Table S1. Parameter settings for MS-DIAL data processing

Parameter	Value	Parameter	Value
Data collection parameters		Identification parameters	
Retention time range	0–15 min	MS1 tolerance	0.02 Da
Mass range	80–1000 m/z	MS2 tolerance	0.025 Da
Centroid parameters		Identification score cut-off	>80%
MS1 tolerance	0.02 Da	Use retention time for scoring	FALSE
MS2 tolerance	0.025 Da	Use retention time for filtering	FALSE
Isotope recognition		Only report the top hit	TRUE
Maximum charged number	2	Adduct ion setting	
Peak detection parameters		Positive ion mode	[M+H]+
Smoothing method	Linear weighted moving average	Negative ion mode	[M−H]−
Smoothing level	3 scans	Alignment parameters	
Minimum peak width	5 scans	Retention time tolerance	0.05 min
Minimum peak height	500 amplitude	MS1 tolerance	0.015 Da
Peak spotting parameters		Retention time factor	0.5
Mass slice width	0.1 Da	MS1 factor	0.5
Deconvolution parameters		Peak count filter	0%
Sigma window value	0.5	N% detected in at least one group	50%
MS2Dec amplitude cut-off	10 amplitude	Keep identified and annotated metabolites	TRUE
Exclude after precursor	TRUE	Gap filling by compulsion	TRUE
Keep isotope until	0.5 Da		
Keep original precursor isotopes	FALSE		