



# **Analysis of VOCs in Foodstuffs by GC/Q-Orbitrap**

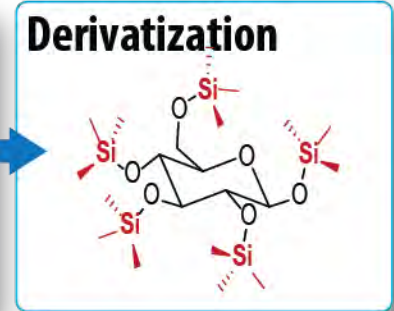
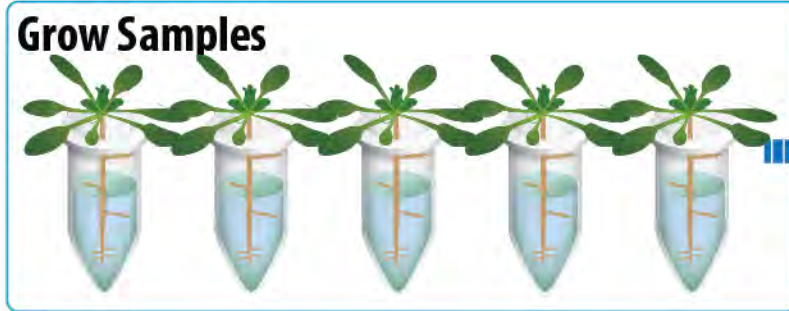
**AJ Balloon, MS Westphall, JJ Coon**



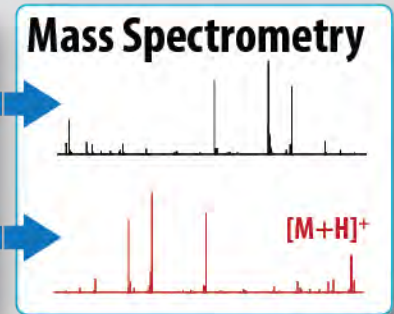
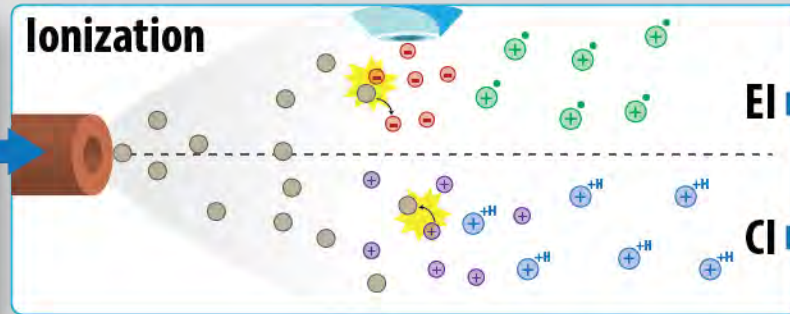
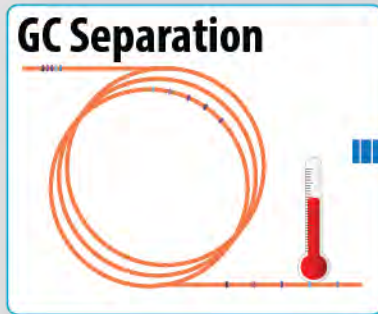
**ThermoFisher**  
SCIENTIFIC

# GC Metabolomics Workflow

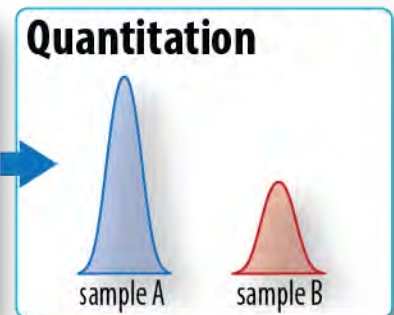
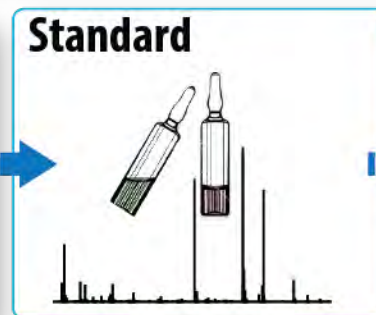
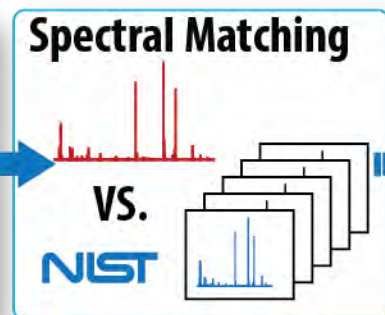
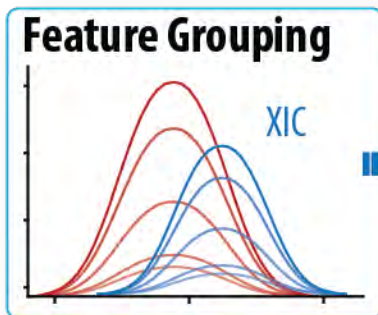
**SAMPLE PREPARATION**



**INSTRUMENTAL ANALYSIS**



**INFORMATICS**





# Metabolomics Standards Initiative Criteria



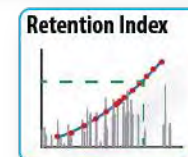
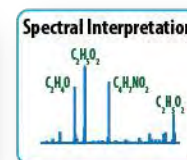
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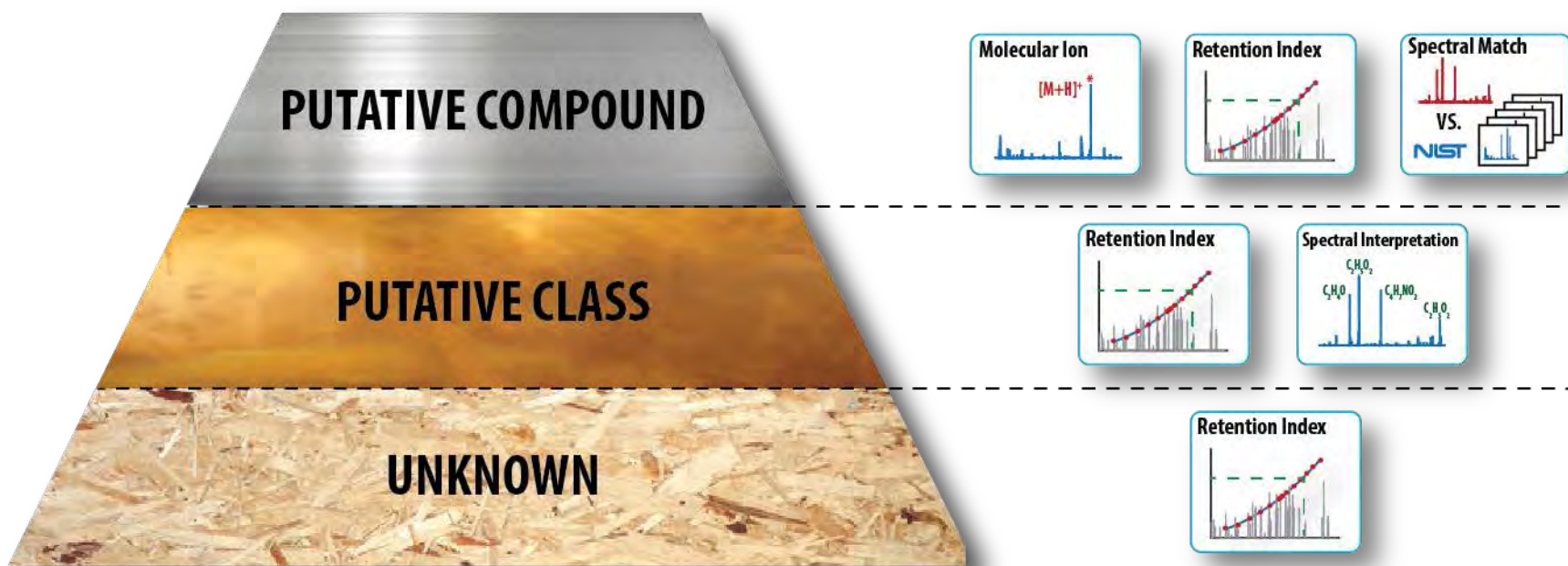
# Metabolomics Standards Initiative Criteria

PUTATIVE CLASS

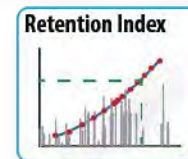
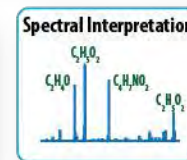
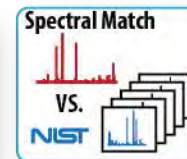
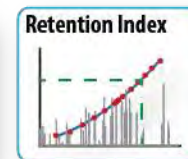
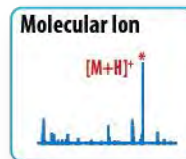
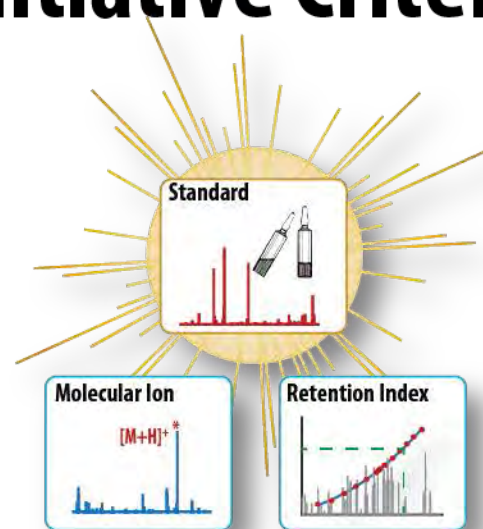
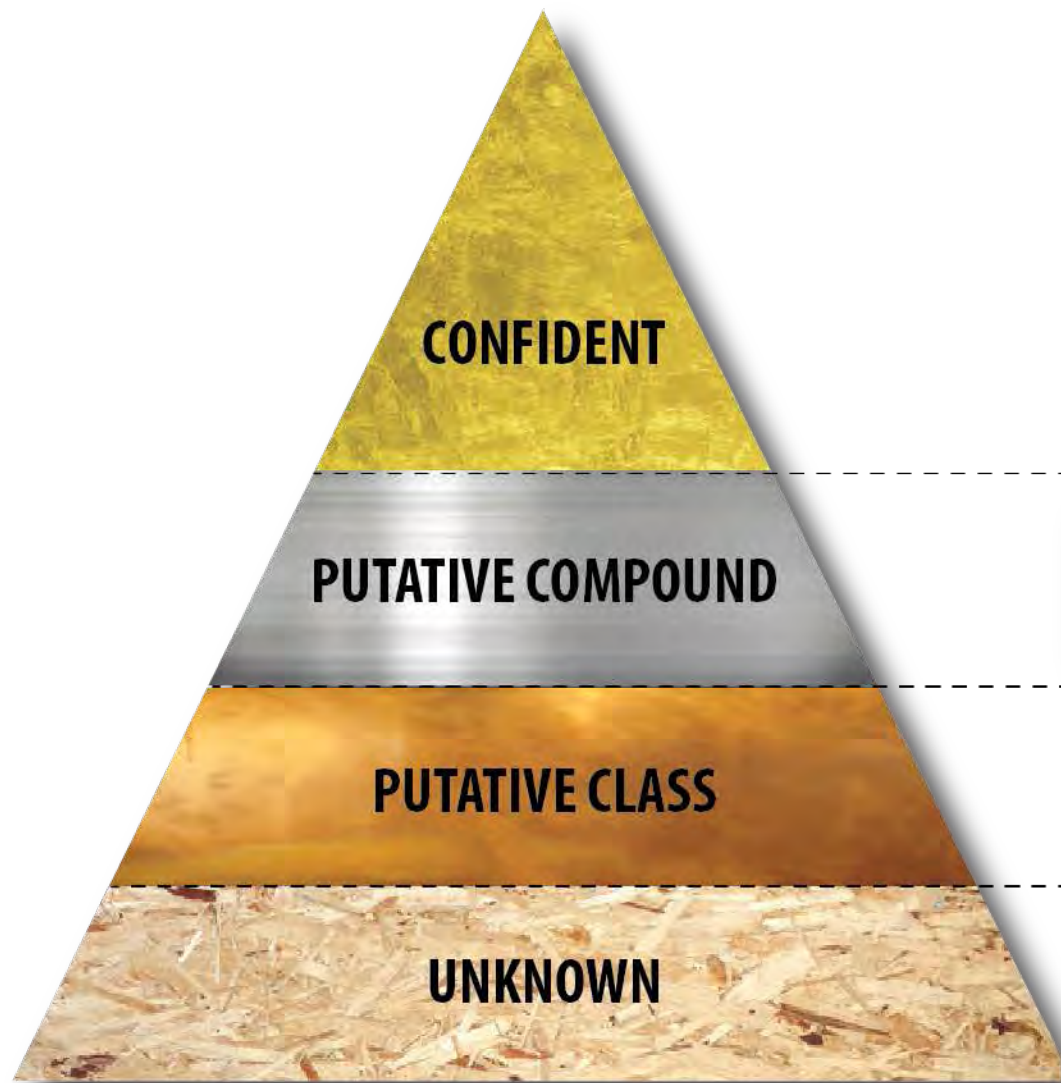
UNKNOWN



# Metabolomics Standards Initiative Criteria



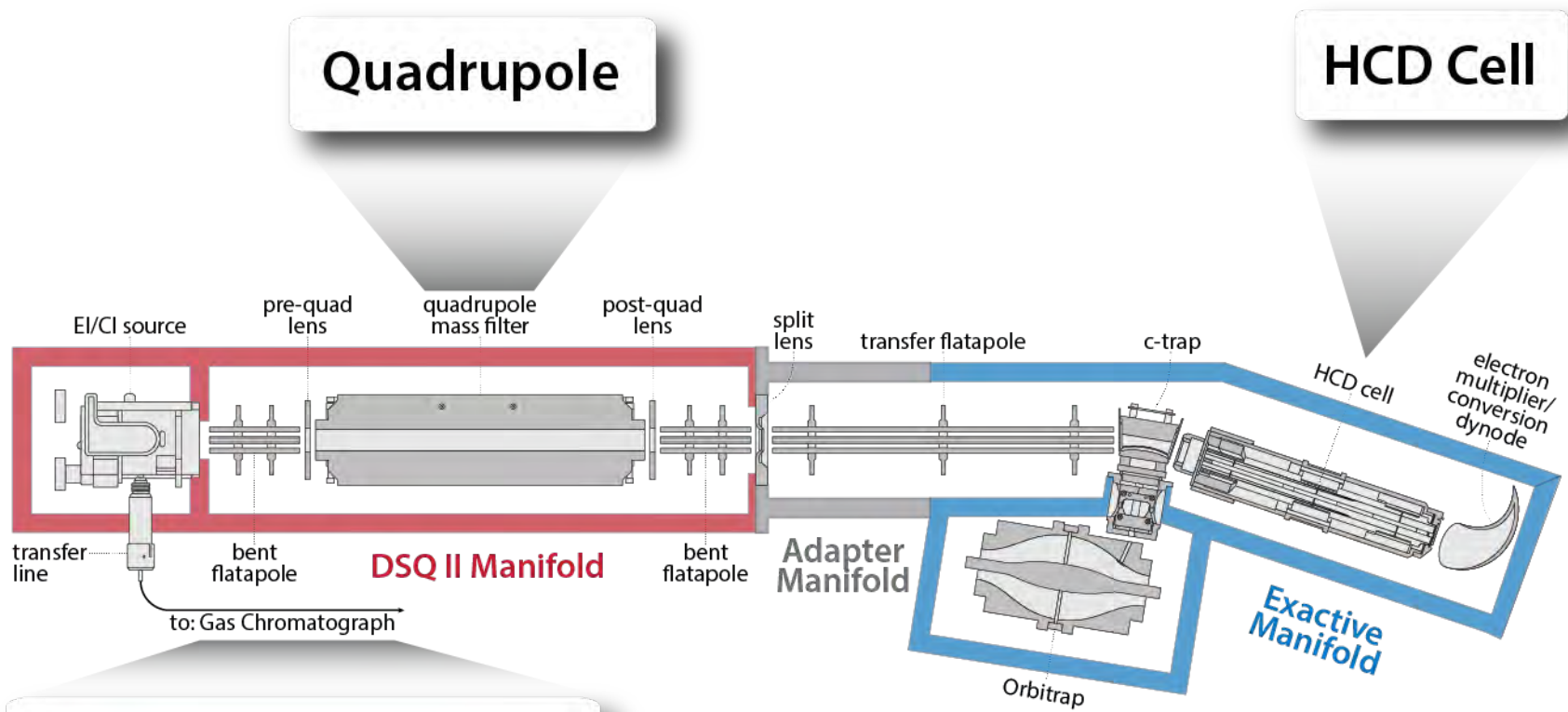
# Metabolomics Standards Initiative Criteria







# The GC/quadrupole-Orbitrap



**Scan Rate = 13.6 Hz**  
**Resolution = 17,500**

**Orbitrap**



# GC/Q - Orbitrap Metabolomics Workflow

**SAMPLE  
PREPARATION**

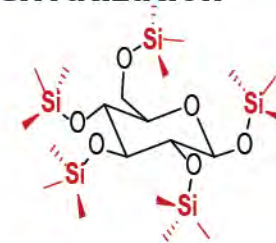
**Grow Samples**



**Extraction**

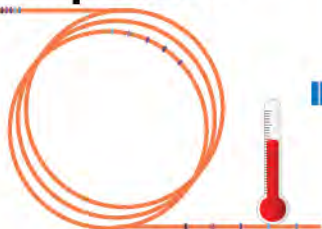


**Derivatization**

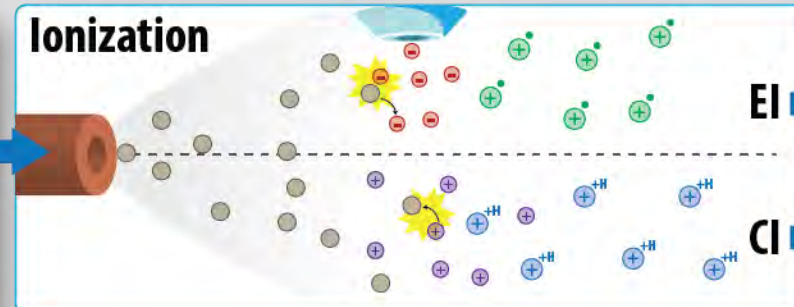


**INSTRUMENTAL  
ANALYSIS**

**GC Separation**



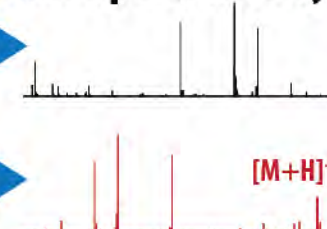
**Ionization**



**EI**

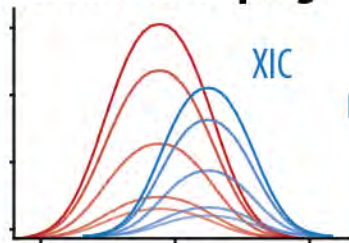
**CI**

**Mass Spectrometry**



**INFORMATICS**

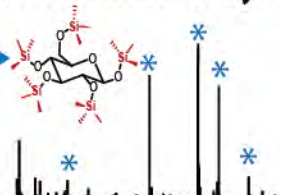
**Feature Grouping**



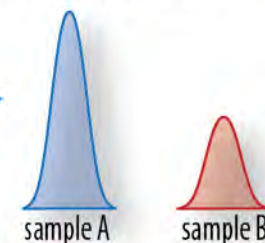
**Spectral Matching**



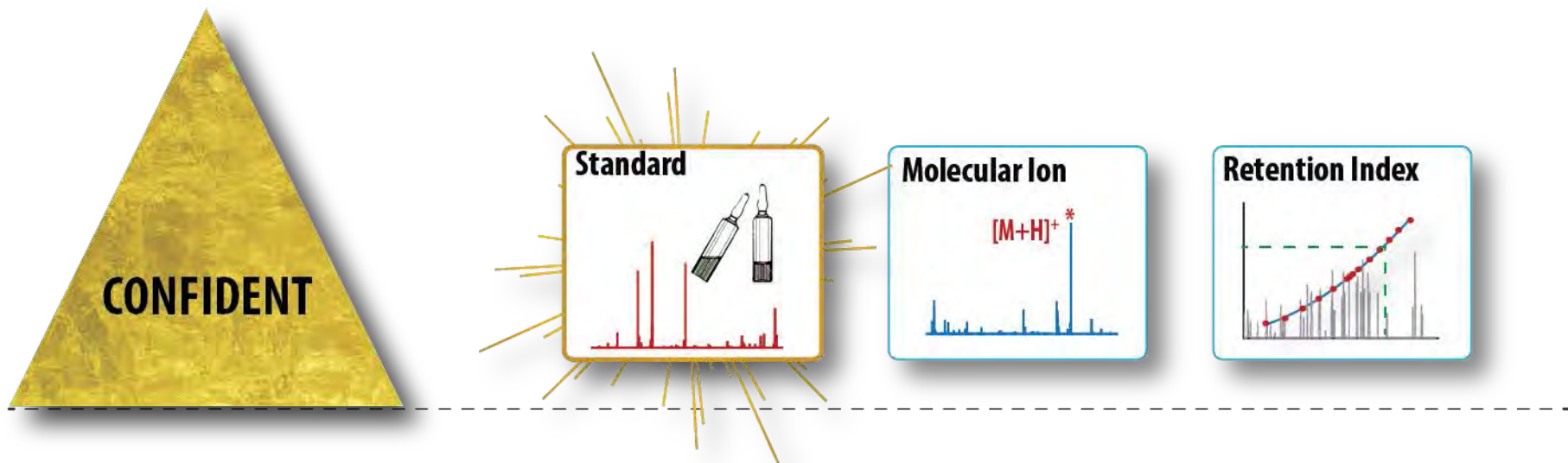
**High Resolution and  
Accurate Mass Analysis**



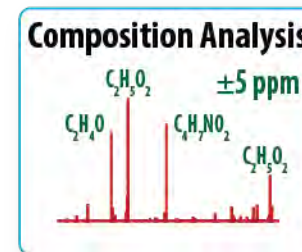
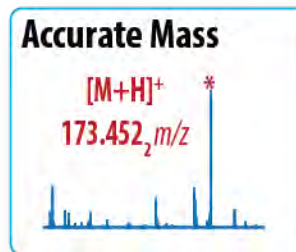
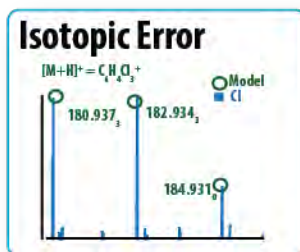
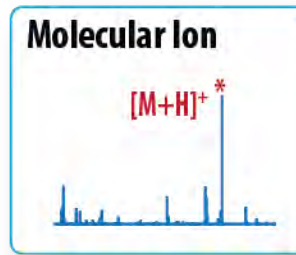
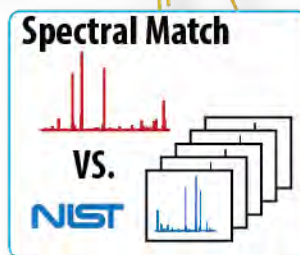
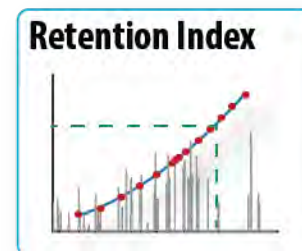
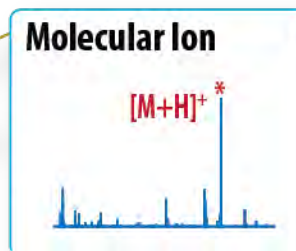
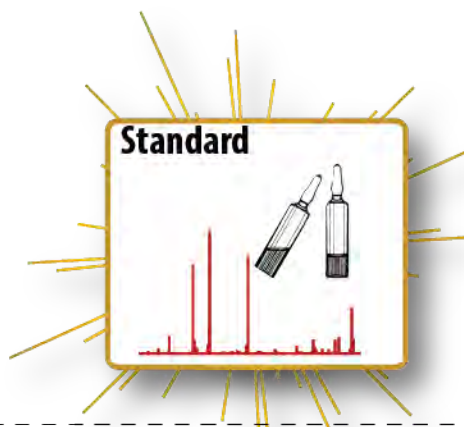
**Quantitation**



# Metabolomics Standards Initiative Criteria



# Metabolomics Standards Initiative Criteria





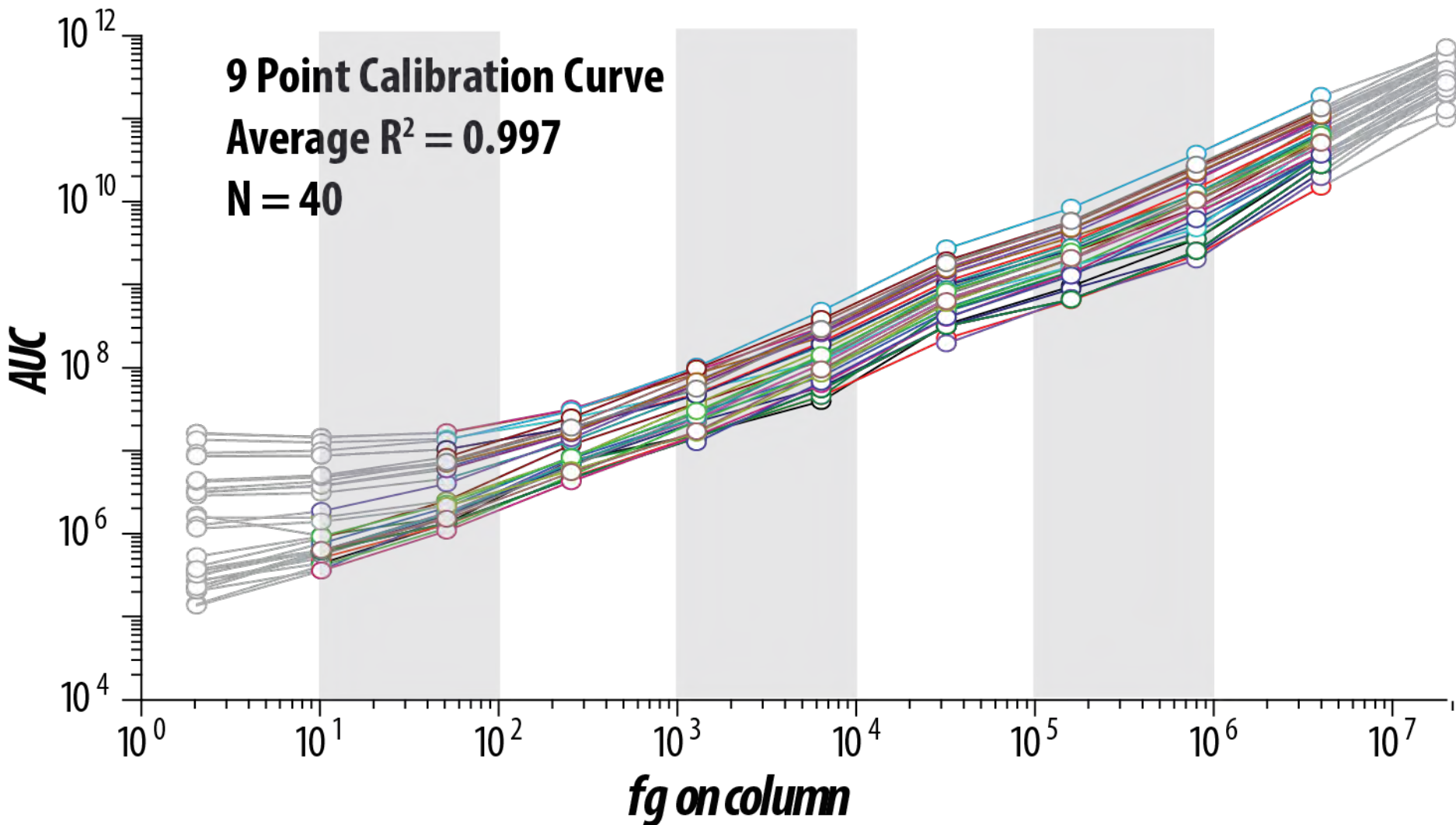
# Dynamic Range

## *Full Scan Electron Impact*

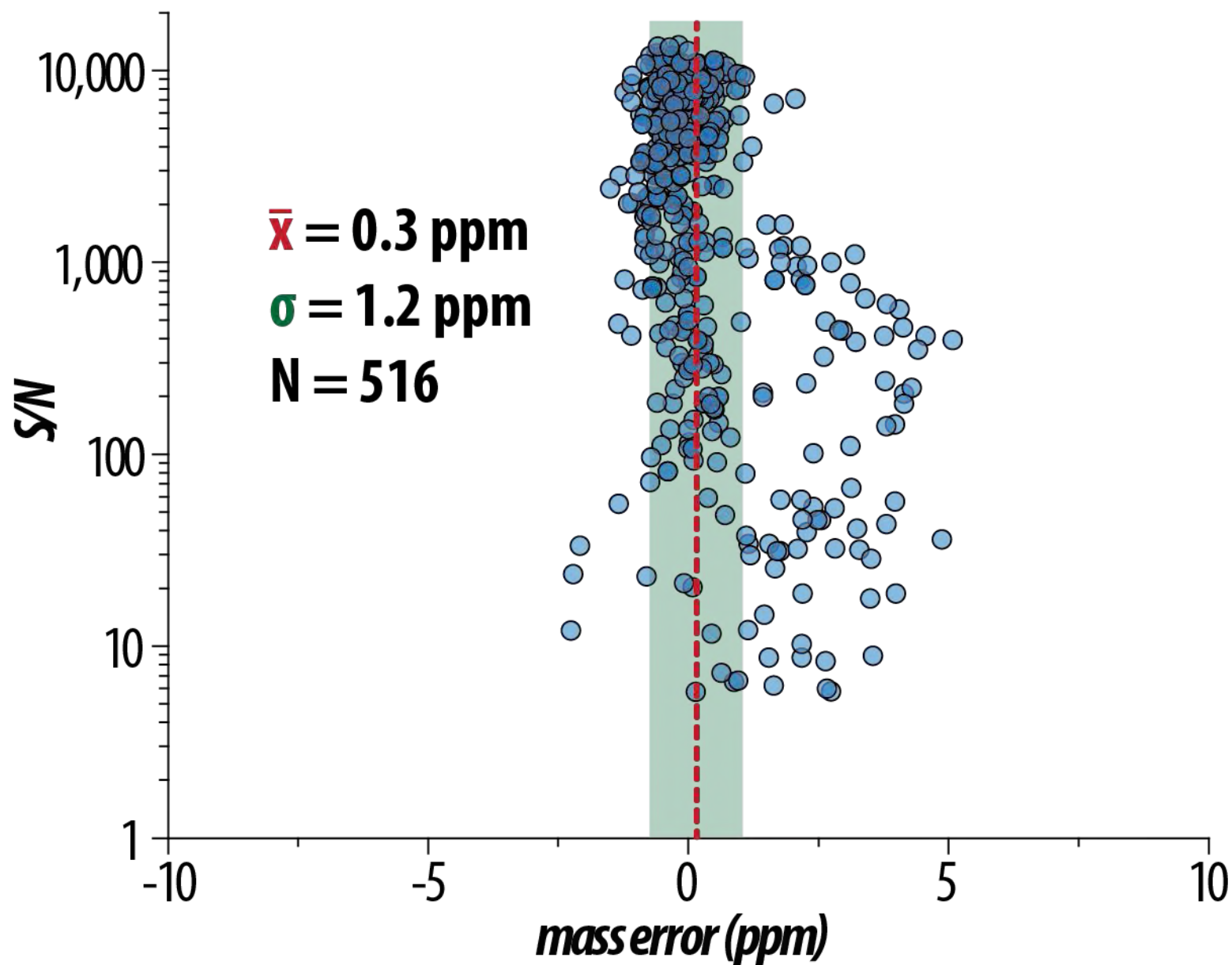
**9 Point Calibration Curve**

**Average  $R^2 = 0.997$**

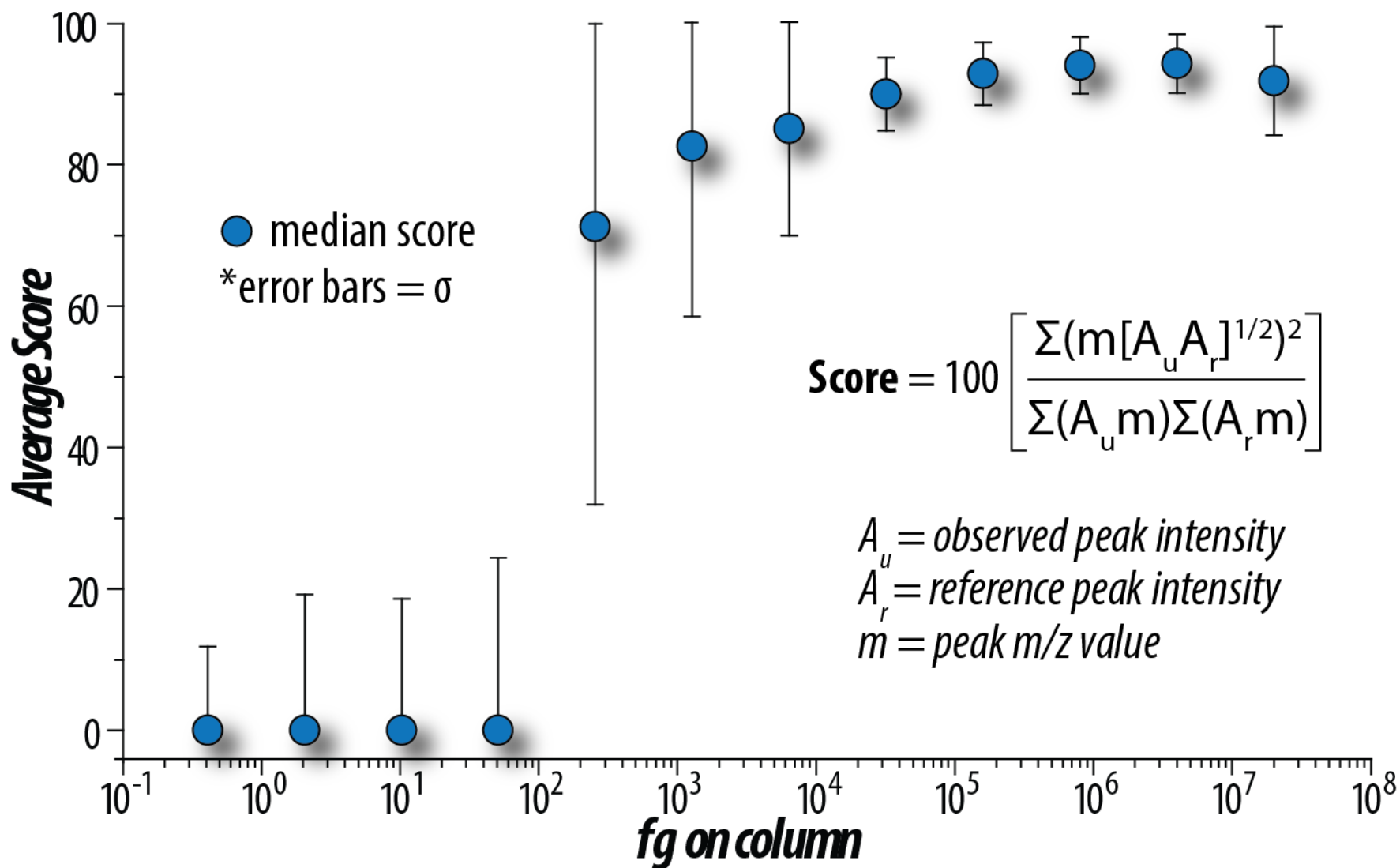
**N = 40**



# Mass Accuracy



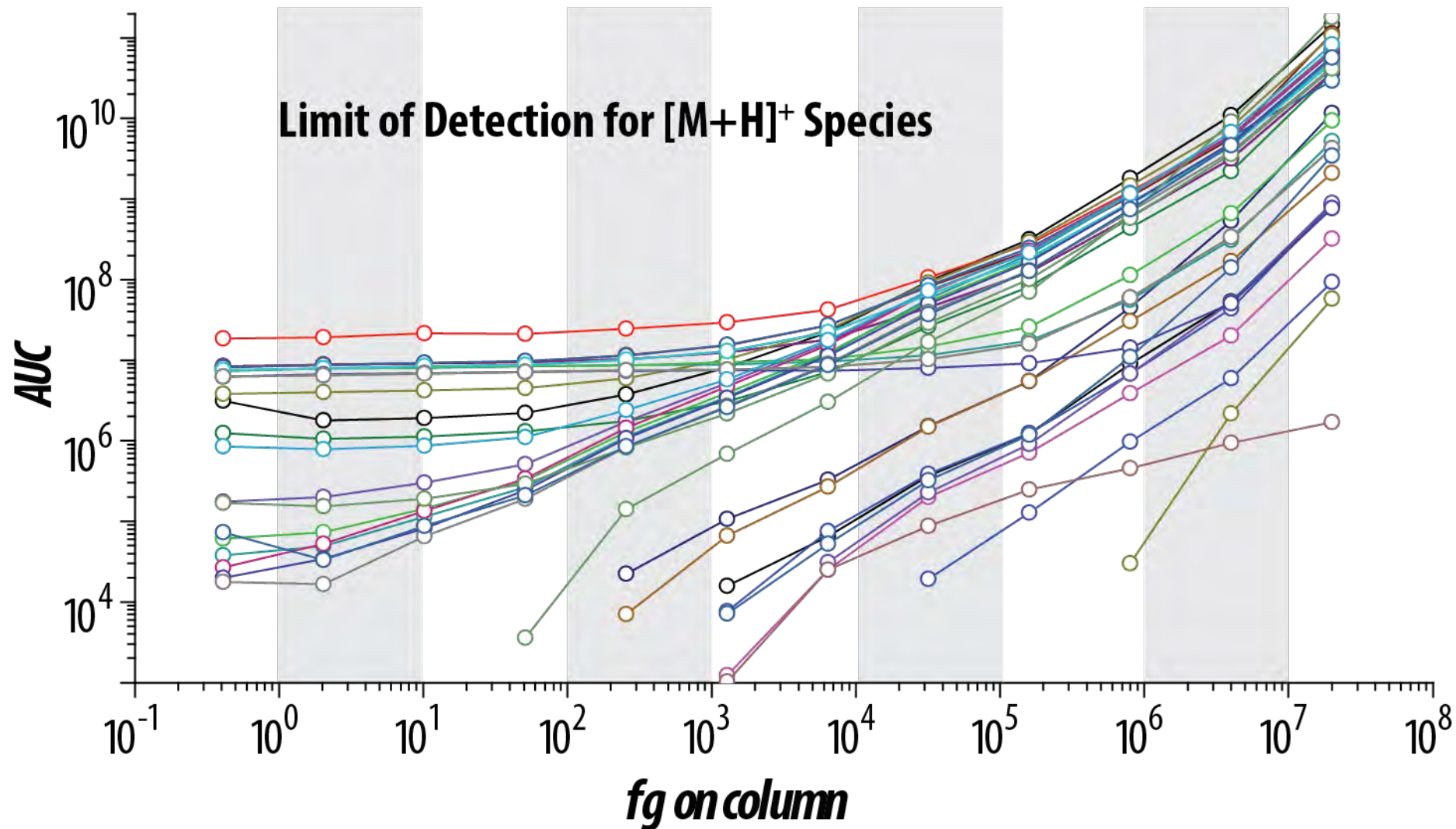
# Spectral Matching





# Precursor Identification

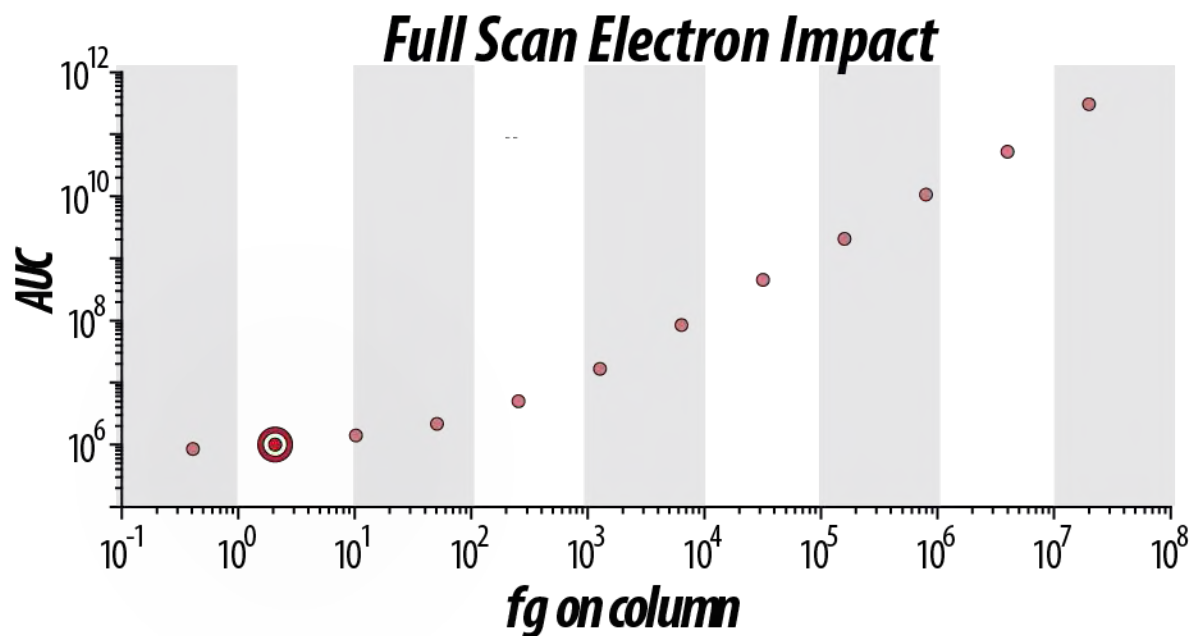
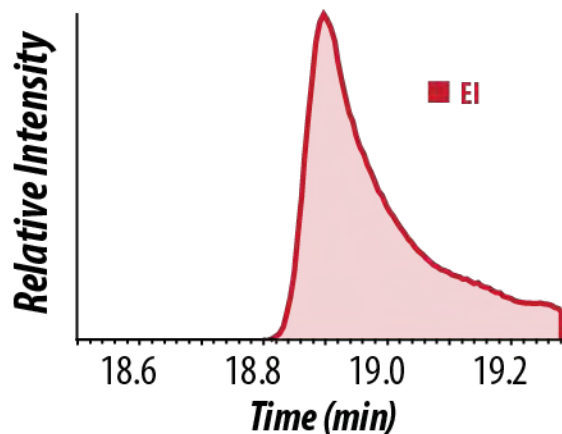
## *Full Scan Methane Ionization*



# Exemplary Workflow

Compound 36

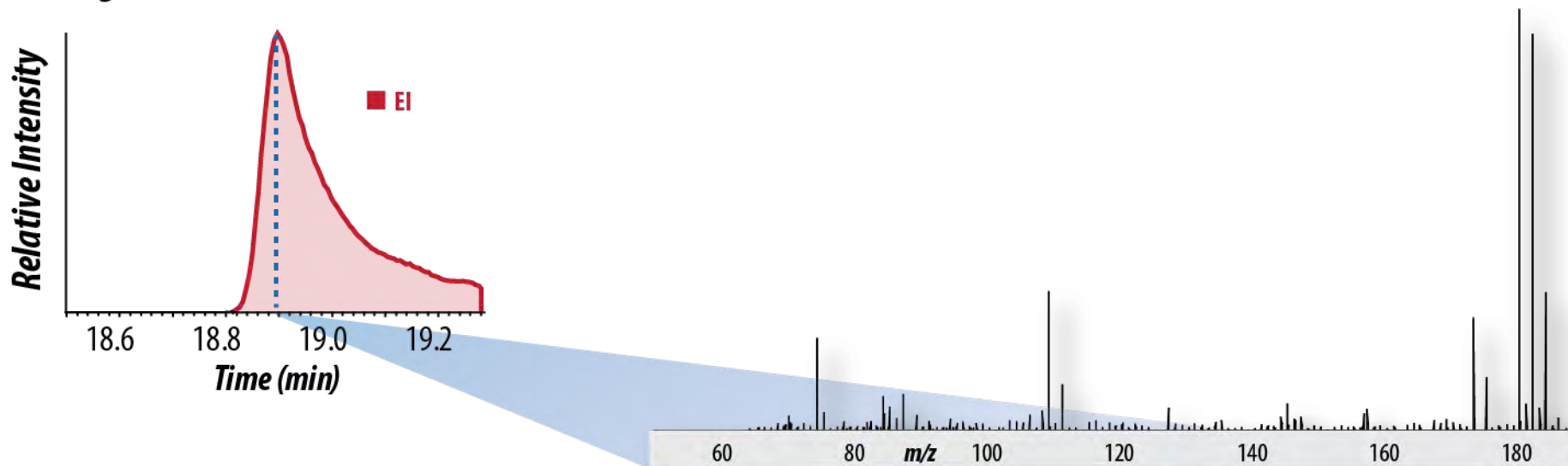
2 fg on column in Full Scan



# Spectral Deconvolution

Compound 36

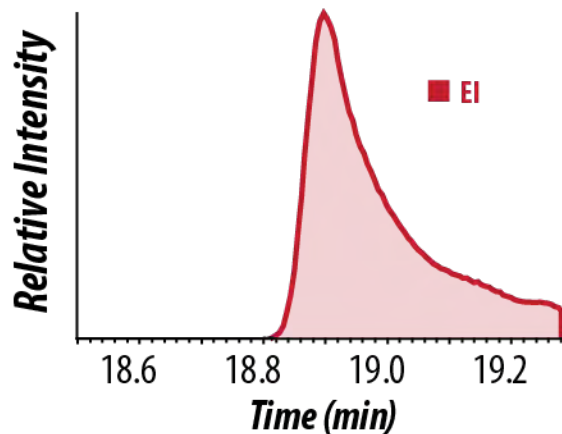
2 fg on column in Full Scan



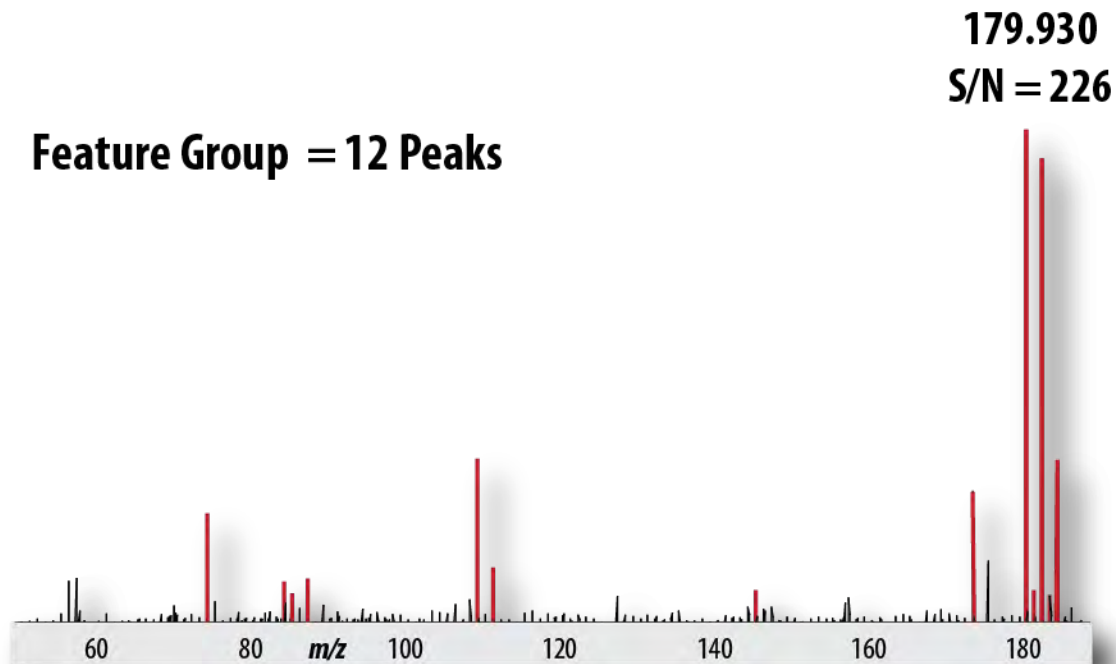


# Spectral Deconvolution

Compound 36  
2 fg on column in Full Scan



Feature Group = 12 Peaks

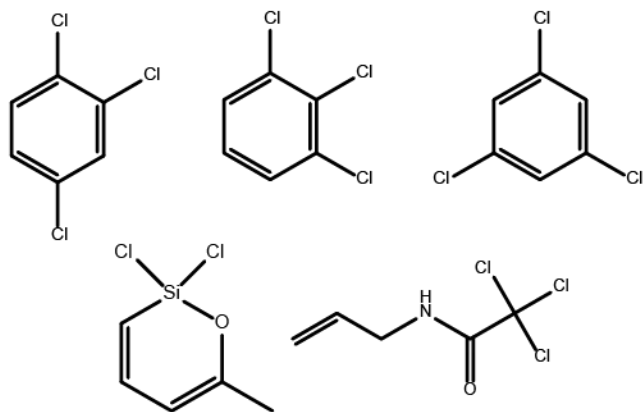
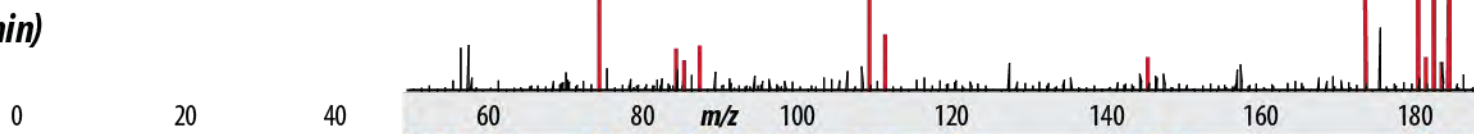
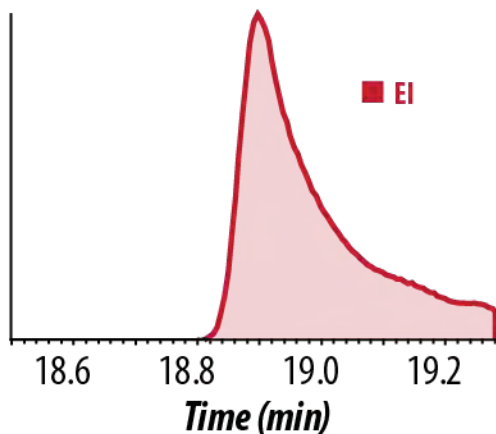


# Spectral Matching

Compound 36  
2 fg on column in Full Scan

179.930  
S/N = 226

Relative Intensity

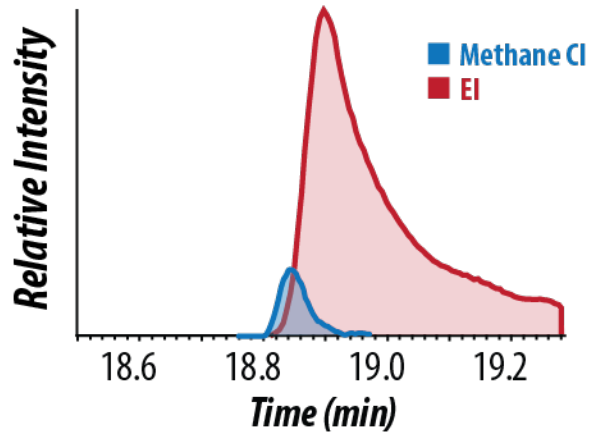


## NIST Spectral Match

- |  | Score |
|--|-------|
| 1. 1,2,3-Trichlorobenzene              | 70.78 |
| 2. 1,3,5-Trichlorobenzene              | 69.51 |
| 3. 1,2,4-Trichlorobenzene              | 67.99 |
| 4. Dichloromethyloxasilacyclohexadiene | 53.17 |
| 5. N-methylallyl-Trichloroacetamide    | 50.02 |

# Precursor Identification

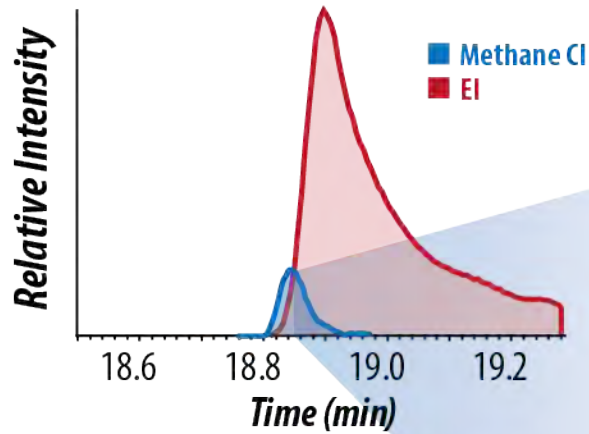
Trichlorobenzene  
2 fg on column in Full Scan



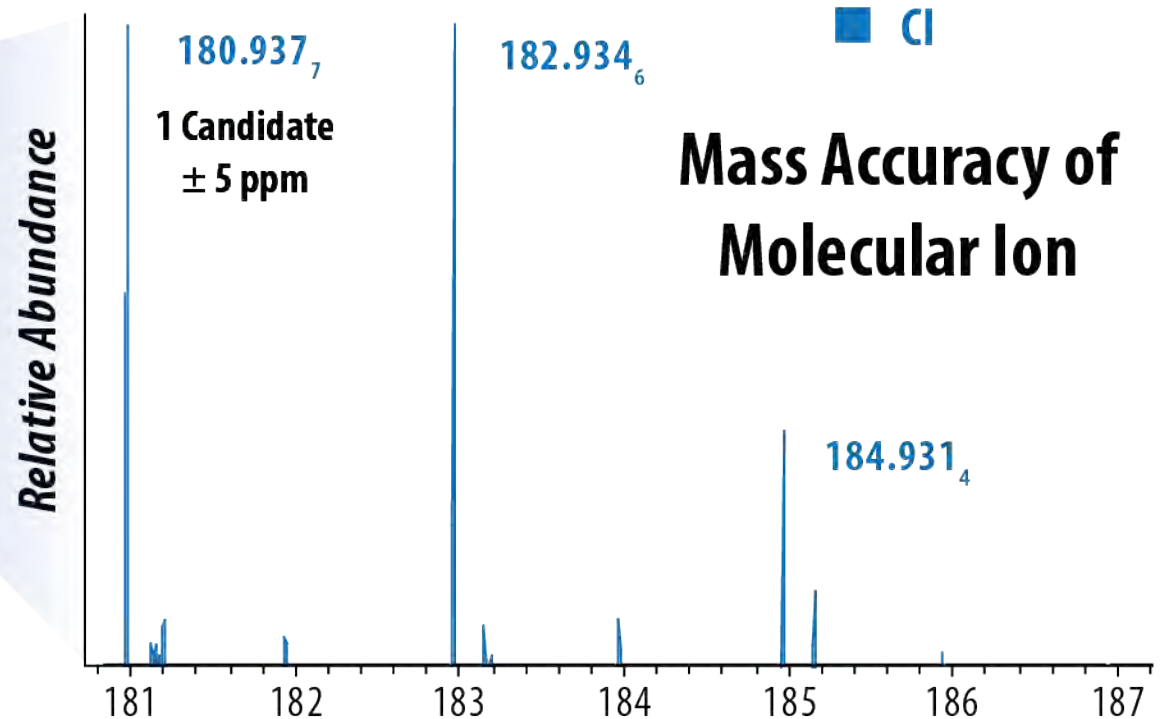


# Precursor Identification

Trichlorobenzene  
2 fg on column in Full Scan

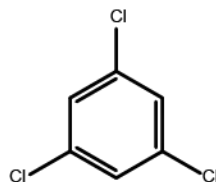
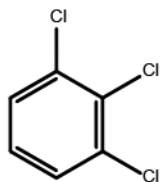
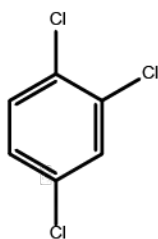
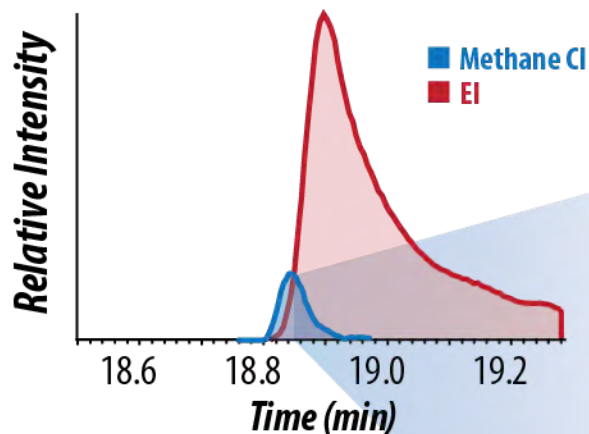


## Isotope Simulation

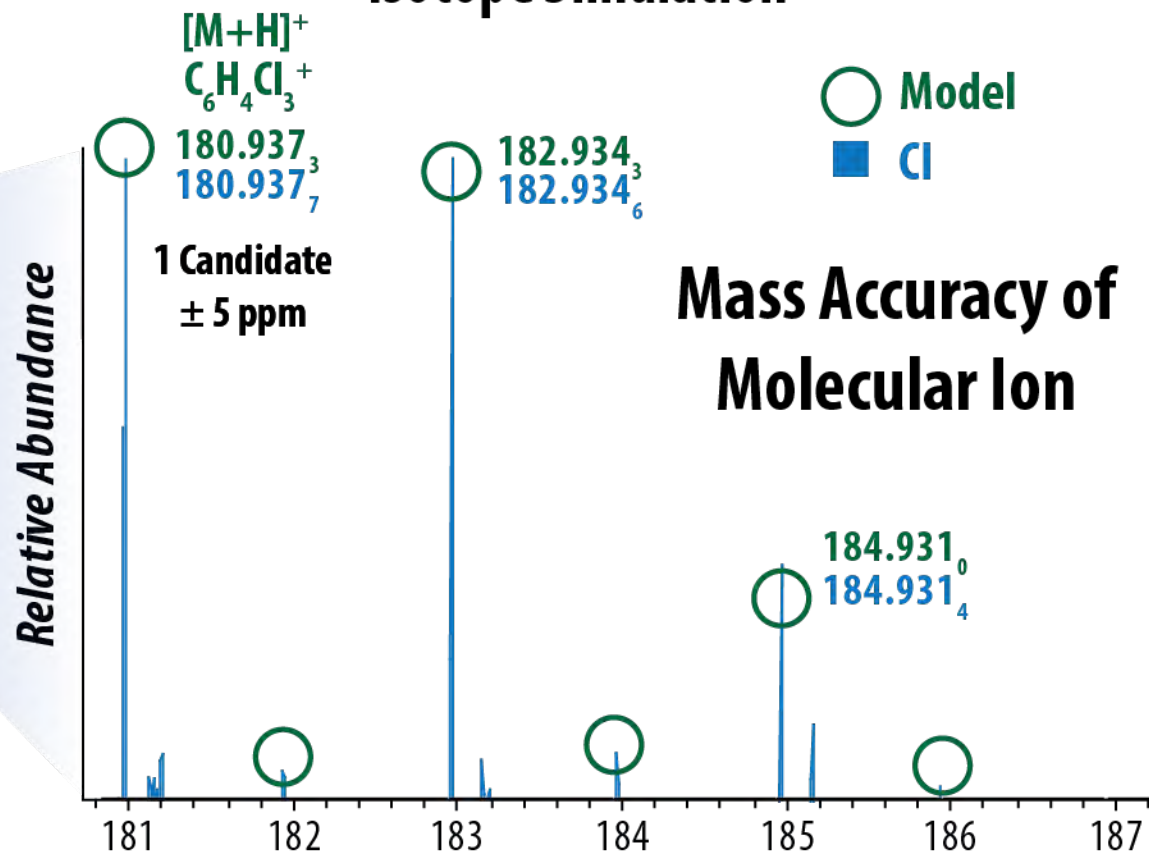


# Precursor Identification

Trichlorobenzene  
2 fg on column in Full Scan

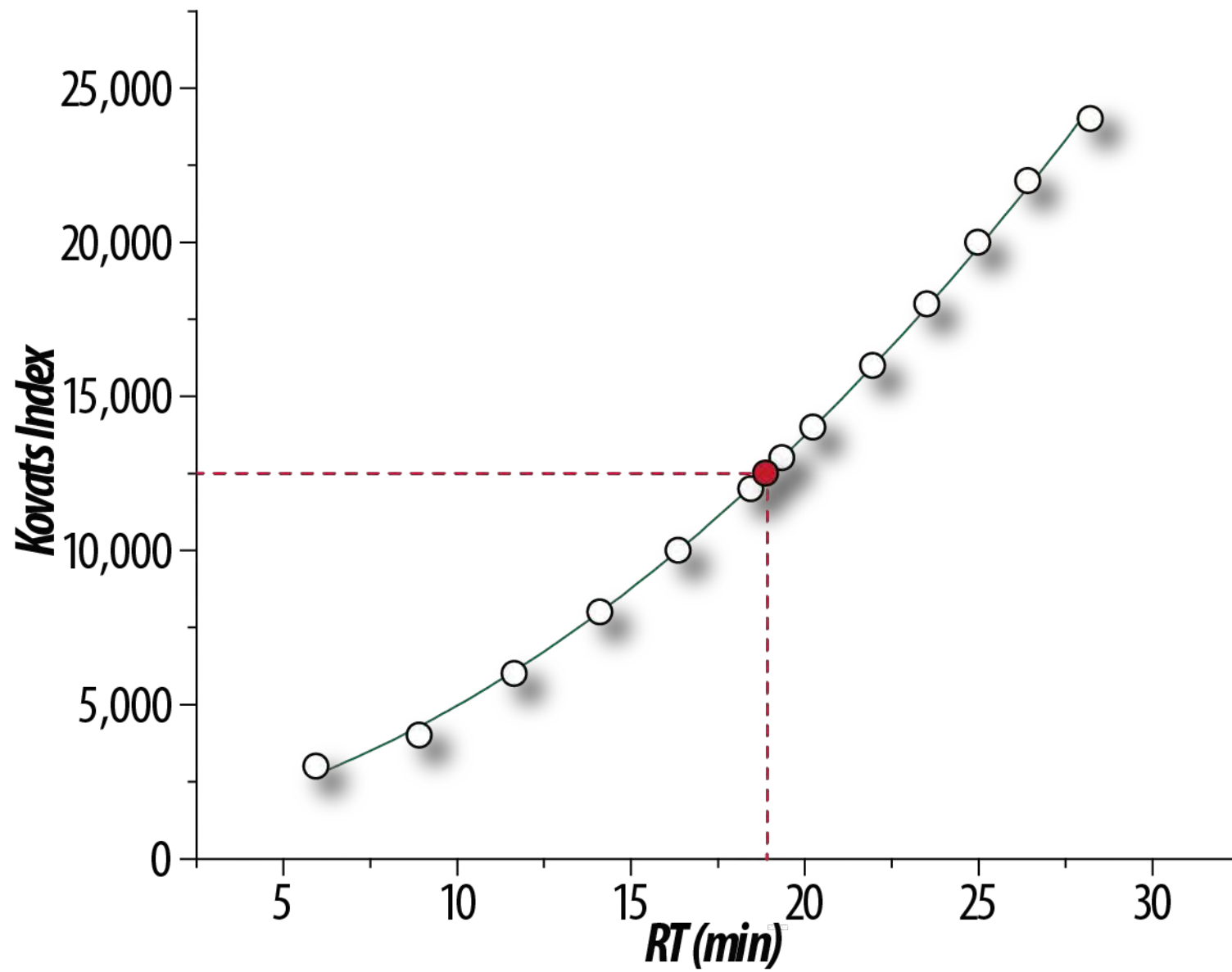


## Isotope Simulation

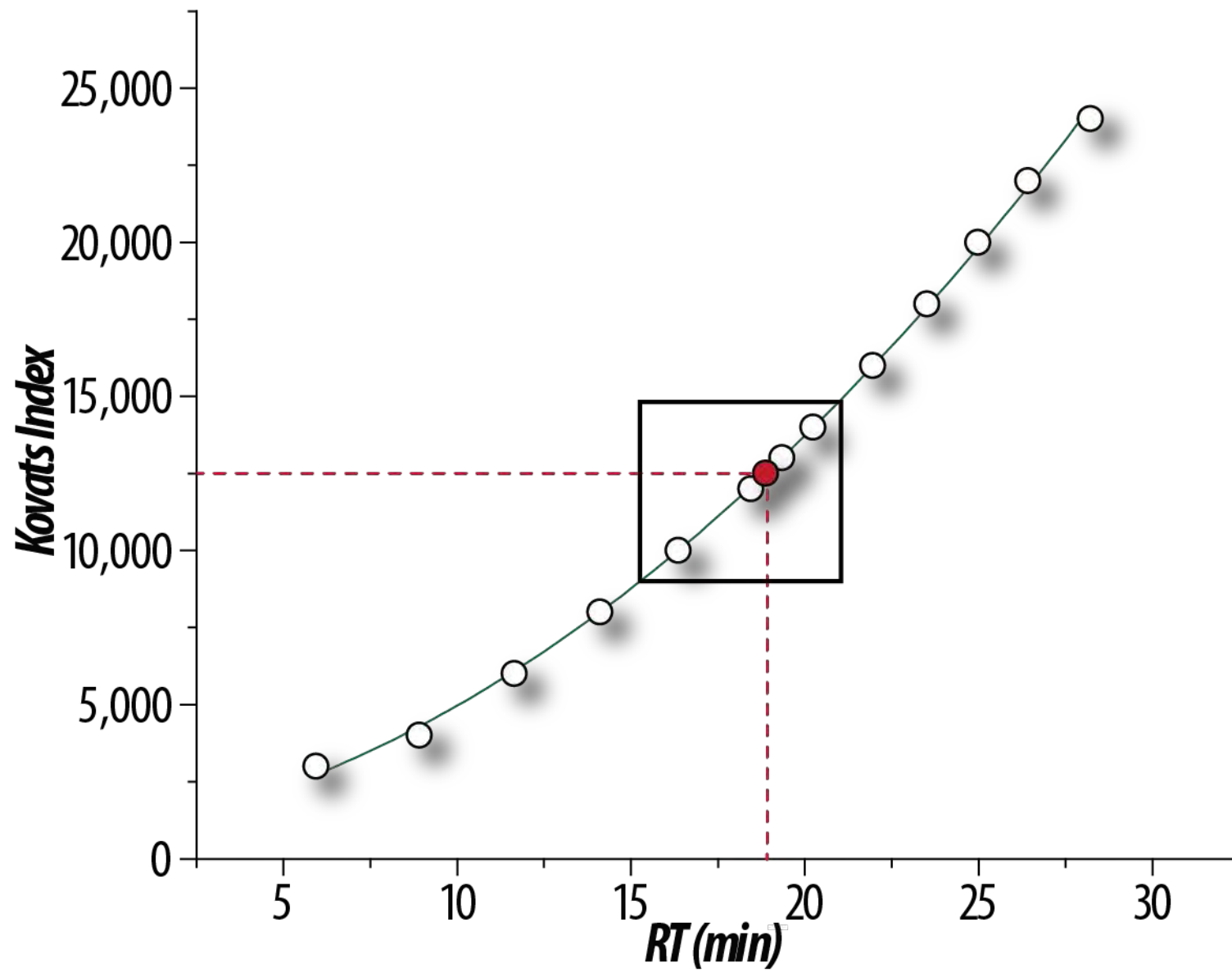


Mass Accuracy of  
Molecular Ion

# Kovat's Retention Indices

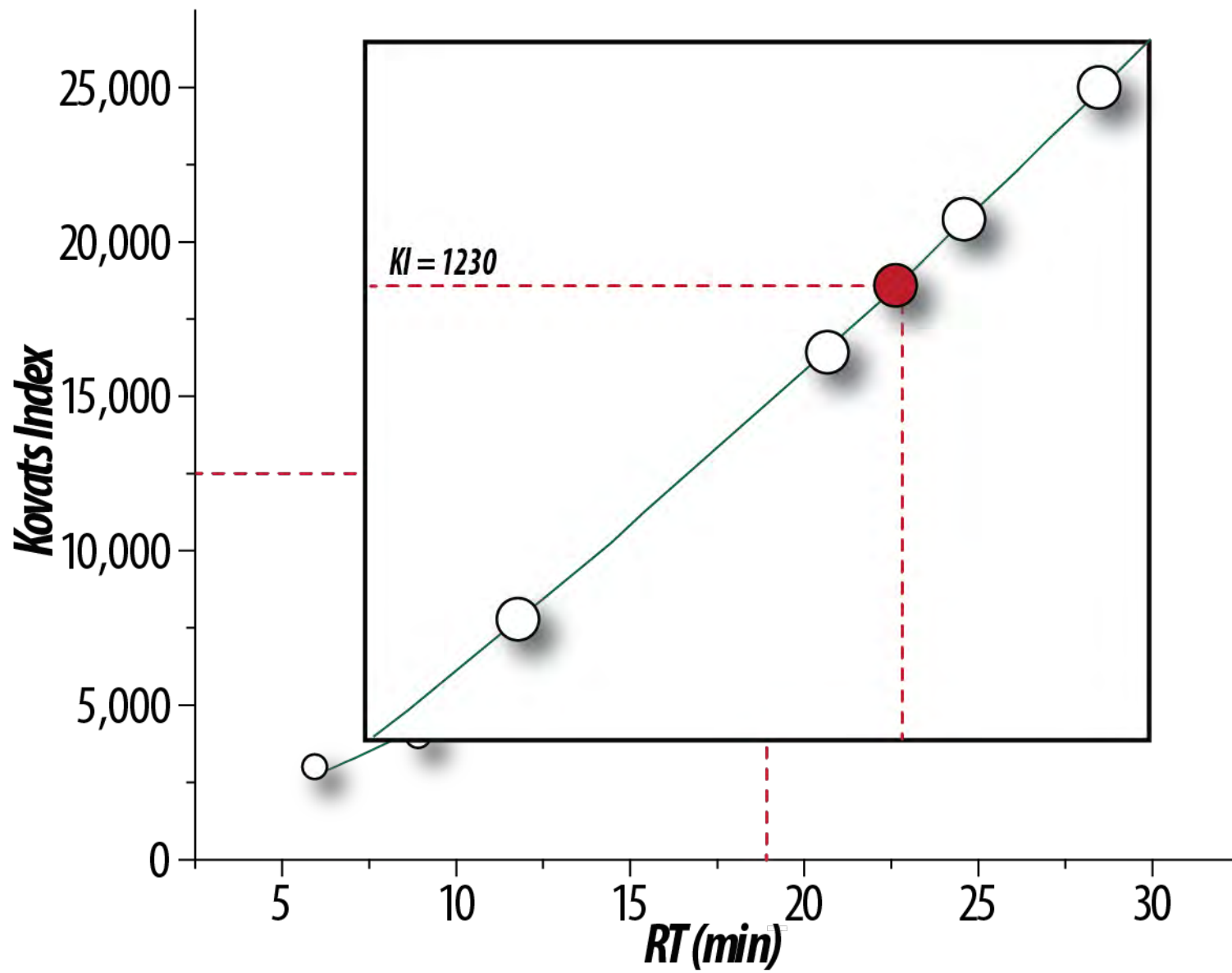


# Kovat's Retention Indices

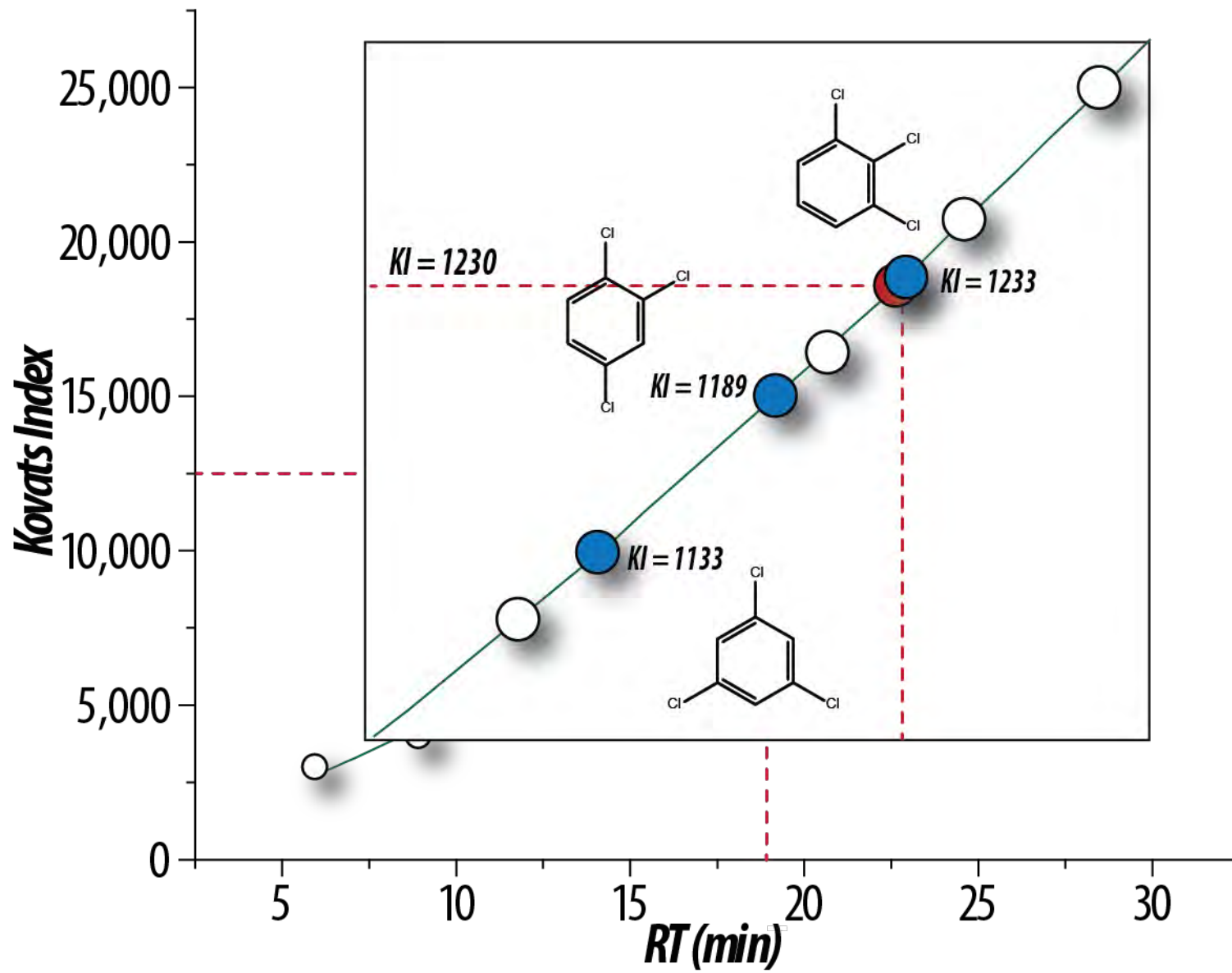




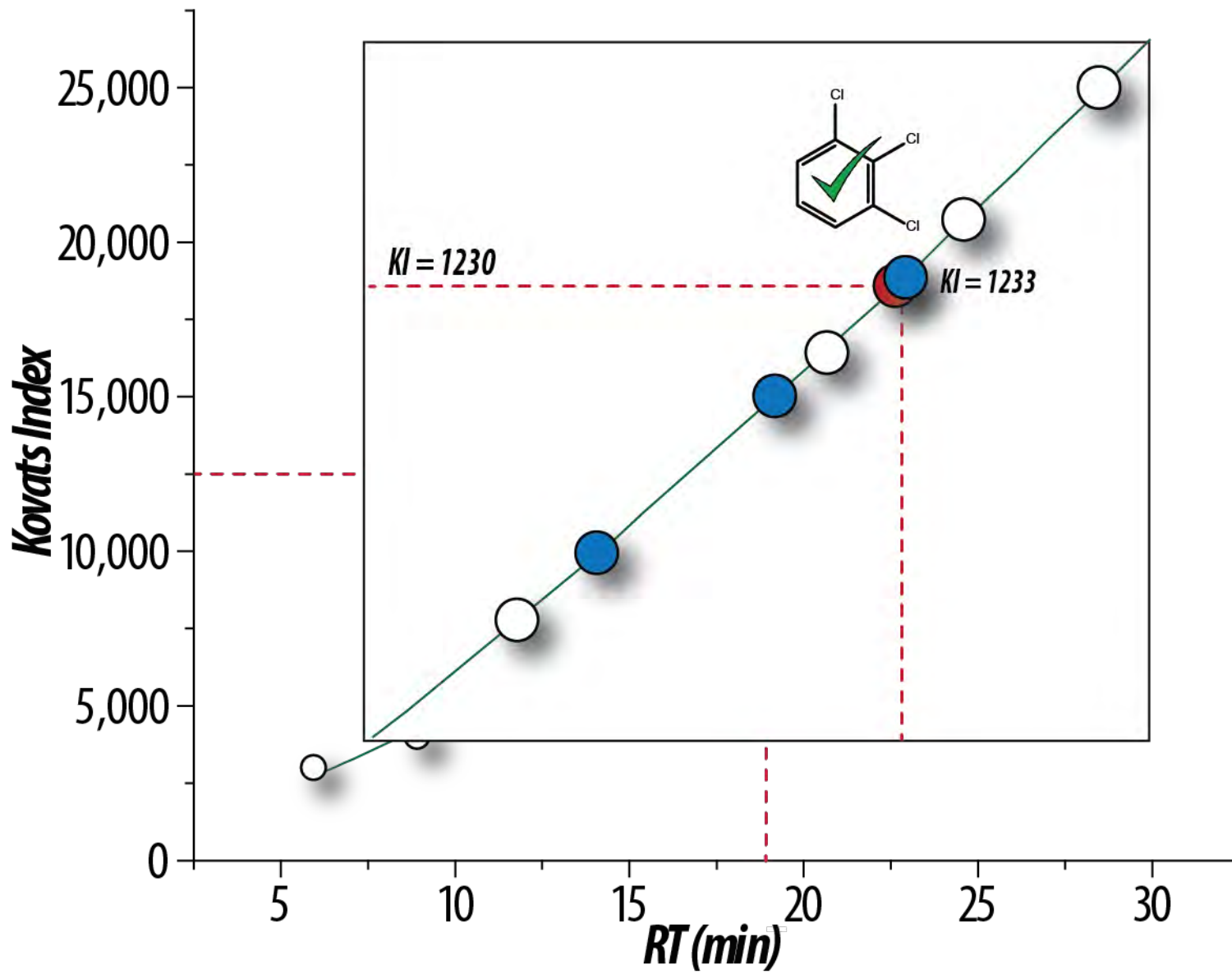
# Kovats's Retention Indices



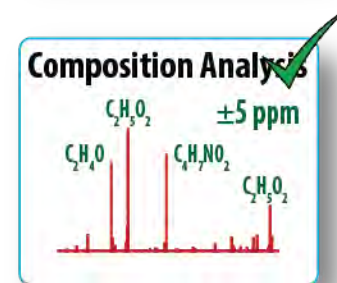
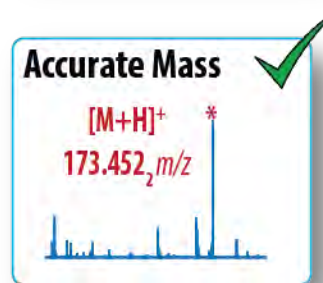
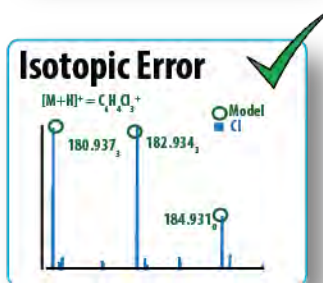
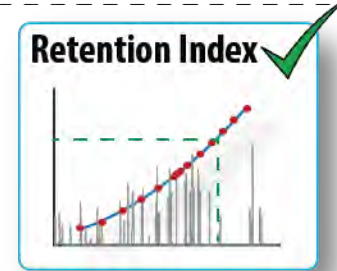
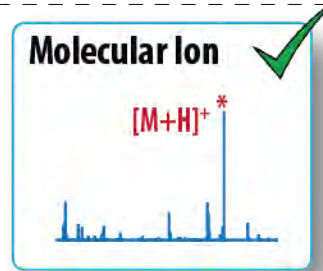
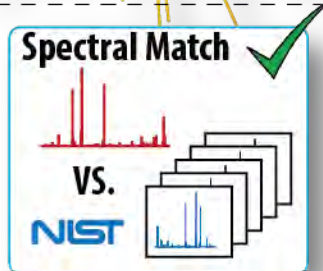
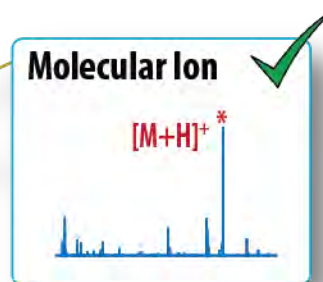
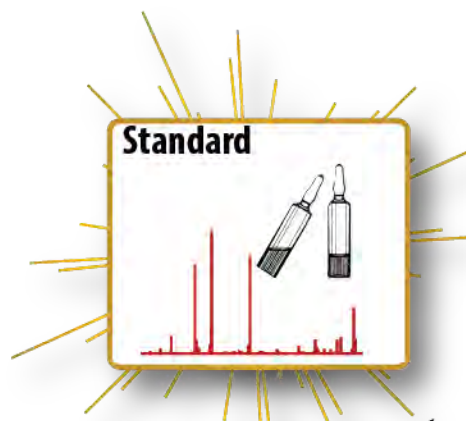
# Kovats's Retention Indices



# Kovats's Retention Indices



# Metabolomics Standards Initiative Criteria





# Quantitative Metabolomics by GC/Quadrupole Orbitrap

AJ Balloon, T Wahlig, JS Cole, NW Kwiecien,  
MS Westphall, M Sussman, JM Ané and JJ Coon

62<sup>ND</sup> ASMS Conference on Mass Spectrometry and Allied Topics  
June 19, 2014 • Baltimore, MD

**METABOLOMICS/LIPIDOMICS: New MS Technologies and Applications**





Derek Bailey  
Allison Balloon  
Molly McDevitt  
Elyse Freiburger  
Alex Hebert

Alan Higbee  
Nick Kwiecien  
Anna Merrill  
Catie Minogue  
Greg Potts

Tim Rhoads  
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Chris Rose  
Matt Rush

Evgenia Shishkova  
Michael Westphall  
Emily Wilkerson  
Clay Williams  
Arne Ulbrich



**Mike Sussman**

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**Taylor Wahlig**

Ané Group



**ThermoFisher**  
SCIENTIFIC