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GC-MS with an Orbitrap? – Yes, with the GC-APPI Interface

Helmut Münster, MasCom Technologies

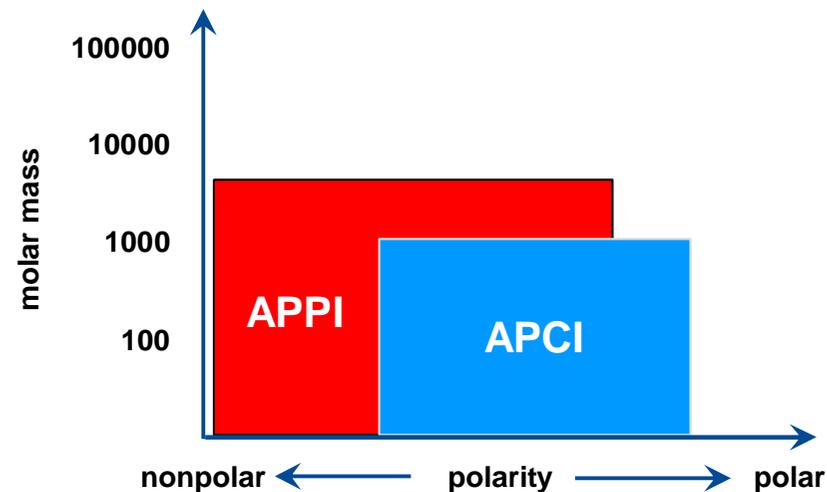
GC-APPI MS

- For many fields of application high resolution and accurate mass (HR/AM) analyses with both GC and LC are needed to allow the analysis of the broadest range of compounds.
- When no dedicated GC-HR/AM instrument is available, the only option is to interface a GC to an HR/AM instrument with an atmospheric pressure ionization (API) source.
- APPI: VUV radiation (124 nm = 10.4 eV).
Has potential to ionize a broader range of compounds than APCI (or ESI) alone, especially non-polar, highly aromatic, or species with electron delocalizations.

GC-APPI is now commercially available.

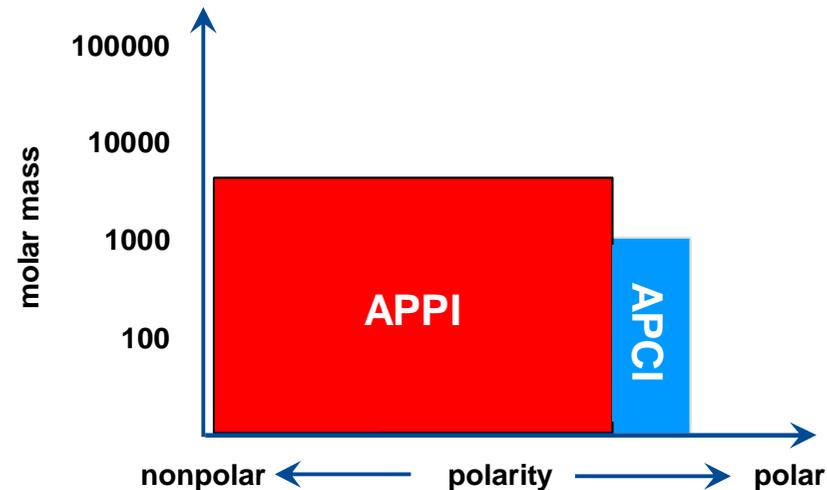
GC-Atmospheric Pressure Chemical Ionization (APCI)

- APCI: Corona discharge (chemical ionization via H_3O^+).
 - Introduced in 1973 by Horning, *et al.* (*Anal Chem*) and since then, fully commercialized; current ionization method of choice for GC-API.
 - Requires very strict control of source and environment to prevent ionization and corona/plasma fluctuations due to changing environmental and analyte gas compositions.
 - Can produce unpredictable, complex spectra due to extensive chemical reactions of the environmental, matrix, and analyte constituents.
 - Favors relatively polar compounds with ionization by protonation.



GC-Atmospheric Pressure Photo-ionization (APPI)

- APPI: VUV radiation (124 nm = 10.4 eV).
 - Ionization region can be hermetically isolated from surrounding environment, thus potentially promising high stability, low background, and low adduct formation.
 - Has potential to ionize a broader range of compounds than APCI (or ESI) alone, especially non-polar, highly aromatic, or species with electron delocalizations.
 - *As yet, GC-APPI has started being used in research – the capabilities of GC-APPI are not yet fully explored.*



Haapala, et al.
Luosujärvi, et al.
Luosujärvi, et al.

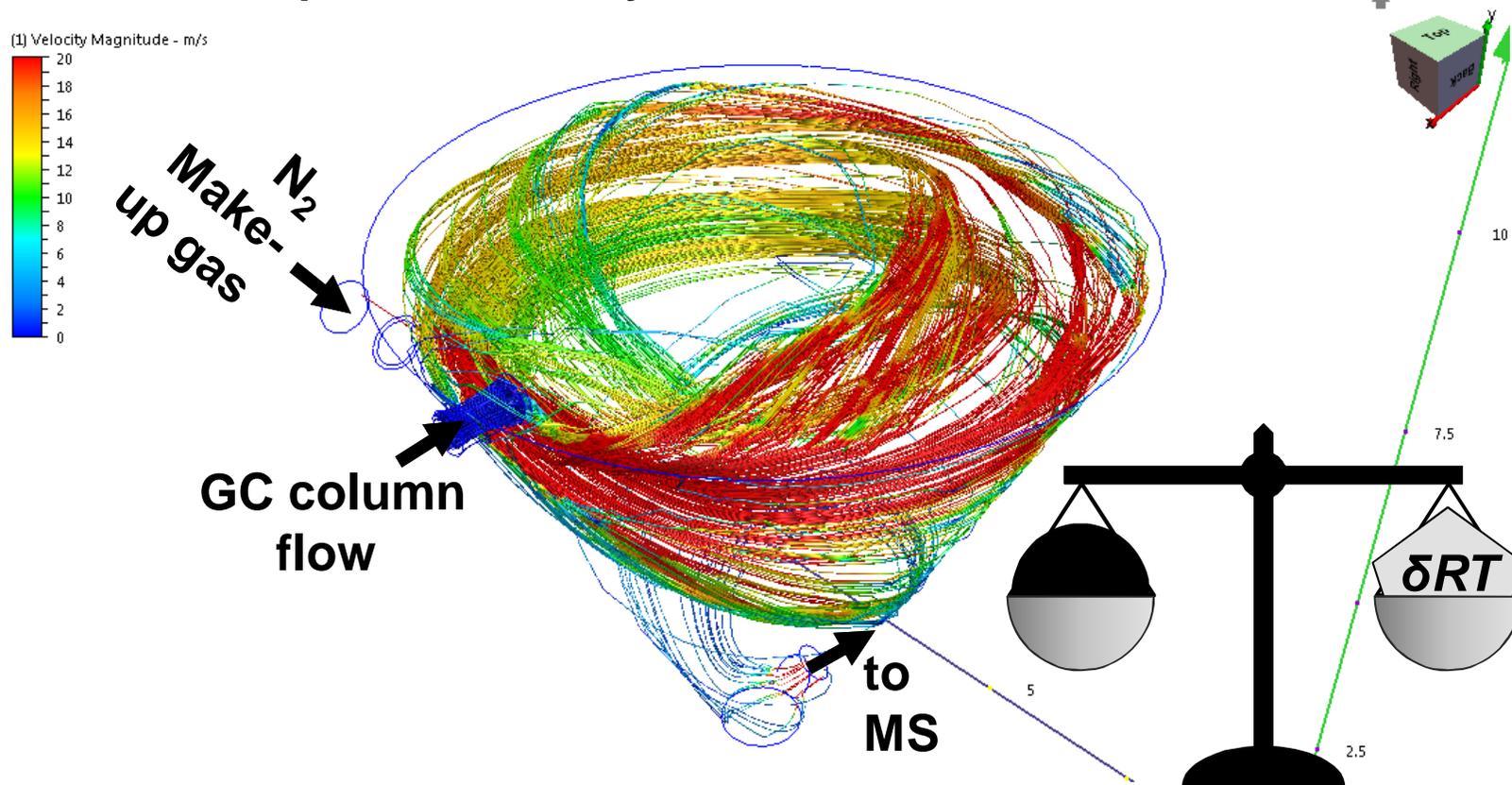
Anal Chem 2007
Rapid Comm Mass Spectrom 2008
J Amer Soc Mass Spectrom 2010

Hintikka, et al.
Lee, et al.
Souminen, et al.

J Chromatogr A 2010
Mass Spectrom Lett 2012
Anal Chim Acta 2013

GC-APPI ionization region vortex flow

Computation fluid dynamic simulation of the column flow

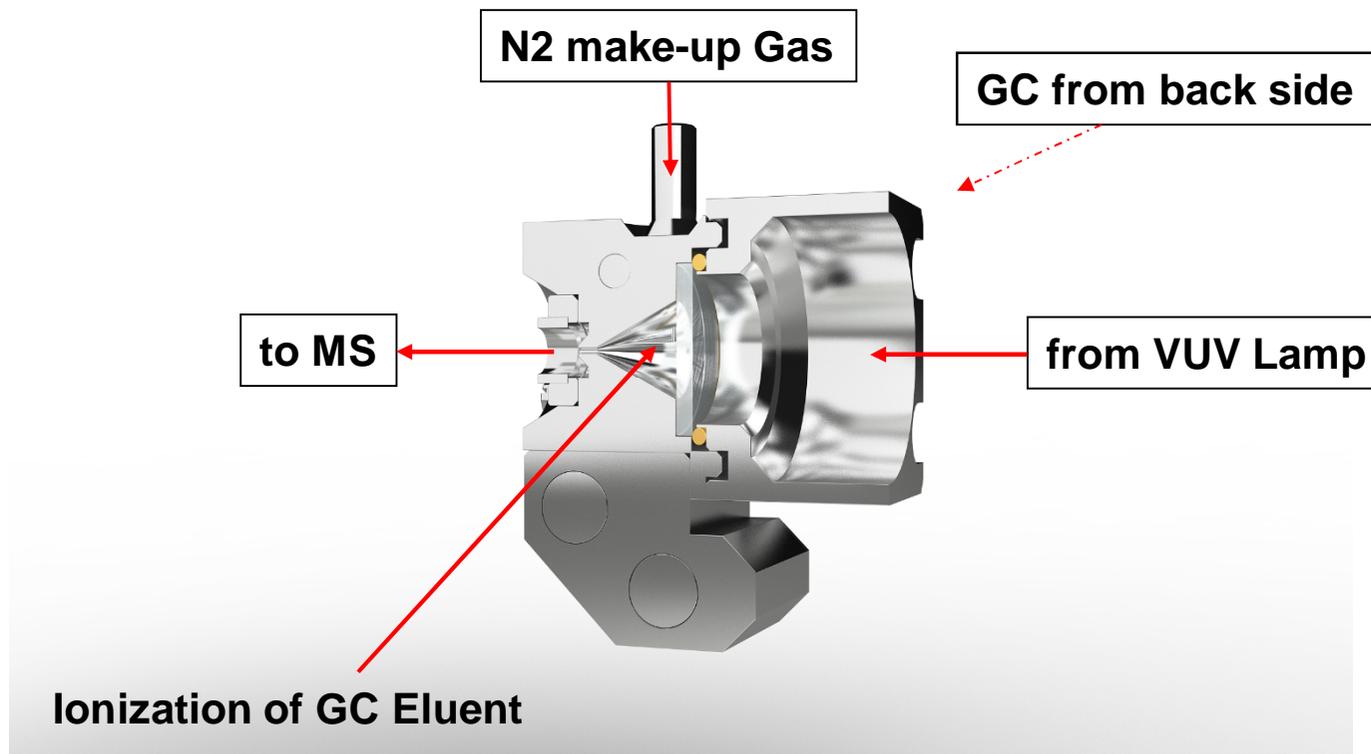


The vortex flow path strikes a balance between chromatographic fidelity and residence time of the compound for higher ionization efficiency.

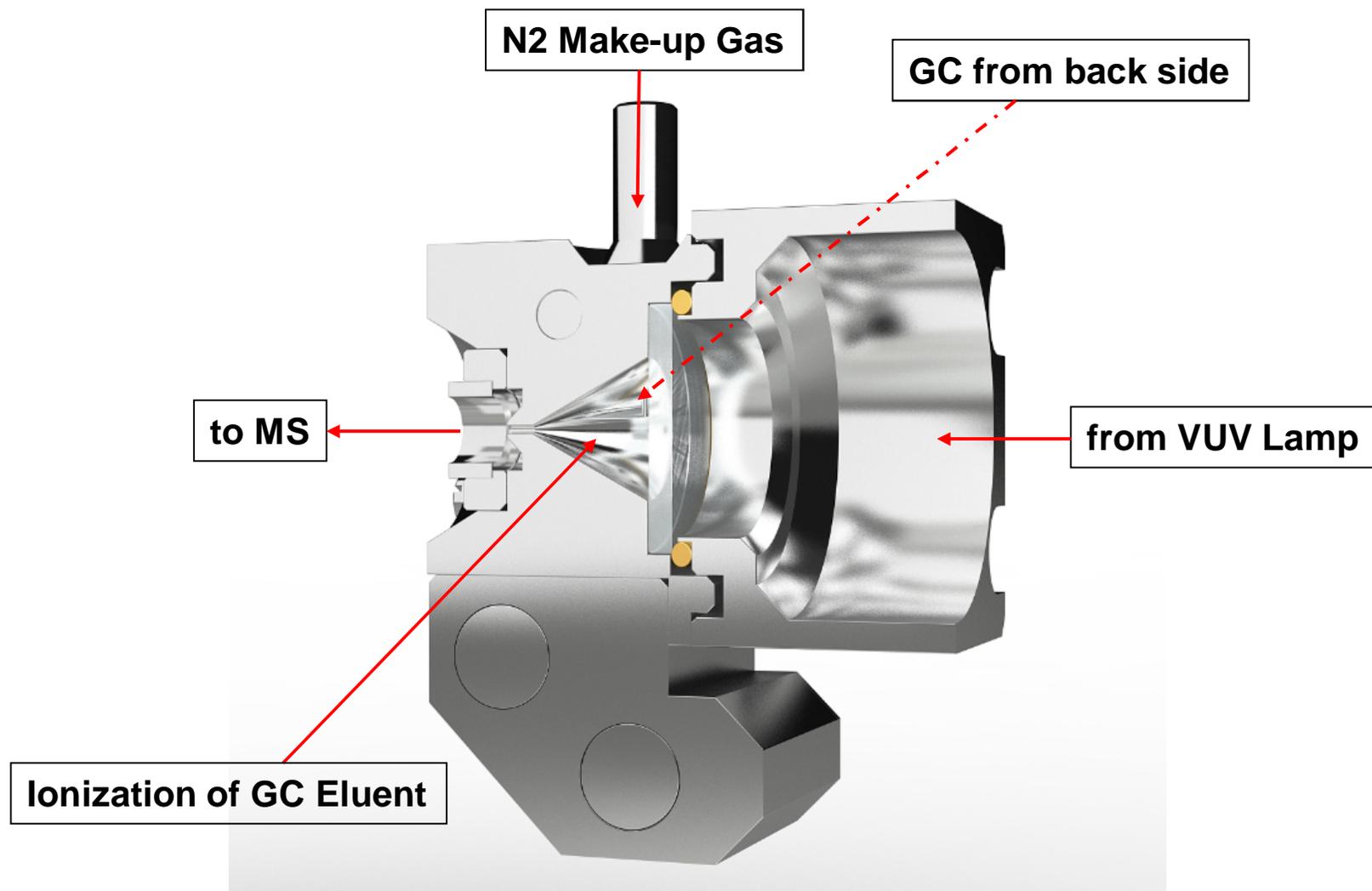
Slide used with permission from A. Peterson, Thermo Fisher Scientific

GC-APPI Interface

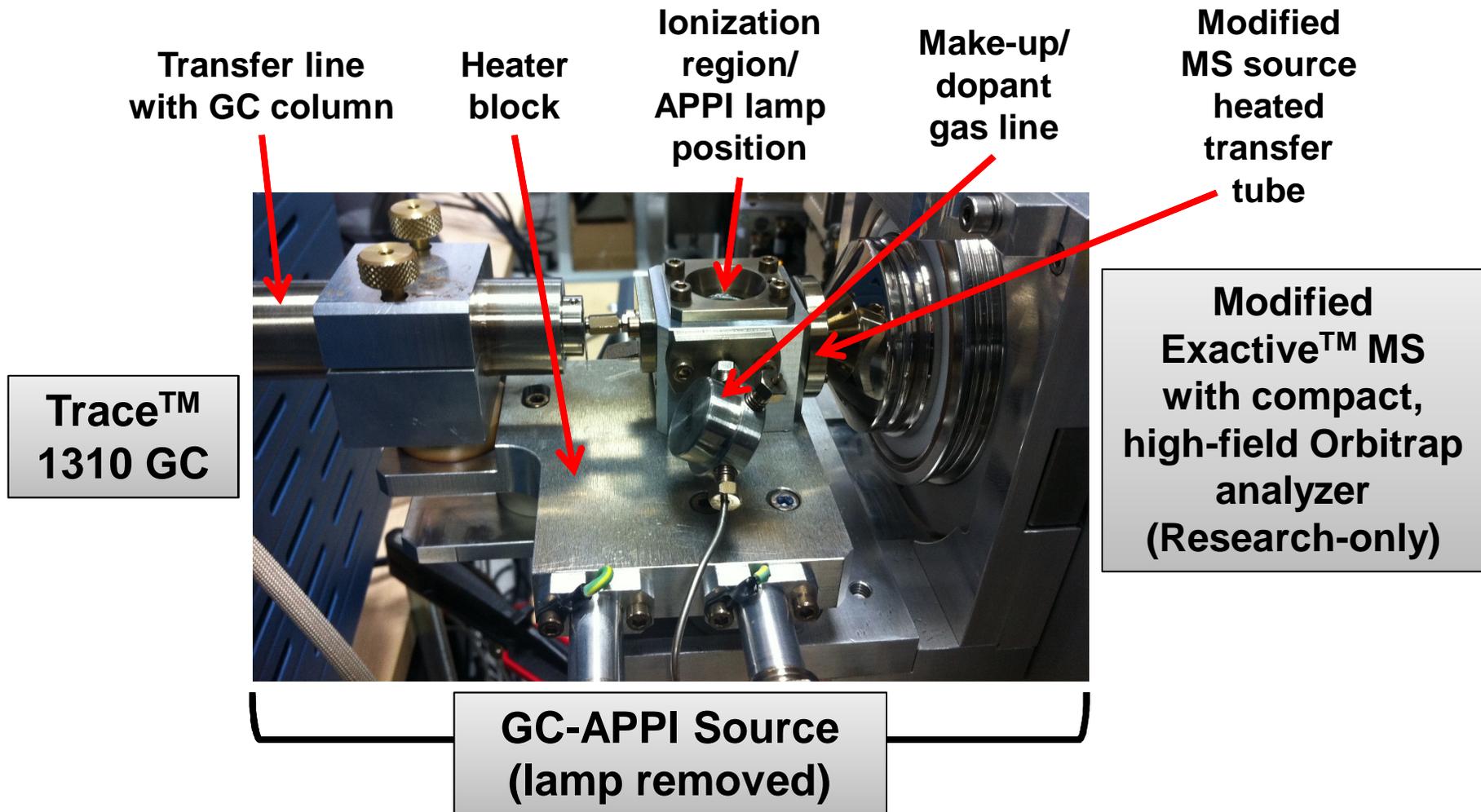
- *The GC-APPI source employs the concept of a sealed, clean ionization region flushed with highly pure N₂*



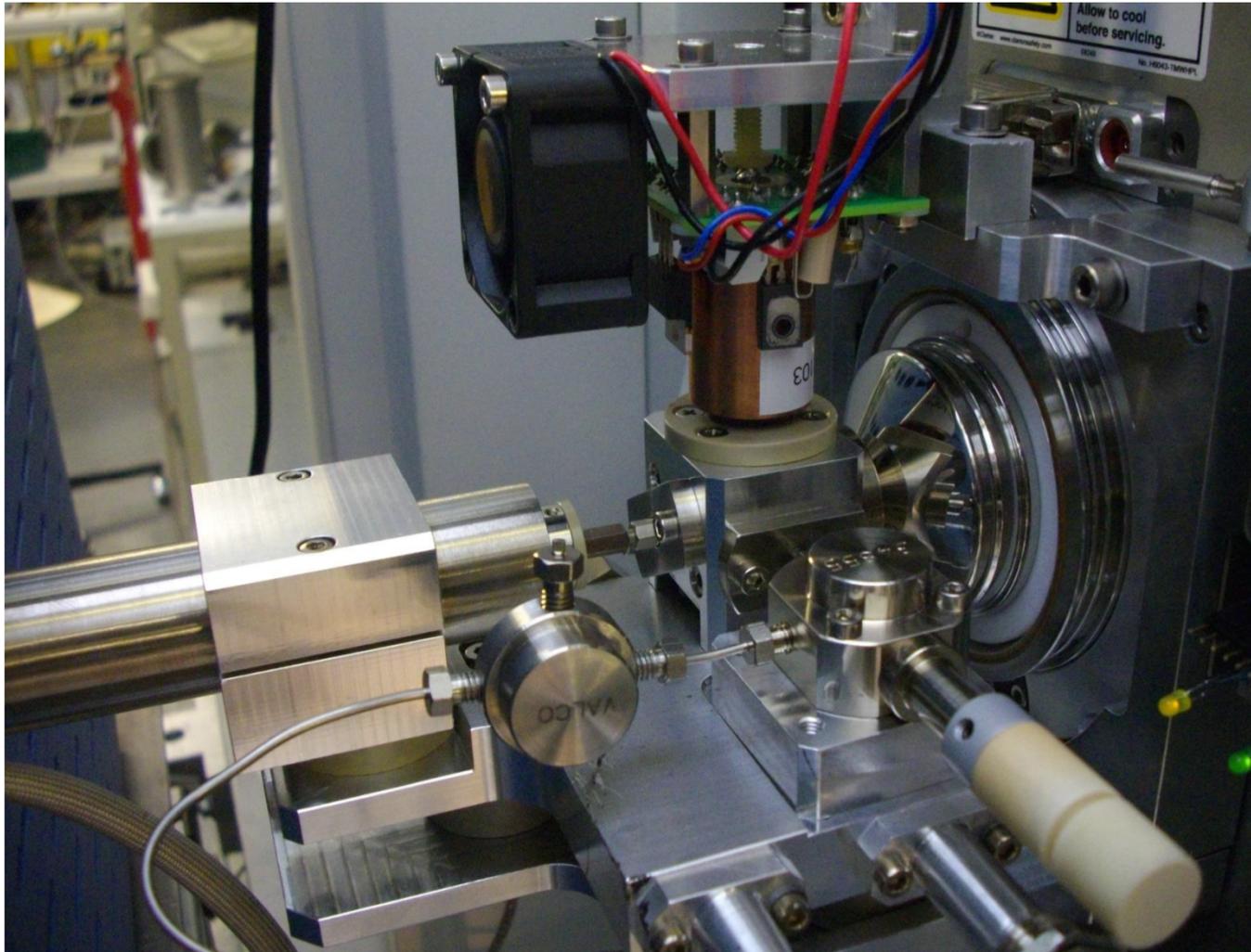
GC-APPI Interface



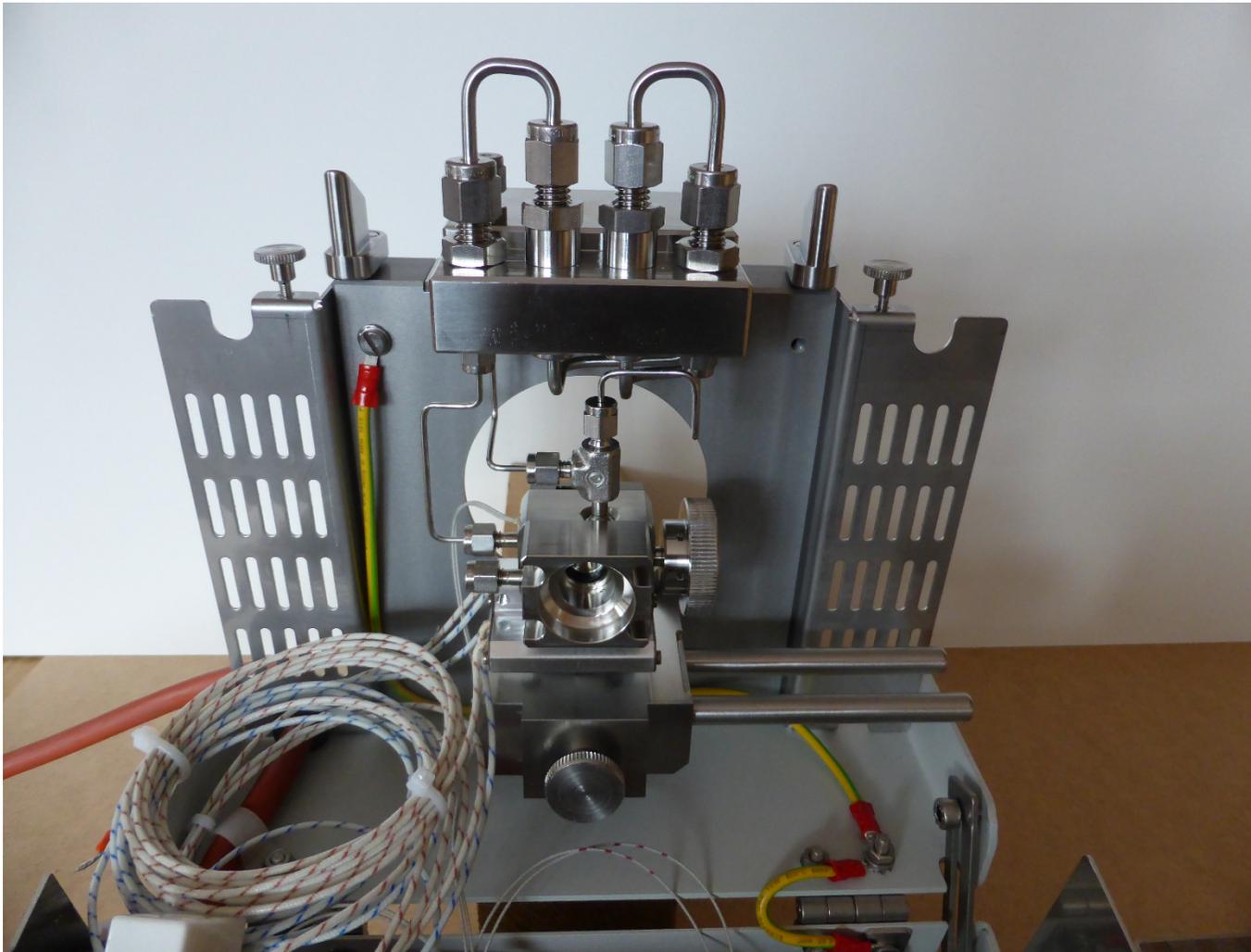
GC-APPI/Orbitrap MS setup in R&D



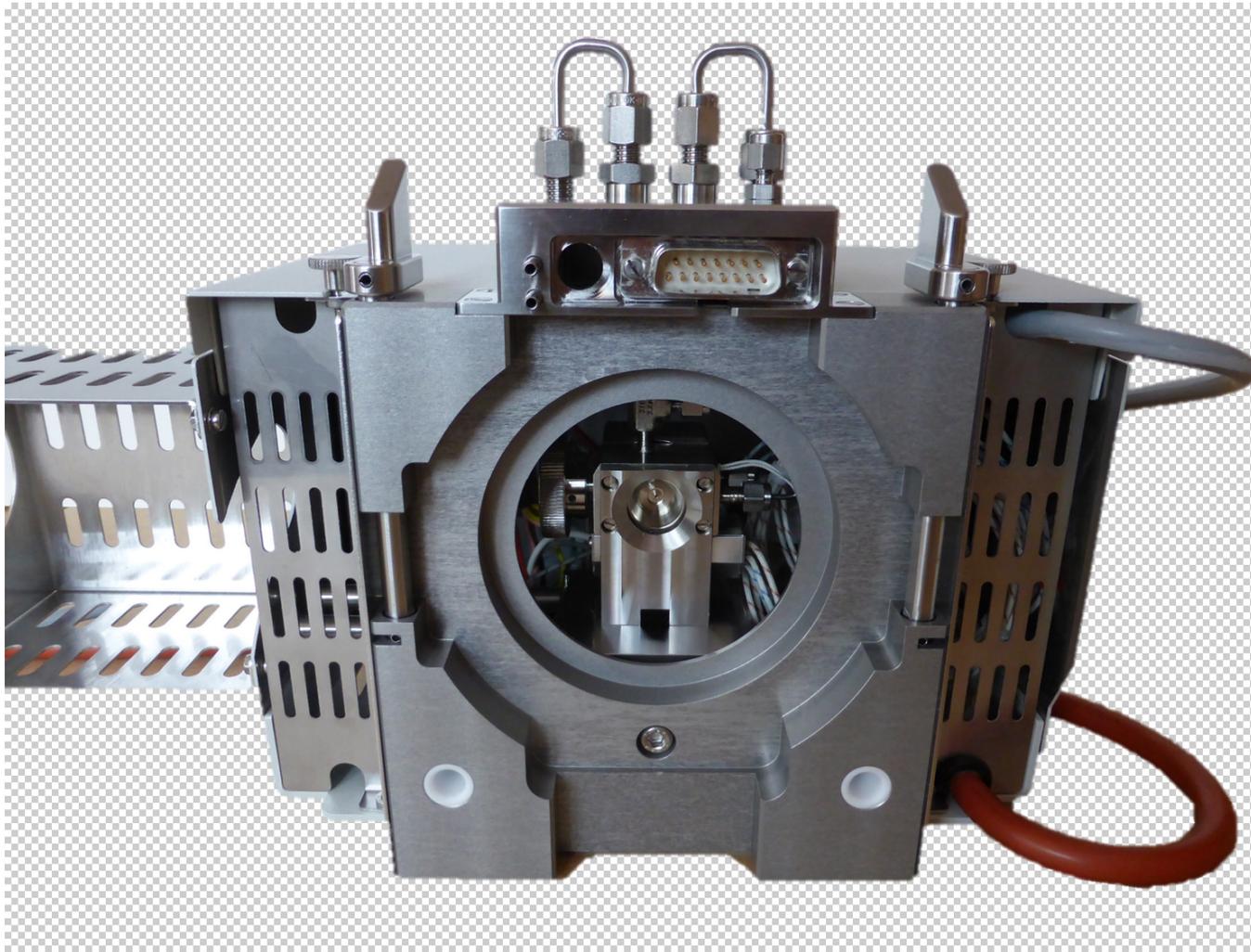
GC-APPI/Lamp MS setup in R&D with Lamp



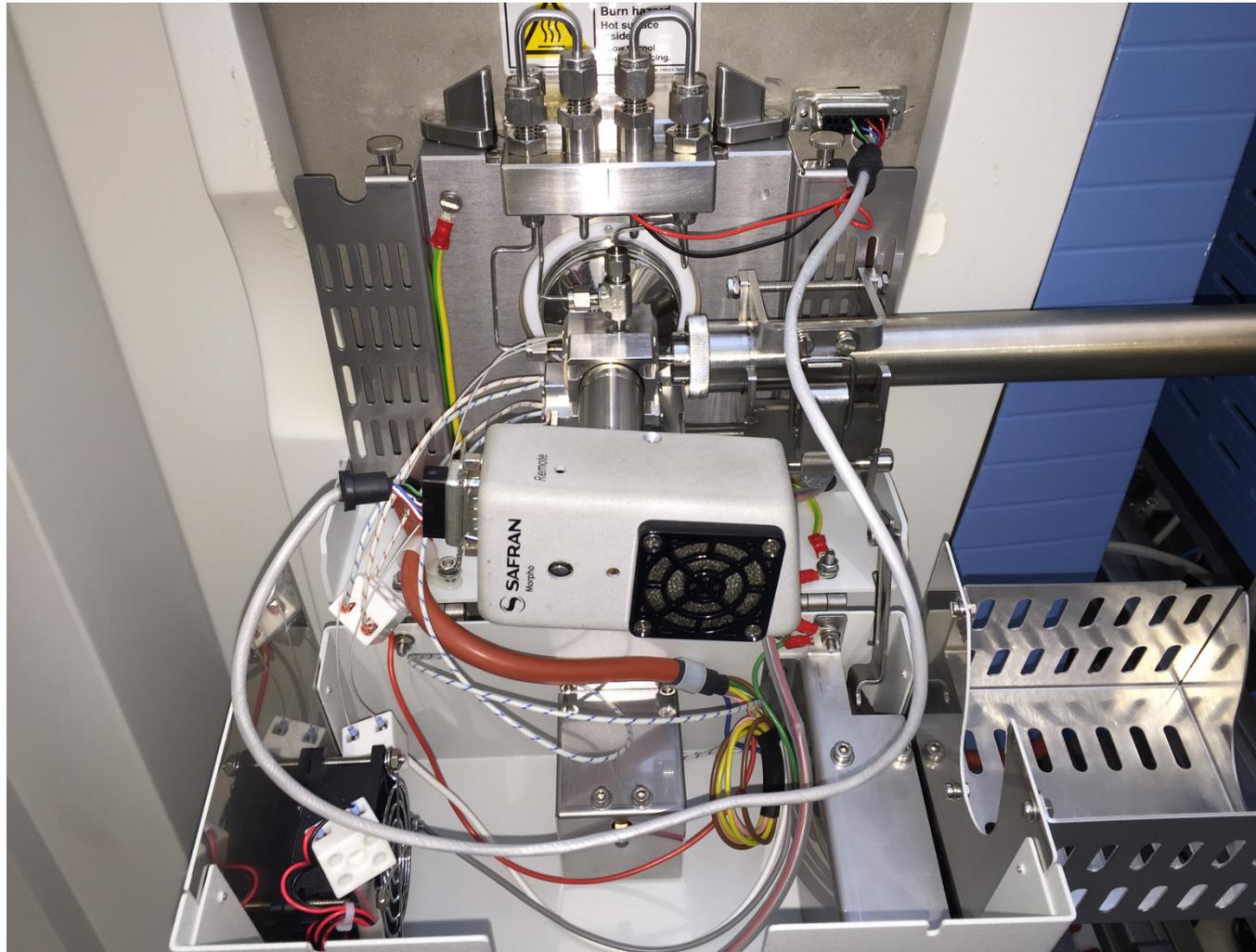
GC-APPI Interface - Prototype



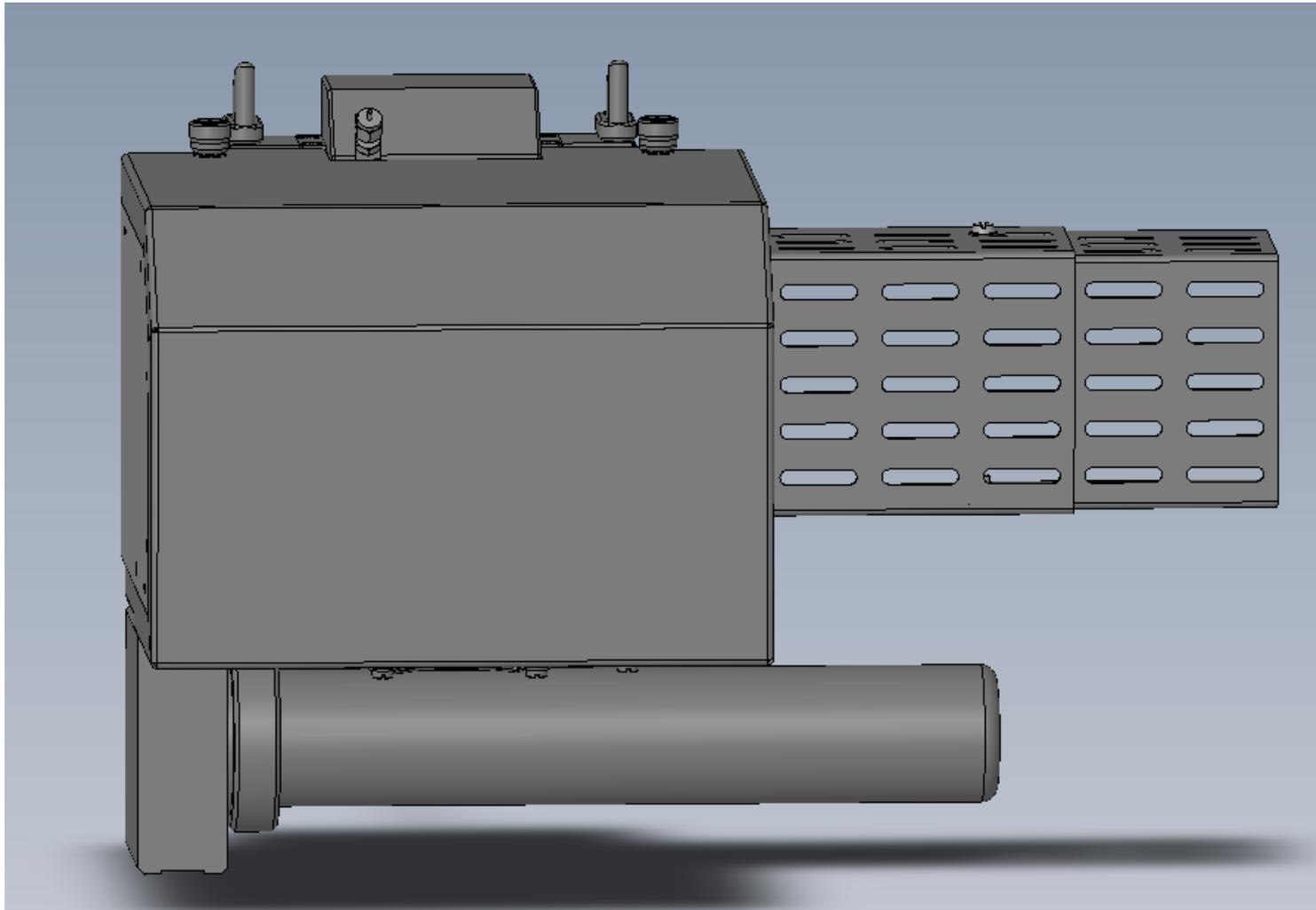
GC-APPI Interface - Prototype



GC-APPI Interface - Prototype



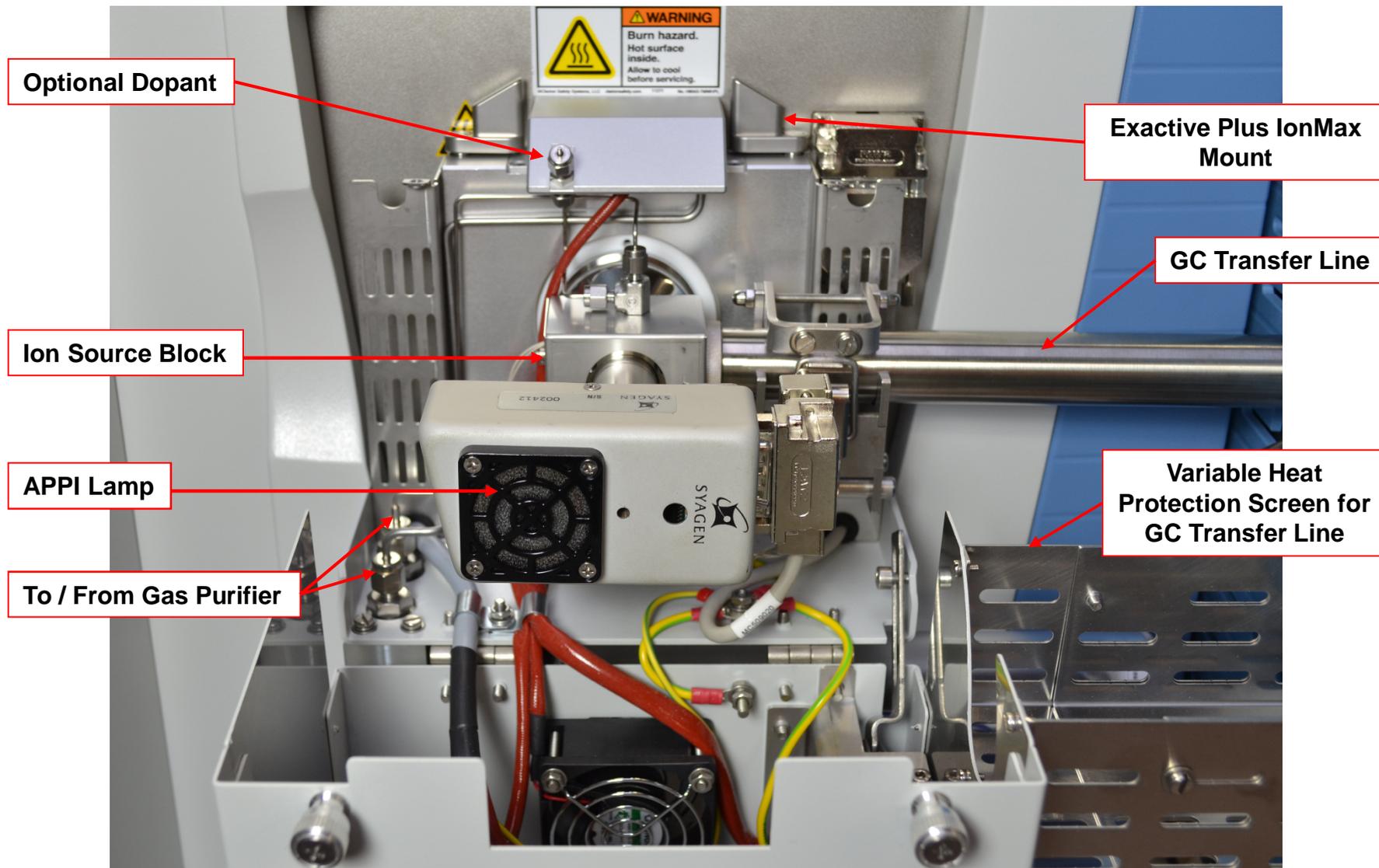
GC-APPI Interface – Final Version



GC-APPI Interface – Final Version



GC-APPI Interface – Final Version - Details



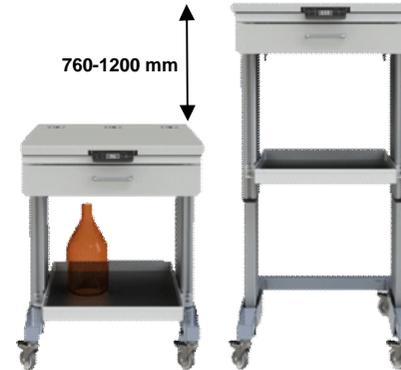
GC-APPI Interface – Final Version



GC-APPI Interface – Optional Items



Trace 1310 GC with Transfer Line



Adjustable GC Table



Transfer Line



**Power Supply for Ion Source Block Heaters,
necessary if no Thermo GC is used.**

GC-APPI Measurements: EPA8270 Mix

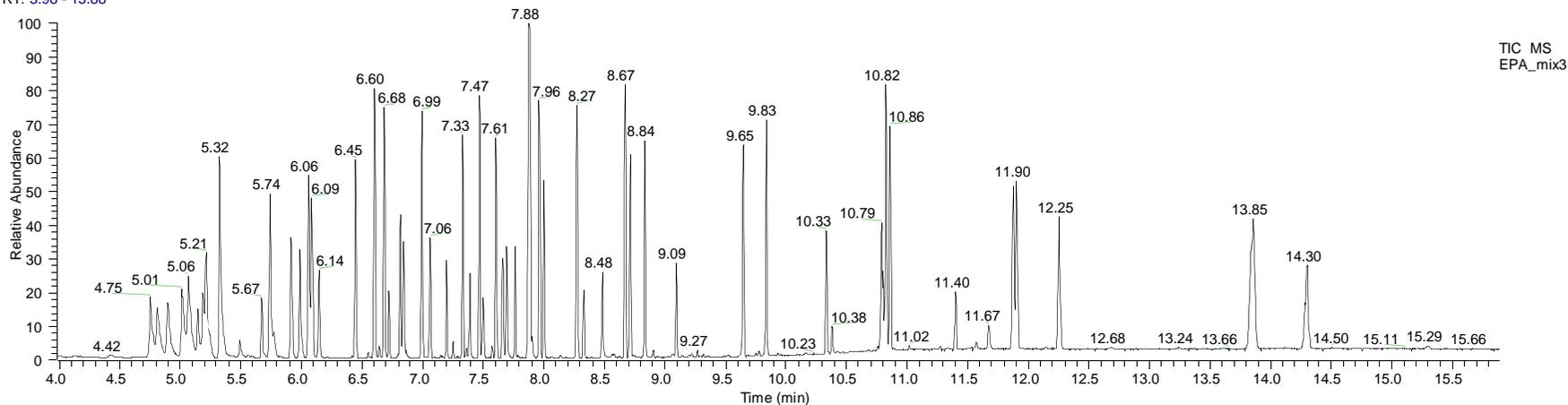
Experimental Conditions

- Sample:** EPA8270 (74 Compounds @ 0.1 ng/uL)
- Injection:** 1 uL
- GC-MS:** Exactive Plus with GC-APPI Interface, Trace 1310 GC and RSH Autosampler
- MS:** APPI Source Temperature – 300 deg C, without Dopant
Scan Range 50-500 amu @ R=35.000 (4 Hz Cycle Time)
- GC:** SSL Injector – Temperature 300 deg C
Oven – 50 deg C for 1.5 min – 320 deg C with 30 deg C / min.
Flow – 1.5 mL/min.
Transfer Line Temperature – 300 deg C

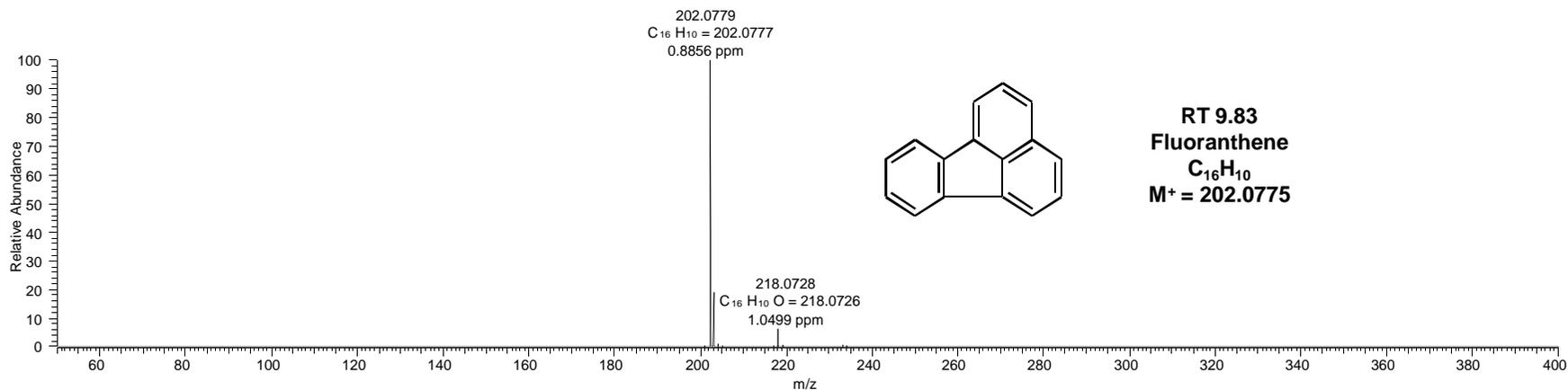
GC-APPI Measurements – EPA 8270 Mix

C:\a_Data\...\GC-APPI\data\EPA_mix3
new column 30mDB5 0.25 0.25

RT: 3.98 - 15.88

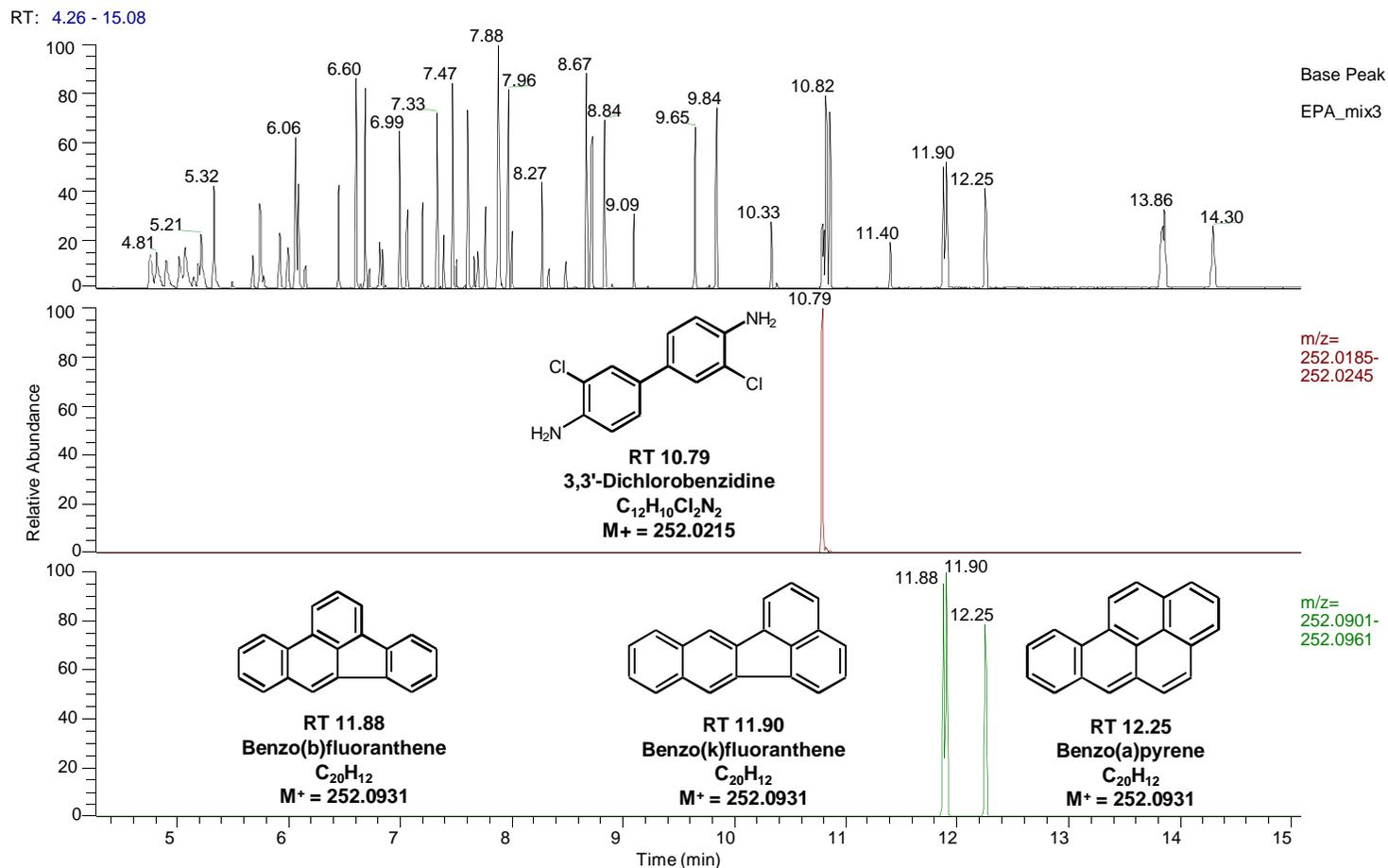


EPA_mix3 RT: 9.83



Measurement done @ 35,000 Resolution Power

GC-APPI Measurements – EPA 8270 Mix



Measurement done @ 35,000 Resolution Power

GC-APPI Measurements – EPA 8270 Mix

Analyte	Formula	Exact Mass	Detect Mass
N-Nitrosodimethylamine	C ₂ H ₆ N ₂ O	74.0474	
Pyridine	C ₅ H ₅ N	79.0416	
Aniline	C ₆ H ₇ N	93.0572	M ⁺
Phenol	C ₆ H ₆ O	94.0412	M ⁺
2-Methylphenol	C ₇ H ₈ O	108.0568	M ⁺
3-Methylphenol	C ₇ H ₈ O	108.0568	M ⁺
4-Methylphenol	C ₇ H ₈ O	108.0568	M ⁺
Benzyl Alcohol	C ₇ H ₈ O	108.0568	M ⁺
Benzoic Acid	C ₇ H ₆ O ₂	122.0361	
2,4-Dimethylphenol	C ₈ H ₁₀ O	122.0724	M ⁺
Nitrobenzene	C ₆ H ₅ NO ₂	123.0314	M ⁺
4-Chloroaniline	C ₆ H ₆ ClN	127.0183	M ⁺
2-Chlorophenol	C ₆ H ₅ ClO	128.0023	M ⁺
Naphthalene	C ₁₀ H ₈	128.0619	M ⁺
N-Nitrosodi-n-propylamine	C ₆ H ₁₄ N ₂ O	130.1098	M+H ⁺
2,4-Dinitrotoluene	C ₇ H ₆ N ₂ O	134.0474	M ⁺
2,6-Dinitrotoluene	C ₇ H ₆ N ₂ O	134.0474	M ⁺
2-Nitroaniline	C ₆ H ₆ N ₂ O ₂	138.0423	M ⁺
3-Nitroaniline	C ₆ H ₆ N ₂ O ₂	138.0423	M ⁺
4-Nitroaniline	C ₆ H ₆ N ₂ O ₂	138.0423	M ⁺
Isophorone	C ₉ H ₁₄ O	138.1036	M+H ⁺
2-Nitrophenol	C ₆ H ₅ NO ₃	139.0263	M ⁺
4-Nitrophenol	C ₆ H ₅ NO ₃	139.0263	M ⁺
Bis(2-chloroethyl) Ether	C ₄ H ₈ Cl ₂ O	141.9946	
4-Chloro-3-methylphenol	C ₇ H ₇ ClO	142.0179	M ⁺
1-Methylnaphthalene	C ₁₁ H ₁₀	142.0775	M ⁺

Analyte	Formula	Exact Mass	Detect Mass
2-Methylnaphthalene	C ₁₁ H ₁₀	142.0775	M ⁺
1,2-Dichlorobenzene	C ₆ H ₄ Cl ₂	145.9685	M ⁺
1,3-Dichlorobenzene	C ₆ H ₄ Cl ₂	145.9685	M ⁺
1,4-Dichlorobenzene	C ₆ H ₄ Cl ₂	145.9685	M ⁺
Acenaphthylene	C ₁₂ H ₈	152.0619	M ⁺
Acenaphthene	C ₁₂ H ₁₀	154.0775	M ⁺
Bis(2-chloroethoxy)methane	C ₅ H ₁₀ Cl ₂ O ₂	156.0102	
2,4-Dichlorophenol	C ₆ H ₄ Cl ₂ O	161.9634	M ⁺
2-Chloronaphthalene	C ₁₀ H ₇ Cl	162.0230	M ⁺
Fluorene	C ₁₃ H ₁₀	166.0775	M ⁺
Carbazole	C ₁₂ H ₉ N	167.0728	M ⁺
1,3-Dinitrobenzene	C ₆ H ₄ N ₂ O ₄	168.0165	M ⁺
Dibenzofuran	C ₁₂ H ₈ O	168.0568	M ⁺
Diphenylamine	C ₁₂ H ₁₁ N	169.0884	M ⁺
Bis(1-chloroisopropyl) Ether	C ₆ H ₁₂ Cl ₂ O	170.0258	
Anthracene	C ₁₄ H ₁₀	178.0775	M ⁺
Phenanthrene	C ₁₄ H ₁₀	178.0775	M ⁺
1,2,4-Trichlorobenzene	C ₆ H ₃ Cl ₃	179.9296	M ⁺
2,4-Dinitrophenol	C ₆ H ₄ N ₂ O ₅	184.0114	M ⁺
Dimethyl Phthalate	C ₁₀ H ₁₀ O ₄	194.0571	M ⁺
2,4,5-Trichlorophenol	C ₆ H ₃ Cl ₃ O	195.9245	M ⁺
2,4,6-Trichlorophenol	C ₆ H ₃ Cl ₃ O	195.9245	M ⁺
4,6-Dinitro-2-methylphenol	C ₇ H ₆ N ₂ O ₅	198.0270	M ⁺
N-Nitrosodiphenylamine	C ₁₂ H ₁₀ N ₂ O	198.0786	M ⁺
Fluoranthene	C ₁₆ H ₁₀	202.0775	M ⁺
Pyrene	C ₁₆ H ₁₀	202.0775	M ⁺

Analyte	Formula	Exact Mass	Detect Mass
4-Chlorophenyl Phenyl Ether	C ₁₂ H ₉ ClO	204.0335	M ⁺
Diethyl Phthalate	C ₁₂ H ₁₄ O ₄	222.0883	F ⁺
Benz(a)anthracene	C ₁₈ H ₁₂	228.0931	M ⁺
Chrysene	C ₁₈ H ₁₂	228.0931	M ⁺
2,3,4,6-Tetrachlorophenol	C ₆ H ₂ Cl ₄ O	229.8856	M ⁺
Hexachloroethane	C ₂ Cl ₆	233.8129	
4-Bromophenyl Phenyl Ether	C ₁₂ H ₉ BrO	247.9829	M ⁺
3,3'-Dichlorobenzidine	C ₁₂ H ₁₀ Cl ₂ N ₂	252.0215	M ⁺
Benzo(a)pyrene	C ₂₀ H ₁₂	252.0931	M ⁺
Benzo(b)fluoranthene	C ₂₀ H ₁₂	252.0931	M ⁺
Benzo(k)fluoranthene	C ₂₀ H ₁₂	252.0931	M ⁺
Hexachlorobutadiene	C ₄ Cl ₆	257.8129	M ⁺
Pentachlorophenol (PCP)	C ₆ HCl ₅ O	263.8467	M ⁺
Hexachlorocyclopentadiene	C ₅ Cl ₆	269.8129	M ⁺
Benzo(g,h,i)perylene	C ₂₂ H ₁₂	276.0931	M ⁺
Indeno(123-cd)pyrene	C ₂₂ H ₁₂	276.0931	M ⁺
Dibenz(a,h)anthracene	C ₂₂ H ₁₄	278.1087	M ⁺
Di-n-butyl Phthalate	C ₁₆ H ₂₂ O ₄	278.1507	M+H ⁺
Hexachlorobenzene	C ₆ Cl ₆	281.8129	M ⁺
Butyl Benzyl Phthalate	C ₁₉ H ₂₀ O ₄	312.1351	M+H ⁺
Bis(2-ethylhexyl) Phthalate	C ₂₄ H ₃₈ O ₄	390.2755	M+H ⁺
Di-n-octyl Phthalate	C ₂₄ H ₃₈ O ₄	390.2755	M+H ⁺

> 88% detected

GC-APPI Measurements – Dioxins (TCDD)

Experimental Conditions

Sample: $^{13}\text{C}_{12}$ -Tetra-Chloro-Dibenzo-Dioxin (TCDD) @ 5 pg/uL

Injection: 1 uL

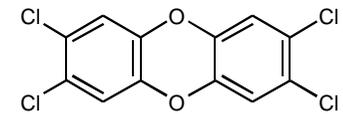
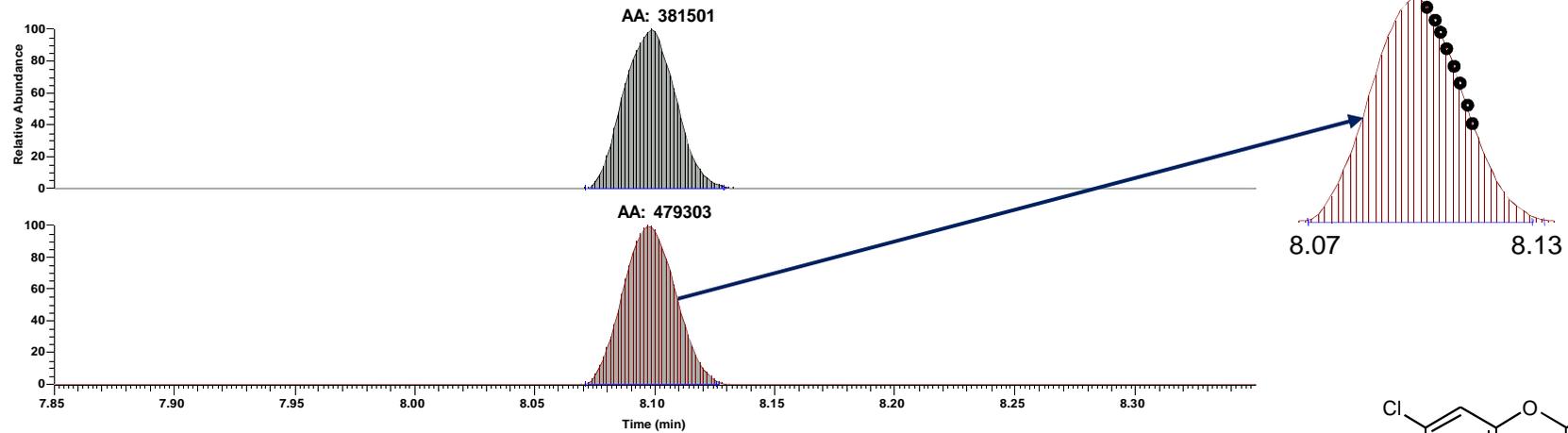
GC-MS: Exactive with GC-APPI Interface, Trace 1310 GC

MS: APPI Source Temperature – 300 deg C, with Dopant (CS_2)
Scan Range 50-500 amu @ R=10.000 (10 Hz Cycle Time)

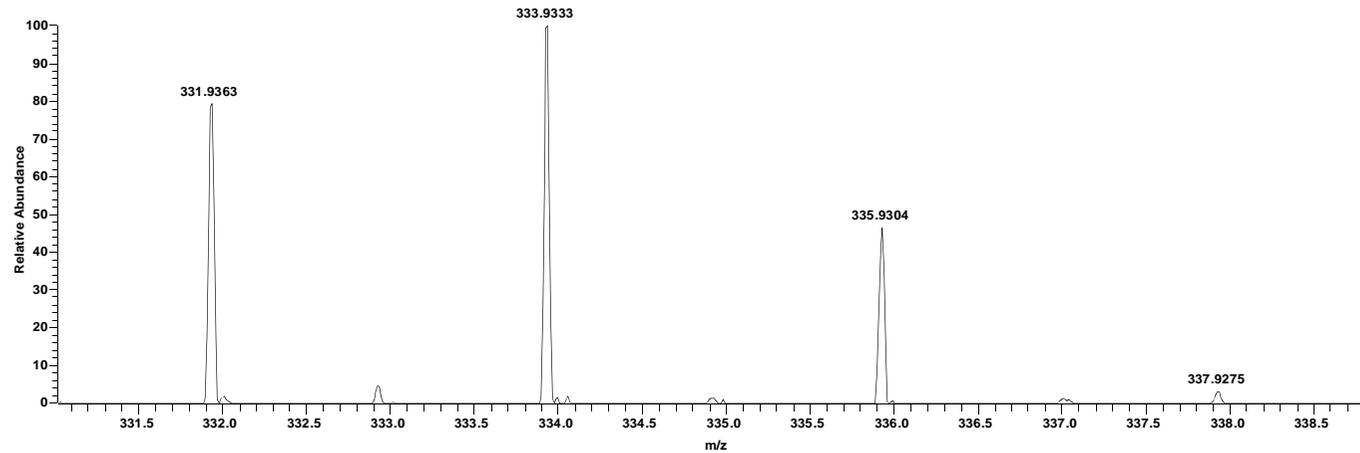
GC: SSL Injector – Temperature 300 deg C
Oven – 120 deg C for 1.5 min – 320 deg C with 30 deg C / min.
Flow – 1.5 mL/min.
Transfer Line Temperature – 300 deg C

GC-APPI Measurements – Dioxins (TCDD)

5 pg $^{13}\text{C}_{12}$ -TCDD on column



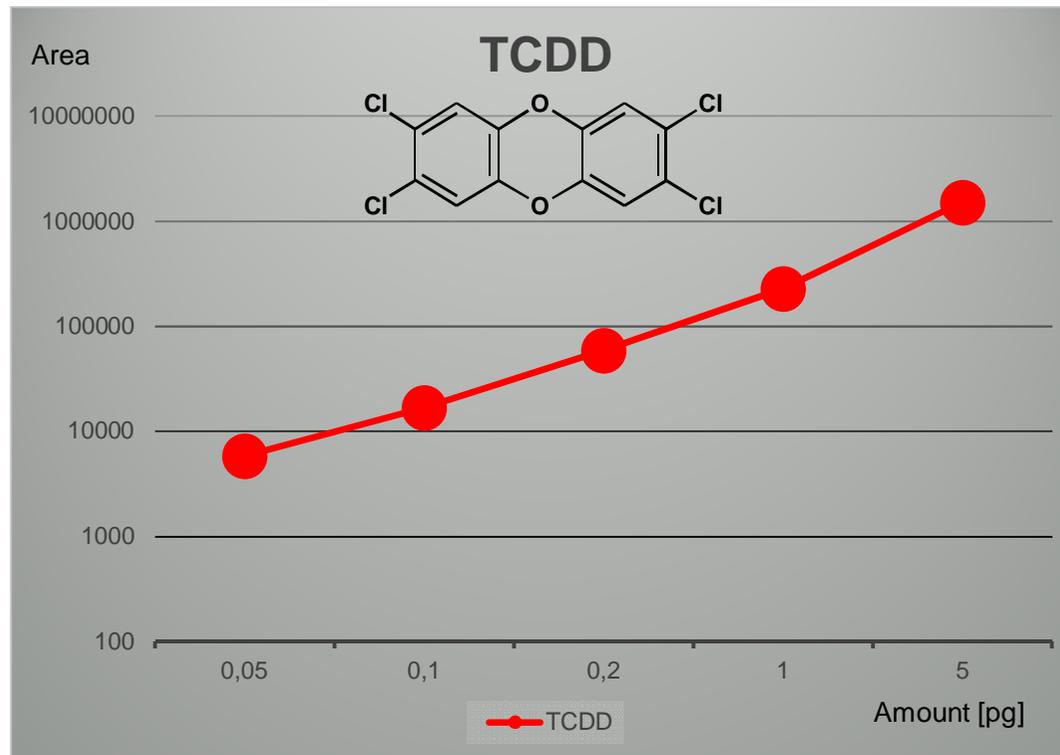
$^{13}\text{C}_{12}$ -2,3,7,8-TCDD



Measurement done @ 10,000 Resolution Power

GC-APPI Measurements – Dioxins (TCDD)

0.05 pg to 5 pg 2378-TCDD on column



Measurement done @ 35,000 Resolution Power

GC-APPI Measurements - Pesticides

Experimental Conditions

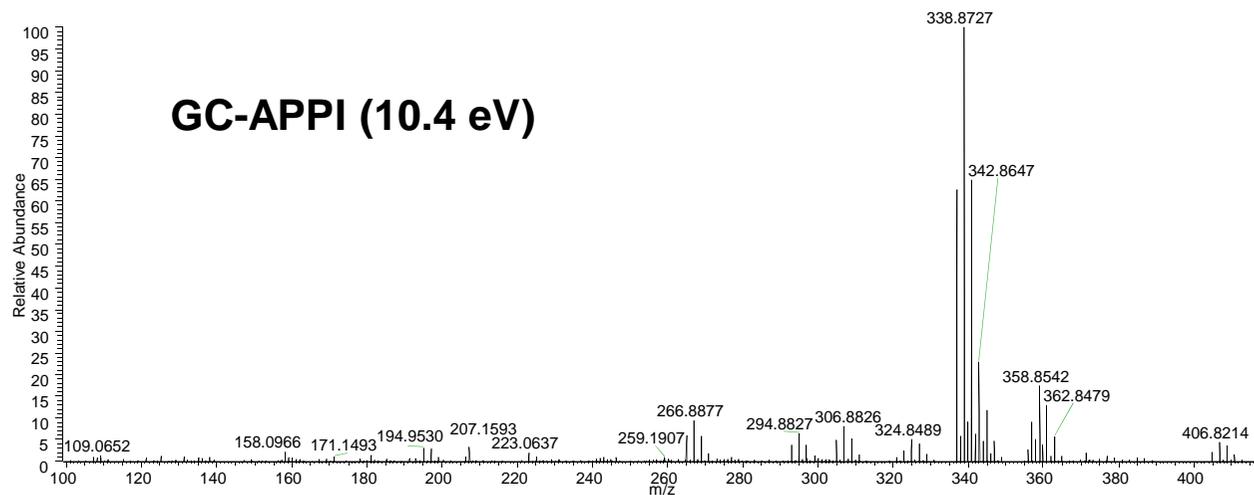
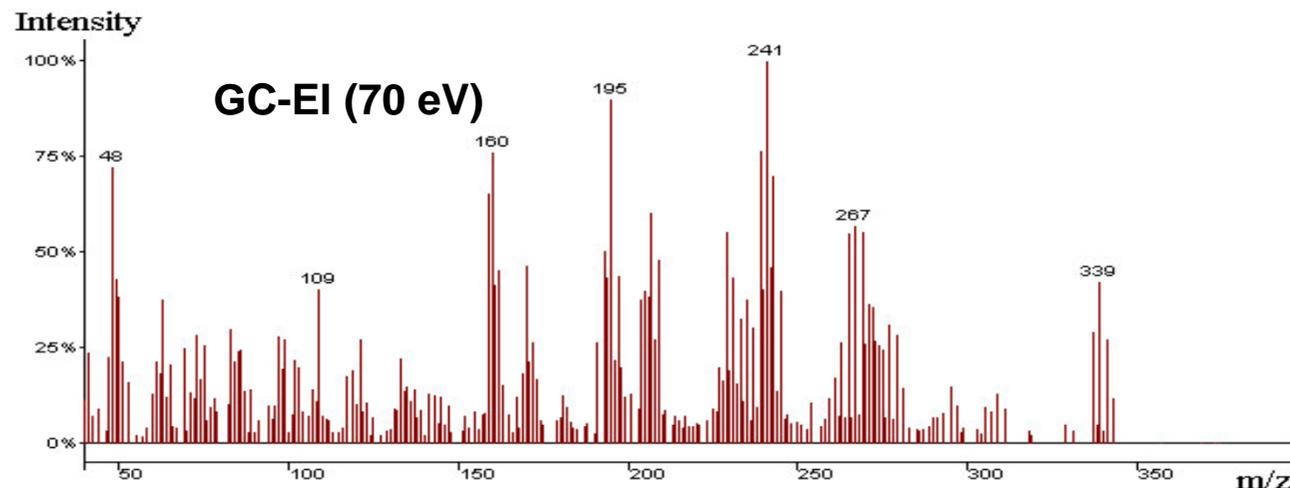
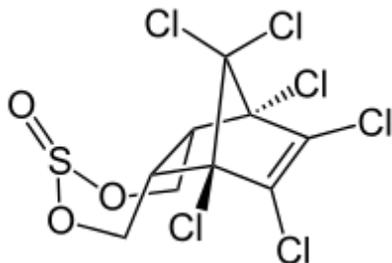
- Samples:** Endosulfan beta @ 1 ng/uL in Aceton
Endosulfan Sulfat @ 1 ng/uL in Aceton
Pesticide Mix12 @ 1 ng/uL in Aceton,
- Injection:** 1 uL
- GC-MS:** Exactive Plus with GC-APPI Interface, Trace 1310 GC and RSH Autosampler
- MS:** APPI Source Temperature – 200 deg C, without Dopant
Scan Range 100-600 amu @ R=35.000 (4 Hz Cycle Time)
- GC:** SSL Injector – Temperature 250 deg C
Oven – 40 deg C for 1.5 min – 300 deg C with 20 deg C / min.
Flow – 1.3 mL/min.
Transfer Line Temperature – 250 deg C

Endosulfan was used worldwide as pesticide. The annual production in the 1980s was about 9000 tons. Today endosulfan is banned in many countries but still in use i.e. in China and India. [Source: Wikipedia]

GC-EI Measurements – Endosulfan-alpha

Comparison of GC-EI with GC-APPI

RT 11.79
Endosulfan I (alpha)
 $C_9H_6Cl_6O_3S$
 $M^+ = 405.7977$

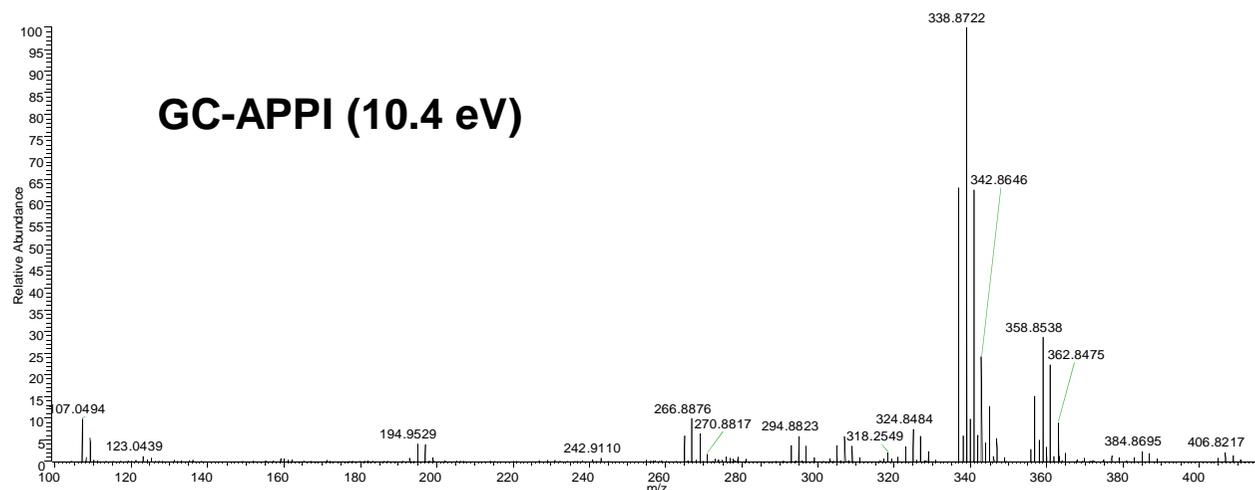
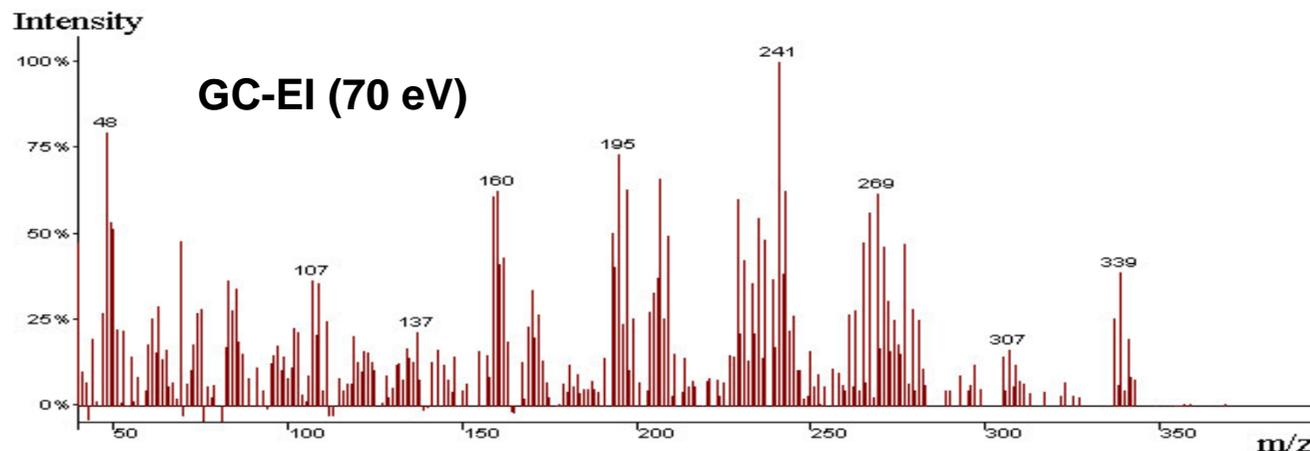
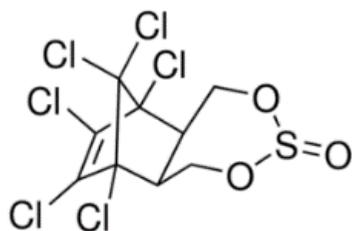


Measurement done @ Low Resolution Power

GC-EI Measurements – Endosulfan-beta

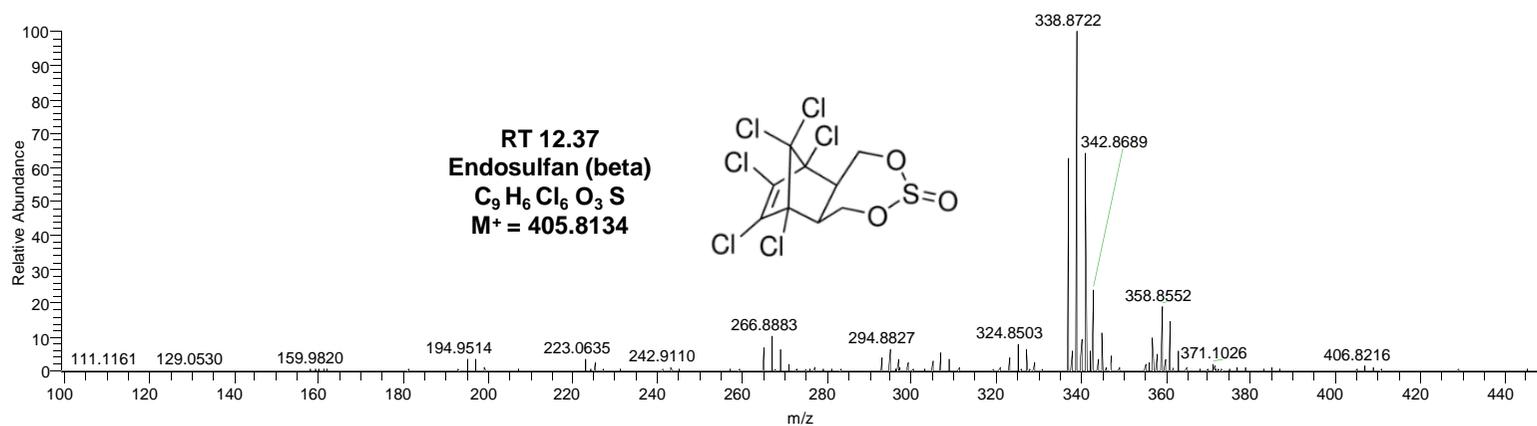
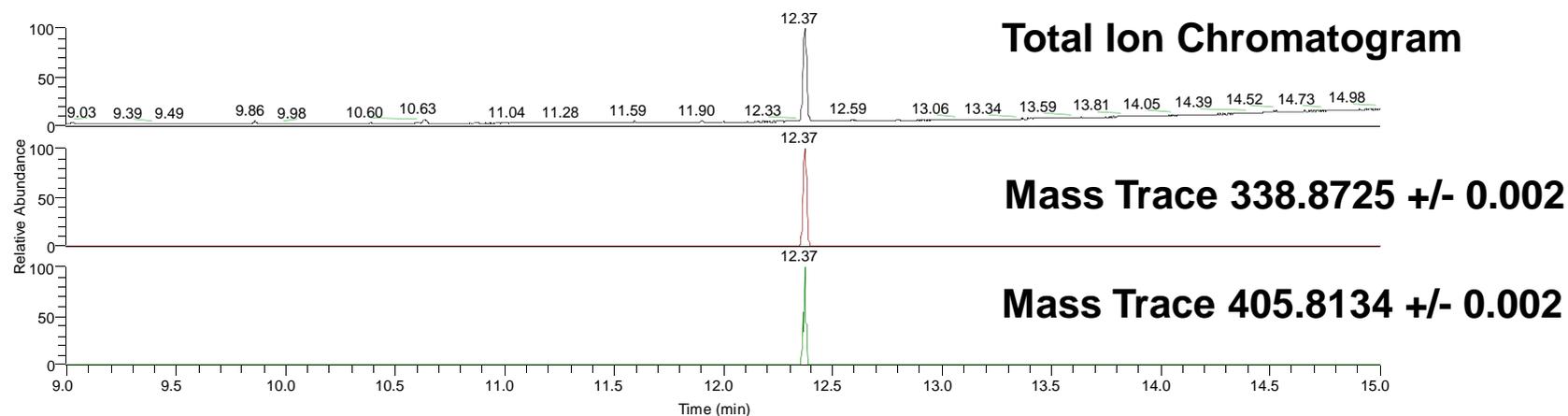
Comparison of GC-EI with GC-APPI

RT: 11.39
Endosulfan-beta
 $C_9H_6Cl_6O_3S$
405.8134



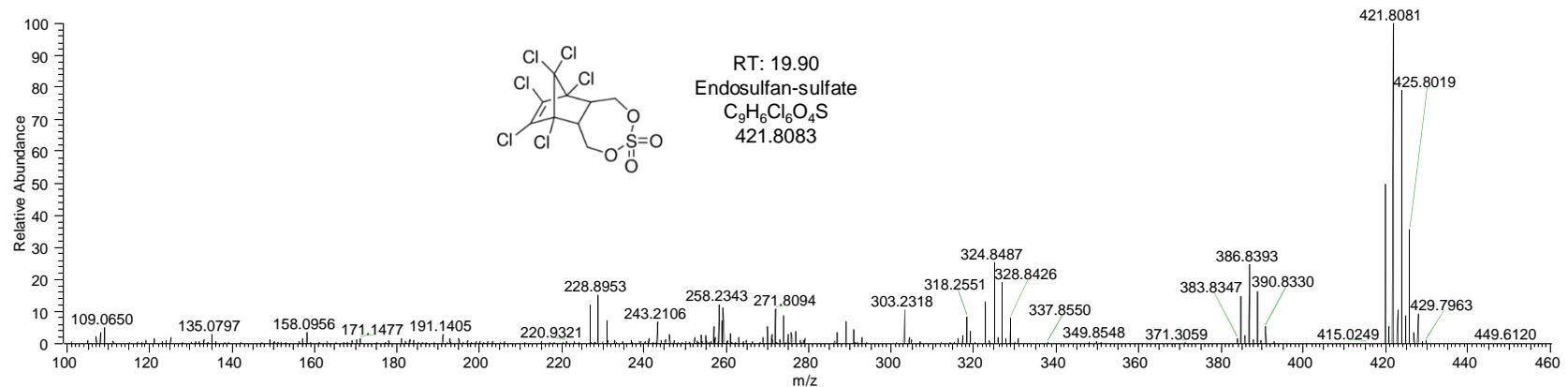
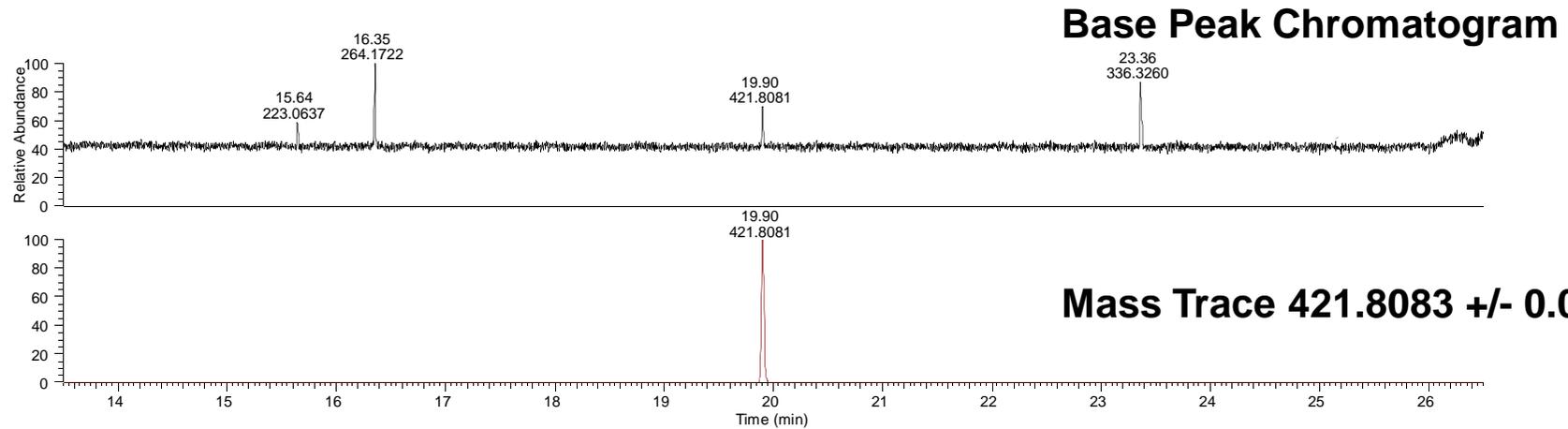
Measurement done @ Low Resolution Power

GC-APPI Measurements – Endosulfan beta



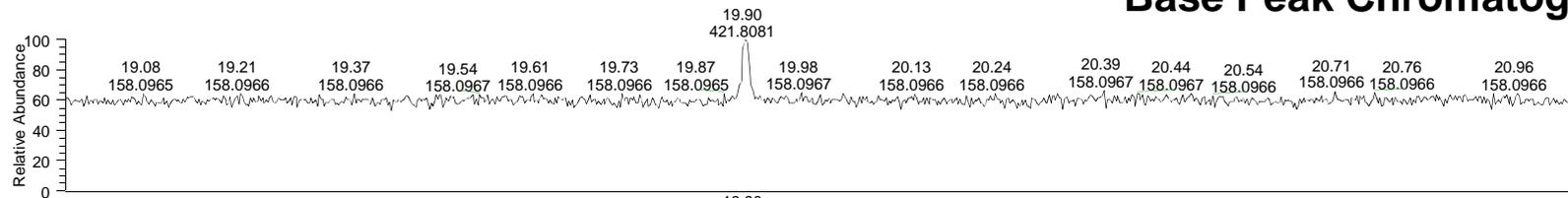
Measurement done @ 35,000 Resolution Power

Sample Endosulfan-Sulfate 1 ng/uL in Acetone

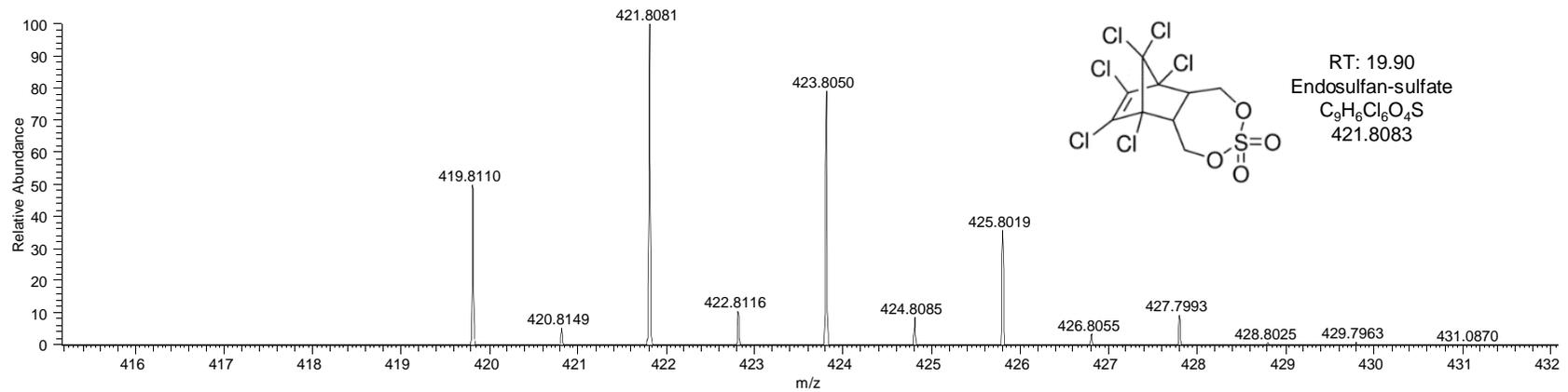
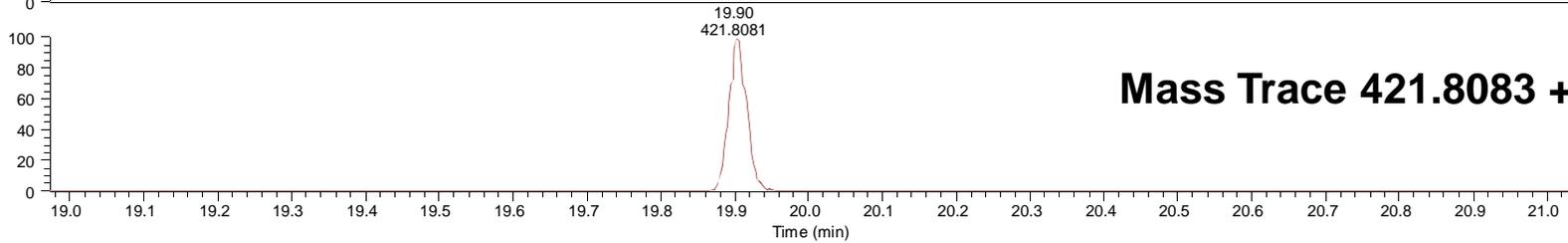


Sample Endosulfan-Sulfate 1 ng/uL in Acetone

Base Peak Chromatogram

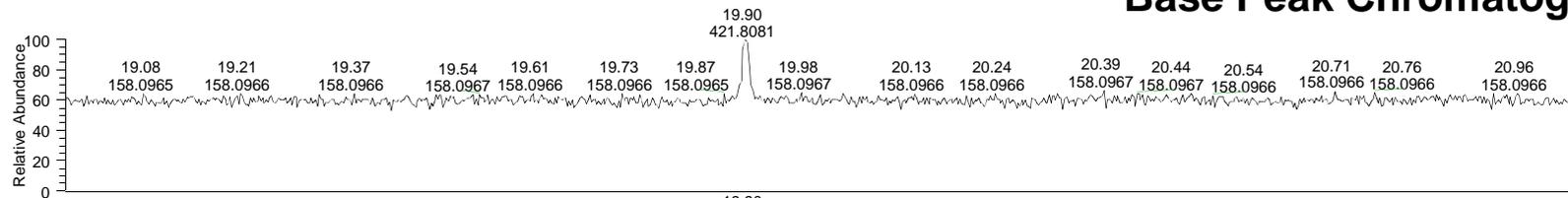


Mass Trace 421.8083 +/- 0.002

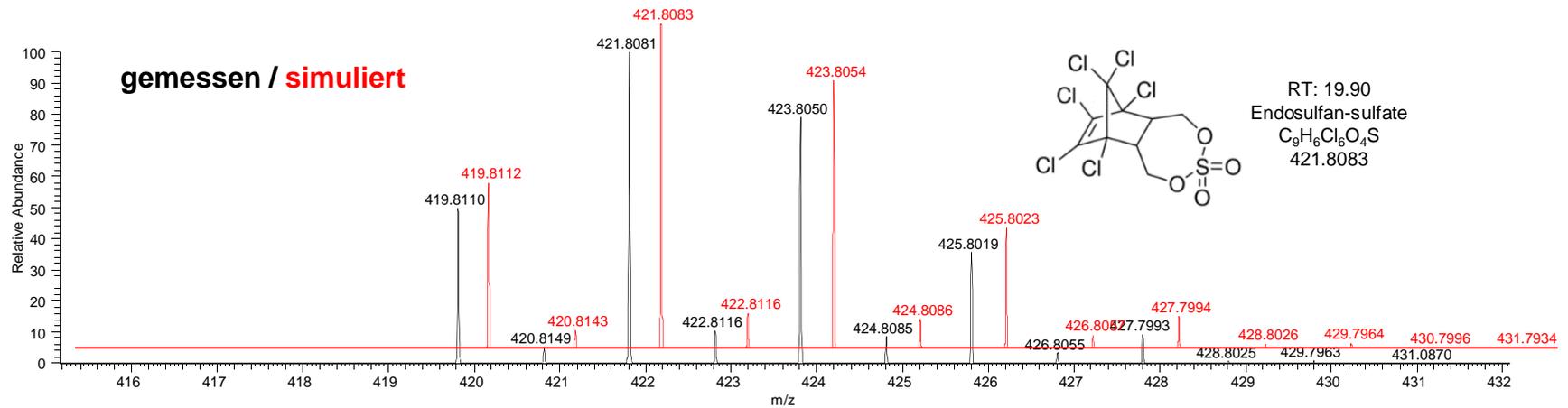
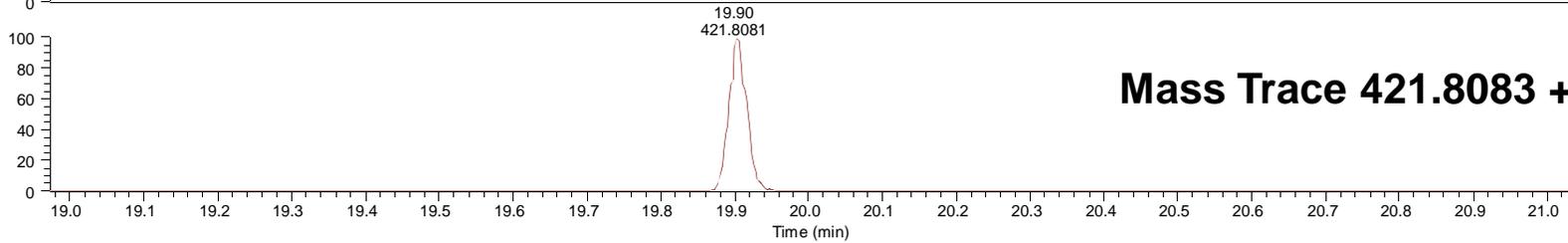


Sample Endosulfan-Sulfate 1 ng/uL in Acetone

Base Peak Chromatogram



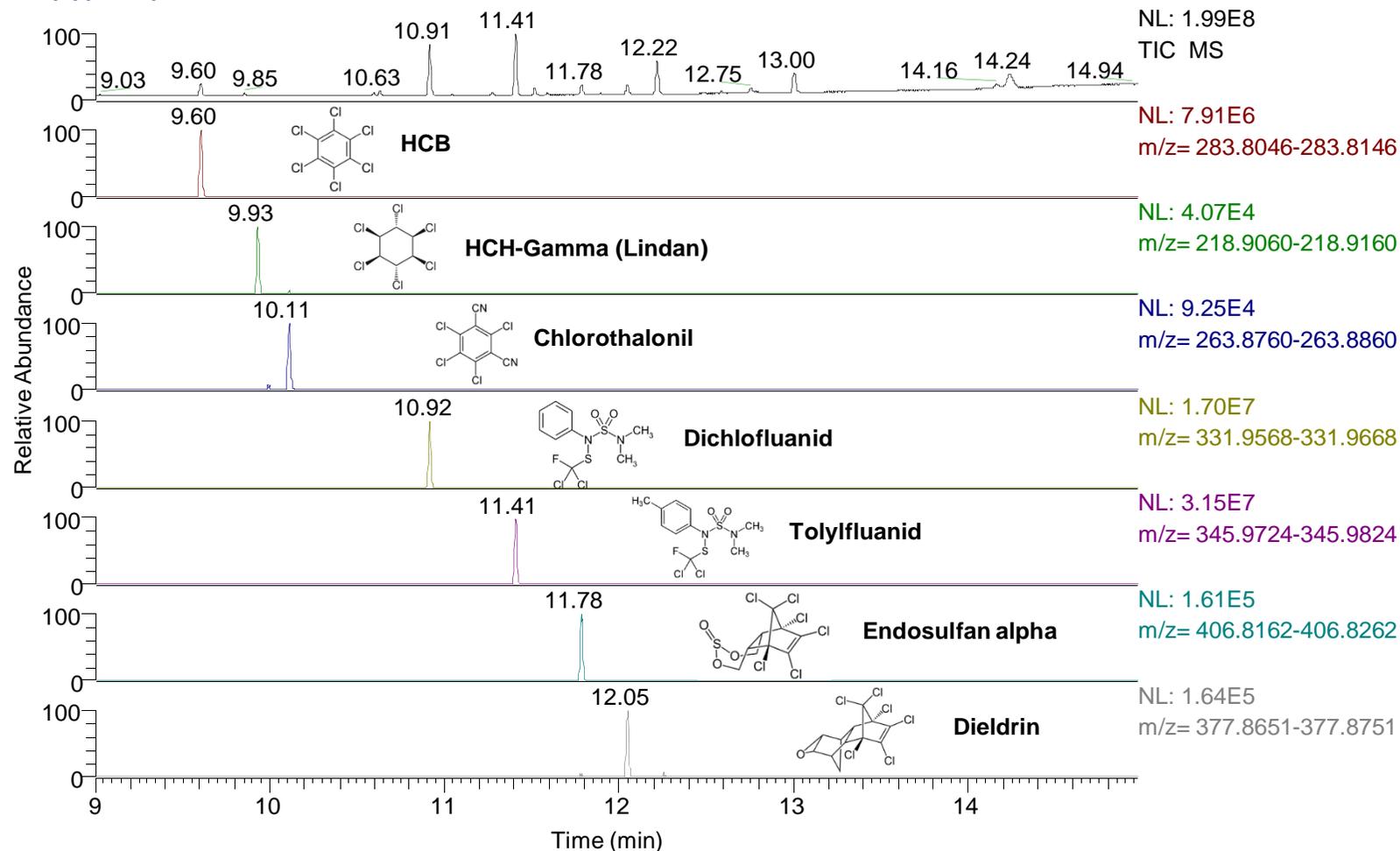
Mass Trace 421.8083 +/- 0.002



GC-APPI Measurements – Pesticide Mix12

MIX 12 Pesticides without Dopant - 1ng/1uL in Aceton

RT: 9.00 - 14.97

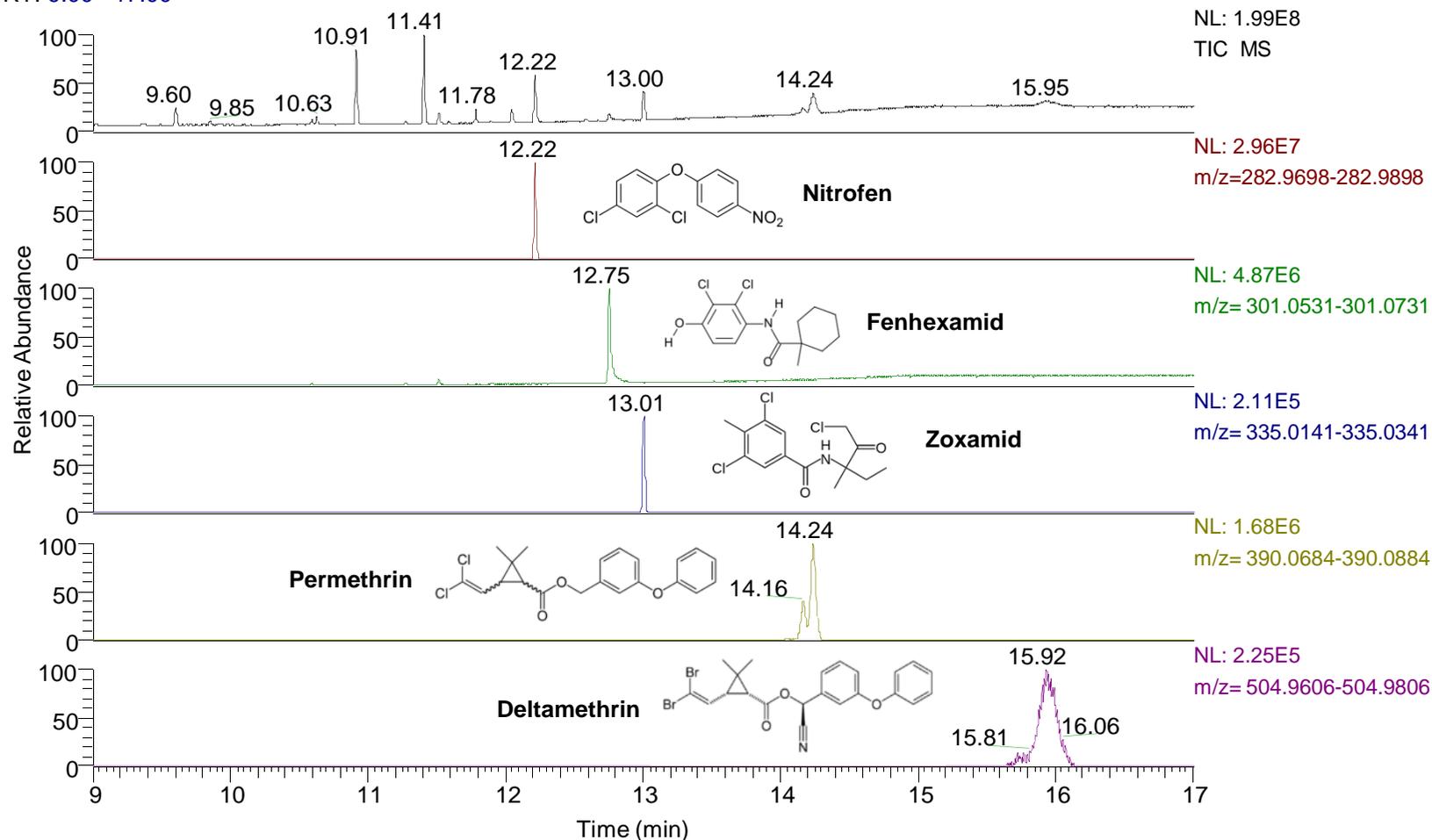


Measurement done @ 35,000 Resolution Power

GC-APPI Measurements – Pesticide Mix12

MIX 12 Pesticides without Dopant - 1ng/1uL in Aceton

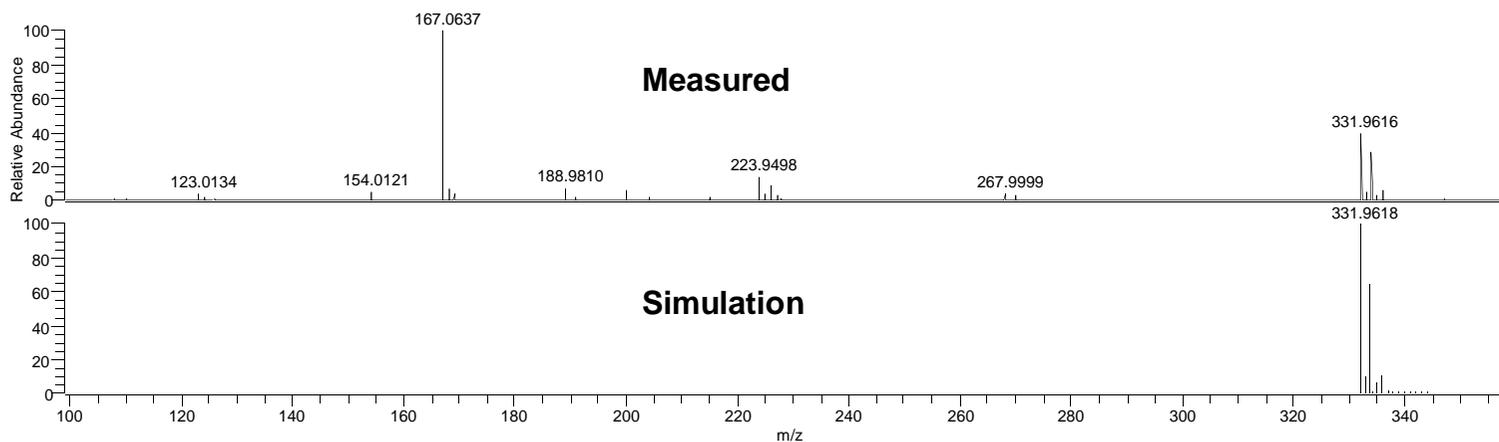
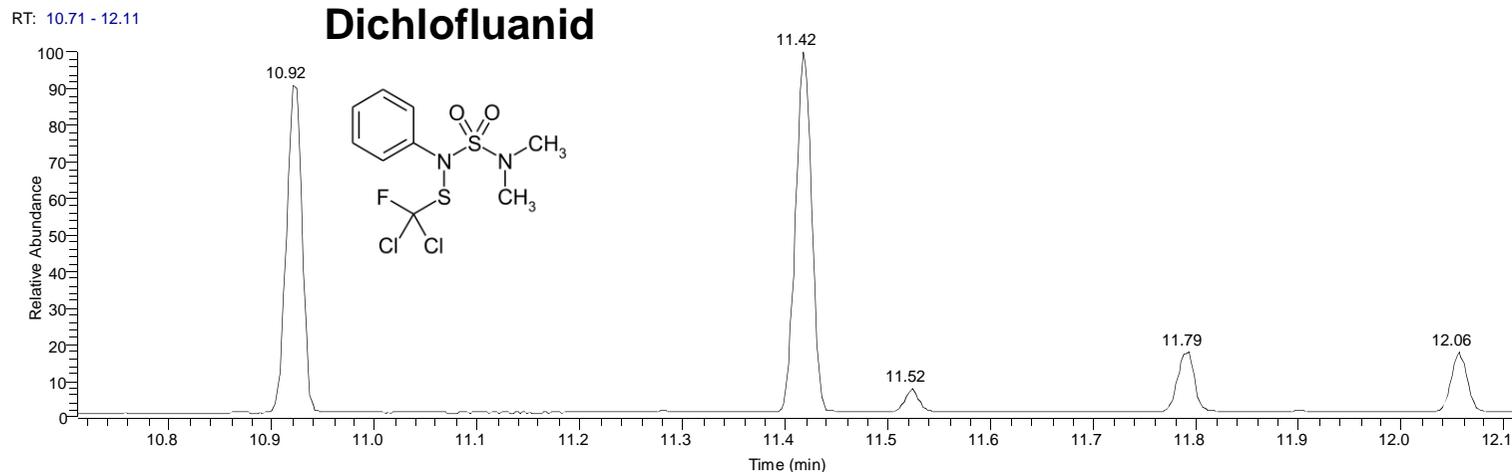
RT: 9.00 - 17.00



Measurement done @ 35,000 Resolution Power

GC-APPI Measurements – Pesticide Mix12

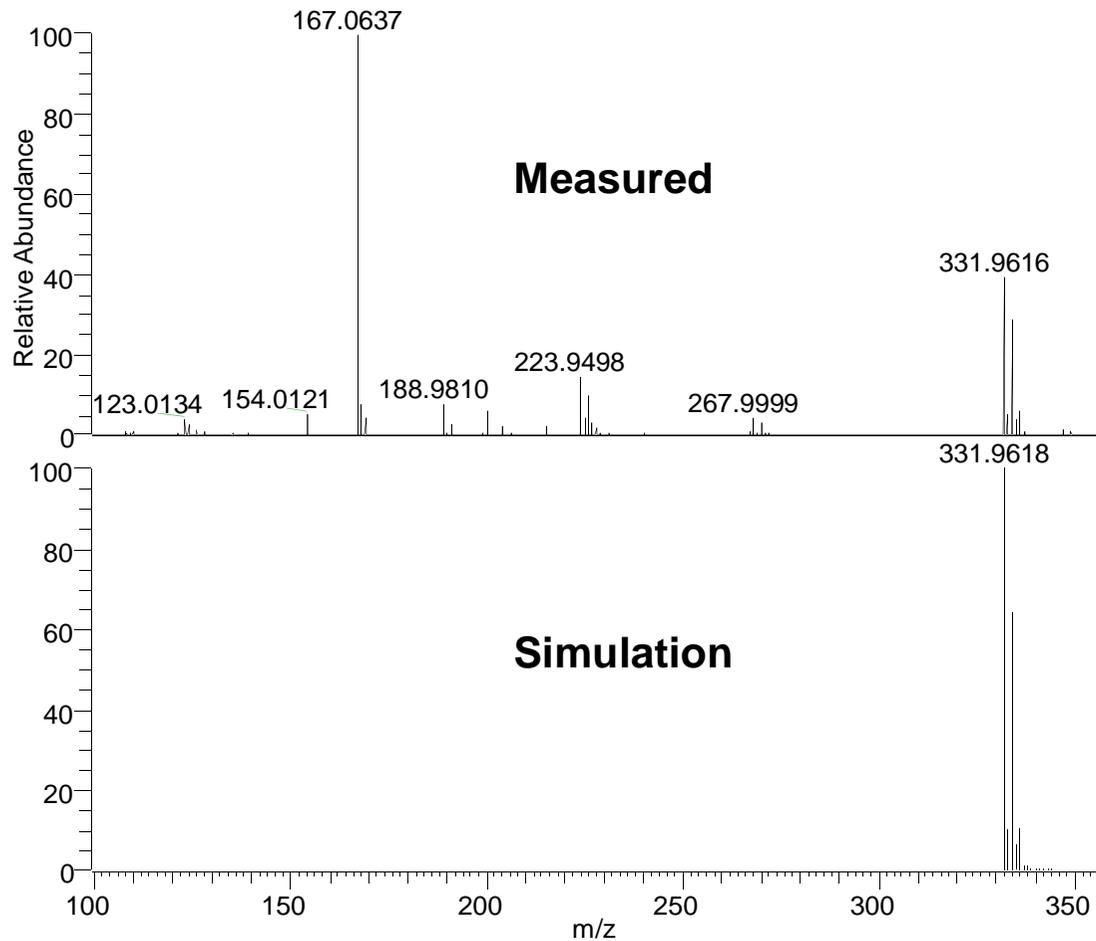
MIX 12 Pesticides without Dopant - 1ng/1uL in Aceton



Measurement done @ 35,000 Resolution Power

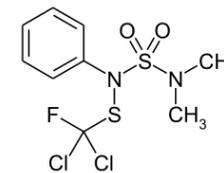
GC-APPI Measurements – Pesticide Mix12

MIX 12 Pesticides without Dopant - 1ng/1uL in Aceton



Dichlofluanid

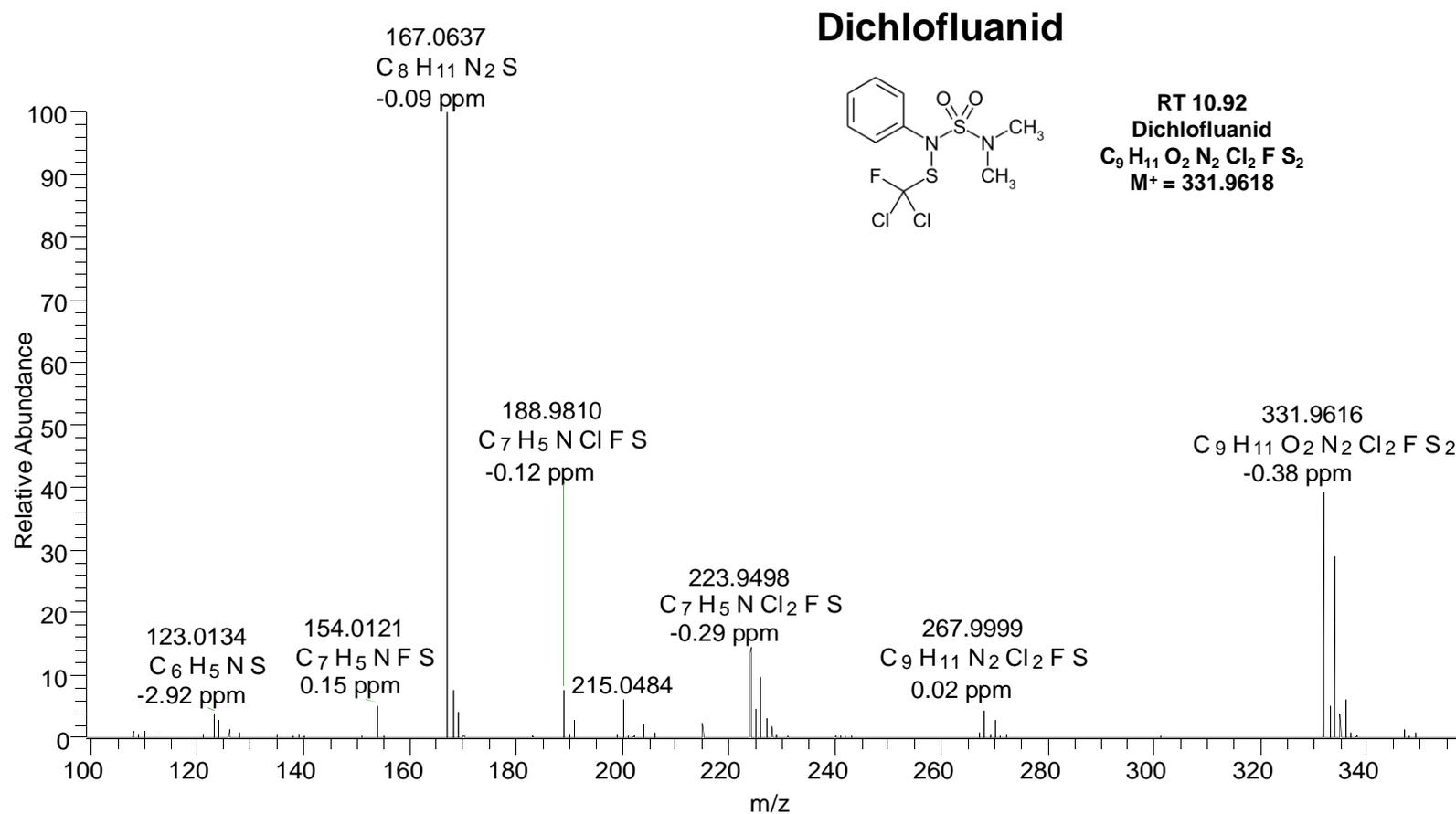
RT 10.92
Dichlofluanid
 $C_9H_{11}O_2N_2Cl_2F S_2$
 $M^+ = 331.9618$



Measurement done @ 35,000 Resolution Power

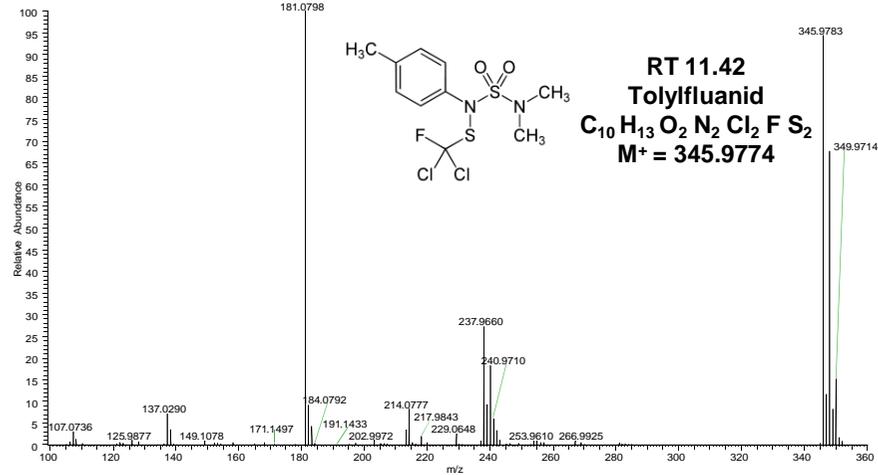
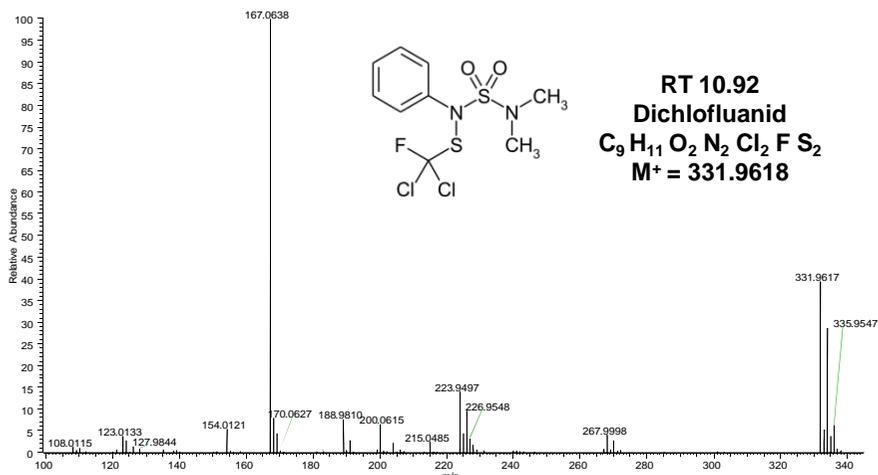
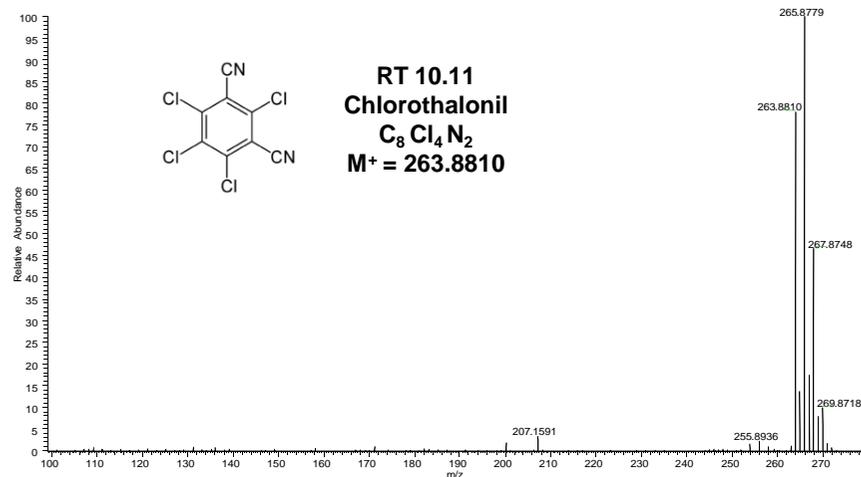
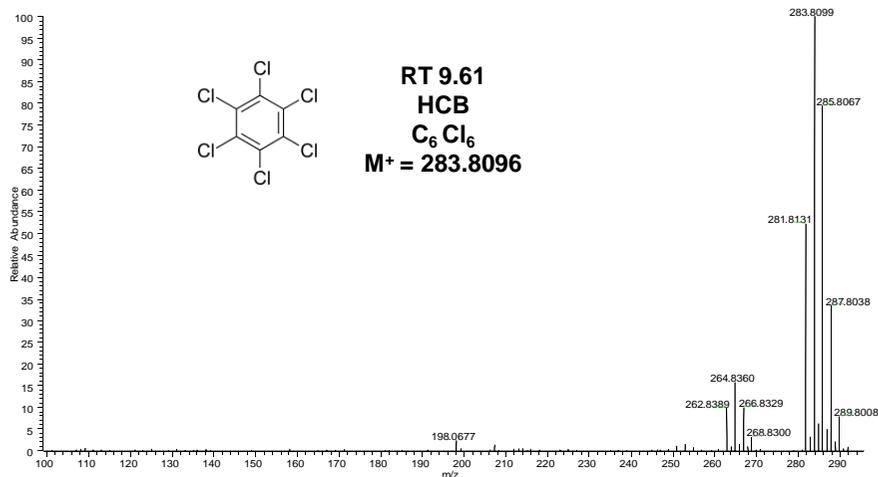
GC-APPI Measurements – Pesticide Mix12

MIX 12 Pesticides without Dopant - 1ng/1uL in Aceton



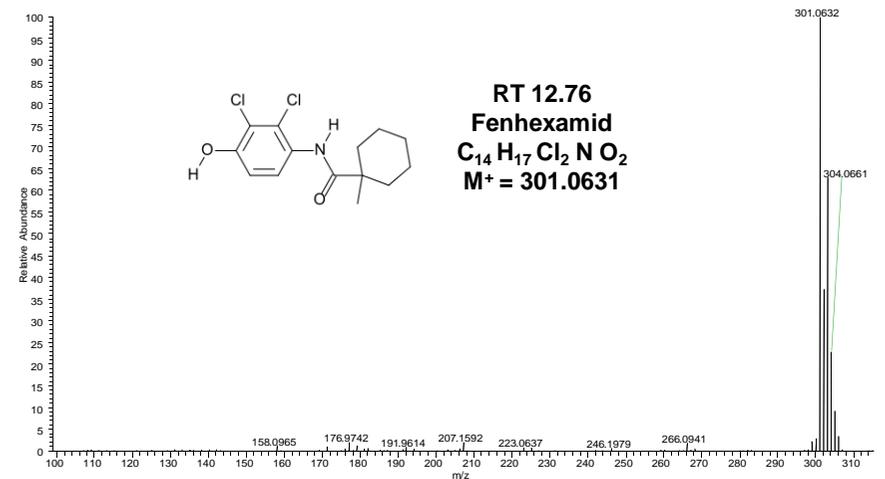
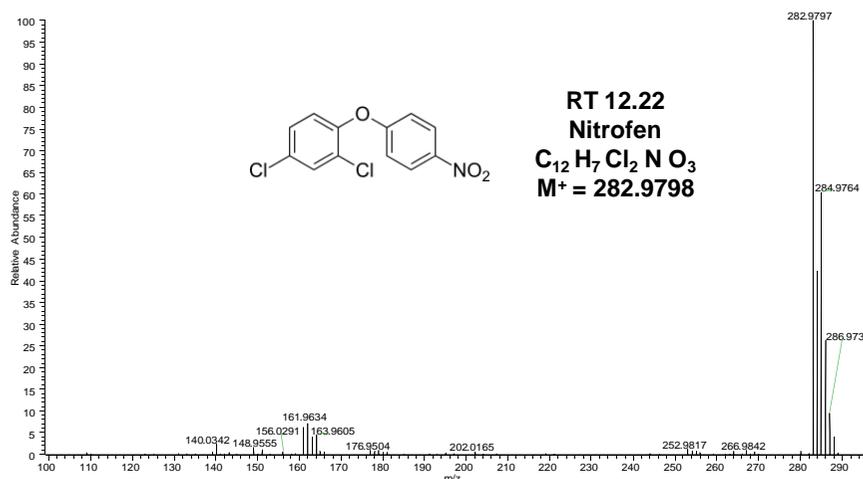
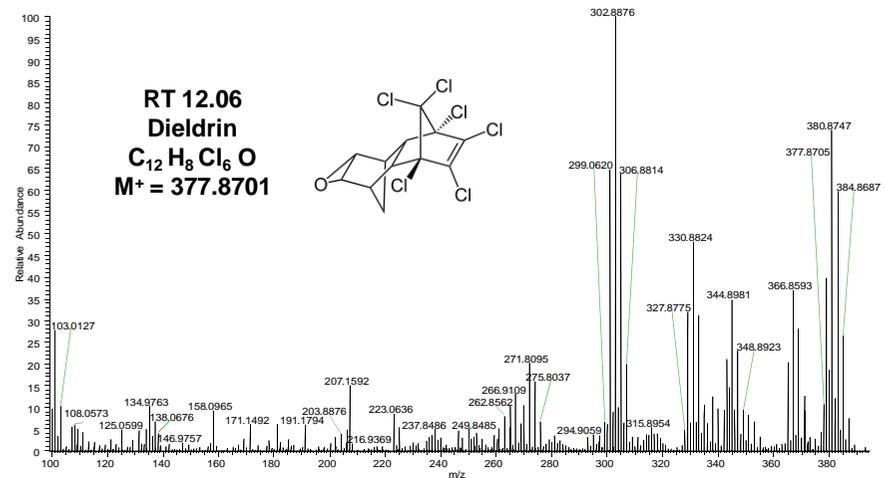
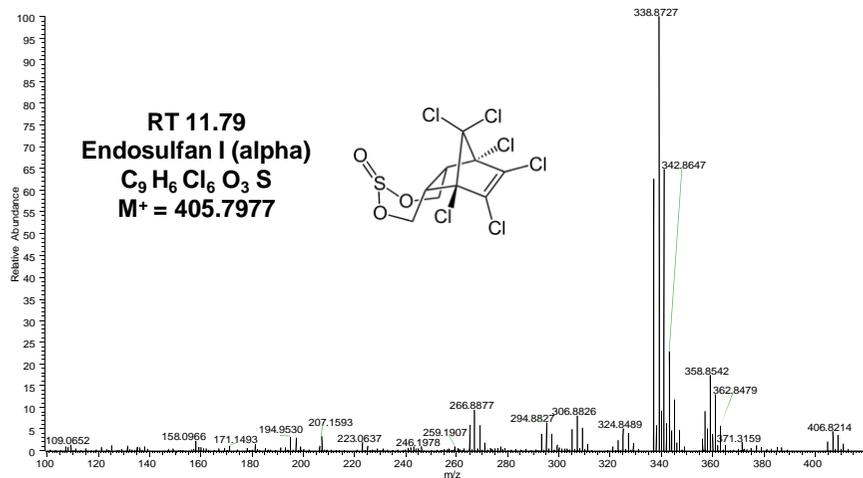
Measurement done @ 35,000 Resolution Power

GC-APPI Measurements – Pesticide Mix12



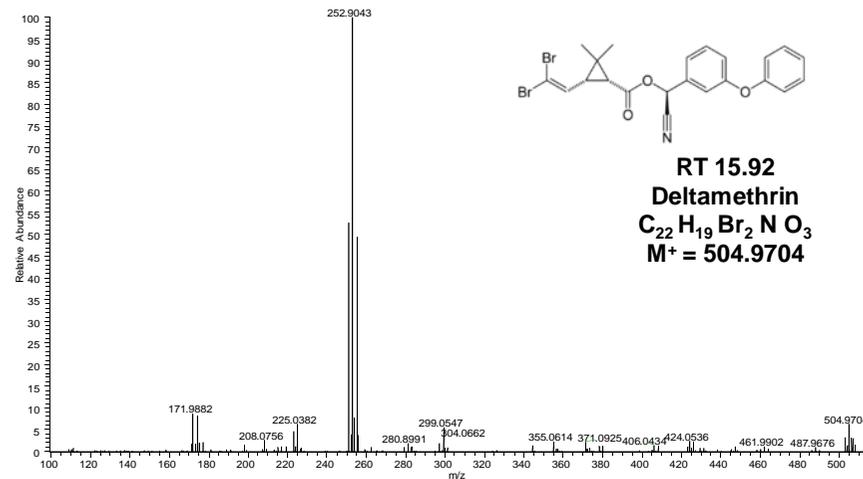
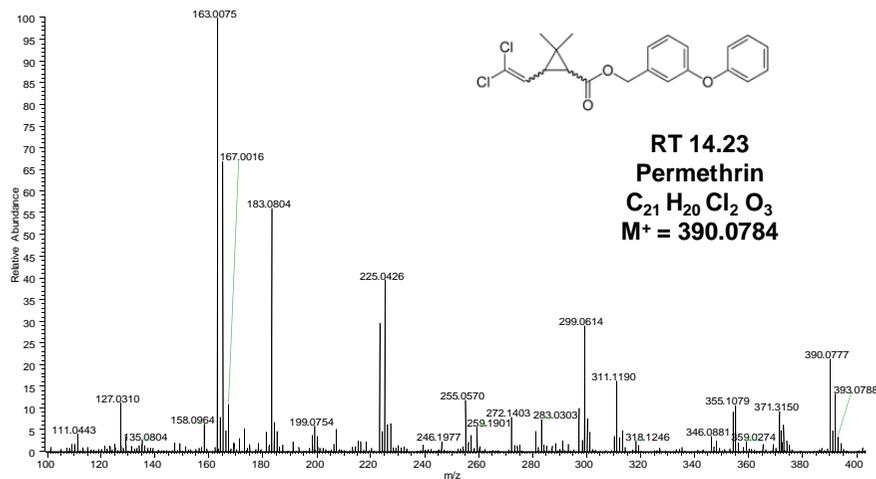
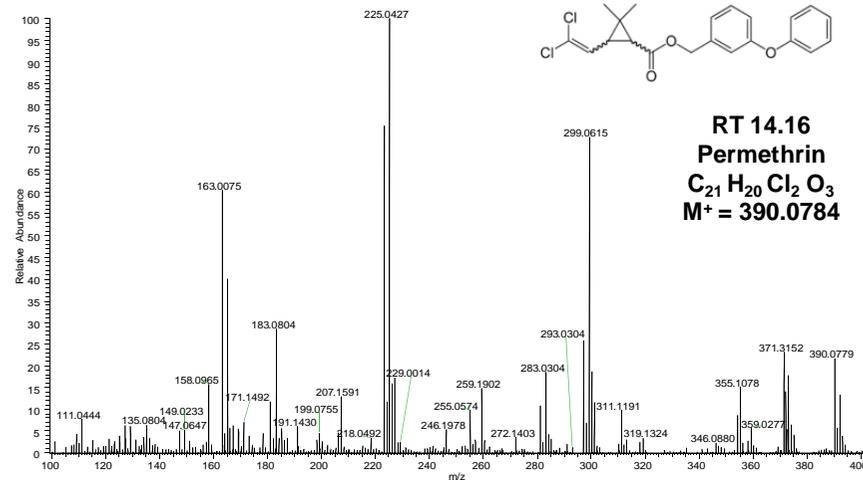
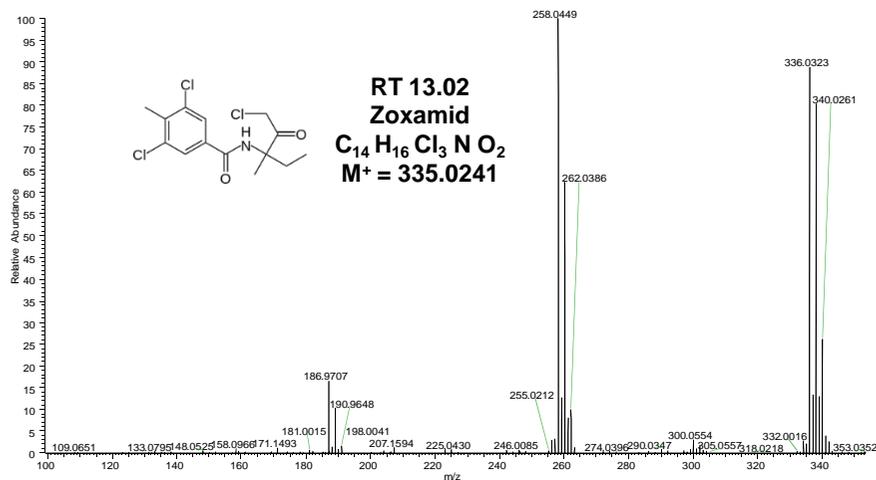
Measurement done @ 35,000 Resolution Power

GC-APPI Measurements – Pesticide Mix12



Measurement done @ 35,000 Resolution Power

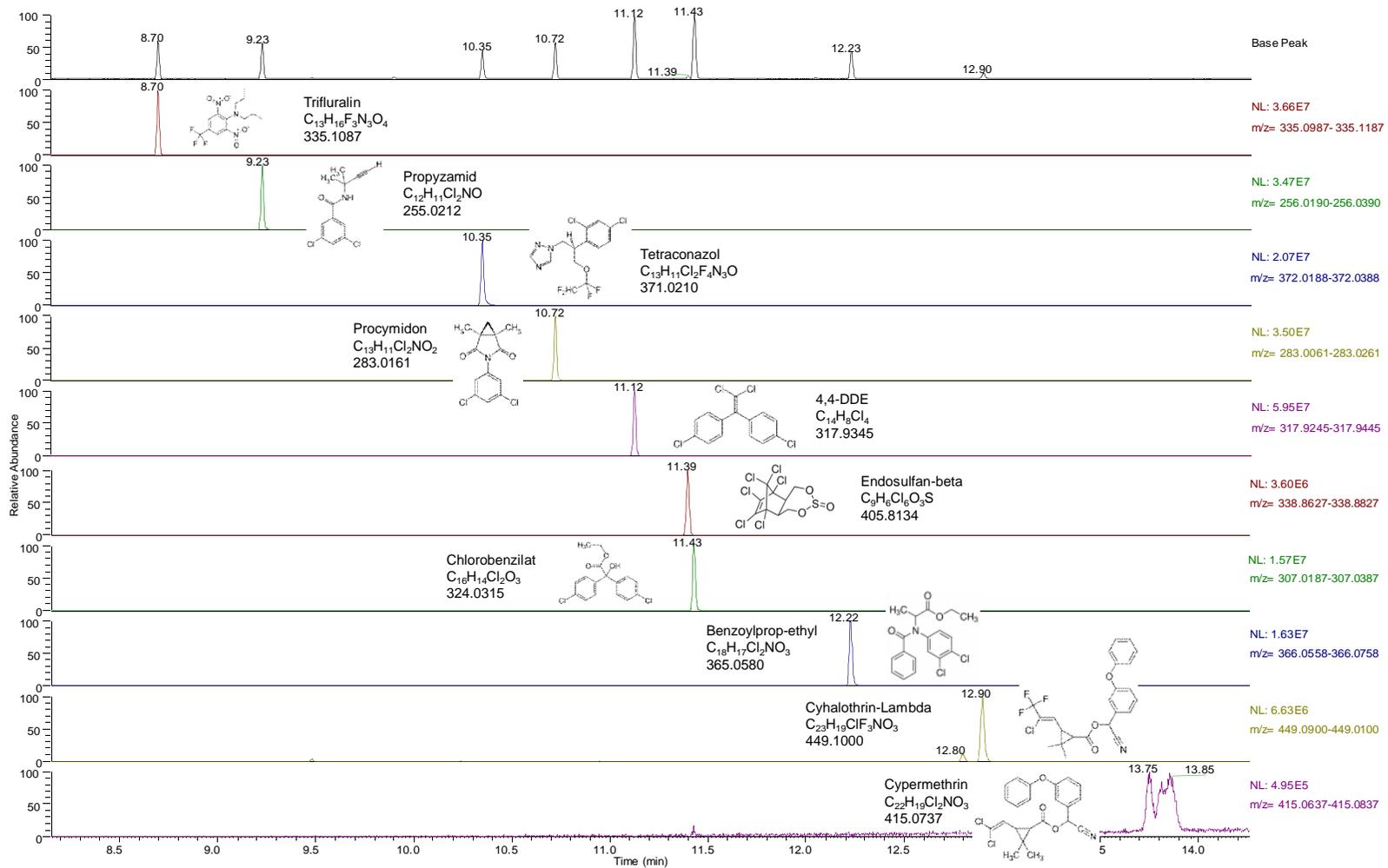
GC-APPI Measurements – Pesticide Mix12



Measurement done @ 35,000 Resolution Power

GC-APPI Measurements – Pesticide MixB10

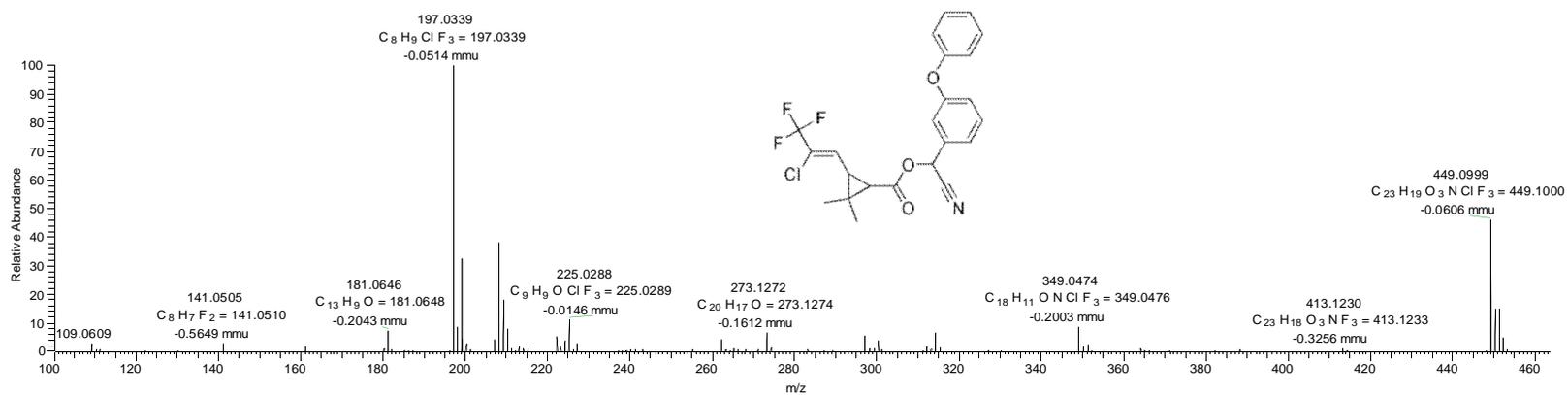
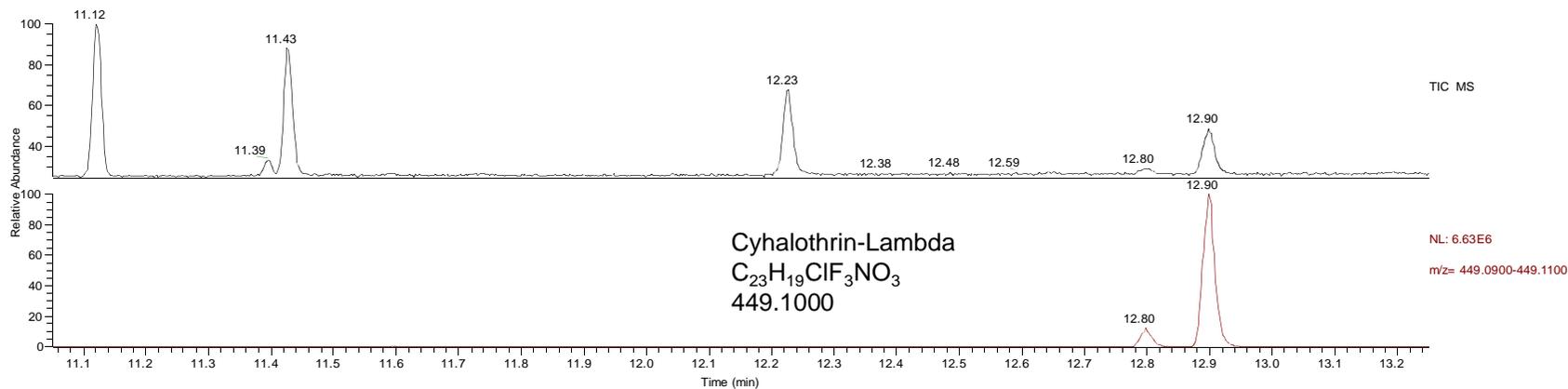
MIX B10 Pesticides without Dopant - 1ng/1uL in Aceton



Measurement done @ 35,000 Resolution Power

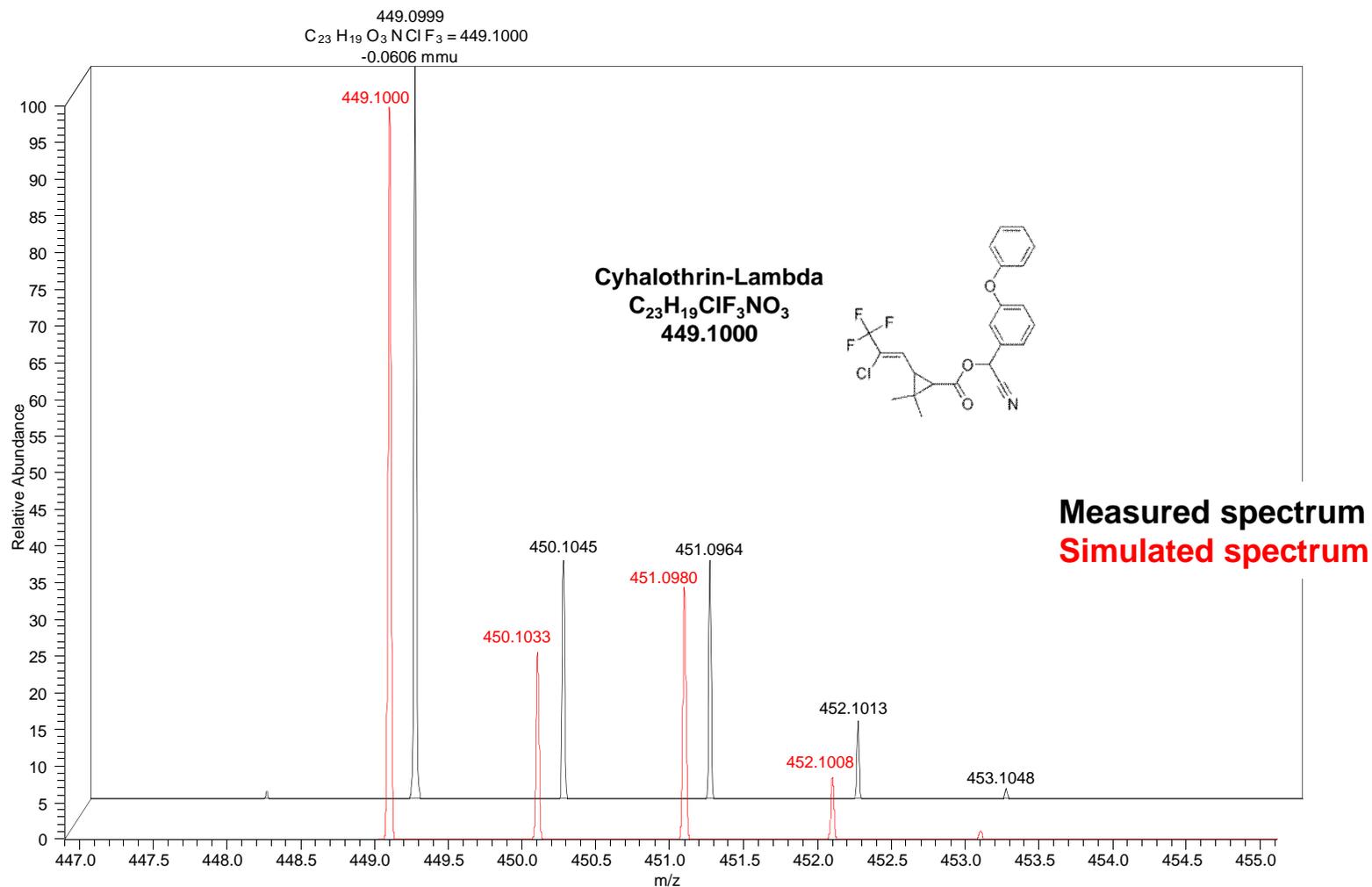
GC-APPI Measurements – Pesticide MixB10

MIX B10 Pesticides without Dopant - 1ng/1uL in Aceton



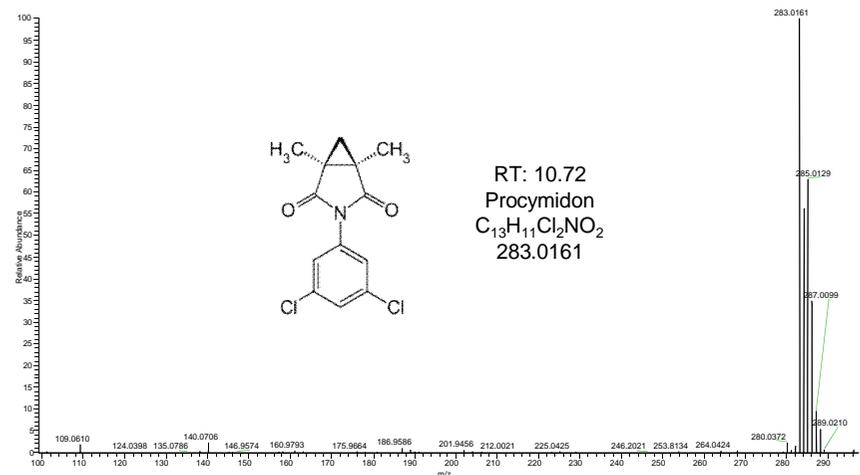
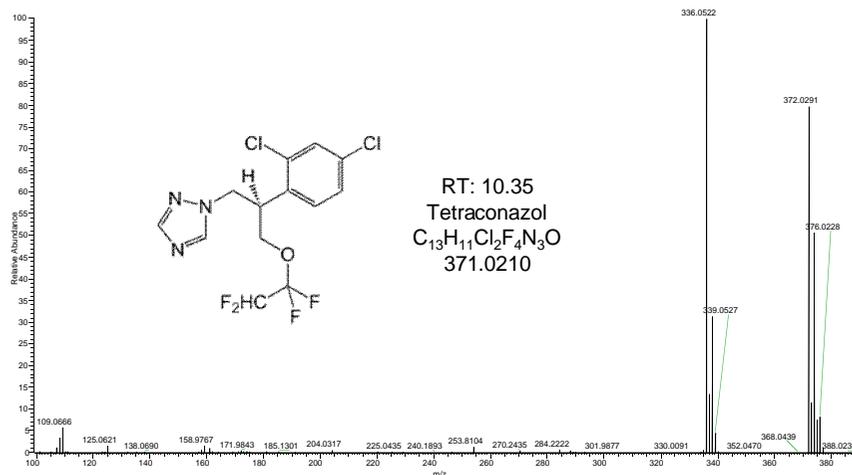
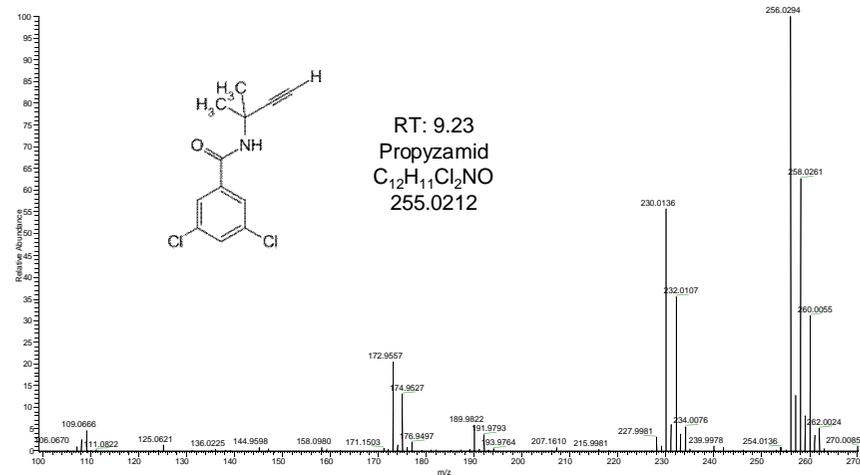
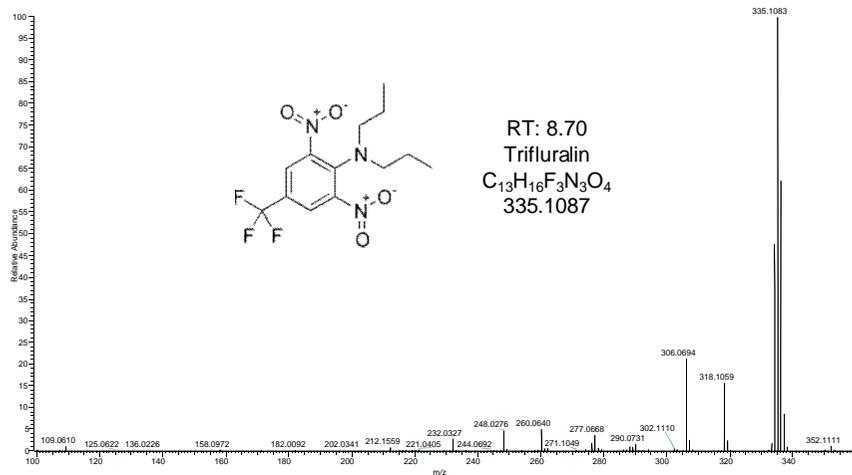
Measurement done @ 35,000 Resolution Power

GC-APPI Measurements – Pesticide MixB10



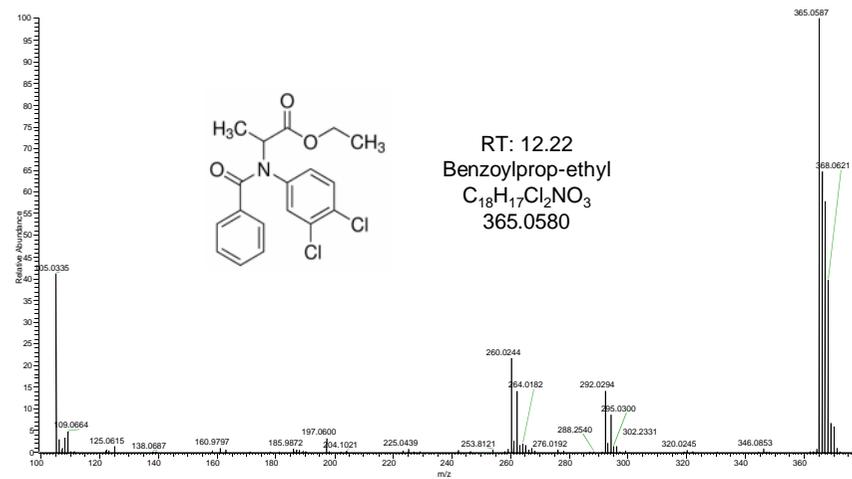
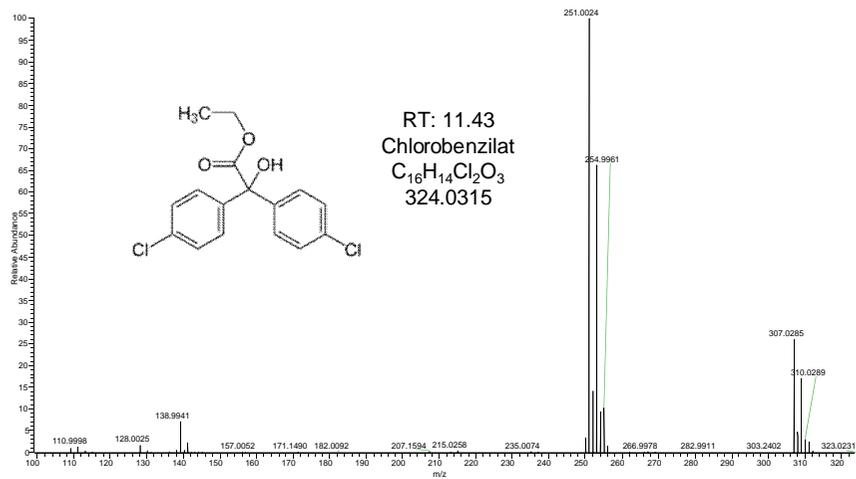
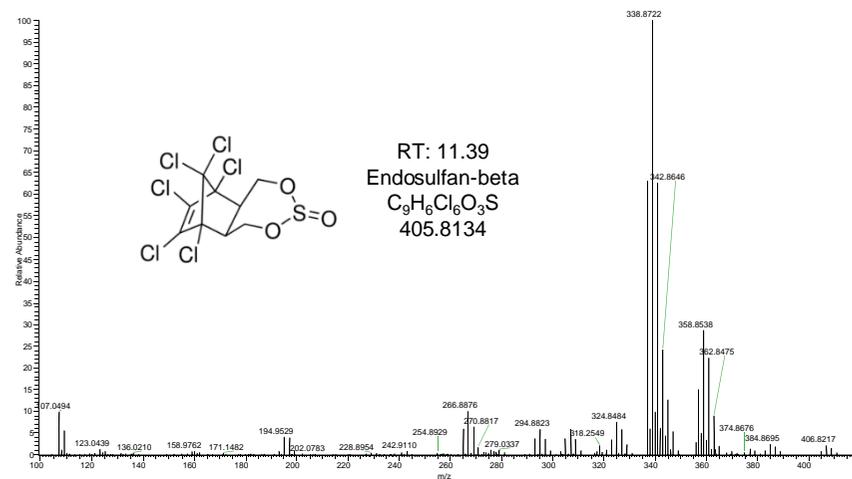
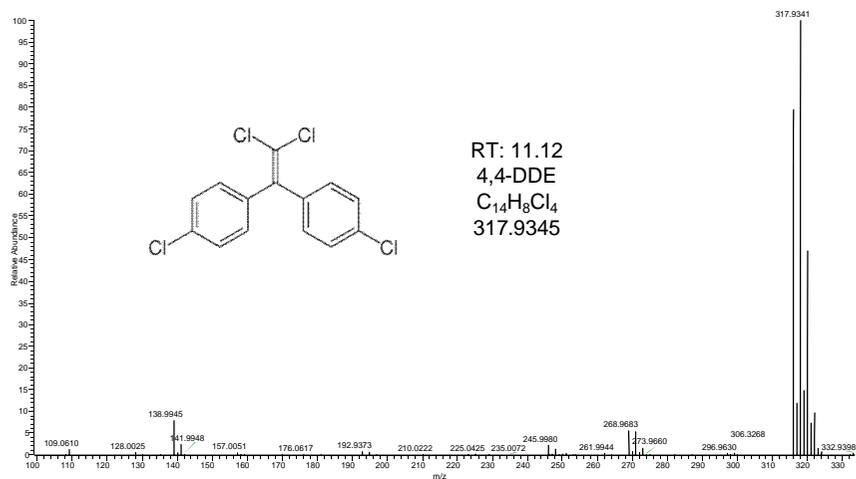
Measurement done @ 35,000 Resolution Power

GC-APPI Measurements – Pesticide Mix12



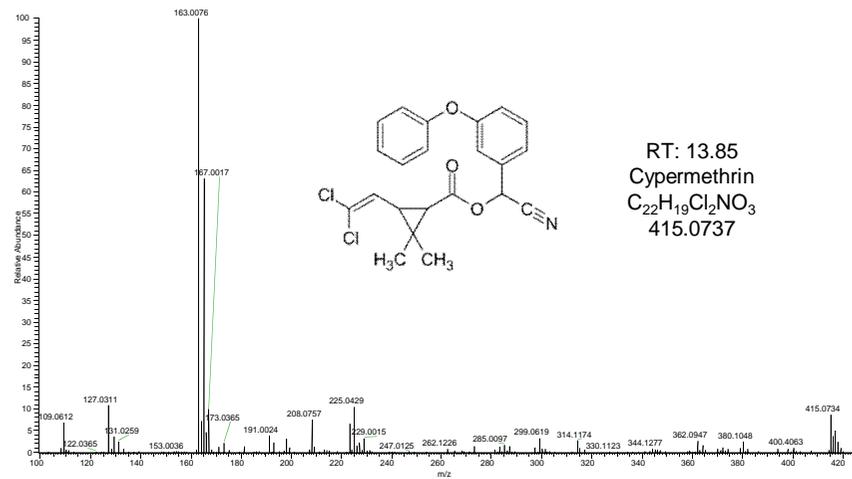
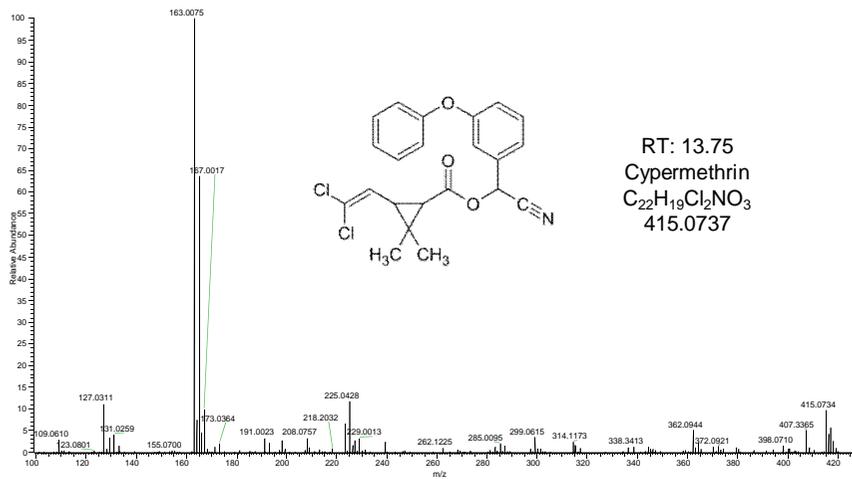
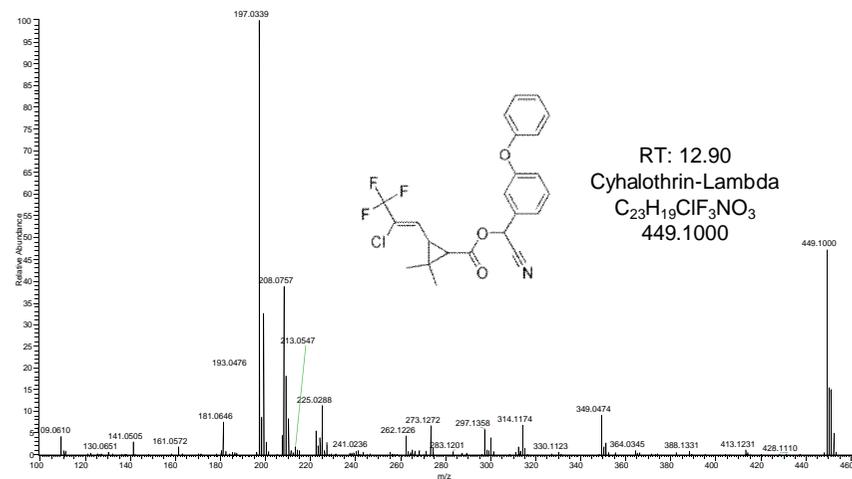
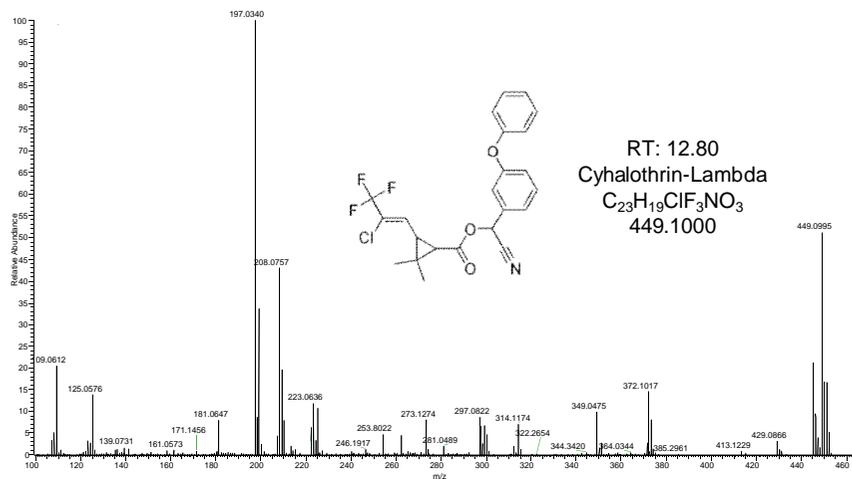
Measurement done @ 35,000 Resolution Power

GC-APPI Measurements – Pesticide Mix12



Measurement done @ 35,000 Resolution Power

GC-APPI Measurements – Pesticide Mix12



Measurement done @ 35,000 Resolution Power

Experimental Conditions

- Samples:**
- 1) TDCPP 1 ng/uL in Acetone (1,3-Dichloro-2-propanol phosphate)
 - 2) Endosulfan-Sulfate 1 ng/uL in Acetone
 - 3) Blank Extract – matrix wine
 - 4) Spiked Extract (1ng/uL spiked) - matrix wine
- Injection:** 1 uL for each measurement
- GC-MS:** Exactive Plus with GC-APPI Interface, Trace 1310 GC and RSH Autosampler
- MS:** APPI Source Temperature – 250 deg C, without Dopant
Scan Range 100-600 amu @ R=35.000 (4 Hz Cycle Time)
- GC:** Column 15m DB5, 0.25 ID, 0.25 Film
SSL Injector – Temperature 250 deg C
Oven – 40 deg C for 1.5 min – 300 deg C with 10 deg C / min.
Flow – 1 mL/min.
Transfer Line Temperature – 250 deg C

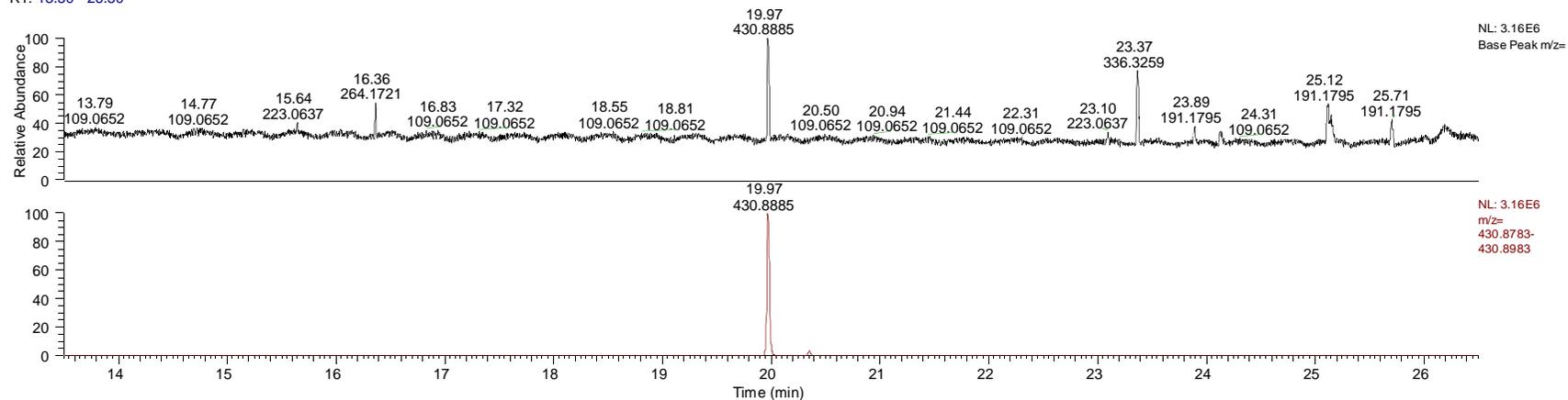
Sample TDCPP 1 ng/uL in Acetone

C:\Xcalibur\...PosterPoster_samples_01
TDCPP 1ng/ul in Aceton w/o dop.

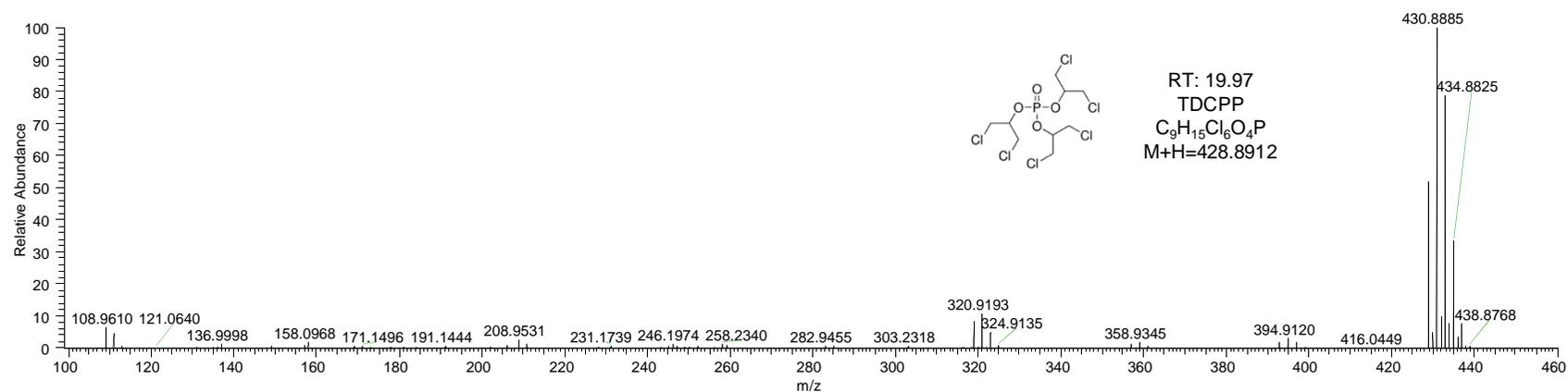
01.04.2016 14:43:02

TDCPP

RT: 13.50 - 26.50



Poster_samples_01 RT: 19.94-20.00 NL: 1.27E6



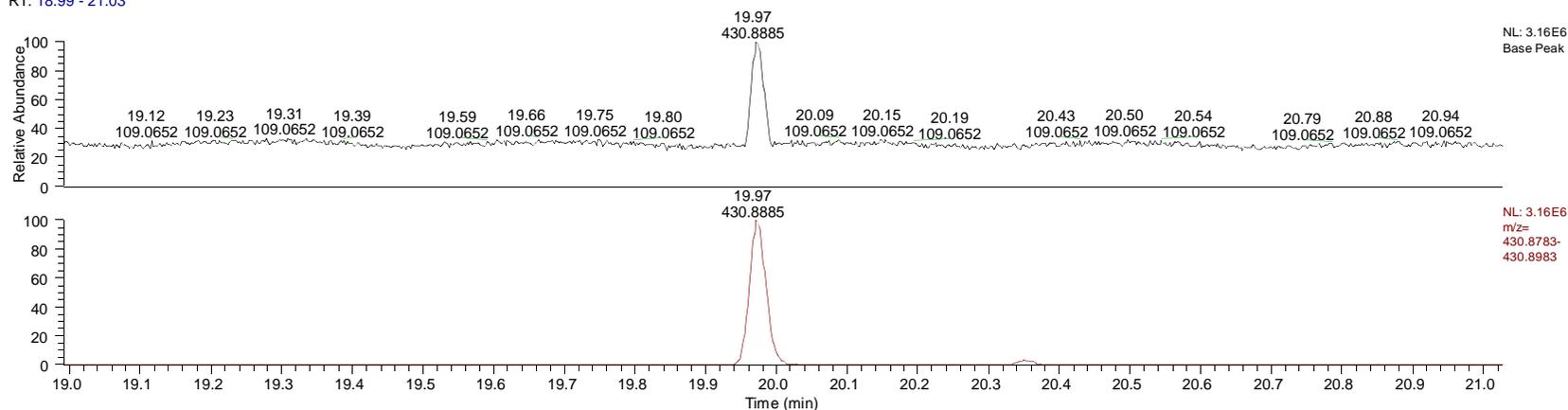
Sample TDCPP 1 ng/uL in Acetone

C:\Xcalibur\...\Poster\Poster_samples_01
TDCPP 1ng/ul in Aceton w/o dop.

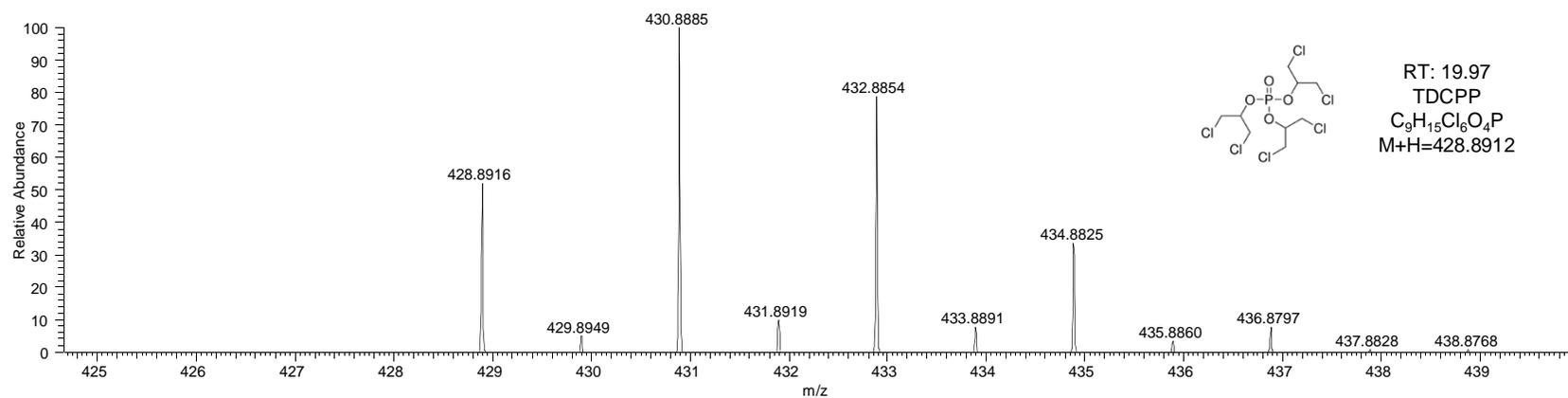
01.04.2016 14:43:02

TDCPP

RT: 18.99 - 21.03



Poster_samples_01 RT: 19.94-20.00 NL: 1.27E6



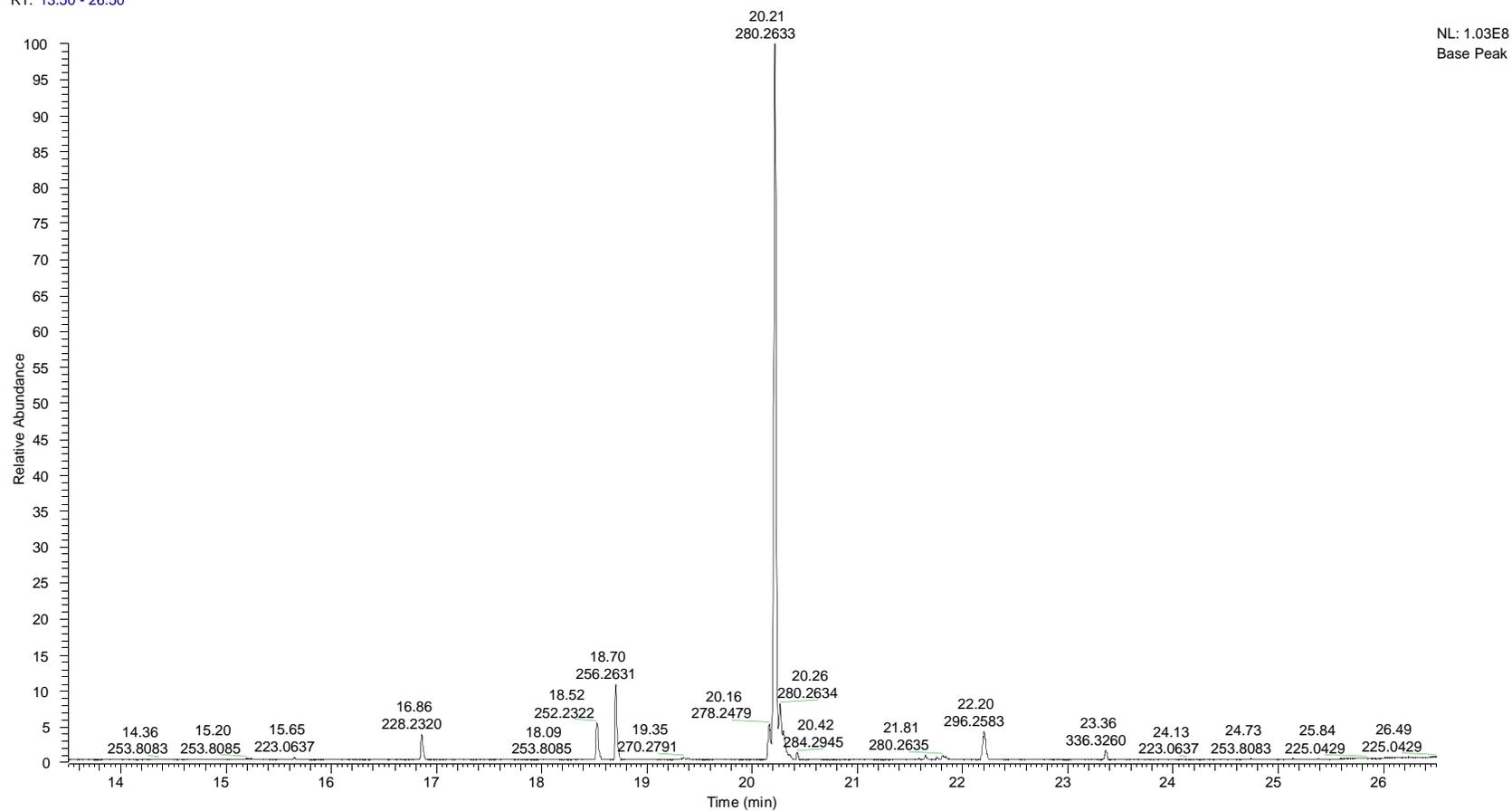
Sample Blank Extract

C:\Xcalibur\...\Poster\Poster_samples_03
Blank Extract in Aceton w/o dop.

01.04.2016 16:02:30

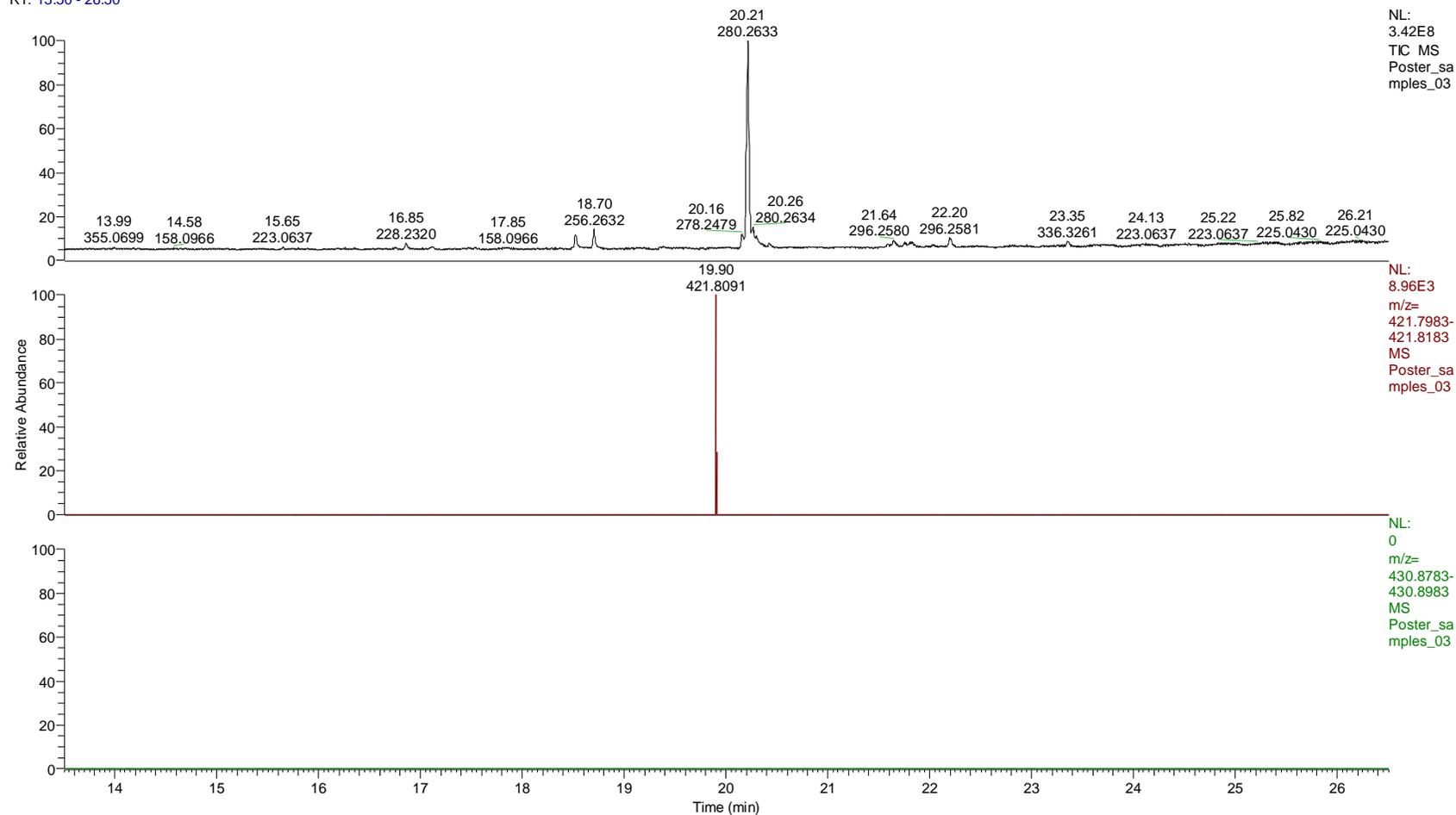
Blank-Extract

RT: 13.50 - 26.50

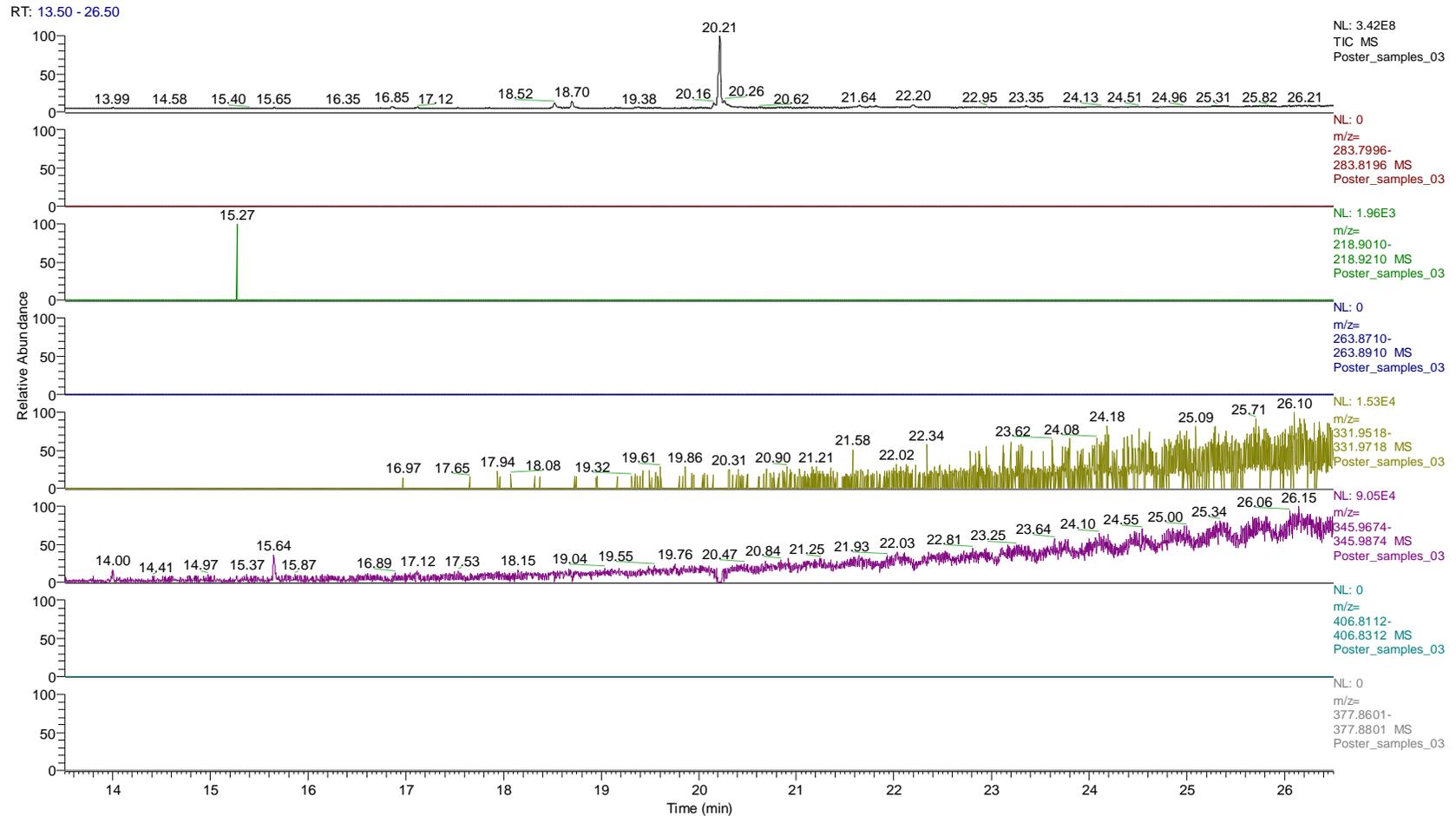


Sample Blank Extract

RT: 13.50 - 26.50

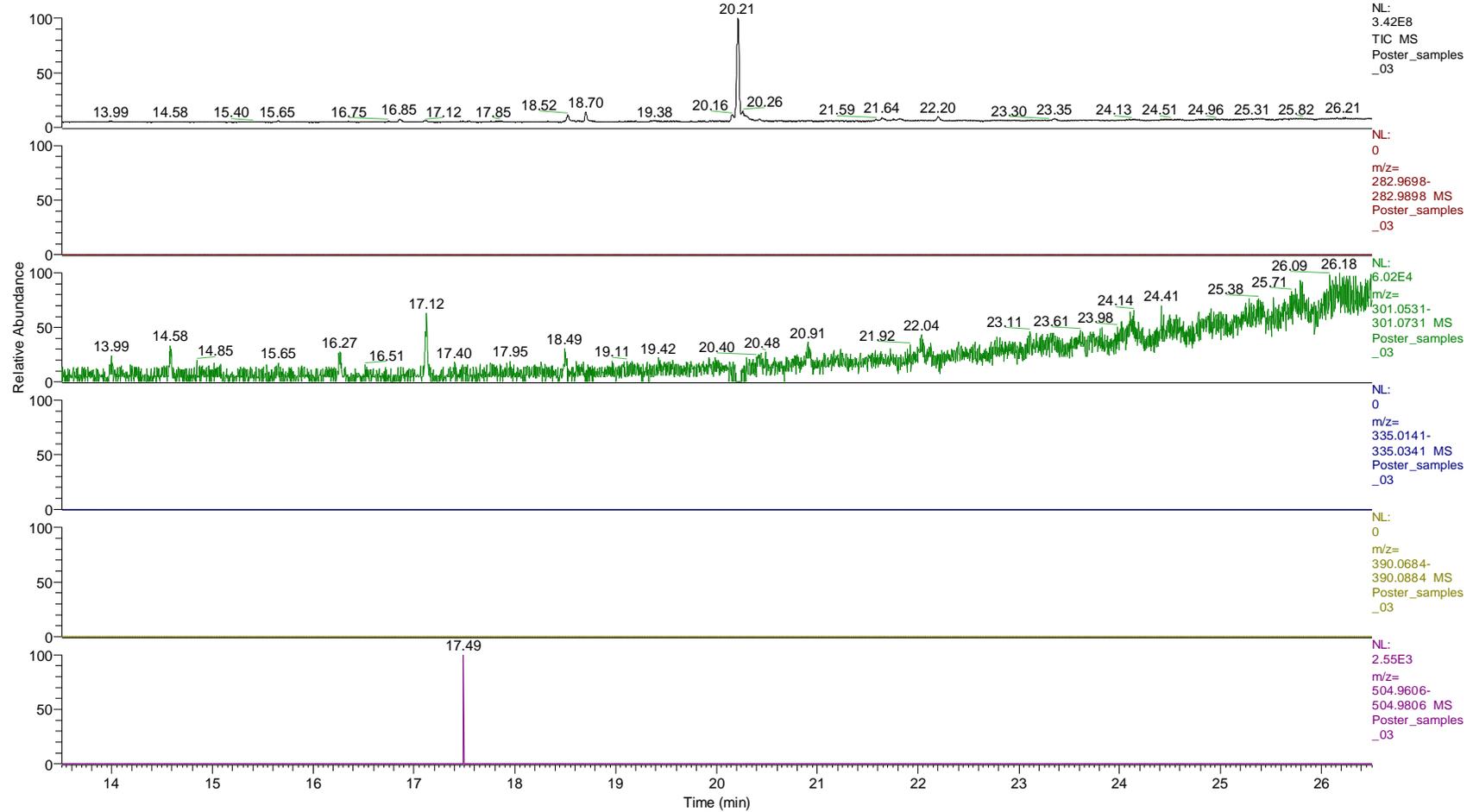


Sample Blank Extract



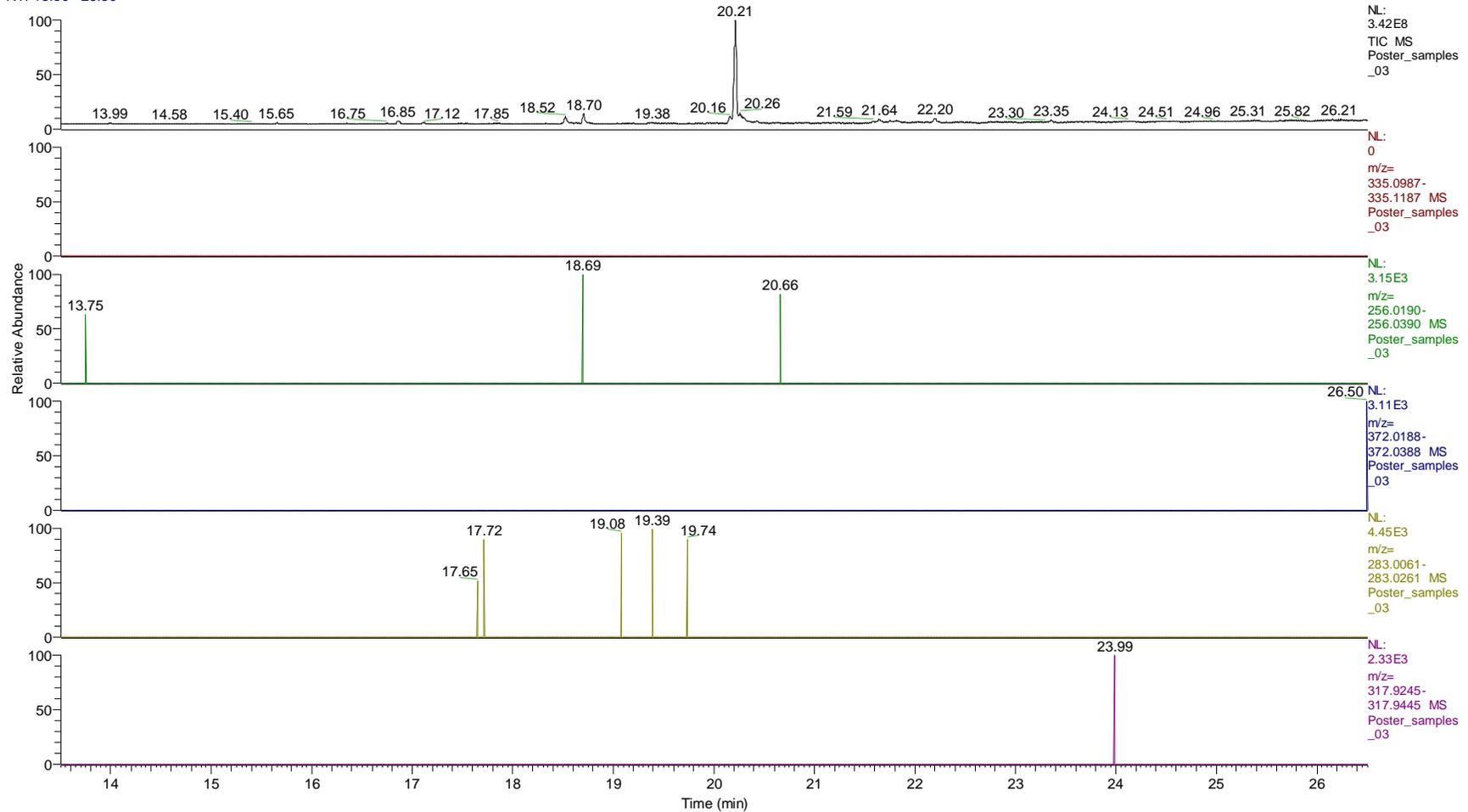
Sample Blank Extract

RT: 13.50 - 26.50

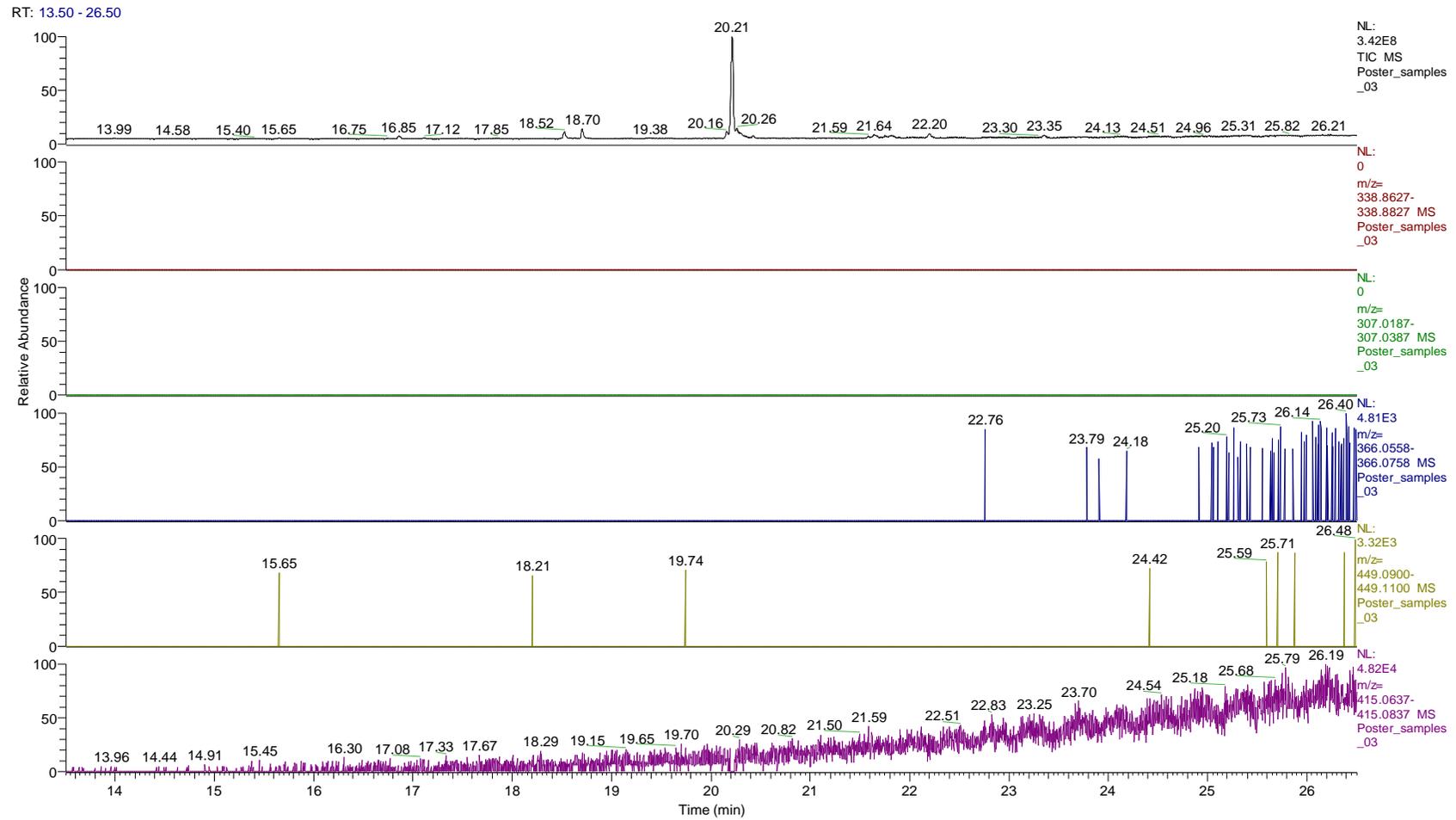


Sample Blank Extract

RT: 13.50 - 26.50



Sample Blank Extract



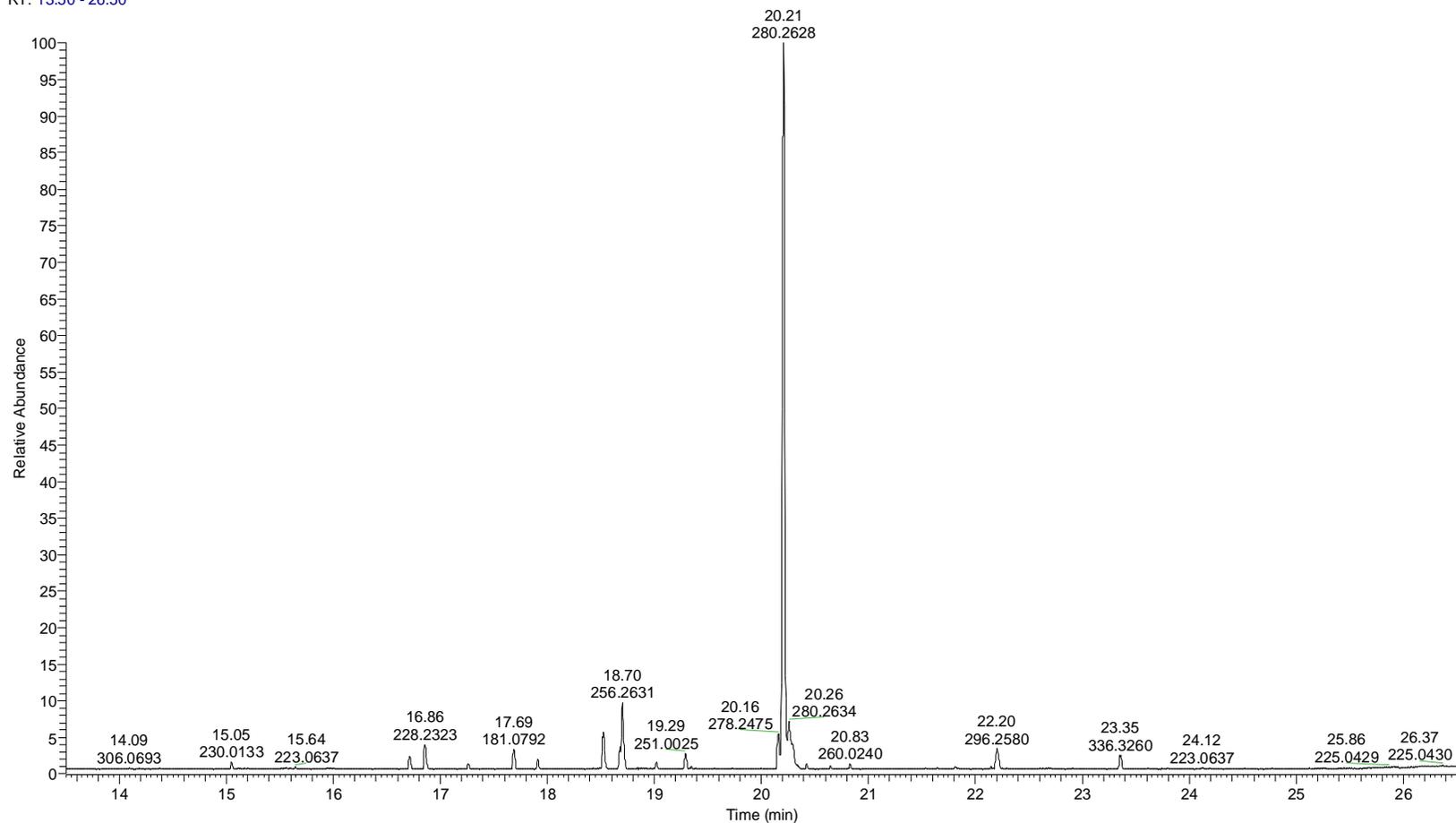
Sample Spiked Extract

C:\Xcalibur\...\Poster\Poster_samples_04
Spiked Extract 0.1ng/ul in Aceton w/o dop.

01.04.2016 16:43:08

Spiked-Extract

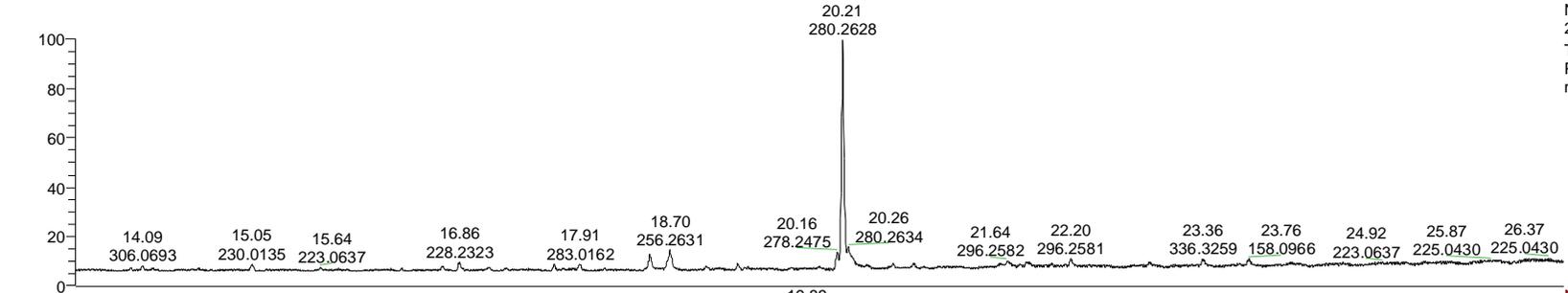
RT: 13.50 - 26.50



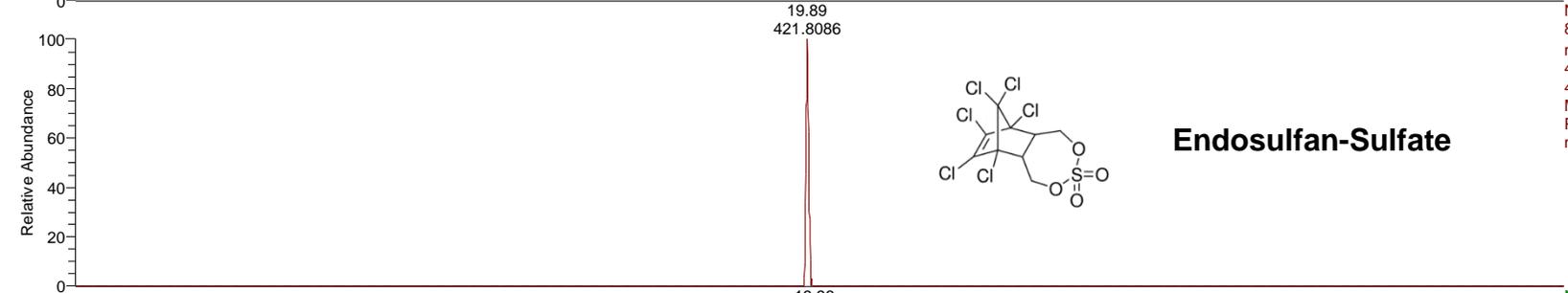
NL:
7.50E7
Base Peak
m/z=
100.0000-
600.0000
MS
Poster_sampl
es_04

Sample Spiked Extract

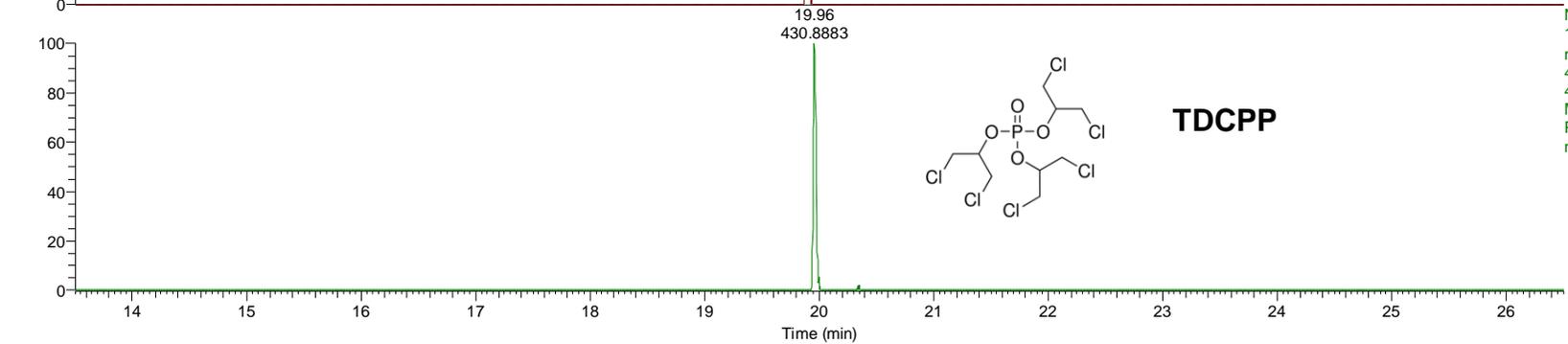
RT: 13.50 - 26.50



NL:
2.59E8
TIC MS
Poster_sam
ples_04



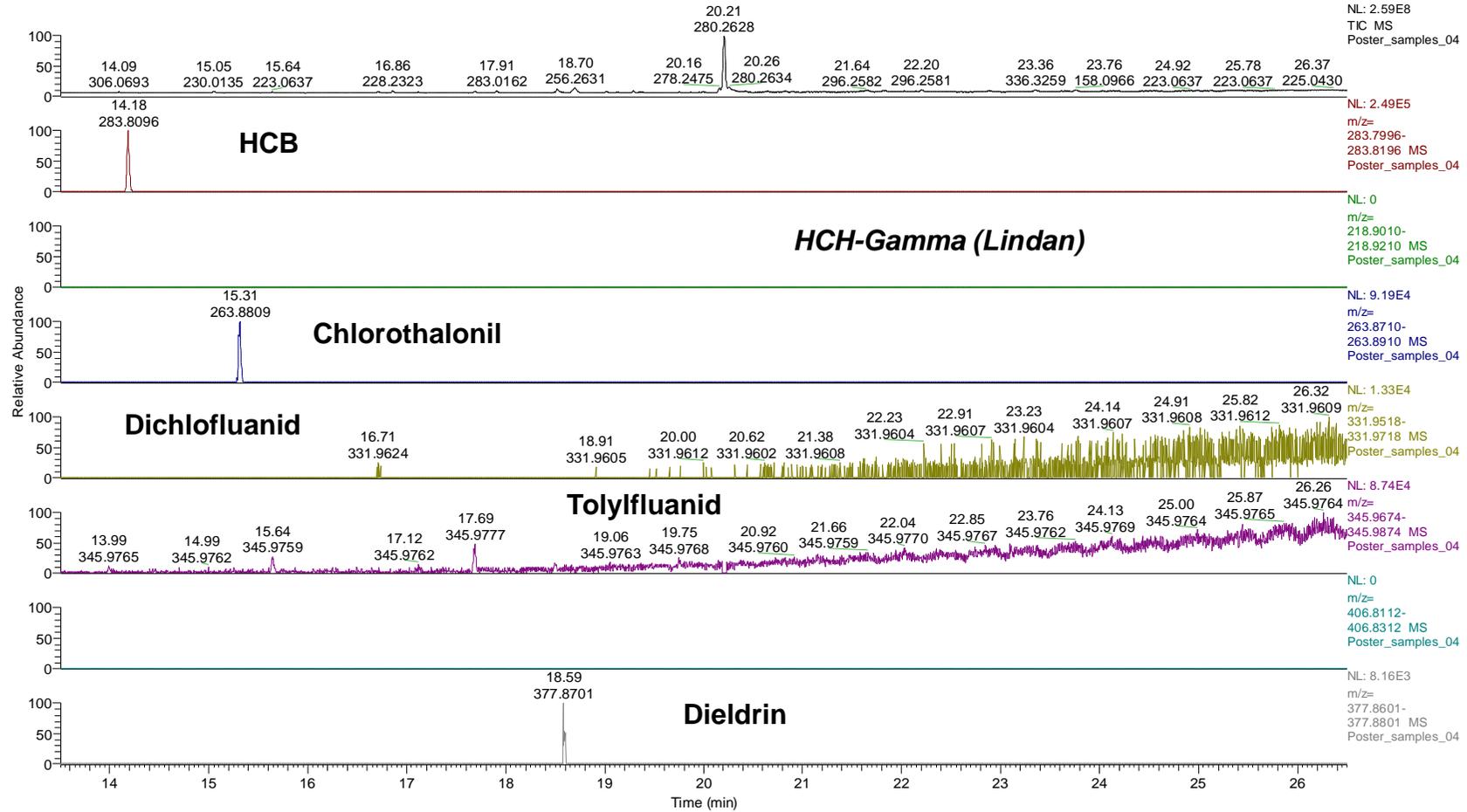
NL:
8.28E4
m/z=
421.7983-
421.8183
MS
Poster_sam
ples_04



NL:
1.33E5
m/z=
430.8783-
430.8983
MS
Poster_sam
ples_04

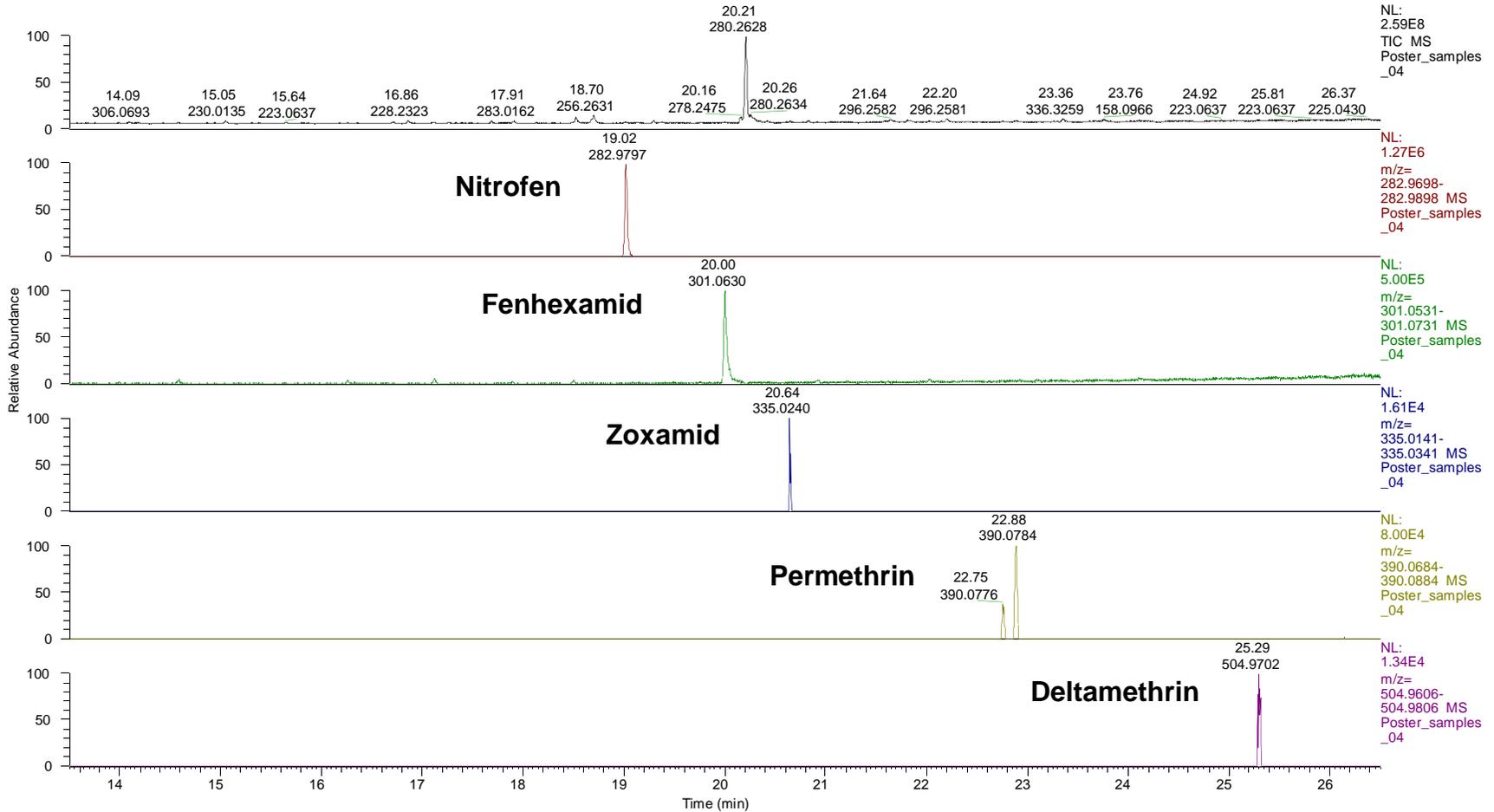
Sample Spiked Extract

RT: 13.50 - 26.50



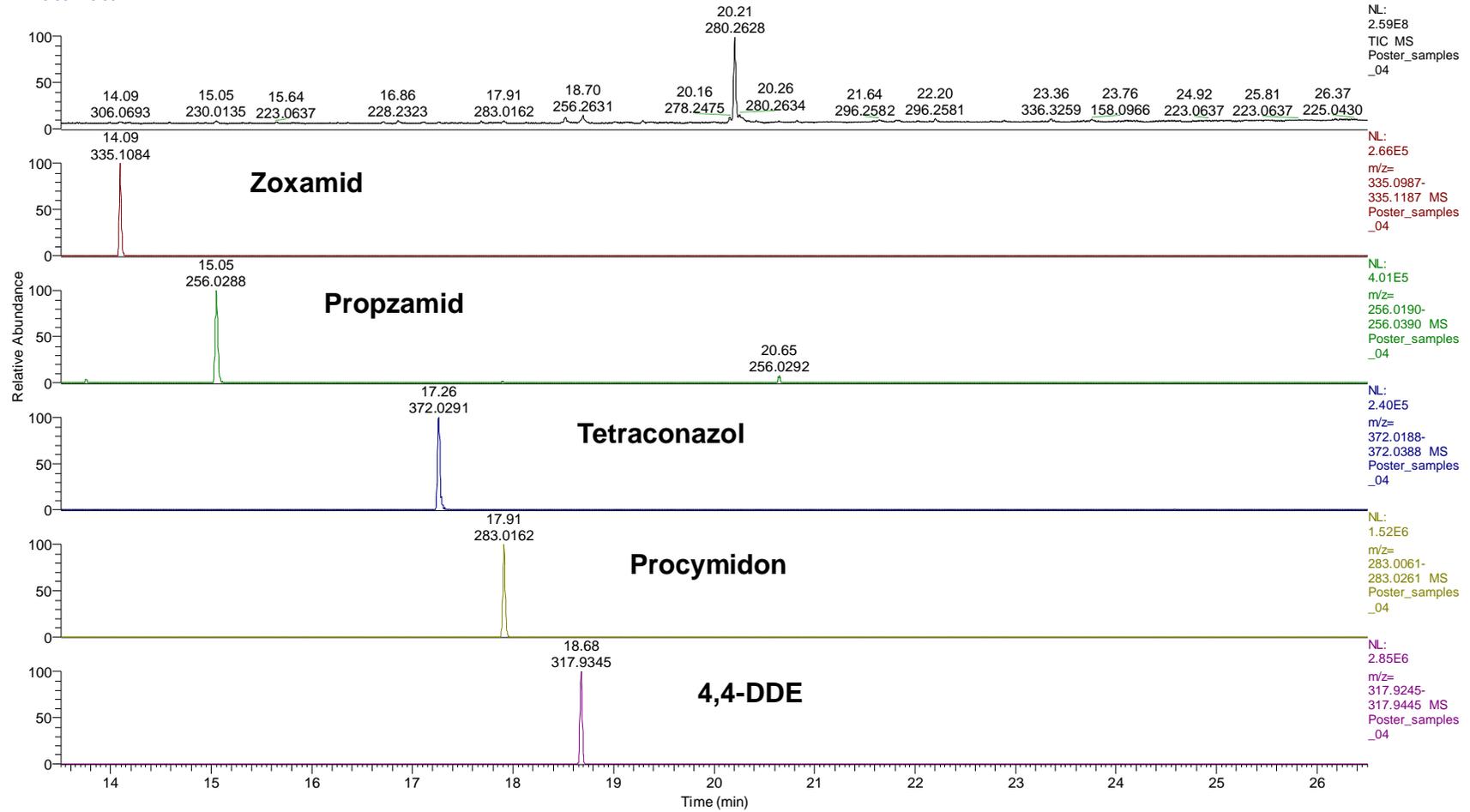
Sample Spiked Extract

RT: 13.50 - 26.50

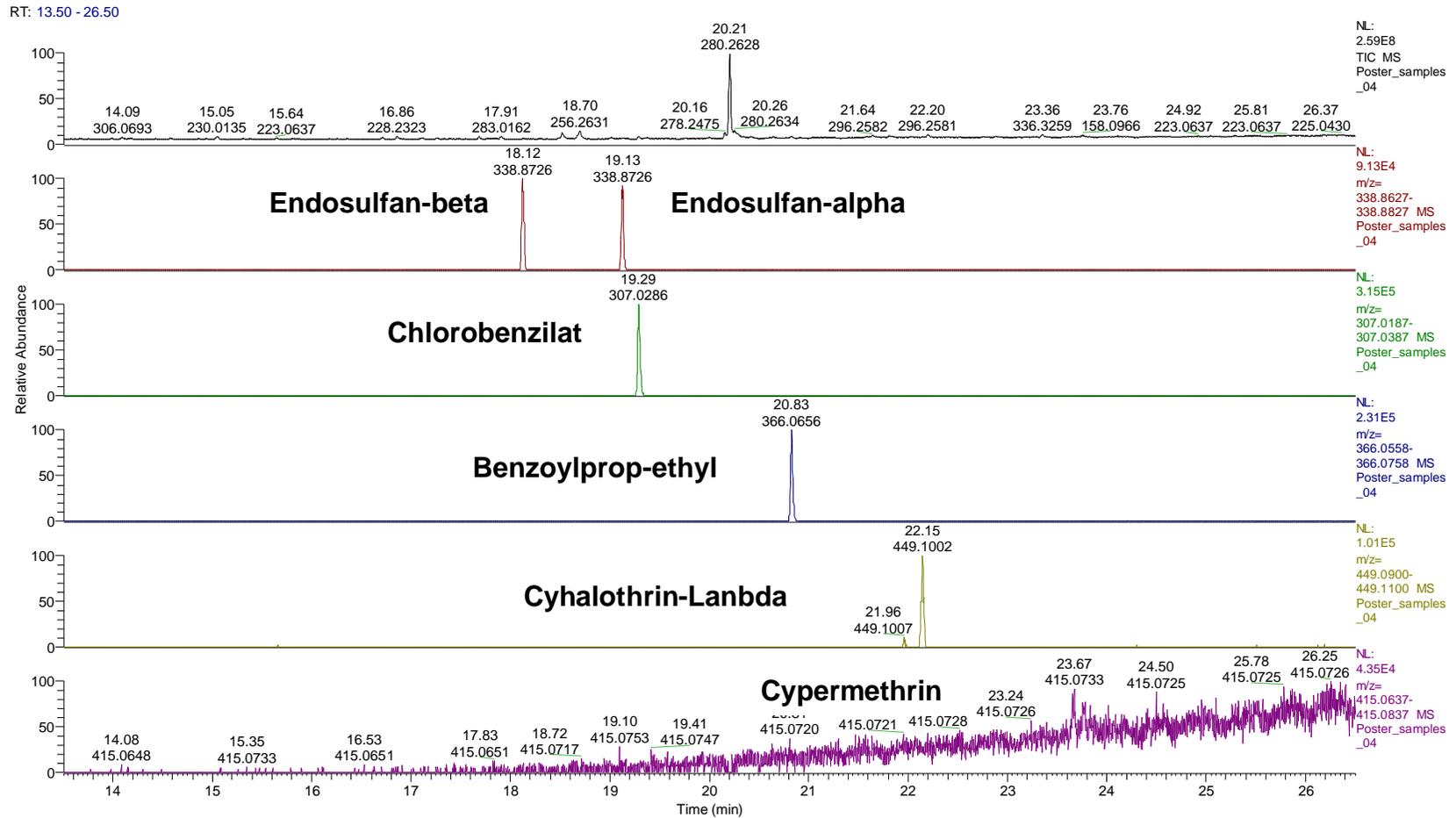


Sample Spiked Extract

RT: 13.50 - 26.50



Sample Spiked Extract



Spiked Sample Extract - Repeated Experiment

Samples: Spiked Extract (0.1 ng/uL spiked) – Matrix Wine

Injection: 1 uL

GC-MS: Exactive Plus with GC-APPI Interface, Trace 1310 GC and RSH Autosampler

MS: APPI Source Temperature – 250 deg C, without Dopant
Scan Range 100-600 amu @ R=35.000 (4 Hz Cycle Time)

GC: SSL Injector – Temperature 250 deg C
Oven – 40 deg C for 1.5 min – 300 deg C with 20 deg C / min.
Flow – 1.3 mL/min.
Transfer Line Temperature – 250 deg C

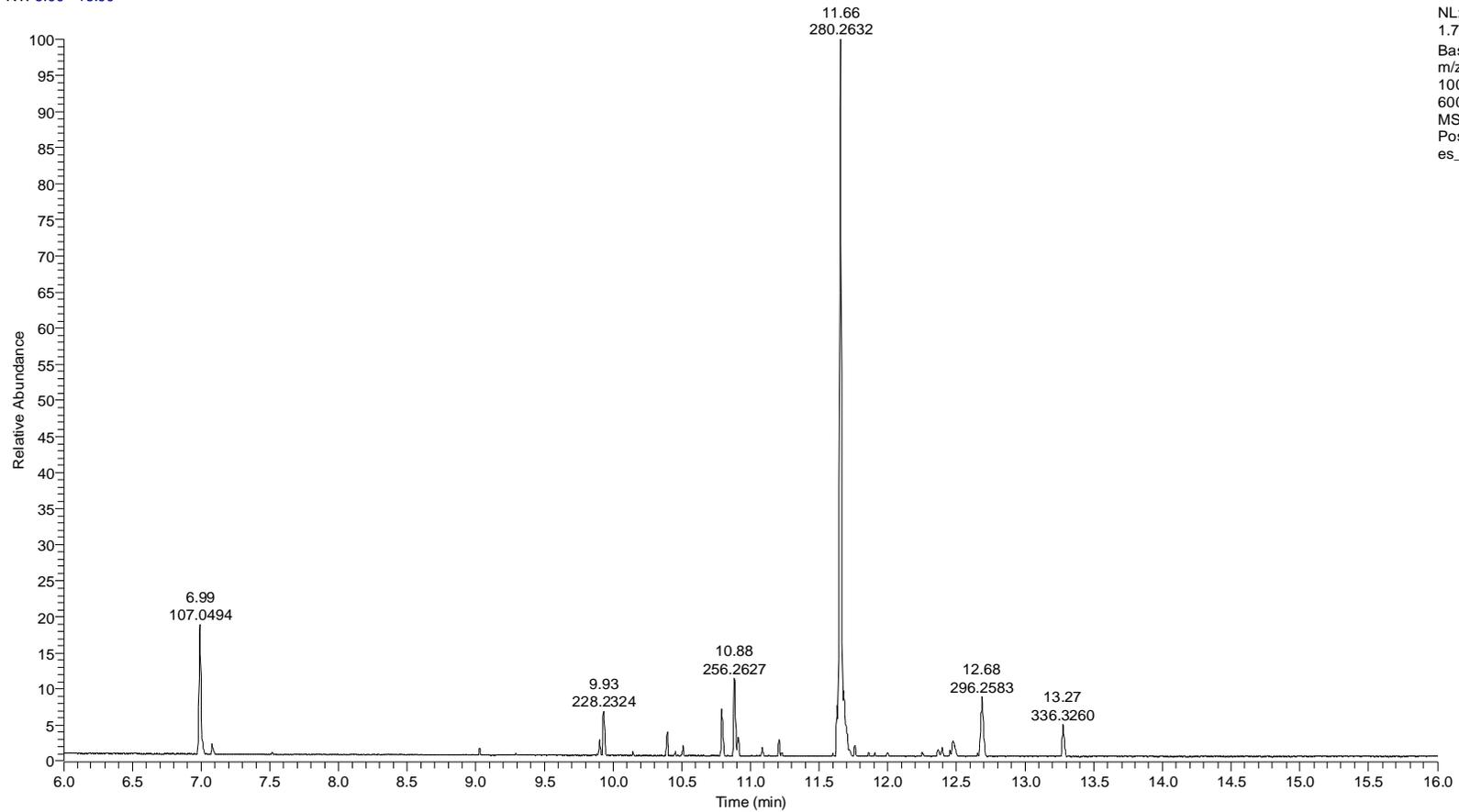
Sample Spiked Extract

C:\Xcalibur\...\Poster\Poster_samples_06
Spiked Extract 0.1ng/ul in Aceton w/o dop.

04.04.2016 08:51:01

Spiked-Extract

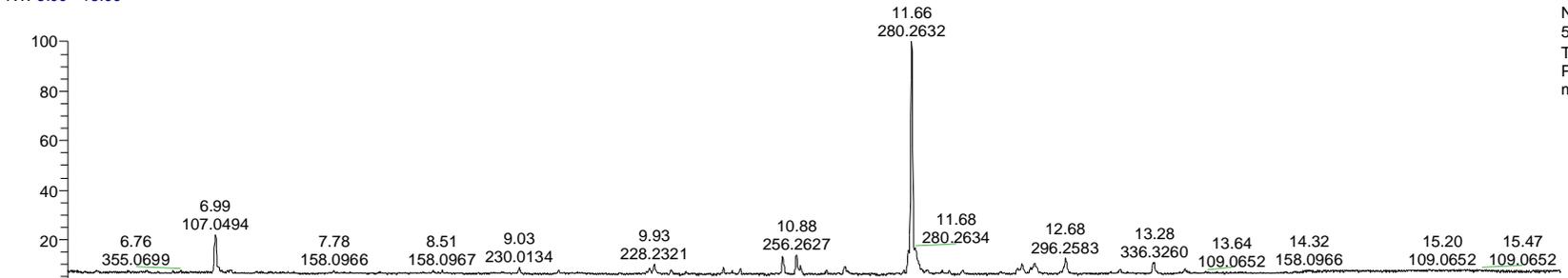
RT: 6.00 - 16.00



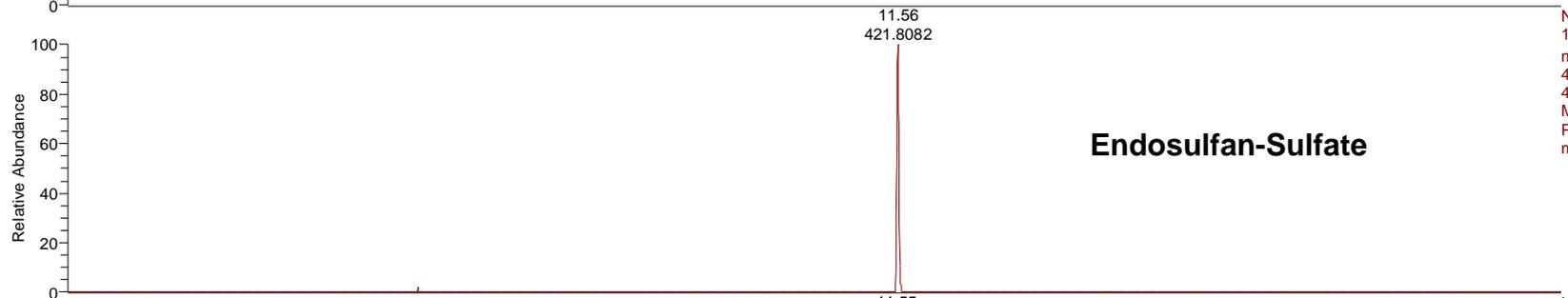
NL:
1.76E8
Base Peak
m/z=
100.0000-
600.0000
MS
Poster_sampl
es_06

Sample Spiked Extract

RT: 6.00 - 16.00

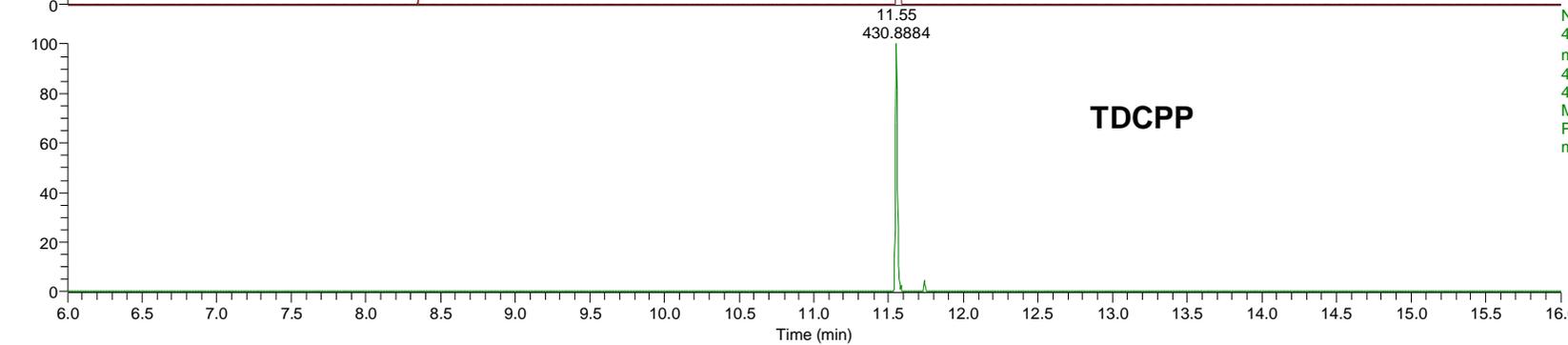


NL:
5.93E8
TIC MS
Poster_sam
ples_06



Endosulfan-Sulfate

NL:
1.64E5
m/z=
421.7983-
421.8183
MS
Poster_sam
ples_06



TDCPP

NL:
4.48E5
m/z=
430.8783-
430.8983
MS
Poster_sam
ples_06

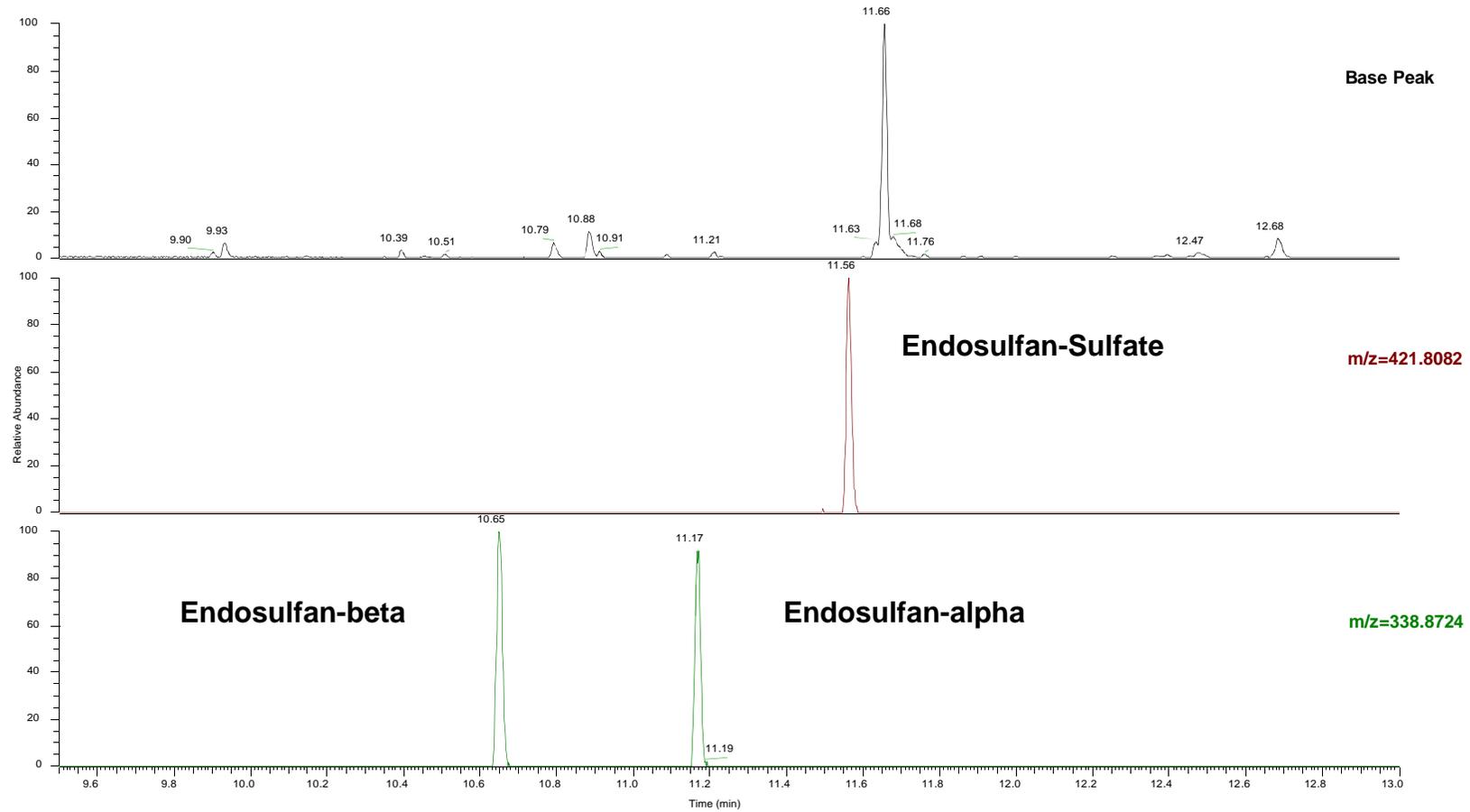
Sample Spiked Extract

C:\Xcalibur\...\Poster\Poster_samples_06
Spiked Extract 0.1ng/ul in Aceton w/o dop.

04.04.2016 08:51:01

Spiked-Extract

RT: 9.50 - 13.00



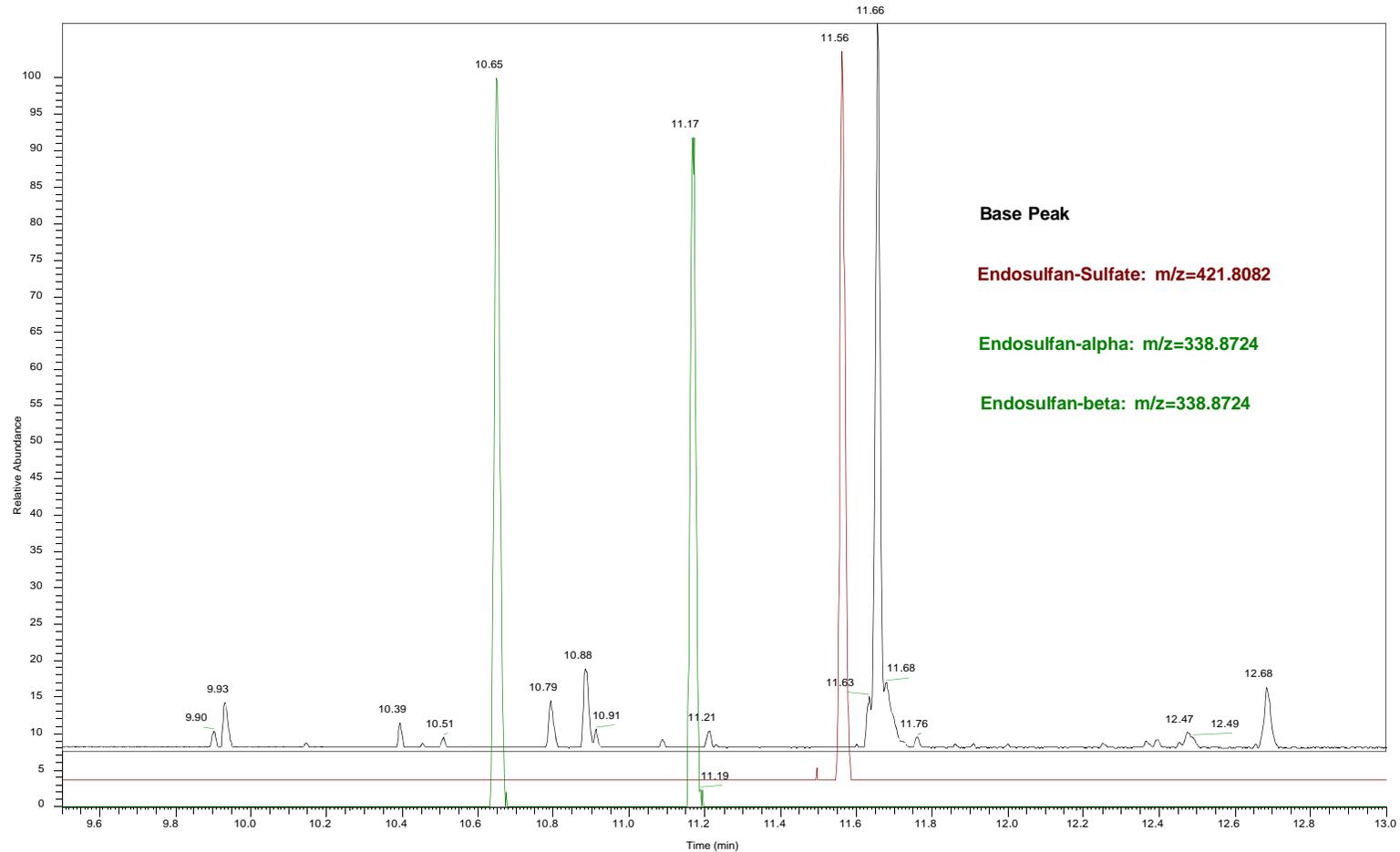
Sample Spiked Extract

C:\Xcalibur...\Poster\Poster_samples_06
Spiked Extract 0.1ng/ul in Aceton w/o dop.

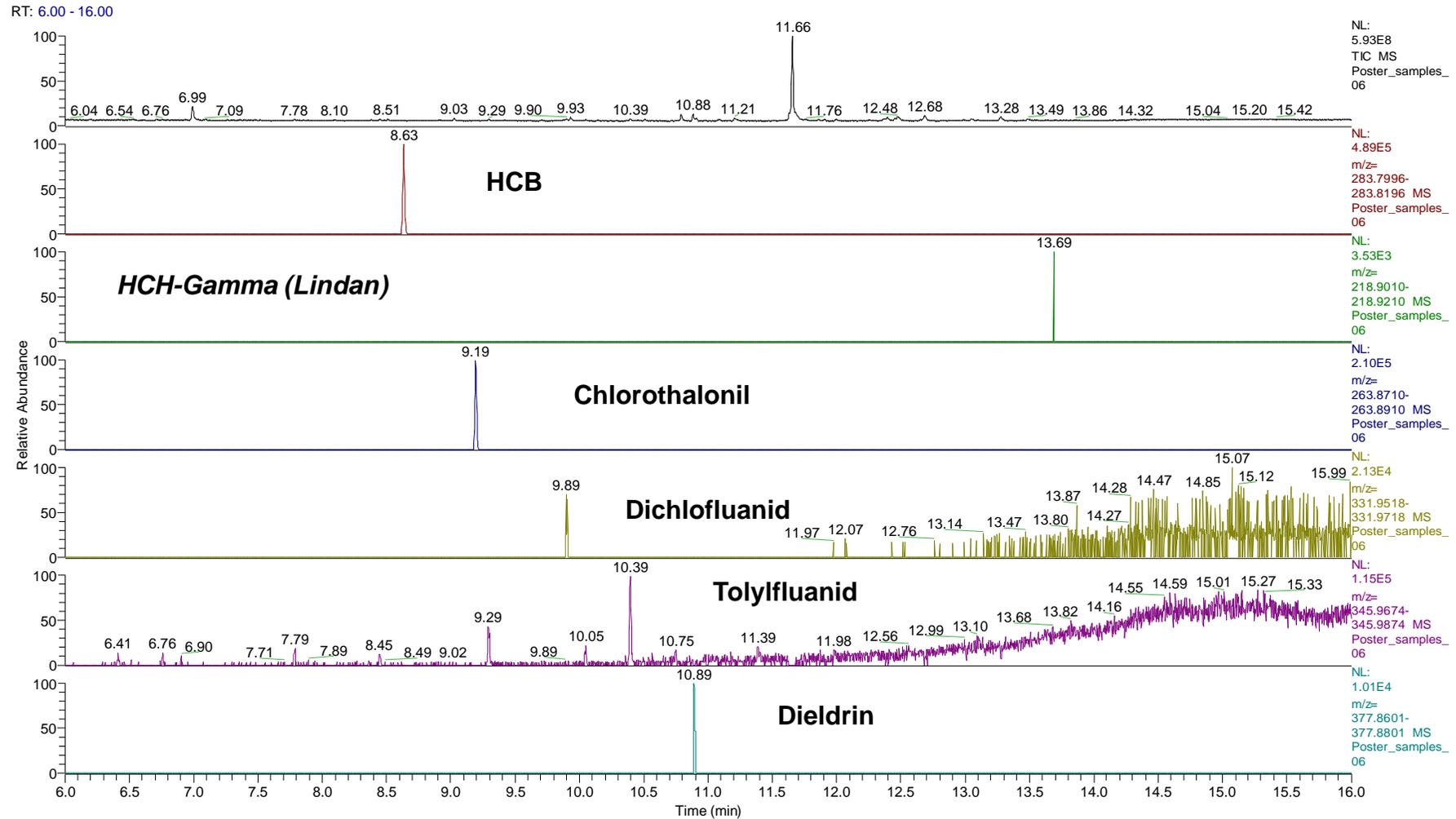
04.04.2016 08:51:01

Spiked-Extract

RT: 9.50 - 13.00

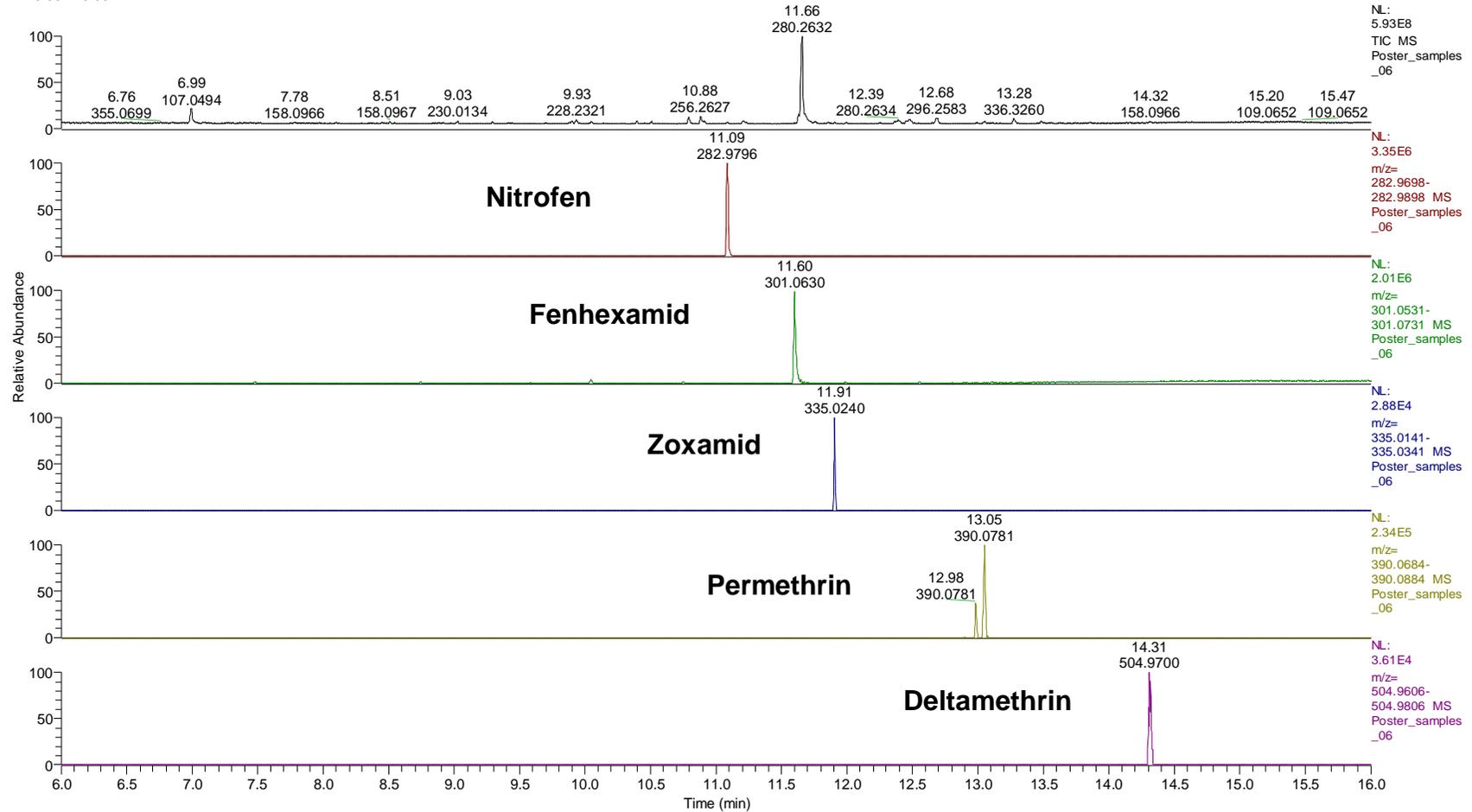


Sample Spiked Extract



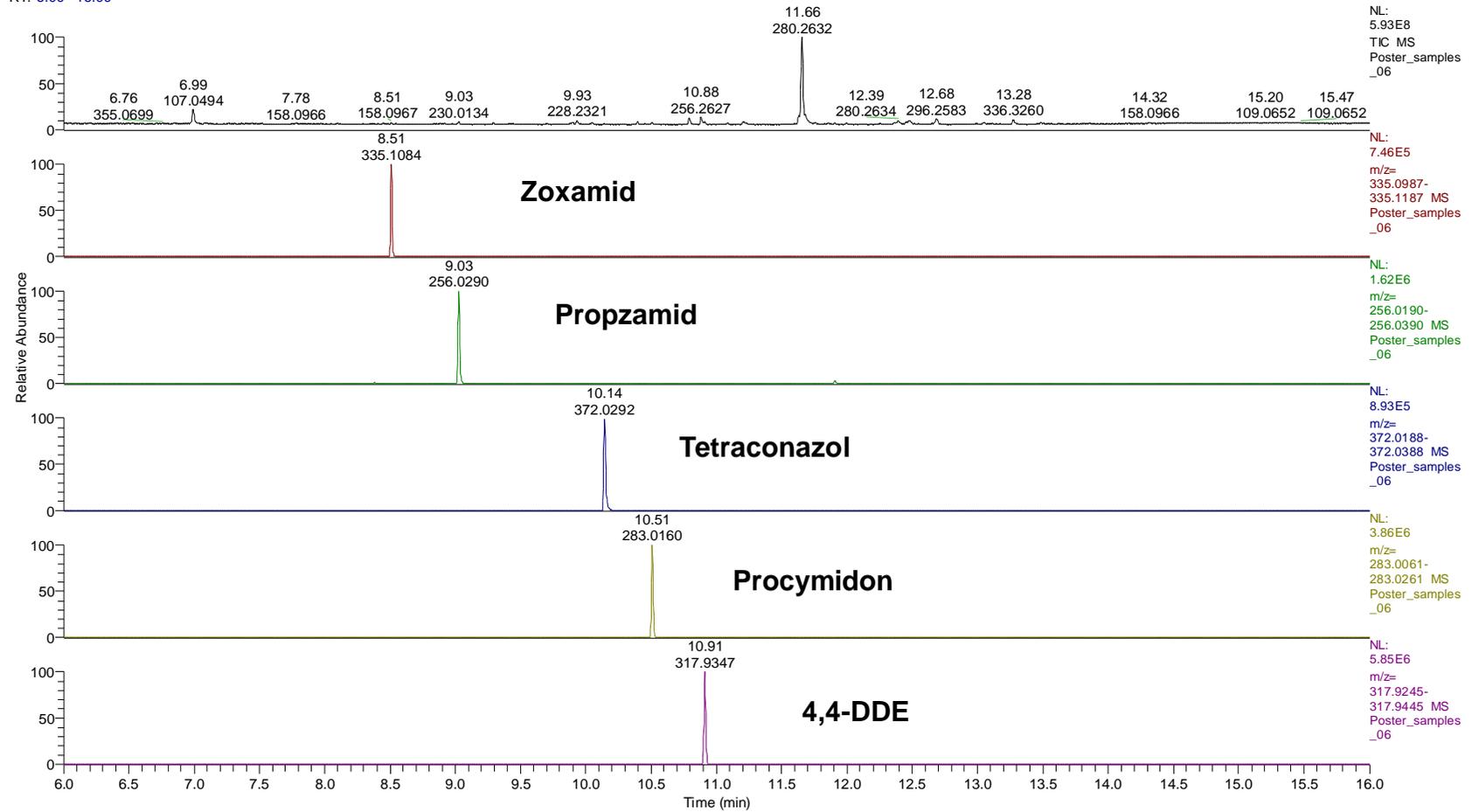
Sample Spiked Extract

RT: 6.00 - 16.00

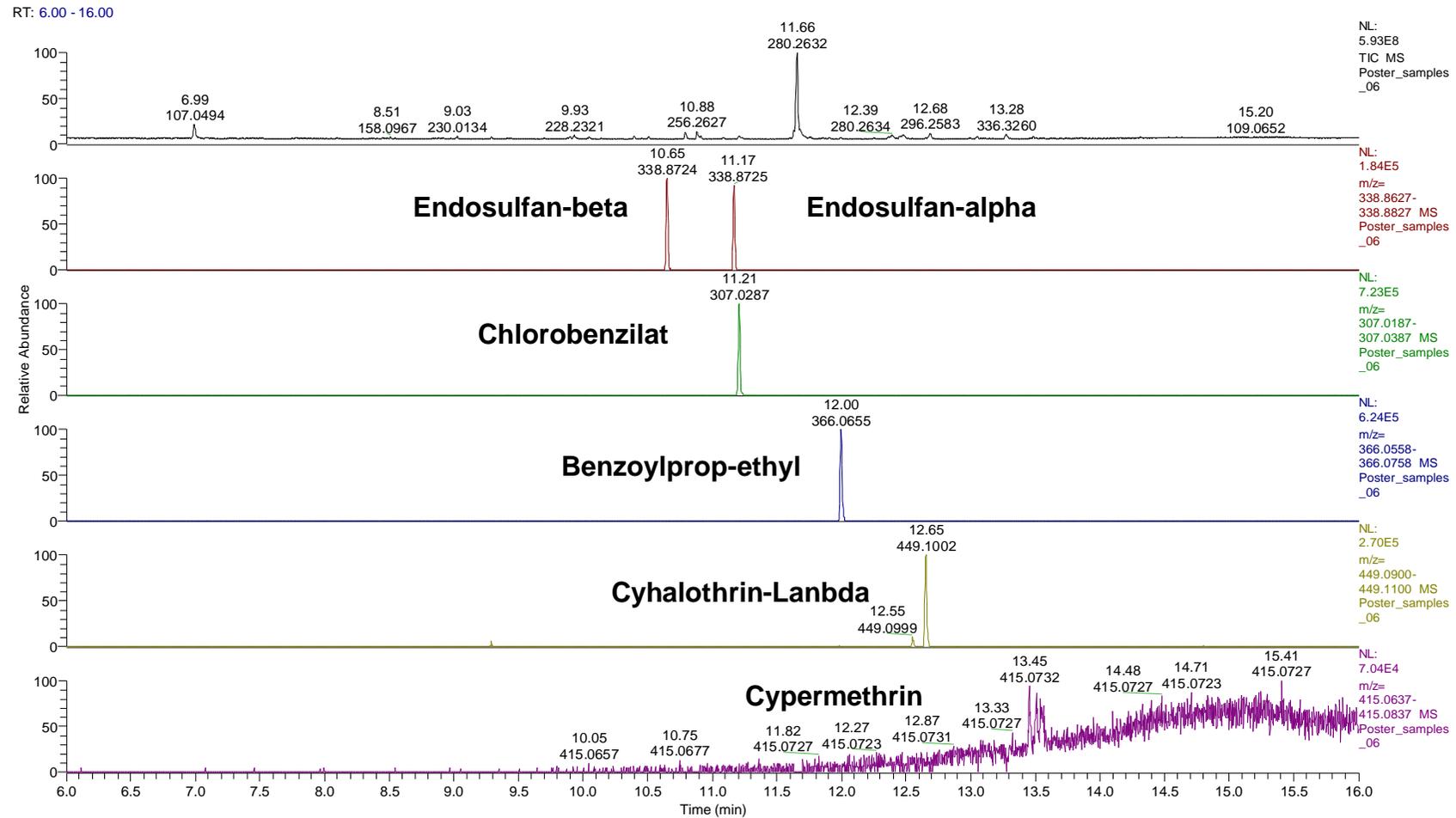


Sample Spiked Extract

RT: 6.00 - 16.00

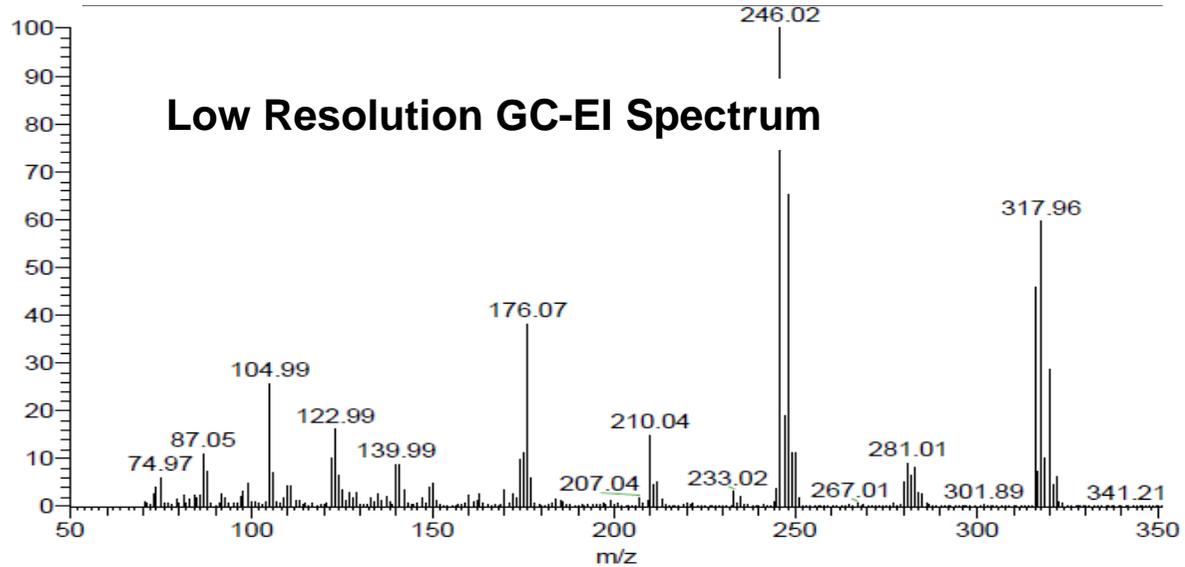
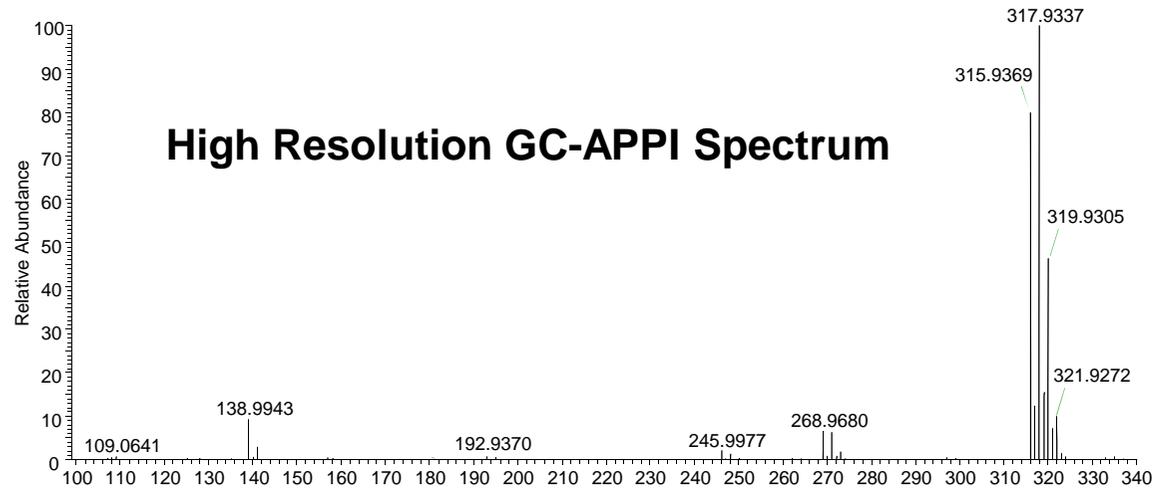
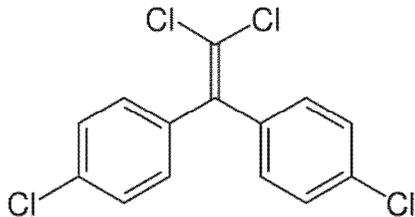


Sample Spiked Extract



GC-EI Measurements – DDE

pp-DDE
 $C_{14}H_8Cl_4$



GC-APPI Offerings

Instrument	GC-APPI Interface	Trace 1310 GC	Trace GC Ultra
Q Exactive	yes	yes	yes
Q Exactive HF	yes	yes	yes
Q Exactive Focus	yes	yes	yes
Exactive Plus	yes	yes	yes
Exactive	yes	yes	yes
LTQ Orbitrap	yes	no	yes
LTQ Orbitrap Discovery	yes	no	yes
LTQ Orbitrap XL	yes	no	yes
LTQ Orbitrap Velos	yes	yes	yes
Orbitrap Velos Pro	yes	yes	yes
Orbitrap Elite	yes	yes	yes
Orbitrap Fusion	yes	yes	yes
Orbitrap Fusion Lumos	yes	yes	yes

For other Thermo instruments with IonMax sources or for using other GCs please contact your sales person or MasCom Technologies directly.

GC-APPI on Orbitrap Fusion Lumos



GC: Thermo Fisher Trace 1310 GC
MS: Thermo Fisher Orbitrap Fusion Lumos™
Source: MasCom Technologies GC-APPI
DS: Windows 7 with Xcalibur 4.1

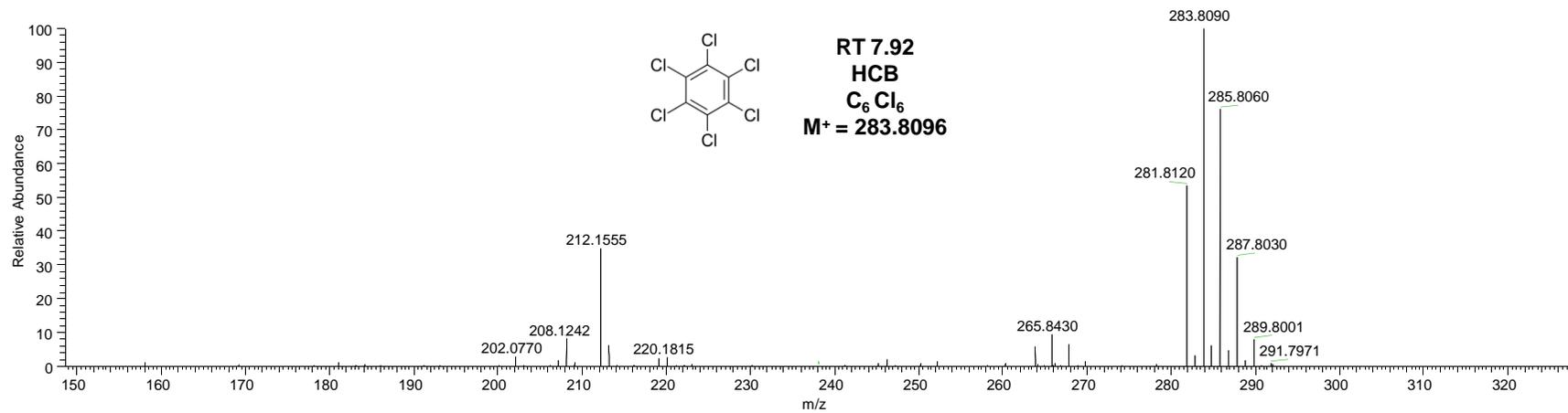
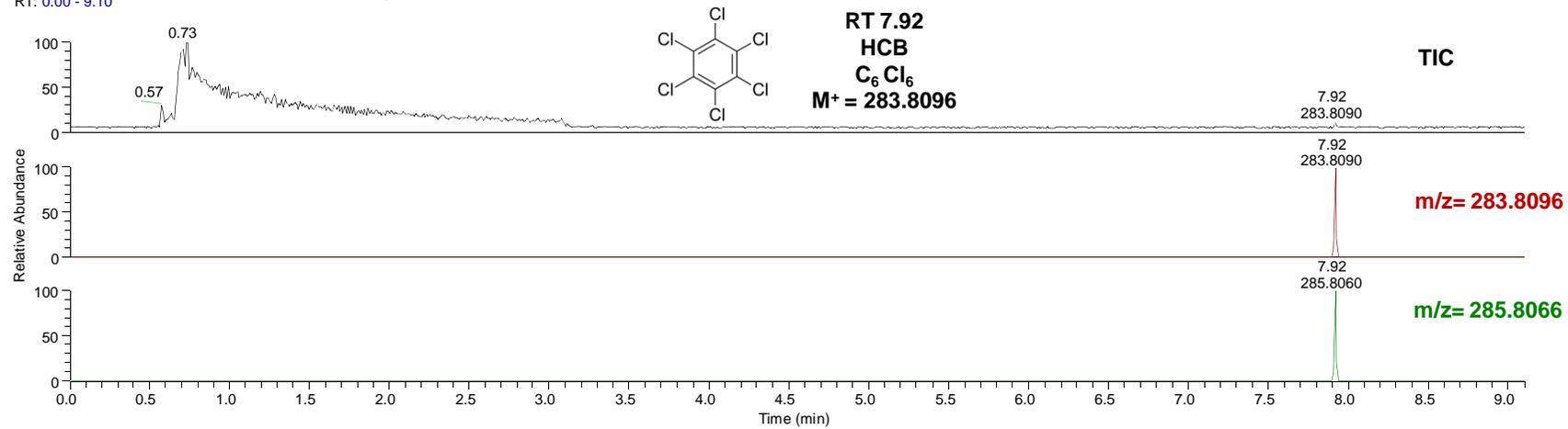
GC-APPI on Fusion Lumos

C:\Xcalibur\data\Lucchi\hcb-fusion1
first measurement on Fusion Lumos MS R=240,000

03/28/18 15:56:47

HCB - 1ng

RT: 0.00 - 9.10

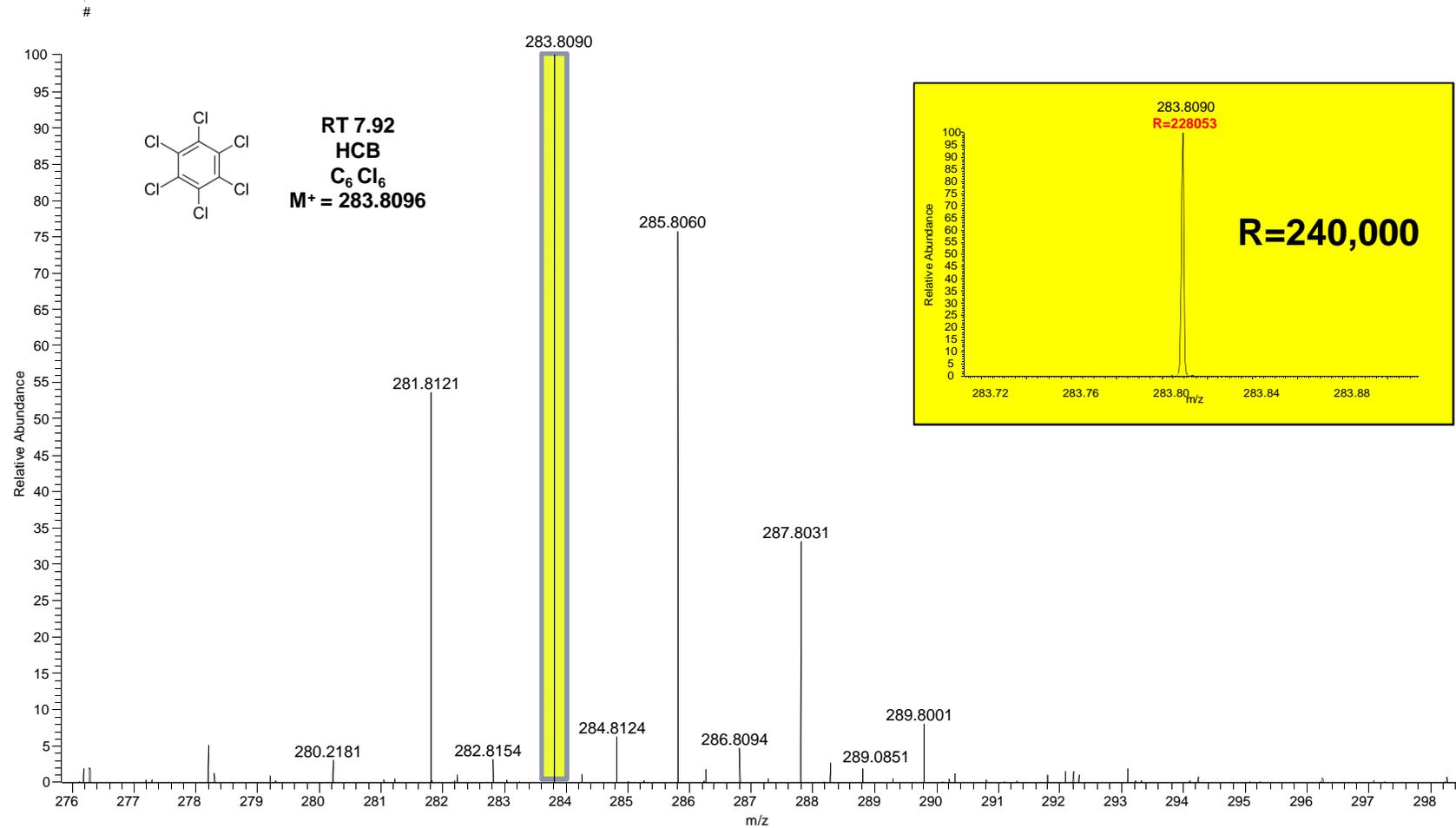


GC-APPI on Fusion Lumos

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first measurement on Fusion Lumos MS R=240000

03/28/18 15:56:47

HCB - 1ng



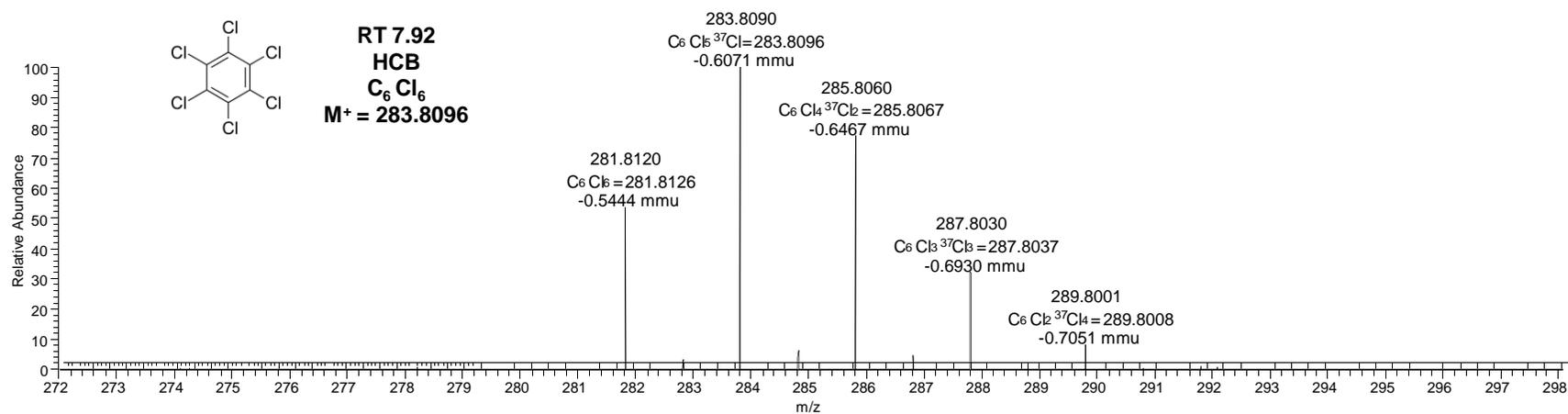
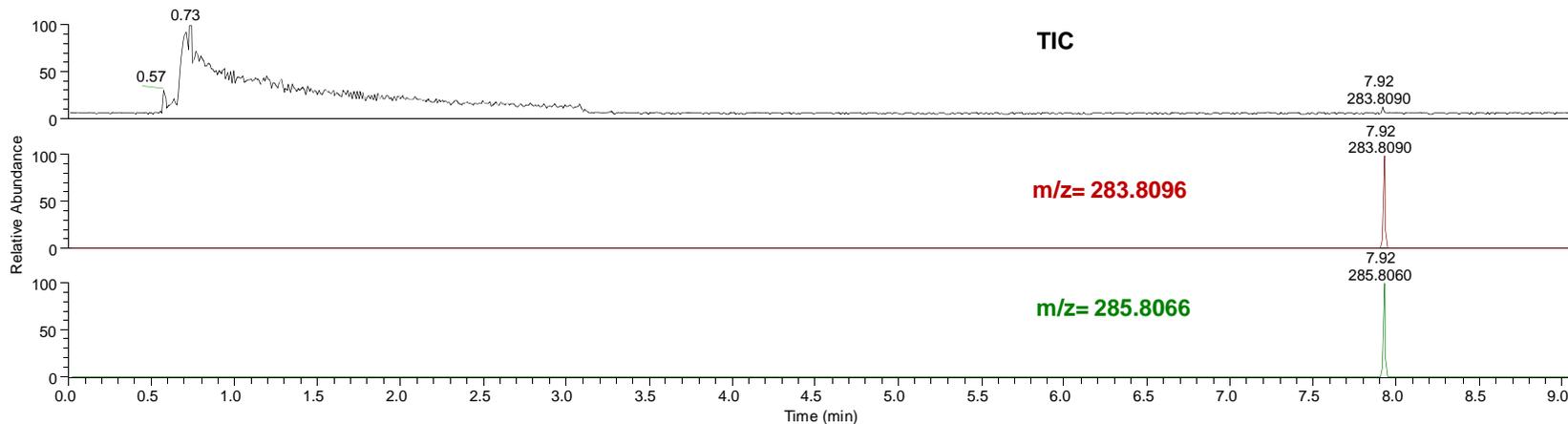
GC-APPI on Fusion Lumos

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first measurement on Fusion Lumos MS R=240,000

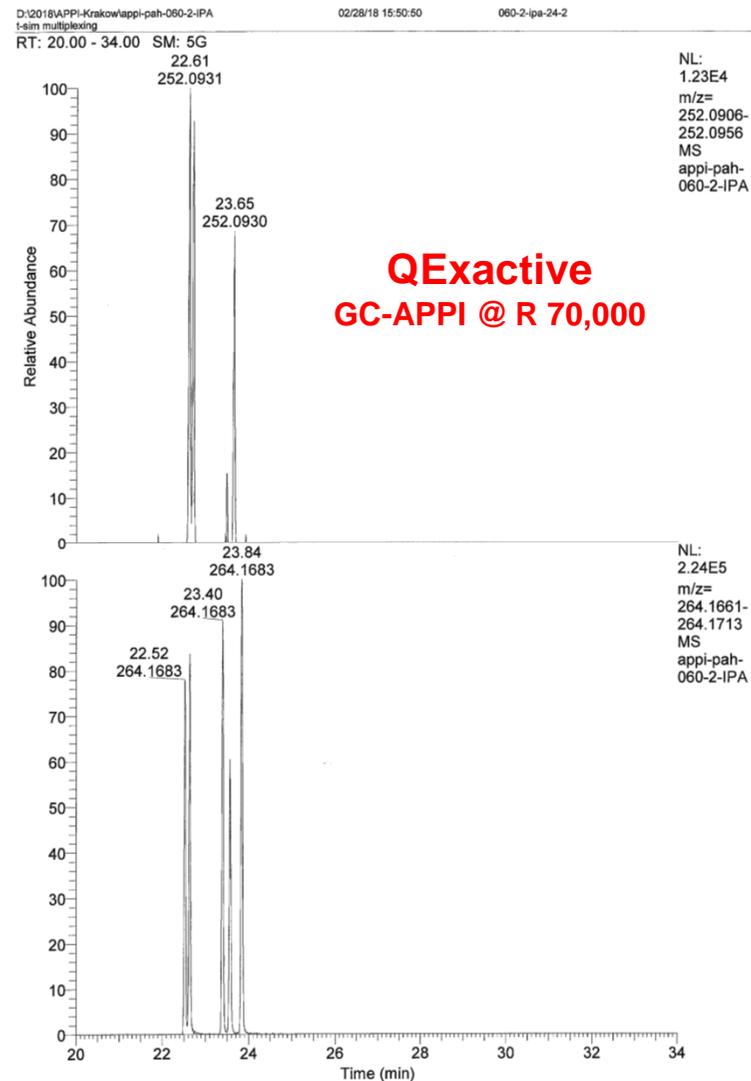
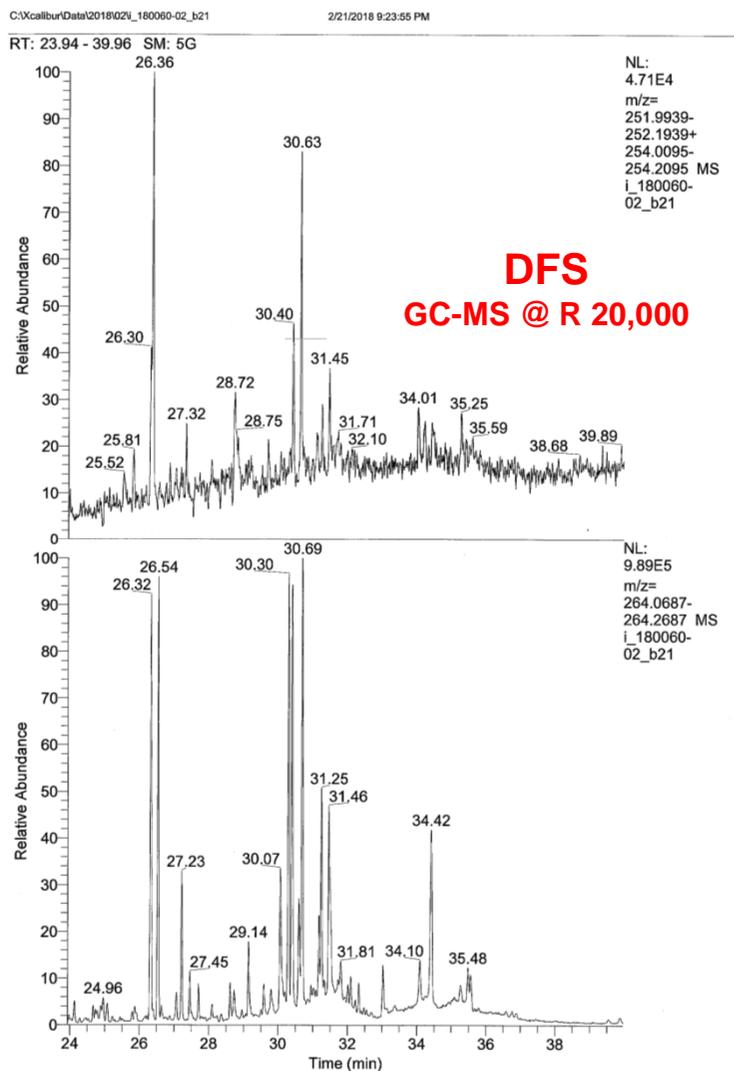
03/28/18 15:56:47

HCB - 1ng

RT: 0.00 - 9.10



DFS versus GC-APPI for PAH



Summary

- The source **preserves the high-fidelity of GC separations** and Orbitrap mass analysis speed provides a sufficient number of scans per peak for quantitation.
- The GC-APPI source ionizes a **broad range of compound**, > 80% of EPA8270 compounds ionized.
- Ionization is depressed as **chlorination** increases, enhanced as **aromaticity** increases.
- **Ionization is softer relative to EI** with less fragmentation observed; some compounds form **readily-explainable adducts**.
- Intact species usually form by **direct ionization** (and have high ionization efficiencies).
- HR/AM, provided by the Orbitrap mass analyzer, **cut through matrix interferences** even at low analyte amounts on column.

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