



Research article

Global metabolome changes induced by environmentally relevant conditions in a marine-sourced *Penicillium restrictum*

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Supplementary Table S1. Parameters used for automatic peak picking using MZmine 2

Step	Parameter	Positive ionization mode	Negative ionization mode
(1)	Crop filter		
	Retention time	0.66–45 min	0–45 min
(2)	Mass detection		
	Mass detection, mass detector	Centroid	Centroid
	Noise level	2.1E4	1.2E4
	Scans MS level	1	1
(3)	Chromatogram builder		
	Algorithm	ADAP Chromatogram builder	ADAP Chromatogram builder
	Min group size in \neq of scans	2	2
	Group intensity threshold	6E4	2E4
	Min highest intensity	2.1E4	1E4
	m/z tolerance	30 ppm	20 ppm
(4)	Chromatogram deconvolution		
	Algorithm	Wavelets ADAP	Wavelets ADAP
	S/N threshold	10	10
	S/N estimator	Intensity window SN	Intensity window SN
	Minimum feature height	20	100
	Coefficient/area threshold	150	110
	Peak duration range	0.0–10	0.0–10
	RT wavelet range	0.0–0.20	0.0–0.07
(5)	Isotope peak grouper		
	m/z tolerance	30 ppm	20 ppm
	Retention time tolerance	1.8 min	0.5 min
	Maximum charge	2	2
	Representative isotope	Lowest m/z	Lowest m/z
(6)	Normalisation		
	m/z tolerance	30 ppm	20 ppm
	RT tolerance	1.8 min	0.5 min
	Minimum standard intensity	2E5	1E4
(7)	Join aligner		
	Algorithm	Ransac aligner	Ransac aligner
	m/z tolerance	0.0 m/z or 30 ppm	50 ppm
	RT tolerance	1.8 absolute (min)	0.7 absolute (min)
	RT tolerance after correction	1.8 absolute (min)	0.7 absolute (min)
	Ransac iterations	200,000	20,000
	Minimum number of points	50.0%	50.0%
	Threshold value	1	1
	Linear model		
(8)	Peak list rows filters		
	Minimum peaks in a row	4	4
(9)	Grap filling		
	Algorithm	Peak finder (multithreaded)	Peak finder (multithreaded)
	Intensity tolerance	50%	30%
	m/z tolerance	30 ppm	20 ppm
	Retention time tolerance	1.8 min absolute	0.7 min absolute