

Metabolomic Profiling (LC–MS²) of Flowers and Bee Honey of Dzidzilche (*Gymnopodium floribundum* Rolfe) and Jabin (*Piscidia piscipula* L. Sarg.) from Yucatán, México

SUPPLEMENTARY MATERIAL

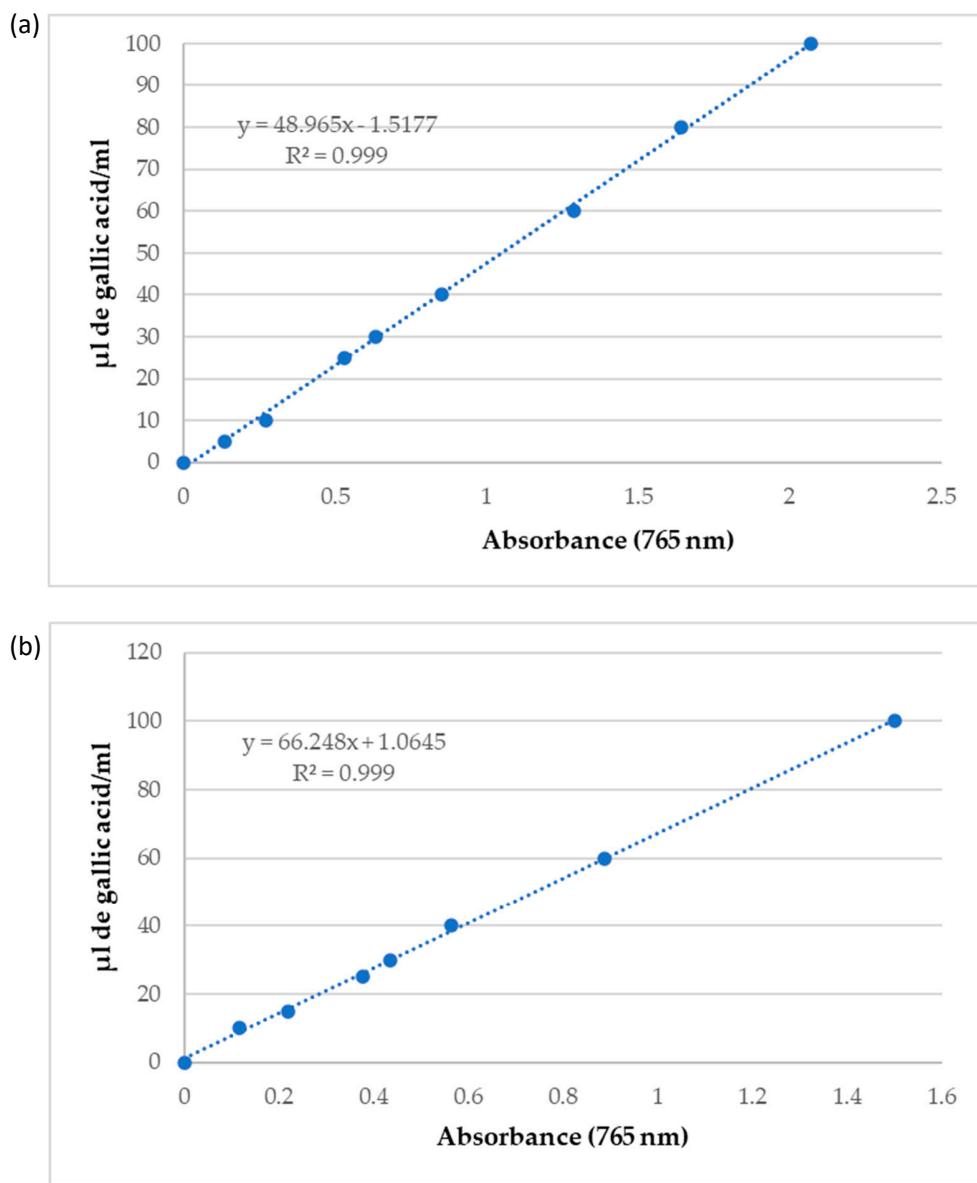


Figure S1. Calibration curve for Total polyphenol content in (a) flower samples and (b) honey samples.

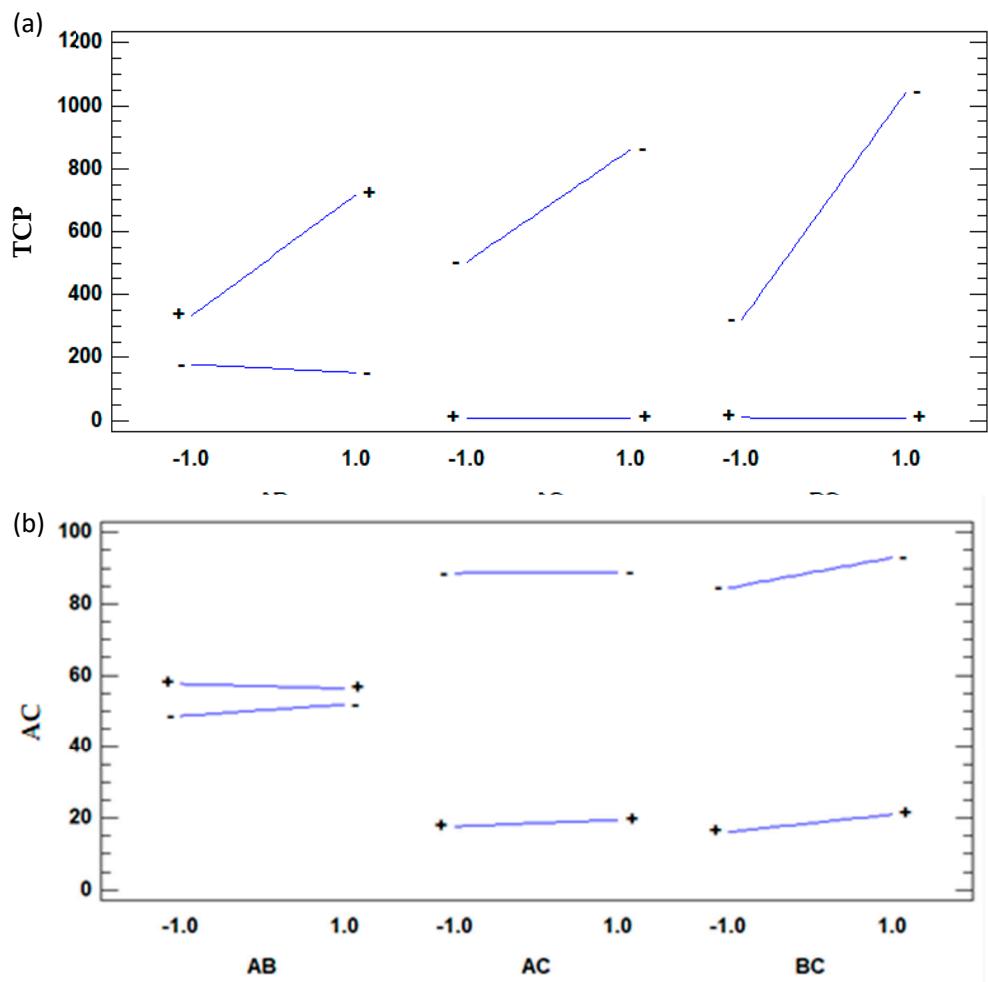


Figure S2. Interaction chart of (a) total polyphenol content and (b) antioxidant capacity.
Abbreviations: A = botanical origin; B = Geographical origin; C = raw material.

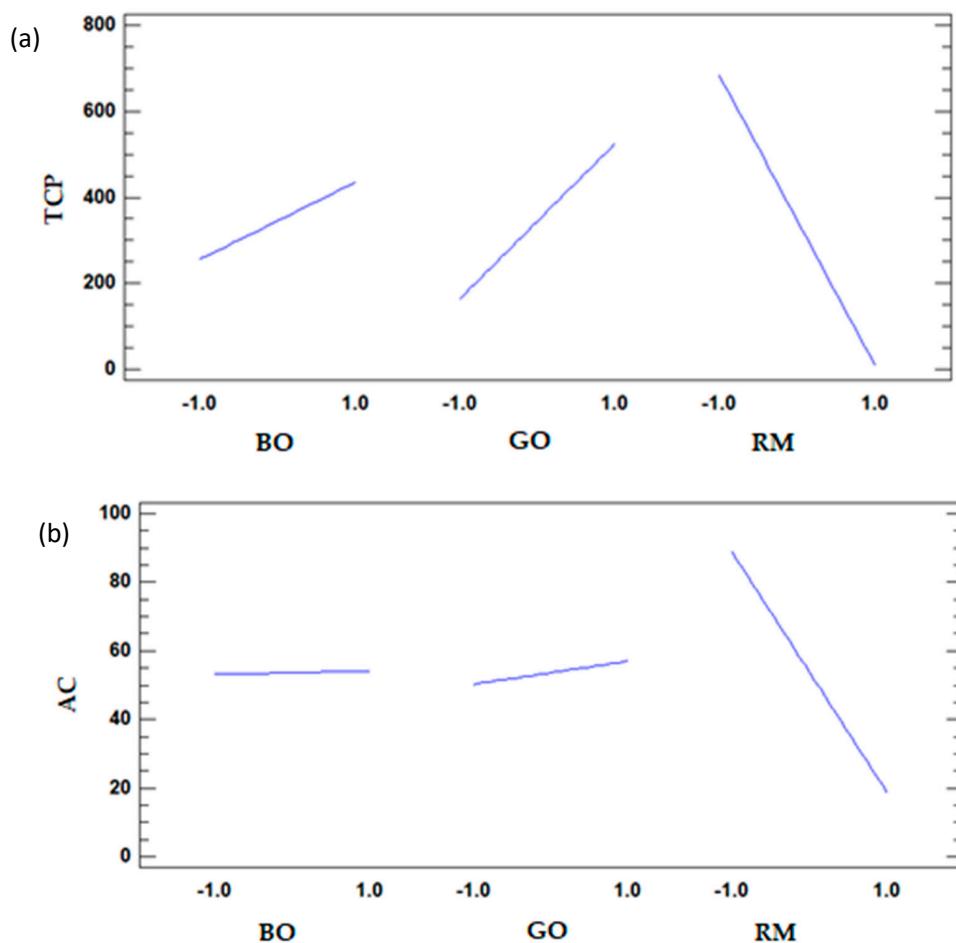


Figure S3. Main Effect plot of (a) total polyphenol content and (b) antioxidant capacity.
Abbreviations: BO = botanical origin; GO = Geographical origin; RM = raw material.

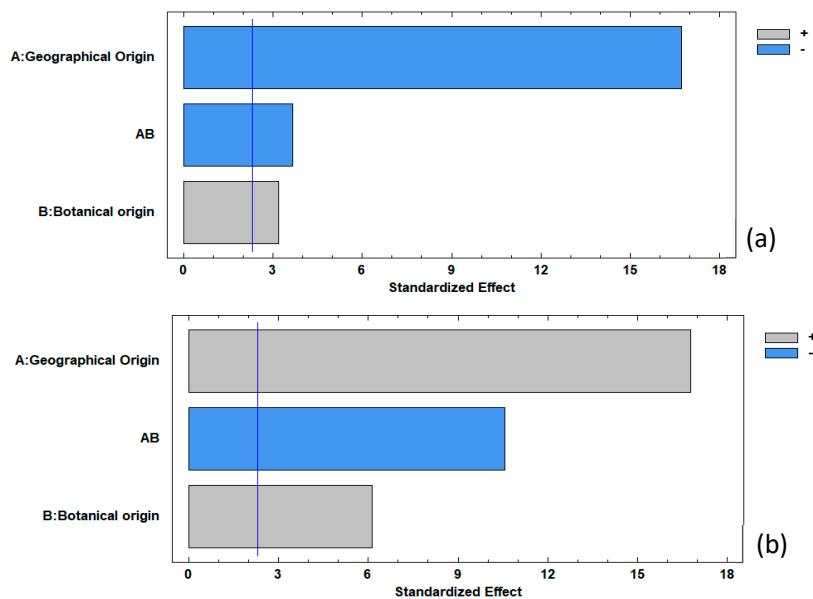


Figure S4. Pareto chart of (a) Total polyphenol content and (b) Antioxidant capacity in honey.

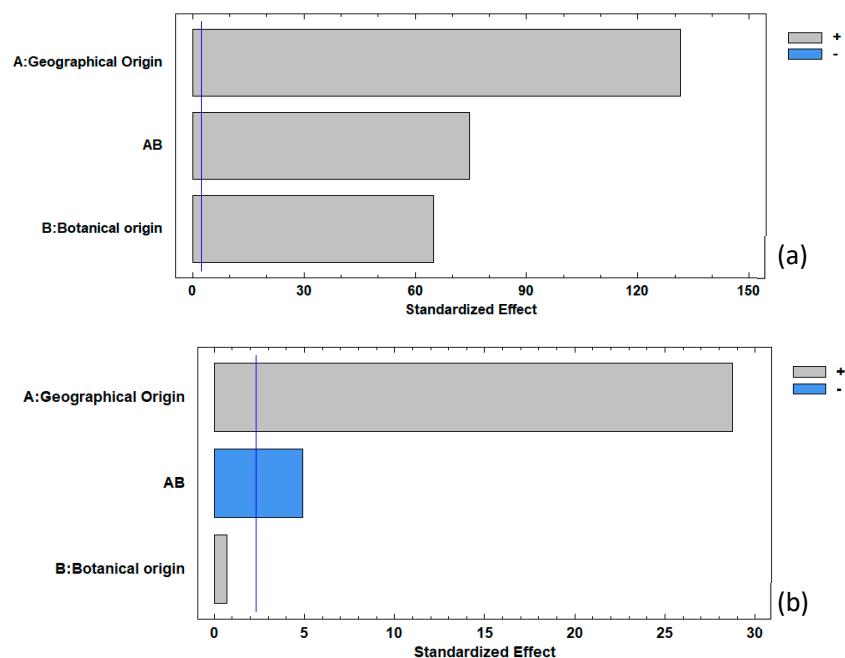


Figure S5. Pareto chart of (a) Total polyphenol content and (b) Antioxidant capacity in flower.

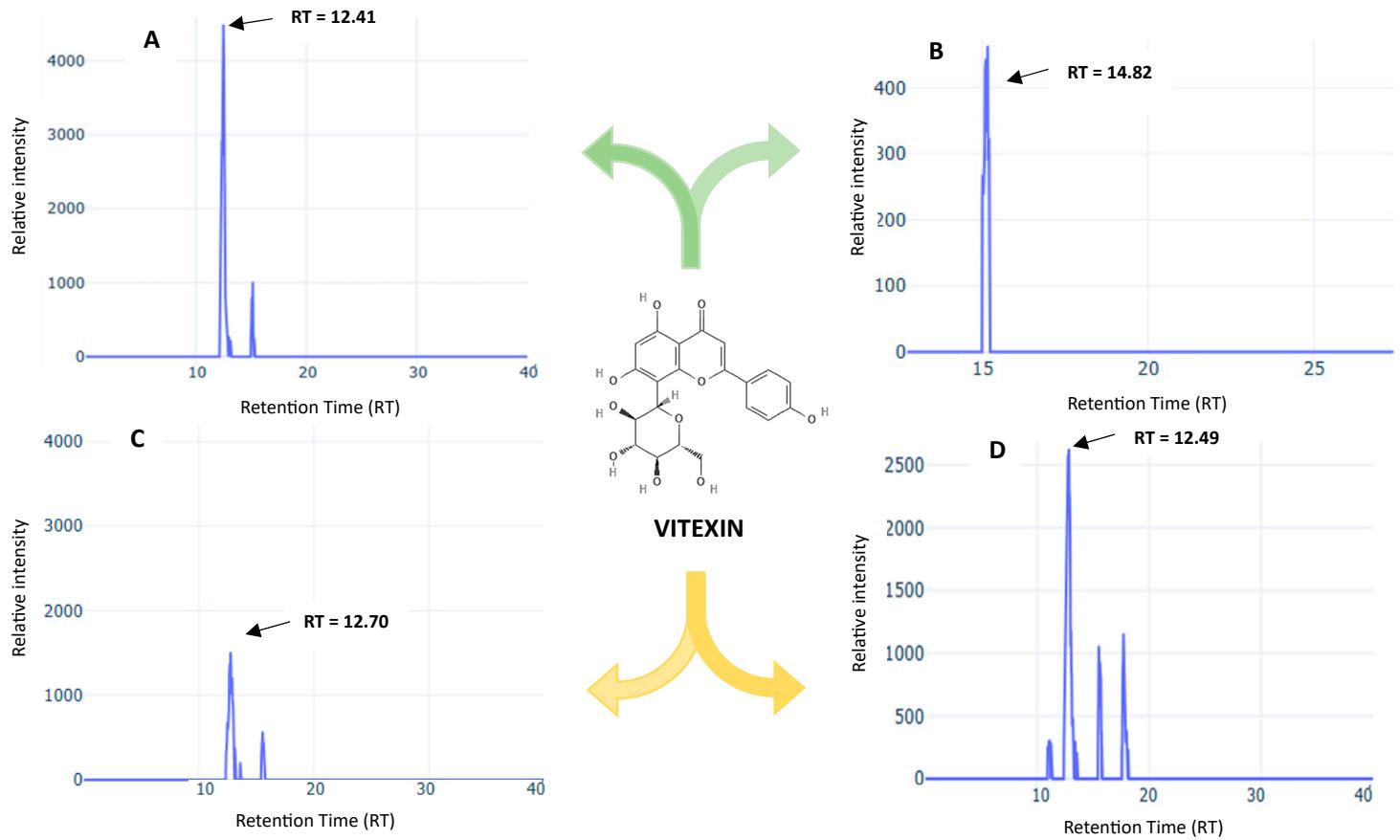


Figure S6. Representative chromatogram used for the analysis of vitexin. A) Extracted ion chromatogram for *Gymnopodium floribundum* flower from Acanceh; B) Extracted ion chromatogram for *Gymnopodium floribundum* honey from Acanceh; C) Extracted ion chromatogram for *Gymnopodium floribundum* flower from Tahdziu; D) Extracted ion chromatogram for *Gymnopodium floribundum* honey from Tahdziu.

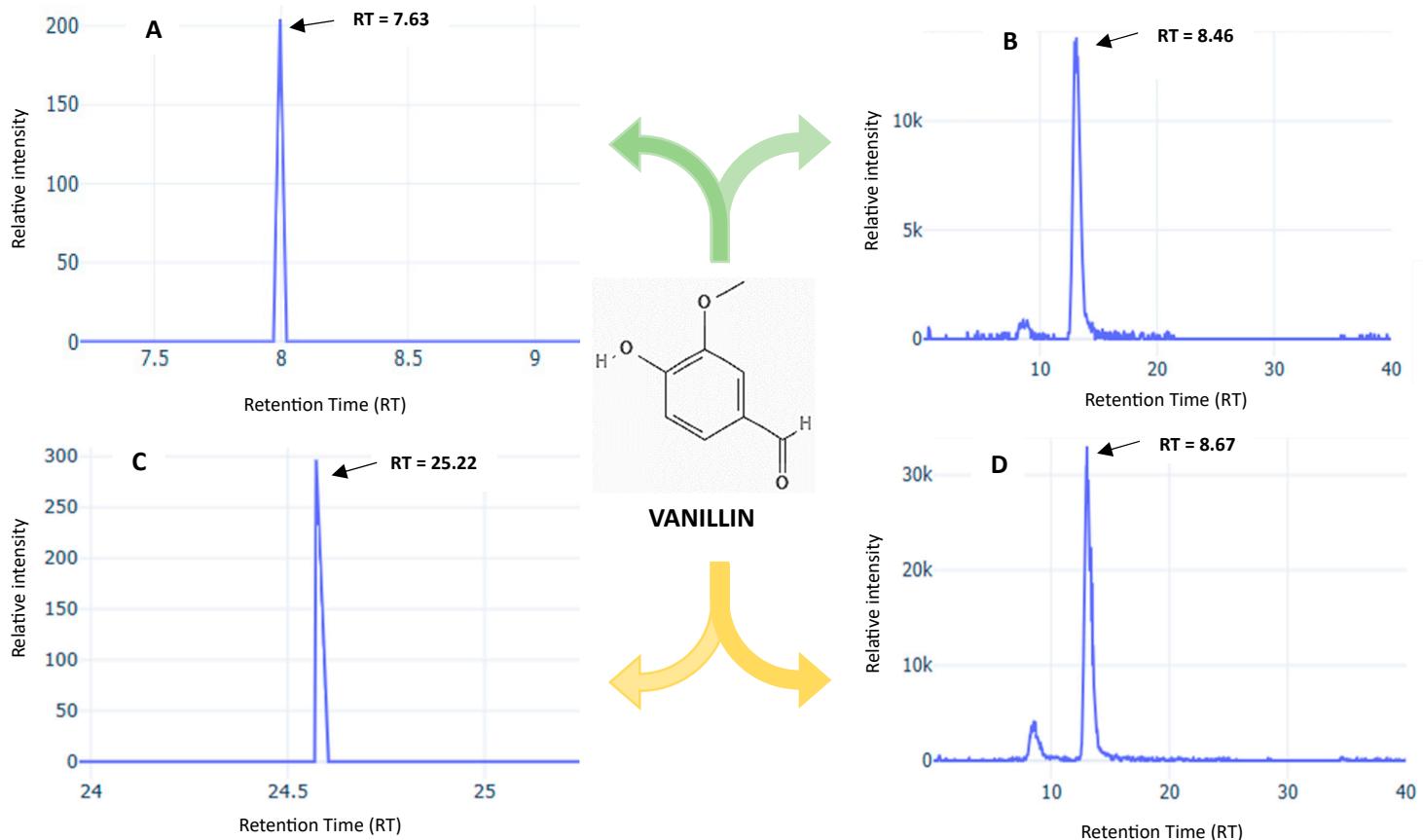


Figure S7. Representative chromatogram used for the analysis of vanillin. A) Extracted ion chromatogram for *Piscidia piscipula* flower from Acanceh; B) Extracted ion chromatogram for *Piscidia piscipula* honey from Acanceh; C) Extracted ion chromatogram for *Piscidia piscipula* flower from Tahdziu; D) Extracted ion chromatogram for *Piscidia piscipula* honey from Tahdziu.

Table S1. List of metabolites putatively annotated using spectral libraries and in-silico predictions in honey.

Chemical class	Compound Name	Molecular	Annotation
BENZENE AND SUBSTITUTED DERIVATIVES	Phenylacetic Acid	C8H8O2	GNPS
	4-Hydroxybenzoic acid	C7H6O3	GNPS
	Benzylideneacetone	C10H10O	GNPS
	3-Methoxybenzoic acid	C8H8O3	GNPS
	Veratric acid	C9H10O4	CSI:FingerID
	3-Methylsalicylic acid	C8H8O3	GNPS
CARBOXYLIC ACIDS AND DERIVATIVES	Phenylalanine	C9H11NO2	GNPS
	Tyrosine	C9H11NO3	GNPS
	N-(Phenylacetyl)phenylalanine	C17H17NO3	CSI:FingerID
	N-Fructosyl-isoleucine	C12H23NO7	GNPS
	N-Fructosyl-phenylalanine	C15H21NO7	CSI:FingerID
	N-Jasmonoyl-leucine	C18H29NO4	GNPS
	N-(1-Deoxy-1-fructosyl) phenylalanine	C15H21NO7	GNPS
	N-Acetyl-phenylalanine	C11H13NO3	GNPS
	2-{[4-Amino-3-(3-Hydroxyprop-1-Yn-1-Yl)-1h-Pyrazolo[3,4-D]pyrimidin-1-Yl]methyl}-5-Methyl-3-(2-Methylphenyl) quinazolin-4(3h)-One	C25H21N7O2	GNPS
FATTY ACYLS	Decanedioic acid	C10H18O4	CSI:FingerID
	Palmitoleic acid	C16H30O2	GNPS
FLAVONOIDS	Naringin	C27H32O14	GNPS
	Vitexin	C21H20O10	GNPS
	Quercitrin	C21H20O11	GNPS
	Quercetin-3-O-rhamnoside	C21H20O11	GNPS
	Kaempferol-3-rhamninoside	C33H40O19	GNPS
	Quercetin	C15H10O7	GNPS
	Afzelin	C21H20O10	GNPS
	3,5-Dihydroxy-2-(4-hydroxyphenyl)-7-[(3,4,5-trihydroxy-6-methyltetrahydro-2H-pyran-2-yl) oxy]-4H-1-benzopyran-4-one	C21H20O10	GNPS
	3"-O-L-Rhamnopyranosylastragalin	C27H30O15	GNPS
GLYCEROLIPIDS	TAG (16:0/16:0/18:1)	C53H100O6	GNPS
	TAG (16:0/18:1/18:1)	C55H102O6	GNPS

	1-Hexadecanoyl-sn-glycerol	C19H38O4	GNPS
GLYCEROPHOSPHOLIPIDS	PE (16:0/18:1(9Z))	C39H76NO8P	GNPS
	PC (18:1(9Z) /18:3(6Z,9Z,12Z))	C44H80NO8P	MolDiscovery
ISOFLAVONOIDS	Puerarin	C21H20O9	GNPS
L-DAPS (FENOLIC ACID)	Chalcone	C15H12O	GNPS
L-DAPS	3-(4-Hydroxy-phenyl)-1-phenyl-prop-2-en-1-one	C15H12O2	GNPS
ORGANOOXYGEN COMPOUNDS	Fructose	C6H12O6	GNPS
	Glucose	C6H12O6	GNPS
	Dianthoside	C12H16O8	GNPS
	Celllobiose	C12H22O11	GNPS
	Sucrose	C12H22O11	GNPS
	Maltotriose	C18H32O16	GNPS
	p-Formylphenol	C7H6O2	GNPS
	2,4,7,9-Tetramethyl-5-decyne-4,7-diol	C14H26O2	GNPS
OXEPANES	Levoglucosan	C6H10O5	GNPS
	6-methyl-10,12-dioxatricyclo [7.2.1.0 _{2,7}] dodec-4-en-8-one	C11H14O3	GNPS
PHENOLS	[6]-Gingerol	C17H26O4	GNPS
	Vanillin	C8H8O3	GNPS
	Moupinamide	C18H19NO4	GNPS
PRENOL LIPIDS	Abscisic acid	C15H20O4	GNPS
	Abscisic acid	C15H20O4	GNPS
	Abscisic acid	C15H20O4	GNPS
	[6-acetyloxy-4-[[3-acetyloxy-4,5-dihydroxy-6-(hydroxymethyl)oxan-2-yl]oxymethyl]-7-(acetyloxymethyl)-7-hydroxy-4a,5,6,7a-tetrahydro-1H-cyclopenta[c]pyran-1-yl] 3-methylbutanoate	C27H40O15	MolDiscovery
PTERIDINES AND DERIVATIVES	Lumichrome	C12H10N4O2	GNPS
	Riboflavin	C17H20N4O6	GNPS
PYRANS	Maltol	C6H6O3	GNPS
STILBENES	Resveratrol	C14H12O3	GNPS

Note: L-DAPs = Linear 1,3-diarylpropanoids

Table S2. List of metabolites putatively annotated using spectral libraries and in-silico predictions in flour flower.

CHEMICAL CLASS	COMPOUND NAME	MOLECULAR FORMULA	ANNOTATION TOOL
AURONE FLAVONOIDS	Bracteatin	C15H10O7	GNPS
	(2Z)-4,6-dihydroxy-2-[(4-hydroxy-3,5-dimethoxyphenyl)methylidene]-1-benzofuran-3-one	C17H14O7	GNPS
BZD	Tyramine	C8H11NO	GNPS
BENZOPYRANS	Ergochrom DD	C32H34O16	MolDiscovery
CARBOXYLIC ACIDS AND DERIVATIVES	N-Methyl-L-tryptophan	C12H14N2O2	GNPS
	Tyrosine	C9H11NO3	GNPS
	Phenylalanine	C9H11NO2	GNPS
	Chicoric acid	C22H18O12	GNPS
	Asparagine	C4H8N2O3	CSI:FingerID
	Proline	C5H9NO2	CSI:FingerID
CAD	Moupinamide	C18H19NO4	GNPS
FATTY ACYLS	Palmitoleic Acid	C16H30O2	GNPS
FLAVONOIDS	Procyanodin B5-3'-O-gallate	C37H30O16	MolDiscovery
	2-(3,4-dihydroxyphenyl)-6,8-bis[2-(3,4-dihydroxyphenyl)-3,7,8-trihydroxy-3,4-dihydro-2H-chromen-5-yl]-3,4-dihydro-2H-chromene-3,5,7-triol	C45H38O18	MolDiscovery
	Tangeretin	C20H20O7	GNPS
	Retusin	C19H18O7	GNPS
	Procyanodin B2	C30H26O12	GNPS
	Peonidin-3-glucoside	C22H23O11	GNPS
	Aromadendrin	C15H12O6	GNPS
	Astragalin	C21H20O11	GNPS
	Rutin	C27H30O16	GNPS
	Isorhamnetin 3-galactoside	C22H22O12	GNPS
	Quercetin	C15H10O7	GNPS
	Taxifolin-3-glucoside	C21H22O12	GNPS
	3-[3,4-Dihydroxy-6-(hydroxymethyl)-5-[3,4,5-trihydroxy-6-	C27H30O17	GNPS

	(hydroxymethyl) oxan-2-yl]oxyoxan-2-yl]oxy-2-(3,4-dihydroxyphenyl)-5,7-dihydroxychromen-4-one		
	(2S,3S)-3,5,7-trihydroxy-2-[4-hydroxy-3-[(2S,3R,4S,5S,6R)-3,4,5-trihydroxy-6-(hydroxymethyl) oxan-2-yl] oxyphenyl]-2,3-dihydrochromen-4-one	C21H22O12	GNPS
	(2S,3S)-3,5,7-trihydroxy-2-[4-hydroxy-3-[(2S,3R,4S,5S,6R)-3,4,5-trihydroxy-6-(hydroxymethyl) oxan-2-yl] oxyphenyl]-2,3-dihydrochromen-4-one	C21H22O12	GNPS
	Rhamnetin 3-sophoroside	C28H32O17	GNPS
	(-)Epicatechin gallate	C22H18O10	GNPS
	3,5-Dihydroxy-2-(4-hydroxyphenyl)-7-[3,4,5-trihydroxy-6-(hydroxymethyl) oxan-2-yl]oxy-2,3-dihydrochromen-4-one	C21H22O11	GNPS
	Luteolin 7-(6"-malonylglucoside)	C24H22O14	GNPS
	6"-O-(3-Hydroxy-3-methylglutaroyl)astragalin	C27H28O15	GNPS
	Reinutrin	C20H18O11	GNPS
	Kaempferol	C15H10O6	GNPS
	Hesperidin	C28H34O15	GNPS
	Luteolin-4'-o-glucoside	C21H20O11	GNPS
	Kaempferol 3-robinobioside	C27H30O15	GNPS
	3,5-dihydroxy-2-(4-hydroxyphenyl)-7-[(2S,3R,5S,6R)-3,4,5-trihydroxy-6-(hydroxymethyl) oxan-2-yl] oxychromen-4-one	C21H20O11	GNPS
	Isovitexin	C21H20O10	GNPS
	Isorhamnetin	C16H12O7	GNPS
	(+)-Catechin	C15H14O6	GNPS

	Isotrifolin	C21H20O12	GNPS
	Luteolon	C15H10O7	GNPS
	2'-O-galloylhyperin	C28H24O16	GNPS
	Taxifolin	C15H12O7	GNPS
	3,6,3',4'-Tetramethoxyflavone	C19H18O6	GNPS
	3,3',4',5,7-Pentahydroxyflavanone-7-Methyl ether, 5-O-D-glucopyranoside	C22H24O12	Dereplicator+
GLYCEROLIPIDS	1-Hexadecanoyl-sn-glycerol	C19H38O4	GNPS
GLYCEROPHOSPHOLIPIDS	DHPE	C37H74NO8P	MolDiscovery
	PE (16:0/17:0)	C38H76NO8P	MolDiscovery
	PE (15:0/16:0)	C36H72NO8P	MolDiscovery
	1-Palmitoyl-sn-glycerol	C42H82NO8P	GNPS
IND	Tryptophan	C11H12N2O2	GNPS
ISOFLAVONOIDS	11-Hydroxytephrosin	C23H22O8	GNPS
	Amorphigenin	C23H22O7	GNPS
	6-Hydroxysumatrol	C23H22O8	GNPS
	6a, 12a-Dehydrovillosin	C23H20O8	Dereplicator+
	Gelomulide N	C24H32O7	GNPS
ORGANONITROGEN COMPOUNDS	Phytosphingosine	C18H39NO3	GNPS
	D-Cellobiose	C12H22O11	GNPS
	D-Glucose	C6H12O6	GNPS
	D-Fructose	C6H12O6	GNPS
	(2S,3S,4S,5R,6R)-6-(3-benzoyloxy-2-hydroxypropoxy)-3,4,5-trihydroxyoxane-2-carboxylic acid	C16H20O10	GNPS
	Chlorogenic acid	C16H18O9	GNPS
	Pinitol	C7H14O6	CSI:FingerID
OXEPANES	Levoglucosan	C6H10O5	GNPS
PRENOL LIPIDS	7b,9-Dihydroxy-3-(hydroxymethyl)-1,1,6,8-tetramethyl-5-oxo-1,1a,1b,4,4a,5,7a,7b,8,9-decahydro-9ah-cyclopropa[3,4]benzo[1,2-e]azulen-9a-yl acetate	C22H30O6	GNPS
	3-Isolongifolol	C15H26O	GNPS
	2-[2-[5-[4-[4,5-Dihydroxy-6-methyl-3-(3,4,5-trihydroxy-6-methyloxan-2-yl) oxyoxan-2-yl]oxy-1,2,4a,5-tetramethyl-	C50H84O22	GNPS

	2,3,4,7,8, 8a-hexahydronaphthalen-1-yl]-3-methylpent-1-en-3-yl]oxy-5-hydroxy-6-methyl-3-(3,4,5-trihydroxy-6-methyloxan-2-yl) oxyoxan-4-yl]oxy-6-methyloxane-3,4,5-triol		
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Note: BZD = Benzene and substituted derivatives. CAD = Cinnamic acids and derivatives. IND = Indoles and derivatives