

# **GCXGC – qMS**

## **toegepast voor de organische screening van luchtstalen**

Hendrik Van De Weghe

Grobbendonk  
14 oktober 2005

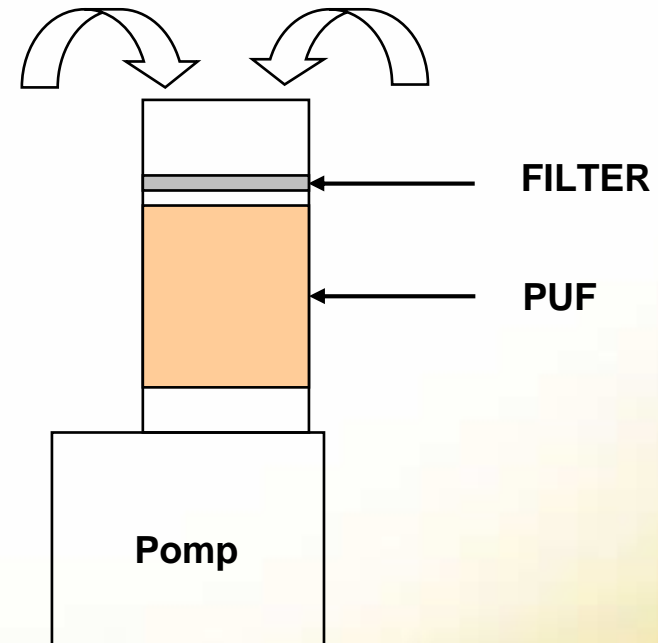


# **GCXGC – DSQ**

- **Aanleiding : Inventarisatiestudie  
PAK in lucht (AMINAL)**
- **Staalname en GC/MS-analyse**
- **GCXGC-DSQ**



## STAALNAME : GPS-1 medium volume sampler



## ANALYSE

- Extractie : Soxhlet
- Fractionering SPE (500 mg silica)
  - F1 : 2 ml hexaan (Alifaten)
  - F2 : 3 ml hexaan/dcm 4/1 (PAK, AlkylPAK)
  - F3 : 6 ml dcm (nitroPAK, oxyPAK)
- Meting GC/MS SCAN (F2 en F3) (screening)
- Meting GC/HRMS (nitro-PAK)



# INVENTARISATIESTUDIE POLYAROMATISCHE KOOLWATERSTOFFEN IN LUCHT

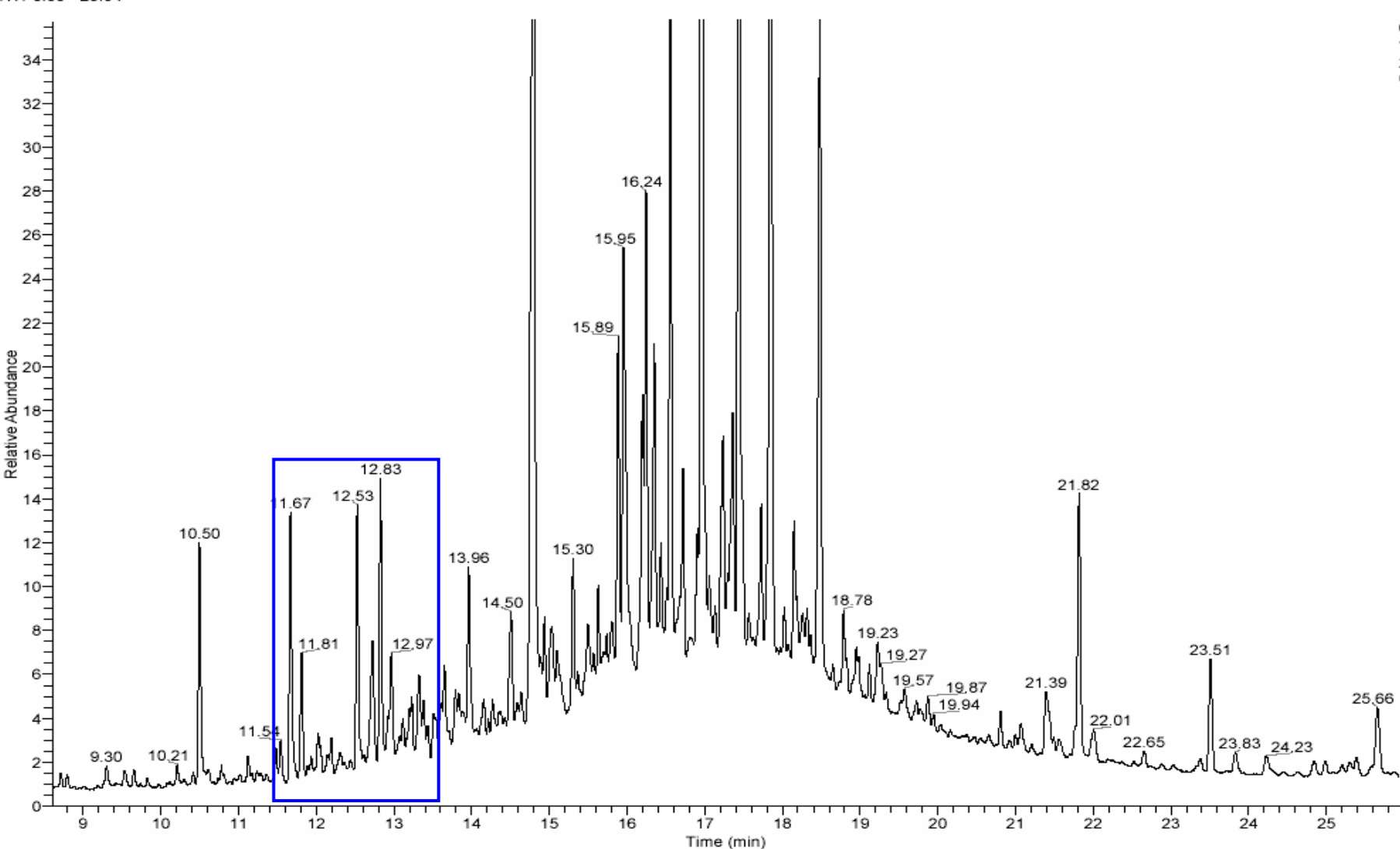
## GC/MS-chromatogram (PUF, F2)

D:\IOR700\_TRACE2005\Data\20050622\_09

22/06/05 20:28:05

2005-3293 puf/2

RT: 8.60 - 25.94



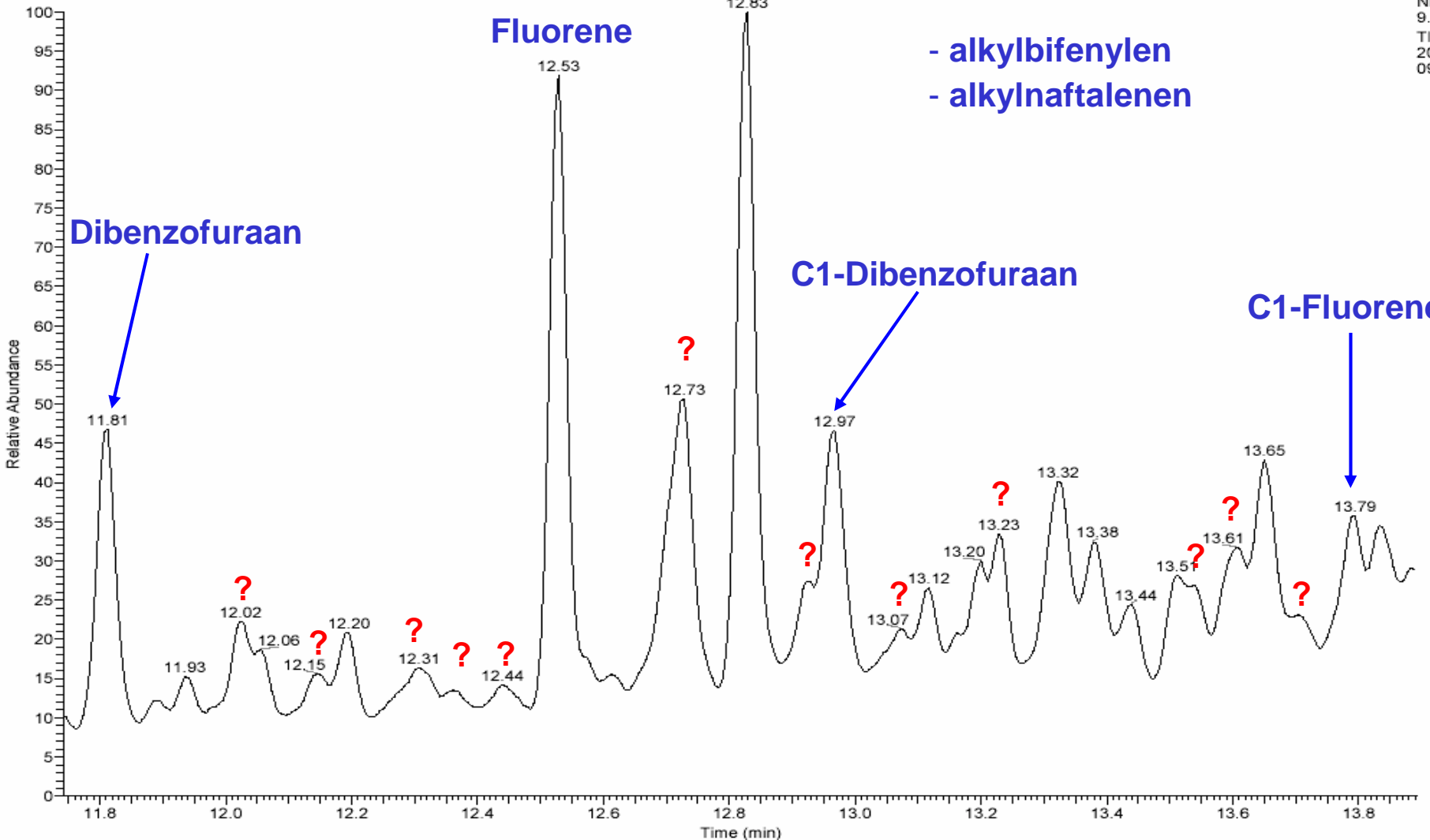
NL:  
6.55E7  
TIC MS  
20050622\_  
09

# INVENTARISATIESTUDIE POLYAROMATISCHE KOOLWATERSTOFFEN IN LUCHT

## GC/MS-chromatogram (PUF, F2)

2005-3293 put/2/5/5/Data/20050622\_09

RT: 11.74 - 13.89

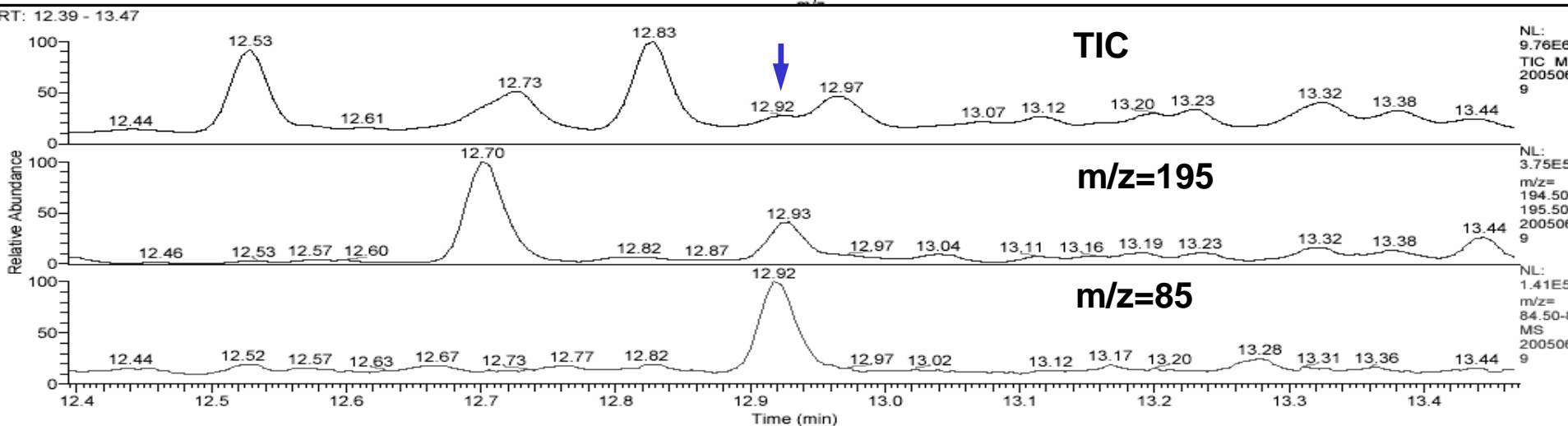
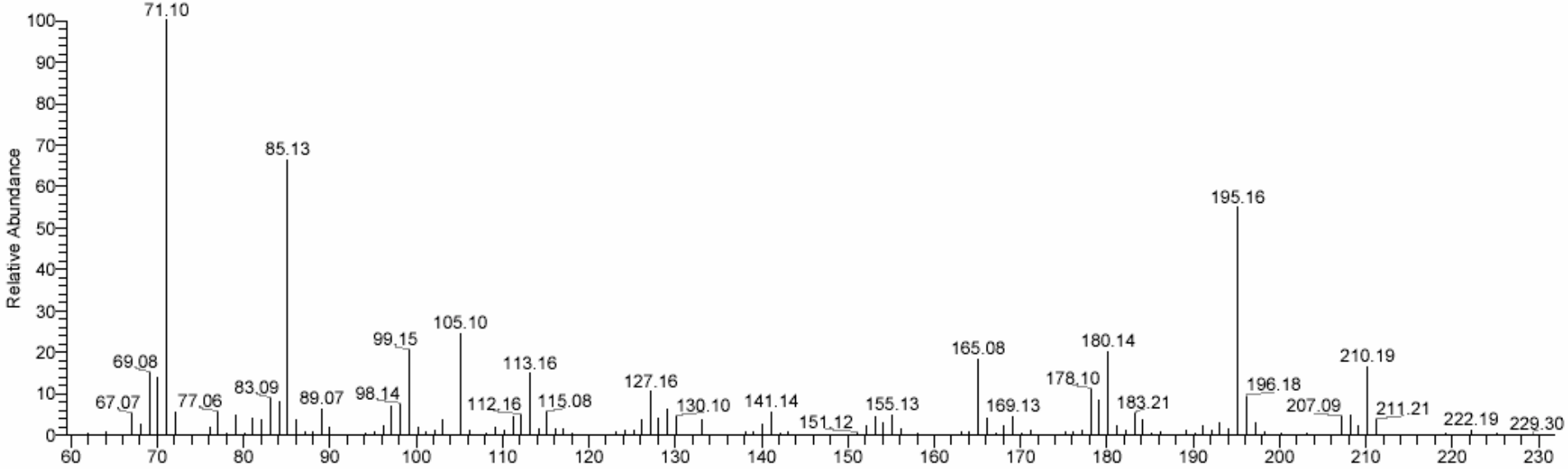


NL:  
9.76E6  
TIC MS  
20050622\_09

# INVENTARISATIESTUDIE POLYAROMATISCHE KOOLWATERSTOFFEN IN LUCHT

## Probleem: coëlutie

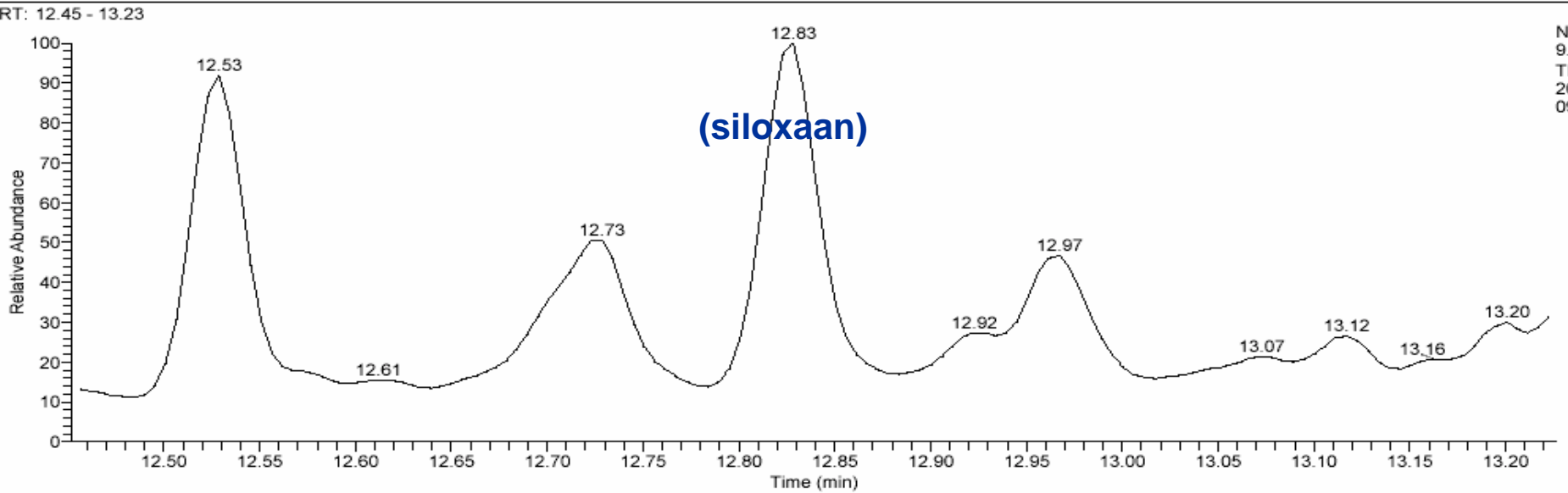
20050622\_09 #1246 RT: 12.92 AV: 1 SB: 1 12.88 NL: 1.87E5  
T: {0;0} + c EI det=450.00 Full ms [ 60.00-375.00]



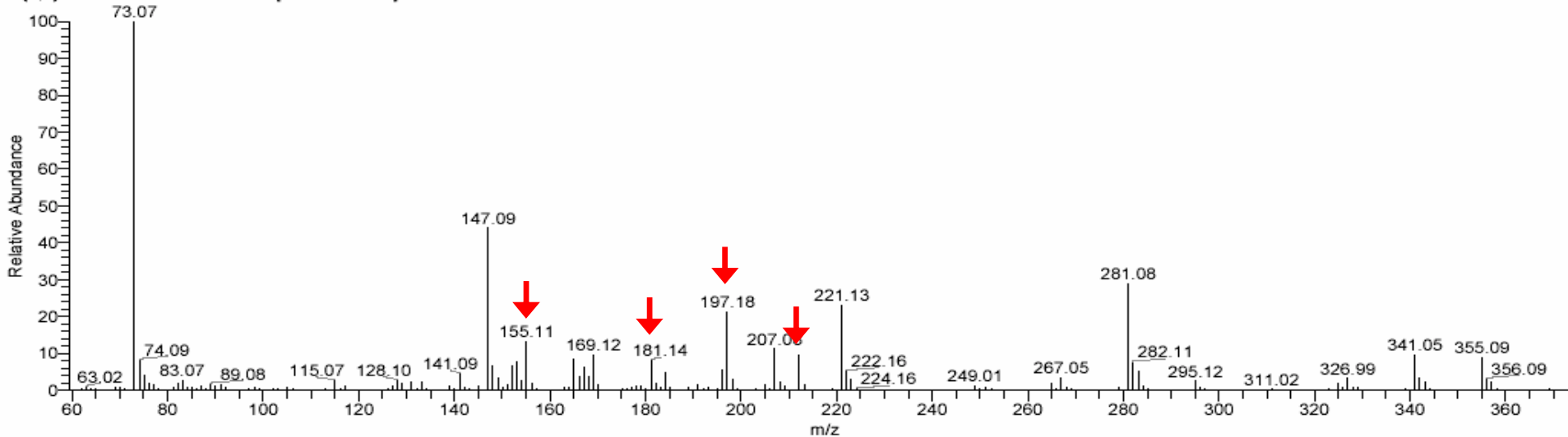
NL: 9.76E6  
TIC MS  
200506  
9  
NL: 3.75E5  
m/z=  
194.50-  
195.50  
200506  
9  
NL: 1.41E5  
m/z=  
84.50-8  
MS  
200506  
9

# INVENTARISATIESTUDIE POLYAROMATISCHE KOOLWATERSTOFFEN IN LUCHT

## Probleem: coëlutie

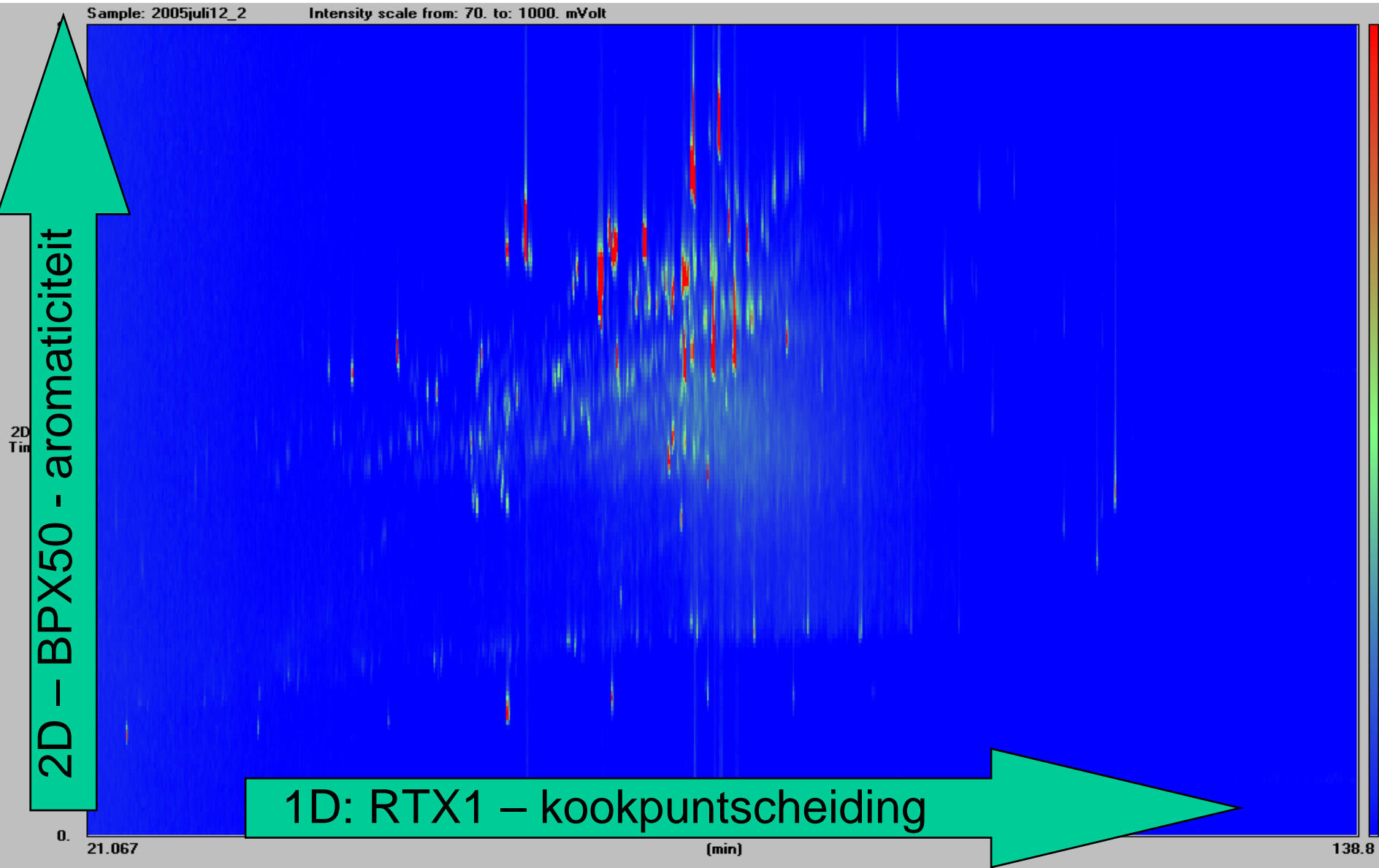


20050622\_09 #1230 RT: 12.83 AV: 1 SB: 1 12.88 NL: 1.66E6  
T: {0:0} + c EI det=450.00 Full ms [ 60.00-375.00]

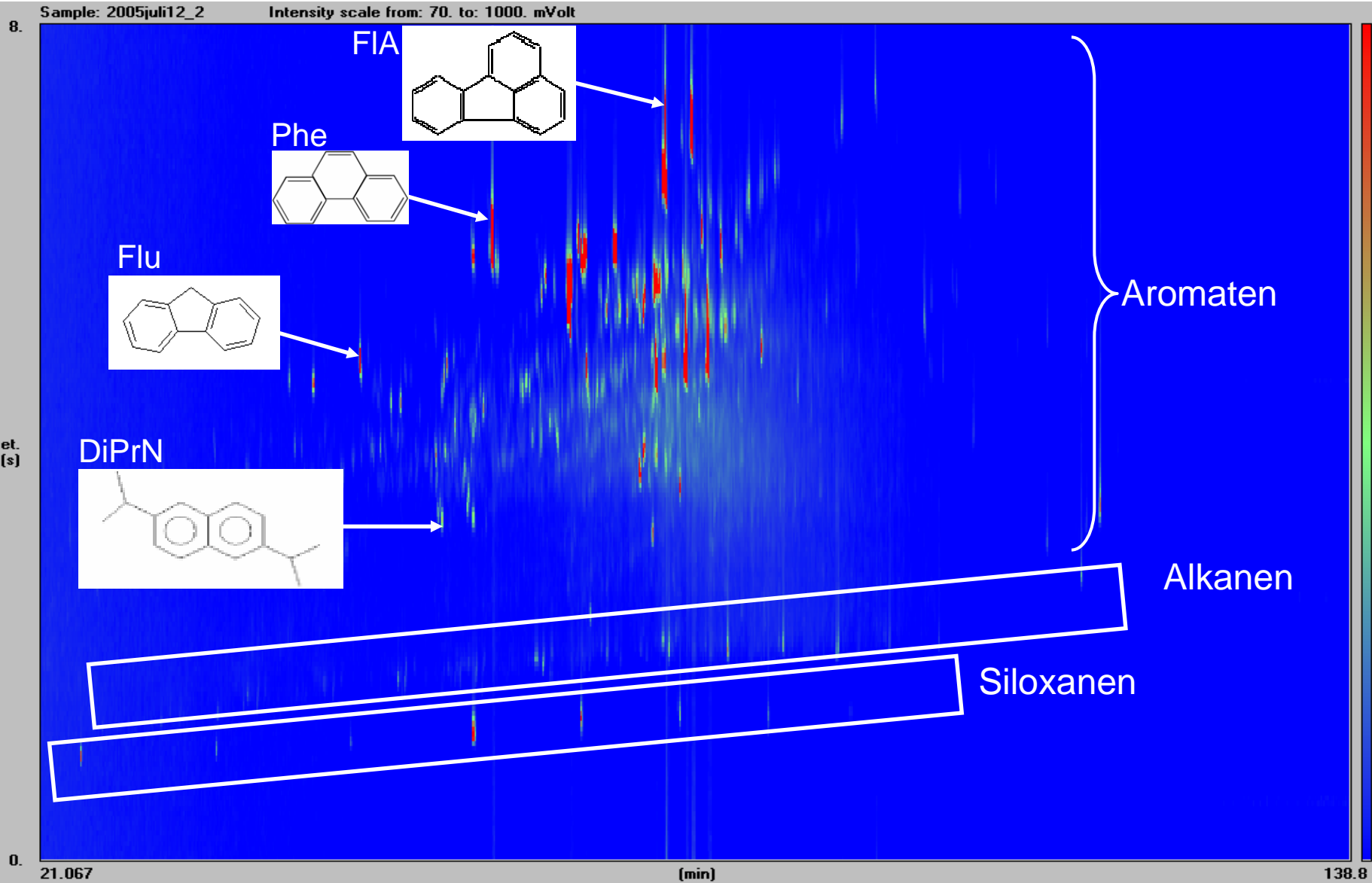




GCXGC/qLRMS-chromatogram (PUF, F2)



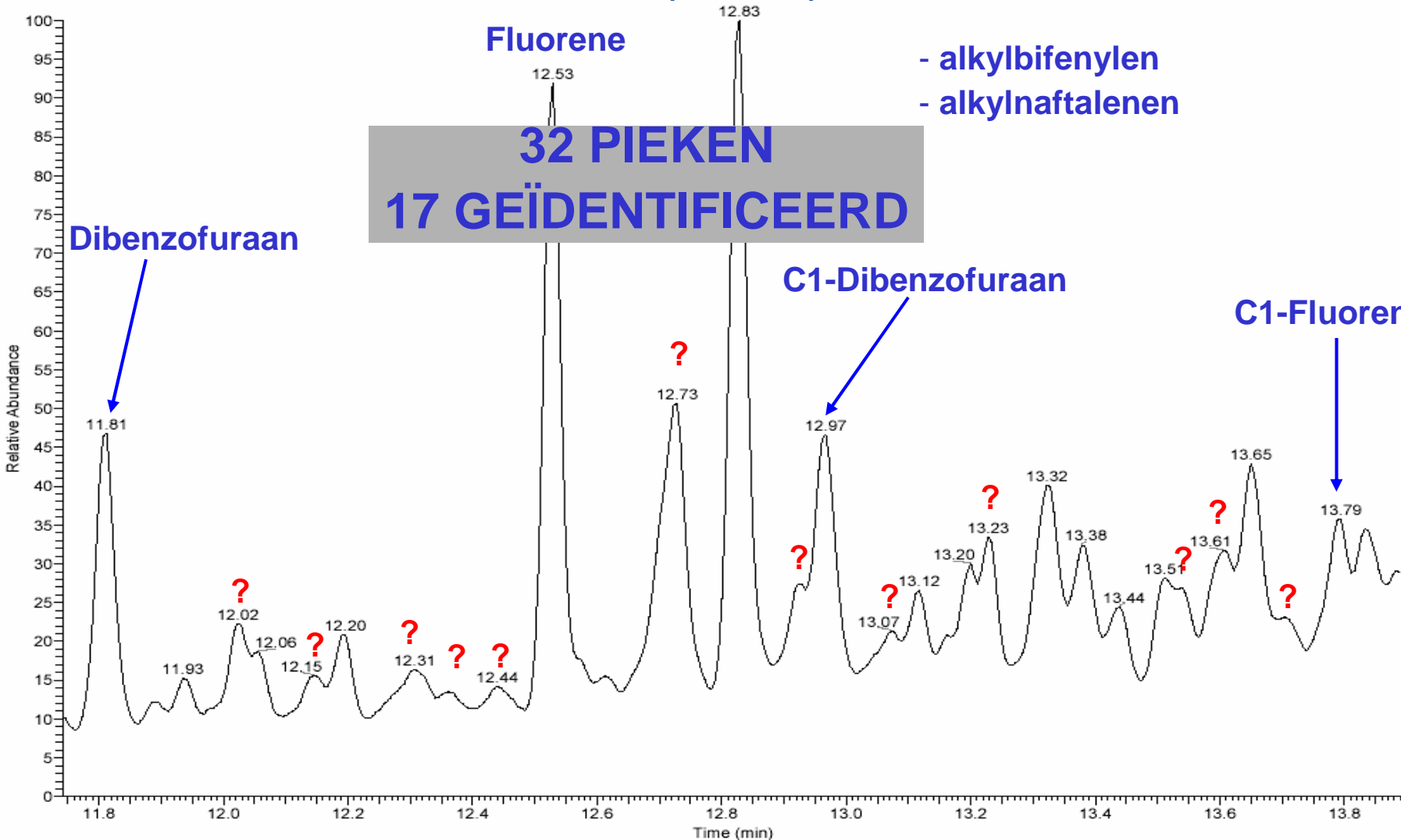
## GCXGC/MS-chromatogram (PUF, F2)



## GC/MS-chromatogram (PUF, F2) (dibenzofuran – C1-fluorene)

2005-3293 put/2\5\5\Data\20050622\_09

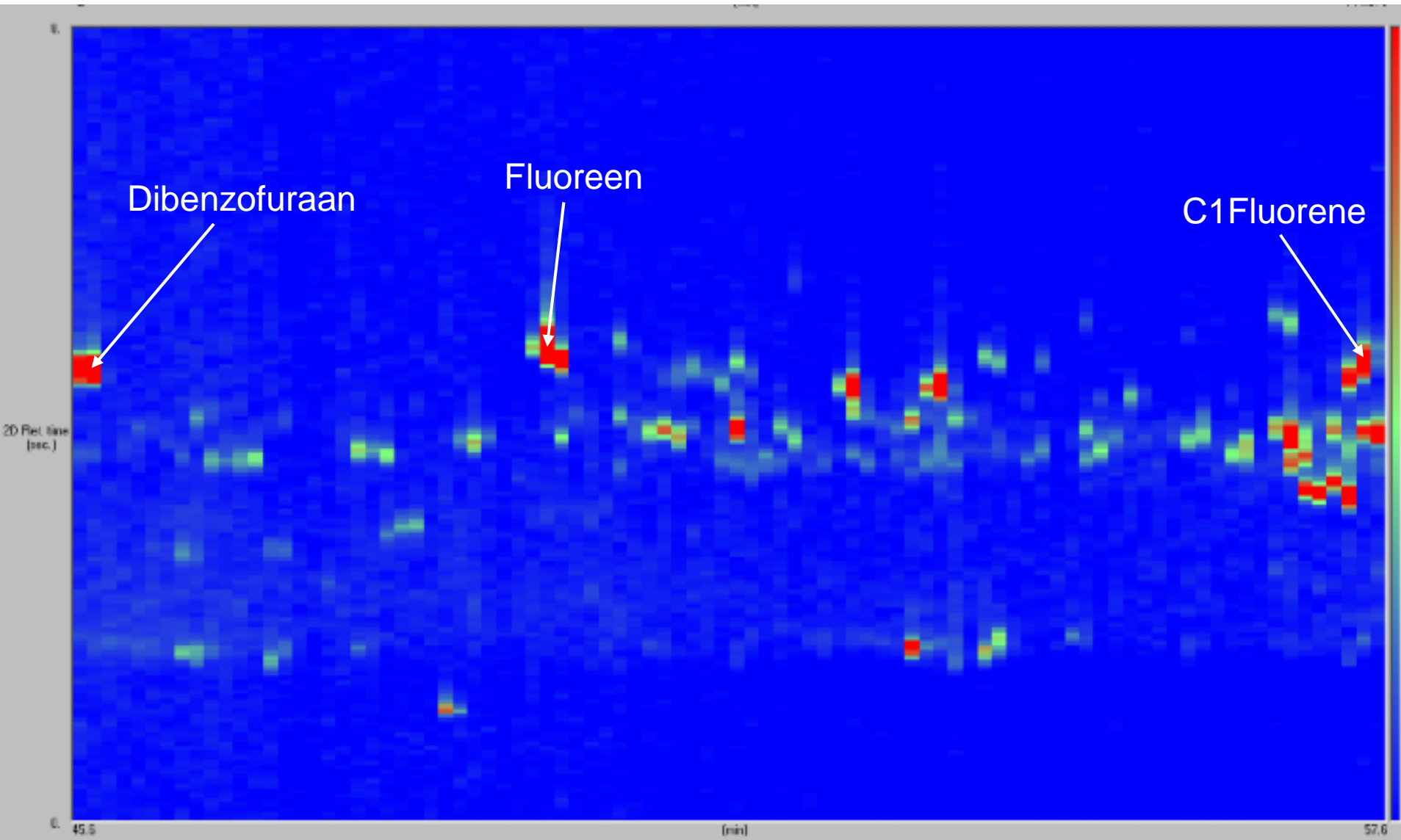
RT: 11.74 - 13.89



NL:  
9.76E6  
TIC MS  
20050622\_09

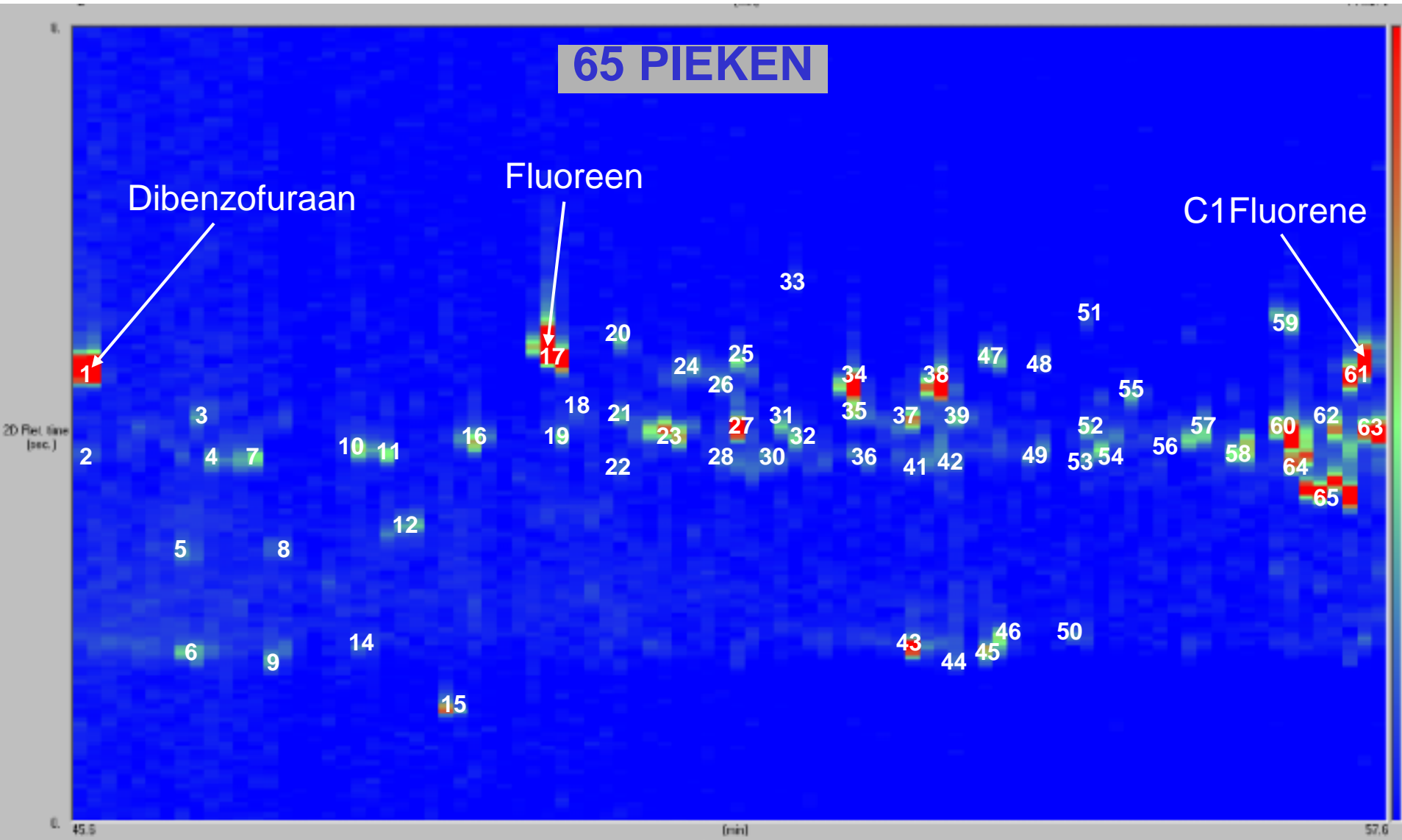
# INVENTARISATIESTUDIE POLYAROMATISCHE KOOLWATERSTOFFEN IN LUCHT

## GCXGX/MS-chromatogram (PUF, F2) (dibenzofuran – C1-fluorene)



# INVENTARISATIESTUDIE POLYAROMATISCHE KOOLWATERSTOFFEN IN LUCHT

## GCXGX/MS-chromatogram (PUF, F2) (dibenzofuran – C1-fluorene)



## GCXGX/MS-chromatogram (PUF, F2) (dibenzofuran – C1-fluorene)

**65 PIEKEN**  
**57 GEÏDENTIFICEERD**

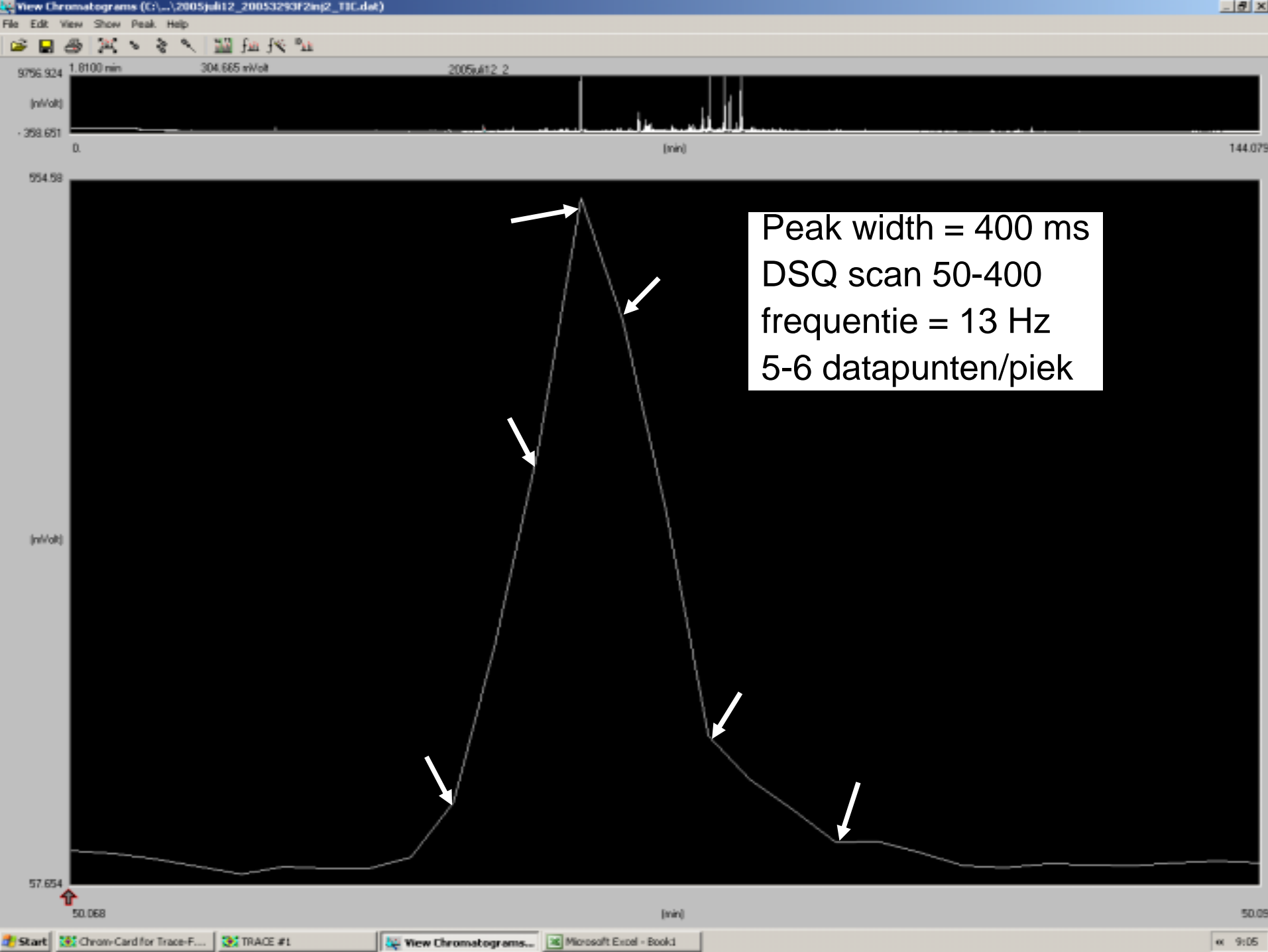
1.	dibenzofuran	23.	C2-bifenyl	45.	n-hexadecane
2.	C3-naftalene	24.	dihydrofluorene	46.	n.i.
3.	C2-bifenyl	25.	dihydrofluorene	47.	C1-dibenzofuran
4.	C3-naftalene	26.	C1-fluorene	48.	n.i.
5.	ditert.butylhydroxytoluene	27.	C2-bifenyl	49.	C4-naftalene
6.	pentadecene	28.	n.i.	50.	n.i.
7.	C3-naftalene	29.	C4-naftalene	51.	methyldiphenylamine
8.	n.i.	30.	methylenebis(C1benzene)	52.	propanediylbis(benzene)
9.	n-pentadecane	31.	C2-bifenyl	53.	C4-naftalene
10.	C3-naftalene	32.	n.i.	54.	C4-naftalene
11.	C3-naftalene	33.	methylphenylpyridine	55.	dimethyl(phenylmethyl)benzene
12.	n.i.	34.	C1-dibenzofuran	56.	C4-bifenyl
13.	C5-hexahydronaftalene	35.	methylenebis(C1benzene)	57.	ethyl(phenylmethyl)benzene
14.	alkene	36.	C4-naftalene	58.	C4-naftalene
15.	siloxane	37.	C2-bifenyl	59.	diphenylethene
16.	C3-naftalene	38.	C1-dibenzofuran	60.	C4-bifenyl
17.	fluorene	39.	methylenebis(C1benzene)	61.	C1-fluorene
18.	C3-naftalene	40.	C3-bifenyl	62.	C4-naftalene
19.	C2-bifenyl	41.	C4-naftalene	63.	C4-naftalene
20.	isopropenylnaftalene	42.	C4-naftalene	64.	C5-naftalene
21.	C3-naftalene	43.	hexadecene	65.	C6-naftalene
22.	C4-naftalene	44.	n.i.		

# BESLUIT

**GCXGC + qLRMS :**  
**zeer krachtige combinatie voor screening complexe stalen**  
**maar...**

- Beperkingen software
- Beperkingen hardware







**VRAGEN ?**



# DECONVOLUTION?

D:\VITO\DATA\AMDIS\20050622\_09.RAW

Run Rescale Info...

