

Excellent

Isotopocule ratios obtained on ESI-Orbitrap MS instrument that are fine-tuned for IRMS acquisition. Using isotopically characterized reference materials that are available for inter-laboratory comparisons and scale correction.

Level 1

High

Absolute

Good

Isotopocule ratios are calibrated using sample/standard comparison and applying the best practices (e.g., the principle of identical treatment). Data are publically available for re-analysis.

Level 2

High

Relative

Basic

Isotopocule ratios are determined using IRMS-relevant sample preparation, data acquisition, and signal-to-noise data.

Level 3

Known but low

None

Exploratory

Isotopocule ratios are determined using ion intensity signals or related metabolomics or proteomics procedures.

Level 4

Often unknown

None

Level of precision

Level of accuracy

