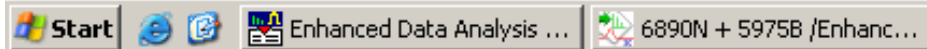


Software for GC/MS



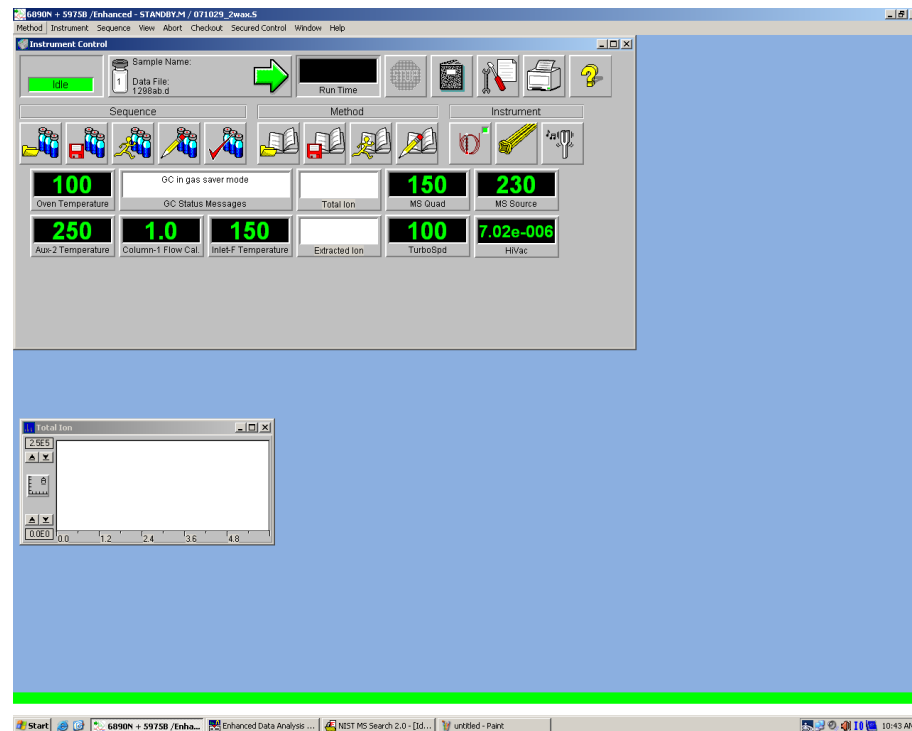
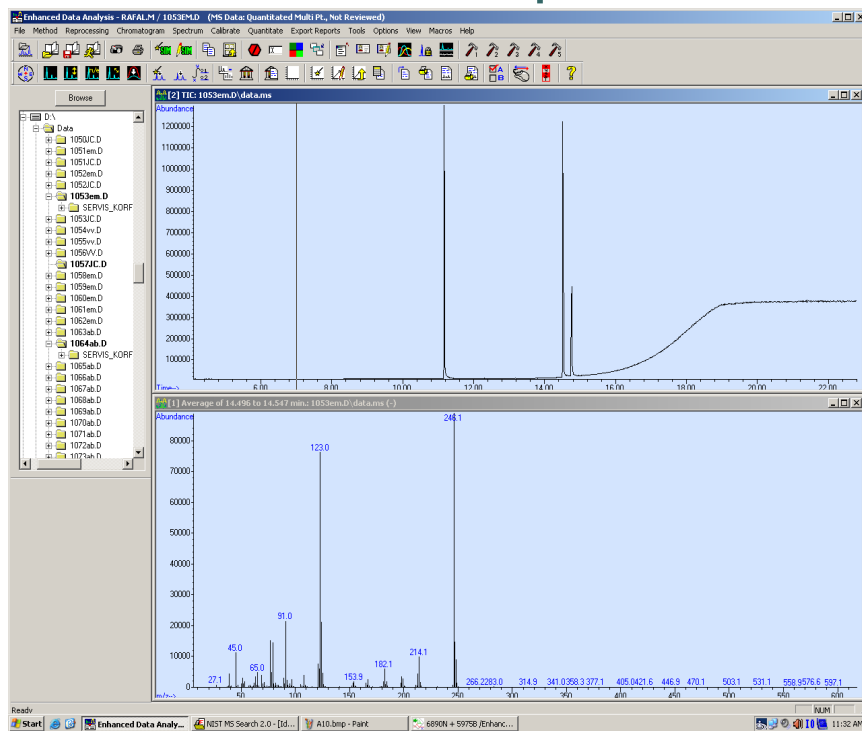
ChemStation

estery TIC.pdf



Interpretation

Measurement



Run measurement

6890N + 5975B → „Sequence“ → „Edit Sequence“

The screenshot displays the software interface for the 6890N + 5975B system. The title bar reads "6890N + 5975B /Enhanced - STANDBY.M / DEFAULT.S". The menu bar includes "Method", "Instrument", "Sequence", "View", "Abort", "Checkout", "Secured Control", "Window", and "Help". The "Sequence" menu is open, with "Edit Sequence..." circled in red. Other menu items include "Load Sequence...", "Save Sequence", "Save Sequence As...", "Run Sequence...", "Print Sequence...", "Import Sequence Information from CSV File...", "Simulate Sequence", "Position and Run Sequence...", "View Sequence Log ...", "View Sequence Quality Log", "Print Sequence Log", "Configure Sequence Table...", "Batch Mode...", and "Additional Sequence Options...".

The main interface shows the "Instrument Control" panel on the left with a green "Idle" status. Below it are two temperature displays: "Oven Temperature" at 100 and "Aux-2 Temperature" at 250. The central area features a "Run Time" display, a "STOP" button, and a toolbar with icons for a book, a wrench, a printer, and a question mark. Below the toolbar are sections for "Method" and "Instrument" with various icons. At the bottom, there are six data displays: "Total Ion", "Extracted Ion", "MS Quad" (150), "TurboSpd" (100), "MS Source" (230), and "HiVac" (7.03e-006).

Sample Log Table

Sample Log Table

Data Path: Method Path:

	Type	Vial	Sample	Method / Keyword	Data File	Comment / KeywordString	Multiplier	Level	Update RF	Update RT	Update OI	Up <u>Δ</u> I
1	Blank	1	Hexan	WAX_EST2	NC1275		1.00000		No Update	No Update	No Update	No Up
2	Sample	2	14:0,18:1	WAX_EST2	NC1276	WAX 1	1.00000		No Update	No Update	No Update	No Up
3	Sample	3	16:1,16:1	WAX_EST2	NC1277	WAX 2	1.00000		No Update	No Update	No Update	No Up
4	Sample	4	18:1,14:1	WAX_EST2	NC1278	WAX 3	1.00000		No Update	No Update	No Update	No Up
5												
6												
7												
8												
9												
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35												

Sheet1

Start | 6890N + 5975B /Enhanc... | Sample Log Table | Enhanced Data Analysis ... | NIST MS Search 2.0 - [Id... | untitled - Paint | 10:35 AM

Overwrite previous sequence

Sample Log Table

Data Path: D:\DATA

	Type	Vial	Sample	Met Key
1	Blank	1	Hexan	WAX_EST
2	Sample	2	14:0,18:1	WAX_EST
2	Sample	2	16:1,16:1	WAX_EST
2	Sample	2	18:1,14:1	WAX_EST
13				
14				
15				
16				

Mark rows by mouse
→ right click
→ „Delete Rows“

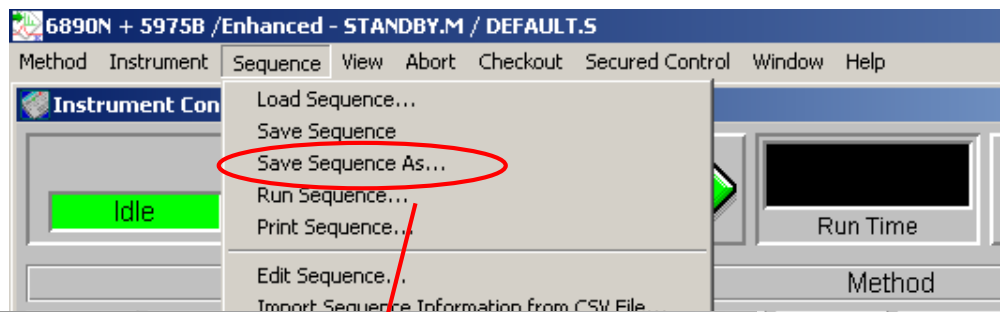
Fill the Sample Log Table

After filling → OK

Nizke – Low
Vysoke – High

Methods	Inlet temperature	split	range	Temperature program
AS_M-nizke_C-nizke	200°C	10:1	to 600 m/z	40°C(2min) →8°C/min do 200→15°C/min do 320°C (3min)
AS_M-nizke_C-vysoke	200°C	50:1	to 600 m/z	40°C (2min) →8°C/min do 200→15°C/min do 320°C (3min)
AS_M- vysoke _C-nizke	230°C	10:1	to 800 m/z	60°C(2min) →10°C/min do 320°C (10min)
AS_M- vysoke _C-vysoke	230°C	50:1	to 800 m/z	60°C(2min) →10°C/min do 320°C (10min)

Save sequence



The main screenshot shows the software interface with the 'Save Sequence' dialog box open. The dialog box is titled 'Save Sequence' and shows the 'Save in:' path as 'sequence'. The file list contains various sequence files, including '071029_1wax.S', '071029_2wax.S', and '071029_4wax.S'. The 'File name:' field is set to '071029_4wax.S' and is circled in red. The 'Select' button is also circled in red. A red arrow points from the 'Save Sequence As...' option in the menu above to the '071029_4wax.S' file in the list.

The background interface shows the 'Instrument Control' window with the 'Idle' status, 'Run Time' button, and various temperature and flow rate displays. The 'Total Ion' and 'Extracted Ion' monitors are also visible.

Run sequence

The screenshot displays the 'Start Sequence' dialog box in a chromatography software interface. The dialog box is titled 'Start Sequence 071029_2wax.S Last Modified: Mon Oct 29 11:03:09 2007'. It contains the following elements:

- Method Sections To Run:** Radio buttons for 'Full Method' (selected) and 'Reprocessing Only'. A checkbox for 'Overwrite Existing Data Files' is unchecked.
- On A Barcode Mismatch:** Radio buttons for 'Inject Anyway' (selected) and 'Don't Inject'.
- Sequence Comment:** A text field containing 'wax'.
- Operator Name:** A text field containing 'Cervenkova'.
- Data File Directory:** A text field containing 'D:\DATA\'. A 'Browse...' button is located to the right.
- Buttons:** 'Run Sequence', 'OK', 'Cancel', 'Help', and 'More>>'.

Red circles highlight the 'Run Sequence...' menu item in the 'Sequence' menu and the 'Run Sequence' button in the dialog box. A red arrow points from the menu item to the dialog box.

„Solvent delay“

Always NO !!!!!!!!!!!!!!!!!!!!!

The screenshot shows the Instrument Control software interface. At the top, the window title is "6890N + 5975B /Enhanced - STANDBY_AS.M / 071029_2wax.5". Below the title bar, the status bar indicates "Sequence 071029_2wax.5 is running...".

The main interface is divided into several sections:

- Run Section:** A "Run" button, a sample name "Hexan", data file "0000w.d", and a "Run Time: 7.33" display.
- Sequence, Method, and Instrument Sections:** Each section contains icons representing different parameters or actions.
- Parameter Displays:** A grid of numerical displays for various parameters: Oven Temperature (138), GC Status Messages, Total Ion, MS Quad (150), MS Source (230), Aux-2 Temperature (250), Column-1 Flow Cal. (1.0), Inlet-F Temperature (150), Extracted Ion, TurboSpd (100), and HiVac (7.02e-006).

An "Acquisition" dialog box is overlaid on the interface, asking: "Override solvent delay [3.75 minutes]?". The dialog includes a warning: "Warning: Overriding solvent delay may shorten filament lifetime." and two buttons: "Yes" and "No". The "No" button is circled in red, indicating the correct response.

At the bottom, there are two small windows: "Total Ion" showing a value of 2.5E5 and "Extracted Ion" showing a value of 2.5E2.

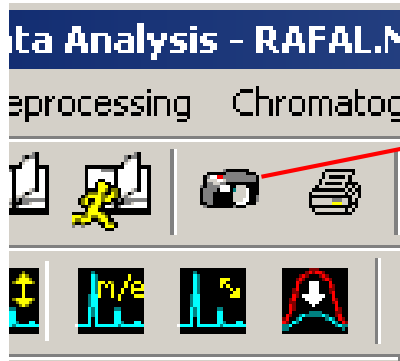


Interpretation

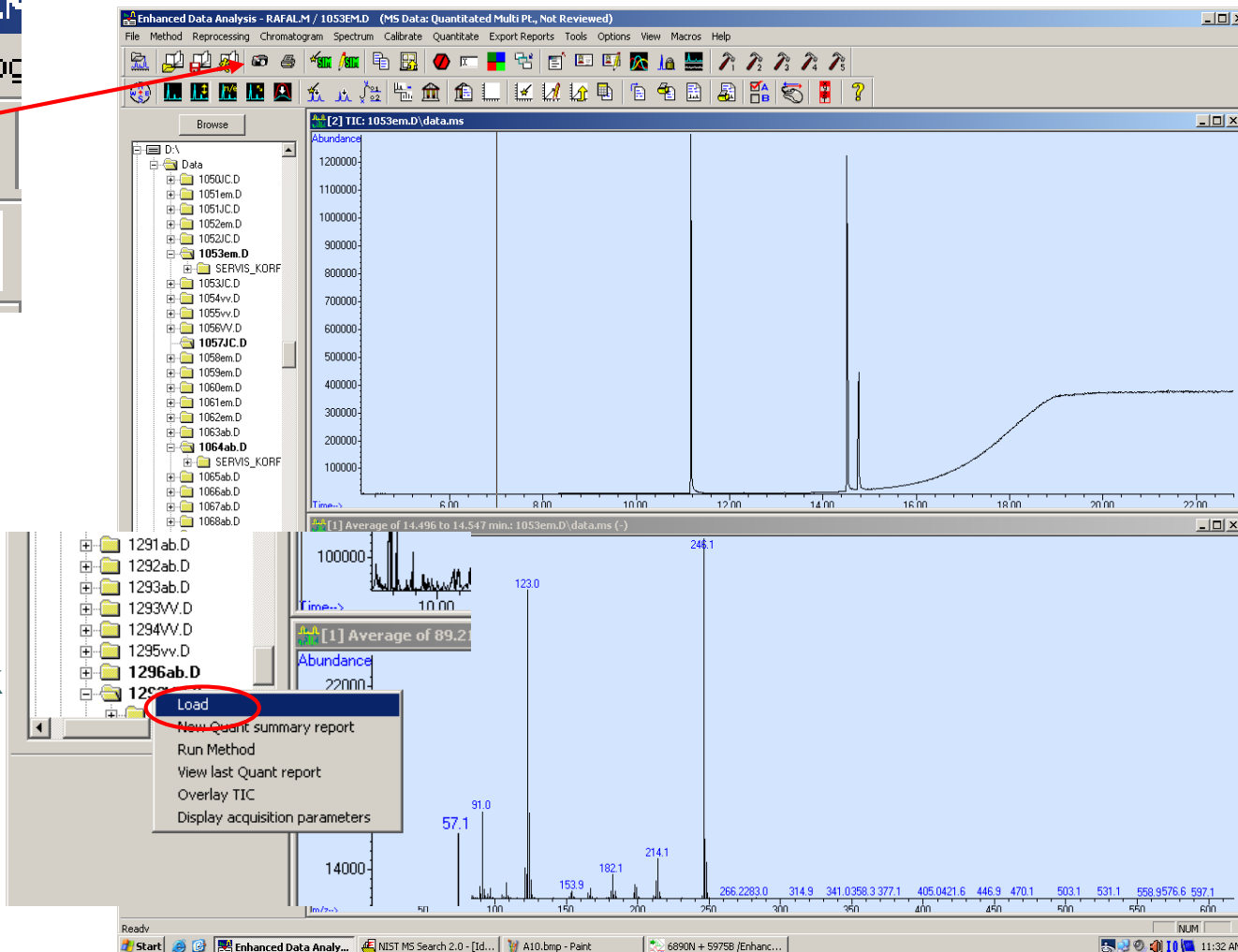
- You can install *ChemStation*: download data from D/DATA/....
 - By *ftp*: (from *Total Commander*)
 - By USB flash disk
 - Licenses of *ChemStation* – J. Cvačka
- You can use *ChemStation* in lab 107
- Back-up your data (yourself)

Load data

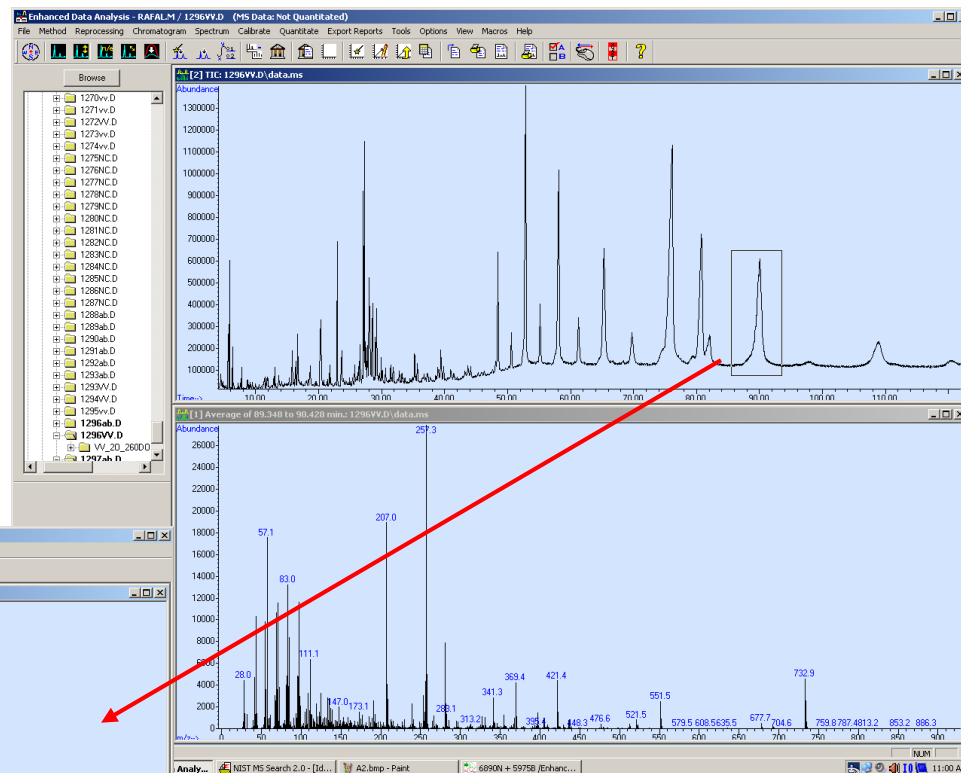
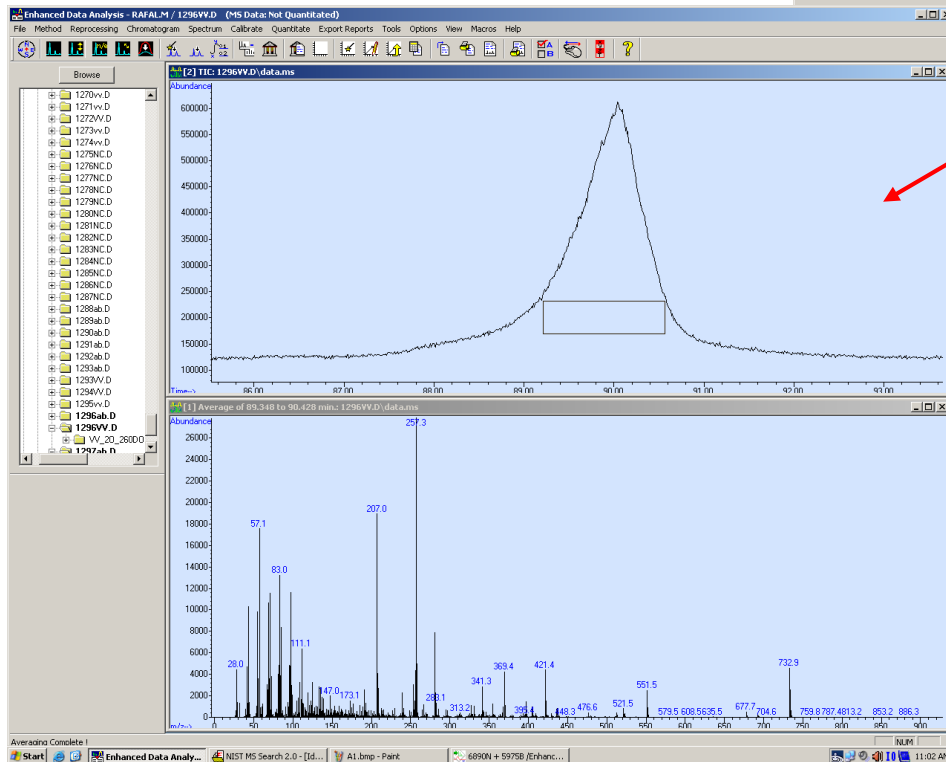
For running analysis – „Take Snapshot“



Load finished
analysis → right click
→ „Load“

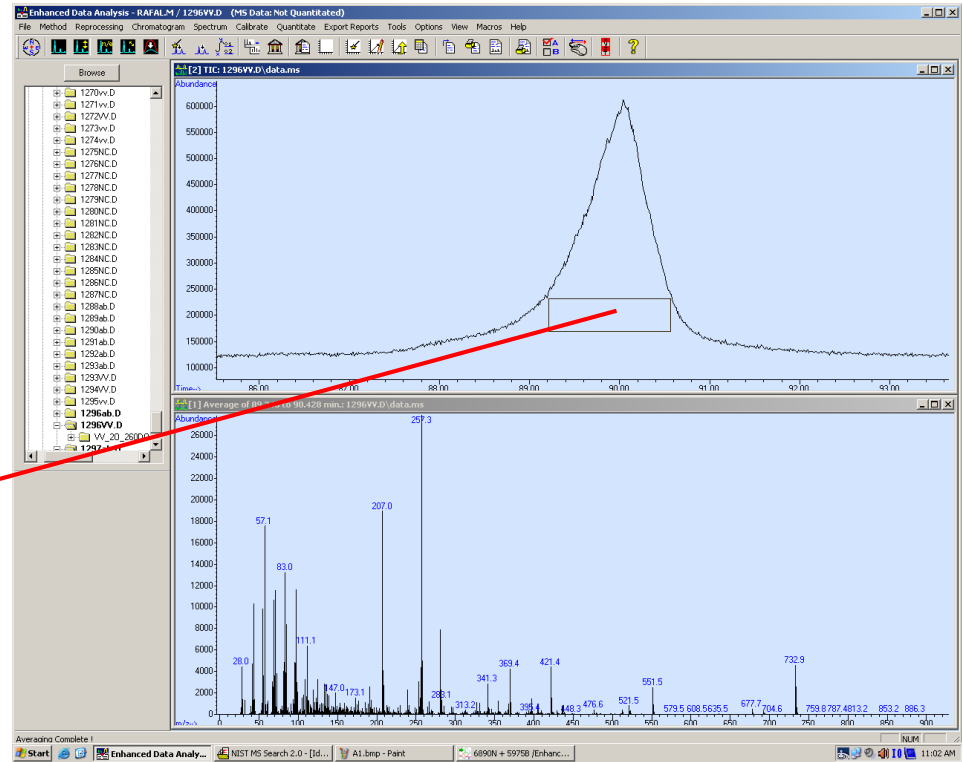
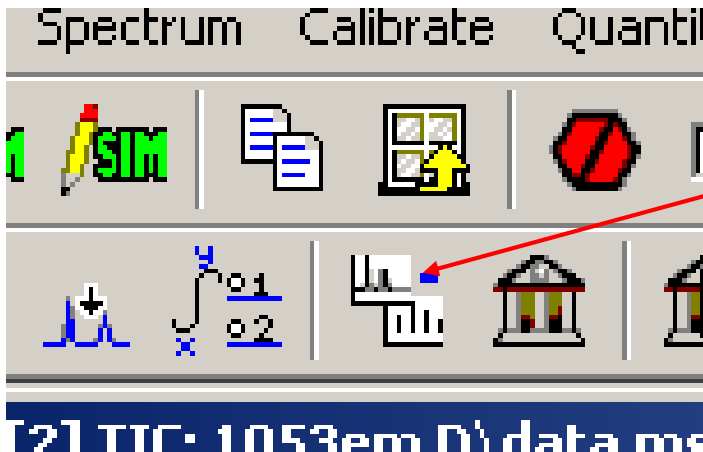


Zoom peak



Zoom by left click
(back – double-click by left click)

Load spectrum and subtract background



1. Load spectrum from peak
2. Load spectrum near the peak
3. Click on „Subtract“

Load spectrum by left click

NIST search

NIST MS Search 2.0 - [Ident, Presearch Default - InLib = -1163, 95 spectra]

File Search View Tools Options Window Help

1. Average of 74.172 to 74.649 min.: 1296VV.D

#	Lib.	Match	R.Match	Prob.	Name
1	M	631	761	42.5	Hexadecanoic acid, octadecyl ester
2	M	610	724	18.1	Hexadecanoic acid, hexadecyl ester
3	M	593	747	9.86	Hexadecanoic acid, tetradecyl ester
4	M	590	682	8.71	Hexadecanoic acid, eicosyl ester
5	M	561	748	2.47	Hexadecanoic acid, dodecyl ester
6	M	550	724	1.69	Hexadecanoic acid, cyclohexyl ester
7	R	548	628	1.56	Hexadecanoic acid, 2-(octadecyloxy)ethyl ester
8	M	542	594	1.22	Dodecyl cis-9,10-epoxycaradecanoate
9	M	528	596	0.76	9-Hexadecenoic acid, eicosyl ester, (Z)
10	M	525	754	0.67	1-Disopropylglycidyldecane
11	M	522	593	0.60	17-Perilatricontene
12	M	522	562	0.60	Docosanoic acid, 1,2,3-propanetriyl ester
13	ms	521	603	0.57	Average of 68.967 to 69.325 min.: 00001
14	M	515	570	0.45	Palmitic acid, 2-(tetradecyloxy)ethyl ester
15	R	514	577	0.43	Octadecanoic acid, octadecyl ester
16	M	512	672	0.40	Isotridecyl alcohol, trimethylsilyl derivative
17	M	511	553	0.38	Oleic acid, eicosyl ester
18	M	505	562	0.30	Hexadecanoic acid, 2-(hexadecyloxy)ethyl ester
19	M	503	719	0.28	1-Dimethyl(4-chloromethyl)silyloxytridecanol
20	M	503	553	0.28	Triarac hinc
21	R	500	581	0.24	Oleic acid, 3-(octadecyloxy)propyl ester
22	M	500	540	0.24	Octadecanoic acid, eicosyl ester
23	M	499	547	0.23	Octadecane, 1-[2-(hexadecyloxy)ethoxy]
24	M	498	559	0.22	9-Octadecenoic acid (Z), octadecyl ester
25	M	496	836	0.21	Docosanoic acid, docosyl ester
26	M	496	577	0.21	9-Hexadecenoic acid, octadecyl ester
27	R	494	629	0.19	1-Hexacosanol
28	M	493	683	0.18	1-Hexacosanol
29	M	493	548	0.18	1-Butyl-dimethyl(4-methyl-dodecyl-oxy)-sil
30	M	492	652	0.17	Lanosta-7(11)-dien-18-oic acid, 22,25-d
31	M	492	584	0.17	Boron, [4-][dimethyl(1-methyl-1-butyl)silyl
32	M	492	553	0.17	1-Hentetracosanoic acid
33	M	491	547	0.17	Distearylthiodipropionate
34	M	490	570	0.16	Octadecanoic acid, 2-(octadecyloxy)ethyl ester
35	M	489	585	0.15	9-Octadecene, 1,1'-[1,2-ethanediyloxy]bis
36	M	488	589	0.15	Nerone, 4,8,5-dihydro-
37	M	487	587	0.14	Bacteriochlorophyll-a-stearyl
38	M	487	587	0.14	9-Hexadecenoic acid, hexadecyl ester

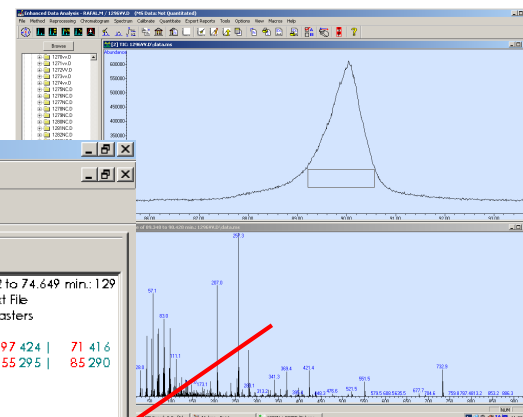
Names Structures InLib = -1163, Hit List

Lib. Search Other Search Names Compare Librarian MSMS

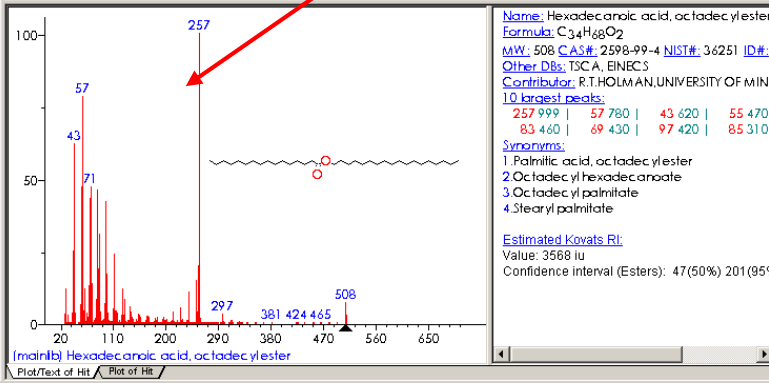
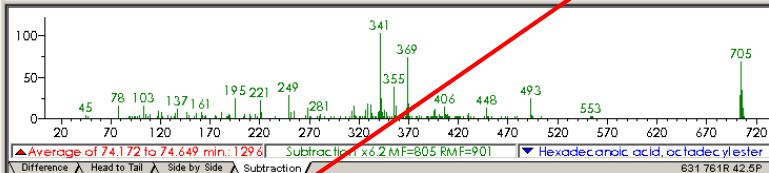
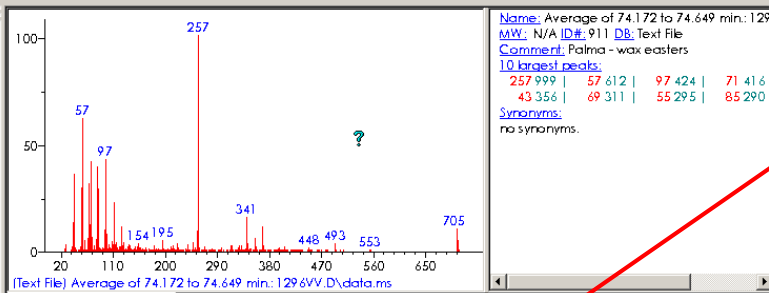
For Help, press F1

Ident Ident

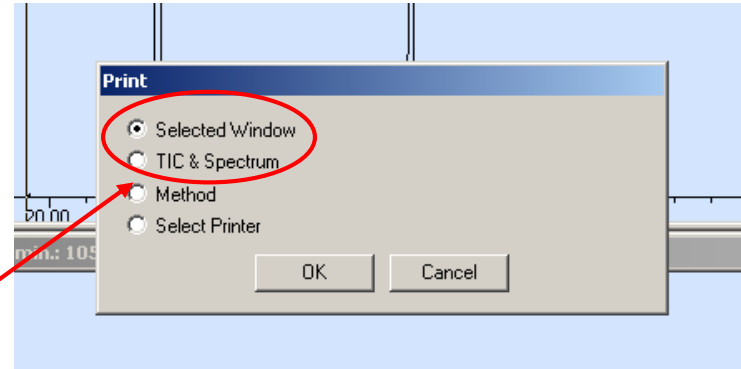
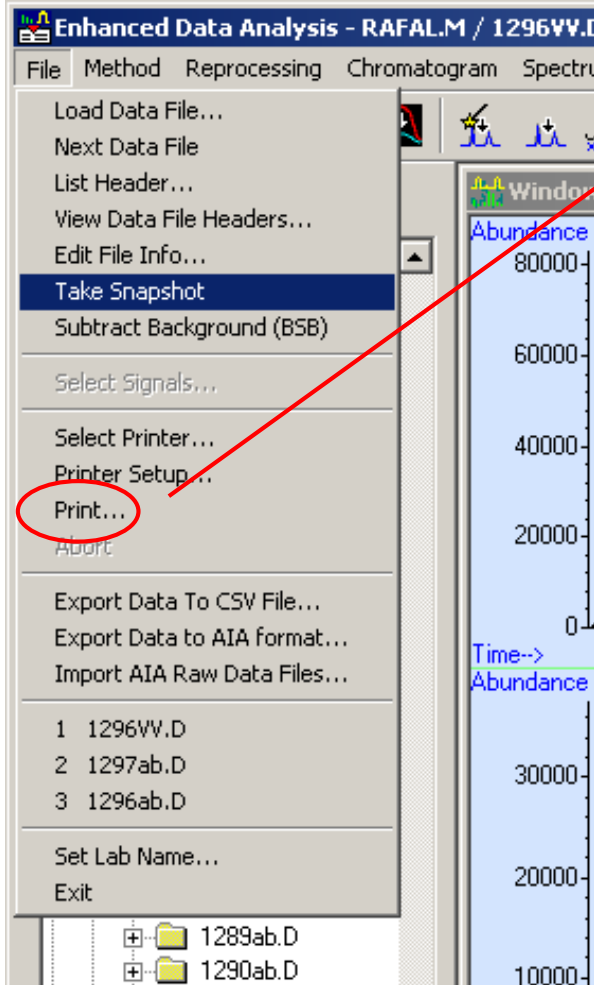
Start 6890N + 5975B /Enhanc... Enhanced Data Analysis ... NIST MS Search 2.0 - ... 1:02 PM



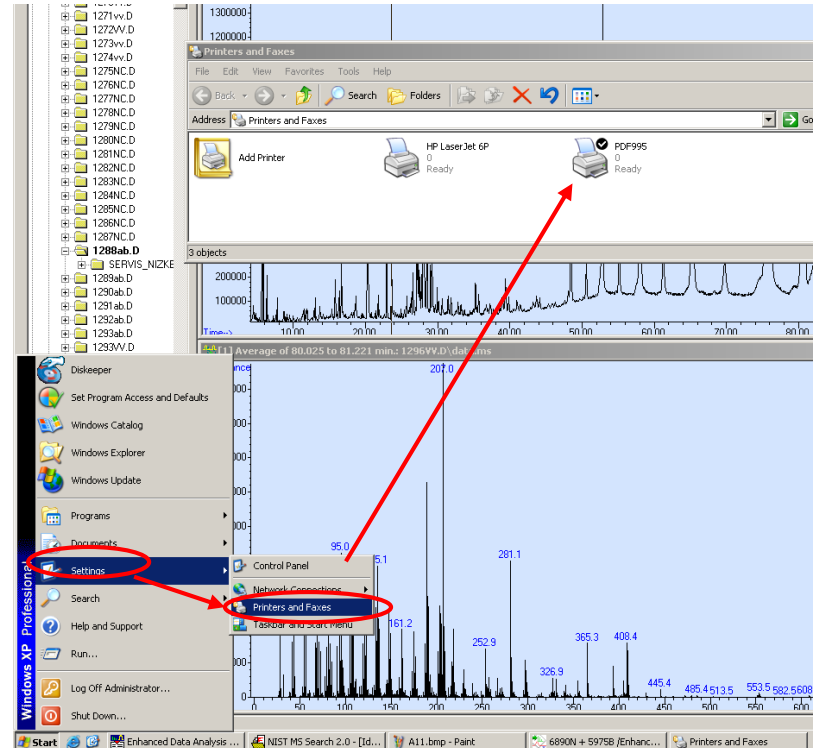
Right double-click on spectrum



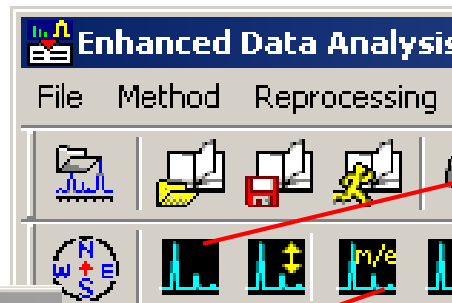
Print to PDF or paper



Set printer as Default



Extracted ion chromatogram



Enhanced Data Analysis - RAFAL.M / 1296VV.D (MS Data: Not Quantitated)

File Method Reprocessing Chromatogram Spectrum Calibrate Quantitate Export Reports Tools Options View

Extracted Ion Chromatograms

Time Range: 4.097 to 121.995 minutes

Ions

1: 57.10	4:
2: 620.80	5:
3:	6:

Use m/z range from - 0.30 to + 0.30

OK Cancel Help

1286NC.D
1287NC.D
1288ab.D
1289ab.D
1290ab.D
1291ab.D
1292ab.D

Ion 57.10 (56.80 to 57.40): 1296VV.D\data.ms

Ion 620.80 (620.50 to 621.10): 1296VV.D\data.ms

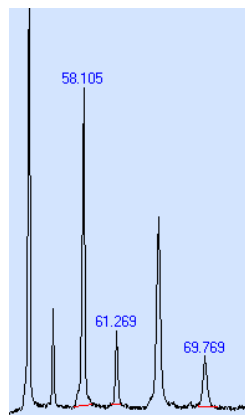
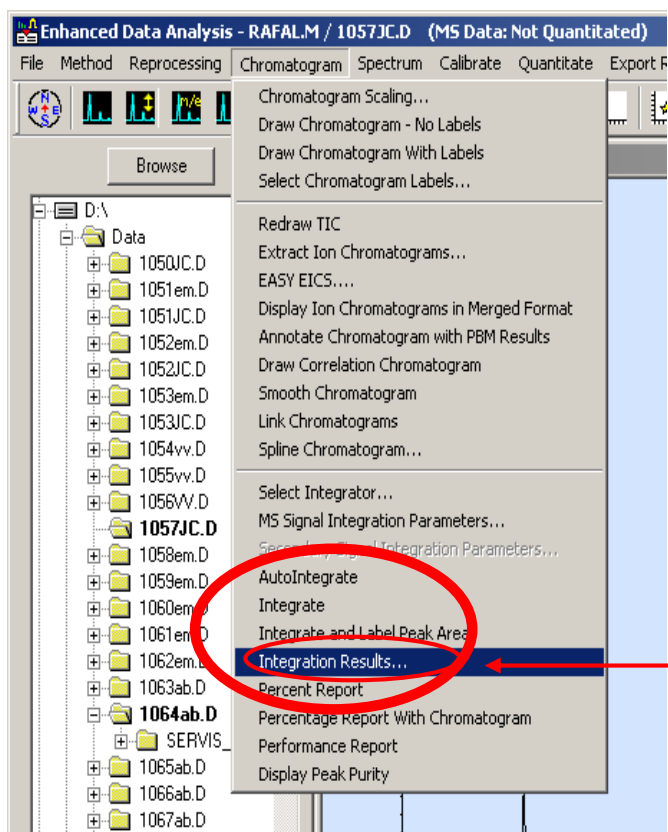
Average of 09.212 to 90.564 min.: 1296VV.D\data.ms

28.1 57.1 83.0 111.1 127.1 173.1 207.0 257.3 283.1 313.1 341.3 363.4 383.1 421.4 450.9476.5 521.5 551.5 579.5 608.5 635.6661.7 692.7 732.8 761.1 790.6 835.2861.4886.6

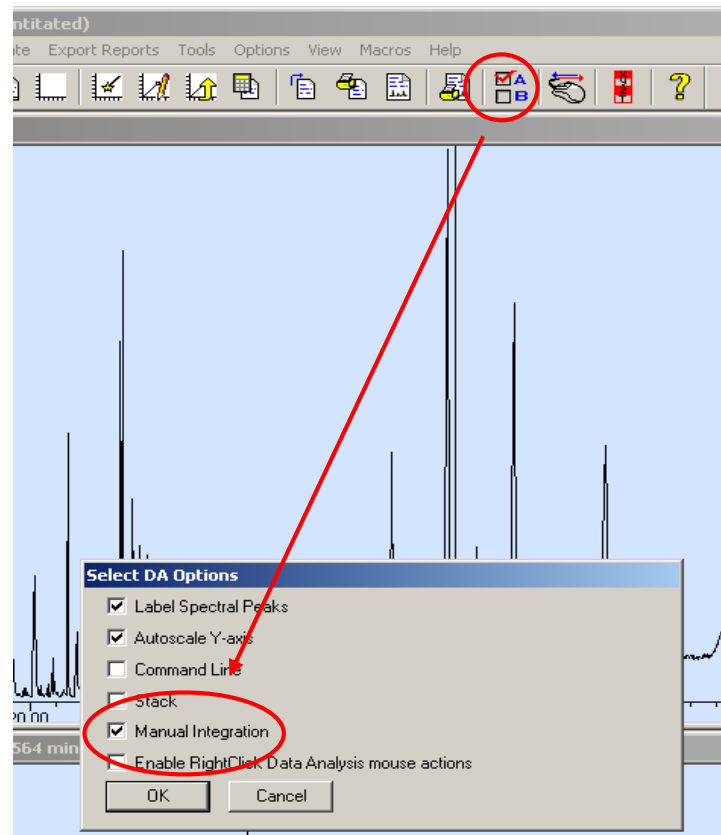
Start Enhanced Data Analy... NIST MS Search 2.0 - [Id... AS.bmp - Paint 6890N + 5975B /Enhanc... NUM 11:09 AM

Integration

Automatic integration



Manual integration



Right click - draw line on base of the peak

Overlay chromatogram

The screenshot illustrates the steps to overlay chromatograms in MSD ChemStation. The main window is titled "Enhanced Data Analysis - RAFAL.M / 1296VV.D (MS Data: Not Quantitated)". A dialog box titled "Select Files for TIC Overlay: 1296VV.D" is open, showing a list of available data files and files selected for processing. The "Available Data Files" list includes files like 1290ab.D, 1291ab.D, 1292ab.D, 1293ab.D, 1294ab.D, 1295VV.D, 1295wv.D, 1296ab.D, 1297ab.D, 1288ab.D, and 1294VV.D. The "Files Selected for Processing" list includes D:\Data\1294VV.D and D:\Data\1296VV.D. A "Select Overlay Mode" dialog box is also visible, with "TIC" selected. The main window shows a chromatogram plot with two traces overlaid, labeled "TIC: 1296VV.D\data.ms" and "TIC: 1294VV.D\data.ms".

File	Sample Name	File	Sample Name
1290ab.D	blank other	D:\Data\1294VV.D	Palma - wax easters
1291ab.D	Arbek_VH221_1	D:\Data\1296VV.D	Palma - wax easters
1292ab.D	blank CHCl3		
1293ab.D	Severa_LS048.D		
1294ab.D	blank		
1295VV.D	blank CHCl3		
1295wv.D	blank CHCl3		
1296ab.D	blank CHCl3		
1297ab.D	Ubik. rozkladne pro...		





- For help do not hesitated to contact staff of MS department

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- **Office : A, JV, 1.85**

- **(Josef Cvačka)**

- **Tel. 303,**
- **Office: A, JV, 1.90**