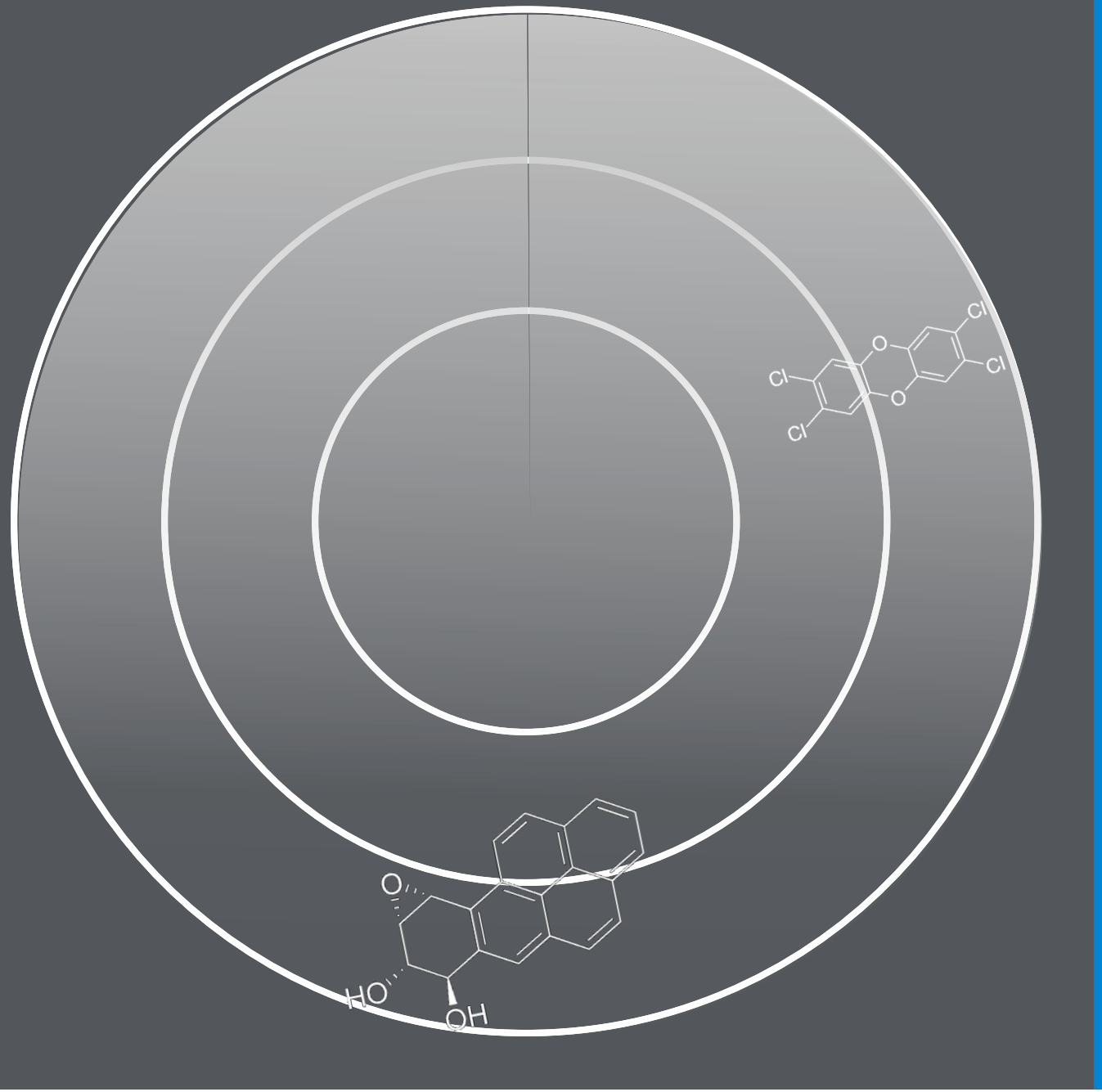
The Era of Mass Surveillance

Identify Suspects, Confirm Targets and Explore Unknowns with GC/Q-TOF

Nathan Eno
GC/Q-TOF Product Manager

Kai Chen, Ph.D.
GC/MS Application Scientist



Agilent

Panoramic Technology for Full Spectrum Surveillance

High Resolution and Mass Accuracy

Reproducible Spectral Performance

Simultaneous
High Resolution and
Wide Dynamic Range

Flexible Agilent
7890B GC

Sensitive Low Energy EI

MassHunter Acquisition

MassHunter Qualitative Analysis

MassHunter Quantitative Analysis

MassHunter PCDL Manager

Online Resources

MassHunter Qualitative Analysis

Molecular Structure Correlator

Actionable Results

MassHunter Unknowns Analysis

MassHunter Profinder / Unknowns Analysis

Mass Profiler Professional

Target Quantitation

Linearity and Detection Limit Performance for Targeted Assays

Agilent MassHunter Quantitative Analysis (for TOF) - 20170929 - Avocado Scan.batch.bin

File | Home | View | Method | Tools | Help

Edit | New | Open | Append | Save | Save As | Method Report | Validate | Exit — Method

Method Setup Tasks | Advanced Tasks | Duplicate Compounds | Manual Setup Tasks | Update | Swap Qualifier With Quantifier | Outlier Setup Tasks | Calibration Curve — Method Setup Tasks

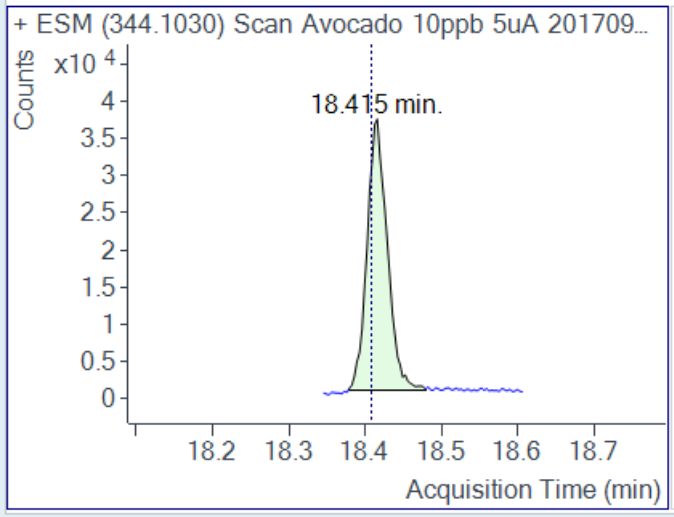
Library Method | Setup Reference Library | Setup Reference Pattern Library — Library

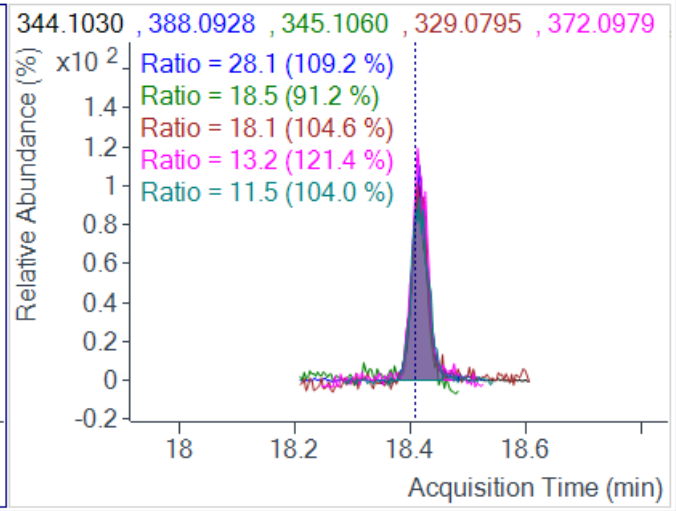
Batch Table

Sample: 10 ppb Avocado | Sample Type: <All> | Compound: Azoxystrobin | ISTD:

Sample				Azoxystro...	Azoxystrobin Results							Qualifier (388.0928) Results				Qualifier (345.1060) Results				
	Name	Type	Level	Exp. Conc.	RT	Resp.	MI	Calc. Conc.	Final Conc.	Accuracy	Mass Accuracy	Ratio	Mass Accuracy	S/N	MI	Ratio	Mass Accuracy	S/N	MI	Ratio
	2 ppb Avocado	Cal	2	2.0000	18.415	11667	☐	2.0805	2.0805	104.0	-1.9689	29.6	-0.7354	7.38	☐	22.4	-0.7069	3.61	☐	15.8
	5 ppb Avocado	Cal	3	5.0000	18.417	32806	☐	4.3995	4.3995	88.0	-2.5398	29.7	-1.8039	16.99	☐	19.5	-3.0019	4.66	☐	18.3
▶	10 ppb Avocado	Cal	4	10.0000	18.415	67221	☐	8.1748	8.1748	81.7	-1.4376	28.1	-1.2841	26.68	☐	18.5	-0.0052	6.28	☐	18.1
	20 ppb Avocado	Cal	5	20.0000	18.417	143907	☐	16.5874	16.5874	82.9	-0.0917	27.0	0.3633	50.71	☐	19.0	0.6008	21.55	☐	15.4
	50 ppb Avocado	Cal	6	50.0000	18.418	424513	☐	47.3703	47.3703	94.7	-1.7079	24.8	-1.7057	77.07	☐	18.4	-1.7582	39.17	☐	15.0
	100 ppb Avocado	Cal	7	100.0000	18.418	858975	☐	95.0315	95.0315	95.0	-0.8646	26.6	-0.6051	455.66	☐	19.3	-1.0061	48.39	☐	16.1
	200 ppb Avocado	Cal	8	200.0000	18.419	1845131	☐	203.2142	203.2142	101.6	-1.5004	26.5	-0.7792	1020.33	☐	20.5	-1.3373	104.66	☐	16.2
	500 ppb Avocado	Cal	9	500.0000	18.420	4638419	☐	509.6419	509.6419	101.9	-0.0104	27.6	0.8329	1648.86	☐	21.2	-0.2021	257.53	☐	16.2

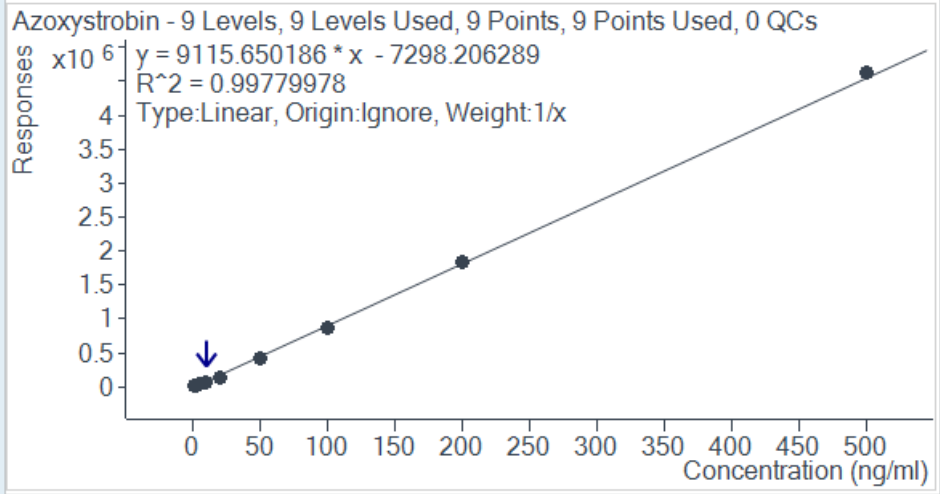
Compound Information



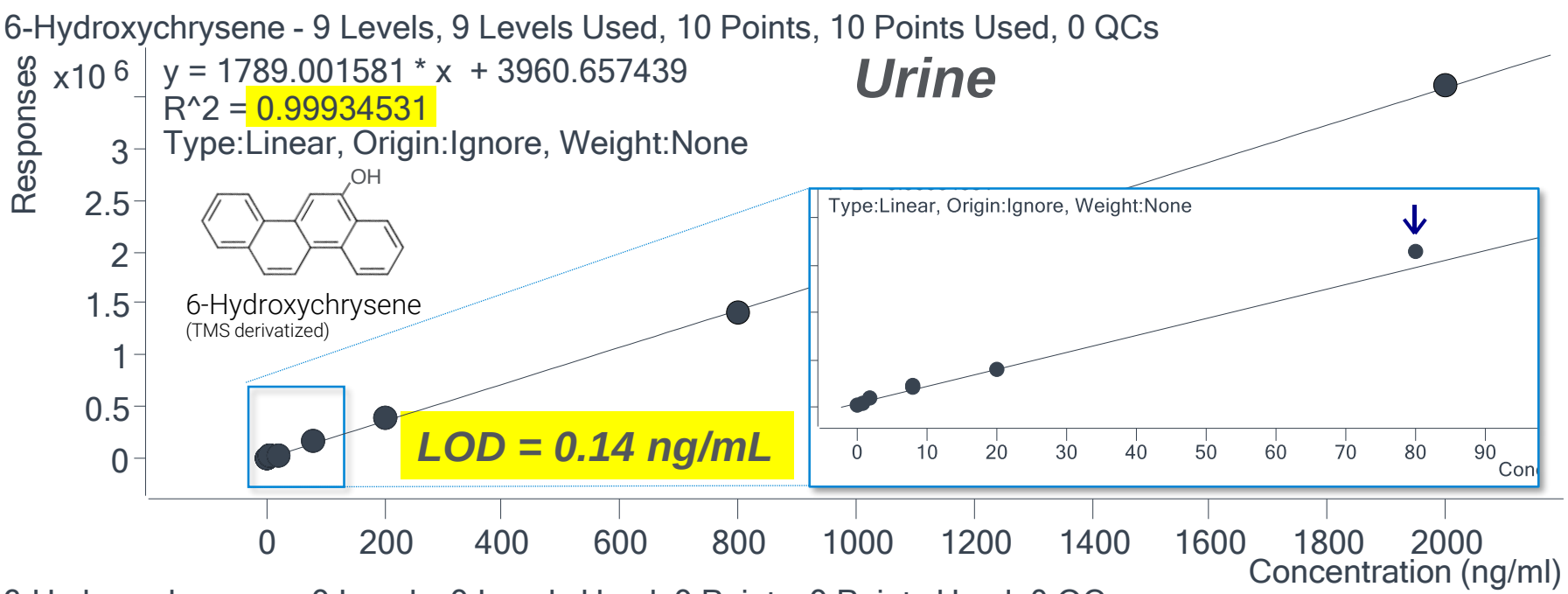


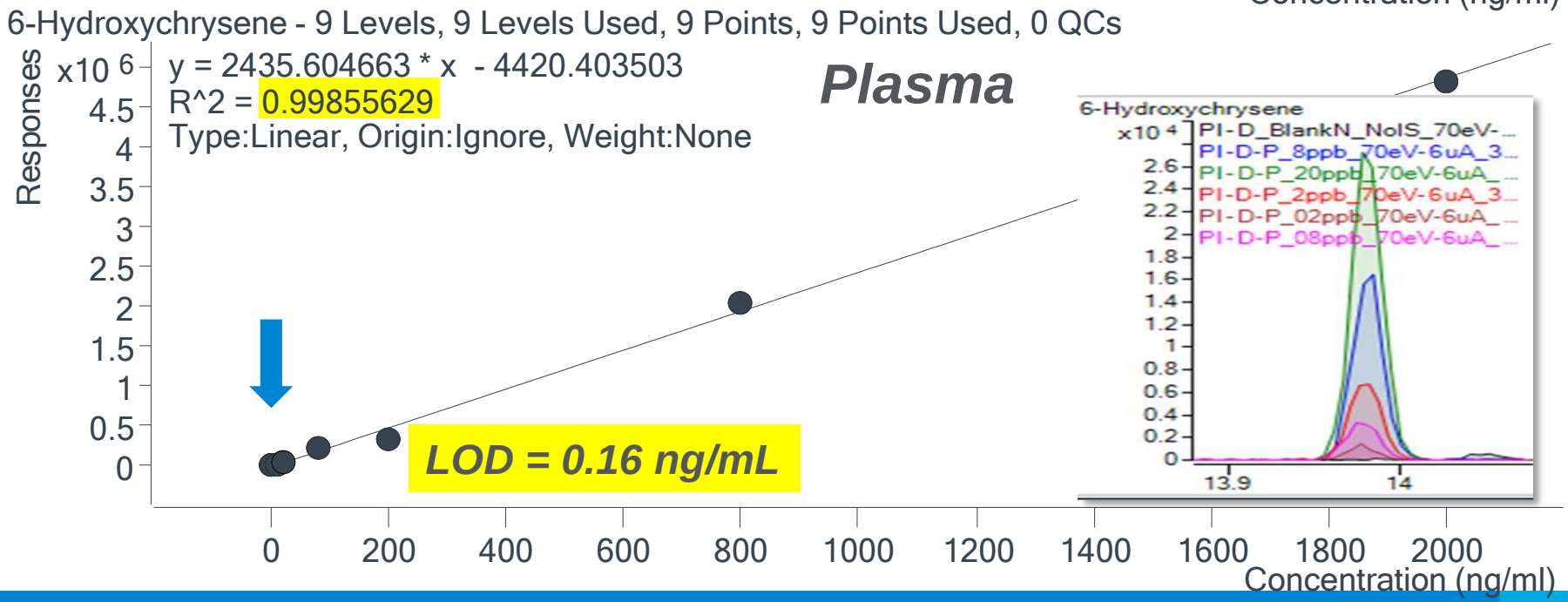
Calibration Curve

Type: Linear | Origin: Ignore | Weight: 1/x | ISTD | QC



Processed | 10 ppb Avocado | Azoxystrobin | 9 Samples (9 total) | AGILENT\kaichen

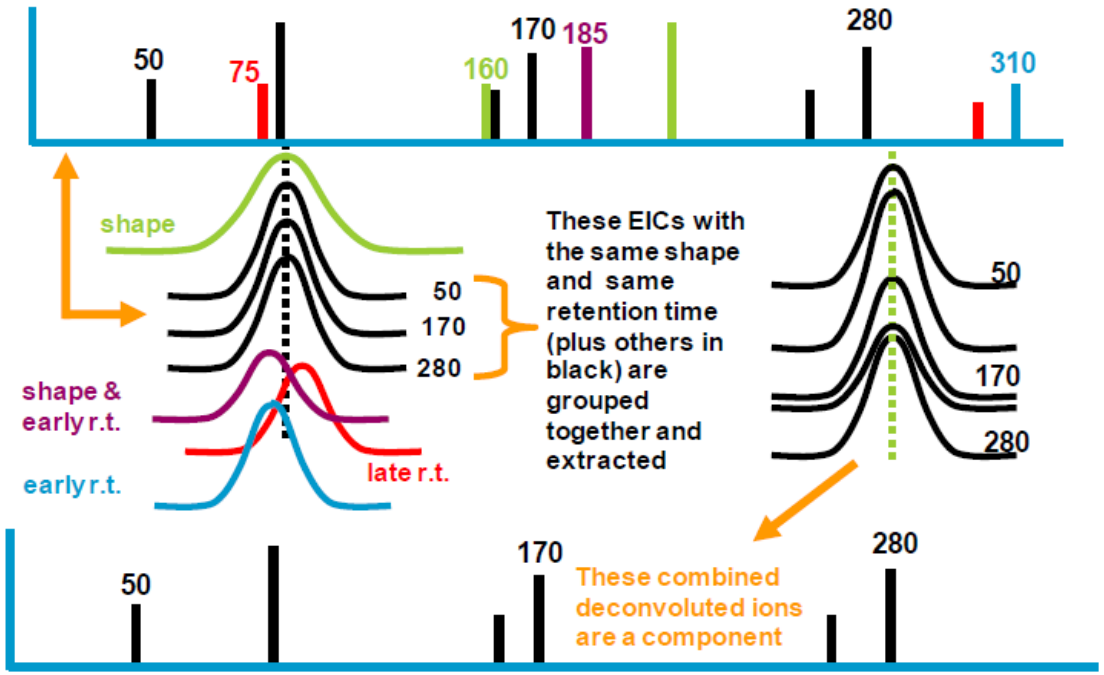




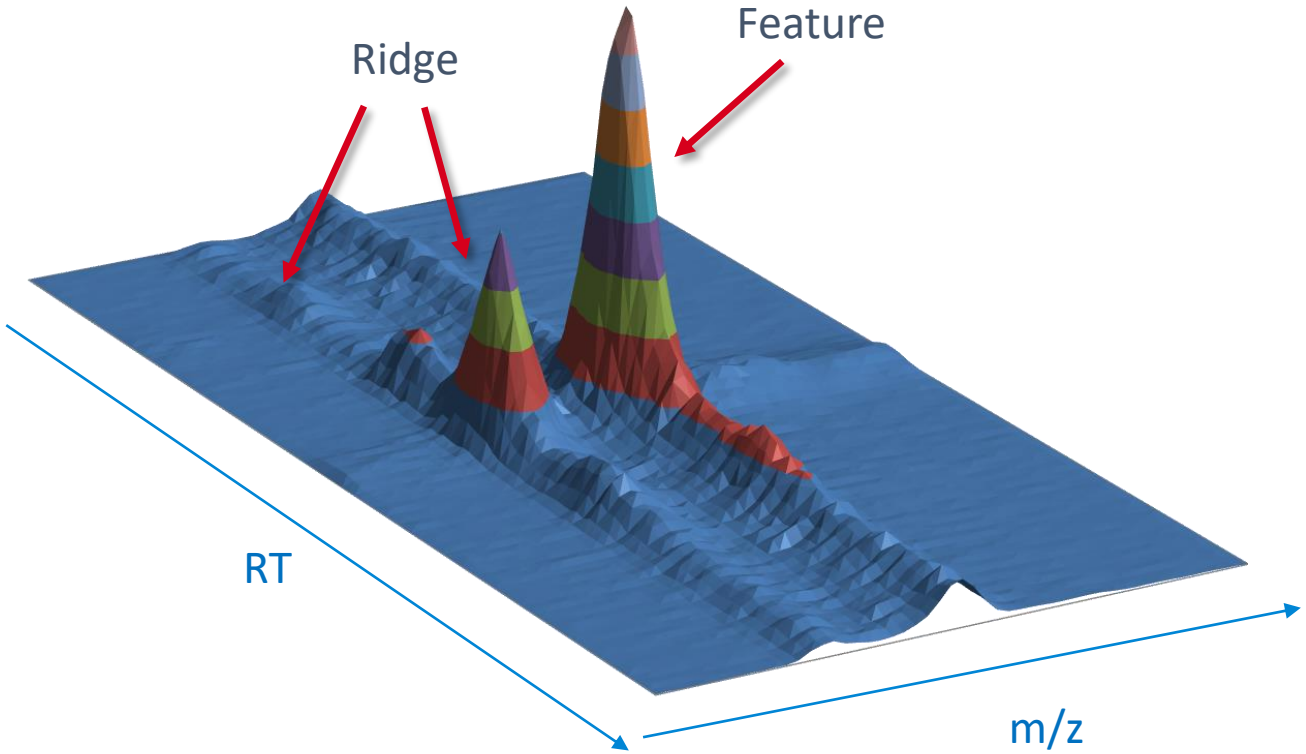
LOD (ng/mL) per matrix

Compound name	Urine	Plasma
Naphthalene	0.52	0.38
Acenaphthylene	0.42	0.74
Acenaphthene	0.98	1.28
1-Hydroxynaphthalene	0.48	0.47
2-Hydroxynaphthalene	0.28	0.20
Fluorene	1.12	0.26
Phenanthrene	0.35	0.18
Anthracene	0.36	0.26
1,6-Dihydroxynaphthalene	0.34	0.16
2,7-Dihydroxynaphthalene	0.13	0.10
3-Hydroxyfluorene	0.22	0.36
2-hydroxyfluorene	0.25	0.21
4-Hydroxyphenanthrene	0.39	0.42
Fluoranthene	0.30	0.19
3-Hydroxyphenanthrene	0.60	0.27
1-Hydroxyphenanthrene	0.34	0.30
9-Hydroxyphenanthrene	0.50	0.33
Pyrene	0.42	0.10
Benzo(a)anthracene	0.16	0.23
Chrysene	0.26	0.09
6-Hydroxychrysene	0.14	0.16
Benzo(b)fluoranthene	0.38	0.26
Benzo(k)fluoranthene	0.38	0.27
Benz(a)pyrene	0.61	0.30
Indeno(1,2,3-cd)pyrene	0.65	0.35
Dibenz(a,h)anthracene	0.51	0.09
9-Hydroxybenzo(a)pyrene	0.47	0.34
Benzo(ghi)perylene	0.89	0.36
7,8-Hydroxybenzo(a)pyrene	6.65	3.63

SureMass Signal Processing



Conventional Deconvolution
(Nominal Mass)



SureMass Signal Processing
(Profile Accurate Mass)

Suspect Screening

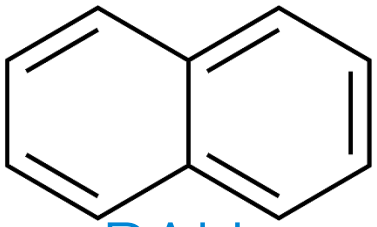
Analytical Performance Factors for Confident Compound Detection

Fingerprint image adapted from
The Photographer - Own work, CC BY-SA 3.0,
https://commons.wikimedia.org/w/index.php?curid=8251516

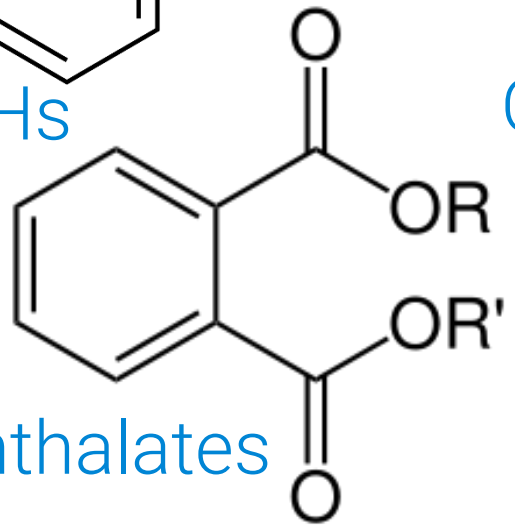
Suspect Surveillance – Now with even broader scope

GC/Q-TOF Pesticides & Environmental Pollutants PCDL – now with *1000+ compounds*:

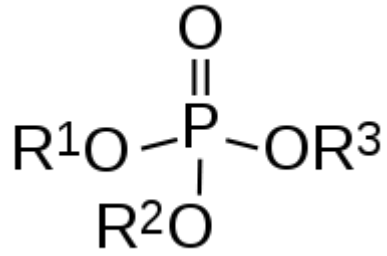
- High Resolution Spectra
- Expert, human curation
- Better compound alignment with US EPA 8270 targets and Agilent GC/TQ MRM database



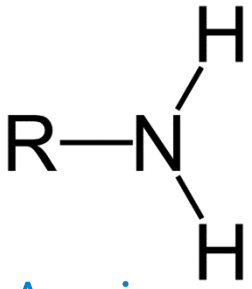
PAHs



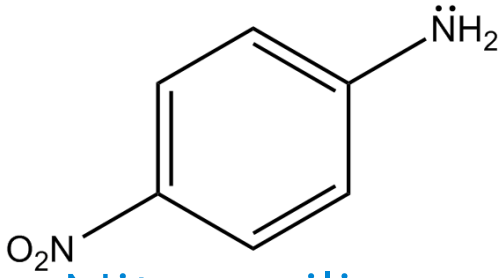
Phthalates



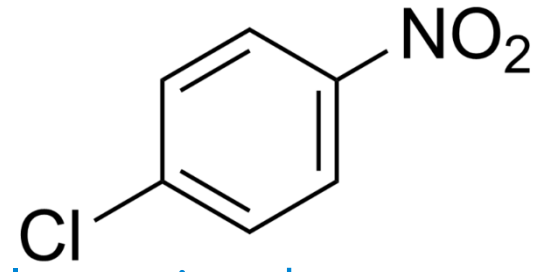
Organophosphates



Amines



Nitroanilines



Chloronitrobenzenes

Agilent MassHunter Qualitative Analysis Workflows B.08.00 - Training_Apr18_GCQTOF_Target Screening.m

File Launch Edit View Find Identify Method Configuration Tools Help

Compound List: 1018 found, 32 shown, filtered on Flags (Tgt), FIs Conf.

Compound Identification		General				Target/Suspect Screening					
Name	CAS	Formula	m/z	Area	RT	RT Diff (Tgt)	Score (Frag Coelution)	Score (Frag Ratio)	Flags (Tgt)	FIs Conf.	FragMassDiff(ppm)
Diisobutylphthalate	84-69-5	C16 H22 O4	149.0233	93135	8.832	0.015	98.63	97.94	Qualified	5	0.68
Dimethomorph (E)	110488-70-5	C21 H22 Cl N O4	387.1241	21210	18.48	0.029	99.75	99.17	Qualified	6	2.42
Dimethomorph (Z)	113210-98-3	C21 H22 Cl N O4	387.1242	16614	18.79	0.09	99.8	99.73	Qualified	6	2.66
Fludioxonil	131341-86-1	C12 H6 F2 N2 O2	248.0394	27773	11.55	0.024	99.35	99.5	Qualified	6	0.6
Isophorone	78-59-1	C9 H14 O	138.104	20234	4.166	0.037	89.3	92	Qualified	5	1.03
Mefenoxam	70630-17-0	C15 H21 N O4	279.1414	1119	9.342	0.007	89.32	97.21	Qualified	5	0.11
Metalaxyl	57837-19-1	C15 H21 N O4	206.1176	12522	9.342	0.014	87.35	99.25	Qualified	6	0.11
Pentachlorobenzoni	20925-85-3	C7 Cl5 N	274.8437	23680	8.27	0.008	99.17	99.98	Qualified	6	0.3
Phenanthrene-D10	1517-22-2	C14 D10	188.1404	66032	8.396	0.089	98.69	99.81	Qualified	6	0.28
Phenol	108-95-2	C6 H6 O	94.0413	10093	3.506	0.097	97.14	98.8	Qualified	6	0.67
Thiamethoxam	153719-23-4	C8 H10 Cl N5 O3	212.0488	8652	10.29	0.023	87.04	87.71	Qualified	5	0.57
TPPA / Triphenyl ph	115-86-6	C18 H15 O4 P	326.07	14125	13.37	0.025	99.85	99.51	Qualified	6	0.81
Triethylphosphate	78-40-0	C6 H15 O4 P	155.0468	19149	4.099	-0.033	95.97	99.5	Qualified	6	0.36
Triisobutylphosphat	126-71-6	C12 H27 O4 P	98.9842	60751	6.088	-0.019	95.64	99.66	Qualified	5	0.65

Compound Identification Results: Cpd 322: Fludioxonil; C12 H6 F2 N2 O2; 11.551

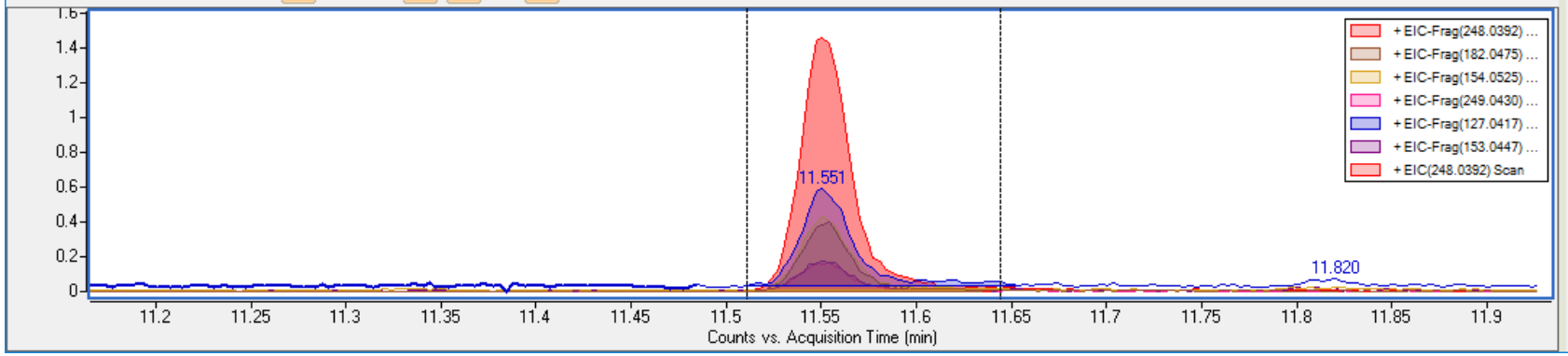
ID Techniques Applied

FBF-FragConfim

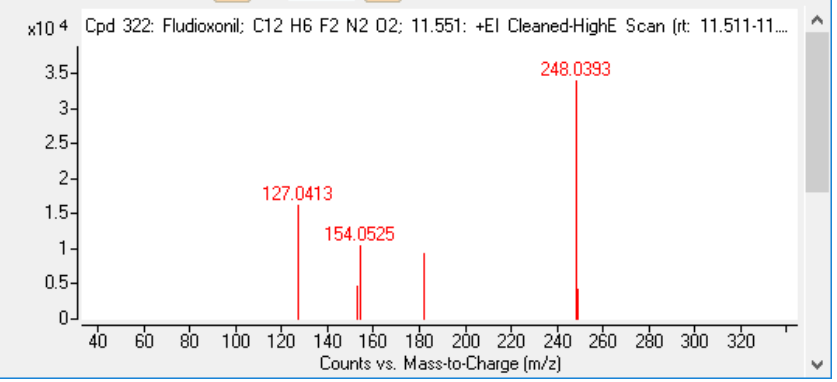
Best	Name	Formula	m/z	Mass	Mass (Tgt)	Diff (ppm)	Score
◉	Fludioxonil	C12 H6 F2 N2 O2	248.0394	248.0399	248.0397	-0.72	

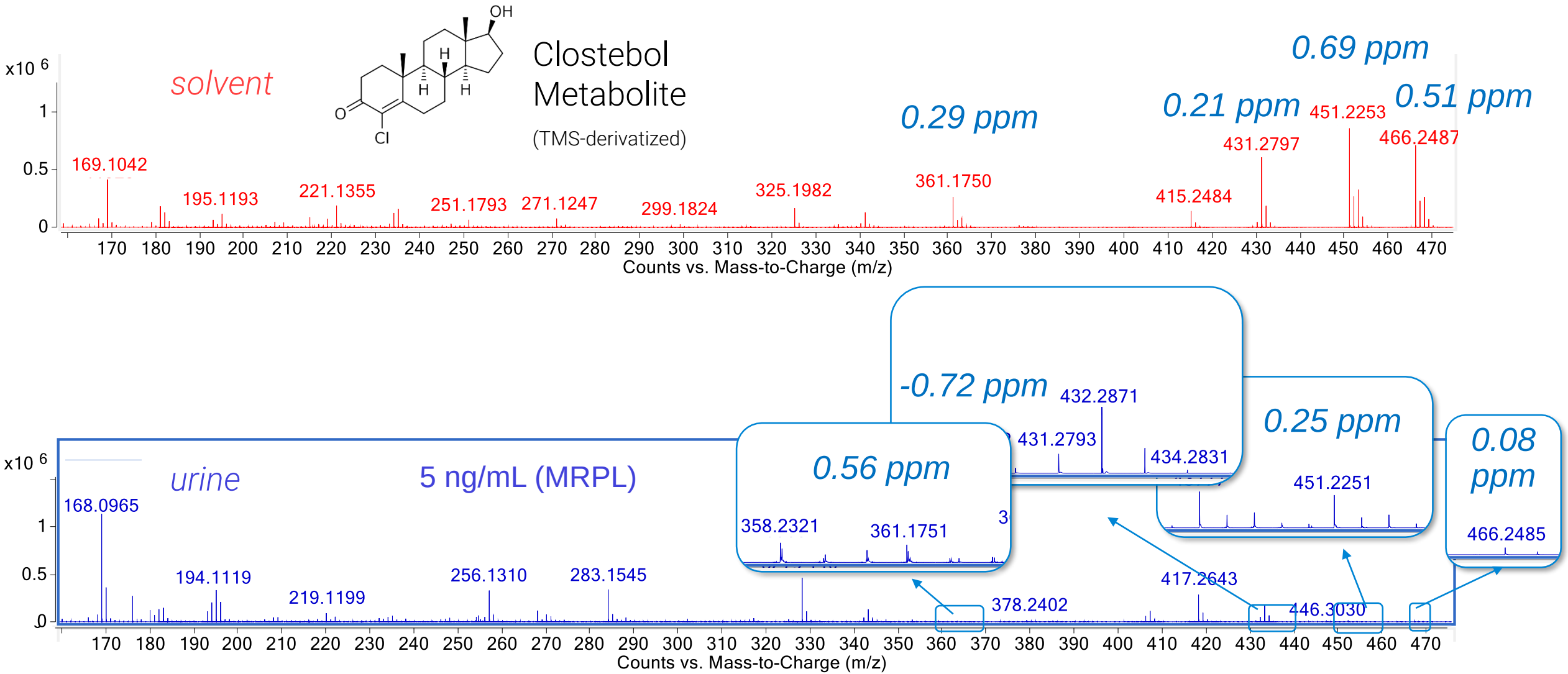
m/z	mz(Lib)	FragMassDiff(ppm)	Flags(FIs)	Abundance(Lib)	SNR	Height
127.0413	127.0417	2.6	Qualified	51.9	11.6	561
153.0448	153.0447	0.4	Qualified	16.7	16.4	1667
154.0525	154.0525	0.3	Qualified	39.8	40.1	4212
182.0475	182.0475	0	Qualified	30.6	92.1	3952
248.0393	248.0392	0.6	Reference ion	100	363.9	14577
249.0424	249.043	2.4	Qualified	14.6	39.2	1596

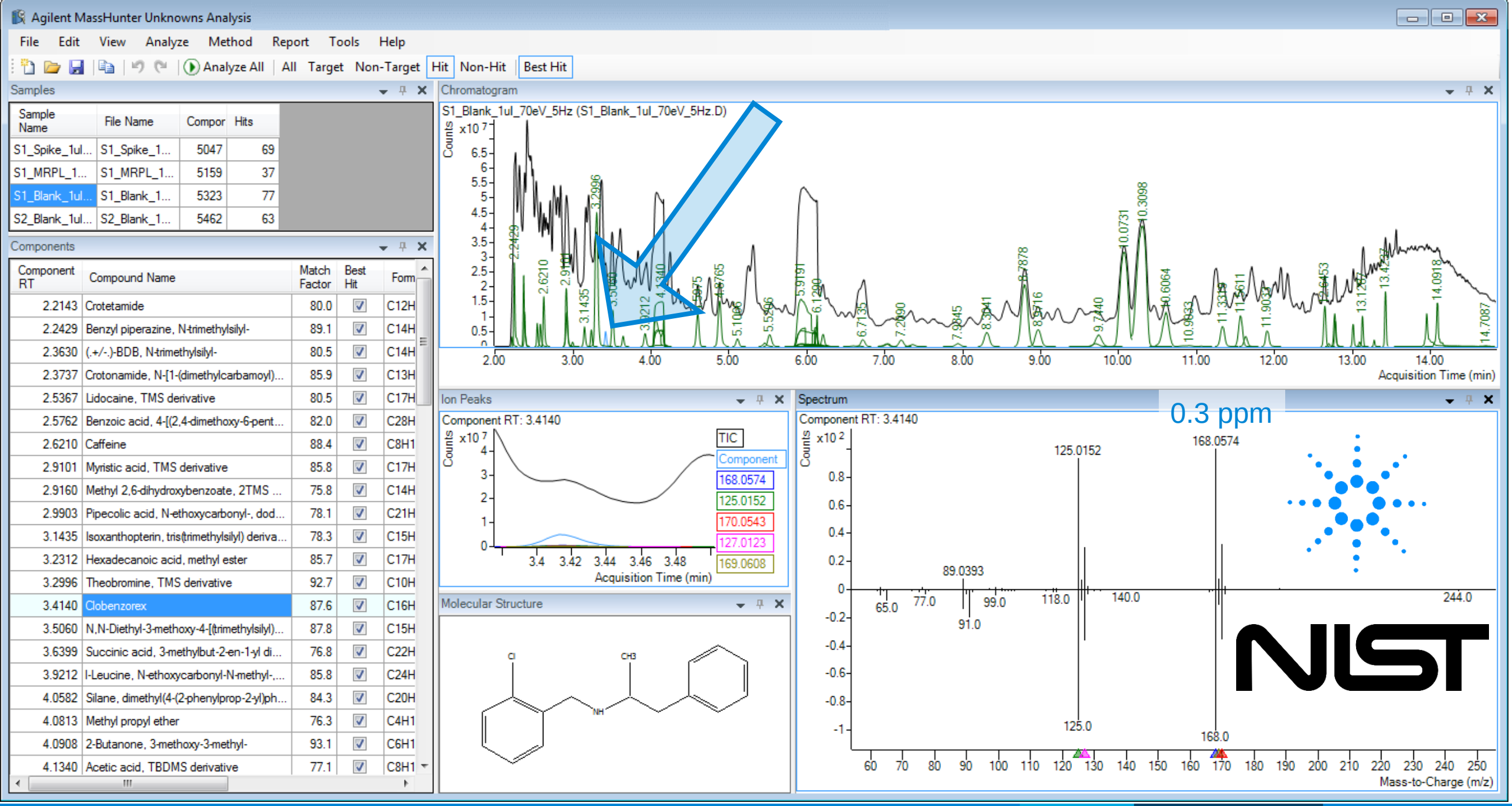
Compound Chromatogram Results (zoomed)



Compound Fragment Spectrum Results (zoomed)

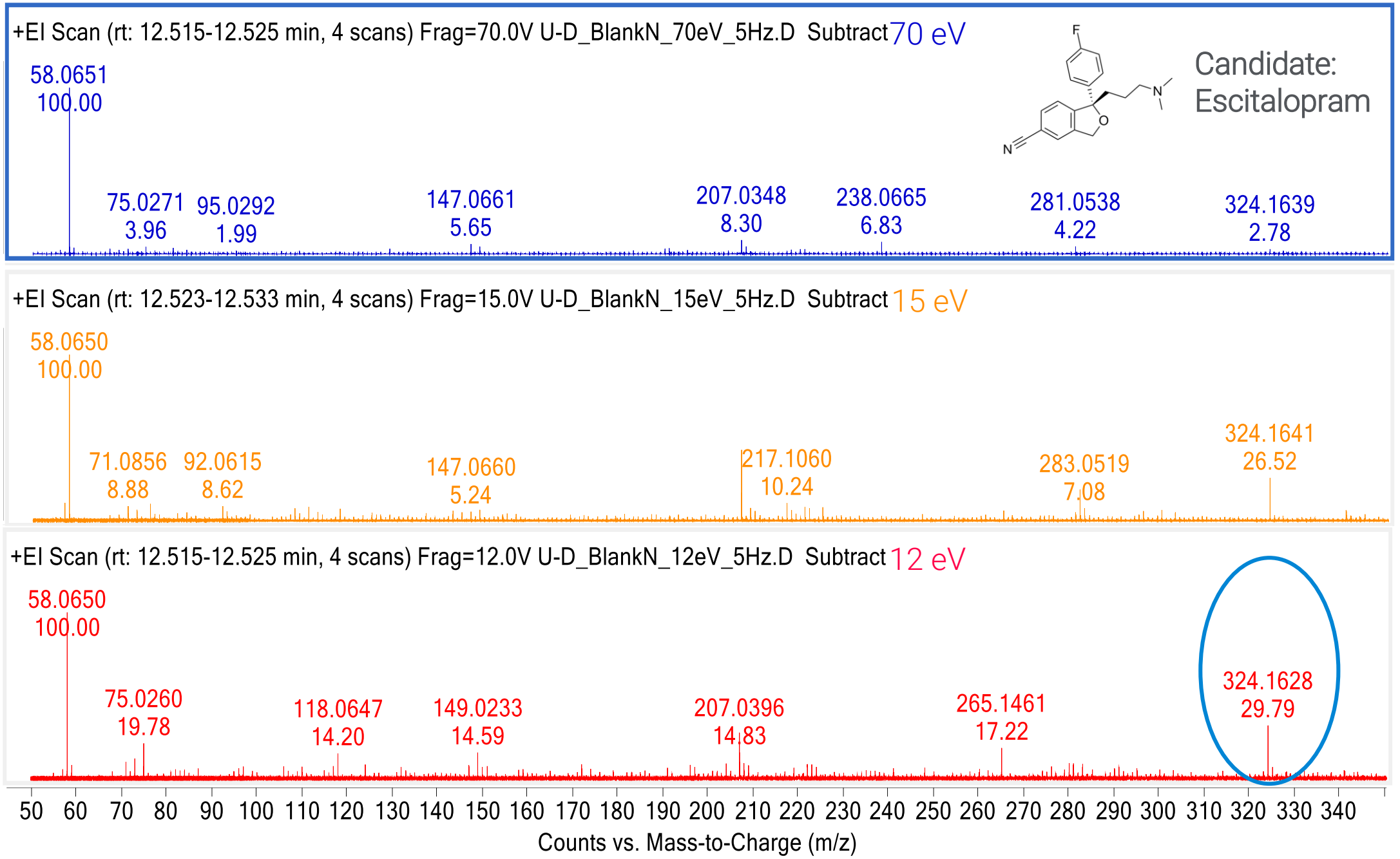



Clostebol Metabolite
(TMS-derivatized)
OH
H
H
H
O
Cl
solvent
x10 6
1
0.5
0
169.1042
195.1193
221.1355
251.1793
271.1247
299.1824
325.1982
361.1750
415.2484
431.2797
451.2253
466.2487
0.29 ppm
0.21 ppm
0.69 ppm
0.51 ppm
170 180 190 200 210 220 230 240 250 260 270 280 290 300 310 320 330 340 350 360 370 380 390 400 410 420 430 440 450 460 470
Counts vs. Mass-to-Charge (m/z)
urine
5 ng/mL (MRPL)
x10 6
1
0.5
0
168.0965
194.1119
219.1199
256.1310
283.1545
358.2321
361.1751
378.2402
417.2643
431.2793
432.2871
434.2831
446.3030
451.2251
466.2485
-0.72 ppm
0.56 ppm
0.25 ppm
0.08 ppm
170 180 190 200 210 220 230 240 250 260 270 280 290 300 310 320 330 340 350 360 370 380 390 400 410 420 430 440 450 460 470
Counts vs. Mass-to-Charge (m/z)


Agilent MassHunter Unknowns Analysis
File Edit View Analyze Method Report Tools Help
Analyze All All Target Non-Target Hit Non-Hit Best Hit
Samples
Sample Name | File Name | Compor | Hits
S1_Spike_1ul... | S1_Spike_1... | 5047 | 69
S1_MRPL_1... | S1_MRPL_1... | 5159 | 37
S1_Blank_1ul... | S1_Blank_1... | 5323 | 77
S2_Blank_1ul... | S2_Blank_1... | 5462 | 63
Components
Component RT | Compound Name | Match Factor | Best Hit | Form
2.2143 | Crotetamide | 80.0 | C12H
2.2429 | Benzyl piperazine, N-trimethylsilyl- | 89.1 | C14H
2.3630 | (.+/-.)-BDB, N-trimethylsilyl- | 80.5 | C14H
2.3737 | Crotonamide, N-[1-(dimethylcarbamoyl)... | 85.9 | C13H
2.5367 | Lidocaine, TMS derivative | 80.5 | C17H
2.5762 | Benzoic acid, 4-[(2,4-dimethoxy-6-pent... | 82.0 | C28H
2.6210 | Caffeine | 88.4 | C8H1
2.9101 | Myristic acid, TMS derivative | 85.8 | C17H
2.9160 | Methyl 2,6-dihydroxybenzoate, 2TMS ... | 75.8 | C14H
2.9903 | Pipecolic acid, N-ethoxycarbonyl-, dod... | 78.1 | C21H
3.1435 | Isoxanthopterin, tris(trimethylsilyl) deriva... | 78.3 | C15H
3.2312 | Hexadecanoic acid, methyl ester | 85.7 | C17H
3.2996 | Theobromine, TMS derivative | 92.7 | C10H
3.4140 | Clobenzorex | 87.6 | C16H
3.5060 | N,N-Diethyl-3-methoxy-4-[(trimethylsilyl)... | 87.8 | C15H
3.6399 | Succinic acid, 3-methylbut-2-en-1-yl di... | 76.8 | C22H
3.9212 | l-Leucine, N-ethoxycarbonyl-N-methyl-,... | 85.8 | C24H
4.0582 | Silane, dimethyl(4-(2-phenylprop-2-yl)ph... | 84.3 | C20H
4.0813 | Methyl propyl ether | 76.3 | C4H1
4.0908 | 2-Butanone, 3-methoxy-3-methyl- | 93.1 | C6H1
4.1340 | Acetic acid, TBDMS derivative | 77.1 | C8H1
Chromatogram
S1_Blank_1ul_70eV_5Hz (S1_Blank_1ul_70eV_5Hz.D)
Counts x10 7
Acquisition Time (min)
Ion Peaks
Component RT: 3.4140
Counts x10 7
TIC
Component
168.0574
125.0152
170.0543
127.0123
169.0608
Acquisition Time (min)
Molecular Structure
Spectrum
0.3 ppm
Component RT: 3.4140
Counts x10 2
125.0152
168.0574
89.0393
91.0
125.0
168.0
Mass-to-Charge (m/z)
NIST

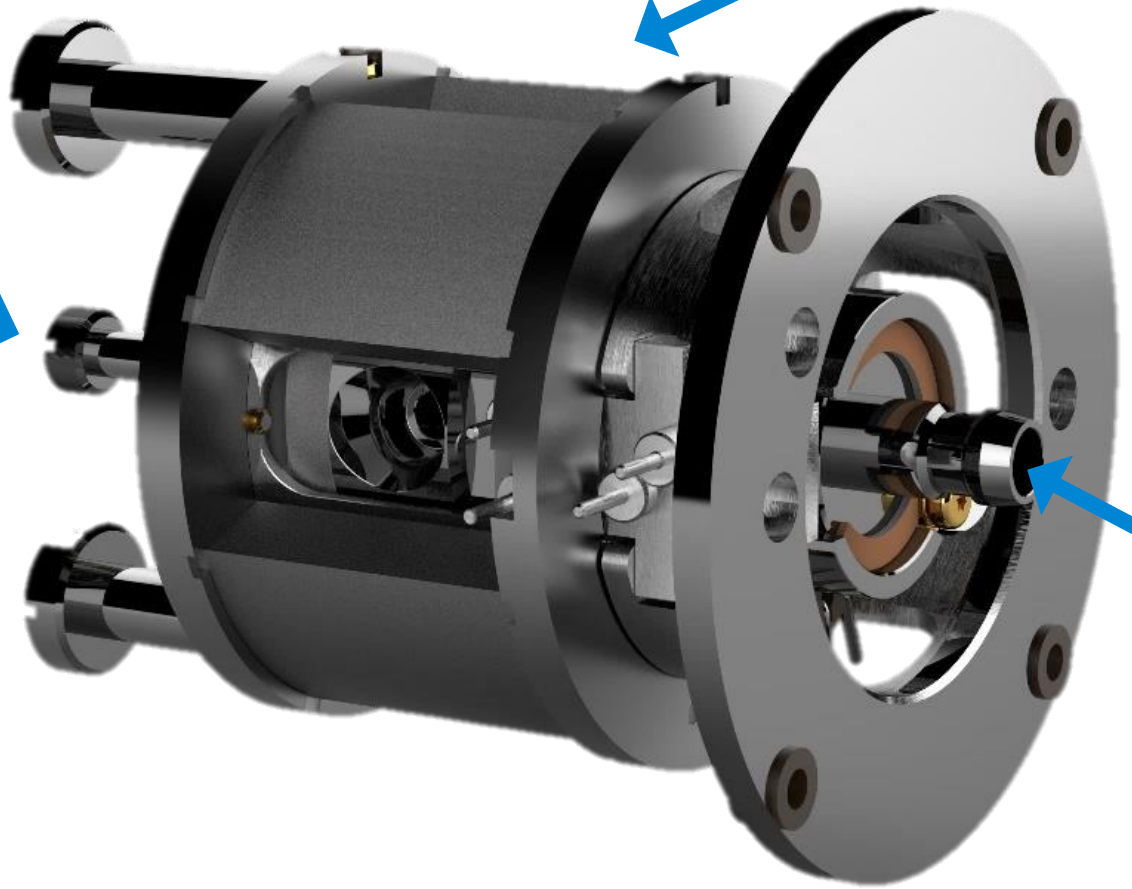
Unknowns Identification

Extensive Functionality and Tools for Identification and Elucidation


+EI Scan (rt: 12.515-12.525 min, 4 scans) Frag=70.0V U-D_BlankN_70eV_5Hz.D Subtract
70 eV
58.0651
100.00
75.0271
3.96
95.0292
1.99
147.0661
5.65
207.0348
8.30
238.0665
6.83
281.0538
4.22
324.1639
2.78
Candidate:
Escitalopram
+EI Scan (rt: 12.523-12.533 min, 4 scans) Frag=15.0V U-D_BlankN_15eV_5Hz.D Subtract
15 eV
58.0650
100.00
71.0856
8.88
92.0615
8.62
147.0660
5.24
217.1060
10.24
283.0519
7.08
324.1641
26.52
+EI Scan (rt: 12.515-12.525 min, 4 scans) Frag=12.0V U-D_BlankN_12eV_5Hz.D Subtract
12 eV
58.0650
100.00
75.0260
19.78
118.0647
14.20
149.0233
14.59
207.0396
14.83
265.1461
17.22
324.1628
29.79
50 60 70 80 90 100 110 120 130 140 150 160 170 180 190 200 210 220 230 240 250 260 270 280 290 300 310 320 330 340
Counts vs. Mass-to-Charge (m/z)

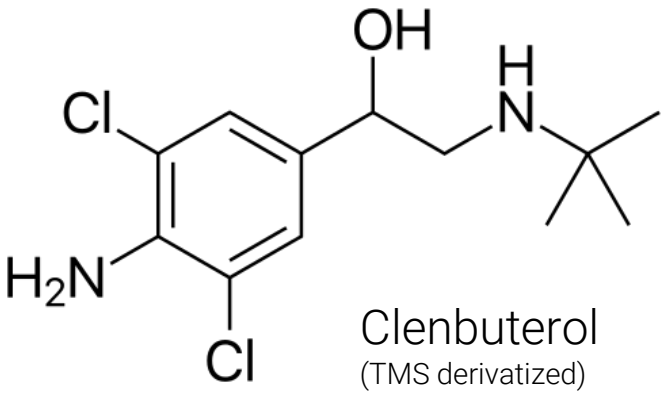
High Strength
Axial Magnet

Centered Filament

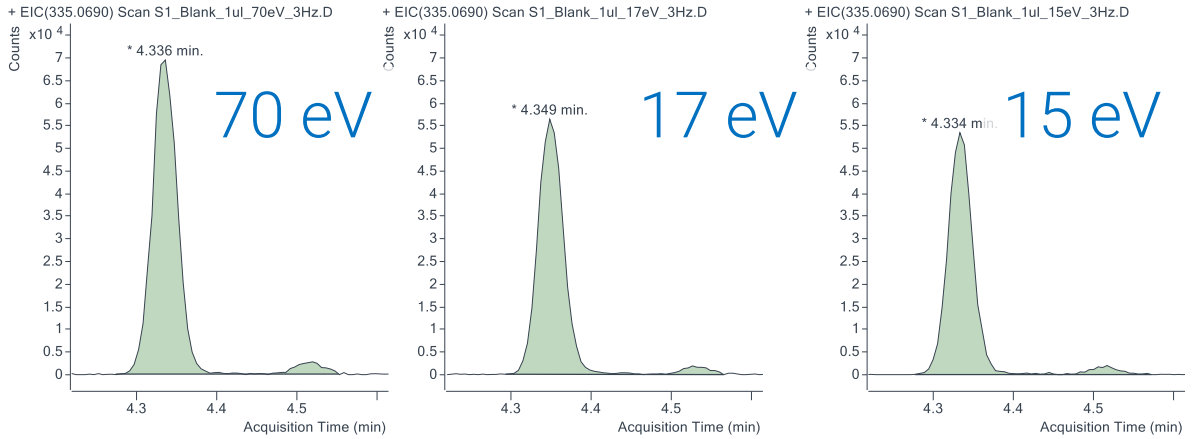


Optimized
Lens Design

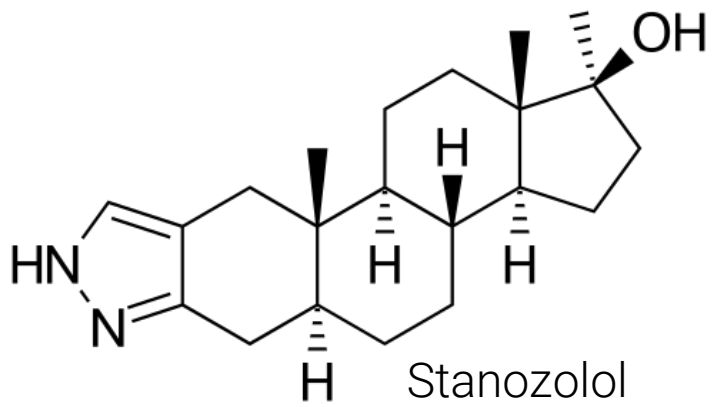
Proprietary
Low Energy EI Source



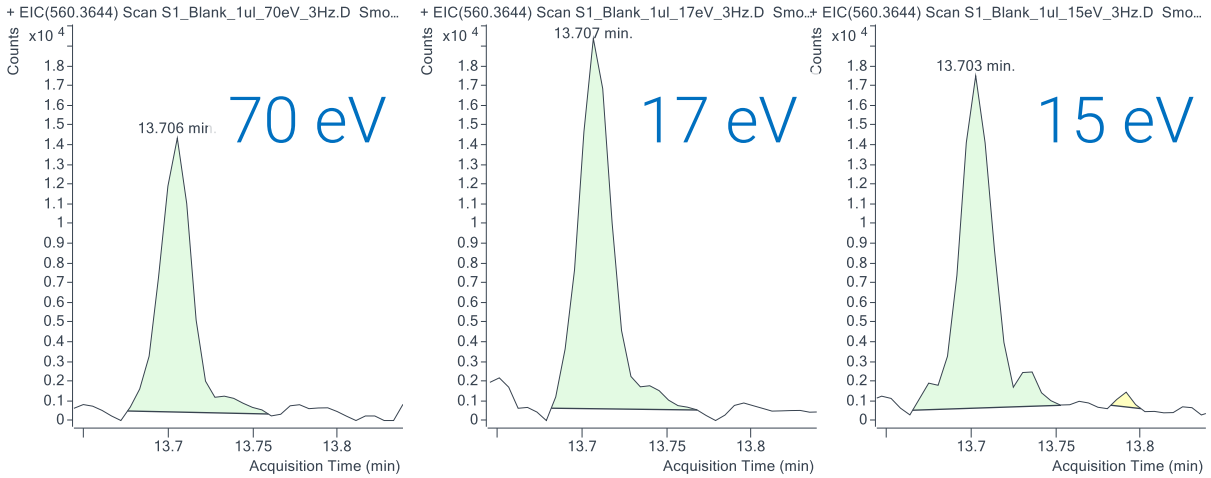
Clenbuterol
(TMS derivatized)



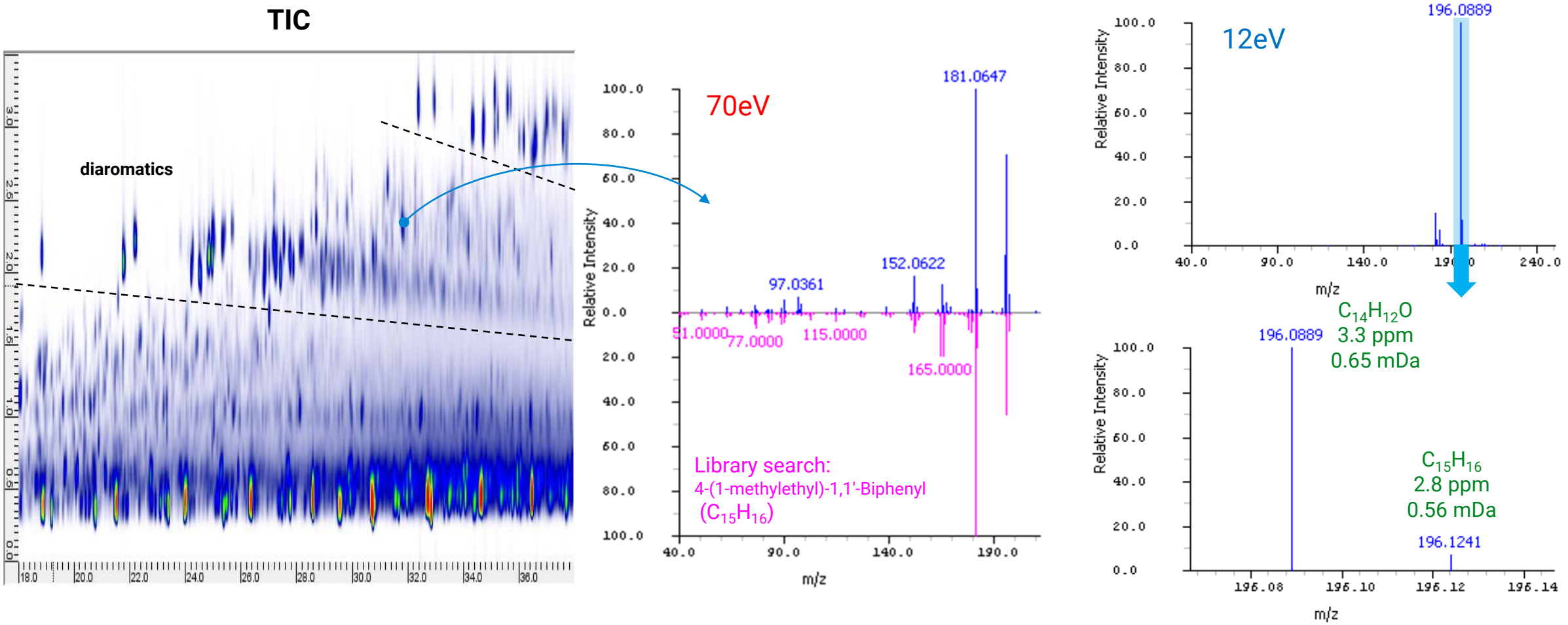
Clenbuterol (335.0690), MRPL = 0.2 ng/ml

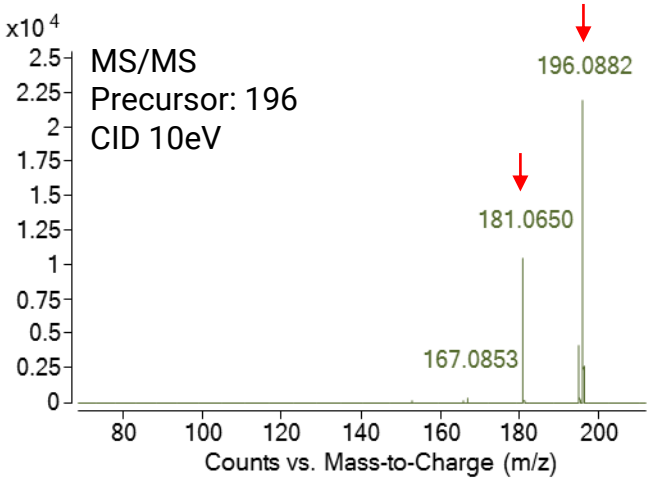


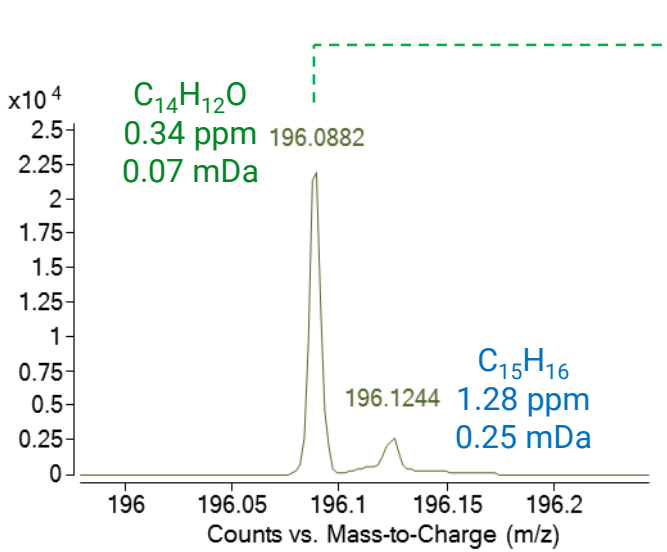
Stanozolol
(TMS derivatized)

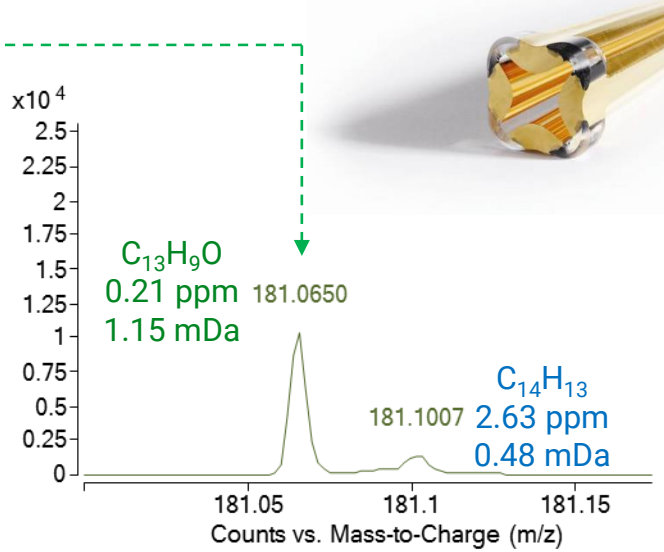


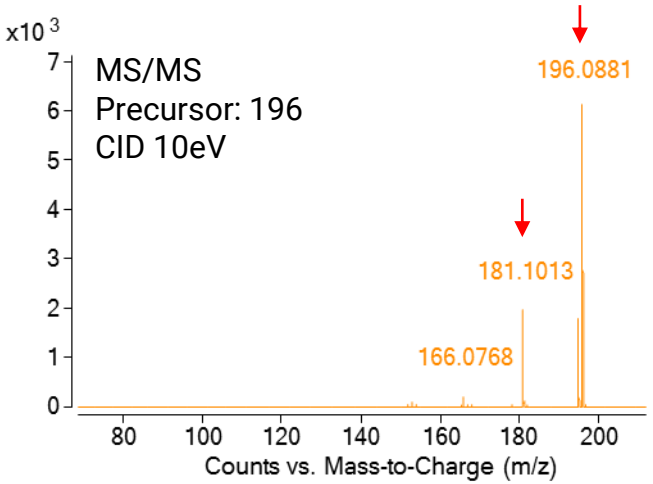
4-OH-Stanozolol (560.3644), MRPL = 5 ng/ml

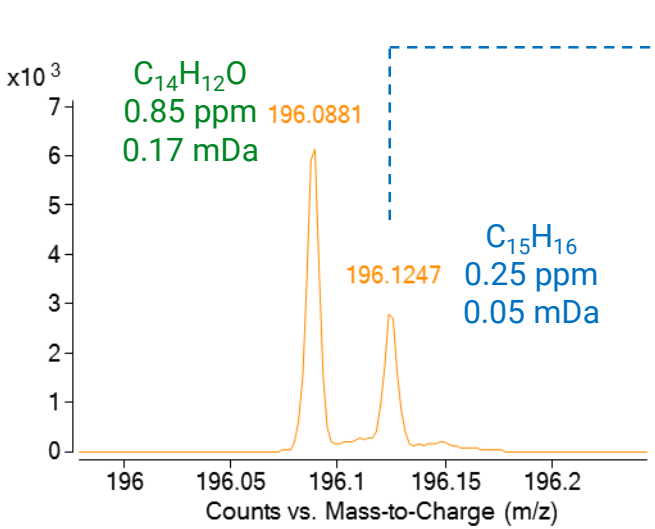

TIC
diaromatics
70eV
181.0647
152.0622
97.0361
91.0000
77.0000
115.0000
165.0000
Relative Intensity
m/z
Library search:
4-(1-methylethyl)-1,1'-Biphenyl
(C15H16)
12eV
196.0889
C14H12O
3.3 ppm
0.65 mDa
C15H16
2.8 ppm
0.56 mDa
196.1241

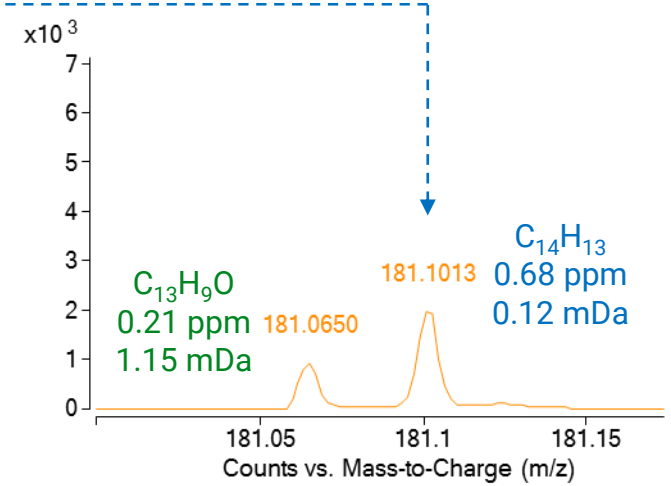

x10 4
MS/MS
Precursor: 196
CID 10eV
196.0882
181.0650
167.0853
Counts vs. Mass-to-Charge (m/z)

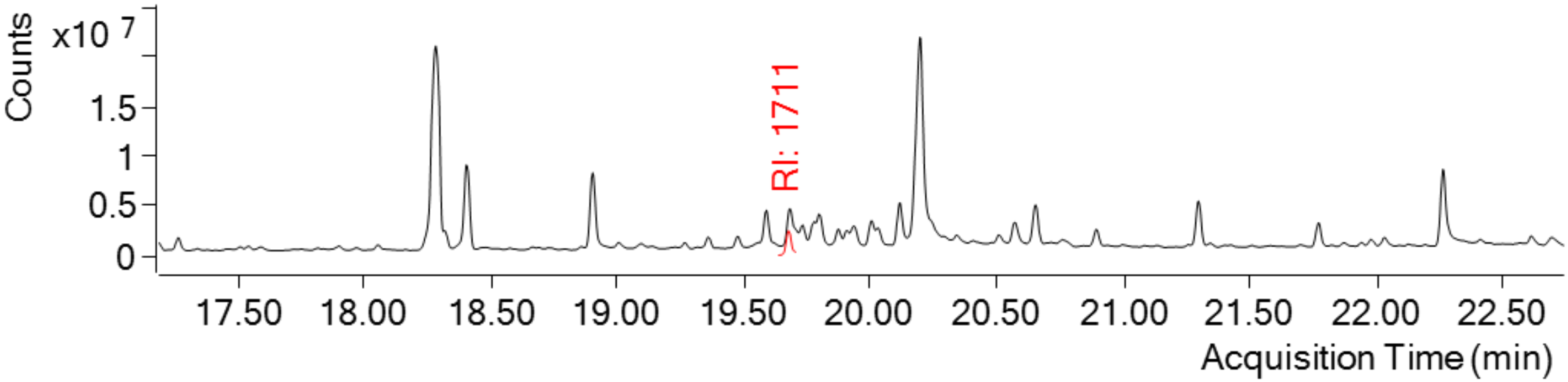

- CH3
x10 4
C14H12O
0.34 ppm
0.07 mDa
196.0882
196.1244
C15H16
1.28 ppm
0.25 mDa
Counts vs. Mass-to-Charge (m/z)


x10 4
C13H9O
0.21 ppm
1.15 mDa
181.0650
181.1007
C14H13
2.63 ppm
0.48 mDa
Counts vs. Mass-to-Charge (m/z)

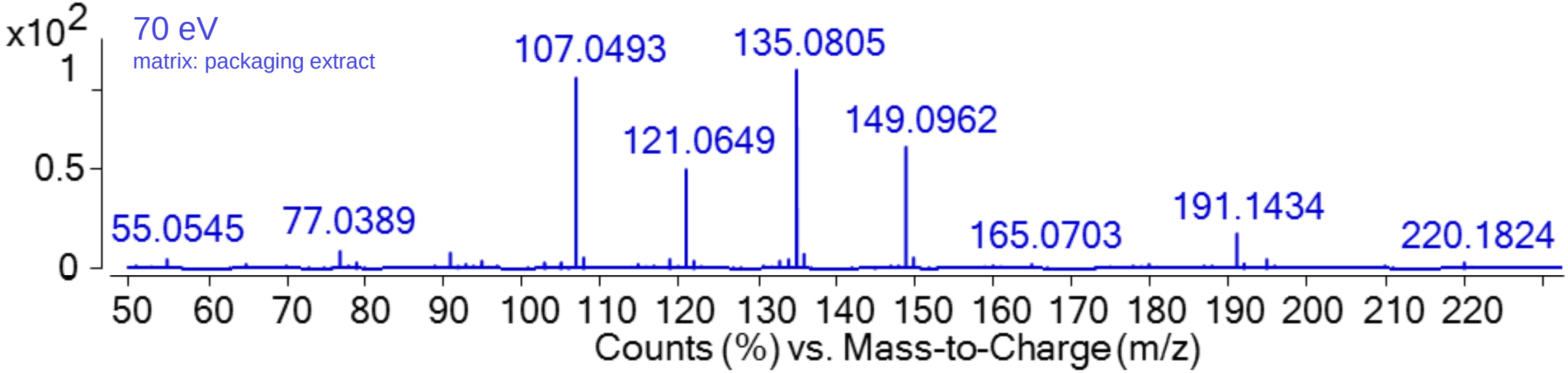

x10 3
MS/MS
Precursor: 196
CID 10eV
196.0881
181.1013
166.0768
Counts vs. Mass-to-Charge (m/z)

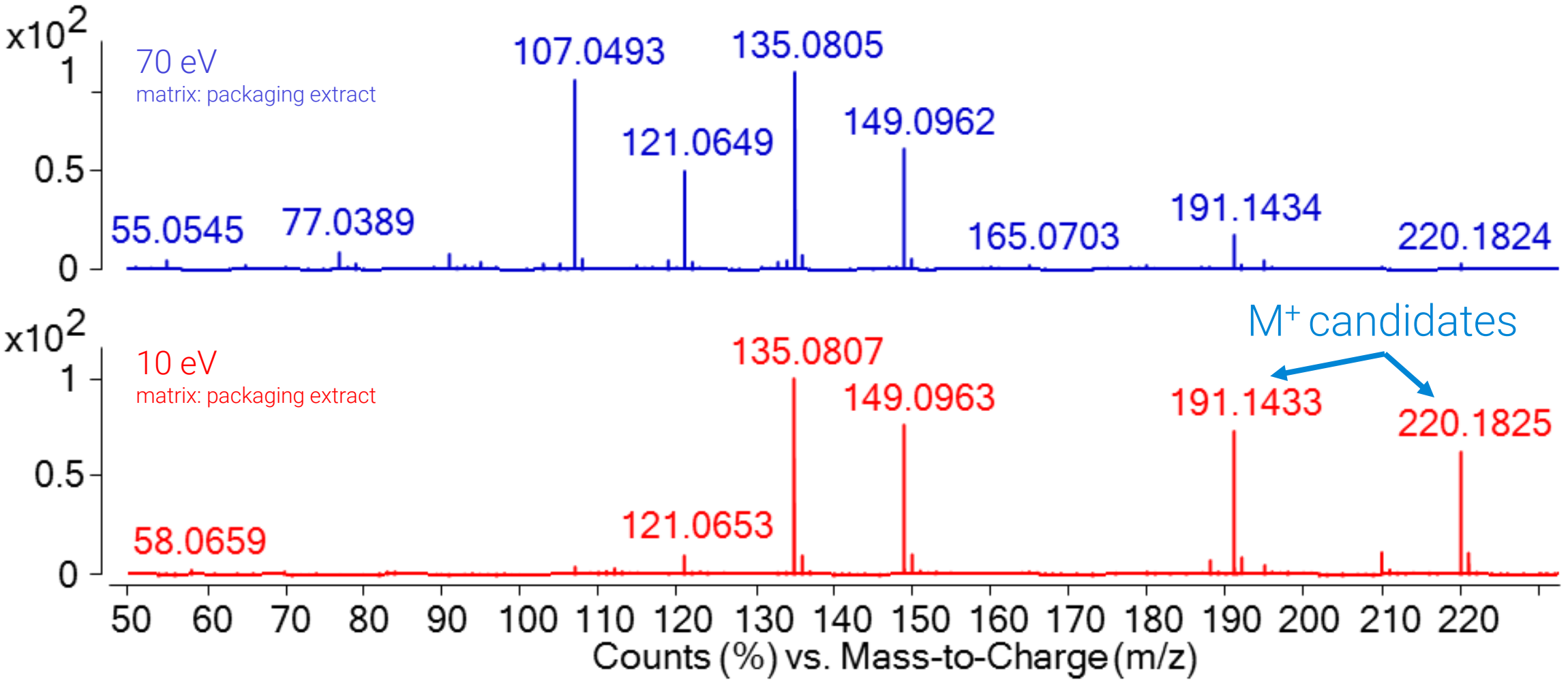

- CH3
x10 3
C14H12O
0.85 ppm
0.17 mDa
196.0881
196.1247
C15H16
0.25 ppm
0.05 mDa
Counts vs. Mass-to-Charge (m/z)

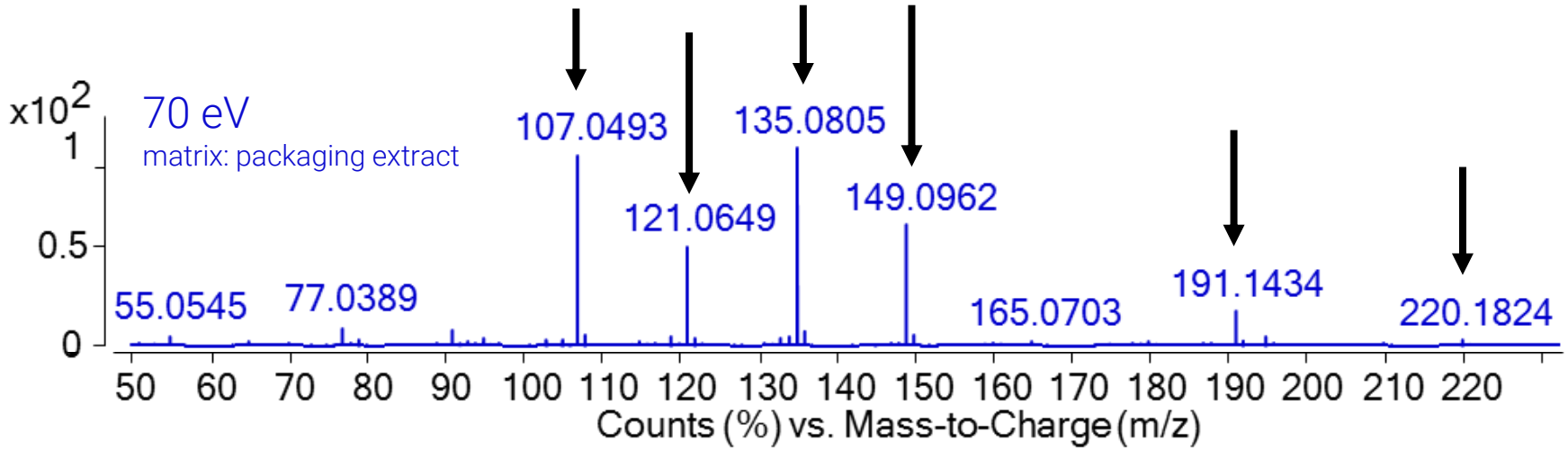

x10 3
C13H9O
0.21 ppm
1.15 mDa
181.0650
181.1013
C14H13
0.68 ppm
0.12 mDa
Counts vs. Mass-to-Charge (m/z)


Counts
x10 7
1.5
1
0.5
0
RI: 1711
17.50
18.00
18.50
19.00
19.50
20.00
20.50
21.00
21.50
22.00
22.50
Acquisition Time (min)

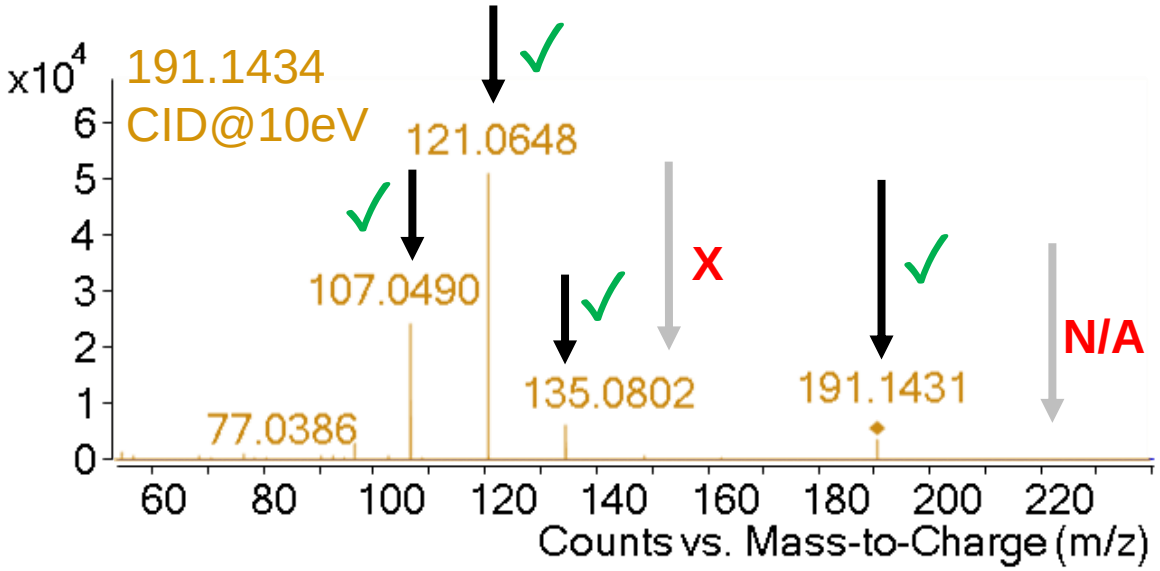
Compound ID = ???


x10 2
1
0.5
0
70 eV
matrix: packaging extract
107.0493
135.0805
121.0649
149.0962
55.0545
77.0389
165.0703
191.1434
220.1824
50
60
70
80
90
100
110
120
130
140
150
160
170
180
190
200
210
220
Counts (%) vs. Mass-to-Charge (m/z)

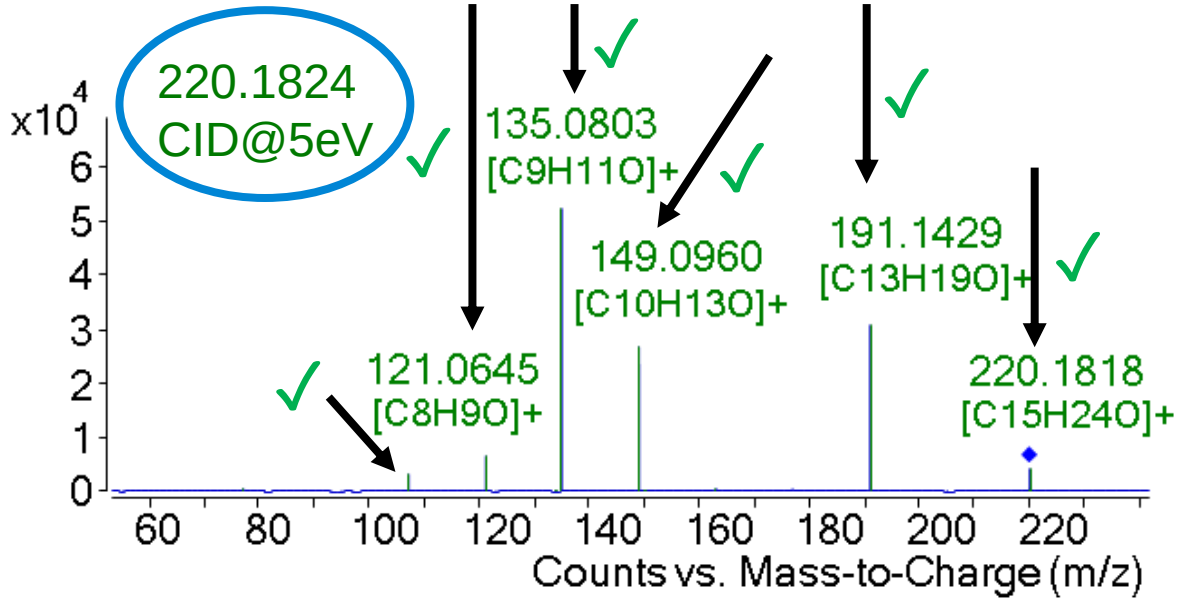

x10^2
1
0.5
0
70 eV
matrix: packaging extract
107.0493
135.0805
121.0649
149.0962
55.0545
77.0389
165.0703
191.1434
220.1824
x10^2
1
0.5
0
10 eV
matrix: packaging extract
M+ candidates
135.0807
149.0963
191.1433
220.1825
121.0653
58.0659
50 60 70 80 90 100 110 120 130 140 150 160 170 180 190 200 210 220
Counts (%) vs. Mass-to-Charge (m/z)

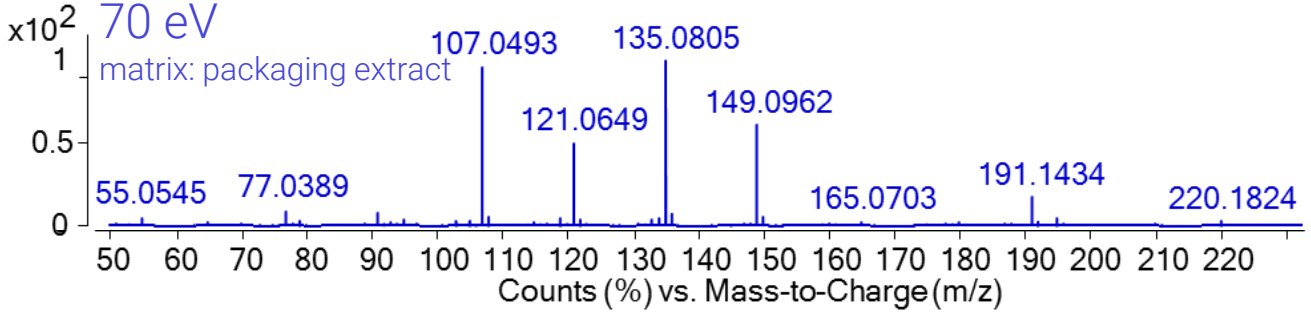


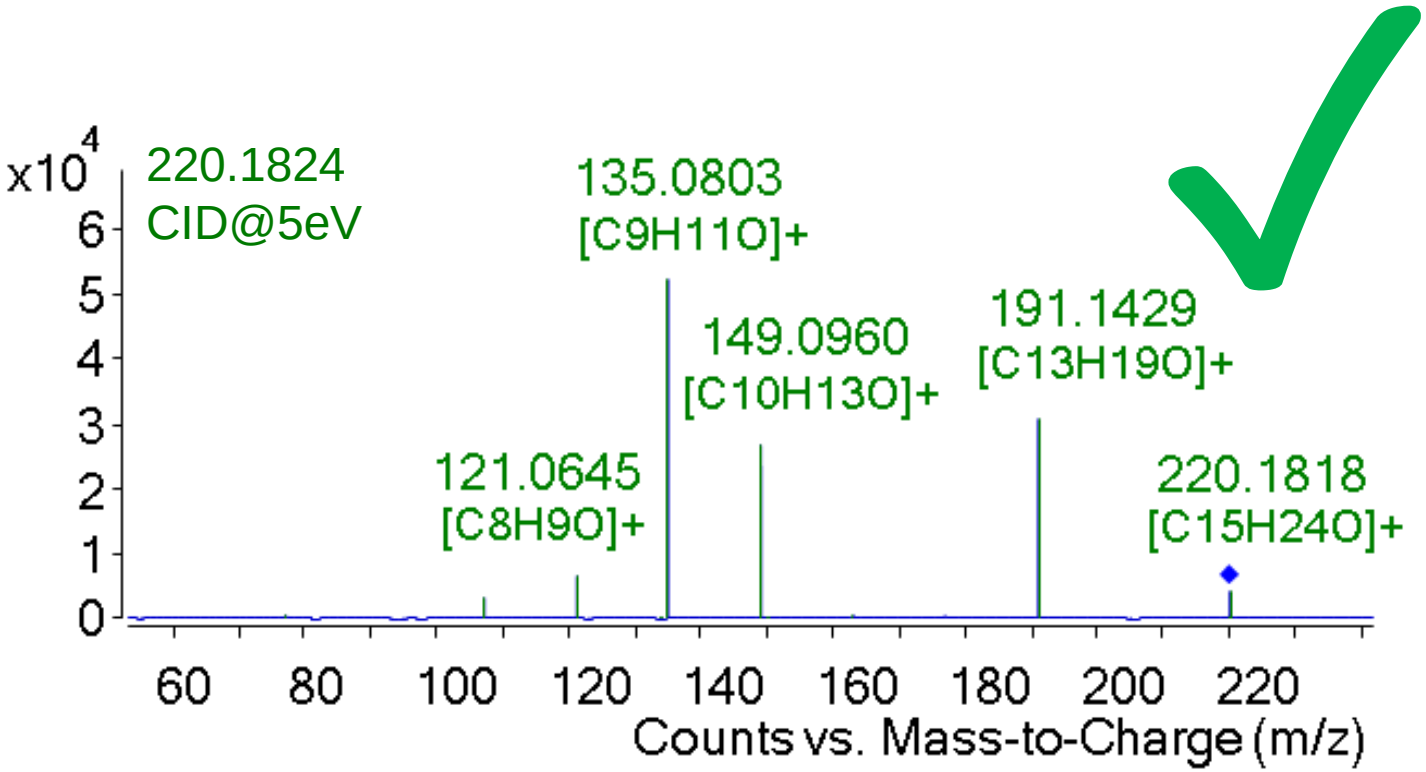
Candidate #1



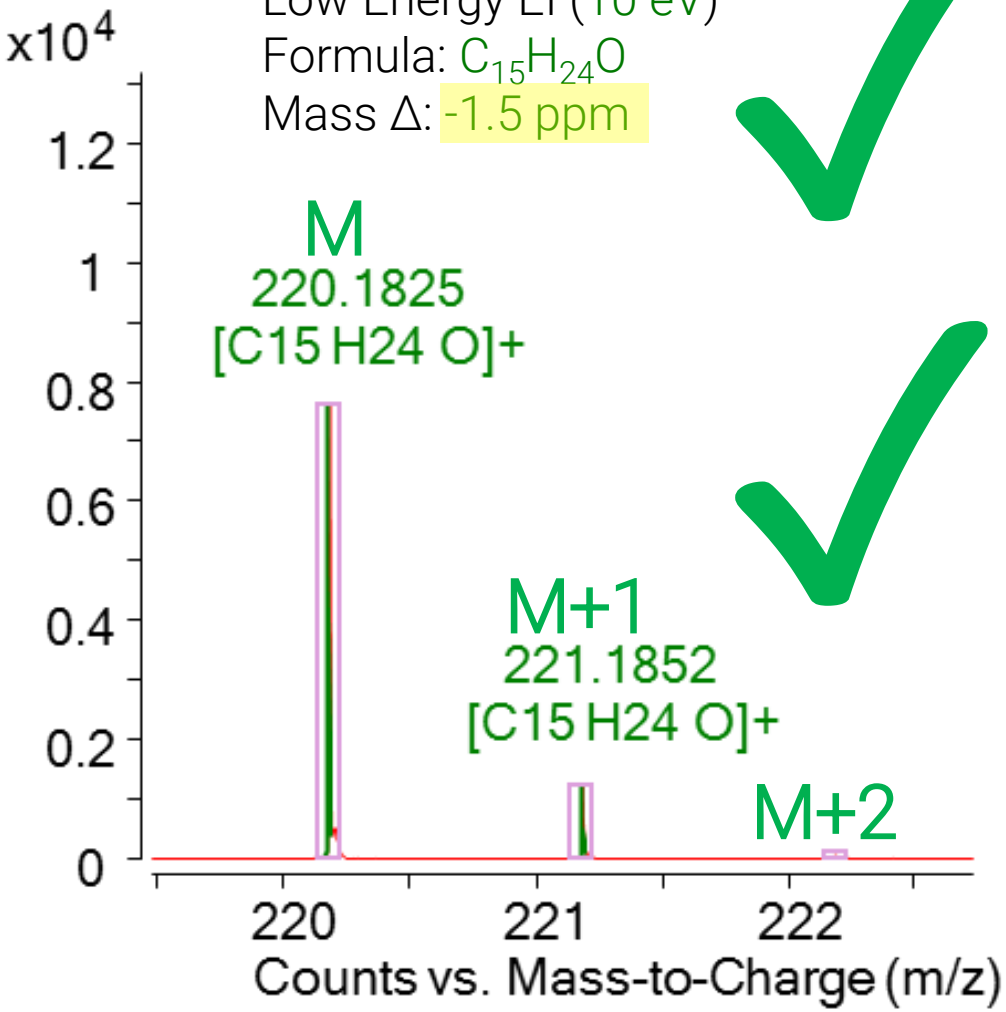
Candidate #2

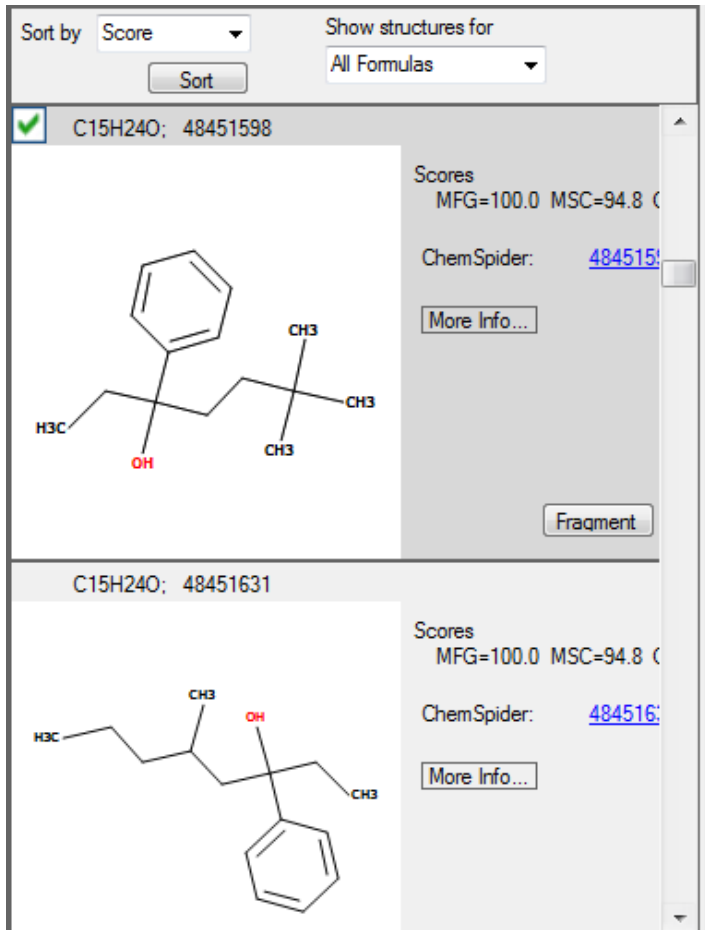


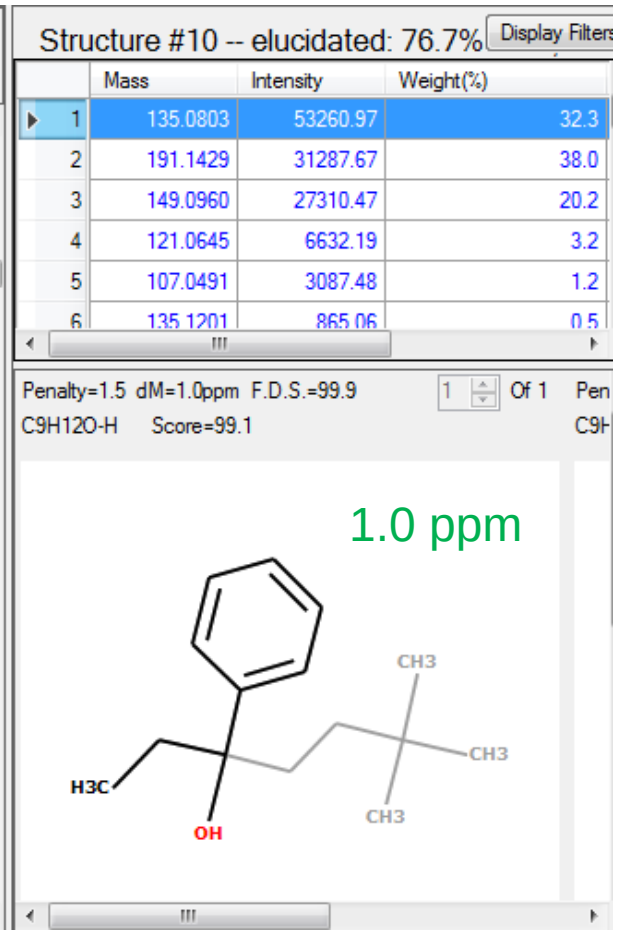


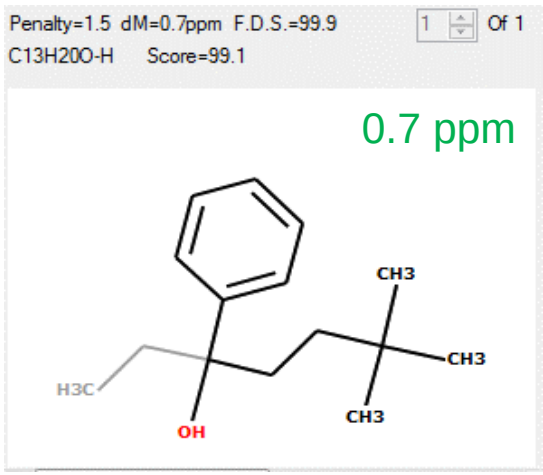


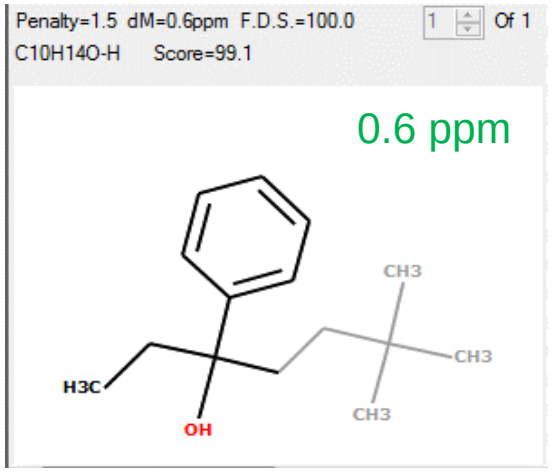
Low Energy EI (10 eV)
Formula: $C_{15}H_{24}O$
Mass Δ: -1.5 ppm

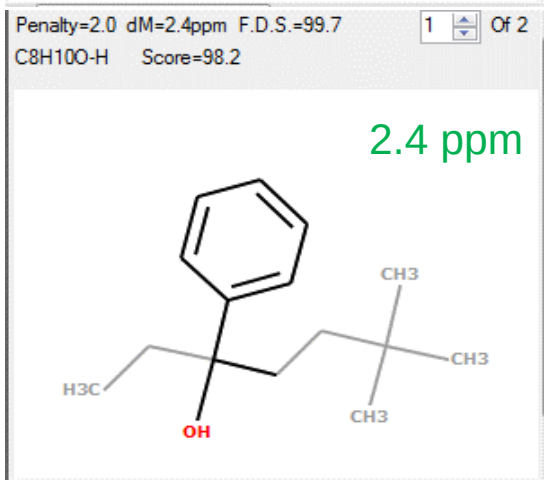


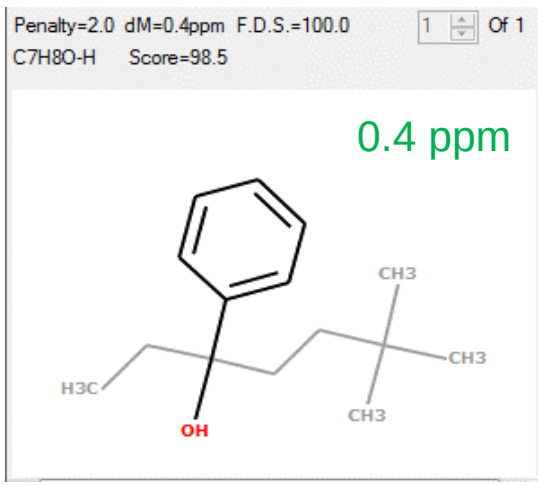








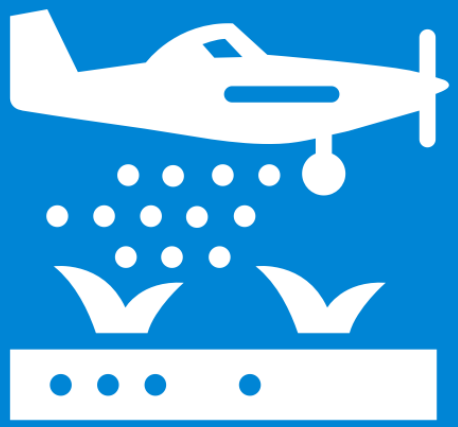




Candidate: Benzenemethanol derivative

Case Study: Food Safety

Full Spectrum Accurate Mass Data for Targets, Suspects and Unknowns



Safeguarding food supply is challenging

- 1000+ pesticides in use or remain in environment
- Other environmental pollutants are also of concern
- Thousands of possible contaminants/food pairs
- High sensitivity and selectivity needed to meet “Default” MRLs in “dirty” extracts
- Growing interests in broadest scope and even untargeted screening for risk assessment

Challenges for our customers

How much of each calibrated target compound is present?

Dozens of Compounds

e.g., 100~200 Targets

Are other target residues present?

100’s of Compounds

e.g., 800 Targets

Is there anything else in my sample?

1000’s of Compounds

Workflow Strategy

Acquire full-spectrum data

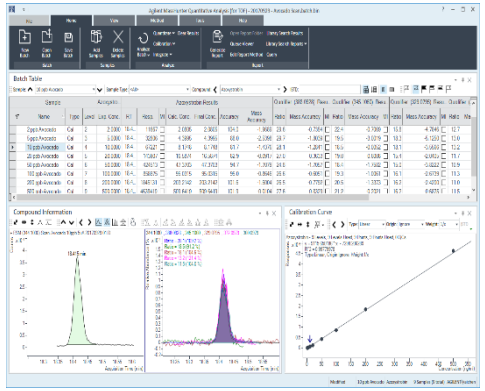
Targeted Method

Calibrate?

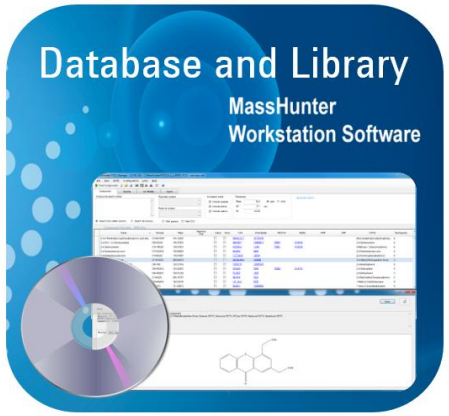
Yes

No

Targeted Quantitative Screening



Suspect Screening

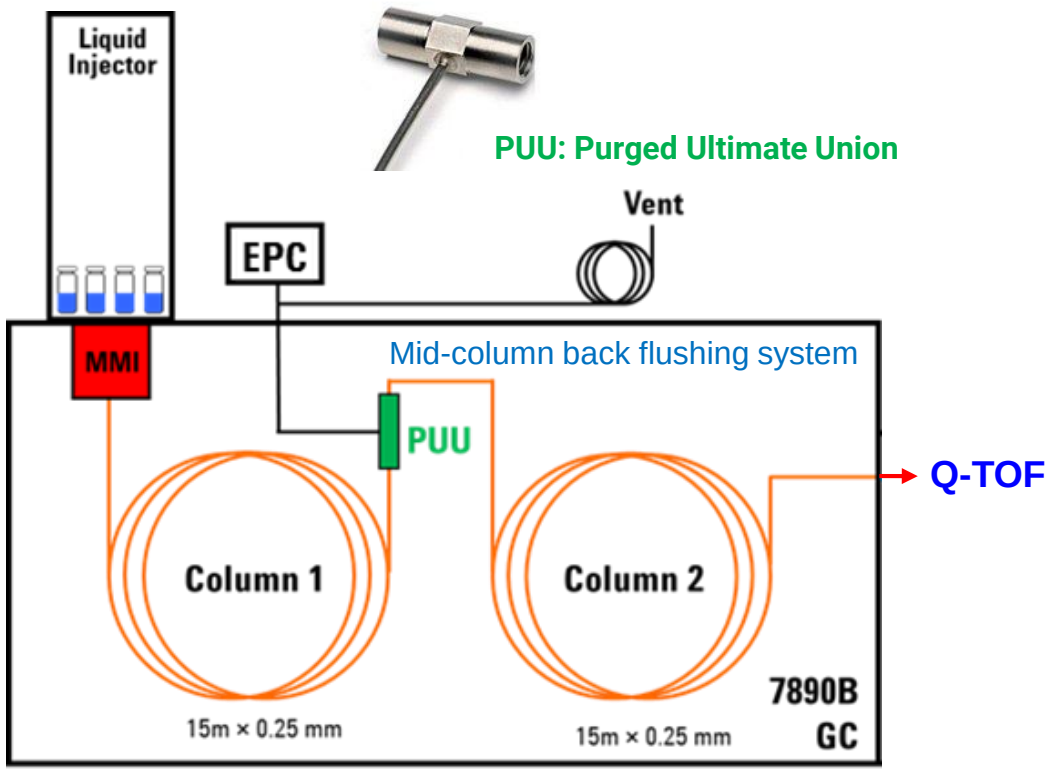


Untargeted Screening

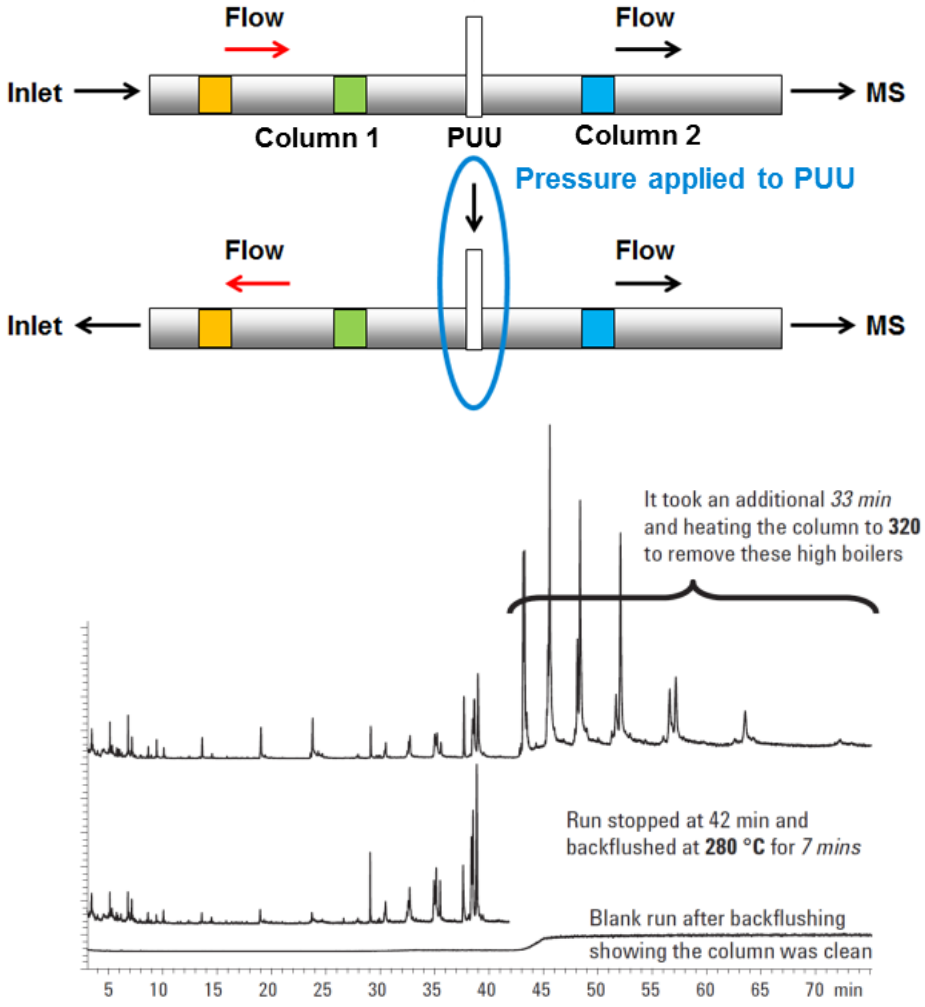
NIST

Deconvolution followed by matching public libraries

Configuration Optimized with Backflushing



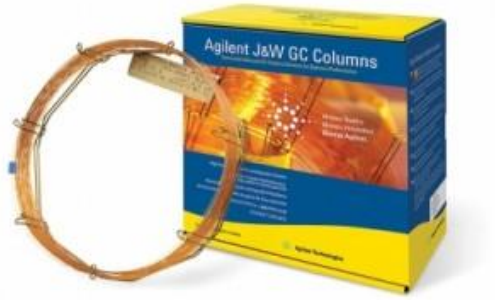
- ✓ Reduced run times
- ✓ Longer column lifetime
- ✓ Less ion source contamination



7250 GC/Q-TOF Method Parameters

Agilent 7890 GC	
Parameter	**Value**
Inert flow path configuration	Mid-column backflush
Columns	Agilent HP-5ms UI, 15 m, 0.25 mm id, 0.25 µm film (two each)
Inlet	MMI, 4 mm UI liner single taper w wool
Injection volume	1~2 µL
Injection mode	Cold Splitless 60 °C for 0.2 minutes 600 °C/min to 300 °C, hold 330 °C, post run
Inlet flow (column 1)	1.0 mL/min (**Chlorpyrifos-methyl locked at 9.143 min**)
PUU flow (column 2)	column 1 flow + 0.2 mL/min
Oven temperature program	60 °C (hold 1 min) then 40 °C/min to 170 °C, then 10 °C/min to 310 °C (hold 3 min) **Run time 20.75 min**
Transfer line	280 °C
Midcolumn Backflush	
Timing	5 min duration during post-run
Oven temperature	310 °C
Aux EPC pressure	~50 psi
Inlet pressure	~2 psi

Agilent 7250 Q-TOF	
Parameter	**Value**
Source temperature	280 °C (70 eV), 250 (°C)
Quad temperatures	150 °C
Collison cell gas flows	1 mL/min N_2 4 mL/min He
Electron energy	70 eV (Standard EI), 15 eV (Low energy EI)
Acquisition mass range	45-550 m/z
Spectral acquisition rate	5 spectra/sec



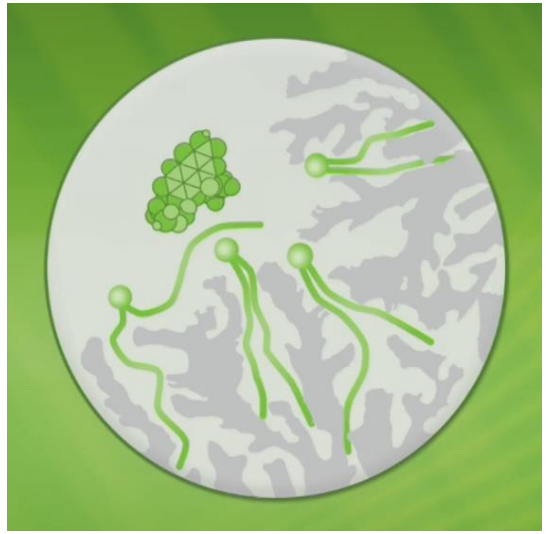
Method Evaluation

Targeted Quantitative Screening

Sample Preparation

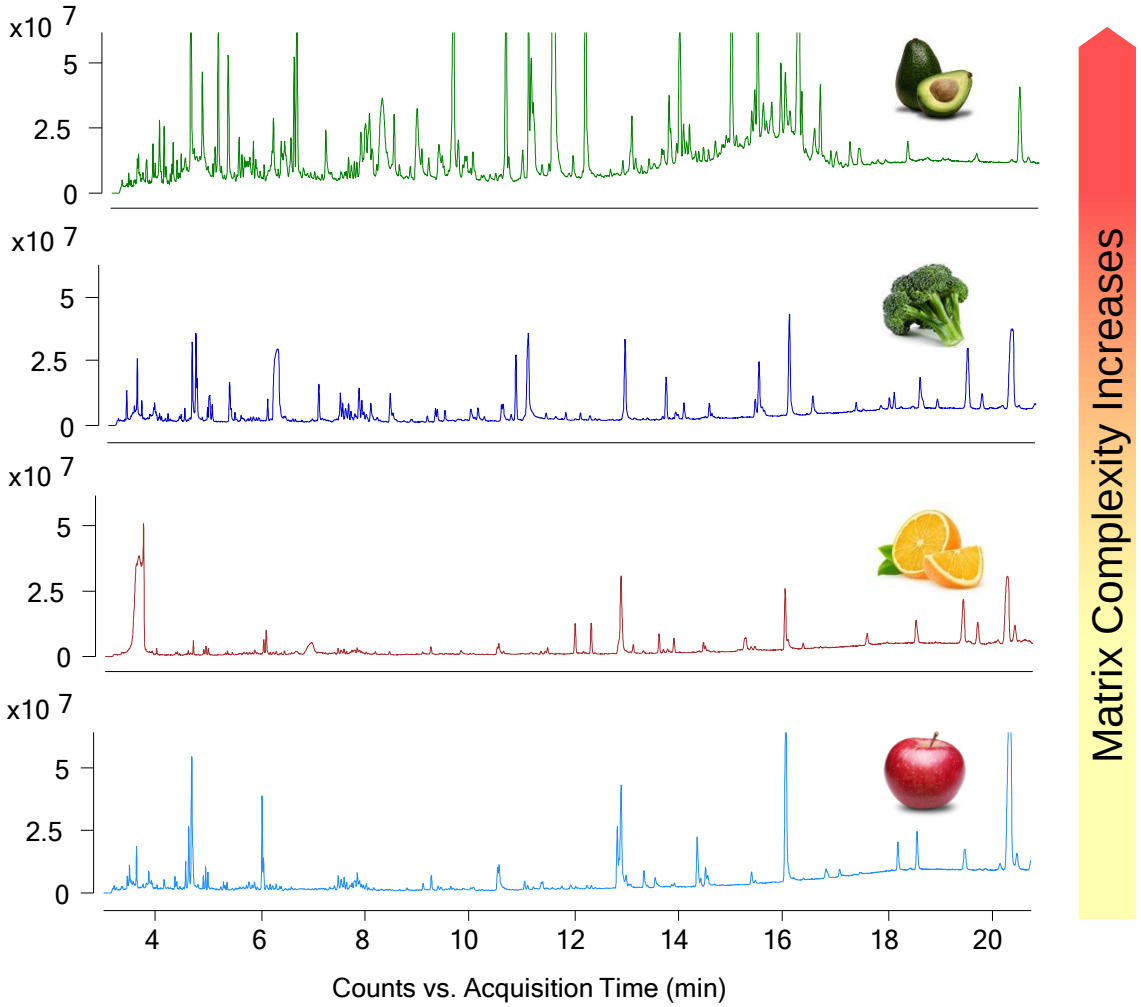
Matrix	Extraction	dSPE Cleanup
	QuEChERS (EN)	EMR-Lipid
	QuEChERS (EN)	Pigment matrix
	QuEChERS (EN)	Fruit/Vegetable
	QuEChERS (EN)	Fruit/Vegetable

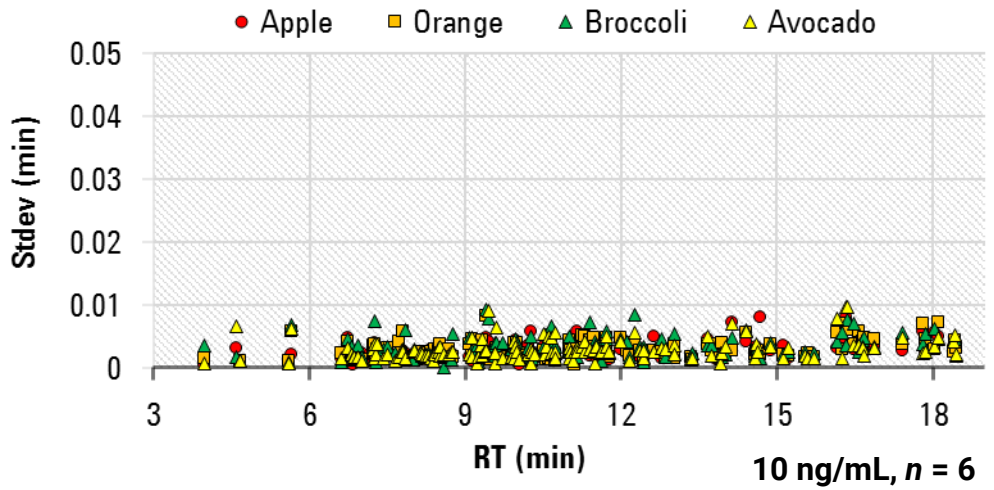
- Blank food matrices spiked with pesticides for method development and calibration
- A mixture of 140+ pesticides represent OCs, OPs, carbamates, triazoles and pyrethroids, etc.
- 6 replicates

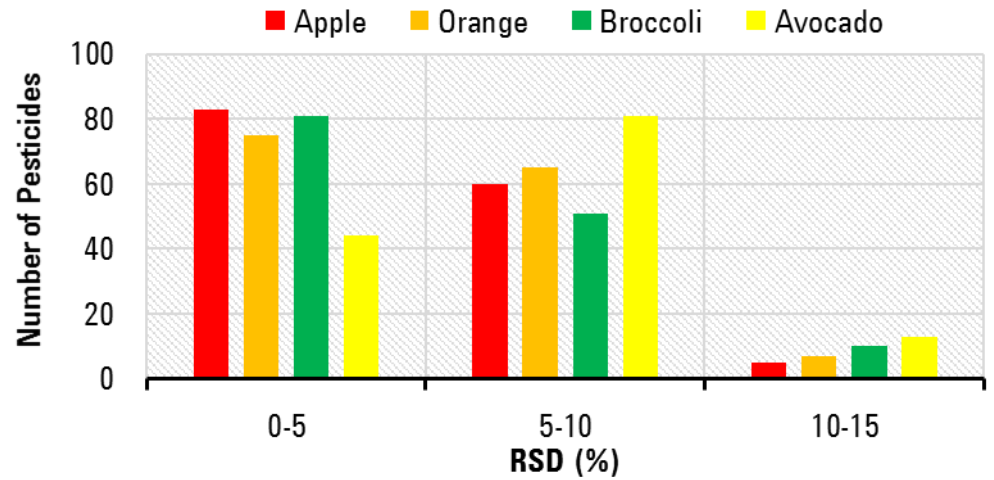


Replicate Precision

Targeted Quantitative Screening





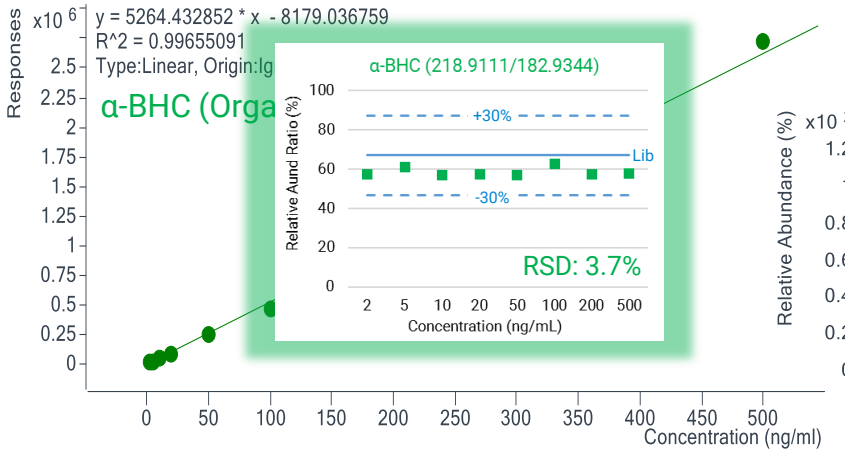


Matrix Matched Calibration

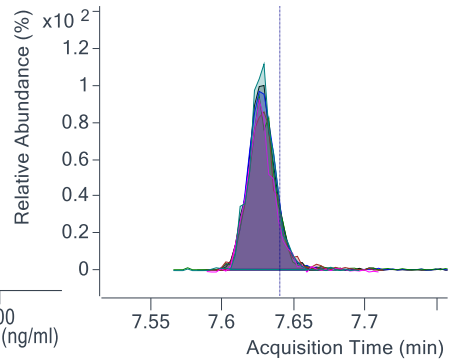
Targeted Quantitative Screening

2-500 ng/mL

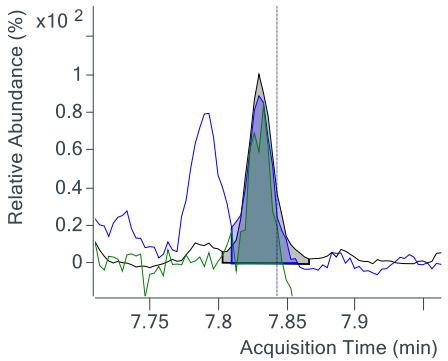
α-BHC - 8 Levels, 8 Levels Used, 8 Points, 8 Points Used, 0 QCs



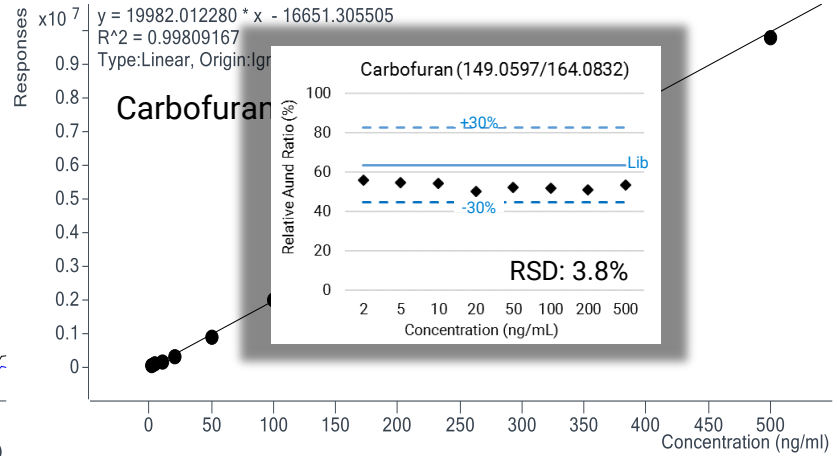
α-BHC 5 ng/mL



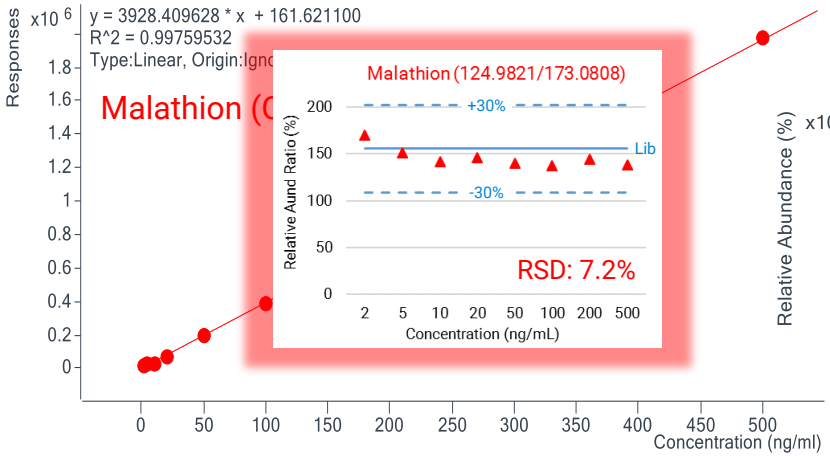
Carbofuran 5 ng/mL



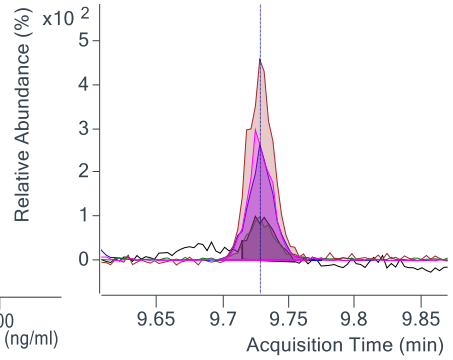
Carbofuran - 8 Levels, 8 Levels Used, 8 Points, 8 Points Used, 0 QCs



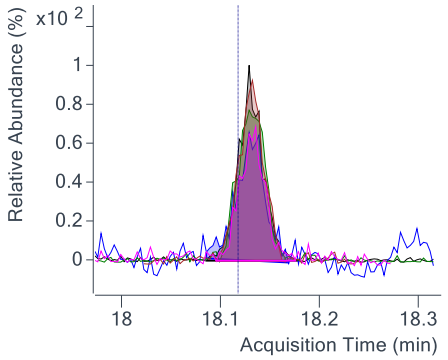
Malathion - 8 Levels, 8 Levels Used, 8 Points, 8 Points Used, 0 QCs



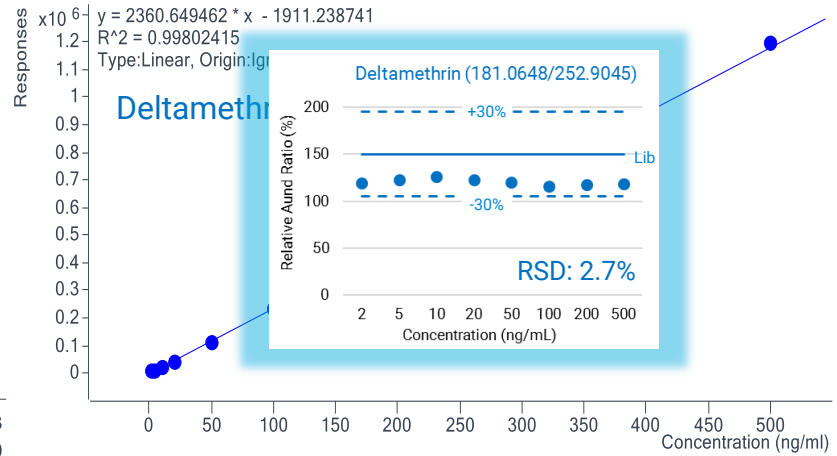
Malathion 5 ng/mL



Deltamethrin 5 ng/mL

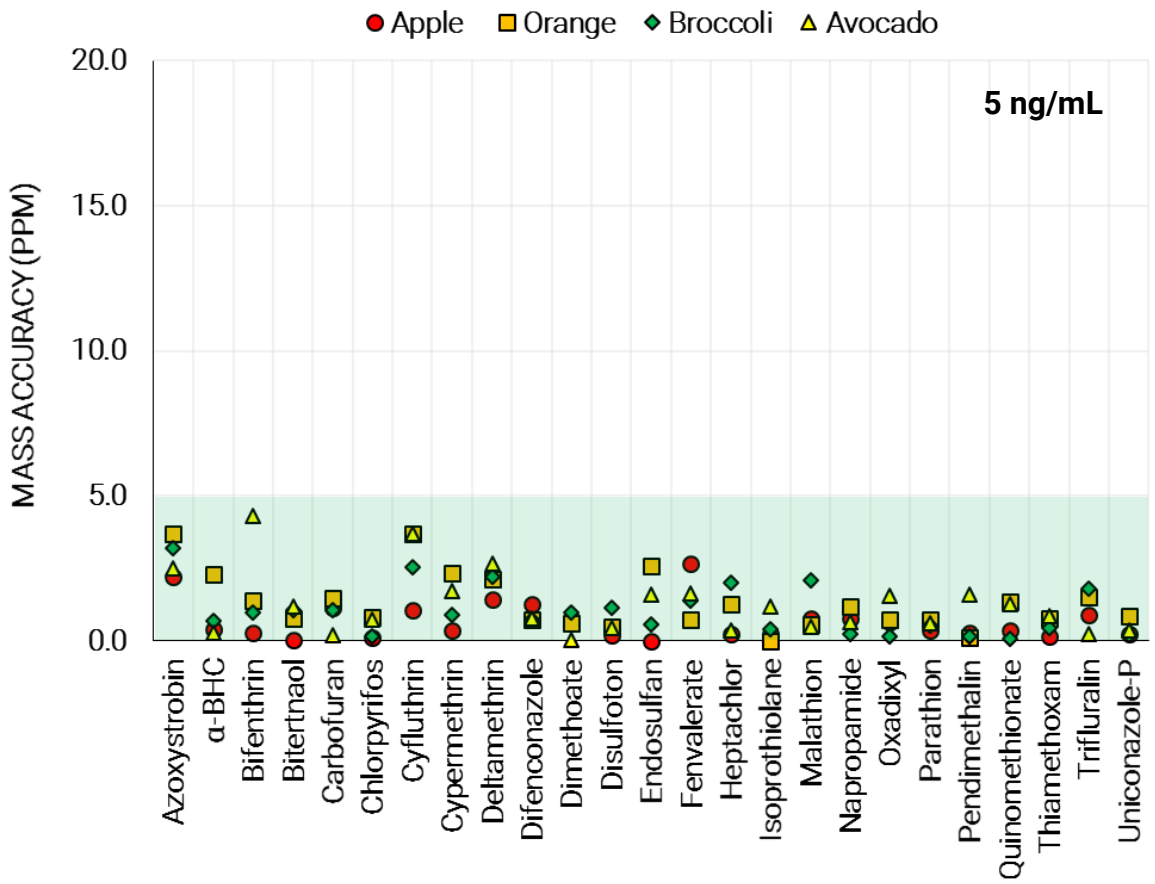


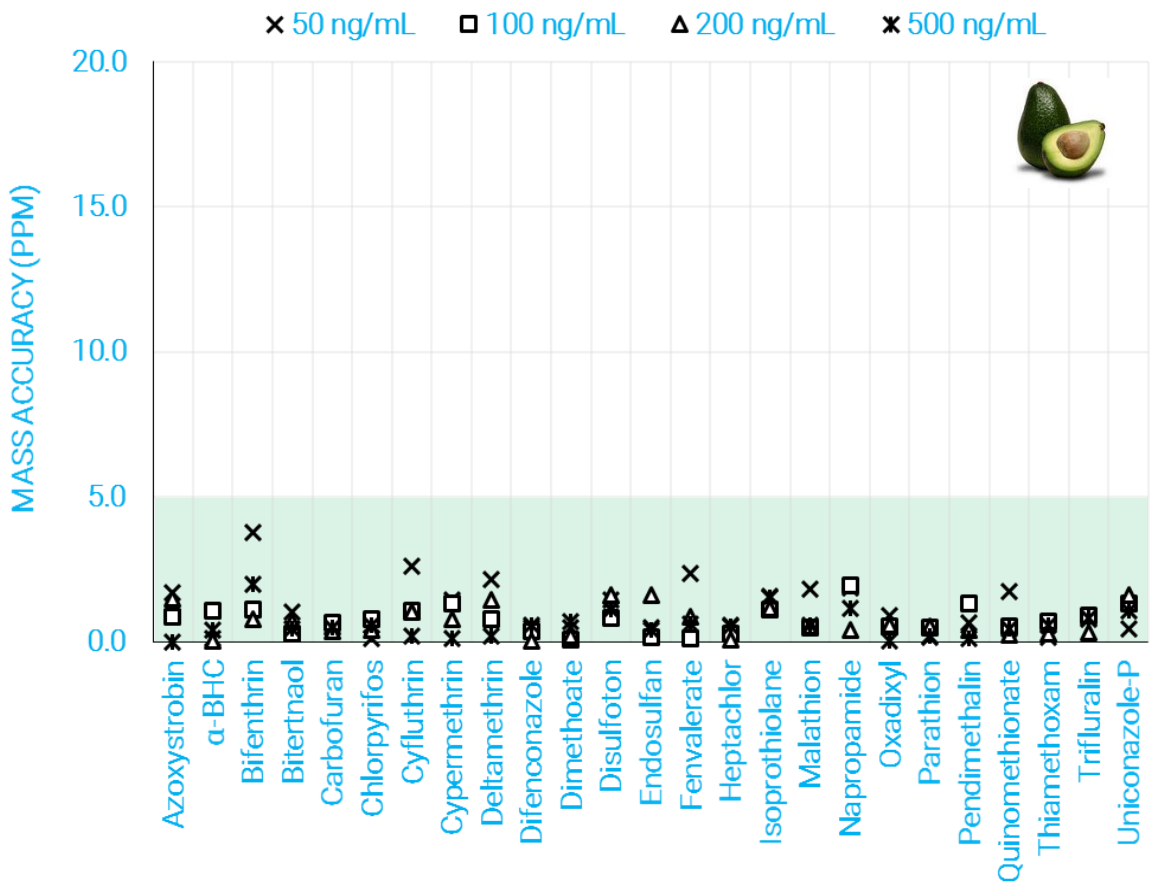
Deltamethrin (Decamethrin) - 8 Levels, 8 Levels Used, 8 Points, 8 Points Used, 0 QCs



Confidence Enhanced by Mass Accuracy

Targeted Quantitative Screening





Identify Suspect and Confirm Target

Targeted Quantitative Screening + **Suspect Screening**

Guideline to Identify Compounds

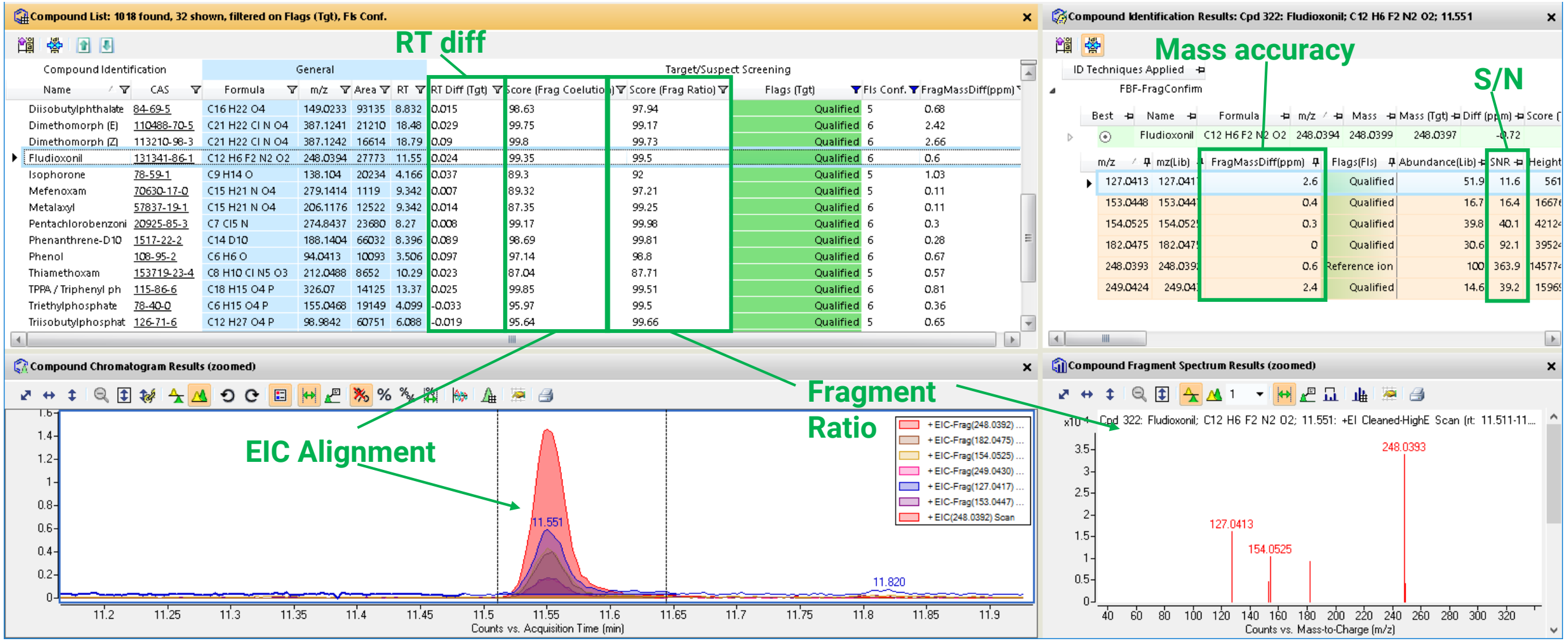
EU SANTE/11813/2017 Guidelines

MS detector/Characteristics		Acquisition	Requirements for identification	
Resolution	Typical systems (examples)		minimum number of ions	other
Unit mass resolution	Single MS quadrupole, ion trap, TOF	full scan, limited m/z range, SIM	3 ions	S/N ≥ 3[d] Analyte peaks from both product ions in the extracted ion chromatograms must fully overlap. Ion ratio from sample extracts should be within **±30% (relative)** of average of calibration standards from same sequence
	MS/MS triple quadrupole, ion trap, Q-trap, Q-TOF, Q-Orbitrap	selected or multiple reaction monitoring (SRM, MRM), mass resolution for precursor-ion isolation equal to or better than unit mass resolution	2 product ions	
Accurate mass measurement	High resolution MS: (Q-)TOF (Q-)Orbitrap FT-ICR-MS sector MS	full scan, limited m/z range, SIM, fragmentation with or without precursor-ion selection, or combinations thereof	2 ions with mass accuracy ≤ 5 ppm[a, b, c]	S/N ≥ 3[d] Analyte peaks from precursor and/or product ion(s) in the extracted ion chromatograms must fully overlap. Ion ratio: see D12

[a] preferably including the molecular ion, (de)protonated molecule or adduct ion
[b] including at least one fragment ion
[c] < 1 mDa for m/z < 200
[d] in case noise is absent, a signal should be present in at least 5 subsequent scans

How to Confirm Identification

Suspect Screening



Targeted Screening

Real samples from the Supermarket

Targeted Quantitative Screening + **Suspect Screening**

Sample	Compound name	RT diff (min)	Score Coelution	Score Frag ratio	Mass diff (ppm)	Amount (ng/mL)
	2,6-Dimethylphathalene	-0.006	97.87	88.53	0.21	ID only
	Azobenzene	0.051	91.18	67.01	0.54	ID only
	Benzylbenzoate	0.014	77.62	62.55	0.59	ID only
	Biphenyl	-0.002	97.05	86.43	1.34	ID only
	Boscalid	0.026	93.56	97.75	1.00	ID only
	DPA / Diphenylamine	0.003	98.54	99.8	0.51	ID only
	Eugenol	-0.003	93.08	86.83	1.02	ID only
	Fludioxonil	0.022	99.82	91.88	0.41	ID only
	Flutriafol	0.016	85.66	80.75	3.62	ID only
	Phenanthrene	0.005	86.57	95.45	0.29	ID only
	Pyraclostrobin	0.02	98.41	93.29	0.8	ID only
	Pyrimethanil	0.007	99.32	97.68	4.41	ID only
	Thiabendazole	0.012	99.67	99.37	0.22	ID only
	2,6-Dimethylphathalene	-0.004	99.44	63.82	0.17	ID only
	Anthraquinone	0.009	94.04	87.87	0.19	ID only
	Imazalil	0.028	88.91	84.45	1.05	ID only
	Propiconazole	0.023	97.29	99.45	0.24	ID only
	Pyrimethanil	0.013	99.12	97.68	4.69	ID only
	Thiabendazole	0.017	88.02	99.29	0.18	ID only
	Thiamethoxam	0.024	86.58	88.41	1.61	2.46
	Tri(2-chloroethyl)phosphate	-0.008	82.55	75.39	2.85	ID only

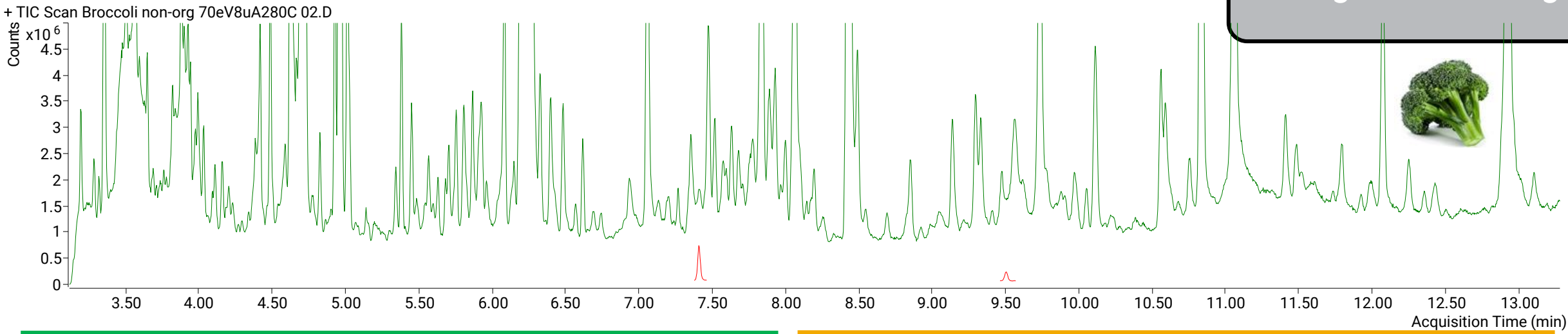
Sample	Compound name	RT diff (min)	Score Coelution	Score Frag ratio	Mass diff (ppm)	Amount (ng/mL)
	1,2,3,5-tetrachlorobenzene	0.008	88.8	85.1	0.48	ID only
	1-aminonaphthalene	0.021	96.6	72.3	0.96	ID only
	Anthraquinone	0.011	78.2	84.7	0.52	ID only
	Azobenzene	0.049	86.1	64.1	0.51	ID only
	Azoxystrobin	0.028	99.5	99.6	2	878
	Benzyl benzoate	0.009	74.3	55.8	0.07	ID only
	Boscalid	0.027	90.7	99.5	0.7	ID only
	Cyfluthrin	0.051	84.3	79.9	0.49	13.6
	Cyhalothrin	0.025	96.1	84.2	1.68	43
	Chlorthal-dimethyl	0.013	93.6	99.9	0.84	ID only
	Dimethomorph (E & Z)	0.029	99.8	99.2	2.42	972
	Fludioxonil	0.024	99.4	99.5	0.6	ID only
	Metalaxyl	0.014	87.4	99.3	0.11	ID only
	p,p'-DDE	0.015	90.8	87.2	1.7	4.65
	Pentachlorobenzonitrile	0.008	99.2	100	0.3	ID only
	Permethrin	0.022	99.5	98.9	1.8	61.3
	Phenathrene	0.003	91.8	97	1.08	ID only
	Pyraclostrobin	0.018	97.8	92.8	0.38	ID only
	Thiabendazole	0.023	88.7	86.7	0.35	ID only
	Thiamethoxam	0.023	87	87.7	0.57	2.46
	Triphenylmethane	0.016	84.4	85.7	0.29	ID only

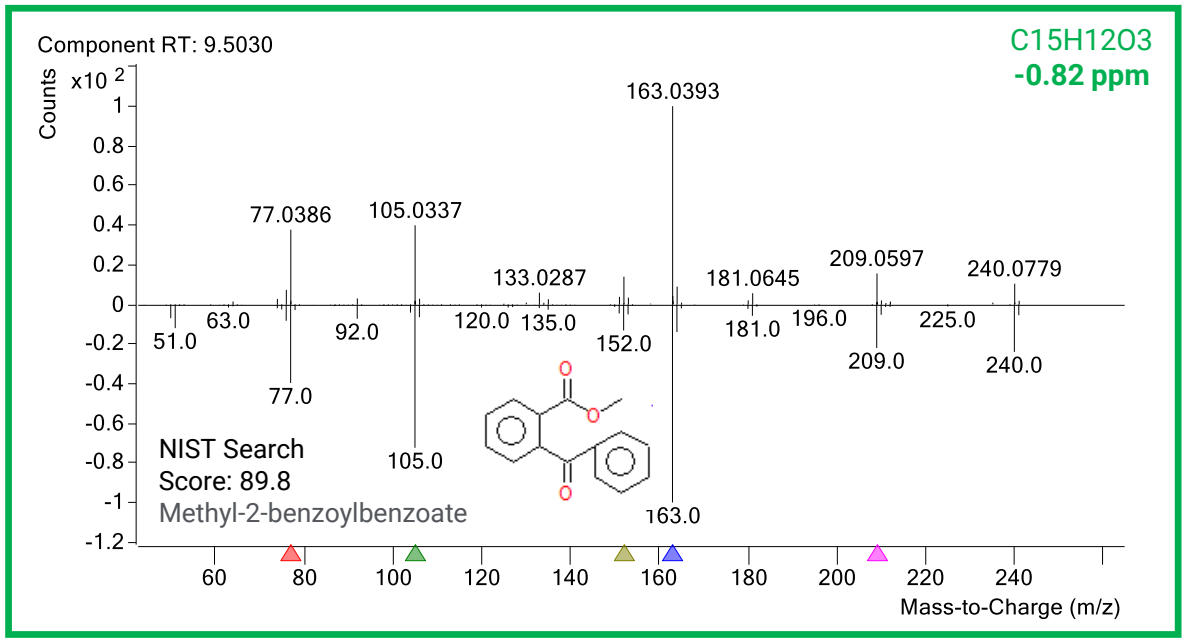
Explore Unknown

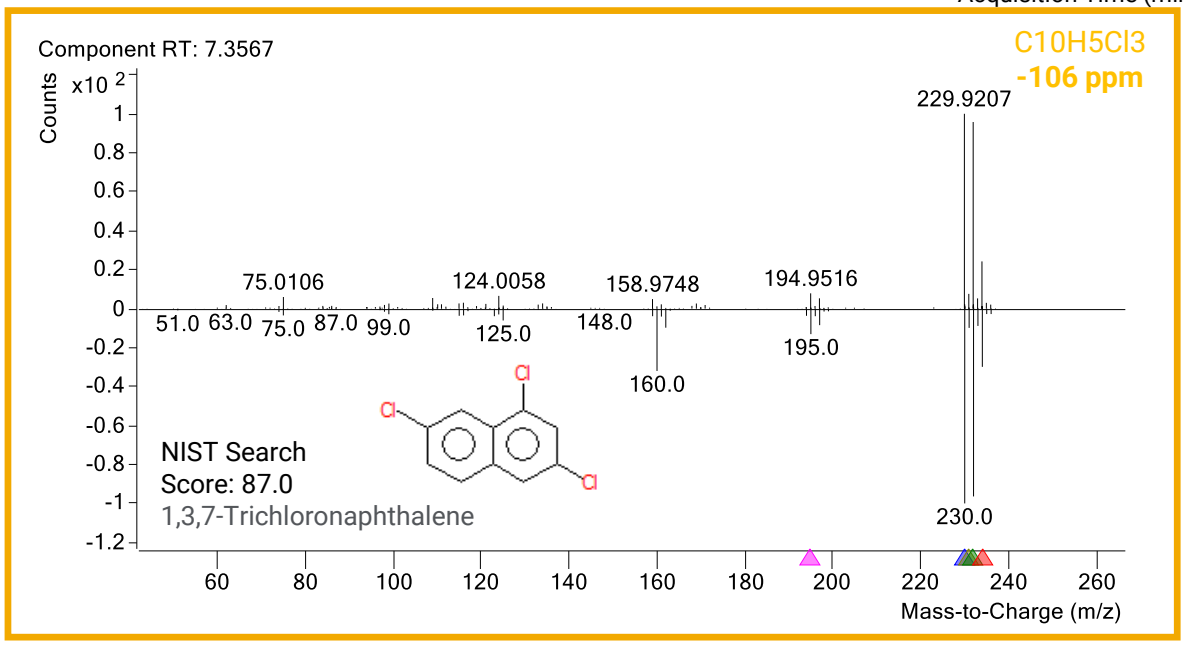
Untargeted Screening

Untargeted Screening (NIST)

Untargeted Screening





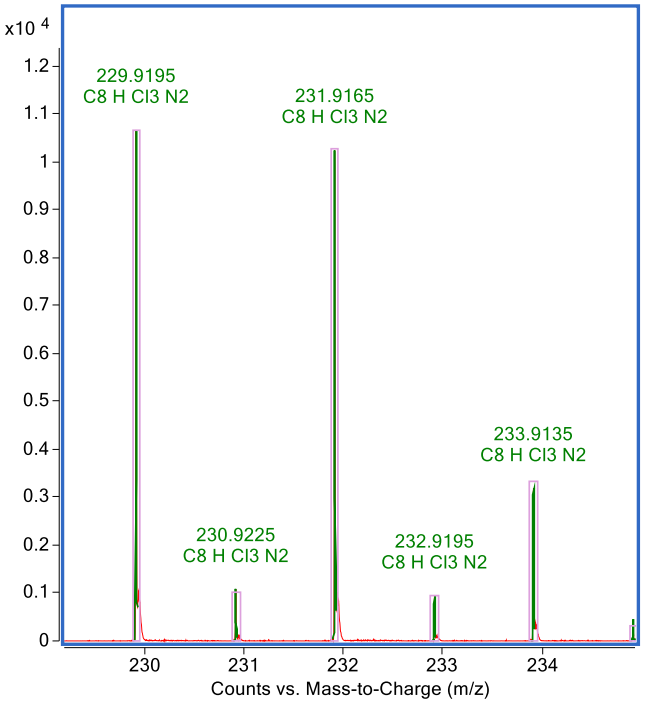


Elucidate structures…..

low energy EI, MS/MS and accurate mass

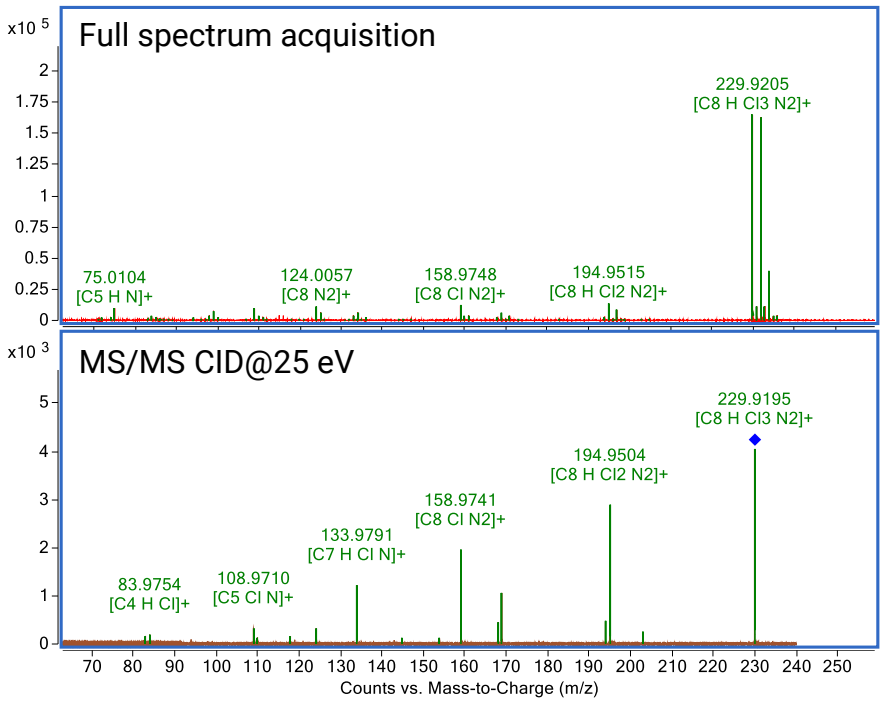
Untargeted Screening

Step 1: Confirm M+

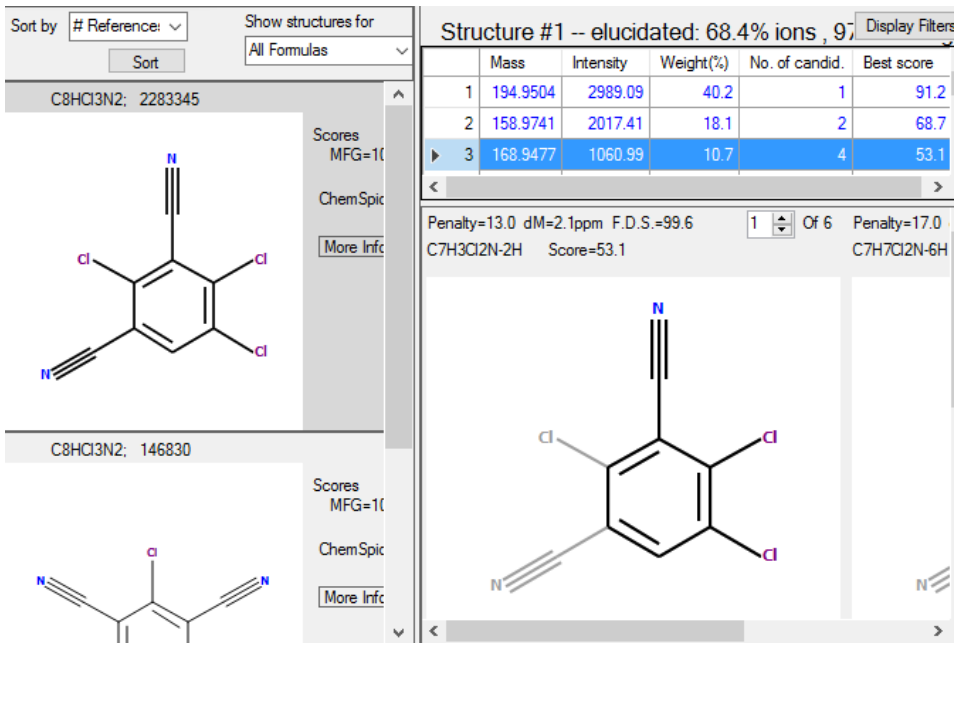


Low energy EI (15 eV)

Step 2: Confirm fragment ions



Step 3: Structure elucidation on candidate



C8-H-Cl3-N2 turns out to be 2,4,5-Trichloroisophthalonitrile.
That is not NIST. It is in fact a degradation product of Chlorothalonil

7250 GC/Q-TOF

- Mass Accuracy
- Isotopic Fidelity
- MS/MS Performance
- Low Energy EI Capability
- MassHunter Software

Identify. Quantify. Simplify

Thank You!

- MP 238 *Analysis of **polycyclic aromatic hydrocarbons (PAH) and hydroxylated PAH metabolites** in plasma and urine*
- MP 284 *Screening of **contaminants in food** and natural products*
- TP 180 *Low Energy EI and High Resolving Power Instrumentation for the Analysis of **Arson Samples***
- TP 213 *Targeted and Untargeted Analysis of **Pesticides and Other Contaminants in Fruits and Vegetables***
- WP 280 *Analysis of **doping and forensic drugs** in urine*
- ThP 286 *Analysis of **halogenated polycyclic aromatic hydrocarbons in atmosphere***
- ThP 295 *Combination of **chemical ionization (CI) and low electron energy ionization** capabilities*