

# Analysis of Pesticides Using TOF and Q-TOF Mass Spectrometry for Accurate Mass Determination

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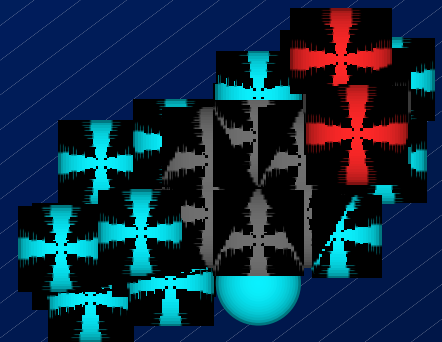
*E.M. Thurman, Imma Ferrer,*

*Ed Furlong*

*Pittsburg Analytical Conference*

*New Orleans*

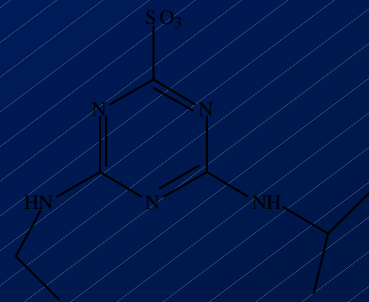
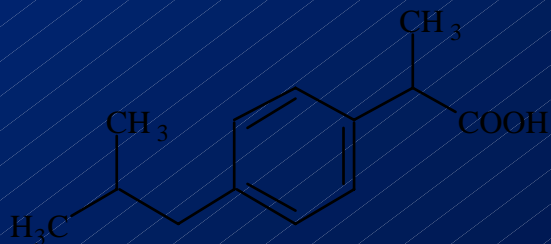
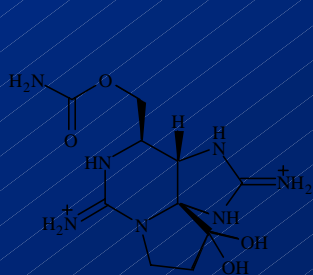
*March 11-15, 2002*



# Emerging Contaminants

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- New compounds: pesticide degradates, algal toxins, pharmaceuticals, hormones, personal-care products, organometallics, and surfactants
- Unequivocal ID required using mass spectrometry
- New environmental methods: LC/TOF accurate mass, LC/MS/MS (Q/TOF, Ion Trap, and Triple Quad)

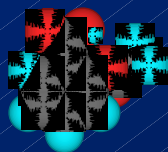


# Types of LC/MS... Instrumentation

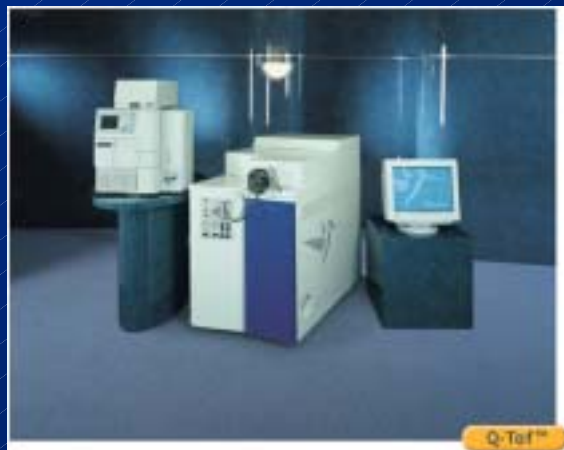
1. TOF
2. Q-TOF
3. Ion Trap



TOF

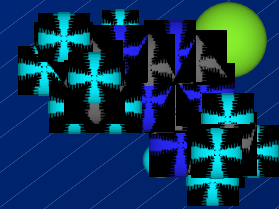


Q-TOF



Trap

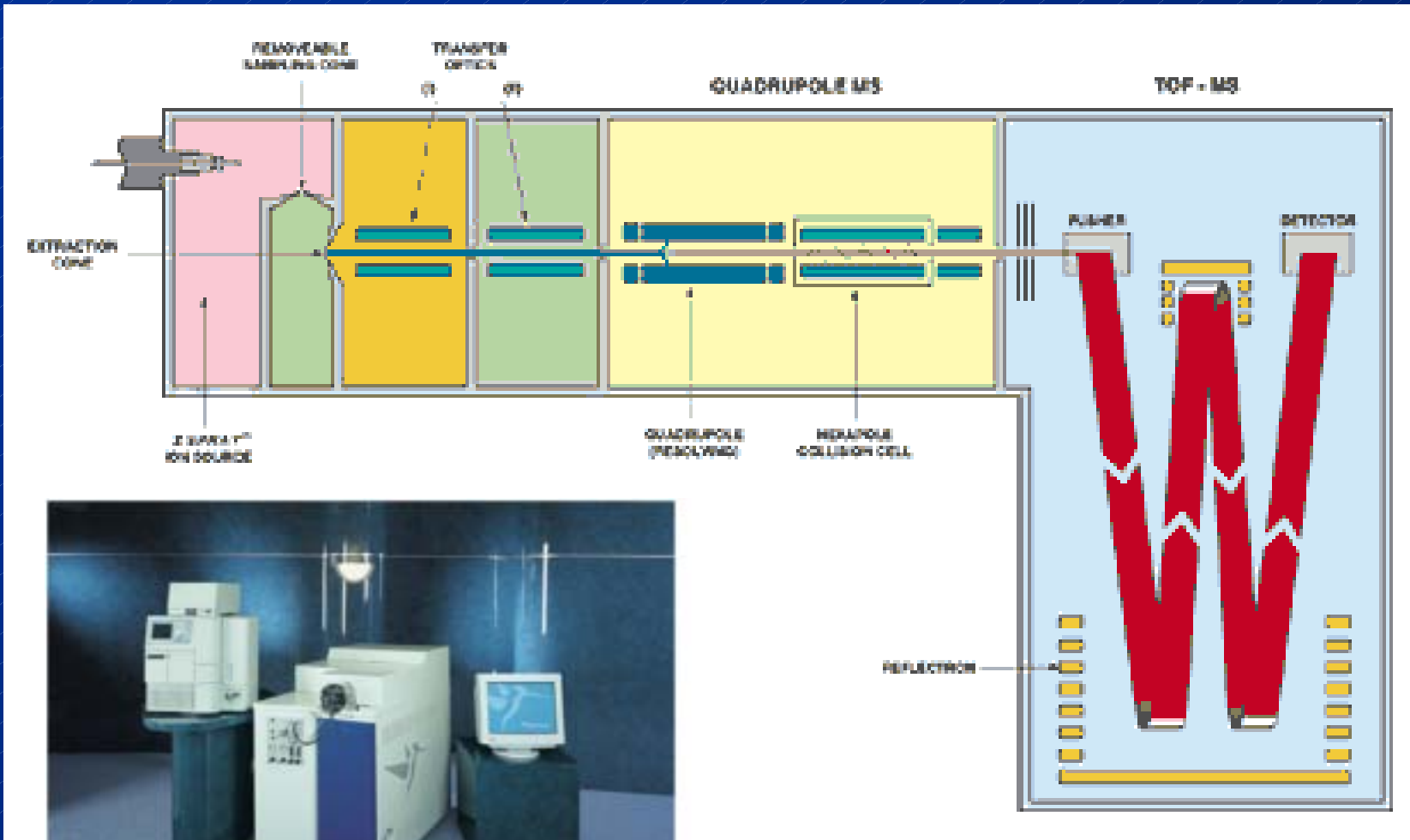
# How LC/MS TOF Works



LC/MS TOF



# How Q-TOF Works



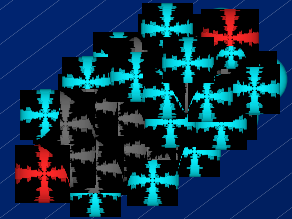
Unique Feature is High Resolution of Fragment Ions

# Q-TOF Spectra

- 1. Atrazine by Q-TOF, atrazine by TOF, compared to lc/ms spectra and gc/ms spectra
- 2. Do same spectra for sulfamethazine or tetracycline.
- 3. Some conclusions on the Q-TOF data
  - Accuracy compared to just TOF
  - Comparison to just LC/MS
  - Comparison to other ms/ms instruments

# How Ion trap works

1. The ion trap holds all the ions in the source until it is full, a beaker for ions.
2. Ions are ejected and measured, this is LC/MS.
3. One mass is held in the trap and fragmented, then fragments are ejected, this is MS/MS. Repeating his process gives MS<sup>n</sup>th.



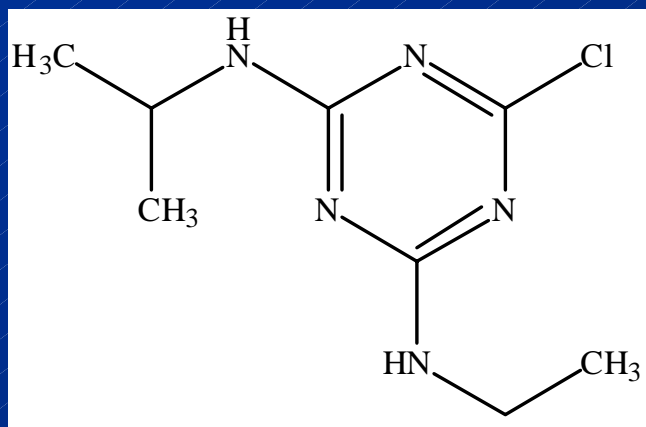
Unique feature is MS<sup>n</sup>th.

# Ion-Trap Spectra

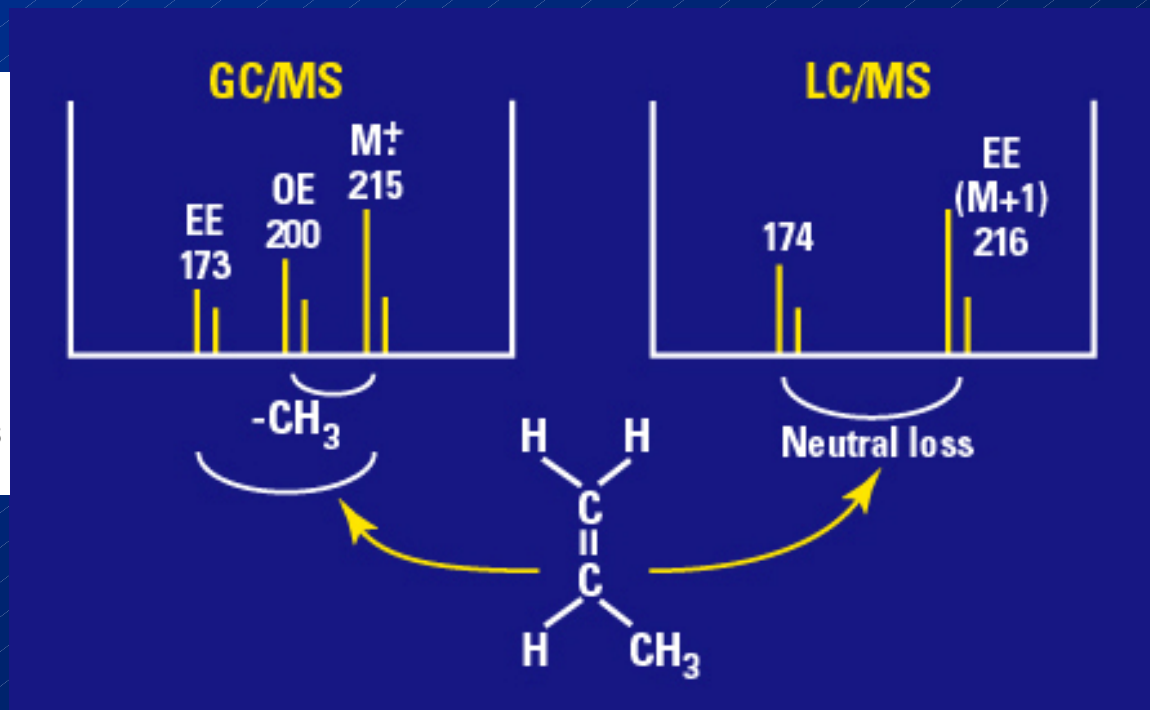
- 1. Atrazine by IT
- 2. Do same spectra for sulfamethazine or tetracycline.
- 3. Some conclusions on the IT data
- 4. Show unique feature of MSnth.



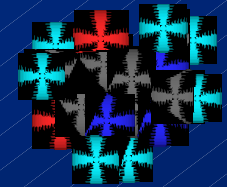
# Fragmentation of Pesticides



Atrazine  $M^+ = 215$



# How Triple Quadrupole Works



- Q1 and Q3 are single quadrupoles
- Q2 is the collision cell where fragmentation takes place with Rf voltage and collision gas

Unique feature is the neutral Loss experiment.



# Operation of Triple Quadrupole MS/MS

<b>Instrument</b>	<b>MS 1</b>	<b>Collision Cell</b>	<b>MS 2</b>
Daughter ion spectrum	Static parent ion selection	RF only, passes all masses	Scanning
Multiple reaction monitoring	Static parent ion selection	RF only, passes all masses	Static daughter ion mass selection
Constant neutral loss	Scanning synchronised with MS 2	RF only, passes all masses	Scanning synchronised with MS 1
Parent ion spectrum	Scanning	RF only, passes all masses	Static daughter ion mass selection

# Triple-Quad Spectra

- 1. Atrazine by TQ, atrazine by Q-TOF,
- 2. Do same spectra for sulfamethazine or tetracycline.
- 3. Some conclusions on the TQ data
- 4. Show unique features and 4 types of operation mode for our samples.

# Comparison of MS/MS Instruments

Instrument	Unique features	Advantages	Disadvantages
Q-TOF	Accurate mass of fragment ions	Sensitive in MS/MS for product ion scan, accurate mass for fragment ID.	Very expensive, Quasi selected reaction monitoring, neutral loss not possible
Triple Quadrupole	Neutral Loss Experiment	Sensitive Instrument for quantitation with SRM. Neutral loss for discovering unknowns	Expensive, not sensitive in scan mode
Ion Trap	MS <sup>nth</sup>	High sensitivity in scan, Inexpensive cost, Real time spectra, MS <sup>nth</sup>	Quantitation less reliable for difficult matrices, neutral loss experiment not possible

# LC/MS/MS Summary

1. Advantages of LC/MS/MS over LC/MS
2. Unique features of each of the three instruments for pesticides and pharmaceuticals.
3. Conclusions on when to use each of these instruments.

