

Supporting information for “Communicating mass spectrometry quality information in mzQC with Python, R, and Java”

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Supplementary Table 1: QC metrics considered during the analysis and their accession numbers in the PSI-MS controlled vocabulary. The last column refers to the programming language used to compute the metrics.

Accession	Metric	Programming Language
MS:1000505	base peak intensity	Java
MS:1002404	count of identified proteins	Python
MS:1003044	number of missed cleavages	Python
MS:1003250	count of identified peptidofoms	Python
MS:1003251	count of identified spectra	Python
MS:4000060	number of MS2 spectra	Python
MS:4000069	m/z acquisition range	Java
MS:4000070	retention time acquisition range	Java
MS:4000071	number of chromatograms	Java
MS:4000104	total ion currents	Java
MS:4000132	MS1 ion collection time mean	R
MS:4000133	MS1 ion collection time sigma	R
MS:4000137	MS2 ion collection time mean	R
MS:4000138	MS2 ion collection time sigma	R
MS:4000178	precursor ppm deviation mean	Python
MS:4000179	precursor ppm deviation sigma	Python
MS:4000180	table of missed cleavage counts	Python
MS:4000181	identified MS2 quarter RT fraction	Python