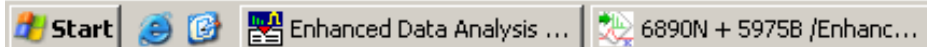


Software pro GC/MS



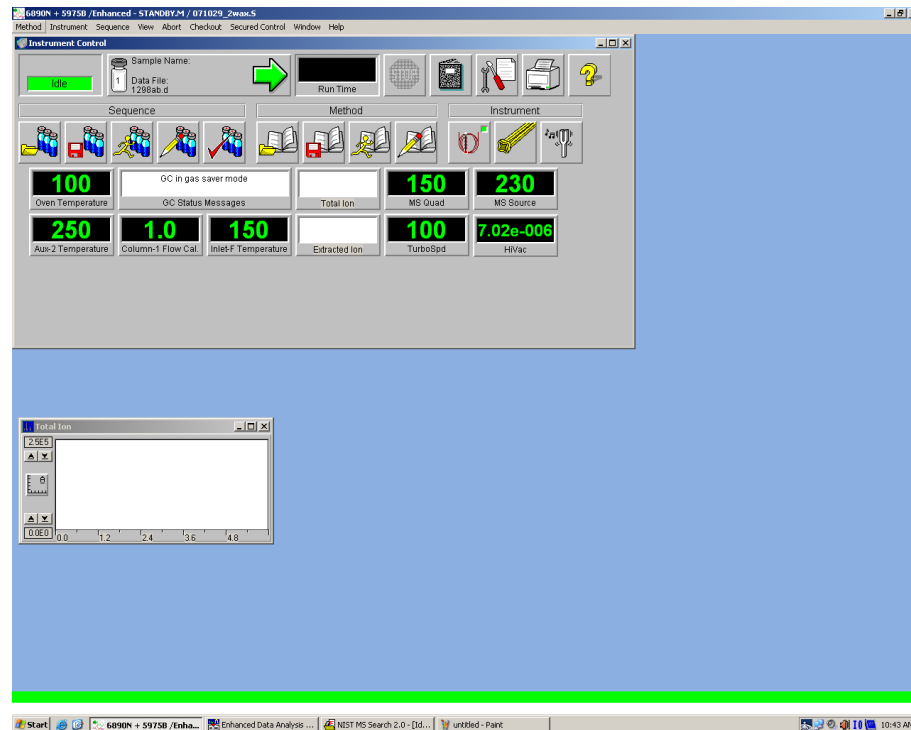
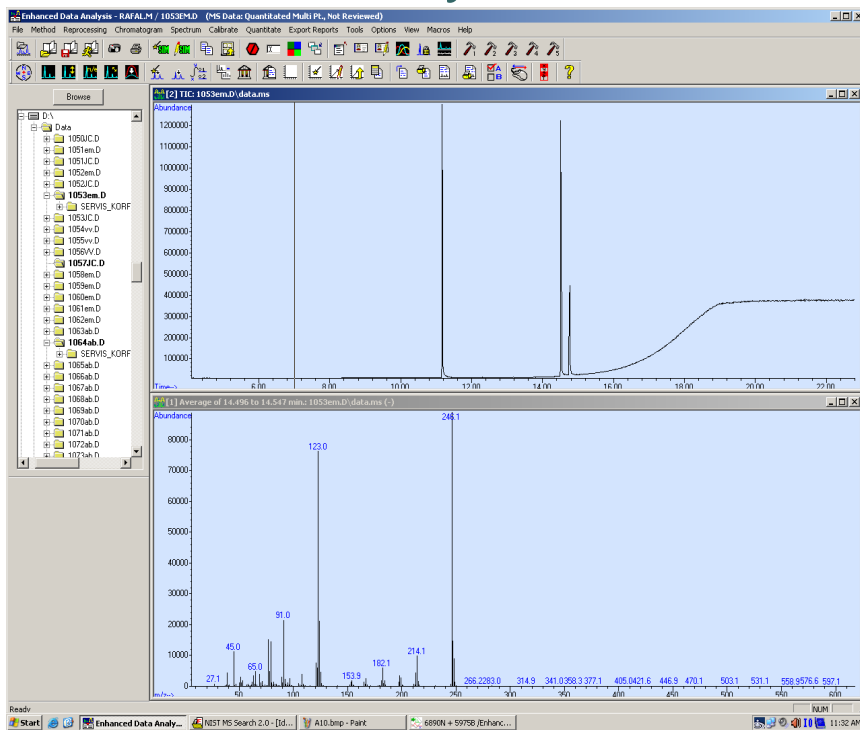
ChemStation

estery TIC.pdf



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, with "Edit Sequence..." circled in red. The interface also shows a status bar with "Idle", a list of sequences (1 Ubik bitrex 2 071106.S, 2 Ubik bitrex 071106.S, 3 Hrbek+Severa 071101.S, 4 Blank ether 071101.S), and various instrument parameters: Oven Temperature (100), Aux-2 Temperature (250), Total Ion, Extracted Ion, MS Quad (150), TurboSpd (100), MS Source (230), and HiVac (7.03e-006).

6890N + 5975B /Enhanced - STANDBY.M / DEFAULT.S

Method Instrument Sequence View Abort Checkout Secured Control Window Help

Instrument Control

Idle

100
Oven Temperature

250
Aux-2 Temperature

1 Ubik bitrex 2 071106.S
2 Ubik bitrex 071106.S
3 Hrbek+Severa 071101.S
4 Blank ether 071101.S

View Sequence Log ...
View Sequence Quality Log
Print Sequence Log

Configure Sequence Table...
Batch Mode...
Additional Sequence Options...

Run Time

Method

Instrument

Total Ion

Extracted Ion

MS Quad

TurboSpd

MS Source

HiVac

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												
10												
11												
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31												
32												
33												
34												
35												

Sheet1

Start | 6890N + 5975B /Enhanc... | Sample Log Table | Enhanced Data Analysis ... | NIST MS Search 2.0 - [Id... | untitled - 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
1				
1				
1				
1				
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

- 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												
8												
9												
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31												
32												
33												
34												
35												

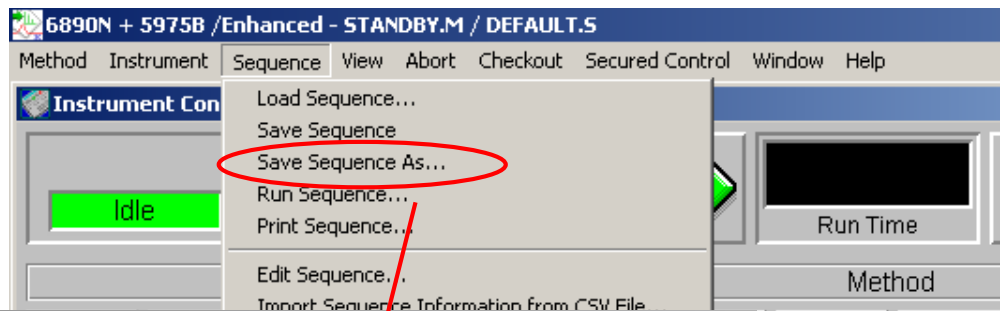
Blank nebo vzorek ?
 poloha vzorku v autosampleru
 popis vzorku
 metoda
 datový soubor
 popis vzorku

Po vyplnění a kontrole → OK

Read Barcode OK Cancel Help

název metody	teplota nástřiku	split*	hmotnostní rozsah	teplotní program
AS_M-nizke_C-nizke	200°C	10:1	do 600 m/z	40°C(2min) →8°C/min do 200→15°C/min do 320°C (3 min)
AS_M-nizke_C-vysoke	200°C	50:1	do 600 m/z	40°C (2min) →8°C/min do 200→15°C/min do 320°C (3 min)
AS_M- vysoke _C-nizke	230°C	10:1	do 800 m/z	60°C(2min) →10°C/min do 320°C (10 min)
AS_M- vysoke _C-vysoke	230°C	50:1	do 800 m/z	60°C(2min) →10°C/min do 320°C (10 min)

Uložte sekvenci



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:' location as 'sequence'. The file list includes various sequence files, with '071029_2max.S' selected. The 'File name:' field is also set to '071029_2max.S', and the 'Select' button is circled in red. The background interface shows the 'Instrument Control' window with a 'Run Time' button and various temperature and flow rate displays.

Instrument Control

Sample Name: 1
Data File: 1298ab.d

Run Time

Sequence

Method

Instrument

Save Sequence

Save in: sequence

File name: 071029_2max.S

Save as type: Custom (*.S)

Select

Cancel

Total Ion

2.5E5

Spustíte analýzu

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" (circled in red); and "Data File Directory" with the text "D:\DATA\". At the bottom of the dialog box, the "Run Sequence" button is circled in red. The background interface shows various controls, including a "Run Time" display showing "100", and several icons for sequence and method management.

„Solvent delay“

Vždy NO !!!!!!!!!!!!!!!!

The screenshot displays the Instrument Control software interface. At the top, the window title is "6890N + 5975B /Enhanced - STANDBY_AS.M / 071029_2wax.5" and the status bar indicates "Sequence 071029_2wax.5 is running...". The main control panel includes a "Run" button, sample information (Sample Name: Hexan, Data File: 0000w.d), a large digital display showing "1.33" with "Run Time: 7.33" below it, and a red "STOP" button. Below these are sections for "Sequence", "Method", and "Instrument" with various icons. A central dashboard 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 Total Ion, "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 two small data windows: "Total Ion" showing "2.5E5" and "Extracted Ion" showing "2.5E2".

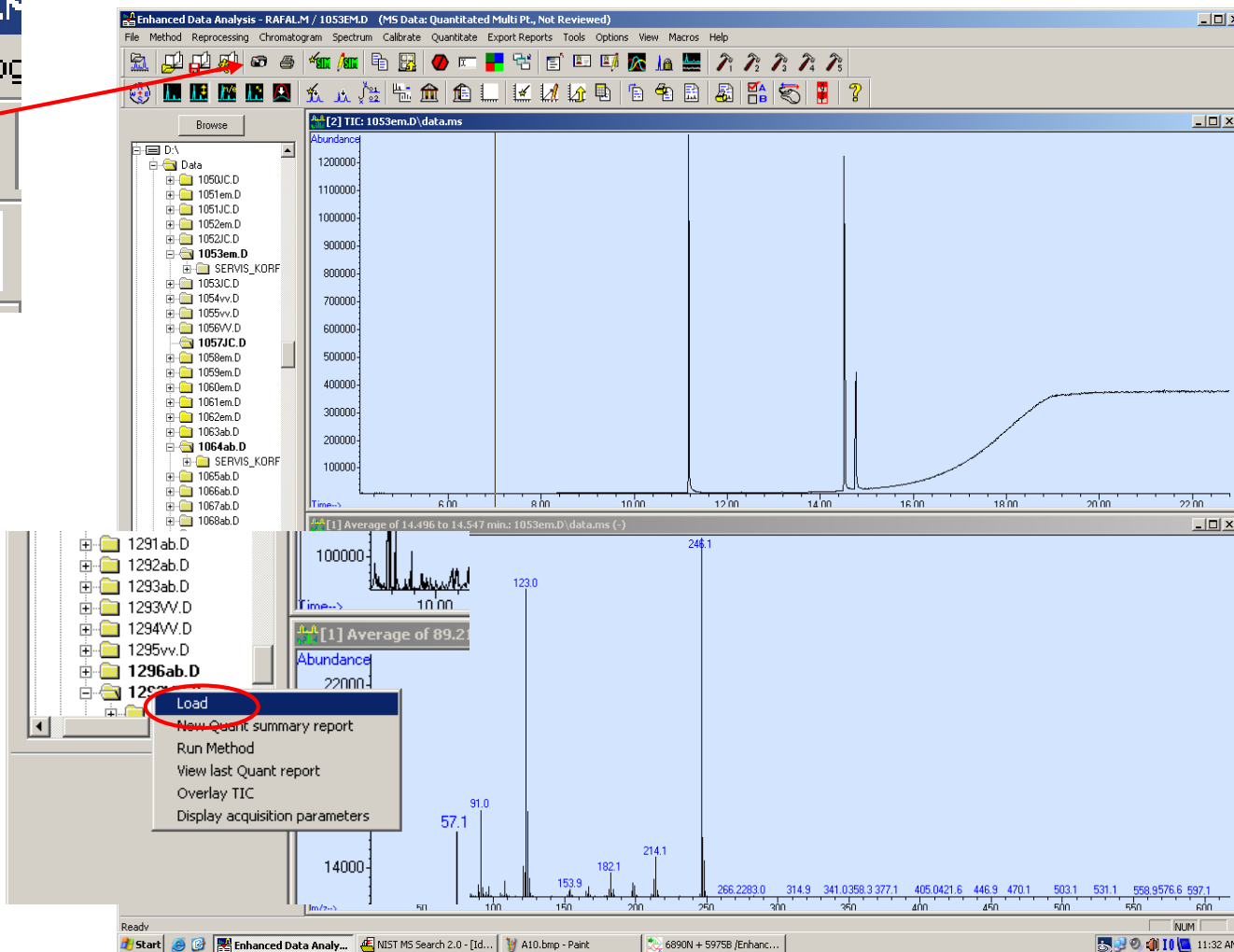
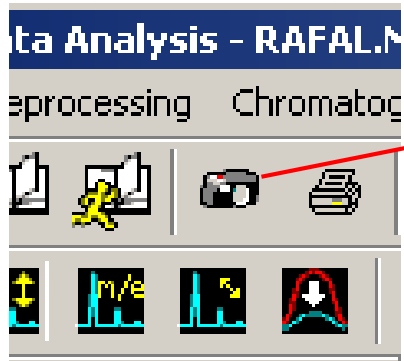


Vyhodnocení

- 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

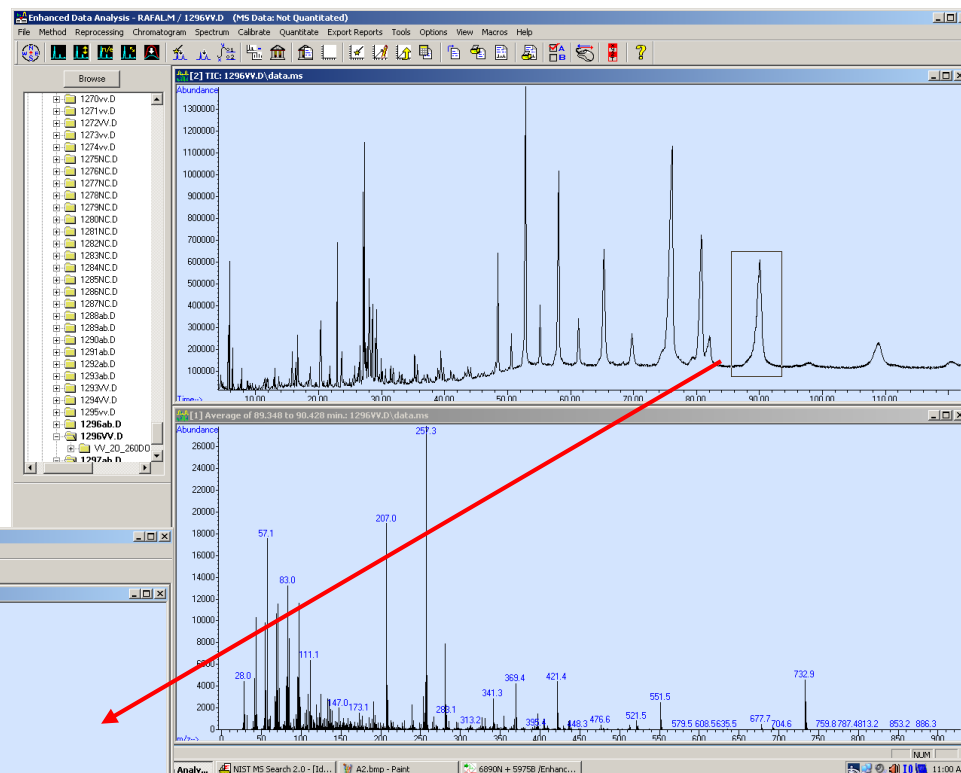
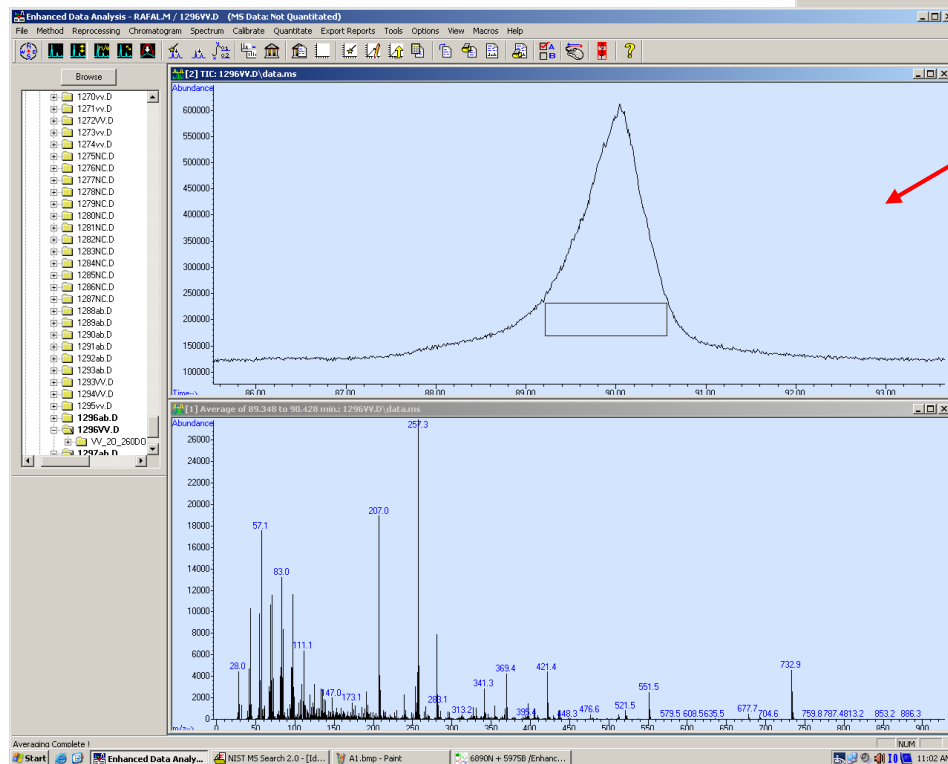
Otevření naměřených dat

Otevření probíhající analýzy – „Take Snapshot“



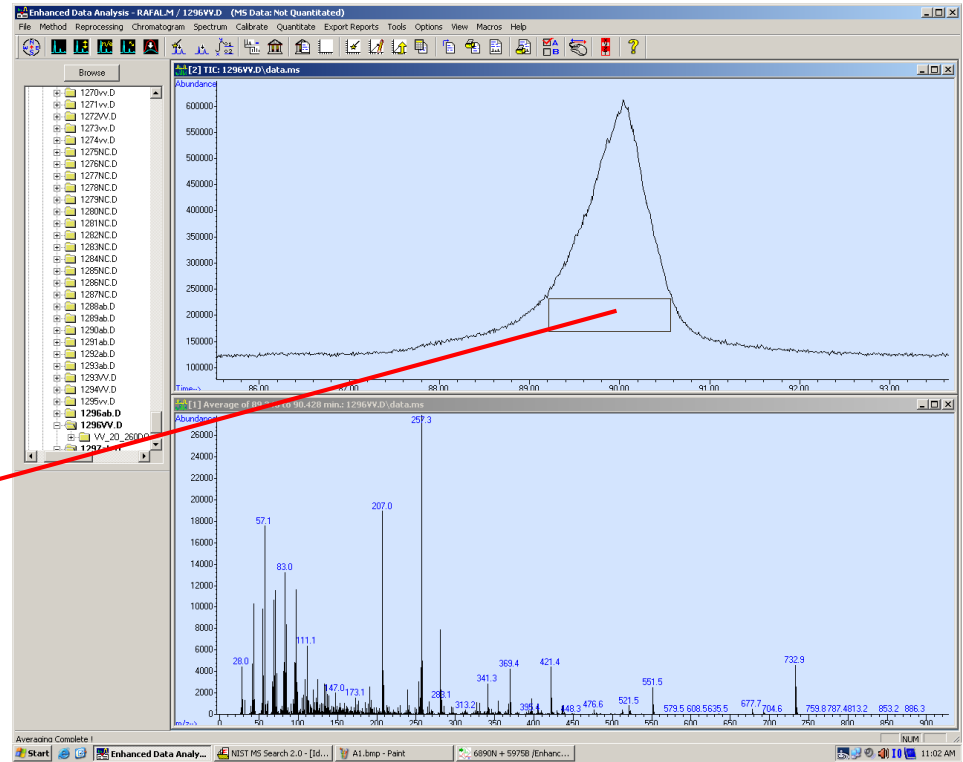
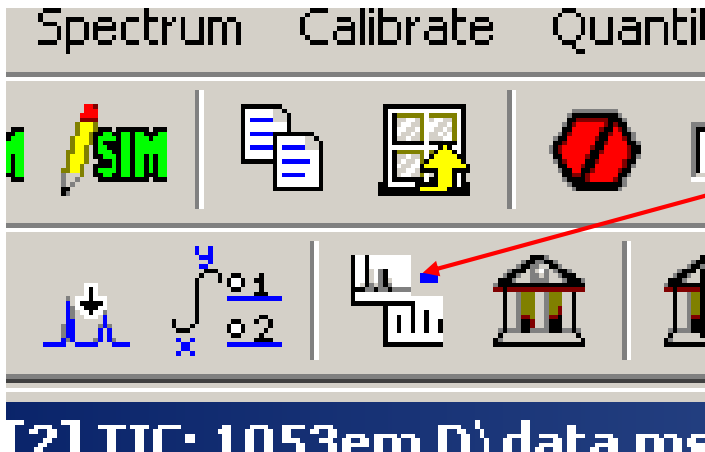
Otevření doměřené analýzy → Pravé tlačítko myši na souboru → „Load“

Zvětšení píku



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

Sejmутí spektra a odečtení pozadí



Odečtení pozadí

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

Sejmутí 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-Disopropylsilyloxydodecane
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)silyloxytridecane
20	M	503	553	0.28	Triarac line
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-Butyl-dimethyl(4-methyl-dodecyloxy)silane
29	M	493	548	0.18	Lanosta-7(11)-dien-18-oic acid, 22,25-diacetate
30	M	492	652	0.17	Boron, [4-(dimethyl(1-methyl-1-butyl)silyloxy)phenyl]boronic acid
31	M	492	584	0.17	1-Hentetracosanoic acid
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-ethanedithiobis(4-oxo)]
35	M	489	585	0.15	Neroline, 4,8,5-dihydro
36	M	488	589	0.15	Bacteriocinophorin-17B
37	M	487	587	0.14	9-Hexadecenoic acid, hexadecyl ester

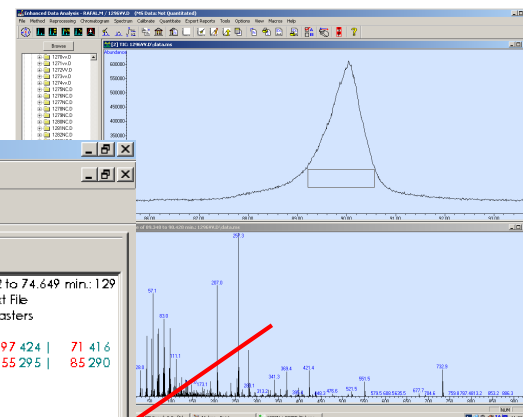
Names Structures InLib = -1163, Hit List

Lib. Search Other Search Names Compare Librarian MSMS

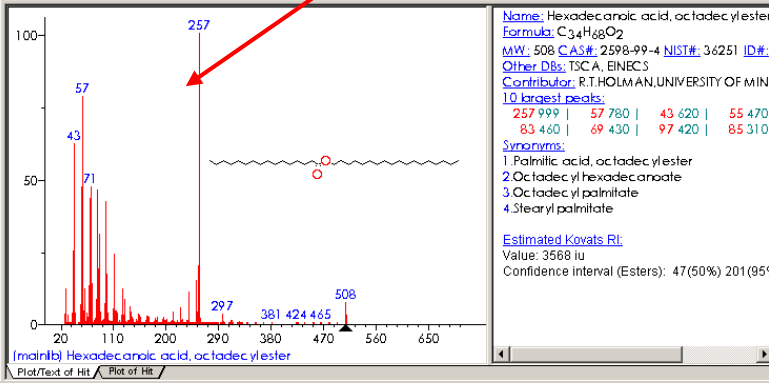
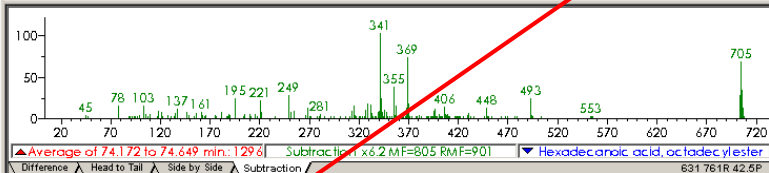
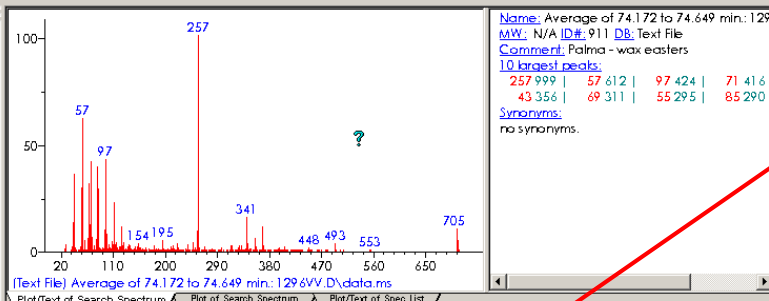
For Help, press F1

Ident Ident

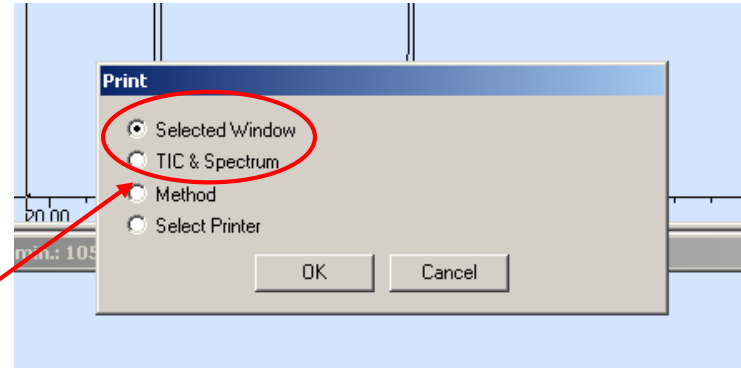
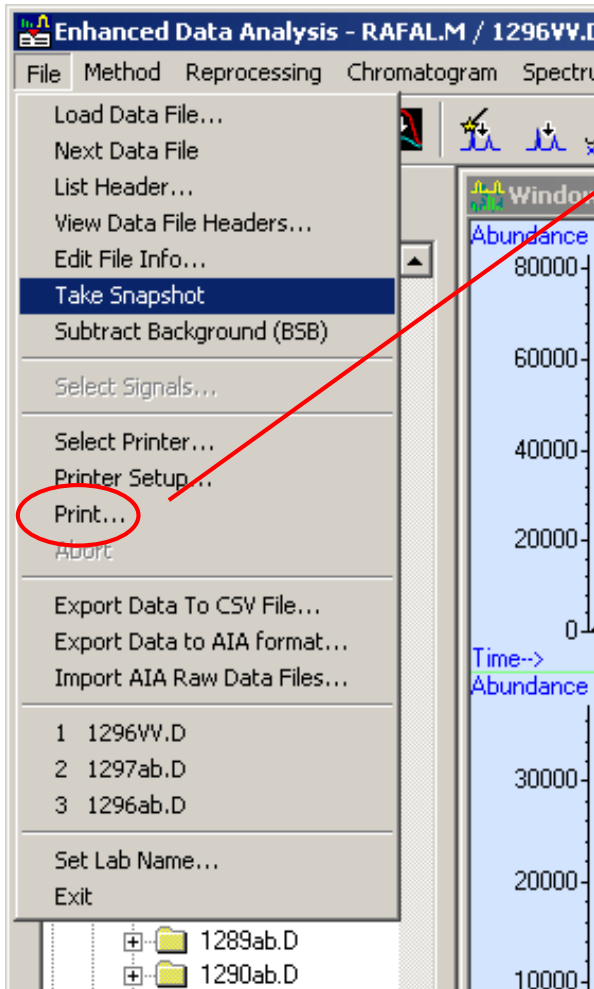
Start 6890N + 5975B /Enhanc... Enhanced Data Analysis ... NIST MS Search 2.0 ... 1:02 PM



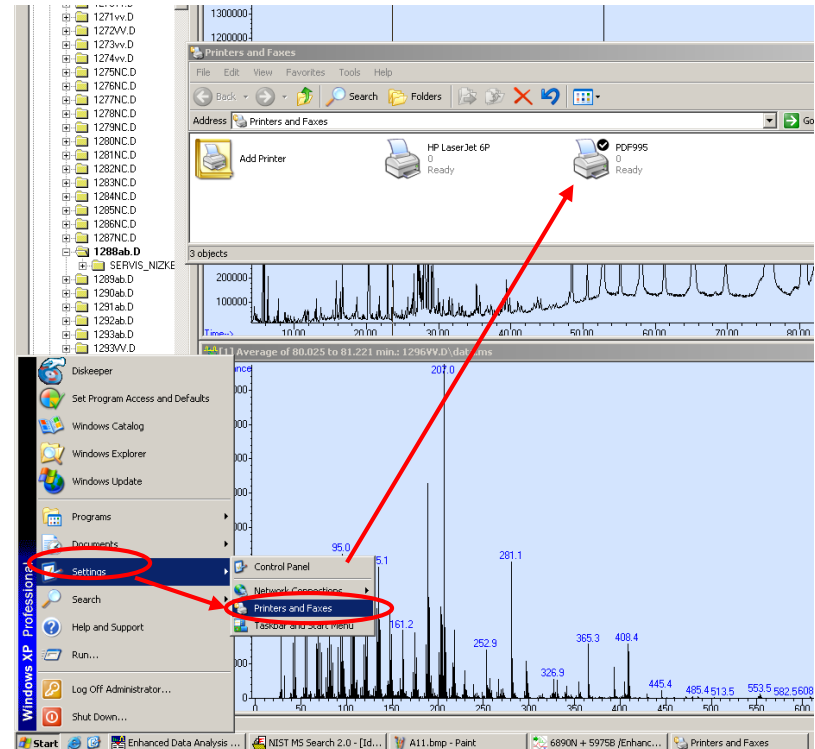
Dvojklik pravým tlačítkem myši na spektrum



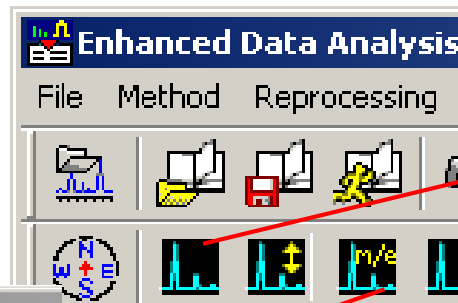
Tisk na papír nebo do PDF



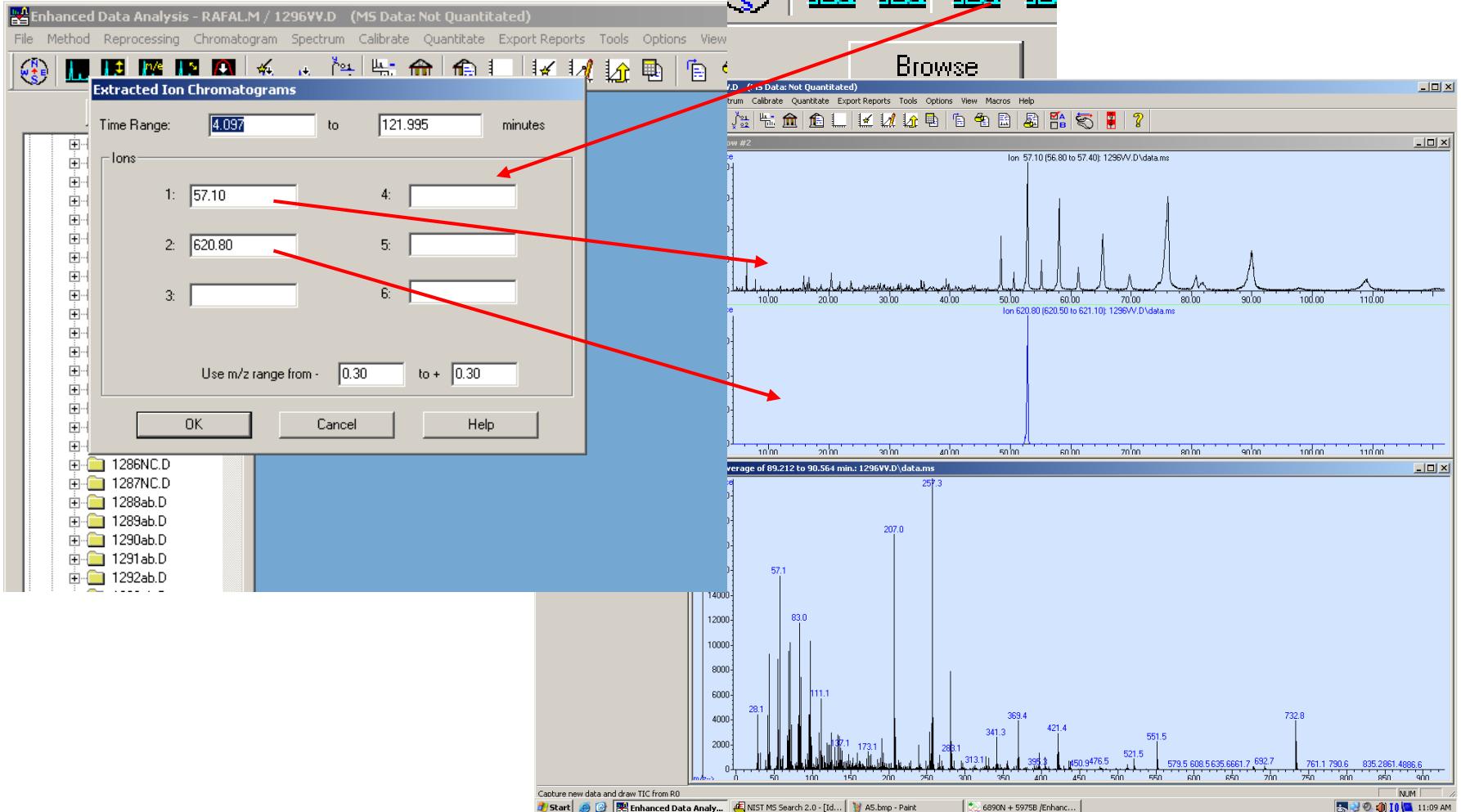
Pozn: Požadovanou tiskárnu nastavit „defaultně“ v nastavení počítače



Zobrazení extrahovaného chromatogramu

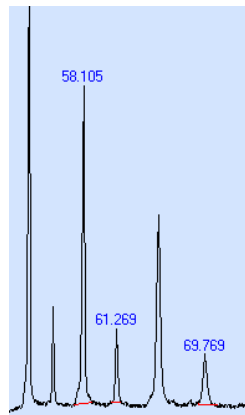
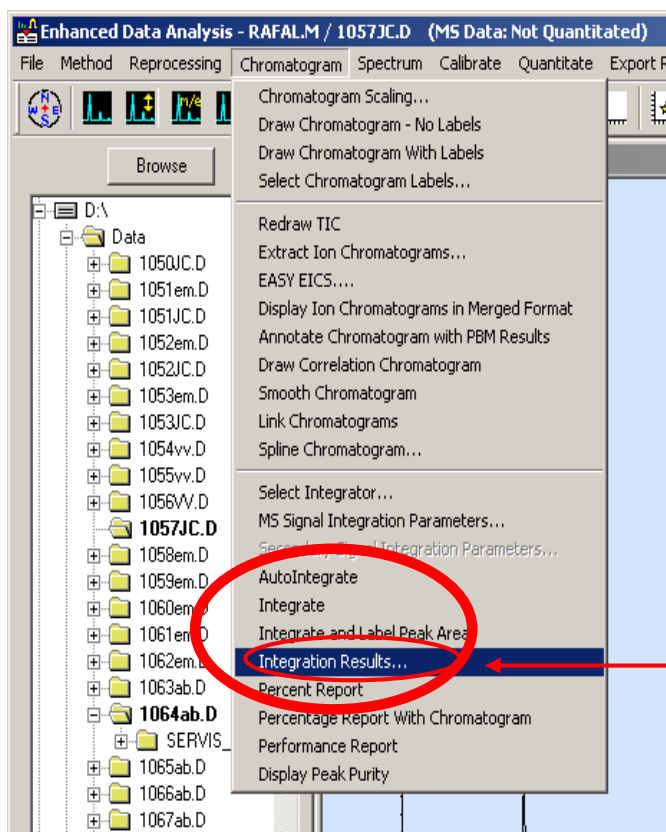


Návrat k „TICu“

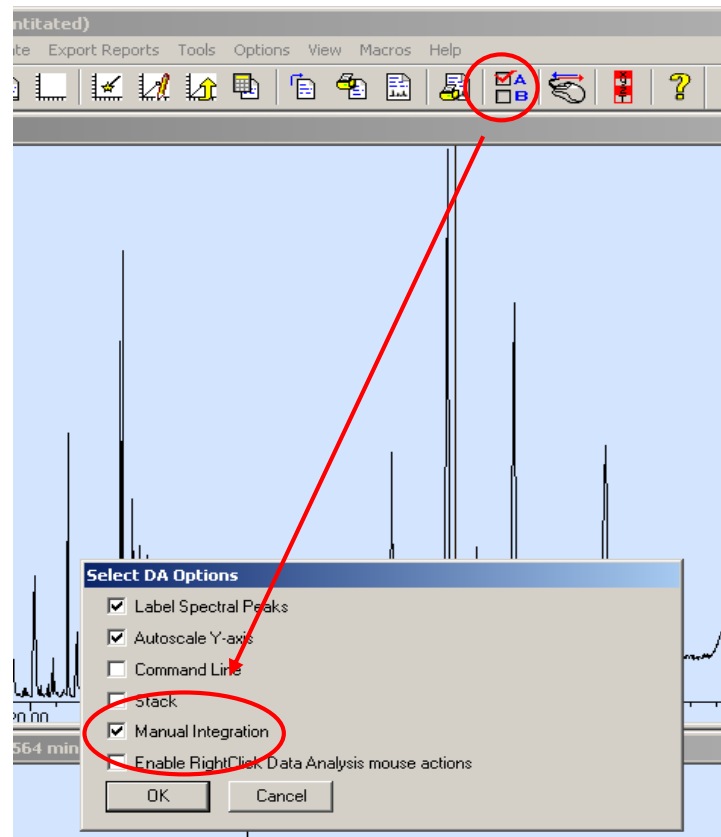


Integrace

Automatická integrace



Manuální integrace

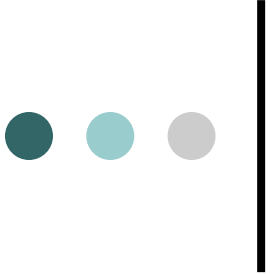


Integrace – potáhnutí pravým tlačítkem myši při základně píku

Překrývání chromatogramů

The image illustrates the process of overlaying chromatograms in MSD ChemStation. The main window shows the 'Select Files for TIC Overlay: 1296VV.D' dialog box, which is used to select files for processing. The 'Available Data Files' list includes files such as 1290ab.D, 1291ab.D, 1292ab.D, 1293ab.D, 1294ab.D, 1295VV.D, 1296VV.D, 1297NC.D, 1298ab.D, 1299ab.D, 1290ab.D, 1291ab.D, 1292ab.D, 1293ab.D, and 1294VV.D. The 'Files Selected for Processing' list includes files such as D:\Data\1294VV.D and D:\Data\1296VV.D. The 'Process' button is highlighted with a red circle. 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'. The y-axis is labeled 'Abundance' and ranges from 0 to 1400000. The x-axis is labeled 'Time-->' and ranges from 0 to 110.00. A red arrow points from the 'Process' button in the dialog box to the chromatogram plot.

File	Sample Name	File	Sample Name
1290ab.D	blank other	D:\Data\1294VV.D	Palma - wax easters
1291ab.D	Prbek_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		
1296VV.D	blank CHCl3		
1297NC.D	blank CHCl3		
1298ab.D	Ubik. rozkladne pro...		
1299ab.D			

- 
- **V případě problémů s měřením kontaktujte pracovníky oddělení MS**
 - **Vladimír Vrkoslav**
 - **Tel. 347**
 - **místnost : A, JV, 1.85**
 - **(Josef Cvačka)**
 - **Tel. 303,**
 - **místnost: A, JV, 1.90**