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Infection by a foliar endophyte elicits novel arabidopside-based plant defence reactions in its host, Cirsium arvense

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Metabolite number	Retention time	<i>m/z</i> observed ion	Ion species	Formula of ion	<i>m/z</i> calculated ion	ppm difference	<i>m/z</i> fragment ions	Formula of fragment	<i>m/z</i> calculated ion	ppm difference	Identity of metabolite
I	3.99	351.2149	M+Na	C ₁₈ H ₃₂ O ₅ Na	351.2147	0.6					
	3.99	327.2152	M-H	C18H31O5	327.2171	-5.8	171.1020 183.1387 211.1332 229.1445	$\begin{array}{c} C_9H_{15}O_3\\ C_{11}H_{19}O_2\\ C_{12}H_{19}O_3\\ C_{12}H_{21}O_4\end{array}$	171.1021 183.1385 211.1334 229.1440	-0.6 1.1 -0.9 2.1	9,12,13-trihydroxyoctadecadienoic acid (9,12,13-TriHODE)
	4.23	353.2308	M+Na	C ₁₈ H ₃₄ O ₅ Na	353.2305	1.1					9,12,13-trihydroxyoctadecenoic acid (9,12,13-TriHOME)
Π	4.23	329.2315	M-H*	C18H33O5	329.2328	-3.9	171.1020 183.1387 211.1335 229.1445	C9H15O3 C11H19O2 C12H19O3 C12H21O4	171.1021 183.1385 211.1334 229.1440	-0.6 1.1 0.4 2.1	
	8.52	731.4340	M+Na	C ₃₉ H ₆₄ O ₁₁ Na	731.4346	-0.8					
ш	8.52	707.4334	M-H	C39H63O11	707.4370	-5.1	167.1440 179.0560 211.1338 253.0925 277.2162 447.2231 513.3069	$\begin{array}{c} C_{11}H_{19}O\\ C_6H_{11}O_6\\ C_{12}H_{19}O_3\\ C_9H_{17}O_8\\ C_{18}H_{29}O_2\\ C_{21}H_{35}O_{10}\\ C_{27}H_{45}O_9 \end{array}$	167.1436 179.0556 211.1334 253.0923 277.2168 447.2230 513.3064	2.3 2.2 1.8 0.8 -2.1 0.2 1.0	dihydrojasmonic/octadecatrienoic acid ester of monogalactosyldiacylglycerol (MGDG dihydroJA/18:3)
IV	4.30	462.2852	M+H	C ₂₆ H ₄₀ NO ₆	462.2856	-0.8	164.0712 274.1809 302.1759 320.1861	C9H10NO2 C17H24NO2 C18H24NO3 C18H26NO4	164.0712 274.1807 302.1756 320.1862	0.0 0.7 0.9 -0.3	unidentified metabolite
	4.60	713.3348	M+Na	C33H54O15Na	713.3360	-1.6	349.2378	C21H33O4	349.2379	-0.2	oxophytodienoic acid ester of digalactosylmonoacylglycerol (DGMG OPDA/H)
v	4.60	689.3381	M-H	C33H53O15	689.3384	-0.4	165.1287 291.1958 415.1453	C11H17O C18H27O3 C15H27O13	165.1279 291.1960 415.1452	4.8 -0.6 0.2	
VI	5.05	551.2803	M+Na	C27H44O10Na	551.2832	-5.2	349.2375	C21H33O4	349.2379	-1.1	oxophytodienoic acid ester of monogalactosylmonoacylglycerol (MGMG OPDA/H)
	5.05	527.2857	М-Н	C27H43O10			165.1281 181.1226 247.2067 253.0921 291.1960	C11H17O C11H17O2 C17H27O C9H17O8 C18H27O3	165.1279 181.1229 247.2062 253.0923 291.1960	1.2 -1.6 0.2 -0.7 0.0	
	8.73	991.5542	M+Na	C51H84O17Na	991.5606	-6.4					oxophytoenoic acid ester of
VII	8.73	967.5612	M-H*	C51H83O17	967.5630	-1.8	167.1442 293.2123 397.1345	C11H19O C18H29O3 C15H25O12	167.1436 293.2117 397.1346	3.5 0.2 -0.2	digalactosyldiacylglycerol (DGDG dihydroOPDA/dihydroOPDA)

Supporting Information Table S1 Metabolite markers identified in leaves of Cirsium arvense infected with the endophyte C. cochlioides

							415.1449	C15H27O13	415.1452	-0.7	
							691.3550	C33H55O15	691.3541	1.3	
	8.76	987.5350	M+Na	C51H82O17Na	987.5293	5.7					
							165.1285	C11H17O	165.1279	3.6	oxophytodienoic acid ester of
VIII	8.76	963.5322	М-Н	C51H79O17	963.5317	0.5	291.1962	C ₁₈ H ₂₇ O ₃	291.1960	0.6	digalactosyldiacylglycerol (DGDG OPDA/OPDA)
							397.1346	C15H25O12	397.1346	0.0	
							415.1449	C15H27O13	415.1452	-0.7	
							689.3386	C33H53O15	689.3384	0.2	
IX	9.78	811.4983	M+Na	C45H72O11Na	811.4972	1.3					oxophytodienoic/octadecatrienoic acid esters of monogalactosyldiacylglycerol (MGDG OPDA/18:3)
	9.78	787.5012	М-Н	C45H71O11	787.4996	0.2	165.1282	C11H17O	165.1279	1.8	
							277.2162	C18H29O2	277.2168	-2.1	
							291.1960	C18H27O3	291.1960	0.0	
							527.2856	C27H43O10	527.2856	0.0	
X	9.87	813.5162	M+Na	C45H74O11Na	813.5129	4.0					oxophytodienoic/octadecadienoic acid esters of monogalactosyldiacylglycerol (MGDG OPDA/18:2)
	9.87	789.5156	6 M-H*	C45H73O11	789.5153	0.3	279.2314	C18H31O2	279.2314	0.0	
							291.1961	C18H27O3	291.1960	0.3	
							527.2864	C27H43O10	527.2856	1.5	

Extracts of plant tissues were analysed by UPLC-QTOFMS in +ESI and –ESI modes and fragment data were obtained using collision-induced dissociation. *, Ions corresponding to the formate adduct were also present.