

Analytical and Bioanalytical Chemistry

Electronic Supplementary Material

Spatially resolved metabolic distribution for unraveling the physiological change and responses in tomato fruit using matrix-assisted laser desorption/ionization–mass spectrometry imaging (MALDI–MSI)

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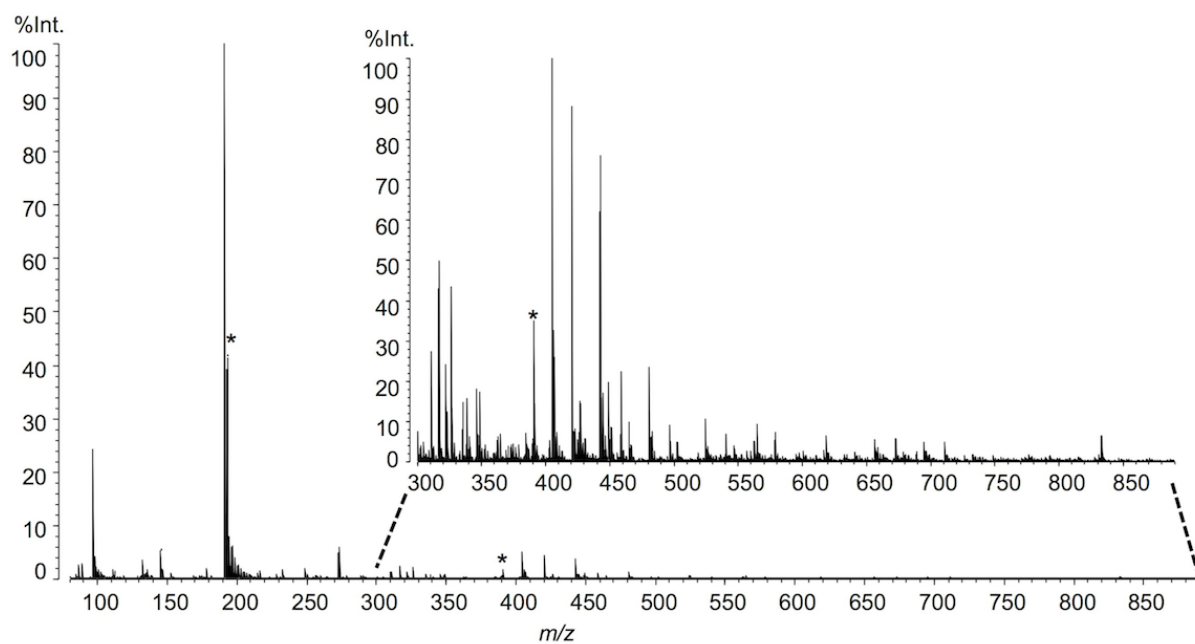


Fig. S1 Overview of the averaged mass spectrum acquired from the direct analysis of MR tomato fruit thin section. Whole averaged mass spectrum acquired from MR tomato thin-sections ($m/z = 80-890$). Enlarged spectra from whole averaged mass spectra data ($m/z = 300-890$). Asterisk marks; matrix-derived peaks (matrix: 9-AA)

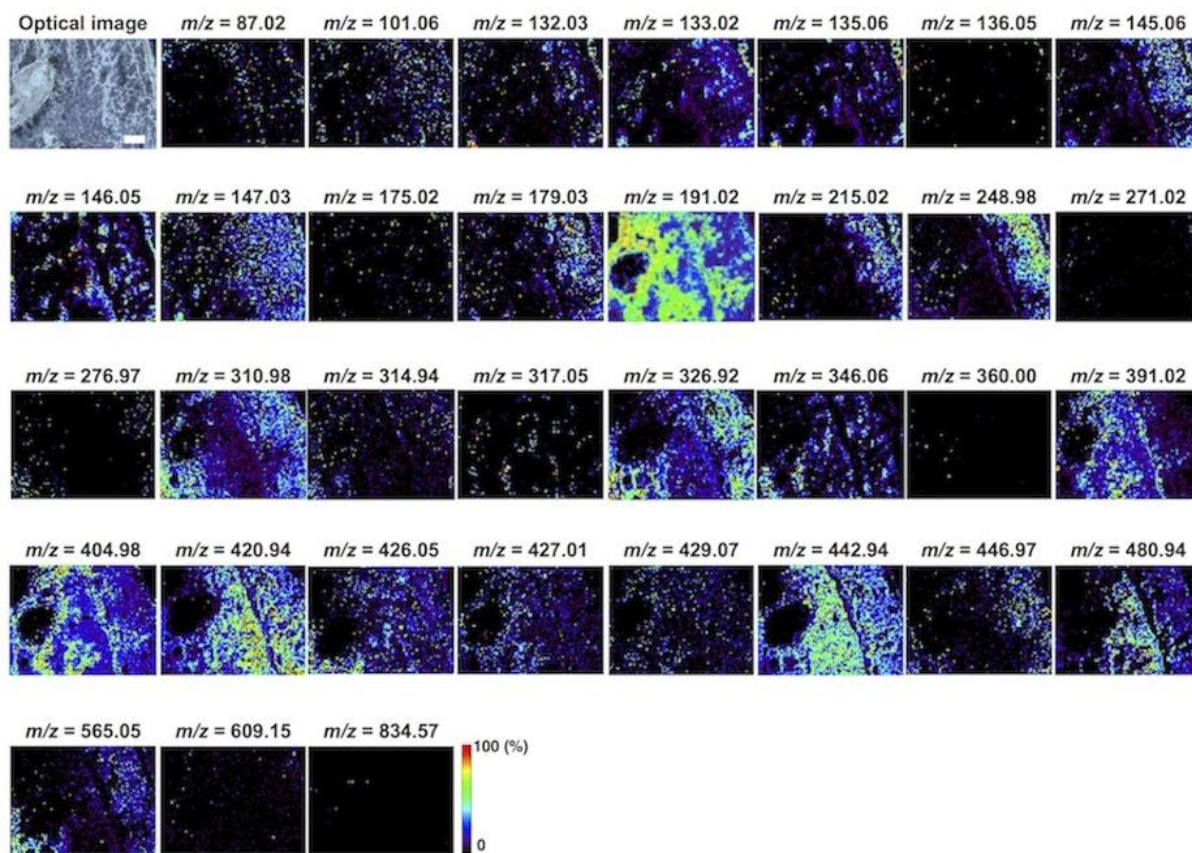


Fig. S2 In situ compounds imaging of MR tomato fruit section. Visualization of unique distributions of 34 compounds derived from metabolites in the MR tomato fruit section. Scale bar = 1.0 mm

Table S1 Mass-to-charge ratio, molecular species and fragmentations observed on the tomato fruit section

<i>m/z</i>	<i>Molecular species</i>	<i>Fragments observed</i>	<i>Formula</i>
87	pyruvate	44	C ₃ H ₄ O ₃
132	aspartate	115, 88	C ₄ H ₇ NO ₄
133	malate	115	C ₄ H ₆ O ₅
145	glutamine	127	C ₅ H ₁₀ N ₂ O ₃
146	glutamate	128, 102	C ₅ H ₈ NO ₄
147	citramalate	129, 101, 87	C ₅ H ₈ O ₅
179	caffeate	135	C ₉ H ₈ O ₄
191	citrate	173, 111	C ₆ H ₈ O ₇
346	AMP	211, 151, 97	C ₁₀ H ₁₄ N ₅ O ₇ P
565	UDP-glucose	403, 323	C ₁₅ H ₂₄ N ₂ O ₁₇ P ₂

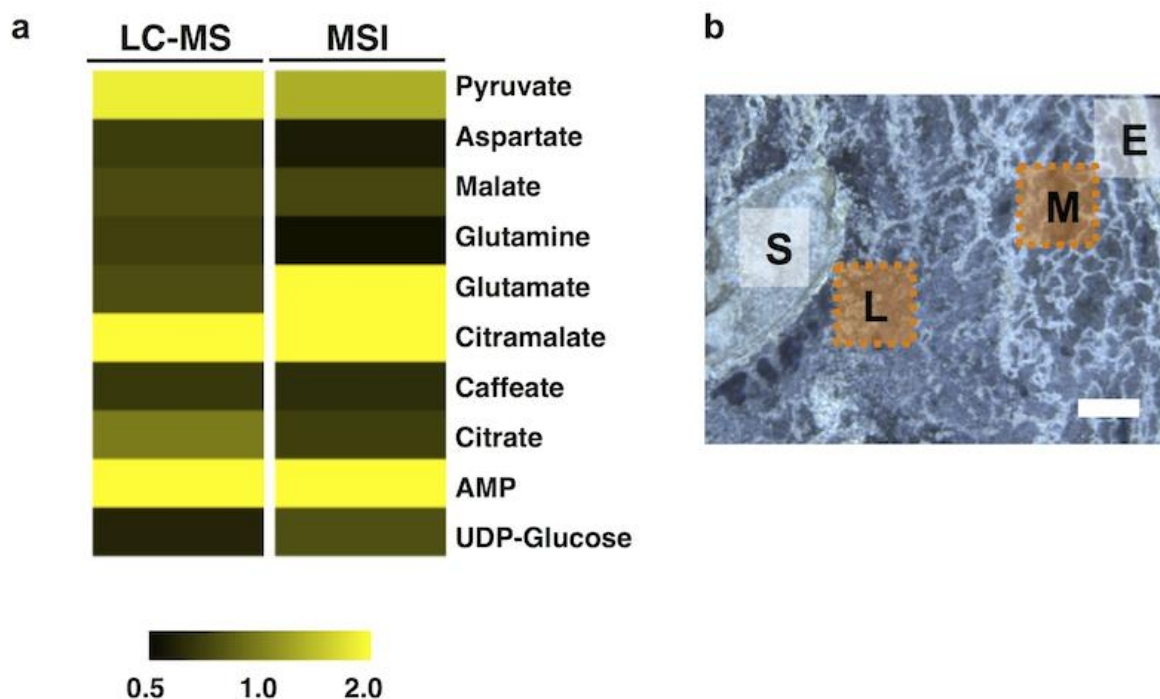


Fig. S3 A comparison of the average concentration/intensity between the whole tissue regions and partial tissue regions. **a** In the heat map, 10 common metabolites ratio detected by LC-MS and MSI. The ratio of the average intensity (locule/pericarp) in LC-MS data (left column). The ratio of the average intensity (locule/mesocarp) obtained from ROIs (L) and (M), which are indicated in the panel **b**, in MALDI-MSI data (right column). **b** Optical image of thin-section of the MR tomato fruit. E; epicarp, M; mesocarp, L; locule, S; seed. Scale bar = 1.0 mm

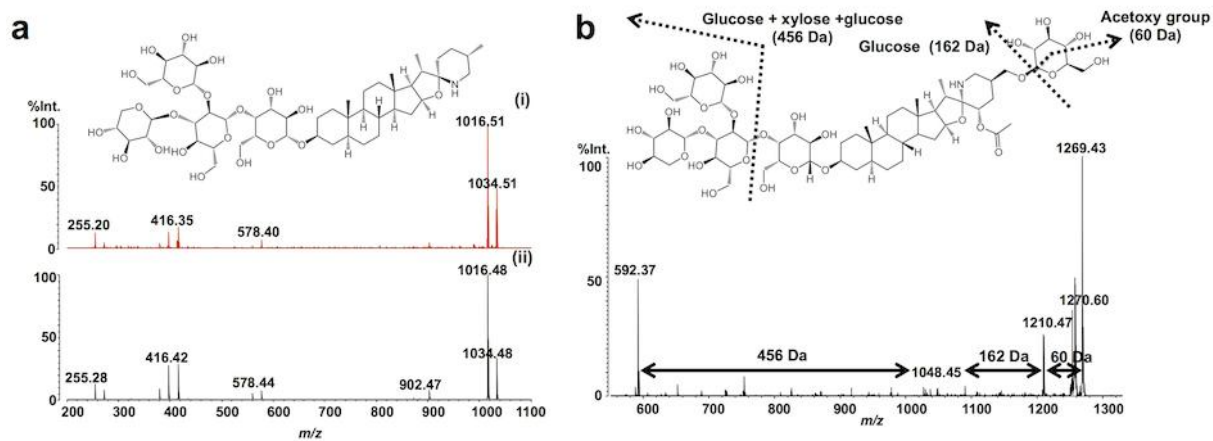


Fig. S4 Identification or estimation of compounds derived from glycoalkaloids by comparing with MS/MS data. **a** Identification of MS peaks of $m/z = 1034.55$ ($[M+H]^+$) as tomatine by comparing with MS/MS spectra between tomato fruit section and standard compound. (i) The MS/MS spectrum acquired from the tomato fruit section. (ii) The MS/MS spectrum of tomatine acquired from standard sample. **b** Estimation of MS peaks of $m/z = 1270.60$ ($[M+H]^+$) as esculoside A by MS/MS data. The fragments were referred from [25]