



# QCProt.V1 - Plot Description and Significance

Developed By - Sanjay S

Plot Name	Description	QC Significance
TIC Trace	Displays total ion current (TIC) intensity over retention time (RT).	Reflects chromatographic performance and overall signal stability; sudden drops or fluctuations indicate spray or LC instability.
BPC Trace	Plots intensity of the most abundant ion in each scan over RT.	Shows chromatographic peak quality and signal consistency; abrupt changes imply source or detector instability.
Scan Count per MS Level	Bar chart of total MS1 and MS2 scans acquired.	Verifies acquisition duty cycle consistency; imbalance may indicate acquisition errors or incomplete runs.
MS1 vs MS2 Ratio	Pie chart of MS1 and MS2 scan proportions.	Confirms balanced acquisition and fragmentation behavior across scans.
MS2 per Minute	Histogram of MS2 scan counts per minute of RT.	Evaluates fragmentation consistency; missing bins or drops suggest pauses or failed cycles.
Intensity Distribution (log10 TIC)	Histogram of log-transformed TIC intensities.	Assesses signal intensity, dynamic range and detector sensitivity.
Dynamic Range	Ratio of maximum to median TIC intensity.	Evaluates detector linearity and ionization consistency across the run.
m/z Density Distribution	Histogram of observed m/z values across scans.	Checks precursor mass range coverage; truncated ranges imply acquisition issues.
Charge State Distribution	Histogram of precursor charge states (MS2).	Evaluates ionization and fragmentation quality; irregular charge ratios indicate method or ion source issues.
MS2 Intensity Boxplot	Boxplot of mean MS2 fragment intensities per scan.	Reflects fragmentation efficiency and detector consistency.



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Fragment Count per Spectrum	Histogram of number of fragment peaks per MS2 spectrum.	Assesses spectral complexity; too few = poor fragmentation, too many = noisy spectra.
TIC per Scan	TIC intensity plotted against scan index.	Detects drift or acquisition inconsistencies throughout the run.
Noise Proxy Distribution	Histogram of 10th percentile fragment intensities.	Measures baseline noise; elevated values indicate contamination or unstable source.
Ion Flux Drift	Rolling mean TIC over retention time.	Monitors long-term signal stability; drift indicates source aging or gradient instability.
Overlaid TIC Traces	Overlay of TIC traces across all samples.	Compares chromatographic consistency and intensity reproducibility between runs.
TIC Correlation Heatmap	Pairwise Pearson correlation of binned TIC intensities.	Quantifies reproducibility between samples; low correlation reveals batch effects.
RT Density Overlay	Kernel density of RT distributions across runs.	Checks LC retention reproducibility; RT shifts indicate gradient or column issues.
Combined BPC Overlay	Overlaid base peak chromatograms for all runs.	Reveals intensity consistency and chromatographic performance differences.
Scan Count per MS Level (Grouped)	Grouped bar of MS1 and MS2 scan counts per sample.	Ensures acquisition settings are uniform across all runs.
MS1 vs MS2 Ratio (Stacked Bar)	Stacked bar of MS1 and MS2 scan percentages per sample.	Validates balanced acquisition across all injections.
MS2 per Minute Overlay	Overlay of MS2 scan frequency per minute across runs.	Highlights acquisition pauses or inconsistent fragmentation rates.



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Intensity Histogram Overlay	Overlay of log10 TIC intensity distributions across samples.	Checks for consistent detector response and sensitivity across runs.
Dynamic Range per Sample	Bar plot of dynamic range (max/median TIC) for each sample.	Detects variations in detector response or sample loading.
m/z Density Overlay	Overlaid m/z distributions for all runs.	Ensures identical precursor coverage across all samples.
Charge State Heatmap	Heatmap of charge-state counts (samples Å— charge).	Identifies ionization inconsistencies or charge bias across runs.
MS2 Intensity Boxplot (Across Samples)	Boxplot of average MS2 intensities for each sample.	Compares fragmentation efficiency and detector performance reproducibility.
Fragment Count Overlay	Overlay of fragment count histograms across samples.	Assesses spectral complexity consistency between runs.
Normalized TIC per Scan Overlay	TIC normalized to [0Å€1] overlaid for all runs.	Highlights chromatographic shape similarity independent of intensity.
Noise Proxy Overlay	Overlay distributions of 10th percentile fragment intensities.	Evaluates noise baseline uniformity across all injections.
Ion Flux Drift Overlay	Overlay of rolling mean TIC traces for all runs.	Reveals shared signal drift patterns or gradient inconsistencies.
RT Density Overlay (Numbered)	RT density distribution (numbered MultiQC variant).	Provides visual fingerprint of retention behavior across all runs.