



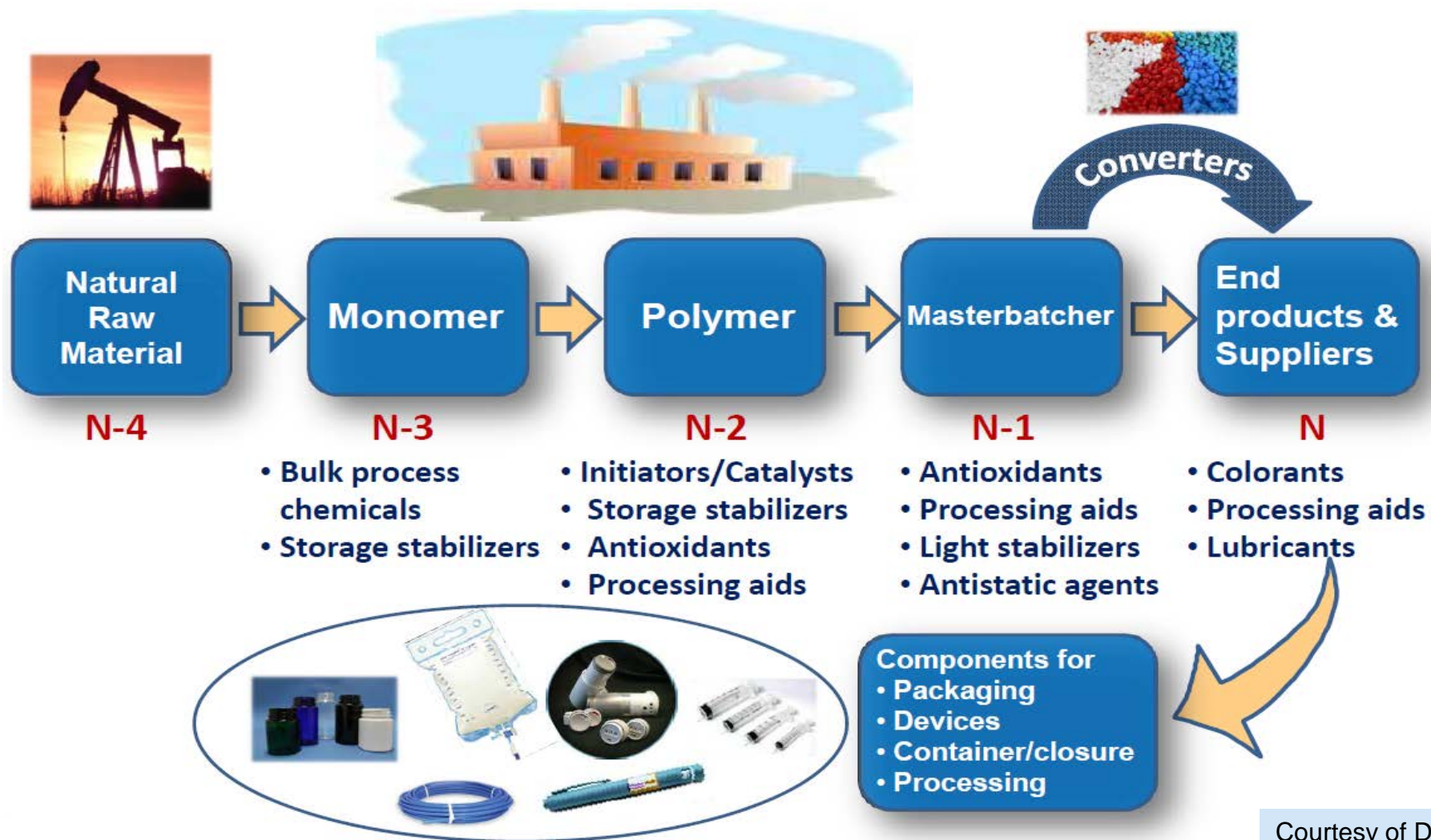
**ThermoFisher**  
S C I E N T I F I C

## The Doctor Did Not Prescribe Irgafos: A Solution for Extractables and Leachables Analysis

The world leader in serving science

- Introduction
  - Why conduct Extractables & Leachable (E&L) analysis?
  - Industries need Extractable & Leachable analysis
  - Regulations and guidelines from agencies and industry consortiums
- Thermo Scientific™ solutions for extractable & leachable analysis
  - Multiple instrumentations and technologies
    - ASE, CAD
    - GCMS
    - LCMS
    - ICP-MS
  - Data analysis software and database/spectral library

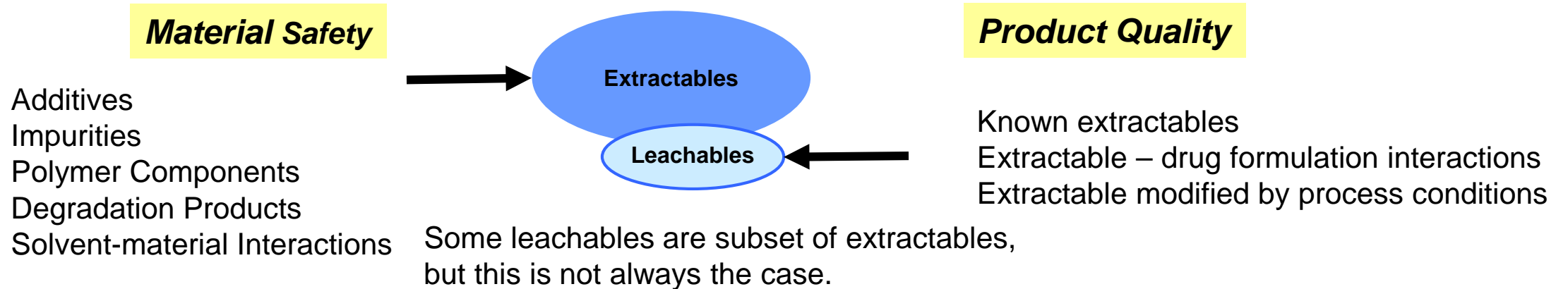
## Polymer Supply Chain for Pharmaceutically Relevant Materials



Courtesy of Doug Kiehl, Eli Lilly

# Definitions

- Extractable (E)
  - Compounds that migrate from the surface under more aggressive conditions of exposure (solvent, time, and temperature). Controlled extraction study
- Leachable (L)
  - Compounds that migrate from the contact surface to drug formulation under normal conditions of exposure. Bioproduction, formulated drug, or device simulants

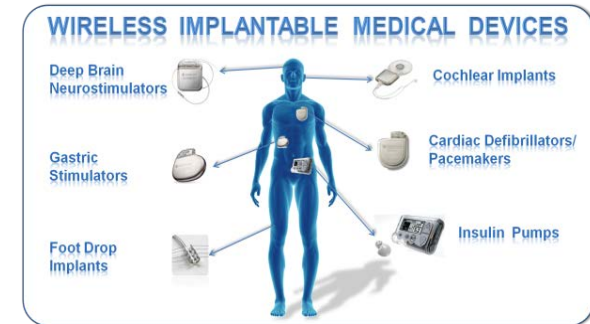


Safety/risk assessment → Regulatory submission → Market

# The Broad Market of Extractable & Leachable Analysis



Single-use systems for bioproduction and storage



Medicine container/packaging, implant and diagnostic devices



Food packaging



Printing ink and adhesives



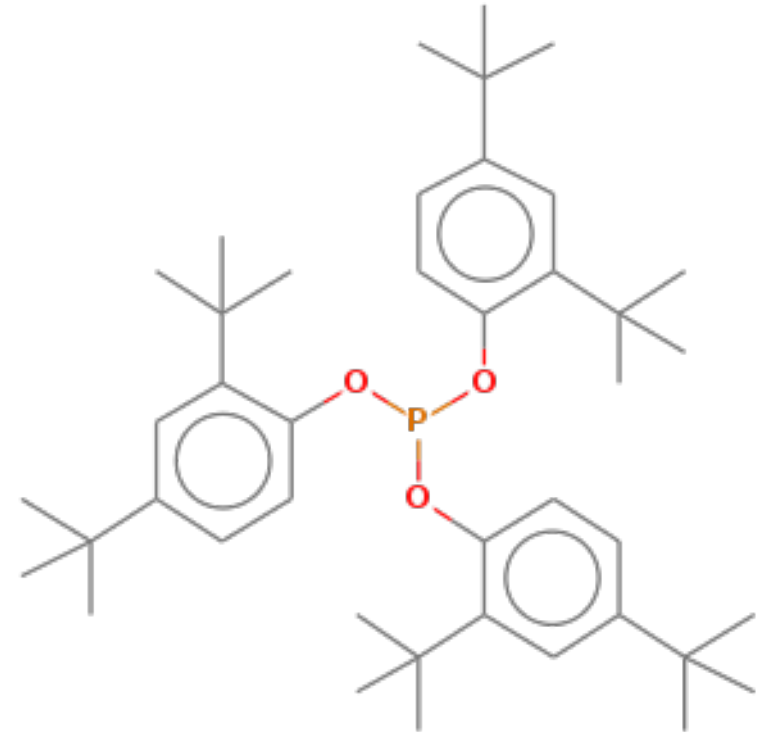
Wearable consumer electronic products

# What is Irgafos?

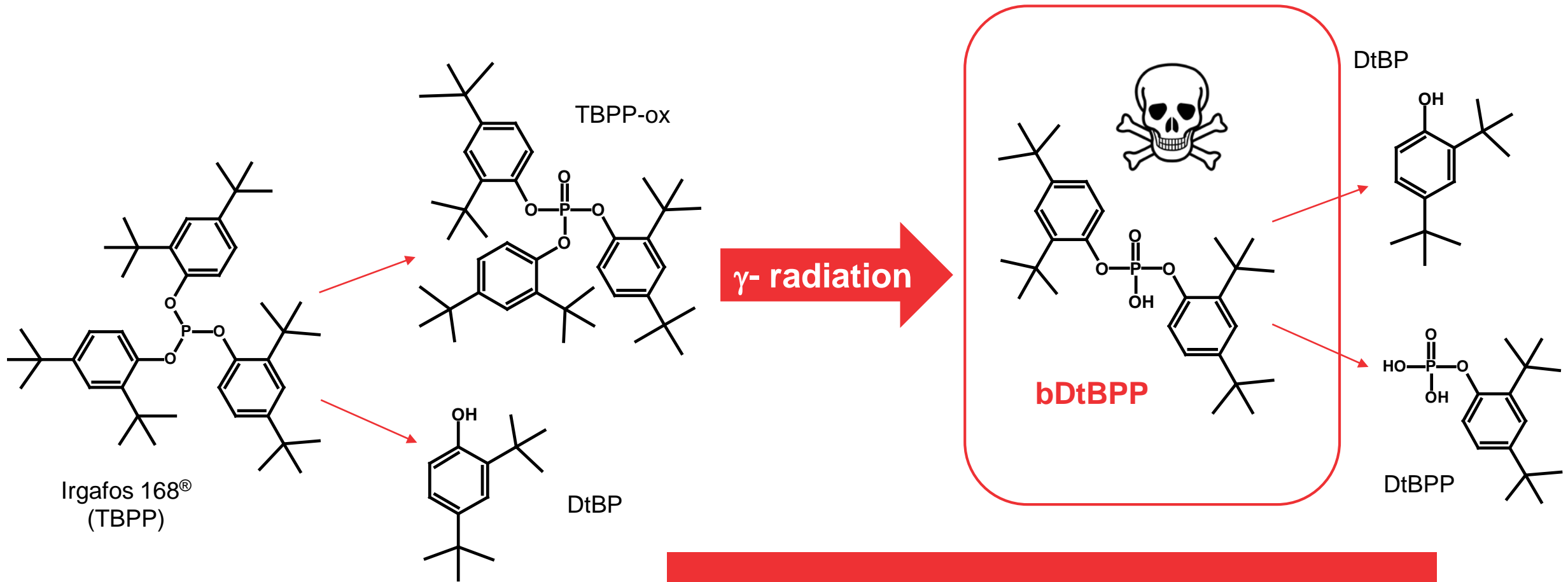
Trade name - **Irgafos® 168 (BASF)**  
*tris(2,4-di-tert.-butylphenyl)phosphite.*

- Polymer additive stabilizer
- Protects plastic from thermooxidative degradation
- Improves the strength and durability
- Used in a range of plastic films

including **Single Use BioProcess films**



# Irgafos 168 is safe – until you irradiate it



**BioProcess bags are sterilized with  $\gamma$ -radiation**

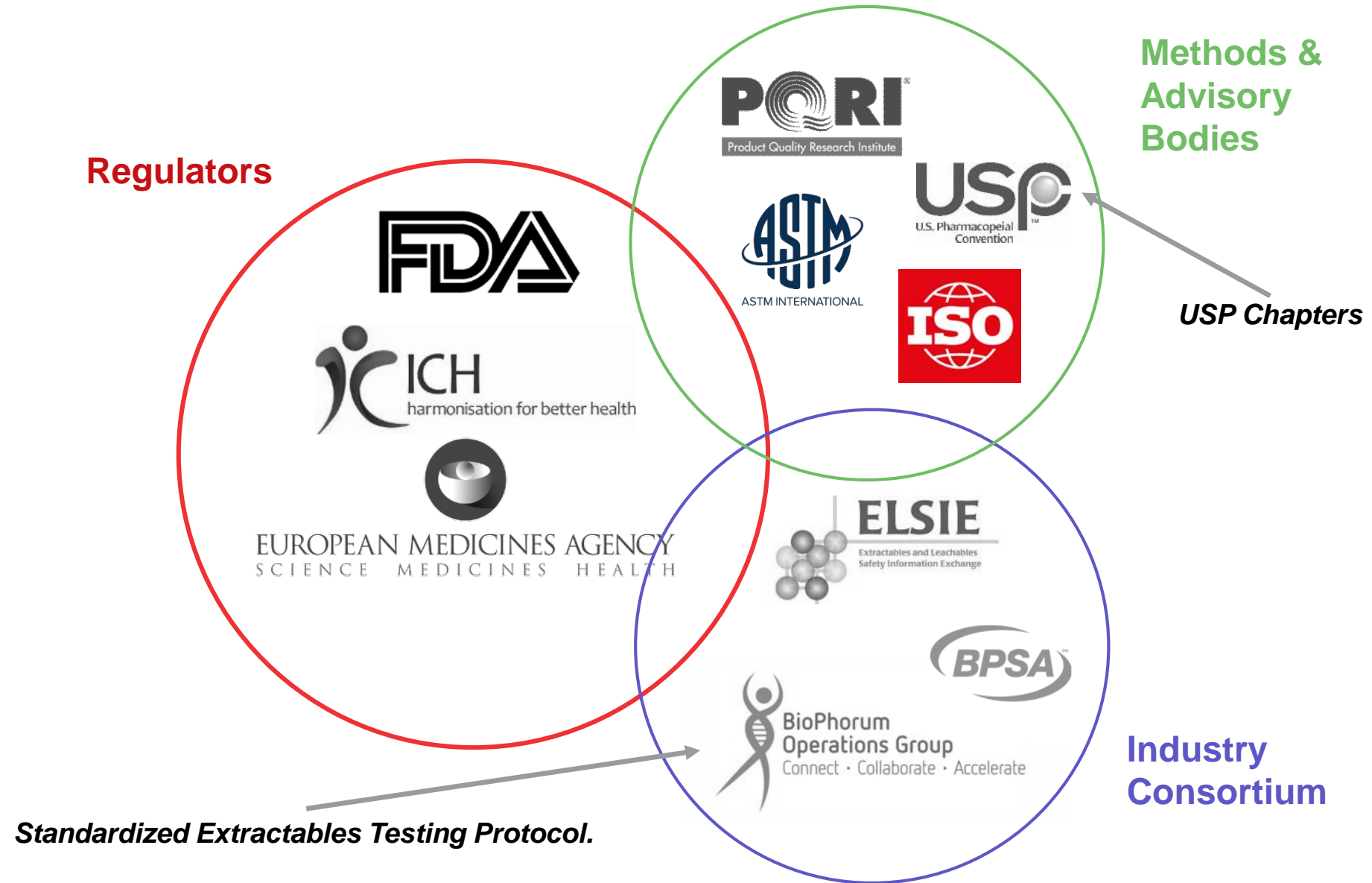
<sup>1</sup> Fouyer K et al (2012) *Anal. Chem.* 84 (20): 8642-8649.

# The Importance and Challenges of E&L Analyses

- Safety
  - Extractables and Leachables are chemical impurities- they could contaminate medicine, food, and drink, affect product quality, and cause adverse effects for consumers.
- Regulations
  - E&L analyses are highly regulated and required for marketing approval of new products.
  - More regulations have been promulgated along the way and will continue into the future.
- E&L analysis is challenging and complex
  - It requires multiple instruments, expertise, data processing software, and database.
  - It needs both identification and quantitation. Unknown structure elucidation is challenging.
  - It must start at early stage to be ready for product launch.

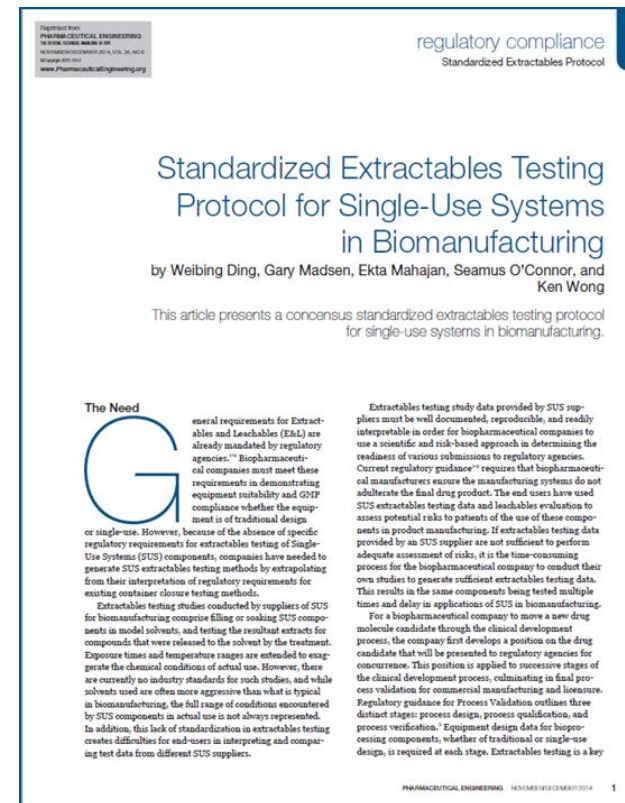


# E&L Regulatory and Method landscape



# Industry Group: BioPhorum Operations Group (BPOG) The Global Community

<http://www.biophorum.com/>



BPOG members are leading biopharmaceutical companies around the world to create an environment where the global biopharmaceutical industry can collaborate and accelerate their rate of progress, for the benefit of all.

Many Technical Resources on their website <http://www.biophorum.com/>

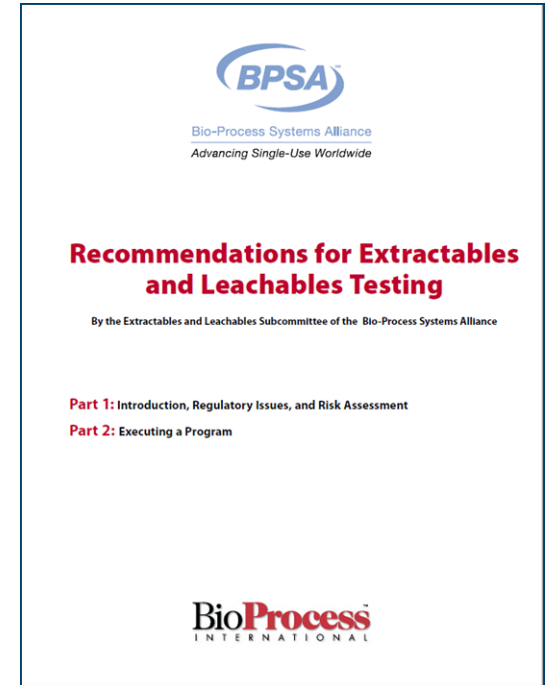
# Industry Group: Bio-Process Systems Alliance (BPSA) - Published Technical Guides



BPSA members include industry-leading manufacturers of single-use biological processing products. BPSA is encouraging and accelerating the adoption of technologies used in the production of biopharmaceuticals and vaccines.

Many Technical Guides on their website [bpsalliance.org/](https://bpsalliance.org/)

## BPSA Members





International Organization  
for Standardization

## ISO 10993

### Biological Evaluation of Medical Devices

Sample preparation and Extraction

- Part 12: Sample preparation and reference materials

Material Characterization

- Part 18: Chemical characterization of materials
  - GCMS - SVOC
  - LCMS – NVOC
  - ICP- MS Elemental impurities
  - Other analytical methods – FTIR...



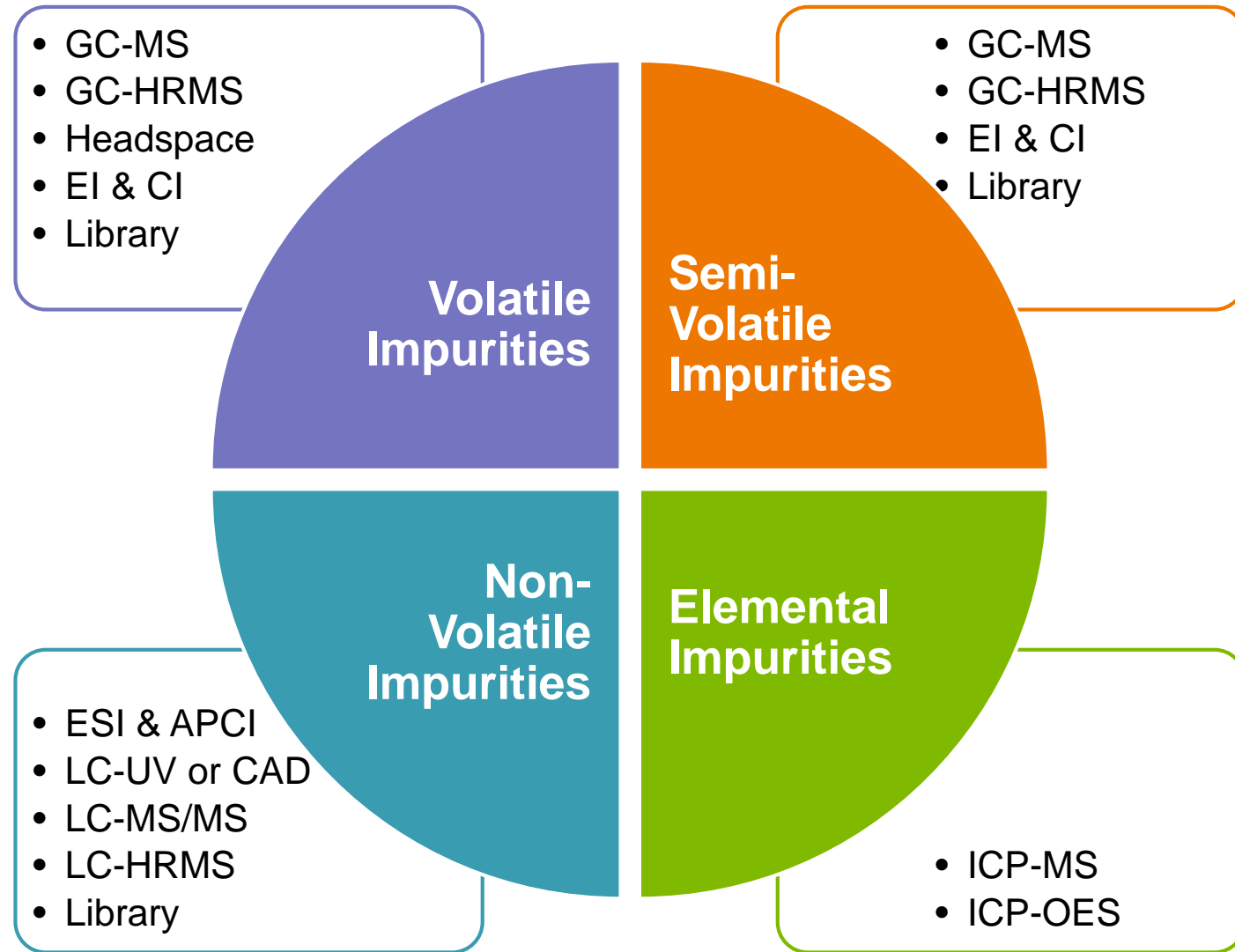
ASTM  
INTERNATIONAL

## ASTM D7210

### Standard Practice for Extraction of Additive in Polyolefin Plastics

- USP <1663> lists ASE as a possible option to perform extractable studies
- ASTM D7210 also lists ASE as one of the options to extract antioxidants from polymeric matrices.

# Analysis of Extractables & Leachables



# Thermo Scientific Instruments, Software, Consumables for Impurity ID & E&L Analysis



Solvent Extraction



FTIR



GCMS-Single Quad



GCMS-Triple Quad



Orbitrap GC-MS/MS



ICP-MS

## Consumables



## UHPLC



Charged Aerosol  
Detection



IC

## LCMS- Non Volatiles



LCMS-Triple Quad



Hybrid Orbitrap LC-MS/MS



## Software & Database



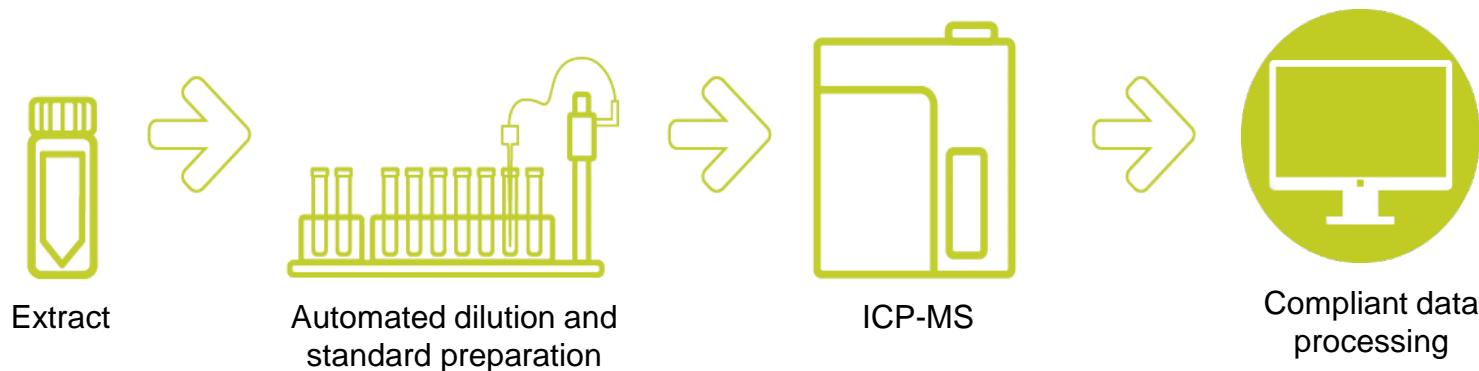
## Thermo Scientific™ iCAP™ RQ ICP-MS



Thermo Scientific™ Qtegra™ ISDS software.  
Integrated CFR compliance tools kit  
Full USP 233 & ICH Q3D method capabilities  
Compliance with USP <232>/<233>



## Thermo Scientific™ iCAP™ 7000 Plus ICP-OES



Using an in-line autodilution and autocalibration system significantly lowers the risk of human error and contamination of the samples, standards, or blanks.

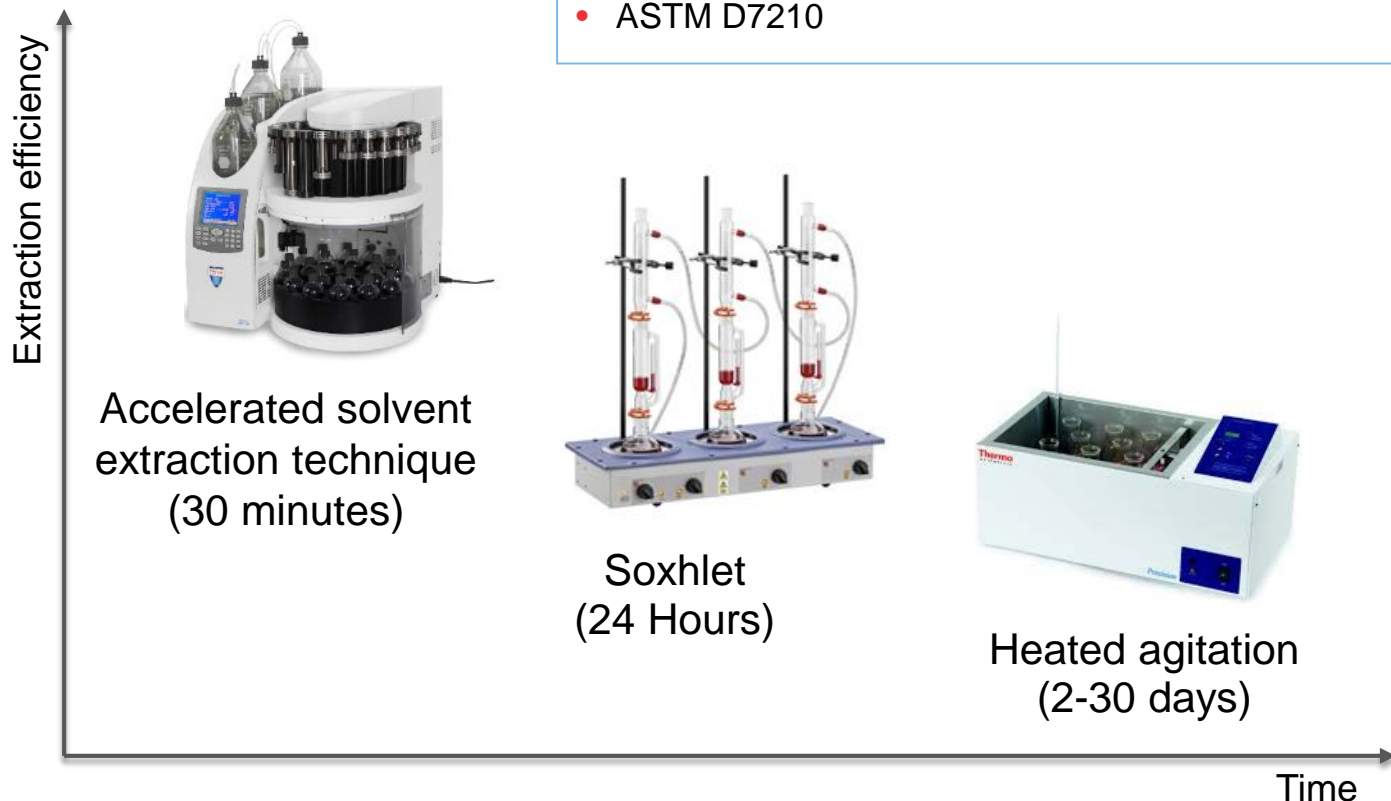
# Principle and Best Practices Recommended

## Guidelines list ASE as an option for extractable studies:

- USP Chapter <1663> & <1664>
- Product Quality Research Institute (PQRI)
- BioPhorum Operations Group (BPOG)
- ASTM D7210

## Advantage

- Automated with intelligent solvent management system
- Reduce extraction times
- Reduce solvent consumption
- Increase extraction efficiency
- Nitrogen flush gas prevents the oxidation of the extractables
- Working very well for wide range of polymers, especially for ultra high molecular weight cross linked polyethylene -Dr. Vas



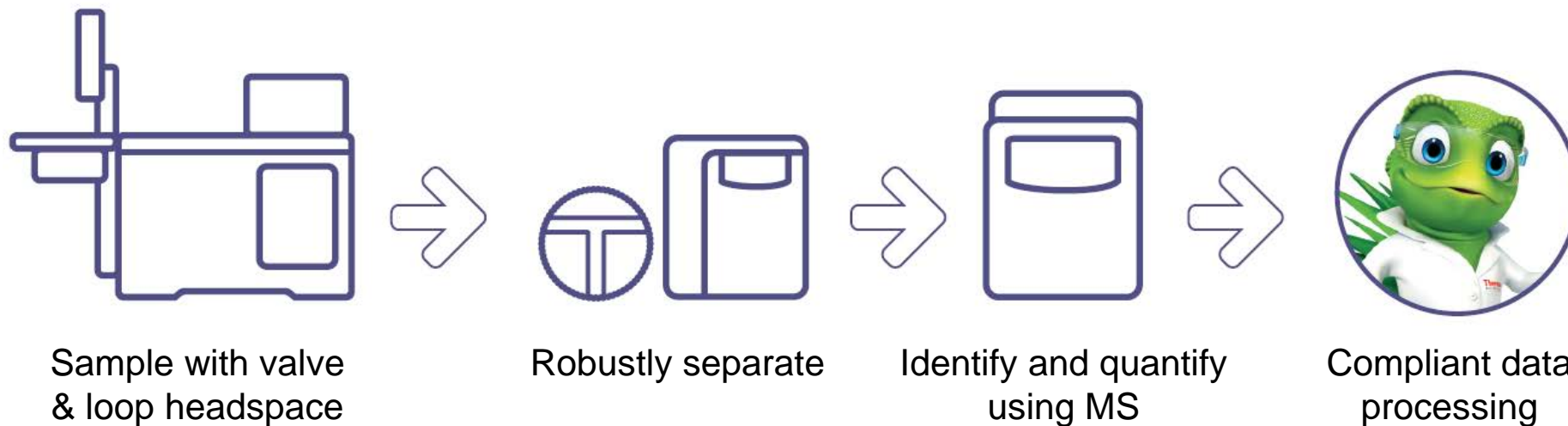


# Comparison of Soxhlet vs. Thermo Scientific Dionex ASE 350 System

Parameter	Soxhlet	Thermo Scientific™ Dionex™ ASE™ 350 System
Extract solvent used per sample (mL)	160	<30
Total extraction time per sample (min)	1440	<30
Extracted compounds	Same	Same
Extracts peak Intensity Ratio Accelerated Solvent Extraction/Soxhlet		<b>1.4x to 90x</b>

**Dionex ASE 350 system delivers faster extractions using less solvent**

# Volatile Impurities Workflow



- Analogous to **USP 467** Residual solvents workflow
- Molecules are generally known, or simple to identify
- **Routine compliant quantification**



# Complete Technologies for Volatile Impurities



Thermo Scientific™ TriPlus™ 300 Headspace Sampler



Thermo Scientific™ Trace™ 1310 GC



Thermo Scientific™ TraceGOLD™ TG-624SiIMS GC Columns



Thermo Scientific™ ISQ™ Series GC-MS

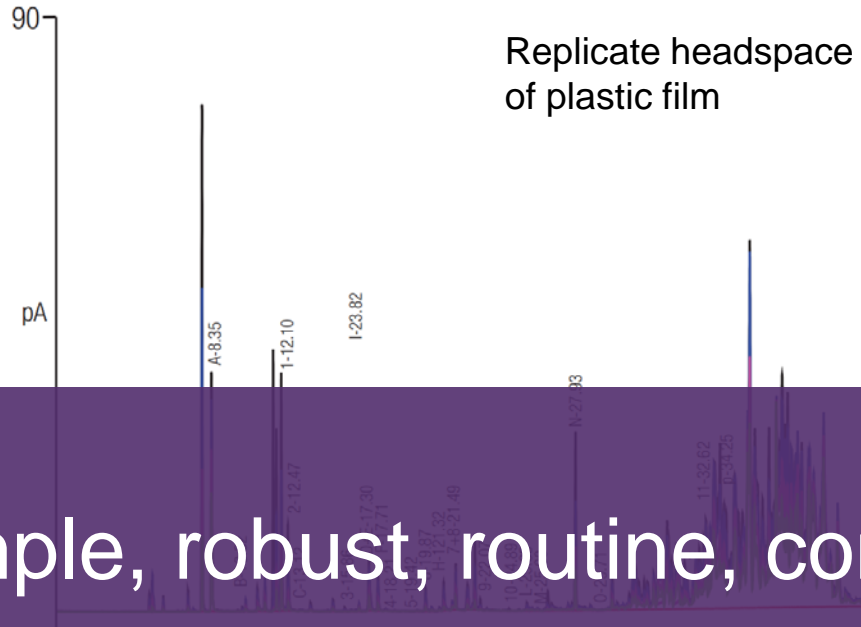


Thermo Scientific™ Chromeleon™ CDS Software



Thermo Scientific™ AppsLab Library

# Volatiles Headspace Analysis

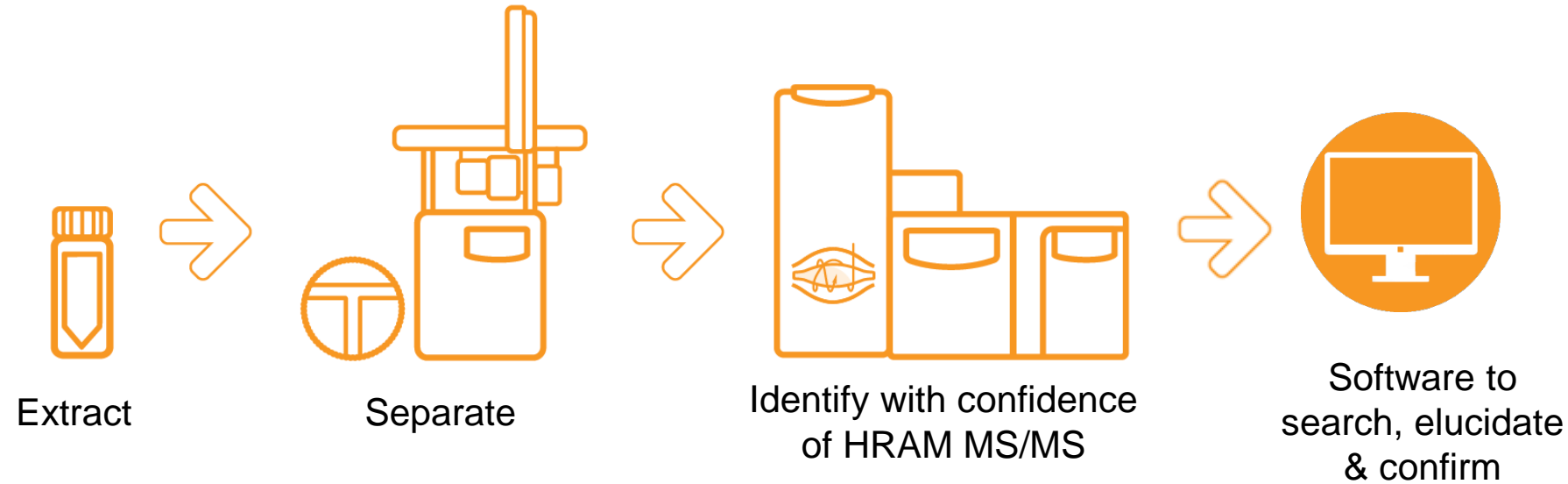


- Methods available on AppsLab
- One click Chromeleon eWorkflow
- Full **quantitative** and **qualitative** mass spectral analysis

- Simple, robust, routine, compliant analysis
- Methods freely downloadable



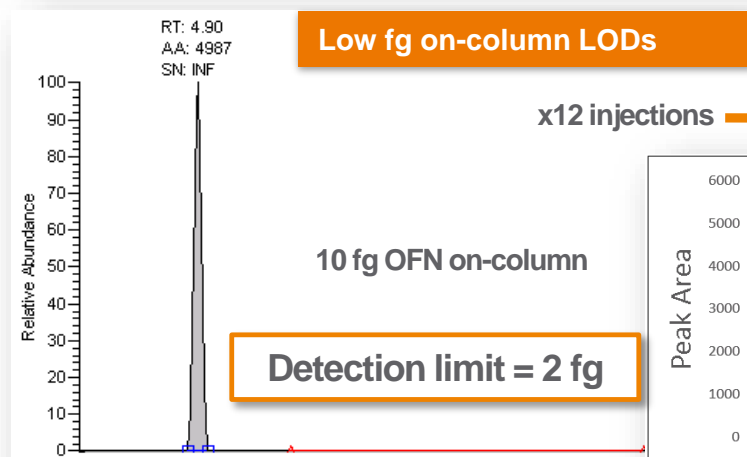
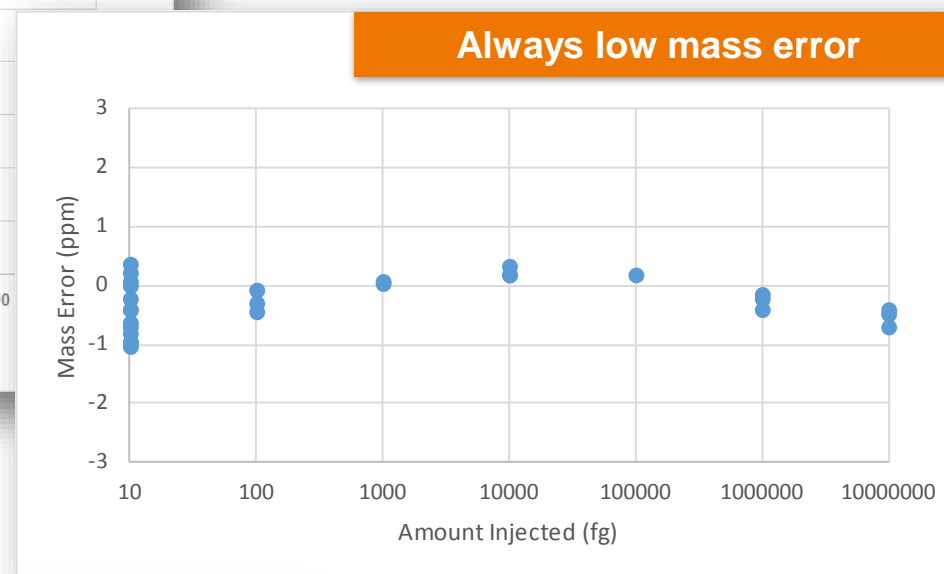
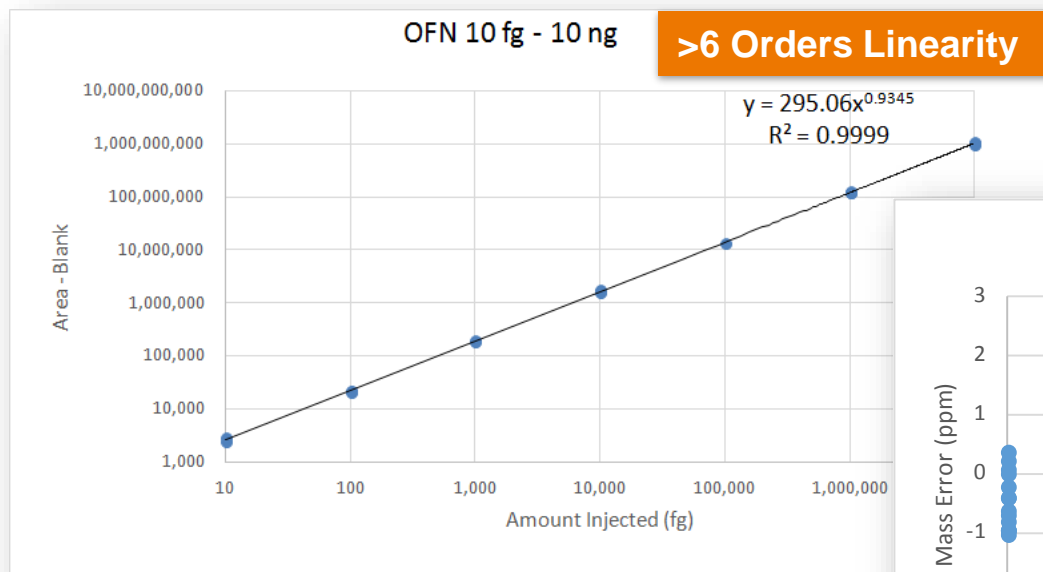
# High Resolution GCMS for Impurity Identification and Quantification Workflow



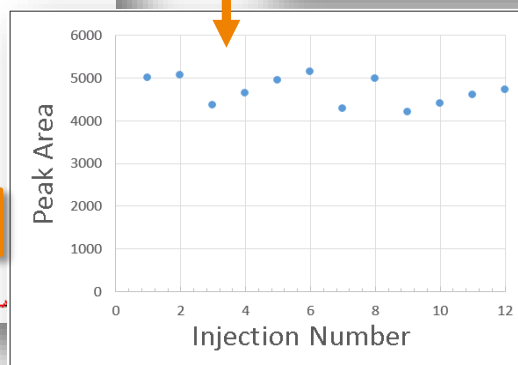
- Deconvolve, identify and quantify even the narrowest GC peaks
  - Unambiguously calculate empirical formulae
  - No need to average scans
  - Simplify data review and report
- 
- Thermo Scientific™ Q Exactive™ GC Orbitrap™ GC-MS/MS system
  - Thermo Scientific™ TraceFinder™ software



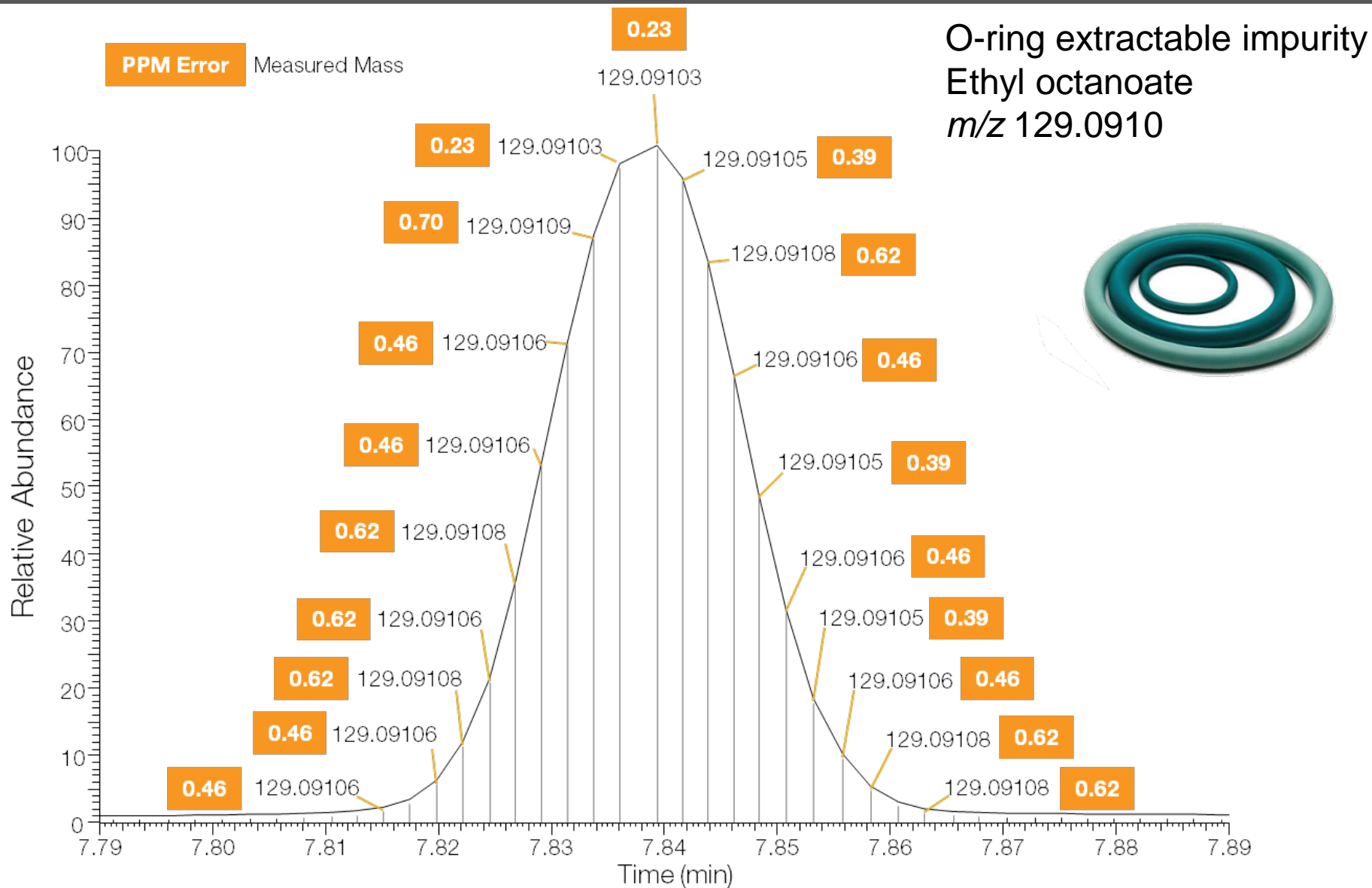
# Detect, Quantify and Identify at Any Concentration



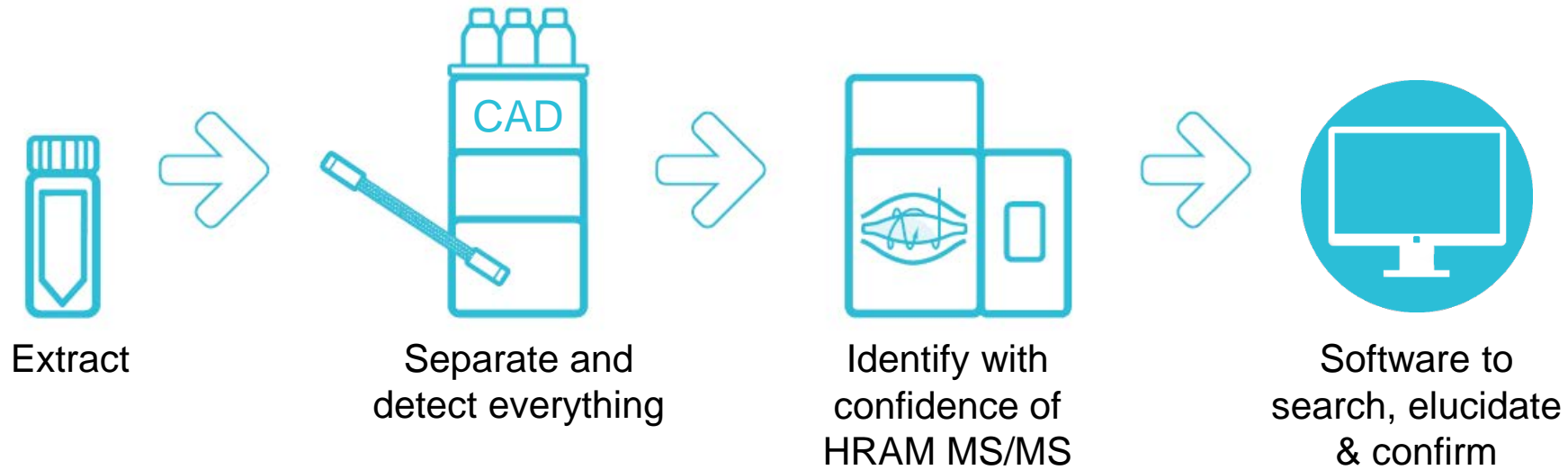
x12 injections



# Scan Speed and Accurate Mass Error Across a Peak



# Non-Volatiles Unknown Identification Workflow

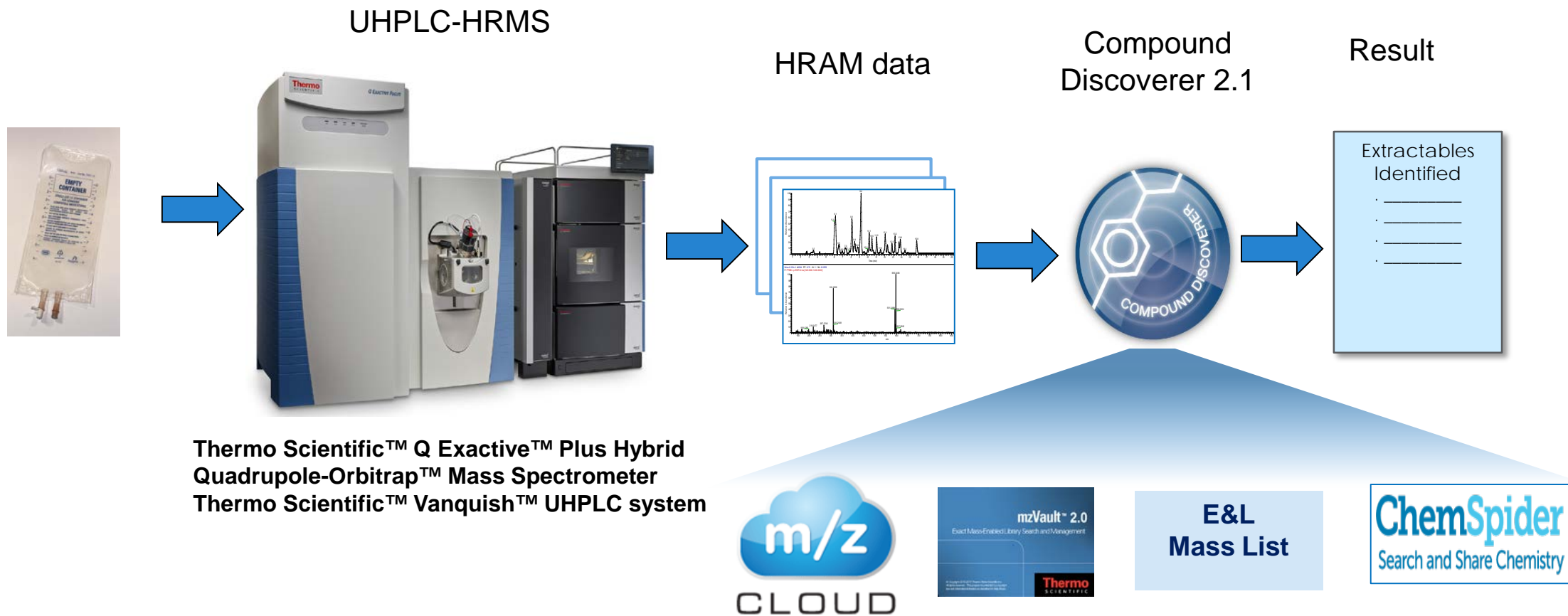


- Catch everything with orthogonal detection
- Detect in both positive and negative ion mode
- Have absolute confidence in elemental composition
- Get full sub-structural information
- Search wide variety of data sources in parallel





# LC-HRMS Analysis for IV Bag Extractables



# MS Method: High Resolution Accurate Mass Untargeted Screening

- **HRAM untargeted screening with polarity switching**
- ESI/APCI full scan MS and data-dependent top 3 MS/MS data with polarity switching using 70K & 17.5K resolution for FMS and HCD MS<sup>2</sup> respectively. Stepped NCE: 30, 45, 60.

**Positive**                      **Negative**

The screenshot displays the ThermoFisher software interface for configuring mass spectrometry methods. It is divided into several sections:

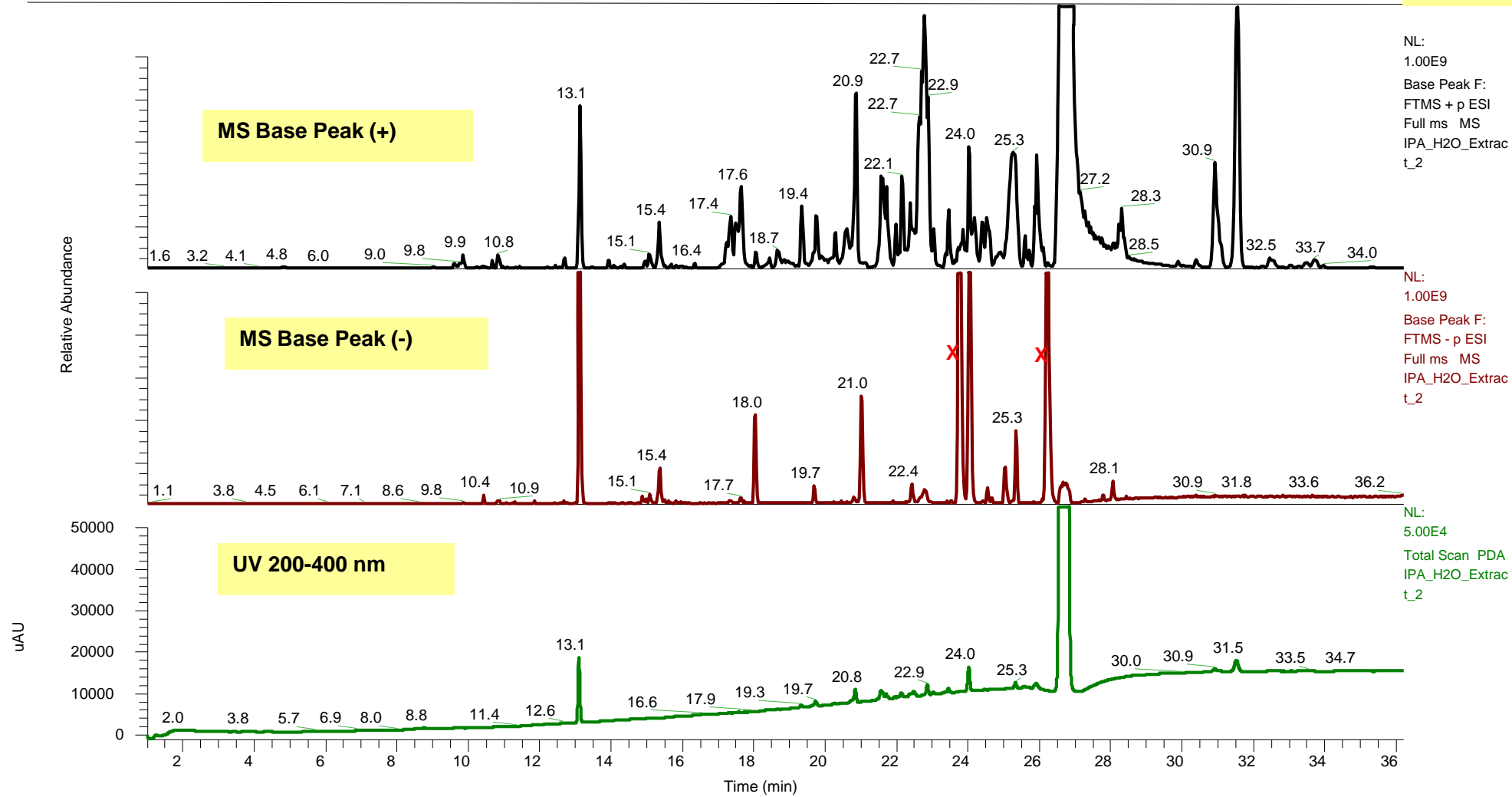
- Global Lists:** Includes Lock Masses, Inclusion, Exclusion, Neutral Loss, and Tag Masses.
- Chromatogram:** Shows a scan range from 0 to 30 minutes with peaks labeled 'Top3'.
- Experiments:** Lists various methods such as Full MS - SIM, AIF, Full MS / dd-MS<sup>2</sup> (TopN), Targeted SIM, Targeted-MS<sup>2</sup>, Targeted-SIM / dd-MS<sup>2</sup>, and DIA.
- Properties of the method:** Two panels show settings for Positive and Negative polarity. Both include Global Settings (User Role: Advanced, Use lock masses: off, Lock mass injection: off, Chrom. peak width: 8 s), Time (Method duration: 42.00 min), and Customized Tolerances (+/-).
- Properties of Full MS / dd-MS<sup>2</sup> (TopN):** Two panels show detailed settings for Full MS and dd-MS<sup>2</sup> / dd-SIM. The Full MS settings include Microscans (1), Resolution (70,000), AGC target (3e6), Maximum IT (100 ms), Scan range (120 to 1500 m/z), and Spectrum data type (Profile). The dd-MS<sup>2</sup> / dd-SIM settings include Microscans (1), Resolution (17,500), AGC target (1e5), Maximum IT (50 ms), Loop count (3), MSX count (1), TopN (3), Isolation window (1.6 m/z), Isolation offset (0.0 m/z), Fixed first mass (50.0 m/z), NCE / stepped NCE (20, 40, 60), and Spectrum data type (Profile).
- dd Settings:** Both panels show Underfill ratio (5.0 %), Intensity threshold (1.0e5), Apex trigger (2 to 3 s), Charge exclusion (off), Peptide match (off), Exclude isotopes (on), and Dynamic exclusion (5.0 s).

# IV Bag IPA-H2O Extract - Positive Negative Full Scan, MSMS and UV in One Run

D:\SGS-E&L\SGS-IVBag\IPA\_H2O\_Extract\_2

Accucore C18 2.1x100 2.6 um A: H2O/0.05% HAc/5 mM NH4AC B: ACN/0.05% HAc/5mM NH4Ac

Zoom-in View



X = present in the blank

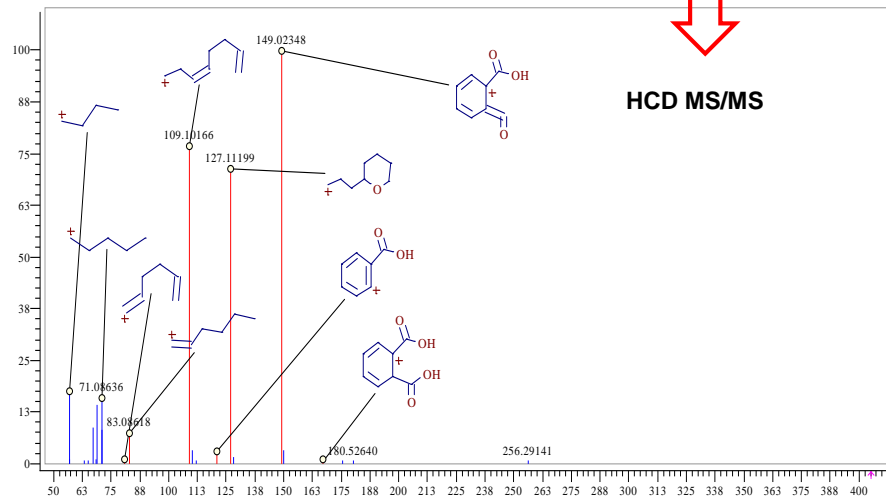
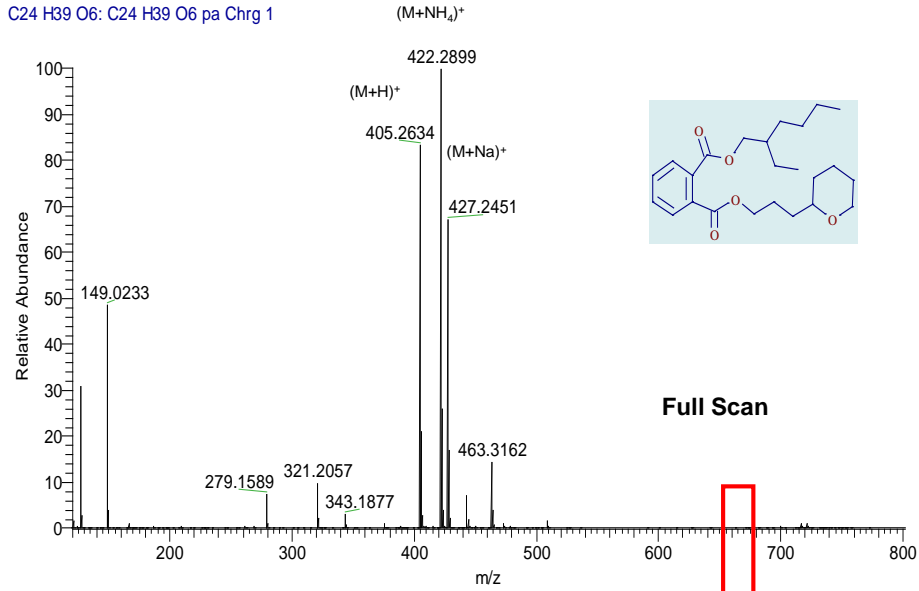
# Full Scan and HCD MS/MS Data for Component ID and Structure Elucidation

G:\Old Passport\...IPA\_H2O\_Extract\_1

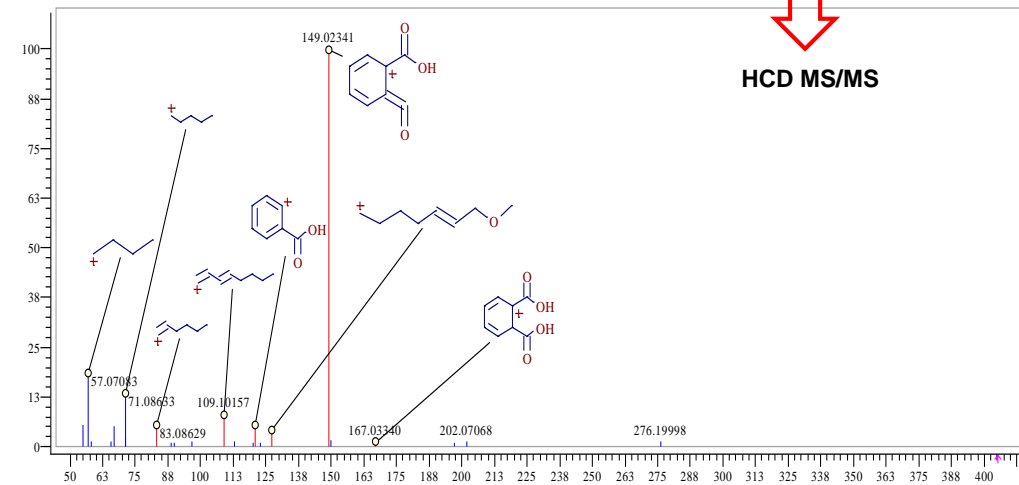
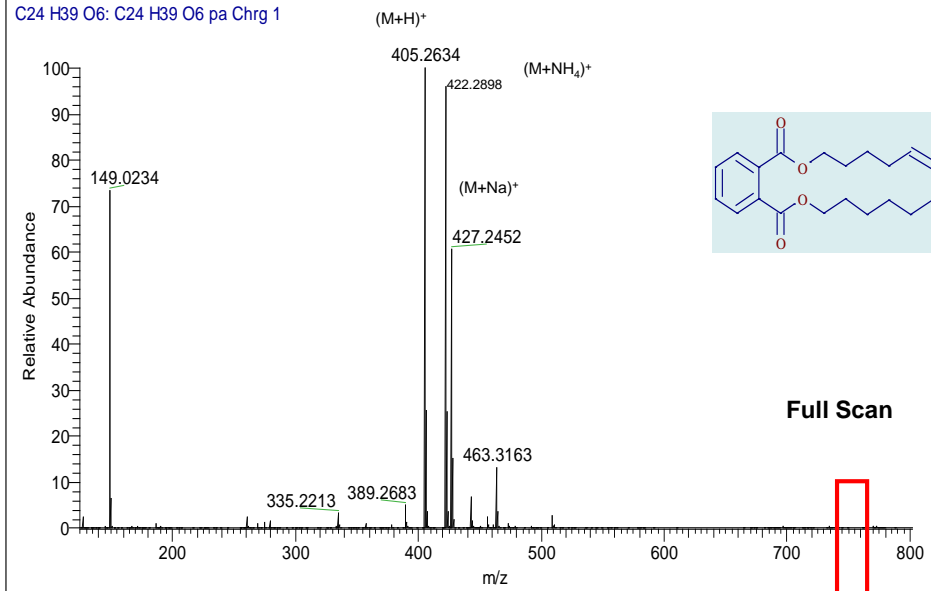
01/18/16 07:08:13

Accucore C18 2.1x100 2.6 um A: H2O/0.05% HAc/5 mM NH4Ac B: ACN/0.05% HAc/5mM NH4Ac

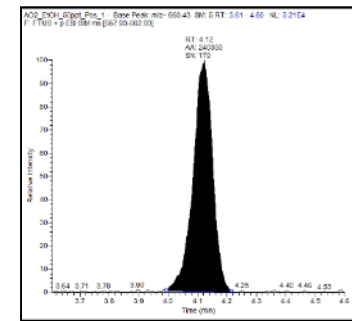
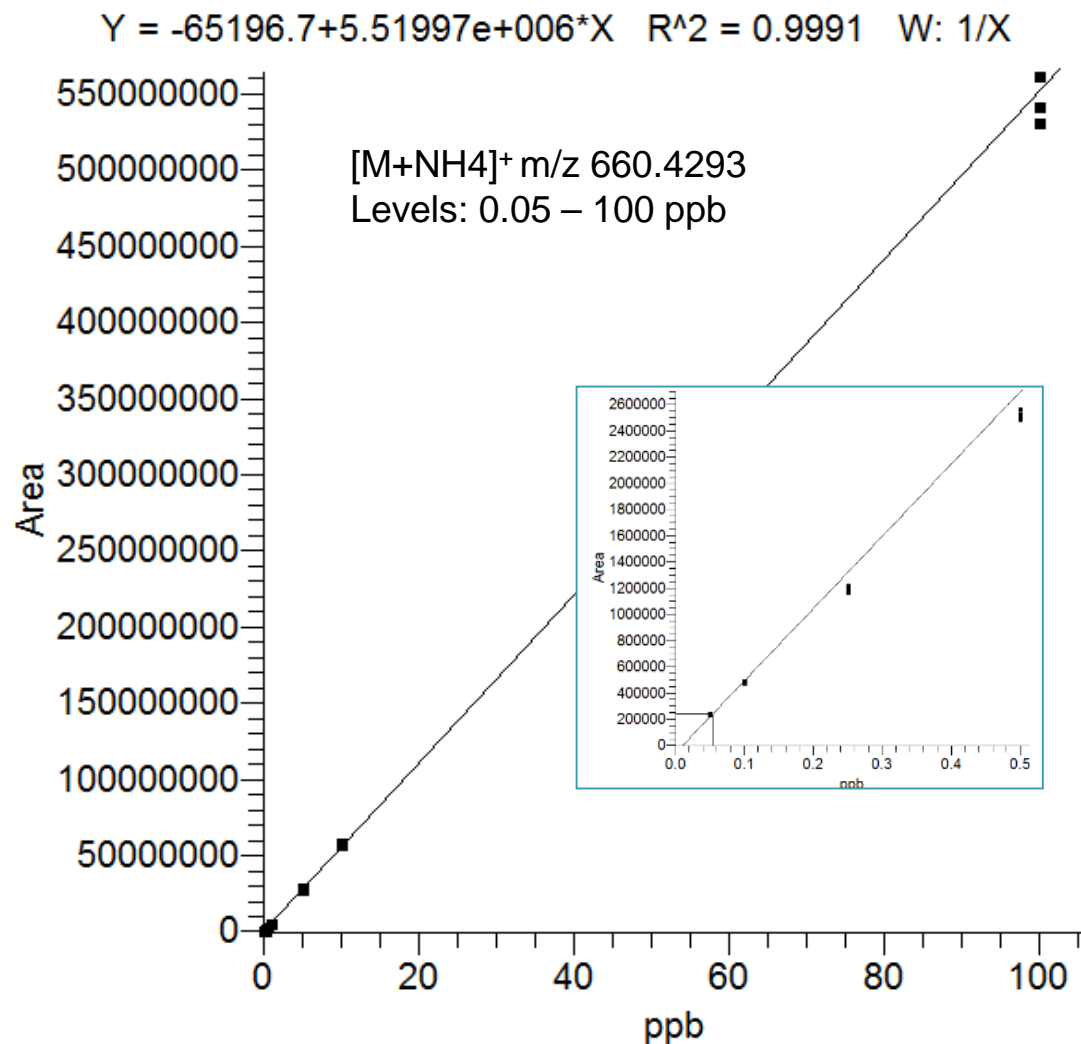
C24 H39 O6: C24 H39 O6 pa Chrg 1



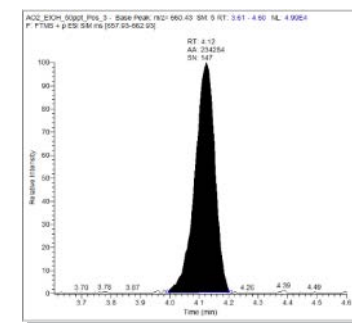
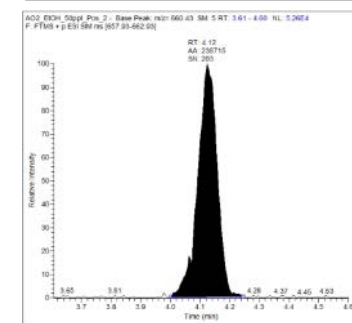
C24 H39 O6: C24 H39 O6 pa Chrg 1



# Quantify Non-Volatile Extractables – Irganox1035



+VE



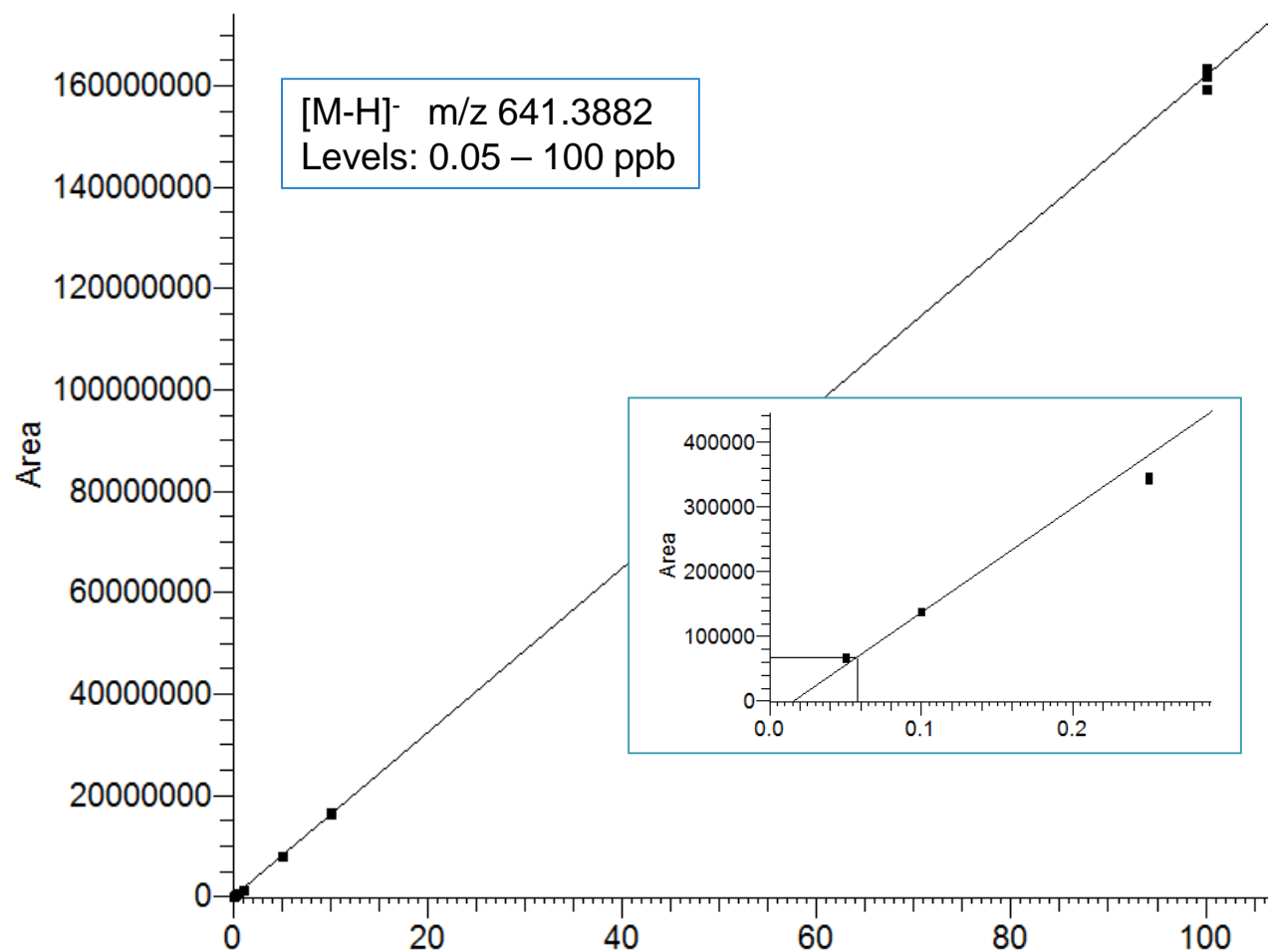
50 ppt  
(Triple Injections)

Detect in positive and negative ion mode in the same run

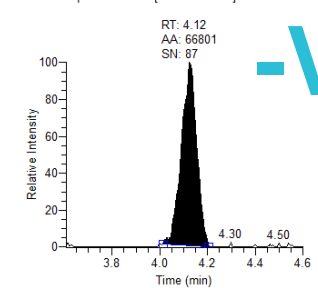
# Quantify Non-Volatile Extractables – Example Irganox1035

cas 41484-35-9

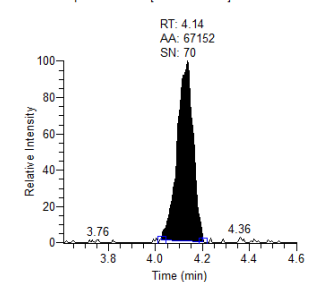
$$Y = -27525.8 + 1.61911e+006 * X \quad R^2 = 0.9998 \quad W: 1/X$$



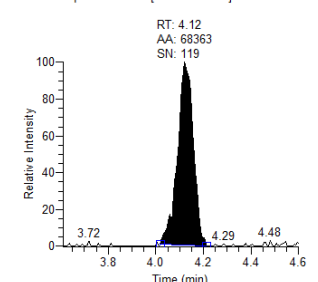
AO2\_EtOH\_50ppt\_Neg\_1 - Base Peak: m/z= 641.39 ...  
F: FTMS - p ESI SIM ms [638.89-643.89]



AO2\_EtOH\_50ppt\_Neg\_2 - Base Peak: m/z= 641.39 ...  
F: FTMS - p ESI SIM ms [638.89-643.89]



AO2\_EtOH\_50ppt\_Neg\_3 - Base Peak: m/z= 641.39 ...  
F: FTMS - p ESI SIM ms [638.89-643.89]



50 ppt  
(Triple Injections)

Full sensitivity in negative ion mode

# See What You're Missing with Charged Aerosol Detection

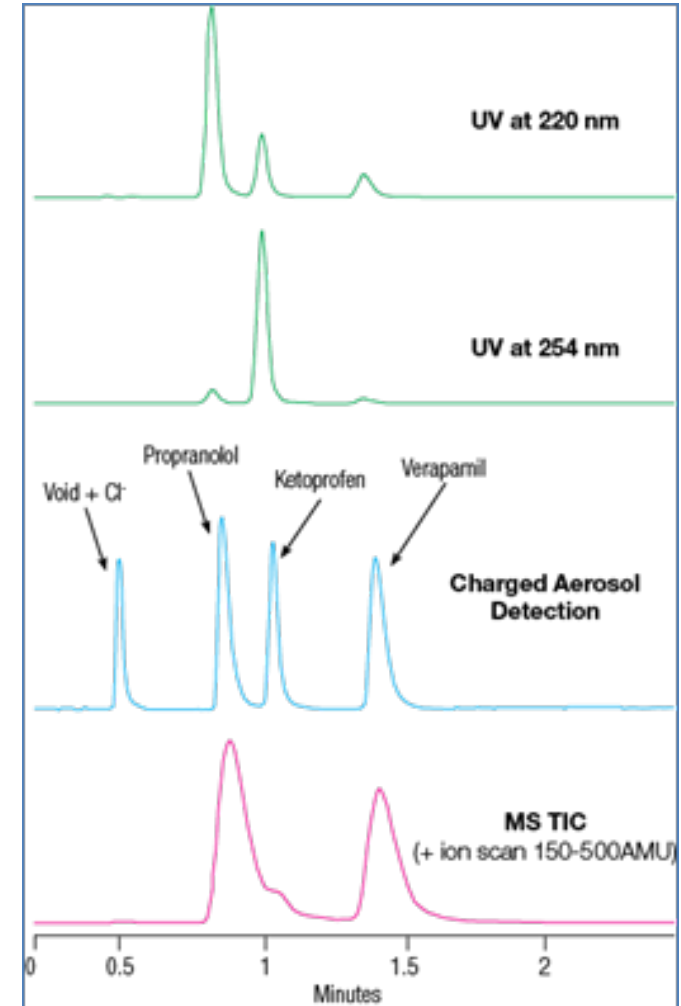


**Thermo Scientific™  
Vanquish™ Charged  
Aerosol Detector**



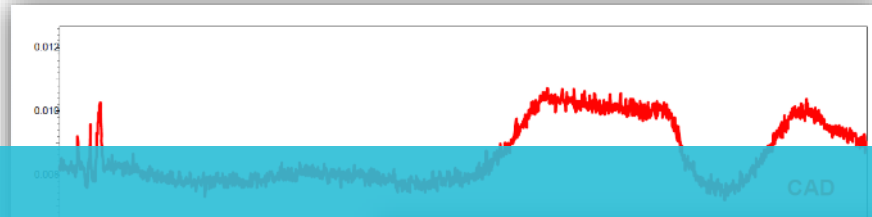
- Detect components without chromophore
- Quantify without exact standards
  - Relative quantification due to consistent response
  - Use virtually any standard for simplified AET calculations
- Consistent analyte response
- Four orders dynamic range
- USP <1663> listed

Comparison of Charged Aerosol  
Detection Result to UV and MS

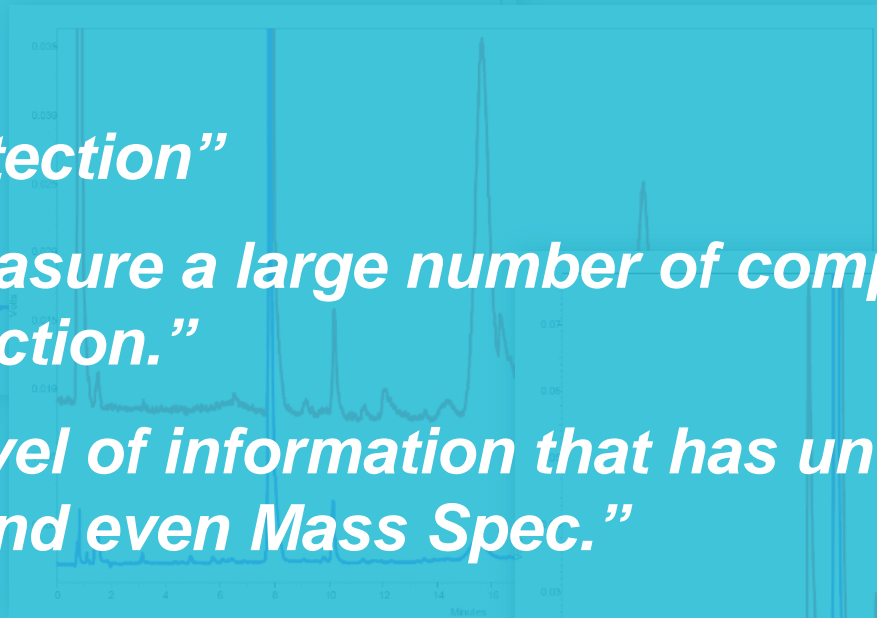


# CAD for Extractables and Leachables

IPA blank



Rubber



Butyl Rubber



- *“Virtually universal detection”*
- *“able to detect and measure a large number of compounds that were completely transparent to UV detection.”*
- *“CAD can provide a level of information that has until now been lacking with methods such as UV and even Mass Spec.”*

Data from ESA Biosciences, Inc., Chelmsford, MA



# Data Analysis Software, Database and Spectral Library for E&L Analysis



Thermo Scientific™ Compound Discoverer™ 2.1



Thermo Scientific™ TraceFinder™ Targeted Screening and Quan



Thermo Scientific™ Mass Frontier™ Spectral Interpretation software



mzCloud is a trademark of HighChem LLC, Slovakia



mzVault™ 2.0 Library Search and Manager



E&L Compound Database



## mzCloud™ Database: Free and cloud-based (www.mzcloud.org)

- Advanced high resolution mass spectral database
- Very high quality data: using standardized acquisition, highly curated data
- Identifying compounds, even when they are not present in the library, through substructure search

Server location : US

search for compounds... Search

Home About Features App Database Partners Contact

mzCloud is a state of the art mass spectral database that assists analysts in identifying compounds in areas such as life sciences, metabolomics, pharmaceutical research, toxicology, forensic investigations, environmental analysis, food control and various industrial applications. mzCloud™ features a freely searchable collection of high resolution/accurate mass spectra using a new third generation spectra correlation algorithm.

Online access to the database is free of charge and no registration is required.

[read more...](#)

Enter Database

New mzCloud App!

Search for Compounds by Name or ID

Search

7,384 (+90) compounds    11,507 (+98) trees    2,624,208 (+21,002) spectra    707,074 QM models    [view more statistics](#)

mzCloud is a trademark of HighChem LLC, Slovakia

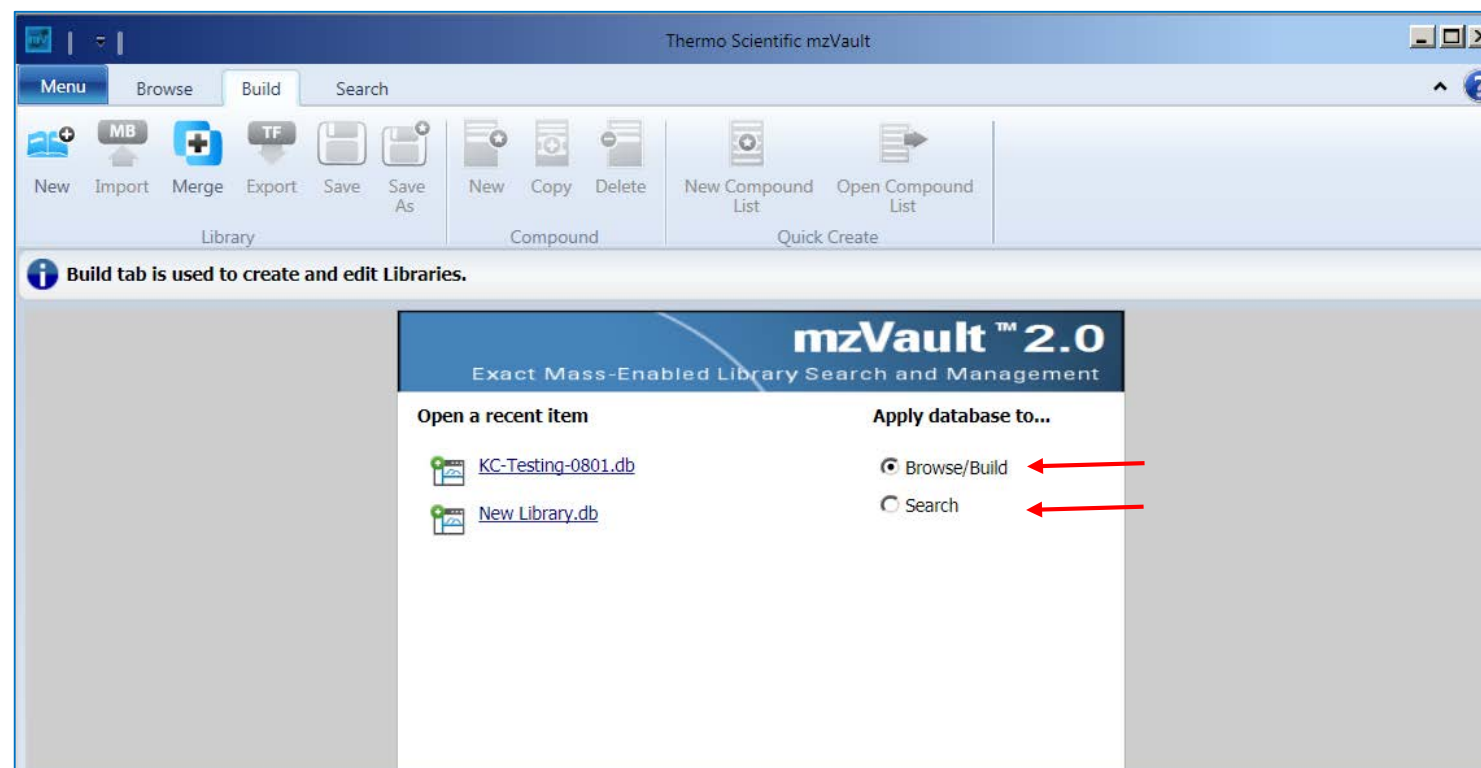
The screenshot displays the mzCloud Spectral Library interface. On the left, a navigation menu is visible with a red box around the 'Search' section, which includes options like 'Spectrum', 'Tree', 'Structure', 'Monoisotopic Mass', 'Peak', 'Precursor', and 'Name'. A callout bubble points to this menu with the text 'Search by different terms'. The main area shows a 'Reference Library' with search results for various compounds, including 'Irganox 1035' and 'Accelerator BBTS'. A callout bubble points to the search results with the text 'Metadata available for selected library entry'. The 'Spectral Tree' section shows a stack of spectra, with a callout bubble pointing to it and the text 'Spectral tree'. The 'Recalibrated Spectrum' section displays a mass spectrum with several peaks annotated with chemical structures and their m/z values (e.g., 57.06988, 133.06479, 203.14304, 219.17434, 231.13796, 665.38463). A callout bubble points to these annotations with the text 'Recalibrated spectra fragment ions annotation'. The 'Breakdown Curves' section shows multiple colored curves representing different fragmentation pathways, with a callout bubble pointing to them and the text 'Breakdown curves'. The 'Structure' section shows the chemical structure of the selected compound, C<sub>38</sub>H<sub>58</sub>O<sub>6</sub>S. At the bottom, a callout bubble points to the 'Metadata' and 'Quantum Chemical Annotations' sections with the text 'Permanent citable links for entry, tree, and spectra'.

mzCloud is a trademark of HighChem LLC, Slovakia



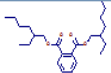
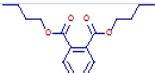
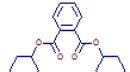
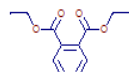
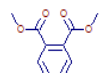
## Exact Mass-Enabled Library Search and Management

- Local mzCloud
- Creation of custom library
- Searching library



# E&L Compound Database in Thermo Scientific Compound Discoverer 2.1

This Excel sheet database contains ~2000 common E&L related compounds. This is a “living document” and new E&L related compounds are added periodically.

Commercial Name	Chemical Name	Class	CAS No.	Chemical Formula	Formula weight	[M-H] <sup>-</sup>	[M-H] <sup>-</sup>	M+NH <sub>4</sub> <sup>+</sup>	M+Na <sup>+</sup>	M+K <sup>+</sup>	Structure	mzCloud link
dioctyl phthalate	ethylhexylphthalate	PL	117-81-7	C <sub>24</sub> H <sub>38</sub> O <sub>4</sub>	390.27701	391.28429	389.26973	408.31083	413.26623	429.24017		<a href="https://mzcloud.org/DataViewer.aspx#CRReference2">https://mzcloud.org/DataViewer.aspx#CRReference2</a>
Dibutyl phthalate	Dibutyl phthalate	PL	84-74-2	C <sub>16</sub> H <sub>22</sub> O <sub>4</sub>	278.1518	278.15908	277.14452	296.18562	301.14102	317.11496		<a href="https://mzcloud.org/DataViewer.aspx#CRReference2">https://mzcloud.org/DataViewer.aspx#CRReference2</a>
	Dicyclohexyl phthalate		84-61-7	C <sub>20</sub> H <sub>26</sub> O <sub>4</sub>	330.18311	331.19039	329.17583	348.21693	353.17233	369.14627		<a href="https://mzcloud.org/DataViewer.aspx#CRReference2">https://mzcloud.org/DataViewer.aspx#CRReference2</a>
	Diethyl phthalate		84-66-2	C <sub>12</sub> H <sub>14</sub> O <sub>4</sub>	222.08921	223.09649	221.08193	240.12303	245.07843	261.05237		<a href="https://mzcloud.org/DataViewer.aspx#CRReference2">https://mzcloud.org/DataViewer.aspx#CRReference2</a>
	Dimethyl phthalate		131-11-3	C <sub>10</sub> H <sub>10</sub> O <sub>4</sub>	194.05791	195.06519	193.05063	212.09173	217.04713	233.02107		<a href="https://mzcloud.org/DataViewer.aspx#CRReference2">https://mzcloud.org/DataViewer.aspx#CRReference2</a>

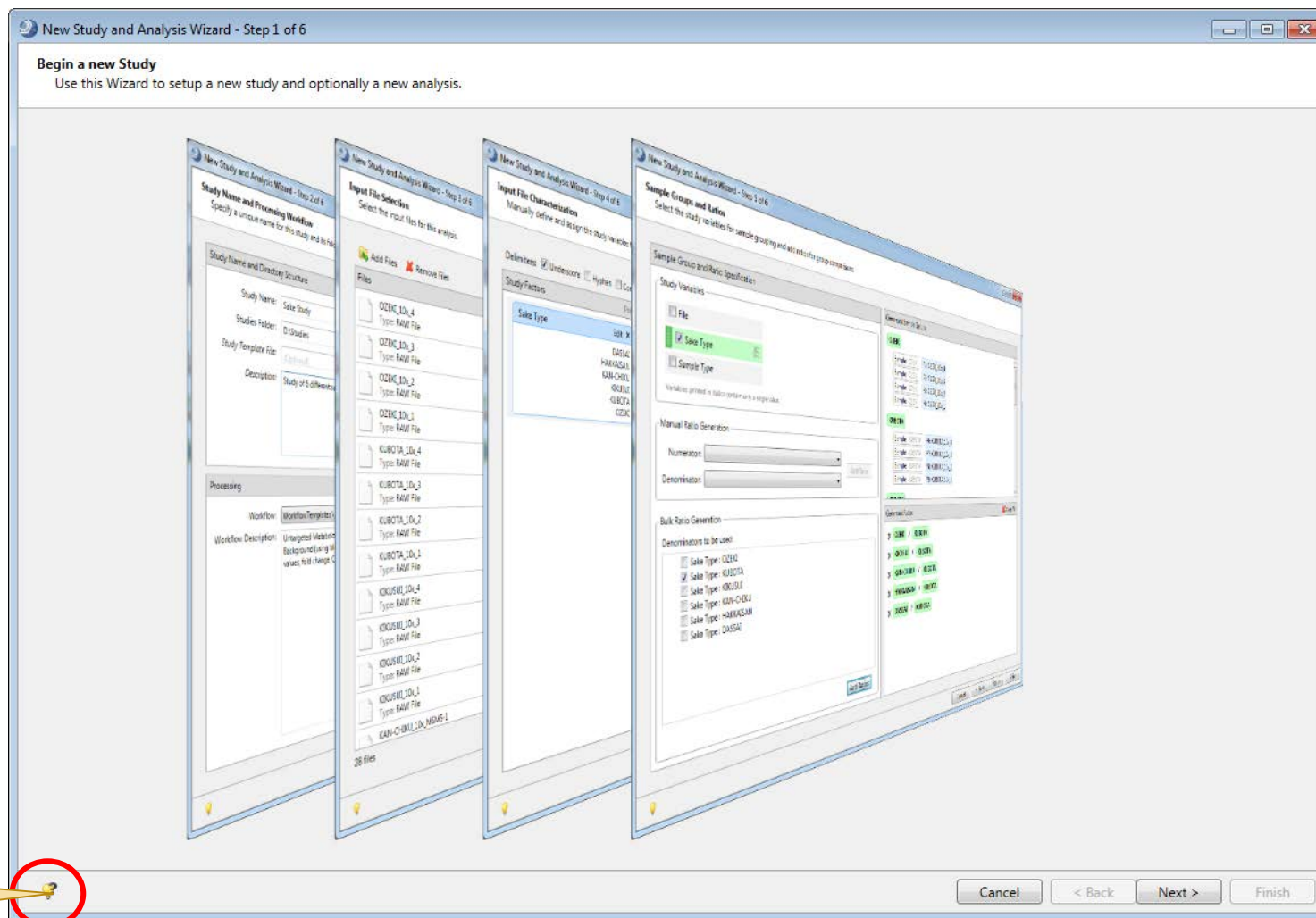
This database has been added to Compound Discoverer as “E&L Mass List”.

# Thermo Scientific Compound Discoverer 2.1: Compound ID and Structure Elucidation

- Compound Discoverer is a small molecule structure analysis software package.
  - It processes high HRAM data generated by Thermo Scientific™ Orbitrap™ MS (LCMS & GCMS)
- It uses flexible node-based processing workflow and HRAM data, isotope pattern matching, conduct component extraction and elemental composition prediction. The component structures are identified using the following techniques:
  - **Known compound ID** through multiple database searching and fragment spectral matching.
  - **Known unknown compound ID** - ChemSpider molecular formula and molecule weight search: using “Structure Proposals” feature to interrogate the fragmentation allows identification of the correct structure.
  - **Total unknown structure elucidation** - For components without database search results, the predicted compositions, MS/MS fragment ions, and similarity search result (mzCloud fragment ions matches) are used to propose putative structure. De Novo structure ID
  - **Validity check of the proposed structure** - Using “FISh Scoring” feature, searching the embedded “HighChem Fragmentation Library”. FISh stands for “Fragment Ion Search”
- Differential analysis for different lots, batch, or type of sample analyses



# Thermo Scientific Compound Discoverer 2.1: Wizard for Processing Workflow Build



Description  
for each step

Creating a study and analysis using the guided “New Study and Analysis Wizard” and built-in workflow templates.

# Node-Based Processing Workflow

The screenshot displays the Compound Discoverer 2.1.0.398 interface. The main window shows a workflow titled "Pharma Label IPA-Extract-one" with a description: "Untargeted E&L workflow without statistics: Find and identify unknowns-Performs retention time alignment, unknown compound detection, and compound grouping across all samples. Predicts elemental compositions for all compounds, and hides chemical background (using Blank samples). Identifies compounds using mzCloud".

The interface is divided into several sections:

- Workflow Nodes:** A list of nodes on the left side, categorized into six main groups:
  1. Input / Output: Export Spectra, Input Files
  2. Data Processing: Align Retention Times, Filter By Mass Defect, Filter By Scan Event, Filter Centroids, Select Spectra
  3. Tracer: Create Analog Trace, Create FISH Trace, Create Mass Trace, Create Pattern Trace
  4. Expected Compounds: FISH Scoring, Find Expected Compounds, Generate Expected Compounds, Group Expected Compounds, Mark Background Compounds
  5. Unknown Compounds: Compound Class Scoring, Detect Unknown Compounds, Fill Gaps, Group Unknown Compounds, Map to BioCyc Pathways (beta), Map to KEGG Pathways, Mark Background Compounds, Normalize Areas, Pattern Scoring, Predict Compositions, Search ChemSpider, Search Mass Lists, Search mzCloud, Search mzVault
  6. Comparison: Merge Features
- Workflow Tree:** A central diagram showing the flow of the workflow. The nodes are:
  - Input Files (Start)
  - Parallel branches: Create Analog Trace, Select Spectra, Create Analog Trace
  - Align Retention Times
  - Parallel branches: Detect Unknown Compounds, Create Mass Trace, Create Mass Trace
  - Group Unknown Compounds
  - Parallel branches: Search Mass Lists, Search mzCloud, Search ChemSpider, Predict Compositions, Mark Background Compounds
  - Merge Features (intermediate node)
- Post-Processing Nodes:** Assign Compound Annotations

Red circles highlight the "Study Definition" tab and the "Workflow Tree" section in the image.



# Result View – Data Interpretation

The screenshot displays the Compound Discoverer 2.1.0.398 interface. The top window shows a chromatogram with a peak at 7.618 minutes. The right window shows a mass spectrum with a base peak at m/z 391.22949. The bottom window shows a table of compounds with columns for Name, Formula, Annotation Sc, FISH Coverage, Molecular Weight, RT [min], Area, # ChemSpider Re, # mzCloud F, mzCloud Best Mat, Mass List, and mzCloud. A red arrow points to the 'Hide Related Tables' button in the bottom left corner.

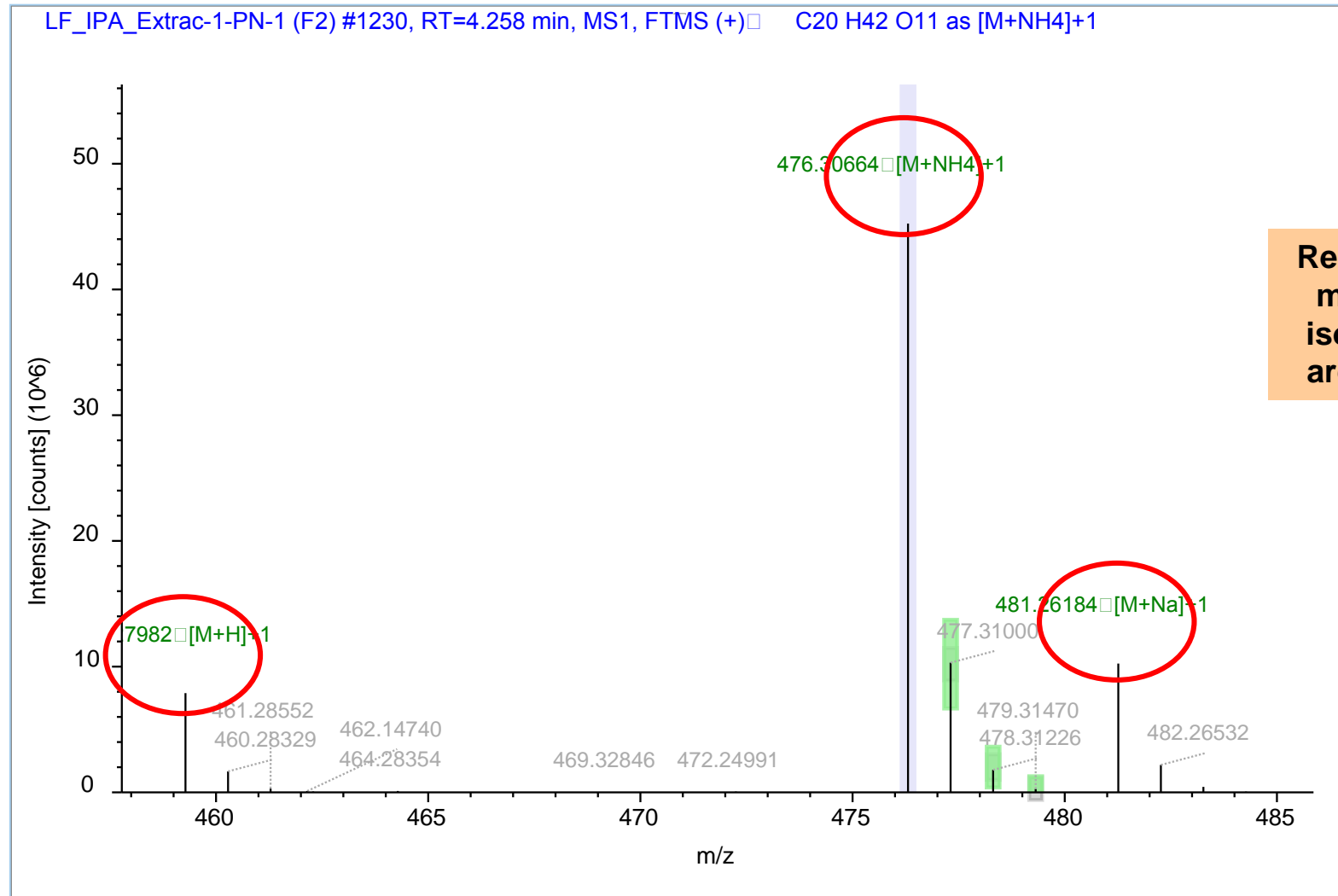
Checked	Name	Formula	Annotation Sc	FISH Coverage	Molecular Weight	RT [min]	Area (Ma	# ChemSpider Re	# mzCloud F	mzCloud Best Mat	Mass List	mzCloud
<input type="checkbox"/>	Oleamide	C18 H35 N O	■■■		264.24510	17.335	146255525	112	4	98.5		
<input type="checkbox"/>	Melamine	C3 H6 N6	■■■		126.06560	0.472	106680600	7	5	100.0		
<input checked="" type="checkbox"/>	Hexamethoxymethyl melamine	C15 H30 N6 O6	■■■		390.22225	7.621	106255412	3	3	98.7		
<input type="checkbox"/>	Eicosapentaenoic acid	C20 H30 O2	■■■		302.22429	16.490	96918439	710	10			
<input type="checkbox"/>	6-Propyl-2-naphthol	C13 H14 O	■■■		186.10445	9.903	89008975	397	12			
<input type="checkbox"/>	Methamphetamine	C10 H15 N	■■■		149.12048	1.070	87923353	297	4	93.7		
<input type="checkbox"/>	pro-ser-arg	C14 H26 N6 O5	■■■		358.19619	7.621	82384299	4	6			

Checked	Molecular Weight	RT [min]	FWHM [min]	Max. # MI	# Adducts	Area	Study File ID
<input type="checkbox"/>	390.22219	7.619	0.045	4	2	106255412	F6
<input type="checkbox"/>	390.22232	7.624	0.048	4	2	98027607	F3

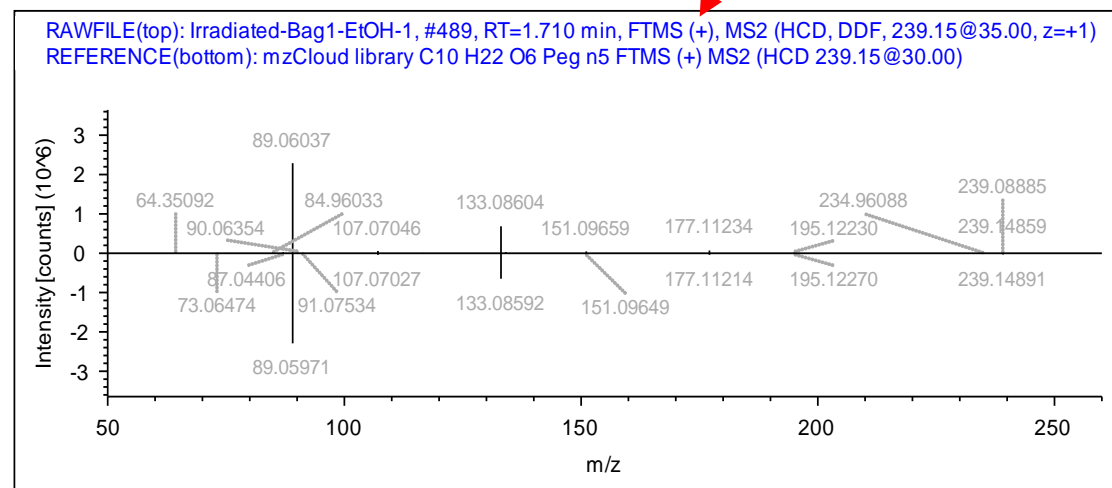
Sub-tables

# Component Detection with Adducts Grouping



# Known Compound ID Through mzCloud™ Database Search

#	Checked	mzCloud ID	Formula	Structure	Molecular Weight	Best Match	Name
1	<input checked="" type="checkbox"/>	1819	C10 H22 O6		238.14164	99.9	Peg n5
2	<input checked="" type="checkbox"/>	22	C16 H22 O4		278.15181	99.9	Dibutyl phthalate
3	<input checked="" type="checkbox"/>	2033	C16 H22 O4		278.15181	99.9	Diisobutylphthalate
4	<input checked="" type="checkbox"/>	20	C24 H38 O4		390.27701	99.9	Bis(2-ethylhexyl) phthalate
5	<input checked="" type="checkbox"/>	2688	C9 H21 N O3		191.15214	99.0	Trisopropanolamine
6	<input checked="" type="checkbox"/>		C24 H38 O4		390.27701	98.5	Dioctyl phthalate



mzCloud™ Mirror plot

mzCloud is a trademark of HighChem LLC, Slovakia

# Unknown Structure Elucidation Using Compound Annotation Editor and FISh Scoring

The screenshot displays the Compound Discoverer 2.0.0.261 interface. The main window shows a mass spectrum plot with intensity (counts) on the y-axis (0 to 2.5 x 10<sup>6</sup>) and m/z on the x-axis (50 to 400). A prominent peak is labeled at m/z 32.100. The mass spectrum is annotated with various fragment ions, including C4 H9 [M-e]+1, C6 H13 O [M-e]+1, C6 H16 O5 P [M-e]+1, and C12 H28 O6 P [M-e]+1. A yellow callout box labeled "Fragment ions auto annotation" points to these annotations.

In the center, a "Custom Explanation Editor" window is open, showing a chemical structure of a phosphonate ester. Below the structure, the "FISh Scoring" tab is active, with the following settings:

- Apply FISh scoring
- Annotate full spectrum tree
- Use fragmentation libraries
- Use libraries for full spectrum tree
- High accuracy mass tolerance: 10 ppm
- Low accuracy mass tolerance: 400 mmu
- S/N threshold: 10

At the bottom of the editor, "Save" and "Cancel" buttons are visible.

Below the mass spectrum, a table of "Selected Traces" is shown:

Change	RT [min]	FWHM [min]	Best SFit [%]	Max. # MI	# Adducts	Area	Study File ID	FISh Coverage
	32.115		45	4	4	40802637	F56	76.92

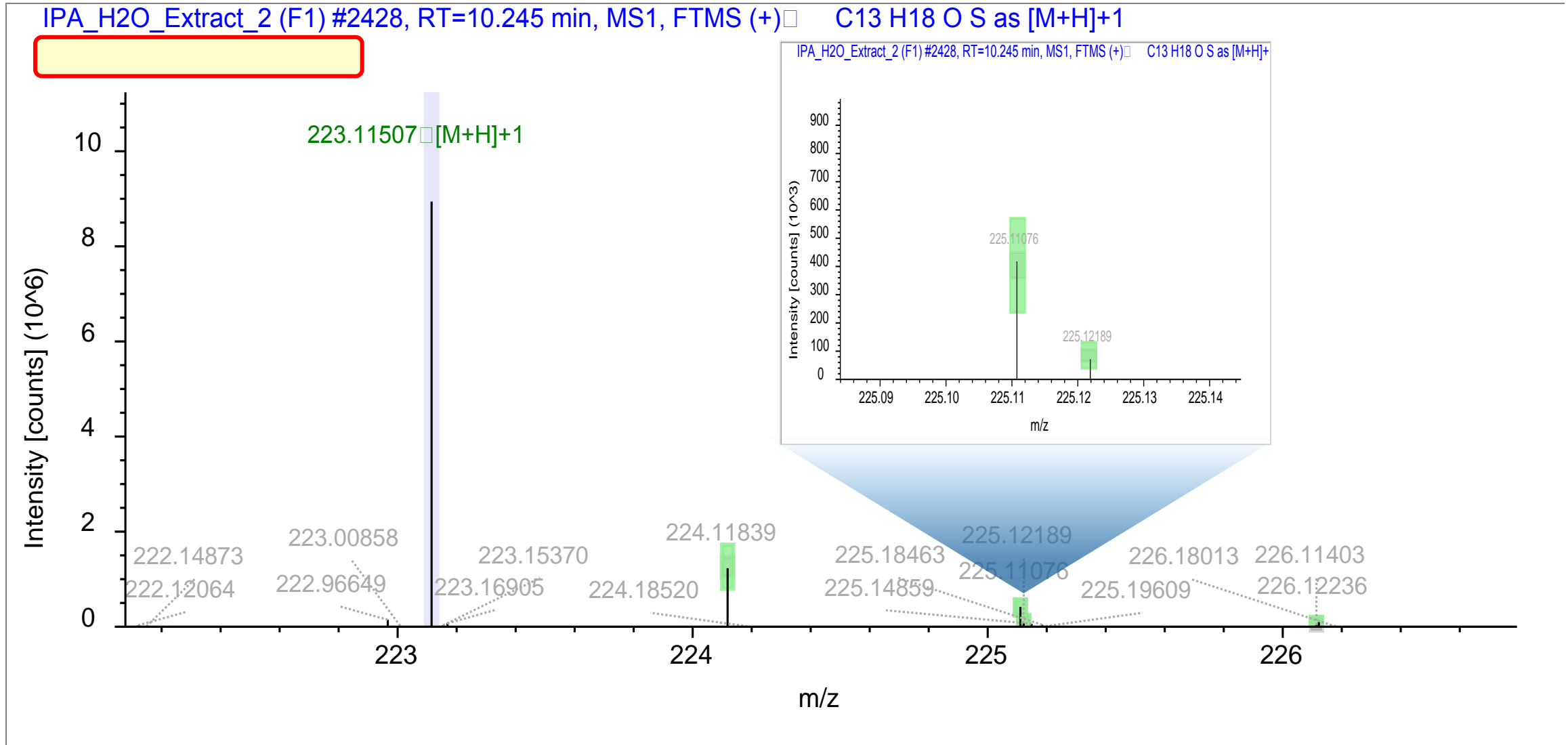
A yellow callout box labeled "Custom Explanation" points to this table.

At the bottom of the interface, a table of "FISh Coverage" is shown:

FISh Coverage	Study File ID
91.67	F56
70.00	F56
66.67	F56
75.00	F56

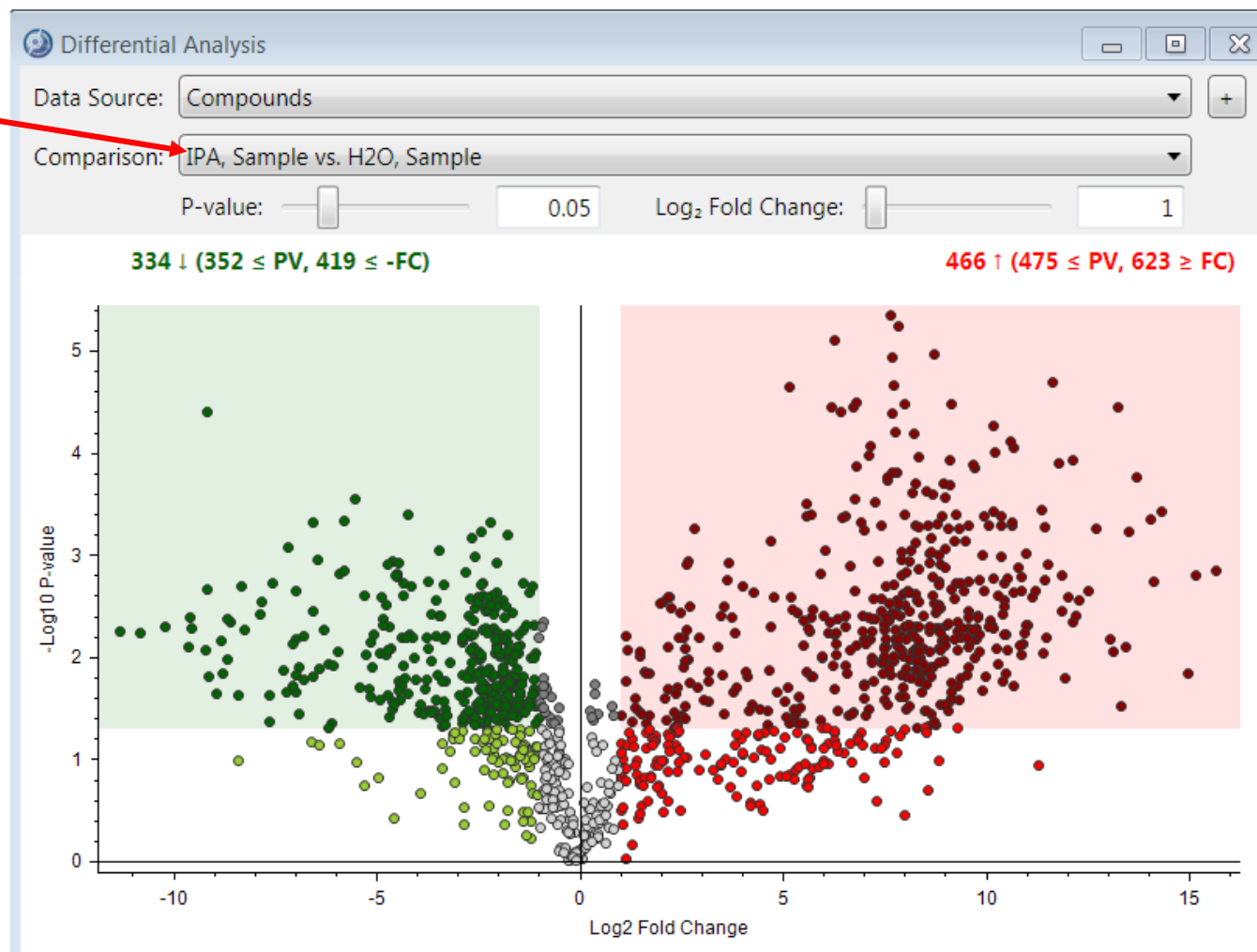
A yellow callout box labeled "Peak Consolidation" points to this table.

# Unknown Structure Elucidation Starting from CD 2.1 "Predicted Compositions"



# Thermo Fisher Compound Discoverer 2.1 Differential Analysis Feature: Volcano Plot

Using the interactive volcano plot to find compounds that are significantly different between two sample groups



# Thermo Scientific Compound Discoverer (CD) Home Page

<http://mycompounddiscoverer.com>

**Compound Discoverer**  
Integrated solutions for small molecule structure identification

thermo scientific

HOME WHAT IS COMPOUND DISCOVERER? HELP BUTTON REQUEST FEATURE... RESOURCES TUTORIALS

## Compound Discoverer 2.1 Released! Get your Demo here.

JUL 31 Posted by [Tim Stratton](#)

**For current Compound Discoverer 2.0 users:**  
The electronic upgrade to Compound Discoverer 2.1 is free! Follow the download instructions below and use the instructions for the CD 2.0 to CD 2.1 upgrade.

**For new users:**  
To download the Compound Discoverer 2.1 Demo (CD 2.1 demo), go to the Thermo Scientific Software Portal (Flexera) and download it from the "Compound Discoverer 2.1 Demo" folder.  
[CLICK HERE FOR DETAILS.](#)

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Tags: [Information](#) Comments Off

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## Compound Discoverer at ASMS 2017

APR 14 Posted by [Tim Stratton](#)

Thanks to everyone who was able to join us at this years Compound Discoverer Users Meeting and parallel Node Developer Workshop at ASMS this year!

We've already heard great feedback from several people and, because of that, we plan to make these meetings a regular occurrence and improve them even more in the future.

Download a DEMO copy, and watch the tutorials videos here.

## Join the Fun! *Cache a Chromeleon* Game

- Use your mobile device to complete challenges and earn a Charlie Chromeleon plush toy!
- If you are playing, you have earned points for attending this seminar. Be sure to scan the barcode on the desk outside the door.
- Ask booth staff for more details on how to play.





Thank You

Please join me in the  
**Mass Spectrometry**  
section of our booth where I'll  
address additional comments and questions.