

# Software for GC/MS

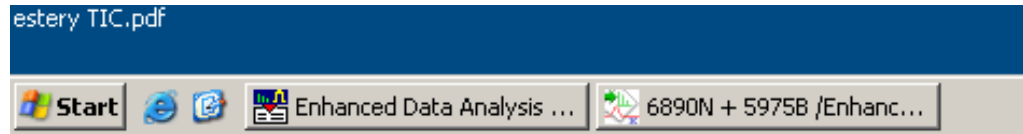


**Building A**  
**Ground floor SV**  
**Lab 107**



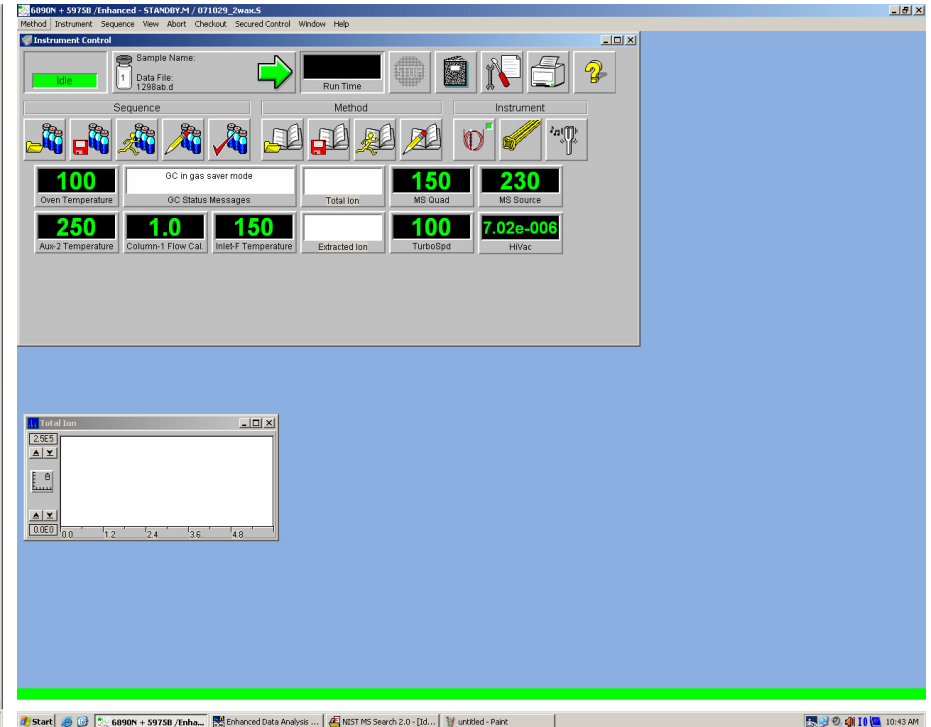
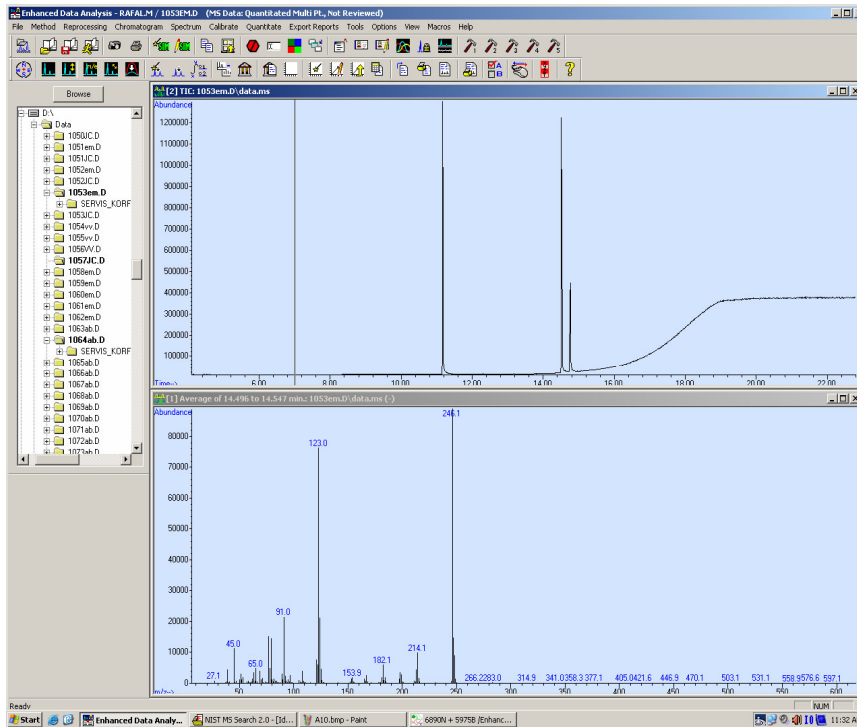


# ChemStation



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. The interface also shows a "Run Time" button, a "Method" section with icons for loading and editing sequences, and an "Instrument" section with various icons. On the left, there are temperature readouts: "100 Oven Tempera" and "250 Aux-2 Tempera". The main display area shows several data points: "Total Ion", "Extracted Ion", "MS Quad" (150), "MS Source" (230), "TurboSpd" (100), and "HiVac" (7.03e-006).

# Sample Log Table

Sample Log Table

Data Path:  Browse...

Method Path:  Browse...

	Type	Vial	Sample	Method / Keyword	Data File	Comment / KeywordString	Multiplier	Level	Update RF	Update RT	Update OI	Up <u>Δ</u> L
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												
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Sheet1

Read Barcode OK Cancel Help

Start 6890N + 5975B /Enhanc... Sample Log Table Enhanced Data Analysis ... NIST MS Search 2.0 - [Id... untitle - 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				

Context menu options:

- Copy
- Cut
- Paste
- Insert Row
- Delete Rows
- Fill Column & increment
- Fill Column, NO increment
- Repeat Row & increment
- Repeat Row, NO increment

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

# Fill the Sample Log Table

Sample Log Table

Data Path: D:\DATA Browse...

Method Path: C:\MSDCHEM\1\METHODS Browse...

	Type	Vial	Sample	Method / Keyword	Data File	Comment / KeywordString	Multiplier	Level	Update RF	Update RT	Update OI	Update 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_EST1	NC1276	WAX 1	1.00000		No Update	No Update	No Update	No Up
3	Sample	3	16.1,16.1	WAX_EST1	NC1277	WAX 2	1.00000		No Update	No Update	No Update	No Up
4	Sample	4	18.1,14.1	WAX_EST1	NC1278	WAX 3	1.00000		No Update	No Update	No Update	No Up
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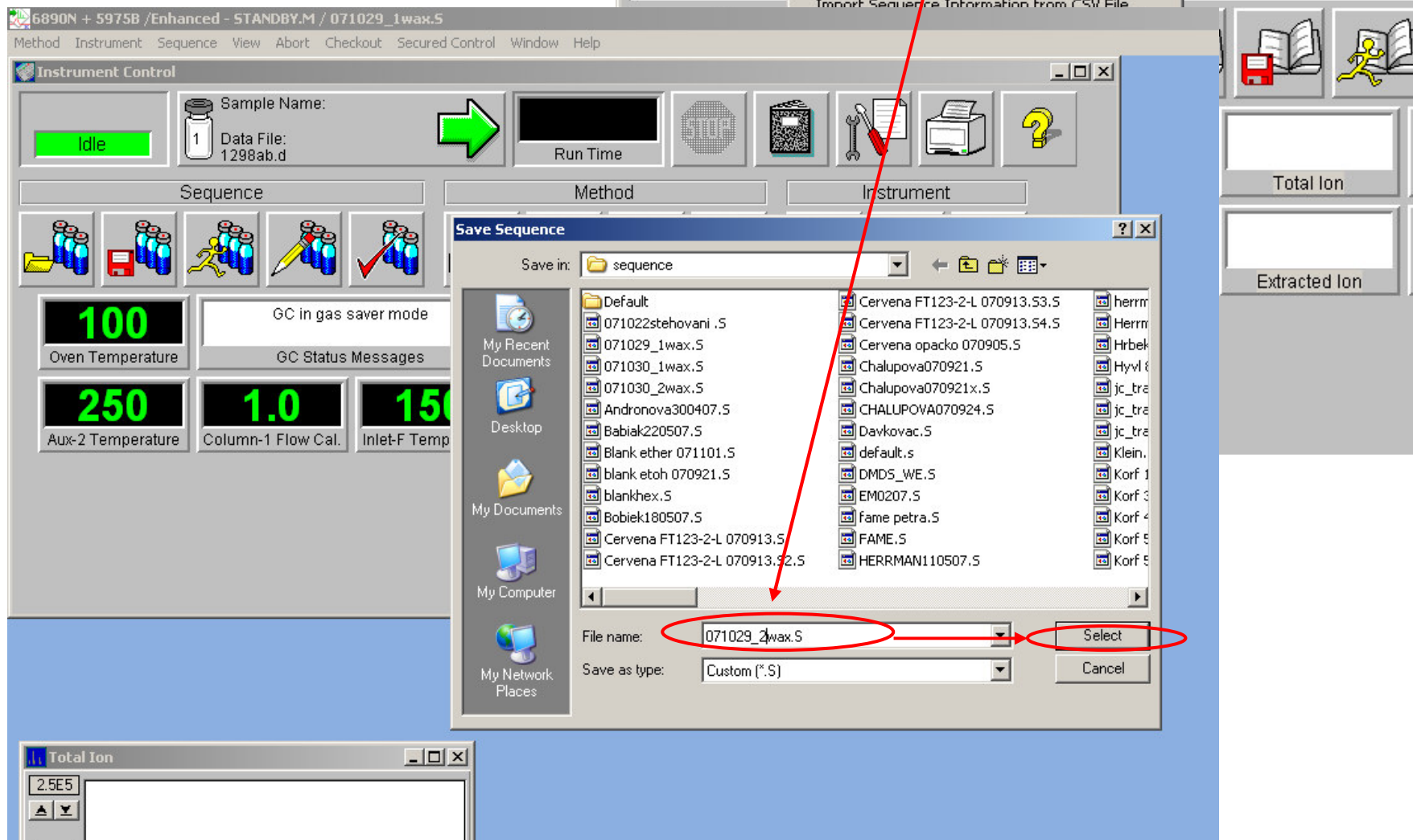
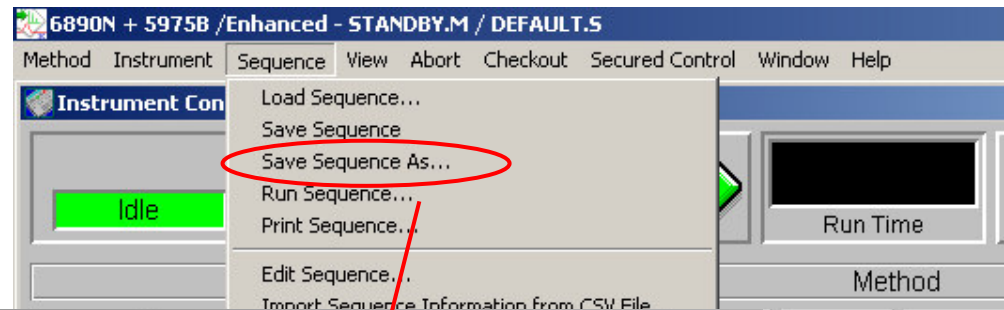
After filling -> OK

Read Barcode OK Cancel Help

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





# Run sequence

The image displays a software interface for instrument control. The main window is titled "6890N + 5975B /Enhanced - STANDBY.M / DEFAULT.S". A menu is open, showing options like "Load Sequence...", "Save Sequence...", and "Run Sequence...". The "Run Sequence..." option is circled in red. Below the main window, a "Start Sequence 071029\_2wax.S" dialog box is open. This dialog box has several sections: "Method Sections To Run" with radio buttons for "Full Method" (selected) and "Reprocessing Only"; "On A Barcode Mismatch" with radio buttons for "Inject Anyway" (selected) and "Don't Inject"; "Sequence Comment" with the text "wax"; "Operator Name" with the text "Cervenkova"; and "Data File Directory" with the text "D:\DATA\". The "Run Sequence" button at the bottom of the dialog box is also circled in red. A red arrow points from the "Run Sequence..." menu option to the "Run Sequence" button in the dialog box. The background interface shows various controls, including a "Run Time" display, "Method" and "Instrument" tabs, and a "Total Ion" display.





„Solvent delay“

**Always NO !!!!!!!!!!!!!!!!!!!!!**

The screenshot shows the Instrument Control software interface. At the top, it displays the sample name 'Hexan' and data file '0000w.d'. A large green digital display shows '1.33' with 'Run Time: 7.33' below it. A 'Run' button is visible on the left. Below the main display are sections for 'Sequence', 'Method', and 'Instrument' with various icons. A central panel shows several numerical readouts: '138' for Oven Temperature, '250' for Aux-2 Temperature, '1.0' for Column-1 Flow Cal., '150' for Inlet-F Temperature, '150' for MS Quad, '100' for TurboSpd, '230' for MS Source, and '7.02e-006' for HiVac. An 'Acquisition' dialog box is open in the foreground, asking 'Override solvent delay [3.75 minutes]?' with a warning: 'Warning: Overriding solvent delay may shorten filament lifetime.' The 'No' button in this dialog is circled in red. At the bottom, there are windows for 'Total Ion' (showing 2.5E5) and 'Extracted Ion' (showing 2.5E2).

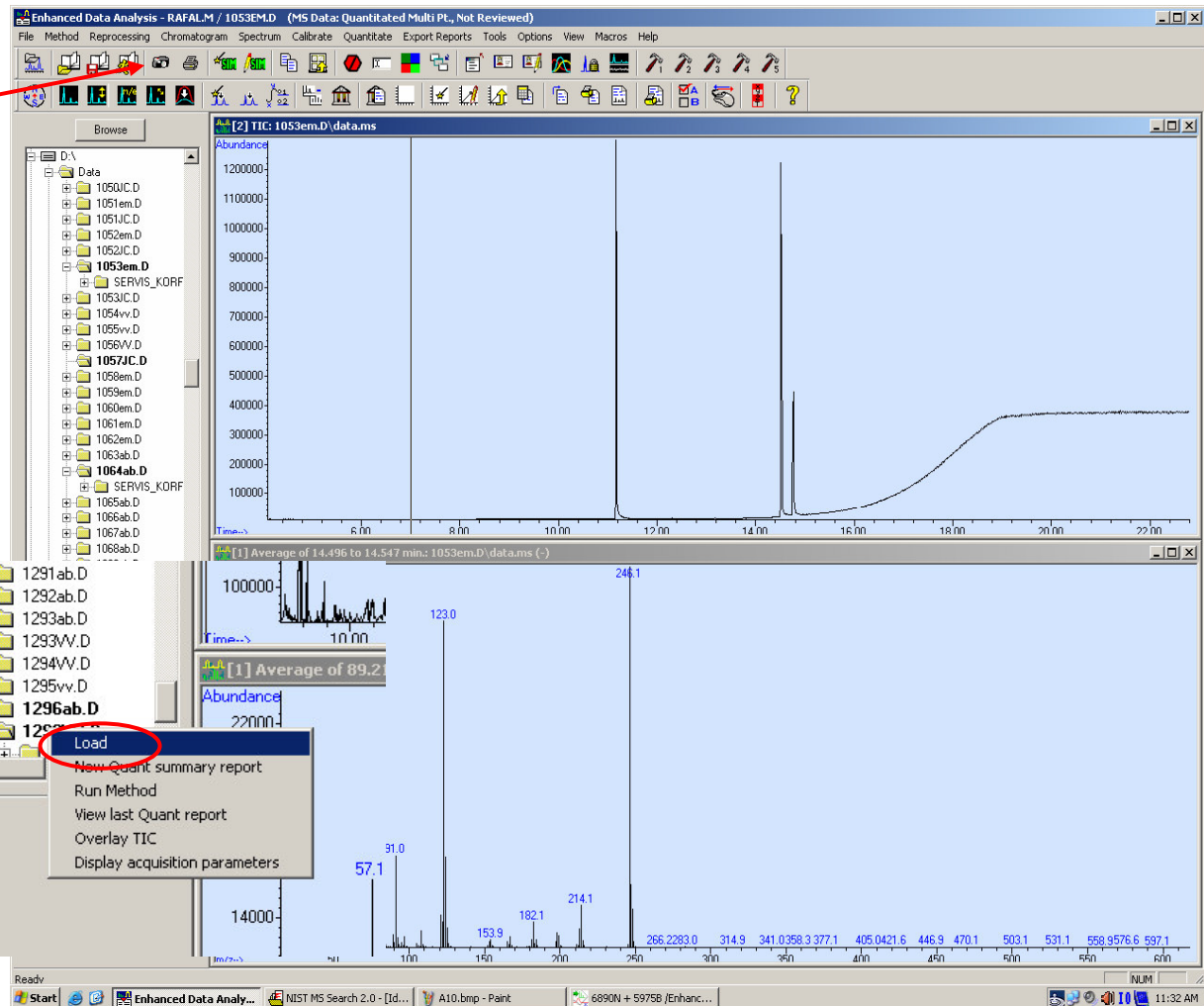
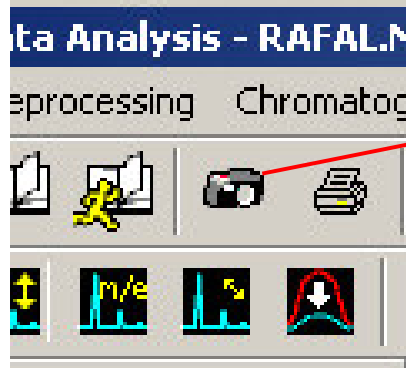


## Interpretation

- 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

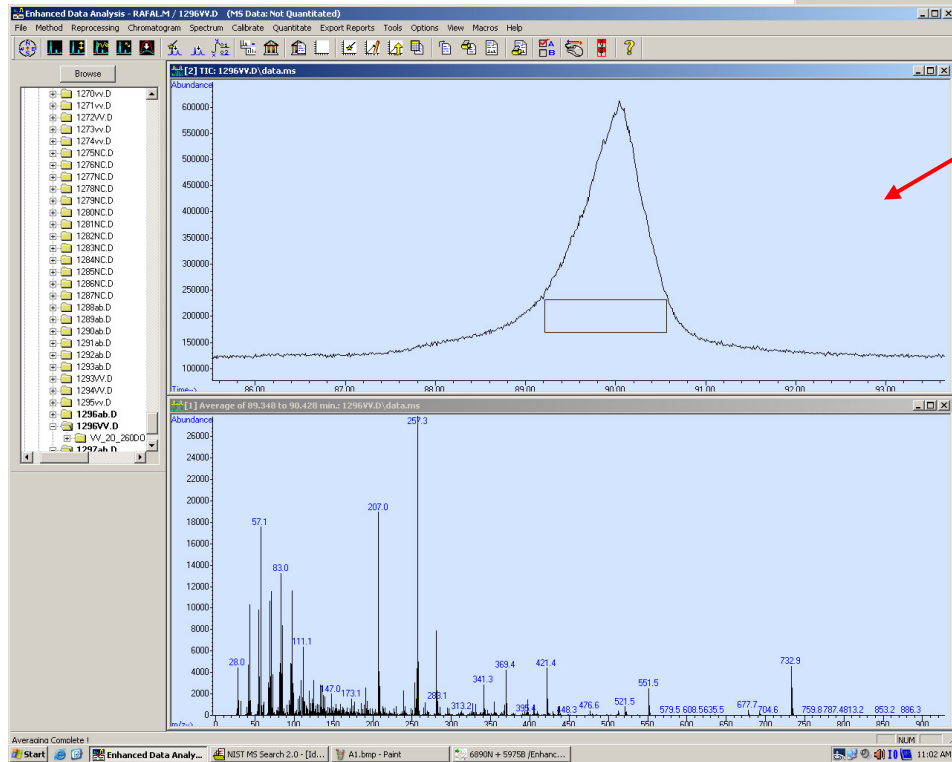
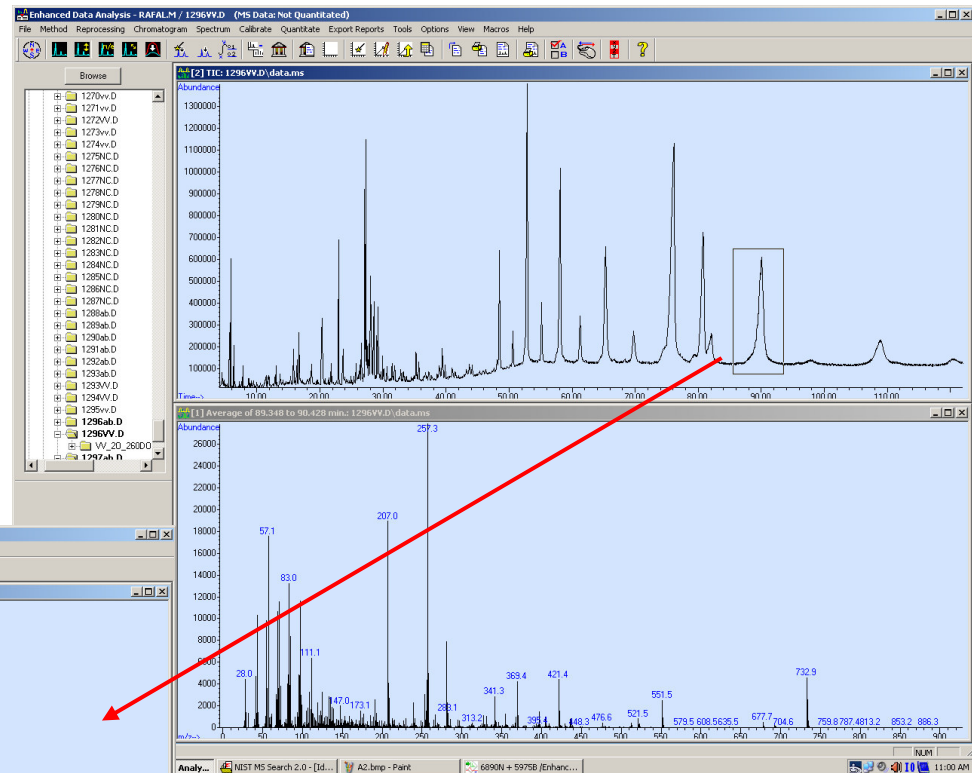
For running analysis – „Take Snapshot“



Load finished  
analysis → right click  
→ „Load“

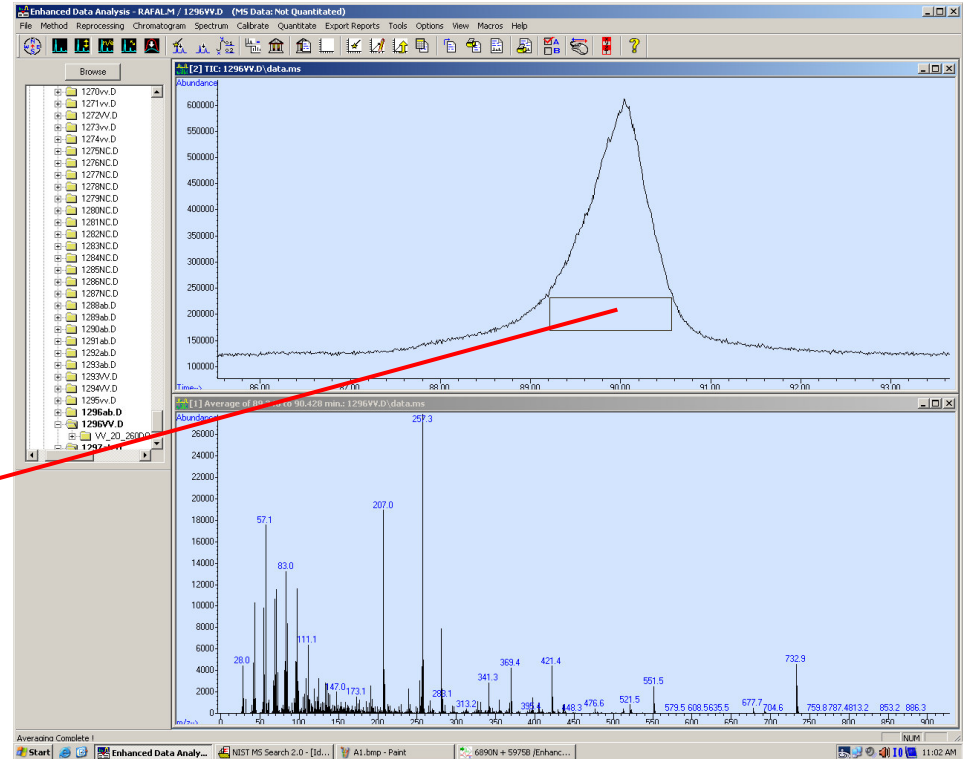
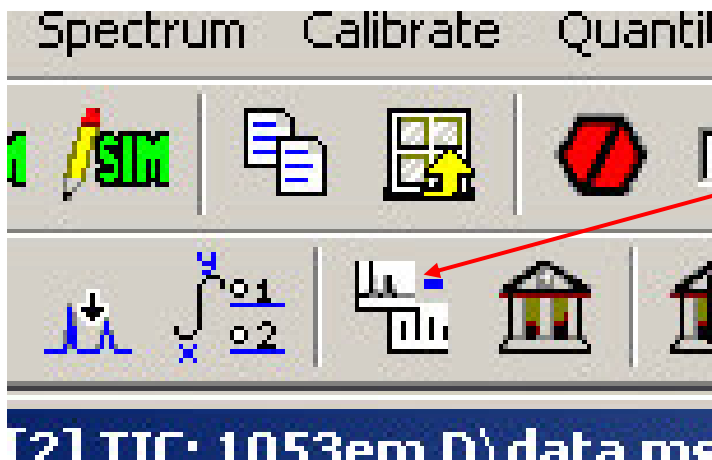


# Zoom peak



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

# Load spectrum and subtract background



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	1.89	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-epoxyoctadecanoate
9	M	528	596	0.76	9-Hexadecenoic acid, eicosyl ester, (Z)-
10	M	525	754	0.67	1-Diisopropylsilyloxydodecane
11	M	522	593	0.60	17-Perfluorooctadecane
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(chloromethyl)silyloxytridecane
20	M	503	553	0.28	Triarac fine
21	R	500	581	0.24	Oleic acid, 3-(octadecyloxy)propyl ester
22	M	500	540	0.24	Oleic acid, 3-(octadecyloxy)propyl ester
23	M	499	547	0.23	Octadecane, 1-[2-(hexadecyloxy)ethyl]oxy
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-Butyldimethyl(4-methyl)dodecylsilyloxy
29	M	493	548	0.18	Lanosta-7(11)-dien-18-ol acid, 22,25-diacetate
30	M	492	652	0.17	Boron, [4-]dimethyl(1-methyl-1-butyl)silyloxy
31	M	492	584	0.17	1-Hentetracontanol
32	M	492	553	0.17	Distearylthiodipropionate
33	M	491	547	0.17	Octadecanoic acid, 2-(octadecyloxy)ethyl ester
34	M	490	570	0.16	9-Octadecene, 1,1'-[1,2-ethanedithiyl]bis-
35	M	489	585	0.15	Neroneine, 4,8,5-dihydro-
36	M	488	589	0.15	Bacteriocinophorol-1-stearyl
37	M	487	587	0.14	9-Hexadecenoic acid, hexadecyl ester

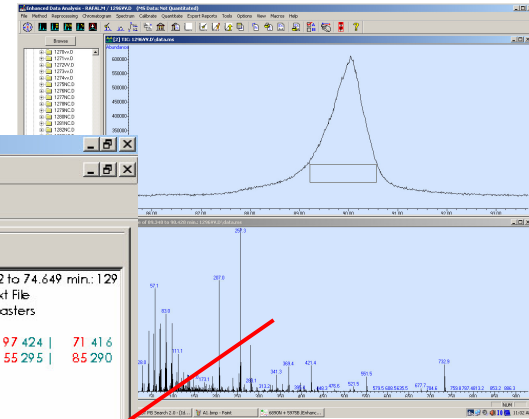
Names Structures InLib = -1163, Hit List

Lib. Search Other Search Names Compare Librarian MSMS

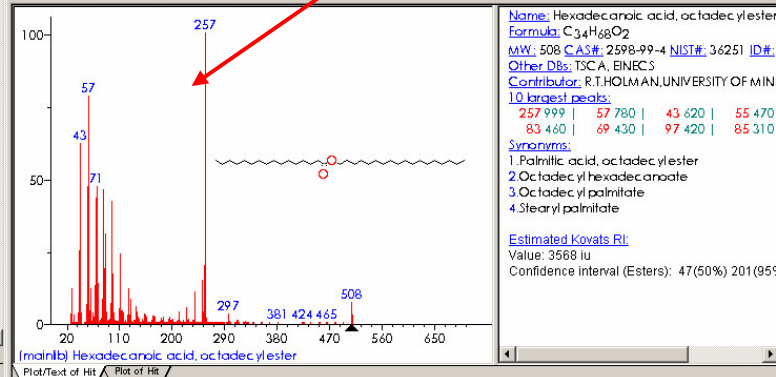
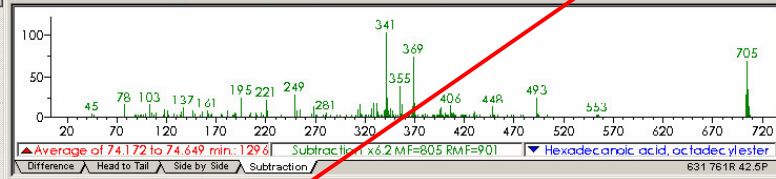
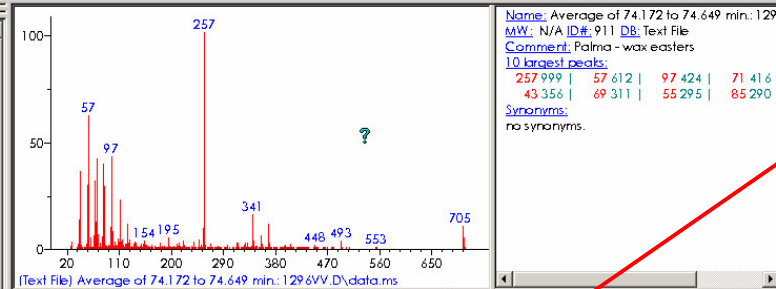
For Help, press F1

Ident Ident

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

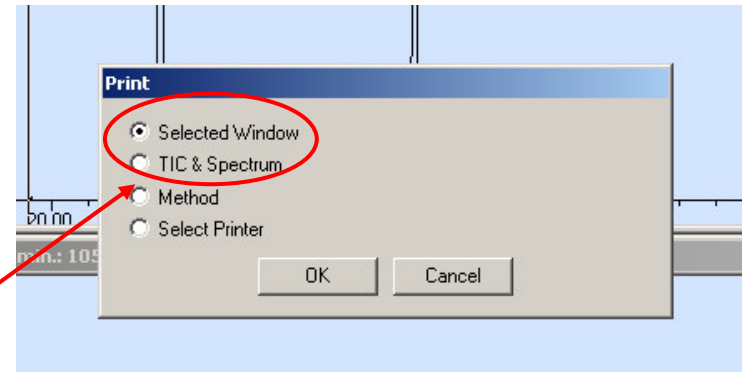
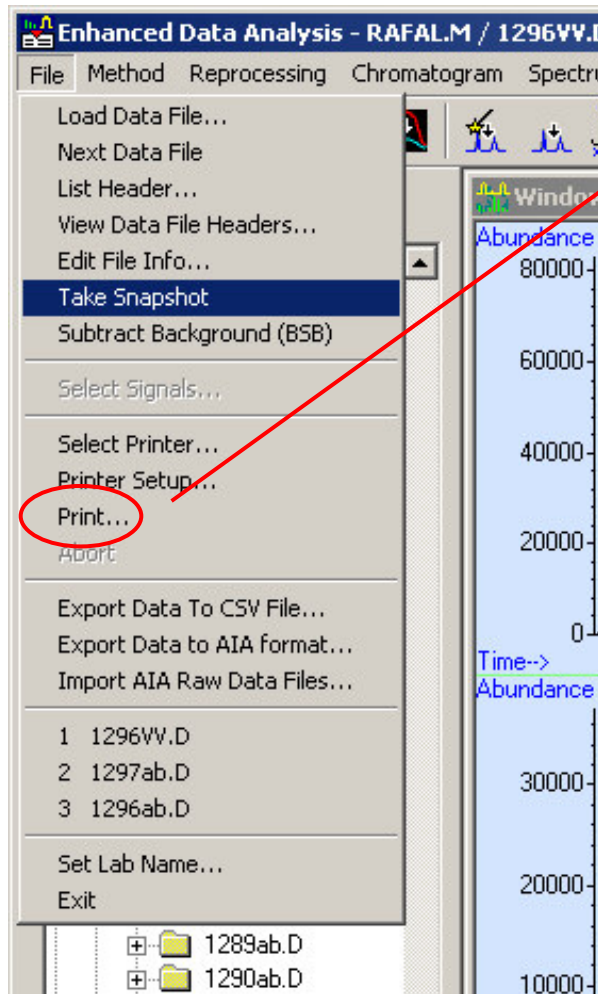


Right double-click on spectrum

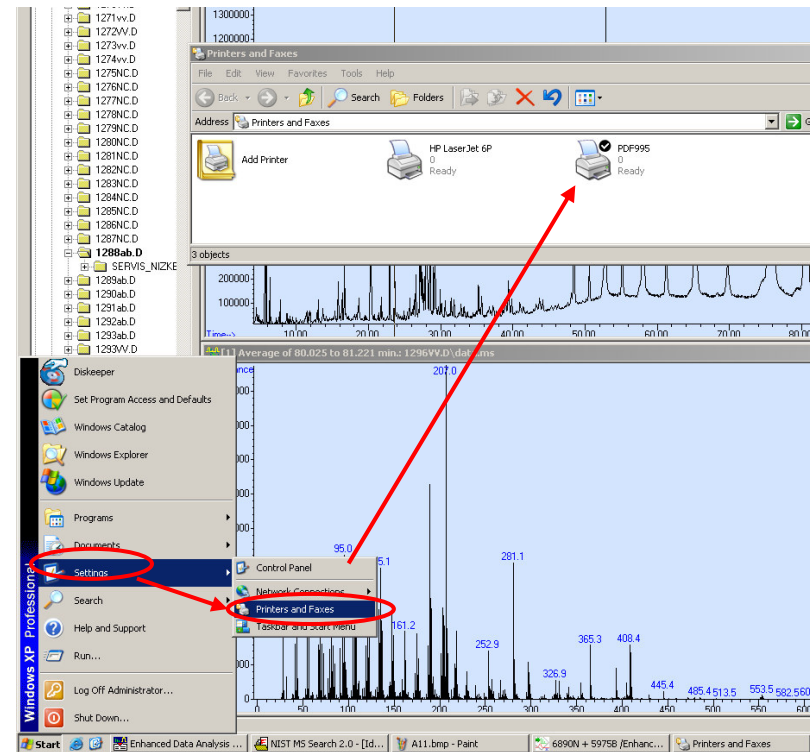




# Print to PDF or paper

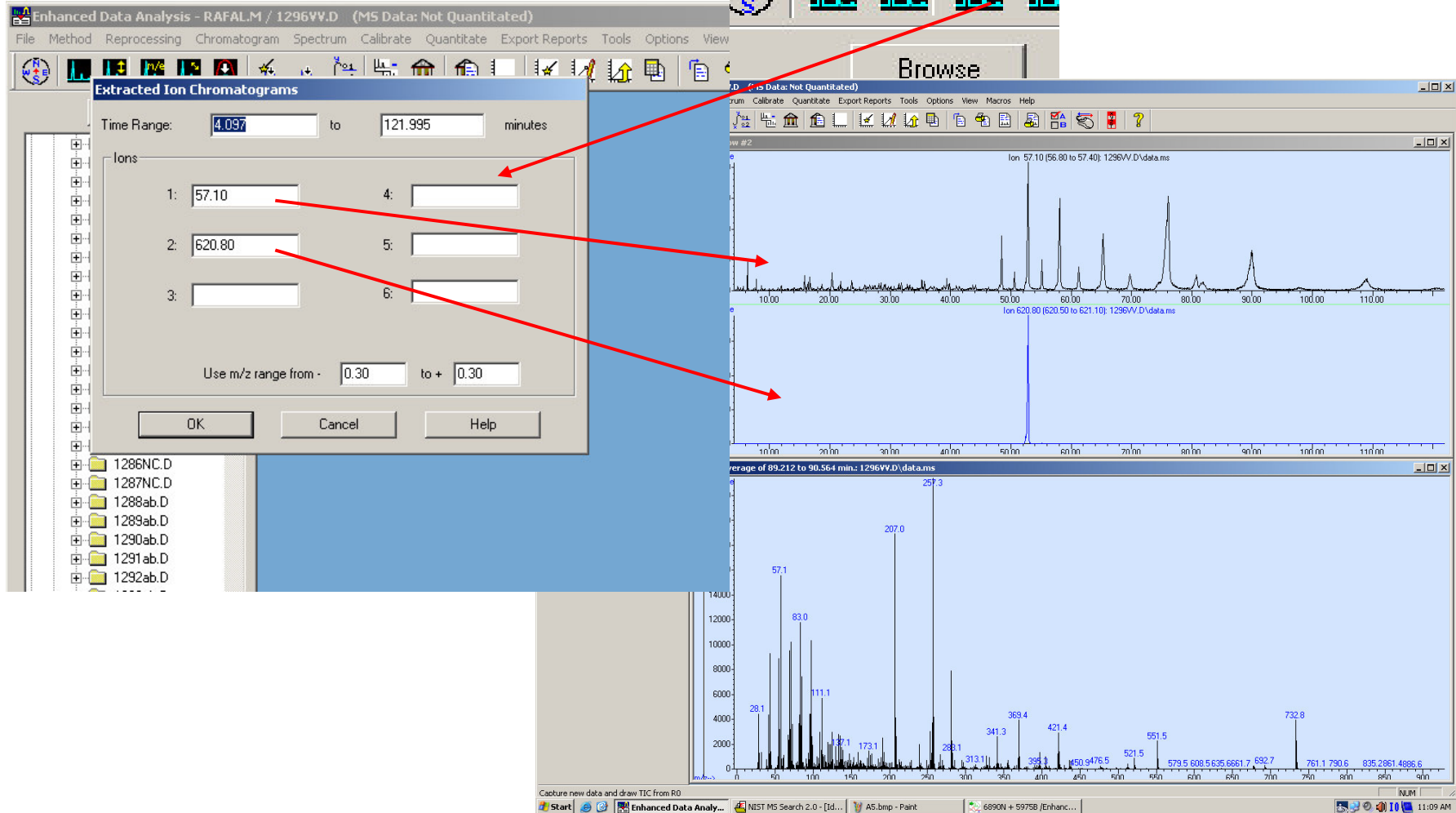
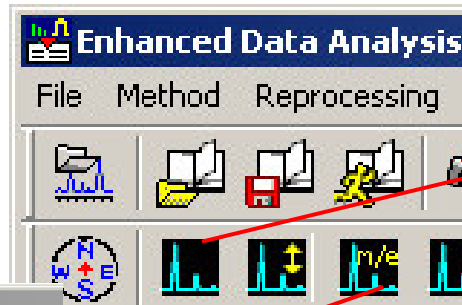


## Set printer as Default





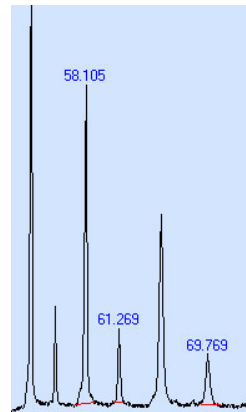
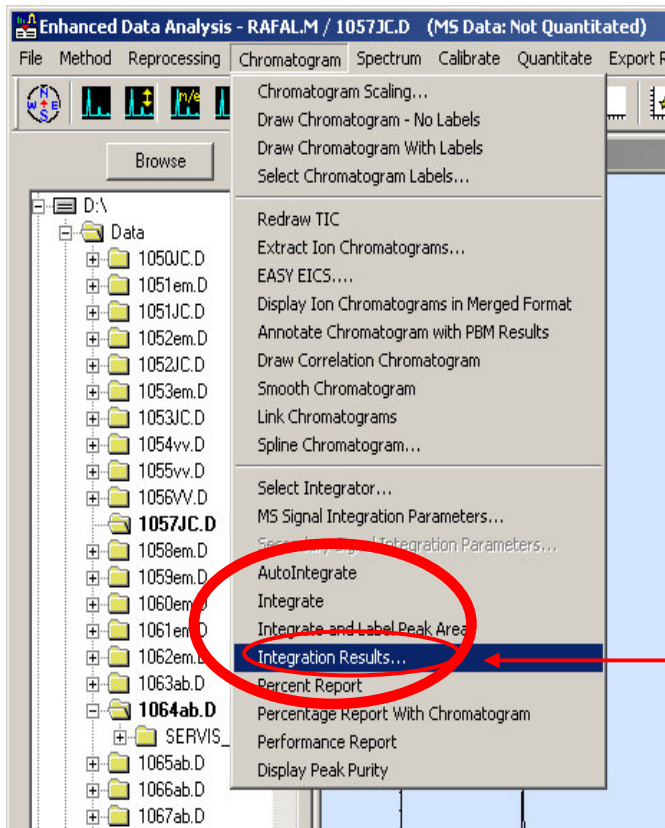
# Extracted ion chromatogram



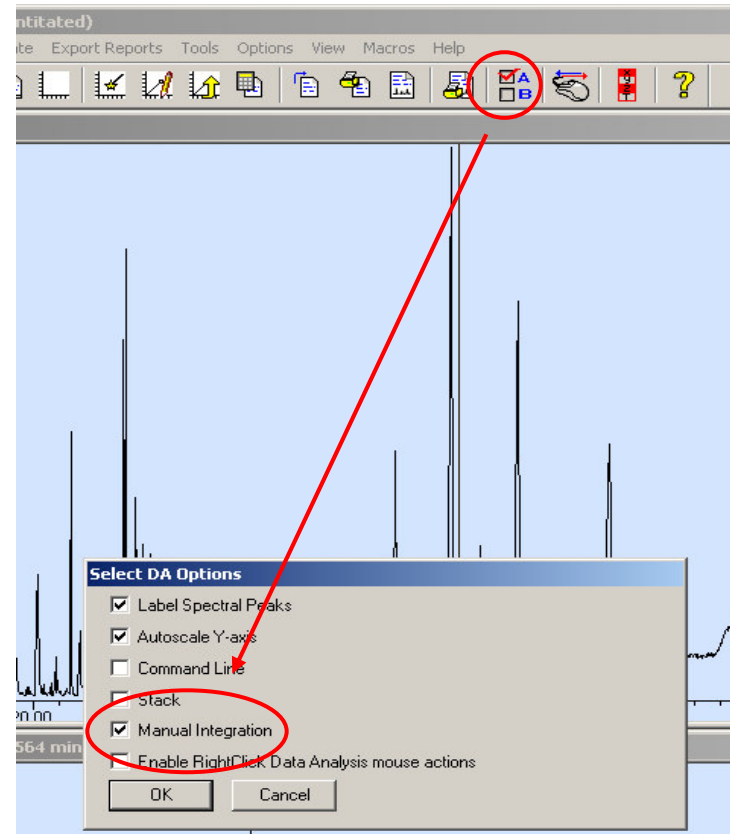


# Integration

## 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 shows the 'Select Files for TIC Overlay: 1296VV.D' dialog, where files are selected from the 'Available Data Files' list and moved to the 'Files Selected for Processing' list. The 'Process' button is highlighted. A secondary dialog, 'Select Overlay Mode', is shown with 'TIC' selected. The bottom window displays the resulting overlaid chromatogram, showing two traces: TIC: 1296VV.D\data.ms (black) and TIC: 1294VV.D\data.ms (blue).

File	Sample Name
1290ab.D	blank, smet
1291ab.D	ribek_VH221_1
1292ab.D	blank, CHC3
1293ab.D	Severa_LS049_01
1293VV.D	blank
1295VV.D	blank, CHC3
1296ab.D	blank, CHC3
1297ab.D	Ubik_rozkladne pro

File	Sample Name
D:\Data\1294VV.D	Palma - wax easters
D:\Data\1296VV.D	Palma - wax easters