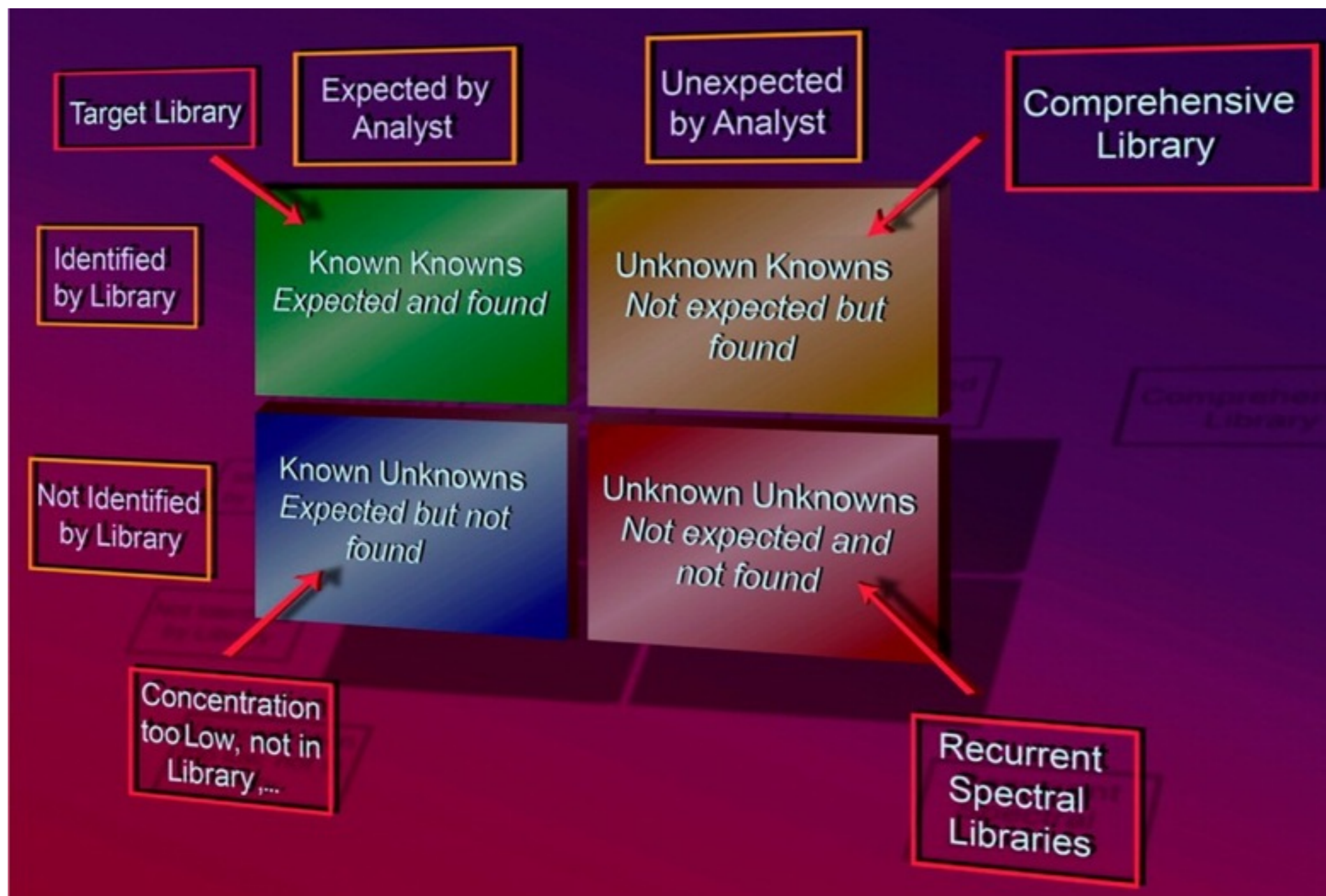


Construct Consensus Mass Spectra for Unknown Metabolites

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Introduction

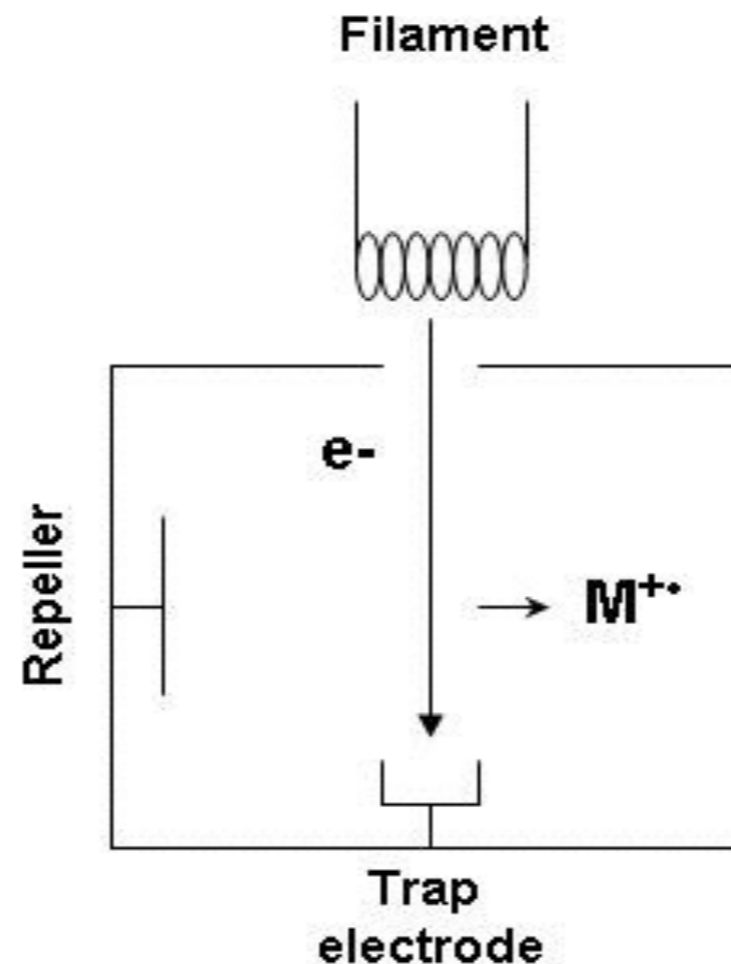


Introduction

- **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.**

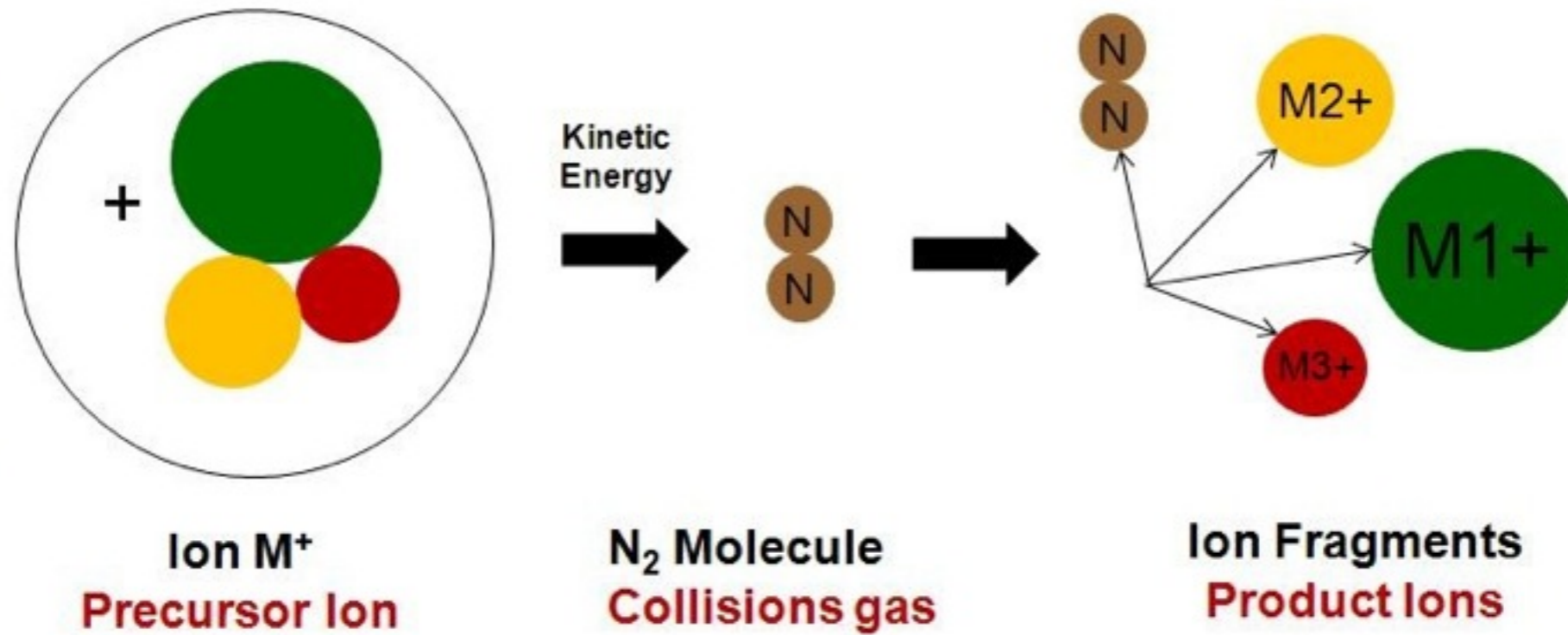
EI-GC-MS spectra

- 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**



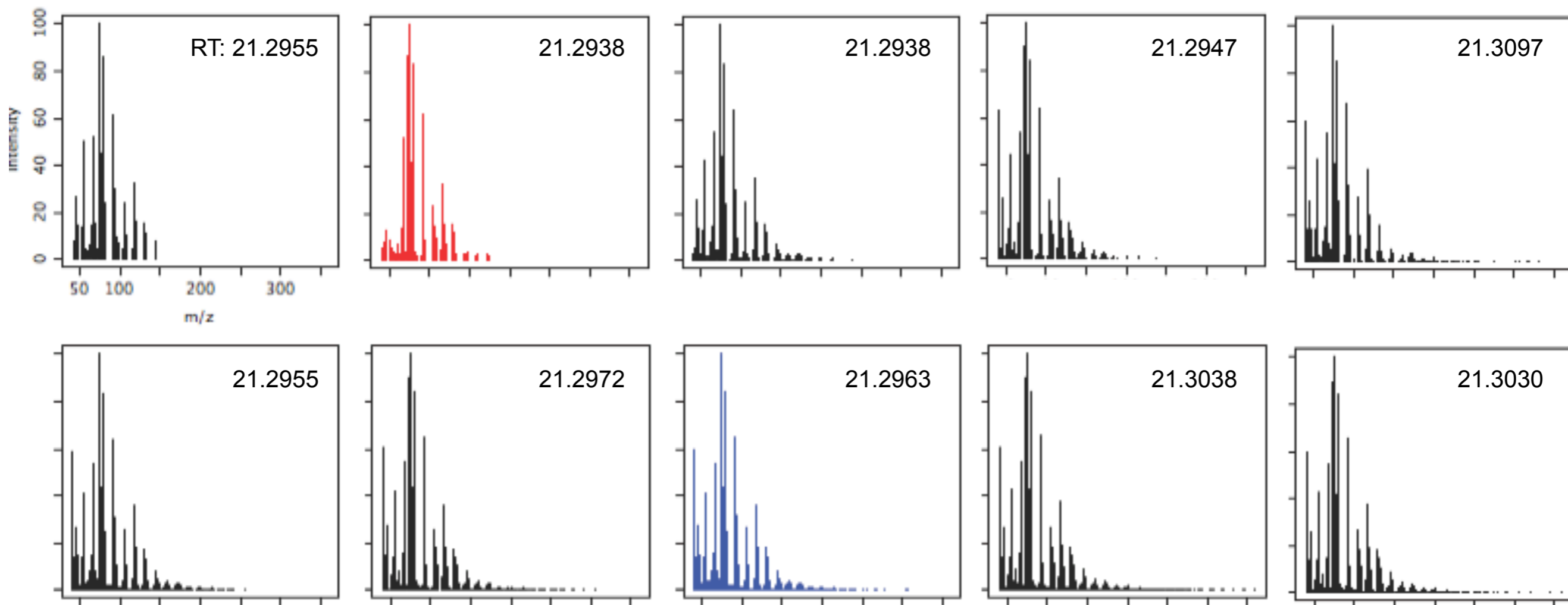
Spectrum variation

- **Causes**

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

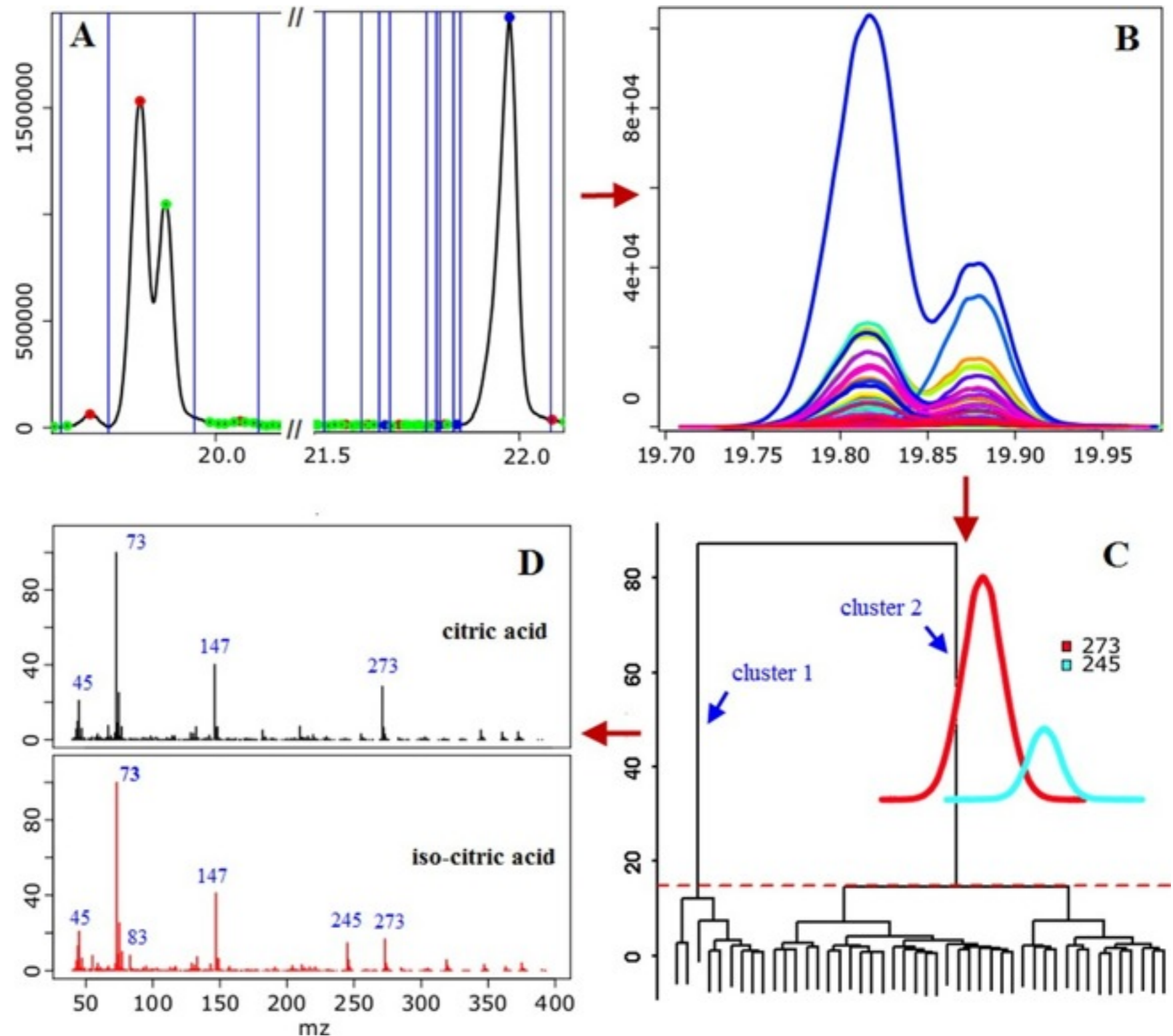
- **As instrument sensitivity improves and lower concentration compounds are observed, the problem of spectrum variation worsens.**

Recurrent spectra



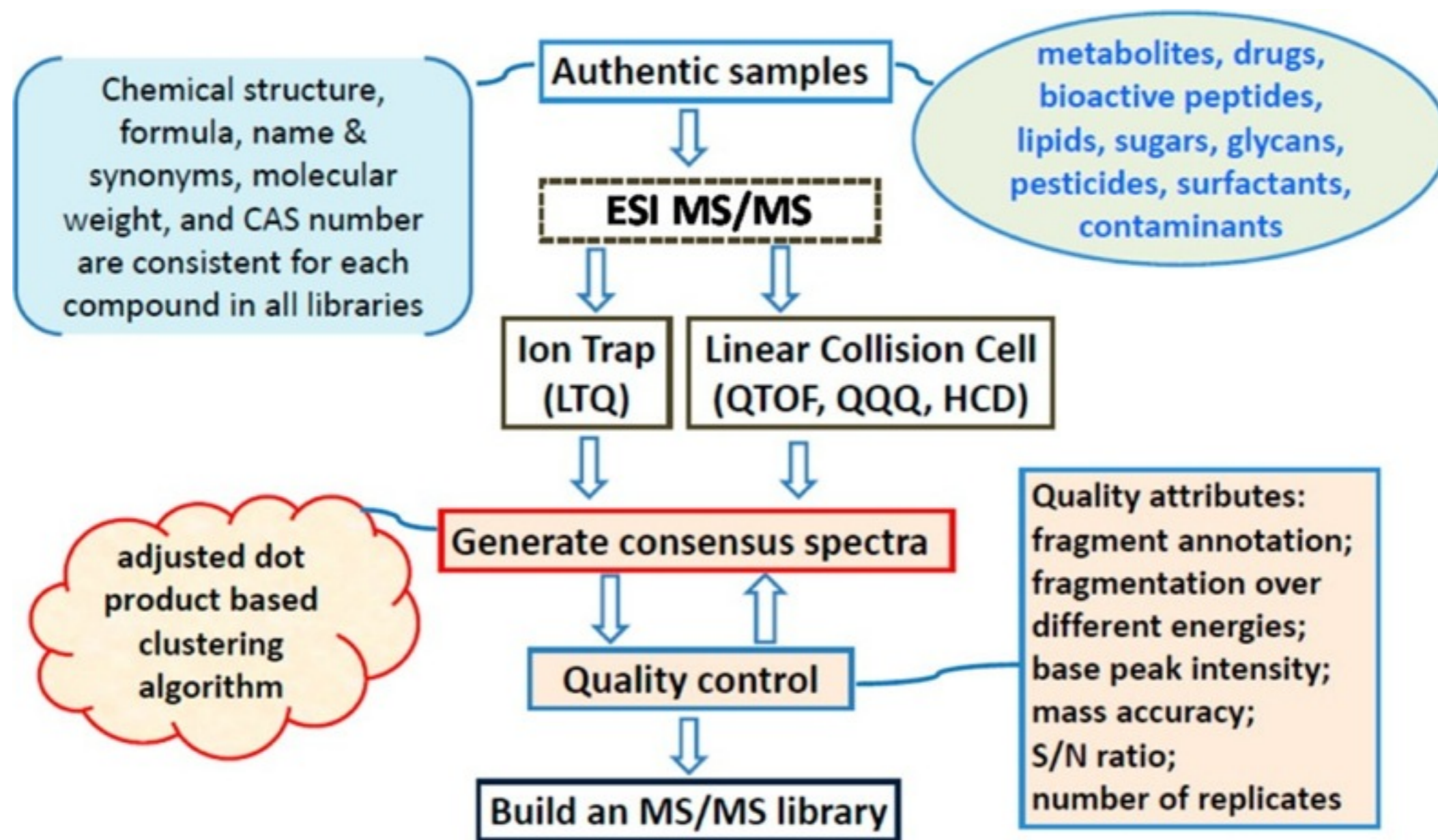
Consensus spectra building

deconvolution

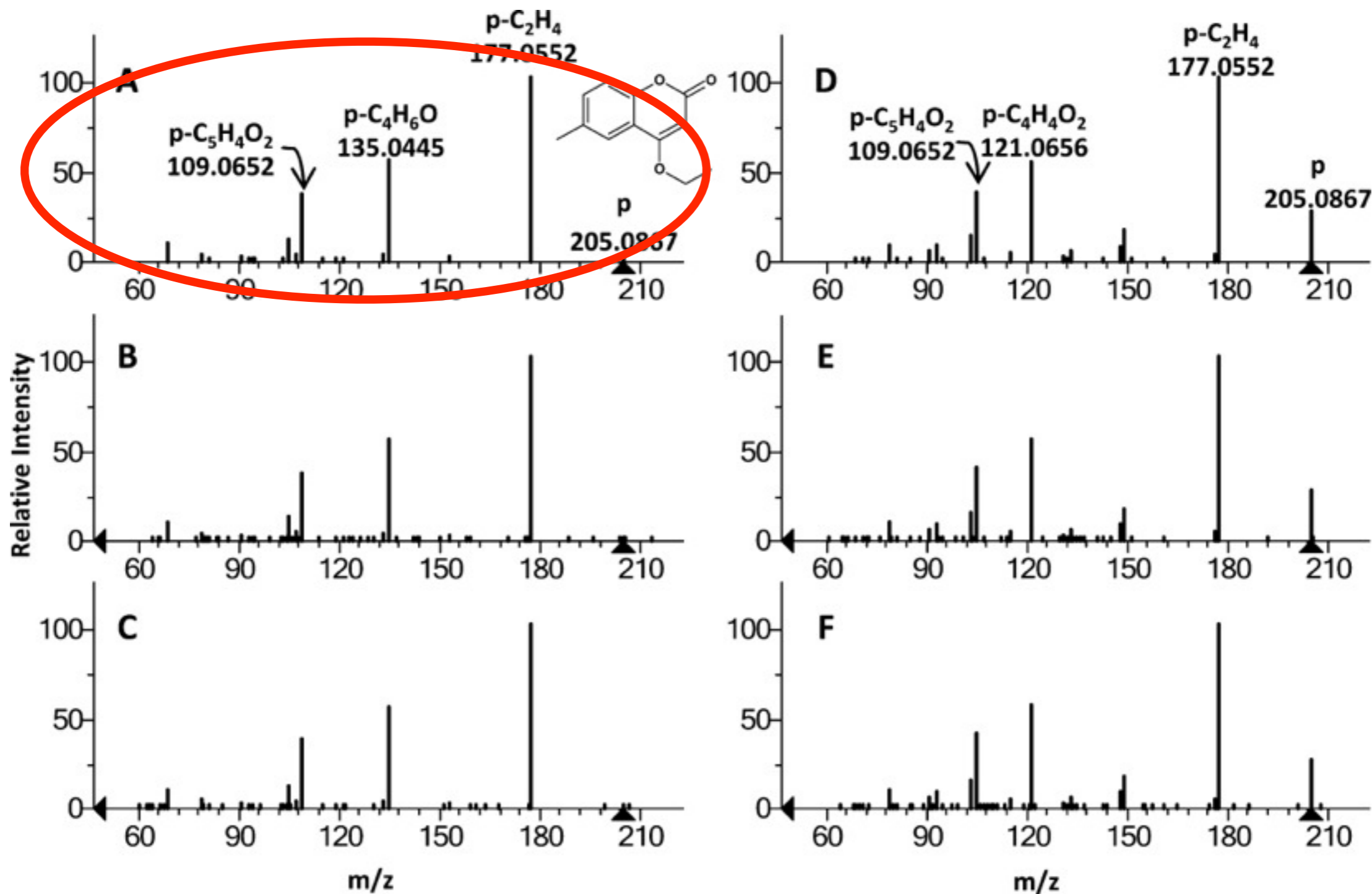


Consensus spectra building

spectra clustering and quality control



Consensus spectra building



With consensus spectra built, then what?