

Table S7. Identified key metabolites of the asparagus samples with their LC-MS data, which show a dependency due to different origins.

Tentative compound	Proposed formula	Adduct	RT [min]	<i>m/z</i> measured	<i>m/z</i> calculated	Error [ppm]	Relevant fragments
Glycolipids							
Glucose-linoleate	C ₂₄ H ₄₂ O ₇	[M+Na] ⁺	5.1	465.2818	465.2823	0.9	202.11; 145.05
Glycerolipids							
DG(36:2)	C ₃₉ H ₇₂ O ₅	[M+NH ₄] ⁺	14.0	638.5720	638.5718	-0.4	341.30; 337.27
DG(36:3)	C ₃₉ H ₇₀ O ₅	[M+NH ₄] ⁺	13.2	636.5566	636.5562	-0.7	339.29; 337.27
DGDG(36:4)	C ₅₁ H ₈₈ O ₁₅	[M+Na] ⁺	9.7	963.5998	963.6015	-1.8	617.51; 599.50; 337.27
DGDG(36:5)	C ₅₁ H ₈₆ O ₁₅	[M+NH ₄] ⁺	9.1	956.6298	956.6305	-0.7	615.50; 597.49; 337.27; 335.26
TG(52:3)	C ₅₅ H ₁₀₀ O ₆	[M+Na] ⁺	18.9	879.7421	879.7412	1.0	601.52; 577.52; 575.50
TG(52:5; 20)	C ₅₅ H ₉₆ O ₈	[M+Na] ⁺	15.1	907.6981	907.6997	1.8	597.49; 575.50; 574.49
TG(53:3)	C ₅₆ H ₁₀₂ O ₆	[M+Na] ⁺	18.7	893.7562	893.7569	0.7	/
TG(54:4;20)	C ₅₇ H ₁₀₂ O ₈	[M+NH ₄] ⁺	16.3	932.7909	932.7913	-0.4	617.54
TG(54:6;20)	C ₅₇ H ₉₈ O ₈	[M+Na] ⁺	15.1	933.7143	933.7154	1.2	617.51; 599.50; 337.27
TG(54:6;30)	C ₅₇ H ₉₈ O ₉	[M+NH ₄] ⁺	14.1	944.7536	944.7520	1.4	613.48; 599.50
TG(54:7;10)	C ₅₇ H ₉₆ O ₇	[M+Na] ⁺	15.5	915.7037	915.7048	1.2	893.72; 613.48; 599.50
TG(54:7;20)	C ₅₇ H ₉₆ O ₈	[M+NH ₄] ⁺	15.8	926.7442	926.7443	-0.1	611.47; 599.50
TG(55:5)	C ₅₈ H ₁₀₂ O ₆	[M+Na] ⁺	18.3	917.7585	917.7569	-1.7	615.53; 599.50
TG(58:4)	C ₆₁ H ₁₁₀ O ₆	[M+NH ₄] ⁺	19.6	956.8651	956.8641	-1.1	659.60; 599.50
TG(58:5)	C ₆₁ H ₁₀₂ O ₆	[M+H] ⁺	18.7	931.7767	931.7749	1.9	652.56; 629.55; 599.50
Phospholipids							
PC(16:0)	C ₂₄ H ₅₀ NO ₇ P	[M+H] ⁺	4.8	496.3407	496.3398	1.9	184.07
PC(O-22:0)	C ₃₀ H ₆₂ NO ₇ P	[M+H] ⁺	7.7	580.4336	580.4337	-0.1	184.07
Phytosterols							
Brassicasterol derivative	C ₅₆ H ₈₅ NO ₄	[M+NH ₄] ⁺	16.2	853.6807	853.6817	-1.2	381.30
Campesterol derivative	C ₅₆ H ₁₀₀ O ₇	[M+NH ₄] ⁺	17.6	902.7811	902.7807	-0.4	383.36
Cycloartenol derivative I	C ₄₆ H ₈₀ O ₂	[M+NH ₄] ⁺	18.3	682.6499	682.6497	-0.4	409.38; 191.18

Table S7– continued.

Cycloartenol derivative II	C ₄₈ H ₈₀ O ₂	[M+NH ₄] ⁺	17.8	706.6505	706.6497	-1.2	409.38; 191.18
Cycloartenol derivative III	C ₄₈ H ₈₂ O ₂	[M+NH ₄] ⁺	18.4	708.6652	708.6653	-0.1	409.38; 191.18
Sitosterol derivative	C ₄₄ H ₈₂ O ₅	[M+Na] ⁺	16.0	713.6041	713.6054	-1.8	397.38
Stigmasterol derivative I	C ₃₃ H ₅₆ O ₆	[M+Na] ⁺	7.8				395.37
Stigmasterol derivative II	C ₄₀ H ₆₈ O ₂	[M+NH ₄] ⁺	13.6	571.3965	571.3969	-0.7	
Stigmasterol derivative III	C ₄₂ H ₇₂ O ₂	[M+NH ₄] ⁺	14.8	598.5559	598.5558	0.2	395.37
Stigmasterol derivative IV	C ₅₇ H ₁₀₀ O ₇	[M+Na] ⁺	17.3	626.5864	626.5871	1.1	395.37
Ubiquinones							
Coenzyme Q9	C ₅₄ H ₈₂ O ₄	[M+NH ₄] ⁺	16.5	812.6558	812.6551	-0.8	197.08
Coenzyme Q10	C ₅₉ H ₉₀ O ₄	[M+NH ₄] ⁺	17.5	880.7191	880.7177	1.5	197.08
Waxes							
Wax monoester	C ₃₄ H ₆₄ O ₂	[M+NH ₄] ⁺	14.7	522.5240	522.5245	0.9	/

Abbreviations: DG, diacylglycerol; DGDG, digalactosyldiacylglycerol; PC, phosphatidylcholin; TG, triacylglycerol