

QC Group	QC Metric Name	Level	Description
Area Ratio	Area2SumRatioCV	Transition	CV of the transition AUC to sum of transition AUCs across all samples for each transition.
Area Ratio	PeakGroupRatioCorr	Peak group	Correlation coefficient of transition AUC to sum of transition AUCs between endogenous and standard isotopes for each peak group for each sample.
Area Ratio	PairRatioConsistency	Transition pair	Consistency of the transition AUC to sum of transition AUCs between endogenous and standard isotopes for each transition pair for each sample
Area Ratio	MeanIsotopeRatioConsistency	Transition	Consistency of the transition AUC to sum of transition AUCs of the same isotope label across all samples for each transition for each sample.
Jaggedness	TransitionJaggedness	Transition	Jaggedness score for each transition for each sample. Jaggedness score is defined as the fraction of time points across a peak where the signal changes direction, excluding the peak apex.
Jaggedness	IsotopeJaggedness	Isotope	Mean of jaggedness scores of peaks with similar isotope label in a peak group for each sample.
Jaggedness	PeakGroupJaggedness.m	Peak group	Mean of jaggedness scores of all peaks in a peak group for each sample.
Symmetry	TransitionSymmetry	Transition	Symmetry score for each transition for each sample. Symmetry score is defined as the Pearson correlation coefficient between left and right half of the peak intensities.
Symmetry	IsotopeSymmetry	Isotope	Mean of symmetry scores of peaks with similar isotope label in a peak group for each sample.
Symmetry	PeakGroupSymmetry.m	Peak group	Mean of symmetry scores of all peaks in a peak group for each sample.
Similarity	PairSimilarity	Transition pair	Similarity score for each transition pair for each sample. Pair similarity score is defined as the Pearson

			correlation coefficient between peak intensities of two peaks.
Similarity	IsotopeSimilarity	Isotope	Mean of similarity scores of peak pairs with similar isotope label in a peak group for each sample.
Similarity	PeakGroupSimilarity.m	Peak group	Mean of similarity scores of all peak pairs in a peak group for each sample.
Modality	TransitionModality	Transition	Modality score for each transition for each sample. Modality score is defined as the largest unexpected dip in the peak, normalized by peak height.
Modality	IsotopeModality	Isotope	Mean of modality scores of peaks with similar isotope label in a peak group for each sample.
Modality	PeakGroupModality.m	Peak group	Mean of modality scores of all peaks in a peak group for each sample.
Shift	TransitionShift	Transition	Elution shift score for each transition for each sample. Elution shift score is defined as the difference between time at max intensity of each peak and the median of time at max intensities of all the peaks in the peak group normalized by the peak base width.
Shift	PairShift	Transition pair	Elution pair shift score for each transition pair for each sample. Shift score between two peaks is defined as the difference between the time at max intensities of the two peaks normalized by the peak base width.
Shift	IsotopeShift	Isotope	Mean of transition shift scores of peaks with similar isotope label in a peak group for each sample.
Shift	PeakGroupShift	Peak group	Mean of transition shift scores of all peaks in a peak group for each sample.
FWHM	TransitionFWHM	Transition	FWHM for each transition for each sample. (FWHM: full-width at half-max)
FWHM	TransitionFWHM2base	Transition	FWHM to peak base width ratio for each transition for each sample.

FWHM	IsotopeFWHM	Isotope	Mean of FWHM of peaks with similar isotope label in a peak group for each sample.
FWHM	IsotopeFWHM2base	Isotope	Mean of FWHM to peak base width ratios of peaks with similar isotope label in a peak group for each sample.
FWHM	PeakGroupFWHM.m	Peak group	Mean of FWHM of all peaks in a peak group for each sample.
FWHM	PeakGroupFWHM2base.m	Peak group	Mean of FWHM to peak base width ratios of all peaks in a peak group for each sample.
FWHM	PairFWHMConsistency	Transition pair	Consistency of the FWHM between endogenous and standard isotopes for each transition pair for each sample:
FWHM	MeanIsotopeFWHMConsistency	Transition	Consistency of the FWHM of the same isotope label across all samples for each transition for each sample.
Retention Time	MeanIsotopeRTConsistency	Transition	Consistency of the peak retention time of the same isotope label across all samples for each transition for each sample.
Intensity	TransitionMaxIntensity	Transition	Maximum peak intensity of each transition for each sample.
Intensity	TransitionMaxBoundaryIntensity	Transition	Maximum peak intensity at the peak boundary of each transition for each sample.
Intensity	TransitionMaxBoundaryIntensityNormalized	Transition	Maximum peak intensity at the peak boundary normalized by maximum peak intensity of each transition for each sample.