

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