

Supplementary Table S1. Deconvolution parameters used for Orbitrap GC-MS data.

Tool	Function	Parameter	Value
XCMS v3.6	xcmsSet	useOriginalCode	true
		method	machtedFilter
		fwhm	3
		step	0.001
		steps	2
		max	1000
		snthresh	3
		mzdiff	0.002
		method	Density
		bw	5
		mzwid	0.002
		minsamp	1
		minfrac	0.5
		max	1000
	retcor	method	obiwarp
	group (2)	method	density
		bw	2
		mzwid	0.002
		minsamp	1
		minfrac	0.5
		max	1000
	fillpeaks	-	-
CAMERA v1.4	xsAnnotate	sample	NA
		polarity	positive
	groupFWHM	sigma	6
		perfwfm	2
		intval	maxo
	groupCorr	cor_eic_th	0.8
custom script		calcCaS	true
		min.clustersize	20