

Supplemental Table S3. Putative identification of metabolic markers from accurate m/z values detected by UPLC-qTOF-MS^E

¹ Accurate m/z values and retention times (RT), detected by UPLC-qTOF-MS^E, and sorted by their corresponding P value³.

² VIP scores from OPLS-discriminant analyses of the elicitors treatments (Fig. 6) and the *nadC* Q experiment (Fig. S8).

³ P values represent levels of significance across the entire dataset (ANOVA, FDR).

⁴ Predicted parameters from the METLIN database using the detected accurate m/z .

⁵ Putative metabolites and their corresponding pathways were validated by information from the PubMed chemical database.

Adducts: type of ion generated by electrospray ionization; Δ ppm: difference between observed and theoretical monoisotopic masses;

PA: Phosphatidic acid; PC: Phosphatidylcholine; PE: Phosphatidylethanolamine; PI: Phosphatidylinositol; PS: Phosphatidylserine.

Detected m/z ¹	RT (min) ¹	<i>nadC</i> ²	Elicitors ²	P value ³	Adducts ⁴	Predicted mass ⁴	Δ ppm ⁴	Putative compound ⁴	Putative Formula ⁴	Putative Pathway ⁵
447.053	1.0	11.4	10.5	< 1E-16	<i>m-H</i>	448.061	1	Glucobrassicin	C16H20N2O9S2	Glucosinolates
137.024	1.0	1.7	11.1	< 1E-16	<i>m-H</i>	138.032	3	Salicylic acid	C7H6O3	SA
299.077	1.0	2.1	14.9	< 1E-16	<i>m-H</i>	300.085	0	Salicylic acid beta-D-glucoside	C13H16O8	SA
223.061	1.8	6.8	13.6	< 1E-16	<i>m-H</i>	224.069	0	Sinapic acid	C11H12O5	Phenylpropanoids
791.495	6.4	10.4	1.8	< 1E-16	<i>m-H</i>	792.506	4	Sulfoquinovosyldiacylglycerol	C41H76O12S	Lipids
175.119	0.4	11.1	5.7	< 1E-16	<i>m+H</i>	174.112	0	Arginine	C6H14N4O2	Amino acids
363.141	1.8	3.3	13.7	< 1E-16	<i>m+Na</i>	340.079	3	Sinapoyl malate	C15H16O9	Phenylpropanoids
756.529	7.0	19.4	1.3	< 1E-16	<i>m+H</i>	755.547	32	PC (15:0/19:3)	C42H78NO8P	Lipids
786.489	5.9	9.1	1.7	< 1E-16	<i>m+H</i>	785.500	22	PE (18:3/22:6)	C45H72NO8P	Lipids
363.069	1.8	2.4	14.8	< 1E-16	<i>m+Na</i>	340.079	0	Sinapoyl malate	C15H16O9	Phenylpropanoids
477.064	1.3	5.3	9.2	3.1E-15	<i>m-H</i>	478.072	0	4-Methoxyglucobrassicin	C17H22N2O10S2	Glucosinolates
381.080	0.4	1.3	10.1	8.9E-15	<i>m+Na</i>	358.090	2	Dihydrocaffeic acid 3-O-glucuronide	C15H18O10	Phenylpropanoids
476.108	2.5	7.7	12.9	8.0E-12	<i>m-H</i>	477.116	1	8-Methylthiooctyl glucosinolate	C16H31NO9S3	Glucosinolates
339.072	1.8	3.1	14.3	9.7E-12	<i>m-H</i>	340.079	0	Sinapoyl malate	C15H16O9	Phenylpropanoids
759.477	6.2	10.3	1.1	9.3E-11	<i>m+NH4</i>	794.495	6	PI (12:0/19:1)	C40H75O13P	Lipids
781.512	6.9	12.2	1.2	3.5E-09	<i>m+H</i>	780.506	1	Sulfoquinovosyldiacylglycerol	C40H76O12S	Lipids
819.453	5.0	4.7	8.2	4.3E-09	<i>m+FA-H</i>	774.432	27	PI (12:0/18:4)	C39H67O13P	Lipids
377.086	0.9	6.7	5.2	1.2E-08	<i>m+Na-2H</i>	356.111	1	1-O-Feruloylglucose	C16H20O9	Phenylpropanoids
809.425	5.0	3.2	6.6	1.7E-08	<i>m+Na-2H</i>	788.448	3	PI (13:0/18:4)	C40H69O13P	Lipids
385.114	1.3	8.5	12.2	1.7E-08	<i>m-H</i>	386.121	0	1-O-Sinapoylglucose	C17H22O10	Phenylpropanoids
615.169	2.4	3.0	7.7	5.3E-08	<i>m+Na</i>	592.179	0	1,2-Bis-O-sinapoyl-beta-D-glucoside	C28H32O14	Phenylpropanoids
202.180	0.4	2.4	8.1	2.7E-07	<i>m+H</i>	201.173	0	11-amino-undecanoic acid	C11H23NO2	Lipids
591.172	2.4	6.0	5.0	3.5E-06	<i>m-H</i>	592.179	0	1,2-Bis-O-sinapoyl-beta-D-glucoside	C28H32O14	Phenylpropanoids
798.448	5.0	3.7	11.1	8.1E-06	<i>m+Na</i>	775.442	20	PS (18:4/18:4)	C42H66NO10P	Lipids
420.046	0.9	6.7	9.9	9.7E-06	<i>m-H</i>	421.054	0	Glucocerucin	C12H23NO9S3	Glucosinolates
613.410	5.0	2.4	7.7	1.1E-05	<i>m+H</i>	612.379	38	PA (12:0/18:4)	C33H57O8P	Lipids
797.444	5.0	5.5	16.9	1.5E-05	<i>m+Na</i>	774.432	28	PI (12:0/18:4)	C39H67O13P	Lipids
492.103	1.1	6.2	5.1	2.3E-05	<i>m-H</i>	493.111	1	Glucohirsutin	C16H31NO10S3	Glucosinolates
795.233	1.3	1.6	9.3	5.6E-05	<i>m+Na</i>	772.243	1	Alhagidin	C34H44O20	Lipids/Flavonoids
326.379	7.1	5.4	10.2	1.6E-03	<i>m+NH4</i>	308.344	2	13R-Methyl-6E-heneicosene	C22H44	Lipids
326.379	5.6	4.8	6.8	1.6E-03	<i>m+NH4</i>	308.344	2	13R-Methyl-6E-heneicosene	C22H44	Lipids
436.040	0.4	10.4	2.6	7.9E-03	<i>m-H</i>	437.048	2	Glucoraphanin	C12H23NO10S3	Glucosinolates
326.379	4.9	3.2	6.3	8.9E-03	<i>m+NH4</i>	308.344	2	13R-Methyl-6E-heneicosene	C22H44	Lipids