

Mobile Mass Spectrometer in daily use – Experiences made by non-scientific operators



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E²M – Enhanced Environmental Mass Spectrometer

small, lightweight, rugged, sensitive



Measurement principle:

Quadrupole Mass Filter

Vacuum System:

Ion getter pump < 10^{-6} mbar

Electron source:

Electron Impact, 70 eV

Filament:

dual

Inlet:

Silicone membrane, heated

Mass range:

1 ... 520 da

Scan rate:

7500 da/s, resolution 0.1 da

External Power Supply:

18 ... 32 VDC

Power Consumption:

250 Watt (switch-on: 500 W)

Transputer Interface:

Ethernet (100 Mbit/s)

Dimensions:

436 x 368 x 442 (L x W x H)

Volume:

58 litres

Weight:

38 kg

Specification:

CE, IP42, IEC 61000, IEC 60068-2 and 2-2, CISPR 16-1 and 16-2, IEC 60068-2-6, -2-27

Various Use of the System



MS Monitoring System

- SIM and Fullscan
- direct sample introduction



GC/MS System

- Fullscan
- Pre separation for complex samples
- Various sample introduction



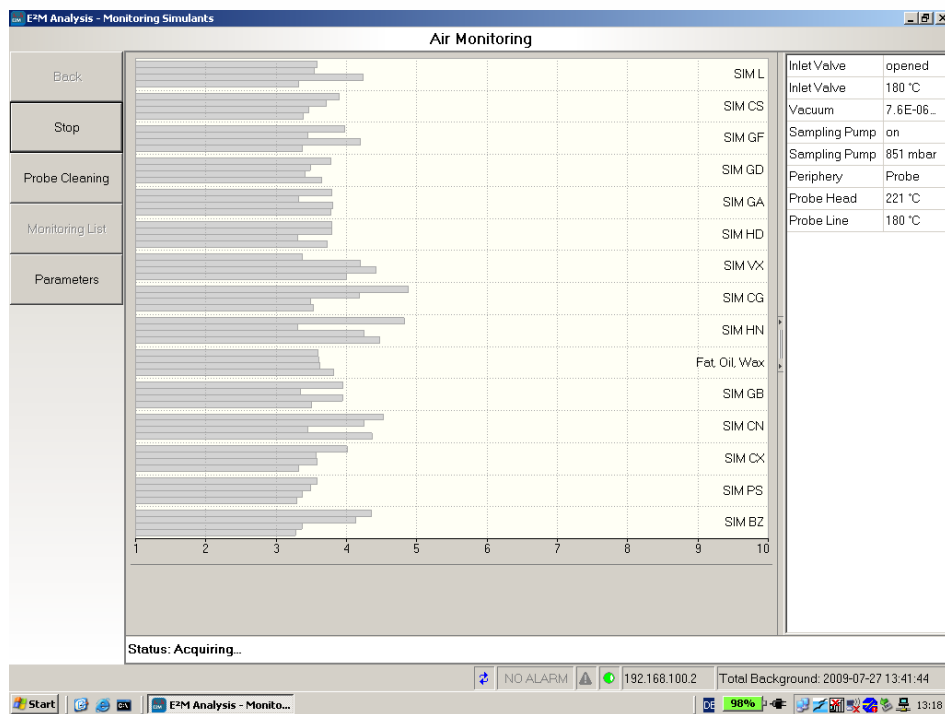
MS Monitoring System



Air/Surface Probe

- direct measurement of air and surface contaminations
- separately heated probe head and probe line
- programmable up to 240 ° C
- 3.5 m length, flexible
- exchangeable probe head membranes

MS Monitoring System



- Selected Ion Monitoring
- Very sensitive
- Several SIM libraries available, adaptable by the user
- Up to 20 substances simultaneously
- Vertical bar graph
- Colour coded signals
- Identification in alarm window



Air Monitoring

Back

Stop

Probe Cleaning

Monitoring List

Parameters



Inlet Valve	opened
Inlet Valve	180 °C
Vacuum	7.6E-06...
Sampling Pump	on
Sampling Pump	851 mbar
Periphery	Probe
Probe Head	221 °C
Probe Line	180 °C

Status: Acquiring...



NO ALARM



192.168.100.2

Total Background: 2009-07-27 13:41:44

Air Monitoring

- Back
- Stop
- Probe Cleaning
- Monitoring List
- Parameters



Inlet Valve	opened
Inlet Valve	180 °C
Vacuum	7.4E-06...
Sampling Pump	on
Sampling Pump	851 mbar
Periphery	Probe
Probe Head	221 °C
Probe Line	180 °C

Alarm: Diethylmalonate (SIM HD), 5.33;

Status: Acquiring...



ALARM



192.168.100.2

Total Background: 2009-07-27 13:41:44

Air Monitoring

Back

Stop

Probe Cleaning

Monitoring List

Parameters

Alarm List

Begin	End	Compound	Max. Intensity
2009-08-28 13:19:35	2009-08-28 13:19:43	Diethylmalonate (SIM HD)	5.36

Clear

Hide

1 2 3 4 5 6 7 8 9 10

Status: Acquiring...

SIM L

SIM CS

SIM GF

IM GD

IM GA

IM HD

SIM VX

IM CG

IM HN

I, Wax

IM GB

IM CN

SIM CX

SIM PS

SIM BZ

Inlet Valve	opened
Inlet Valve	180 °C
Vacuum	7.4E-06...
Sampling Pump	on
Sampling Pump	851 mbar
Periphery	Probe
Probe Head	221 °C
Probe Line	180 °C



ALARM



192.168.100.2

Total Background: 2009-07-27 13:41:44

GC/MS System

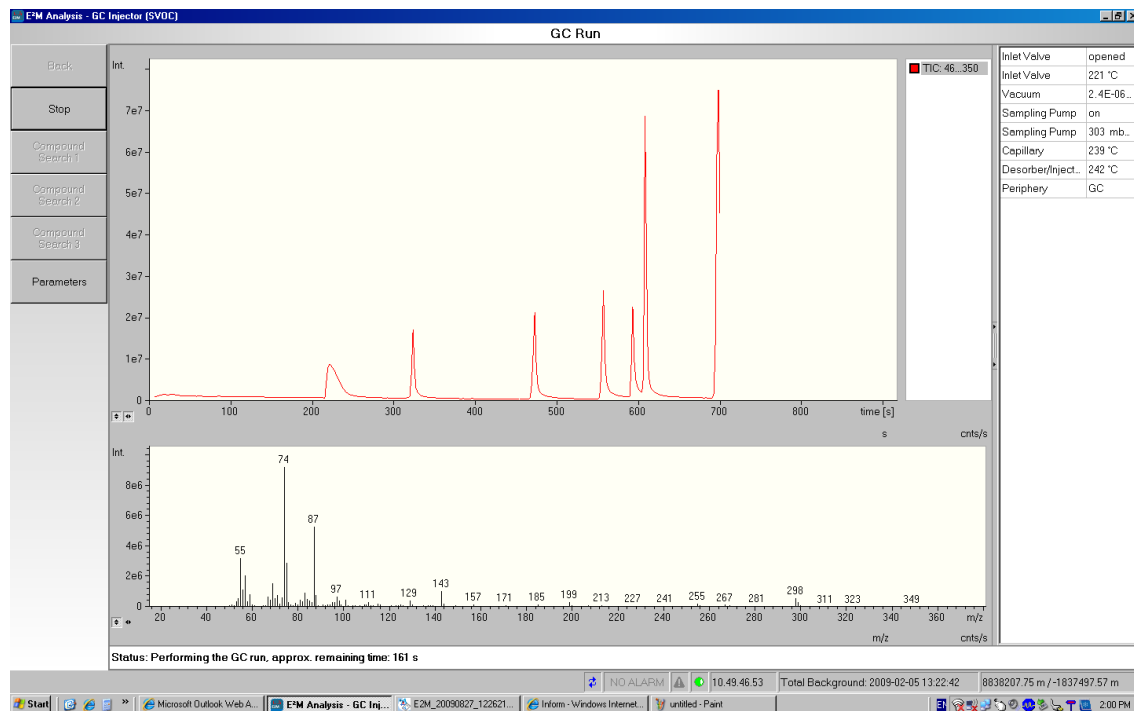


- temperature controlled gas flow
- 3 programmable **temperature gradients** ($T_{\max}$: 240 ° C)
- **Carrier gas:** ambient air
- **GC-capillary:** type depends on application
robust metal capillaries
Standard: MXT®-5, 12 m, ID 0.32 mm
film thickness 1 µm or
MXT®-1, 15 m, ID 0.32 mm
film thickness 5 µm
- **Injector:**
 - a) Thermo desorber (various sampling material, tubes)
 - b) Split injector (liquid)
 - c) SPME thermo desorption

GC/MS System



- Chromatogram window
- Mass spectrum window
- Automated identification at the end of the run



GC Run

Back

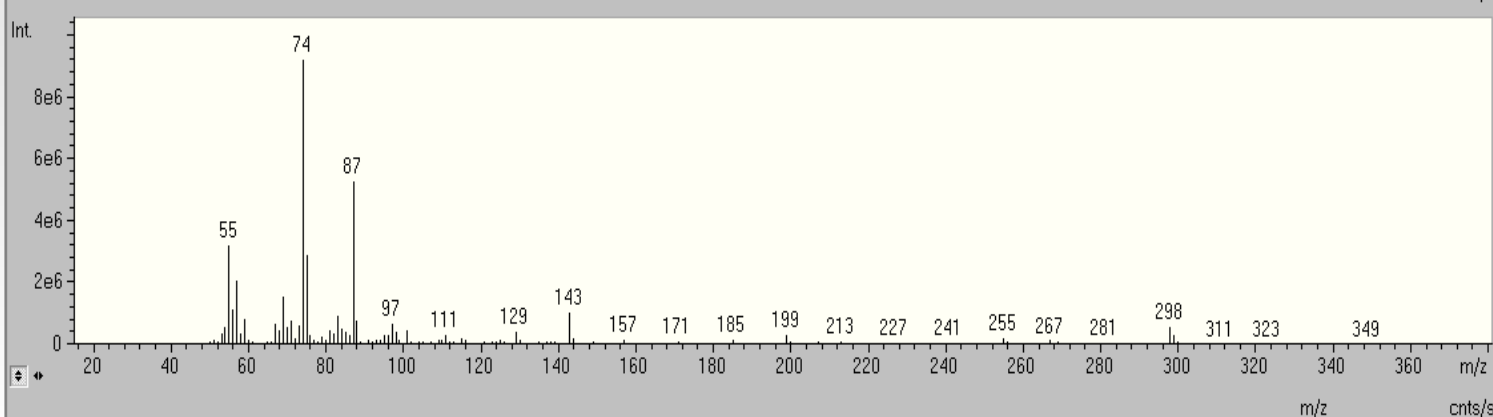
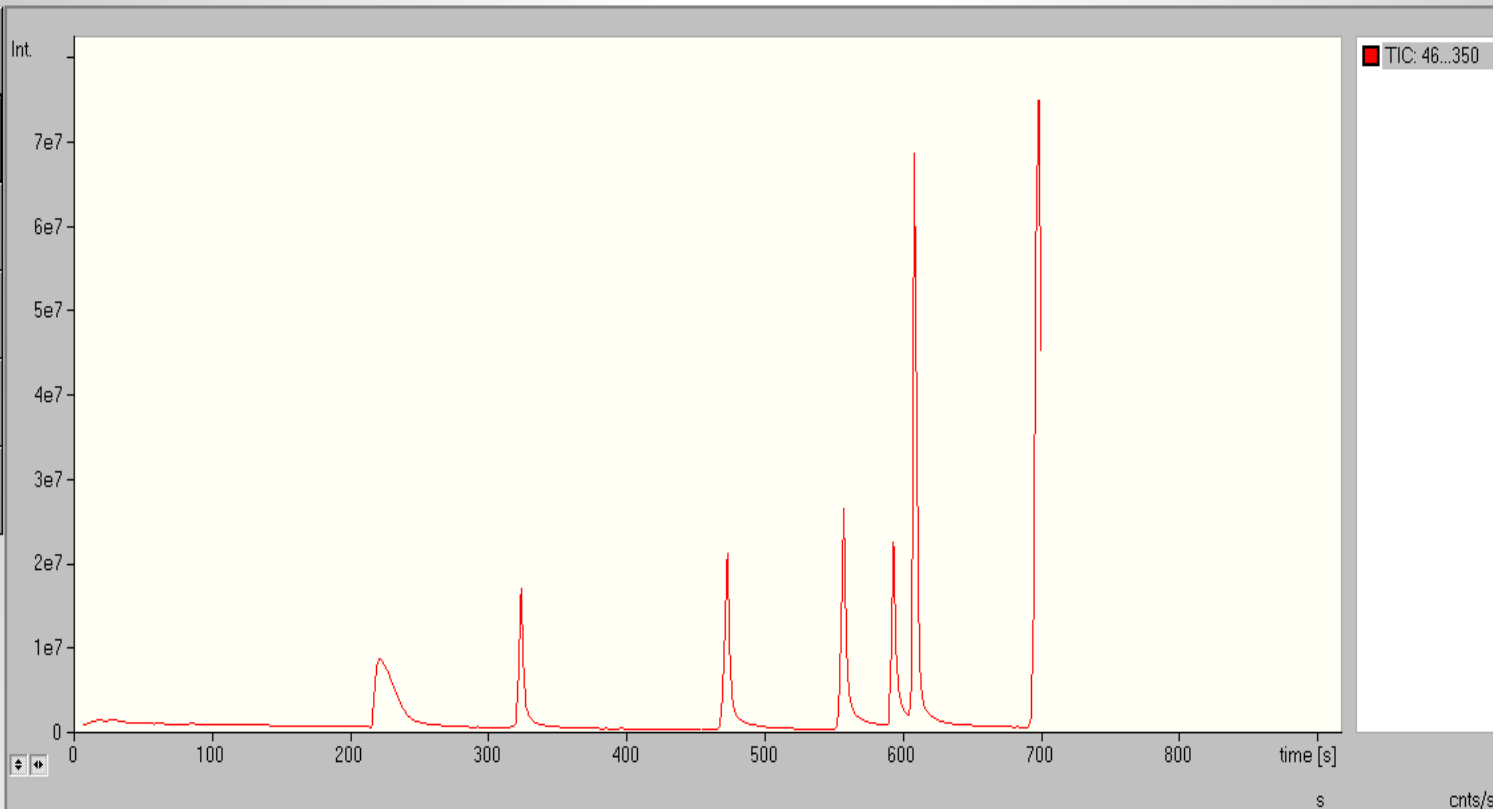
Stop

Compound Search 1

Compound Search 2

Compound Search 3

Parameters



Inlet Valve	opened
Inlet Valve	221 °C
Vacuum	2.4E-06...
Sampling Pump	on
Sampling Pump	303 mb...
Capillary	239 °C
Desorber/Inject...	242 °C
Periphery	GC

Status: Performing the GC run, approx. remaining time: 161 s



NO ALARM



10.49.46.53

Total Background: 2009-02-05 13:22:42

8838207.75 m / -1837497.57 m



Microsoft Outlook Web A...

E*M Analysis - GC Inj...

E2M_20090827_122621...

Inform - Windows Internet...

untitled - Paint

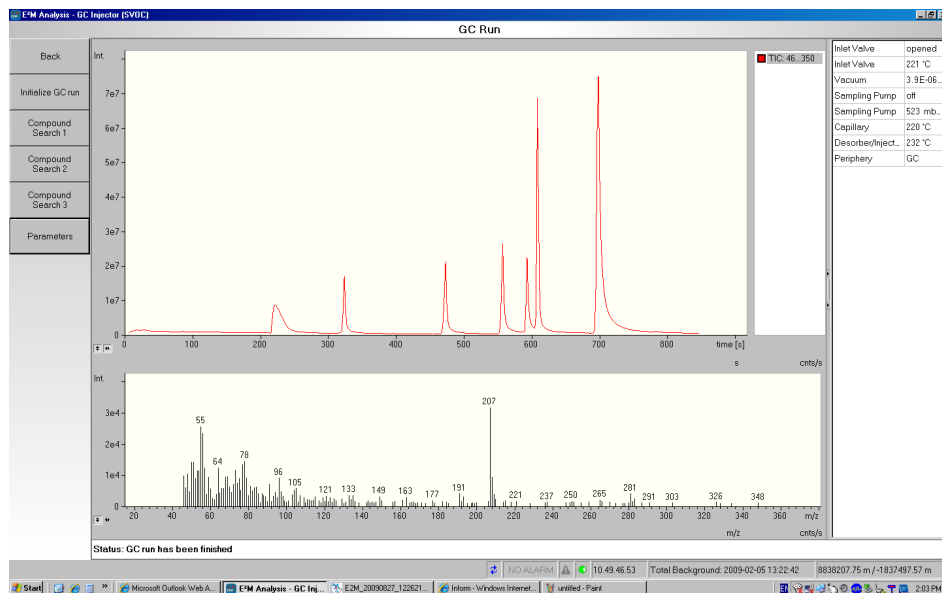


2:00 PM

GC/MS System

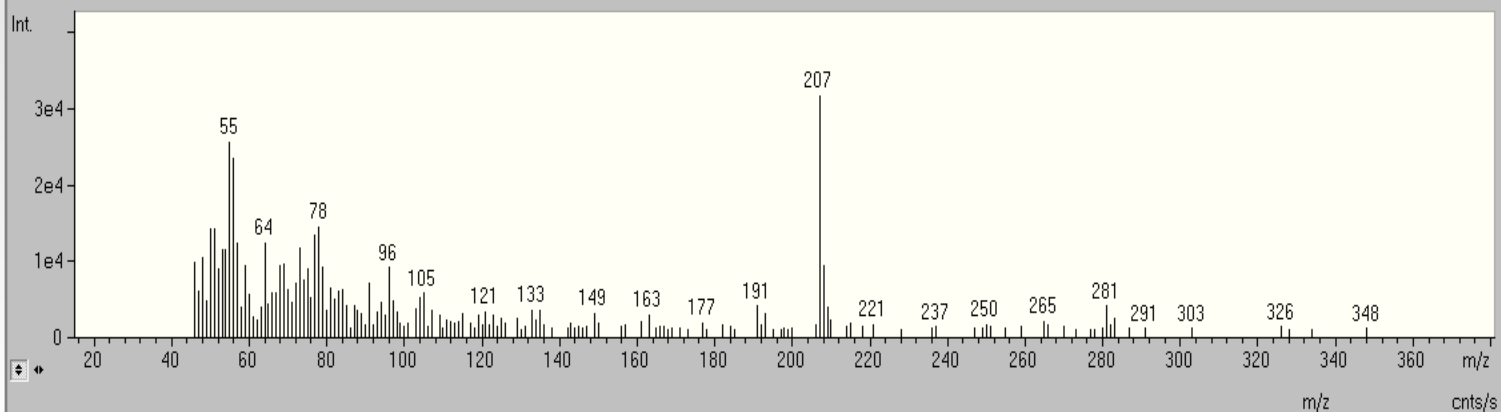
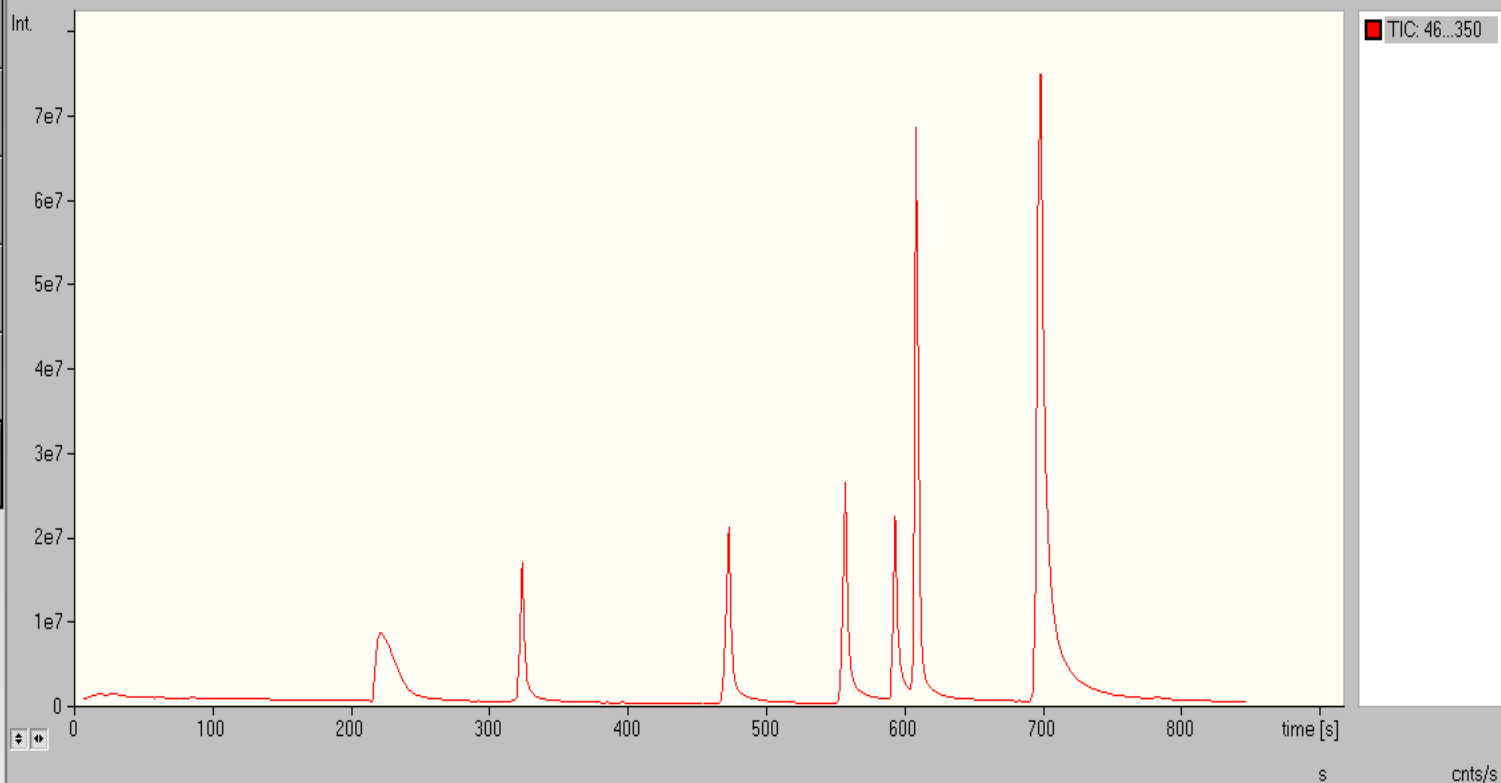


- Fully automated identification within seconds
- Up to 3 different identification procedures (sensitivity, library used)
- File information displayed
- Convertible to pdf files
- Copy CAS# available for use in several first responder data bases



GC Run

- Back
- Initialize GC run
- Compound Search 1
- Compound Search 2
- Compound Search 3
- Parameters



Inlet Valve	opened
Inlet Valve	221 °C
Vacuum	3.9E-06...
Sampling Pump	off
Sampling Pump	523 mb...
Capillary	220 °C
Desorber/Inject...	232 °C
Periphery	GC

Status: GC run has been finished



NO ALARM

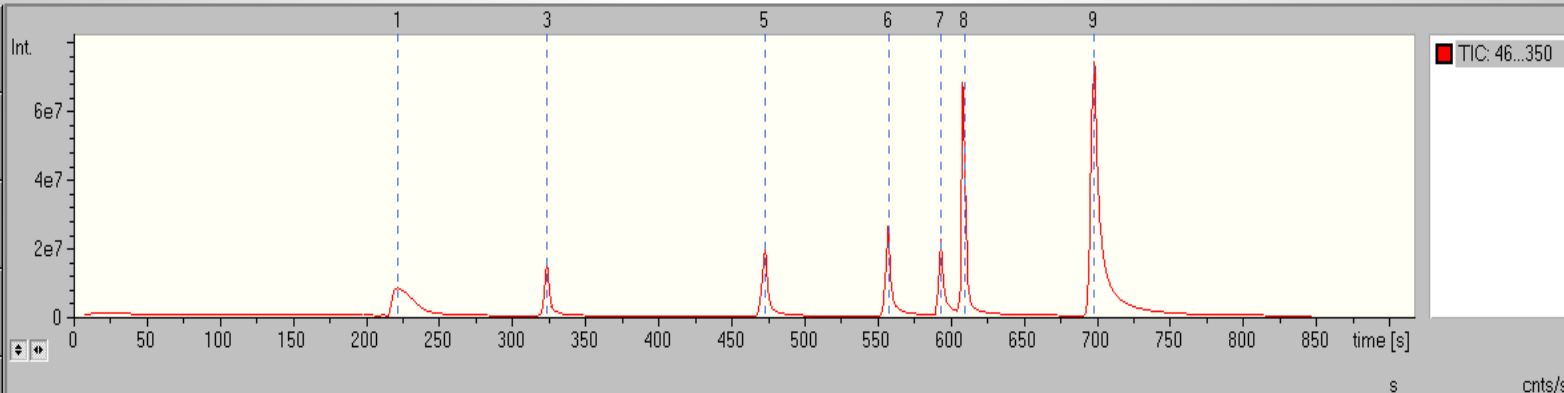


10.49.46.53

Total Background: 2009-02-05 13:22:42

8838207.75 m / -1837497.57 m

GC Run



Method	GC Injector (SVOC)
DataAnalysis Method	E2M_TIC_3Hit.m
Date/Time	8/28/2009 1:46:00 PM
Sample ID	Screenshot_2
Sampling Time [min]	0.0
Sampling Method	Injector
Operator	FRL
Organization	BDAL
Coordinates	8838207.75 m / -1837497.57 m
Location	Appli
Comment	injection 1 uL DB5-Mix

No.	Retention time [s]	Area	CAS #	Compound	Formula	Purity	Library
1	221.7	118...	756-79-6	Dimethyl methylphosphonate	C3H9O...	939.0	TIC
3	323.7	581...	123-25-1	Butanedioic acid, diethyl ester	C8H14...	965.0	TIC
5	472.8	846...	131-11-3	Dimethyl phthalate	C10H1...	928.0	TIC
6	557.3	800...	84-66-2	Diethyl Phthalate	C12H1...	922.0	TIC
7	593.2	491...	126-73-8	Tributyl phosphate	C12H2...	808.0	TIC
8	609.1	191...	132-65-0	Dibenzothiophene	C12H8S	890.0	TIC
9	697.9	394...	112-61-8	Octadecanoic acid, methyl ester	C19H3...	898.0	TIC

Status: Analysis is complete

Report View

Previous

Next

Copy CAS #

PDF Report



NO ALARM



10.49.46.53

Total Background: 2009-02-05 13:22:42

8838207.75 m / -1837497.57 m

Mass Spectrometer used by non scientific users

Typical non scientific users



- Fire fighter specialists
- First responder
- Mobile forensic investigators
- Police



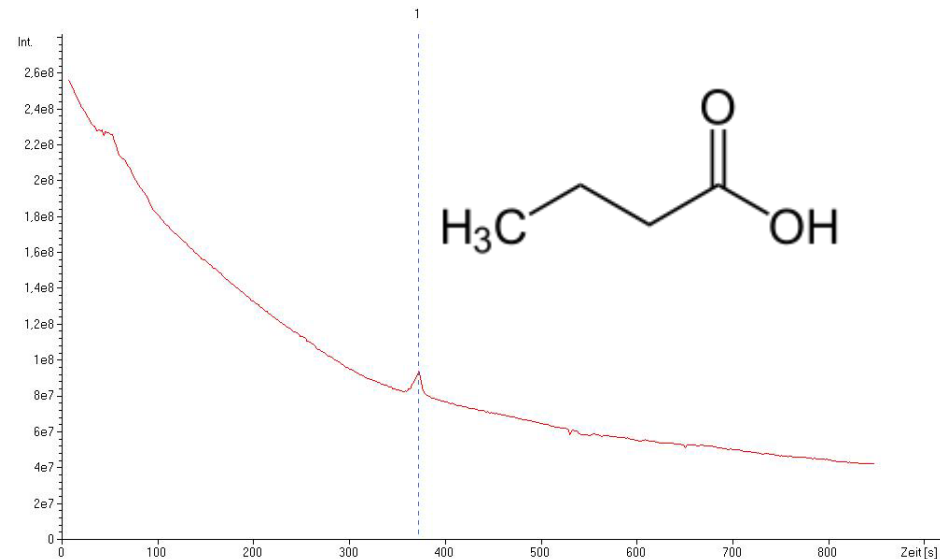
Sample preparation – source of problems



Butyric Acid in Dance Club



- Attack with butyric acid in dancing club in Leipzig
→ odor pollution, evacuation necessary
- Fire fighter specialists Leipzig
- Samples of ambient air taken by hand pump, sampling tubes
- Identification of the agent by GC/MS System
- Identification of the source (sports bag) → further investigations by police



Airport Lübeck – Supervisory impaired



- Rusted containers from 2nd world war with chlorosulfonic acid below ground cause fog
→ all flights stopped
- Task force Hamburg
- Identification by MS Monitoring System
- Instrument partially destroyed due to highly acidic character
- Pre check with pH stripes essential



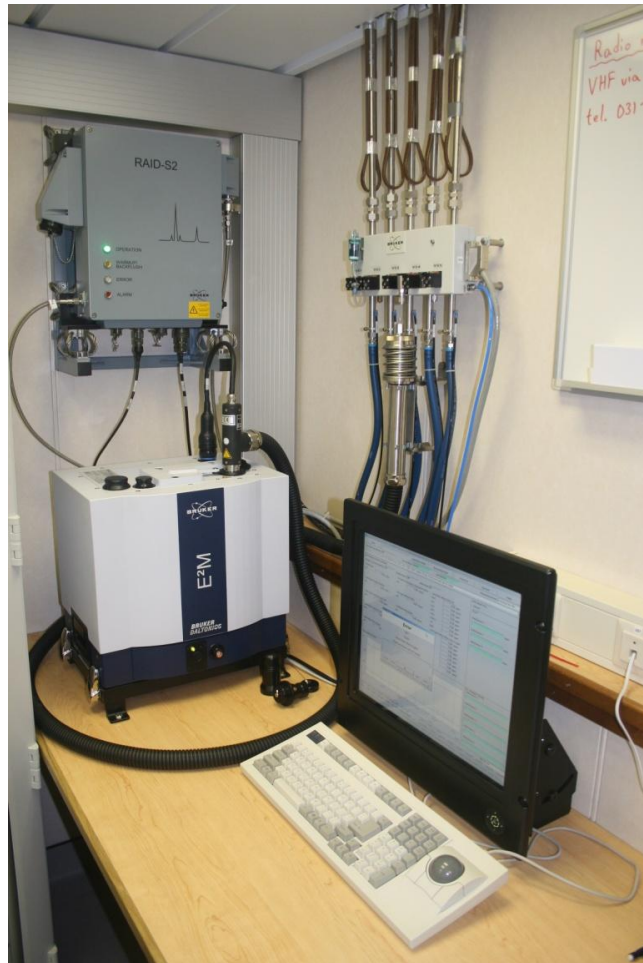
Shine on River



- Shine on popular river in Leipzig
- Fire fighter specialists Leipzig
- Analysis of water by purge and trap and GC/MS negative
- Analysis of sediment by solid-liquid-extraction with Methanol and GC/MS
 - identification of an old plant protective agent
- Old barrel found by divers



Swedish Coast Guard Ship



- Integration into gas detection system
- Combination with other sensors
- Gas detection 24/7 fullscan



Ground contamination



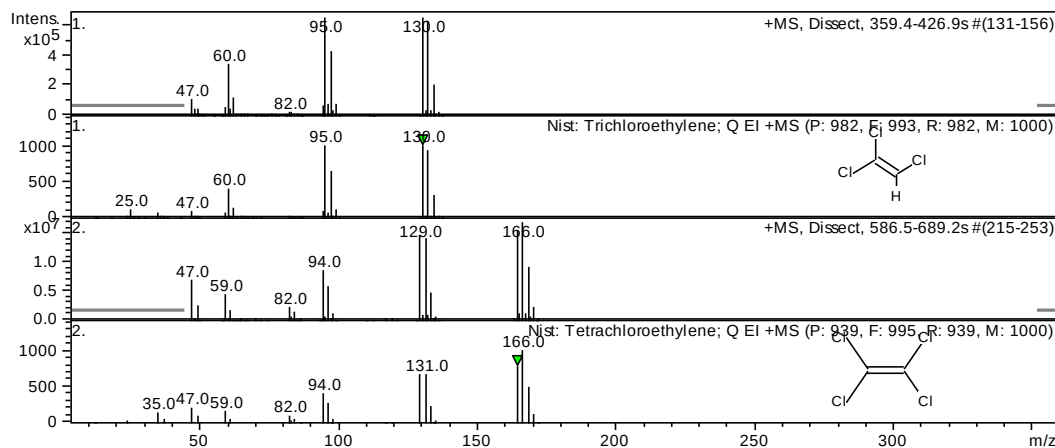
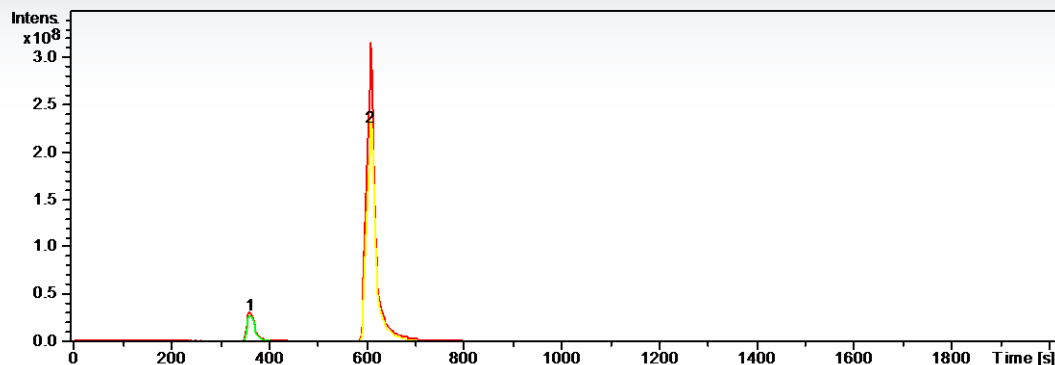
**Ruin of a fur-manufacturing company
in Niedersachsen**

**Wide area contamination with
chlorinated hydrocarbons**

**On-site Measurements with MM2 to
determine risks and area together with
police and federal office of ground
protection**



Ground contamination

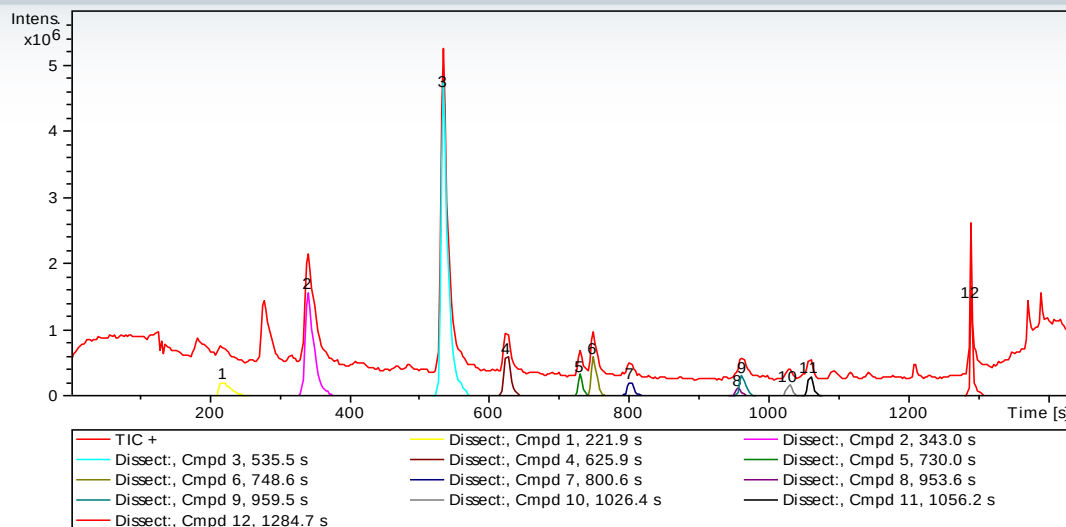


Sampling of ground air
(down to 7 m)

Identified substances in ground air

#	RT [s]	Area	Compound Name	Library	CAS#	Purity'
1	365.1	545080091	Trichloroethylene	Nist	79-01-6	985
2	610.3	5053466991	Tetrachloroethylene	Nist	127-18-4	918

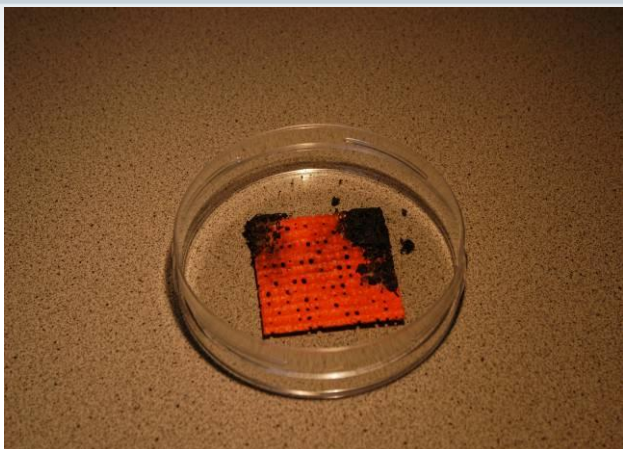
Dump Air



Identified substances in dump air

#	RT [s]	Area	Compound Name	Library	CAS#	Purity'
1	221.9	3739195	Carbon disulfide	Nist	75-15-0	979
2	343.0	23245934	Furan, tetrahydro-	Nist	109-99-9	816
3	535.5	56298844	Toluene	Nist	108-88-3	977
4	625.9	6321778	Tetrachloroethylene	Nist	127-18-4	960
5	730.0	2585451	Ethylbenzene	Nist	100-41-4	915
6	748.6	5263568	Benzene, 1,3-dimethyl-	Nist	108-38-3	996
7	800.6	2026941	p-Xylene	Nist	106-42-3	912
10	1026.4	1494777	Benzene, 1,3,5-trimethyl-	Nist	108-67-8	919
11	1056.2	2559744	Benzene, 1,3-dichloro-	Nist	541-73-1	948
12	1284.7	8775766	Naphthalene	Nist	91-20-3	986

Combustion Air Sample

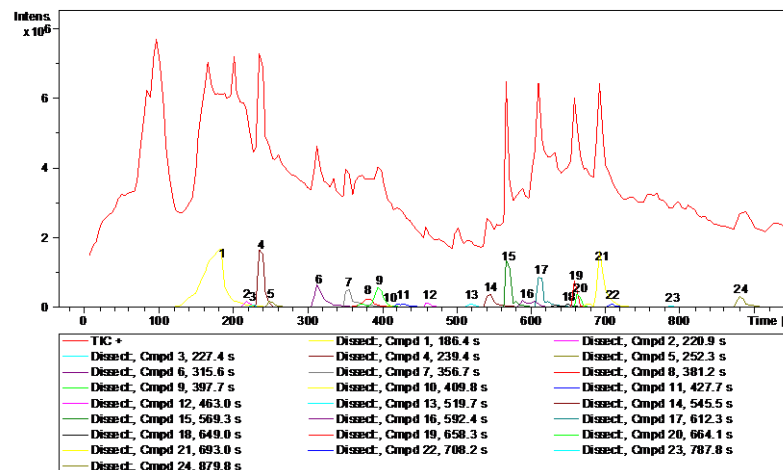


1 stroke



Combustion gas sample:

Material: unknown
Product information: during combustion only
CO₂ produced



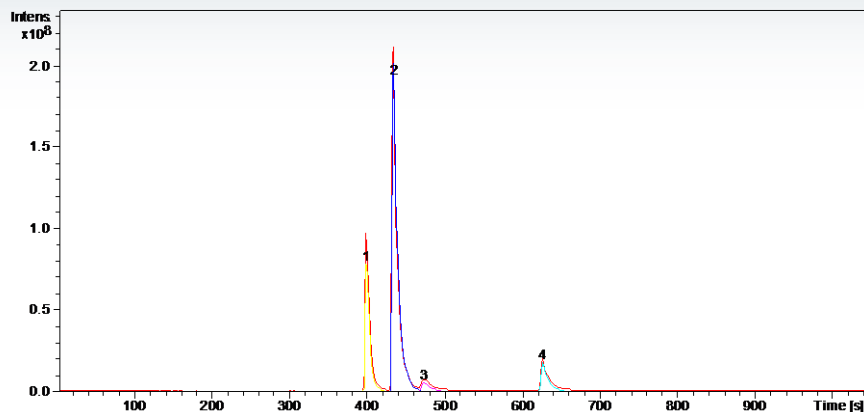
Result: Combustion Air Sample



Identified subsatnces in combustion gas

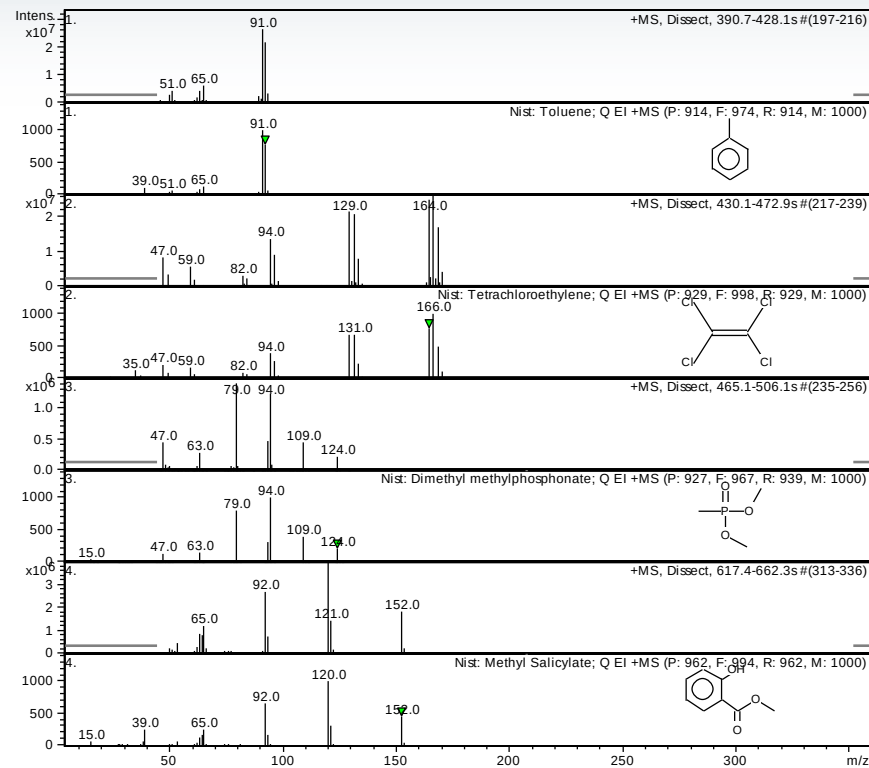
#	RT [s]	Area	Compound Name	Library	CAS#	Purity'
1	186.4	57537182	Phenol	Nist	108-95-2	984
2	220.9	2022382	Benzaldehyde	Nist	100-52-7	914
3	227.4	687206	1,3-Dioxane, 4-phenyl-	Nist	772-00-9	807
4	239.4	16755153	1-Hexanol, 2,2-dimethyl-	Nist	2370-13-0	988
5	252.3	1986960	2-Pyrimidinamine	Nist	109-12-6	933
6	315.6	9612901	Diaminopyridine	Nist	4318-76-7	953
7	356.7	8595473	Naphthalene	Nist	91-20-3	986
8	381.2	5364933	1-Phenoxypropan-2-ol	Nist	770-35-4	938
9	397.7	9831706	Neodecanoic acid	Nist	26896-20-8	934
10	409.8	325468	Indole	Nist	120-72-9	890
11	427.7	2082647	Benzocycloheptatriene	Nist	264-09-5	898
12	463.0	1304697	Biphenyl	Nist	92-52-4	935
13	519.7	1338885	Biphenylene	Nist	259-79-0	974
14	545.5	5314064	Hexanoic acid, 1-naphthyl ester	Nist	28749-24-8	978
15	569.3	13251392	Benz[cd]indol-2(1H)-one	Nist	130-00-7	955
16	592.4	4434952	Fluorene	Nist	86-73-7	975
17	612.3	10571146	Phenoxazine	Nist	135-67-1	760
18	649.0	1708473	Pyridine, 2-(2-phenylethenyl)-	Nist	714-08-9	968
19	658.3	6165698	1,10b(2H)-Dihydropyrano [3,4,5-jk]fluorene	Nist		954
20	664.1	3489942	Dibutyl phthalate	Nist	84-74-2	966
21	693.0	19305061	Isopropyl Palmitate	Nist	142-91-6	773
22	708.2	945927	Naphthalene, 2-phenyl-	Nist	612-94-2	956
23	787.8	338389	2-(2-Benzothiazolyl)benzofurane	Nist	69976-47-2	765
24	879.8	4409451	2-Ethylhexyl trans-4- methoxycinnamate	Nist	83834-59-7	962

SPME from Tedlar-bag



PDMS – SPME-fibre

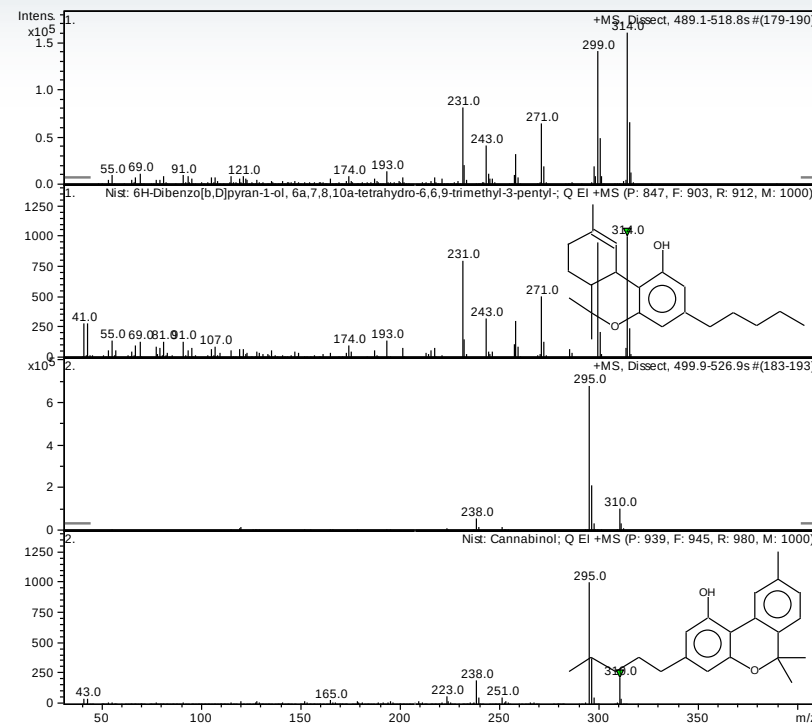
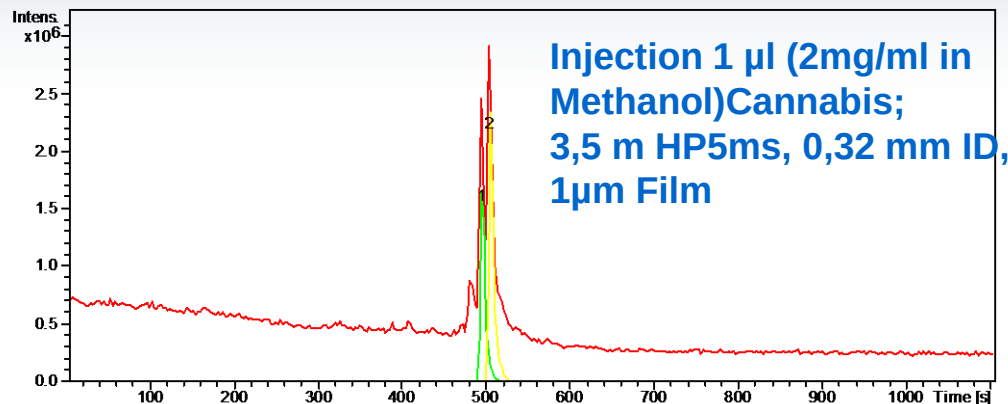
Gas sample from Tedlar-Bag
(10 min sampling time)



Identified substances

#	RT [s]	Area	Compound Name	Library	CAS#	Purity'
1	400.0	522697770	Toluene	Nist	108-88-3	914
2	434.6	1679381101	Tetrachloroethylene	Nist	127-18-4	929
3	473.9	68186097	Dimethyl methylphosphonate	Nist	756-79-6	927
4	625.7	184068834	Methyl Salicylate	Nist	119-36-8	962

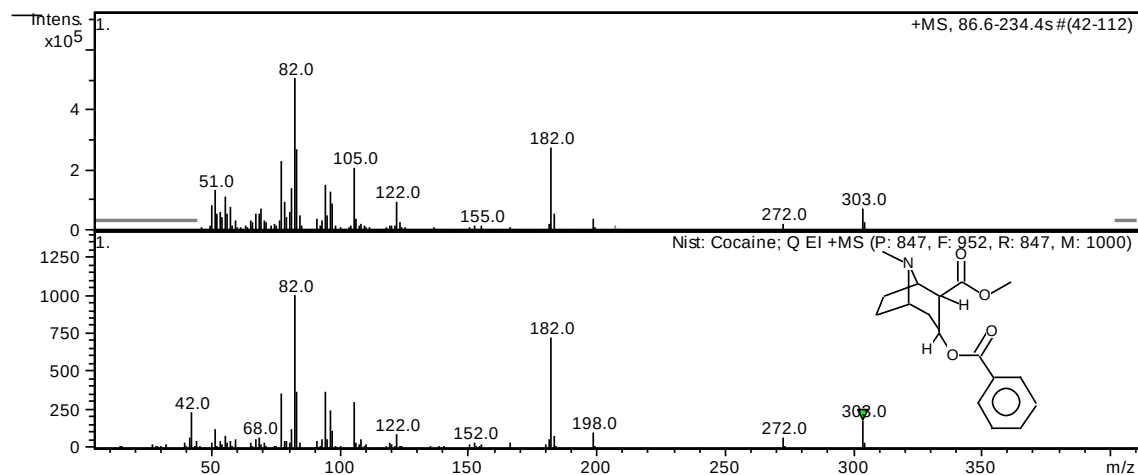
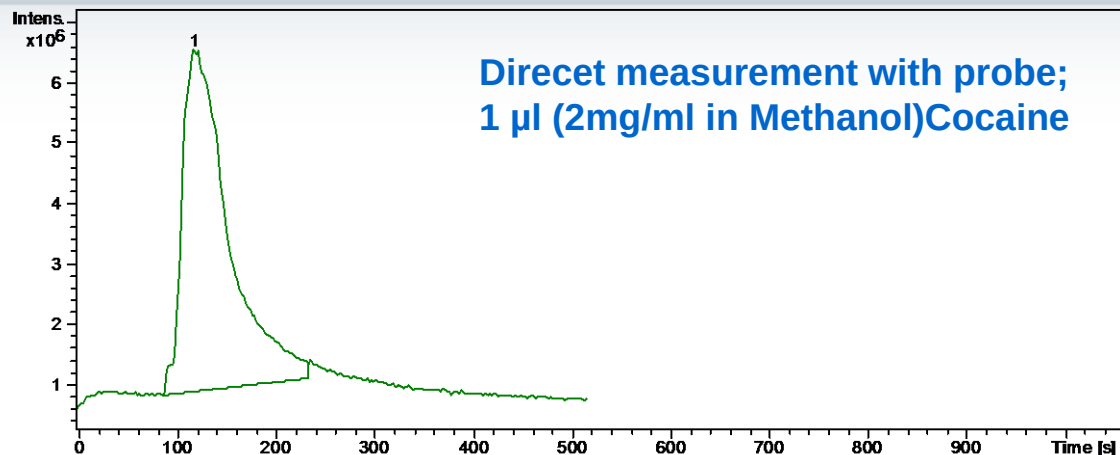
Drugs: Cannabis



Identified substances

#	RT [s]	Area	Compound Name	Library	CAS#	Purity'
1	495.5	11662059	Tetrahydrocannabinol (THC)	Nist	33086-25-8	847
2	505.8	15867883	Cannabinol	Nist	521-35-7	939

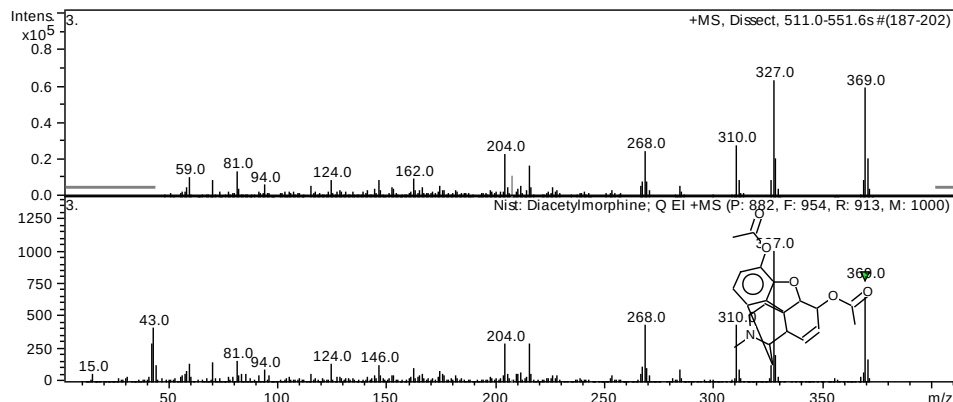
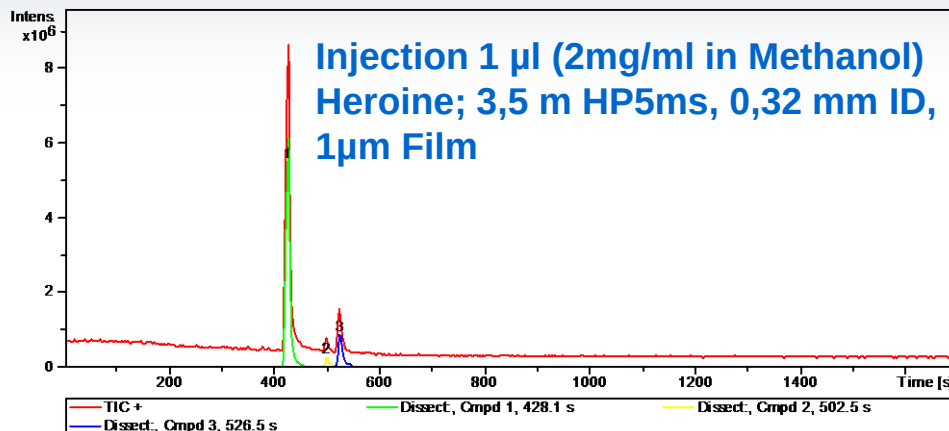
Drugs: Cocaine



Identified substances

#	RT [s]	Area	Compound Name	Library	CAS#	Purity'
1	119.8	304612217	Cocaine	Nist	50-36-2	847

Drugs: Heroin (Street sample)



Identified substances

#	RT [s]	Area	Compound Name	Library	CAS#	Purity
1	428.1	55787740	Novocaine	Nist	59-46-1	941
2	502.5	1991596	Acetylcodein	Nist		716
3	526.5	8490099	Diacetylmorphine (Heroin)	Nist	561-27-3	882

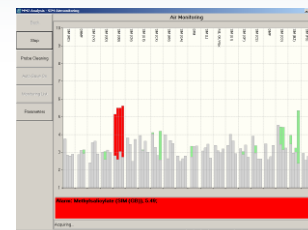
Military Reconnaissance Mission



Reconnaissance Mission

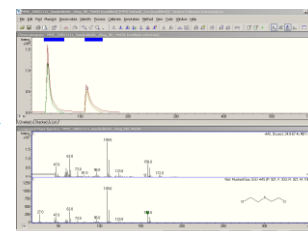


Monitoring



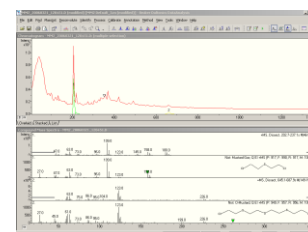
Response time: 3 – 20 sec

Spectra Series with Identification



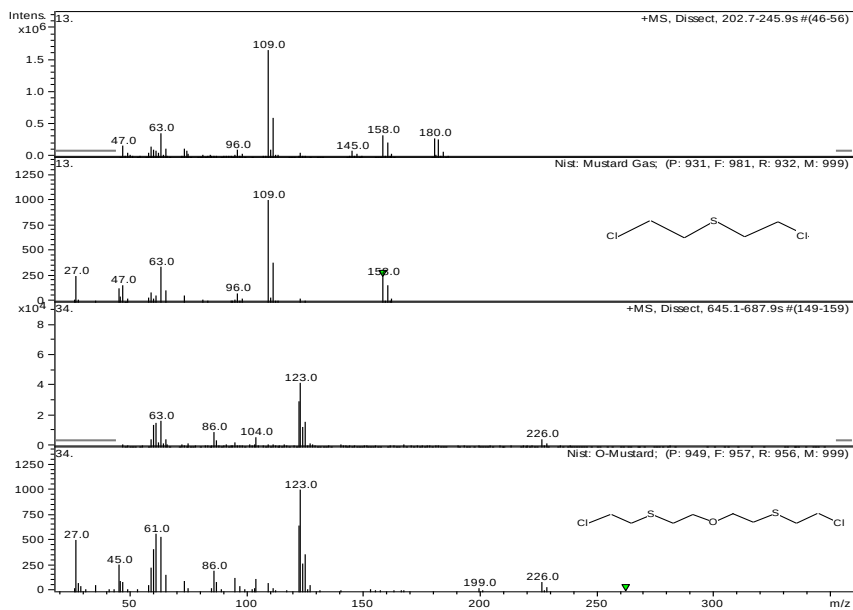
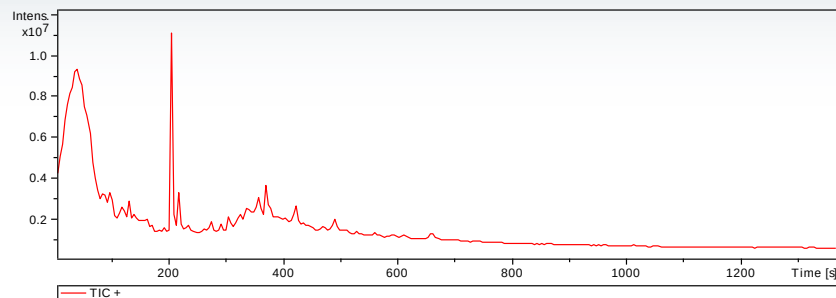
Analysis time: 2 – 3 min

GC Analysis with Identification



Analysis time: 10 -15 min

Military Reconnaissance Mission

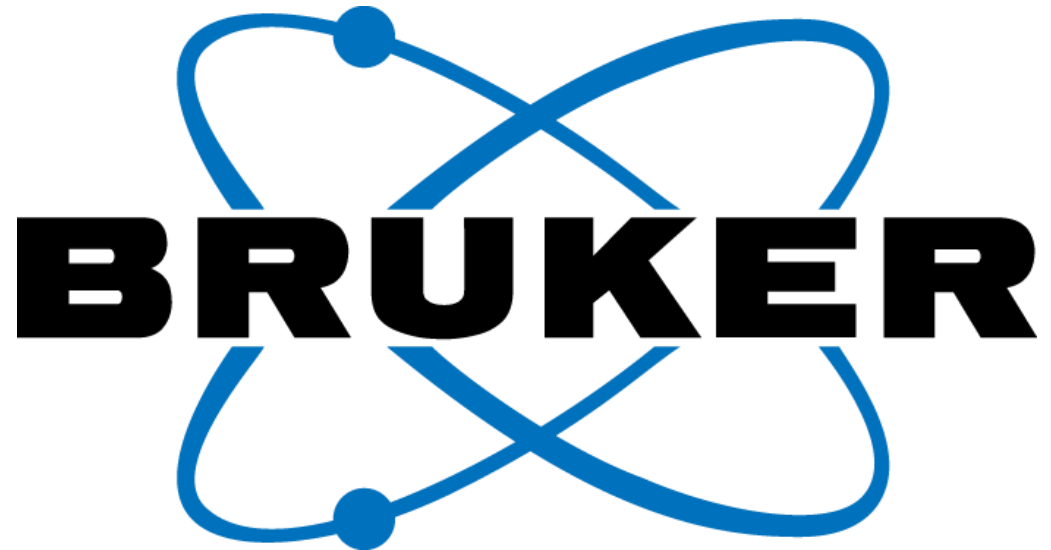


Things to take care on



- Good initial education and training necessary to use all available components and options
- Standard operation procedures may help to handle correctly
- Basic chemical knowledge essential (also to protect the instrument against damage)





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