different or absent if using a different version of the software. It is assumed that the reader is familiar with GCxGC theory and the use of ChromaTOF software for GCxGC, as covered in, "An Introduction to LECO's Comprehensive Two-Dimensional Gas Chromatography (GCxGC) with ChromaTOF Software".

Introduction

Classifications is a feature of the data processing package for GCxGC of LECO's proprietary ChromaTOF software. Classifications utilize the structured nature of a GCxGC chromatogram to organize related analytes into user defined groups. Classifications may also be used to selectively process, or exclude, regions of the chromatogram. In this work, the creation and implementation of Classifications will be covered.

Background

One of the notable characteristics of a GCxGC chromatogram is its structured nature. Homologous series tend to form bands in the Contour Plot. A homologous series is a group of chemical compounds that differ by a simple structural unit. An example of a homologous series would be 2-pentanone, 2-hexanone, 2-heptanone, 2-octanone and 2-nonanone, where each compound differs by the addition of a methylene (-CH₂-) unit. Another example of a homologous series would be benzene, toluene, ethyl benzene, propyl benzene, and butyl benzene. Figure 1 shows an example of how a homologous series, in this case the n-alkanes, appears in a Contour Plot. The red dashed line highlights the band formed by the series.

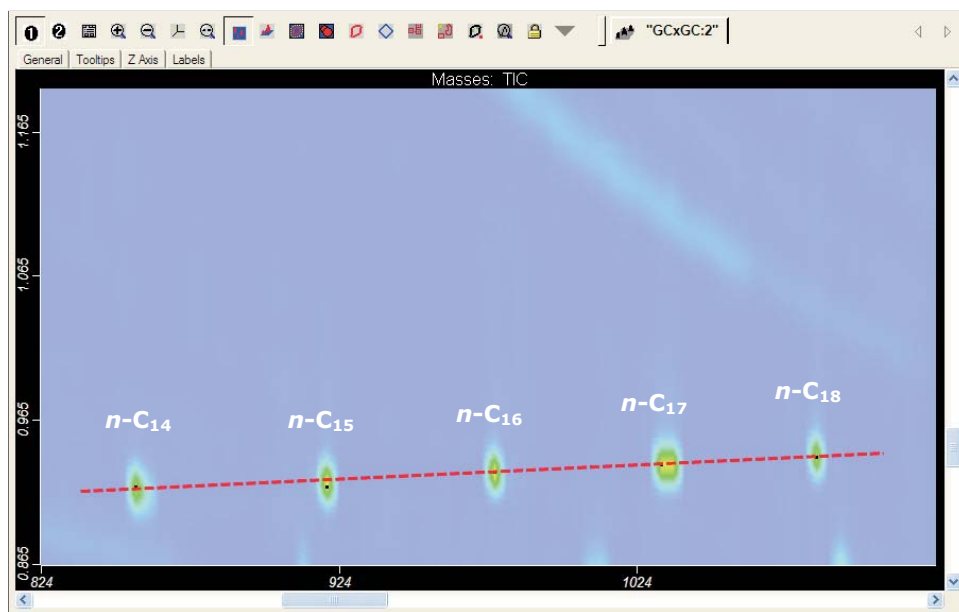


Figure 1: An example of how a homologous series, in this case the n-alkanes would appear in a Contour Plot. Note the "band" (the red dashed line) formed by the components in the series.

The tendency for homologous series to form structured features in the Contour Plot, when combined with the increased chromatographic resolution, provides the analyst with a powerful tool to aid in categorizing and filtering the Peak Tables resulting from the analysis of complex samples. Specific geographic regions of the Contour Plot can be designated as the "address" for a certain compound or related group of compounds. Peaks that occur inside one of these regions are assigned to the Classification associated with that region. Peaks in the Peak Table can be sorted and/or filtered by Classifications, allowing for more efficient management of large amounts of data obtained from complex samples.

Creating a Classification Region

A standard is used to construct a Classification. To create a new Classification, select Classifications in the Database Pane. Right-click in the File Pane and select "New". When the new Classification appears in the File Pane, it may be re-named. In this case, the sample Classification was re-named "Intro to Classifications". Figure 2 shows the step-by-step procedure for creating a new Classification.

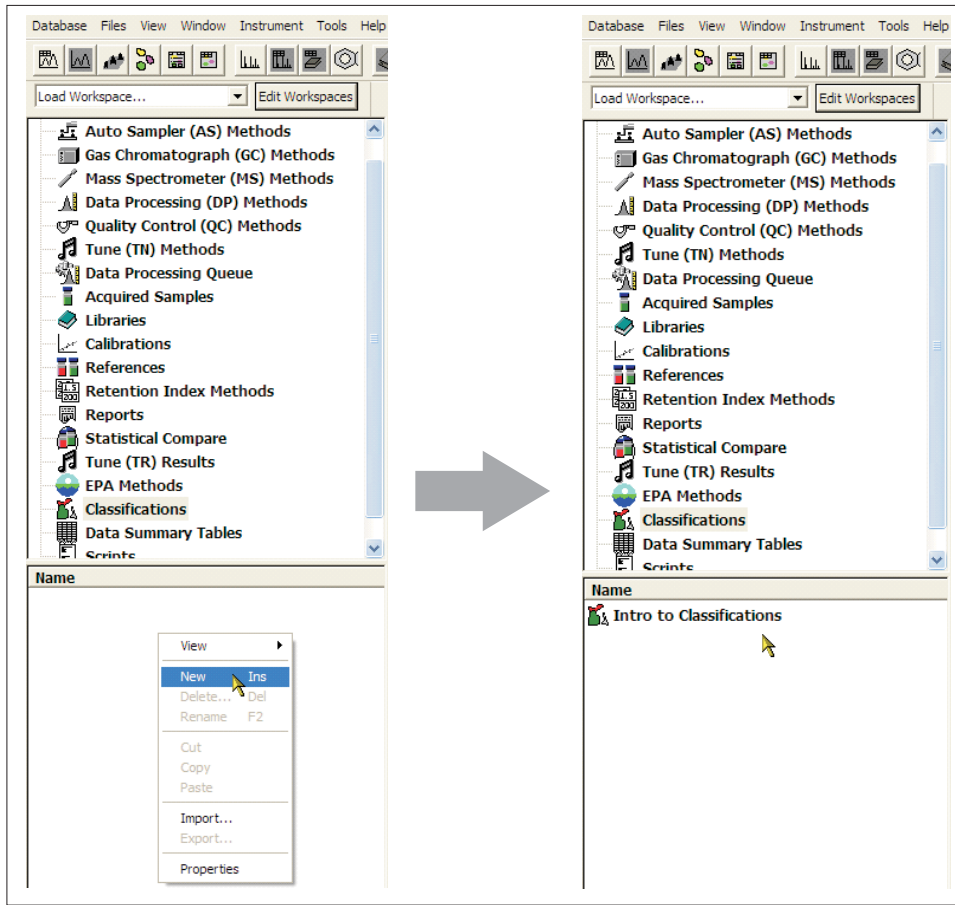


Figure 2: The step-by-step procedure for creating a new Classification.

The next step is to set-up the workspace with the necessary windows for creating and editing Classifications. Only two windows are mandatory; the Classifications Window and the 3D Image Window. Several other windows are useful in the process of editing and creating Classifications. There is no "wrong" way to organize the workspace. As with other sections of the ChromaTOF software, the workspace is easily configurable to whatever layout the user finds most efficient for them. Figure 3 shows an example of a workspace configured for working with Classifications.

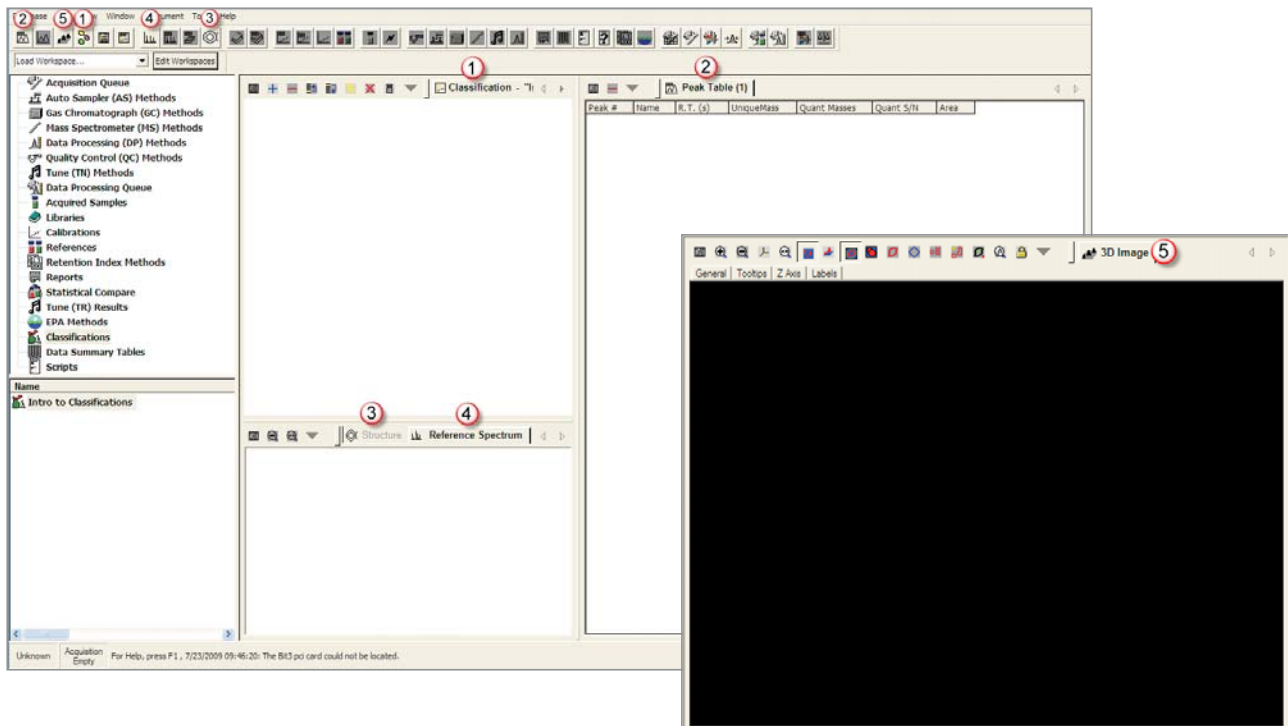


Figure 3: An example of a workspace configured for working with Classifications. Individual windows, and the buttons used to select those windows, are highlighted. The 3D Image is usually detached and placed on the second monitor.

Once the workspace has been configured, a standard must be selected for use as a template for creating the Classification. It is important to remember that a Classification is only valid for samples run under identical conditions. To assign a sample as the standard for a Classification, right-click in the Classification window and select "Set Standard". A window will appear listing the available samples from Acquired Samples. Select the desired sample as the standard. It is important to note that the standard should be a sample that has been previously data processed. Figure 4 shows the step-by-step procedure for setting sample "raw diesel_1" as a standard for the Classification.

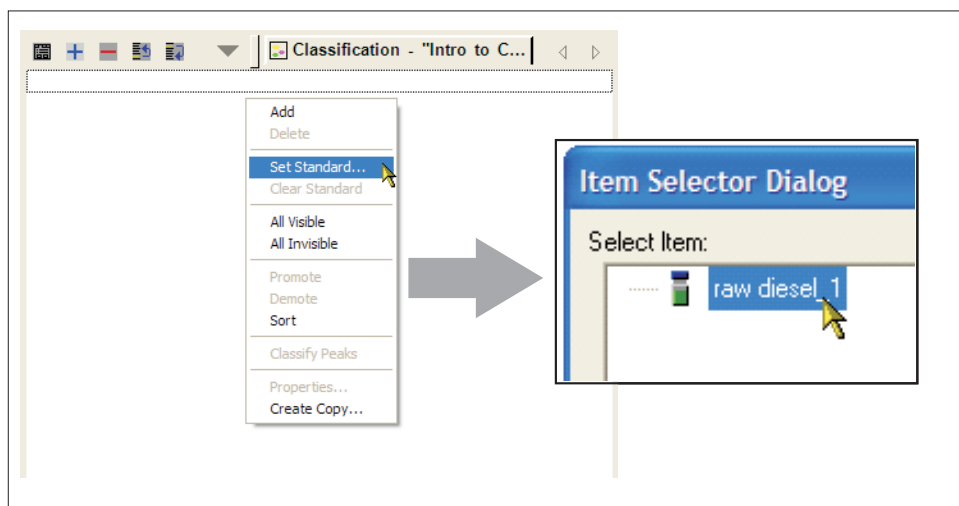


Figure 4: The step-by-step procedure for setting sample "raw diesel_1" as a standard for the Classification.

When the standard has been selected, the windows shown in Figure 3 should now be populated with the information from the sample that was selected as the standard. Figure 5 shows the windows from Figure 3 populated with the data from the sample "raw diesel_1".

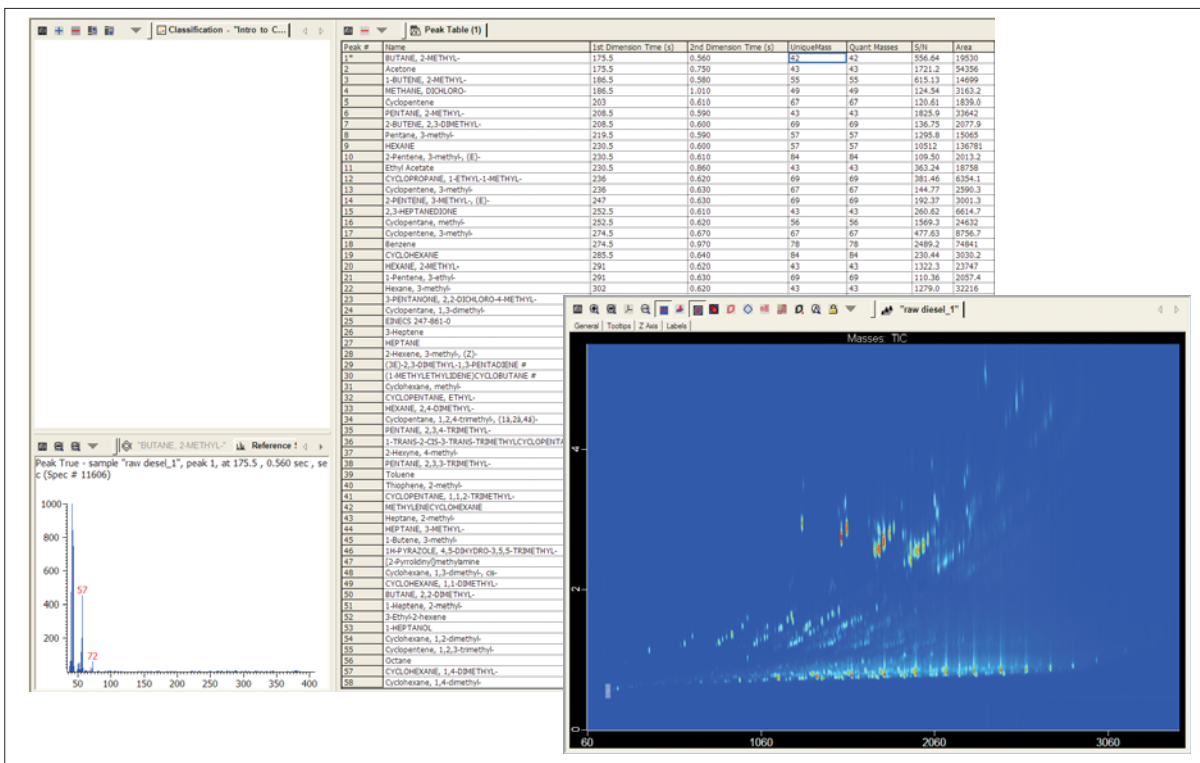


Figure 5: The windows from Figure 3 populated with the data from sample "raw diesel_1".

At this point, the Classification is set-up and ready for the analyst to begin adding Classes. The first step is to add a "blank" Class. To add a new Class, the analyst can either right-click in the Classification window and select "Add", or click on the blue "+" in the top left corner of the Classification Window. Figure 6 shows the addition of a new Class by using the blue plus sign. The first Class created will be for the C3-substituted benzenes.

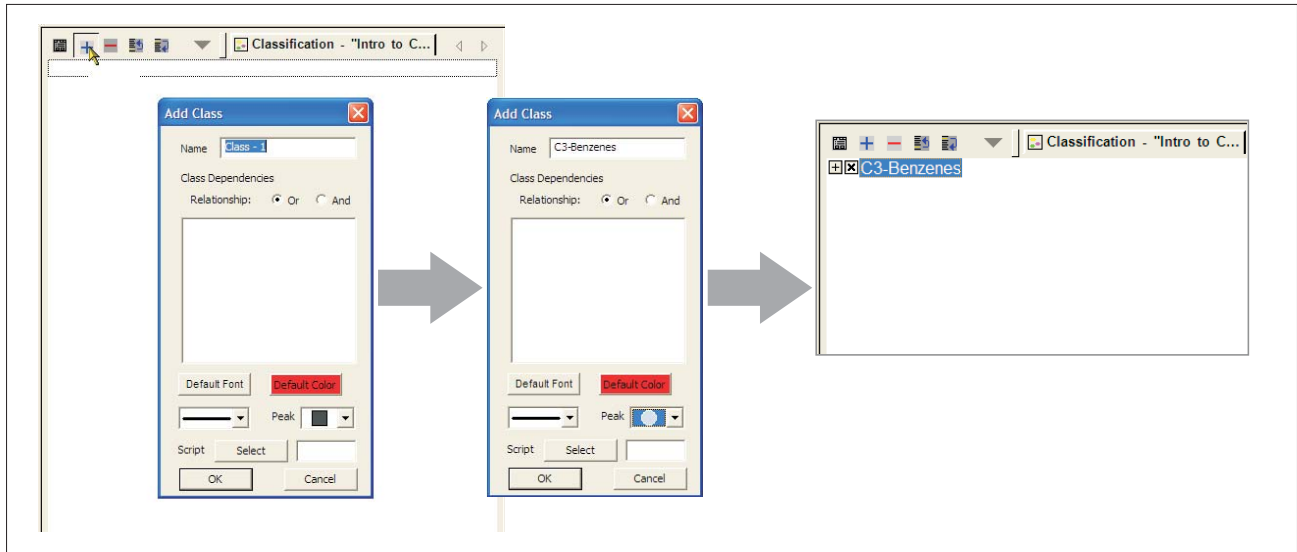


Figure 6: The step-by-step directions for creating a new Classification Region for the C3-substituted benzenes and utilizing circular red Peak Markers.

The "Add Class" window appears and contains entries for the name of the new Class, the color that will be used to identify the new Class, the style and color of Peak Marker to be used for the new Class, and an entry for a Script to be applied to the new Class. The use of Scripts will not be covered in this work.

The next step is to make sure that the "View Classification Regions" is enabled. It is located at the top of the 3D Image. Figure 7 shows the View Classification Regions in the enabled position. Toggling of this button will alternate between showing and hiding Classification Regions.

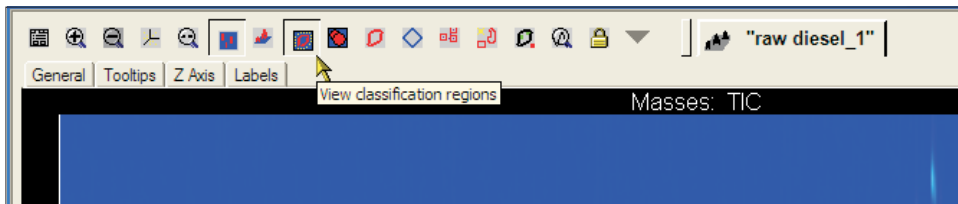


Figure 7: The top of the 3D Image showing "View Classification Regions" enabled.

Defining the boundaries of a Classification Region is a manual process. It is entirely up to the analyst to decide the placement, orientation and overall shape of the Classification Region. The first step in establishing the Classification Region is for the analyst to identify the grouping of the related peaks which will comprise the Classification. Figure 8 shows a zoomed-in view of the area of the chromatogram where the C3-substituted benzenes are located. The orange-dashed line highlights the "band" formed by this group of compounds in the Contour Plot.

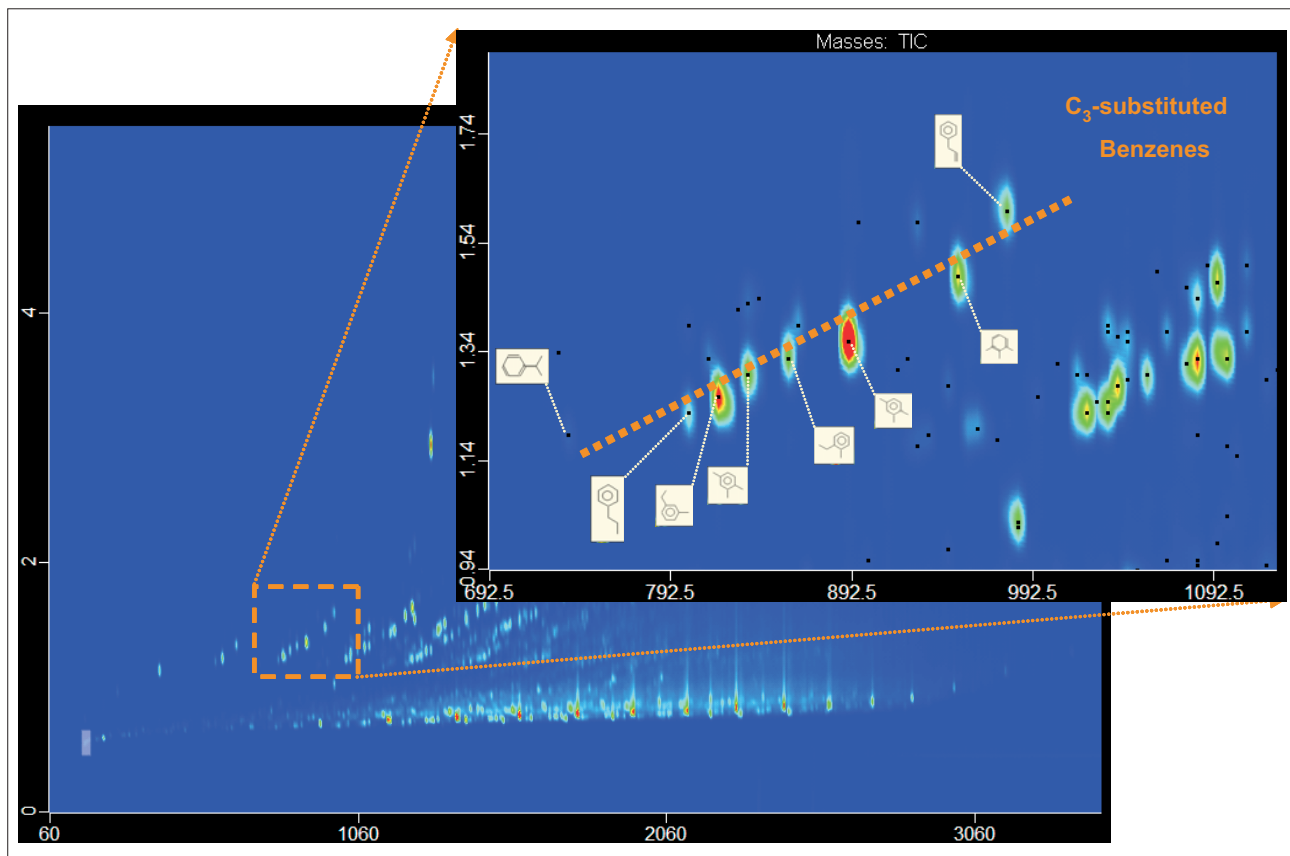


Figure 8: A zoomed-in view of the area of the chromatogram where the C₃-substituted benzenes are located. The orange-dashed line highlights the "band" formed by this group of compounds in the Contour Plot.

The two styles of Classification Region are Curved Regions and Polygonal Regions. To draw or edit a region, the appropriate Edit Region button must be enabled. The buttons are found at the top of the 3D Image window and are shown in Figure 9.

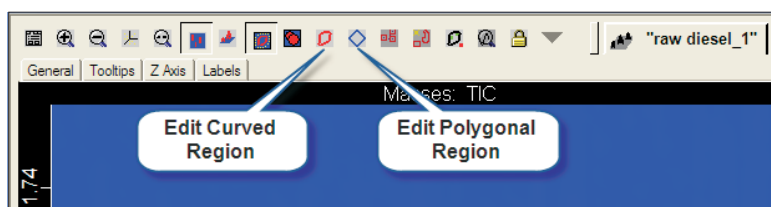


Figure 9: The top bar of the 3D Image window with the Edit Curved Region and Edit Polygonal Region buttons highlighted.

In this first example, a Curved Region will be created for the C₃-substituted benzenes. The Contour Plot is zoomed-in to the area where the Classification Region will be drawn and the Edit Curved Regions button is enabled (see Figure 10). Next, the Class that the region will be drawn for is highlighted in the Classification Window (see Figure 11). If the Class is not highlighted, the Classification Region will be labeled as "Unassigned".

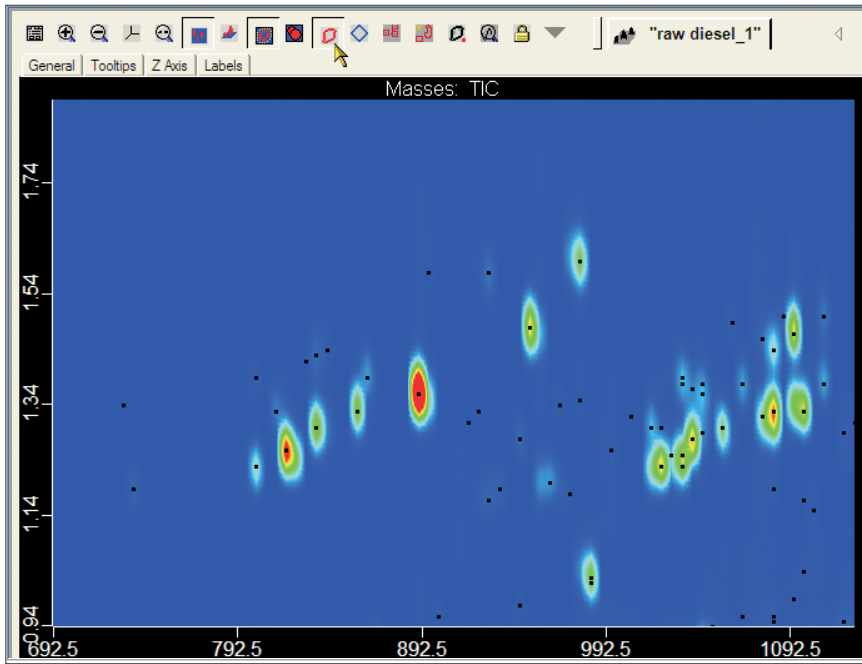


Figure 10: The Contour Plot is zoomed-in to the area where the Classification Region will be drawn and the Edit Curved Regions button is enabled.

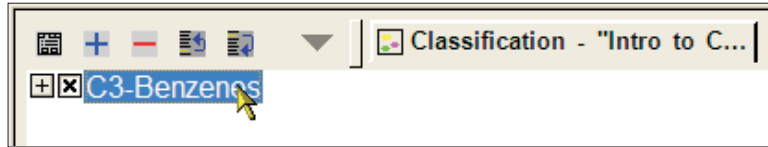


Figure 11: The Class that the region will be drawn for is highlighted in the Classification Window.

The drawing of the curved region will start with the creation of a line, similar to the dashed-orange line in Figure 8, drawn along the axis of the band. The line will serve as the long axis of the ellipse-shaped curved region. The line is drawn by holding the left mouse button down, in the 3D Image, at the point where the line should start (see Figure 12A), followed by releasing the left mouse button at the point where the line should end (see Figure 12B). When the left mouse button is released, the line should be visible. As the cursor is moved down, the ellipse will expand perpendicular to the line and as the cursor is moved up, the ellipse will contract perpendicular to the line (see Figure 12C). When the size of the ellipse is approximately that desired by the analyst, a single left-click will fix the size of the ellipse (see Figure 12D).

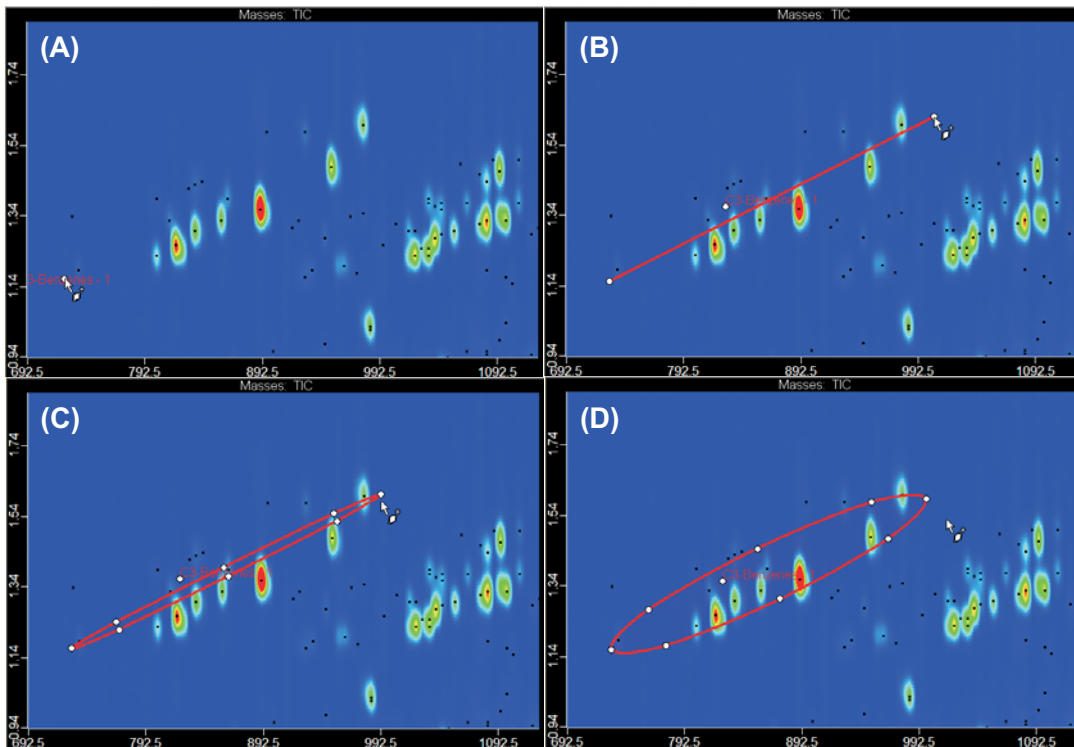


Figure 12: An example of the four step process to create a Curved Classification Region.

Any peak whose Peak Marker falls inside of the Classification Region will now be assigned to that Class. In Figure 13, it can be observed that two peaks, which were not identified as C₃-substituted benzenes in Figure 8, have been inaccurately assigned to the C₃-Benzenes Class and one peak, which was identified as a C₃-substituted benzene in Figure 8, has been missed. It is possible to fine tune the shape of the Classification Region to exclude the false inclusions and include the missed peak. When Edit Curved Regions is enabled and the Class is selected, the Classification Region will have white editing marks around it (see Figure 14A). By left-clicking on an editing mark, it is possible to drag it to a new location, thereby modifying the shape of the Classification Region (see Figure 14B and 14C). Figure 14D shows the Classification Region for C₃-Benzenes modified to exclude the false positives and include the missed peak. To add additional editing marks, left-click on the outline of the Classification Region and an editing mark will be placed in that position on the Classification Region (see Figure 15).

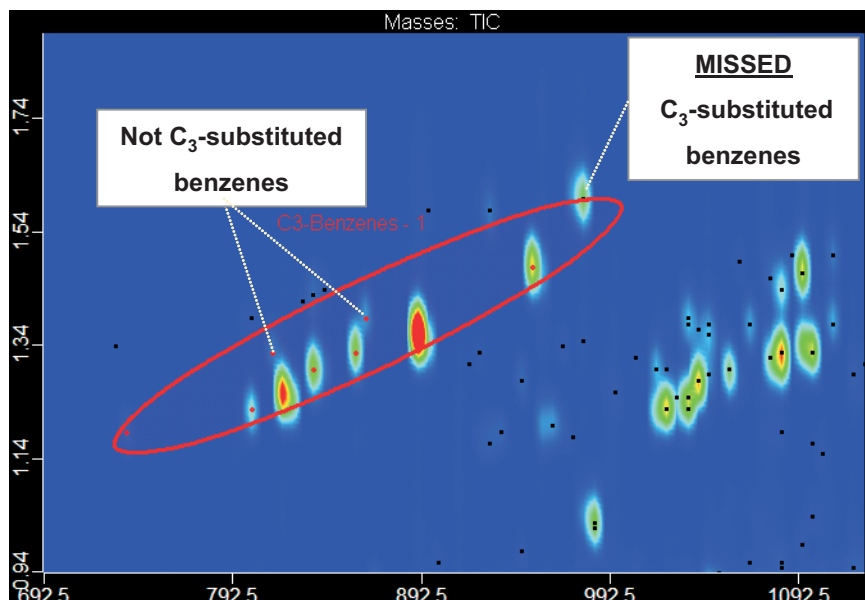


Figure 13: The Classification Region for C₃-Benzenes showing two false positives and a missed peak.

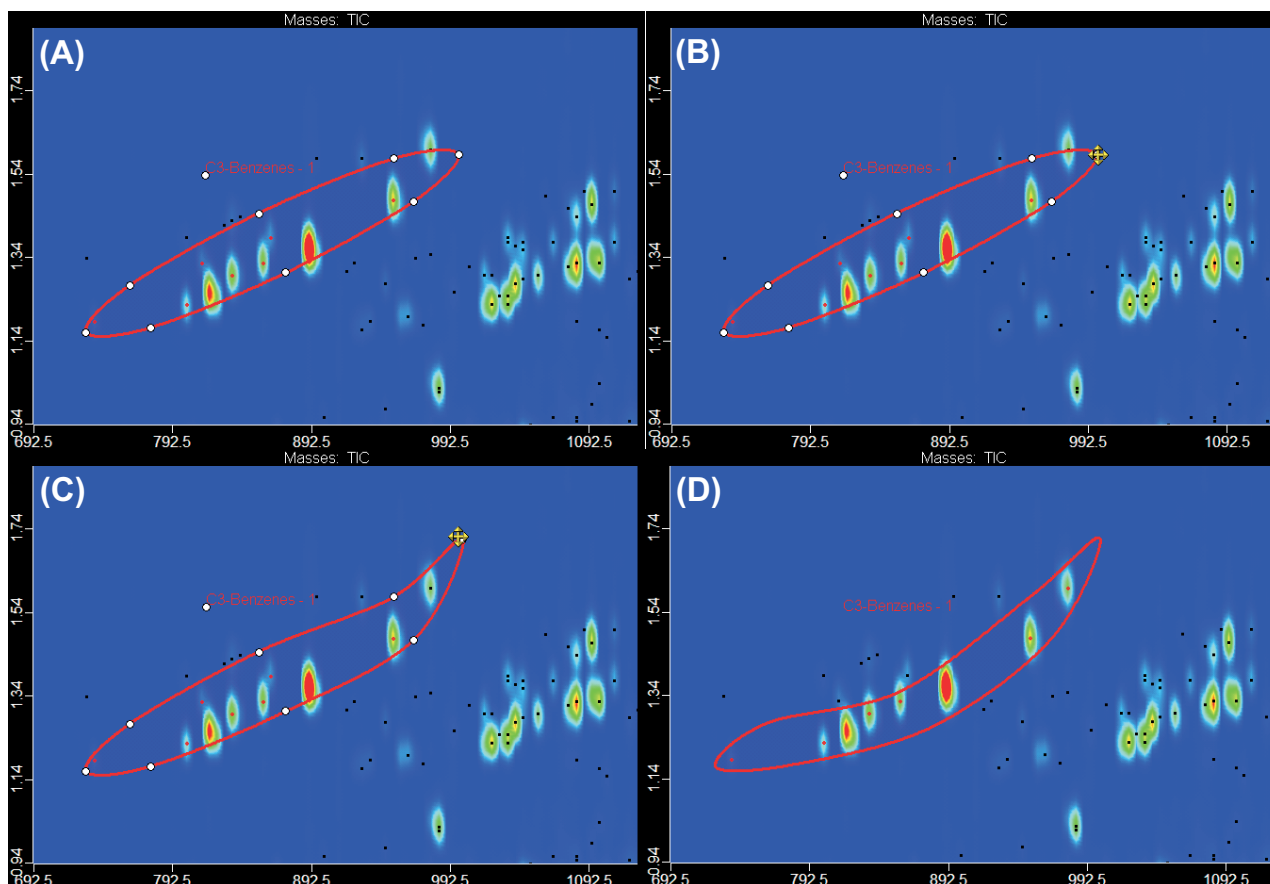


Figure 14: Modification of the Classification Region for C₃-Benzenes to exclude the false positives and include the missed peak.

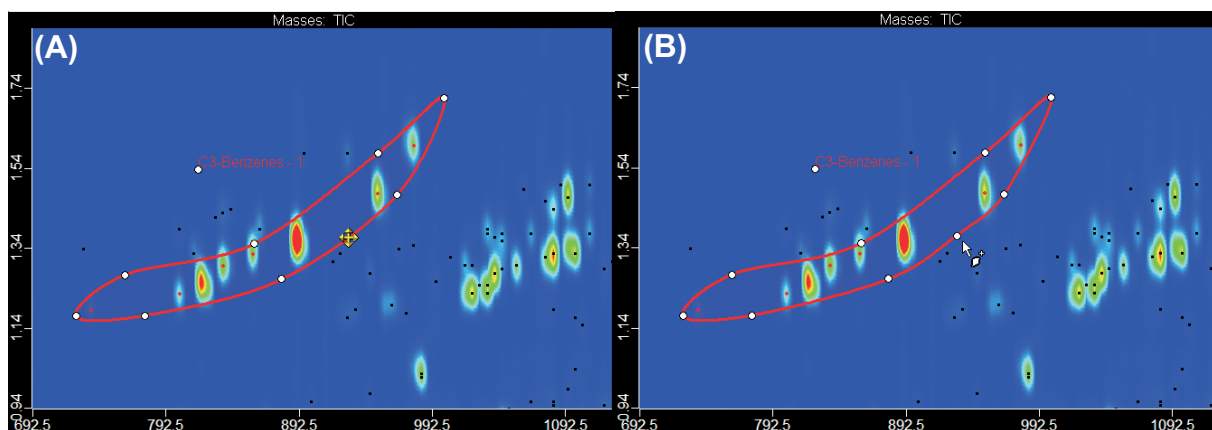


Figure 15: An example showing the addition of an editing mark. To add additional editing marks, left-click on the outline of the Classification Region (A) and an editing mark will be placed in that position on the Classification Region (B).

It is also possible to draw multiple Classification Regions for a single class. To create additional Classification Regions for a Class, highlight the Class in the Classification Window and repeat the steps for creating a Classification Region as shown in Figure 12. Figure 16 shows the addition of Classes for C4-substituted benzenes and Thiophenes. The Thiophene Class has two distinct Classification Regions, Thiophenes-1 and Thiophenes-2.

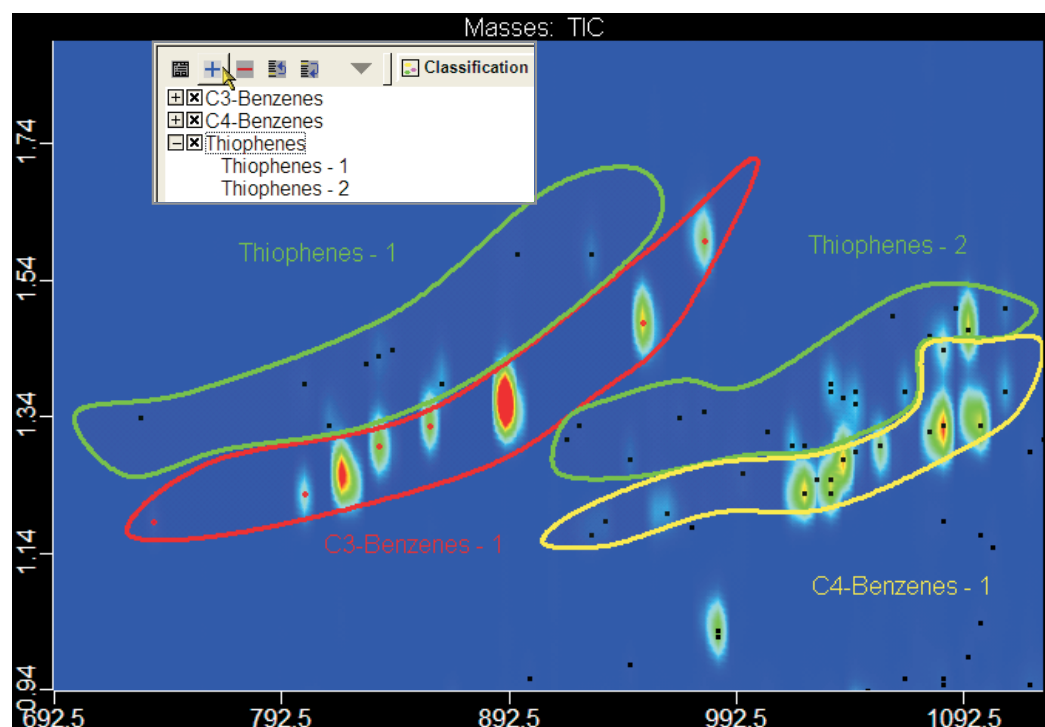


Figure 16: An example of two Classes with single Classification Regions and a single Class with two Classification Regions.

When the Classification Regions have been configured as desired, the Classification can be applied to the standard. To apply the Classification to the standard, press the "Classify the sample's peaks" button in the top toolbar of the 3D Image. When the Classification is applied, the Peak Markers of all of the peaks whose Peak Markers fall within a Classification Region are changed to the specifications made when the Class was created (see Figure 17). In a Contour Plot with multiple Classification Regions, it can become very cluttered. It is possible to hide the Classification Regions by selecting the "View Classification Regions" button in the top toolbar of the 3D Image. Toggling this button will alternate between showing and hiding the Classification Regions. The color coded Peak Markers remain. An example of the region shown in Figure 17, with the Classification Regions hidden, is shown in Figure 18A. That region is highlighted in the full Contour Plot in Figure 18B.

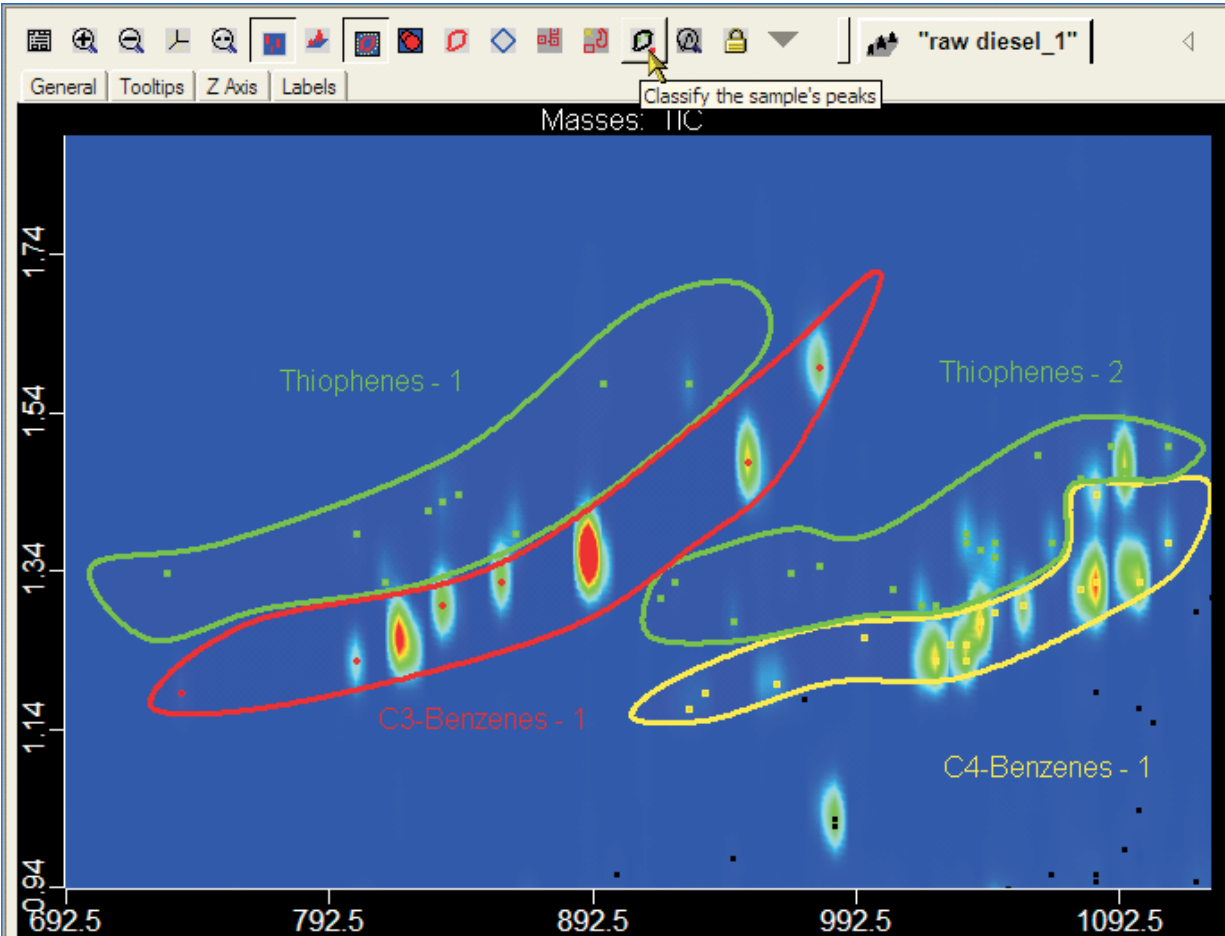


Figure 17: An example showing the result of applying the Classification to the standard. Note that the Peak Markers within a Classification Region have changed color to match that of the Classification Region.

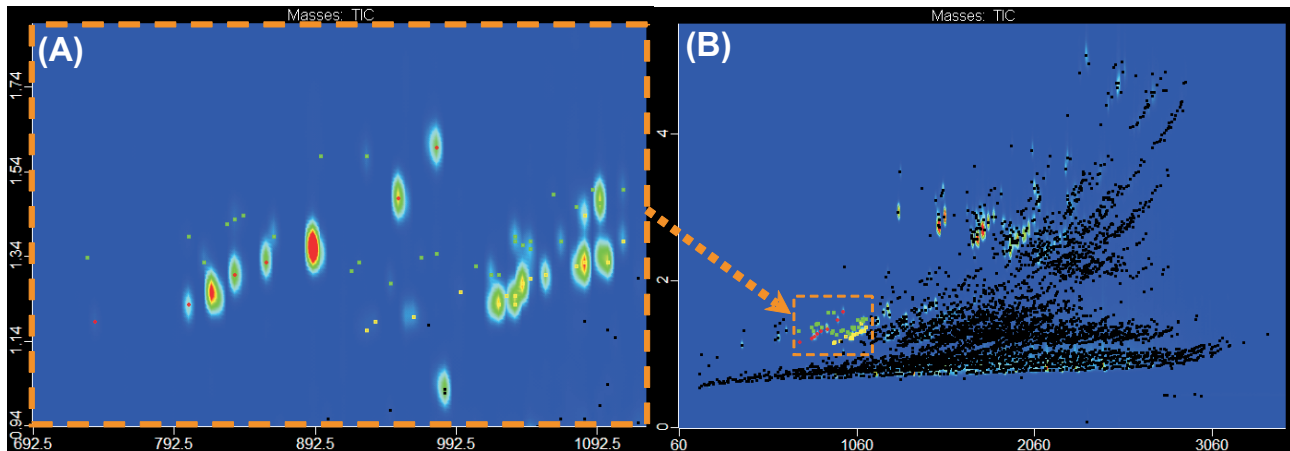


Figure 18: An example of the region shown in Figure 17, with the Classification Regions hidden (A) and that region highlighted in the full Contour Plot (B).

The second style of Classification Region is the Polygonal Classification Region. The drawing of the polygonal region begins directly with the outline of the region, unlike the process for creating a curved region. First, select the "Edit Polygonal Regions" button at the top of the toolbar in the 3D Image and then the Class that the region will be associated with must be highlighted (see Figure 19).

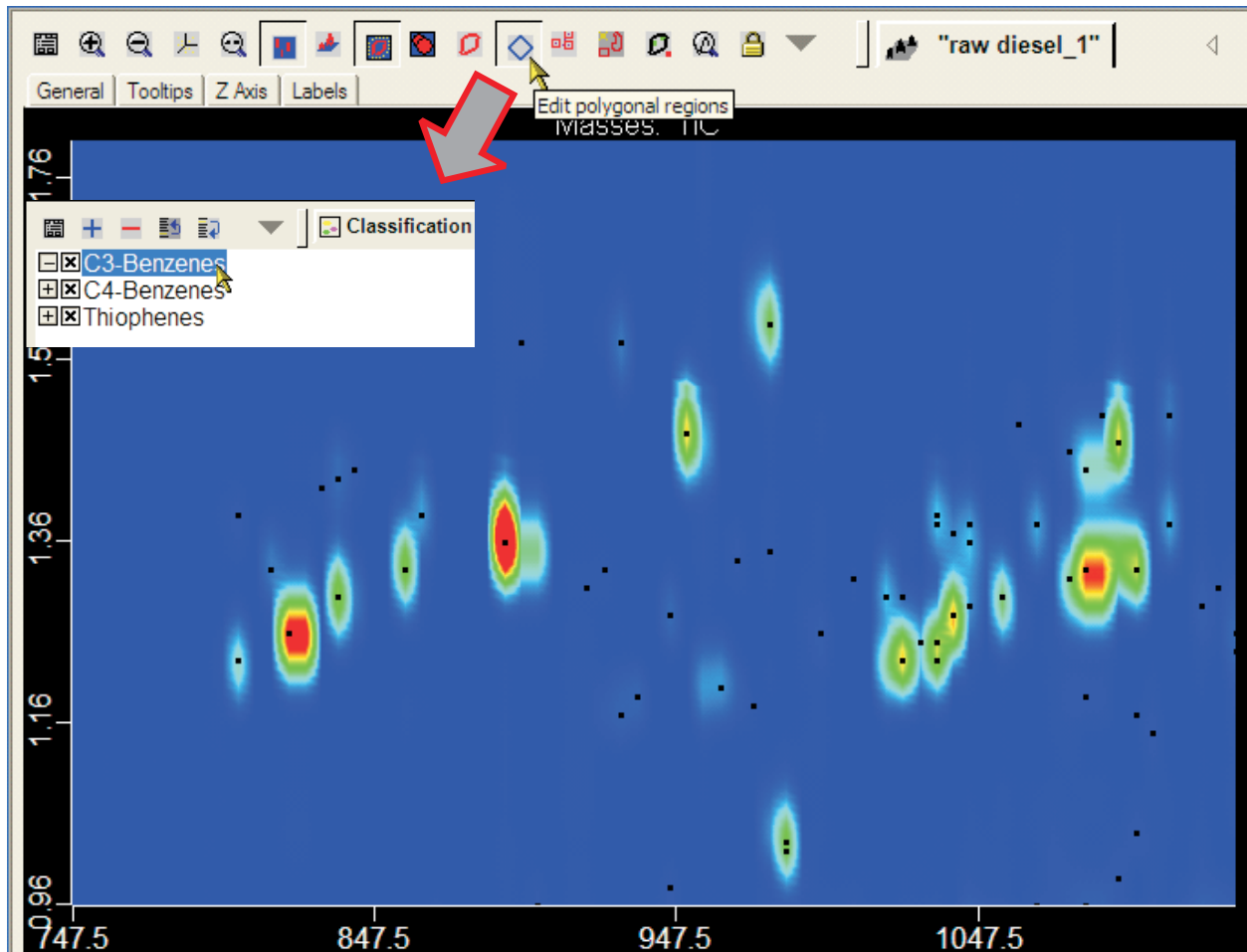


Figure 19: The Contour Plot is zoomed-in to the area where the Classification Region will be drawn and the Edit Polygonal Regions button is enabled.

Begin defining the outline of the region by holding the left mouse button down at the point where the outline should start. Then move the cursor to the next point in the outline and release the left mouse button. At this point, the Classification Region will resemble a line with an editing point at each end (see Figure 20A). Continue to the next desired point in the outline and left-click. This will place another editing point and a line will continue from that point back to the origin, forming a triangle (see Figure 20B). The addition of each new editing point will add another side to the polygon with the boundary continuing from the last editing point to the origin (see Figure 20C). To complete the definition of the Polygonal Classification Region, left-click on the first editing point at the origin (see Figure 20D). The Classification is then applied to the standard in the same way as it was with the Curved Classification Region.

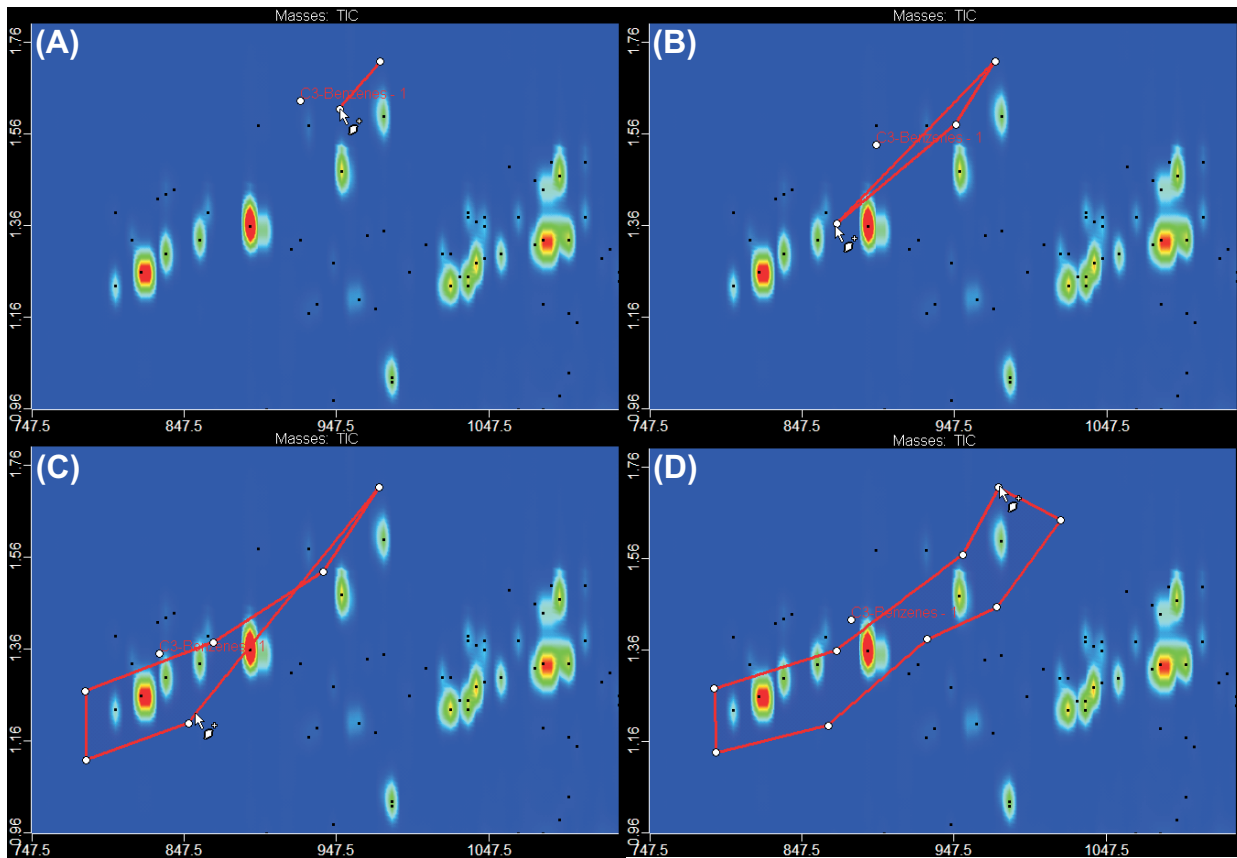


Figure 20: An example showing the creation of a Polygonal Classification Region.

When the Classification is applied to the sample, besides modifying the Peak Markers, it also assigns the entries in the Peak Table to a Class. To view this information, the Classifications column must be set to "show" in the columns tab in properties of the Peak Table. If the Peak Marker falls inside of a Classification Region, it is assigned to the Class associated with that region. If the peak does not fall inside of a Classification Region, the entry for that peak is left blank. Figure 21 shows a section of the Peak Table for the standard and Classifications used in Figure 17.

The peaks may be sorted by their Classifications. This gives the analyst the ability to effectively filter a large number of peaks into manageable sections. In the example's Peak Table, more than 4100 peaks are present. To sort by Classifications, highlight the Classifications column and right-click, then select sort. This will sort the Peak Table and group peaks with the same Classification together. An example is shown in Figure 22.

Peak #	Name	Classifications	R.T. (s)	UniqueMas	Quant Mas	S/N	Area
139	PENTALENE, OCTAHYDRO-		802.5, 0.840	82	82	186.14	7969.4
140	3,5-Octadien-2-one, (E,E)-		802.5, 0.860	39	39	116.95	9699.4
141	Benzene, propyl-	C3-Benzenes	802.5, 1.230	91	91	5826.2	191382
142	Thiophene, 2-propyl-	Thiophenes	802.5, 1.390	97	97	550.02	19591
143	HEPTANE, 3-ETHYL-2-METHYL-		808, 0.700	57	57	1600.2	45325
144	ETHYLPROPYLCYCLOPENTANE		808, 0.730	69	69	438.82	43672
145	Camphene		808, 0.880	93	93	817.65	27192
146	1,1,2,3-TETRAMETHYLCYCLOHEXANE		813.5, 0.750	69	69	344.82	10355
147	(S,E)-3-METHYL-2-METHYLENE-4-HEXENAL		813.5, 0.800	109	109	108.20	2682.8
148	Thiophene, 2-(1-methylethyl)-	Thiophenes	813.5, 1.330	111	111	1409.8	40928
149	CYCLOBUTANE, 1,2-DIETHYL-, TRANS-		819, 0.740	56	56	179.87	5029.0
150	4-OCTENE, 2,6-DIMETHYL-, [S-(Z)]-		819, 0.760	69	69	437.30	13016
151	Unknown 10		819, 0.780	109	109	53.285	1172.1
152	Unknown 11		819, 0.790	95	95	113.94	3613.7
153	1H-Indene, octahydro-, trans-		819, 0.850	82	82	125.30	4436.2
154	Benzene, 1-ethyl-3-methyl-	C3-Benzenes	819, 1.260	105	105	19811	753003
155	1-DECENE		824.5, 0.750	57	57	430.72	8360.8
156	1-HEXENE, 5-METHYL-		830, 0.770	56	56	799.02	23552
157	2,2,5,5-TETRAMETHYL-3-HEXENE		830, 0.780	69	69	1506.7	48164
158	Cyclohexene, 1-propyl-		830, 0.850	81	81	133.66	4272.8
159	2-ETHYL-5-METHYLTHIOPHENE #	Thiophenes	830, 1.420	111	111	229.70	6233.1
160	DECANE, 5-METHYL-		835.5, 0.700	57	57	953.27	18014
161	1-HEXENE, 3-METHYL-		835.5, 0.750	69	69	420.28	13009
162	TOSYLATE OF 2,2-DIMETHYL-5-HEXEN-1-OL		835.5, 0.760	111	111	135.70	2649.1
163	4-Ethyl-2-hexynal		835.5, 0.790	67	67	165.67	5849.2
164	Benzene, 1,2,4-trimethyl-	C3-Benzenes	835.5, 1.300	105	105	9318.5	305218
165	Thiophene, 2-(1-methylethyl)-	Thiophenes	835.5, 1.430	111	111	1038.2	31790
166	CYCLOHEXANE, 2-ETHYL-1,3-DIMETHYL-		841, 0.760	69	69	729.34	18737
167	2-HEXYNAL, 4-ETHYL-		841, 0.780	96	96	117.18	2945.1
168	CYCLOPROPANE, 1-METHYL-2-(1-METHYLETHYL)-3-(1-M		841, 0.840	82	82	290.90	6833.6
169	Thiophene, 2-(1-methylethyl)-	Thiophenes	841, 1.440	111	111	309.54	9774.2
170	3-NONENE, 2-METHYL-		846.5, 0.760	69	69	580.59	28246
171	Unknown 12		846.5, 0.770	111	111	273.57	5125.1
172	1,5-DIMETHYLCYCLOHEXENE-5-CARBOXALDEHYDE		846.5, 0.780	109	109	113.37	2494.5

Figure 21: An example of a Peak Table for a sample that has had Classifications applied to it.

Peak #	Name	Classifications	S/N	Area
139*	PENTALENE, OCTAHYDRO-		186.14	7969.4
140	3,5-Octadien-2-one, (E,E)-		116.95	9699.4
141	Benzene, propyl-	C3-Benzenes	5826.2	191382
142	Thiophene, 2-propyl-	Thiophenes	550.02	19591
143	HEPTANE, 3-ETHYL-2-METHYL-		1600.2	45325
144	ETHYLPROPYLCYCLOPENTANE		438.82	43672
145	Camphene		817.65	27192
146	1,1,2,3-TETRAMETHYLCYCLOHEXANE		344.82	10355
147	(S,E)-3-METHYL-2-METHYLENE-4-HEXENAL		108.20	2682.8
148	Thiophene, 2-(1-methylethyl)-	Thiophenes	1409.8	40928
149	CYCLOBUTANE, 1,2-DIETHYL-, TRANS-		179.87	5029.0
150	4-OCTENE, 2,6-DIMETHYL-, [S-(Z)]-		437.30	13016
151	Unknown 10		53.285	1172.1
152	Unknown 11		113.94	3613.7
153	1H-Indene, octahydro-, trans-		125.30	4436.2
154	Benzene, 1-ethyl-3-methyl-	C3-Benzenes	19811	753003
155	1-DECENE		430.72	8360.8
156	1-HEXENE, 5-METHYL-		799.02	23552
157	2,2,5,5-TETRAMETHYL-3-HEXENE		1506.7	48164
158	Cyclohexene, 1-propyl-		133.66	4272.8
159	2-ETHYL-5-METHYLTHIOPHENE #	Thiophenes	229.70	6233.1
160	DECANE, 5-METHYL-		953.27	18014
161	1-HEXENE, 3-METHYL-		420.28	13009
162	TOSYLATE OF 2,2-DIMETHYL-5-HEXEN-1-OL		135.70	2649.1
163	4-Ethyl-2-hexynal		165.67	5849.2
164	Benzene, 1,2,4-trimethyl-	C3-Benzenes	9318.5	305218
165	Thiophene, 2-(1-methylethyl)-	Thiophenes	1038.2	31790
166	CYCLOHEXANE, 2-ETHYL-1,3-DIMETHYL-		729.34	18737
167	2-HEXYNAL, 4-ETHYL-		117.18	2945.1
168	CYCLOPROPANE, 1-METHYL-2-(1-METHYLETHYL)-3-(1-M		290.90	6833.6
169	Thiophene, 2-(1-methylethyl)-	Thiophenes	309.54	9774.2
170	3-NONENE, 2-METHYL-		580.59	28246
171	Unknown 12		273.57	5125.1
172	1,5-DIMETHYLCYCLOHEXENE-5-CARBOXALDEHYDE		113.37	2494.5

Figure 22: An example of how to sort a Peak Table by the Classifications of its peaks.

Classifications are implemented as part of the Data Processing (DP) Method. To add Classifications to the DP Method, go to the Task Selection List at the beginning of the method and make sure there is a check in the box next to Classifications (see Figure 23). At the bottom of the DP Method, add the Classifications to use by clicking on the Add button (see Figure 24).

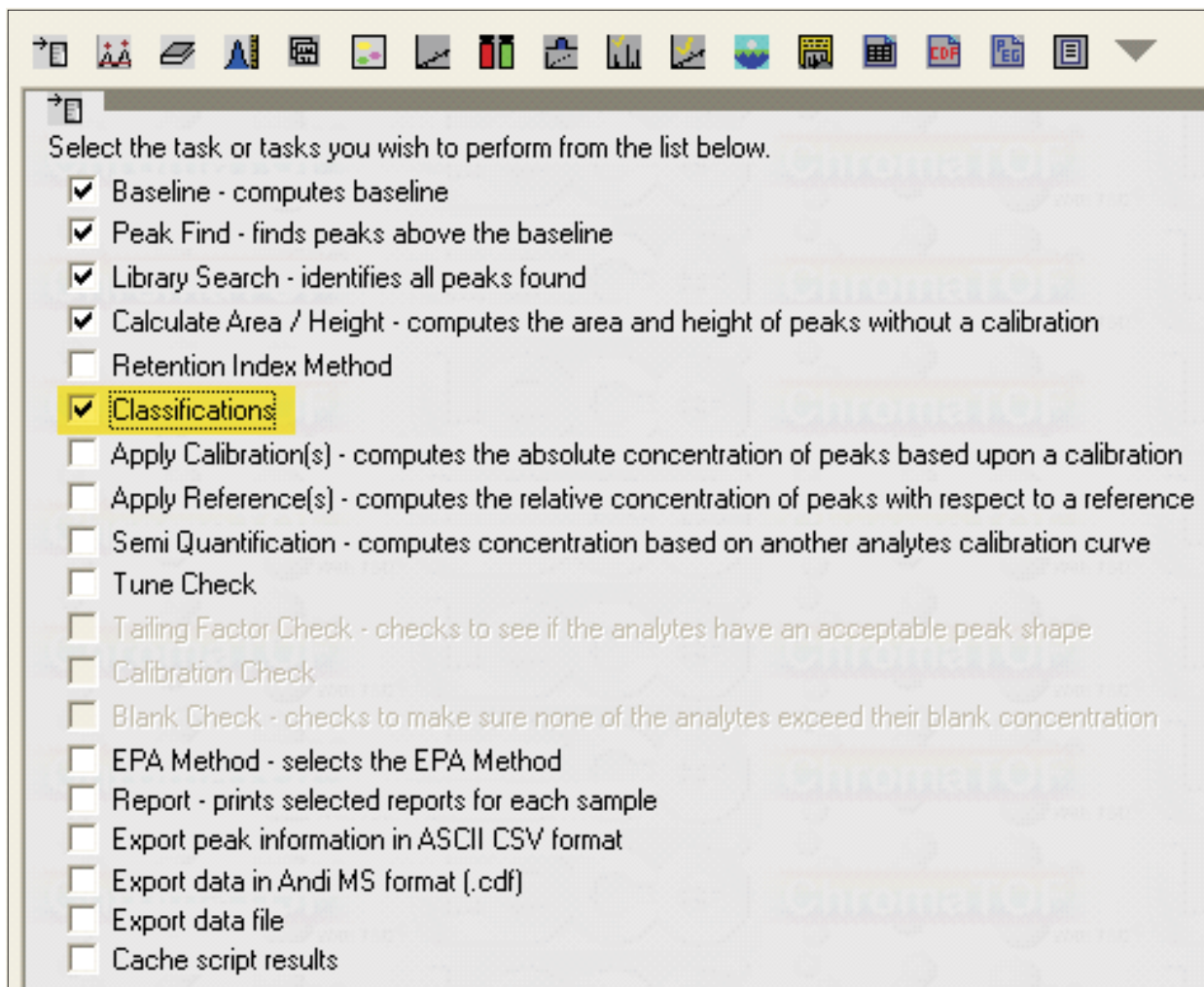


Figure 23: The Task Selection List at the beginning of the DP Method with the check-box enabling Classifications highlighted.

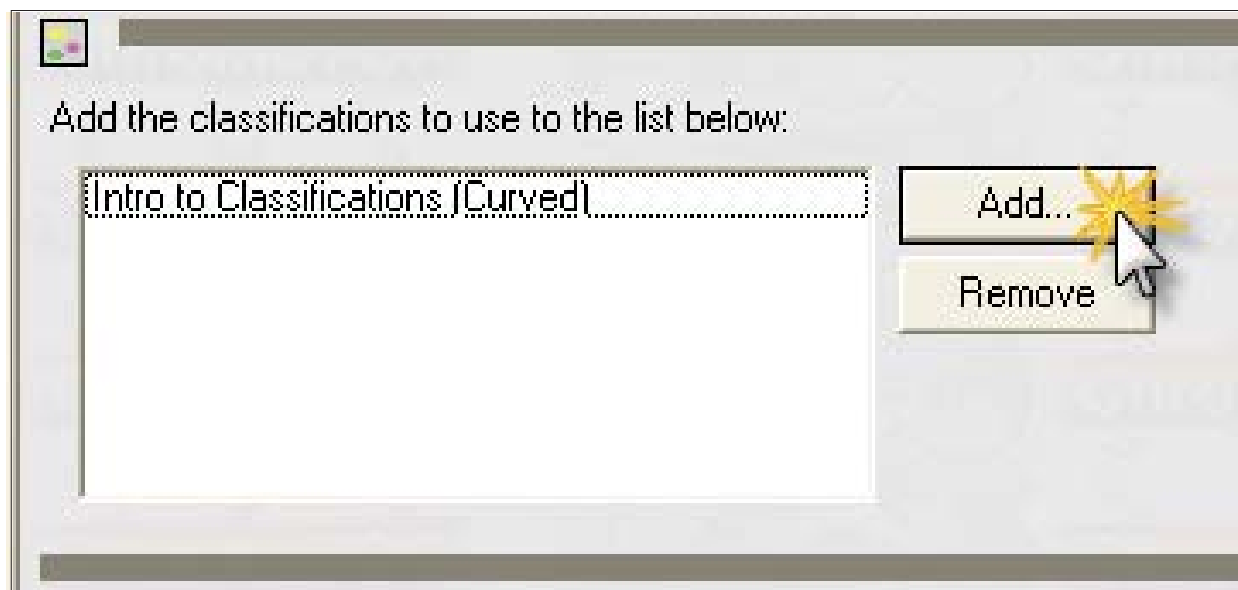


Figure 24: The list of Classifications to be used. It is located at the bottom of the DP Method.

Another application of Classification Regions is the Exclusion Region. When an Exclusion Region is specified, the Data Processing Method does not process peaks in that area. This type of Classification Region is often used to exclude peaks that would result from the solvent and/or column bleed. Exclusion Regions should be created in a separate Classifications file from regular Classifications Regions because they are utilized in a different way. Figure 25 shows the Contour Plot of a petroleum-type sample with 4215 peaks. The regions for the solvent and column bleed are drawn in the same way as regular Classification Regions (see Figure 26). To change the Classification Region to an Exclusion Region, double-click inside of the region's boundaries. The area of the region will become filled with a cross-hatched pattern, indicating that it is now an Exclusion Region (see Figure 27). To implement the Exclusion Regions, go to the GCxGC Parameters section of the DP Method and select "Filter Peaks by Classification" (see Figure 28). When the sample is data processed with the Exclusion Regions, the exclusion of solvent and column bleed peaks reduces the number of peaks in the Peak Table from 4215 to 3281 (see Figure 29). By filtering the Peak Table in this way, the peaks not associated with the actual sample can be excluded, thereby reducing the amount and increasing the relevancy of information the analyst must work up.

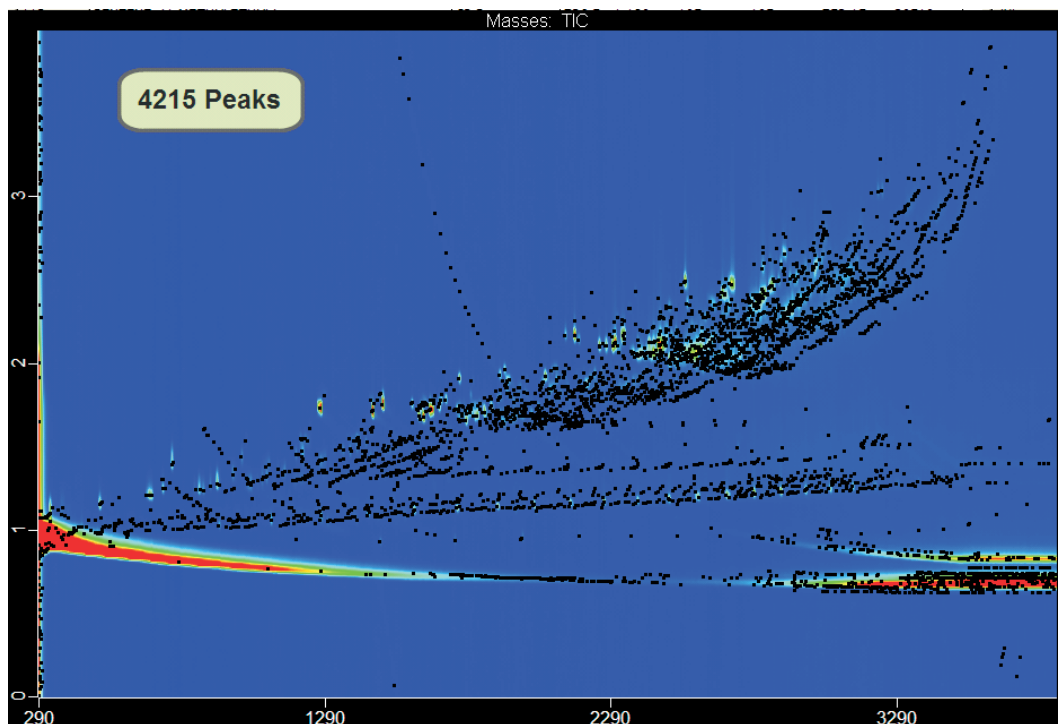


Figure 25: The Contour Plot of a petroleum-type sample with 4215 peaks.

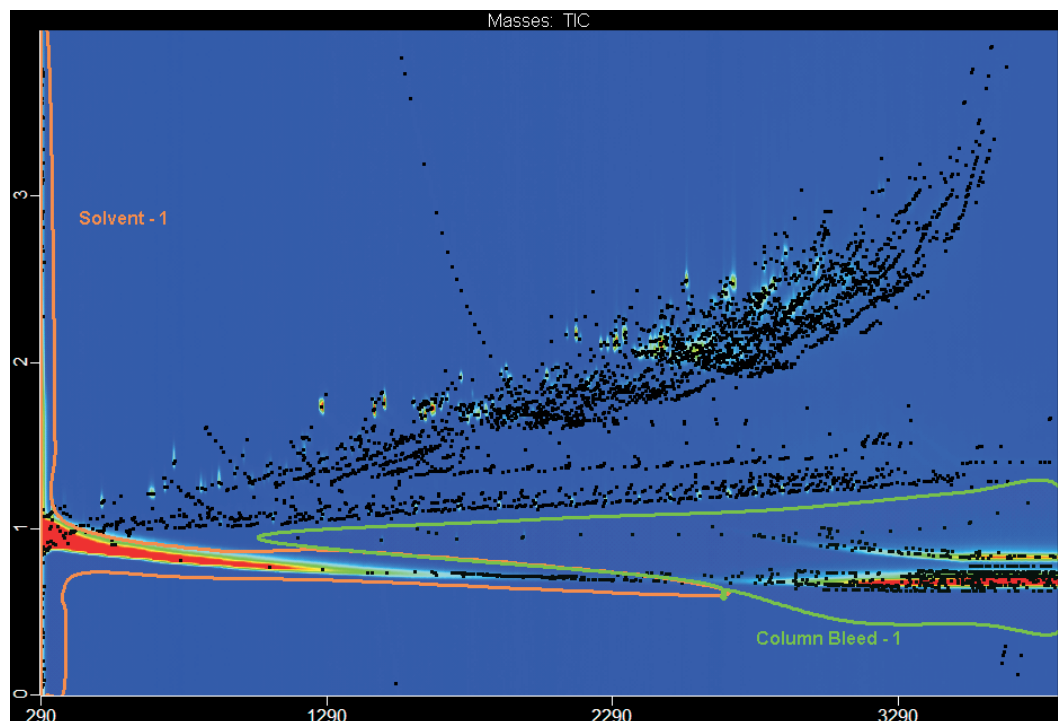


Figure 26: The regions for the solvent and column bleed are drawn in the same way as regular Classification Regions.

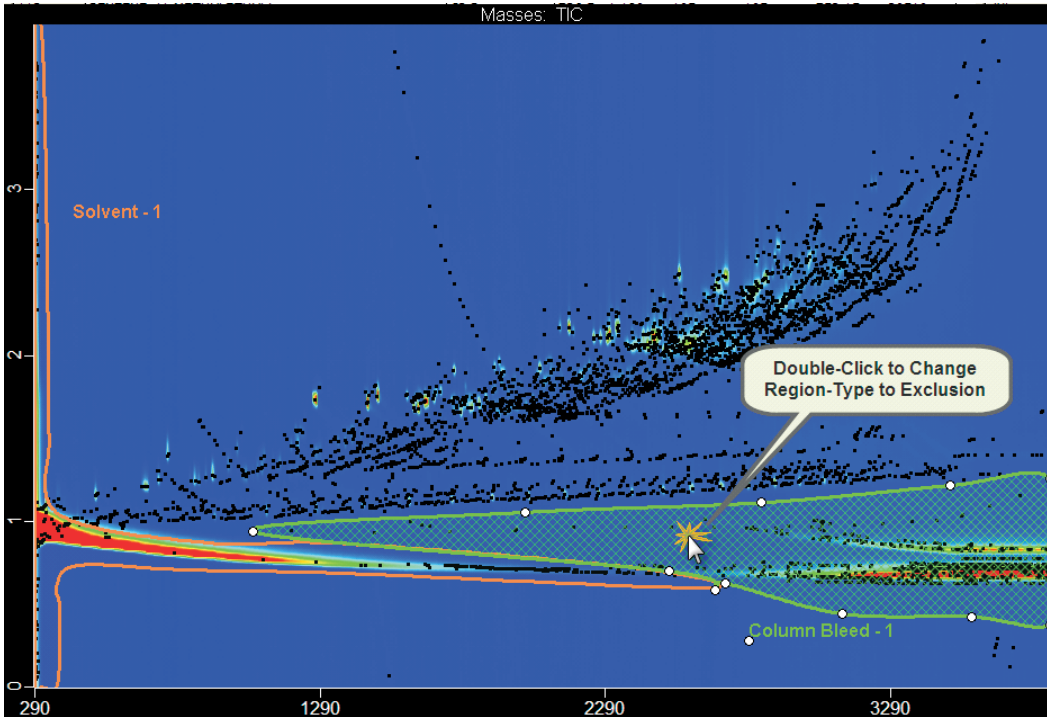


Figure 27: Converting the Classification Regions to Exclusion Regions.

GCxGC Parameters

Match Required to combine:

Override the allowed second dimension R.T shift for combine

Early

Late

Enter the peak width in seconds below (first dimension):

Peak widths broaden throughout the chromatographic run

Peak Width	Retention Time
<input type="text" value="16"/>	<input type="text"/>
<input type="text"/>	<input type="text"/>

Subpeak Settings

Minimum S/N: Enter the minimum required S/N for the subpeak to be retained.

Integration Approach:

Traditional

Adaptive

Filter peaks by classification

Exclusion	<input type="button" value="Add"/>
 	<input type="button" value="Remove"/>

Figure 28: An example of the GCxGC Parameters section of the DP Method. This is where Exclusion Regions are implemented by utilizing the "Filter Peaks by Classification" feature.

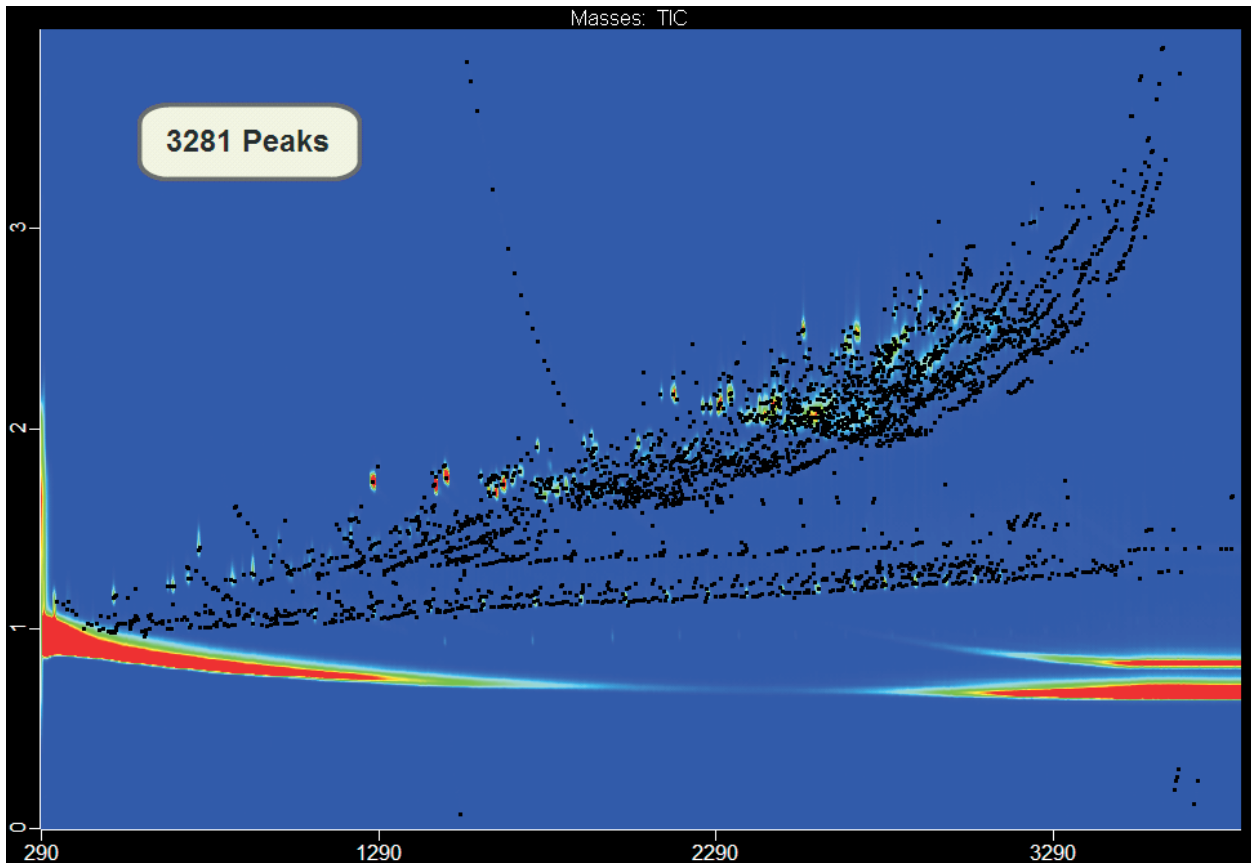


Figure 29: The sample after having been filtered using Exclusion Regions. The exclusion of solvent and column bleed peaks reduces the number of peaks in the Peak Table from 4215 to 3281.

Another feature of Classifications is the Classifications Summary. The Classifications Summary allows for the comparison of the contributions of the various Classes to each other or the entire sample. To utilize Classification Summaries, two tabs are opened in Classifications. They are Classifications Summary Configuration and Classifications Summary View. Figure 30 shows these tabs and the location of the buttons used to open them.

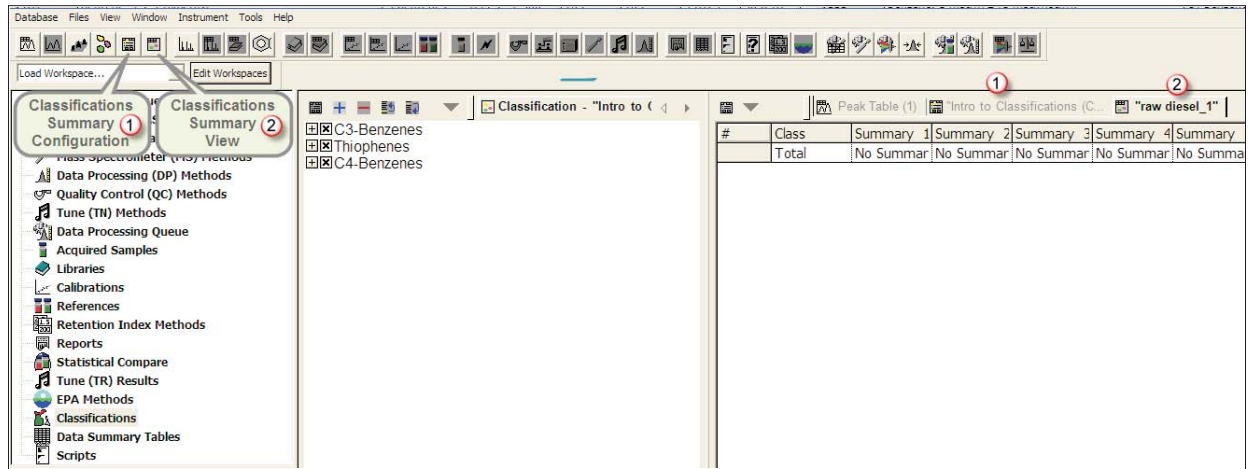


Figure 30: Classifications with the Classifications Summary Configuration and Classifications Summary View windows open and the buttons used to open them indicated.

Select the Classifications Summary Configuration tab and right-click in the window. From the drop down menu, select Add Summary. A pop-up window will then ask you to assign a name to the Summary. The column for the new Summary will appear to the right of the Class columns in the window. An example showing the addition of a Summary named "Sub-Benzenes in Total" is shown in Figure 31. Figure 32 shows the addition of another Summary named "Sub-Benzenes Composition".

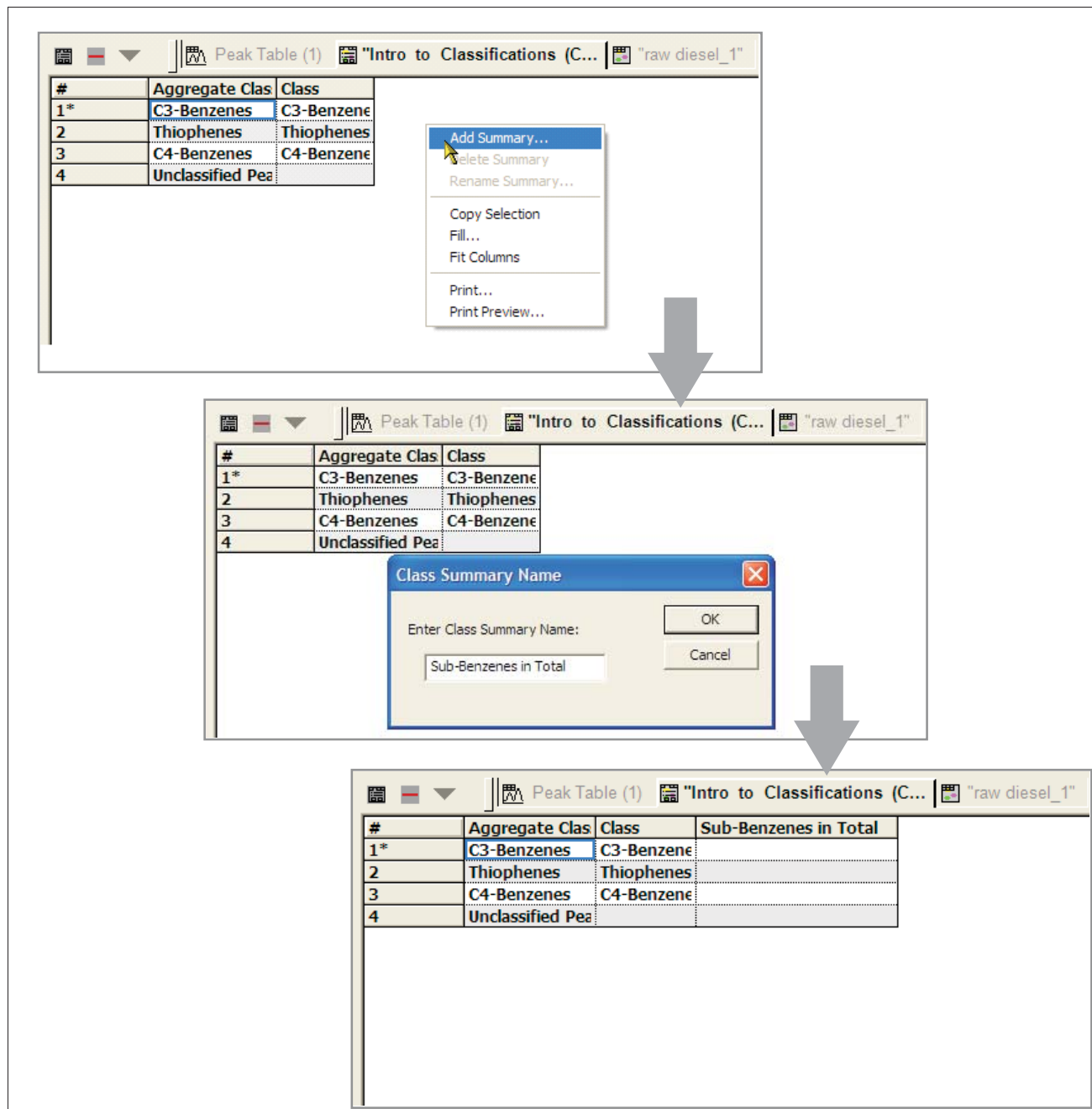


Figure 31: An example showing the addition of a Summary named "Sub-Benzenes in Total".

#	Aggregate Clas	Class	Sub-Benzenes in Total	Sub-Benzenes Composition
1*	C3-Benzenes	C3-Benzene		
2	Thiophenes	Thiophenes		
3	C4-Benzenes	C4-Benzene		
4	Unclassified Pea			

Figure 32: An example showing the addition of a second Summary named "Sub-Benzenes Composition".

The Summary will contain a row for each of the existing Classes, as well as a row for the Class "Unclassified Peaks". This Class will consist of the sum of all of the peaks which are not included in any of the other Classes. The next step is to choose which Classes should be included in the Summary and which Quant Masses should be used in calculating the contribution. Figure 33 shows an example where the contributions of the substituted benzenes are compared to the contributions of all other Classes. This Summary is titled "Sub-Benzenes in Total". The Deconvoluted Total Ion Chromatogram (DTIC) is specified as the Quant Mass.

#	Aggregate Class	Class	Sub-Benzenes in Total	Sub-Benzenes Composition
1*	C3-Benzenes	C3-Benzenes	DTIC	
2	Thiophenes	Thiophenes	DTIC	
3	C4-Benzenes	C4-Benzenes	DTIC	
4	Unclassified Peaks		DTIC	

Figure 33: An example where the contributions of the substituted benzenes are compared to the contributions of all other Classes. This Summary is titled "Sub-Benzenes in Total". The Deconvoluted Total Ion Chromatogram (DTIC) is specified as the Quant Mass.

Figure 34 shows an example where the contributions of each of the individual Classes of substituted benzenes are compared to the total amount of substituted benzenes. This Summary is titled "Sub-Benzenes Composition". The DTIC is specified as the Quant Mass. Quant Masses are only entered for a Class if that Class is to be included in that particular Summary.

#	Aggregate Class	Class	Sub-Benzenes in Total	Sub-Benzenes Composition
1*	C3-Benzenes	C3-Benzenes	DTIC	DTIC
2	Thiophenes	Thiophenes	DTIC	
3	C4-Benzenes	C4-Benzenes	DTIC	DTIC
4	Unclassified Peaks		DTIC	

Figure 34: An example where the contributions of each of the individual Classes of substituted benzenes are compared to the total amount of substituted benzenes. This Summary is titled "Sub-Benzenes Composition". The Deconvoluted Total Ion Chromatogram (DTIC) is specified as the Quant Mass.

To view the Summaries, select the Classifications Summary View tab (see Figure 35).

#	Class	Summary 1	Summary 2	Summary 3	Summary 4	Summary 5
*	Total	No Summar	No Summar	No Summar	No Summar	No Summar

Figure 35: An example of the Classifications Summary View prior to the application of the Classification to the standard.

The Classification must then be applied to the standard in the same way as in Figure 17. The Classifications Summary can be configured to make comparisons of contribution based on peak area, percentage peak area, peak count, or percentage peak count. The default setting is percentage peak area. Figure 36 shows the Classifications Summary View after application of the Classification to the standard.

#	Class	Sub-Benzenes in Total	Sub-Benzenes Composition	Summary 3	Summary 4	Summary 5
1*	C4-Benzenes	0.773	49.457	No Summar	No Summar	No Summar
2	Thiophenes	0.265		No Summar	No Summar	No Summar
3	C3-Benzenes	0.790	50.543	No Summar	No Summar	No Summar
	Unclassified	98.173		No Summar	No Summar	No Summar
	Total	100.000	100.000	No Summar	No Summar	No Summar

Figure 36: The Classifications Summary View after application of the Classification to the standard.

To change the comparison from percentage peak area to percentage peak count for the Sub-Benzenes in Total Summary, right-click and select "Properties". Then select the "Class Summaries Data" tab and select "Peak Count % in each class". Figure 37 shows this process step-by-step.

The figure illustrates the process of changing the comparison type for Class Summaries in three steps:

- Step 1:** The user right-clicks on the 'Sub-Benzenes in Total' column of the table. A context menu appears with options: Copy Selection, Fit Columns, Print Preview..., Print..., and Properties. The 'Properties' option is selected.
- Step 2:** The 'Class Summary' dialog box is open. The 'Class Summary Data' tab is selected. Under 'Data To Display', the radio button for 'Peak Count % in each class' is selected.
- Step 3:** The resulting table shows the 'Sub-Benzenes in Total' values updated to percentages: 0.39, 0.68, 0.19, 98.73, and 100.00.

Figure 37: An example of the step-by-step-process for changing the comparison type for the Class Summaries.

Figure 38 shows the same Summaries compared by Peak Count in each class.

#	Class	Sub-Benzenes in Total	Sub-Benzenes Composition	Summary 3	Summary 4	Summary 5
1	C4-Benzenes	16	16	No Summar	No Summar	No Summar
2	Thiophenes	28		No Summar	No Summar	No Summar
3	C3-Benzenes	8	8	No Summar	No Summar	No Summar
	Unclassified	4051		No Summar	No Summar	No Summar
	Total	4103	24	No Summar	No Summar	No Summar

Figure 38: The same Summaries as in Figure 37 now compared by Peak Count.

Conclusions

Classifications are valuable tools for working with the complex data obtained from GCxGC analyses. They provide the analyst the ability to selectively filter and organize GCxGC Peak Tables and more effectively manage the data. The examples shown in this work are intended to provide an introduction to the implementation and use of the Classifications feature. More advanced features and capabilities are covered in the LECO training class for the Pegasus 4D GCxGC-TOFMS.



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