

## Metabolite Identification

### Mass Accuracy

- Sub-5 ppm for confident ID
- High-resolution mass spec
- Elemental formula prediction

### Isotope Patterns

- Natural isotope distribution
- Confirm molecular formula
- Chlorine/bromine signatures

### MS/MS Matching

- Fragment ion patterns
- Spectral library search
- In-silico fragmentation

### Standards Confirmation

- Authentic chemical standards
- Retention time matching
- Gold standard for identification