

Preparing GC Chromatograms from Bruker Workstation for Publication

by:

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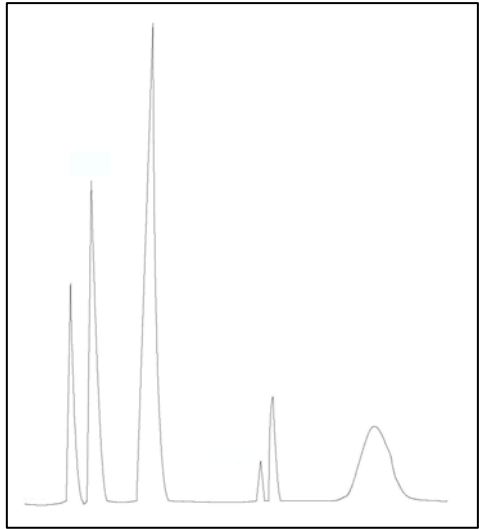
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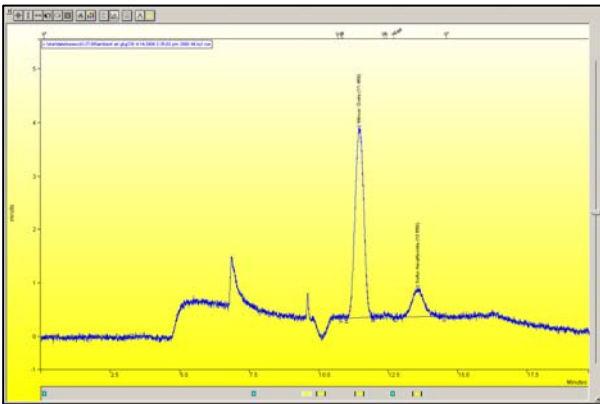
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Display of chromatograms in technical write-ups and presentations helps to better illustrate results from chromatographic experiments through a picture, instead of data in tables or through verbiage. Some attempts to translate chromatograms into a useful electronic form have included hand-tracings, often assisted with a French curve template, but here original peak shapes and noise characteristics are lost or severely distorted. Scanning paper copies or taking “print screens” usually includes extraneous labeling details that detract from the relevant information, and chromatograms cannot be reformatted to accentuate important aspects of the chromatogram.

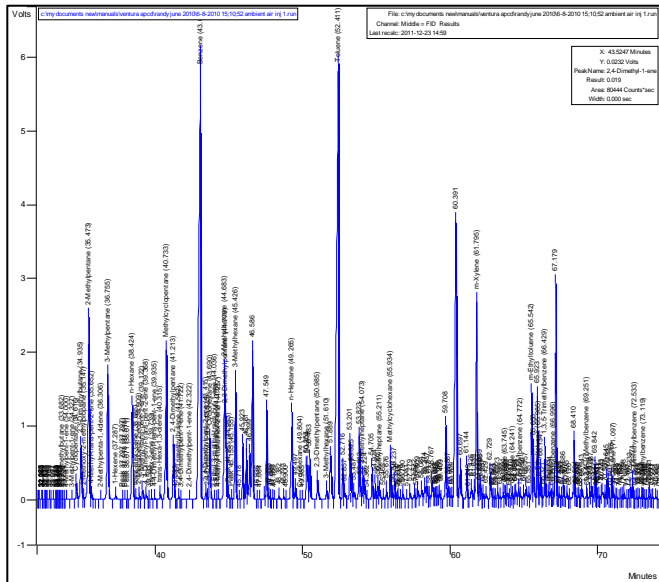


Typical hand-drawn chromatogram with distorted peak shapes and misrepresented noise.

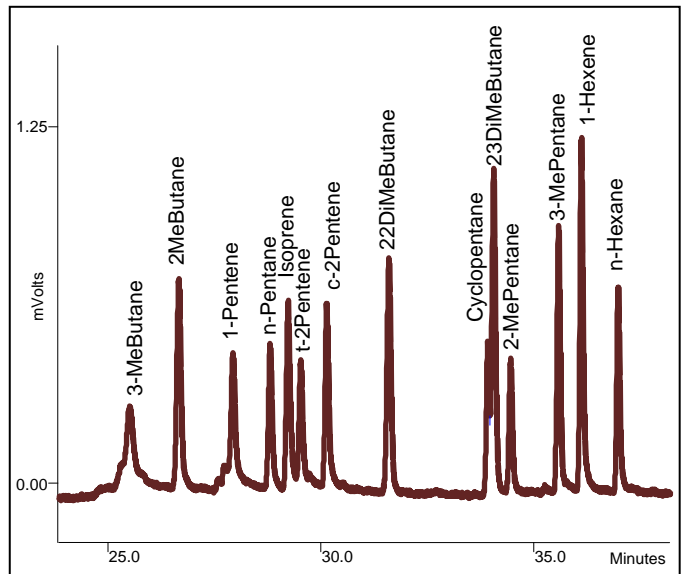


Chromatogram generated from Interactive Graphics with PrtScn key is limited to original formatting.

Bruker Workstation provides an ability to transfer generated chromatograms into Microsoft Windows Metafile formats (.WMF) that then can be readily edited to achieve the desired presentation for insertion into a working document. Without some alterations, a chromatogram occasionally can be overwhelmed with unimportant details that obscure the purpose of the figure. Elements in the figure can be changed or deleted to emphasize the salient points of the chromatogram.



Converting a chromatogram into a Metafile without editing can yield a picture that is inundated with too many details and gives no readability to most of the labeling.



Details in metafiles can be edited with various tools in Microsoft Word to emphasize only the important information, to match with discussions in the associated text.

The following discussions provide several approaches to convert GC .RUN data files from Bruker Workstation into formats that can be readily edited and then inserted into Microsoft Word or PowerPoint. Advantages of each are summarized in Table I.

1. Conversion through Interactive Graphics. This operation offers the most adaptability for generating a concise chromatogram for insertion into a document.

a) Locate target chromatograms and open with Workstation Toolbar → Interactive Graphics → File → New Chromatogram...

b) Adjust time and amplitude intervals for a relevant portion of chromatogram layout and choose preferred trace settings with View → Preferences → Layout and Trace Settings.¹

c) Select Edit → Copy Picture to File... to generate a .WPF file, and name file appropriately.

d) Insert picture .WPF into Word or Power Point document by Insert → Picture.

e) Right click anywhere in the picture and choose Edit Picture and set Drawing Tools Format → Text Wrapping → Square.

f) Right click anywhere in picture and delete highlighted blank object to expose items underneath. This is an empty rectangle that must be removed before access to text boxes.

g) To change color and intensity of chromatogram tracing, highlight all chromatogram data points and right click anywhere in picture to select Format AutoShape... → Colors and Lines and adjust as needed.

h) To change font sizes and orientations of a text box, highlight text box and right click to choose Edit Text. Then right click to select Font and adjust as desired.

i) To take out unnecessary text boxes, highlight and delete.

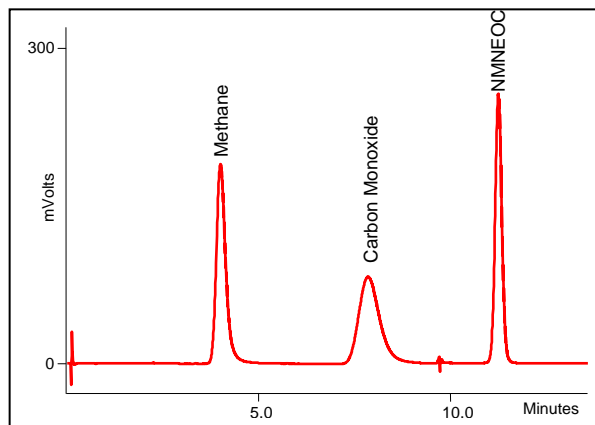
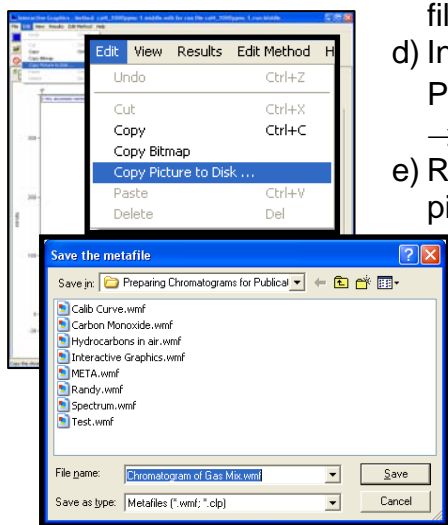
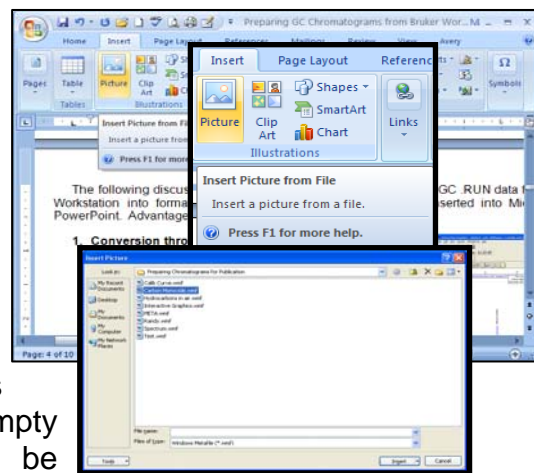
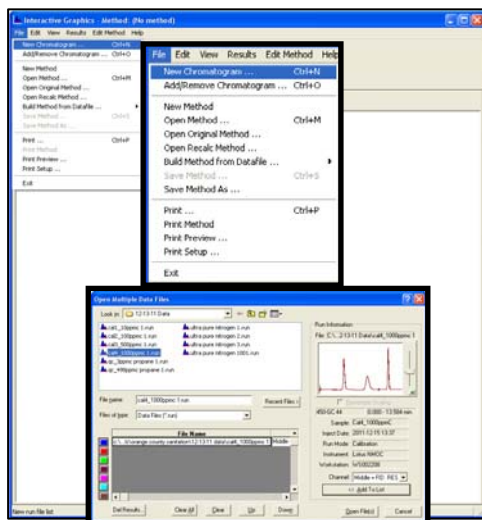
j) Remove peak start/end markers by highlighting and delete.

k) Add comments by highlighting picture and choosing Insert → Text Box → Draw Text Box and highlight area location for text box. Then enter text and adjust font and color as needed.

l) Combine all objects into a single one by selecting Home → Select → Select Objects and highlight all objects within Format Drawing Canvas and then right click to select Grouping → Group.

m) Resize chromatogram object as needed to fit into document.

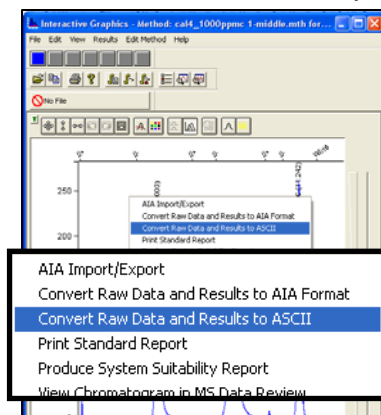
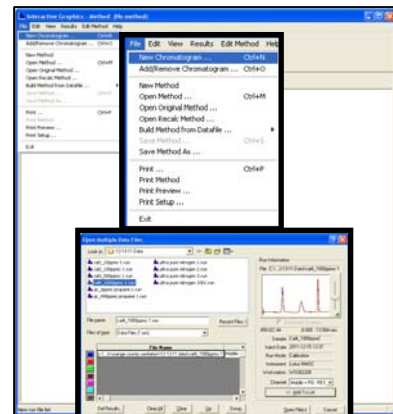
n) Save document.



¹ If all boxes in Layout and Trace Settings are unchecked, the displayed chromatogram will appear as if it had come from a stripchart recorder, with no labeling.

2. Generation from ASCII Raw Data and Microsoft Excel. This process allows custom computations on the raw data points, but lacks coordinate labeling and other formatting found with the others.

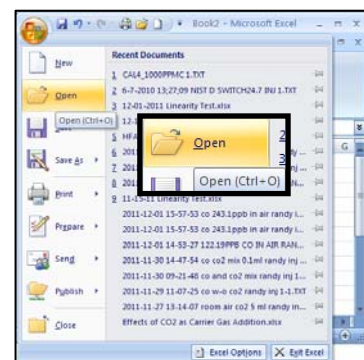
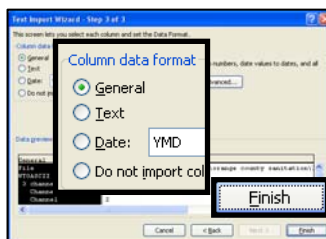
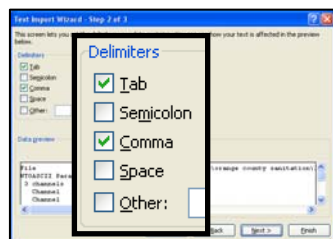
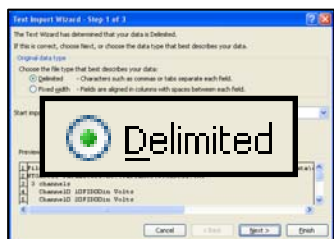
a) Locate target chromatograms and open with Workstation Toolbar → Interactive Graphics → File → New Chromatogram...



b) Right click anywhere in the active chromatogram and select Convert Raw Data and Results to ASCII. A TXT file is automatically created with the same name and folder as the .RUN file.

c) Open this .TXT in Microsoft Excel by selecting File of type → Text Files.

d) Text Import Wizard will open, then select Delimited → Next, and check both Tab and Comma, then Finish.



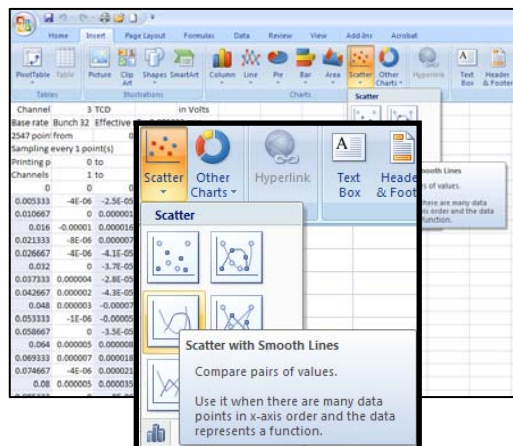
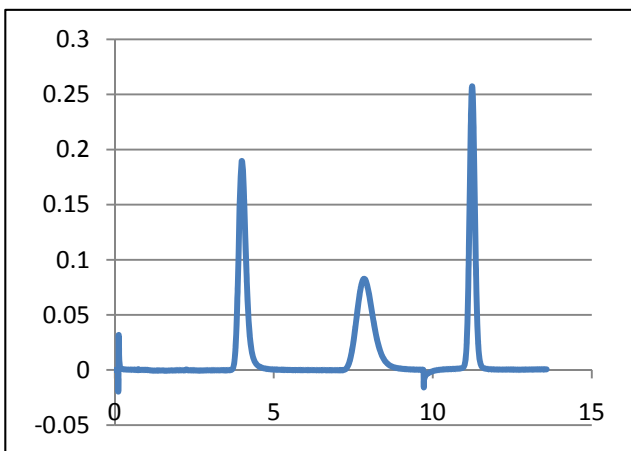
e) Highlight desired retention times and matching amplitudes in worksheet.² If data from multiple channels were originally collected, then extra columns for signal amplitudes are displayed.

f) Select Insert → Scatter Chart → Scatter with Smooth Lines.

g) Highlight chart and select Chart Tools and format as needed.

h) Right click anywhere on chart and select Copy, and Paste into Word or PowerPoint document.

i) Save document.



Channel	B	C
Channel	3	TCD
Base rate	3.125	Bunch 32
Effective r		0
2547 points from		
Sampling every 1 point(s)		
Printing p	0	to
Channels	1	to
0.0000	0.000000	0.000000
0.0053	-0.000004	-0.000025
0.0107	0.000000	0.000001
0.0160	-0.000010	0.000016
0.0213	-0.000008	0.000007
0.0267	-0.000004	-0.000041
0.0320	0.000000	-0.000037
0.0373	0.000004	-0.000028
0.0427	0.000002	-0.000043
0.0480	0.000003	-0.000070
0.0533	-0.000001	-0.000050
0.0587	0.000000	-0.000035
0.0640	0.000005	0.000008
0.0693	0.000007	0.000018
0.0747	-0.000004	0.000021
0.0800	0.000005	0.000035
0.0853	0.000000	-0.000008
0.0907	0.000004	-0.000002
0.0960	0.000003	0.000009
0.1013	0.000003	0.000015
0.1067	-0.000675	-0.002617
0.1120	-0.000216	-0.019473

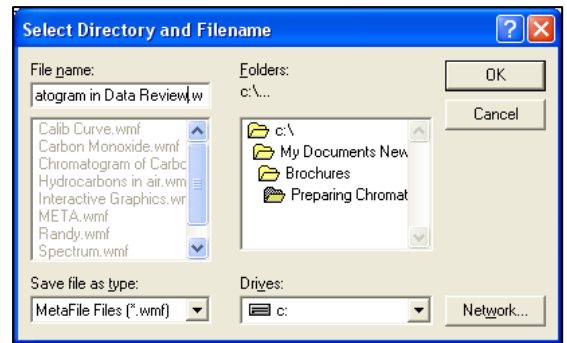
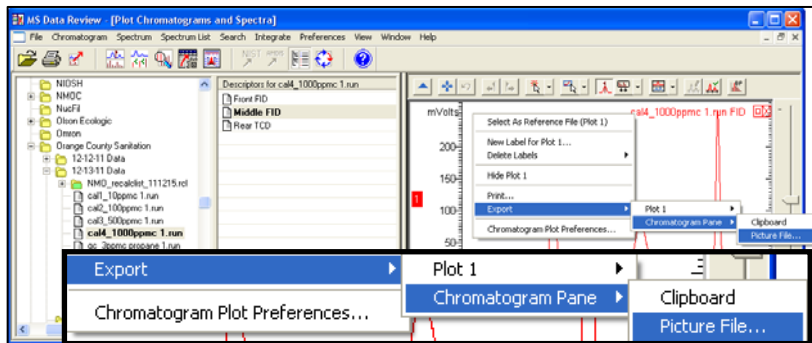
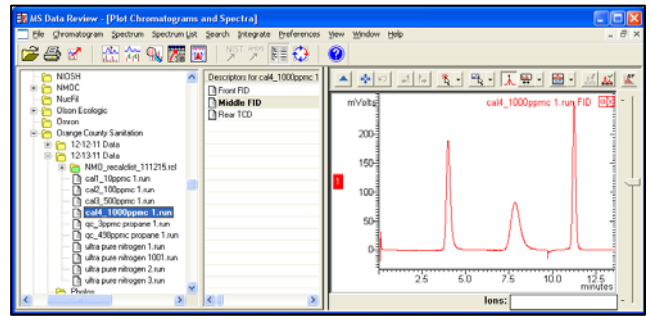
² Note that retention times (minutes) in the first column are reported to four decimal places - the only such listing in Bruker Workstation. Units for amplitudes are volts to six decimal places.

3. Creation with MS Data Review. Even though MS Data Review is designed for mass spec data, .RUN files can be opened and displayed here. Although these steps do not allow any recalculations or detailed formatting of the data, as offered in Interactive Graphics, chromatograms can be tiled to view up to 20 chromatograms at a time, and can be normalized to allow direct comparisons of peak shapes.

a) Open Review/Process MS Data icon from Workstation Toolbar and locate/click on target chromatogram .RUN file in tree on left side of window to open in pane on right.

b) Adjust time and amplitude intervals for a relevant portion of chromatogram.

c) Right click anywhere on chromatogram and select Export → Chromatogram Pane → Picture File... and then select Directory and Filename as needed to relocate readily later.



d) Insert picture .WPF saved in step c) into Word or Power Point document by Insert → Picture.
 e) Right click anywhere in the picture and choose Edit Picture and set Drawing Tools Format → Text Wrapping → Square, to allow image to be moved within document at will.

f) To change color and intensity of chromatogram tracing, highlight all data points and right click anywhere in picture to select Format AutoShape... → Colors and Lines, and adjust as needed.

g) To change font size and orientation of a text box, highlight text box and right click to choose Edit Text. Then right click to select Font and adjust as desired.

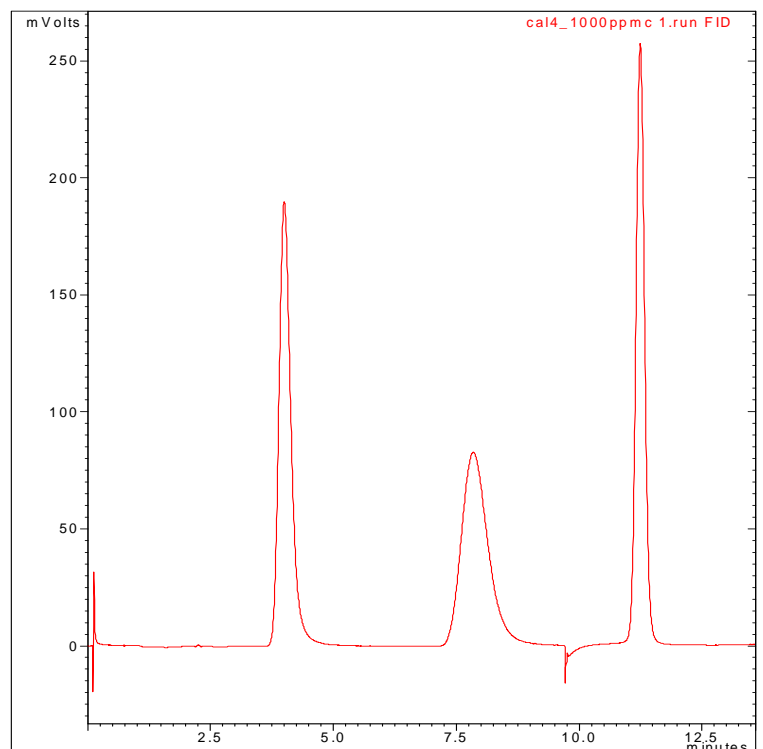
h) To remove unnecessary text boxes, highlight and delete.

i) Add comments by highlighting picture and choosing Insert → Text Box → Draw Text Box and highlight area location for text box. Then enter text and adjust font and color as needed.

j) Combine all objects into a single one by selecting Home → Select → Select Objects and highlight all objects within Format Drawing Canvas and then right click to select Grouping → Group.

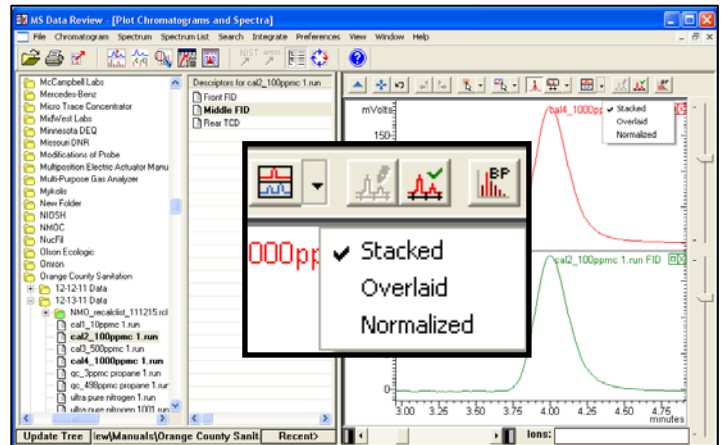
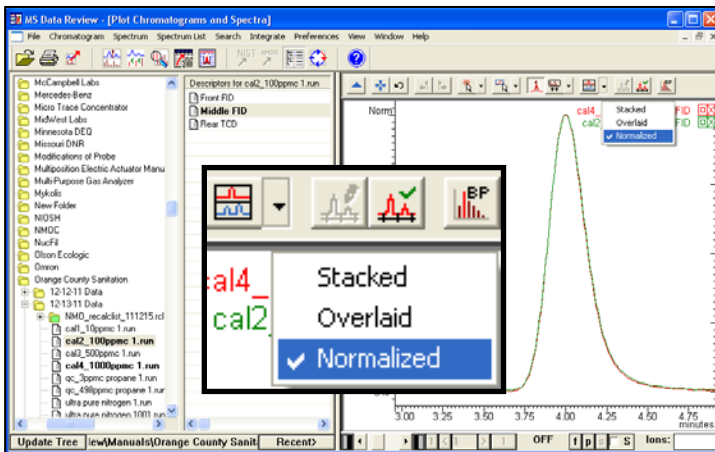
k) Resize chromatogram display as needed to fit into document.

l) Save document.

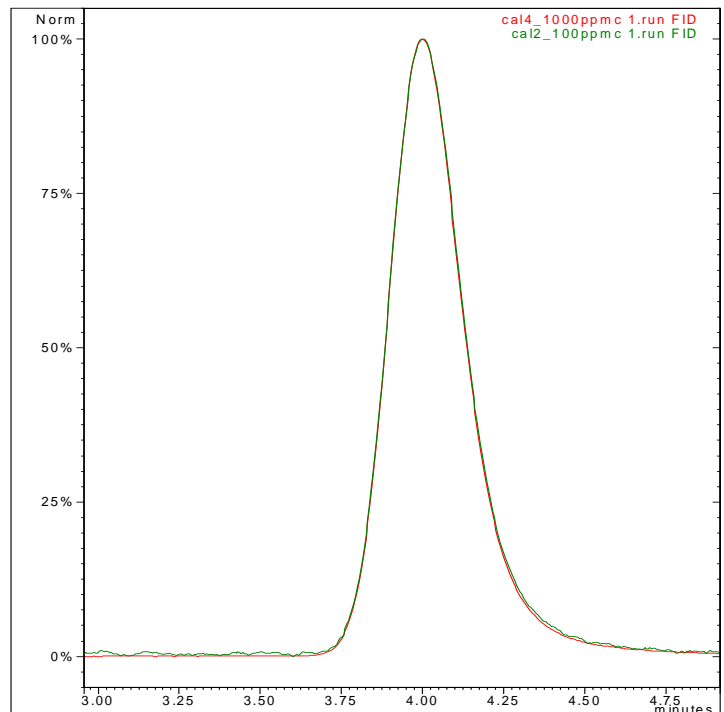


3A. Tile and Overlay of Multiple Chromatograms with MS Data Review. Normalizing GC chromatograms is only available in MS Data Review. This can be employed, for example, to compare peak shapes of an analyte with different concentrations.

- Open Review/Process MS Data icon from Workstation Toolbar and locate/click on target chromatogram .RUN files in tree on left side of window by Ctrl + mouse clicks to open in pane on right.
- Default presentation is “stacked”. To change to “overlay” or “normalize”, select with Chromatogram → Set Chromatogram Display and choose format.

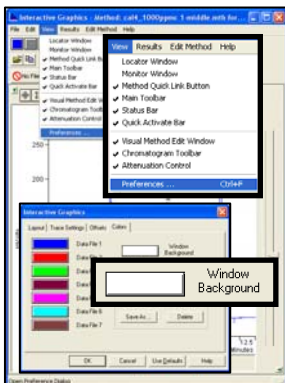


- Right click anywhere on chromatogram and select Export → Chromatogram Pane → Picture File... and then select Directory and Filename as needed to relocate readily later.
- Insert picture .WPF saved in step c) into Word or Power Point document by Insert → Picture.
- Right click anywhere in the picture and choose Edit Picture and set Drawing Tools Format → Text Wrapping → Square.
- To change color and intensity of chromatogram tracing, highlight all data points and right click anywhere in picture to select Format AutoShape... → Colors and Lines and adjust as needed.
- To change font size and orientation of a text box, highlight text box and right click to choose Edit Text. Then right click to select Font and adjust as desired.
- To remove unnecessary text boxes, highlight and delete.
- Add comments by highlighting picture and choosing Insert → Text Box → Draw Text Box and highlight area location for text box. Then enter text and adjust font and color as needed.
- Combine all objects into a single one by selecting Home → Select → Select Objects and highlight all objects within Format Drawing Canvas and then right click to select Grouping → Group.
- Resize chromatogram display as needed to fit into document.
- Save document.



4. **Display by PrtScn.** This operation is by far the easiest to execute, but lacks any ability to change formatting, other than what is available in Interactive Graphics.

a) Locate target chromatograms and open with Workstation Toolbar → Interactive Graphics.



b) Adjust time and amplitude intervals for a desired portion of chromatogram layout and choose preferred trace settings with View → Preferences → Layout and Trace Settings.

c) Set background color to white with View → Preferences → Colors → Window Background.

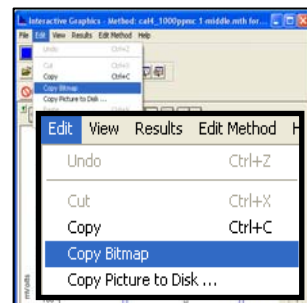
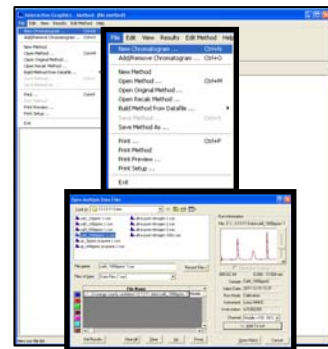
d) Use Edit → Copy Bitmap to capture image.

e) Open Word or PowerPoint document and Edit → Paste.

f) Right click anywhere inside bitmap image and select Text Wrapping → Square, to allow image to be moved within document at will.

g) Resize as needed by grabbing hold of any corner or edge.

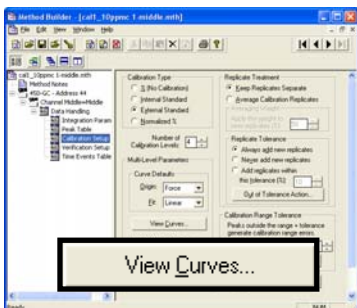
h) Save document.



Insertion of Calibration Curve

Loads of information on calibration data are included in the Bruker Workstation calibration curves and can be transferred intact into Microsoft Word or PowerPoint as outlined below.

A. Open target method with View/Edit Methods in Toolbar.



B. Locate Channel → Data Handling → Calibration Setup → View Curves... and select analyte curve to transfer. If error message “No Calibrated Peaks in Peak Table” appears, then calibration has not been performed for that peak.

C. Pick Export... at top of window, and enter appropriate Amount Units, then OK.

D. Select Export → To Picture File

E. Choose Directory and File name as needed to relocate readily later.

F. Insert picture.WPF saved in step E) into Word or Power Point document by Insert → Picture.

G. Right-click anywhere in picture and select Size. Then uncheck “Lock aspect ratio” and set Height to 7.5 and Width to 6 to provide undistorted picture of curve. Reset “Lock aspect ratio” to keep new ratio intact.

H. Right-click anywhere in picture and choose Edit Picture to permit editing of text boxes.

I. Resize as needed by grabbing hold of any corner or edge.

J. Save document.

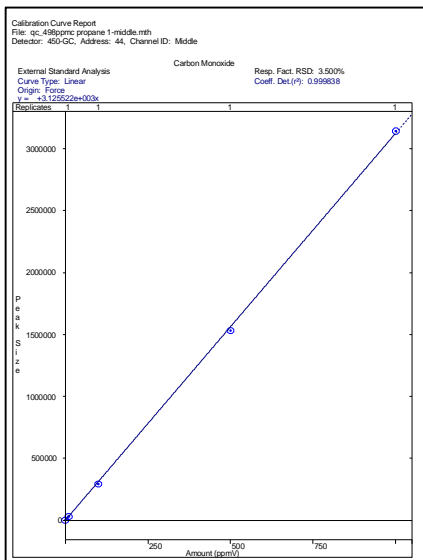
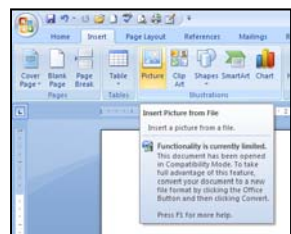
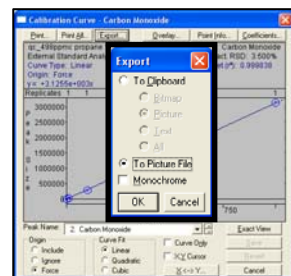
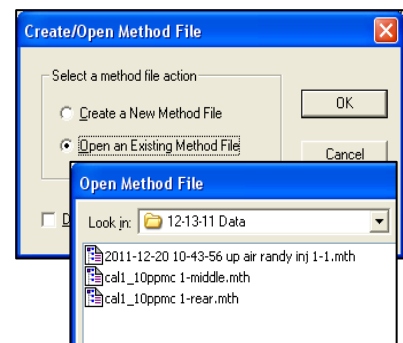


Table I.

The four methods to generate chromatograms from Bruker Workstation for insertion into Microsoft Word or PowerPoint have distinct differences in abilities to accomplish desired effects.

Approach	Original Axis Labeling	Original Text	Original Peak Names	Original Retention Times	Edit Original Labeling	Add User Labeling	Change Color + Line Size
1. Interactive Graphics	✓	✓	✓	✓	✓	✓	✓
2. ASCII Raw Data						✓	✓
3. MS Data Review	✓				✓	✓	✓
4. Print Screen	✓	✓	✓	✓			

Approach	Baseline Drawn	Normalize Chromatograms	Tile Display	Offset Chromatograms	Perform Computations on Data	Maximum Displayed
1. Interactive Graphics	✓		✓	✓		7
2. ASCII Raw Data				✓	✓	many
3. MS Data Review		✓	✓			20
4. Print Screen	✓		✓	✓		7

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