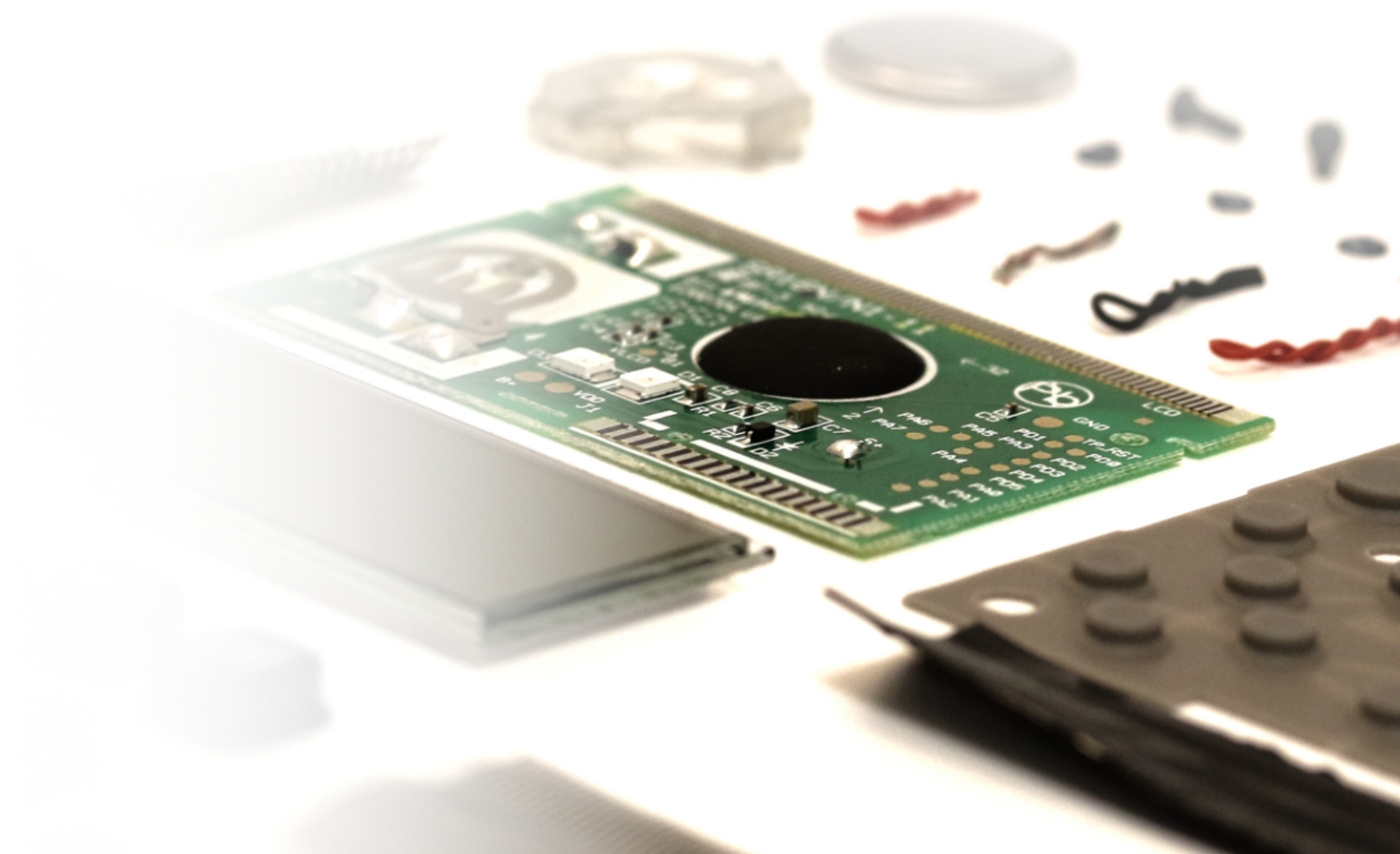


Webinar - Materials Matching

Laboratory equipment and Ai

Presented by:
Bruce Calder
VP Consulting

August 26 2026



Situations

This material is **not working** the way it **used to**

I have a **new supplier** of a material. **Is it the same** as the current material?

Why is my **competitor's** material working **differently** than mine?

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Overview - Agenda

- New Claigan Services
- Situations
- TD-MS
- Time Slicer program
- Ai
- Examples
- Q&A



Claigan Services LCA



LIFE CYCLE ASSESSMENT (LCA) SERVICES

Measuring Your Product's True Environmental Footprint

As the demand for transparent, quantifiable environmental data surges, understanding the precise carbon footprint of your products is no longer optional. Claigan's comprehensive Life Cycle Assessment (LCA) services break down the complexities of measuring emissions so you can make informed, sustainable design decisions and maintain global compliance.

WHAT IS A LIFE CYCLE ASSESSMENT?

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We examine every critical stage, including:

- Raw material extraction and refinement.
- Complex product manufacturing.
- Distribution and transportation networks.
- Product use, maintenance, and end-of-life disposal.

UNDERSTANDING THE CO2 EMISSIONS ASSOCIATED WITH YOUR PRODUCT GIVES YOU A MEASURABLE VIEW OF ITS ENVIRONMENTAL IMPACT.

UNDERSTANDING YOUR GHG EMISSIONS PROFILE

To effectively measure environmental impact, companies must categorize their Greenhouse Gas (GHG) footprint into specific scopes.

Scope 1: direct emissions generated by the company, (i.e. combustion by company-owned vehicles or escaped refrigerants).

Scope 2: indirect emissions stemming from energy purchased by the company.

Scope 3: indirect emissions across a company's full value chain, covering the full lifecycle of your products and contributing factors like employee travel.

CLAIGAN'S EXPERT LCA METHODOLOGY

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GET IN TOUCH



- Claigan LCA services
 - GHG
 - LCA
 - EPD
- **We are really good at these :-)**

- [For more information](#)

Claigan Services

Packaging EPR Reporting



US Packaging EPR Data Generation

Are you compliant with California and Oregon's passed deadlines?

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- Lots of deadlines
 - Especially in the US
 - California
 - Oregon
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Solution

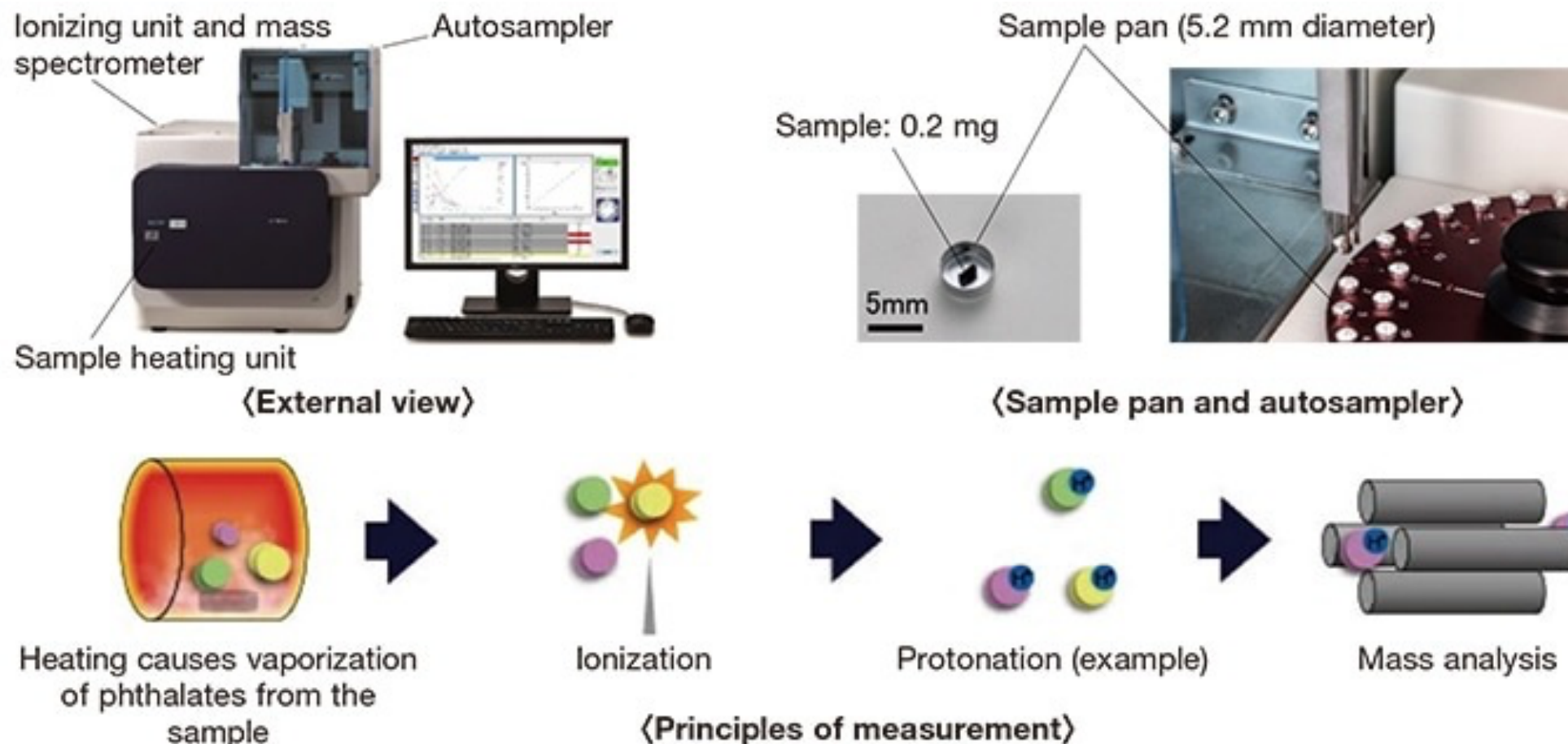
- **Claigan ‘Time Slicer’ Program**
- **Full Range Mass Spectroscopy**
 - Over 16 different temperate / time conditions
 - >300,000 data points per measurement
- **Combined with the ‘magic’ of Ai.**

Historical Issue

- **Large mass spectroscopy data sets**
 - Too big for humans
 - Even with specialized knowledge
- **Ai has no problem with huge data sets**
 - Especially if looking for **differences** in data sets
 - Ie. **Material Matching**

Thermal Desorption Mass Spectrometry (TD-MS)

- **HMI 000A**



- Gives you
 - Mass spectroscopy (weights of ions)
 - At different temperatures
 - **Without** complicated solvents

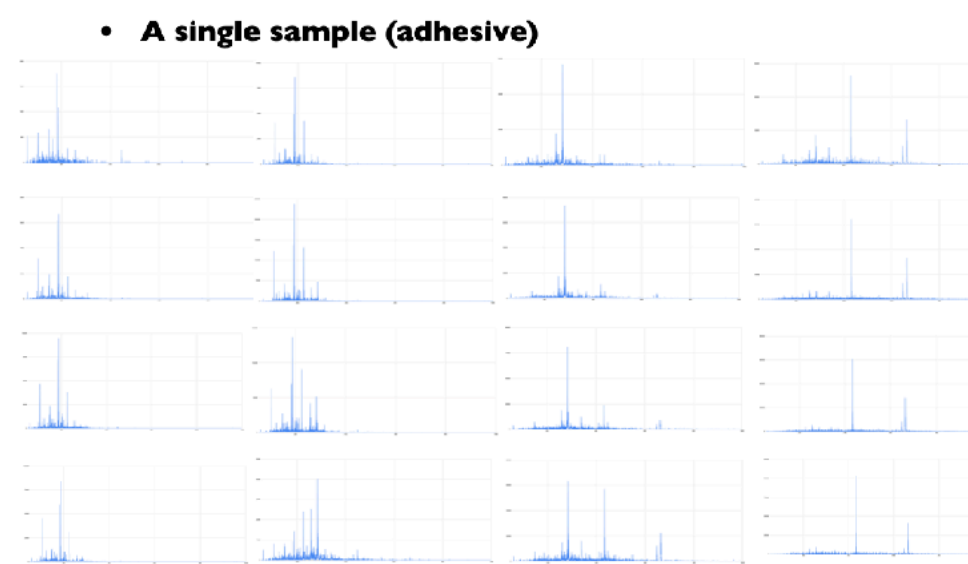
Claigan Time Slicer Data Set

- **A single sample (adhesive)**



Claigan Time Slicer Data Set

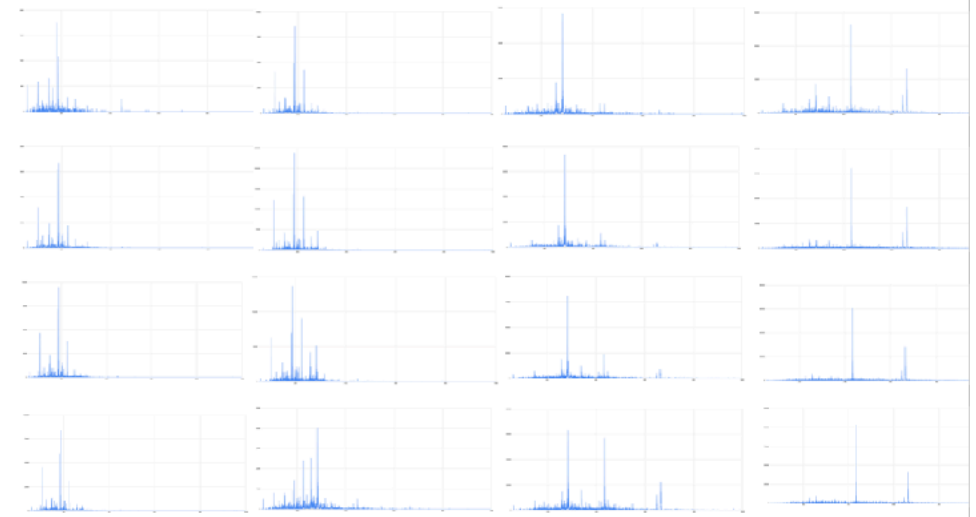
- **Processing**
- **Too much for humans**
 - w/o a lot of time and cost
- **How about library matching?**
 - Still way too much data and too many degradation products
 - Slow, uncertain, expensive, and high skill scientists
 - And very hard to explain to ‘normal people’



Claigan Time Slicer Data Set

- **Ai** is great with large data sets
 - Especially for comparisons

• A single sample (adhesive)



- **Ai**
 - Excels at differences in large data sets
 - Fast
 - Much more approachable answers for ‘normal people’
- **Cutting edge**
 - None of this was possible a year ago

Examples

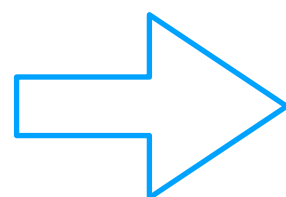
- **This sounds cool, but really?**
- Time for **Examples**

Examples

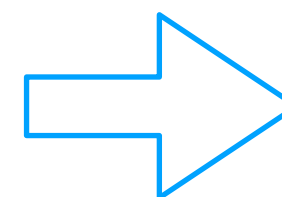
- **Ai**
 - Gemini Pro
 - *However, most advanced Ai can perform the job*
- Samples
 - Interlab standard for phosphated flame retardants
 - Polyimide tube under different process conditions

Materials Matching Process

Submit
Question into
AI



Review output

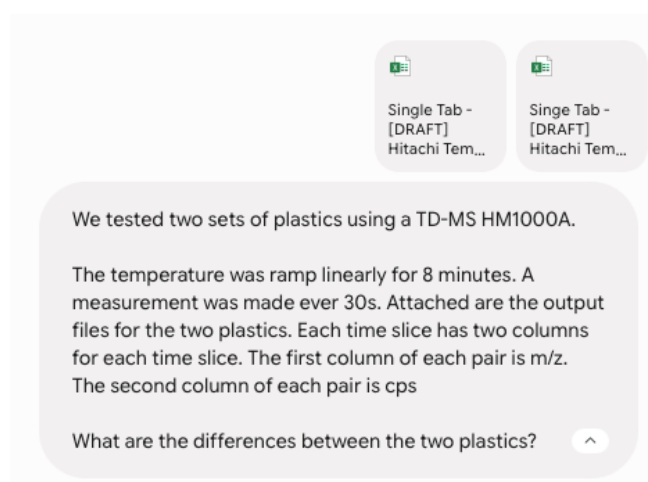


Actions

- Two - Single tab raw data files
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 - *Identify likely chemicals from data provided*
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 - *Deep dives*

- **Expert**
 - Review actual data
 - Ai will tell you **exactly** what to look at
 - *Feedback to material owner*



First Example

Interlaboratory Sample

- **Simple control samples**
 - Two (2) inter laboratory samples
 - With different low levels of phosphated flame retardants



- **Should** be a very simple example of materials matching

First Example

Interlaboratory Sample

- Testing completed
- Files and question below submitted into Ai



Single Tab -
[DRAFT]
Hitachi Tem...



Singe Tab -
[DRAFT]
Hitachi Tem...

We tested two sets of plastics using a TD-MS HM1000A.

The temperature was ramp linearly for 8 minutes. A measurement was made every 30s. Attached are the output files for the two plastics. Each time slice has two columns for each time slice. The first column of each pair is m/z. The second column of each pair is cps

What are the differences between the two plastics?



First Example

Interlaboratory Sample

- Answer to starting question

	Sample 1	Sample 2
Dominant m/z Peaks	279, 167, 392, 280	548, 547, 305, 436
Likely Additive Class	Standard Phthalate (e.g. DEHP)	Alternative Plasticizer (e.g. TOTM)
Outgassing Onset	~150 seconds	~210 seconds
Peak Signal Intensity	~50,000,000 cps	~36,000,000 cps
Plateau Time	~330 seconds	~390 seconds

Surprise!

Not so simple...

e.g. is not good enough

First Example

Interlaboratory Sample

- Refining generalities

can you be more specific on the chemical differences instead of (e.g.)?

Chemical Identification

- Plastic 1 (Restricted Plasticizer):** The primary chemical in the first file is **Bis(2-ethylhexyl) phthalate**, universally known as **DEHP**.
- Plastic 2 (Compliant Alternative):** The primary chemical in the second file is **Trioctyl trimellitate**, commonly known as **TOTM**.

Chemical identification

Science / details

Mass Spectrometry Evidence

- DEHP Fragmentation (Plastic 1):** DEHP has a molecular weight of 390.5 g/mol, which shows up as the protonated molecular ion at **m/z 391** (and its isotope at 392). When the molecule fragments in the mass spectrometer, it loses its eight-carbon side chains (octene, mass 112). Losing one side chain creates the massive dominant peak at **m/z 279**. Losing both side chains leaves protonated phthalic acid at **m/z 167**.
- TOTM Fragmentation (Plastic 2):** TOTM has a heavier molecular weight of 546.8 g/mol, appearing as the primary protonated ion at **m/z 547** (and its isotope at 548). Similar to DEHP, it also breaks apart by losing octene side chains. A single loss yields the peak at **m/z 435**, and a double loss yields **m/z 323**. A subsequent loss of a water molecule from that structure produces the highly prominent **m/z 305** peak.

First Example

Interlaboratory Sample

- Deep dive

can you review for phosphated flame retardants?

Both datasets contain substantial signal intensities at m/z 327, which is the primary protonated ion $[M + H]^+$ for Triphenyl phosphate (TPHP or TPP), a very widely used non-halogenated organophosphate flame retardant.

Chemical identification

Science / details

Here is the supporting chemical evidence for this identification:

- **Molecular Mass:** TPHP has a molecular formula of $C_{18}H_{15}O_4P$ and a molar mass of 326.28 g/mol, yielding a strong positive ion peak at m/z 327.
- **Isotopic Confirmation:** In both plastics, the m/z 327 peak is accompanied by an m/z 328 peak that is roughly 26% to 28% of the primary peak's intensity. This perfectly aligns with the expected natural abundance of Carbon-13 for an 18-carbon molecule, heavily supporting the presence of TPHP.

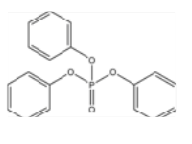
But still need details

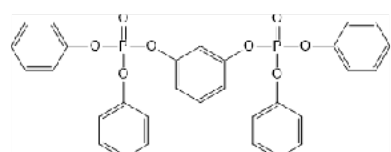
First Example

Interlaboratory Sample

- Refining generalities

Are there any other phosphated flame retardant differences between the two samples?

Additive	Plastic 1 (Restricted)	Plastic 2 (Compliant)
 Triphenyl phosphate (TPHP)	Present (High Concentration)	Present (Lower Concentration)
TDCPP (Chlorinated OPFR)	Present	Absent
RDP (Non-Halogenated OPFR)	Absent	Present



‘Trick substance for interlab’
Dimer (double) of TPP

Science / details

Could create **false positives**

Chemical identification

1. Presence of a Chlorinated Flame Retardant in Plastic 1

In addition to TPHP, Plastic 1 (the DEHP formulation) contains Tris(1,3-dichloro-2-propyl) phosphate (TDCPP).

- Mass Spec Signature:** TDCPP is characterized by significant peaks at m/z 431 and m/z 433 (due to the presence of chlorine isotopes).
- Data Comparison:** Plastic 1 shows massive accumulated counts for m/z 431 (over 7.6 million cps), starting its outgassing precisely at the 180-second mark alongside the DEHP.
- Plastic 2 Status:** Plastic 2 is virtually free of this compound, registering only trace background noise for these specific m/z values. This is an important distinction, as TDCPP is highly scrutinized and frequently regulated due to toxicity concerns.

2. Presence of a Heavy Non-Halogenated Flame Retardant in Plastic 2

Conversely, Plastic 2 (the TOTM formulation) compensates for the lack of TDCPP by utilizing a heavier, non-halogenated alternative: Resorcinol bis(diphenyl phosphate) (RDP).

- Mass Spec Signature:** RDP is a large oligomeric flame retardant with a primary characteristic fragment at m/z 575.
- Data Comparison:** Plastic 2 shows significant accumulation of the m/z 575 ion (over 1.5 million cps). Because it is a heavy molecule, it requires more thermal energy to volatilize; the outgassing for RDP in your 8-minute ramp does not begin until the 180–210 second window and doesn't peak until the very end of the test (450–480 seconds).
- Plastic 1 Status:** Plastic 1 registers zero significant counts for RDP.

Not as simple example as originally thought!!!

Second Example

Interlaboratory Sample

- **Polyimide tubes**
 - Two (2) process variations



- **Should** also be a very simple example of materials matching

Second Example

Polyimide Tubes

- Testing completed
- Files and question below submitted into Ai

 Single Tab -
[DRAFT]
Hitachi Tem...

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We tested two polyimide tubes using a TD-MS HM1000A.

The temperature was ramp linearly for 8 minutes. A measurement was made every 30s. Attached are the output files for the two plastics. Each time slice has two columns for each time slice. The first column of each pair is m/z. The second column of each pair is cps

What are the differences between the two tubes? ^

First Example

Interlaboratory Sample

- Answer to starting question

3. Key Compound/Mass (m/z) Differences

When breaking down the data by specific mass-to-charge ratios (m/z), a few key signatures drive the differences between the two tubes:

- **$m/z \sim 100$ Group (e.g., 99.8 - 100.4):** Process A emits drastically more of these fragments. Between minutes 6 and 8, Process A's emissions for this mass group skyrocket to roughly 27,500 CPS, while Process B remains much more subdued (peaking around 14,500 CPS). Hitachi Temp and Time Slicer - Polyimide Tube - Process A.xlsx", "Single Tab - [DRAFT] Hitachi Temp and Time Slicer - Polyimide Tube - Process B.xlsx"]
- **$m/z \sim 113.7$ Group:** Process A shows significant, erratic emission spikes for this fragment at higher temperatures (especially in Slices 10, 14, and 16). Process B keeps this fragment largely suppressed. Hitachi Temp and Time Slicer - Polyimide Tube - Process A.xlsx", "Single Tab - [DRAFT] Hitachi Temp and Time Slicer - Polyimide Tube - Process B.xlsx"]
- **$m/z \sim 59$ Group:** Both tubes show high outgassing for $m/z \sim 59$, but their timing differs. Process B actually experiences a sharp early emission spike for this mass range around the 90–120 second mark (Slice 4) which is not mirrored as intensely by Process A. Hitachi Temp and Time Slicer - Polyimide Tube - Process A.xlsx", "Single Tab - [DRAFT] Hitachi Temp and Time Slicer - Polyimide Tube - Process B.xlsx"]

A good start

But still too general

First Example

Interlaboratory Sample

- Refining generalities

what do you think the substances at 100 m/ and 114 m/z are?

m/z ~100: N-Methyl-2-pyrrolidone (NMP)

- What it is:** NMP is one of the most ubiquitous and essential solvents used in the synthesis of polyimides.
- Why it fits:** NMP has a molecular weight of 99.13 g/mol. In mass spectrometry, it frequently appears as a molecular ion at m/z 99, or as a protonated ion at m/z 100 depending on how the molecules are ionized in the instrument.

m/z ~114: N-Ethyl-2-pyrrolidone (NEP)

- What it is:** NEP is a chemical cousin to NMP. It is frequently used as a drop-in replacement, co-solvent, or additive in polymer processing—especially as manufacturers seek alternatives to NMP for regulatory and environmental reasons.
- Why it fits:** NEP has a molecular weight of 113.16 g/mol, which aligns perfectly with the m/z 113.7 signature found in your data.

Chemical identification

Science / details

First Example

Interlaboratory Sample

- Deep dive

can you summarize the differences?

Total Outgassing Volume

- **Process A:** Exhibits significantly higher total outgassing throughout the heating cycle (~584,000 total counts).
- **Process B:** Is much cleaner overall, releasing roughly 28% fewer volatile compounds (~422,000 total counts).

High-Temperature Stability

- **Process A:** Degrades or releases heavily trapped volatiles as temperatures peak (minutes 6 to 8 of the test), with emissions spiking over 100,000 CPS.
- **Process B:** Demonstrates superior thermal stability at higher temperatures, with peak emissions reaching only about half of Process A's maximum.

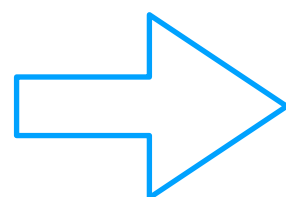
Residual Solvent Content

- **Process A:** Retains high levels of heavy molecular fragments, strongly pointing to trapped manufacturing solvents. Specifically, it shows massive spikes for $m/z \sim 100$ (likely N-Methyl-2-pyrrolidone or NMP) and $m/z \sim 113.7$ (likely N-Ethyl-2-pyrrolidone or NEP).
- **Process B:** Effectively minimizes these heavy solvent residuals, suggesting a much more thorough curing, drying, or washing process.

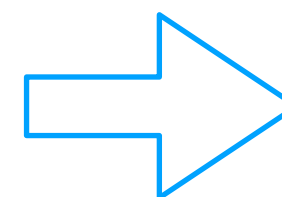
Great for analysis of
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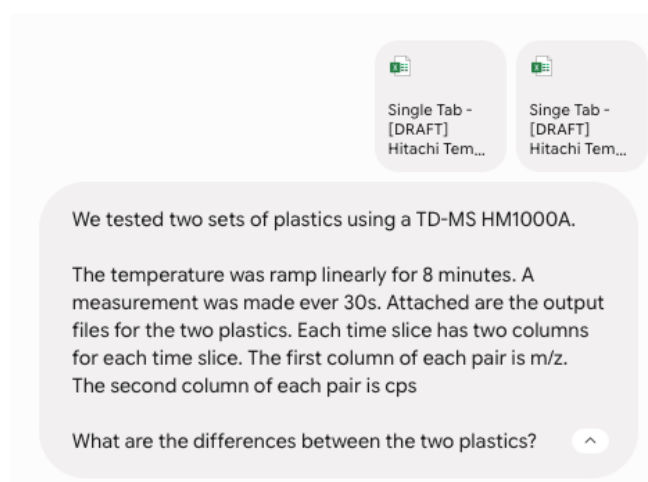


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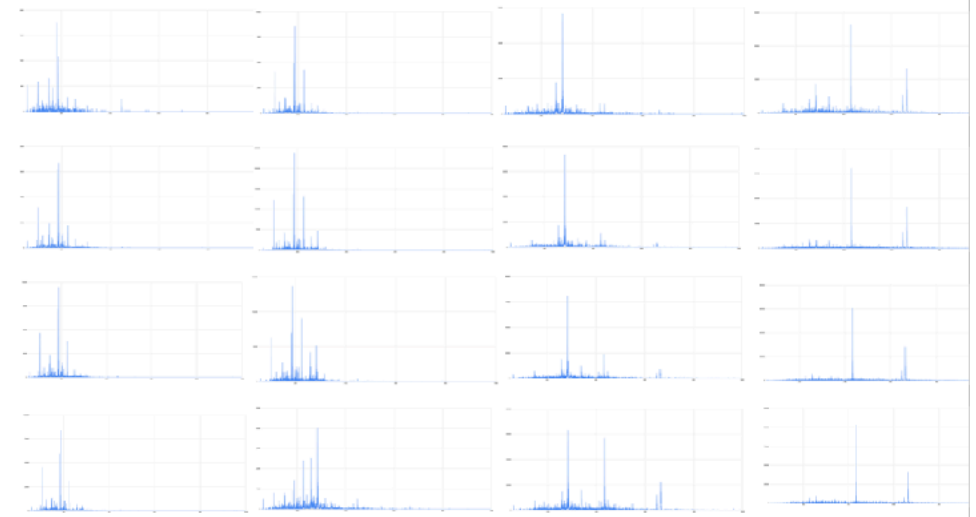
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Q&A