



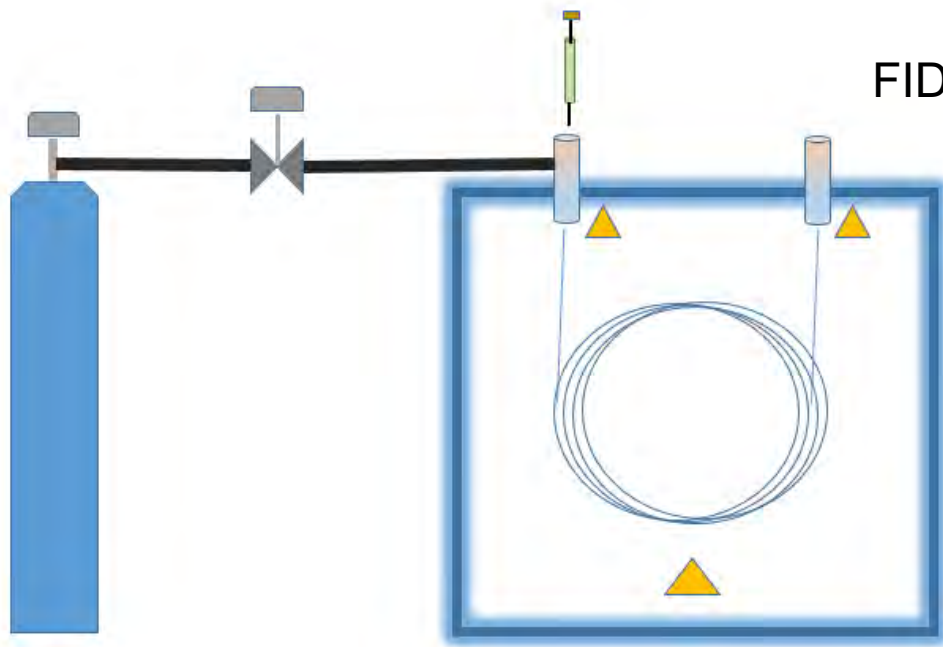
ThermoFisher
S C I E N T I F I C

New technology of GCMS

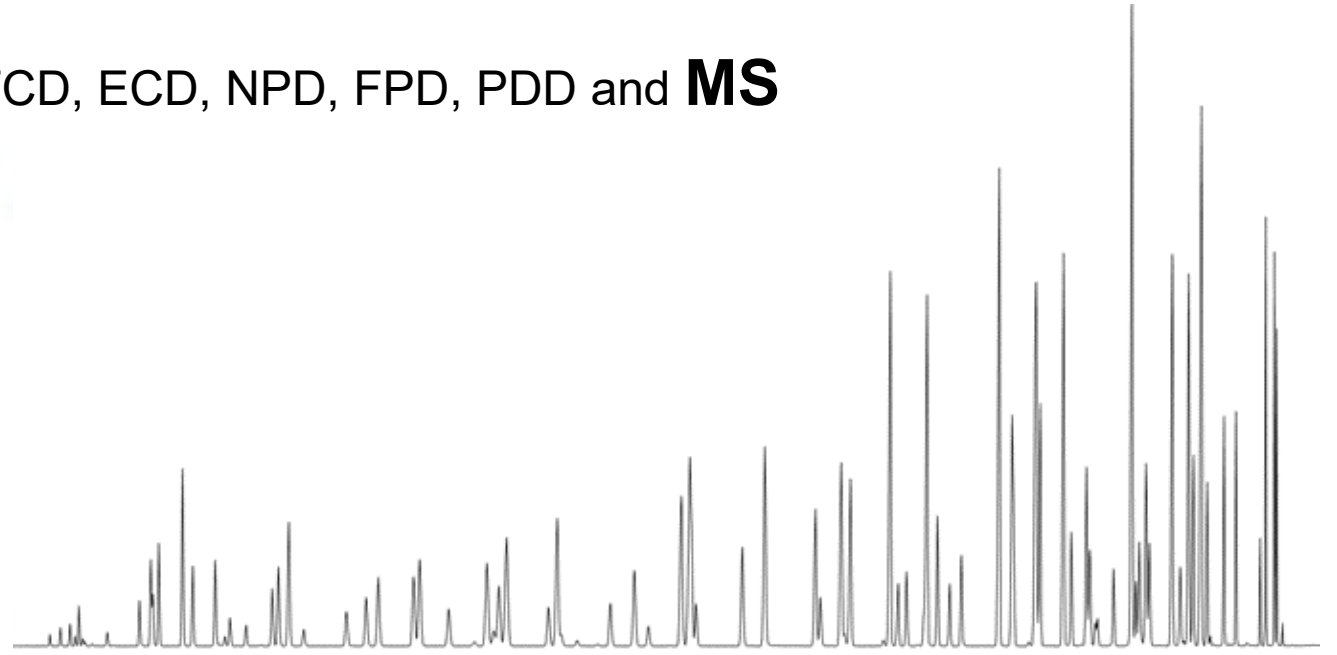
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Basic of Gas chromatography

- Gas Chromatography (GC) : Chromatography technique which gas is used as mobile phase
- Sample will be injected into the system, Injection port where all components are vaporized and swept into the column
- Sample components will then be separated according to the interaction with stationary phase and eluted to detector.

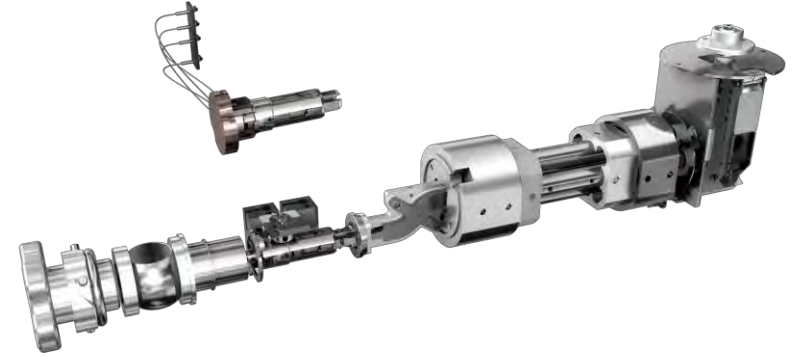


FID, TCD, ECD, NPD, FPD, PDD and **MS**



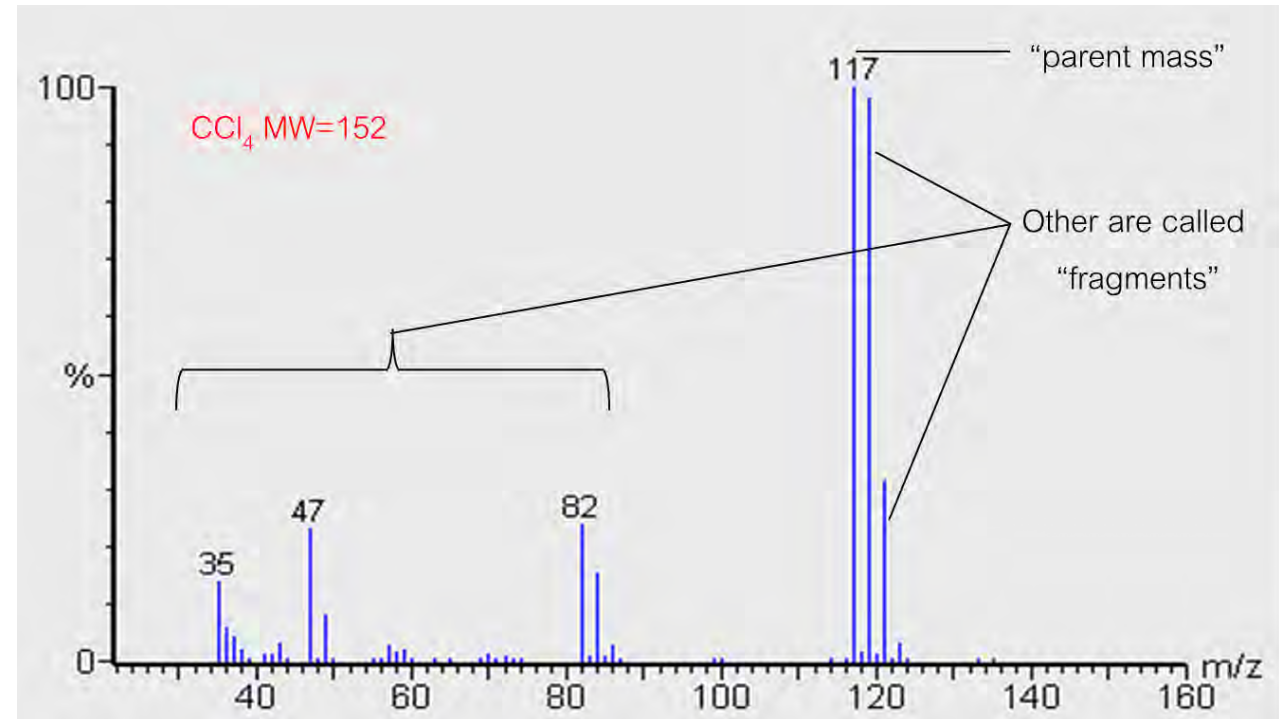
Why GC/MS?

- Universal and specific
 - ✓ Full scan for unknown sample
 - ✓ SIM, MIM for specific (interested) mass
- High Sensitivity
 - ✓ ppt level
- Provides identification with standard or library spectrum
- Interference-free quantitation (SIM or MIM)
- Isotopic information
- Confirmation of other conventional detectors



What is Mass Spectrometry?

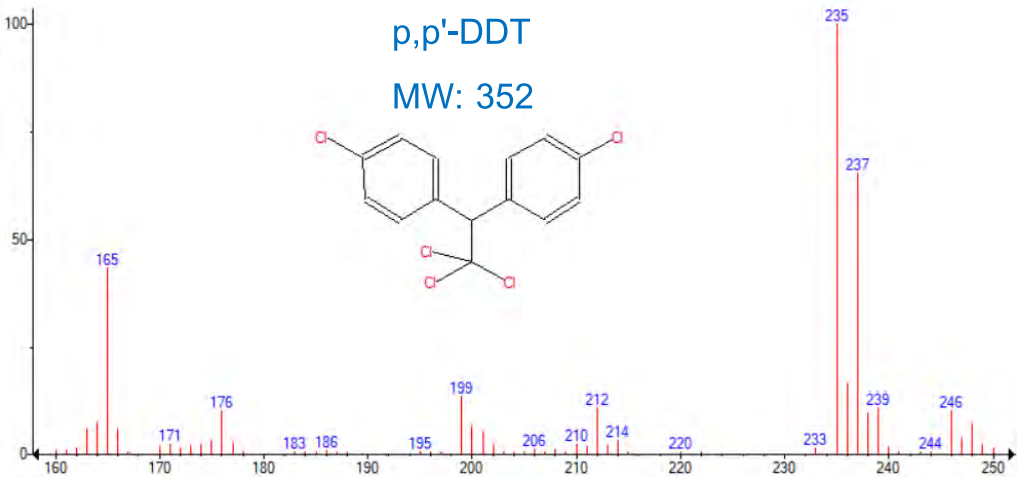
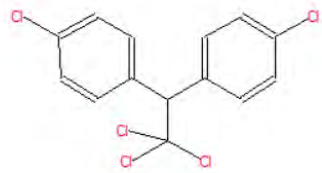
- The production of ions that are subsequently separated or filtered according to their mass-to-charge (m/z) ratio and detected.
- The resulting mass spectrum is a plot of the (relative) abundance of the produced ions as a function of the m/z ratio.”



Mass Spectrum

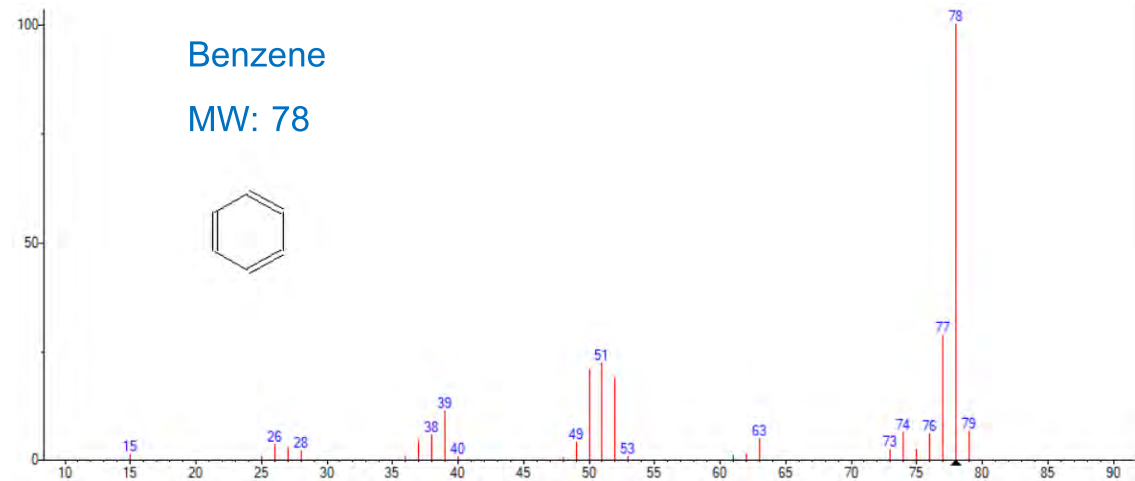
p,p'-DDT

MW: 352



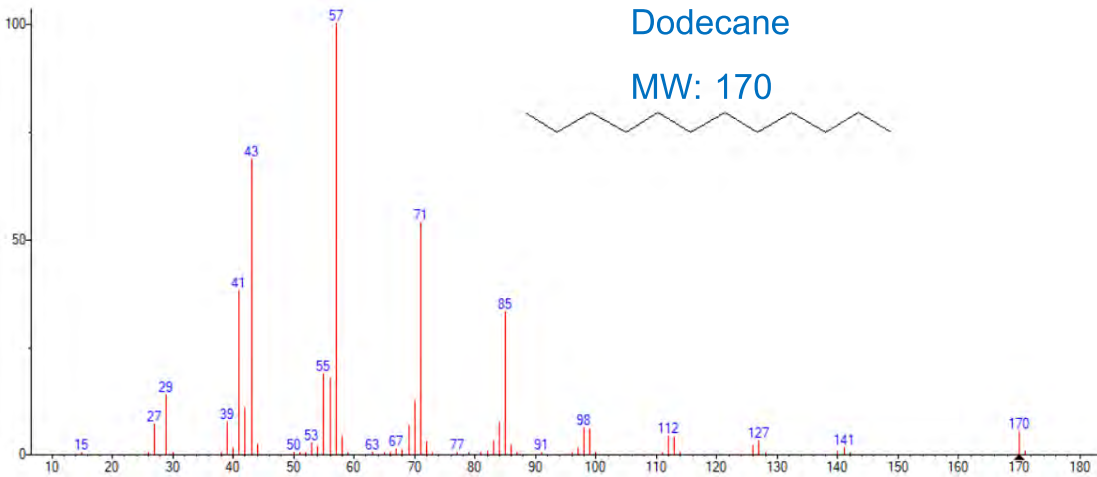
Benzene

MW: 78



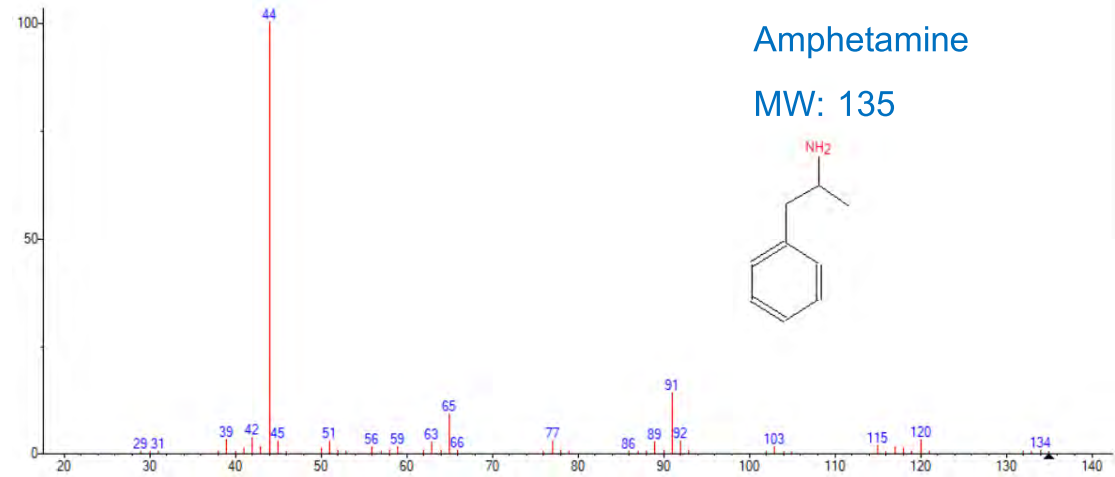
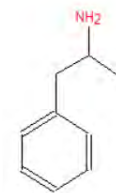
Dodecane

MW: 170



Amphetamine

MW: 135

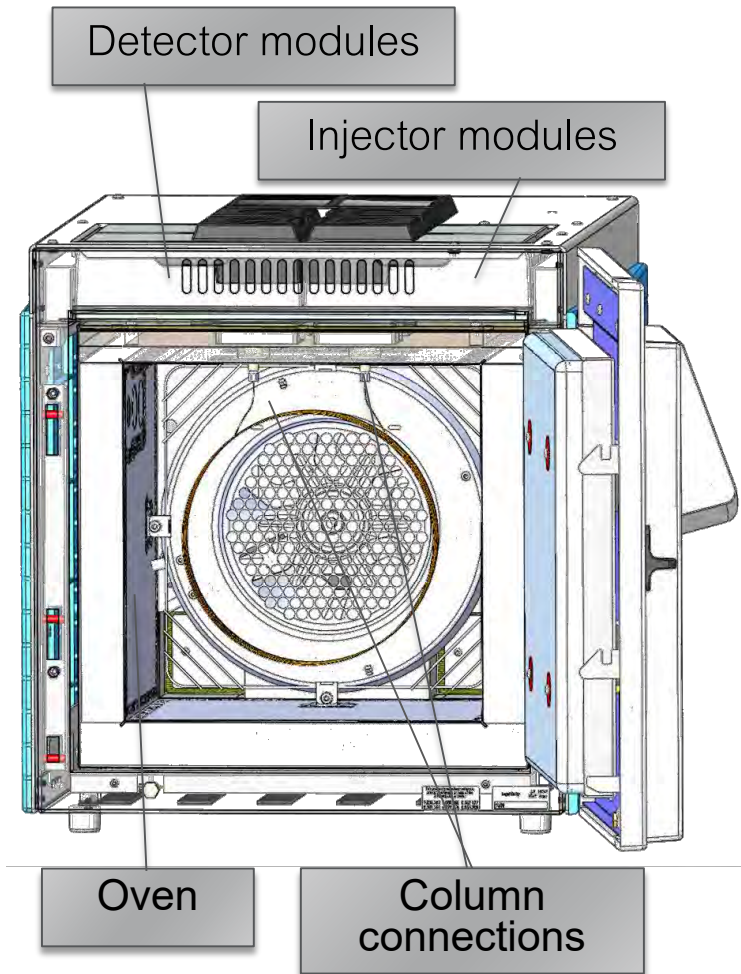


Trace1300 Series GC features to boost productivity and laboratory efficiency

- Capillary iConnect Injector Modules
 - SSL, PTV, On-Column
- Integrated Backflush
 - iConnect SSL and PTV injectors module with integrated BKF capabilities
- Large Volume Injection capabilities
 - With PTV and SSL injector
- iConnect Helium Saver module
 - Proprietary solution to save Helium consumption during operation
- iConnect Detector Modules
 - FID, TCD, ECD, NPD, FPD, PDD
- Retention Time Alignment
 - Easy and quick approach to keep data consistency
- No-vent Module (for NOVPI MS systems)
 - In GCMS operation, it allows to disconnect the column without venting the MS



A New Modular GC System

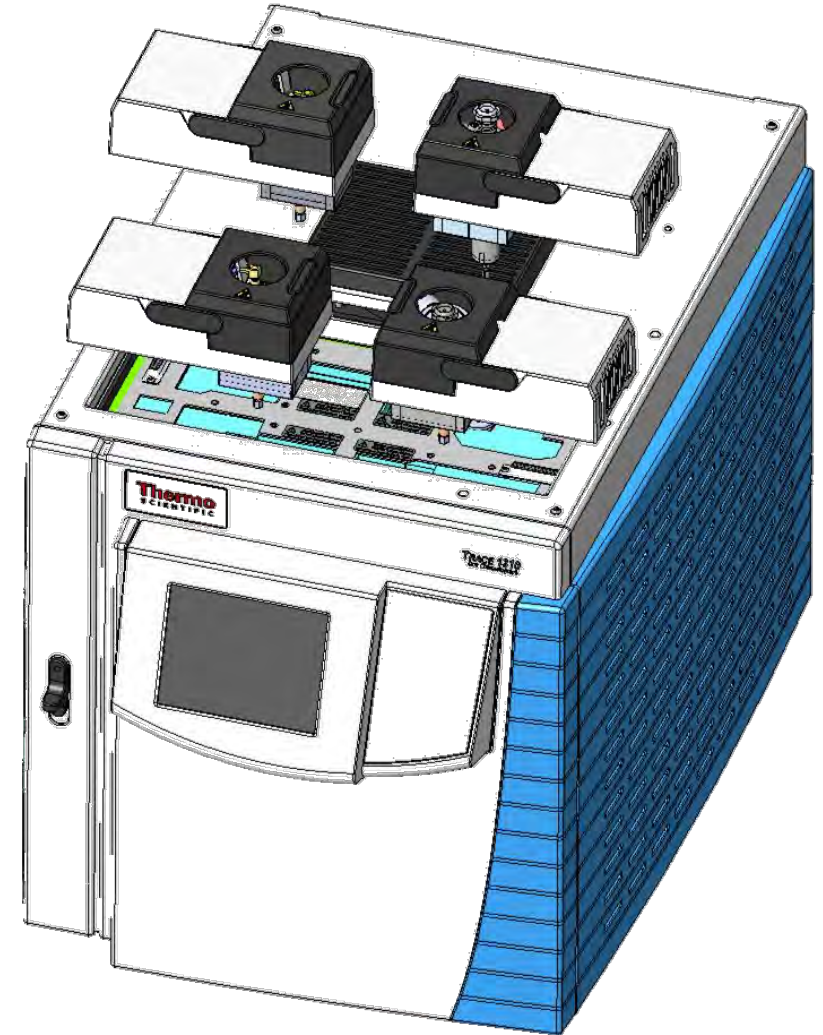


- Inj/det modules fit on the oven top and enter the oven with column connection terminals
- Gas and electrical connections are provided on the top deck base
- User- exchangeable modules in two minutes:
 - Tailor configuration to applications
 - Upgrade systems to ensure productivity growth
 - Inlets: SSL; SSL with Backflush; PTV; PTV with Backflush
 - Detectors: FID; TCD; ECD; NPD



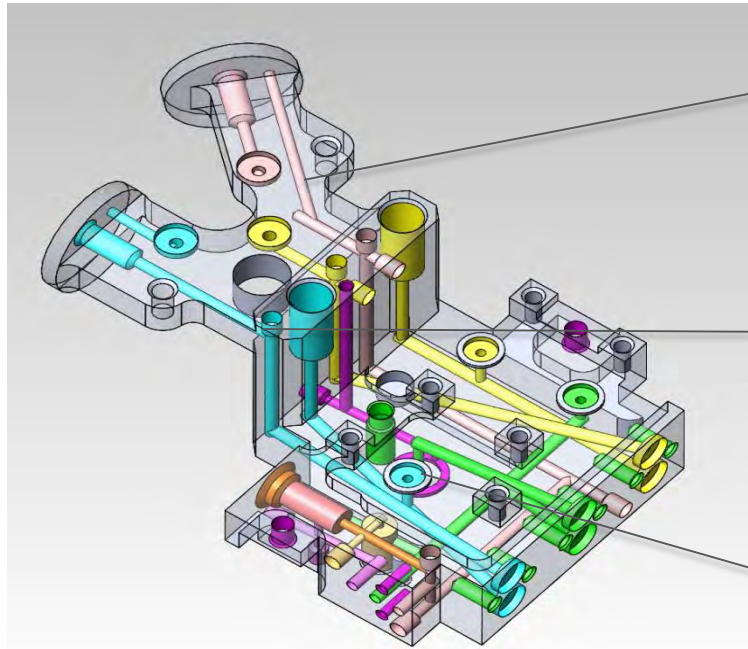
Modular GC: Main Design Challenges

- Miniaturization of components
 - ✓ Miniaturization of electronics board
 - ✓ Miniaturization of pneumatic circuits and components
- Temperature constrains
 - ✓ Housing modules with electronics on an oven running up to 450°C
 - ✓ Compact modules with electronics and with high temperature injector and detector bodies
- Ensuring reliable connections
 - ✓ Gas connections
 - ✓ Electrical connections



Miniaturized Injectors / Detectors Manifolds

- All pneumatic circuit is integrated in the manifold allowing miniaturization.
- No or minimum use of tubing or fittings minimizing risks of leaks.



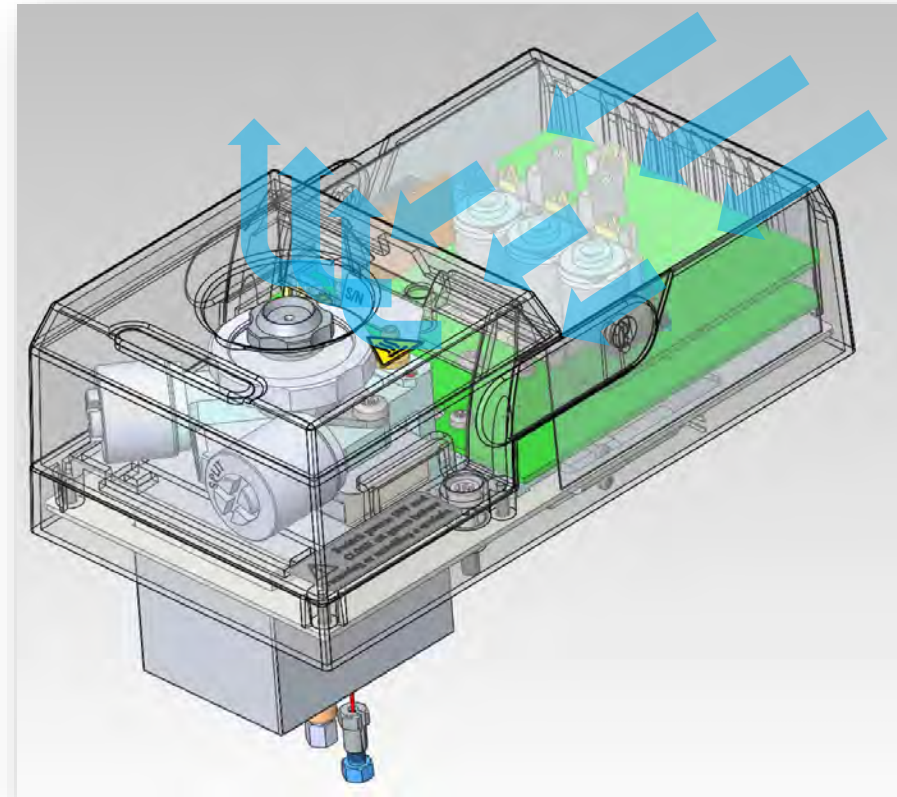
All gas channels are machined into the manifold

Flow restrictors are housed directly into the manifold. Manifold temperature is measured in real time and used for proper flow compensation

Seal to valve and sensor is made by high quality o-rings

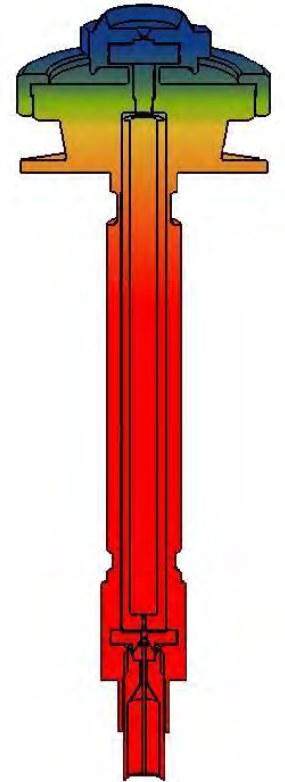
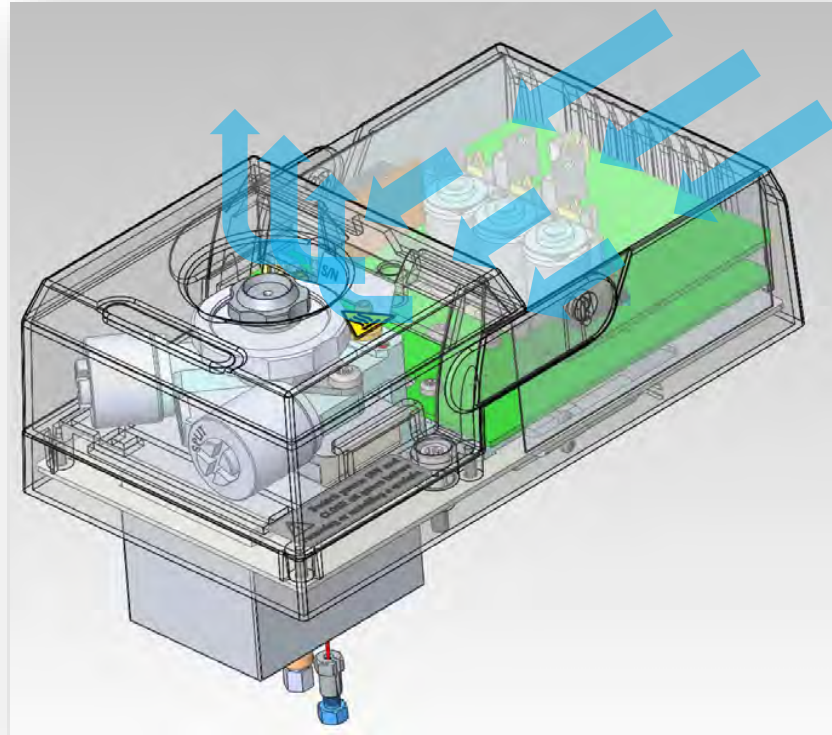
SSL Injector Module Active Cooling

- Forced air enters the module from its back side and keep electronics cool
- Air is then vented through the injector box hole creating a barrier against the heat produced by the hot injector
- The air vent helps in keeping the septum head cool without affecting the internal inlet temperature profile
- Module base is cooled by the cold oven top deck copper plate
- Same air path is used for detectors



SSL Injector Module Active Cooling

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- Same air path is used for detectors



Backflush: built-in for iC-SSL and iC-PTV

- Injector can operate as standard SSL and PTV or reversing the carrier gas flow direction in the inlet, venting from the split line possible "undesired" analytes.
- SSL/PTV BKF can be used as a standard inlets just capping the BKF line

- Back-flush option included in the module without additional plumbing
- Self adjusted carrier flow during backflush for easier operation and method set up
- No need for additional auxiliary gas for backflush operation





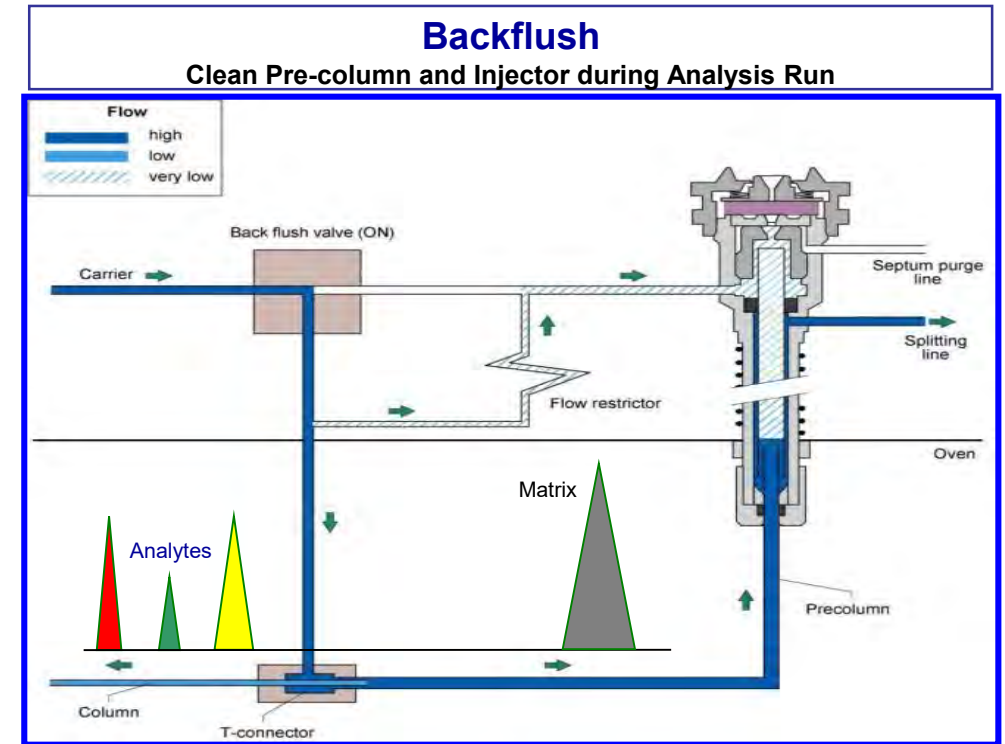
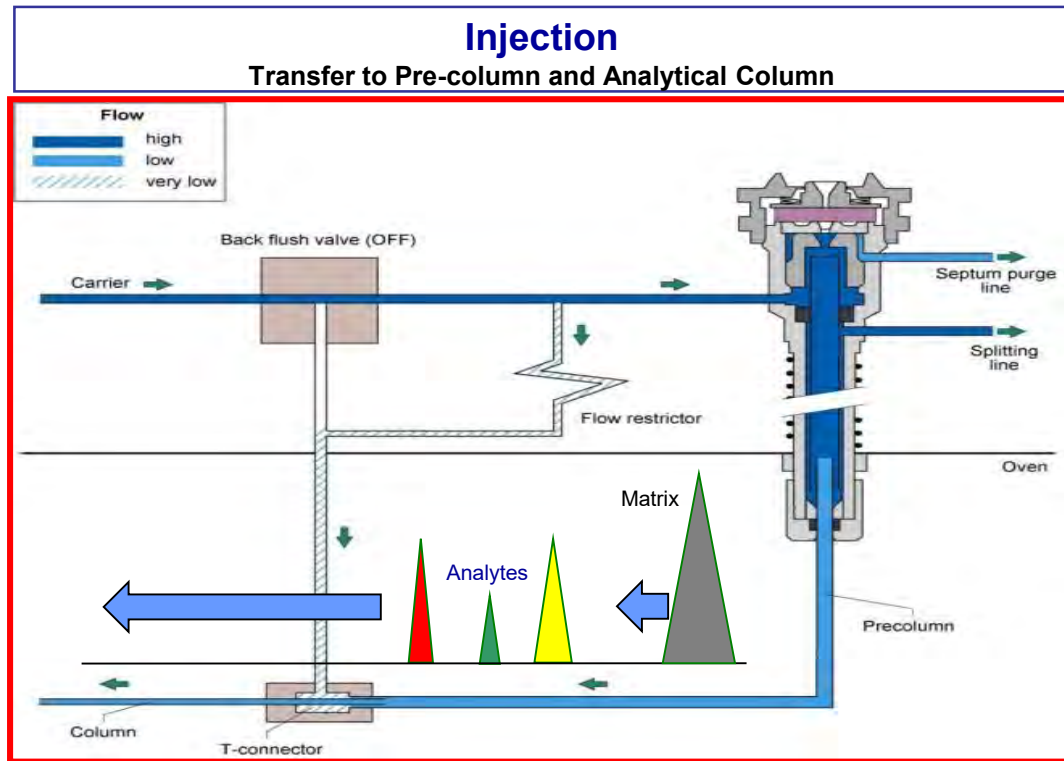
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Instant connect SSL and PTV injector with Backflush

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Backflush Option : Integrated Solution with PTV and SSL

- Instant connect SSL and PTV injector with backflush capabilities to shorten analysis time and keep the analytical column and the detector cleaner
- Entire pneumatic circuit is integrated in the injector module for a self adjusted carrier flow rate during BKF
- No tubing nor fittings are used, minimizing risks of leaks and method complexity
- Very useful for dirty samples (poor clean-up) (i.e. biological/food extracts)



Shorten the analysis time and preserve from matrix contamination

Pear Extracted with Ethyl Acetate

- **No Backflush**

Relative Abundance

- **With Backflush**

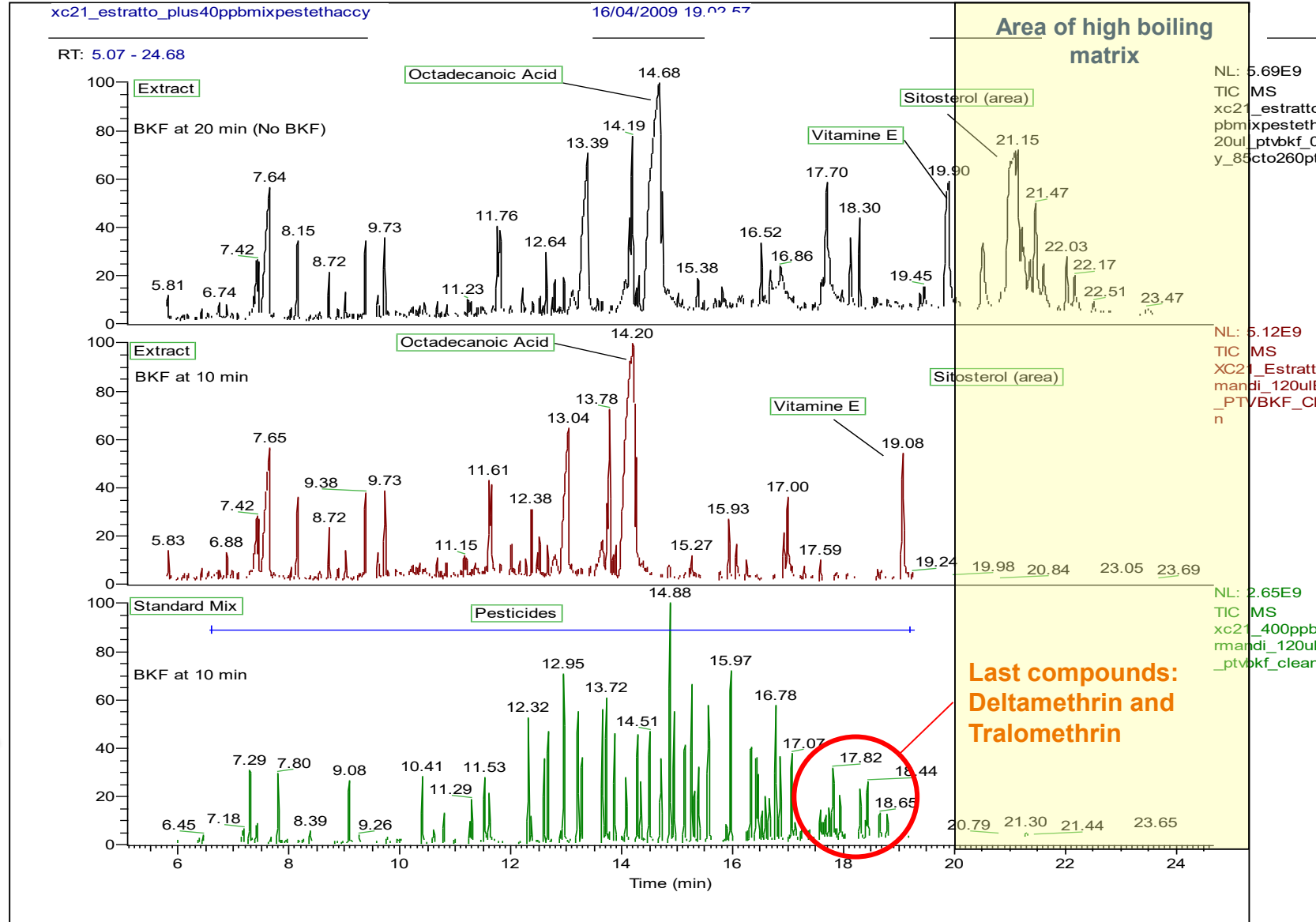
- Transfer time 10 min

Relative Abundance

- **Pesticide standard w BKF**

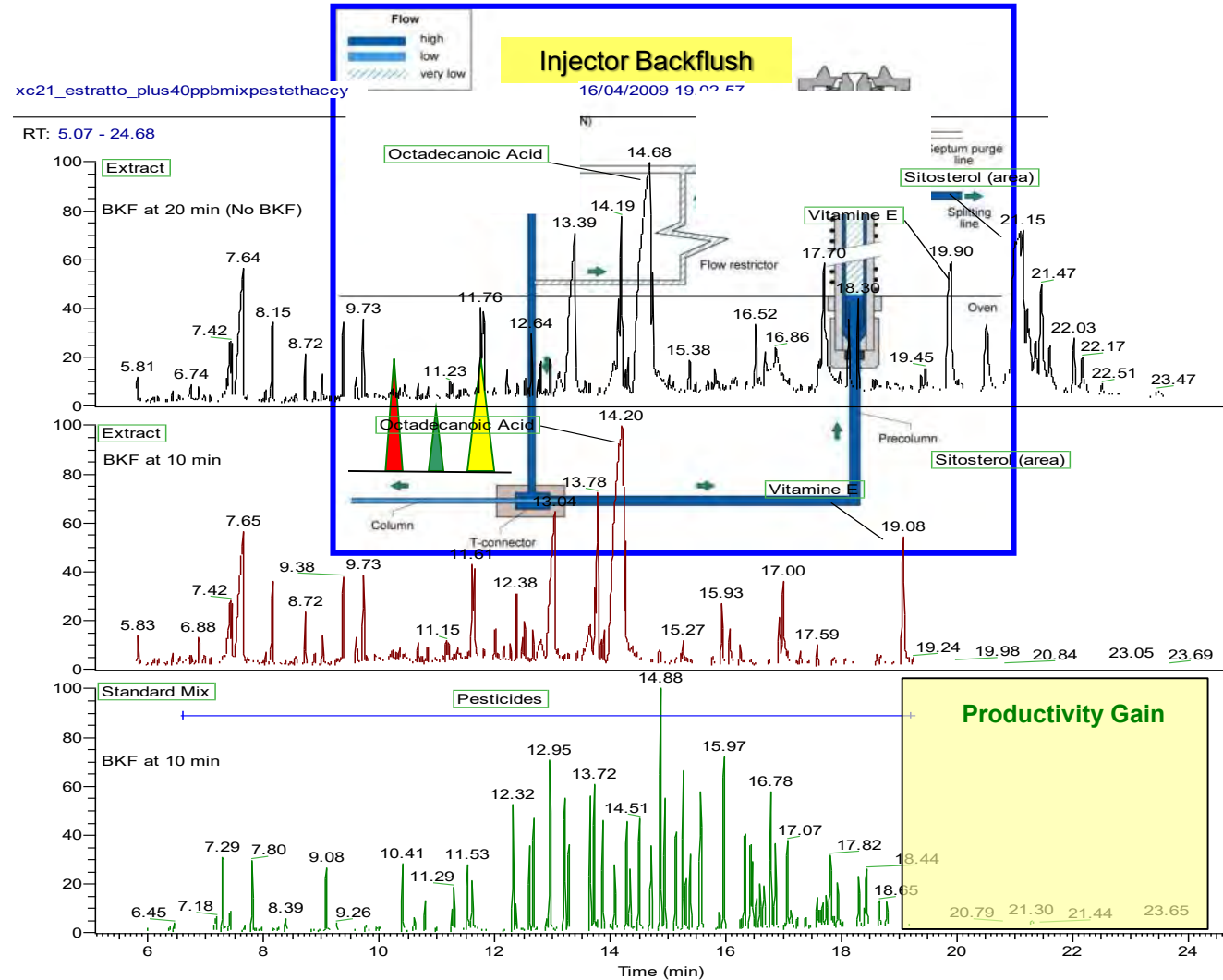
- Transfer time 10 min

Relative Abundance



Benefits - Injector Backflush Increases Productivity

- Reduce sample prep procedure
 - for multi-component methods
 - e.g. QuEChERS for pesticides
- Use concurrent injector backflush
 - Keep high boiling matrix from the column
 - No need to backflush the whole column
 - Avoid additional clean time after the run
 - Clean the injector as well during the run
 - No need of additional Aux Gas Control
- Stop the run
 - After the last compound of interest
 - Get to the next injection
 - Increase sample throughput

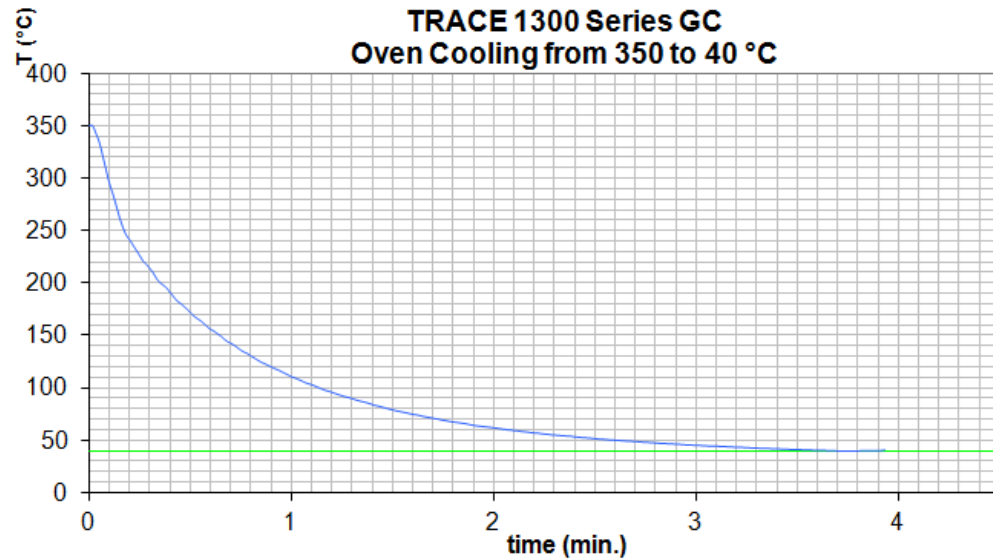


TRACE 1300 series: "1000-holes" capabilities

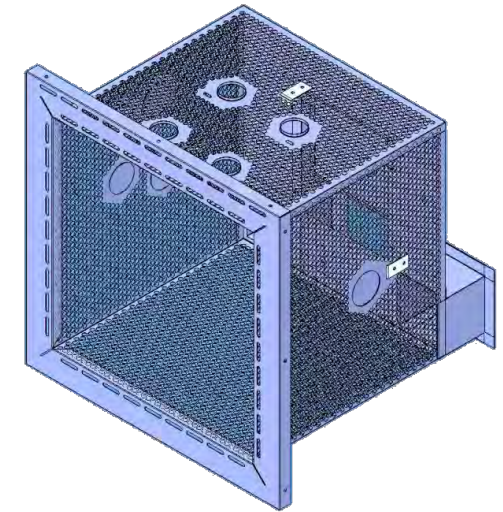
- Quickly recover starting conditions after power off

Warm-up times. From OFF conditions to readiness (minutes)

	TRACE 1300 Series	Brand A
Oven at 50 °C INJ & DET at 250°C	3.5	10.2



- Fast Heating and cooling
- Quickly reaching starting temperature of ambient +3°C
- Cooling from 450 to 50°C in < 4'
- Cooling from 350 to 40°C in < 3.5'





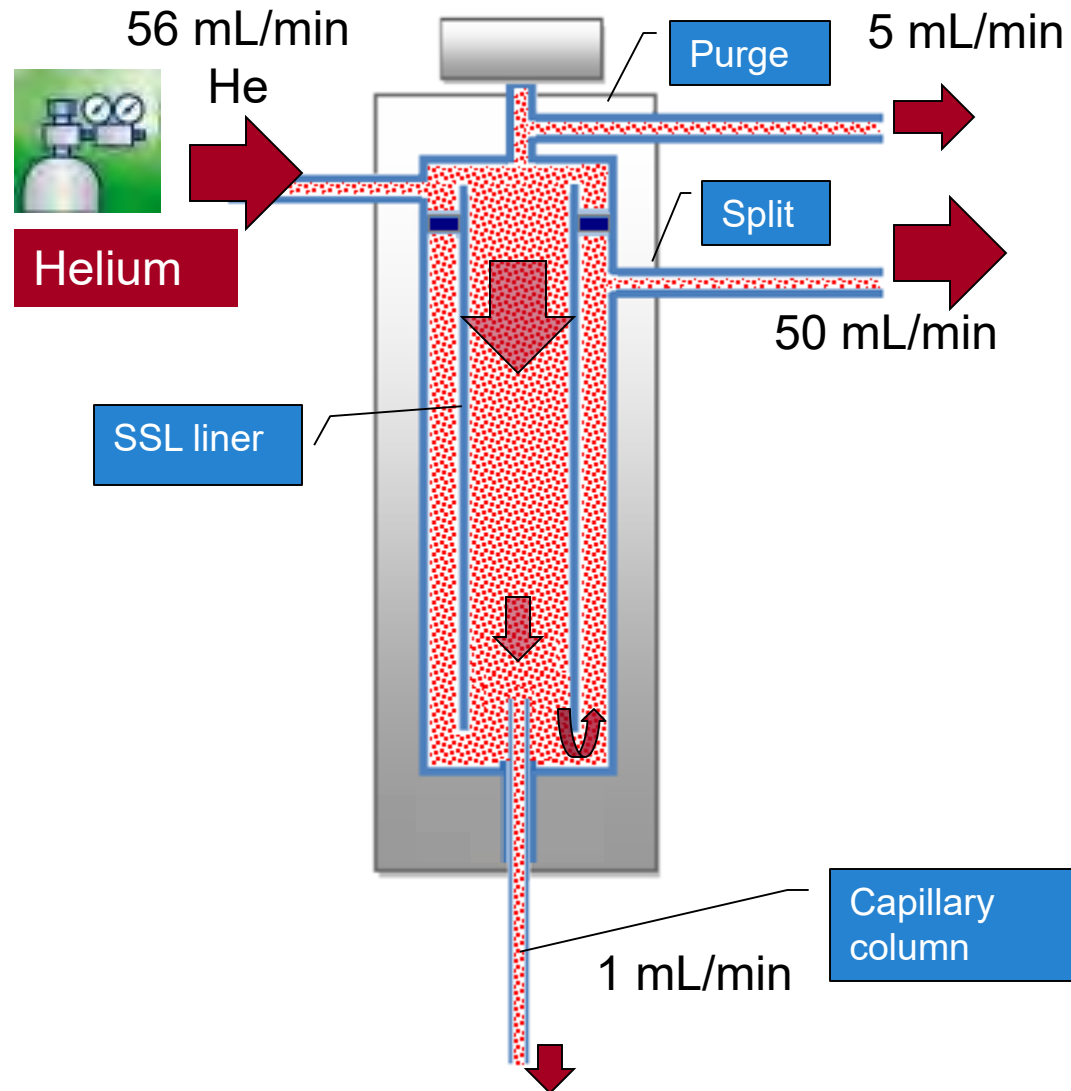
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Instant Connect Helium Saver

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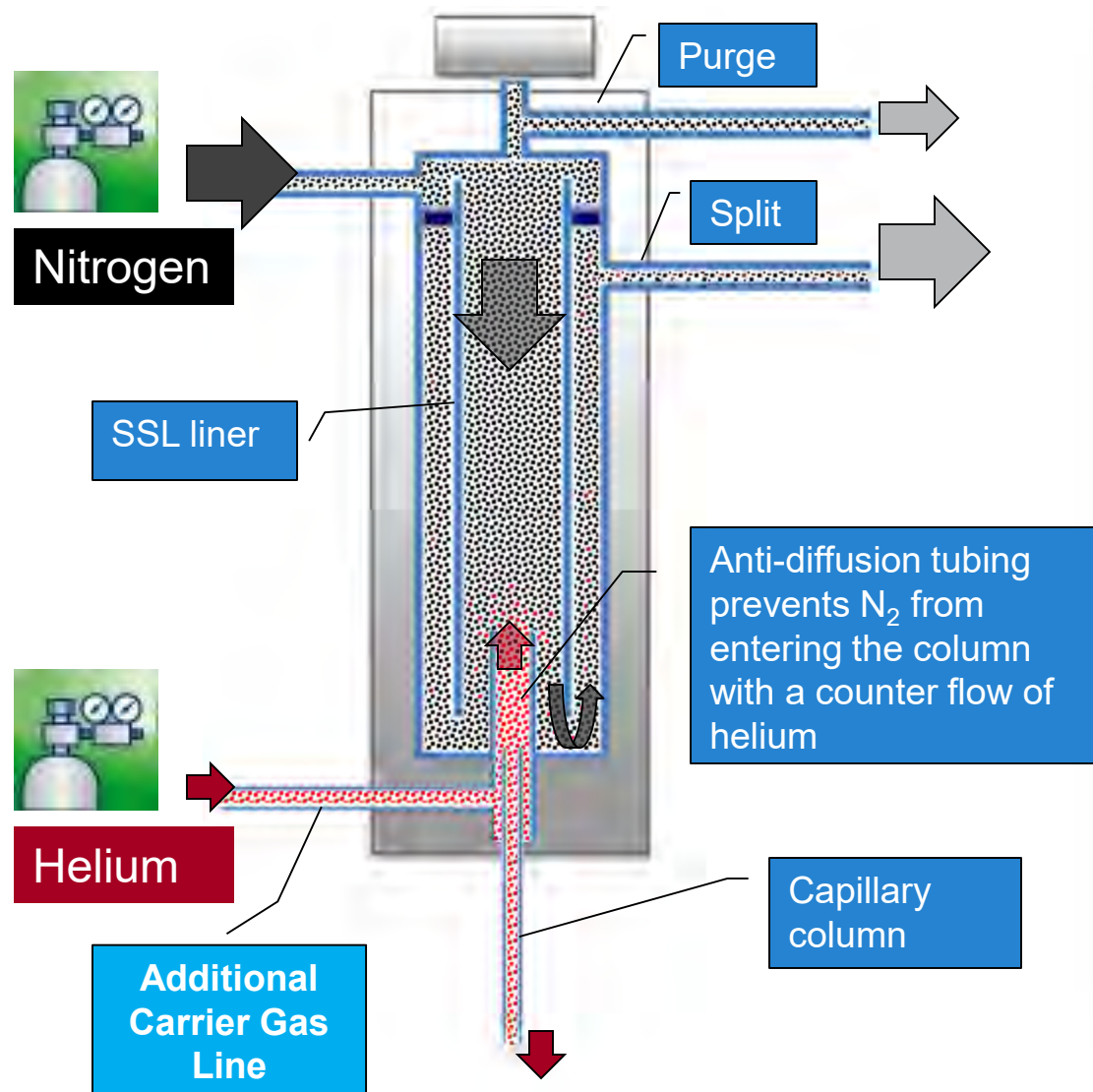
- There are some practical advantages in reducing Helium consumption versus migrating to a different carrier gas
 - There is no need to revalidate methods
 - There are no safety concerns when using Helium in the GC oven
 - There are no concerns about possible negative impact on detector performance (e.g. MS)
- The instant connect helium saver injector is using simultaneously two different gasses
 - Helium carrier gas is only used for separation process
 - A different gas is used to purge the inlet and split sample (e.g. Nitrogen)

Standard Split/Splitless Injector



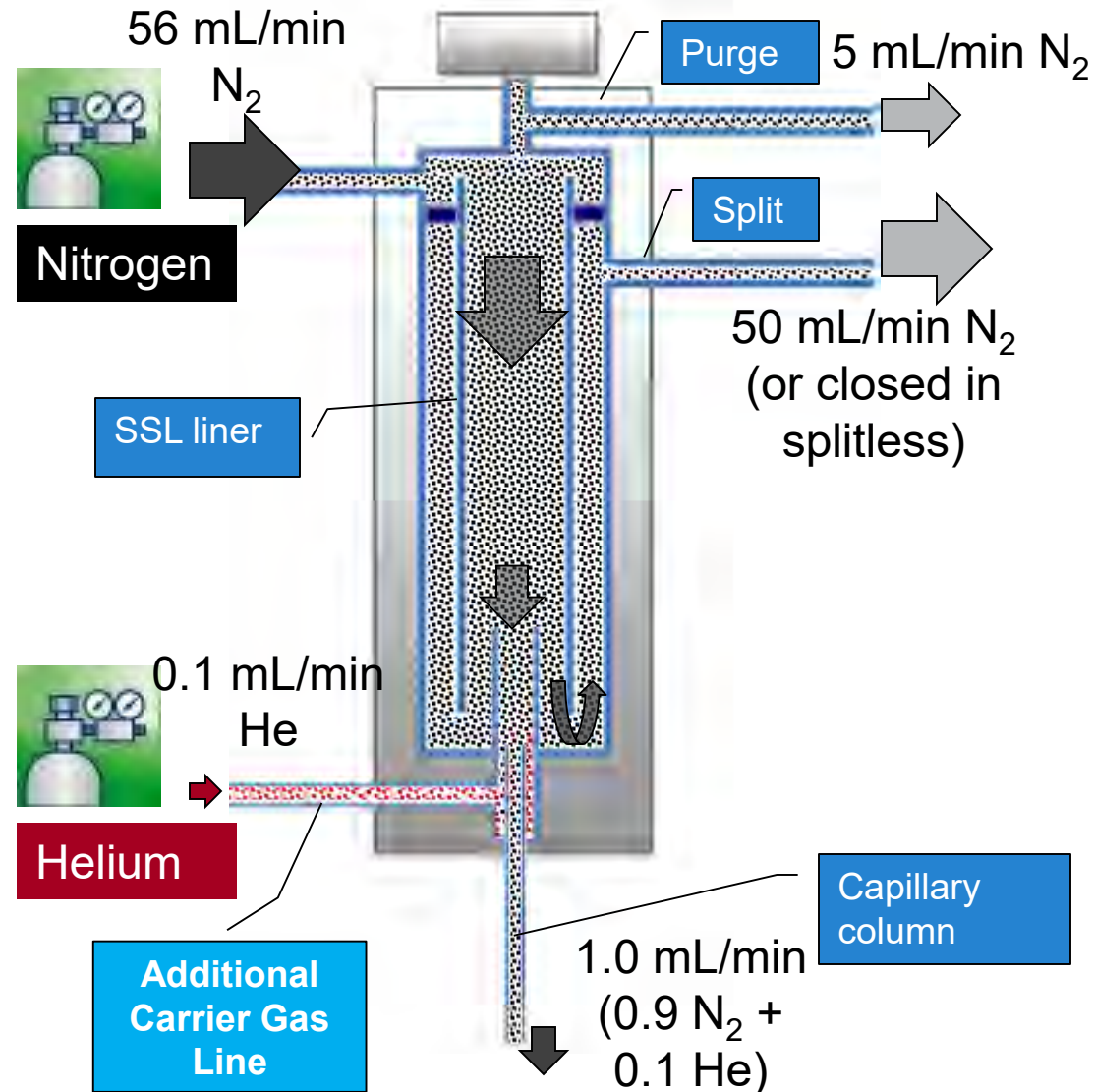
- SSL design almost unchanged since the introduction of capillary columns
- Same gas used for separation carrier, septum/inlet purge and sample splitting
- Typically only ~1/10 - 1/50 of the total flow enters the column
- Purge and split flows cannot be reduced beyond a certain limit without introducing contamination into column/detector:
 - Sample matrix accumulated in liner and lines
 - Septa particles
 - Air diffusing from septa
 - Seals outgassing

Instant Connect Helium Saver Module



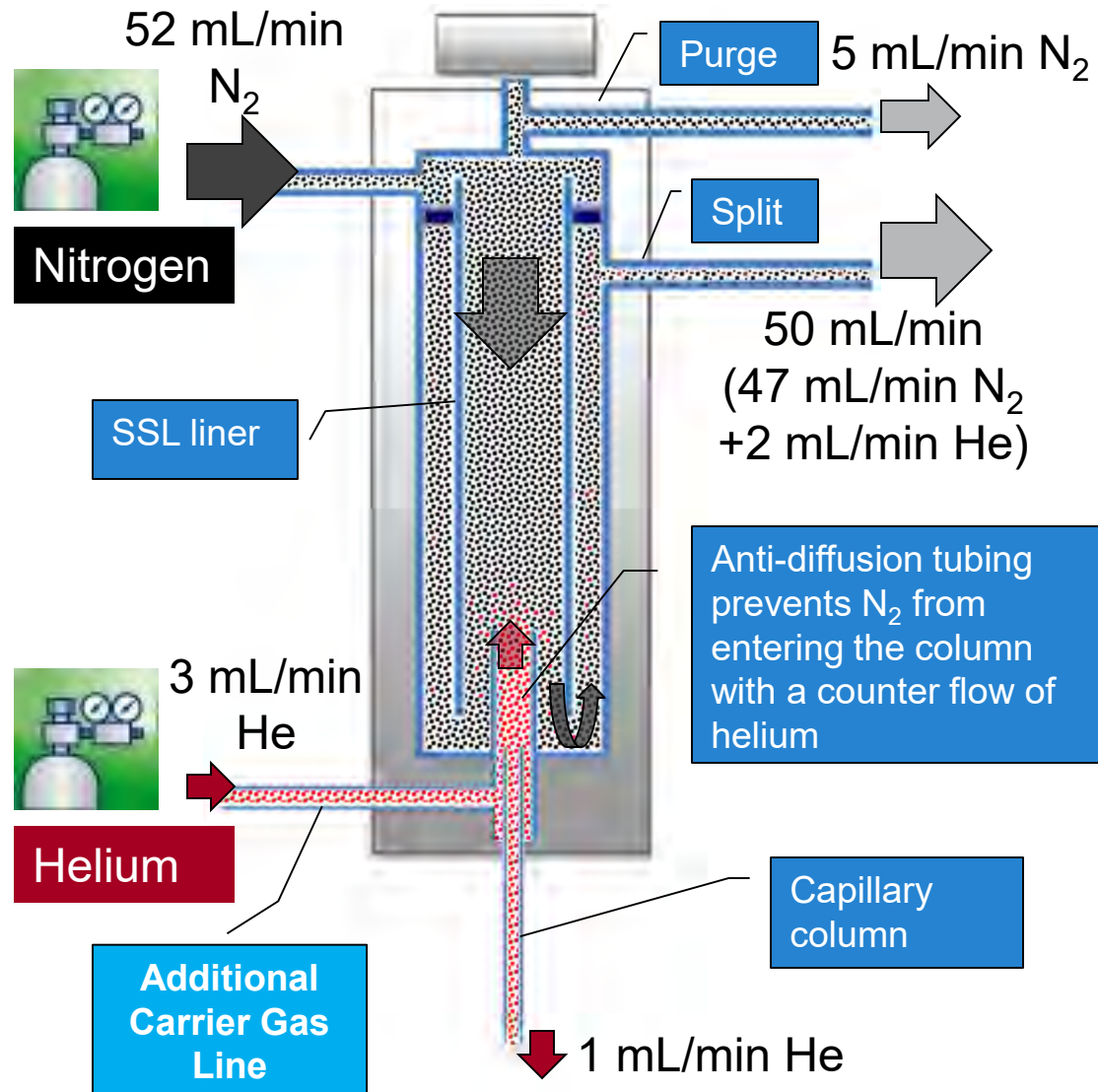
- Inlet supplied with 2 gases
- **Nitrogen** column head pressure settings regulates **Helium** flow
- The additional Helium line doesn't need active regulation and gas can be supplied using calibrated restrictor

How the Helium Saver Module Works: Injection



- During injection period, nitrogen flows into the column for sample introduction
- Helium is supplied at 0.1 mL/min to keep the connection swept and avoid dead volumes effects
- When GC is in stand-by, can be left in this condition with zero consumption of helium
- Separation uses helium

How the Helium Saver Module Works: Operation



- During all “non-injection” periods, Helium is supplied with a flow slightly higher than the column flow
- Helium consumption is only 1/15 – 1/20 of standard Split/Splitless injector



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The unstoppable and Off-axis Mass Spectrometer

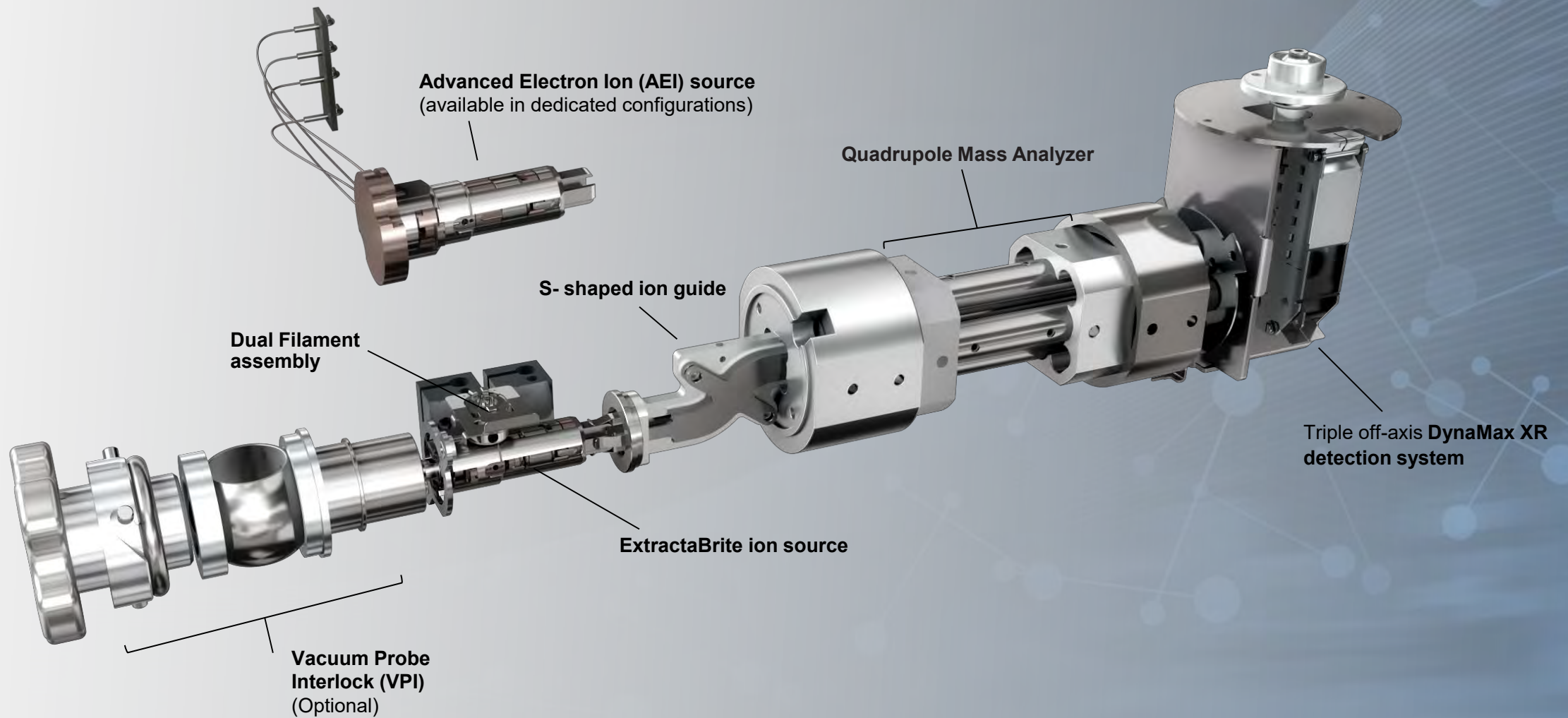
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Mass Spec Components Same for All Product Offerings

New ISQ 7000 Single Quadrupole GC-MS



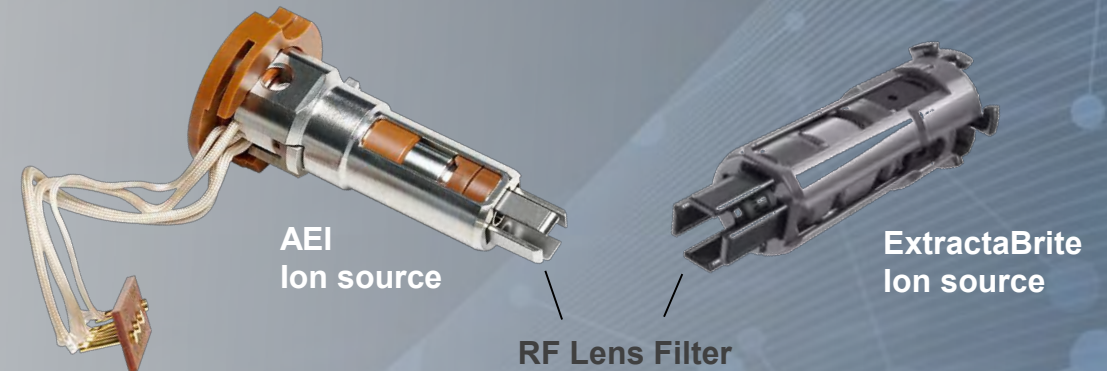
ISQ 7000 GCMS – Designed with Intention



Introducing Advanced Electron Ionization (AEI)

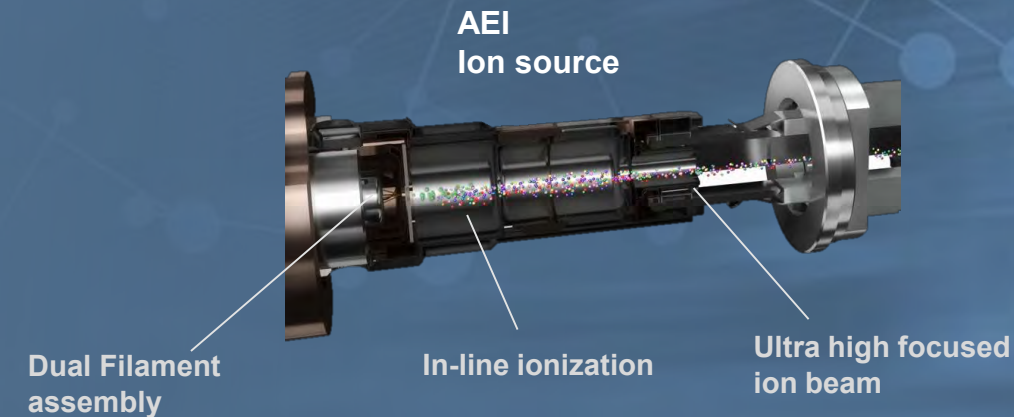
Inheriting from the ExtractaBrite™ ion source

- Highly inert material
- Independent dual heater
- Proprietary RF lenses
- Dual filament design



Adding innovative design for superior sensitivity and robustness

- Highly efficient ionization
- Tightly focused ion beam



Extended uptime for enhanced laboratory efficiency

UNSTOPPABLE



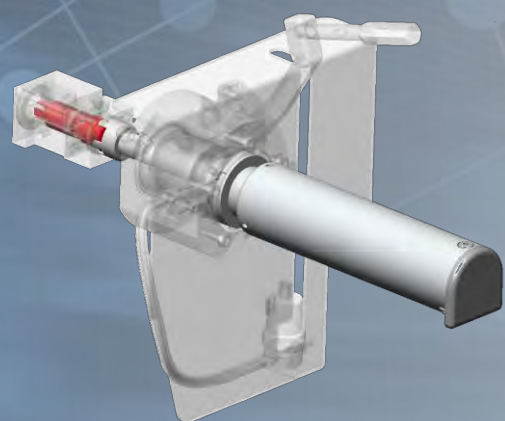
Unstoppable Uptime

What is NeverVent™

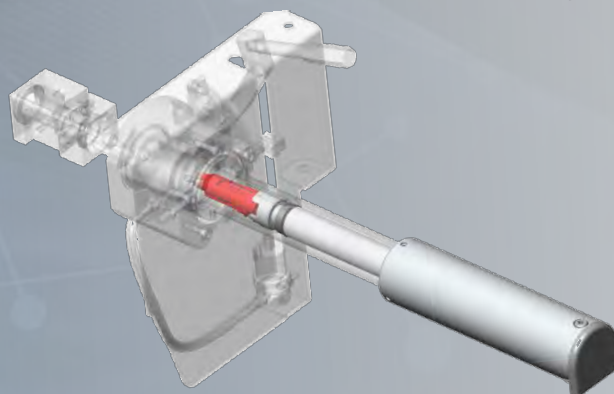


Extends the capability of the Vacuum Probe Interlock (VPI) design with the newly introduced source plug, **V-Lock**

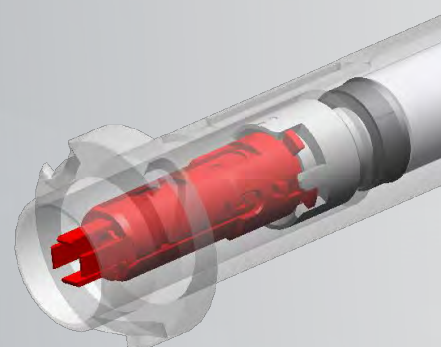
Through the VPI, no need to vent mass spec system for extracting the wireless ExtractaBrite ion source



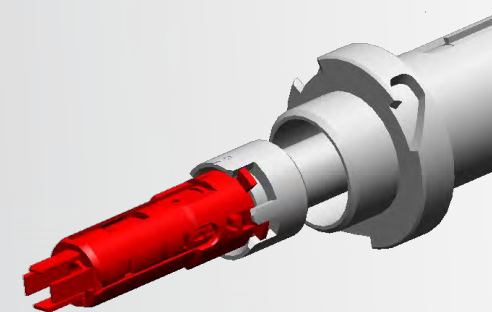
Step 1. Insert removal tool



Step 2. Remove source



Step 3. Hot source is held in tool



Step 4. Push source out of tool

Unstoppable Uptime

What is NeverVent™



Extends the capability of the Vacuum Probe Interlock (VPI) design with the newly introduced source plug, **V-Lock**

Through the VPI and the V-Lock source plug, no need to vent mass spec system to change the analytical column

Through the VPI and the V-Lock source plug, no need to vent mass spec system to make injector maintenance

V-Lock

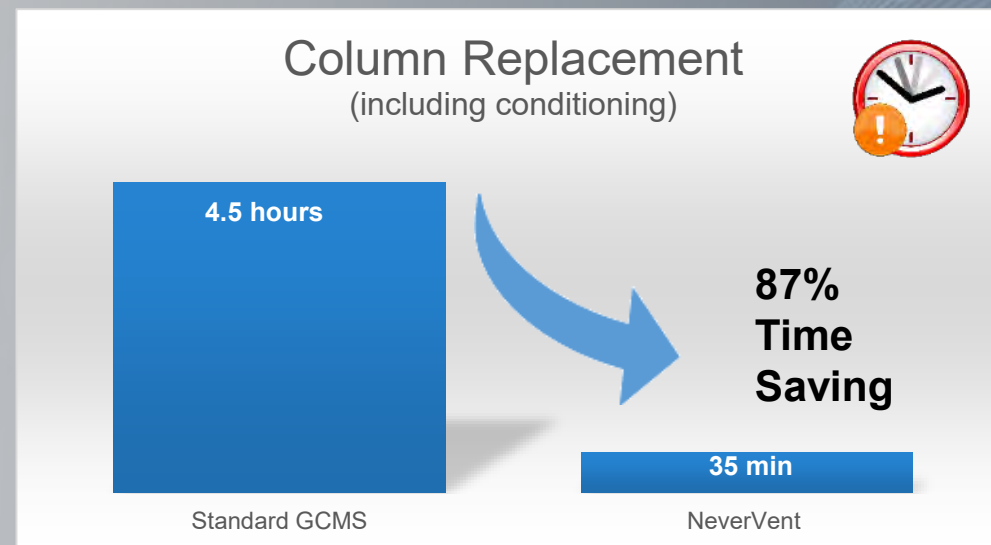
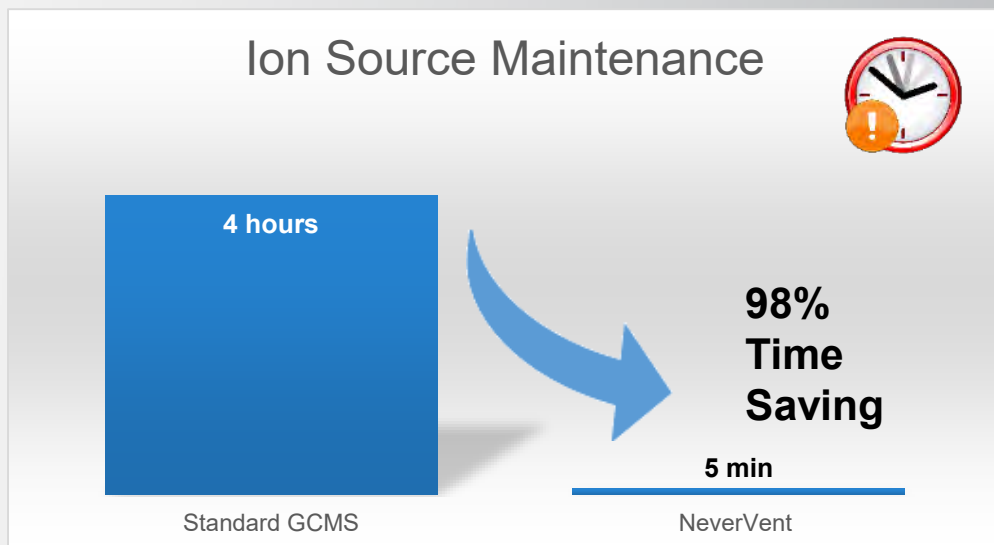
Isolate the MS under vacuum from the GC

No complicated fluidics or extra connections



Unstoppable Uptime

Time saving by using the NeverVent technology



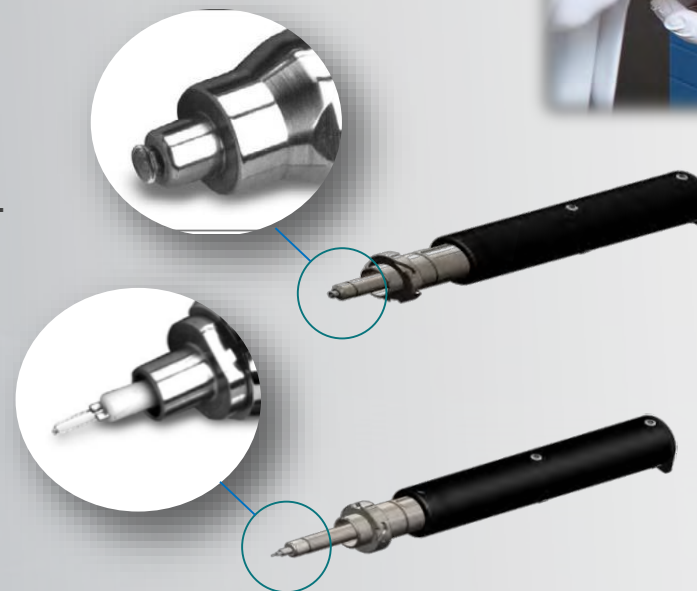
- **NeverVent reduces downtime and maximize sample analysis**
- **Increases the lab efficiency by saving the time otherwise wasted in recovering MS operation**
- **Your time can be spent on producing quality results**

Direct Sample Probe - ideal for materials difficult to elute chromatographically

- Designed to eliminate sample preparation time
- Compatible with all modes of ionization and mass analysis
- Simplified use through the Vacuum Probe Interlock (VPI)

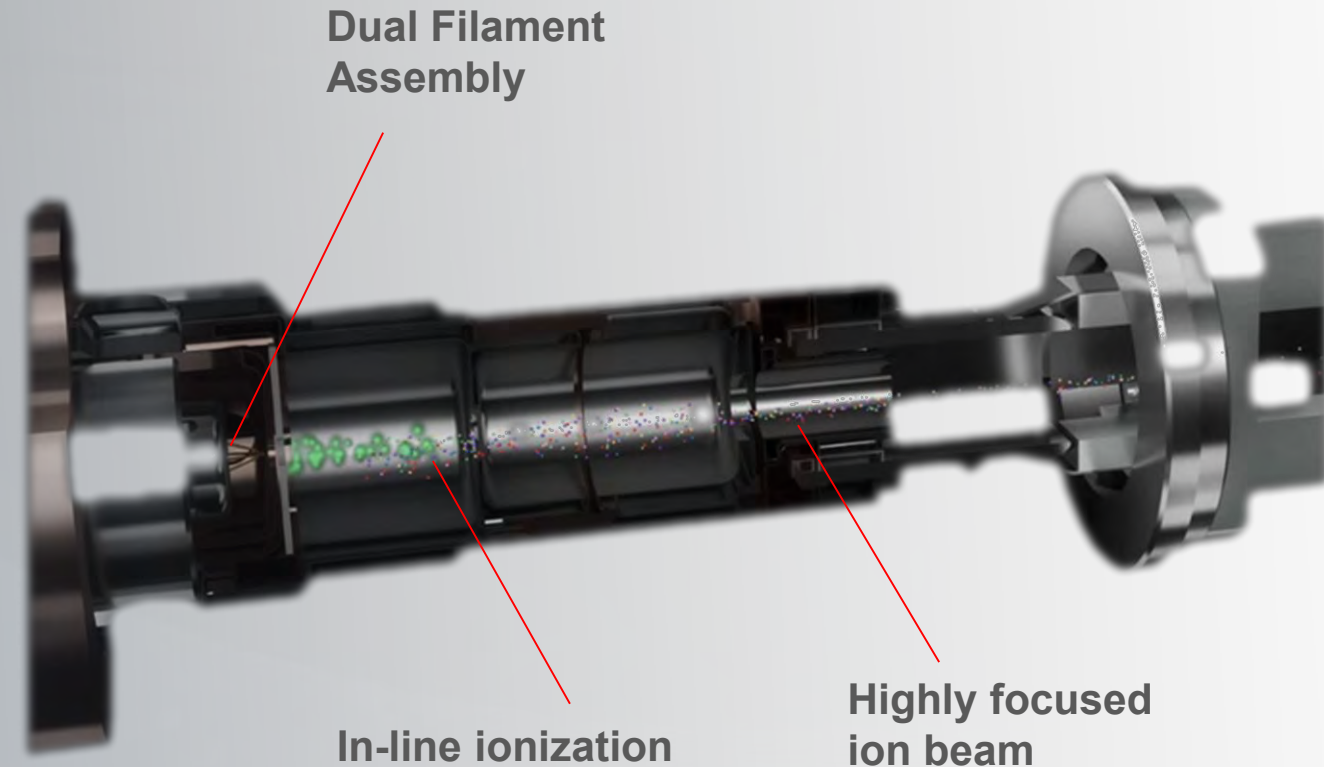
- **Direct Insertion Probe (DIP)** – ideal for solid samples or trace components in solid matrices such as forensic samples, tissue, etc.

- **Direct Exposure Probe (DEP)** – ideal for liquids or solids dissolved in a suitable solvent.



Advance Electron Ionization (AEI) source – extended robustness

- Highly focused ion beam makes this ion source extremely robust
- Maintenance frequency is significantly reduced even with difficult matrices
- Utmost sensitivity is now achieved with extended robustness, ideal for challenging samples



Thermo Scientific™ Chromeleon™ CDS

- Control your entire chromatography lab. It is fully scalable from a single workstation to an enterprise-wide installation
- Control of more than 350 modules from Thermo Fisher Scientific™ and many other vendors
- Quantitative mass spectrometry workflows for all separation techniques and MS variants, all using the same intuitive user interface.
- Boost laboratory efficiency with operational simplicity and intelligent functionality



Thermo Scientific™ TRACE™ 1300 Series GC is part of our family of GC-MS solutions



Thermo Scientific™
TRACE™ 1300
Series GC

Thermo Scientific™
ISQ™ Series MS

Thermo Scientific™
TSQ™ Series MS

Thermo Scientific™
Exactive™
GC-HRMS

Thermo Scientific™
Q Exactive™
GC-HRMS

Thermo Scientific™
DFS™
HRMS

Instant Connect
Modular GC

Single Quadrupole MS

Triple Quadrupole MS

Hybrid Quadrupole-Orbitrap
HRMS

Hybrid Quadrupole-Orbitrap
HRMS

Magnetic Sector HRMS

Detection with Multiple
Detectors

Confirmation by Mass
Spectrum or SIM

High speed and high
capacity MS/MS and
SRM

High Resolution and Accurate
Mass
Full Scan MS

High Resolution and Accurate
Mass
Full Scan & MS/MS

High-Resolution Full Scan and
SIM

The best solutions at every level of specificity



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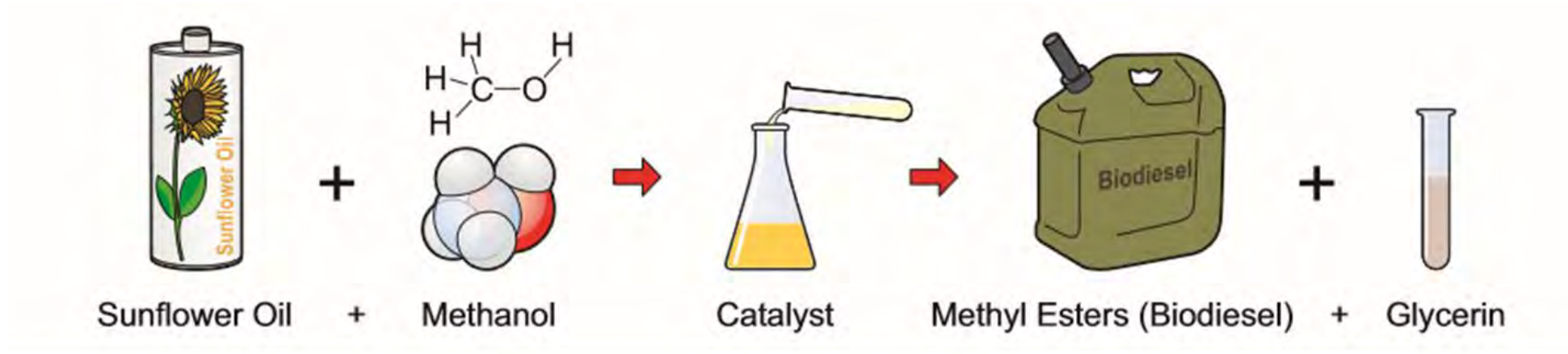
Application on GCMSMS

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GC and GCMS application support.



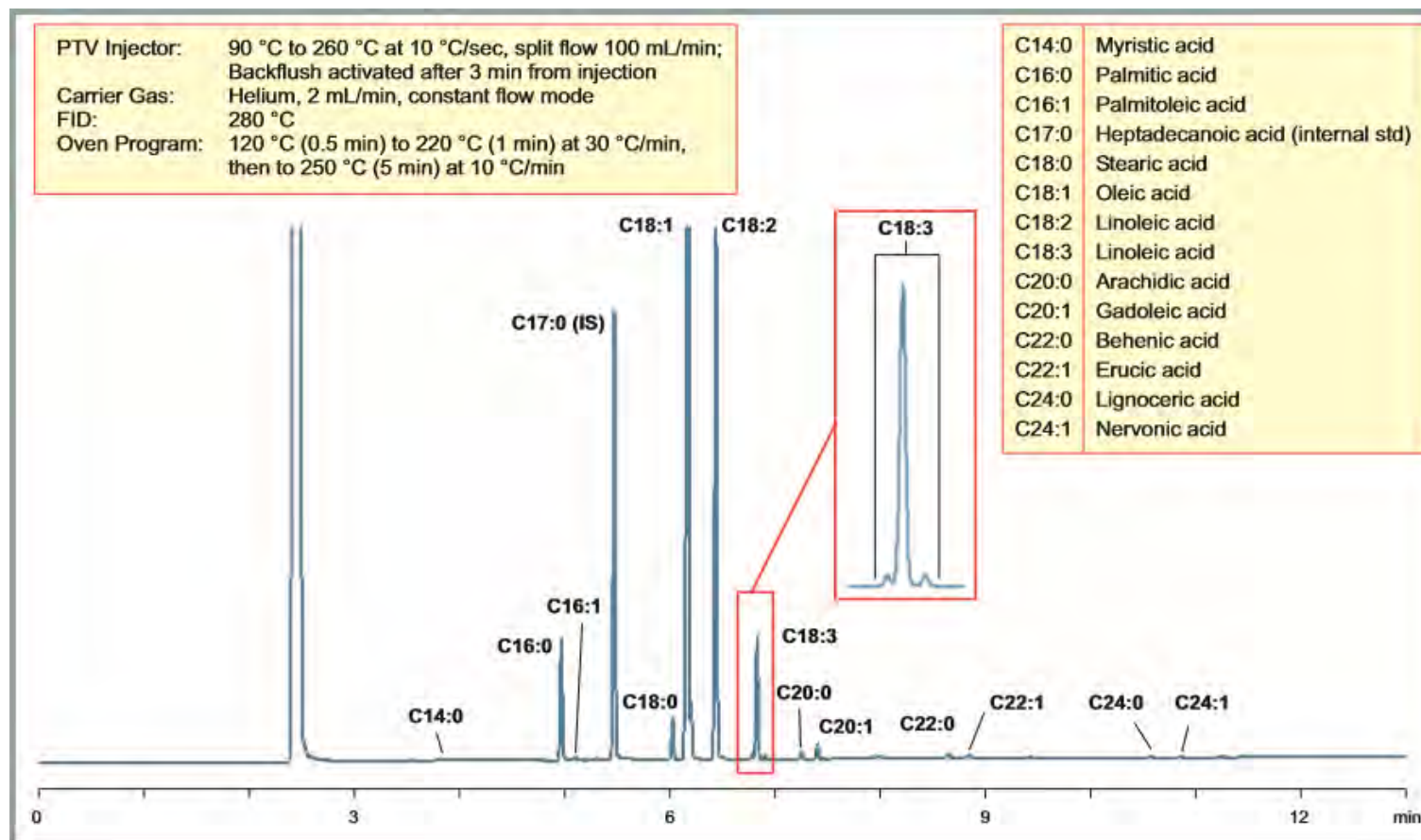
Application : Biodiesel



- Total FAME and Linolenic Acid Methyl Ester : EN 14103
 - Free and Total glycerin : ASTM D6584 / EN 14150
 - Methanol Content : EN 14110

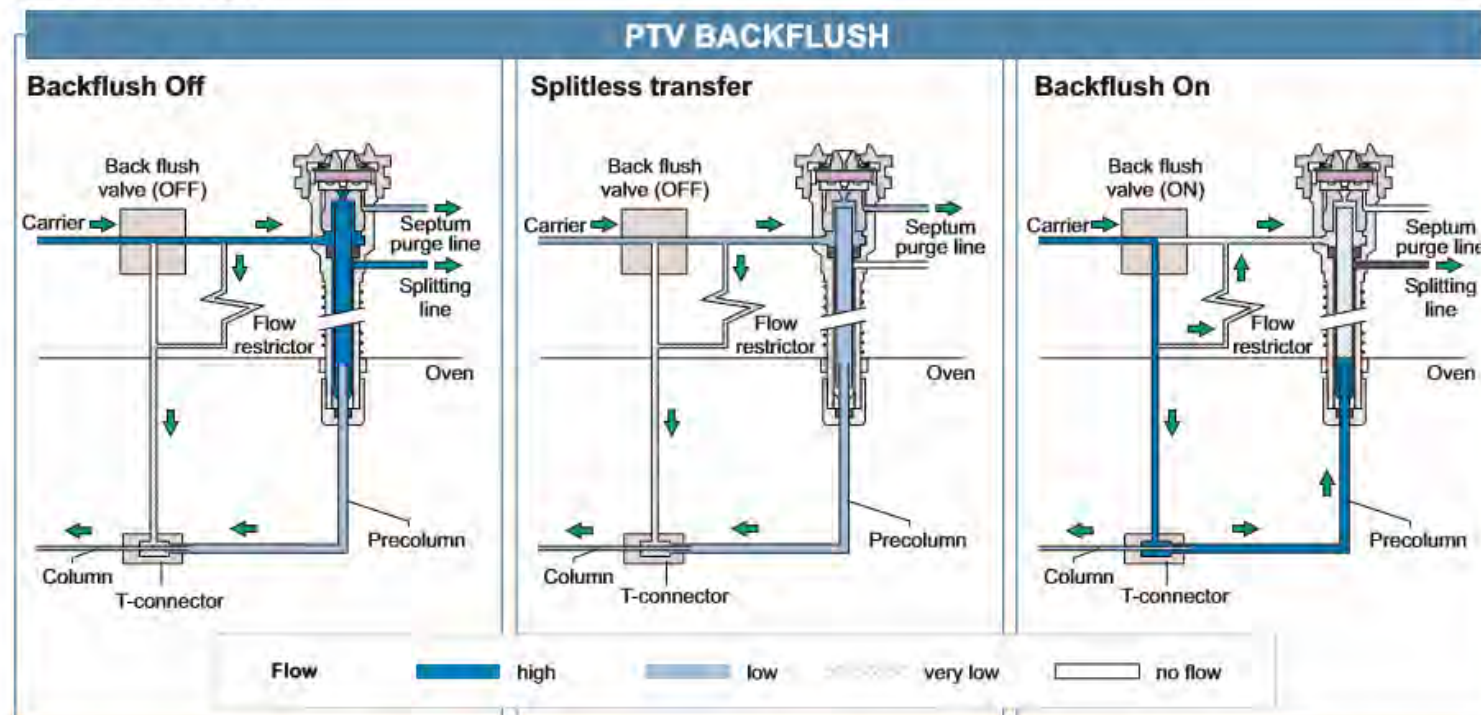
Total FAME and Linolenic Acid Methyl Ester : EN 14103

The cetane number of biodiesel depends on the distribution of fatty acids in the original oil. Thus a reliable characterization of FAME is essential for a more accurate calculation of the cetane index. EN 14103 is a standard method for determination of esters and linolenic acid methyl ester and can be applied to biodiesel analysis. EN 14103 requires GC analysis.



By incorporating the backflush option into the PTV injector, heavy compounds can be vented out of the inlet system, effectively preventing column contamination while still allowing efficient transfer of compounds of interest.

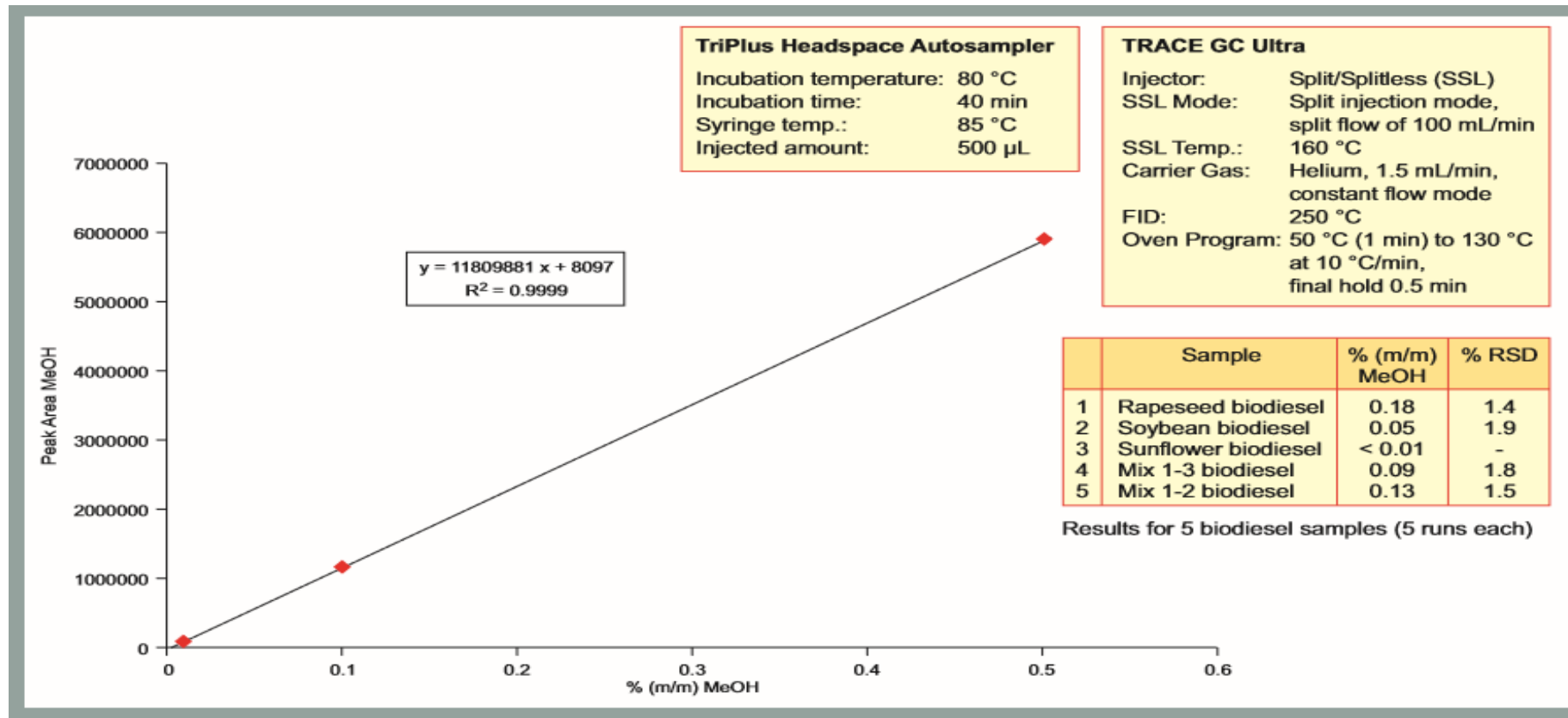
PTV Backflush



PTV Backflush (reverse flow device): the glycerides fraction is vented out without entering the column.

Methanol Content : EN 14110

Methanol in B100 is a matter of safety since even small amounts of this material can reduce the flash point of the biodiesel. Moreover, residual methanol can affect fuel pumps, seals and elastomers and can result in poor combustion properties. EN 14110 requires a headspace GC method, based on either polar or non-polar columns, and is applicable for a concentration range from 0.01% m/m to 0.5% m/m of methanol (MeOH).





Sample Preparation

Dried leaves , fruits or seeds
and other herbal products

Weight 10 g of sample.

Mixed with DE and load
into the extraction cells.

Concentrated Sample and
injection with GC



ASE™ 350

Sample weight	10 g
Extraction solvent	Ethylacetate/cyclo-Hexane 1:1, same as GPC solvent
Temperature	120 °C
Pressure	100 bar
Extraction time	5 min, 1 cycle
Flushing with solvent	60% of cell volume
Flushing with nitrogen	100 s



GC : Condition

Injector PTV	Splitless mode
Base temperature	50 °C
Transfer	10 °C/s to 250 °C, until end of run
Flow	Constant flow, 1.2 mL/min, helium
Analytical column	40 m, ID 0.18 mm, 0.18 µm film, 5%-phenyl phase (5MS type)
Pre-column	5 m, ID 0.18 mm, empty deactivated, no backflush
Column oven	Temperature programmed
Start	70 °C, for 1.50 min
Ramp 1	15 °C/min to 190 °C
Ramp 2	7 °C/min to 290 °C, 12 min
Transfer line	250 °C

MS/MS : Condition

Ion source temperature	220 °C
MRM Detection	Timed SRM mode (see Appendix)

SRM : More than 80 compound

Pesticide Name	RT (min)	Precursor Mass (m/z)	Product Mass (m/z)	Collision Energy (V)
Difluorobenzamid Degradation (isocyanat)	6.93	152.93	90.01	20
Difluorobenzamid Degradation (isocyanat)	6.93	152.93	125.01	20
Carbofuran 1	8.80	149.06	121.05	10
Carbofuran 1	8.80	164.08	149.07	10
Difluorobenzamid Degradation	8.62	141.00	63.11	25
Difluorobenzamid Degradation	8.62	141.00	113.09	15
Biphenyl-d10_ISTD	9.24	160.00	160.16	10
Biphenyl	9.28	154.08	153.08	15
Biphenyl	9.28	153.08	152.08	15
Carbofuran-3-hydroxy 1	10.43	137.05	81.01	18
Carbofuran-3-hydroxy 1	10.43	180.05	137.01	15
Tetrahydrophthalimid	10.84	151.04	79.01	25
Tetrahydrophthalimid	10.84	151.04	122.09	10
O-Phenylphenol	11.00	170.07	141.06	20
O-Phenylphenol	11.00	170.07	115.05	20
Molinate	11.10	187.10	126.07	10
Molinate	11.10	126.07	98.05	5
Chlorfenprop methyl	11.59	196.00	165.00	10
Chlorfenprop methyl	11.59	165.00	137.00	10
Fenobucarb	11.20	121.07	77.05	15
Fenobucarb	11.20	150.09	121.07	10

Propachlor	11.76	176.06	120.04	10
Propachlor	11.76	120.04	92.03	10
Propachlor	11.76	169.06	120.04	10
Propachlor	11.76	196.07	120.04	10
Cyloate	11.98	154.10	83.05	10
Cyloate	11.98	215.13	154.10	5
Diphenylamin	11.49	169.01	168.09	20
Diphenylamin	11.49	169.01	167.09	20
Chloroprotham	12.26	213.06	127.03	15
Chloroprotham	12.26	213.06	171.04	10
Phosmet-oxon	12.09	160.00	132.96	15
Phosmet-oxon	12.09	104.00	75.88	10
Phosmet-oxon	12.09	160.00	76.96	20
Prometon	13.10	225.16	183.13	10
Prometon	13.10	225.16	210.15	10
Carbofuran 2	13.13	149.06	121.05	10
Carbofuran 2	13.13	164.08	149.07	10
Profthuralin	13.22	318.10	198.06	15
Profthuralin	13.22	330.23	252.45	25
Sweep	13.46	187.05	123.95	15
Sweep	13.46	219.11	174.02	18
Trietazine	13.48	229.14	200.14	15
Trietazine	13.48	214.14	186.10	15
Dimethipin	13.53	117.98	57.97	10

Pesticide Name	RT (min)	Precursor Mass (m/z)	Product Mass (m/z)	Collision Energy (V)
Dimethipin	13.53	210.10	76.02	10
Terbutylazin	12.97	214.10	132.06	10
Terbutylazin	12.97	214.10	104.05	10
Propyzamid	13.04	173.01	145.01	15
Propyzamid	13.04	173.01	109.01	18
Propyzamid	13.04	175.02	147.01	15
Propyzamid	13.04	254.02	226.02	15
Isocarbamide	13.67	142.03	70.01	15
Isocarbamide	13.67	142.03	113.01	10
Dinoseb	13.92	211.13	116.99	15
Dinoseb	13.92	211.13	163.11	10
Terbazil	13.42	160.05	76.02	15
Bromocylen	14.37	358.79	242.85	15
Bromocylen	14.37	356.93	241.24	15
Dimethenamid	14.60	230.06	154.04	10
Dimethenamid	14.60	232.06	154.04	10
Dimethachlor	14.61	197.08	148.06	10
Dimethachlor	14.61	199.08	148.06	10
Acetochlor	14.65	174.11	146.15	15
Acetochlor	14.65	223.19	147.17	10
Desmetryn	14.68	213.11	171.08	10
Desmetryn	14.68	213.11	198.10	10
Flurprimidol	14.77	269.12	106.98	20

Alachlor	14.26	188.10	160.07	10
Alachlor	14.26	188.10	130.12	25
Alachlor	14.26	237.14	160.15	10
Metribuzin	14.14	198.08	82.03	20
Metribuzin	14.14	198.08	89.04	16
Propanil	15.00	217.01	161.00	10
Propanil	15.00	219.01	163.00	10
Fipronildesulfanyl	14.15	333.00	231.20	20
Fipronildesulfanyl	14.15	333.00	281.30	20
Carbofuran-3-hydroxy 2	15.02	137.05	81.01	18
Carbofuran-3-hydroxy 2	15.02	180.05	137.01	15
Prometryn	14.49	241.14	184.10	15
Prometryn	14.49	226.13	184.10	12
Tridiphan	15.18	186.94	158.94	15
Tridiphan	15.18	219.09	184.09	20
Ethofumesat	14.80	206.82	160.86	10
Ethofumesat	14.80	285.75	206.82	12
Pentachlor	15.73	141.05	106.05	15
Pentachlor	15.73	239.05	141.05	15
Chlorpyrifos	15.78	257.97	165.98	20
Chlorpyrifos	15.78	314.05	258.18	15
Bromacil	15.03	205.01	188.01	15
Bromacil	15.03	207.01	180.01	15

Pesticide Name	RT (min)	Precursor Mass (m/z)	Product Mass (m/z)	Collision Energy (V)
Anthrachinon	15.44	207.97	151.99	20
Anthrachinon	15.44	180.04	152.05	15
Anthrachinon	15.44	207.97	180.10	10
Nithrothal isopropyl	16.09	236.08	194.07	10
Nithrothal isopropyl	16.09	236.08	148.05	20
Triadimefon	15.41	208.07	181.06	10
Triadimefon	15.41	210.07	183.06	10
Tiocarbazil	16.15	156.08	100.05	8
Tiocarbazil	16.15	279.10	156.07	6
Tetraconazol	15.39	336.02	218.01	20
Tetraconazol	15.39	338.02	220.01	20
Butralin	15.54	266.14	220.11	15
Butralin	15.54	266.14	190.10	15
Dicaphon	15.44	262.00	262.00	9
Dicaphon	15.44	262.00	216.00	13
Crufomat	16.30	256.20	226.15	25
Crufomat	16.30	276.20	182.09	10
Allethrin	16.17	123.07	80.98	10
Allethrin	16.17	136.04	92.98	10
Dinobuton	16.89	163.06	116.04	15
Dinobuton	16.89	211.07	117.04	18
Penconazol	16.89	248.06	157.04	25
Penconazol	16.89	248.06	192.04	15
Pyrifinox 1	16.17	262.03	192.02	20
Pyrifinox 1	16.17	262.03	200.02	20
Pyrifinox 2	16.81	262.03	192.02	20
Pyrifinox 2	16.81	262.03	200.02	20

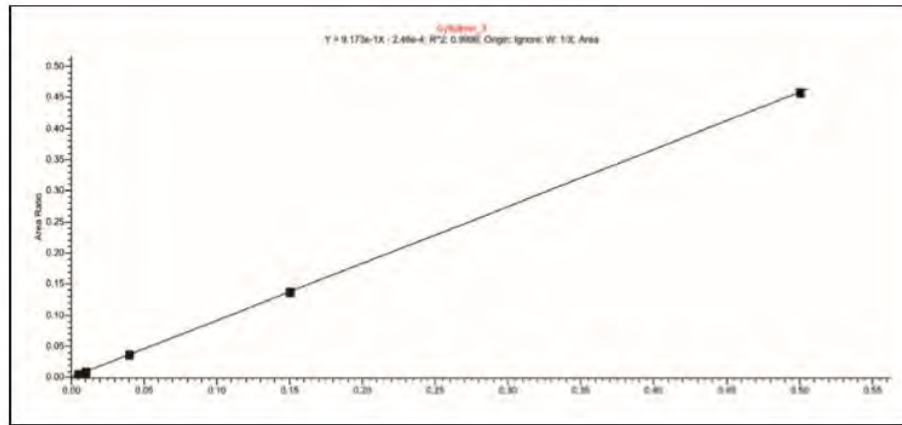
Famphos (Famphur)	20.16	218.07	108.94	15
Famphos (Famphur)	20.16	218.07	126.95	20
Iprodion Degradation	18.63	186.87	123.99	20
Iprodion Degradation	18.63	186.87	159.02	15
Iprodion Degradation	18.63	243.94	187.02	10
Iprodion	20.57	314.06	245.25	15
Iprodion	20.57	186.99	123.87	20
Iprodion	20.57	316.00	247.35	15
Iprodion	20.57	316.00	273.11	10
Propiconazol 1	19.38	259.02	173.02	20
Propiconazol 1	19.38	172.94	144.91	15
Propiconazol 2	19.54	259.02	173.02	20
Propiconazol 2	19.54	172.94	144.91	15
Pyraflufen-ethyl	20.30	412.02	349.02	15
Pyraflufen-ethyl	20.30	349.02	307.02	15
Clodinafop-propargyl	20.36	349.05	266.04	15
Clodinafop-propargyl	20.36	349.05	238.04	15
Lenacil	20.70	153.05	136.06	15

Pesticide Name	RT (min)	Precursor Mass (m/z)	Product Mass (m/z)	Collision Energy (V)
Paclotrazole	17.75	238.11	127.06	15
Chinomethionat	17.78	206.06	147.98	15
Chinomethionat	17.78	234.08	206.06	10
Napropamid	18.07	271.16	128.07	5
Napropamid	18.07	128.07	72.04	10
Flutrialol	18.11	219.07	123.04	15
Flutrialol	18.11	123.04	75.03	15
Flurodifen	18.14	190.02	126.01	10
Flurodifen	18.14	190.02	146.01	5
Bisphenol A	18.17	213.14	119.06	15
Bisphenol A	18.17	213.14	164.99	20
Bisphenol A	18.17	228.15	213.07	10
Chlorfensol_ISTD	18.20	302.00	110.90	20
Hexaconazol	18.22	214.08	159.07	20
Hexaconazol	18.22	214.08	151.98	25
Imazalil	18.24	172.96	144.96	15
Imazalil	18.24	172.96	108.95	25
Isoprothiolan	18.24	203.99	117.95	7
Isoprothiolan	18.24	203.99	84.90	25
Isoprothiolan	18.24	290.06	118.03	15
Flamprop-methyl	18.39	230.05	170.04	10
Flamprop-methyl	18.39	276.06	105.02	10
Kresoximmethyl	18.48	206.10	131.09	15
Kresoximmethyl	18.48	206.10	116.01	10
Buprofezin	18.51	175.08	116.96	20
Buprofezin	18.51	175.08	131.99	15
Buprofezin	18.51	249.16	105.93	20

Pesticide Name	RT (min)	Precursor Mass (m/z)	Product Mass (m/z)	Collision Energy (V)
Azinphosmethyl	22.95	160.00	132.00	10
Azinphosmethyl	22.95	160.00	104.64	10
Pyriproxifen	23.06	136.00	77.92	20
Fenamirol	23.55	251.02	139.01	15
Fenamirol	23.55	330.03	139.01	10
Pyridaben	24.50	364.14	309.12	5
Pyridaben	24.50	309.12	147.06	15
Fluquinconazol	24.59	340.01	298.01	22
Fluquinconazol	24.59	342.01	300.01	22
Etofenprox	26.05	163.09	107.06	16
Etofenprox	26.05	163.09	135.07	10
Etofenprox	26.05	376.14	135.02	30
Etofenprox	26.05	376.14	163.09	10
Silaflofen	26.25	179.00	151.00	7
Silaflofen	26.25	286.13	258.12	15
Difenconazol 1	26.91	323.05	265.04	15
Difenconazol 1	26.91	325.05	267.04	20
Difenconazol 2	27.05	323.05	265.04	15
Difenconazol 2	27.05	325.05	267.04	20
Indoxacarb	28.55	264.02	176.14	10
Indoxacarb	28.55	264.02	148.03	20
Indoxacarb	28.55	321.05	289.34	10

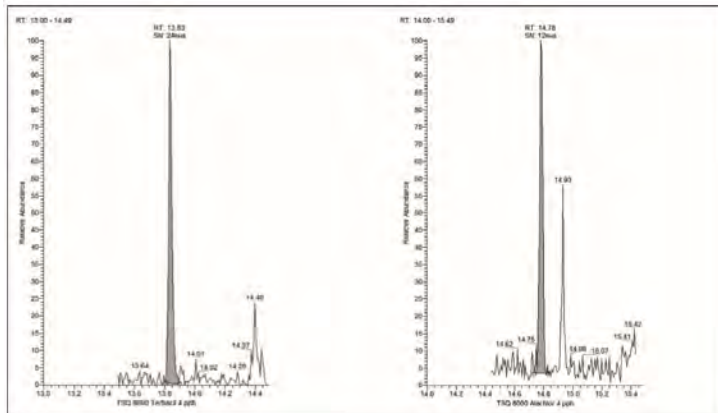
Calibration and Detection limit.

Calibration level : 0.004 µg/mL to 1.0 µg/mL (This range represents an analyte concentration of 0.01 to 2.5 mg/kg in the samples)

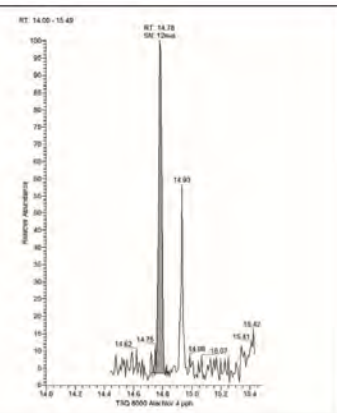


Pesticide	RT [min]	S/N @ 4 ppb
Terbacil	13:83	24
Alachlor	14:78	12
Tolyfluanid	16:75	44
Pyridaben	24:17	83

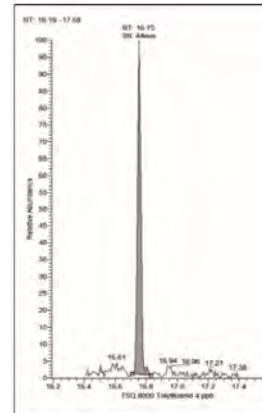
Sensitivity (LOD)



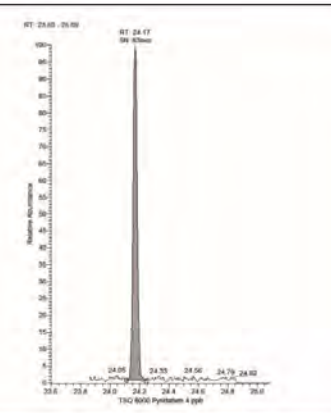
Terbacil



Alachlor



Tolyfluanid



Pyridaben

Sample Matrix	Pesticide Residues Found	Concentration (mg/kg)
Dried Herbs	o-Phenylphenol	0.017
Dried Herbs	Tebuconazol	0.023
Dried Fruit	Diflubenzuron	0.049
Dried Fruit	Myclobutanil	0.023
Dried Fruit	Propargit	0.479
Dried Fruit	Tebuconazol	0.081
Dried Fruit	Difenconazol	0.013
Dried Herbs	Picoxystrobin	0.228
Dried Herbs	Picoxystrobin	0.233
Dried Herbs	o-Phenylphenol	0.011
Herbal Tea	o-Phenylphenol	0.014
Herbal Tea	o-Phenylphenol	0.011
Herbal Tea	Terbutylazin	0.016



Multi-Residue Pesticide Analysis in Herbal Products Using Accelerated Solvent Extraction with a Triple Quadrupole GC-MS/MS System

Uwe-Jochen Hadermann, Jürgen Gammertopf, Thimo Felix Eckardt, Tobias Gerny, Marc Hübner, Jürgen Richter, Hans-Ulrich Pöhlke, Christa Köck, Volkmar Gessler, Germany

Key Words: Pesticides, tea, herbal products, ASE, SBE, MRM, Multi-residue analysis, TQD, MS/MS, MS/MS.

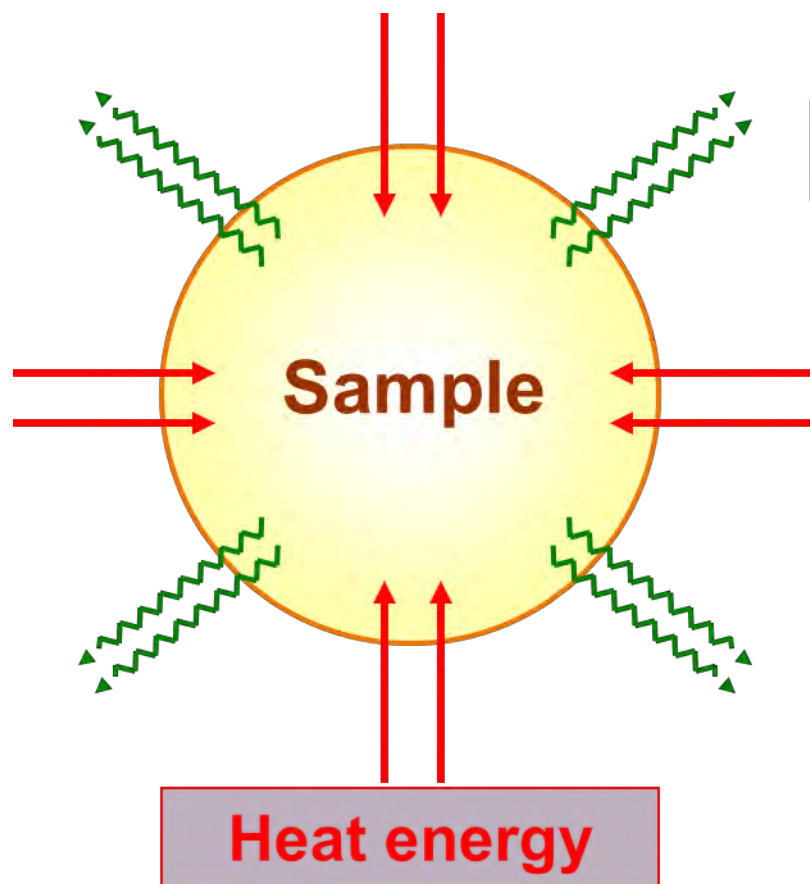
Introduction: The residue analysis of pesticides has developed in recent years into a comprehensive methodology for the detection of many hundreds of potential contaminating compounds. A multi-residue method for herbal products and teas is faced with additional challenges from the worldwide origin of the products and the complex matrix of the dried materials. In the strict quality control of raw materials, the unknown or undeclared local plant protection treatments must be taken into account with a wide variety of potential pesticide contaminations. Dried leaves, fruits or seeds and other herbal products of medicinal use deliver highly complex extracts from the sample preparation due to the rich content of active ingredients, essential oils and the typical high boiling natural polymer compounds from broken cells, leaves or fruit skins. A thorough clean up of the extracted sample can lead to losses of critical analytes of interest. A complete characterization of pesticide and other residue contamination is done by both LC and GC-MS/MS to cover the complete range of functional groups. This application report describes the methodology used for the multi-residue pesticide analysis of herbal products using accelerated solvent extraction (ASE) and gas chromatography (GC) sample preparation with detection and quantitation by the Thermo Scientific TSQ 8000 GC-MS/MS system.

A routine screening method for more than 200 pesticide compounds was applied to a wide variety of different sample types, ranging from regular black tea or apple leaves, to soups like fennel and herbs of medical and fragrant use like thyme and chamomile. The clean-up and reporting was achieved by using the Thermo Scientific TraceFinder quantitation software suite. The sensitivity requirement for this analysis was determined by the regulatory background. The analysis of pesticide residues in tea and herbal products follows the regulations of the European Directorate General for Health and Consumer Affairs (SANCO) for "Method Validation and Quality Control Procedures for Pesticide Residue Analysis in Food and Feed" (1). The sensitivity requirements for these products as referenced in the Code Alimentaire (2) result in maximum residue levels of 0.01 mg/kg for most of the pesticide compounds.

Thermo SCIENTIFIC



Information from polymeric Materials by Heating

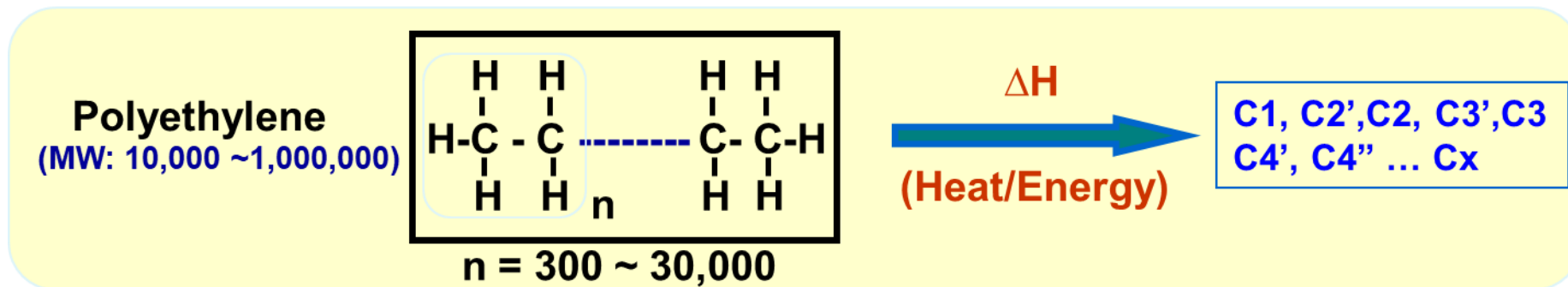
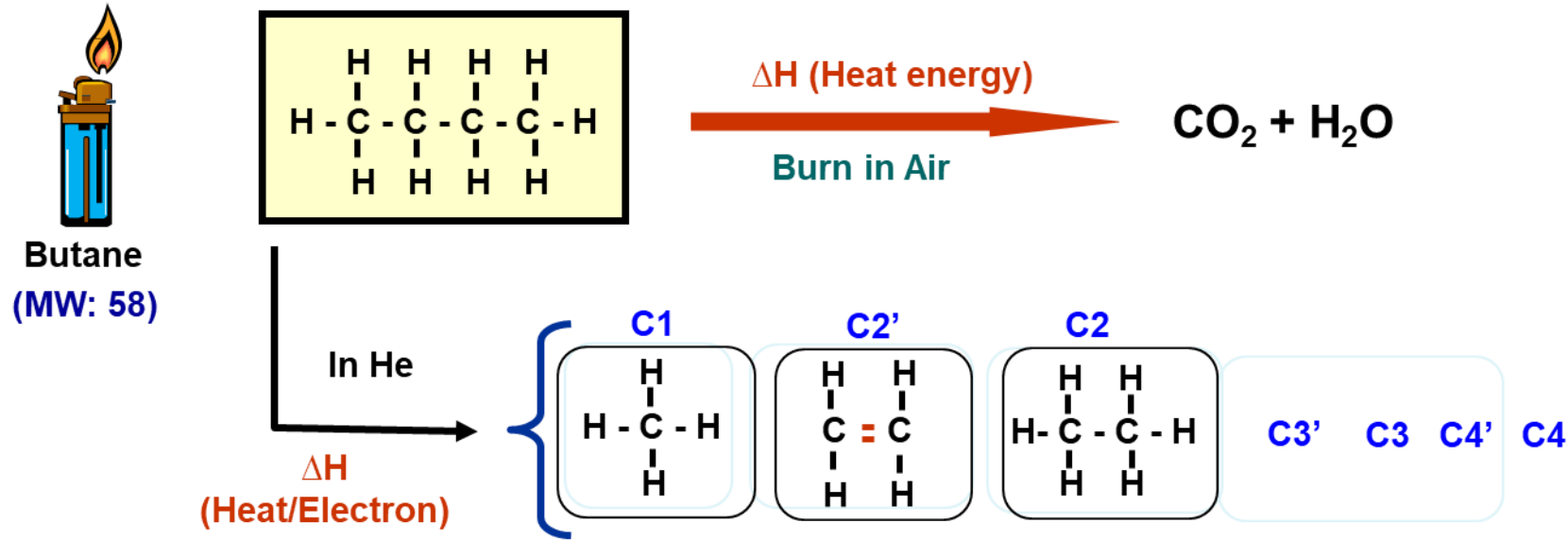


Information

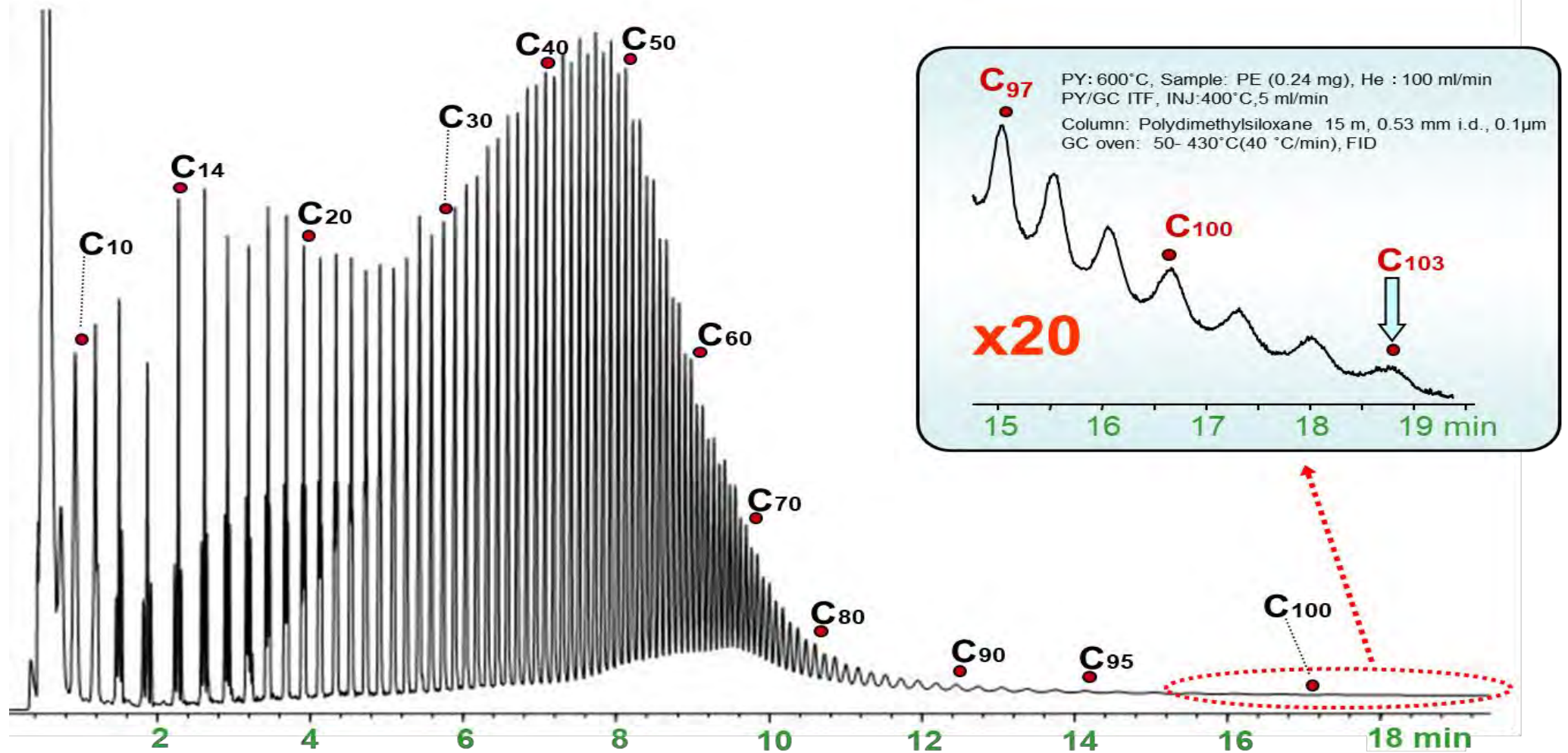
- Weight loss: **TGA**
- Enthalpy change: **DTA, DSC**
- Mechanical change: **TMA, Dilatometry**
- Evolved gas
 - volume: **EGA (volume of gas)**
 - qualification & quantification:

Py-GC/MS
TD-GC/MS
UV/Py-GC/MS
EGA/MS
Py/MS

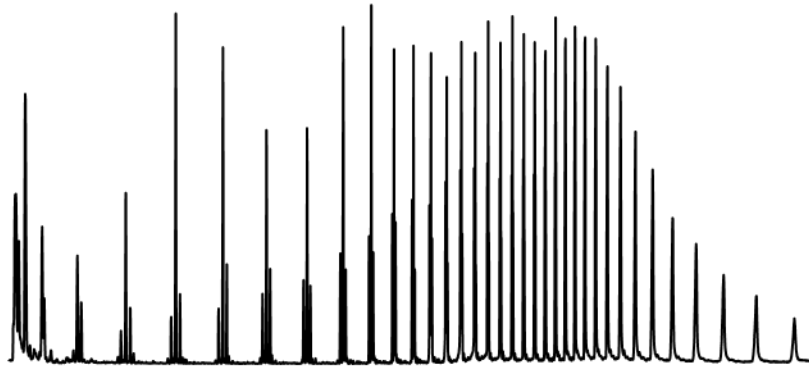
Pyrolysis of Polymeric materials and pyrolyzates



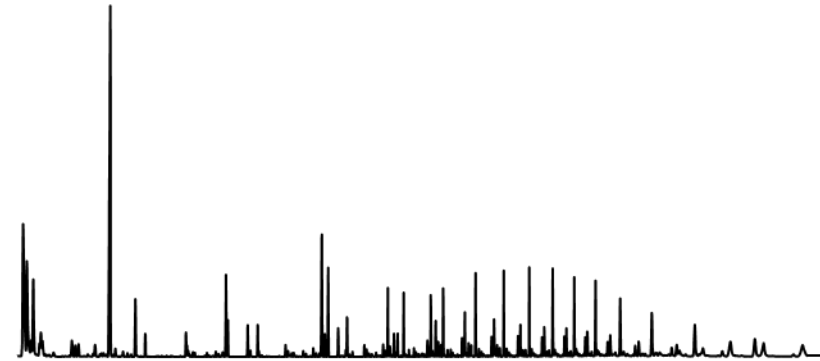
Typical pyrogram of polyethylene at 600°C



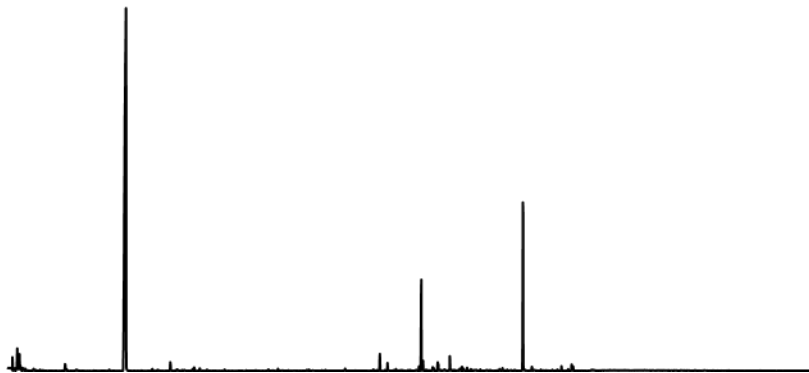
Polyethylene



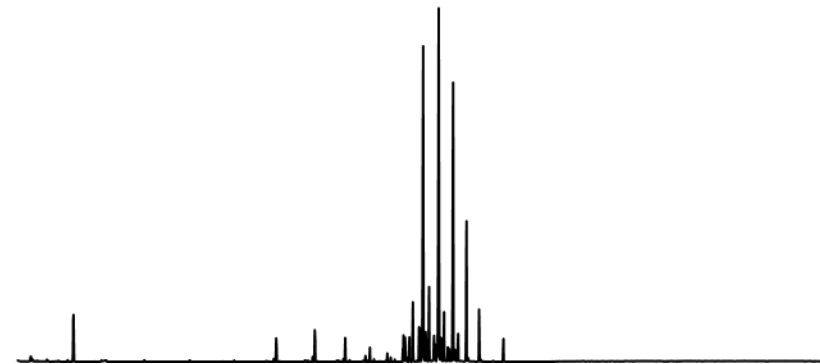
Polypropylene



Polystyrene



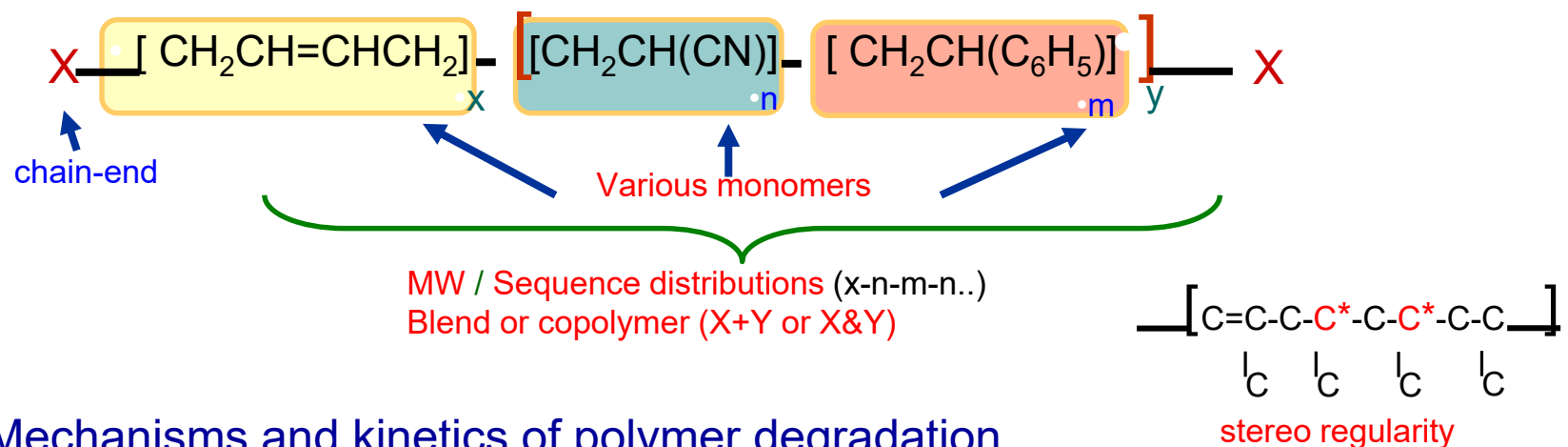
Higher methacrylate copolymer



A: Identification of polymeric materials

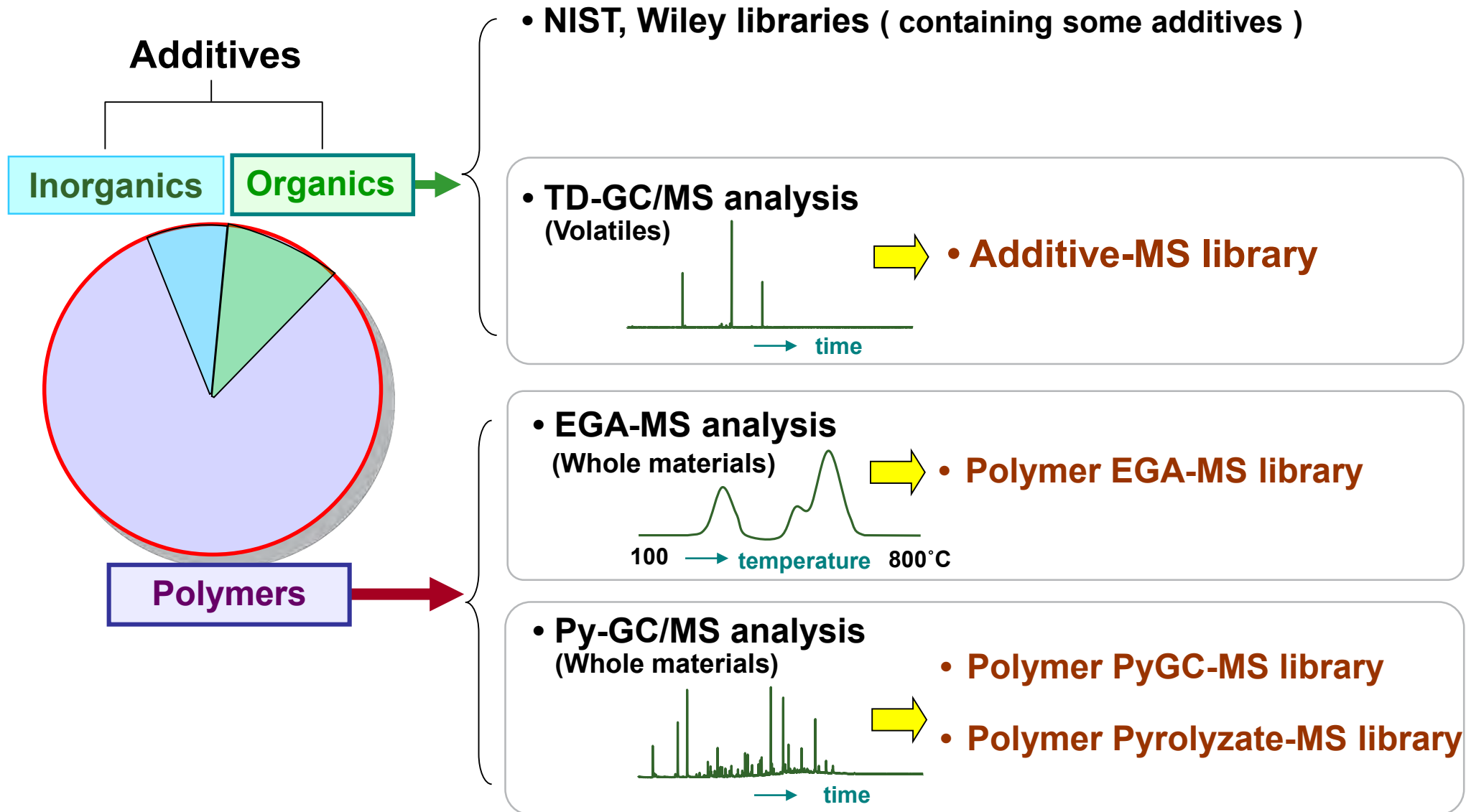
Unknown materials (PP/ PVC/ SBR?)

B: Structural characterization of polymers



C: Mechanisms and kinetics of polymer degradation

D: Qualitative and quantitative analysis of additives



Classification of 700 polymers in the libraries

- 1) Vinyl polymers with ethylene unit
- 2) Polyolefines
- 3) Vinyl polymers with styrene unit
- 4) Vinyl polymers with styrene derivative unit
- 5) Acrylic polymers
- 6) Chlorine containing vinyl polymers
- 7) Fluorine containing vinyl polymers
- 8) Polyvinyl alcohols and its ester polymers
- 9) Diene - elastomers

- 10) Polyamide
- 11) Polyacetals and polyethers
- 12) Thermosetting resines
- 13) Engineering plastics of polyimide and aramide type
- 14) Engineering plastics of polyester type
- 15) Other engineering plastics with phenylene backbone
- 16) Silicone polymers
- 17) Cellulose polymers
- 18) Polyurethanes
- 19) Others

Classification of 494 additives in the library

- 1) Antioxidant
- 2) Ultraviolet absorber,
Light stabilizer
- 3) Metal deactivator
- 4) Stabilizer
- 5) Lubricant
- 6) Plasticizer
- 7) Antistatic additive
- 8) Anti-clouding agents
- 9) Fire retardant
- 10) Blowing agent
- 11) Conductive agent
- 12) Nucleating agent

- 13) Optical characteristic
controlling agent
- 14) Antibacterial, Antifungal agent
- 15) Resin modifier
- 16) Vulcanization accelerator
- 17) Antidegradant

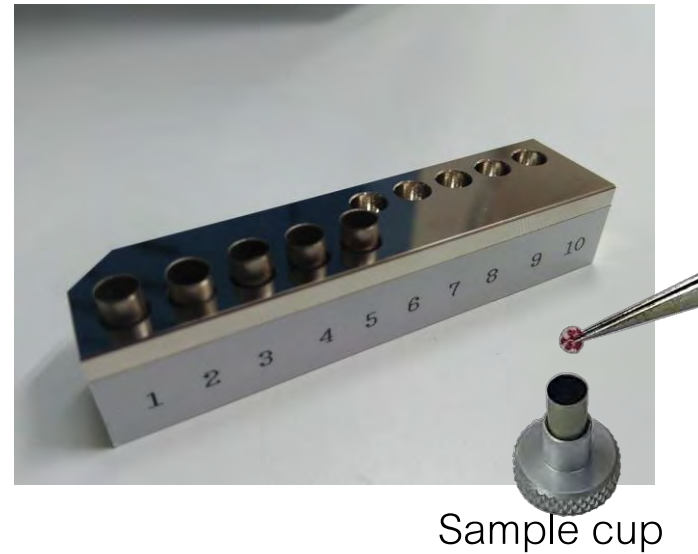
download the complete list from
[http://www.frontier-lab.com/english/
multi-functional-pyrolysis-system/](http://www.frontier-lab.com/english/multi-functional-pyrolysis-system/)

- 1) EGA-MS polymer library : 700 polymers stored
- 2) PyGC-MS polymer library : 700 polymers stored
- 3) Pyrolyzate-MS library : 165 polymers stored
- 4) ADD-MS library : 494 additives stored (136 newly added)
-  Catalog
-  Polymer list
-  Additive list
-  FAQ
- Download Trial Version

ตัวอย่างการวิเคราะห์ด้วย PY-GCMS

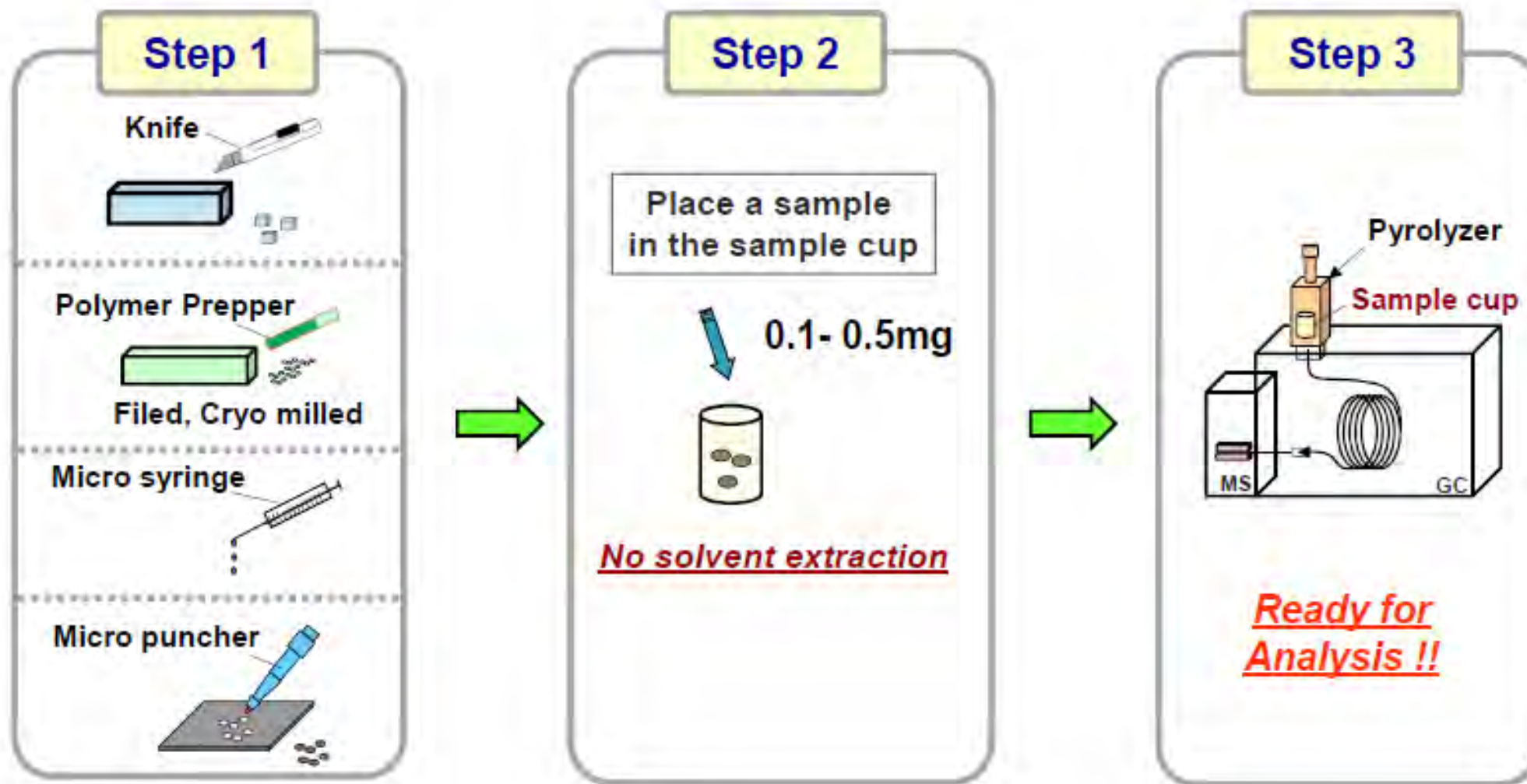
- สภาวะเครื่อง GCMS
 - Injector
 - Temperature 300 °C
 - Split 200:1
 - Carrier gas flow 1.0 ml/min
 - Oven
 - Initial 70 °C hold 1min ramp 1 ; 10 °C/min to 320 °C hold 8 min.
 - MS
 - Temperature 250 °C
 - Scan 35-550 amu.

- สภาวะเครื่อง Pyrolyzer
 - Single-Shot Analysis
 - Furnace Temperature 600 °C
 - Interface Temperature 300 °C

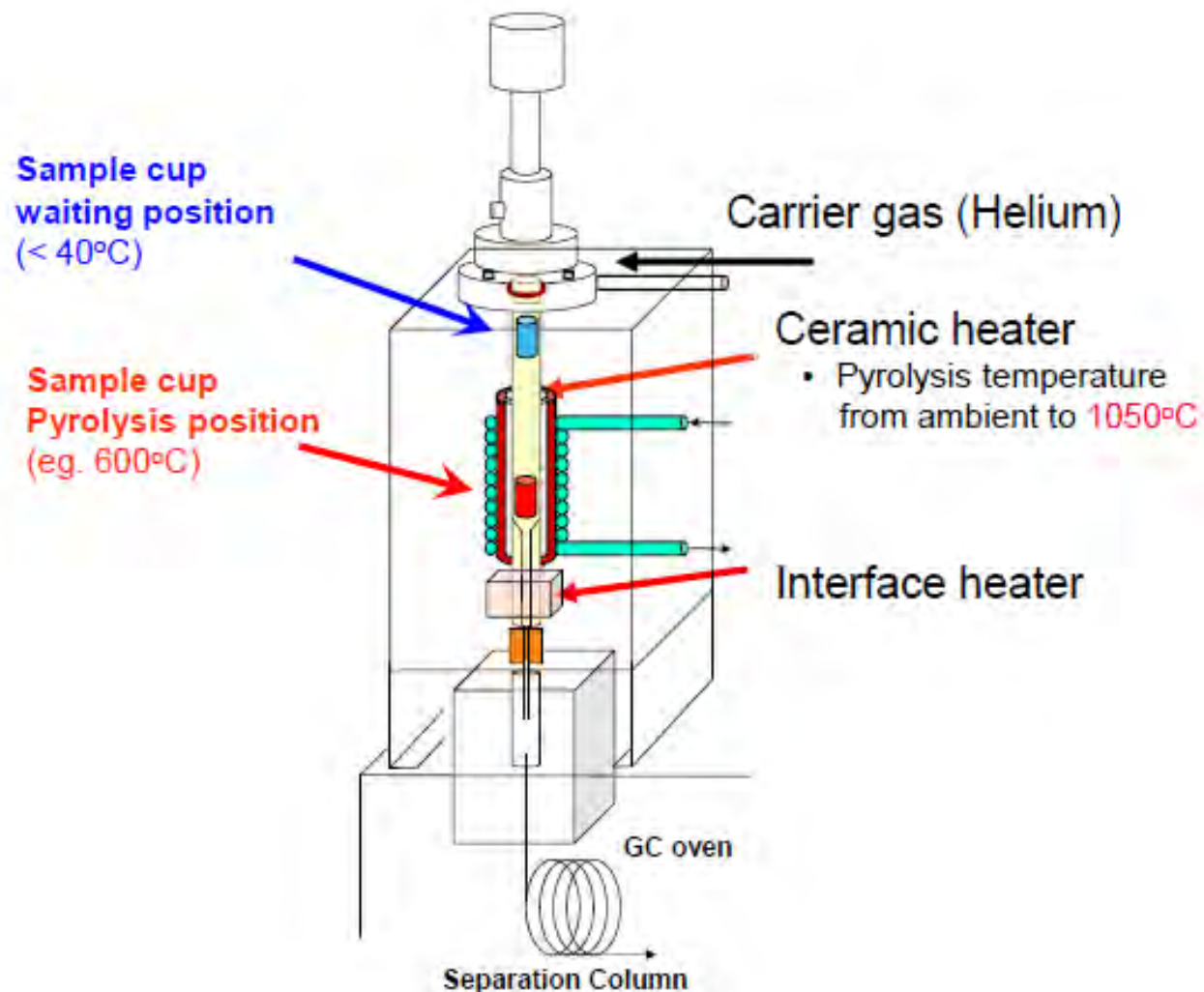


Sample cup

Sample preparation



Schematic diagram of Multi-Shot pyrolyzer EGA/PY-3030D

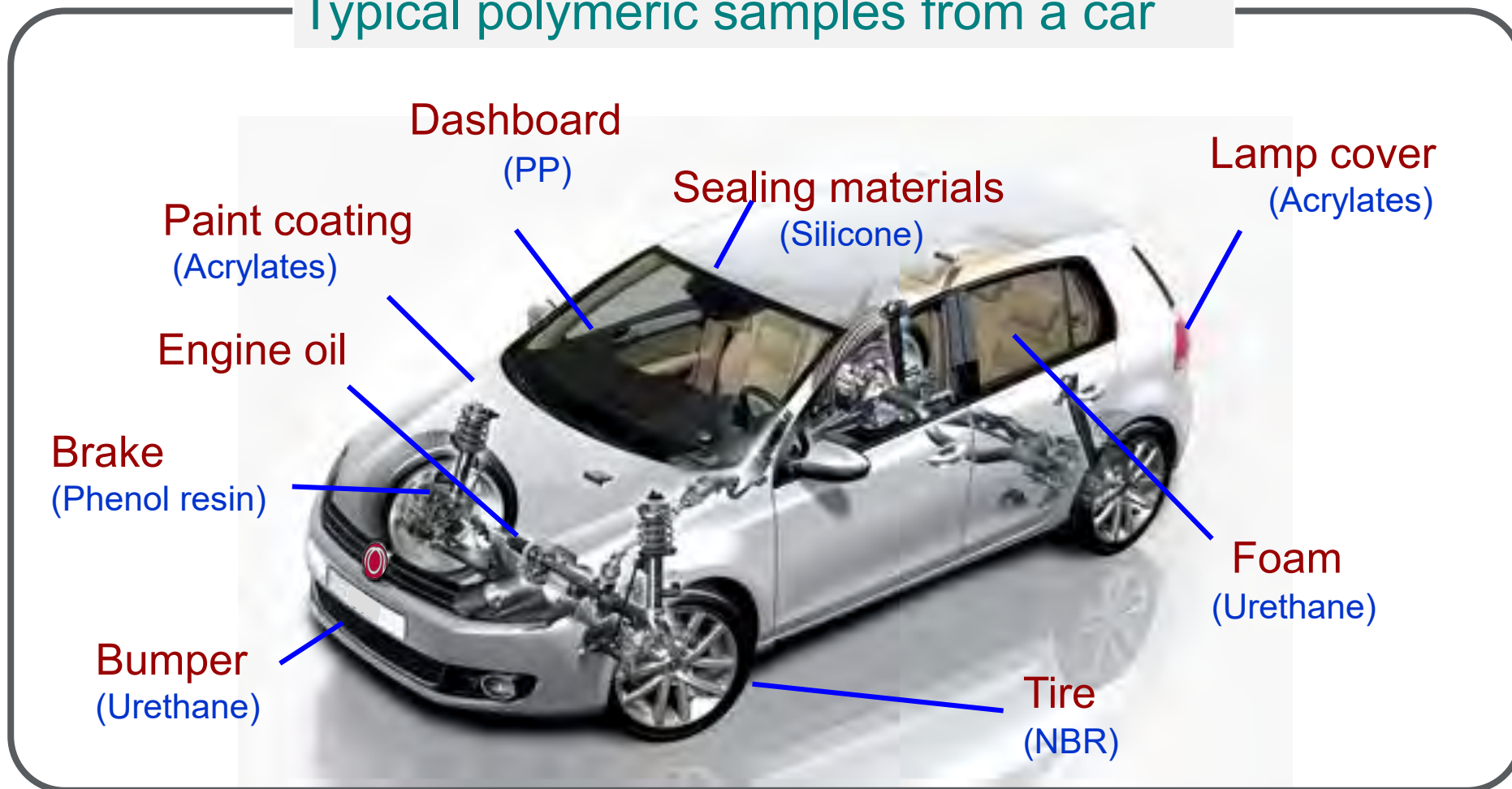


Auto-Shot Sampler

- ▶ 48 samples
- ▶ Extremely Reliable
- ▶ Excellent Reproducibility



Typical polymeric samples from a car



Analysis of phthalate esters in PVC

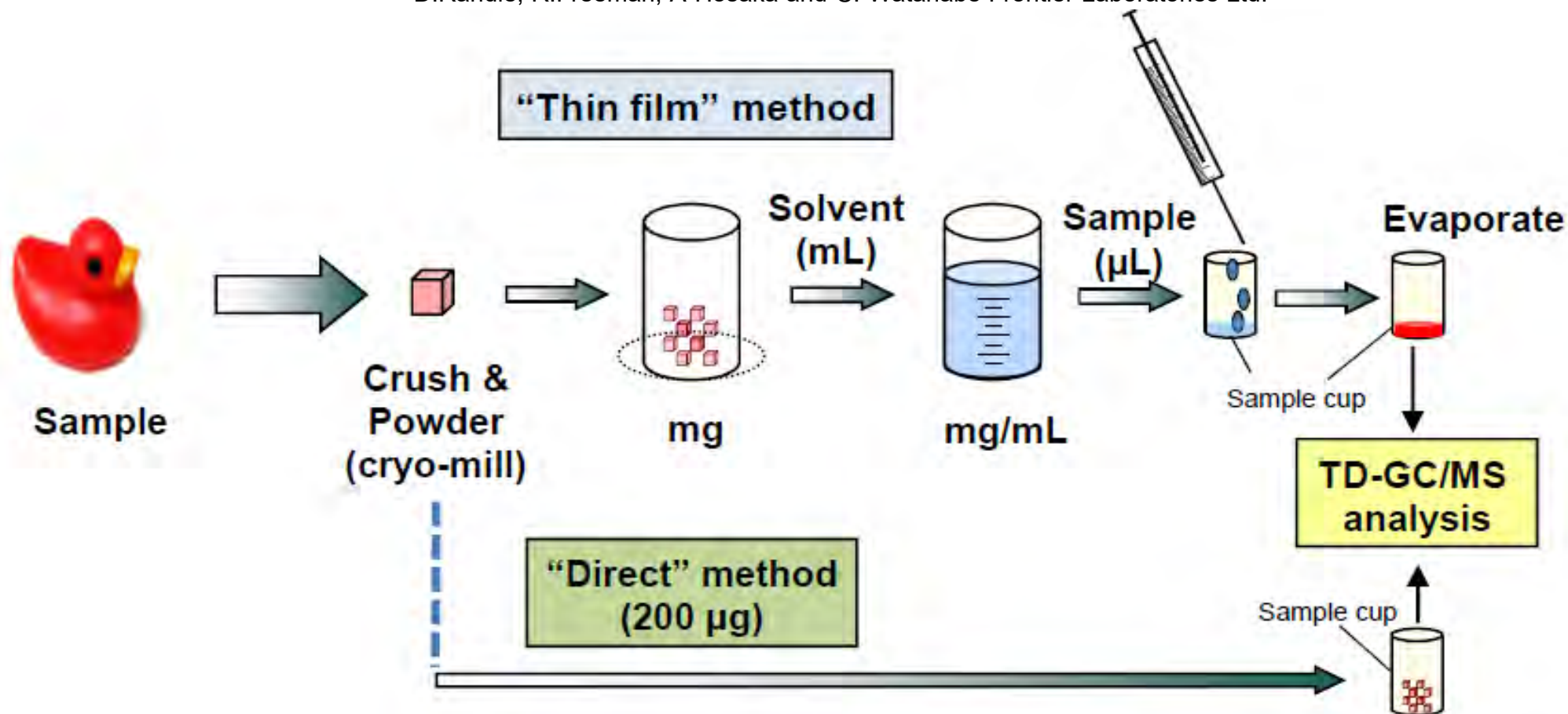
- Thermal Desorption GC/MS has become an official method approved by IEC for the analysis of restricted phthalates in electrotechnical products. Phthalates are widely used as plasticizers in manufacturing plastic products. With regard to additives in plastics used in electrical and electronic equipment, the maximum concentration of the restricted phthalates is **limited to 1000 ppm by the RoHS directive.**
- In March 2017, the thermal desorption GC/MS using a pyrolyzer was adopted as the official method and approved by IEC (International Electrotechnical Commission) for the analysis of certain phthalates in electrotechnical products regulated by the **RoHS directive (IEC 62321-8:2017).**
- The thermal desorption GC/MS method using Frontier Lab products complies with the IEC method.

A fast, easy and “green” thermal desorption-GCMS method for the analysis of phthalate esters in PVC

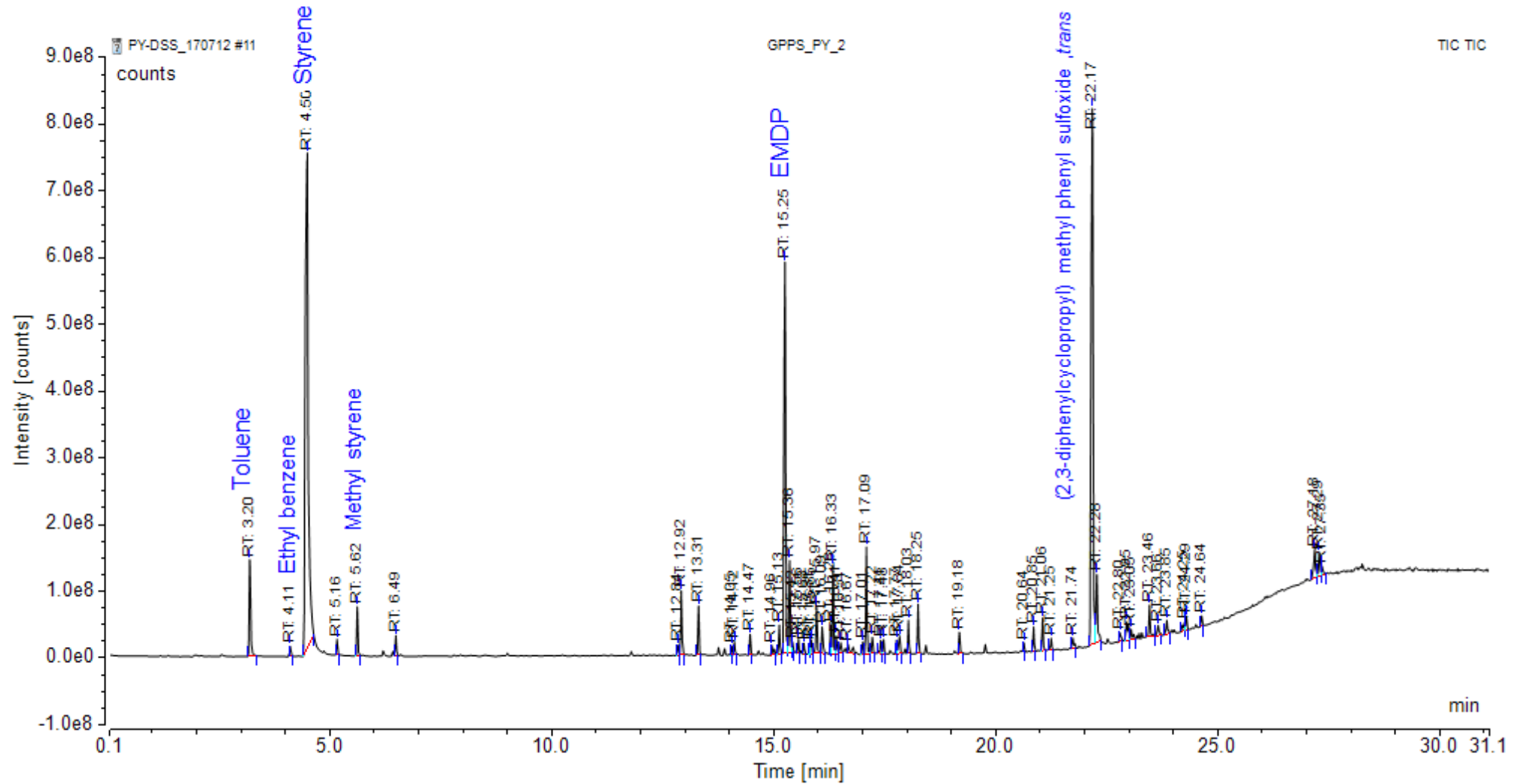
A discussion of the central factors that influence data quality when using ASTM D7823 for the determination of phthalates in polymeric substrates.

Thin Film method provides better quantitative results and sensitivity (due to more sample and homogeneity)

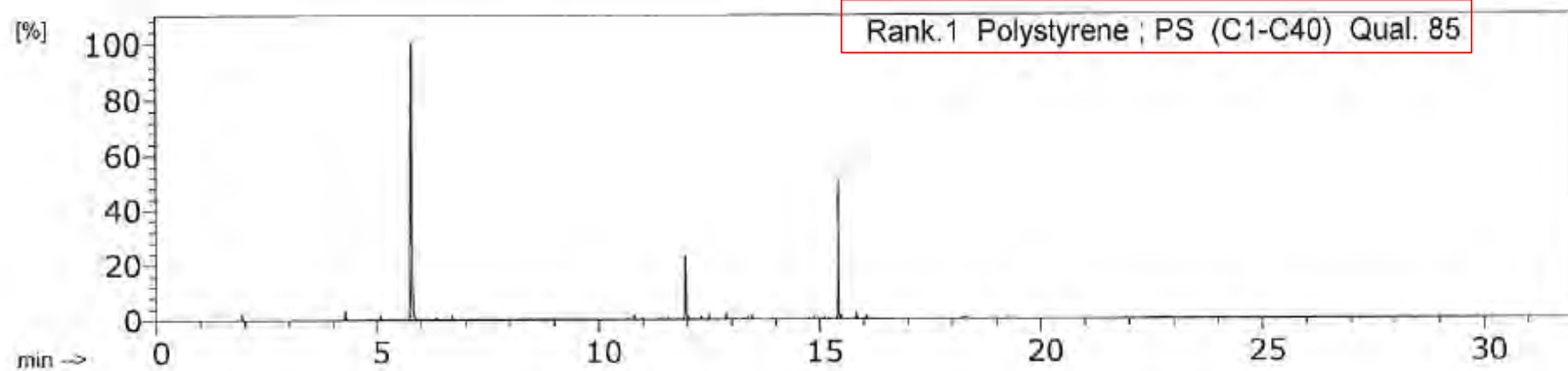
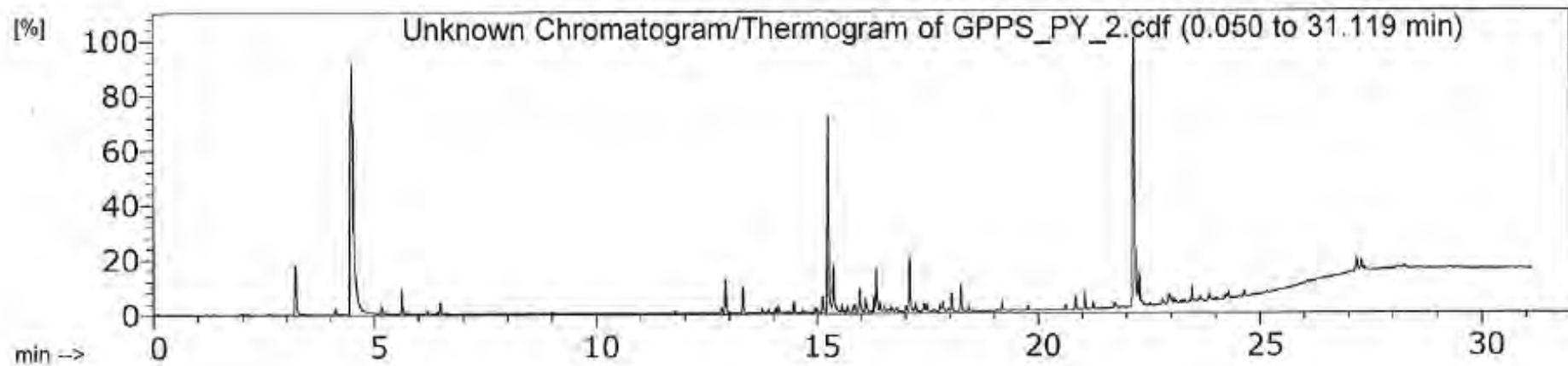
D.Randle, R.Freeman, A Hosaka and C. Watanabe Frontier Laboratories Ltd.



ผลการวิเคราะห์ตัวอย่างที่ 1



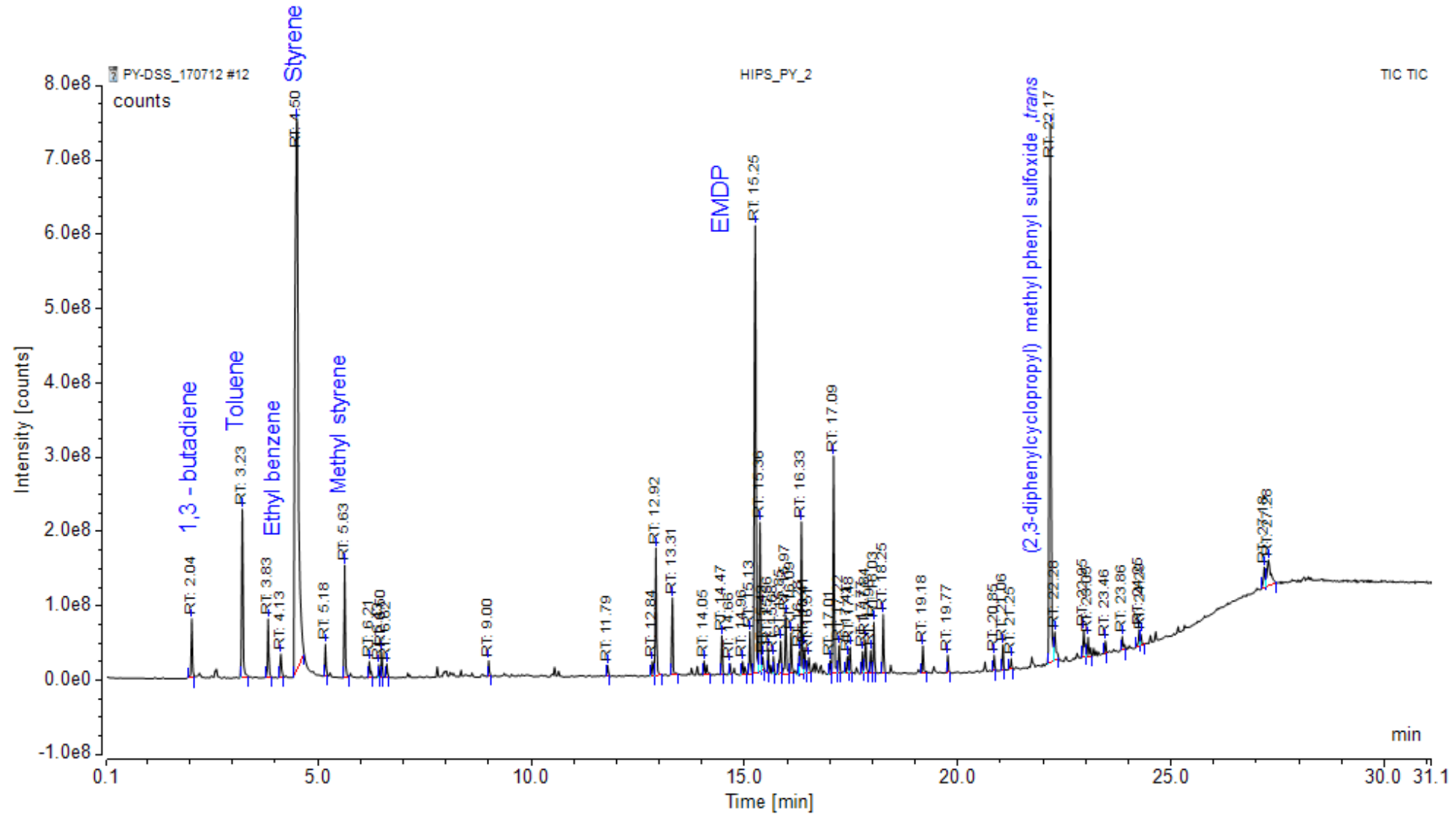
ผลการวิเคราะห์เมื่อเทียบกับฐานข้อมูลด้านพอลิเมอร์ผ่านซอฟต์แวร์ F-Search



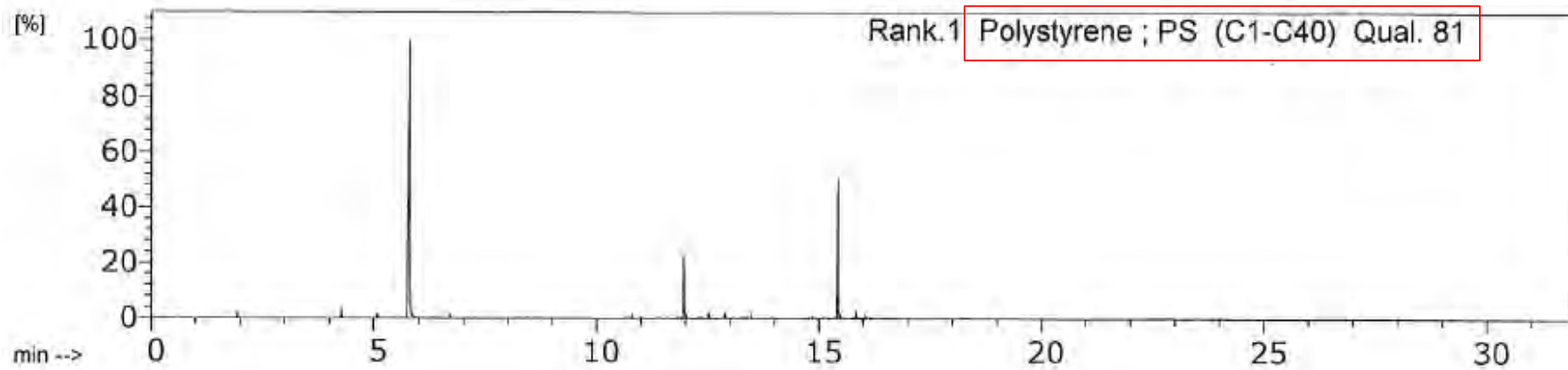
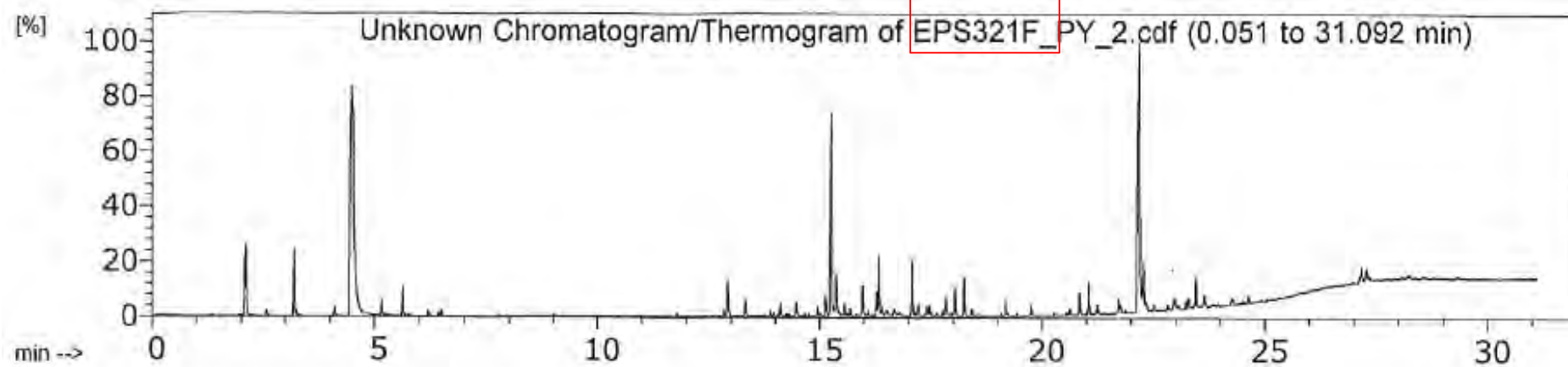
Rank.2 : Styrene-butadiene copolymer ABA block, 85% styrene (C1-C40) Qual. 85

Rank.3 : Acrylonitrile-Butadiene-Styrene copolymer ; ABS (C1-C40) Qual.84

ผลการวิเคราะห์ตัวอย่างที่ 2



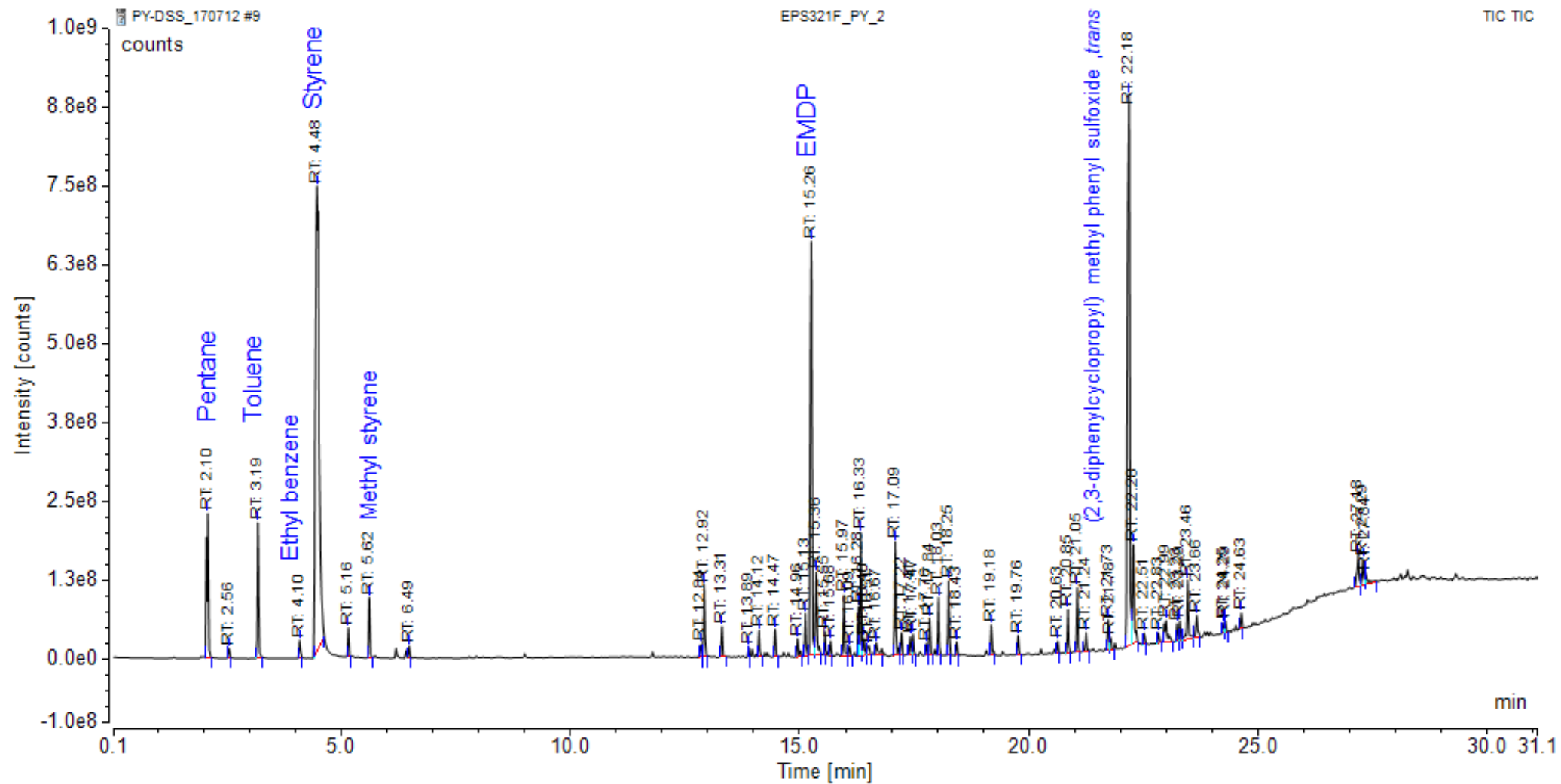
ผลการวิเคราะห์เมื่อเทียบกับฐานข้อมูลด้านพหิเมอร์ผ่านซอฟต์แวร์ F-Search



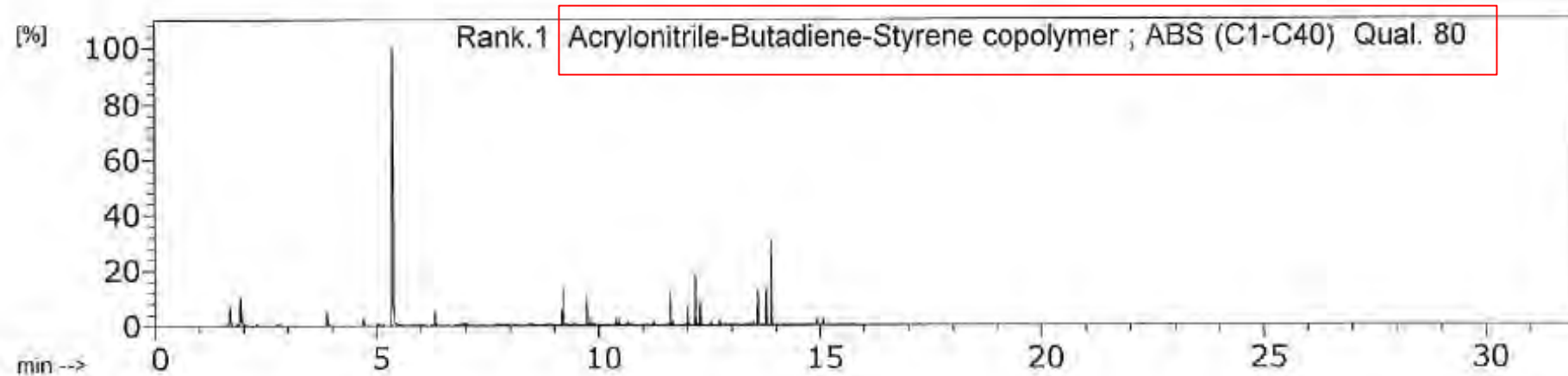
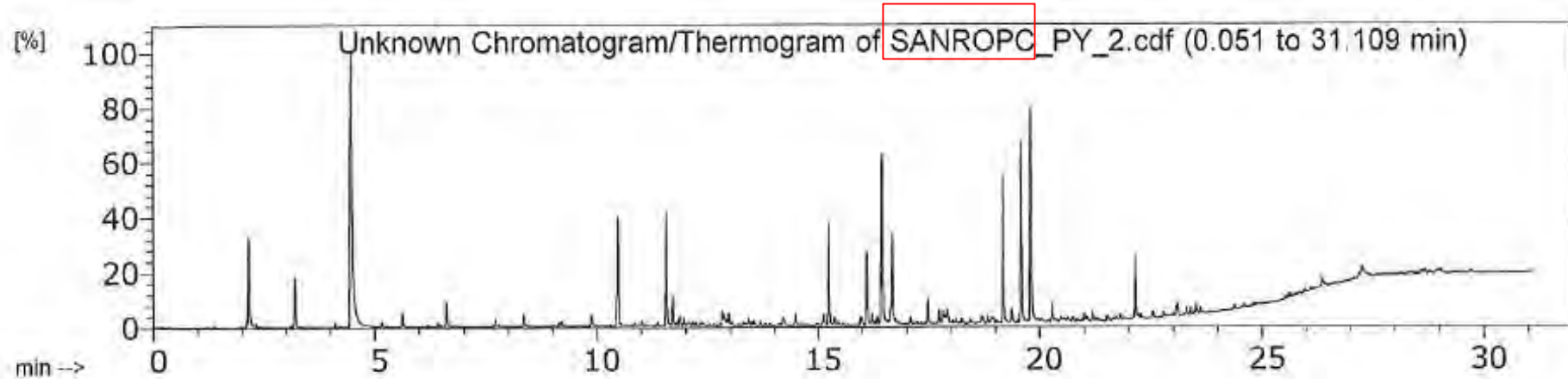
Rank.2 : Acrylonitrile-Butadiene-Styrene copolymer ; ABS (C1-C40) Qual.81

Rank.3 : Styrene-butadiene copolymer ABA block, 85% styrene (C1-C40) Qual. 81

ผลการวิเคราะห์ตัวอย่างที่ 3



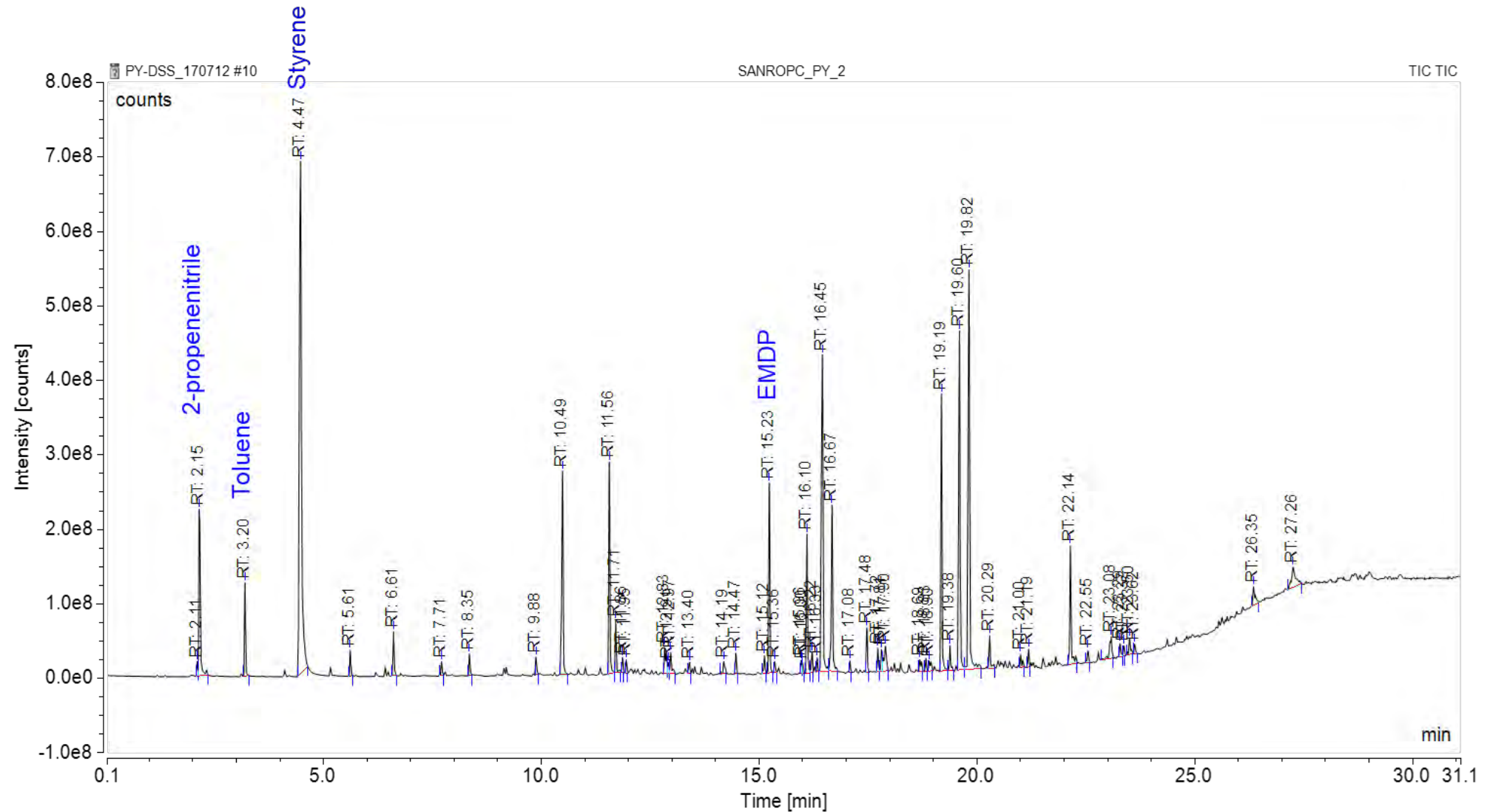
ผลการวิเคราะห์เมื่อเทียบกับฐานข้อมูลด้านพอลิเมอร์ผ่านซอฟต์แวร์ F-Search



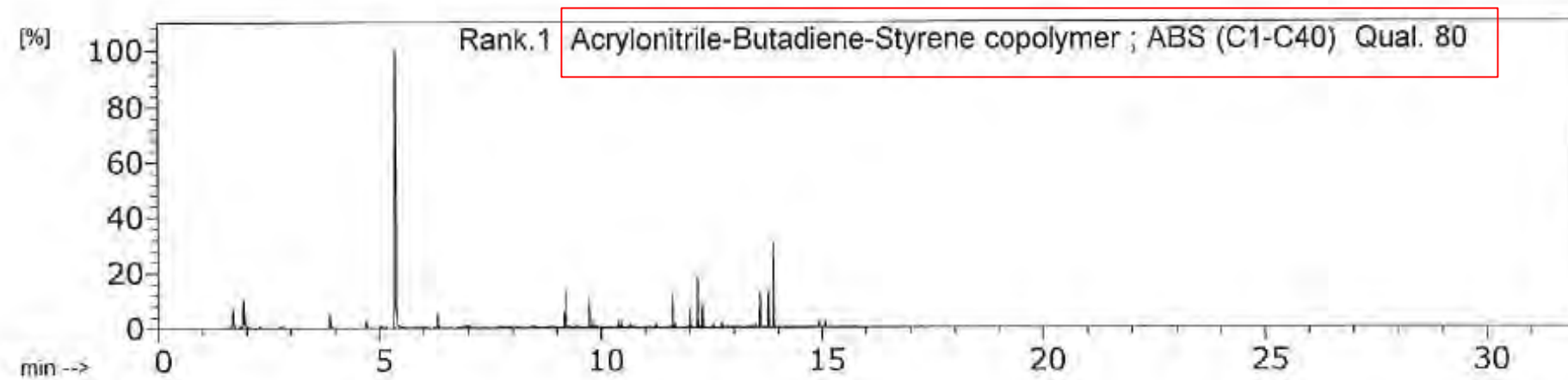
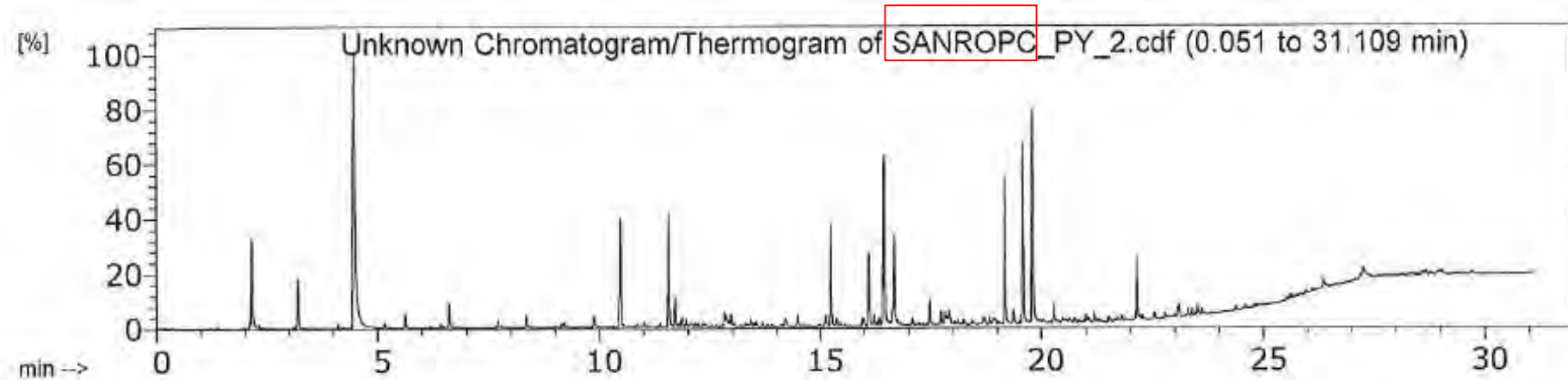
Rank.2 : Acrylonitrile-Butadiene-Styrene copolymer ; ABS (C1-C40) Qual.79

Rank.3 : Acrylonitrile styrene copolymer ; AS (C1-C40) Qual.76

ผลการวิเคราะห์ตัวอย่างที่ 4



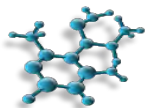
ผลการวิเคราะห์เมื่อเทียบกับฐานข้อมูลด้านพอลิเมอร์ผ่านซอฟต์แวร์ F-Search



Rank.2 : Acrylonitrile-Butadiene-Styrene copolymer ; ABS (C1-C40) Qual.79

Rank.3 : Acrylonitrile styrene copolymer ; AS (C1-C40) Qual.76

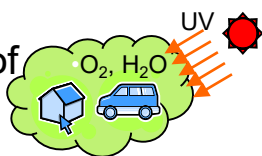
1: Characterization of polymers



2: Quality control



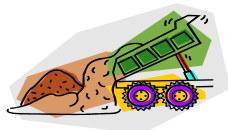
3: Degradation/life evaluation of polymeric materials



4: Recycling of polymeric materials, biomass utilization



5: Organic geochemistry and soil chemistry



6: Clinical science, pathology



7: Biochemistry, microbiology



8: Coal liquefaction, energy conservation



9: Forensic science



10: Wood science, pulp industry



11: Tobacco smoke, toxicology



12: Extraterrestrial science



13: Environmental science



ThermoFisher
S C I E N T I F I C

Analysis PAHs in extender oils



The world leader in serving science

- EU standard specifies a procedure for determination of benzo(a)pyrene and sum of the eight individual polycyclic aromatic hydrocarbons in extender oils. ***listed in Table1***
- Sample Preparation Method : BS EN 16143:2013

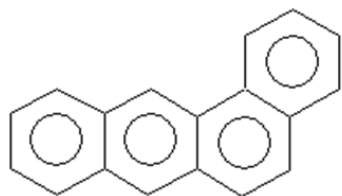
Name of PAH	Abbreviation	CAS Registry number
Benzo(a)pyrene	BaP	50-32-8
Benzo(e)pyrene	BeP	192-97-2
Benzo(a)anthracene	BaA	56-55-3
Chrysene	CHR	218-01-9
Benzo(b)fluoranthene	BbFA	205-99-2
Benzo(j)fluoranthene	BjFA	205-82-3
Benzo(k)fluoranthene	BkFA	207-08-9
Dibenzo(a,h)anthracene	DBahA	53-70-3

Table 1- List of individual PAHs in extender oils

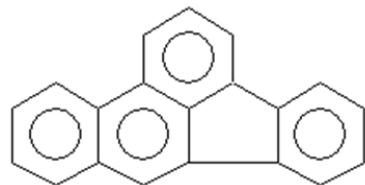
PAHs...

Consists of 8 natives of PAHs

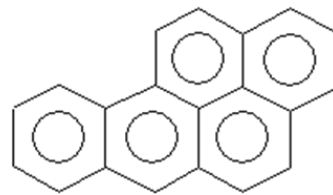
MW range 228-278 amu (16PAHs could be up to 300+)



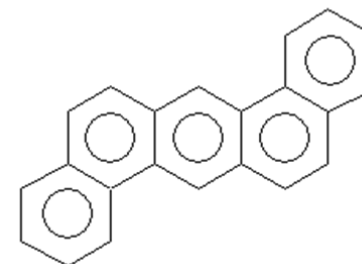
Benzo(a)anthracene



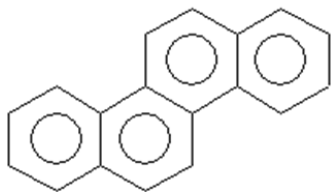
Benzo(b)fluoranthene



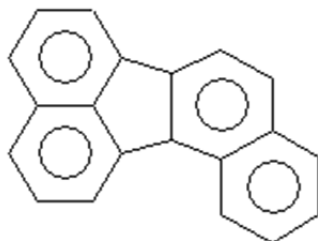
Benzo(a)pyrene



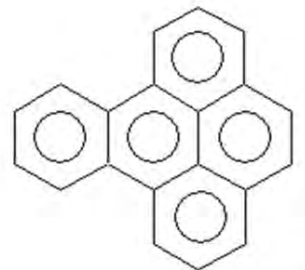
Dibenzo(a,h)anthracene



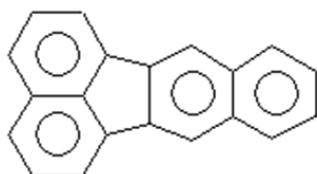
Chrysene



Benzo(j)fluoranthene



Benzo(e)pyrene



Benzo(k)fluoranthene

$C_{18}H_{12}$
MW. 228 g/mol

$C_{20}H_{12}$
MW. 252 g/mol

$C_{20}H_{12}$
MW. 252 g/mol

$C_{22}H_{14}$
MW. 278 g/mol

Sample Preparation Process

(1) Prepares sample solution

Weight Sample 70 ± 0.1 mg into Vol. flask 5 ml

Dissolve with 2 ml of *n*-Pentane and Spike internal Std. (deuterated IS)

(2) Deactivates silica

Deactivate Silica gel by stirring with 7% (m/m) of water for 24 h.

(3) 1st sample extraction (8 Hours)

3.1 Mix deactivated silica (in 2) 5 g with *n*-Pentane

3.2 Load silica gel into chromatographic column (16 cm. L X 1 cm. ID)*

3.3 Flush silica gel with 10 ml *n*-Pentane through the column (discard)

3.4 Load sample (1) into column (before *n*-Pentane vanish form silica gel surface).

3.5 Rinse sample container with 2 ml *n*-Pentane. (not critical) and pour into column.

3.6 Elute sample by Cyclohexane 75 ml (several portion) and collect the eluents.**

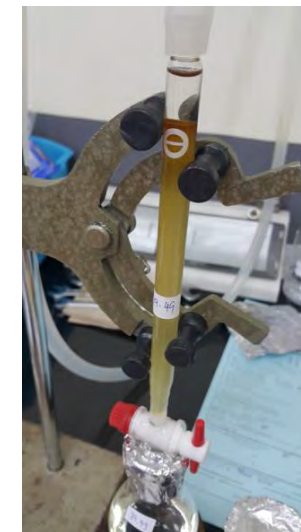
3.7 Evaporate eluent (3.6) under 35 C till final volume 1ml.

*extended length of column to 25 cm. convenient for sample loading

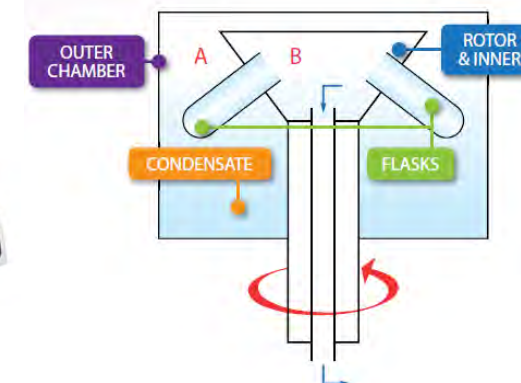
** pressurized with N₂ (1 bar est.) for faster elution



Pack column



Extracting



Sample Preparation Process

(4) Sample clean up (Sephadex LH20) (6 hours)

4.1 Mix 5 g. of Sephadex with IPA .. leave for overnight.

4.2 Load Sephadex into chromatographic column (12 cm L X 2.3 cm ID)

4.3 Add 1 ml IPA into (3.7) and load into column.

4.4 Rinse sample vessel with IPA (1 ml) and load into column.

4.5 Elute with IPA at 1 ml/min, Discard the first 24 ml eluent.

4.6 Collect eluent portion (@24-70 ml) in drying vessel

4.7 Evaporate eluent (4.6) under 35 C till nearly dry.

4.8 Add 2 ml Acetone and evaporate till dry.

4.9 Dissolve with CycloC6 and transfer into 1 ml Vol.Flask

4.10 Add injection standard (DE)* 0.2 ml and make up volume to 1 ml with CycloC6

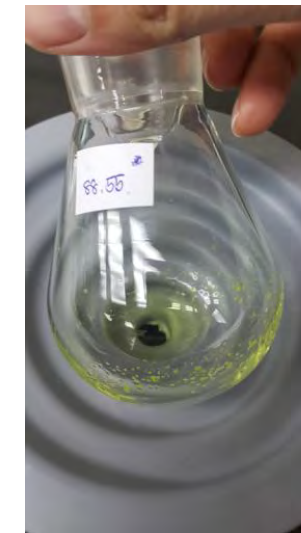
4.11 Make up volume to 1 ml wth Cyclohexane.

4.12 Analyze with GCMSMS.

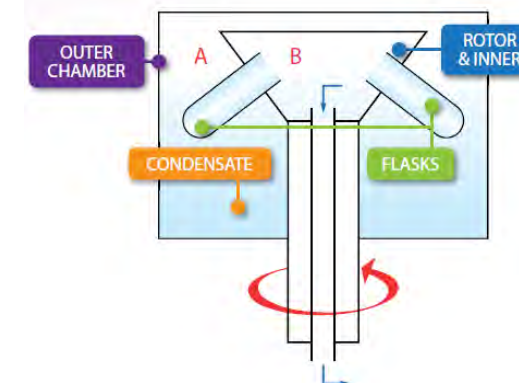
*DE = Decafluorodiphenyl



Fraction
collecting



Dissolved
Solution



GC parameters

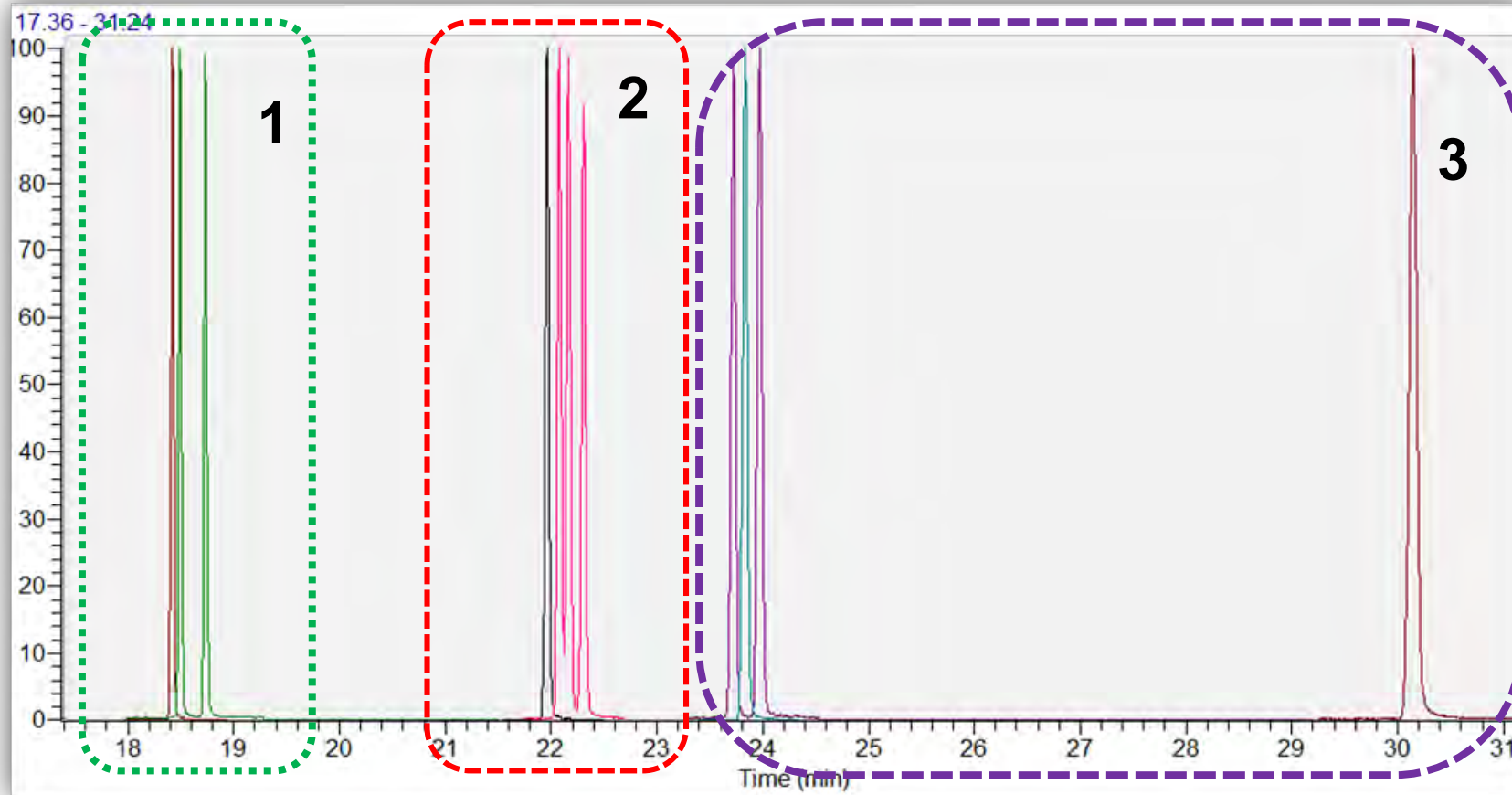
Parameter	Value
GC-column	60 m x 0.25 mm ID x 0.25 μ m
Stationary phase	17% phenyl-methylpolysiloxane
Temperature program	Initial 90 °C hold 1min 20°C /min to 250 °C 4°C /min to 330 °C hold 10 min
Injection	PTV, Splitless
Injection temperature	275 °C
Injection Volume	1 μ L
Carrier gas	He UHP grade 1.2 ml/min

- **Mass Spectrometer : EI – Temp 250 C/ TL Temp 330/**
- **MSMS – SRM Q1 resolution 0.7 FWHM, Q3 Resolution 0.7 FWHM**

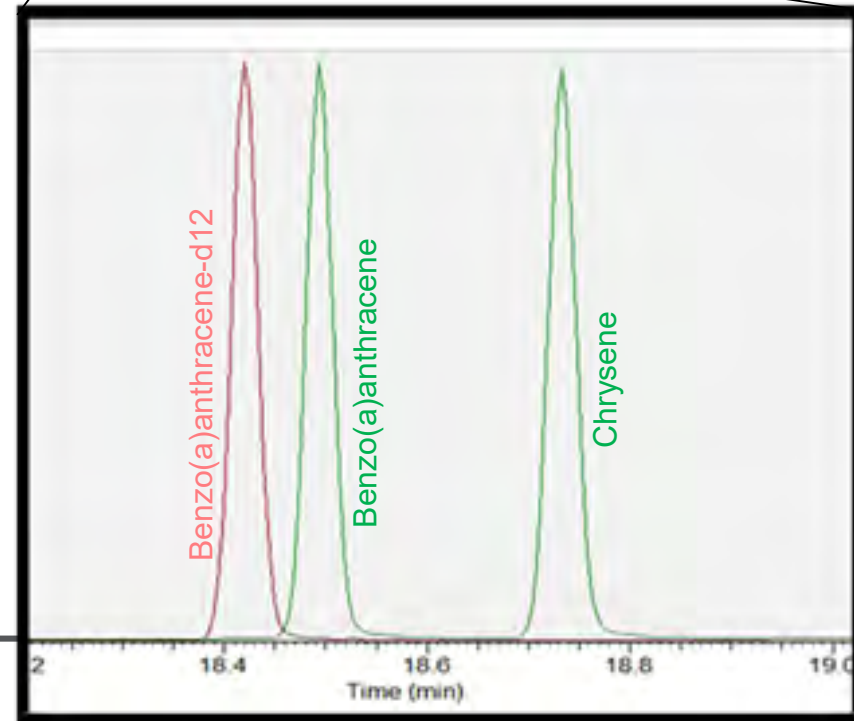
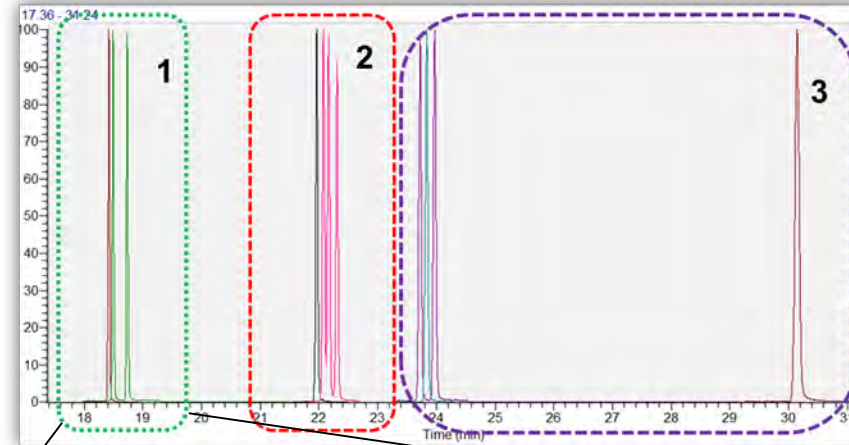
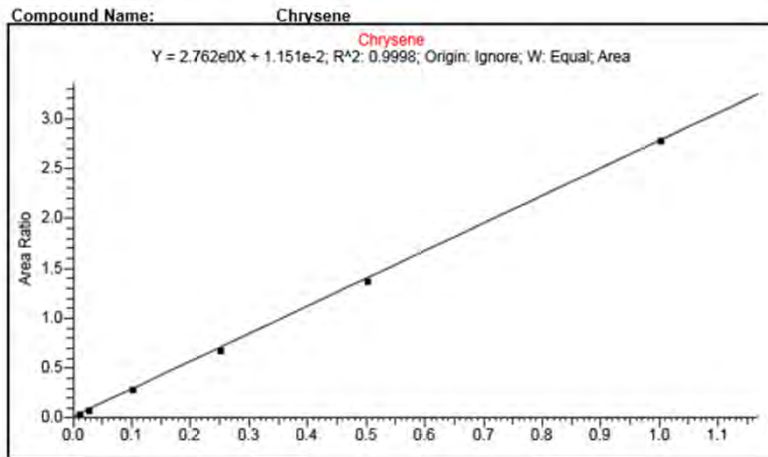
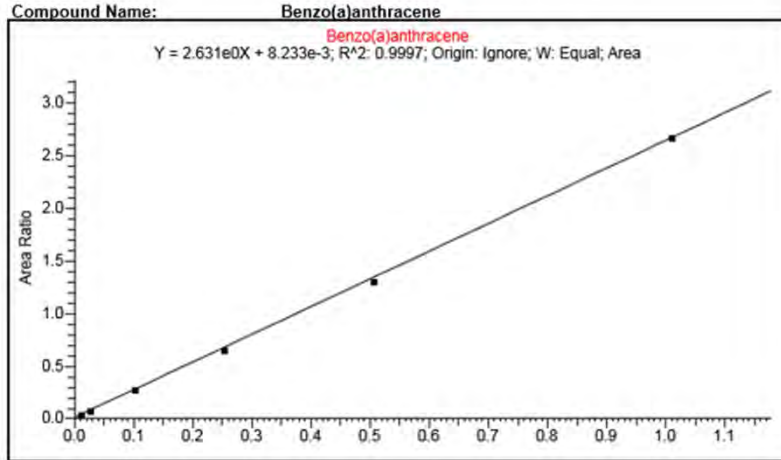
Component	RT	mass	product mass	Collision energy
Decfluorodiphenyl	5.84	333.9	233.9	35
		333.9	264.9	25
Benzo(a)anthracene-D12	18.46	240.1	212.1	25
		240.1	236	30
Benzo(a)anthracene	18.53	228.1	202	25
		228.1	226	30
Chrysene	18.77	228.1	202	25
		228.1	226	30
Benzo(b)Fluoranthene-D12	22.02	264.1	236	30
		264.1	260	35
Benzo(b)fluoranthene	22.13	252.1	226	25
		252.1	250	30
Benzo(k)fluoranthene	22.22	252.1	226.1	25
		252.1	250	35
Benzo(j)fluoranthene	22.36	252.1	226	25
		252.1	250	30
Benzo(e)pyrene	23.78	252.1	226.1	30
		251.1	250	30
Benzo(a)pyrene-D12	23.89	264.2	236.1	30
		264.2	260	35
Benzo(a)pyrene	24.03	252.1	226.1	35
		251.1	250	30
Dibenzo(a,h)anthracene	30.23	278.1	276	35
		278.1	276.2	50

8 PAHs Standard

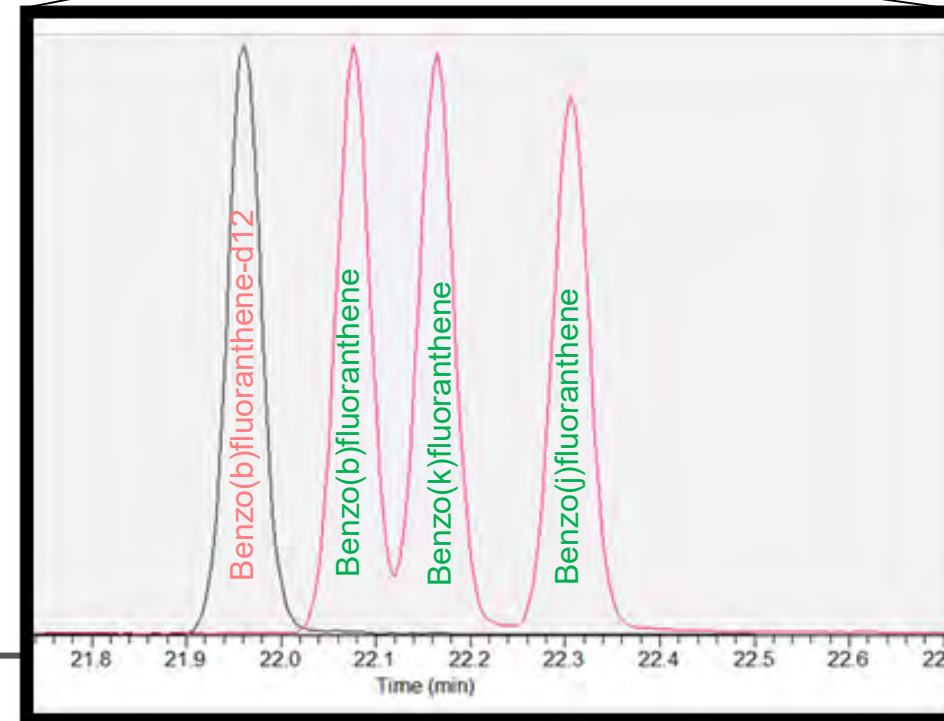
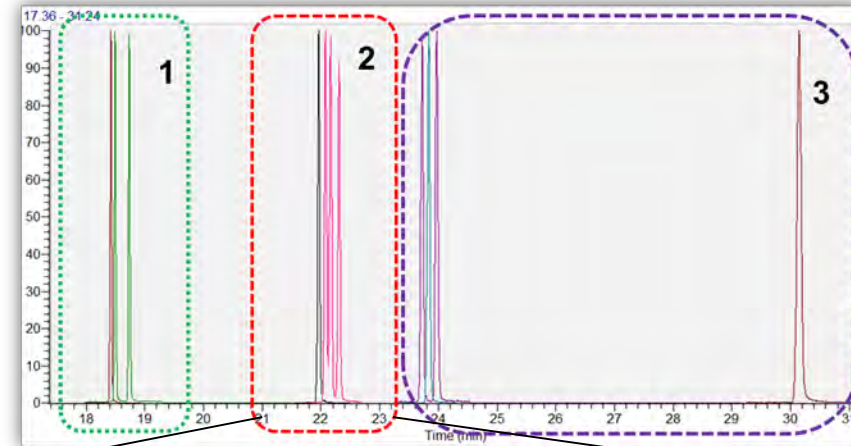
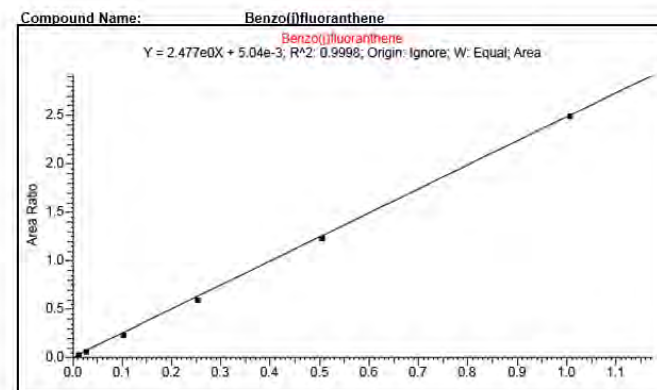
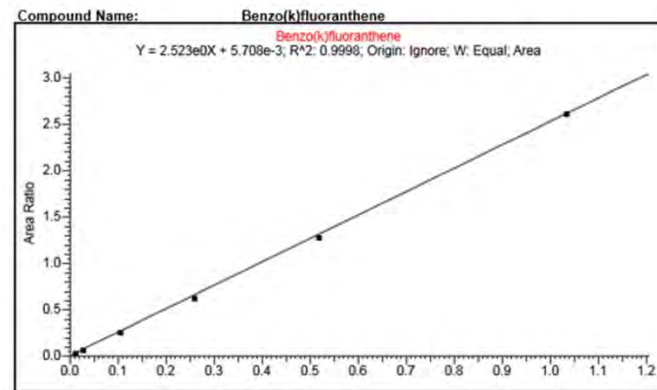
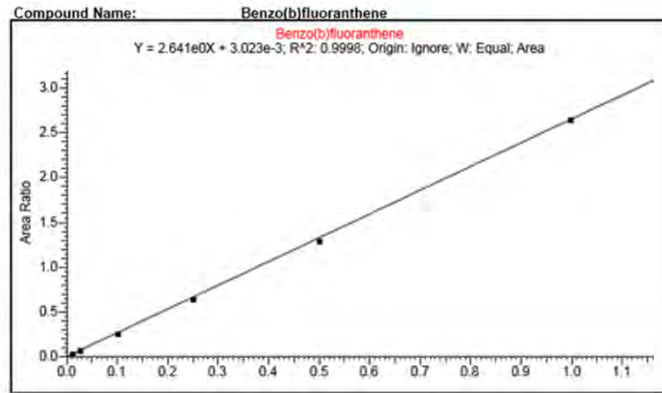
TIC



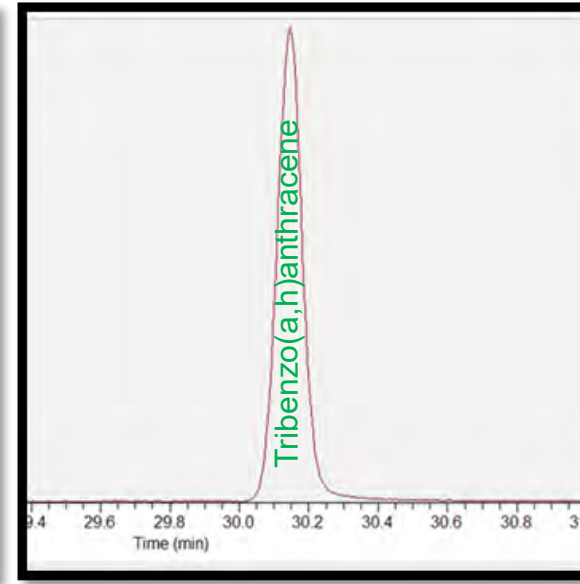
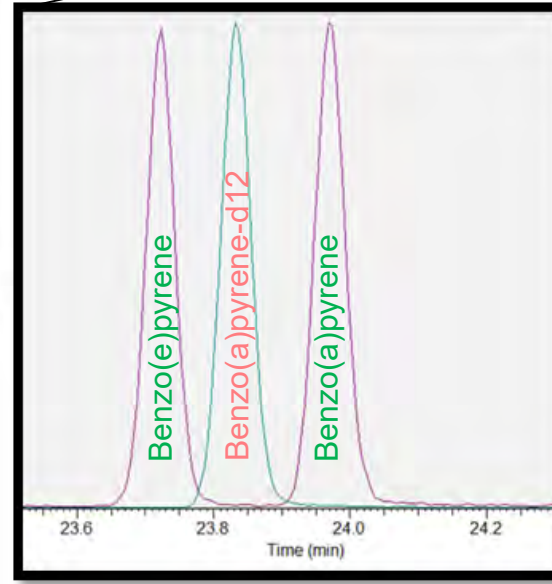
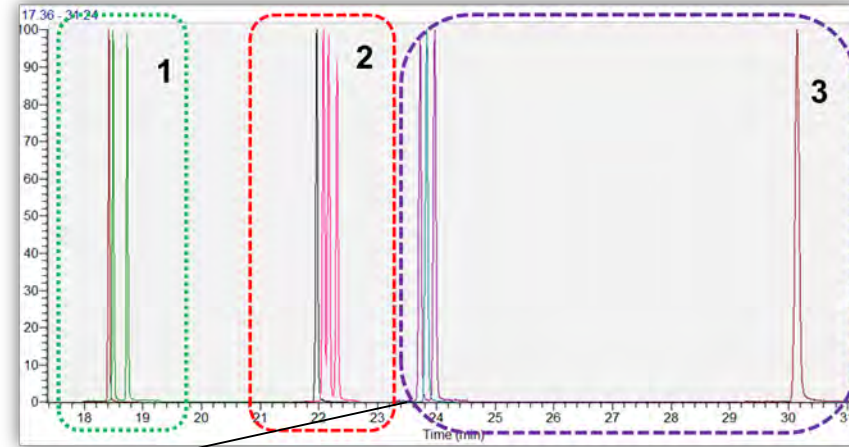
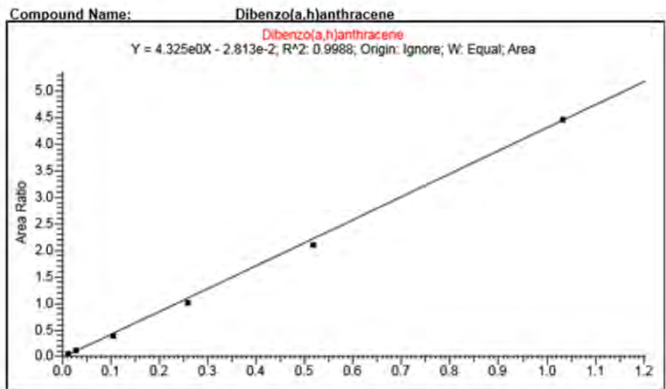
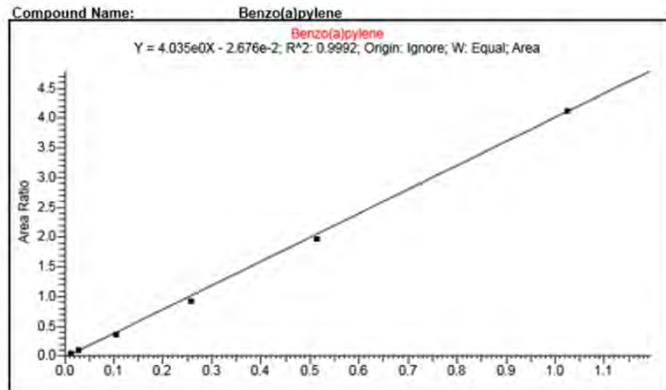
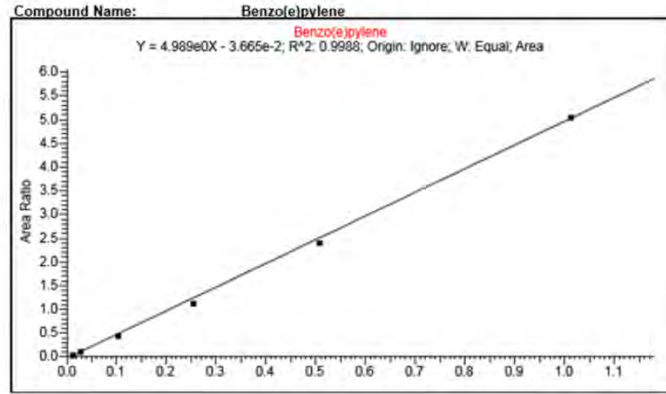
Chromatogram (1) –Standard 8 PAHs with 3 IS(d12)



Chromatogram (2) – Standard 8 PAHs with 3 IS(d12)



Chromatogram (3) – Standard 8 PAHs with 3 IS(d12)



- Calculated from 10 replicate runs of TDAE sample (Treated Distillate Aromatic Extracted)

No.	PAHs (mg/kg)							
	Benzo(a)anthracene	Chrysene	Benzo(b)fluoranthene	Benzo(k)fluoranthene	Benzo(j)fluoranthene	Benzo(e)pyrene	Benzo(a)pyrene	Dibenzo(a,h)anthracene
1	0.226	0.370	0.198	0.186	0.103	-0.507	0.144	0.125
2	0.220	0.367	0.177	0.165	0.117	-0.510	0.130	0.148
3	0.222	0.361	0.184	0.182	0.127	-0.507	0.137	0.124
4	0.236	0.375	0.194	0.178	0.136	-0.511	0.147	0.149
5	0.221	0.372	0.204	0.168	0.118	-0.518	0.129	0.150
6	0.224	0.366	0.189	0.180	0.117	-0.510	0.129	0.142
7	0.236	0.363	0.192	0.194	0.123	-0.535	0.122	0.139
8	0.221	0.368	0.204	0.178	0.133	-0.509	0.126	0.135
9	0.247	0.369	0.181	0.166	0.118	-0.509	0.125	0.144
10	0.231	0.362	0.202	0.169	0.130	-0.507	0.115	0.147
SD	0.0089	0.0045	0.0097	0.0095	0.0097	0.0086	0.0098	0.0095
LOD	0.0267	0.0134	0.0291	0.0285	0.0291	0.0258	0.0294	0.0286
LOQ	0.0891	0.0447	0.0969	0.0951	0.0972	0.0860	0.0980	0.0955

8 compounds of PAHs have LOQ less than 0.1 mg/kg

Peak Confirmation

Benzo(a)anthracene

Chrysene

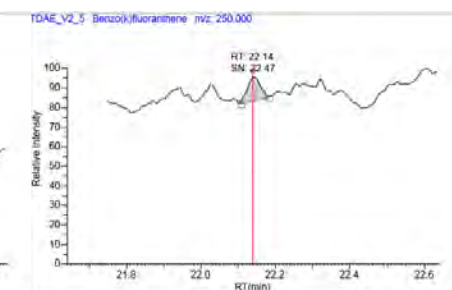
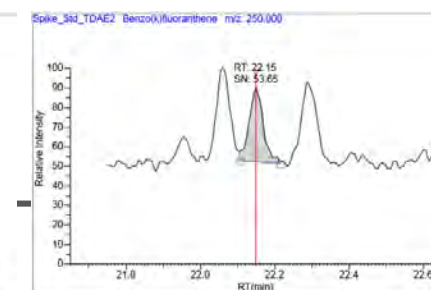
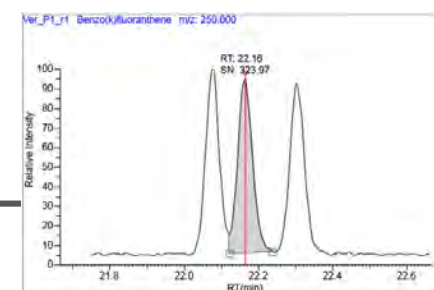
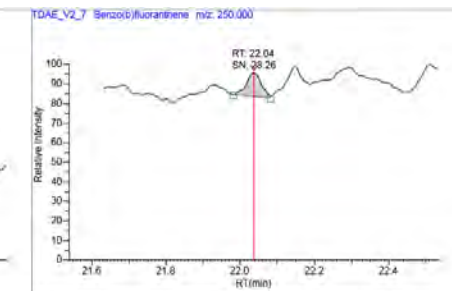
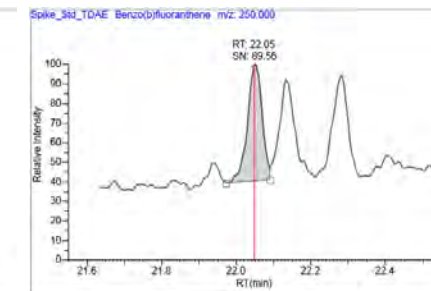
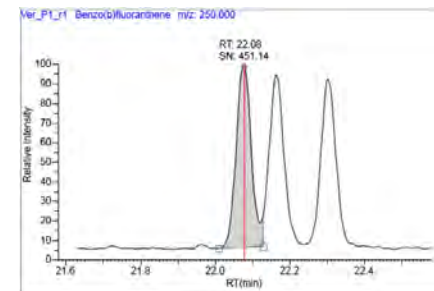
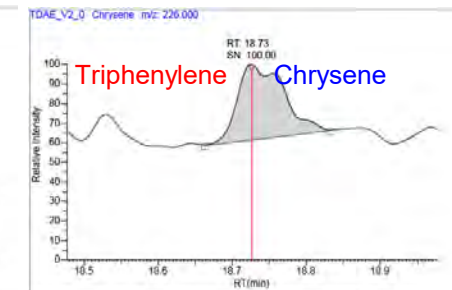
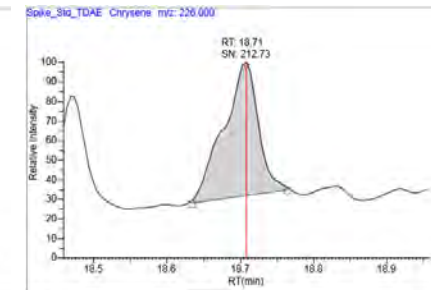
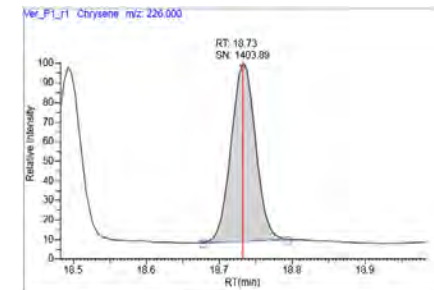
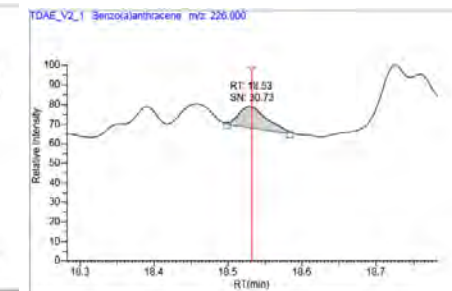
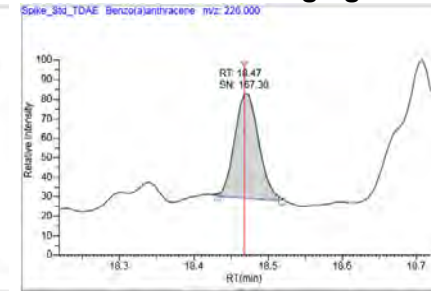
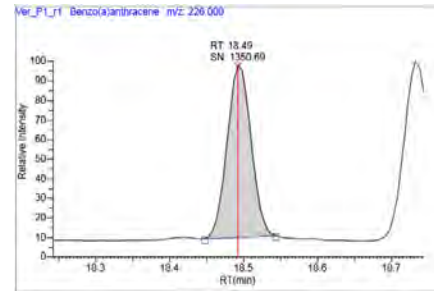
Benzo(b)fluoranthene

Benzo(k)fluoranthene

QC Check

Sample spiked
3 ul of 0.5 mg/kg

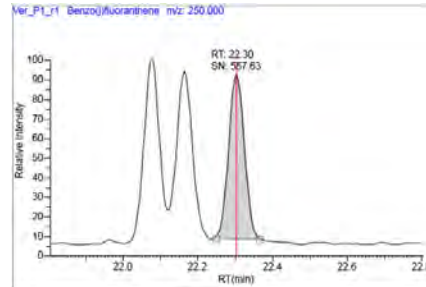
Sample(TDAE)



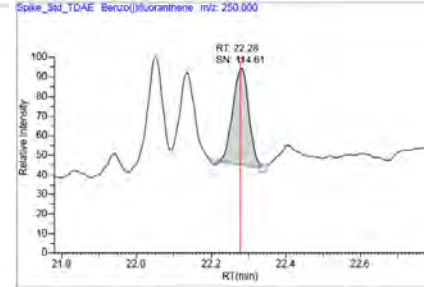
Peak Confirmation

Benzo(j)fluoranthene

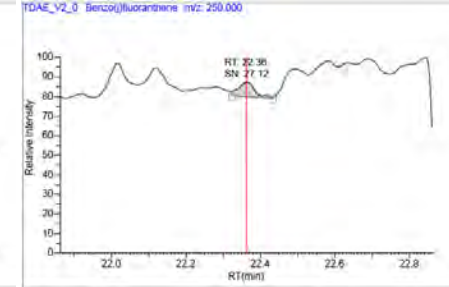
QC Check



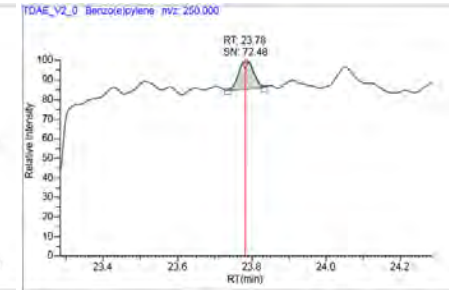
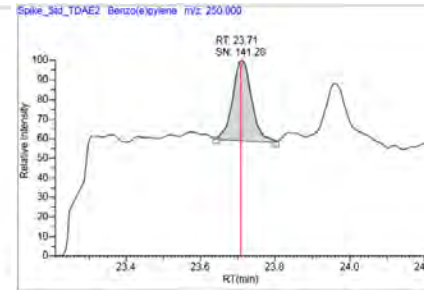
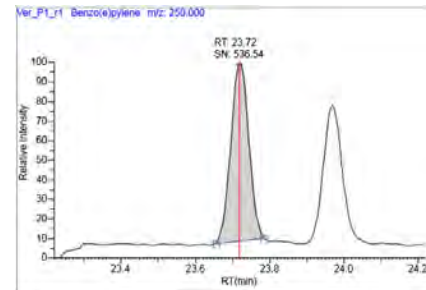
Sample spiked
3 ul of 0.5 mg/kg



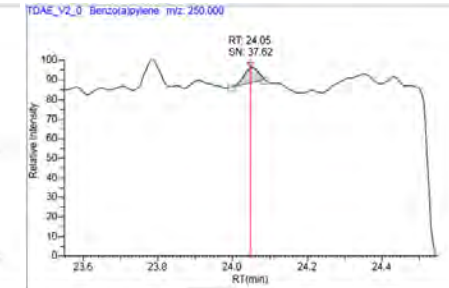
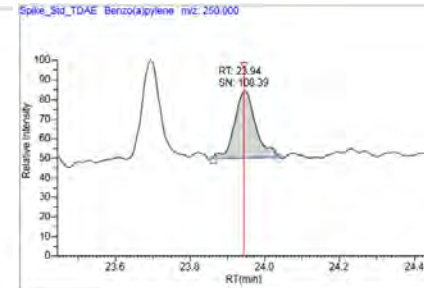
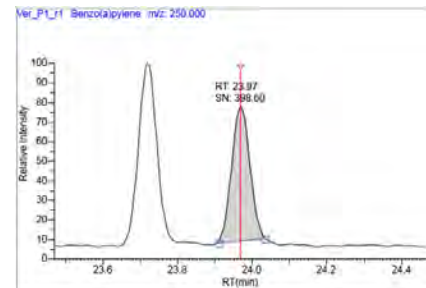
Sample-TDAE



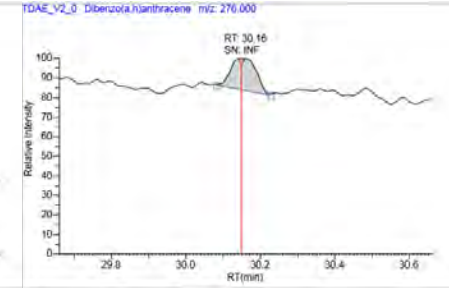
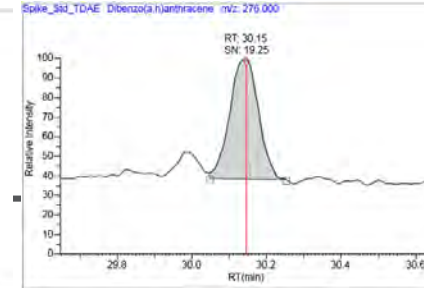
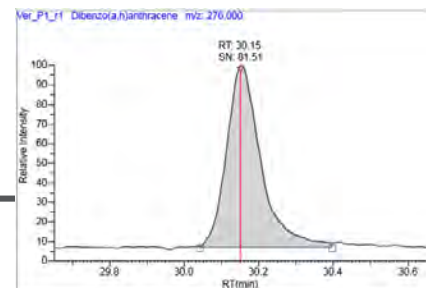
Benzo(e)pyrene



Benzo(a)pyrene



Dibenzo(a,h)anthracene



- Two batches of analysis (2 replicates for each batch) from same sample (RPO)
- Recovery of PAHs : Deuterated IS vs. Injection Standard (Decafluorodiphenyl)
- BIU acceptable recovery is between 50% and 150%

Internal standard	Standard amount (mg)	Sample		Calculated amount (mg)	%Recovery	Acceptable Criteria of %Recovery	Verified
		RPO_V1_Re01	RPO_V1_Re02				
Benzo(a)anthracene-d12	4008	4663.572	4719.434	4691.503	117.05	(50-150)	Pass
Benzo(b)fluoranthene-d12	4216	5684.548	5493.625	5589.087	132.57	(50-150)	Pass
Benzo(a)pyrene-d12	4060	5389.764	5301.968	5345.866	131.67	(50-150)	Pass
		RPO_V2_Re01	RPO_V2_Re02				
Benzo(a)anthracene-d12	4008	3532.543	3532.543	3532.543	88.14	(50-150)	Pass
Benzo(b)fluoranthene-d12	4216	3249.254	3249.254	3249.254	77.07	(50-150)	Pass
Benzo(a)pyrene-d12	4060	3319.878	3319.878	3319.878	81.77	(50-150)	Pass

- Complicated & time consuming sample preparation – requires skills and prone to error
- Improvement in separation (triphenylene vs. chrysene) can be done upon availability of standard (triphenylene).
- Comparison study of purification between the two steps i.e. Silica Gel vs. Silica Gel & Sephadex are not so much different.
- New development on sample prep in order to reduce work loads and improve analysis result.



Simplify

the complexity of dioxin analysis

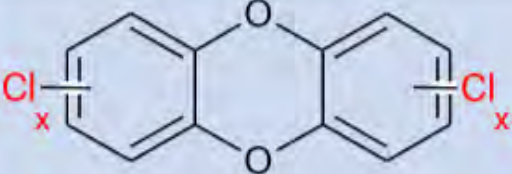
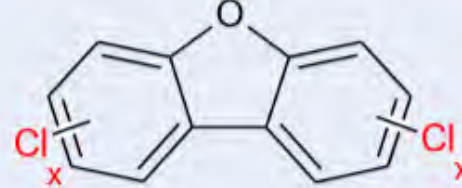
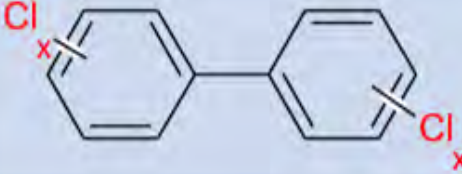
Thermo Scientific Dioxin Analyzer

ThermoFisher
SCIENTIFIC

Introduction to Dioxin & Dioxin Like PCBs

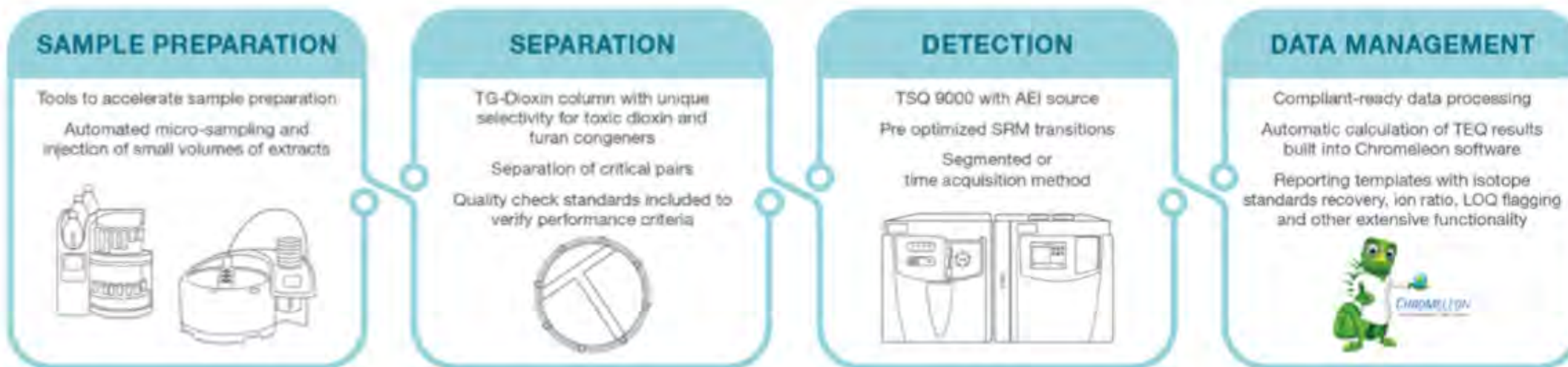
- Identified as toxic by the United Nations due to adverse effects on humans and the ecosystem
- The Stockholm agreement was signed in 2001 and entered into EU Legislation in 2004
- Of the possible 419 PCDD, PCDF and PCB congeners only 29 are recognised as toxic, but each have differing toxicity
- Most toxic: 2,3,7,8-Tetrachlorodibenzo-p-dioxin (TCDD)

- Up to 2012 only Magnetic Sector GC-HRMS was acceptable for analysis

Structure	Abbreviation	# Toxic Congeners
	PCDD	7
	PCDF	10
	PCB	12

Thermo Scientific™ Dioxin Analyzer

The Thermo Scientific™ Dioxin Analyzer is an integrated, sample-to-result GC-MS/MS based, easy to implement, analytical workflow developed to deliver robust and sensitive quantitation of polychlorinated dibenzo-p-dioxins (PCDD), polychlorinated dibenzo furans (PCDF) and dioxin-like polychlorinated biphenyls (dl-PCBs), in food and feed samples in compliance with the latest EU regulations (EU Regulation 664/2017).



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TSQ 9000 Triple Quadrupole GC-MS/MS system with AEI source



Feature

Highly efficient ionization

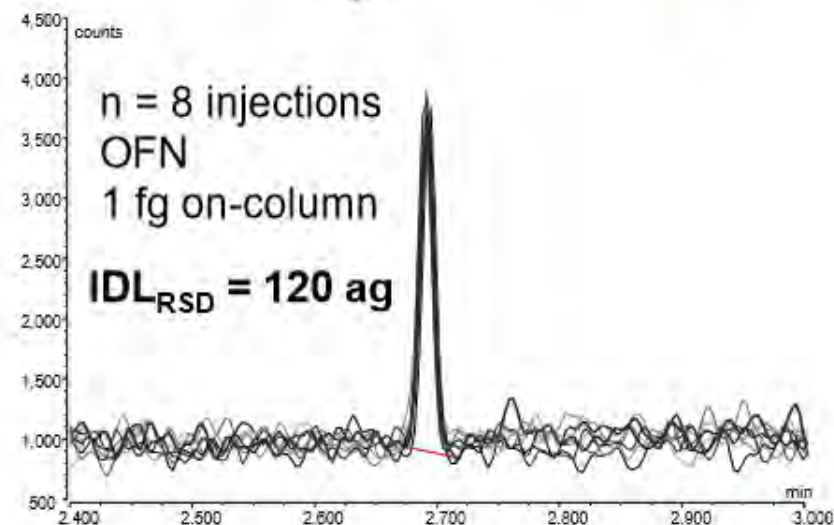
A more tightly focused ion beam

Benefit

A greater ion flux reaching the detector

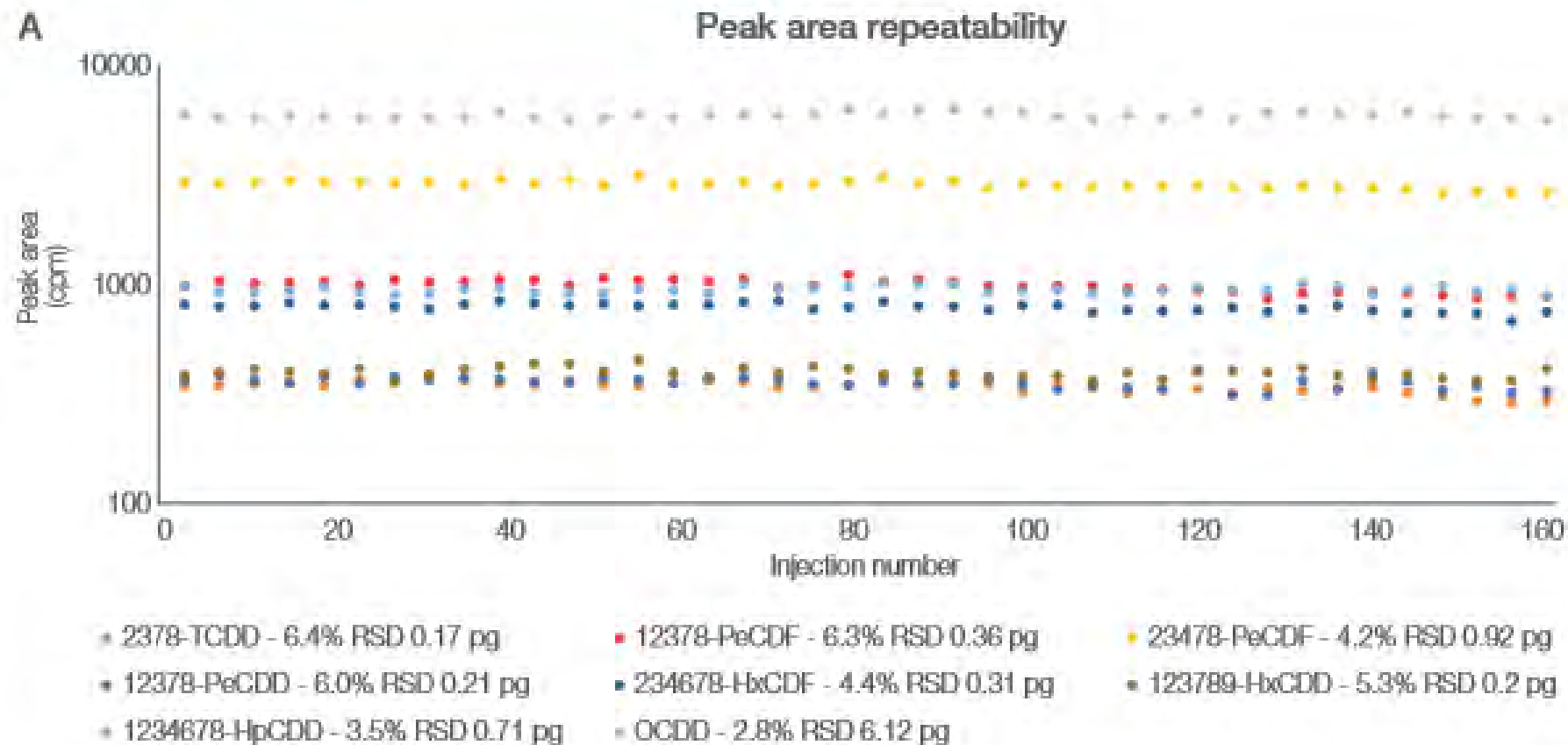
Less ion burn and a higher degree of robustness

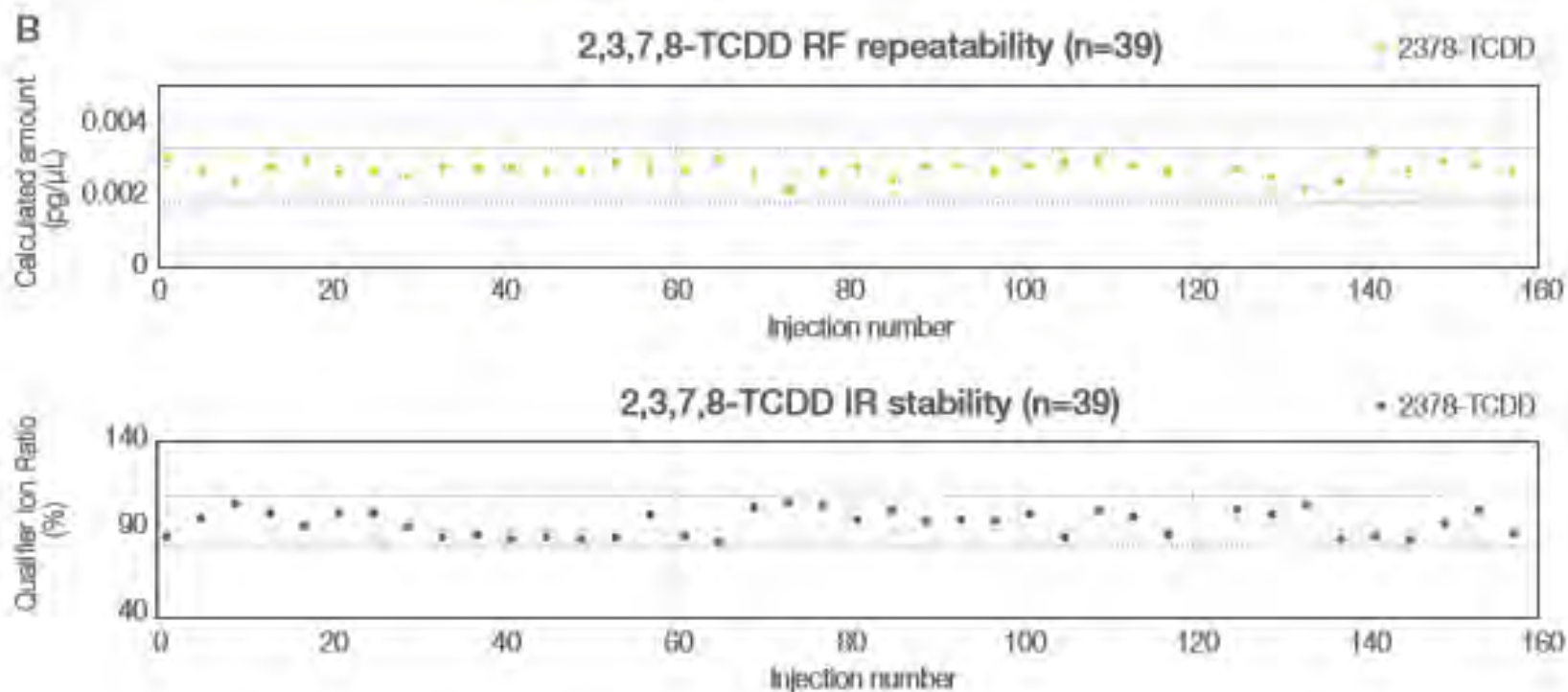
Thermo Scientific™ Advanced Electron Ionization (AEI) source



ThermoFisher
SCIENTIFIC

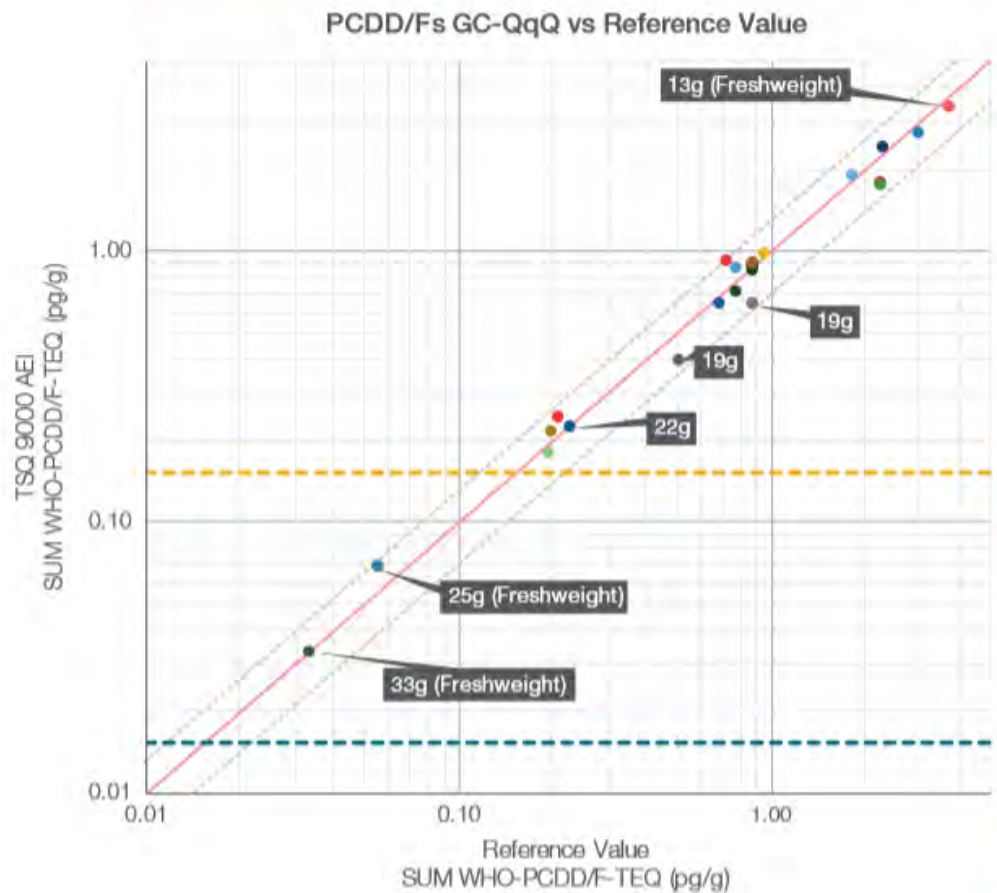
Consistent results over continuous analysis





(A) Absolute peak area repeatability over two weeks of analysis, for selected PCDD/F congeners in pooled matrix sample. Relative standard deviations and amounts on-column (pg) are annotated for each selected congener. **(B)** LOQ Response Factor (RF) deviation (upper plot, calculated as deviation from target amount) and Ion Ratio, IR, (lower plot) for the 10 fg on-column 2,3,7,8-TCDD congener (2.5 fg/μL, 4 μL injection).

Excellent match with EURL results on supplied samples



- QK1 - 1 Mixed fat
- QK1 - 2 Mixed fat
- QK1 - 3 Mixed fat
- QK1 - 4 Mixed fat
- QK1 - 5 Mixed fat
- QK1 - 6 Mixed fat
- QK7 Fish oil
- QK8 Meat
- QK9 Grass meal
- 1201-PLA 1 Pork sausage
- 1201-PLA 2 Pork sausage
- 1202-HEA 1 Whole egg
- 1302-MIA 1 Milk powder
- 1302-MIA 2 Milk powder
- 1501-AFB 1 Sugar beet pulp
- 1501-AFB 2 Sugar beet pulp
- 1601-HFA 1 Fish
- 1601-HFA 2 Fish
- 1401-SEA Sepiolite
- 1701-PFA PFAD
- 1301-FF Feed fat
- 1302-MIB Milk fat
- 9255 Meat
- 9373 Milk
- 9182 Eggs
- 9487 Fish
- 9488 Fish

Dioxin Analyzer Deployment Guide
For TSQ 9000 Mass Spectrometers

Quick Start Settings - Workflow

1. Sample Preparation
2. GC & Autosampler Configuration
3. Injection
4. Chromatography
5. Data Acquisition
6. System Specifications
7. Data Acquisition, Processing, and Reporting

Dioxin Analyzer documentation to guide user step-by-step through all phases of this workflow



Error-free execution of routine analysis

The eWorkflow™ procedures provide a pre-loaded template that captures the unique aspects of a chromatography workflow and guides the operator through a minimal number of choices needed to create a finalized sequence with predefined files and a well-defined method structure. The Dioxin Analyzer eWorkflow includes all pre-optimized SRM transitions, isotope dilution calculation and reporting templates for an error-free execution of the analysis to meet compliance requirements.

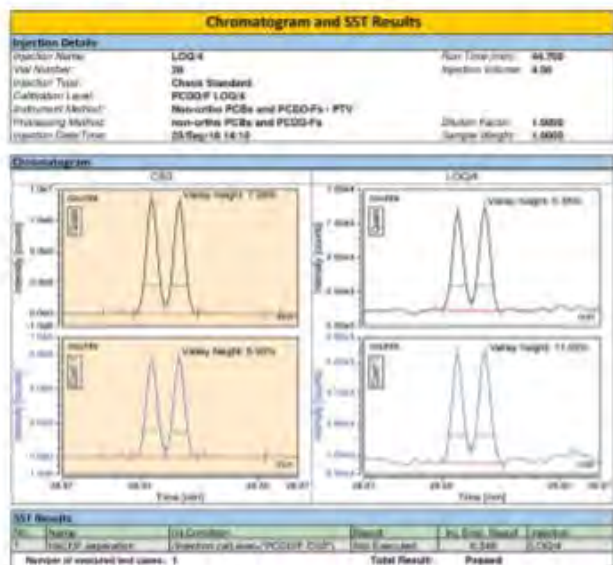
Interactive results pane with real-time updates

Interactive results pane showing ISTD recovery and ion ratio deviation (flagged red if outside limits) and upper, middle and lower-bound congener specific result. Sum WHO-PCDD/F-TEQ result and flag to indicate above/below maximum limit (top right). Ion ratio deviation and congener specific contribution to the WHO-PCDD/F-TEQ (bottom right).

Compliance control at a glance

Compliance tools are available in the results pane and dynamically updated during the data acquisition for easy and immediate checking of results, thus saving time. This template shows for instance, internal standard (ISTD) recovery and ion ratio deviation, using a color-coded flag to visually highlight compliance/noncompliance throughout the sequence. Dynamically updated calculation results for sample Toxicity Equivalent (TEQ) are also shown and color flagged for faster action in case the results are outside of the acceptable limits.

System suitability test report



System suitability results built into the method allow for intelligent run control, ensuring samples are only analyzed if the system passes specification, saving repeat analysis time, acquisition and processing of non-compliant data

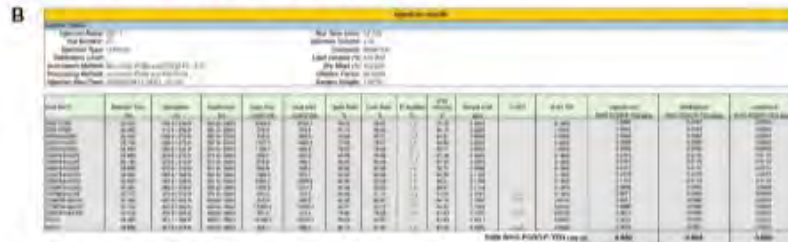
Built-in reporting tool

To simplify data reporting, the Dioxin Analyzer eWorkflow offers a comprehensive template that includes the required results and calculations to meet all quality and compliance requirements. This includes recovery for ¹³C-labeled standards, ion ratio, sum parameters, and LOQ flagging amongst other features. If needed, the Report Designer enables further customization to meet all reporting and charting requirements.

Comprehensive calibration report



Comprehensive sample report template



A. Key information includes average response factor, response factor deviation and ion ratio
 B. Key results include ¹³C-labeled standards recovery, ion ratio, sum parameters, LOQ flagging

Thank you.....

<http://www.scispec.co.th>

The image shows a screenshot of the SciSpec website. At the top, there is a navigation menu with the following items: HOME, OUR PRODUCTS, APPLICATIONS, SCIENCE STUDIO, ABOUT US, CONTACT US, and JOIN US. A search icon is located to the right of the JOIN US link. Below the navigation menu is a large banner for the 'New DUO! Orbitrap TRIBRID ECLIPSE & EXPLOR' product. The banner features the text 'New DUO! Orbitrap' in blue, 'TRIBRID ECLIPSE' in large red letters, and '& EXPLOR' in large blue letters. Below this, it says 'One System, Maximum Ins...' and has a 'Read More...' button with a colorful bar. To the left of the banner is a vertical image of a Thermo Scientific Orbitrap mass spectrometer. Below the banner is a search bar with the text 'ค้นหา แอปพลิเคชัน ที่คุณสนใจ' (Find the application you are interested in) and a search icon. Below the search bar are three colored boxes representing different application areas: a purple box for 'อาหารและสิ่งแวดล้อม' (Food and Environment) with subtext 'Safety, Authenticity, Contaminants', a blue box for 'ชีวโมเลกุล' (Molecular Biology) with subtext 'Genomics, Proteomics, Metabolomics, Lipidomics', and a dark blue box for 'คลีนิกและพิษวิทยา' (Clinical and Toxicology) with subtext 'Toxicology, Clinical, Forensics'. A green arrow points from the 'OUR PRODUCTS' menu item to the search bar.



QUESTIONS ?