

Chromatography

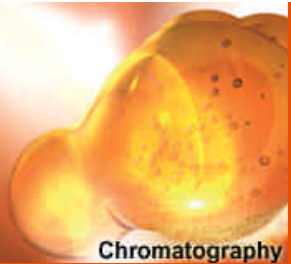
Determination of organic contaminants in water by modern GCMS:

- Standard vs fast
- EI and NCI
- Two columns – one MS

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Product Specialist GC&GCMS

Shimadzu Deutschland GmbH

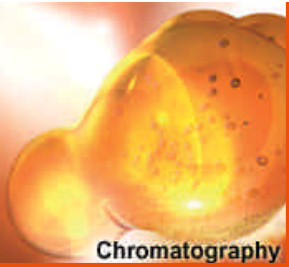


Modern GCMS

- Sensitivity
- Rapid answers
- Ease of use
- Flexibility
- Includes sample prep

- GCMS-QP2010



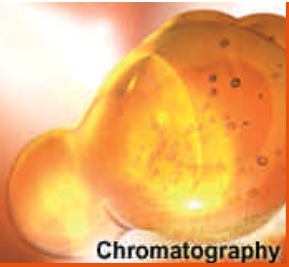


Flexibility

- 1.) Different sample introduction systems
 - PTV/SPL combinations
 - Pyrolysis/SPL

- 2) Different Columns for screening many different analytes

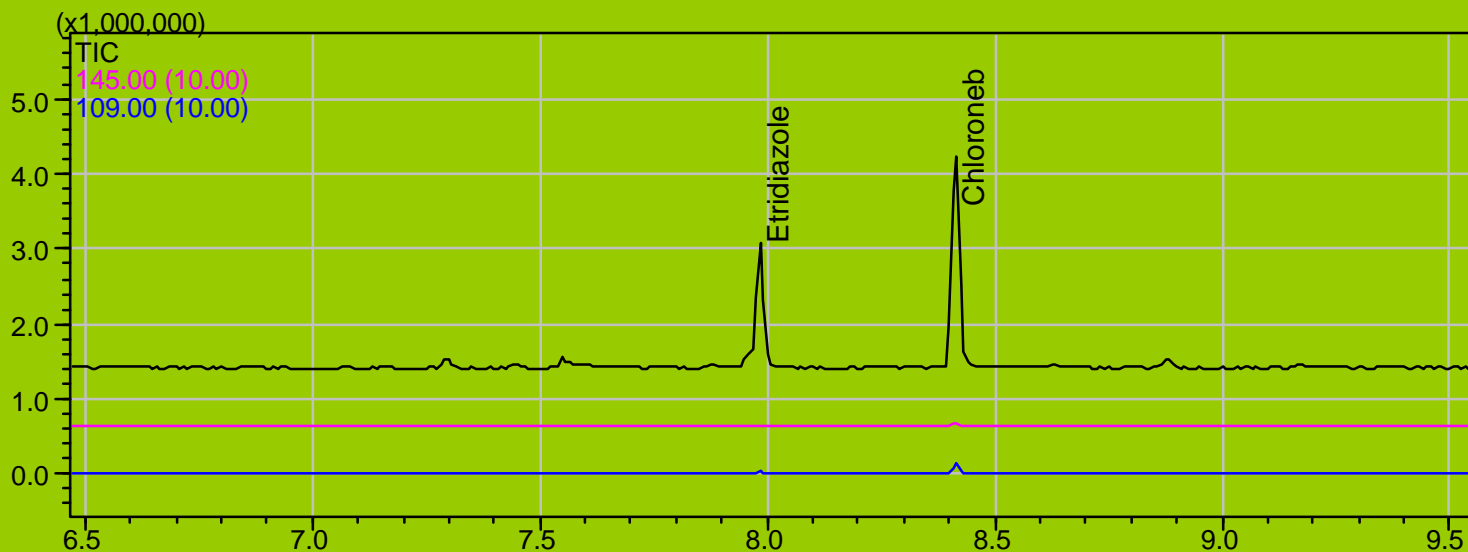
Two column – one MS setup



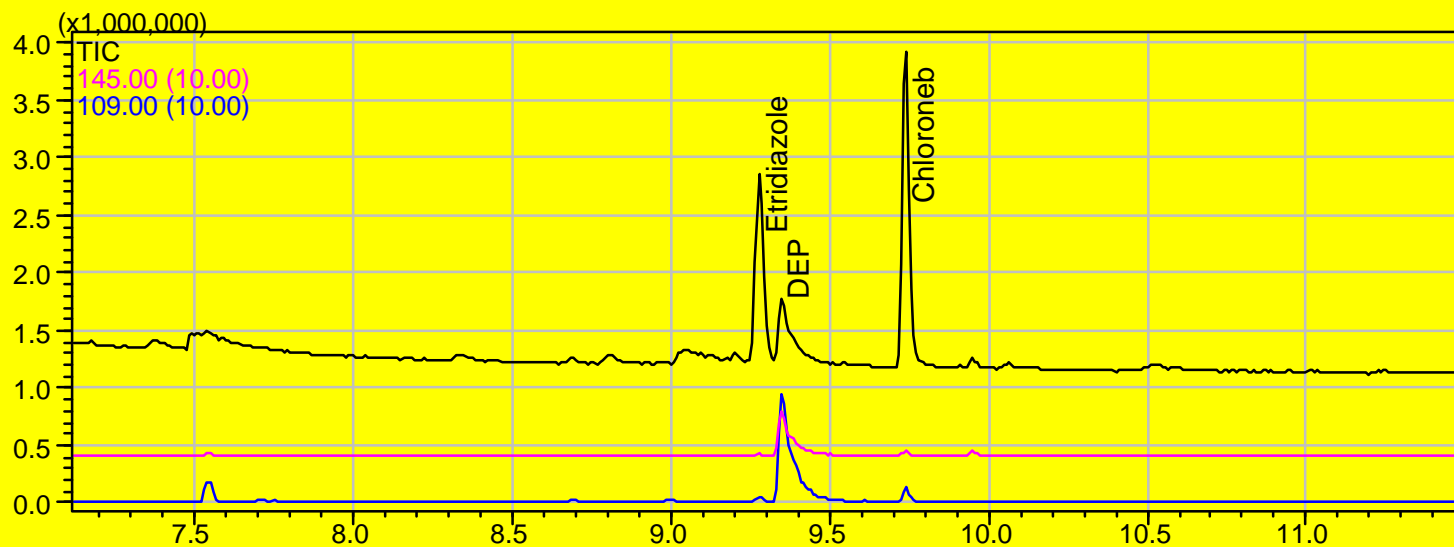
Chromatography

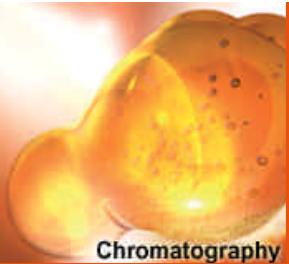
Dual Column - Pesticides

Rtx-5MS
Hot SPLITLESS



Rtx-5MS
PTV





Chromatography

Analytical Conditions

Rtx-5MS SPLITLESS

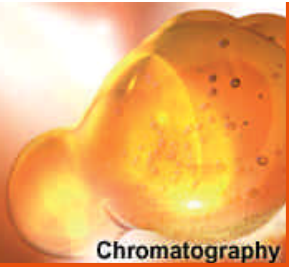
? GCMS QP2010

Column : Rtx-5MS [30m× 0.25mm I.D. df=0.25um]
Injection Mode : Splitless
Injection Temp. : 250 ?
Column Oven Temp. : 35? (1min)? (20? /min)? 140? ? (10? /min)? 280? (3min)
Carrier Gas : He
Flow Control Mode : Linear Velocity (48.6 cm/sec)
Ion Source Temp. : 200?
Interface Temp. : 250?
SCAN
Scan Range : m/z 70~ 360
Interval : 0.5sec

Rtx-5MS PTV

? GCMS QP2010

Column : Rtx-5MS [30m× 0.25mm I.D. df=0.25um]
Injection Mode : PTV
Injection Temp. : 30? (0.5min)? (100? /min)? 280? (17min)
Column Oven Temp. : 35? (1min)? (20? /min)? 140? ? (10? /min)? 280? (3min)
Carrier Gas : He
Flow Control Mode : Linear Velocity (48.6 cm/sec)
Ion Source Temp. : 200?
Interface Temp. : 250?
SCAN
Scan Range : m/z75~ 360
Interval : 0.5sec



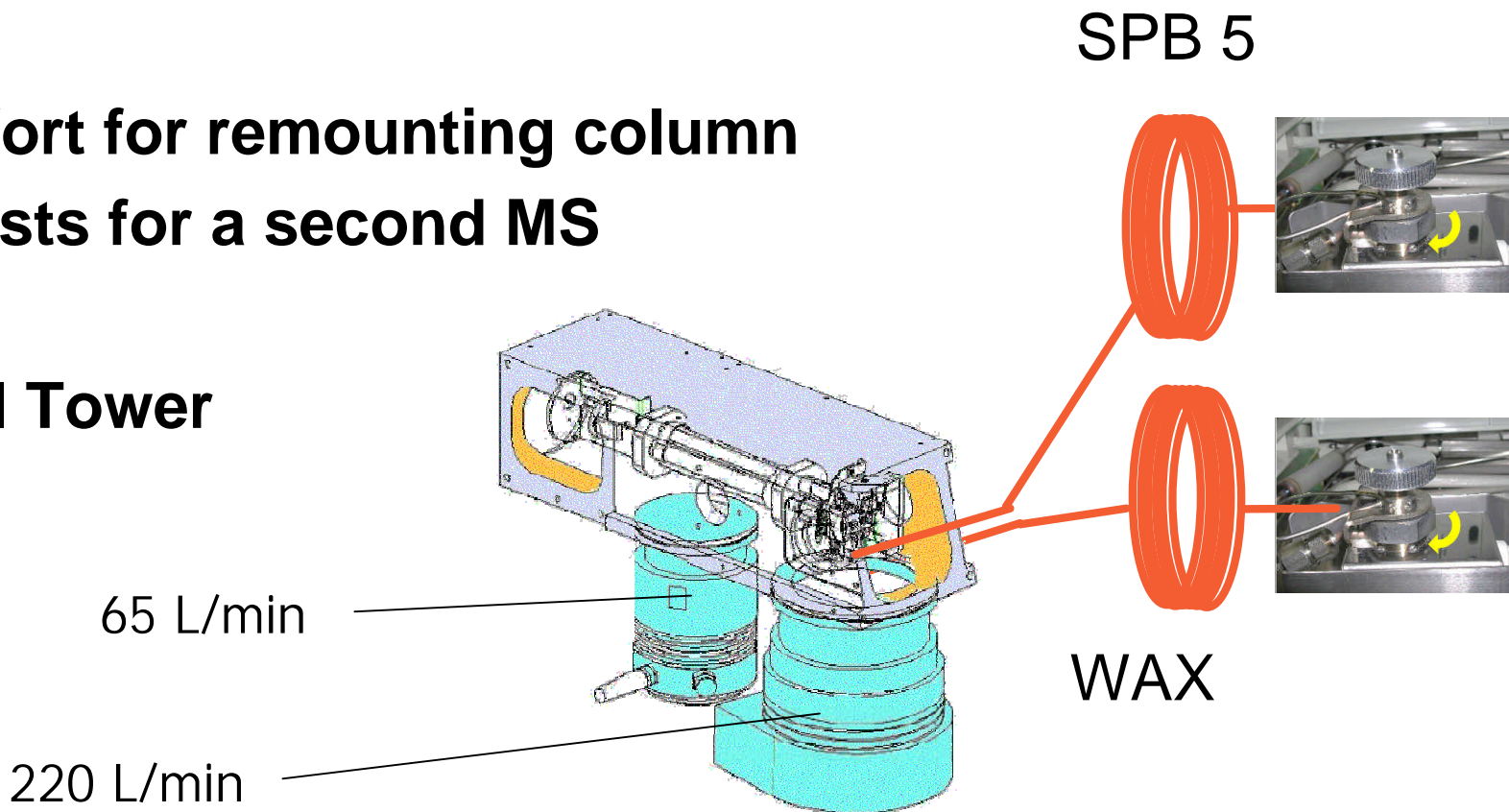
Chromatography

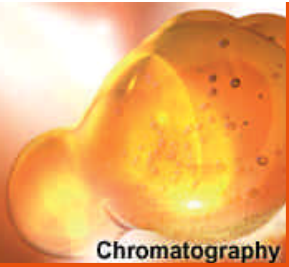
Flexibility

Dual column setup:

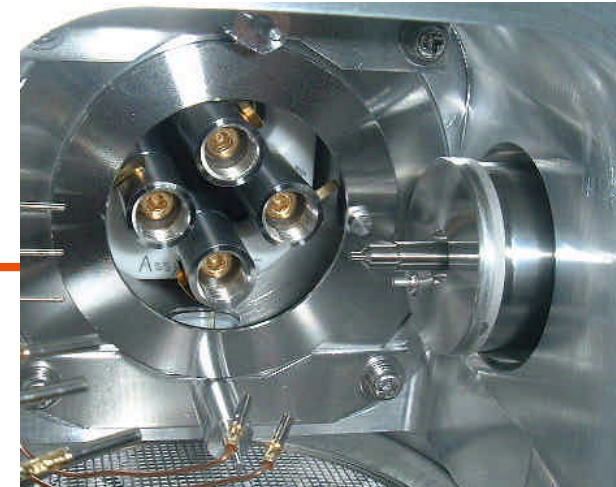
- 2 columns in 1 MS
- saves effort for remounting column
- saves costs for a second MS

AOC-20 Dual Tower
AOC-5000

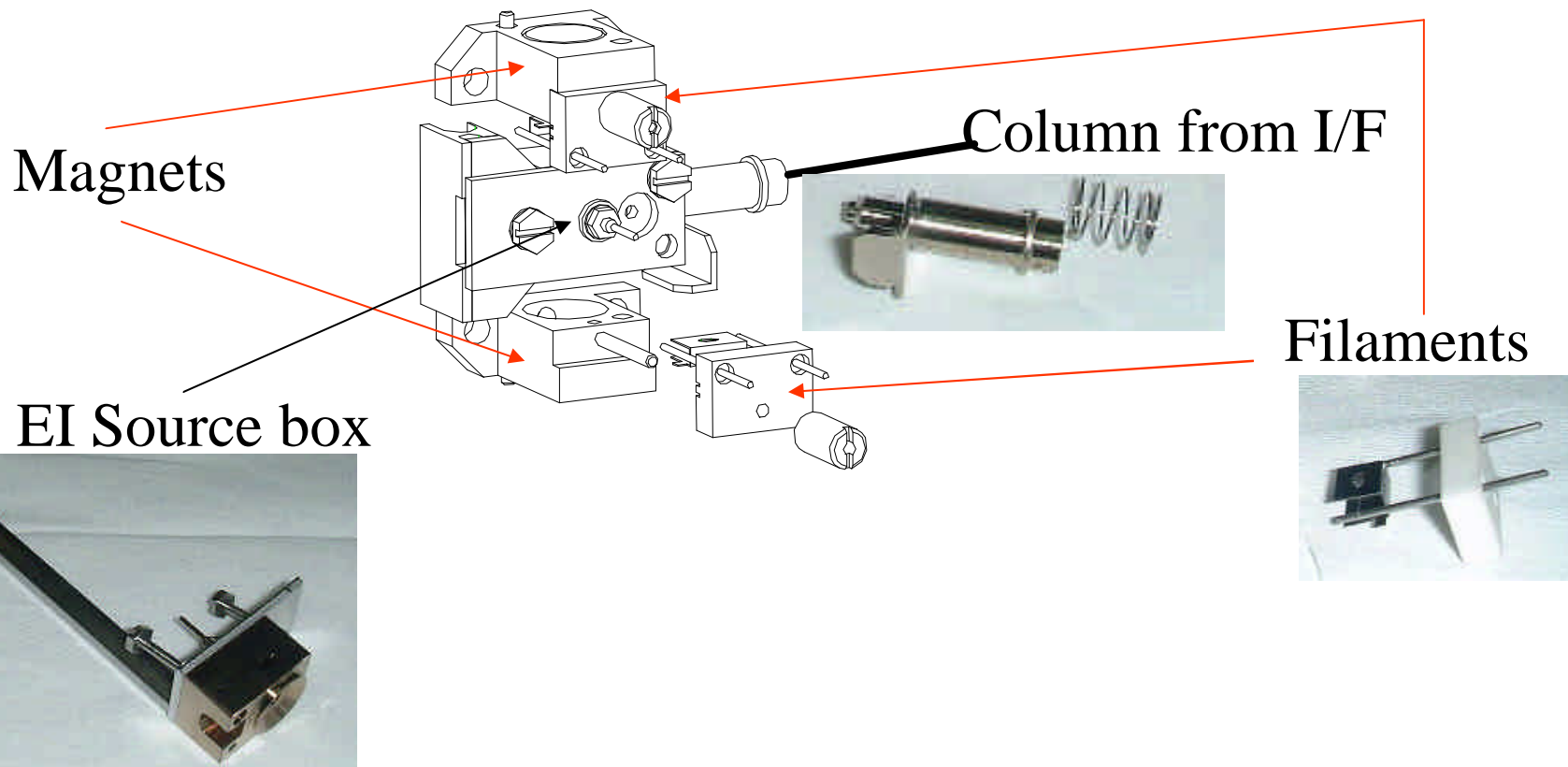


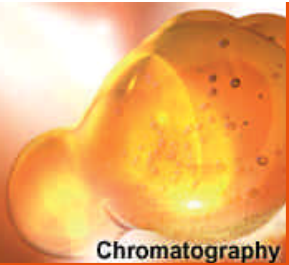


GCMS QP-2010



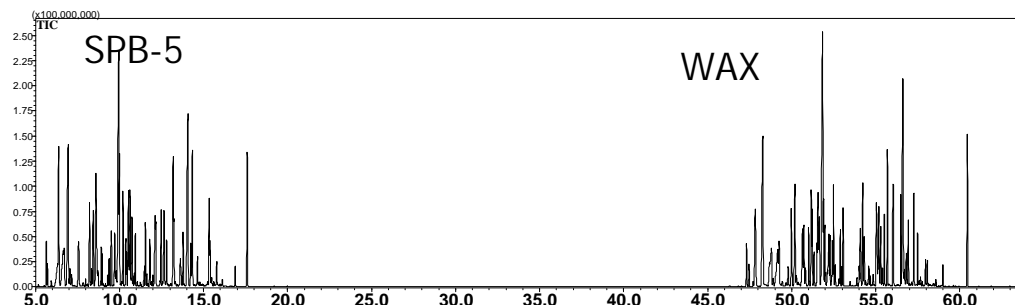
New Ion Source





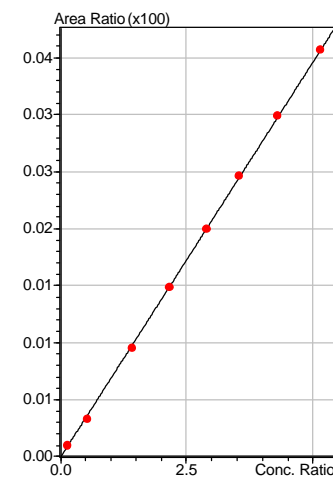
Dual Columns – Flexibility

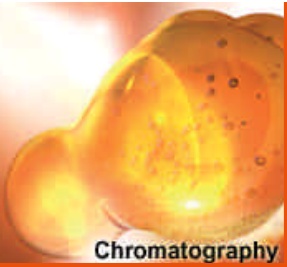
- Allergens:
- Method based on SCAN instead of SIM



- Full Scan Information and confirmation via second column.
- H. Leijds et al: J. Agric. Food Chem. 2005,53,6487

ID	Name	m/z
1	2,3-DICHLOROTOLUENE (Cp Restek rtx-5MS, low)	125.00
2	2,3-DICHLOROTOLUENE (Cp Sil 24 CB, low)	125.00
3	BENZYL ALCOHOL (Cp Restek rtx-5MS)	108.00
4	BENZYL ALCOHOL (Cp Sil 24 CB)	108.00
5	LIMONENE (Cp Restek rtx-5MS)	68.00
6	LIMONENE (Cp Sil 24 CB)	68.00
7	LINALOOL (Cp Restek rtx-5MS)	71.00
8	LINALOOL (Cp Sil 24 CB)	71.00
9	METHYL HEPTIN CARBONATE (Cp Restek rtx-5MS)	123.00
10	METHYL HEPTIN CARBONATE (Cp Sil 24 CB)	123.00
11	CITRONELLOL (Cp Restek rtx-5MS)	81.00
12	CITRONELLOL (Cp Sil 24 CB)	81.00
13	NERAL (Cp Restek rtx-5MS)	69.00
14	NERAL 84 (Cp Restek rtx-5MS)	84.00
15	NERAL (Cp Sil 24 CB)	69.00
16	NERAL 84 (Cp Sil 24 CB)	84.00
17	CINNAMALDEHYDE (Cp Restek rtx-5MS)	131.00
18	CINNAMALDEHYDE (Cp Sil 24 CB)	131.00
19	GERANIOL (Cp Restek rtx-5MS)	93.00
20	GERANIOL (Cp Sil 24 CB)	93.00
21	GERANIAL (Cp Restek rtx-5MS)	69.00
22	GERANIAL 84 (Cp Restek rtx-5MS)	84.00
23	GERANIAL (Cp Sil 24 CB)	69.00
24	GERANIAL 84 (Cp Sil 24 CB)	84.00
25	ANISIC ALCOHOL (Cp Restek rtx-5MS)	138.00
26	ANISIC ALCOHOL (Cp Sil 24 CB)	138.00
27	HYDROXY CITRONELLAL (Cp Restek rtx-5MS)	59.00
28	HYDROXY CITRONELLAL (Cp Sil 24 CB)	59.00
29	CINNAMYL ALCOHOL (Cp Restek rtx-5MS)	134.00
30	CINNAMYL ALCOHOL (Cp Sil 24 CB)	134.00
31	EUGENOL (Cp Restek rtx-5MS)	164.00
32	EUGENOL (Cp Sil 24 CB)	164.00



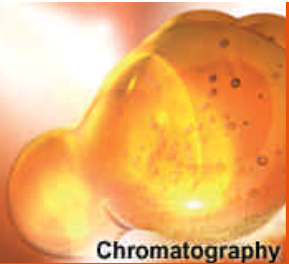


Matrix Water

GCMS analysis according to European Drinking Water Regulations

- volatile hydrocarbons (VOC´s)
- polycyclic aromatic hydrocarbons (PAH´s)
- benzene, toluene und xylene (BTX)
- pesticides and herbicides





Chromatography

Dual Column-Drinking Water

SPL: FS-SE-54

(50m × 0.32mm I.D. df=0.5um)

Analysis of VOCs

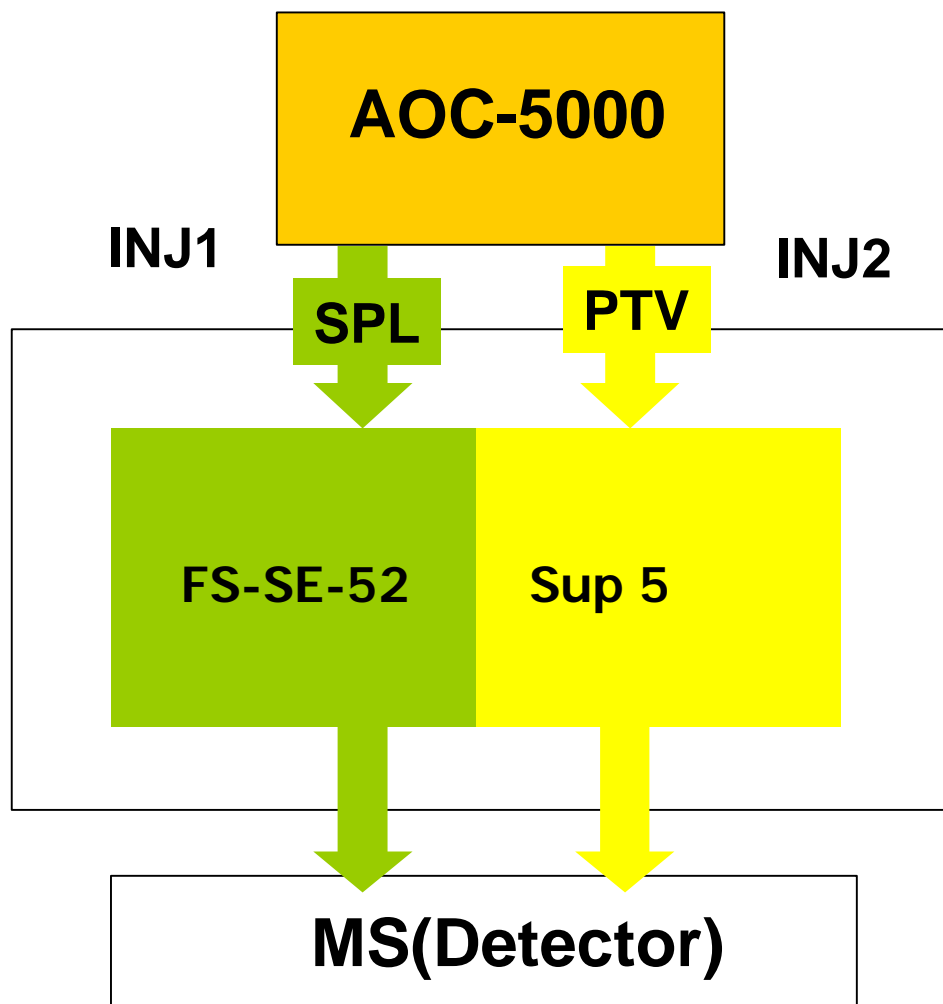
HS&

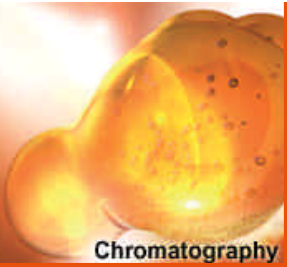
HS-SPME: Carboxen phase

PTV:Supreme 5

(30m × 0.25mm I.D. df=0.25um)

**For analysis of
Pesticides,PCBs...**





Chromatography

Volatile Hydrocarbons (VOC's) - HS

1,2-Dichlorethane:

Concentration: 1 µg/l

Limit for Drinking water: 3 µg/l

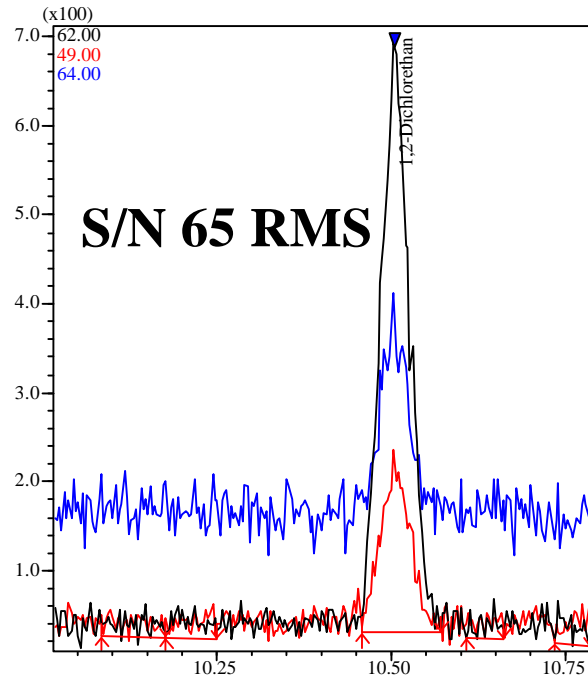
Split 10:1

Scan 48-100, IV=0.4s

Det Gain 1 KV

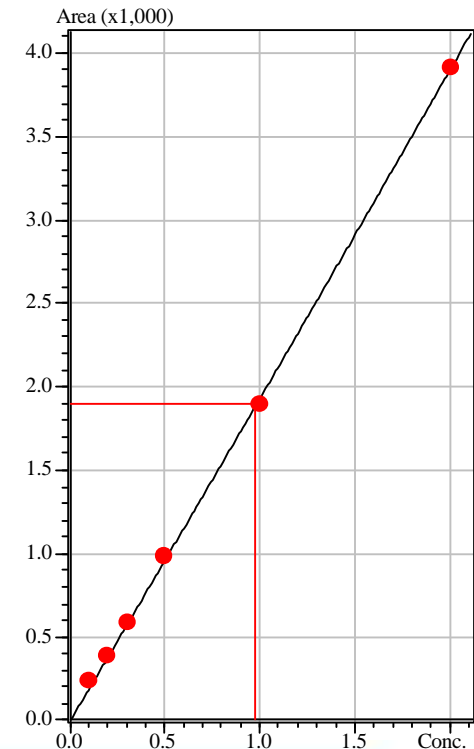
Calibration range: 0.1 µg/l - 10 µg/l

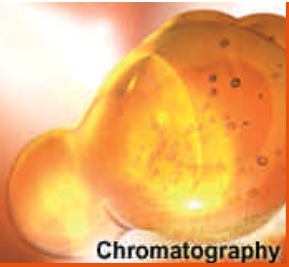
Correlation factor: 0.9997



HS:

80 °C, 60 min





Chromatography

Benzene, Toluene and Xylene

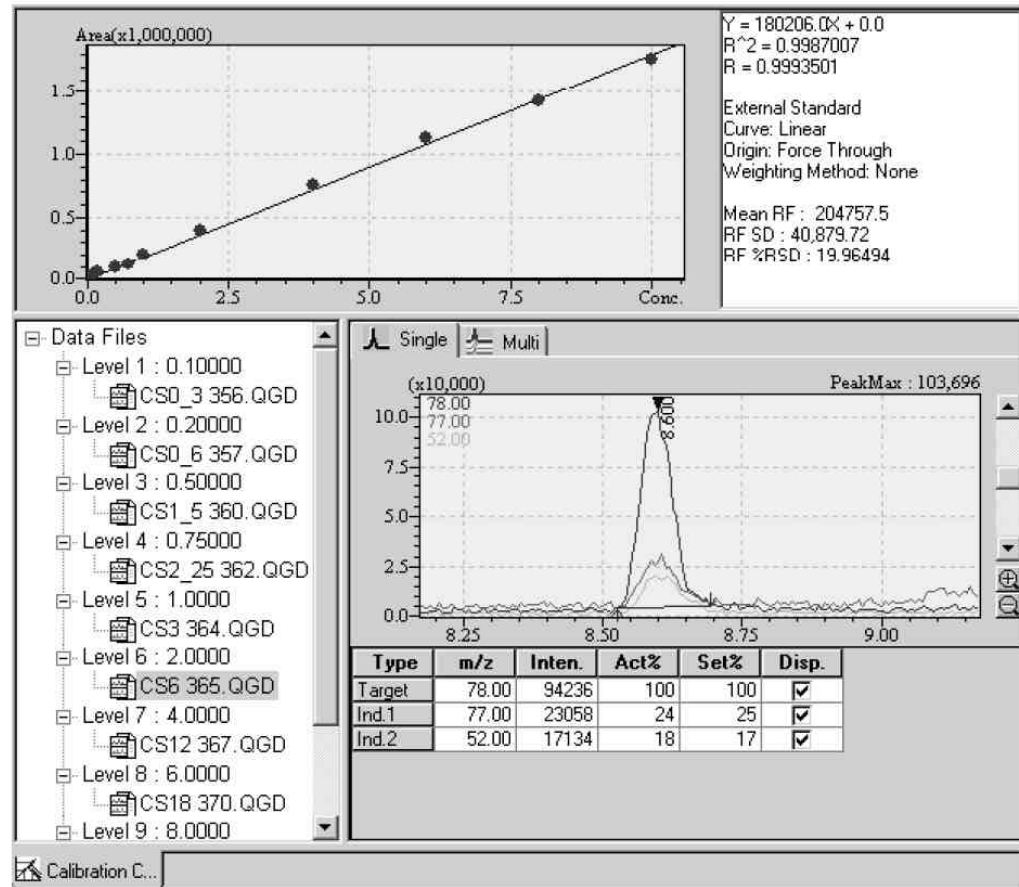
Benzene:

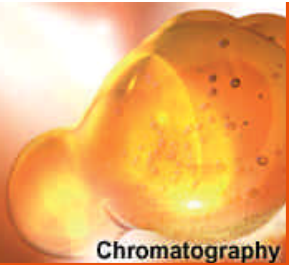
10 point calibration

0,1 – 10 µg/l

Drinking water limit

1 µg/l

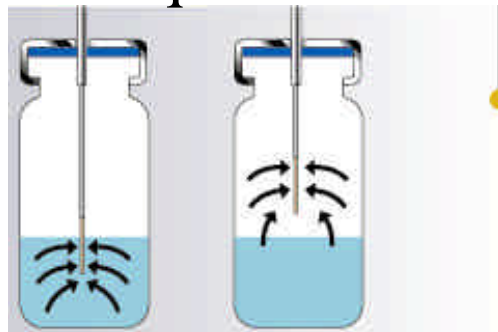




AOC 5000

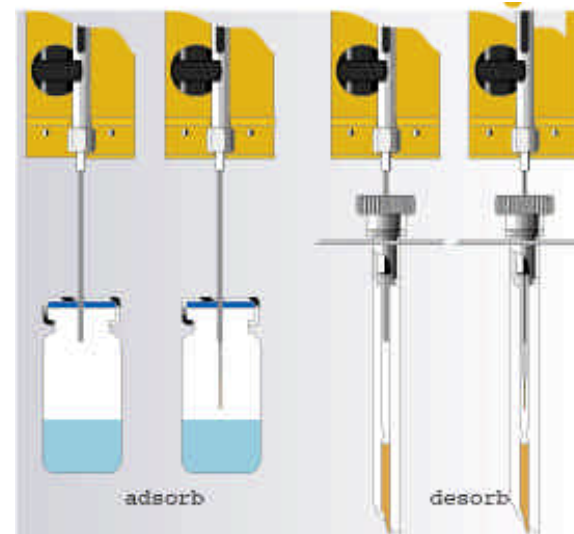
- SPME:

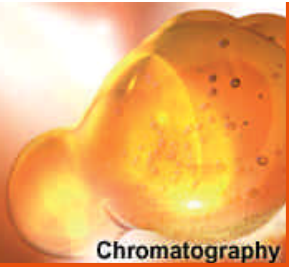
Variable Needle Penetration Depths
for Adsorption in Liquid or Head Space



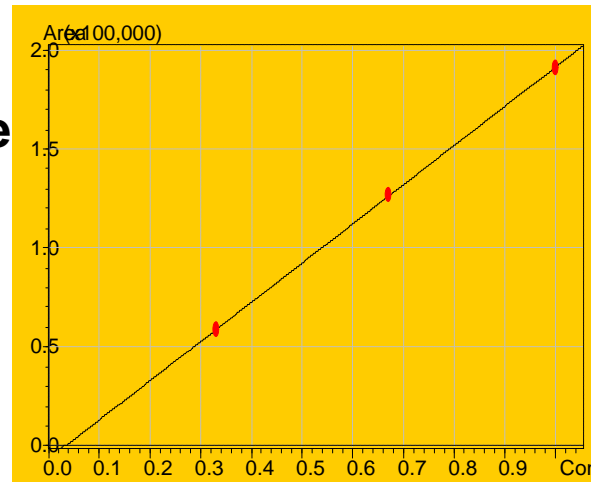
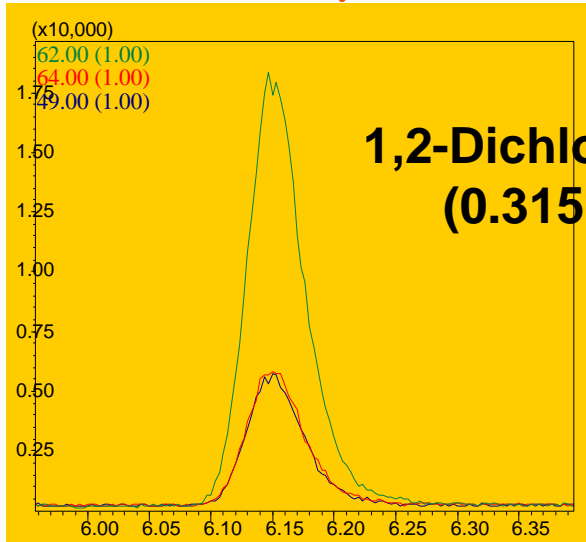
Adsorption
Vial in Agitator

Desorption
in Injector



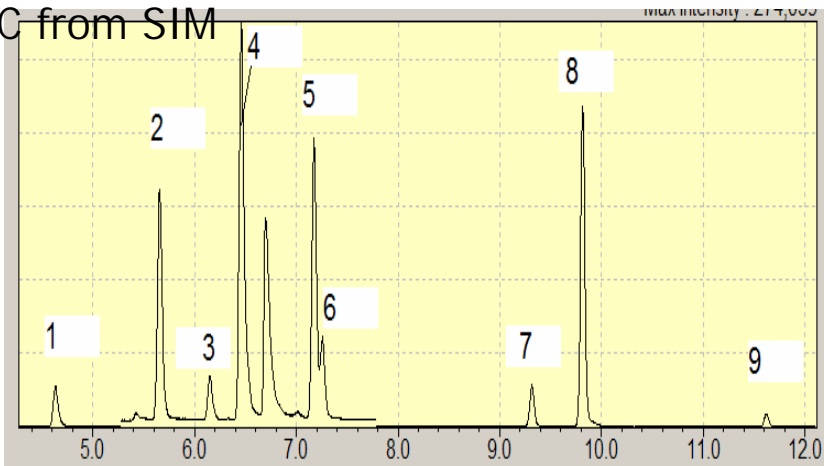


VOCs-HS/SPME (Carboxen)

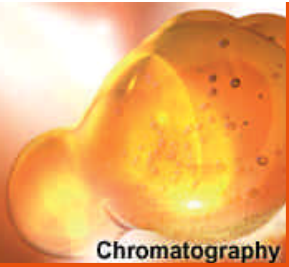


SPME Calibration:
 Ads.: 15 min, 50°C
 Des.: 0.5 min, 280 °C
 Split 5:1
 MS: SIM

TIC from SIM



	conc ug/L	RT		QM
1. Dichlormethan	0.31725	4.635	Target	84.00
2. Trichlormethan	0.31181	5.659	Target	83.00
3. 1,1,1-Trichlorethan	0.31482	6.170	Target	97.00
4. Tetrachlorkohlenstoff	0.31942	6.502	Target	117.00
5. Trichlorethen	0.32500	7.176	Target	130.00
6. Monobromdichlormethan	0.31626	7.259	Target	83.00
7. Dibromchlormethan	0.31184	9.319	Target	129.00
8. Tetrachlorethen	0.33027	9.819	Target	166.00
9. Tribrommethan	0.31332	11.627	Target	173.00



Chromatography

VOCs-HS/SPME (Carboxen)

Data Acquisition Parameters

Select Line1 Line2

GC MS Description

Inj. Port: SPL1 Inj. Heat Port: INJ1

Column Oven Temp.: 40.0 °C °C

Injection Temp.: 280.0 °C

Injection Mode: Split

Sampling Time: 1.00 min

Carrier Gas: He Prim. Press.: 300-500

Flow Control Mode: Linear Velocity

Pressure: 18.1 kPa

Total Flow: 9.0 mL/min

Column Flow: 1.00 mL/min

Linear Velocity: 28.0 cm/sec

Purge Flow: 3.0 mL/min

Split Ratio: 5.0

Detail of Injection Port...

High Press. Injection: Carrier Gas Saver

Splitter Hold: Fan

Split Ratio Program

Program: Column Oven Temperature

	Rate	Final Temperature	Hold Time
0	-	40.0	1.00
1	7.00	135.0	2.00
2	0.00	0.0	0.00
3	0.00	0.0	0.00

Total Program Time: 16.57 min

Column:

Name: FS-SE-54 Thickness: 0.50 um

Length: 50.0 m Diameter: 0.32 mm

Ready Check...

GC Program...

Pre-run Program Time Program

Schließen Hilfe

Data Acquisition Parameters

Select Line1 Line2

GC MS Description

GCMS-QP2010

Ion Source Temp.: 200 °C

Interface Temp.: 250 °C

Detector Voltage: Relative to the Tuning Result Absolute

Solvent Cut Time: 3.5 min

Micro Scan Width: 0 u

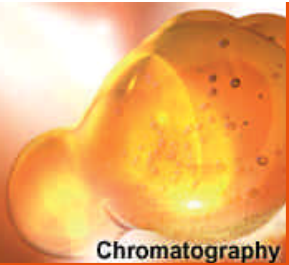
Threshold: 0

Use MS Program

GC Program Time: 16.57 min

	Start Time (min)	End Time (min)	Acq. Mode	Interval (sec)	Scan Speed	Start m/z	End m/z	Ch1 m/z	Ch2 m/z	Ch3 m/z
1	4.13	5.13	SIM	0.20				84.00	49.00	86.00
2	5.13	7.75	SIM	0.20				86.00	83.00	85.00
3	7.75	10.32	SIM	0.20				129.00	127.00	131.00
4	10.32	12.12	SIM	0.20				173.00	133.00	171.00
5	0.00	0.00	Scan	0.00	0	0.00	0.00			

Schließen Hilfe



Line 2: PCBs

- 100 ng/L

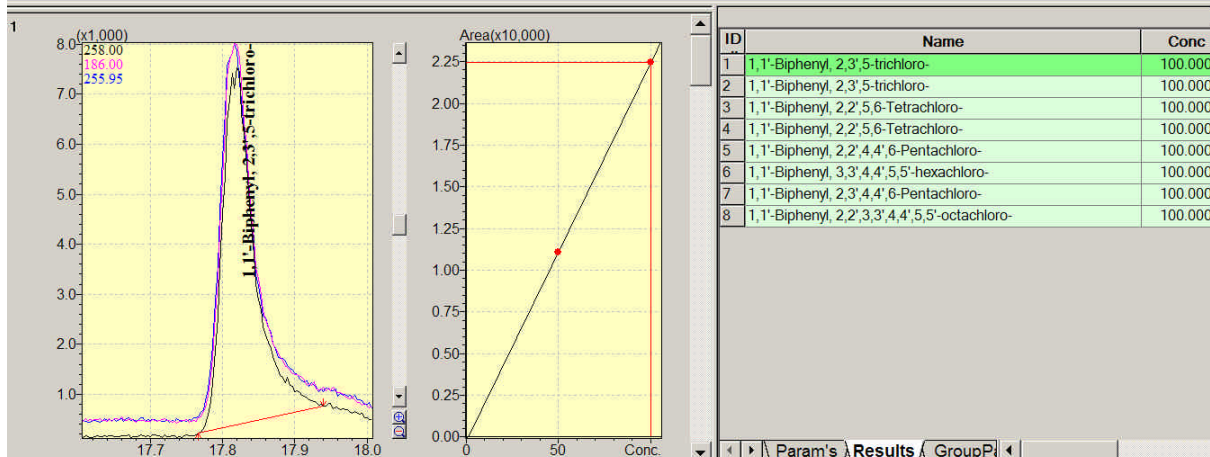
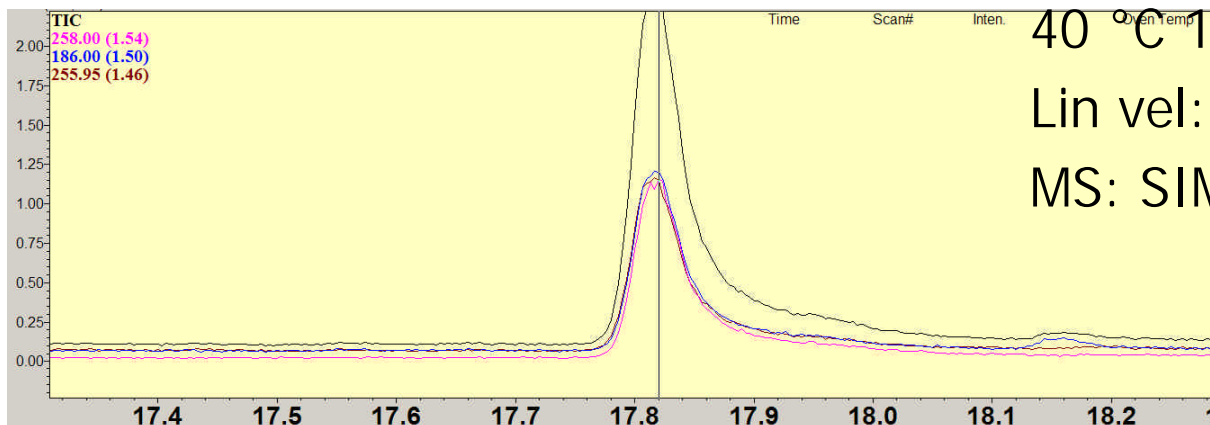
PTV Injection split 50:1

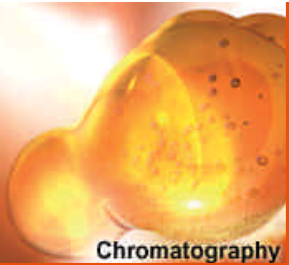
FS 5 30 m, 0.25 mm, 0.25 μ m

40 $^{\circ}$ C 1 min, 10 $^{\circ}$ C/min to 280 $^{\circ}$ C

Lin vel: 40 cm/s

MS: SIM





Triazine Pesticides

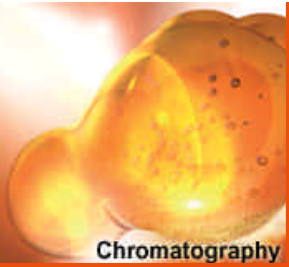
Procedure:

Determination of selected Nitrogen- and Phosphorous compounds, gas chromatographic procedure (DIN EN ISO 10695)

- solid phase extraction (Laborintern: HR-P (3ml/200mg) MN)
- Internal Standards used

Limit according to drinking water regulation, pesticides:

- sum concentration < 500 ng/l
- single components < 100 ng/l



Triazine Pesticides

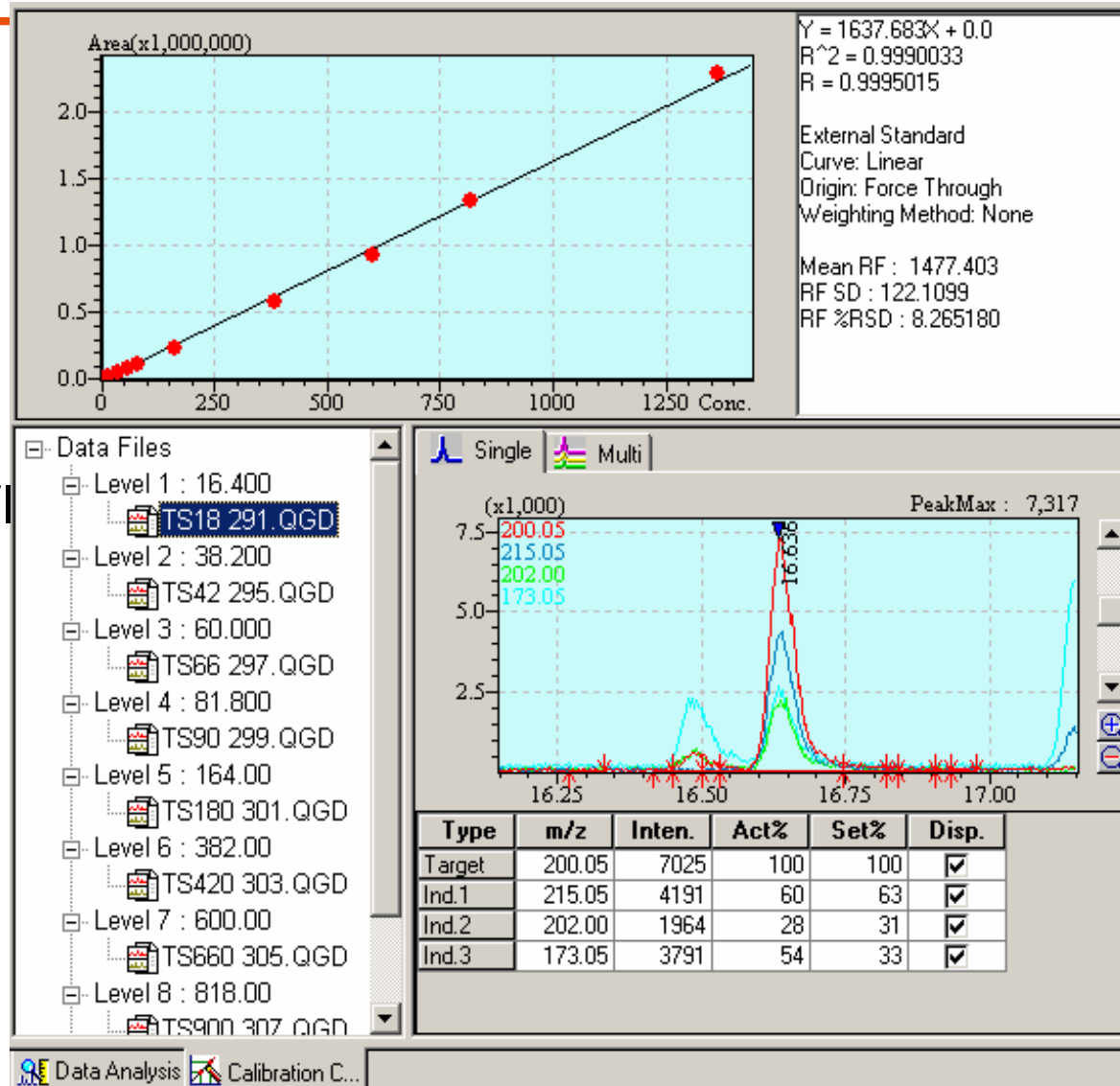
Atrazine

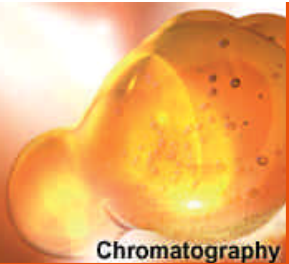
10 level calibration curve:

➤ calibration range: 15-1500 ng/l

➤ limit: 100 ng/l

concentration
determined: 16.4 ng/l



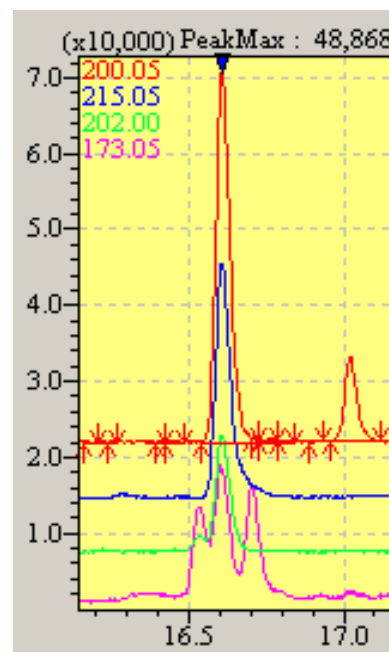


Chromatography

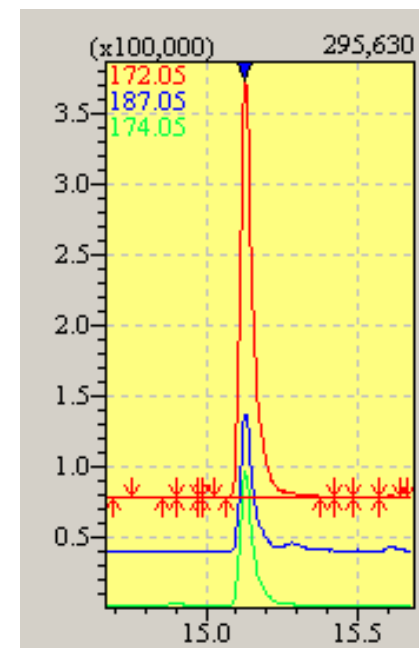
Reliability

Real sample (3 times repetitive measurement)

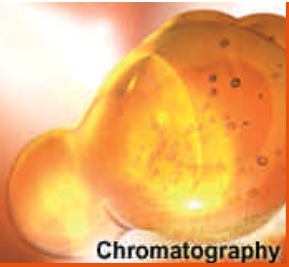
	Real sample (3 repetitions)		
Triazine	MW (µg/l)	Std.dev. (µg/l)	Std.dev. (%)
Atrazine	0,121	0,002	1,7
	MW (µg/l)	Std.dev.. (µg/l)	Std.dev. (%)
Atrazine-desethyl	0,292	0,013	4,4



Atrazine peak in real sample

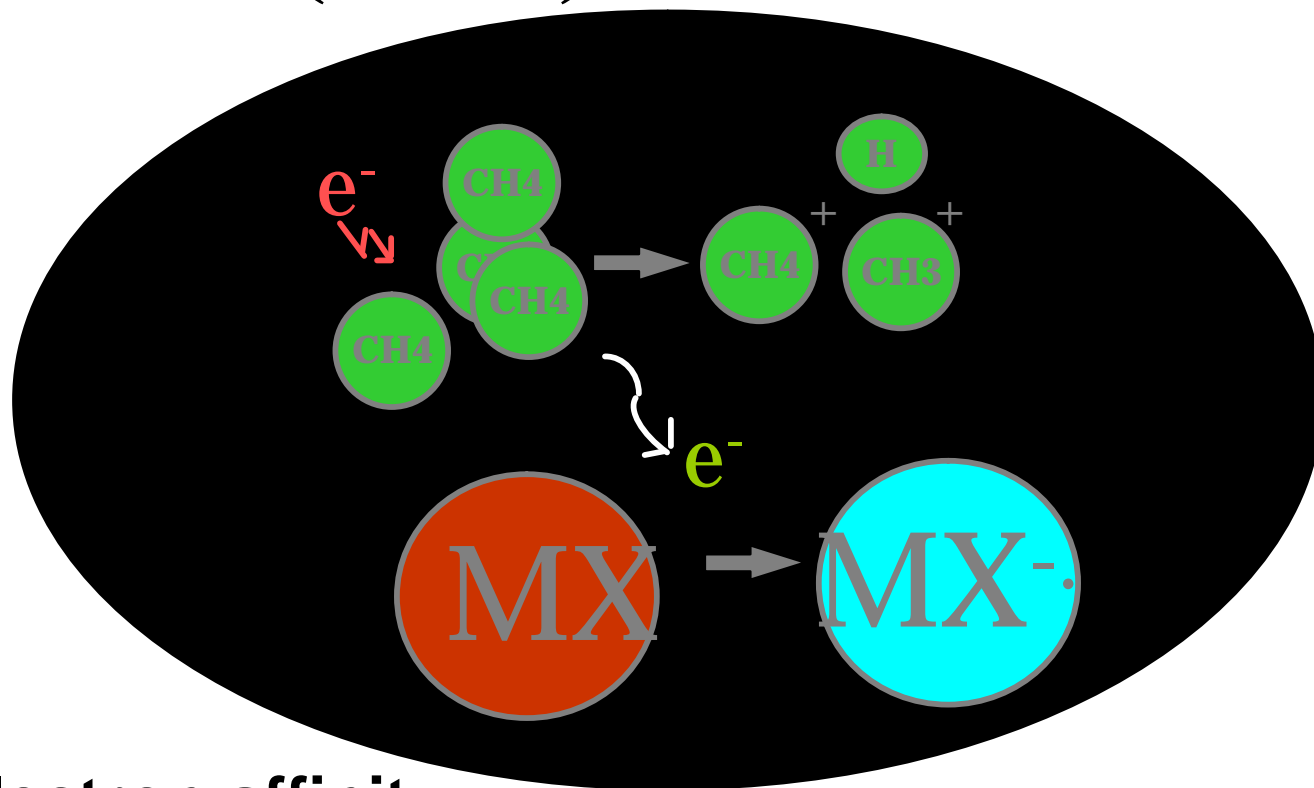


Atrazine-desethyl peak in real sample

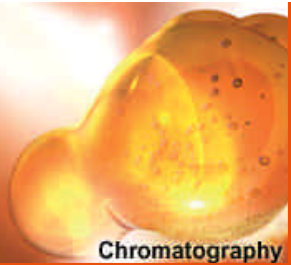


Negative chemical Ionization NCI

- $\text{MX} + \text{e}^- (\sim 0 \text{ eV}) \rightarrow \text{MX}^-$.



**X: High electron affinity
part**

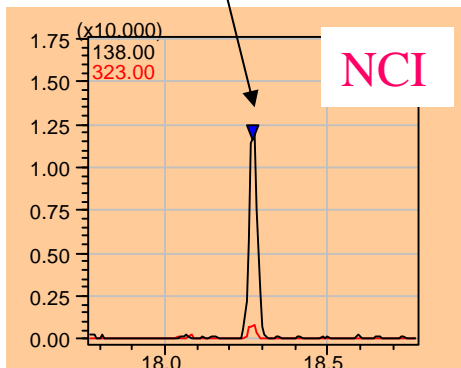
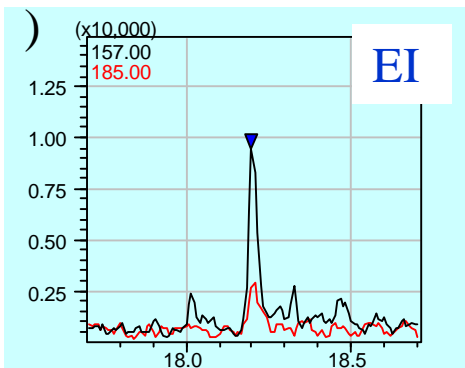


Chromatography

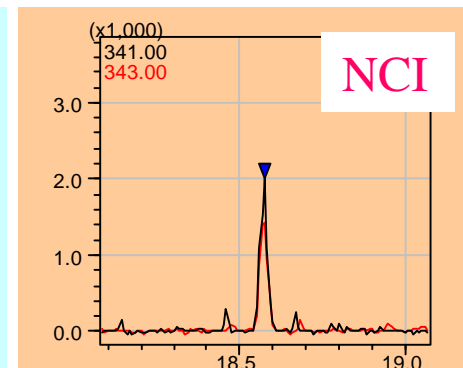
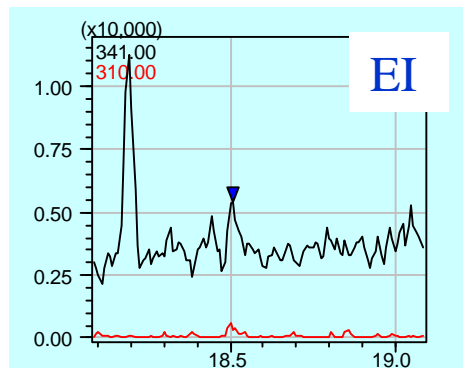
Comparison of Sensitivity NCI/EI

Higher sensitivity in NCI

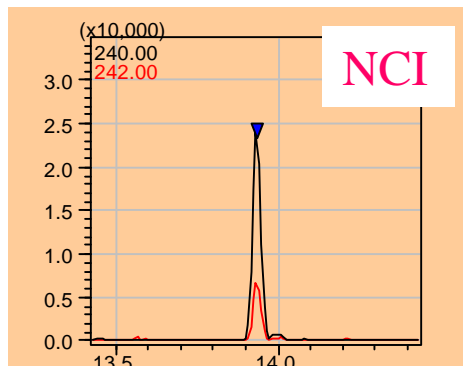
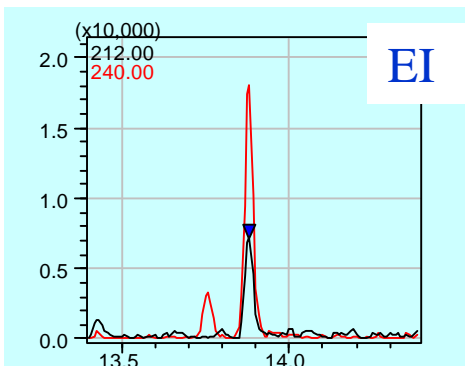
EPN(0.05 μ g/ml)



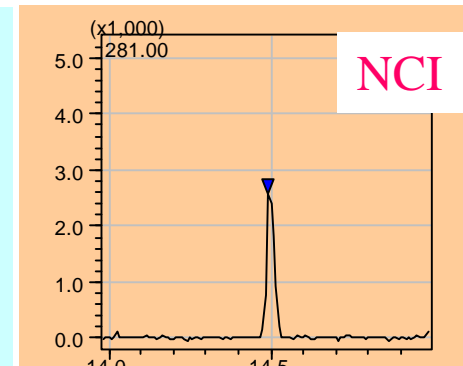
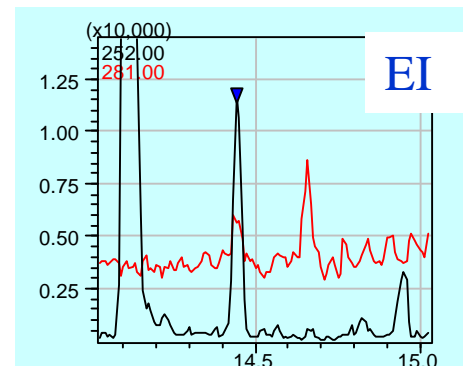
Bifenox(0.025 μ g/ml)



Cyanazin(0.01 μ g/ml)



Pendimethalin(0.025 μ g/ml)

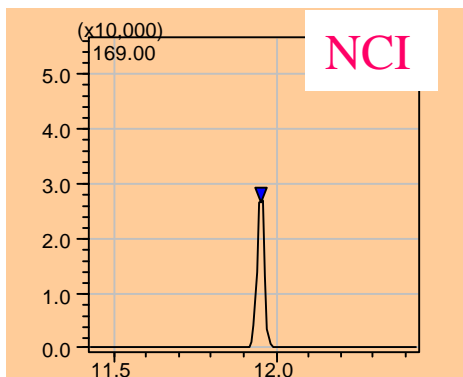
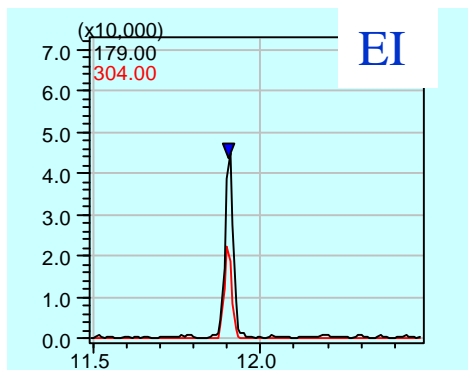




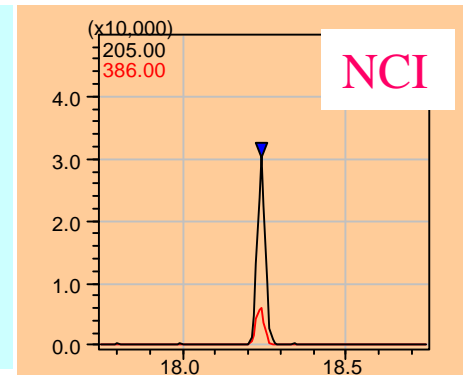
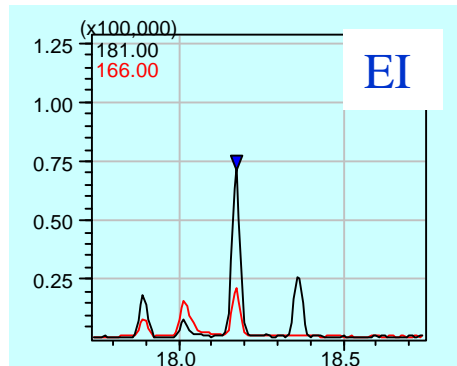
Comparison of Sensitivity NCI/EI

Similar sensitivity

Diazinon(0.05μ g/ml)

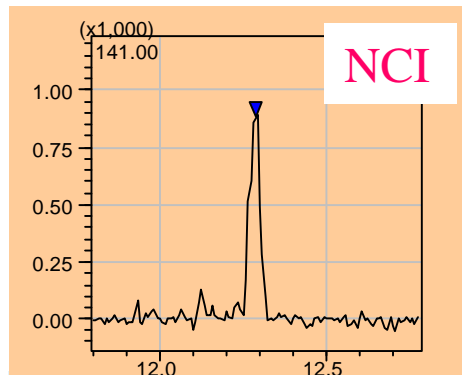
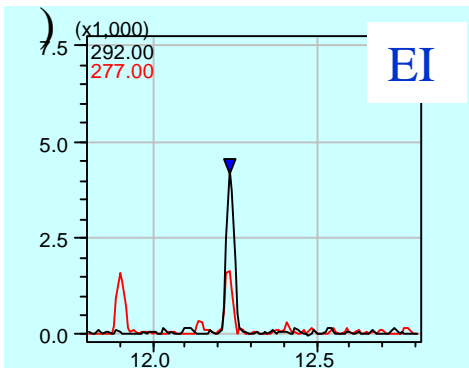


Bifenthrin(0.025μ g/ml)

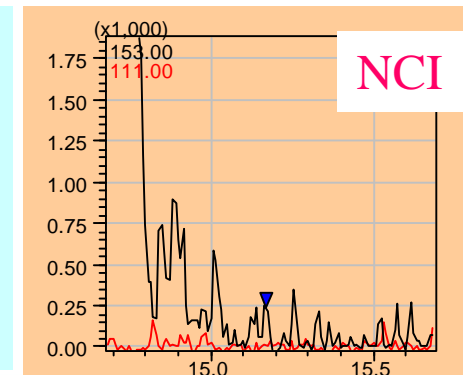
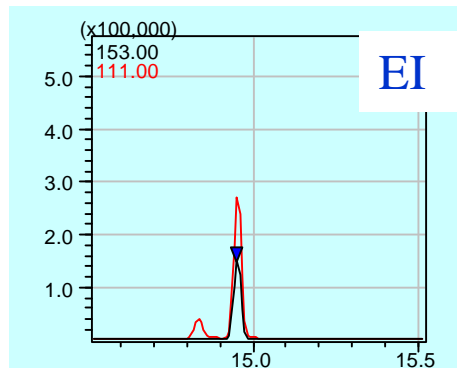


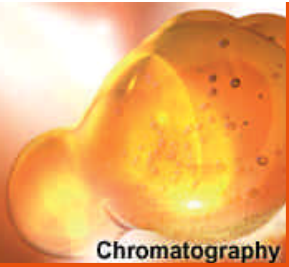
Higher sensitivity in EI

Etrimfos(0.005μ g/ml)



Methoprene(1.0μ g/ml)

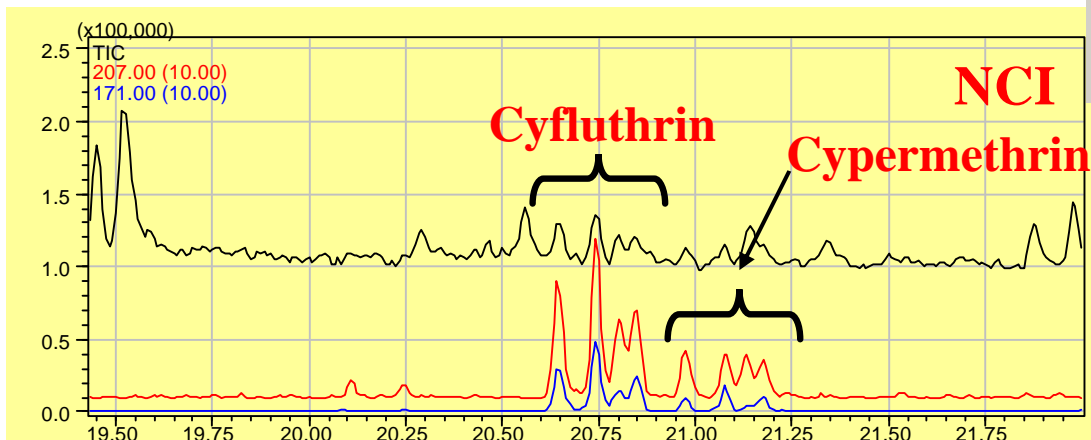
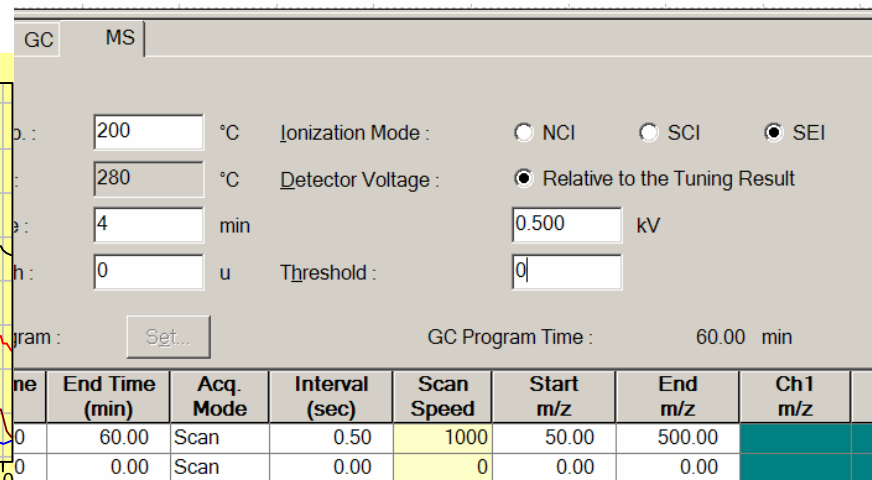
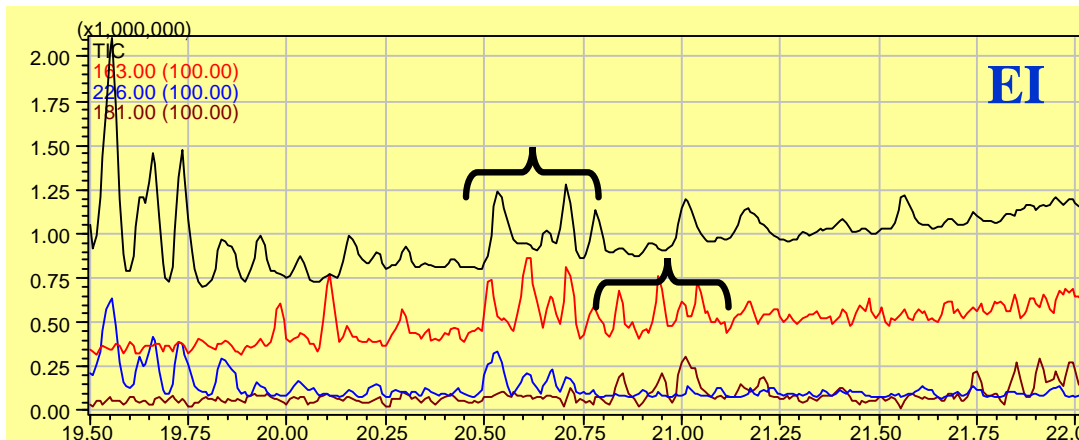




Chromatography

Advantages of NCI

Cyfluthrin 0.5ppm, Cypermethrin 0.25ppm



Combined
NCI/EI Library available

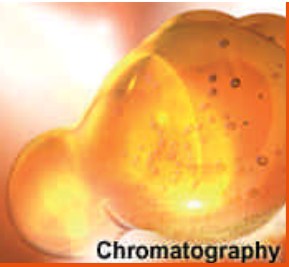
Comparison of the sensitivities in EI and NCI

Higher sensitivity in NCI mode

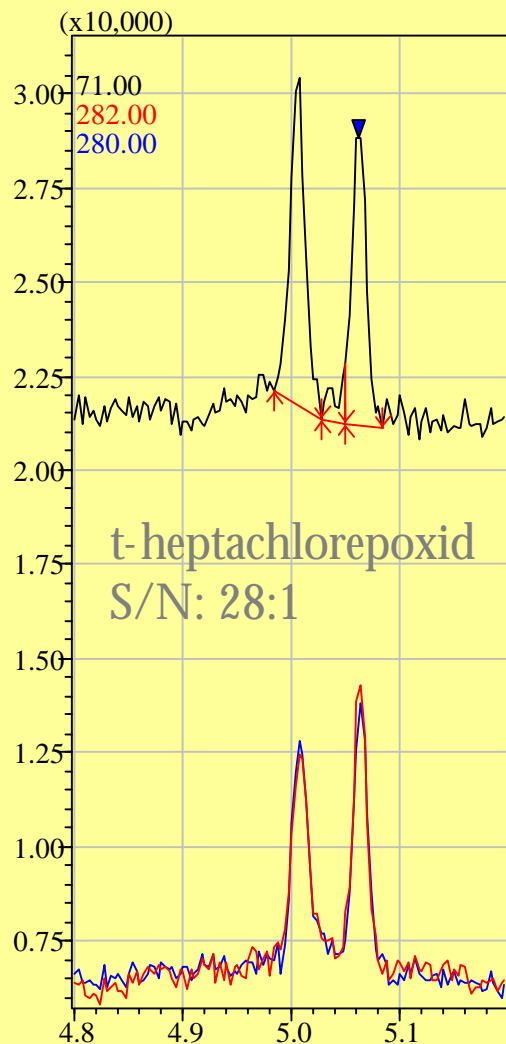
Higher sensitivity in EI mode

Chromatography

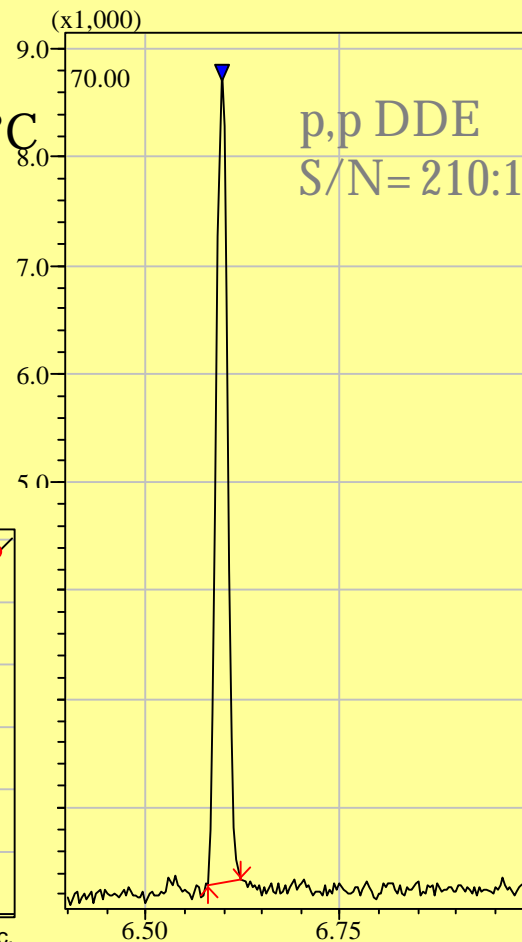
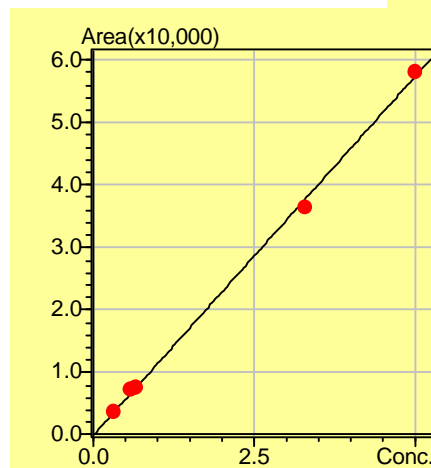
>10 times	2-10 times		Equality			>10 times	
Bifenox	Dichlofluanid	Dicofol bunkaibutu	p,p'-DDT	Aldrin	Fosthiazate	Chlofentezine deg	Mepronil
Fenvalerate	Fenalimol	malathion	Dimethoate	Thiobencarb	Acephate	Methamidophos	Propiconazol
Chlorfenapyr	Pendimethalin	Parathion	delta.-Lindane	Permethrin	Terbacil	EPTC	Lenacil
Cyfluthrin	Dieldrin	Dimethylvinphos	Cafenstrole	Pyributicarb	Pyraclofos	Propamocarb	Tebuconazole
Pyrethrin-2	Edifenphos	Pyrifenox-Z	Fluvalinate-1	p,p'-DDD	Penconazol	Chlorpropham	Etoxazole
MEP	Tefluthrin	Parathion-methyl	Pyrifenox-E	Chlopyrifos	Uniconazolep	Terbufos	Tebufenpyrad
EPN	Cypermethrin	Kresoxim-methyl	Diflufenican	Bitertanol	Fensulfothion	Benfuresate	Pyriproxyfen
Fenpropathrin	Thifluzamide	Folpet	Hxaconazole	Isofenphos	Cyhalofop-buthyl	Dimethenamid	Pyrimidifen
Acrinthrins	Acetamiprid	Cyanazine	Thiometon	Quinalphos	Butachlor	Alachlor	Mefenacet
Trifluralin	PAP ; Phenthoate	Cadusafos	Diazinon	p,p'-DDE		Metolachlor	Triadimenol
Phosalone	Pyrethrin-1	Tolclofos methyl	Prothiofos	Pirimiphos-methyl		Diethofencarb	Etrimfos
Cyhalothrin	Endrin	Pretilachlor	Difenoconazole	o,p'-DDT		Fenthion	Chlorobenzilate
β-CVP	Deltamethrin	Malathion	Pyridaben	Halfenprox		Fludioxonil	Esprocarb
Flucythrinate	beta.-BHC	Captafol	Teraconazole	Ethoprofos		Methoprene	Thenylchlor
Butamifos	alpha.-BHC	Flutolanil	Chinomethionate	Dichlorvos		Paclobutrazol	Tricyclazole
gamma.-BHC			Bifenthrin			Flusilazole	Isoprocarb
Captan			Inabenfide			Cyproconazole	
Imibenconazole			Myclobutanil				

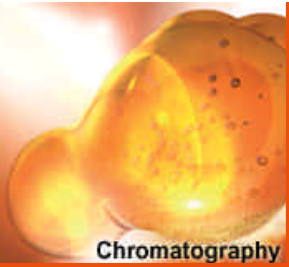


OCP's with fast NCI/GCMS



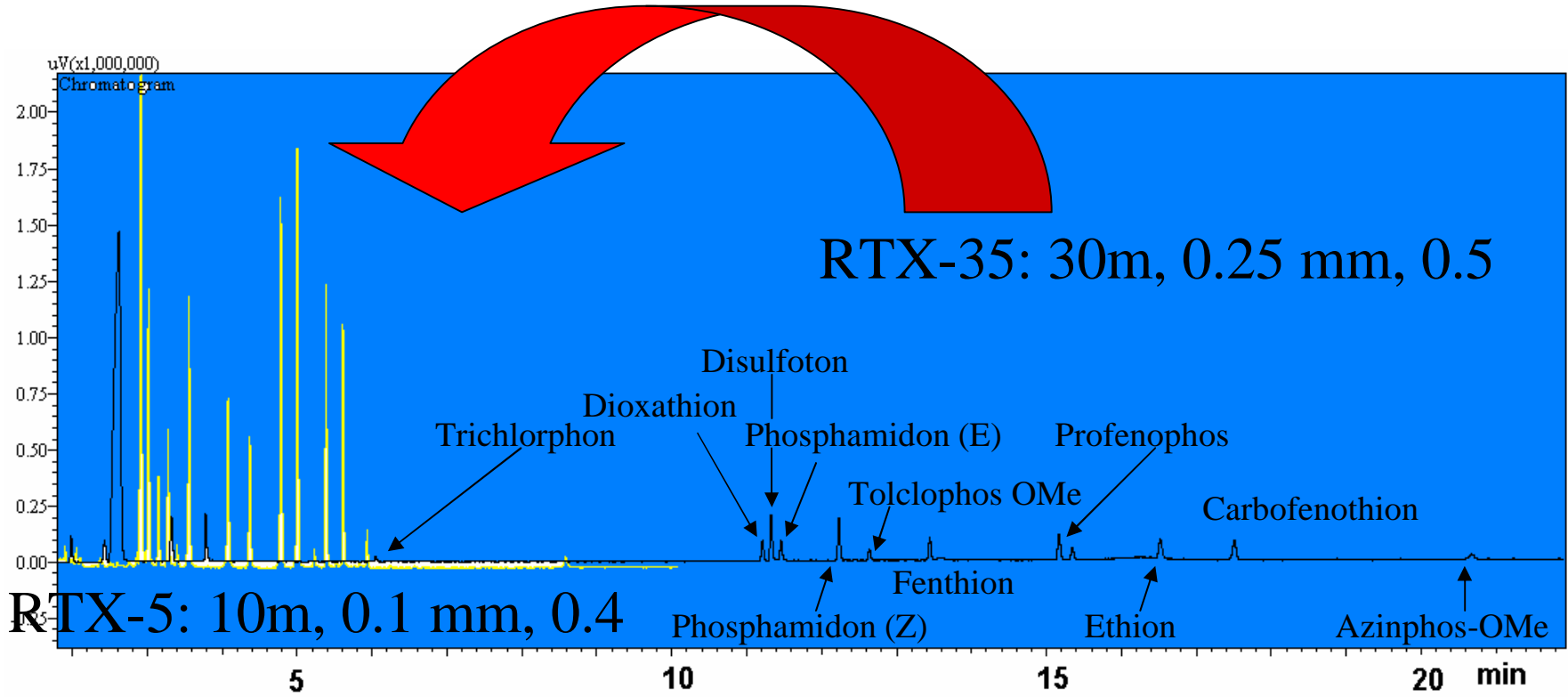
SPB-5 10m, 0.1 mm, 0.1 μ m
80 °C, 1 min, 60°C/min 200 °C
25 °C/min 280 °C
He, 50 cm/s
SIM: 0.6 ppb

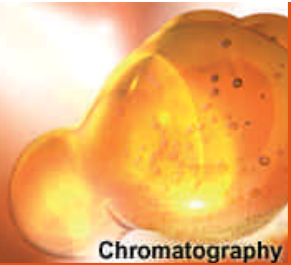




STD vs fast

Phosphor Pesticides: GC-FPD Splitless analysis





Chromatography

Transfer to fast: EI

Program : Column Oven Temperature

	Rate	Final Temperature	Hold Time
0	-	50.0	1.00
1	60.00	280.0	1.00
2	0.00	0.0	0.00
3	0.00	0.0	0.00

Total Program Time : 5.83 min

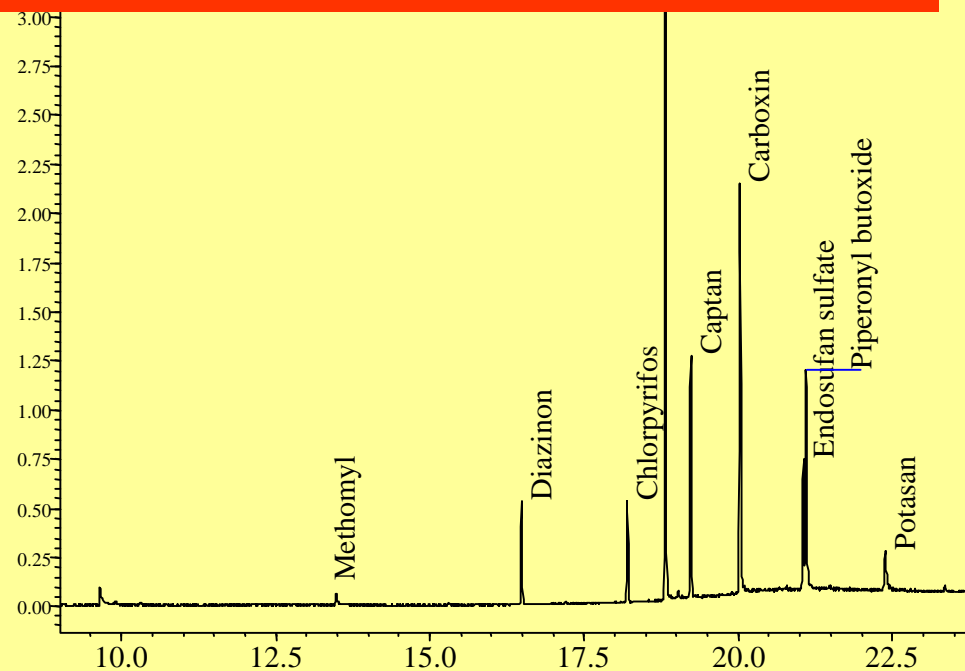
Column

Length : 10.0 m

Diameter : 0.10 mm ID

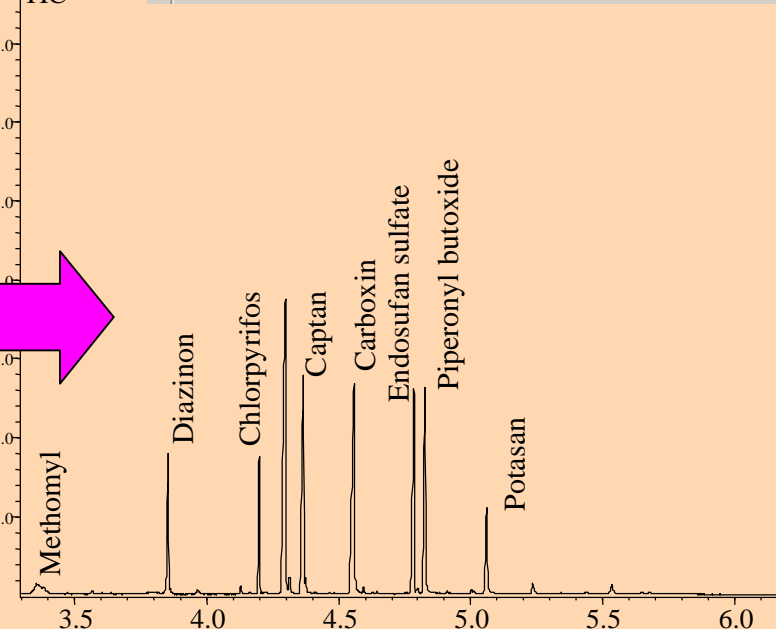
Set...

RTX-5: 30m, 0.25 mm, 0.25 μ m
 He 35 cm/sec, splitless 1 μ l,
 HPI 250 kPa



(x100,000,000)

TIC



RTX-5: 10m, 0.1 mm, 0.1 μ m
 He 60 cm/sec, splitless 1 μ l
 HPI=600kPa



RTX-5: 10m, 0.15 mm, 0.15 μ m
He 35 cm/sec, splitless 1 μ l,
HPI=450kPa

Data Acquisition Parameters

Sampler: GC MS Description

GCMS-QP2010

Ion Source Temp.: 230 °C
Interface Temp.: 290 °C
Solvent Cut Time: 2.5 min
Micro Scan Width: 0 u

Detector Voltage: Relative to the Tuning Result Absolute
0.4 kV
Threshold: 1000

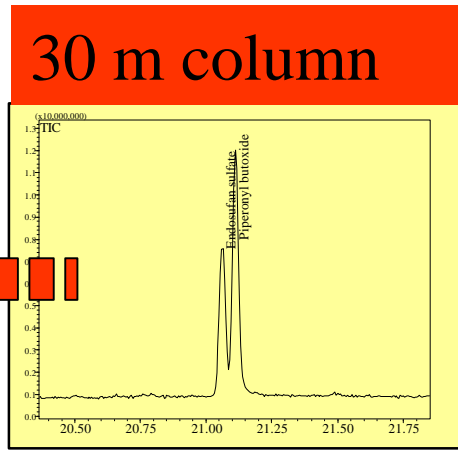
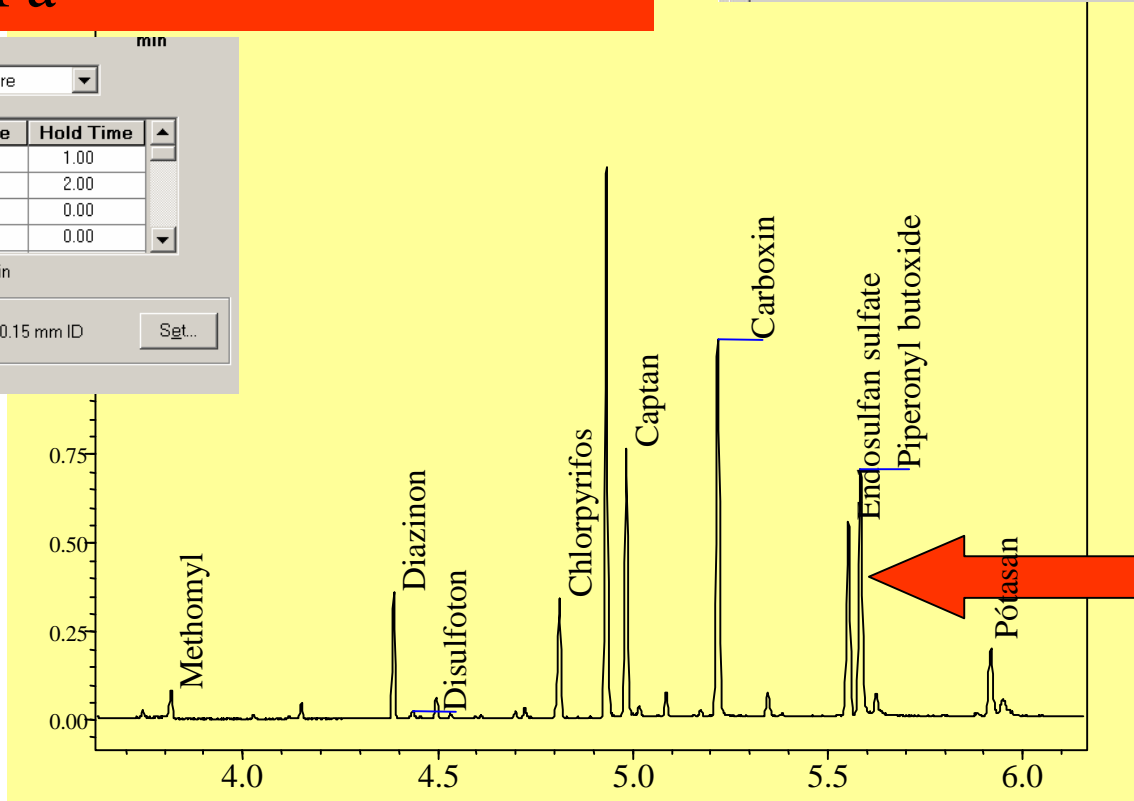
Use MS Program: Set GC Program Time: 7.20 min

	Start Time (min)	End Time (min)	Acq. Mode	Interval (sec)	Scan Speed	Start m/z	End m/z	Ch1 m/z	Ch2 m/z
1	3.00	7.20	Scan	0.08	5000	50.00	400.00		
2	0.00	0.00	Scan	0.00	0	0.00	0.00		

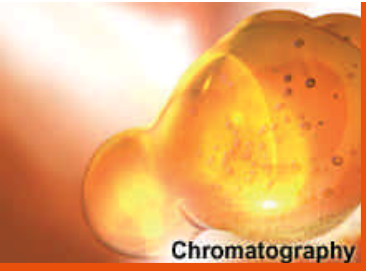
Program: Column Oven Temperature

	Rate	Final Temperature	Hold Time
0	-	70.0	1.00
1	50.00	280.0	2.00
2	0.00	0.0	0.00
3	0.00	0.0	0.00

Total Program Time: 7.20 min
Column Length: 15.0 m Diameter: 0.15 mm ID

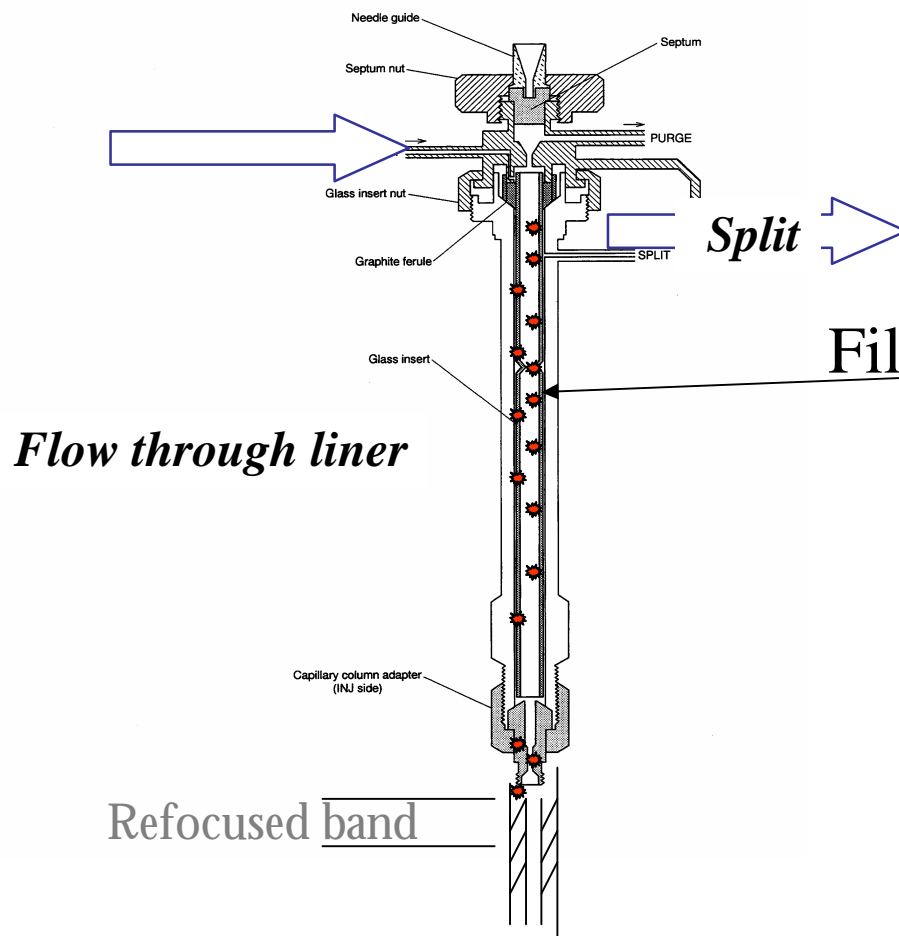


Speed gain with better resolution » 4



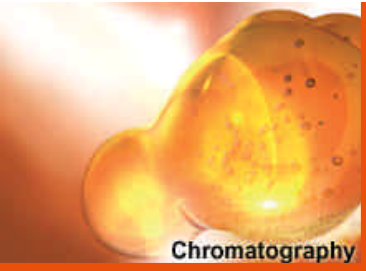
Fast -Sample Transfer

Sample transfer in an SPL injector



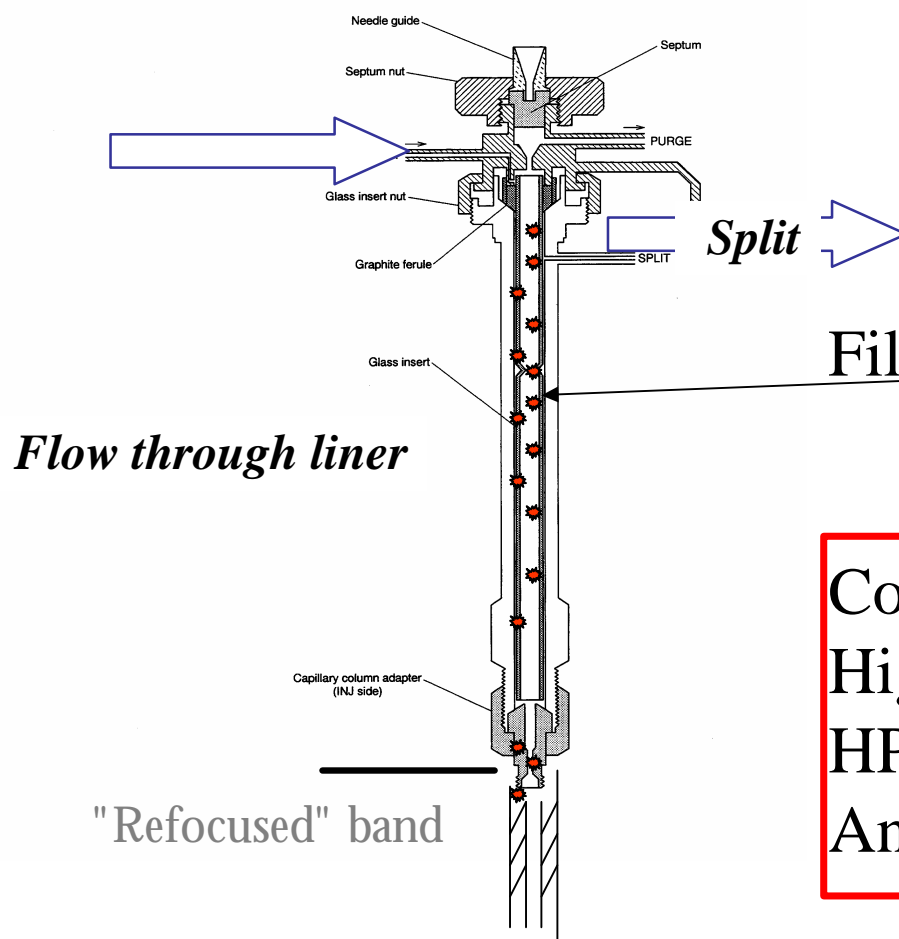
Typ Liner vol ~ 1 ml
Vapour of 1 μ l injected
Between 300-600 μ l

Filled liner with sample



Fast -Sample Transfer

Sample transfer in an SPL injector

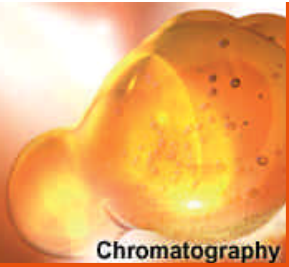


Typ Liner vol ~ 1 ml
Vapour of 1 μ l injected
Between 300-600 μ l

Filled liner with sample

Flow through liner

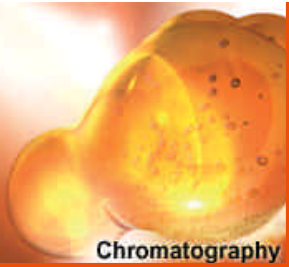
Compensation:
High pressure injection
HPI
And/or small ID liner



Fast GCMS-Detector

Users need for fast GCMS

- 1. - Data Acquisition rate (Sampling Frequency)**
- 2. - Mass Range (Scan speed)**



GCMS-QP2010

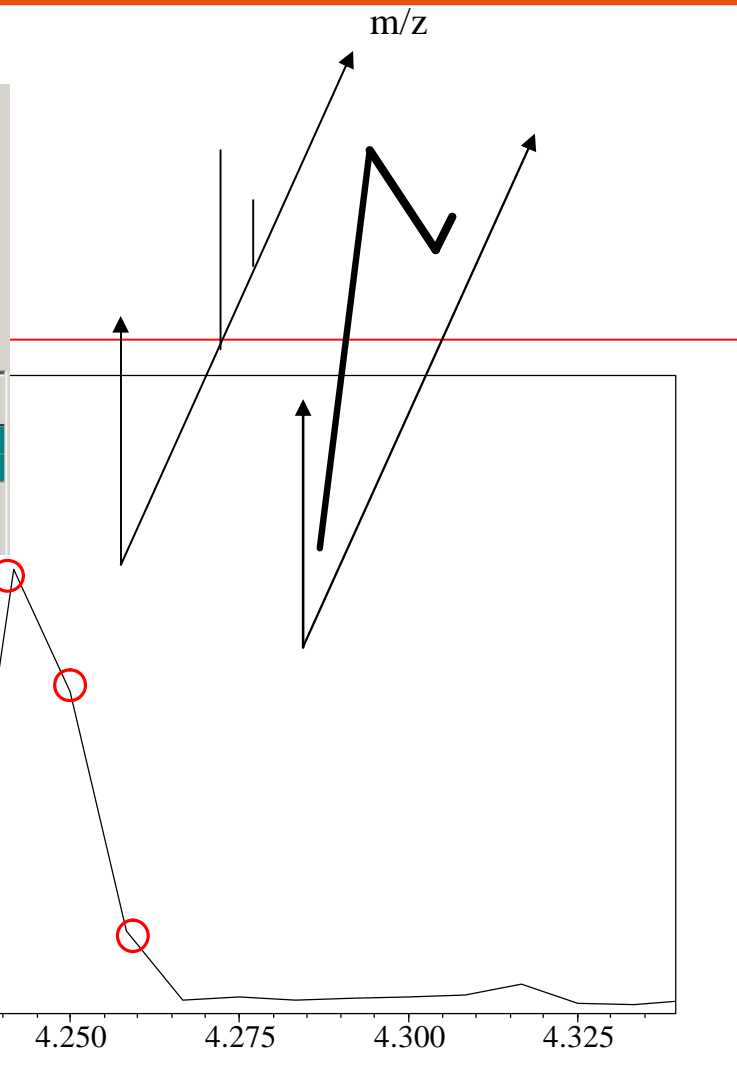
Chromatography

Speed and sampling frequency:

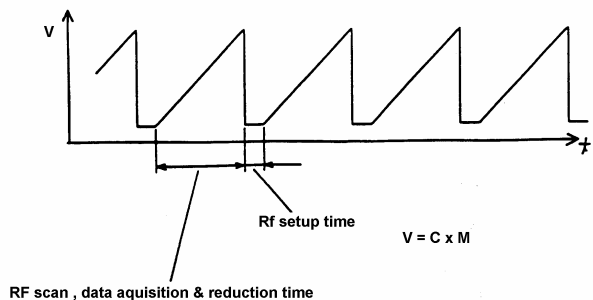
GCMS-QP2010

Ion Source Temp.: 200 °C
 Interface Temp.: 250 °C
 Solvent Cut Time: 3 min
 Micro Scan Width: 0 u
 Detector Voltage: Relative to the Tuning Result Absolute
 Threshold: 0 kV
 GC Program Time: 11.21 min

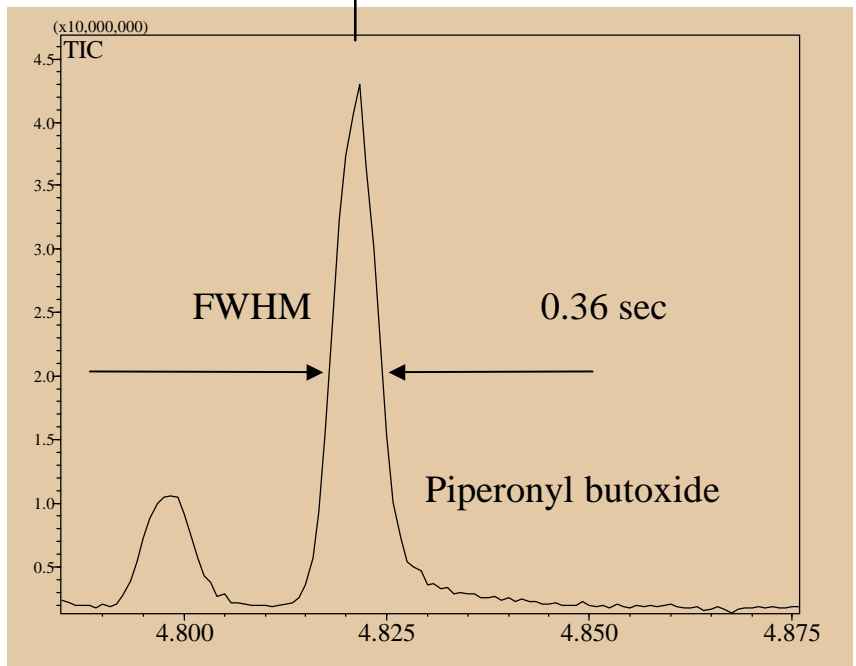
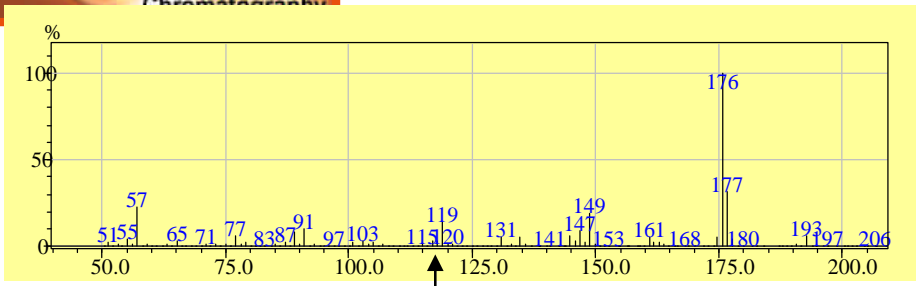
	Start Time (min)	End Time (min)	Acq. Mode	Interval (sec)	Scan Speed	Start m/z	End m/z	Ch1 m/z	Ch2 m/z
1	3.50	10.00	Scan	0.50	208	200.00	300.00		
2	0.00	0.00	Scan	0.00	0	0.00	0.00		



Scan Mode (Spectral acquisition)



Fast GCMS Analysis



Scan range 50-400 amu
20 spectra/sec

- Fast GCMS Analysis needs:
1. High speed Quad scan and low Rf setup time →
 2. High No of spectra/sec FWHM 0.1-0.5 sec:
sampling ≥ 20 Hz [2]
- [2] J. V. Hinshaw, LCGC (2002)vol 15 p. 152

200 °C Ionization Mode : NCI SCI SEI

280 °C Detector Voltage : Relative to the Tuning Result

4 min 0.500 kV

0 u Threshold : 0

Set...

GC Program Time : 60.00 min

End Time (min)	Acq. Mode	Interval (sec)	Scan Speed	Start m/z	End m/z	Ch1 m/z
60.00	Scan	0.05	10000	50.00	400.00	
0.00	Scan	0.00	0	0.00	0.00	

Low interscan setup time needed



Fast GCMS

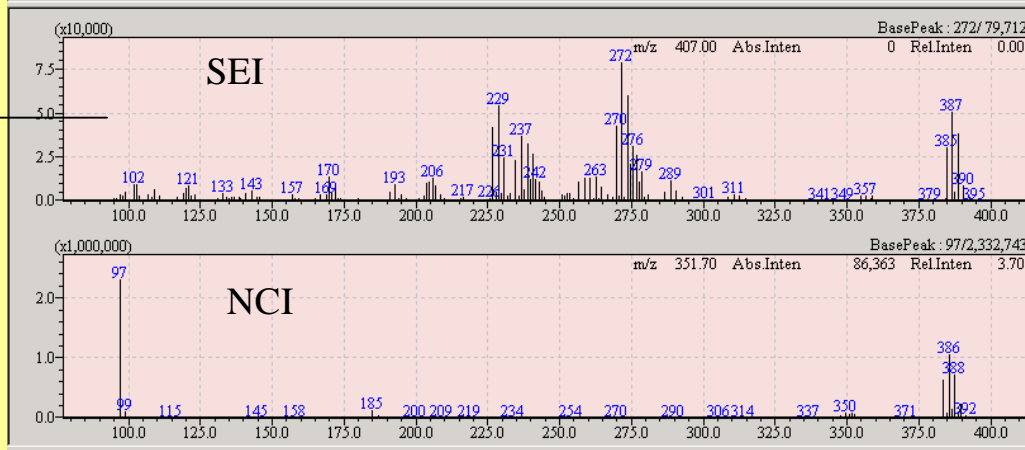
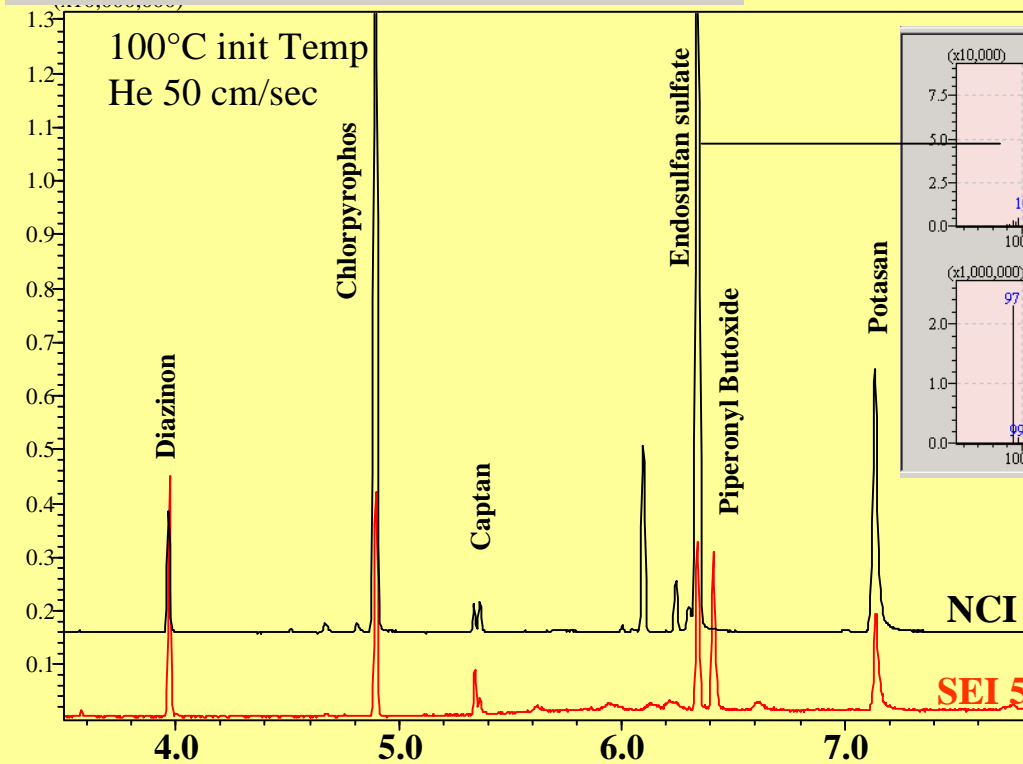
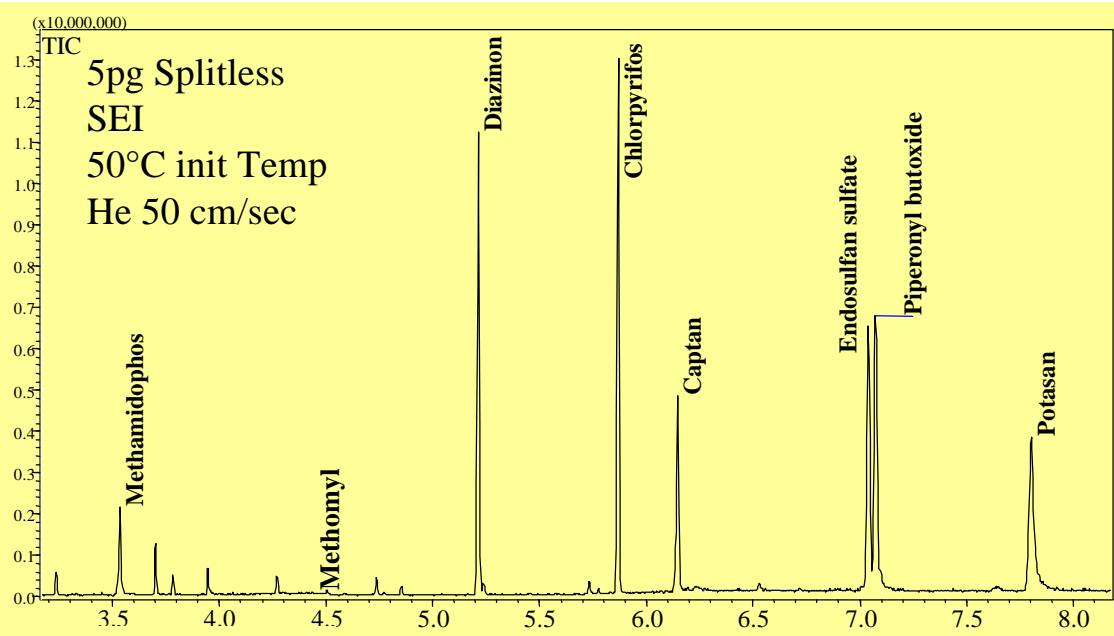
Program : Column Oven Temperature

	Rate	Final Temperature	Hold Time
0	-	50.0	1.00
1	50.00	220.0	0.00
2	20.00	240.0	0.00
3	50.00	280.0	4.00

Total Program Time : 10.20 min

Column

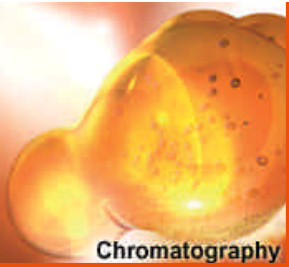
Length : 10.0 m Diameter : 0.10 mm ID



Scan 50 – 400 amu
10000 amu/sec

NCI 50 pg Splitless

SEI 5 ng Split 20:1



Chromatography

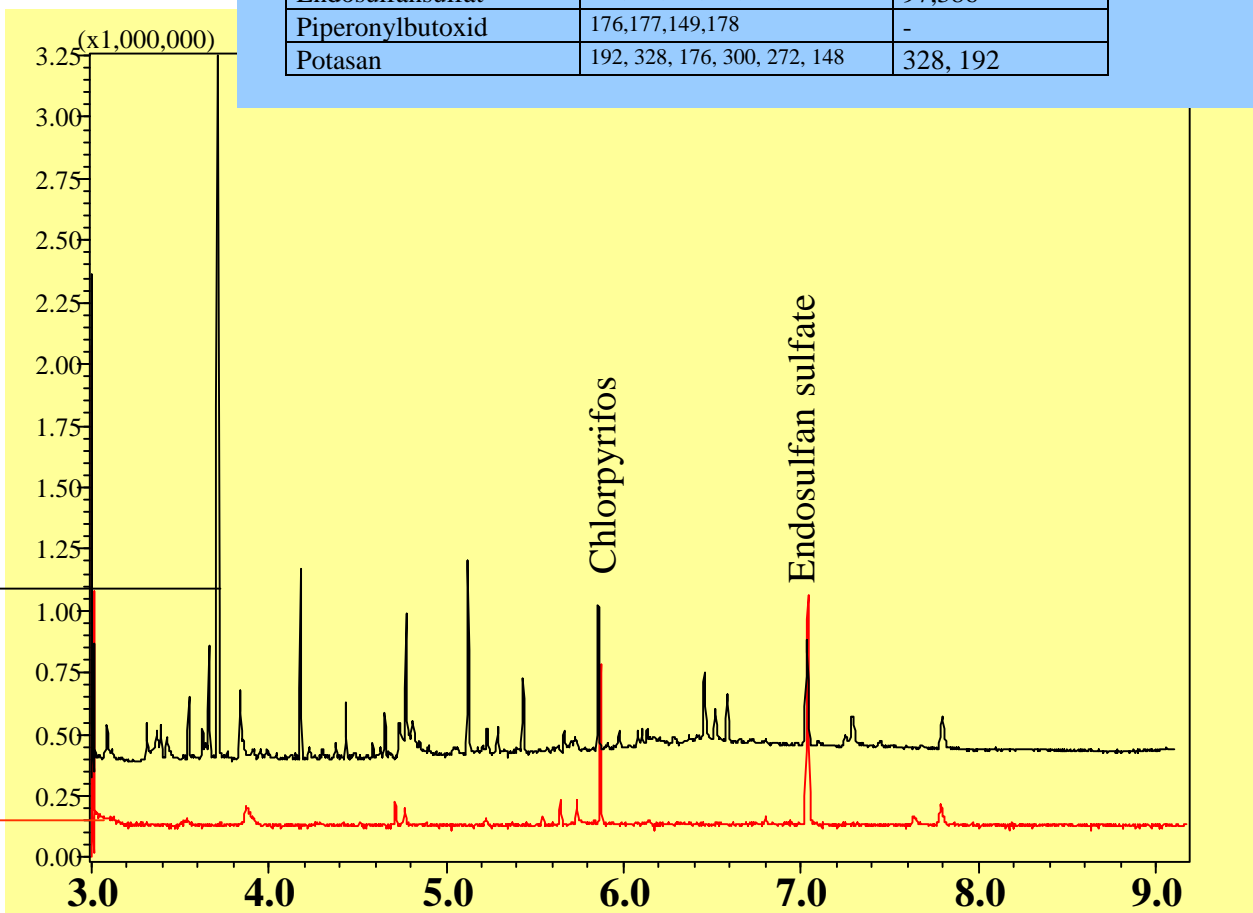
Fast GCMS NCI Scan

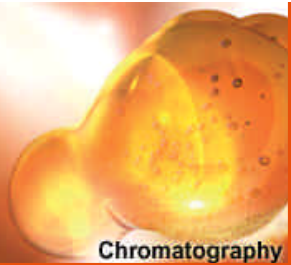
Scan 50 – 400 amu
10000 amu/sec

Substance	EI Peaks (Da)	NCI Peaks (Da)
Methamidophos	94,141,126,111,110,128	-
Methomyl	58,105,88,73,115,162	-
Diazinon	304,179,137,152,276,199	169
Chlorpyrifos-OEt	314,187,258,244,97,125,351	313,315,212,214
Captan	79,117,149,264,301,182,236	150, 149
Endosulfansulfat	229,272,239,207,170,387	97,386
Piperonylbutoxid	176,177,149,178	-
Potasan	192, 328, 176, 300, 272, 148	328, 192

Black Tea

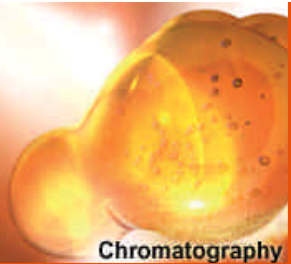
Mix 0.5 pg





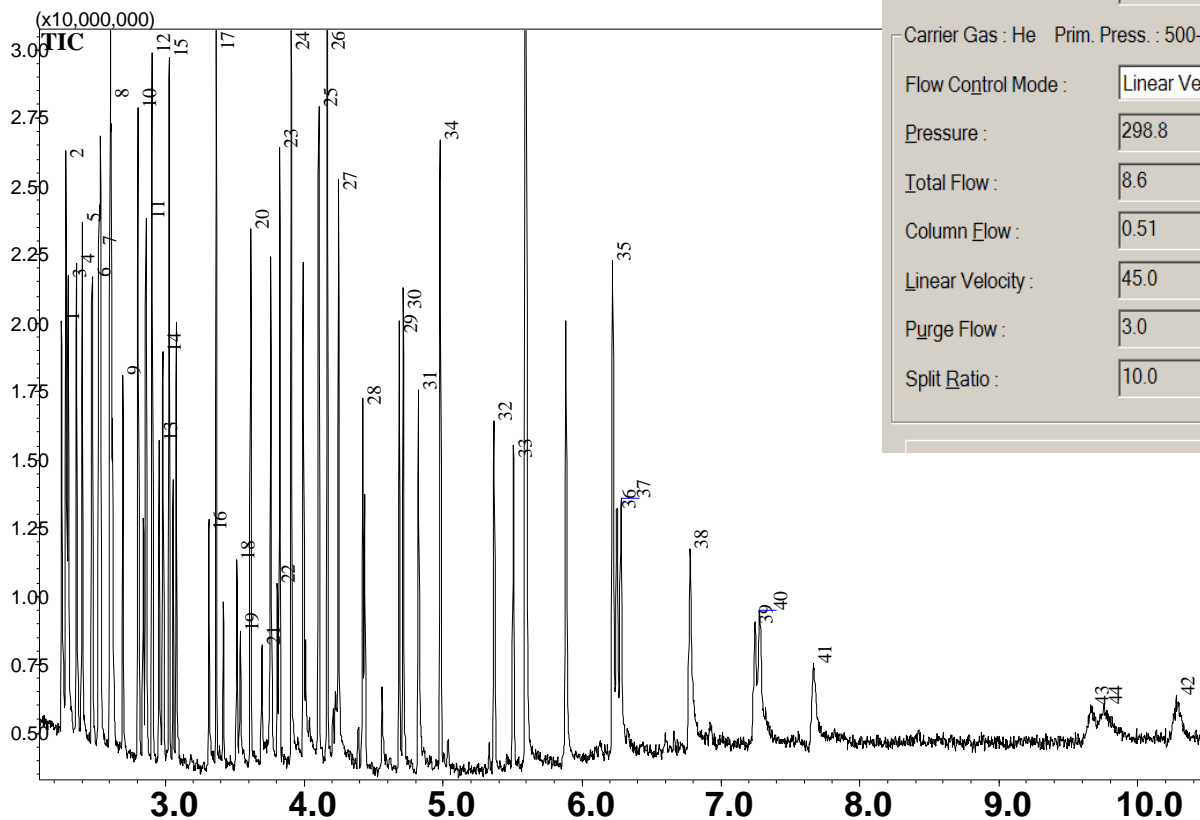
Fast GCMS

What about stability in fast GCMS?



Chromatography

EPA 625 ~100 ppb each



Inj. Port : SPL1 Inj. Heat Port : INJ1

Column Oven Temp. : 50.0 °C

Injection Temp. : 250.0 °C

Injection Mode : Split

Sampling Time : 1.00 min

Carrier Gas : He Prim. Press. : 500-900

Flow Control Mode : Linear Velocity

Pressure : 298.8 kPa

Total Flow : 8.6 mL/min

Column Flow : 0.51 mL/min

Linear Velocity : 45.0 cm/sec

Purge Flow : 3.0 mL/min

Split Ratio : 10.0

Program : Column Oven Temperature

	Rate	Final Temperature	Hold Time
0	-	50.0	1.00
1	50.00	200.0	0.00
2	40.00	280.0	4.50
3	0.00	0.0	0.00

Total Program Time : 10.50 min

Column Name : BPX-5 Thickness : 0.10 um

Length : 10.0 m Diameter : 0.10 mm

Full scan

20-550 amu, 20 Hz

Stability-fast (~100 ppb each)

Adobe Acrobat Professional - [EPA625 repro 20 runs.pdf]

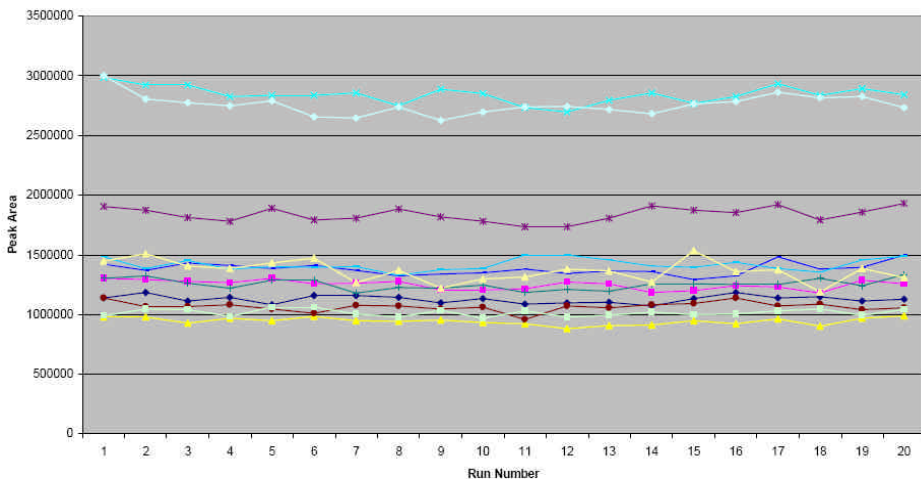
Datei Bearbeiten Anzeige Dokument Werkzeuge Erweitert Fenster Hilfe

Öffnen Speichern Drucken E-Mail Suchen PDF erstellen Überprüfen und kommentieren Schützen Unterschreiben Erweiterte Bearbeitung

Textauswahl 125% Verfahren...

Lesezeichen
Unterschriften
Ebenen
Seiten
Kommentare

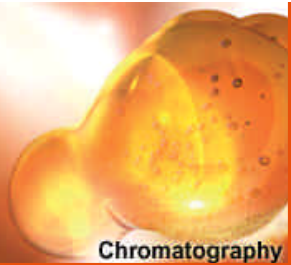
EPA625 Mix Raw Area Reproducibility



Analyte	%RSD
Bis(2-chloroethyl) ether	2.80
Benzene, nitro-	3.14
Phenol, 2,6-dimethyl-	3.15
Naphthalene	2.51
Naphthalene, 1-methyl-	3.24
Naphthalene, 1-chloro-	3.70
Acenaphthene	3.51
Phenanthrene	3.74
Pyrene	3.53
p-Terphenyl-d14	3.07
Benzyl butyl phthalate	2.85
Benz[a]anthracene	6.67

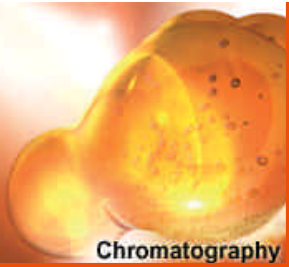
[Result][Area]	Area	Area	Area	Area	Area	Area	Area	Area	Area	Area	Area	Area	Area	Area	Area	Area	Area	Area	Area	Area	%RSD	
ID	Compound Name	Data1	Data2	Data3	Data4	Data5	Data6	Data7	Data8	Data9	Data10	Data11	Data12	Data13	Data14	Data15	Data16	Data17	Data18	Data19	Data20	
1	Bis(2-chloroethyl) ether	1139146	1182013	1113967	1140150	1081284	1156212	1157437	1141603	1097458	1134800	1084879	1093910	1099428	1073088	1133019	1181439	1133088	1149493	1110825	1125086	2.800055
2	Benzene, nitro-	1302209	1293751	1277378	1265401	1304548	1255351	1259185	1275717	1204911	1205095	1214270	1273076	1257205	1183900	1197120	1239604	1230515	1180878	1288636	1254203	3.138704
3	Phenol, 2,6-dimethyl-	978189	978573	928713	965756	948693	985203	948429	943077	954209	933592	923718	881751	906525	910305	949083	921430	961842	903246	969065	986697	3.151739
4	Naphthalene	2985789	2924721	2923380	2823348	2835181	2838027	2857065	2749656	2887519	2851990	2734718	2699079	2796434	2857646	2771581	2824102	2935657	2833813	2892657	2840839	2.505205
5	Naphthalene, 1-methyl-	1906481	1871430	1812136	1780756	1887999	1793750	1807288	1882923	1817975	1779292	1736723	1734569	1806929	1910170	1871317	1855120	1918742	1791355	1859344	1930235	3.236435
6	Naphthalene, 1-chloro-	1138420	1064761	1065953	1081402	1042602	1009634	1073994	1042665	1060885	956554	1069941	1054127	1082008	1090521	1139115	1071928	1085186	1038027	1056149	1067509	3.697509
7	Acenaphthene	1303802	1321125	1258952	1217638	1287686	1287652	1180234	1227517	1220457	1248052	1183998	1209921	1160695	1257092	1257753	1250896	1248339	1303225	1238657	1331505	3.512076
8	Phenanthrene	1419342	1369792	1432920	1411606	1384106	1412126	1369788	1322488	1336174	1351019	1377767	1341298	1364389	1366786	1290405	1323336	1484040	1379111	1394817	1495557	3.736534
9	Pyrene	1482999	1384321	1453515	1377824	1399664	1384922	1402123	1332585	1375134	1384355	1499960	1496656	1458771	1405967	1394787	1438647	1383354	1354634	1455810	1485655	3.534234
10	p-Terphenyl-d14	3002355	2806976	2772407	2748027	2791826	2656789	2647677	2738546	2626883	2699311	2735666	2745378	2715154	2679470	2764430	2784463	2863471	2816936	2827847	2731681	3.074156
11	Benzyl butyl phthalate	986574	1043926	1042076	984518	1060118	1059539	1002950	980366	1034405	966497	1030872	977567	994969	1010706	1000966	1005566	1027150	1045406	993146	1039205	2.849091
12	Benz[a]anthracene	1448135	1505592	1406853	1386661	1428460	1473169	1264298	1370526	1220448	1295750	1312497	1381680	1365872	1273519	1536075	1357571	1372074	1186648	1386109	1305926	6.6671

[Result][RT]	RT	RT	RT	RT	RT	RT	RT	RT	RT	RT	RT	RT	RT	RT	RT	RT	RT	RT	RT	RT	RT	%RSD
ID	Compound Name	Data1	Data2	Data3	Data4	Data5	Data6	Data7	Data8	Data9	Data10	Data11	Data12	Data13	Data14	Data15	Data16	Data17	Data18	Data19	Data20	
1	Bis(2-chloroethyl) ether	2.527	2.525167	2.523667	2.526167	2.5235	2.527833	2.526	2.524	2.523	2.522667	2.524333	2.523333	2.524667	2.523833	2.525	2.523333	2.522333	2.525	2.526667	2.527833	0.066269
2	Benzene, nitro-	2.932333	2.931667	2.931833	2.931667	2.932833	2.930667	2.9315	2.929	2.930167	2.930333	2.930333	2.932167	2.931	2.928833	2.931333	2.930333	2.9315	2.931667	2.930833	2.934	0.041563
3	Phenol, 2,6-dimethyl-	3.086833	3.0865	3.085667	3.085167	3.0855	3.0855	3.085833	3.085167	3.086333	3.084833	3.084	3.083833	3.084833	3.084833	3.086	3.085333	3.086	3.085333	3.085167	3.085167	0.024365
4	Naphthalene	3.2655	3.264333	3.263833	3.263833	3.265167	3.265333	3.265833	3.2645	3.265833	3.264833	3.266167	3.265	3.263833	3.264	3.265333	3.265167	3.264833	3.265833	3.266333	3.265833	0.024531
5	Naphthalene, 1-methyl-	3.6065	3.603667	3.603667	3.604333	3.6045	3.603833	3.604667	3.6045	3.605	3.603233	3.6035	3.604667	3.6035	3.6045	3.605333	3.606	3.604833	3.605	3.605167	3.605167	0.026125
6	Naphthalene, 1-chloro-	3.857333	3.8535	3.854167	3.855	3.856	3.853833	3.854667	3.855333	3.856167	3.854167	3.854333	3.853333	3.8535	3.852333	3.856167	3.853833	3.853833	3.856333	3.855	3.855667	0.032817
7	Acenaphthene	4.149	4.15	4.151167	4.149	4.151333	4.151167	4.15	4.150167	4.149	4.151167	4.152167	4.150667	4.151167	4.151333	4.151667	4.151667	4.1515	4.1515	4.1515	4.150167	0.023107
8	Phenanthrene	4.91	4.907167	4.907	4.909333	4.905667	4.91	4.9085	4.9085	4.91	4.91	4.91	4.9095	4.91	4.909667	4.908667	4.9085	4.908333	4.907	4.908667	4.9075	0.025859
9	Pyrene	5.521167	5.515333	5.516833	5.518333	5.518167	5.5195	5.517	5.517	5.519167	5.5185	5.5155	5.518333	5.517667	5.517167	5.5195	5.5185	5.517	5.518667	5.519833	5.518667	0.026046
10	p-Terphenyl-d14	5.707167	5.705	5.703333	5.7045	5.705333	5.704333	5.704333	5.704333	5.704833	5.7045	5.704	5.705167	5.704833	5.704667	5.706167	5.706167	5.704833	5.7045	5.704667	5.702167	0.018572
11	Benzyl butyl phthalate	5.971833	5.969167	5.967333	5.968833	5.9705	5.967333	5.9715	5.969	5.97	5.970333	5.969	5.972667	5.970667	5.970833	5.972667	5.9715	5.968667	5.967167	5.968833	5.970833	0.030218
12	Benz[a]anthracene	6.458	6.450167	6.448833	6.4505	6.4545	6.451833	6.456	6.456167	6.453167	6.454333	6.45	6.450167	6.451167	6.4515	6.452	6.453167	6.453167	6.450333	6.450667	6.448333	0.039961

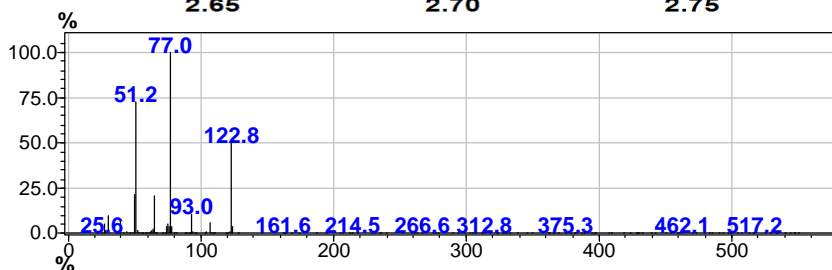
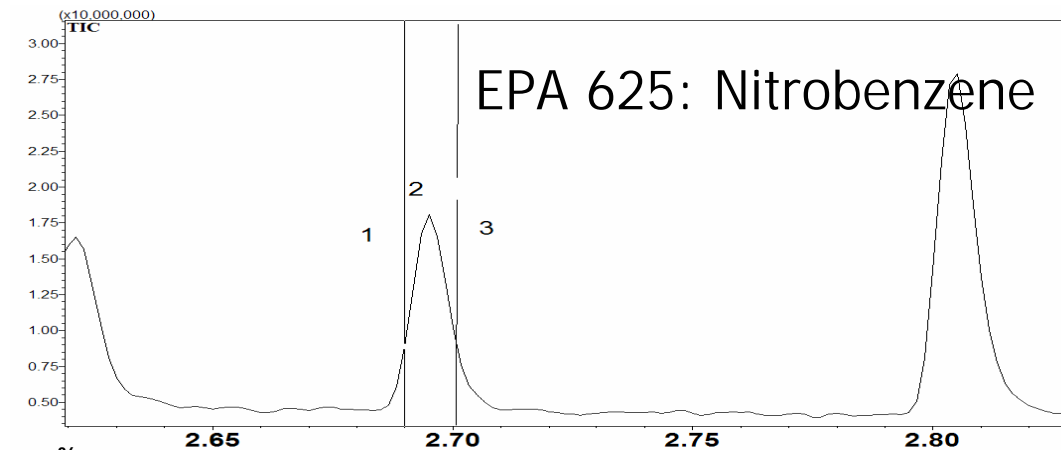


Fast GCMS

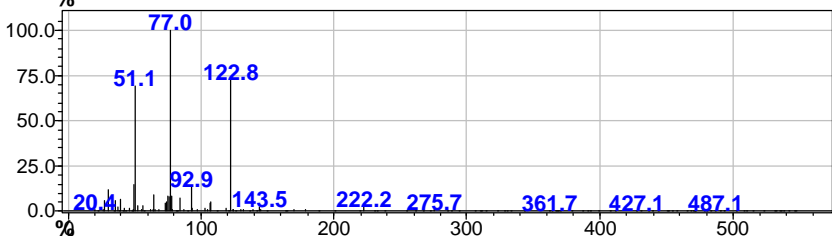
What about spectrum Quality in fast GCMS?



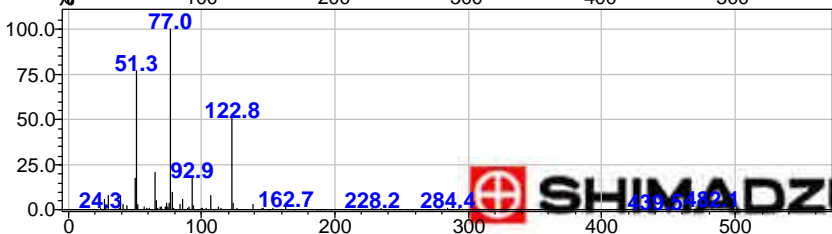
Spectrum Quality Fast GCMS



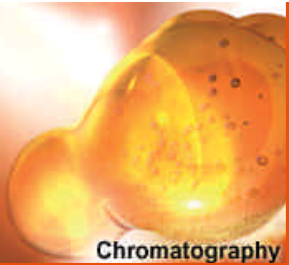
1: SI 89 Wiley



2: SI 93 Wiley



3: SI 88 Wiley



Spectrum Quality fast scanning

1. **Comprehensive two-dimensional gas chromatography in combination with rapid scanning quadrupole mass spectrometry in perfume analysis**

Luigi Mondello *et al*:

Journal of Chromatography A, 1067 (2005) 235–243

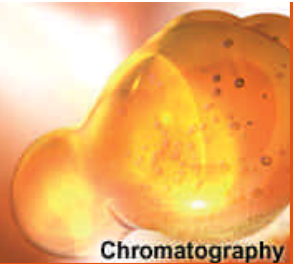
2. **Comprehensive Two-Dimensional Gas Chromatography coupled to rapid-scanning Quadrupole Mass Spectrometer (GC-GC-qMS): Principles and Applications**

Mohamed Adahchour, Menno Brandt, Hans-Ulrich Baier, René J.J. Vreuls and Udo A.Th. Brinkman:

[Journal of Chromatography A](#)

[Volume 1067, Issues 1-2](#) , 4 March 2005, Pages 245-254

Mass Spectrometry: Innovation and Application. Part IV



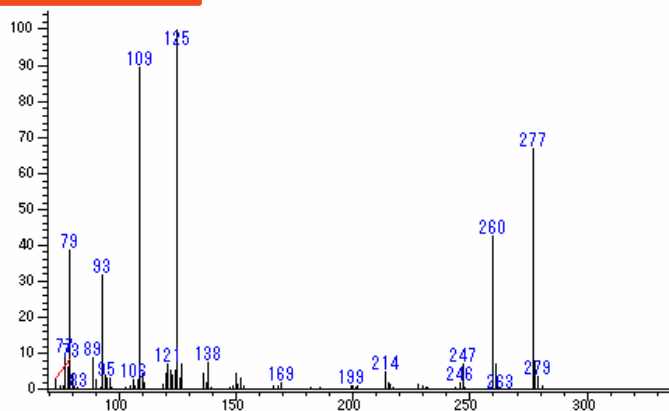
Chromatography

Inert: QP-2010 as default

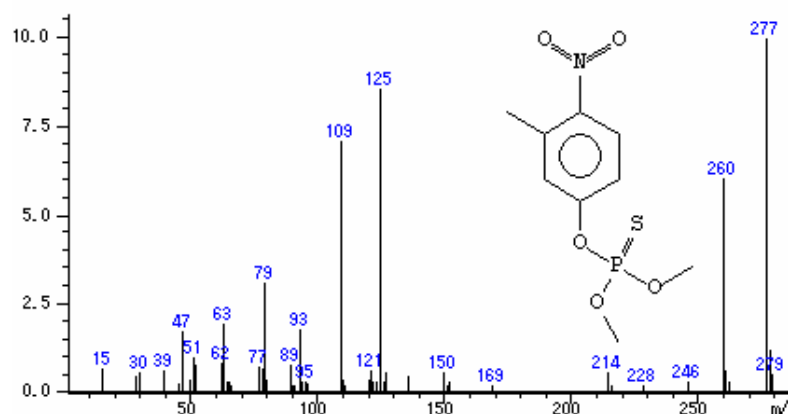
Degradation of PEST in Ion source?

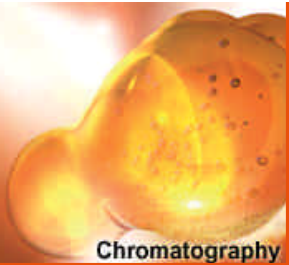
Fenitrothion

QP2010



NIST Lib.

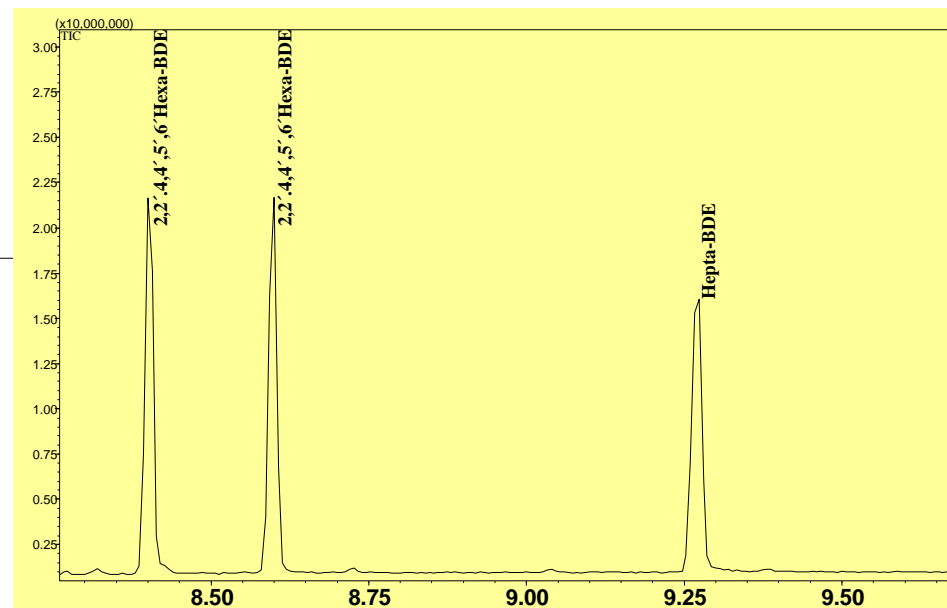
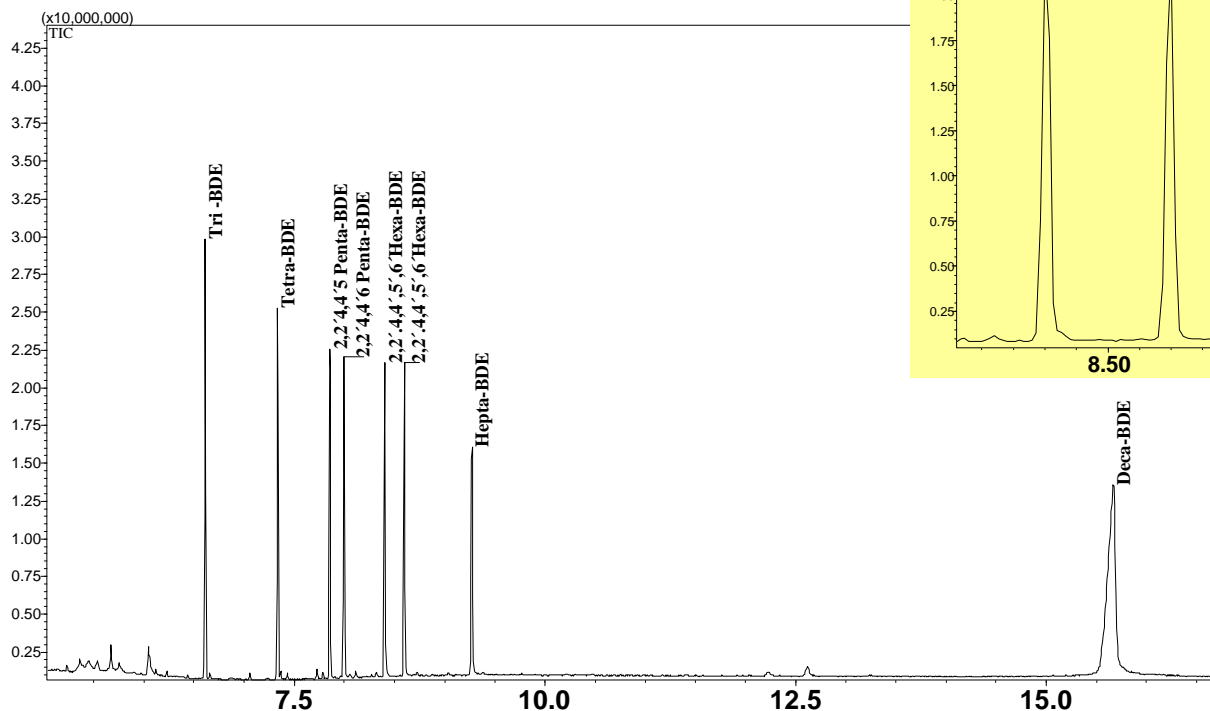




Chromatography

Inert: QP-2010 as default

- Data from the GCMS-QP2010
- Ion Source Temp: 200 °C



Liquid injection in SPL-2010 (270 °C)
Split 5:1, 20 ppm each, Deca 200ppm
Column: UA5-30m-0.25mm, 0.1 film
(Frontier Lab)