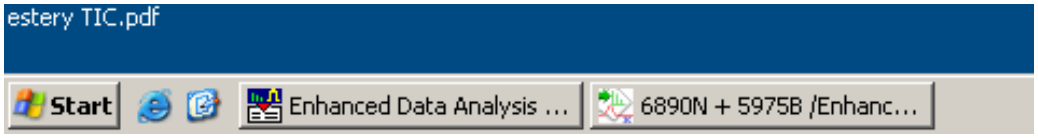
Software for GC/MS

Building A

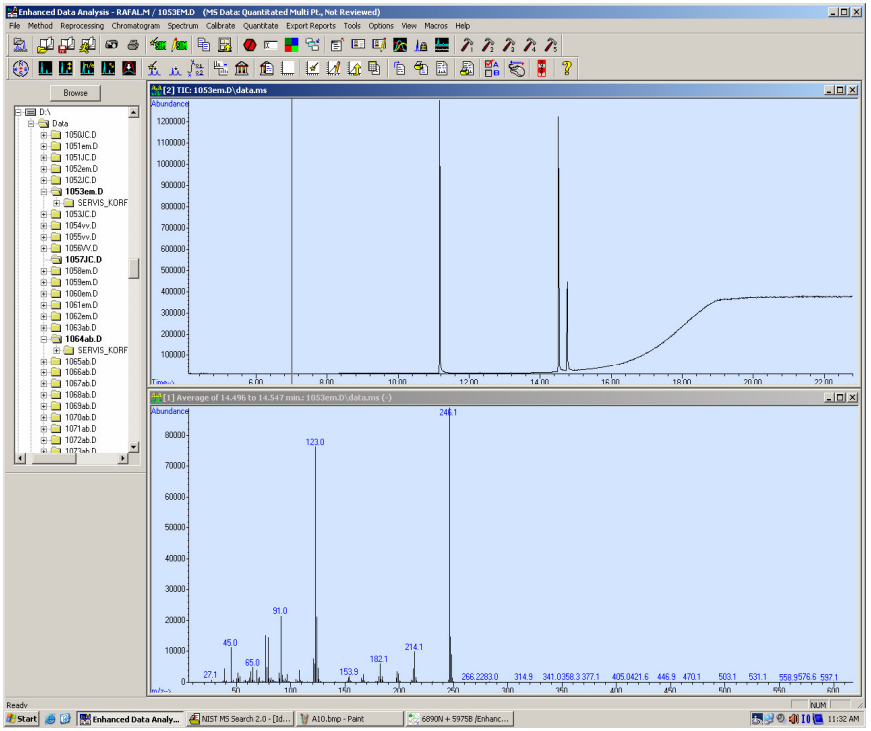
Ground floor SV

Lab 107

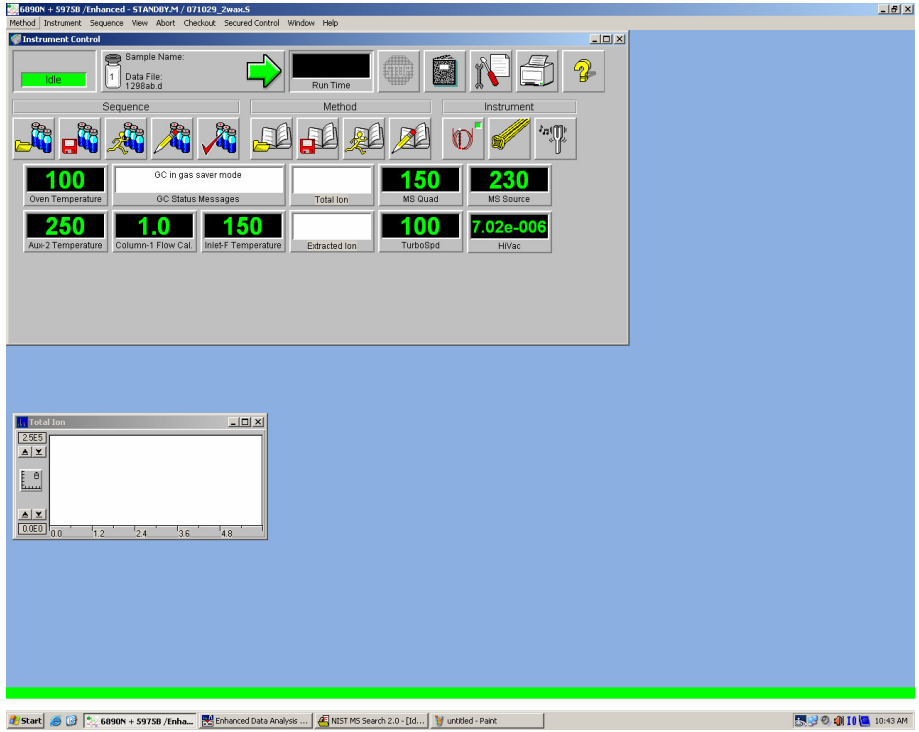
ChemStation



Interpretation

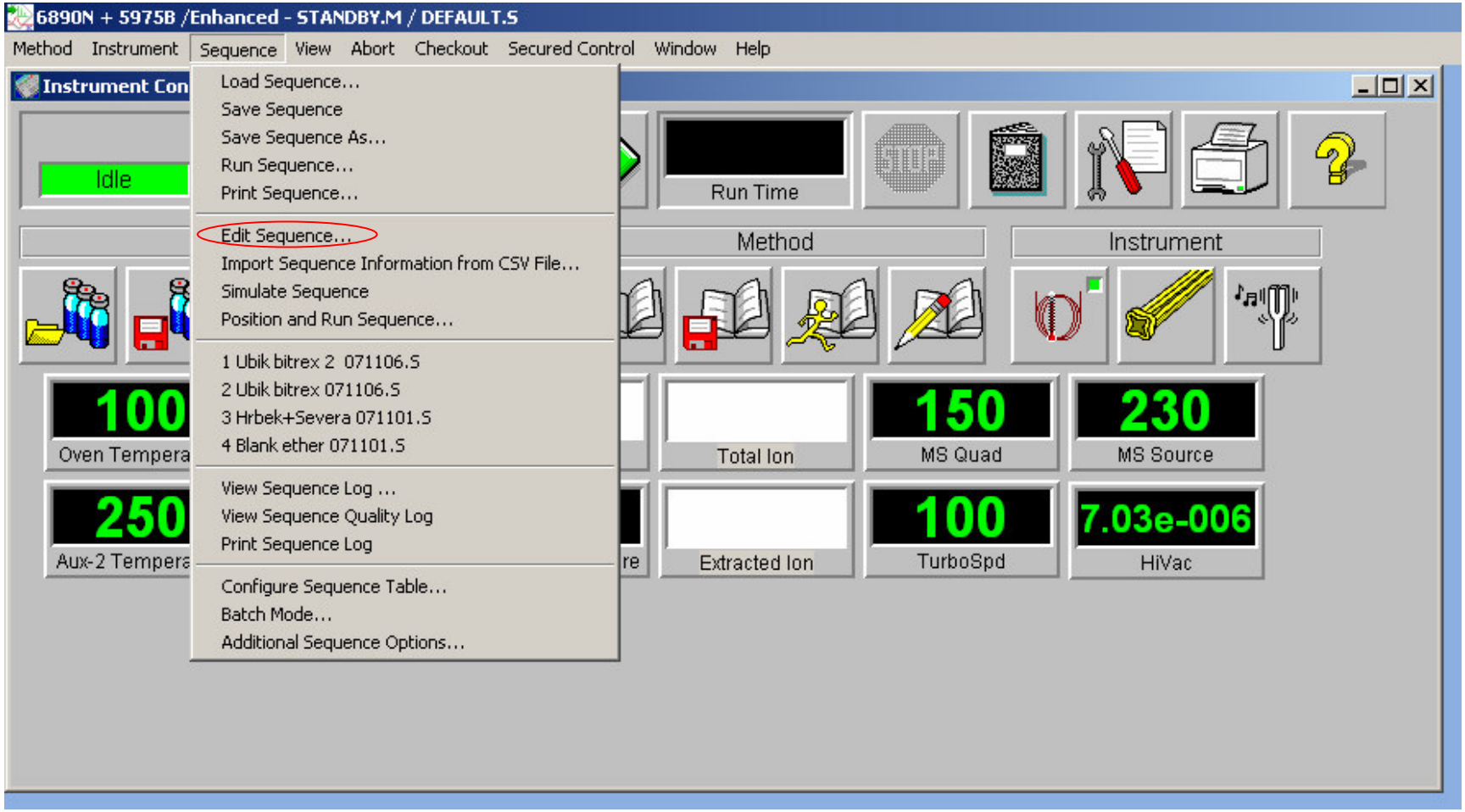


Measurement

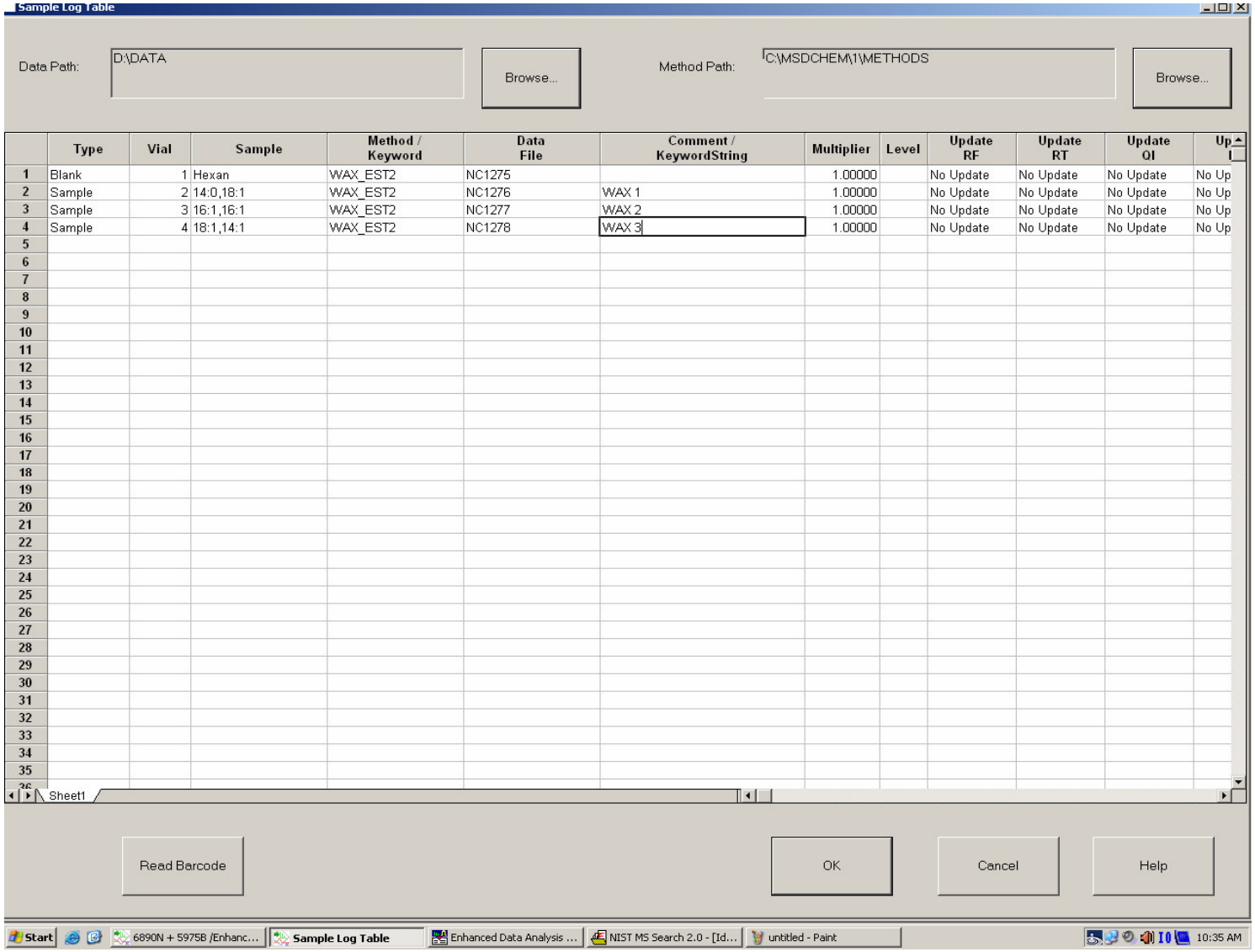


Run measurement

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

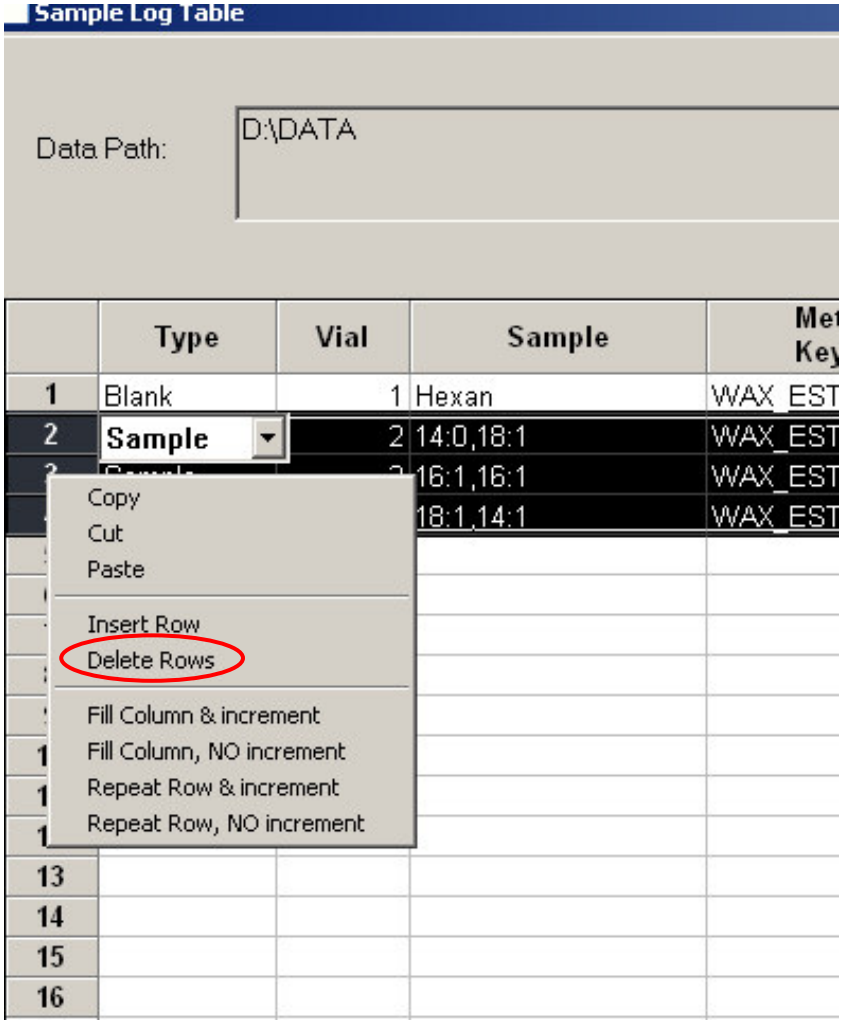


Sample Log Table



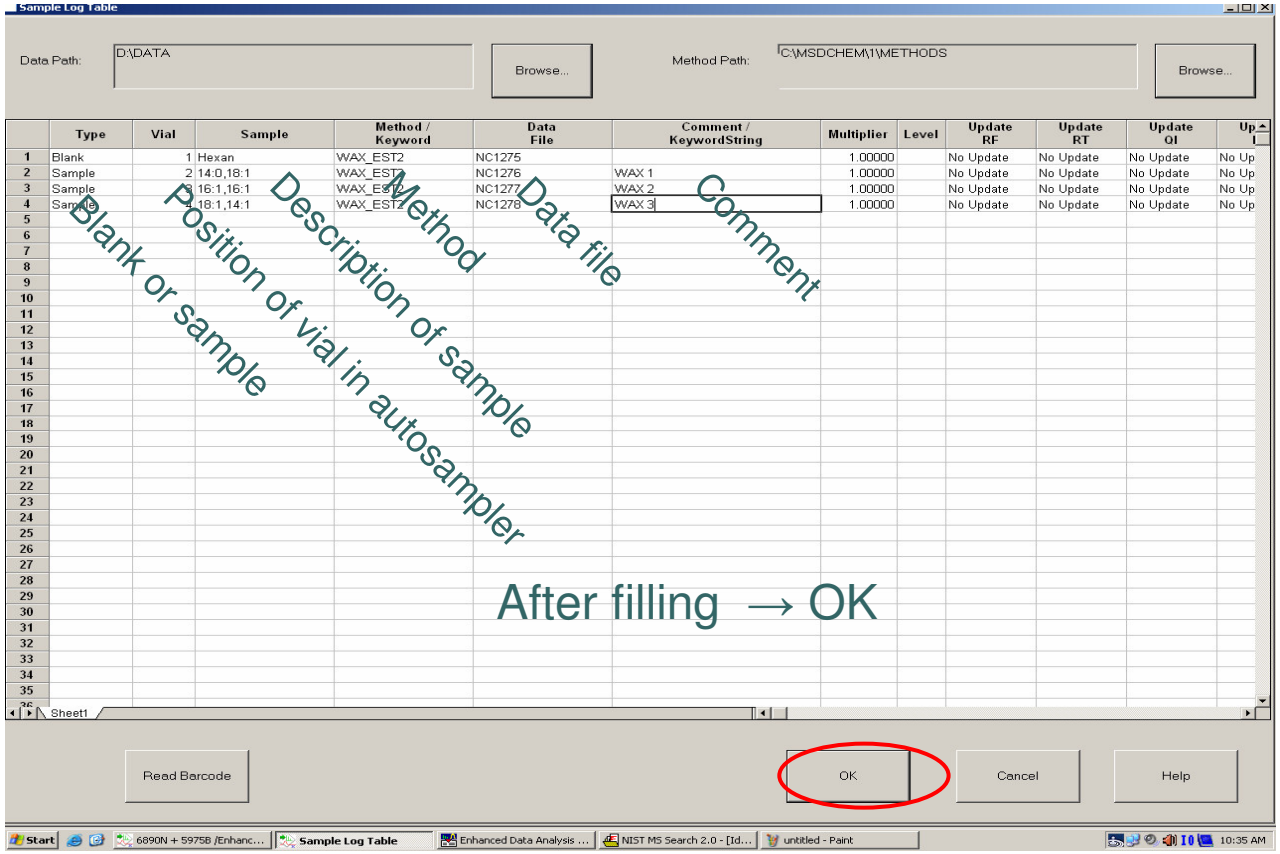
	Type	Vial	Sample	Method / Keyword	Data File	Comment / KeywordString	Multiplier	Level	Update RF	Update RT	Update QI	Up
1	Blank	1	Hexan	WAX_EST2	NC1275		1.00000		No Update	No Update	No Update	No Up
2	Sample	2	14:0,18:1	WAX_EST2	NC1276	WAX 1	1.00000		No Update	No Update	No Update	No Up
3	Sample	3	16:1,16:1	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

Overwrite previous sequence



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

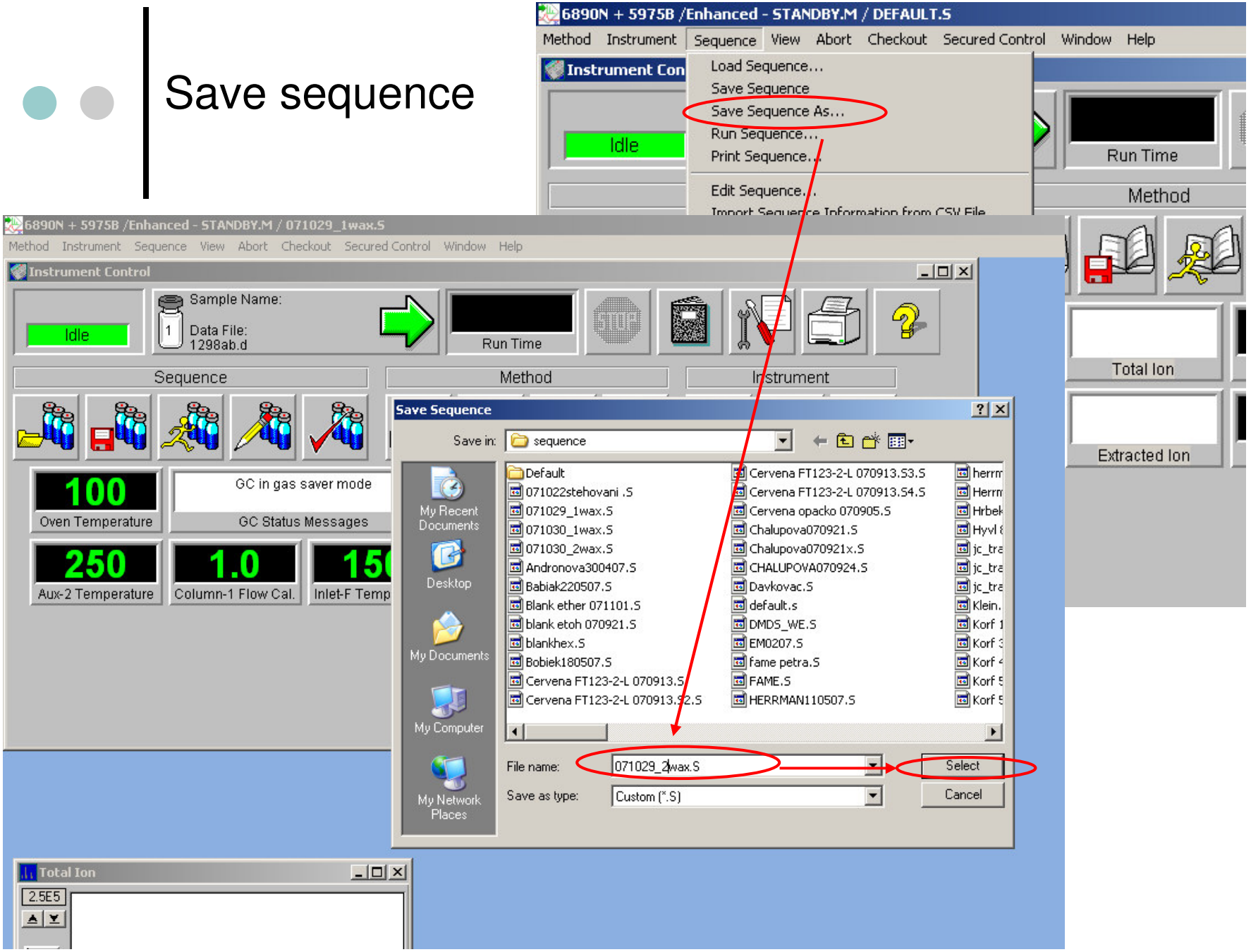
Fill the Sample Log Table



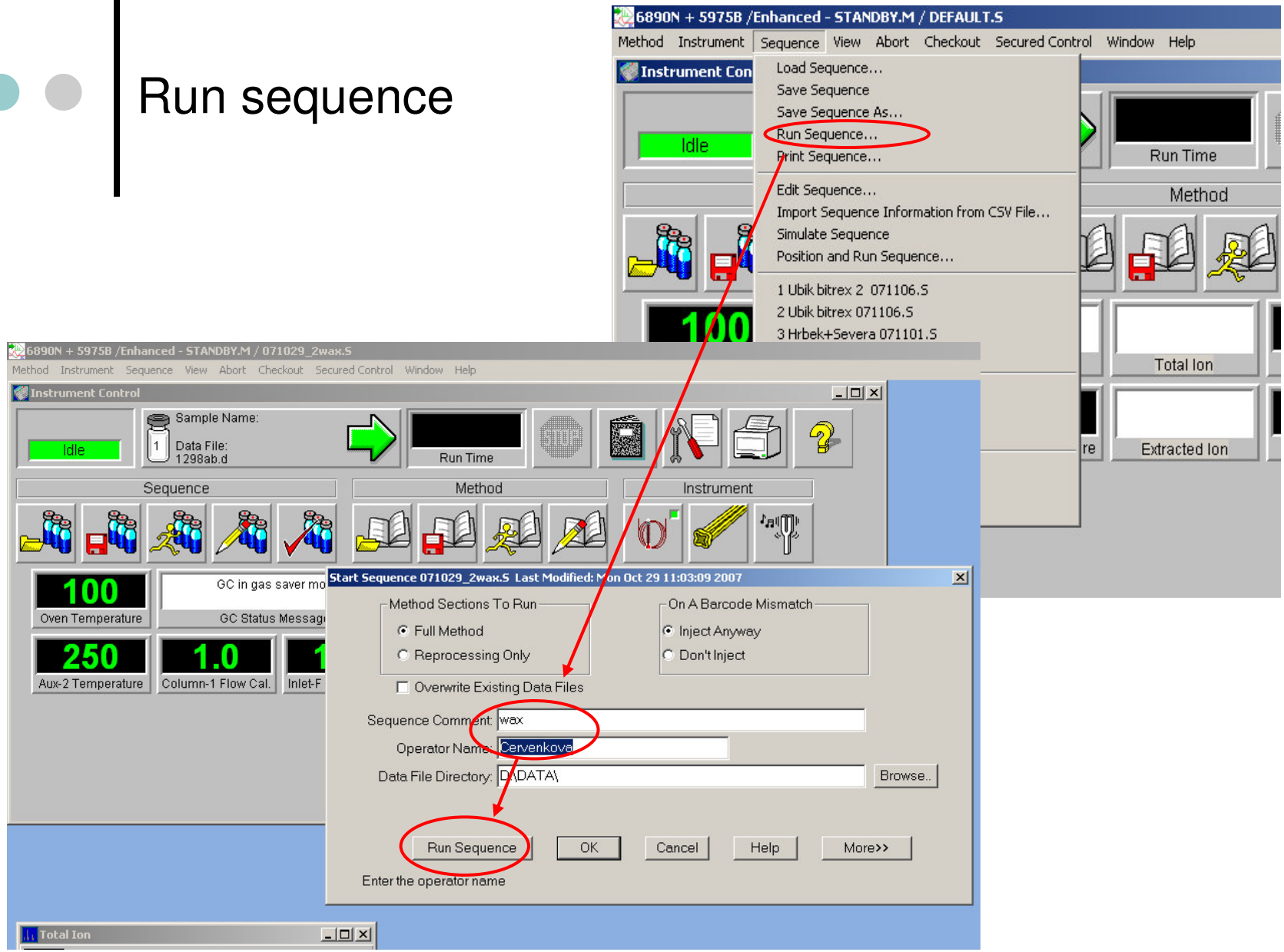
Nizke – Low
Vysoke – High

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

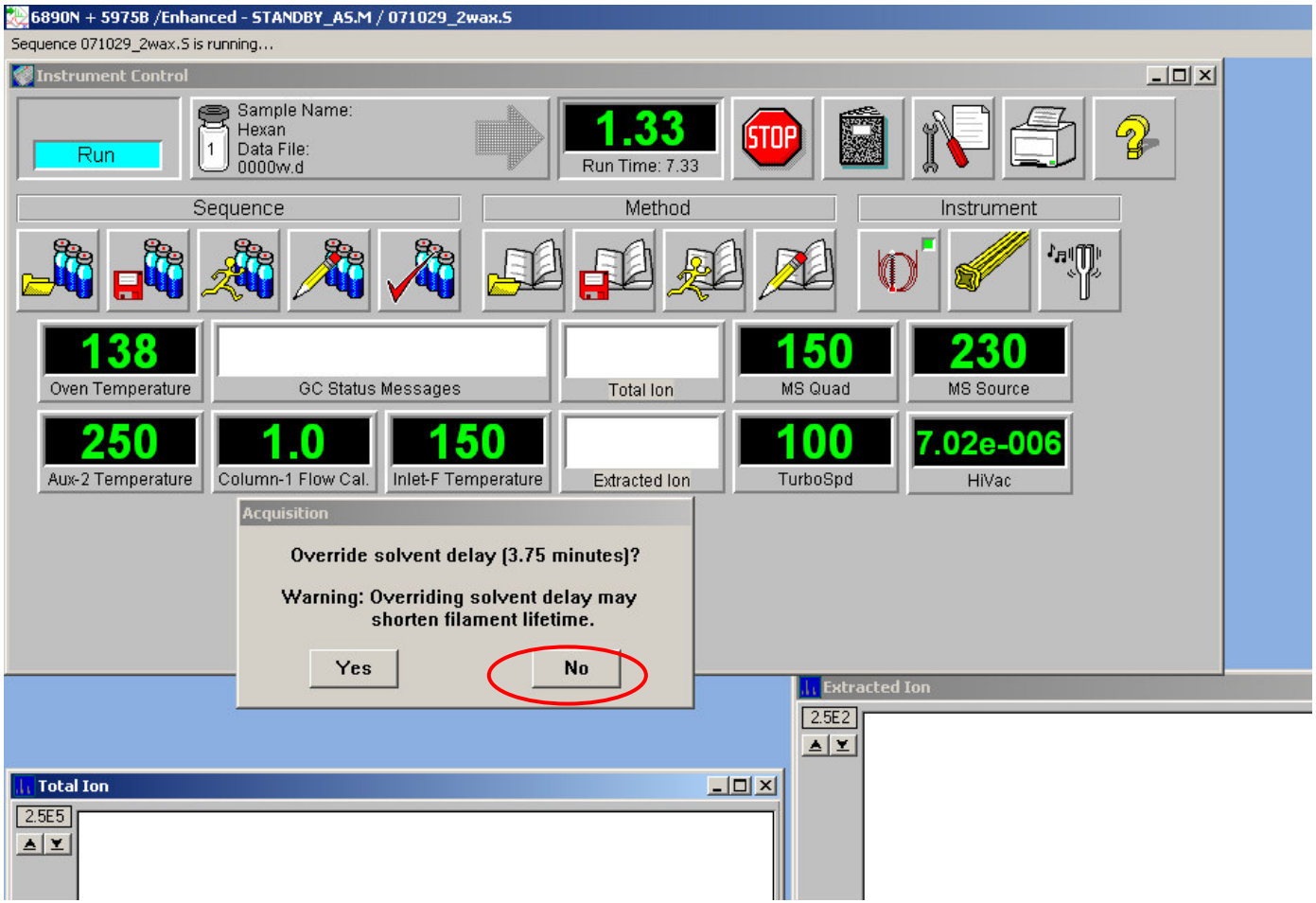


Run sequence



„Solvent delay“

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

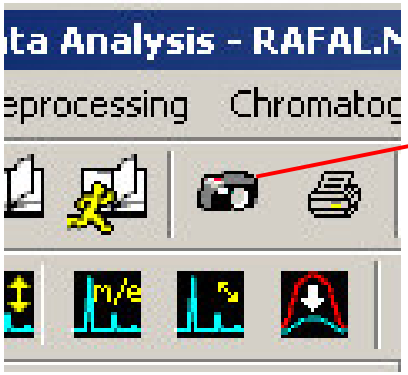


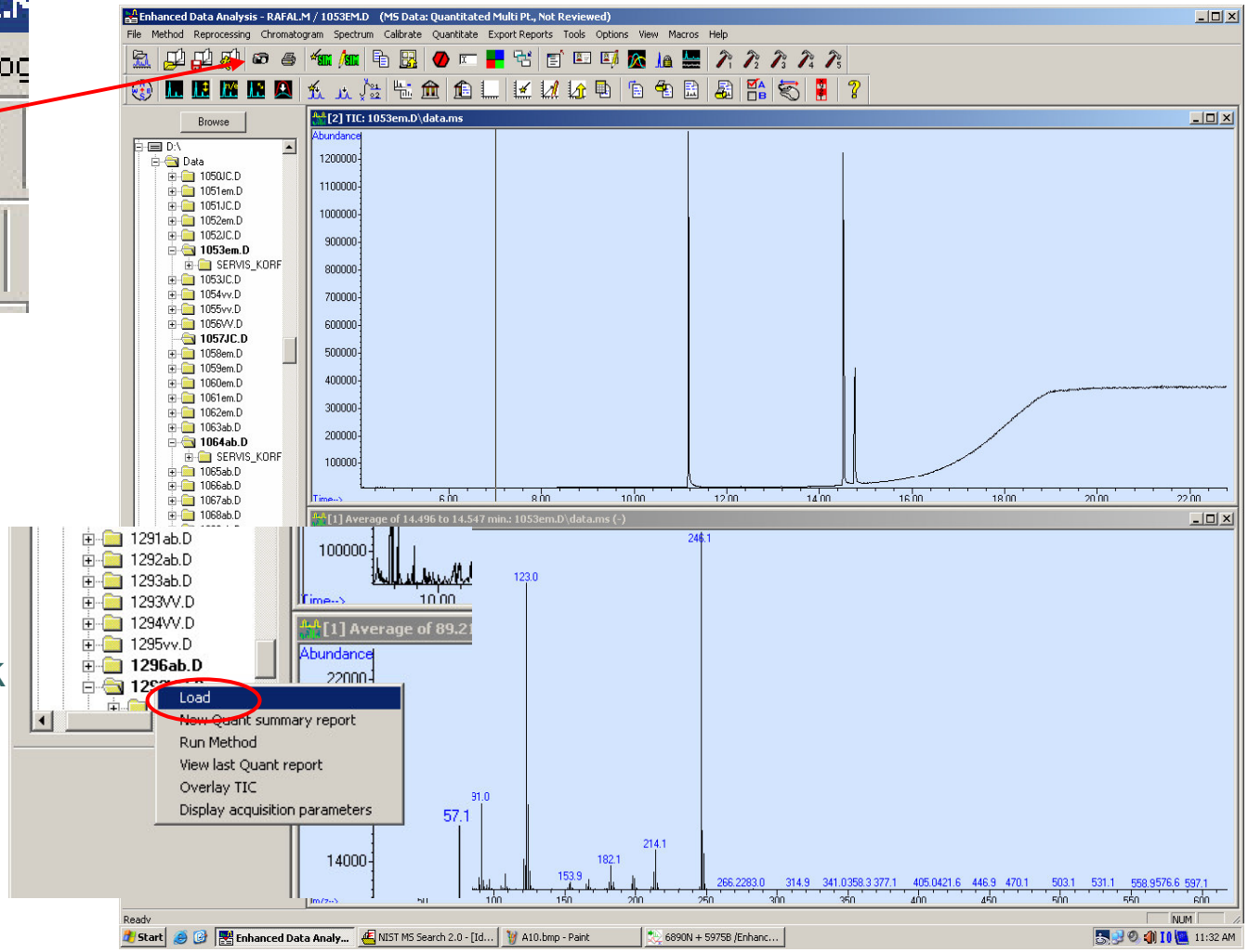
Interpretation

- 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

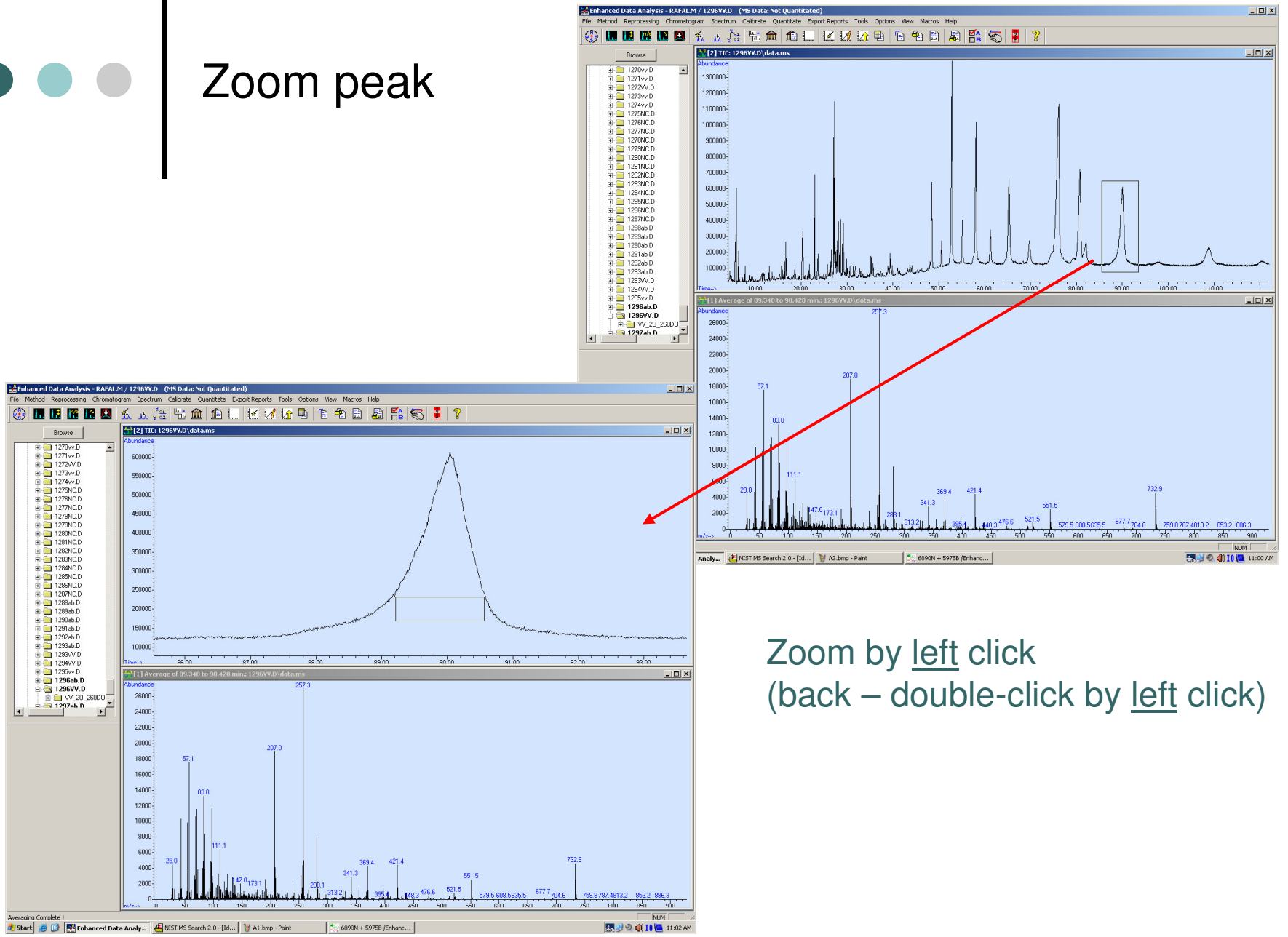
For running analysis – „Take Snapshot“



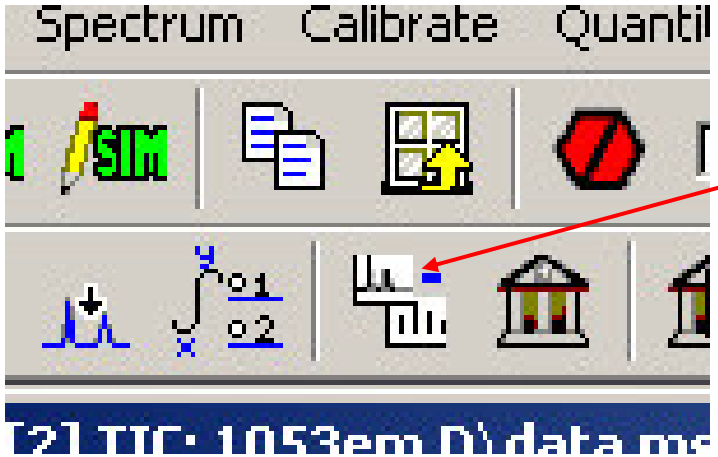


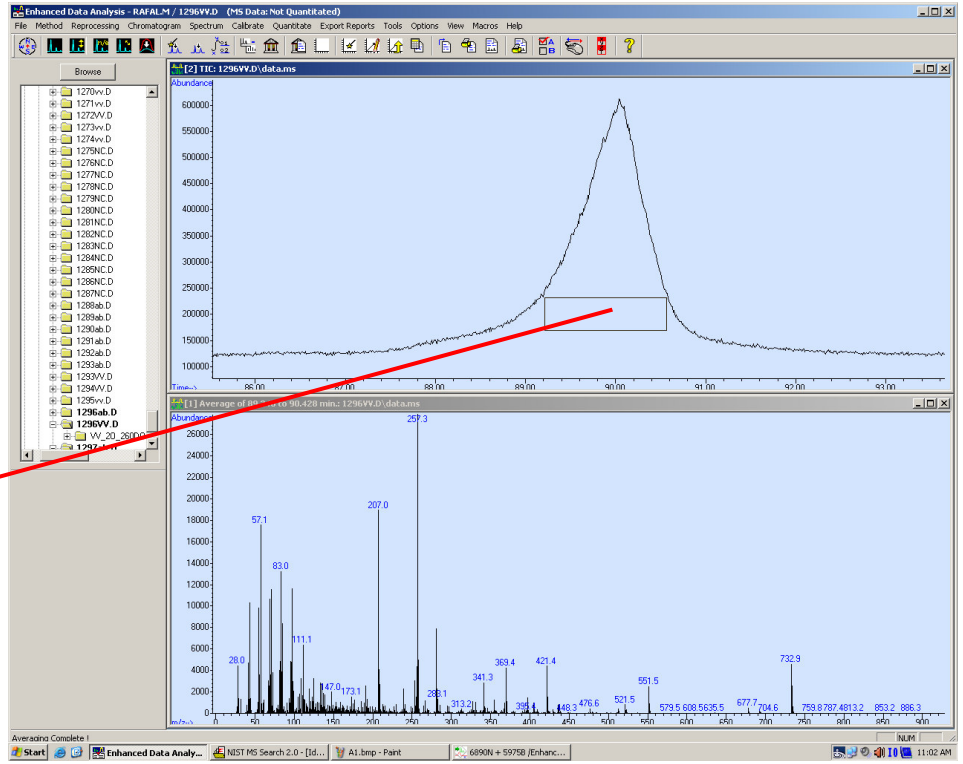
Load finished analysis → right click → „Load“

Zoom peak


Enhanced Data Analysis - RAFAL.M / 1296VV.D (MS Data: Not Quantitated)
[2] TIC: 1296VV.D\data.ms
[1] Average of 89.348 to 90.428 min.: 1296VV.D\data.ms
Zoom by left click
(back – double-click by left click)

Load spectrum and subtract background

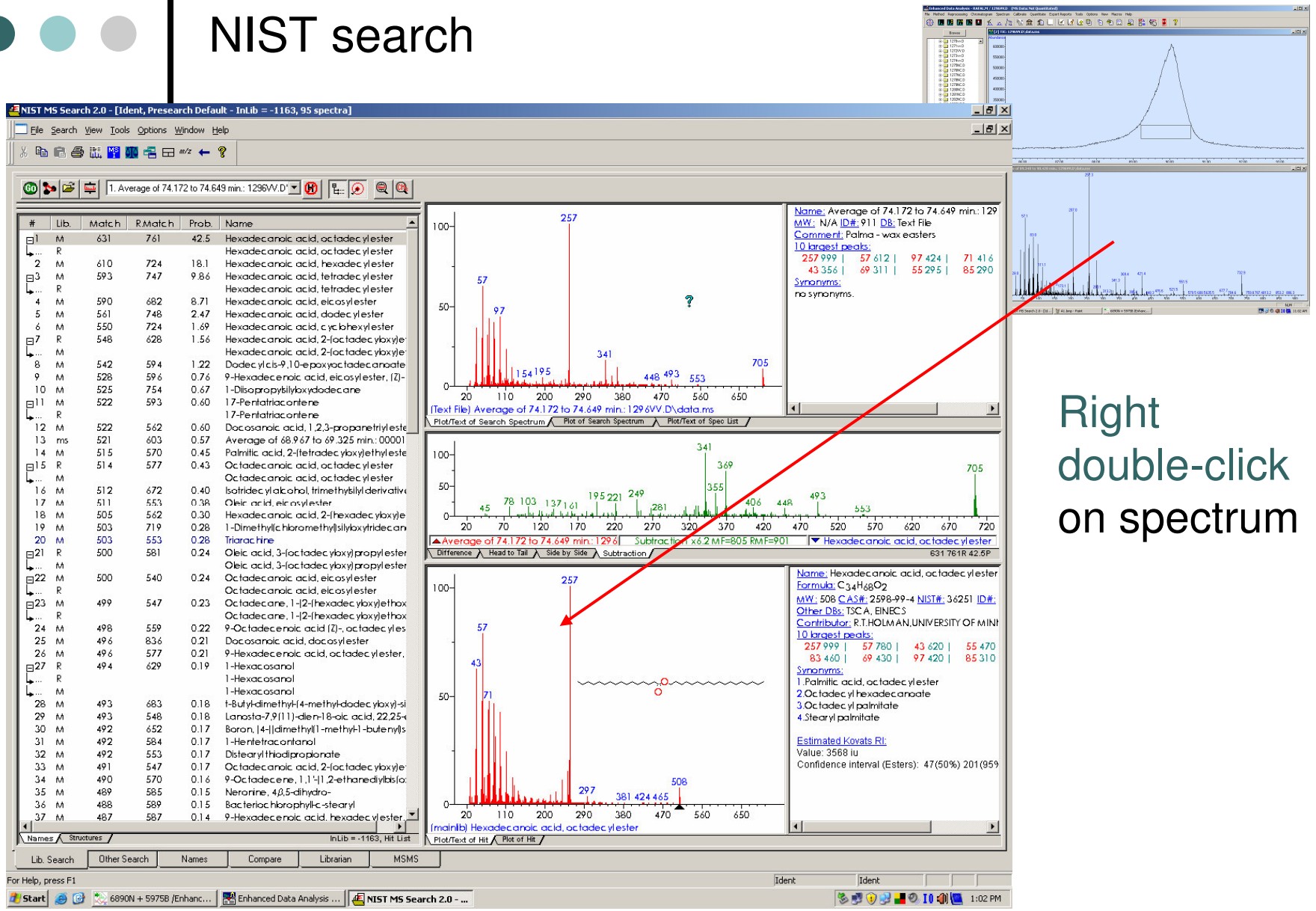




Subtract background
1. Load spectrum from peak
2. Load spectrum near the peak
3. Click on „Subtract“

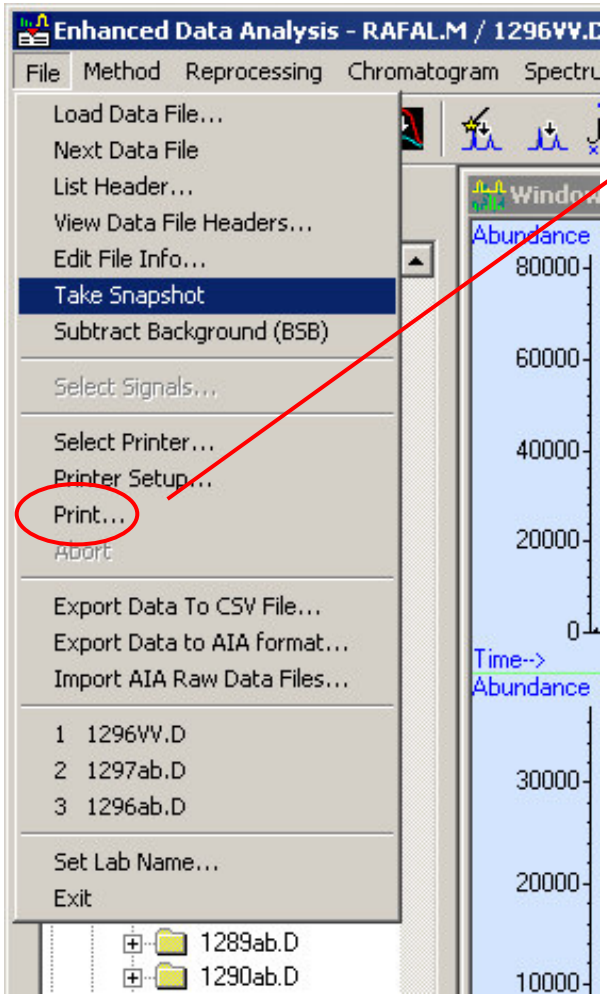
Load spectrum by left click

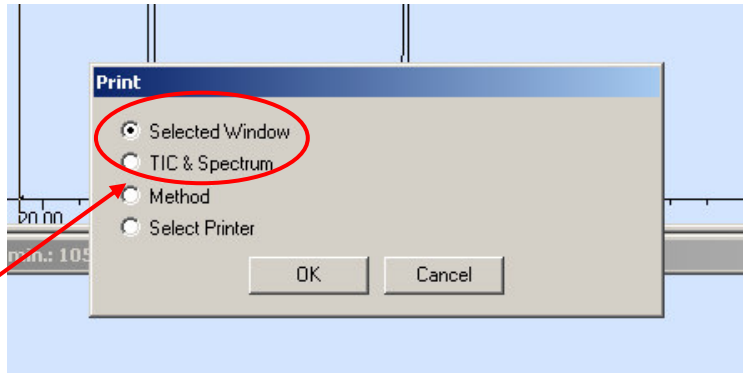
NIST search



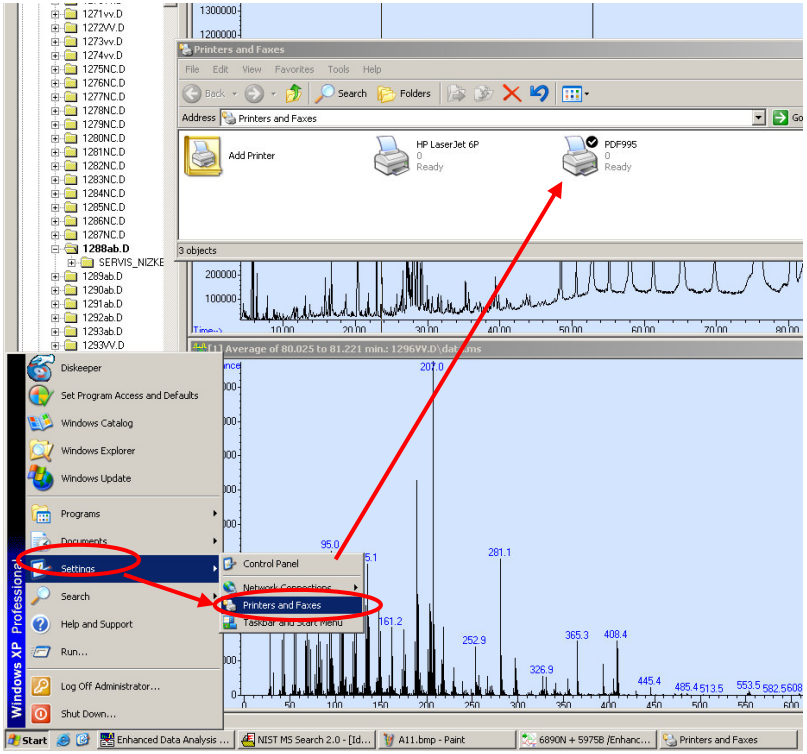
Right double-click on spectrum

Print to PDF or paper

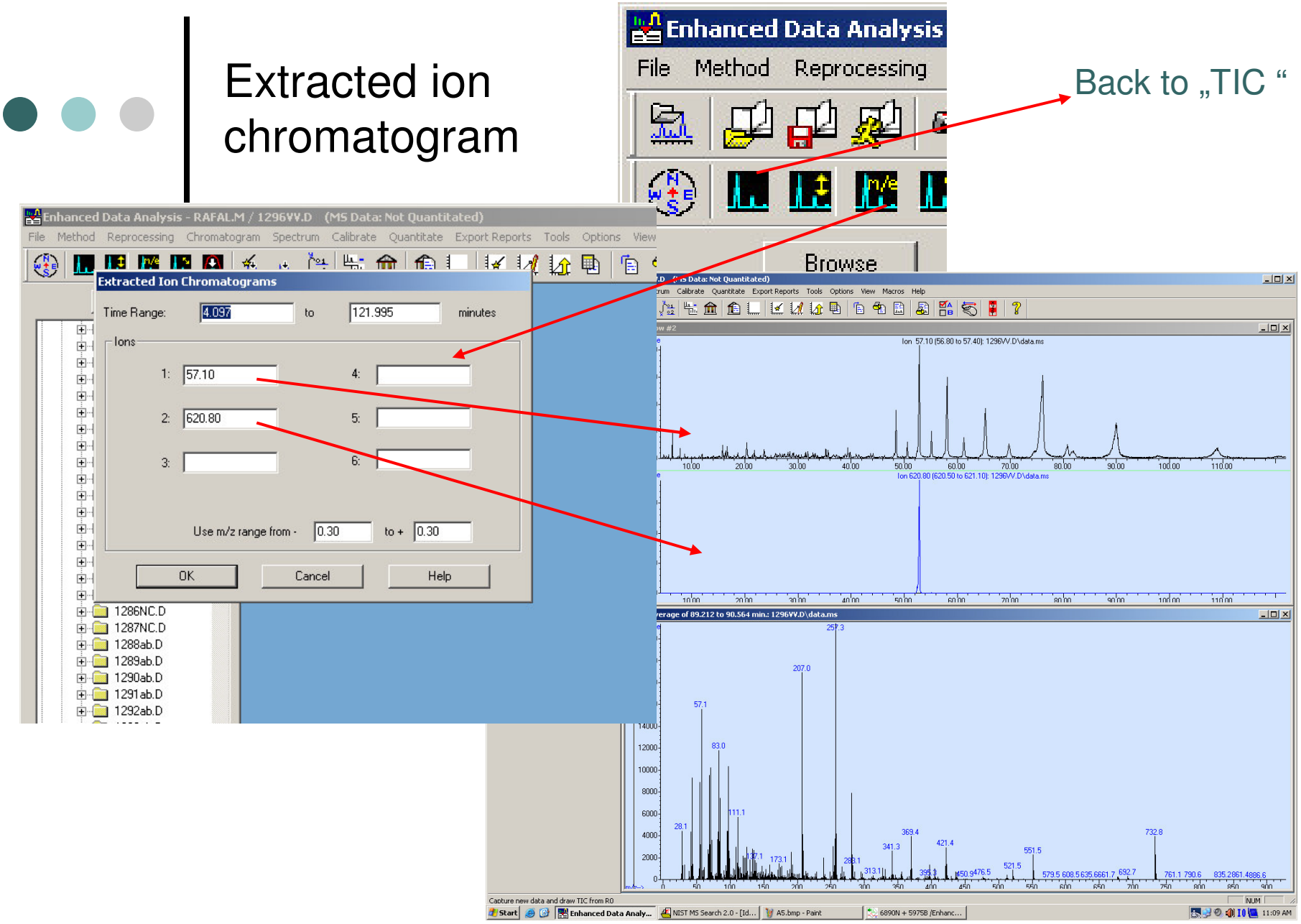




Set printer as Default

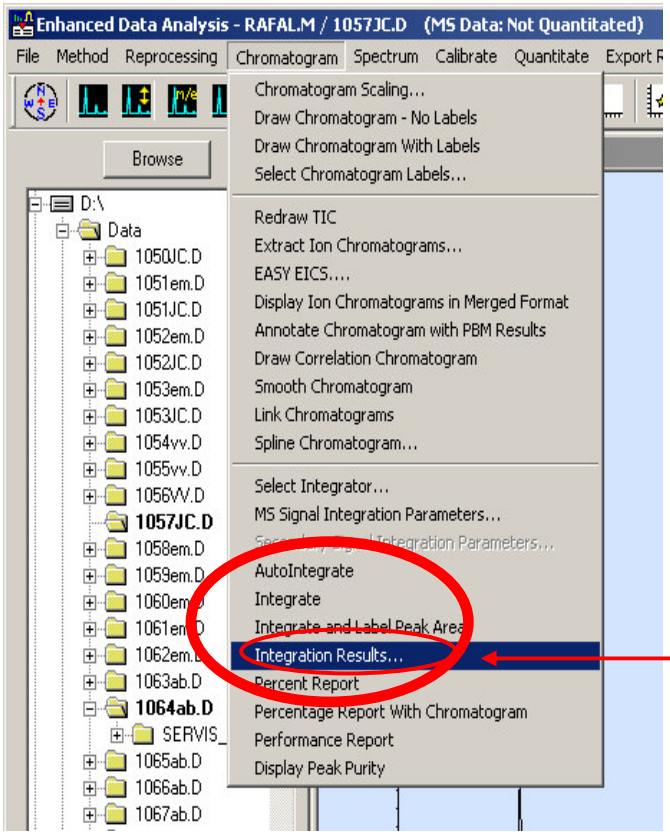


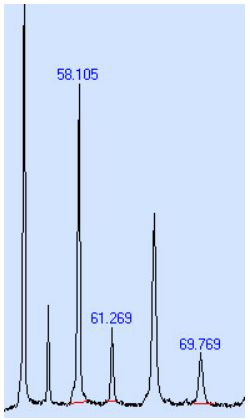
Extracted ion chromatogram



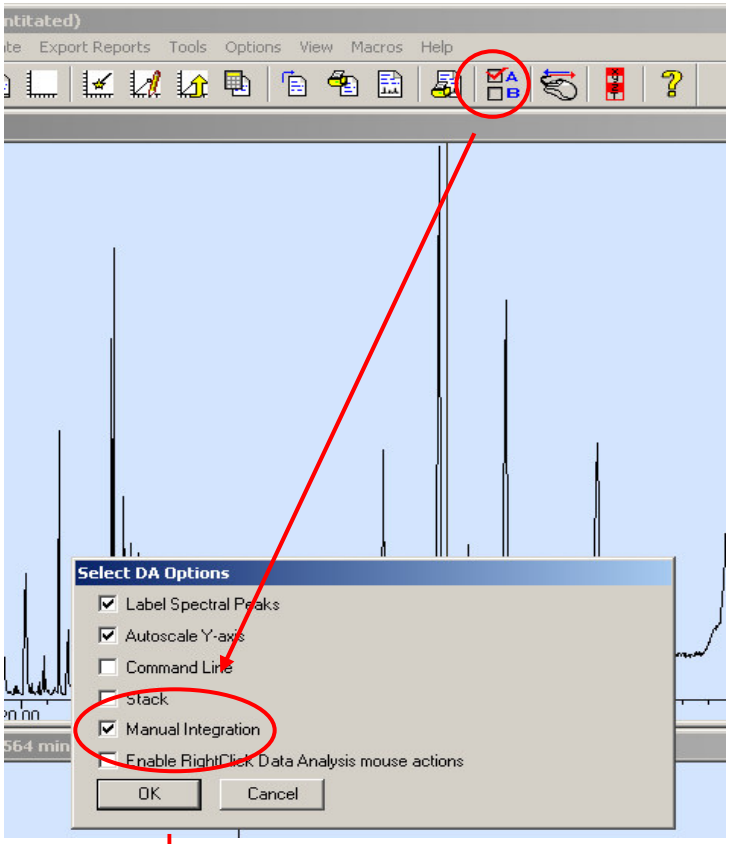
Integration

Automatic integration





Manual integration



Right click– draw line on base of the peak

Overlay chromatogram