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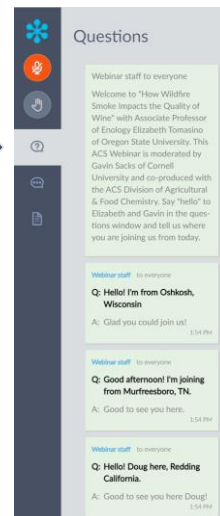
Questions or Comments?

Type them into the questions box!



"Why am I muted?"

Don't worry. Everyone is muted except the Presenter and the Host. Thank you and enjoy the show.



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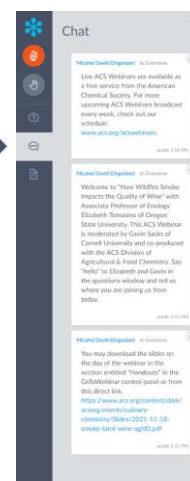
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Chat
Announcements and hyperlinks from our team



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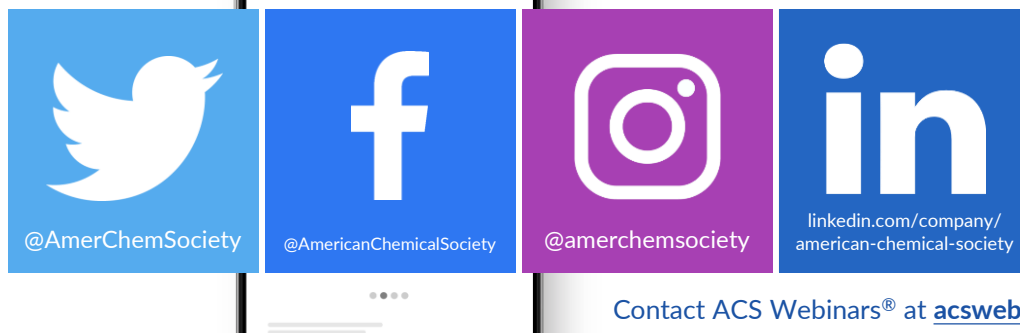


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A Career Planning Tool For Chemical Scientists



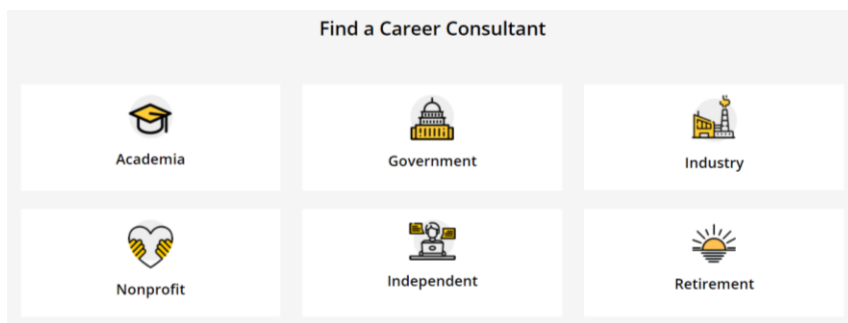
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<https://chemidp.acs.org>

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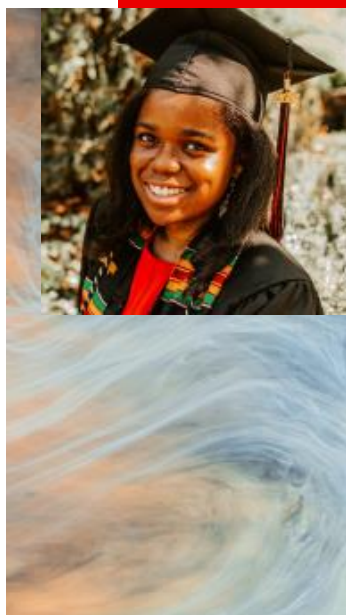
Email us at bridge@acs.org

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ACS Scholar Adunoluwa Obisesan

BS, Massachusetts Institute of Technology, June 2021
(Chemical-biological Engineering, Computer Science & Molecular Biology)



“The ACS Scholars Program provided me with monetary support as well as a valuable network of peers and mentors who have transformed my life and will help me in my future endeavors. The program enabled me to achieve more than I could have ever dreamed. Thank you so much!”

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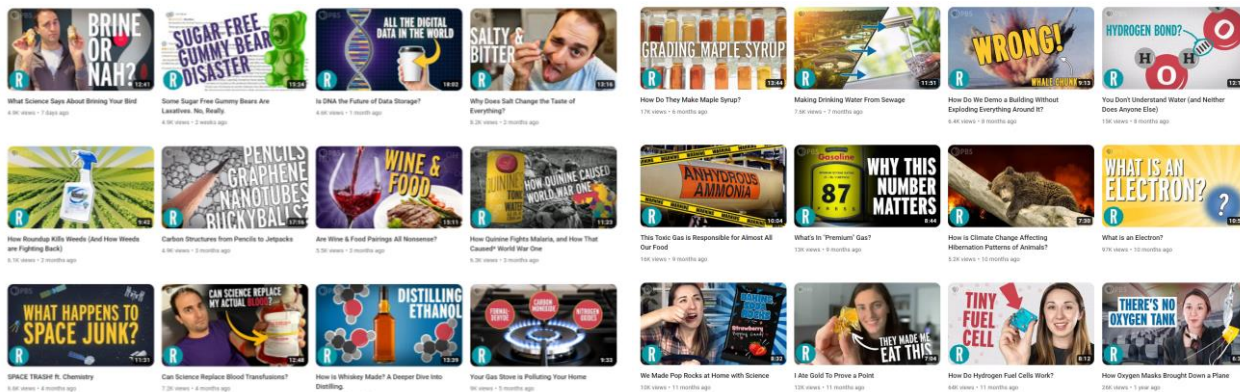
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Bonus Episode
Carolyn Bertozzi and K. Barry Sharpless chat about sharing the 2022 Nobel Prize in Chemistry
December 6, 2022



Bonus Episode
Bioorthogonal, click chemistry clinch the Nobel Prize
October 9, 2022



Episode #40
Lithium mining's water use sparks bitter conflicts and novel chemistry
September 13, 2022



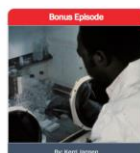
Bonus Episode
Happy 100th birthday, John Goodenough! Stereo Chemistry revisits a fan-favorite interview with the renowned scientist
July 25, 2022



Bonus Episode
Jess Wade on Wikipedia and work-life balance
June 21, 2022



Bonus Episode
The sticky science of why we eat so much sugar
May 31, 2022



Bonus Episode
There's more to James Harris's story
April 27, 2022



Bonus Episode
The helium shortage that wasn't supposed to be
March 24, 2022

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ACS Career Resources



Virtual Office Hours



<https://www.acs.org/careerconsulting.html>

Personal Career Consultations

Jim Tung
Marketing
Lacamas Laboratories
B.S., Biochemistry, University of Oregon
Ph.D., Organic Chemistry, University of Notre Dame

Jim Tung works at Lacamas Laboratories in Portland, OR, currently as a business development manager. He has been with Lacamas for 10 years, working on developing new chemical manufacturing projects. Before that, he was a senior research chemist at Oblet Research in Champaign, IL, performing kilo-scale organic chemistry.

An Oregon native, Jim got his B.S. in biochemistry from the University of Oregon, his Ph.D. in organic chemistry from the University of Notre Dame, with postdoctoral experience at Pfizer's laboratories in La Jolla, CA. He is past chair of the Portland Section of the American Chemical Society and was 2019 general co-chair of NORM 2019. He has interests in process chemistry, labor economics, social media outreach and encouraging career exploration and development for younger chemists.

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Advancing ACS' Core Value of Diversity, Equity, Inclusion and Respect



Resources

Inclusivity Style Guide Designed to help staff and members use language and images that respect diversity in all its forms. →	ACS Webinars on Diversity Covering diversity and inclusion at the workplace →
ACS Publications DEIR Hub See what ACS Publications is doing for fostering inclusivity in scholarly publishing →	ACS Volunteer and ACS Meetings Code of Conduct Fostering a positive and welcoming environment for attendees, volunteers and staff. →
C&EN Trailblazers C&EN highlights scientists from different backgrounds who are making an impact in chemistry. →	NEW! Download DEIR Educational Resources Download this educational guide for additional recommendations on videos, articles, books, podcasts, and more on diversity, inclusion, and related topics. →
Quick Guide: Inclusion Moments Learn more about what Inclusion Moments are and see ideas to host them during your meetings. →	Quick Guide: How to host inclusive in-person events Recommendations and best practices to ensure that your events can accommodate everyone. →

Diversity, Equity, Inclusion, and Respect

**Adapted from definitions from the Ford Foundation Center for Social Justice:

Equity**

Seeks to ensure fair treatment, equality of opportunity, and fairness in access to information and resources for all. We believe this is only possible in an environment built on respect and dignity. Equity requires the identification and elimination of barriers that have prevented the full participation of some groups.

Diversity**

The representation of varied identities and differences (race, ethnicity, gender, disability, sexual orientation, gender identity, national origin, tribe, caste, socio-economic status, thinking, and communication styles, etc.) collectively and as individuals. ACS seeks to proactively engage, understand, and draw on a variety of perspectives.

Inclusion**

Builds a culture of belonging by actively inviting the contribution and participation of all people. Every person's voice adds value, and ACS strives to create balance in the face of power differences. In addition, no one person can or should be called upon to represent an entire community.

Respect

Ensures that each person is treated with professionalism, integrity, and ethics underpinning all interpersonal interactions.

<https://www.acs.org/diversity>

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2439+

Members participated
In Act4Chemistry

Get Involved

1739+

ACS Advocacy
Workshops participants
or enrollees

Enroll in a workshop

49

Years of Public
Policy Fellows

Become a Fellow

2000

Letters sent to
Congress

Take Action

American Chemical Society

<https://www.acs.org/policy>

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Mass Spectrometry Made Simple; or, How to Weigh a Molecule (Even Though There Isn't a Way to Weigh a Molecule)



LEE N. POLITE, PHD

President and Founder, Axion
Analytical Labs, Inc.



BRYAN TWEEDY, BS

Assistant Director, ACS Education,
Office of Career and Professional
Education, American Chemical Society

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Mass Spectrometry Made Simple
or
*How do you weigh a molecule...
even though there is no way to weigh a molecule?*

Dr. Lee N. Polite
Axion Analytical Labs, Inc.
Axion Training Institute, Inc.
info@axionlabs.com

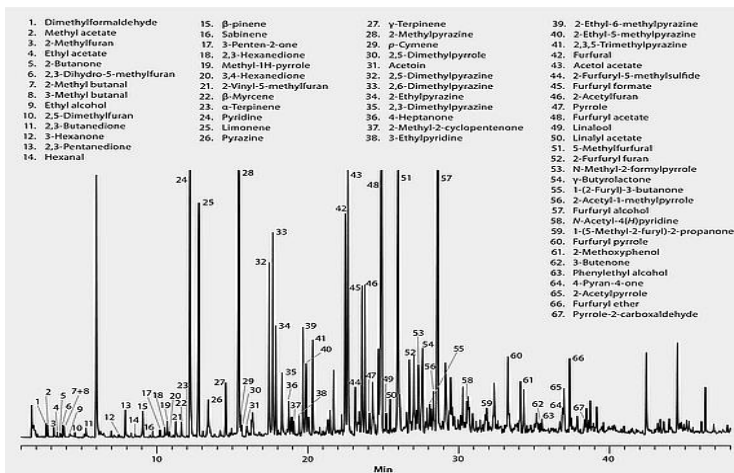
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GC/MS...Why Gas Chromatography?

- Excellent Separation Tool
- Separates complex mixtures into pure compounds (peaks)
- Provides tentative identifications



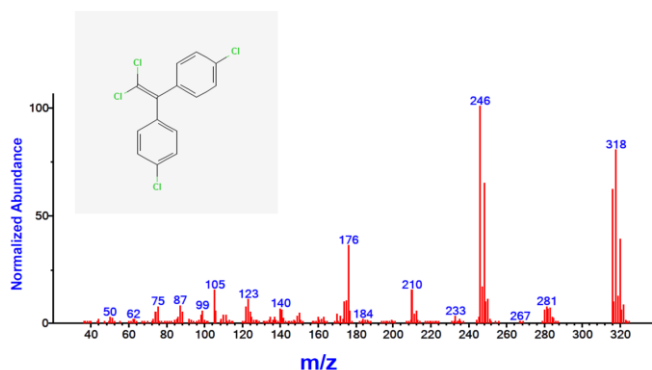
Coffee Analysis
by GC-FID

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GC/MS: Why Mass Spectrometry?

- Excellent Identification Tool - Identify unknown compounds
- Quantify known materials down to trace levels
- Elucidate the structure of molecules (molecular weight)
- Needs only nanograms of samples
- But only works on pure compounds!



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Why GC/MS?

- Combines advantages of both techniques:
 - High resolving power of GC
 - Positive identification of MS
- Requires only small samples (micrograms to picograms)
- Quantitative trace analysis (ppm, ppb)
- Mass range ~2 - 1050 AMU



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Audience Survey Question

ANSWER THE QUESTION ON THE INTERACTIVE SCREEN IN ONE MOMENT

Which phrases would you like to hear Dr. Polite use during his mass spec explanations?
(Select all that apply)

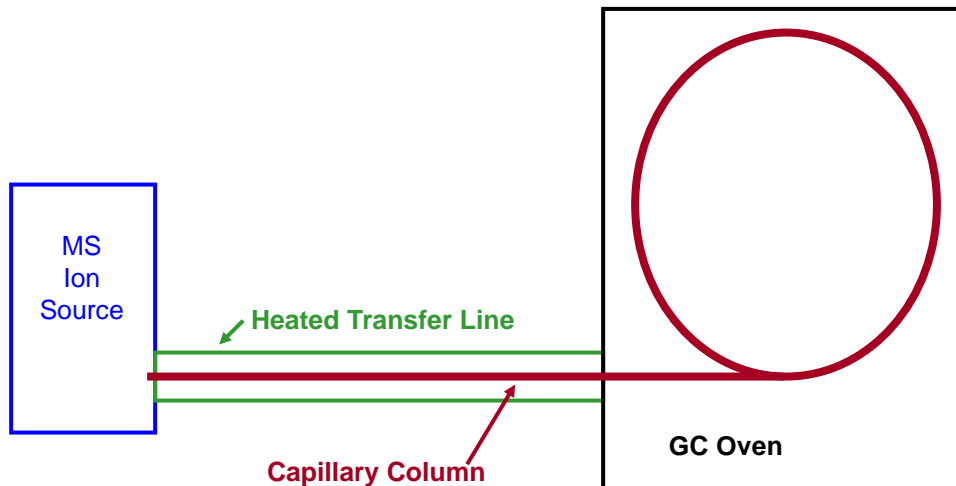
- Le Chatelier's Principle
- Coulombic Explosion
- Clausius Clapeyron Equation
- Blowing up a car and a motorboat

* If your answer is "Other" tell us more in the questions window!

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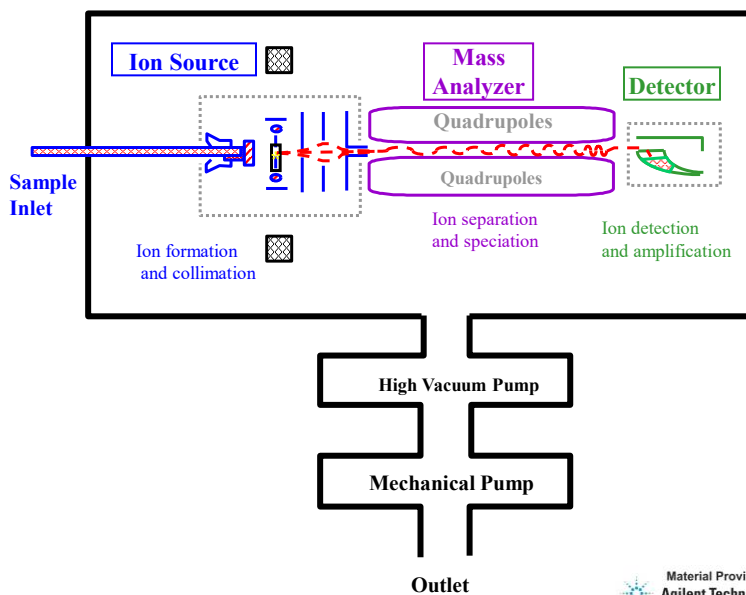
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Why GC/MS? Simple Direct Interface

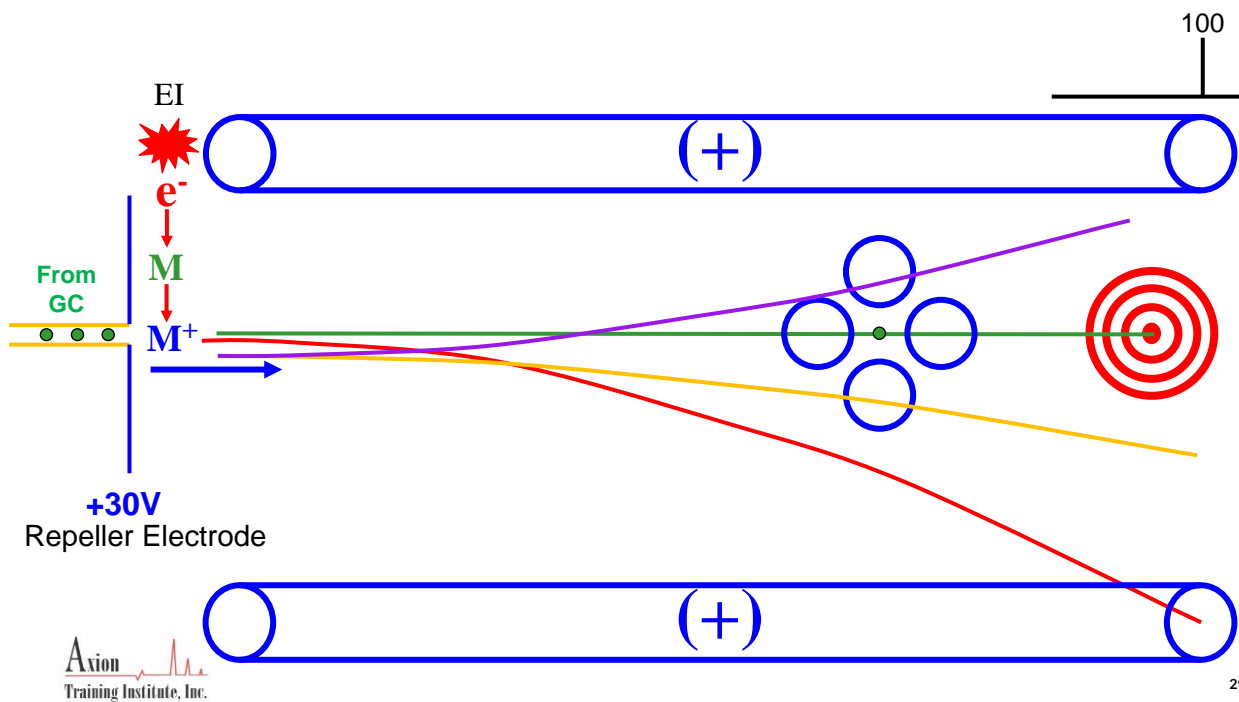


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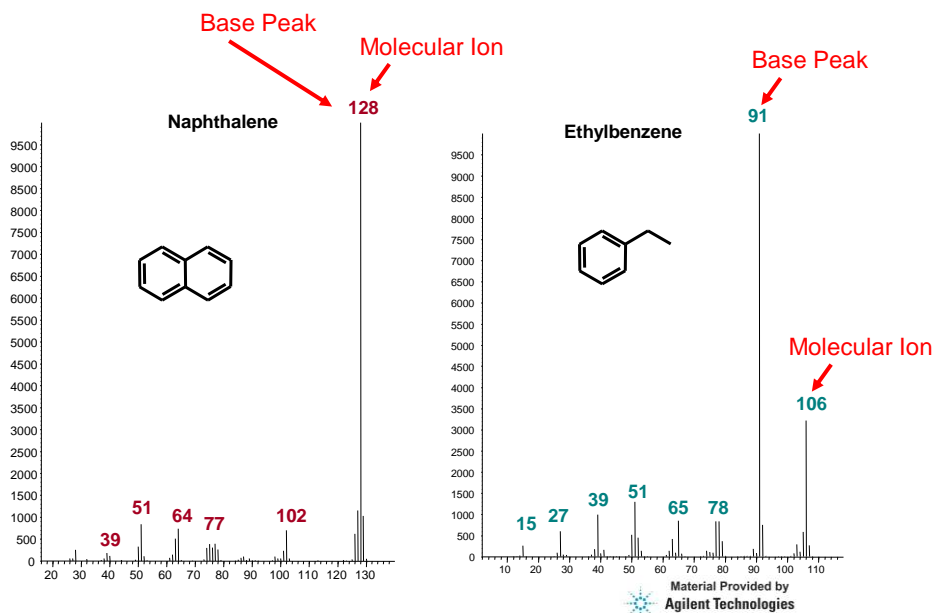
Mass Spectrometer Hardware



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Fragmentation and Interpretation (time for cars and boats!)



Single Quad Modes: Scan and SIM

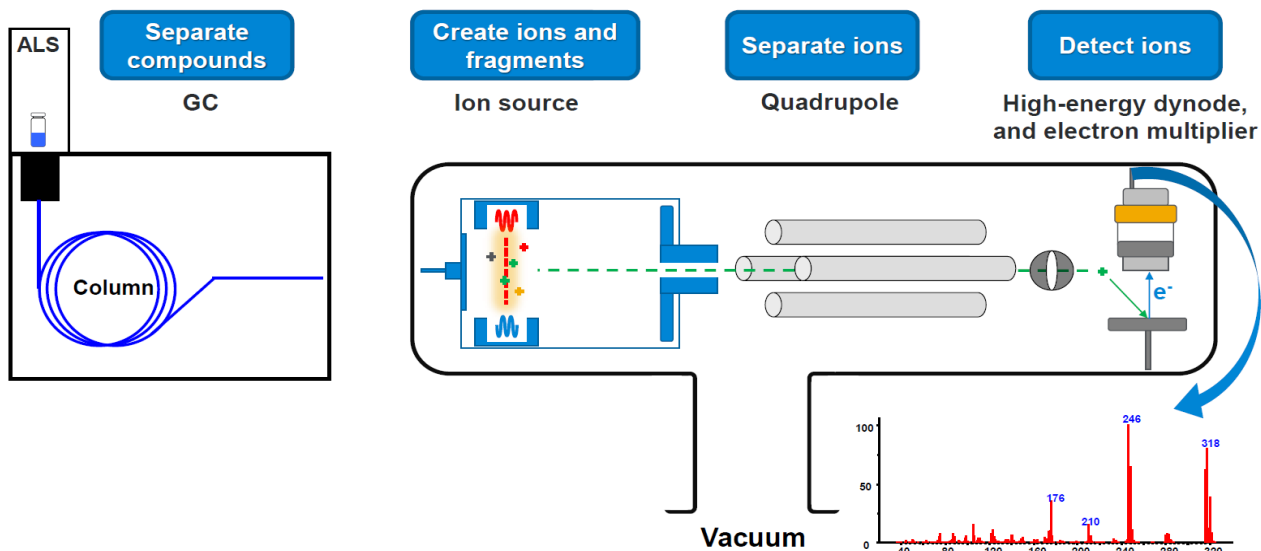
Scan (TIC)

- Scan all masses from 0-1000 amu
- Typically scan from ~40-600
- Produce Searchable spectra
- Identify Unknowns
- Confirm Identities
- Great for identification
- Not great for sensitivity

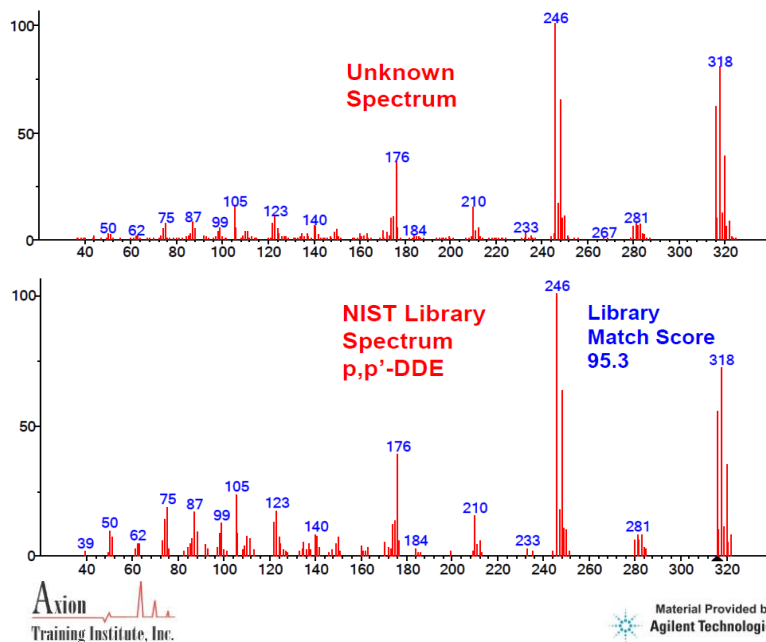
Selective Ion Monitoring (SIM)

- Only monitor a few distinct masses
- Typically, 1 quant ion and 2 qualifiers.
- Spends more time measuring each mass
- Produces lower noise = Higher signal to noise ratio
- Much better sensitivity
- Loss of some identifying information

Single Quad GC/MS

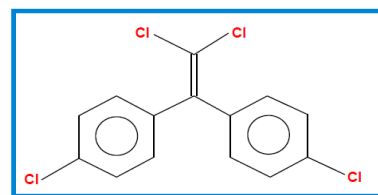


Single Quad GC/MS Library Searching



Searching unknown spectra against NIST or other libraries is widely used for identification of compounds.

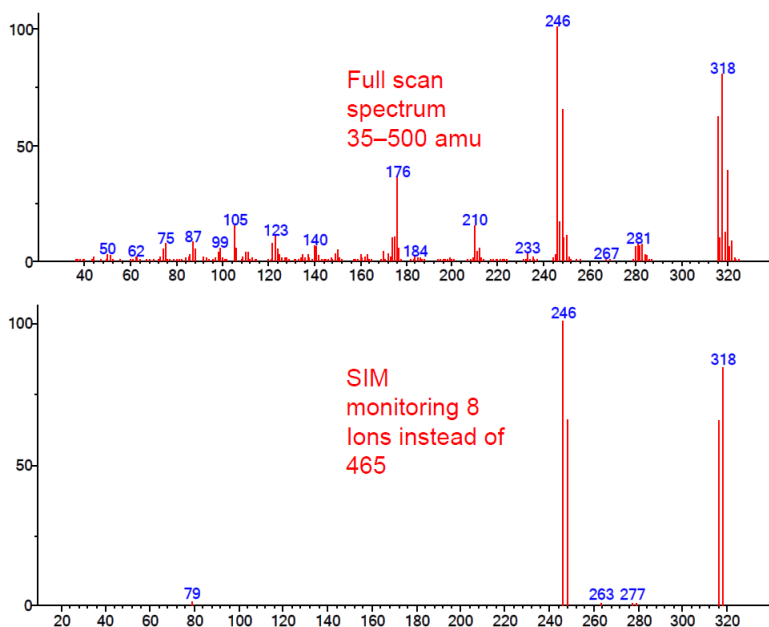
Spectral deconvolution software from NIST (AMDIS) and now MassHunter SureTarget can be used to produce spectra with the ions from overlapping matrix peaks removed.



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Single Quad GC/MS – Selected Ion Monitoring (SIM)



During chromatographic run, quad is programmed to monitor a small number of ions for specific analytes in specific time ranges.

More time is spent measuring each ion vs scan.

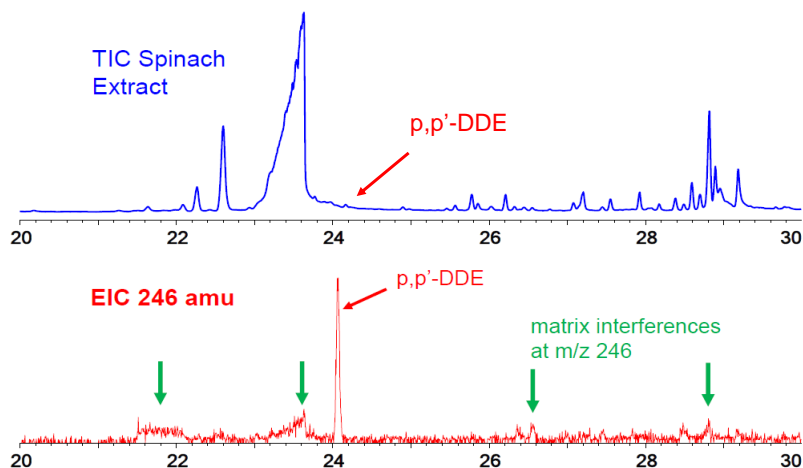
This gives ~10 x better signal-to-noise and better area precision. However, ability to search spectra for unexpected unknowns is lost.

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SIM Makes it Easier to Find Your Compound of Interest



The p,p'-DDE peak is visible in this spinach extract, but the baseline shows that the SQ has only limited selectivity over other matrix compounds that also have m/z 246 as a fragment.

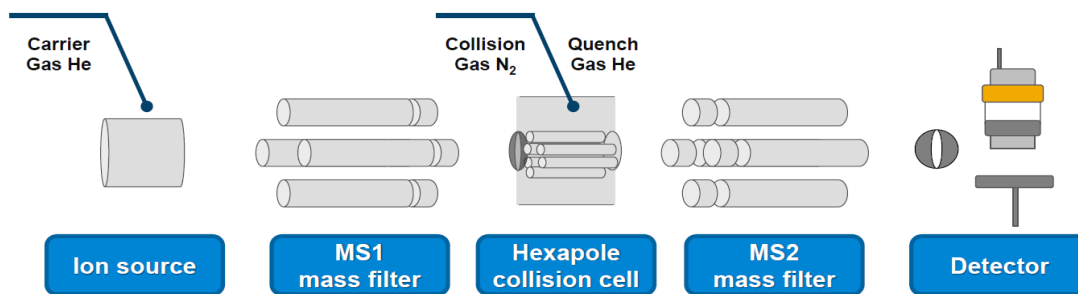
This limits the ability of the SQ to find traces of pesticides in extracts with high levels of matrix interferences.



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Triple Quad GC/MS (QqQ, MS/MS, Tandem MS, etc.)

MS/MS requires multiple mass filters in series



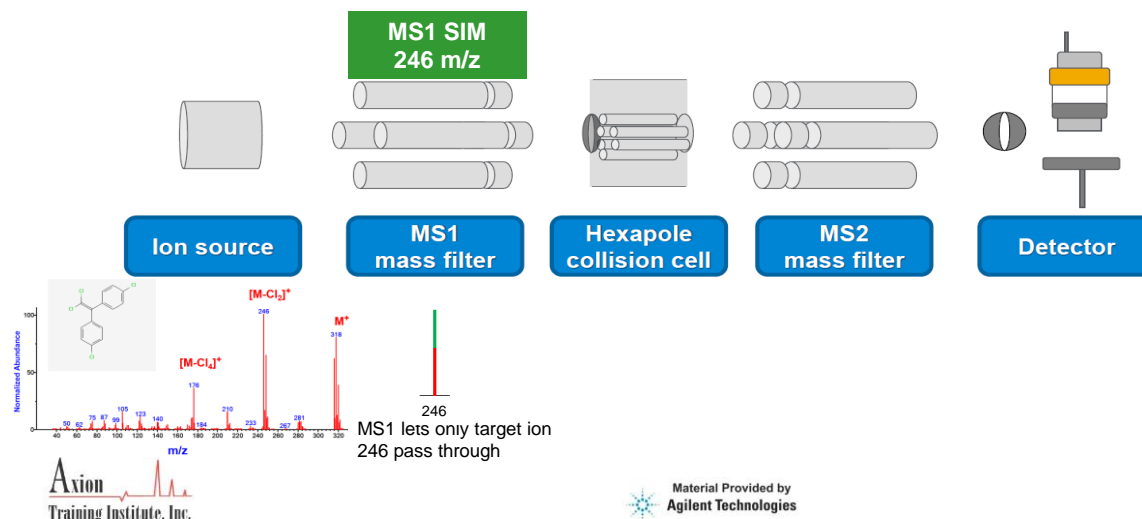
Typical analysis = Selection of precursor ion (MS1) Fragmentation of precursor ion (Collision cell) Selection of fragment ions (MS2) Detection



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Triple Quad GC/MS – Multiple Reaction Monitoring (MRM)

Step 1: Precursor ion of target passed by MS1. Contains fragment ions of mass 246 created from **both** analyte **and** interference molecules.

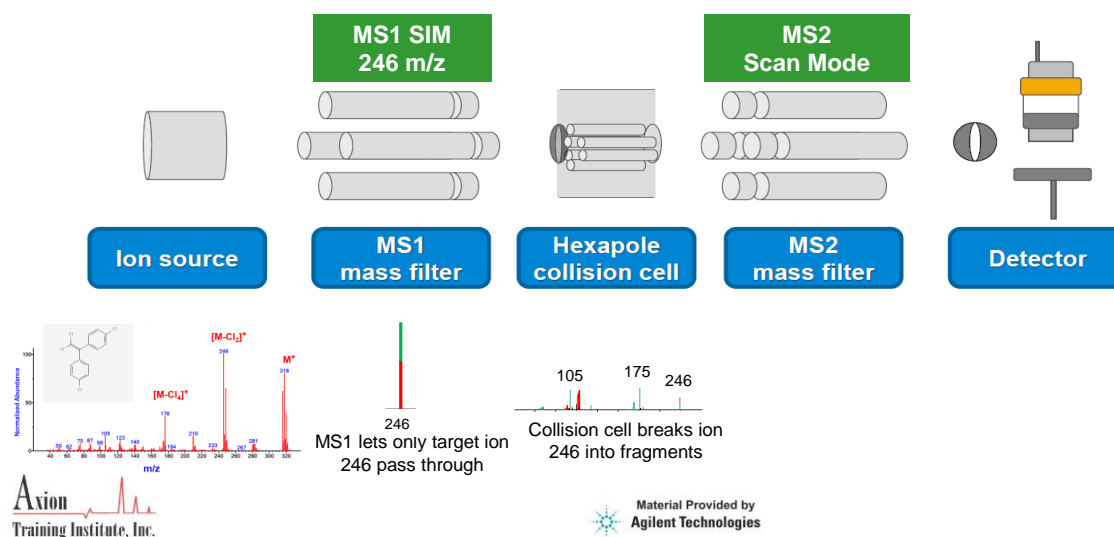


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Triple Quad GC/MS – Multiple Reaction Monitoring (MRM)

Step 2: The collision cell generates ions from the mass **246** fragments from **both** analyte **and** interferences.

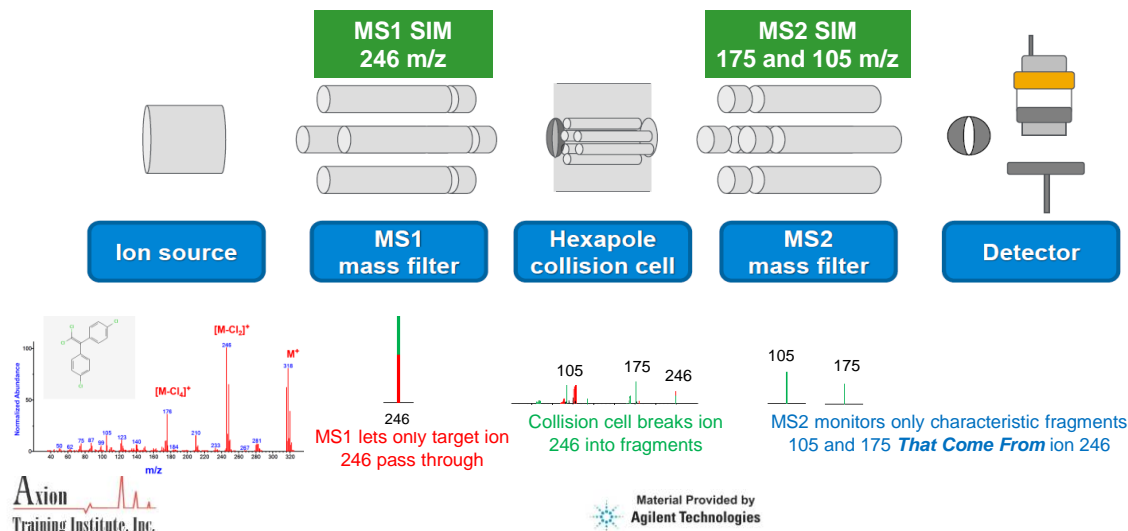


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Triple Quad GC/MS – Multiple Reaction Monitoring (MRM)

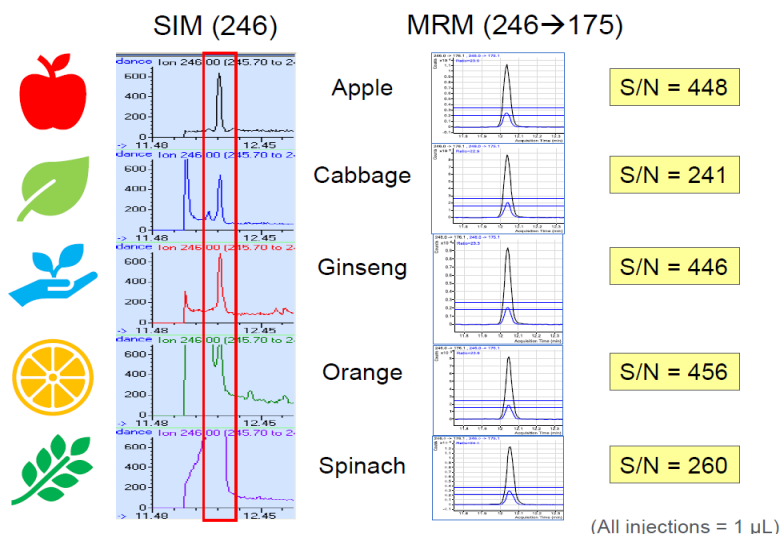
Step 3: MS2 is set to filter for quantification and qualifier product ions **only** formed by the analyte (unique ions.)



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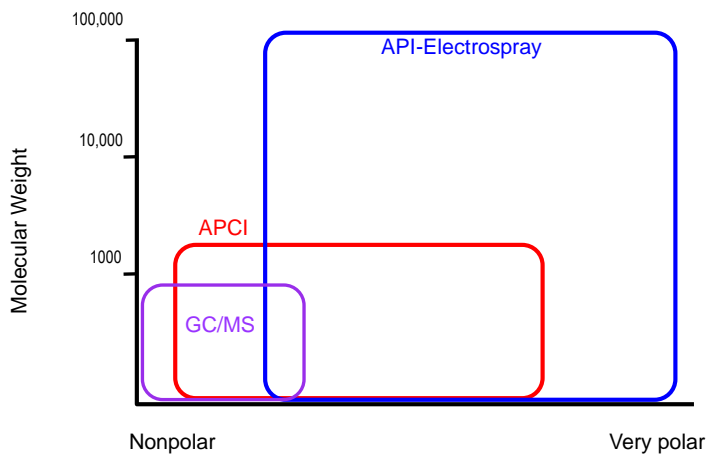
Single Quad SIM vs Triple Quad MRM Data for DDE



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LCMS...It's the same as GC/MS...but Different...and Huge!

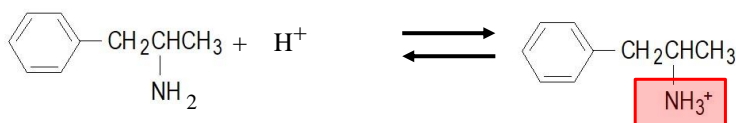


How do you Ionize a Molecule in HPLC? Adjust the mobile phase pH!

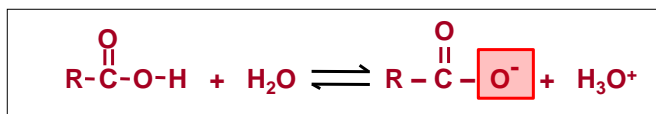
Low pH for Bases like Amphetamine

Neutral at High pH

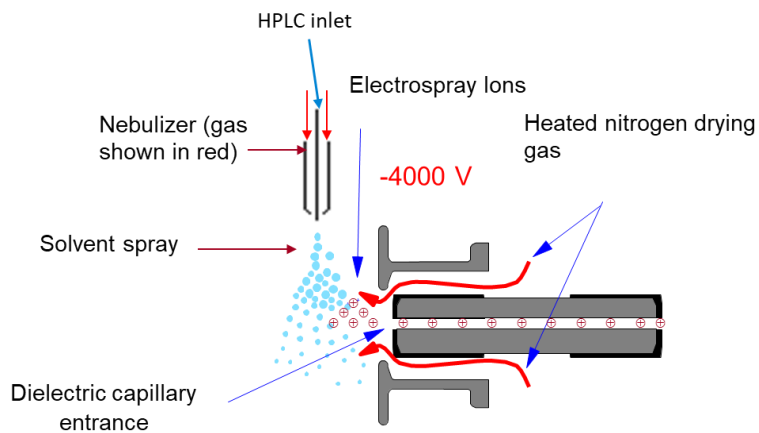
Ionized at Low pH (in acid)



High pH for Acids like Benzoic Acid

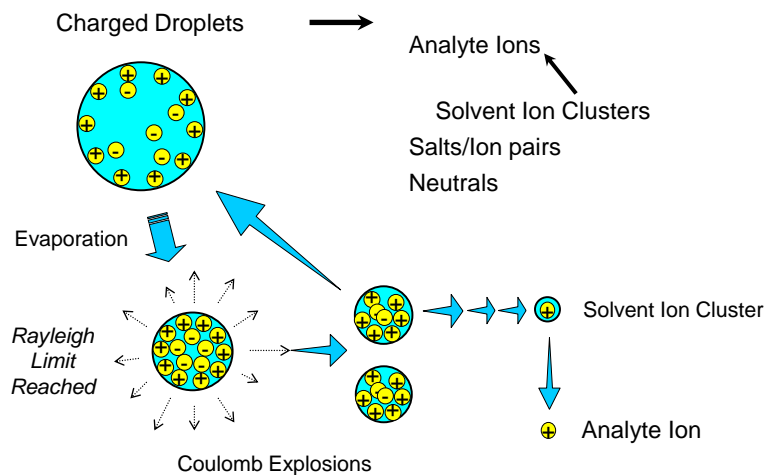


API-Electrospray Ionization



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Theory: API Electro spray



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Conclusions: Which MS Should I choose?




- **Single quad GCMS in the scan mode** to identify (volatile) unknowns
- **Single quad GCMS in the SIM mode** to quantify knowns at low levels (sub ppm)
- **GC triple quad** to quantify volatile knowns at extremely low levels (sub ppb)
- **LC Triple quad** to quantify soluble knowns at extremely low levels
- **LC Q-TOF** to characterize and quantify proteins (proteomics)



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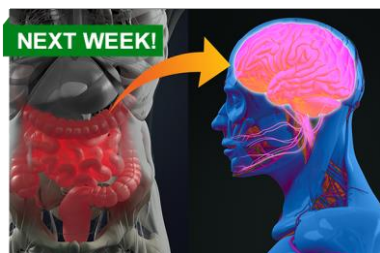


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