

Supplemental Table 1: Selected Parameter Settings for xMSwrapper.apLCMS Function for QExactive

Package	Parameter	Description	Value(s)
apLCMS	Min.run.list	Minimum footprint of a feature in retention time (s)	c(4,3)
	Min.pres.list	Minimum presence of signal over retention time window (p)	c(0.5,0.8)
	Minexp.pct	Minimum prevalence of feature across all spectra (p)	0.1
xMSanalyzer	Max.mz.diff	m/z tolerance for feature matching (ppm)	10
	Max.rt.diff	Retention time tolerance for feature matching (s)	300
	Feat.filt.thresh	Threshold for filtering samples based on CoV (%)	30
	Samp.filt.thresh	Threshold for filtering samples based on correlation between triplicates (p)	0.1

(s) = seconds; (p) = proportion; ppm = parts per million; % = percent