S13 Table. (a) Rules for checking for m/z agreement between 2 ions.

Ion Mode 1	Ion Mode 2	Setting	d
Positive	Positive	No adduct	0
Positive	Positive	Adduct	0 and pairwise m/z differences between the positive ions
Negative	Negative	No adduct	0
Negative	Negative	Adduct	0 and pairwise m/z differences between the negative ions
Positive	Negative	No adduct	m/z difference between [M+H]$^+$ and [M-H]$^-$
Positive	Negative	Adduct	m/z differences between each pair of positive and negative ions
Negative	Positive	No adduct	m/z difference between [M-H]$^-$ and [M+H]$^+$
Negative	Positive	Adduct	m/z differences between each pair of negative and positive ions

S13 Table. (b) m/z values of different adduct ions included in "adduct" settings.

Ion Mode	Ion	m/z value [1]
Positive	M$^+$	m
	[M+H]$^+$	m + 1.007276
	[M+NH$_4$]$^+$	m + 18.033823
	[M+Na]$^+$	m + 22.989218
Negative	[M-H]$^-$	m − 1.007276

m is the mass of the analyte molecule M. Additional or alternative adduct ions may be specified when running the m/z checking algorithm (see documentation on https://github.com/yuhanhsu/PAIRUP-MS).

References

1.   Huang N, Siegel MM, Kruppa GH, Laukien FH. Automation of a Fourier transform ion cyclotron resonance mass spectrometer for acquisition, analysis, and e-mailing of high-resolution exact-mass electrospray ionization mass spectral data. Journal of the American Society for Mass Spectrometry. 1999;10(11):1166-73. doi: 10.1016/s1044-0305(99)00089-6.