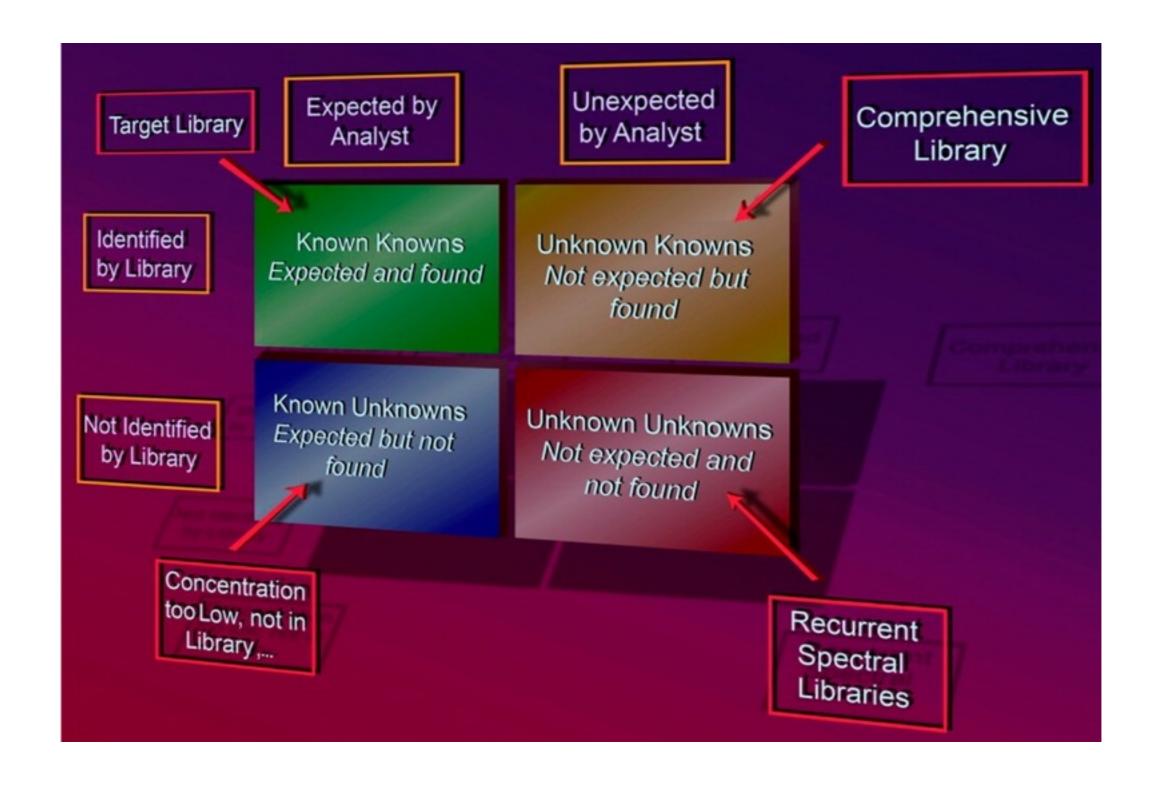
# Construct Consensus Mass Spectra for Unknown Metabolites

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### Introduction



Stein, S., Mass spectral reference libraries: an ever-expanding resource for chemical identification. Analytical chemistry **2012**, 84 (17), 7274-82.

### Introduction

• A sizable fraction of metabolites observed in GC/MS and LC/MS metabolomics are unknown.

• Fragmentation patterns of their ions provide information on the elemental composition and labile bonds of these ions.

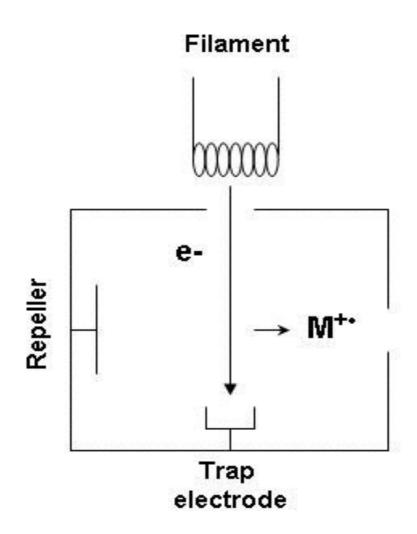
• Fragmentation mass spectra can be used for determining the identity of these unknown compounds.

• The fragmentation mass spectrum of an ion depends on the fragmentation energy.

### EI-GC-MS pectra

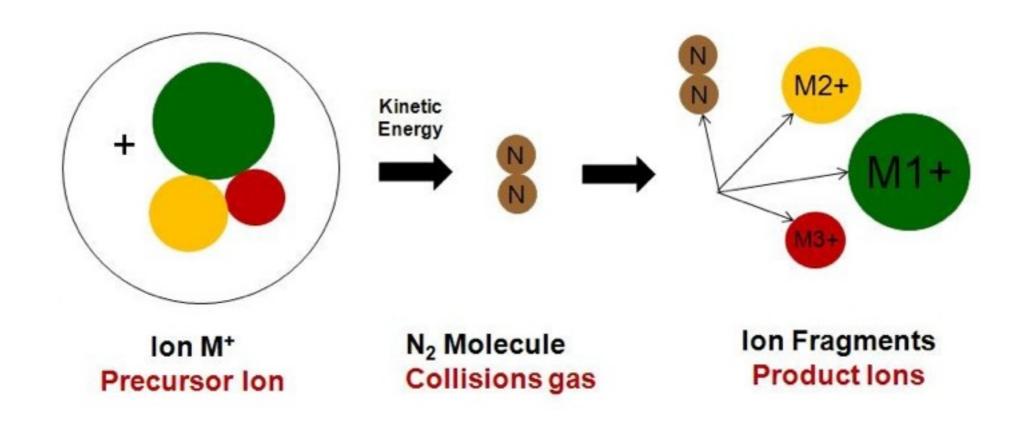
• For electron ionization used for GC/MS, fragmentation occurs following the ejection of an electron in a molecule.

• Fragmentation spectra are highly reproducible at the standard electron energy of 70eV.



### ESI-LC-MS spectra

• CID: collision induced dissociation



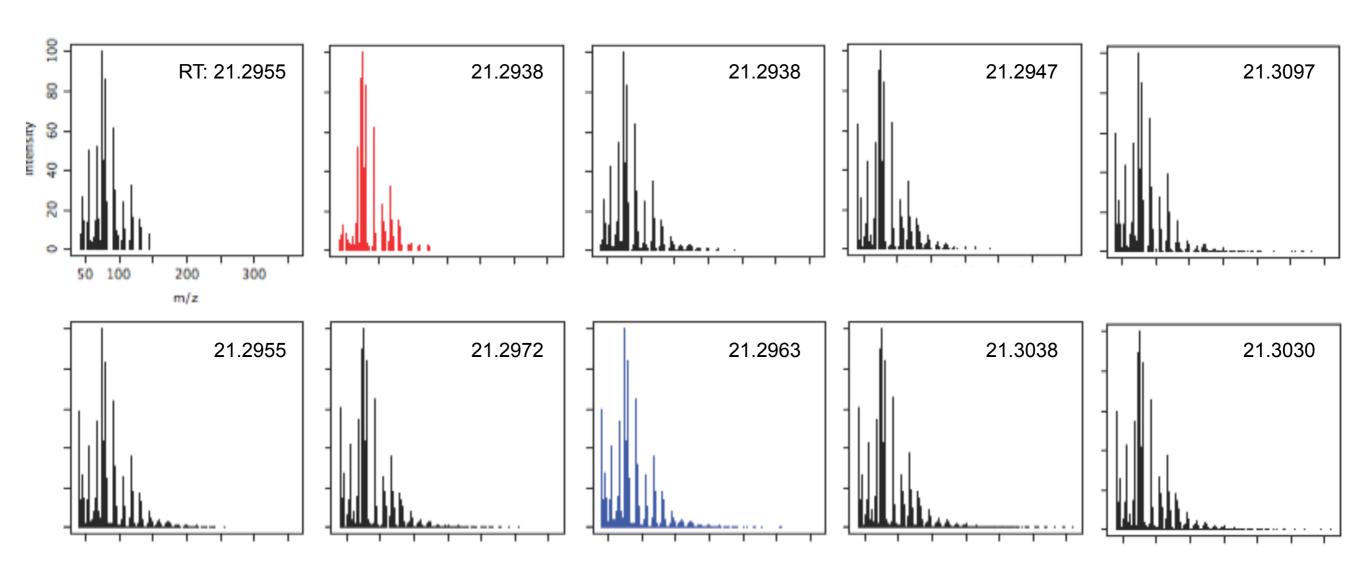
### Spectrum variation

#### Causes

- Low signal strength
- Contaminant peaks
- Co-fragmentation
- Differences in instrument conditions

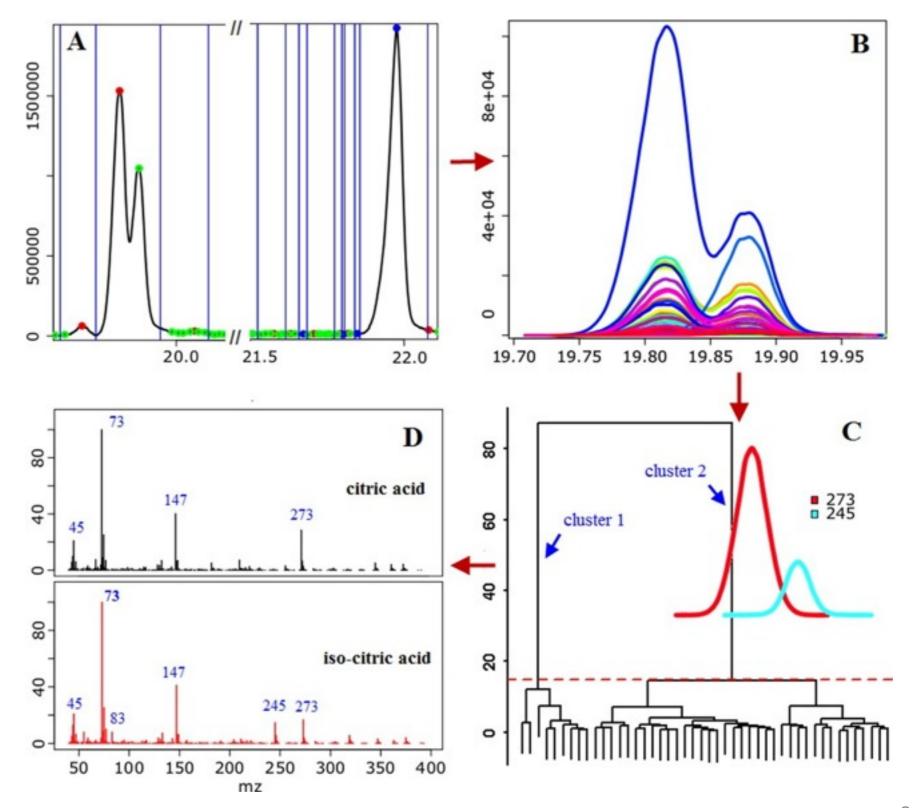
• As instrument sensitivity improves and lower concentration compounds are observed, the problem of spectrum variation worsens.

# Recurrent spectra



# Consensus spectra building

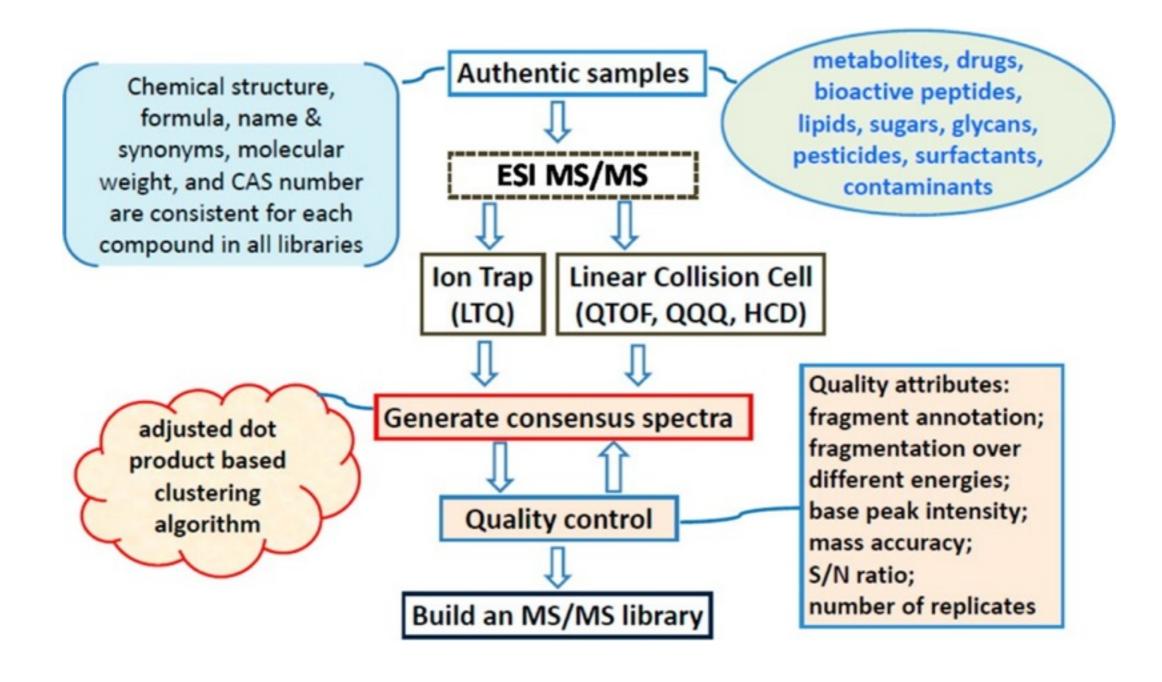
deconvolution



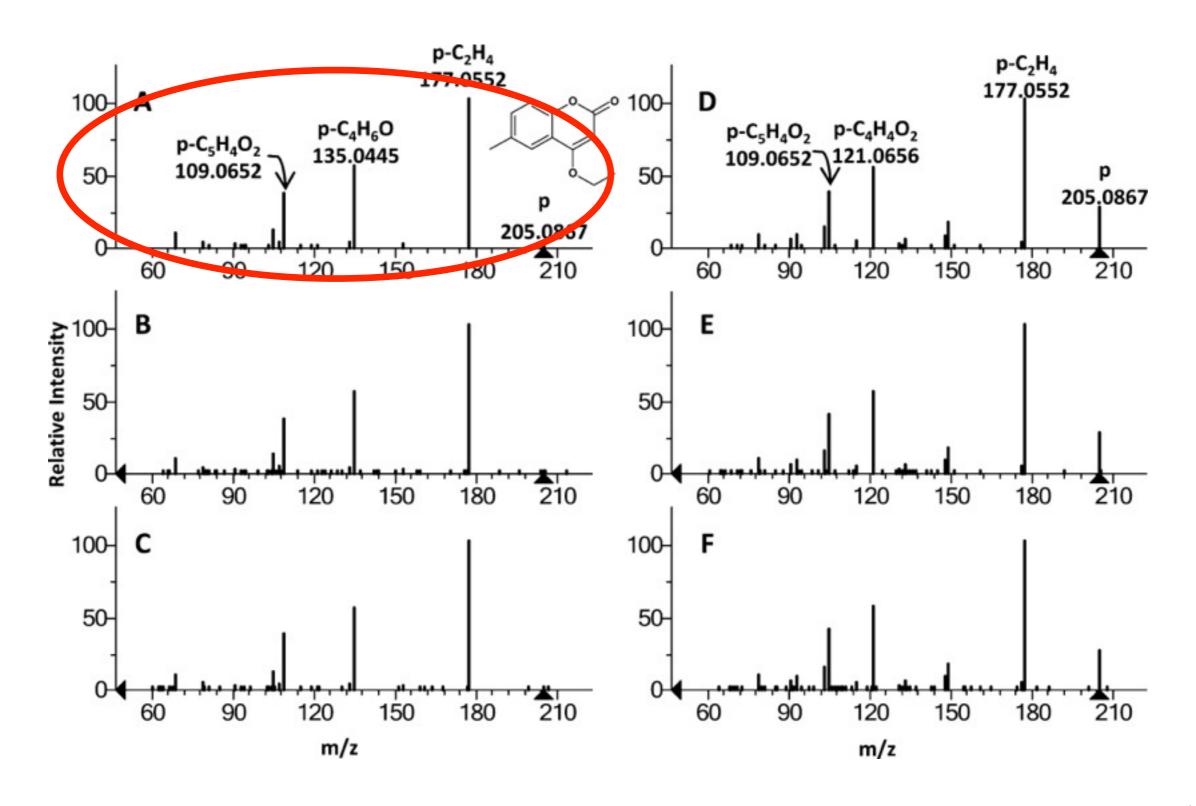
Ni, Y. et al., ADAP-GC 2.0: deconvolution of coeluting metabolites from GC/TOF-MS data for metabolomics studies. Analytical chemistry **2012**, 84 (15), 6619-29.

# Consensus spectra building

#### spectra clustering and quality control



# Consensus spectra building



Yang, X.; Neta, P.; Stein, S. E., Quality control for building libraries from electrospray ionization tandem mass spectra. Analytical chemistry **2014**, 86 (13), 6393-400.

