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SUPPLEMENTARY INFORMATION

Analytical method for metabolites involved in biosynthesis of plant volatile compounds

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Supplemental Table S1 The methods for analysis of metabolites involved in biosynthesis of plant volatile compounds

Metabolites		Analysis methods	Advantage	Disadvantage	Ref
① **Metabolites involved in glycolysis and pentose phosphate pathway**	G6P F6P FBP PEP Pyr 3PG 2PG DHAP GAP 3PG+2PG 1,3-PBG	Spectrophotometer analysis	● low cost and easy analysis	● imprecision	S1, S2, S3, S4, S5, S6
		GC-MS	● high sensitivity ● high reliability	● requirement for derivatization	
		LC-MS	● wide analytical range of metabolites	● lower reproducibility of retention times ● lower accurate quantification	
		CE-MS	● small quantity of sample ● without derivatization step ● high mass accuracy and resolution	● poor migration time reproducibility ● lack of reference libraries	
② **Metabolites involved in formation of volatile phenylpropanoids/benzenoids**	orgainc acid 3-deoxy-arabino-heptulonate 7-phosphate 3-dehydroquinic acid 3-dehydroshikimic acid shikimic acid shikimate 3-phosphate 5-enolpyruvylshikimate-3-phosphate (EPSP) chorismic acid prephenic acid	GC-MS	● high sensitivity	● requirement for derivatization	S7, S8, S9, S10

	phenylpyruvate *trans*-cinnamic acid *para*-coumaric acid 3-hydroxy-3-phenylpropionic acid amino acid L-phenylalanine phenolic acid conjugated coenzyme A *trans*-cinnamoyl CoA 3-hydroxy-3-phenylpropionyl CoA 3-oxo-3-phenylpropionyl CoA	HPLC-PDA	● low cost and easy analysis ● direct analysis	● limited compounds detected ● poor separation	
		HPLC-MS	● direct analysis	● requirement for sample clean-up	
		CE-MS	● simple extraction process ● short analytical time ● small quantity of sample	● lower sensitivity	
③ **Metabolites involved in formation of volatile fatty acid derivatives**	unsaturated fatty acid linoleic acid linolenic acid saturated fatty acid	GC	● high sensitivity ● short analytical time	● lower accurate quantitative ● requirement for derivatization ● time-consuming	S11, S12, S13, S14, S15
		HPLC	● accurate quantitative analysis	● poor retention time reproducibility ● requirement for derivatization ● time-consuming	

			LC-MS	● without derivatization step	● requirement for MS equipment	
		13-Hydroperoxylinolenic acid (12, 13*S*)-epoxylinolenic acid octadecanoid 12-oxo-phytodienoic acid Jasmonic acid	GC-MS	● high sensitivity	● requirement for derivatization	S16, S17, S18, S19
			LC-MS	● direct analysis	● unavailable of internal standards	
④	**Glycosidically bound volatile compounds**	Depend on plant species, such as glycosides constituting aglycons of the 3-hexenol, benzyl alcohol, 2-phenylethanol, methyl salicylate, geraniol and linalool	GC-MS	● easy to identify the structures of aglycone	● requirement for derivatization ● hard to identify the sugar residues	S20, S21, S22
			LC-MS	● direct analysis	● hard to obtain internal standards ● more purification steps	
⑤	**Metabolites involved in formation of carotenoid derived aroma compounds**	Phytoene Lycopene β-carotene δ-carotene	LC-PDA	● well separation ● fast detection of known carotenoid compounds	● complex elution gradient program ● long analysis time	S23, S24
			UPLC-MS	● reduction in analysis time and mobile phase solvent	● poor separation ● requirement for MS equipment	

			consumption ● identification for unknown carotenoids		
⑥ **Metabolites involved in formation of volatile isoprenoids**	DMAPP GPP FPP GGPP	CE	● well separating isoprenoids ● direct analysis	● lower sensitivity	S25, S26
		HPLC-MS	● high sensitivity ● direct detection		

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