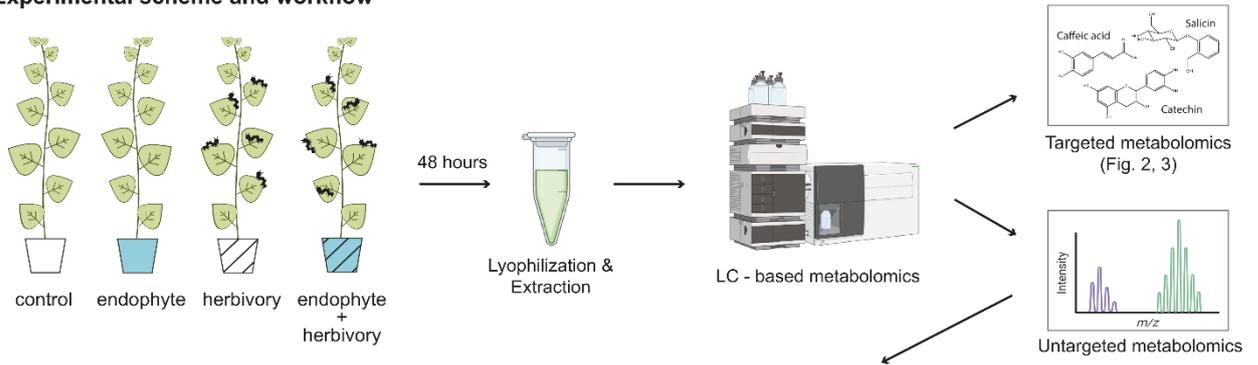
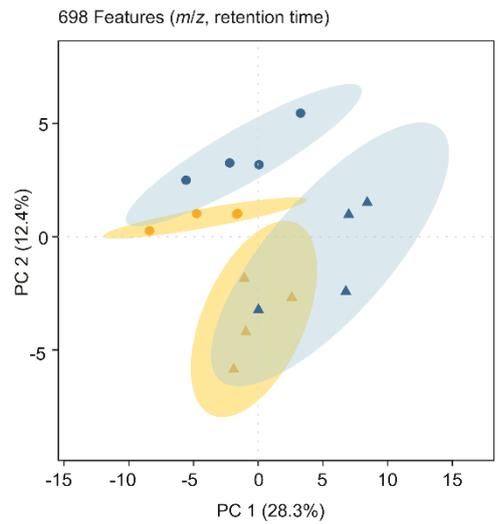


(a) Experimental scheme and workflow

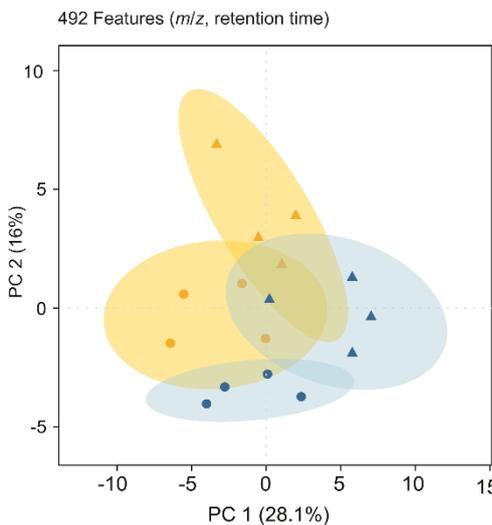


(b) Positive polarity



	control	endophyte	herbivory	endophyte + herbivory	Significant features
					Mass (Da), RT (min), Formula, Putative identification
I					707.2208 0.79 C ₂₇ H ₃₈ N ₂ O ₂₀
					476.1611 0.79 C ₂₇ H ₃₈ NO ₁₅
					107.0492 8.64 C ₁₇ H ₂₆ O ₁₁
					593.1416 9.39 C ₂₉ H ₃₈ O ₁₁
					585.1355 7.83
					505.1105 6.62 C ₂₇ H ₃₆ O ₁₁
					457.2193 6.35
					455.1108 7.77
					429.0945 7.42 C ₂₀ H ₂₂ O ₆
					421.1256 6.93 C ₂₀ H ₂₂ N ₂ O ₅ S ₂
III					349.0683 5.64 C ₁₈ H ₁₈ O ₅
					335.0705 5.64 C ₁₈ H ₁₈ O ₅
					325.0894 1.41 C ₁₇ H ₁₈ N ₂ O ₆
					319.1362 1.38 C ₁₇ H ₁₈ O ₈
					309.0735 4.01 C ₁₇ H ₁₈ N ₂ O ₅
					289.0707 2.80 C ₁₇ H ₁₈ O ₆
					279.1438 2.75 C ₁₇ H ₁₈ O ₇
					227.1278 4.17 C ₁₇ H ₁₈ O ₇
					136.0618 3.11 C ₁₁ H ₁₅ N ₂ O ₅ S ₁
					455.1167 0.76
II					293.0651 0.77
					290.8473 0.72
					206.8859 0.72
					144.1020 0.81 C ₈ H ₁₁ NO ₂
					777.2380 8.17 C ₃₅ H ₃₉ N ₂ O ₃ PS
					564.1384 9.07
					511.1598 9.06 C ₂₇ H ₃₆ O ₁₀
					439.0373 0.75
					112.8957 0.73

(b) Negative polarity



Legend PCA
 ● control ▲ herbivory
 ● endophyte ▲ endophyte + herbivory



	control	endophyte	herbivory	endophyte + herbivory	Significant features
					Mass (Da), RT (min), Formula, Putative identification
III					527.1557 7.82 C ₂₇ H ₃₈ O ₁₁
					331.1035 3.07 C ₁₇ H ₁₈ O ₇
					591.1710 7.82 C ₂₈ H ₃₈ O ₁₄
					839.3348 5.37 C ₂₈ H ₃₈ O ₁₉
					573.1612 8.64 C ₂₇ H ₃₈ O ₁₁
					599.1769 9.39 C ₂₉ H ₃₈ O ₁₁
					585.1612 6.50 C ₂₉ H ₃₈ O ₁₃
					479.1559 7.42 C ₂₇ H ₃₈ O ₁₁
					465.1408 5.76 C ₂₇ H ₃₈ O ₁₁
					461.1451 7.77 C ₂₇ H ₃₈ O ₁₁
II					435.1295 7.41 C ₂₇ H ₃₈ O ₈
					423.1295 6.47 C ₂₇ H ₃₈ O ₁₀
					421.1139 7.26 C ₂₇ H ₃₈ O ₁₀
					421.1138 5.53 C ₂₇ H ₃₈ O ₁₀
					323.1348 2.76 C ₁₇ H ₁₈ O ₇
					277.1293 2.90 C ₁₇ H ₁₈ O ₇
					271.0823 3.49 C ₁₇ H ₁₈ O ₇
					471.0756 0.74 C ₁₇ H ₁₈ N ₂ O ₆ PS ₂
					269.0819 10.32 C ₁₆ H ₁₈ O ₇
					203.0825 3.38 C ₁₇ H ₁₈ N ₂ O ₂
V					431.1347 8.57 C ₂₇ H ₃₈ O ₉
					463.2546 6.35 C ₂₇ H ₃₈ O ₈
					427.1608 6.93 C ₂₇ H ₃₈ O ₁₀
					427.1608 7.23 C ₂₇ H ₃₈ O ₁₀
					405.1190 6.43 C ₂₇ H ₃₈ O ₉
					401.1241 8.48 C ₂₇ H ₃₈ O ₉
					373.1867 6.04 C ₂₇ H ₃₈ O ₈
					355.1034 5.64 C ₁₇ H ₁₈ O ₇
					283.0825 4.19 C ₁₇ H ₁₈ O ₇
					257.0278 1.36 C ₈ H ₁₁ N ₂ O ₅
I					793.1342 0.77
					751.2124 0.92 C ₃₁ H ₃₄ N ₂ O ₁₇ P
					455.1018 0.94 C ₁₇ H ₁₈ N ₂ O ₁₁
					451.0182 0.75
					435.0441 0.75
					415.1244 5.79 C ₁₈ H ₂₄ O ₁₁
					377.0857 0.77
					275.114 2.52 C ₁₇ H ₂₀ O ₇
					227.1288 8.58 C ₁₂ H ₂₀ O ₄