

# Software pro GC/MS



**budova A  
přízemí SV  
místnost 107**



# ChemStation

estery TIC.pdf

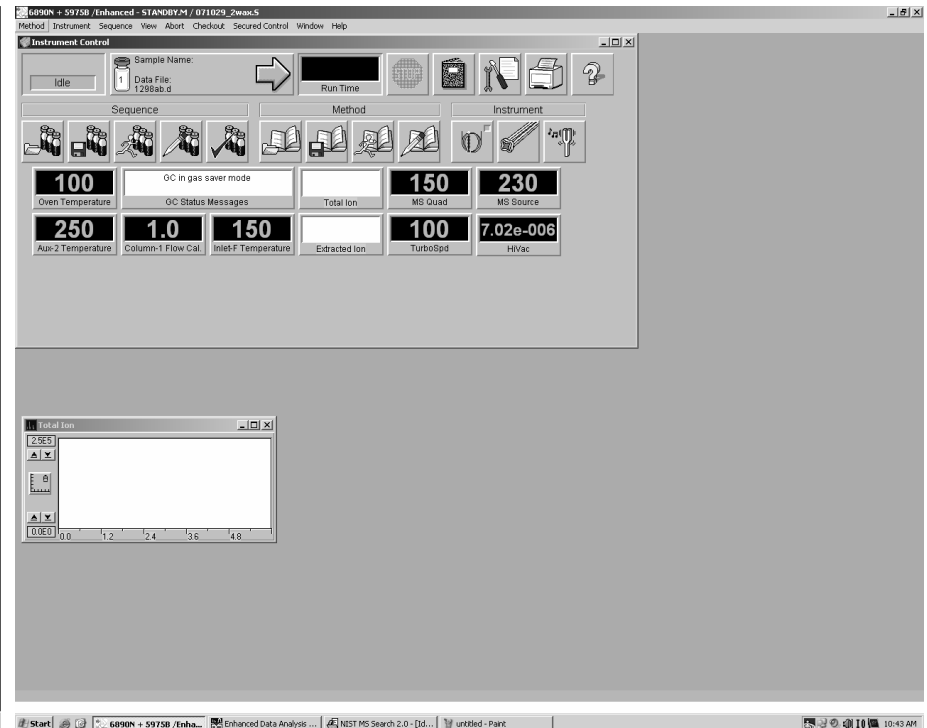
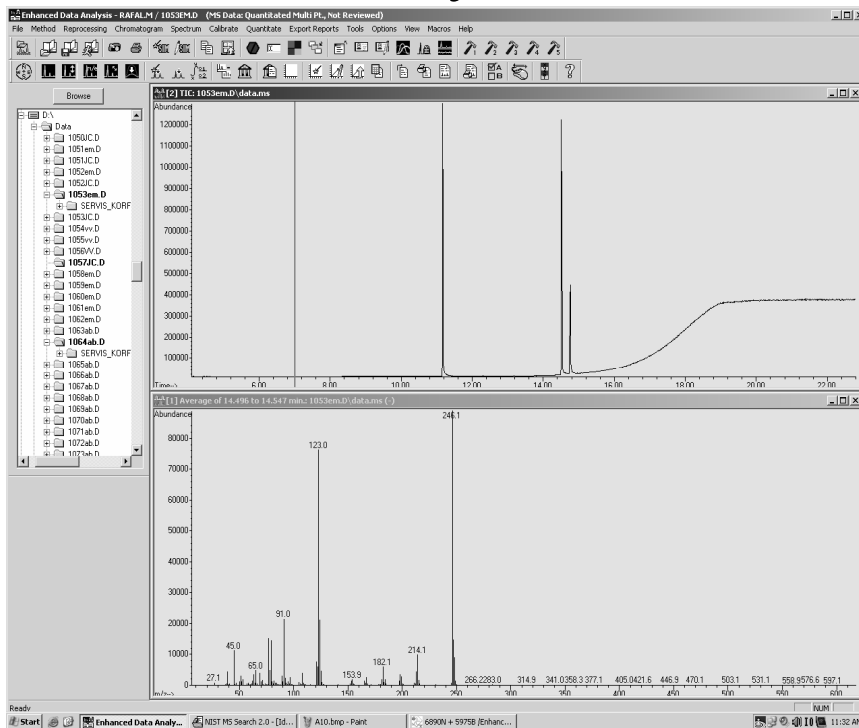
Start

Enhanced Data Analysis ...

6890N + 5975B /Enhanc...

Vyhodnocování

Měření



# Spuštění analýzy

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

The screenshot displays the Agilent ChemStation software interface. 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, showing options such as "Load Sequence...", "Save Sequence", "Save Sequence As...", "Run Sequence...", "Print Sequence...", "Edit Sequence..." (circled in red), "Import Sequence Information from CSV File...", "Simulate Sequence", and "Position and Run Sequence...". Below these are four sequence entries: "1 Ubik bitrex 2 071106.S", "2 Ubik bitrex 071106.S", "3 Hrbek+Severa 071101.S", and "4 Blank ether 071101.S". At the bottom of the menu are "View Sequence Log ...", "View Sequence Quality Log", "Print Sequence Log", "Configure Sequence Table...", "Batch Mode...", and "Additional Sequence Options...".

The main interface features a "Run Time" display, a "STOP" button, and a toolbar with icons for a file, a printer, and a help icon. Below the toolbar are sections for "Method" and "Instrument". The "Method" section contains icons for a book, a book with a floppy disk, a book with a person, and a book with a pencil. The "Instrument" section contains icons for a ball, a test tube, and a musical instrument. The interface also displays several numerical values in large boxes: "100" (Oven Tempera), "250" (Aux-2 Tempera), "150" (MS Quad), "230" (MS Source), "100" (TurboSpd), and "7.03e-006" (HiVac). The "Total Ion" and "Extracted Ion" displays are currently blank.

# 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 $\Delta$ 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												
6												
7												
8												
9												
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34												
35												

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

## Smažte předchozí sekvenci

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 for row 2:

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

označit myší řádky  
→ klik pravým tlačítkem  
→ „Delete Rows“

# Vyplňte tabulku

Sample Log Table

Data Path: D:\DATA Browse... Method Path: C:\MSDCHEM1\METHODS Browse...

	Type	Vial	Sample	Method / Keyword	Data File	Comment / KeywordString	Multiplier	Level	Update RF	Update RT	Update OI	Up_2
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												
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36												

Read Barcode OK Cancel Help

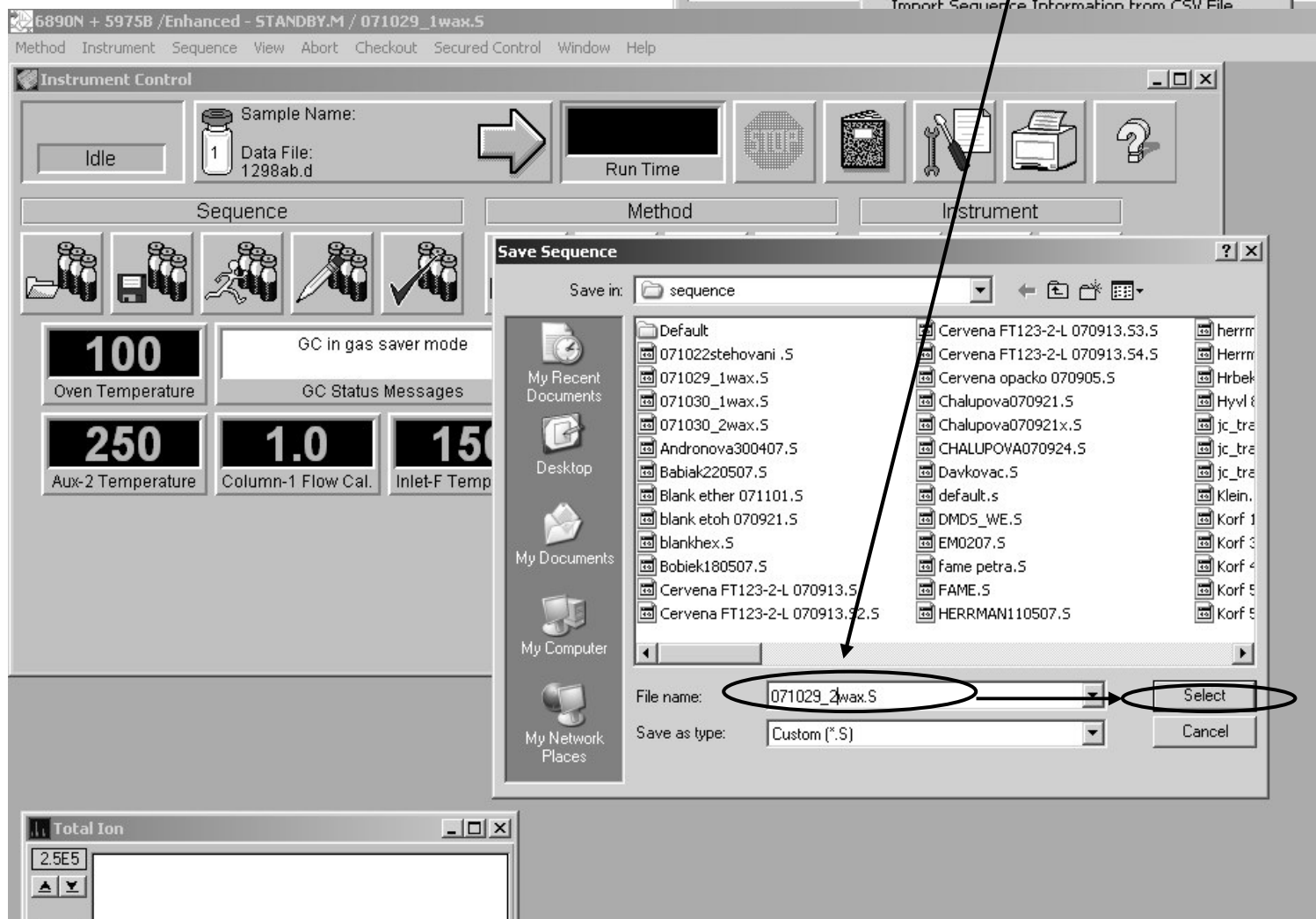
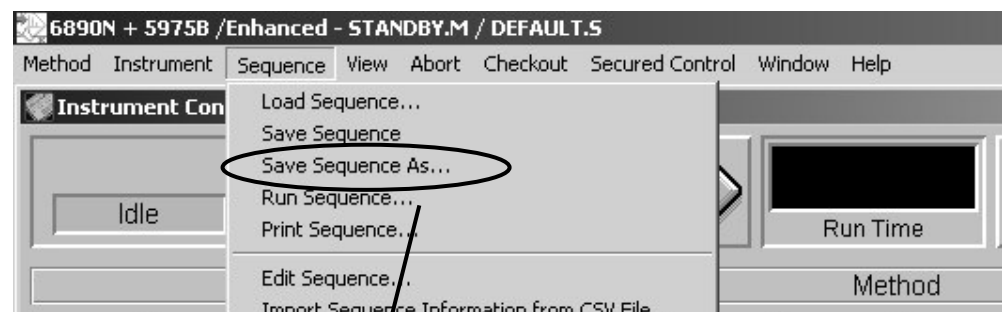
Start 6890N + 5975B /Enhanc... Sample Log Table Enhanced Data Analysis... NIST MS Search 2.0 - [Id... untitled - Paint 10:35 AM

metoda  
 popis vzorku  
 datový soubor  
 popis vzorku  
 poloha vzorku v autosampleru  
 blank nebo vzorek ?

Po vyplnění a kontrole → OK

název metody	teplota nástřiku	split*	hmotnostní rozsah	teplotní program
AS_M-nizke_C-nizke	200°C	10:1	do 600 m/z	40°C(4min) →8°C/min do 200→15°C/min do 320°C (3min)
AS_M-nizke_C-vysoke	200°C	100:1	do 600 m/z	40°C (4min) →8°C/min do 200→15°C/min do 320°C (3min)
AS_M- vysoke _C-nizke	230°C	10:1	do 800 m/z	60°C(4min) →10°C/min do 320°C (3min)
AS_M- vysoke _C-vysoke	230°C	100:1	do 800 m/z	60°C(4min) →10°C/min do 320°C (3min)

# Uložte sekvenci



# Spustíte analýzu

The image displays a chromatography software interface with two main windows. The top window, titled "6890N + 5975B /Enhanced - STANDBY.M / DEFAULT.S", shows a menu with "Run Sequence..." circled. The bottom window, titled "6890N + 5975B /Enhanced - STANDBY.M / 071029\_2wax.S", shows a "Start Sequence" dialog box with "Run Sequence" circled. A red arrow points from the circled menu item to the circled dialog button.

**Start Sequence 071029\_2wax.S Last Modified: Mon Oct 29 11:03:09 2007**

Method Sections To Run

- Full Method
- Reprocessing Only

Overwrite Existing Data Files

On A Barcode Mismatch

- Inject Anyway
- Don't Inject

Sequence Comment: wax

Operator Name: Cervenkova

Data File Directory: D:\DATA\ Browse..

Run Sequence OK Cancel Help More>>

Enter the operator name





„Solvent delay“

**Vždy NO !!!!!!!!!!!!!!!!!!!!!**

6890N + 5975B /Enhanced - STANDBY\_AS.M / 071029\_2wax.S  
Sequence 071029\_2wax.S is running...

Instrument Control

Run    Sample Name: Hexan    Run Time: 7.33    STOP    ?

Data File: 0000w.d

Sequence    Method    Instrument

138    GC Status Messages    Total Ion    150    230  
Oven Temperature    MS Quad    MS Source

250    1.0    150    Extracted Ion    100    7.02e-006  
Aux-2 Temperature    Column-1 Flow Cal.    Inlet-F Temperature    TurboSpd    HiVac

Acquisition

Override solvent delay [3.75 minutes]?  
Warning: Overriding solvent delay may shorten filament lifetime.

Yes    No

Total Ion    2.5E5

Extracted Ion    2.5E2

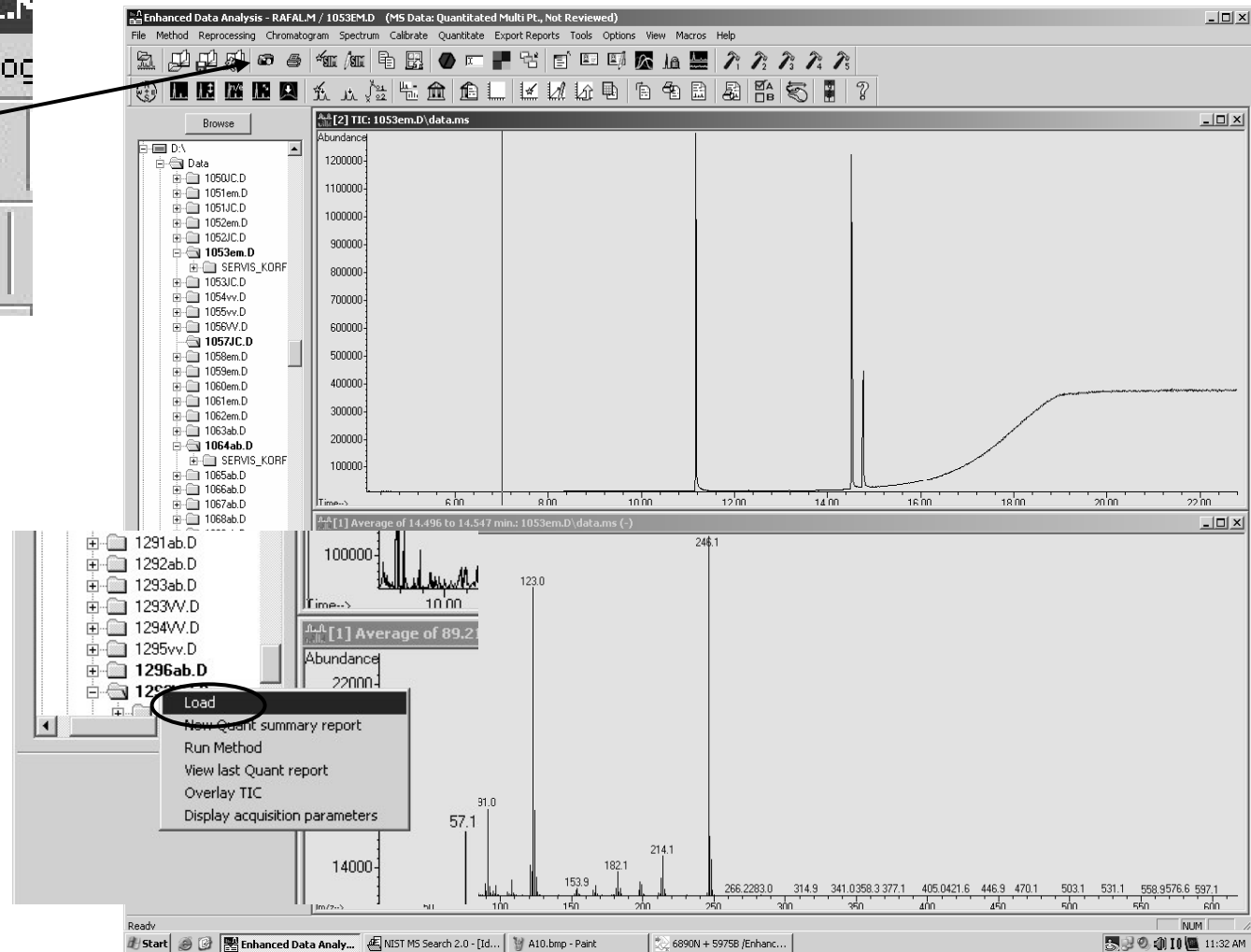
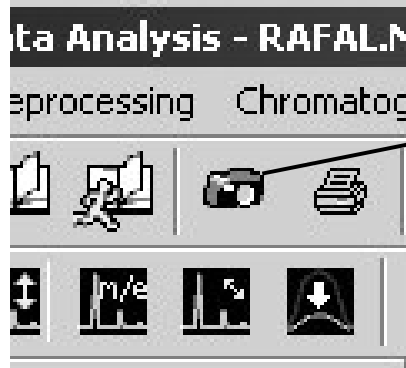


## Vyhodnocení

- Pokud máte k dispozici *ChemStation* :  
stáhnout data z D/DATA/....přes *ftp*: klienta v  
*Total Commander* nebo flash disk
  - Licence na *ChemStation* – J. Cvačka
- Pokud nemáte k dispozici *ChemStation*  
můžete si vyhodnotit svá data na PC v  
místnosti 107
- Naměřená data si zálohujte na svých  
počítačích, budou se průběžně mazat

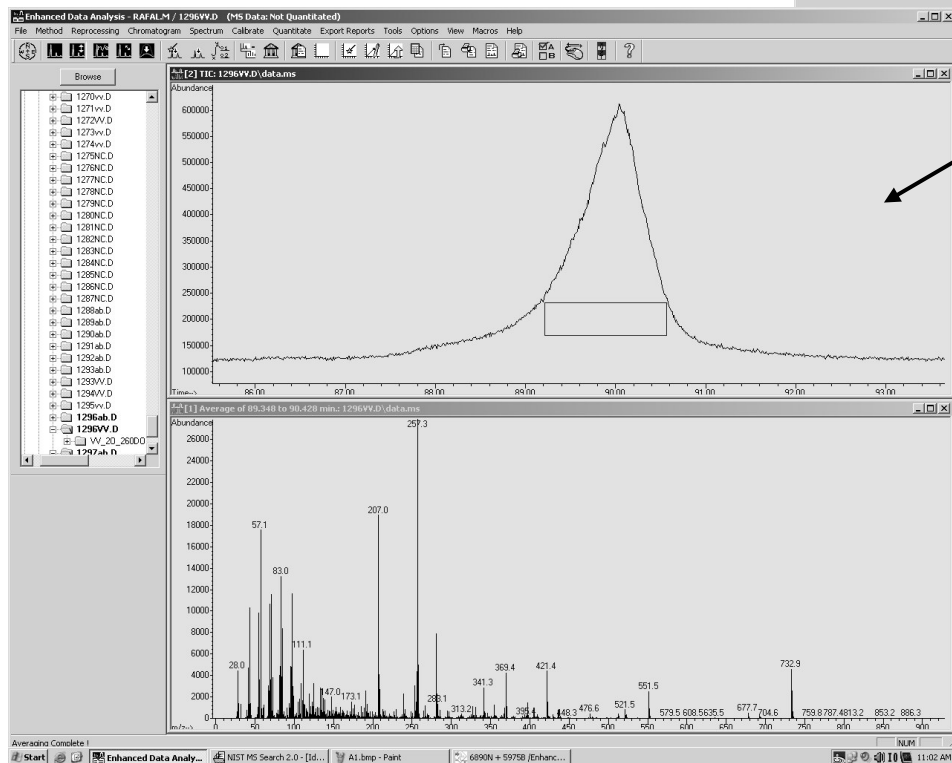
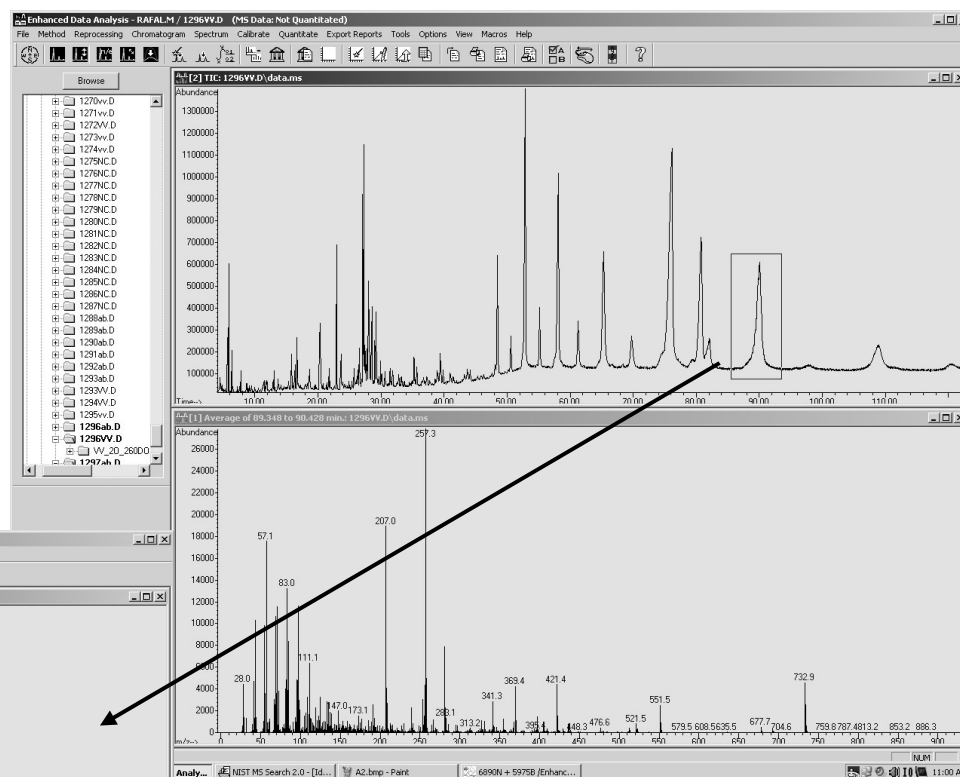
# Otevření naměřených dat

## Otevření probíhající analýzy – „Take Snapshot“



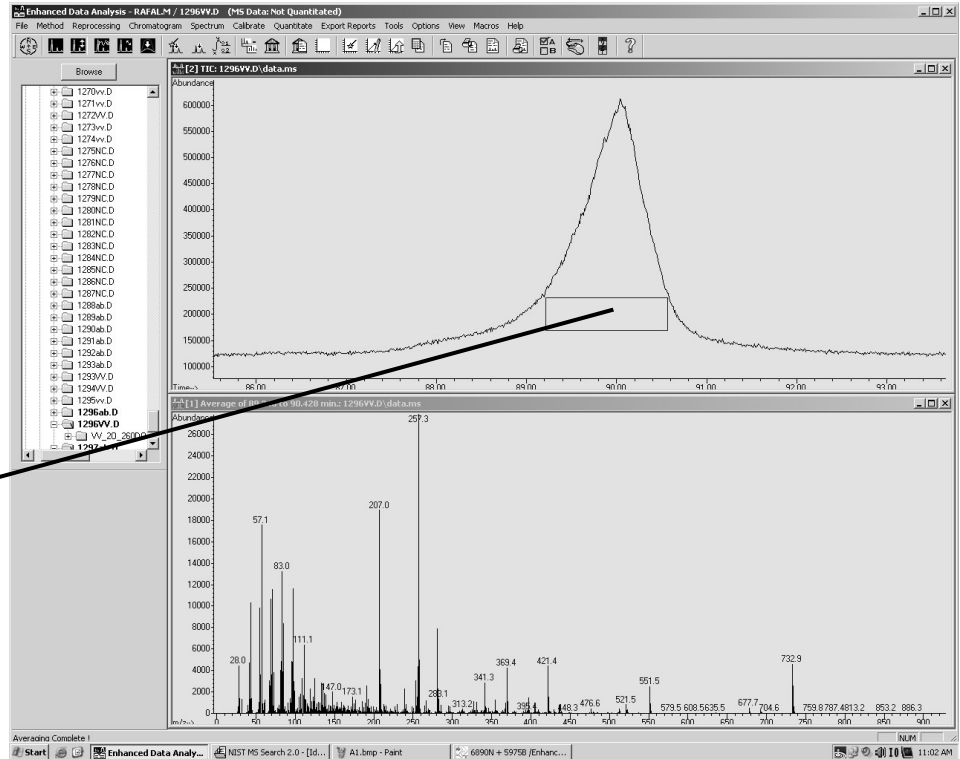
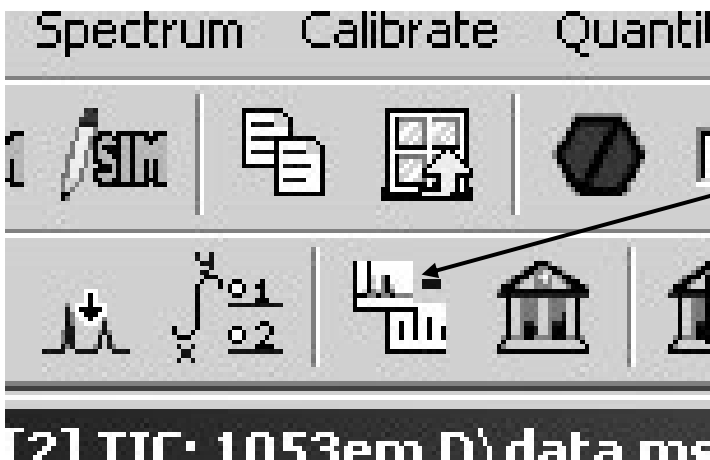
Otevření doměřené analýzy → Pravé tlačítko myši na souboru → „Load“

# Zvětšení píku



Potáhnutí levým tlačítkem myši  
– požadovaná oblast v rámečku  
(zpět – dvojklik levým tlačítkem  
myši)

# Sejmutí spektra a odečtení pozadí



## Odečtení pozadí

1. Sejmout spektrum píku
2. Sejmout spektrum pozadí
3. Kliknout na ikonu „Subtract“

Sejmutí spektra – potáhnutí pravým tlačítkem myši – požadovaná oblast v rámečku  
(zpět – dvojklik levým tlačítkem myši)

# Prohledávání knihovny - NIST

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-epoxycarboxylic acid
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-Perfluorooctane
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-Dimethylchloromethylsilyloxytridecane
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]butane
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-ethanedithiylbis(2-oxo-2-(propan-2-ylideneamino)ethyl)]-
35	M	489	585	0.15	Neroneine, 4,8,5-dihydro-
36	M	488	589	0.15	Bacteriocinophorolide-3-stearyl
37	M	487	587	0.14	9-Hexadecenoic acid, hexadecyl ester

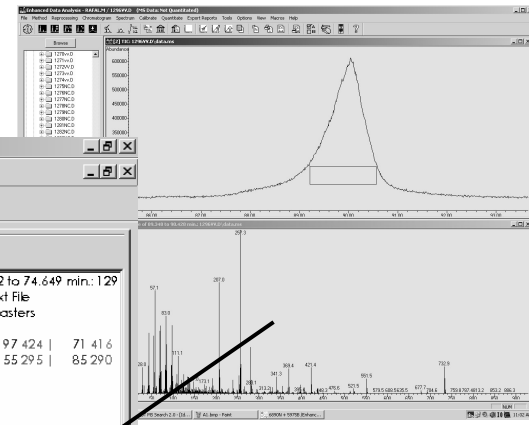
Names Structures InLib = -1163, Hit List

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



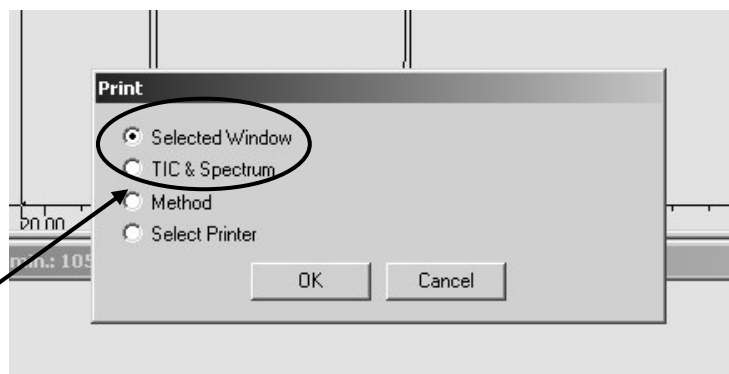
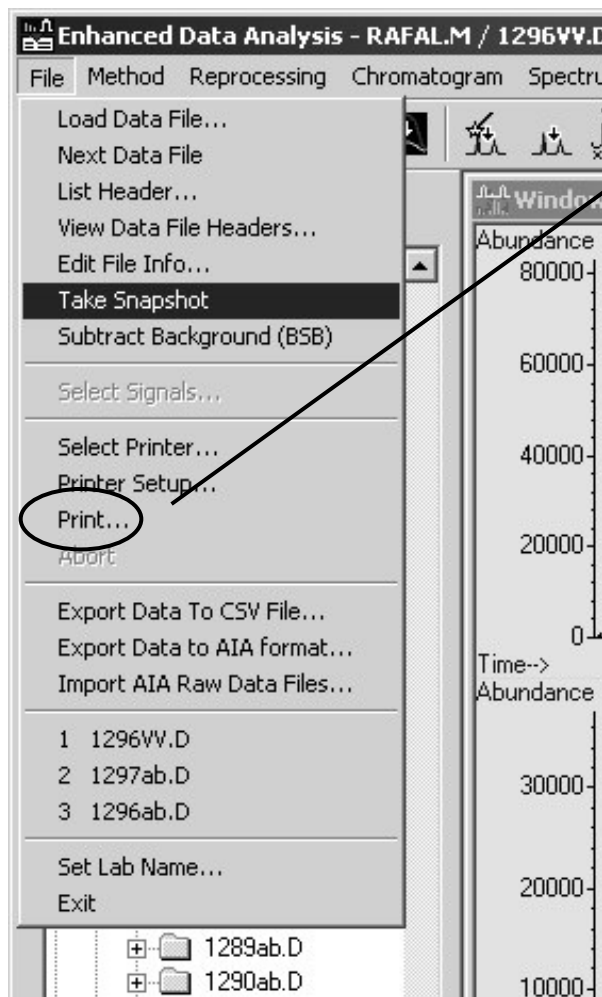
Dvojklik pravým tlačítkem myši na spektrum

Name: Average of 74.172 to 74.649 min.: 129  
MW: N/A ID#: 911 DB: Text File  
Comment: Palma - wax esters  
10 largest peaks:  
257 999 | 57 612 | 97 424 | 71 416  
43 356 | 69 311 | 55 295 | 85 290  
Synonyms:  
no synonyms.

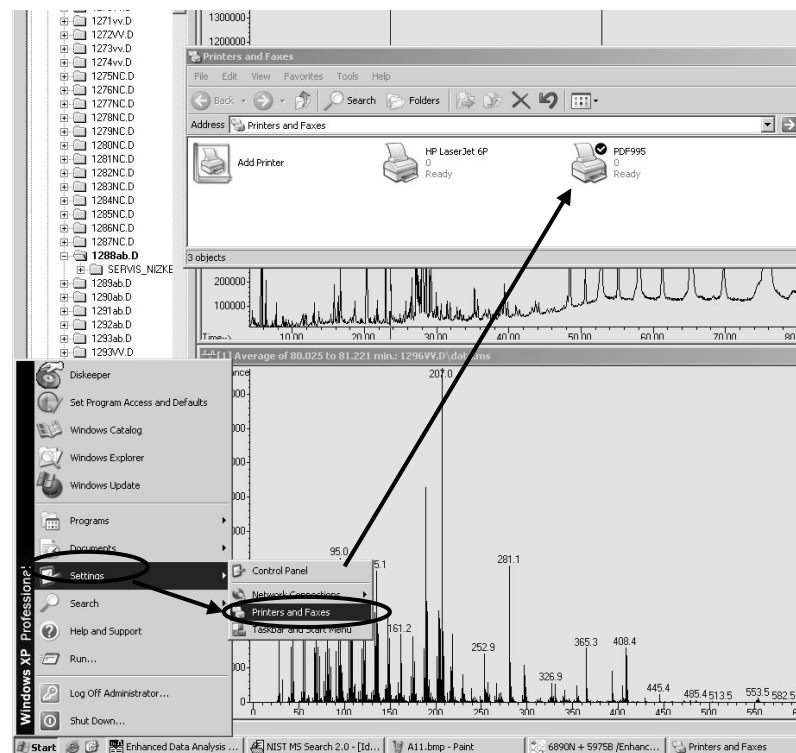
Average of 74.172 to 74.649 min.: 129% Subtraction x3.2 MF=805 RMF=901 Hexadecanoic acid, octadecyl ester

Name: Hexadecanoic acid, octadecyl ester  
Formula: C<sub>34</sub>H<sub>68</sub>O<sub>2</sub>  
MW: 508 CAS#: 2598-99-4 NIST#: 36251 ID#:  
Other DBs: TSCA, EINECS  
Contributor: R.T.HOLMAN, UNIVERSITY OF MINN  
10 largest peaks:  
257 999 | 57 780 | 43 620 | 55 470  
83 460 | 69 430 | 97 420 | 85 310  
Synonyms:  
1. Palmitic acid, octadecyl ester  
2. Octadecyl hexadecanoate  
3. Octadecyl palmitate  
4. Stearyl palmitate  
Estimated Kovats RI:  
Value: 3568 Iu  
Confidence interval (Esters): 47(50%) 201(85%)

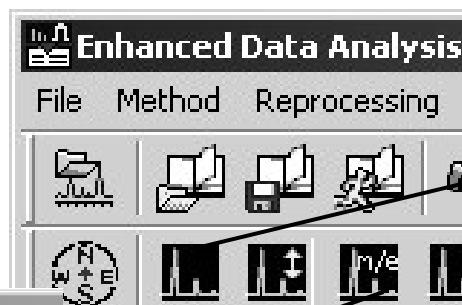
Tisk na papír nebo  
do PDF



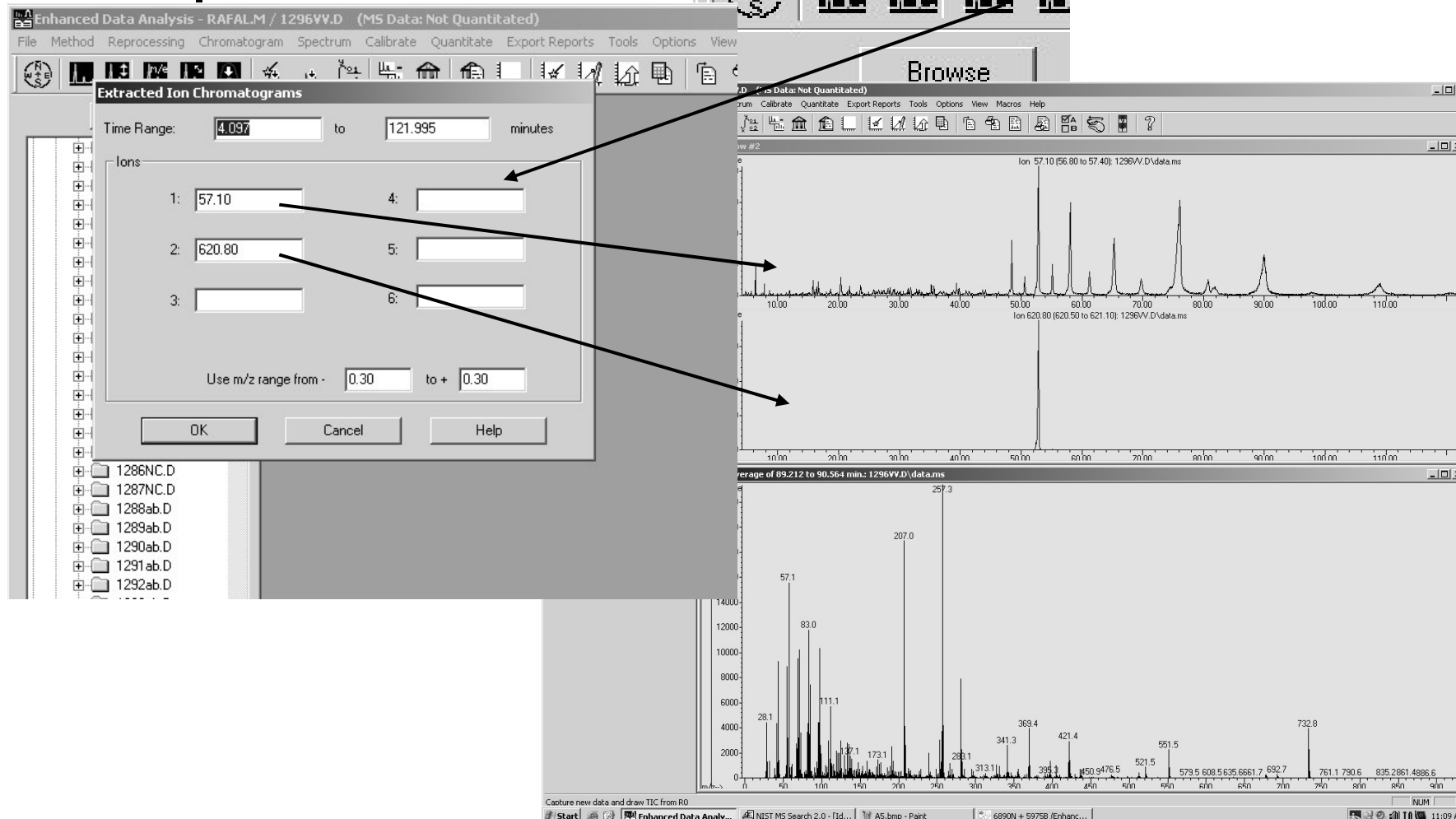
Pozn: Požadovanou tiskárnu nastavit  
„defaultně“ v nastavení počítače



# Zobrazení extrahovaného chromatogramu



Návrat k „TICu“

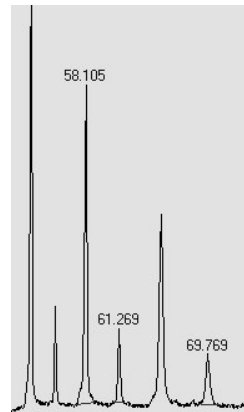
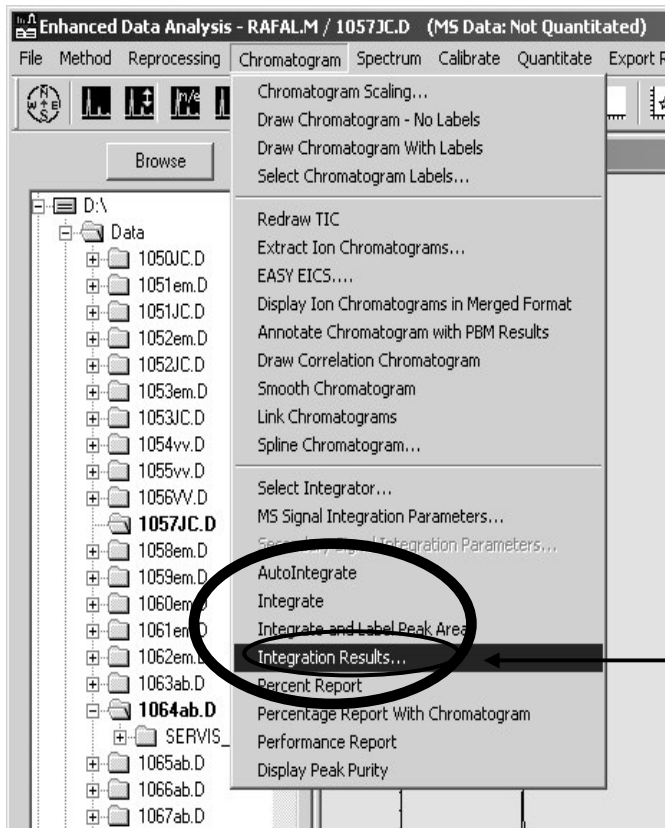




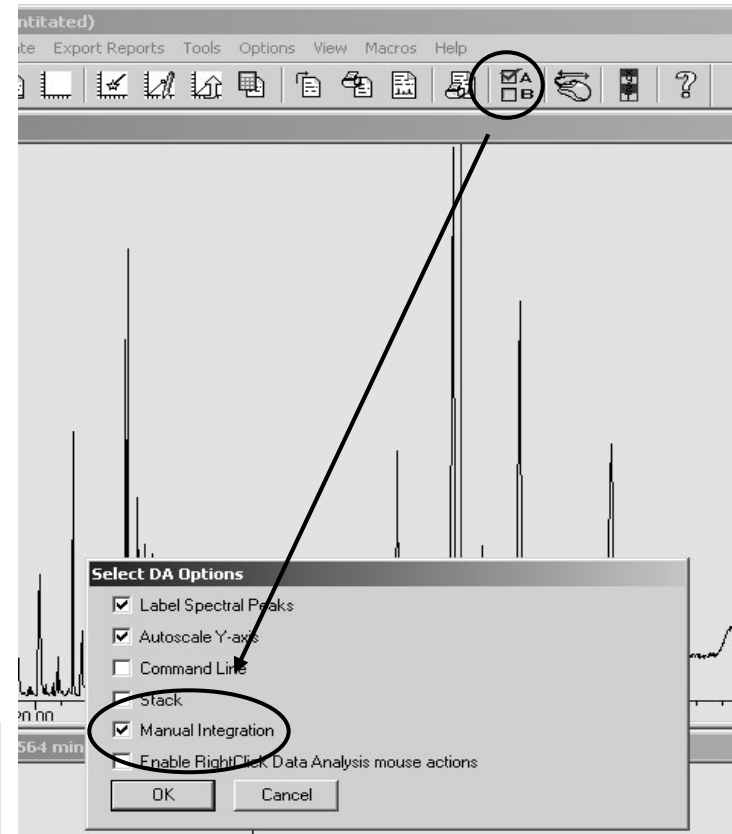


# Integrace

## Automatická integrace



## Manuální integrace



Integrace – potáhnutí pravým tlačítkem myši při základně píku

# Překrývání chromatogramů

The image illustrates the process of overlaying chromatograms in MSD ChemStation. The main window shows a file list on the left with '1288ab.D' and '1294VV.D' highlighted. A dialog box titled 'Select Files for TIC Overlay: 1296VV.D' is open, showing a list of available data files and a list of files selected for processing. The 'Process' button is circled. An inset window shows the 'Select Overlay Mode' dialog with 'TIC' selected. The bottom window shows the resulting overlaid chromatogram with two traces: 'TIC: 1296VV.D\data.ms' and 'TIC: 1294VV.D\data.ms'.

File	Sample Name
1290ab.D	blank, smet
1291ab.D	Prbek_VH221_1
1292ab.D	blank, CHCl3
1293ab.D	Severa, LSD149_01
1293VV.D	blank
1293V.D	blank, CHCl3
1293VV.D	blank, CHCl3
1297ab.D	Ubik, rozkladne pro...

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



# Informační zdroje

- K dispozici jsou
  - Zjednodušený návod k obsluze + informace o metodách
  - Tato přednáška vytištěná a na ploše počítače
  - Manuál k ChemStation na ploše počítače
  - HELP v programu
- **V případě problémů s měřením kontaktujte pracovníky oddělení MS – tel. 302, 492**