

## Supplementary material

**Figure S1.** Summary of lipid metabolism.

**List S1.** Main abbreviations used for lipid species.

**Table S1.** List of detected lipids in leaves of both *ndufs4* and Col0 (Arabidopsis) with loadings of multivariate statistics ( $p_{\text{corr}}$ ) and *P*-value from univariate statistics.

**Table S2.** List of detected lipids in leaves of both *ndufs8* and Col0 (Arabidopsis) with loadings of multivariate statistics ( $p_{\text{corr}}$ ) and *P*-value from univariate statistics.

**Table S3.** List of detected lipids in leaves of both *CMSII* and WT (tobacco) with loadings of multivariate statistics ( $p_{\text{corr}}$ ) and *P*-value from univariate statistics.

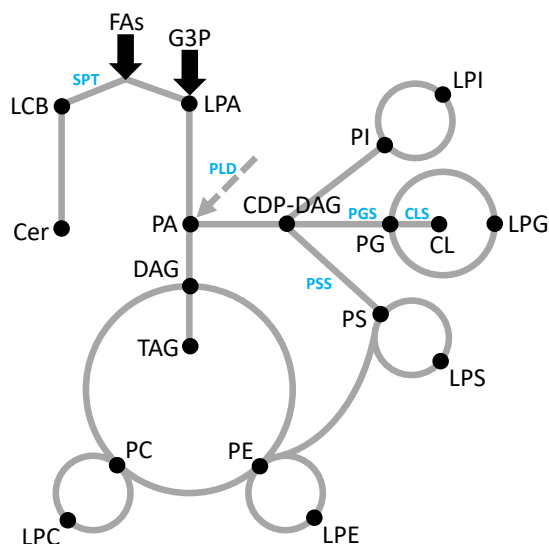
**Table S4.** List of detected lipids in seeds of both *ndufs4* and Col0 (Arabidopsis) with loadings of multivariate statistics ( $p_{\text{corr}}$ ) and *P*-value from univariate statistics.

**Table S5.** List of detected lipids in seeds of both *ndufs8* and Col0 (Arabidopsis) with loadings of multivariate statistics ( $p_{\text{corr}}$ ) and *P*-value from univariate statistics.

**Table S6.** List of detected lipids in seeds of both *CMSII* and WT (tobacco) with loadings of multivariate statistics ( $p_{\text{corr}}$ ) and *P*-value from univariate statistics.

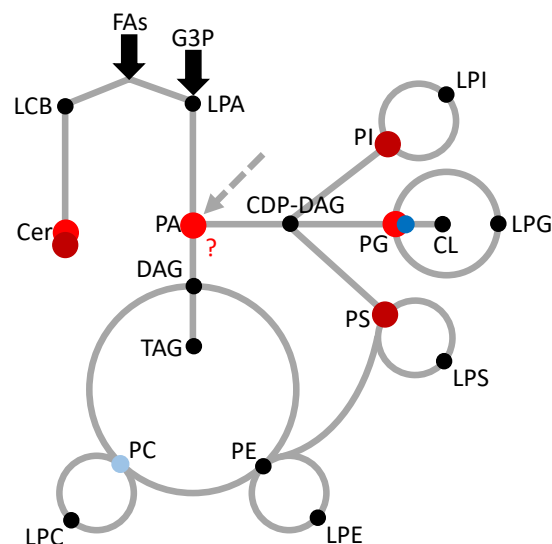
**Table S7.** List of detected lipids in pollen of both *CMSII* and WT (tobacco) with loadings of multivariate statistics ( $p_{\text{corr}}$ ) and *P*-value from univariate statistics.

- CLS – cardiolipin synthase
- PGS – phosphatidylglycerol synthase
- PLD – phospholipase D
- PSS – phosphatidylserine synthase
- SPT – serine palmitoyl-transferase



**In leaves**  
 ● Increase  
 ● Decrease

**In seeds**  
 ● Increase  
 ● Decrease



**Figure S1. Summary of lipid biosynthetic pathways and observed changes in complex I mutants.** (a) pathways with enzymes mentioned in text (in blue). (b) overview of changes observed in mutants with increases (red) and decreases (blue). For simplicity, the biosynthesis of galactolipids (chloroplast) is not shown here. Cer, ceramides; CL, cardiolipins; DAG, diacylglycerol; FAs, fatty acids; G3P, glycerol 3-phosphate; LCB, long chain base; PA, phosphatidic acid; PC, phosphatidyl choline; PE, phosphatidyl ethanolamine; PG, phosphatidyl glycerol; PI, phosphatidyl inositol; PS, phosphatidyl serine; TAG, triglycerides (triacylglycerol). Upper case ‘L’ stands for “lyso”. Grey circles indicate the possibility of cycling between species shown. Phospholipid cleavage and recycling can generate PA, and it is shown with a dashed grey arrow. The link between PE and PS represents the interconversion between PE and PS. In (b), the question mark symbolises uncertainty about the increase in PA (see main text). Changes in pollen (which are limited to data collected in tobacco) are not shown here.

**List S1.** Main abbreviations used for lipid species in the paper.

Abbreviation	Meaning
LPC	Lyso phosphatidyl-choline
PC	Phosphatidyl-choline
LPG	Lyso phosphatidyl-glycerol
PG	Phosphatidyl-glycerol
LPE	Lyso phosphatidyl-ethanolamine
PE	Phosphatidyl-ethanolamine
dMePE	Dimethyl phosphatidyl-ethanolamine
LPI	Lyso phosphatidyl-inositol
PI	Phosphatidyl-inositol
PL	Phospholipids
PS	Phosphatidyl-serine
DG	Diacylglycerol (diglycerides)
TG	Triacylglycerol (triglycerides)
PA	Phosphatidic acid
PMe	Phosphatidyl-methanol
PEt	Phosphatidyl-ethanol
CL	Cardiolipin
Cer	Ceramide
MGDG	Monogalactosyl-diacylglycerol
DGDG	Digalactosyl-diacylglycerol
StE	Stigmasterol ester
PX(n:i, m:j)	Phosphatidyl-X esterified with C <sub>n</sub> and C <sub>m</sub> fatty acid chains, with i and j unsaturations, respectively. Example, PC(18:3, 18:3): phosphatidyl-choline esterified with two C <sub>18</sub> chains carrying 3 unsaturations (linolenic type fatty acid).

**Table S1** : List of  $p_{\text{corr}}$  from OPLS-DA and  $P$ -value from Welsch T-test of *Arabidopsis thaliana* leaf samples *ndufs4* vs *col0*

ID	cat	family	pcorr	pvalue	PE(16:0_18:3)	PL	PE	-1.87E-01	6.51E-01
StE(32:3)	Sterols	StE	-9.99E-01	1.32E-10	Cer(d18:1+hO_26:0)	Cer	Cer	-1.77E-01	6.25E-01
SQDG(16:0_18:2)	GL	SQDG	-9.72E-01	4.85E-06	DGDG(18:3_20:0)	GL	DGDG	-1.63E-01	6.36E-01
MGDG(36:7)	GL	MGDG	-9.71E-01	5.30E-06	DGDG(16:2_18:3)	GL	DGDG	-1.48E-01	6.97E-01
PG(16:0_16:1)	PL	PG	-9.61E-01	1.16E-05	PC(16:0_18:3)	PL	PC	-9.84E-02	8.01E-01
PG(32:3)	PL	PG	-9.57E-01	2.21E-05	PC(33:1)	PL	PC	-7.67E-02	8.93E-01
SQDG(34:5)	GL	SQDG	-9.50E-01	3.05E-05	MGDG(18:2_18:3)	GL	MGDG	-6.80E-02	8.99E-01
PC(16:0_22:5)	PL	PC	-9.33E-01	8.96E-05	TG(18:0_16:0_18:1)	TG	TG	-3.23E-02	9.30E-01
DGDG(16:0_18:2)	GL	DGDG	-9.17E-01	1.76E-04	MGDG(18:1_18:3)	GL	MGDG	-1.93E-02	9.93E-01
MGDG(16:3_18:1)	GL	MGDG	-9.08E-01	3.84E-04	DG(24:0_18:2)	DG	DG	6.07E-03	9.58E-01
DG(18:3_20:2)	DG	DG	-8.97E-01	6.04E-04	AGlcSiE(18:3)	AGlcSiE	AGlcSiE	2.30E-02	9.40E-01
MGDG(16:0_16:3)	GL	MGDG	-8.95E-01	6.35E-04	PC(33:2)	PL	PC	8.56E-02	7.64E-01
SiE(18:2)	Sterols	SiE	-8.94E-01	4.80E-04	MGDG(18:3_19:2)	GL	MGDG	1.43E-01	6.63E-01
SiE(18:3)	Sterols	SiE	-8.86E-01	7.40E-04	PC(33:3)	PL	PC	1.52E-01	6.21E-01
StE(18:2)	Sterols	StE	-8.86E-01	7.41E-04	So(d22:0+pO)	Sterols	So	1.63E-01	7.22E-01
CL(72:12)	PL	CL	-8.83E-01	1.21E-03	DG(15:0_18:2)	DG	DG	1.78E-01	6.09E-01
PG(16:0_18:1)	PL	PG	-8.74E-01	1.15E-03	PC(18:3_18:3)	PL	PC	1.86E-01	5.82E-01
MGDG(16:0_18:3)	GL	MGDG	-8.74E-01	1.21E-03	PC(18:3_18:2)	PL	PC	1.86E-01	6.30E-01
DGDG(16:3_18:3)	GL	DGDG	-8.72E-01	8.24E-04	PE(20:2_18:2)	PL	PE	2.36E-01	5.10E-01
DGDG(16:0_18:1)	GL	DGDG	-8.60E-01	1.41E-03	CerG1(d42:2+2O)	Cer	CerG1	2.86E-01	3.85E-01
SQDG(18:2_18:3)	GL	SQDG	-8.52E-01	1.88E-03	TG(16:0_16:0_18:1)	TG	TG	3.06E-01	3.81E-01
DGDG(16:0_16:0)	GL	DGDG	-8.51E-01	2.04E-03	PE(18:2_18:2)	PL	PE	3.40E-01	3.33E-01
CL(18:3_18:2_14:0_22:6)	PL	CL	-8.38E-01	3.33E-03	PC(32:1)	PL	PC	3.54E-01	2.98E-01
PE(24:1_18:3)	PL	PE	-8.30E-01	3.99E-03	DGDG(18:3_18:3)	GL	DGDG	3.54E-01	3.22E-01
MGDG(16:1_18:1)	GL	MGDG	-8.18E-01	4.29E-03	Cer(d18:1+hO_25:0)	Cer	Cer	3.57E-01	2.99E-01
MGDG(16:1_16:3)	GL	MGDG	-8.18E-01	4.80E-03	CerG1(d18:1+hO_24:0+O)	Cer	CerG1	3.65E-01	2.73E-01
PI(16:1_18:3)	PL	PI	-8.03E-01	7.35E-03	PE(17:0_18:2)	PL	PE	3.83E-01	2.59E-01
SQDG(16:1_18:3)	GL	SQDG	-7.89E-01	7.30E-03	DG(18:1_18:3)	DG	DG	3.89E-01	2.60E-01
DGDG(18:3_20:3)	GL	DGDG	-7.71E-01	6.68E-03	WE(5:0_17:3)	WE	WE	3.90E-01	2.92E-01
TG(18:0_16:0_18:3)	TG	TG	-7.65E-01	1.39E-02	DG(18:0_20:0)	DG	DG	4.19E-01	2.36E-01
PG(16:1_18:3)	PL	PG	-7.49E-01	1.01E-02	DG(18:1_18:2)	DG	DG	4.37E-01	1.78E-01
MGDG(16:3_18:3)	GL	MGDG	-7.32E-01	1.40E-02	PE(24:0_18:2)	PL	PE	4.72E-01	1.59E-01
MGDG(16:2_18:3)	GL	MGDG	-7.32E-01	1.89E-02	DG(18:0_18:0)	DG	DG	4.86E-01	1.51E-01
MGDG(16:0_18:1)	GL	MGDG	-7.31E-01	1.69E-02	DG(16:0_16:0)	DG	DG	4.97E-01	1.44E-01
CerG1(d18:1+hO_25:0+O)	Cer	CerG1	-7.23E-01	2.58E-02	PI(18:0_18:2)	PL	PI	5.01E-01	1.27E-01
SQDG(18:3_18:3)	GL	SQDG	-7.08E-01	2.27E-02	DGDG(18:1_18:3)	GL	DGDG	5.02E-01	1.32E-01
MGDG(16:3_16:3)	GL	MGDG	-6.88E-01	2.61E-02	MGDG(18:0_18:2)	GL	MGDG	5.04E-01	1.15E-01
CerG1(d18:1+hO_27:0+O)	Cer	CerG1	-6.87E-01	3.35E-02	CL(18:2_16:0_16:0_20:1)	PL	CL	5.07E-01	1.37E-01
CerG1(d43:2+2O)	Cer	CerG1	-6.82E-01	3.92E-02	Cer(d18:0+pO_26:0)	Cer	Cer	5.08E-01	1.36E-01
DGDG(16:0_18:3)	GL	DGDG	-6.71E-01	3.22E-02	PE(22:0_18:2)	PL	PE	5.11E-01	1.25E-01
Cer(d18:2_27:0+O)	Cer	Cer	-6.68E-01	3.26E-02	So(d20:0+pO)	Sterols	So	5.46E-01	1.21E-01
DG(18:3_18:3)	DG	DG	-6.50E-01	5.10E-02	PE(15:0_18:2)	PL	PE	5.50E-01	9.27E-02
PI(15:0_18:3)	PL	PI	-6.12E-01	7.37E-02	PI(18:3_18:2)	PL	PI	5.53E-01	9.78E-02
PE(18:3_18:3)	PL	PE	-6.01E-01	7.88E-02	PE(16:0_18:2)	PL	PE	5.78E-01	7.84E-02
Cer(d18:2_26:0+O)	Cer	Cer	-6.00E-01	6.94E-02	TG(18:0_16:0_18:0)	TG	TG	5.96E-01	6.86E-02
PC(34:6)	PL	PC	-5.97E-01	7.70E-02	PE(18:0_18:3)	PL	PE	6.02E-01	5.30E-02
CL(18:3_18:2_16:1_20:4)	PL	CL	-5.92E-01	7.89E-02	DG(16:0_18:1)	DG	DG	6.04E-01	6.13E-02
DGDG(18:3_19:2)	GL	DGDG	-5.82E-01	8.25E-02	DG(16:0_18:2)	DG	DG	6.09E-01	6.53E-02
MGDG(18:3_20:3)	GL	MGDG	-5.65E-01	9.05E-02	DG(18:0_16:0)	DG	DG	6.16E-01	5.83E-02
PE(24:1_18:2)	PL	PE	-5.63E-01	9.99E-02	StE(30:3)	Sterols	StE	6.30E-01	3.61E-02
MGDG(17:3_18:3)	GL	MGDG	-5.58E-01	1.05E-01	CerG1(d18:1+hO_22:0+O)	Cer	CerG1	6.40E-01	4.03E-02
PC(34:5)	PL	PC	-5.40E-01	1.20E-01	PC(16:0_18:1)	PL	PC	6.51E-01	4.03E-02
DG(16:0_18:3)	DG	DG	-5.34E-01	1.25E-01	PI(16:0_18:1)	PL	PI	6.72E-01	2.94E-02
PG(16:1_18:1)	PL	PG	-5.11E-01	1.26E-01	AGlcSiE(18:2)	AGlcSiE	AGlcSiE	6.89E-01	2.90E-02
CerG1(d18:1+hO_23:0+O)	Cer	CerG1	-5.04E-01	1.70E-01	DG(18:0_18:2)	DG	DG	6.91E-01	2.35E-02
DGDG(16:0_18:0)	GL	DGDG	-4.88E-01	1.79E-01	AGlcSiE(18:1)	AGlcSiE	AGlcSiE	6.97E-01	2.12E-02
PC(16:1_18:3)	PL	PC	-4.88E-01	1.78E-01	DG(17:0_18:2)	DG	DG	6.97E-01	2.13E-02
DG(18:3_18:2)	DG	DG	-4.84E-01	1.72E-01	CerG1(d18:1+hO_28:0+O)	Cer	CerG1	7.06E-01	2.49E-02
DGDG(17:0_18:2)	GL	DGDG	-4.76E-01	1.81E-01	TG(18:0_18:0_18:0)	TG	TG	7.09E-01	2.19E-02
PC(38:4)	PL	PC	-4.75E-01	1.52E-01	PG(18:3_18:3)	PL	PG	7.27E-01	1.69E-02
TG(16:0_18:1_18:1)	TG	TG	-4.21E-01	2.46E-01	PE(18:0_18:2)	PL	PE	7.32E-01	1.42E-02
TG(18:1_18:1_18:2)	TG	TG	-3.98E-01	2.77E-01	TG(18:0_16:0_16:0)	TG	TG	7.34E-01	1.49E-02
PE(26:0_18:2)	PL	PE	-3.81E-01	2.83E-01	PG(16:1_18:2)	PL	PG	7.51E-01	1.18E-02
PI(18:3_18:3)	PL	PI	-3.60E-01	3.37E-01	AGlcSiE(18:0)	AGlcSiE	AGlcSiE	7.55E-01	9.42E-03
MGDG(18:3_20:2)	GL	MGDG	-3.48E-01	3.40E-01	MGDG(18:3_18:3)	GL	MGDG	7.65E-01	8.34E-03
PG(16:0_16:0)	PL	PG	-3.47E-01	3.39E-01	DGDG(18:0_18:3)	GL	DGDG	7.93E-01	4.97E-03
PE(18:3_18:2)	PL	PE	-3.30E-01	3.70E-01	PG(18:3_18:2)	PL	PG	8.01E-01	6.79E-03
CL(70:5)	PL	CL	-3.29E-01	3.90E-01	DG(18:4_18:3)	DG	DG	8.03E-01	3.96E-03

MGDG(18:0_18:3)	GL	MGDG	8.08E-01	3.37E-03
Cer(d18:1+hO_24:0)	Cer	Cer	8.18E-01	3.36E-03
Cer(d18:2_24:0+O)	Cer	Cer	8.27E-01	2.34E-03
PC(18:0_18:2)	PL	PC	8.36E-01	2.08E-03
PS(39:1)	PL	PS	8.42E-01	1.82E-03
TG(16:0_14:0_16:0)	TG	TG	8.71E-01	1.11E-03
AGlcSiE(16:0)	AGlcSiE	AGlcSiE	8.73E-01	7.11E-04
TG(16:0_16:0_16:0)	TG	TG	8.84E-01	6.64E-04
DGDG(18:0_18:1)	GL	DGDG	9.17E-01	1.16E-04
PC(17:1_17:1)	PL	PC	9.25E-01	1.65E-04
MGDG(18:3_20:1)	GL	MGDG	9.26E-01	8.50E-05
PE(16:0_18:1)	PL	PE	9.27E-01	9.55E-05
PC(38:3)	PL	PC	9.31E-01	8.95E-05
PC(18:1_18:3)	PL	PC	9.31E-01	1.31E-04

**Table S2** : List of  $p_{\text{corr}}$  from OPLS-DA and  $P$ -value from Welsch T-test of *Arabidopsis thaliana* leaf samples *ndufs8* vs Col0

ID	cat	family	pcorr	pvalue
StE(32:3)	Sterols	StE	-9.98E-01	2.50E-11
SQDG(16:0_18:2)	GL	SQDG	-9.13E-01	2.65E-04
MGDG(36:7)	GL	MGDG	-9.14E-01	2.52E-04
PG(16:0_16:1)	PL	PG	-8.45E-01	2.01E-03
PG(32:3)	PL	PG	6.61E-01	3.38E-02
SQDG(34:5)	GL	SQDG	-5.71E-01	8.79E-02
PC(16:0_22:5)	PL	PC	-2.77E-01	4.10E-01
DGDG(16:0_18:2)	GL	DGDG	-9.18E-01	1.78E-04
MGDG(16:3_18:1)	GL	MGDG	-9.37E-01	6.14E-05
DG(18:3_20:2)	DG	DG	2.24E-01	5.49E-01
MGDG(16:0_16:3)	GL	MGDG	-2.69E-01	4.70E-01
SiE(18:2)	Sterols	SiE	-9.31E-01	7.41E-05
SiE(18:3)	Sterols	SiE	-9.49E-01	2.14E-05
StE(18:2)	Sterols	StE	-9.49E-01	2.13E-05
CL(72:12)	PL	CL	-4.98E-01	1.42E-01
PG(16:0_18:1)	PL	PG	-8.87E-01	6.16E-04
MGDG(16:0_18:3)	GL	MGDG	-9.17E-01	1.84E-04
DGDG(16:3_18:3)	GL	DGDG	-2.61E-01	4.58E-01
DGDG(16:0_18:1)	GL	DGDG	-9.39E-01	4.90E-05
SQDG(18:2_18:3)	GL	SQDG	-8.36E-01	2.93E-03
DGDG(16:0_16:0)	GL	DGDG	-9.66E-01	4.82E-06
CL(18:3_18:2_14:0_22:6)	PL	CL	-3.52E-01	3.16E-01
PE(24:1_18:3)	PL	PE	2.38E-01	5.18E-01
MGDG(16:1_18:1)	GL	MGDG	-8.91E-01	4.98E-04
MGDG(16:1_16:3)	GL	MGDG	-8.20E-01	3.39E-03
PI(16:1_18:3)	PL	PI	5.77E-01	8.05E-02
SQDG(16:1_18:3)	GL	SQDG	-3.32E-01	3.53E-01
DGDG(18:3_20:3)	GL	DGDG	3.82E-02	9.17E-01
TG(18:0_16:0_18:3)	TG	TG	-3.13E-01	3.87E-01
PG(16:1_18:3)	PL	PG	-7.54E-02	8.33E-01
MGDG(16:3_18:3)	GL	MGDG	-6.98E-01	2.42E-02
MGDG(16:2_18:3)	GL	MGDG	-8.85E-01	6.97E-04
MGDG(16:0_18:1)	GL	MGDG	-8.29E-01	2.88E-03
CerG1(d18:1+hO_25:0+O)	Cer	CerG1	-2.98E-01	4.01E-01
SQDG(18:3_18:3)	GL	SQDG	6.88E-01	2.85E-02
MGDG(16:3_16:3)	GL	MGDG	4.52E-01	1.98E-01
CerG1(d18:1+hO_27:0+O)	Cer	CerG1	-4.85E-01	1.59E-01
CerG1(d43:2+2O)	Cer	CerG1	-1.69E-01	6.48E-01
DGDG(16:0_18:3)	GL	DGDG	-9.33E-01	7.97E-05
Cer(d18:2_27:0+O)	Cer	Cer	-8.55E-02	8.00E-01
DG(18:3_18:3)	DG	DG	5.92E-01	6.82E-02
PI(15:0_18:3)	PL	PI	2.24E-01	5.31E-01
PE(18:3_18:3)	PL	PE	-1.04E-01	7.86E-01
Cer(d18:2_26:0+O)	Cer	Cer	3.46E-01	3.36E-01
PC(34:6)	PL	PC	4.92E-01	1.42E-01
CL(18:3_18:2_16:1_20:4)	PL	CL	-2.64E-01	4.58E-01
DGDG(18:3_19:2)	GL	DGDG	4.33E-01	2.05E-01
MGDG(18:3_20:3)	GL	MGDG	7.11E-02	8.61E-01
PE(24:1_18:2)	PL	PE	5.61E-01	9.48E-02
MGDG(17:3_18:3)	GL	MGDG	4.28E-01	2.18E-01
PC(34:5)	PL	PC	5.26E-01	1.18E-01
DG(16:0_18:3)	DG	DG	7.34E-01	1.42E-02
PG(16:1_18:1)	PL	PG	-3.19E-01	3.83E-01
CerG1(d18:1+hO_23:0+O)	Cer	CerG1	-7.91E-02	8.37E-01
DGDG(16:0_18:0)	GL	DGDG	-8.90E-01	5.32E-04
PC(16:1_18:3)	PL	PC	2.96E-01	4.18E-01
DG(18:3_18:2)	DG	DG	5.88E-01	7.42E-02
DGDG(17:0_18:2)	GL	DGDG	-7.86E-01	7.12E-03
PC(38:4)	PL	PC	1.09E-02	9.92E-01
TG(16:0_18:1_18:1)	TG	TG	-7.44E-01	1.43E-02
TG(18:1_18:1_18:2)	TG	TG	-2.49E-01	4.89E-01
PE(26:0_18:2)	PL	PE	-5.84E-02	8.81E-01
PI(18:3_18:3)	GL	PI	6.83E-01	2.80E-02
MGDG(18:3_20:2)	GL	MGDG	2.48E-01	5.01E-01
PG(16:0_16:0)	PL	PG	6.01E-01	5.83E-02
PE(18:3_18:2)	PL	PE	1.19E-01	7.43E-01
CL(70:5)	PL	CL	7.31E-01	1.55E-02
PG(18:4_18:3)	PL	PG	7.93E-01	6.81E-03
TG(18:1_18:1_18:1)	TG	TG	-8.23E-01	3.66E-03
PE(22:0_18:3)	PL	PE	6.93E-01	2.55E-02
DGDG(17:0_18:3)	GL	DGDG	-3.76E-01	2.81E-01
PI(16:0_18:2)	PL	PI	9.07E-02	8.00E-01
PE(16:0_18:3)	PL	PE	5.63E-01	8.70E-02
Cer(d18:1+hO_26:0)	Cer	Cer	-3.77E-02	9.06E-01
DGDG(18:3_20:0)	GL	DGDG	4.31E-01	2.10E-01
DGDG(16:2_18:3)	GL	DGDG	1.97E-01	5.95E-01
PC(16:0_18:3)	PL	PC	2.71E-01	4.35E-01
PC(33:1)	PL	PC	5.66E-01	9.36E-02
MGDG(18:2_18:3)	GL	MGDG	-1.18E-01	7.73E-01
TG(18:0_16:0_18:1)	TG	TG	-5.67E-01	8.74E-02
MGDG(18:1_18:3)	GL	MGDG	-8.90E-01	5.47E-04
DG(24:0_18:2)	DG	DG	5.51E-01	9.57E-02
AGlcSiE(18:3)	AGlcSiE	AGlcSiE	-6.54E-01	3.71E-02
PC(33:2)	PL	PC	6.30E-01	5.30E-02
MGDG(18:3_19:2)	GL	MGDG	7.96E-01	5.54E-03
PC(33:3)	PL	PC	6.06E-01	6.38E-02
So(d22:0+pO)	Sterols	So	-1.25E-01	7.53E-01
DG(15:0_18:2)	DG	DG	5.45E-01	1.05E-01
PC(18:3_18:3)	PL	PC	2.30E-01	5.06E-01
PC(18:3_18:2)	PL	PC	2.25E-01	5.33E-01
PE(20:2_18:2)	PL	PE	4.85E-01	1.62E-01
CerG1(d42:2+2O)	Cer	CerG1	5.30E-01	1.17E-01
TG(16:0_16:0_18:1)	TG	TG	-5.07E-01	1.37E-01
PE(18:2_18:2)	PL	PE	2.63E-01	4.65E-01
PC(32:1)	PL	PC	1.69E-01	6.39E-01
DGDG(18:3_18:3)	GL	DGDG	3.85E-01	2.67E-01
Cer(d18:1+hO_25:0)	Cer	Cer	7.88E-01	6.78E-03
CerG1(d18:1+hO_24:0+O)	Cer	CerG1	4.18E-01	2.30E-01
PE(17:0_18:2)	PL	PE	6.36E-01	4.70E-02
DG(18:1_18:3)	DG	DG	3.67E-01	3.08E-01
WE(5:0_17:3)	WE	WE	-3.75E-01	2.97E-01
DG(18:0_20:0)	DG	DG	-3.82E-01	2.77E-01
DG(18:1_18:2)	DG	DG	6.64E-01	3.67E-02
PE(24:0_18:2)	PL	PE	6.50E-01	4.12E-02
DG(18:0_18:0)	DG	DG	-1.49E-01	6.88E-01
DG(16:0_16:0)	DG	DG	-1.47E-01	6.93E-01
PI(18:0_18:2)	PL	PI	2.14E-01	5.58E-01
DGDG(18:1_18:3)	GL	DGDG	-9.00E-01	3.19E-04
MGDG(18:0_18:2)	GL	MGDG	-6.88E-01	2.72E-02
CL(18:2_16:0_16:0_20:1)	PL	CL	6.93E-01	2.71E-02
Cer(d18:0+pO_26:0)	Cer	Cer	-5.24E-01	1.16E-01
PE(22:0_18:2)	PL	PE	6.58E-01	3.85E-02
So(d20:0+pO)	Sterols	So	6.91E-02	8.28E-01
PE(15:0_18:2)	PL	PE	6.31E-01	5.07E-02
PI(18:3_18:2)	PL	PI	5.21E-01	1.21E-01
PE(16:0_18:2)	PL	PE	5.95E-01	7.06E-02
TG(18:0_16:0_18:0)	TG	TG	-6.37E-01	5.03E-02
PE(18:0_18:3)	PL	PE	-6.08E-02	8.61E-01
DG(16:0_18:1)	DG	DG	3.18E-01	3.77E-01
DG(16:0_18:2)	DG	DG	6.40E-01	4.39E-02
DG(18:0_16:0)	DG	DG	-2.89E-01	4.25E-01
StE(30:3)	Sterols	StE	4.83E-01	1.54E-01
CerG1(d18:1+hO_22:0+O)	Cer	CerG1	6.14E-01	5.81E-02
PC(16:0_18:1)	PL	PC	-8.36E-02	8.00E-01
PI(16:0_18:1)	PL	PI	1.97E-01	5.96E-01
AGlcSiE(18:2)	AGlcSiE	AGlcSiE	4.84E-02	9.10E-01
DG(18:0_18:2)	DG	DG	4.32E-01	2.17E-01
AGlcSiE(18:1)	AGlcSiE	AGlcSiE	-2.36E-01	4.99E-01
DG(17:0_18:2)	DG	DG	7.13E-01	1.98E-02
CerG1(d18:1+hO_28:0+O)	Cer	CerG1	3.50E-01	3.19E-01
TG(18:0_18:0_18:0)	TG	TG	-7.11E-01	2.32E-02
PG(18:3_18:3)	PL	PG	9.69E-01	4.46E-06
PE(18:0_18:2)	PL	PE	5.37E-01	1.12E-01
TG(18:0_16:0_16:0)	TG	TG	-6.58E-01	4.18E-02

PG(16:1_18:2)	PL	PG	9.18E-01	1.62E-04
AGlcSiE(18:0)	AGlcSiE	AGlcSiE	6.34E-01	5.24E-02
MGDG(18:3_18:3)	GL	MGDG	8.70E-01	1.07E-03
DGDG(18:0_18:3)	GL	DGDG	1.27E-01	7.27E-01
PG(18:3_18:2)	PL	PG	8.54E-01	1.74E-03
DG(18:4_18:3)	DG	DG	4.26E-01	2.20E-01
MGDG(18:0_18:3)	GL	MGDG	-4.79E-01	1.58E-01
Cer(d18:1+hO_24:0)	Cer	Cer	8.06E-01	5.31E-03
Cer(d18:2_24:0+O)	Cer	Cer	9.11E-01	2.67E-04
PC(18:0_18:2)	PL	PC	6.25E-02	8.84E-01
PS(39:1)	PL	PS	-8.01E-02	8.06E-01
TG(16:0_14:0_16:0)	TG	TG	-3.33E-01	3.61E-01
AGlcSiE(16:0)	AGlcSiE	AGlcSiE	8.34E-01	2.99E-03
TG(16:0_16:0_16:0)	TG	TG	-3.75E-01	3.00E-01
DGDG(18:0_18:1)	GL	DGDG	5.76E-02	8.89E-01
PC(17:1_17:1)	PL	PC	7.44E-01	1.46E-02
MGDG(18:3_20:1)	GL	MGDG	9.17E-01	1.73E-04
PE(16:0_18:1)	PL	PE	5.28E-01	1.24E-01
PC(38:3)	PL	PC	5.60E-01	1.01E-01
PC(18:1_18:3)	PL	PC	-8.03E-02	8.01E-01

**Table S3** : List of  $p_{\text{corr}}$  from OPLS-DA and  $P$ -value from Welsch T-test of *Nicotiana sylvestris* leaf samples CMSII vs WT.

ID	cat	family	pvalue	pcorr					
PA.18.2_18.2.N	PL	PA	1.39E-09	-9.44E-01	SQDG.18.3_18.3.	GL	SQDG	1.97E-04	-7.32E-01
CerG1.d18.2_28.0_O.	Cer	CerG1	3.79E-09	-9.41E-01	TG.16.0_18.2_18.2.	TG	TG	1.52E-04	-7.30E-01
PA.18.3_18.2.	PL	PA	4.16E-09	-9.34E-01	PMe.18.2_18.2.	PL	PMe	1.91E-04	-7.24E-01
MGDG.18.2_18.3.	GL	MGDG	2.10E-08	-9.16E-01	Cer.d18.0_pO_24.0.	Cer	Cer	6.32E-04	-7.24E-01
Cer.d46.1_hO_O.	Cer	Cer	1.44E-07	-9.11E-01	PG.16.1_18.2.N	PL	PG	4.87E-04	-7.21E-01
CerG1.d18.2_29.0_O.	Cer	CerG1	9.78E-08	-9.06E-01	PE.20.0_18.2.P	PL	PE	3.50E-04	-7.20E-01
Cer.d18.1_hO_27.0_O.	Cer	Cer	1.59E-07	-9.05E-01	PMe.16.1_18.3.	PL	PMe	6.50E-04	-7.02E-01
MGDG.18.1_18.3.	GL	MGDG	4.41E-08	-9.04E-01	PE.18.2_18.2_12	PL	PE	3.93E-04	-6.98E-01
CerG1.d18.2_26.0_O.	Cer	CerG1	2.07E-07	-9.02E-01	PG.18.0_16.0.	PL	PG	8.83E-04	-6.94E-01
CerG1.d18.2_24.0_O.	Cer	CerG1	2.42E-07	-8.98E-01	PMe.16.0_16.0.	PL	PMe	9.58E-04	-6.93E-01
Cer.d18.1_hO_23.0_O.	Cer	Cer	4.13E-07	-8.92E-01	PG.34.5.	PL	PG	1.76E-03	-6.92E-01
Cer.d18.0_pO_22.0_O.	Cer	Cer	9.95E-07	-8.90E-01	Cer.d18.2_24.0_O.	Cer	Cer	7.09E-04	-6.90E-01
Cer.d18.1_hO_24.0_O.	Cer	Cer	1.31E-06	-8.78E-01	DGDG.16.0_18.0.	GL	DGDG	1.42E-03	-6.89E-01
PEt.32.4.	PL	PEt	2.02E-06	-8.76E-01	PA.16.0_18.1.P	PL	PA	8.94E-04	-6.89E-01
CerG1.d18.2_25.0_O.	Cer	CerG1	1.25E-06	-8.71E-01	Cer.d17.1_hO_25.0.	Cer	Cer	9.19E-04	-6.87E-01
MGDG.16.0_18.2.	GL	MGDG	1.22E-06	-8.65E-01	PA.18.1_18.1.	PL	PA	9.33E-04	-6.86E-01
CerG1.d18.2_22.0_O.	Cer	CerG1	2.91E-06	-8.62E-01	CerG1.d18.1_hO_22.0.	Cer	CerG1	1.15E-03	-6.77E-01
PA.16.1_18.3.P	PL	PA	5.02E-06	-8.62E-01	PE.15.0_18.3.	PL	PE	1.23E-03	-6.75E-01
Cer.d18.0_pO_24.0_O.	Cer	Cer	9.10E-06	-8.54E-01	PE.24.0_18.2.	PL	PE	1.19E-03	-6.72E-01
CerG1.d18.2_20.0_O.	Cer	CerG1	3.85E-06	-8.53E-01	TG.18.0_17.0_18.3.	TG	TG	8.49E-04	-6.68E-01
PA.18.2_18.2.P	PL	PA	2.09E-06	-8.53E-01	MGDG.16.3_18.3.	GL	MGDG	1.95E-03	-6.67E-01
Cer.d18.1_hO_26.0.	Cer	Cer	5.76E-06	-8.45E-01	DGDG.18.3_18.3.	GL	DGDG	1.46E-03	-6.67E-01
PA.16.0_18.2.N	PL	PA	7.79E-06	-8.43E-01	PE.18.0_16.1.	PL	PE	1.48E-03	-6.64E-01
Cer.d18.0_pO_22.0.	Cer	Cer	1.36E-05	-8.42E-01	CerG1.d18.1_hO_26.0_O.	Cer	CerG1	1.50E-03	-6.64E-01
Cer.d18.1_hO_25.0_O.	Cer	Cer	7.54E-06	-8.40E-01	CerG1.d18.2_18.0_O.	Cer	CerG1	2.28E-03	-6.63E-01
PA.17.0_18.3.	PL	PA	3.29E-06	-8.37E-01	PE.22.0_18.2.	PL	PE	1.30E-03	-6.63E-01
Cer.d18.0_pO_26.0.	Cer	Cer	1.61E-05	-8.36E-01	DGDG.18.3_20.4.	GL	DGDG	2.80E-03	-6.61E-01
Cer.d18.0_pO_26.0_O.	Cer	Cer	2.67E-05	-8.31E-01	PE.20.0_18.2.N	PL	PE	1.17E-03	-6.61E-01
Cer.d17.1_hO_22.0.	Cer	Cer	9.77E-06	-8.29E-01	PC.38.4.	PL	PC	1.69E-03	-6.60E-01
CerG1.d18.2_31.0_O.	Cer	CerG1	6.37E-06	-8.29E-01	PMe.22.0_18.2.	PL	PMe	1.44E-03	-6.56E-01
DGDG.16.2_18.3.N	GL	DGDG	1.80E-05	-8.20E-01	PMe.20.0_18.2.	PL	PMe	1.41E-03	-6.55E-01
Cer.d18.0_pO_25.0.	Cer	Cer	3.34E-05	-8.17E-01	DGDG.16.0_16.3.	GL	DGDG	2.74E-03	-6.50E-01
DG.16.0_18.2.	DG	DG	2.97E-05	-8.17E-01	DGDG.18.0_18.2.	GL	DGDG	2.08E-03	-6.43E-01
PC.18.2_18.2.P	PL	PC	9.88E-06	-8.16E-01	CerG1.d38.0_O.	Cer	CerG1	3.26E-03	-6.43E-01
Cer.d18.1_hO_23.0.	Cer	Cer	2.86E-05	-8.14E-01	PMe.16.0_16.1.	PL	PMe	3.34E-03	-6.37E-01
PA.18.1_18.2.	PL	PA	1.44E-05	-8.11E-01	PC.36.1.	PL	PC	2.03E-03	-6.36E-01
DG.18.1_18.3.	DG	DG	1.25E-05	-8.10E-01	PI.16.0_18.2.P	PL	PI	3.28E-03	-6.35E-01
Cer.d18.1_hO_22.0_O.	Cer	Cer	3.54E-05	-8.10E-01	PE.15.0_18.1.	PL	PE	2.43E-03	-6.35E-01
Cer.d18.1_hO_26.0_O.	Cer	Cer	4.07E-05	-8.09E-01	PI.16.0_18.2.N	PL	PI	3.16E-03	-6.34E-01
MGDG.16.0_18.1.	GL	MGDG	1.82E-05	-8.09E-01	TG.18.0_18.2_18.3.	TG	TG	2.41E-03	-6.19E-01
MGDG.16.2_18.3_10	GL	MGDG	2.65E-05	-8.03E-01	TG.18.1_18.1_18.2.	TG	TG	2.62E-03	-6.18E-01
PG.16.1_18.2.P	PL	PG	2.85E-05	-8.01E-01	PA.18.0_18.1.	PL	PA	5.52E-03	-6.18E-01
PG.16.0_18.1.P	PL	PG	1.79E-05	-8.00E-01	PI.16.0_20.5.	PL	PI	3.70E-03	-6.11E-01
PG.16.1_18.3.N	PL	PG	5.85E-05	-7.93E-01	DGDG.18.0_18.1.	GL	DGDG	4.86E-03	-6.10E-01
PE.18.2_18.2.	PL	PE	1.51E-05	-7.90E-01	TG.18.1_18.2_18.3.	TG	TG	2.88E-03	-6.09E-01
DGDG.16.0_18.1.	GL	DGDG	5.89E-05	-7.89E-01	CerG1.d18.1_hO_23.0_O.	Cer	CerG1	4.95E-03	-6.04E-01
CerG1.d18.2_23.0_O.	Cer	CerG1	3.73E-05	-7.89E-01	PC.34.1.	PL	PC	4.03E-03	-5.99E-01
DGDG.16.0_18.2.	GL	DGDG	1.07E-04	-7.72E-01	PE.16.0_18.2.P	PL	PE	6.27E-03	-5.98E-01
PA.16.0_18.2.P	PL	PA	8.86E-05	-7.71E-01	PA.16.0_16.1.	PL	PA	8.43E-03	-5.98E-01
DGDG.18.1_18.3.	GL	DGDG	7.34E-05	-7.70E-01	PA.16.1_18.3.N	PL	PA	7.34E-03	-5.97E-01
PA.18.3_18.2_11.1	PL	PA	5.81E-05	-7.70E-01	TG.16.0_18.2_18.3.	TG	TG	3.26E-03	-5.96E-01
PE.16.1_18.3.	PL	PE	5.81E-05	-7.70E-01	PG.16.0_16.0.P	PL	PG	7.07E-03	-5.94E-01
DGDG.16.3_18.3.	GL	DGDG	1.08E-04	-7.67E-01	PE.18.2_23.0.P	PL	PE	6.85E-03	-5.85E-01
CerG1.d44.3_pO.	Cer	CerG1	2.35E-04	-7.65E-01	CerG1.d18.1_hO_25.0_O.	Cer	CerG1	5.42E-03	-5.84E-01
Cer.d17.1_hO_26.0.	Cer	Cer	1.08E-04	-7.65E-01	PA.17.0_18.2.	PL	PA	5.69E-03	-5.83E-01
CerG1.d42.0_O.	Cer	CerG1	2.76E-04	-7.60E-01	PMe.16.0_18.2.	PL	PMe	5.69E-03	-5.83E-01
PA.16.0_18.1.N	PL	PA	1.93E-04	-7.53E-01	DGDG.16.0_16.0.N	GL	DGDG	1.11E-02	-5.78E-01
Cer.d17.1_hO_23.0.	Cer	Cer	1.60E-04	-7.51E-01	PMe.16.0_18.1.	PL	PMe	6.09E-03	-5.78E-01
PG.16.0_18.1.N	PL	PG	1.53E-04	-7.48E-01	DG.18.0_18.0.	DG	DG	1.27E-02	-5.73E-01
PA.18.0_18.2.	PL	PA	2.04E-04	-7.47E-01	TG.58.4.	TG	TG	7.04E-03	-5.69E-01
DGDG.18.2_18.3.	GL	DGDG	1.52E-04	-7.46E-01	TG.18.3_18.2_18.2.	TG	TG	5.34E-03	-5.68E-01
PE.37.1.	PL	PE	1.41E-04	-7.46E-01	DG.18.0_16.0.	DG	DG	1.46E-02	-5.60E-01
DGDG.16.2_18.3.P	GL	DGDG	2.36E-04	-7.43E-01	PMe.18.0_18.2.	PL	PMe	7.89E-03	-5.60E-01
PC.38.1.	PL	PC	1.38E-04	-7.42E-01	DGDG.16.0_16.0.P	GL	DGDG	1.48E-02	-5.57E-01
PI.18.3_18.2.	PL	PI	1.65E-04	-7.39E-01	CerG1.d43.3_pO.	Cer	CerG1	1.84E-02	-5.55E-01
DG.18.0_18.2.	DG	DG	3.21E-04	-7.34E-01	TG.17.0_18.2_18.2.	TG	TG	6.69E-03	-5.51E-01
PG.16.1_18.3.P	PL	PG	2.78E-04	-7.32E-01	TG.19.0_18.2_18.2.	TG	TG	9.58E-03	-5.50E-01
					PE.16.0_18.1.	PL	PE	9.71E-03	-5.50E-01
					AGlcSiE.18.1.	AGlcSiE	AGlcSiE	1.36E-02	-5.38E-01
					DG.18.0_18.1.	DG	DG	1.79E-02	-5.36E-01
					CerG1.d18.1_hO_22.0_O.	Cer	CerG1	1.42E-02	-5.36E-01
					PE.17.1_18.0.	PL	PE	1.29E-02	-5.35E-01
					DG.16.0_18.1.	DG	DG	1.74E-02	-5.33E-01



SQDG.30.0.	GL	SQDG	2.00E-02	-5.29E-01	PA.15.0_18.3.P	PL	PA	8.11E-01	-5.27E-02
DGDG.16.0_18.3.	GL	DGDG	2.26E-02	-5.27E-01	DGDG.18.0_18.3.	GL	DGDG	8.91E-01	-3.45E-02
CerG1.d18.2_16.0_O.	Cer	CerG1	2.13E-02	-5.26E-01	TG.17.0_18.2_18.3.	TG	TG	7.52E-01	-3.35E-02
SQDG.16.0_16.0.	GL	SQDG	2.26E-02	-5.24E-01	LPMe.18.2.	PL	LPMe	8.43E-01	-2.67E-02
DGDG.16.1_18.3.	GL	DGDG	1.88E-02	-5.23E-01	TG.4.0_10.1_13.0.	TG	TG	9.89E-01	-2.32E-02
PG.16.0_16.0.N	PL	PG	2.24E-02	-5.23E-01	LPC.18.2.P	PL	LPC	8.93E-01	-1.84E-02
MGDG.16.0_16.2.	GL	MGDG	3.08E-02	-5.12E-01	AGlcSiE.16.0.	AGlcSiE	AGlcSiE	9.76E-01	-1.74E-02
TG.22.0_18.2_18.3.	TG	TG	1.67E-02	-5.07E-01	LPC.20.0.	PL	LPC	8.95E-01	-1.57E-02
AGlcSiE.17.0.	AGlcSiE	AGlcSiE	2.46E-02	-5.07E-01	LPA.18.1.	PL	LPA	9.42E-01	-8.12E-03
PE.17.1_18.3.	PL	PE	2.09E-02	-4.99E-01	LPMe.17.1.	PL	LPMe	9.46E-01	-6.83E-03
DGDG.17.3_18.3.	GL	DGDG	2.32E-02	-4.98E-01	PE.17.0_18.2.P	PL	PE	9.74E-01	-5.80E-03
SQDG.16.0_18.3.	GL	SQDG	2.65E-02	-4.96E-01	LPG.18.2.P	PL	LPG	9.76E-01	-2.44E-03
PET.30.1.	PL	PET	4.09E-02	-4.94E-01	TG.18.4_16.1_18.4.	TG	TG	9.65E-01	1.25E-03
PE.20.2_18.2.	PL	PE	1.92E-02	-4.92E-01	PC.16.0_16.0.	PL	PC	8.99E-01	1.39E-03
PA.20.1_18.2.	PL	PA	2.44E-02	-4.83E-01	DG.15.0_18.2.	DG	DG	8.81E-01	1.13E-02
MePC.38.7.	PL	MePC	4.04E-02	-4.82E-01	MGDG.16.0_16.3.	GL	MGDG	8.24E-01	1.42E-02
CerG1.d34.3_20.	Cer	CerG1	4.41E-02	-4.75E-01	PMe.20.0_18.3.	PL	PMe	9.91E-01	1.49E-02
PI.16.0_18.3.P	PL	PI	3.23E-02	-4.75E-01	MGDG.18.0_18.1.	GL	MGDG	9.67E-01	1.70E-02
DG.16.0_16.0.	DG	DG	5.27E-02	-4.68E-01	DGDG.17.0_18.3.	GL	DGDG	9.02E-01	1.80E-02
MGDG.18.3_20.2.	GL	MGDG	3.71E-02	-4.65E-01	DGDG.18.3_19.1.	GL	DGDG	9.42E-01	2.47E-02
PC.18.2_18.2.N	PL	PC	3.65E-02	-4.65E-01	LPC.22.0.	PL	LPC	9.90E-01	2.91E-02
SQDG.36.5.	GL	SQDG	5.07E-02	-4.56E-01	LPA.16.1.	PL	LPA	7.74E-01	5.35E-02
PMe.18.0_18.1.	PL	PMe	3.48E-02	-4.54E-01	TG.18.3_18.2_18.3.	TG	TG	9.57E-01	5.59E-02
MGDG.18.0_18.2.	GL	MGDG	5.02E-02	-4.33E-01	DGDG.18.3_20.0.	GL	DGDG	8.78E-01	5.96E-02
PG.16.0_16.1.P	PL	PG	7.61E-02	-4.20E-01	PG.33.1.	PL	PG	7.60E-01	6.22E-02
PMe.18.3_18.2.	PL	PMe	5.38E-02	-4.13E-01	PC.16.0_17.0.	PL	PC	7.25E-01	7.02E-02
PE.16.0p.	PL	PE	7.14E-02	-4.13E-01	DGDG.39.7.	GL	DGDG	6.42E-01	8.93E-02
PE.16.0_18.2.N	PL	PE	6.81E-02	-4.11E-01	MGDG.18.3_20.3.	GL	MGDG	6.22E-01	1.06E-01
AGlcSiE.15.0.	AGlcSiE	AGlcSiE	7.95E-02	-4.10E-01	LPC.18.1.P	PL	LPC	7.01E-01	1.09E-01
TG.24.0_18.2_18.3.	TG	TG	5.85E-02	-4.03E-01	PE.15.0_18.2.	PL	PE	6.63E-01	1.12E-01
CerG1.d18.2_16.0.	Cer	CerG1	8.84E-02	-3.99E-01	SQMG.18.1.	GL	SQMG	7.33E-01	1.15E-01
PG.16.1_18.1.P	PL	PG	7.62E-02	-3.97E-01	DG.19.0_18.2.	DG	DG	5.89E-01	1.21E-01
PE.18.2_23.0.N	PL	PE	8.36E-02	-3.89E-01	PC.34.5.	PL	PC	6.34E-01	1.22E-01
PG.16.1_18.1.N	PL	PG	9.42E-02	-3.81E-01	DG.25.0_18.2.	DG	DG	5.99E-01	1.23E-01
PI.16.0_18.3.N	PL	PI	9.97E-02	-3.79E-01	Cer.d18.2_16.0_O.	Cer	Cer	4.71E-01	1.40E-01
PC.16.0_18.1.	PL	PC	1.01E-01	-3.64E-01	PC.24.2_10.4.	PL	PC	4.85E-01	1.42E-01
MGDG.18.3_18.3.	GL	MGDG	1.23E-01	-3.57E-01	DGMG.16.3.	GL	DGMG	4.84E-01	1.49E-01
CerG1.d18.1_hO_24.0_O.	Cer	CerG1	1.26E-01	-3.55E-01	MGDG.17.2_18.3.	GL	MGDG	5.21E-01	1.57E-01
PE.18.0_18.2.P	PL	PE	1.15E-01	-3.43E-01	AGlcSiE.18.0.	AGlcSiE	AGlcSiE	5.02E-01	1.61E-01
DG.18.4_16.1.	DG	DG	1.65E-01	-3.36E-01	PE.35.5.	PL	PE	5.42E-01	1.61E-01
PG.16.0_16.1.N	PL	PG	1.85E-01	-3.26E-01	PA.18.3_18.3.P	PL	PA	4.87E-01	1.73E-01
MePC.38.6p.	PL	MePC	2.40E-01	-3.24E-01	PE.34.5.	PL	PE	4.87E-01	1.73E-01
AGlcSiE.16.1.	AGlcSiE	AGlcSiE	1.89E-01	-3.21E-01	LPMe.18.1.	PL	LPMe	4.57E-01	1.91E-01
TG.18.0_18.0_18.0.	TG	TG	1.91E-01	-3.17E-01	TG.15.0_18.2_18.2.	TG	TG	4.35E-01	2.11E-01
SQDG.36.3.	GL	SQDG	1.56E-01	-3.15E-01	PA.16.0_18.3_11.9	PL	PA	3.17E-01	2.17E-01
PA.20.0_18.2.	PL	PA	3.28E-01	-2.91E-01	PE.16.1_16.1.	PL	PE	3.17E-01	2.17E-01
SQMG.18.2.	GL	SQMG	2.16E-01	-2.86E-01	LPG.18.3.P	PL	LPG	2.79E-01	2.43E-01
AGlcSiE.20.0.	AGlcSiE	AGlcSiE	2.25E-01	-2.82E-01	DG.18.1_18.2.	DG	DG	2.76E-01	2.48E-01
PC.18.0_18.1.	PL	PC	2.09E-01	-2.74E-01	MGDG.16.0_18.3.	GL	MGDG	2.56E-01	2.51E-01
LPG.16.1.P	PL	LPG	3.01E-01	-2.68E-01	PE.18.3_18.2_11	PL	PE	3.82E-01	2.53E-01
PE.18.0_18.2.N	PL	PE	2.38E-01	-2.62E-01	SiE.18.3_19.6	Sterol	SiE	2.82E-01	2.64E-01
AGlcSiE.25.0.	AGlcSiE	AGlcSiE	2.79E-01	-2.54E-01	DGDG.38.7.	GL	DGDG	2.13E-01	2.70E-01
LPI.16.0.	PL	LPI	2.92E-01	-2.52E-01	MGDG.17.3_18.3.	GL	MGDG	2.31E-01	2.88E-01
AGlcSiE.23.0.	AGlcSiE	AGlcSiE	2.72E-01	-2.50E-01	PMe.16.0_18.3.	PL	PMe	2.17E-01	3.02E-01
PE.22.0_18.3.P	PL	PE	2.49E-01	-2.48E-01	PC.24.0_18.3.P	PL	PC	2.81E-01	3.07E-01
LPI.18.2.	PL	LPI	2.91E-01	-2.39E-01	LPG.16.1.N	PL	LPG	1.67E-01	3.16E-01
MGMG.16.2.	GL	MGMG	3.02E-01	-2.35E-01	PA.16.0_18.3.	PL	PA	1.49E-01	3.16E-01
PC.34.0.	PL	PC	4.46E-01	-2.00E-01	LPG.18.2.N	PL	LPG	1.75E-01	3.28E-01
LPA.18.2.	PL	LPA	3.87E-01	-1.96E-01	MGDG.18.3_19.1.	GL	MGDG	1.63E-01	3.30E-01
AGlcSiE.22.0.	AGlcSiE	AGlcSiE	4.03E-01	-1.94E-01	PA.18.3_18.3.N	PL	PA	1.41E-01	3.46E-01
DG.18.2_23.0.	DG	DG	4.78E-01	-1.78E-01	PS.20.0_18.2.P	PL	PS	1.07E-01	3.52E-01
PC.18.3_18.2.P	PL	PC	4.03E-01	-1.72E-01	TG.12.0e_11.3_11.3.	TG	TG	1.05E-01	3.59E-01
PC.32.0.	PL	PC	5.52E-01	-1.72E-01	PC.18.3_18.2.N	PL	PC	1.29E-01	3.61E-01
DG.14.0_18.3.	DG	DG	5.53E-01	-1.71E-01	DGMG.16.0.	GL	DGMG	7.83E-02	3.99E-01
PC.18.0_18.2.	PL	PC	4.49E-01	-1.68E-01	LPMe.16.0.	PL	LPMe	8.99E-02	3.99E-01
PE.18.3_18.2.	PL	PE	4.07E-01	-1.60E-01	PE.22.0_18.3.N	PL	PE	1.23E-01	4.05E-01
PC.18.0_18.3.P	PL	PC	4.96E-01	-1.51E-01	PC.40.3.	PL	PC	1.26E-01	4.14E-01
PC.16.0_18.2.	PL	PC	5.36E-01	-1.49E-01	PE.20.0_18.3.P	PL	PE	9.07E-02	4.24E-01
DGDG.37.7.	GL	DGDG	5.43E-01	-1.46E-01	DG.26.0_18.2.	DG	DG	6.65E-02	4.25E-01
TG.16.0_17.0_18.3.	TG	TG	4.97E-01	-1.45E-01	LPC.16.0.P	PL	LPC	5.46E-02	4.32E-01
MGMG.18.2.	GL	MGMG	5.18E-01	-1.37E-01	TG.16.1_18.3_18.3.	TG	TG	7.61E-02	4.34E-01
DG.17.0_18.2.	DG	DG	6.50E-01	-1.29E-01	PC.33.2.	PL	PC	6.56E-02	4.37E-01
DG.16.0_22.0.	DG	DG	7.15E-01	-9.79E-02	MGDG.16.0_16.0.	GL	MGDG	4.79E-02	4.38E-01

DG.15.0_18.3.	DG	DG	4.84E-02	4.39E-01	PE.16.0_18.3.P	PL	PE	7.91E-04	7.10E-01
TG.18.3_18.3_20.2.	TG	TG	7.20E-02	4.41E-01	TG.18.3_18.3_20.3.	TG	TG	6.20E-04	7.10E-01
DG.16.0_24.0.	DG	DG	4.25E-02	4.43E-01	MGMG.16.0.	GL	MGMG	3.49E-04	7.13E-01
PMe.18.3_18.3.	PL	PMe	6.07E-02	4.45E-01	PC.16.0_18.3.P	PL	PC	2.42E-04	7.28E-01
LPC.18.0.P	PL	LPC	4.61E-02	4.46E-01	MGMG.18.3.	GL	MGMG	3.07E-04	7.29E-01
MGDG.18.0_18.3.	GL	MGDG	4.38E-02	4.51E-01	DG.30.0_18.0.	DG	DG	2.05E-04	7.32E-01
TG.18.3_17.1_18.3.	TG	TG	6.61E-02	4.57E-01	TG.18.4_18.3_18.3.	TG	TG	3.94E-04	7.34E-01
LPC.18.1.N	PL	LPC	5.07E-02	4.64E-01	TG.18.3_13.0_20.4.	TG	TG	2.90E-04	7.37E-01
PMe.18.0_18.3.	PL	PMe	4.45E-02	4.66E-01	AGlcSiE.18.3.	AGlcSiE	AGlcSiE	2.25E-04	7.38E-01
PA.15.0_18.3.N	PL	PA	3.79E-02	4.70E-01	LPE.18.0.	PL	LPE	2.75E-04	7.39E-01
DG.22.0_18.2.	DG	DG	4.01E-02	4.70E-01	DG.24.0_18.3.	DG	DG	2.42E-04	7.46E-01
DG.18.1_24.0.	DG	DG	3.64E-02	4.72E-01	DG.28.0_16.0.	DG	DG	6.29E-05	7.54E-01
LPG.18.0.	PL	LPG	3.49E-02	4.72E-01	StE.18.3.	Sterol	StE	2.27E-04	7.56E-01
TG.16.0_16.1_18.3.	TG	TG	4.06E-02	4.77E-01	MGDG.16.0_18.0.	GL	MGDG	1.63E-04	7.57E-01
PE.38.5.	PL	PE	5.30E-02	4.79E-01	LPG.18.1.N	PL	LPG	2.62E-04	7.58E-01
DGDG.18.3_19.0.	GL	DGDG	3.08E-02	4.86E-01	DGMG.18.3.	GL	DGMG	1.45E-04	7.59E-01
DG.24.0_18.2.	DG	DG	3.26E-02	4.86E-01	DG.22.0_18.3.	DG	DG	1.58E-04	7.62E-01
DGDG.18.2_24.0.	GL	DGDG	4.82E-02	4.89E-01	PS.20.0_18.3.P	PL	PS	7.22E-05	7.64E-01
TG.15.0_18.2_18.3.	TG	TG	3.48E-02	5.04E-01	DG.19.1_18.3.	DG	DG	6.72E-05	7.66E-01
LPG.16.0.	PL	LPG	2.42E-02	5.08E-01	DG.30.0_16.0.	DG	DG	4.87E-05	7.67E-01
DG.16.0_16.1.	DG	DG	1.70E-02	5.08E-01	LPA.18.0.	PL	LPA	5.10E-05	7.71E-01
LPC.18.2.N	PL	LPC	2.65E-02	5.14E-01	MGMG.18.0.	GL	MGMG	5.31E-05	7.74E-01
TG.16.0_18.3_18.3.	TG	TG	2.65E-02	5.14E-01	PC.32.3.	PL	PC	9.59E-05	7.77E-01
LPE.18.2.	PL	LPE	2.69E-02	5.16E-01	LPC.16.0.N	PL	LPC	7.71E-05	7.77E-01
PE.17.0_18.2.N	PL	PE	3.56E-02	5.17E-01	DG.18.3_23.0.	DG	DG	6.07E-05	7.79E-01
DGDG.18.2_22.0.	GL	DGDG	4.02E-02	5.18E-01	DG.16.0_18.3.	DG	DG	3.60E-05	7.80E-01
PC.8.0e_16.0.	PL	PC	2.74E-02	5.27E-01	LPC.18.0.N	PL	LPC	7.29E-05	7.80E-01
LPC.24.0.	PL	LPC	2.53E-02	5.33E-01	LPS.18.2.	PL	LPS	4.15E-05	7.83E-01
StE.18.2.	Sterol	StE	2.78E-02	5.39E-01	ChE.18.3.	Sterol	ChE	4.33E-05	7.97E-01
TG.17.0_18.3_18.3.	TG	TG	1.72E-02	5.43E-01	PE.16.0_18.3.N	PL	PE	4.56E-05	7.99E-01
DG.16.1_18.3.	DG	DG	8.08E-03	5.57E-01	ChE.18.2.	Sterol	ChE	5.33E-05	8.00E-01
MGMG.16.1.	GL	MGMG	1.56E-02	5.60E-01	LPC.17.0.	PL	LPC	2.39E-05	8.10E-01
dMePE.18.3_18.2.	PL	dMePE	1.67E-02	5.60E-01	DG.17.0_18.3.	DG	DG	1.19E-05	8.13E-01
PE.20.3_18.2.	PL	PE	1.67E-02	5.60E-01	PS.20.0_18.3.N	PL	PS	8.58E-06	8.14E-01
DG.18.4_18.3.	DG	DG	9.76E-03	5.65E-01	PE.18.3_18.3_8	PL	PE	2.46E-05	8.15E-01
LPG.18.1.P	PL	LPG	1.13E-02	5.69E-01	PC.33.3.	PL	PC	1.56E-05	8.23E-01
DG.26.0_16.0.	DG	DG	6.45E-03	5.71E-01	PC.16.0_18.3.N	PL	PC	7.17E-06	8.26E-01
DG.18.3_20.3.	DG	DG	7.69E-03	5.71E-01	PE.18.0_18.3.P	PL	PE	8.85E-06	8.39E-01
PC.33.1.	PL	PC	8.68E-03	5.73E-01	PE.18.3_18.3.	PL	PE	1.39E-05	8.40E-01
MGMG.16.3.	GL	MGMG	7.13E-03	5.75E-01	LPI.18.3.	PL	LPI	8.18E-06	8.40E-01
LPG.18.3.N	PL	LPG	9.49E-03	5.75E-01	DG.19.0_18.3.	DG	DG	1.51E-06	8.48E-01
PC.19.0_18.2.	PL	PC	9.33E-03	5.87E-01	PC.18.0_18.3.N	PL	PC	2.54E-06	8.50E-01
SQMG.18.0.	GL	SQMG	7.17E-03	5.94E-01	PC.19.1_16.0.	PL	PC	3.49E-06	8.60E-01
DG.18.3_18.3.	DG	DG	5.25E-03	5.98E-01	SQMG.18.3.	GL	SQMG	1.60E-06	8.62E-01
PE.18.3_20.2.	PL	PE	1.16E-02	5.99E-01	LPS.18.3.	PL	LPS	8.87E-07	8.66E-01
DG.19.1_16.0.	DG	DG	3.62E-03	6.10E-01	PS.16.0_18.3.	PL	PS	3.68E-07	8.79E-01
LPE.16.0.	PL	LPE	5.03E-03	6.14E-01	PE.17.0_18.3.	PL	PE	1.24E-06	8.79E-01
LPMe.18.3.	PL	LPMe	3.46E-03	6.15E-01	LPE.18.3.	PL	LPE	7.57E-07	8.81E-01
PS.20.0_18.2.N	PL	PS	2.15E-03	6.23E-01	CerG1.d18.1_hO_24.0.	Cer	CerG1	8.82E-07	8.83E-01
CerG1.d43.0_pO_20.	Cer	CerG1	3.94E-03	6.26E-01	PC.18.3_18.3.N	PL	PC	2.57E-07	8.87E-01
PE.20.0_18.3.N	PL	PE	5.66E-03	6.32E-01	PS.18.0_18.3.	PL	PS	1.16E-07	8.88E-01
PC.16.0_16.1.	PL	PC	2.89E-03	6.37E-01	MGDG.18.3_24.0.	GL	MGDG	7.81E-07	8.89E-01
MGDG.16.0_22.0.	GL	MGDG	3.80E-03	6.40E-01	PC.18.3_18.3.P	PL	PC	1.91E-07	8.92E-01
DG.17.1_18.3.	DG	DG	2.30E-03	6.40E-01	LPC.18.3.N	PL	LPC	8.24E-08	9.05E-01
PE.18.0_18.3.N	PL	PE	3.98E-03	6.44E-01	PC.19.0_18.3.	PL	PC	4.44E-09	9.28E-01
SiE.18.2.	Sterol	SiE	3.33E-03	6.53E-01	LPC.18.3.P	PL	LPC	1.53E-09	9.35E-01
SQMG.16.0.	GL	SQMG	1.98E-03	6.54E-01	PC.17.0_18.3.	PL	PC	8.40E-09	9.38E-01
StE.25.2.	Sterol	StE	1.70E-03	6.57E-01	PC.15.0_18.3.	PL	PC	3.80E-09	9.41E-01
TG.53.9.	TG	TG	1.79E-03	6.65E-01					
PC.35.1.	PL	PC	2.05E-03	6.67E-01					
TG.14.0_18.3_18.3.	TG	TG	1.16E-03	6.70E-01					
MGDG.16.0_24.0.	GL	MGDG	1.91E-03	6.72E-01					
TG.18.3_18.3_18.3.	TG	TG	1.53E-03	6.78E-01					
TG.15.0_18.3_18.3.	TG	TG	1.45E-03	6.78E-01					
MGDG.17.0_18.3.	GL	MGDG	8.72E-04	6.80E-01					
DG.20.0_18.3.	DG	DG	8.53E-04	6.85E-01					
TG.19.1_18.3_18.3.	TG	TG	1.44E-03	6.89E-01					
LPA.16.0.	PL	LPA	7.02E-04	6.89E-01					
LPMe.15.0.	PL	LPMe	6.94E-04	6.89E-01					
LPA.18.3.	PL	LPA	7.73E-04	6.92E-01					
PC.24.0_18.3.N	PL	PC	2.31E-03	7.02E-01					
PC.20.1_18.2.	PL	PC	7.37E-04	7.03E-01					
PC.17.0_18.2.	PL	PC	7.06E-04	7.08E-01					

**Table S4** : List of  $p_{\text{corr}}$  from OPLS-DA and  $P$ -value from Welsch T-test of *Arabidopsis thaliana* seed samples *ndufs4* vs Col0

ID	family	cat	pcorr	pvalue					
DGMG(18:2)	DGMG	GL	-9.97E-01	1.03E-09	PI(34:5)	PI	PL	-9.00E-01	1.39E-04
DGDG(18:3_20:3)	DGDG	GL	-9.96E-01	1.57E-09	WE(3:0_20:3)	WE	WE	-9.00E-01	2.16E-04
LPC(20:2)	LPC	PL	-9.95E-01	4.16E-10	PE(22:0_18:2)	PE	PL	-8.99E-01	1.19E-04
DGDG(18:3_20:2)	DGDG	GL	-9.93E-01	3.91E-08	PC(40:4)	PC	PL	-8.96E-01	1.83E-04
DGDG(18:2_20:1)	DGDG	GL	-9.92E-01	2.04E-08	DG(16:0_18:2)	DG	DG	-8.95E-01	2.62E-04
LPC(20:3)	LPC	PL	-9.91E-01	4.97E-09	Cer(d18:0+pO_24:0)	Cer	Cer	-8.90E-01	4.64E-04
LPE(20:1)	LPE	PL	-9.91E-01	2.34E-09	PE(17:1_16:0)	PE	PL	-8.88E-01	3.14E-04
LPC(20:1)	LPC	PL	-9.88E-01	2.61E-08	WE(3:0_20:4)	WE	WE	-8.88E-01	3.15E-04
PG(20:1_18:2)	PG	PL	-9.88E-01	6.26E-08	PG(16:1_20:2)	PG	PL	-8.86E-01	3.99E-04
DGMG(18:3)	DGMG	GL	-9.87E-01	1.39E-07	PC(42:3)	PC	PL	-8.83E-01	2.85E-04
LPC(18:2)	LPC	PL	-9.87E-01	4.22E-08	LPE(24:0)	LPE	PL	-8.82E-01	4.04E-04
LPE(18:2)	LPE	PL	-9.87E-01	1.42E-08	DG(18:1_18:2)	DG	DG	-8.81E-01	3.60E-04
DGDG(16:0_18:3)	DGDG	GL	-9.86E-01	2.56E-07	PE(22:1_18:2)	PE	PL	-8.78E-01	2.53E-04
PG(16:0_20:1)	PG	PL	-9.86E-01	1.93E-07	PG(16:0_18:1)	PG	PL	-8.77E-01	4.07E-04
LPE(16:1)	LPE	PL	-9.84E-01	8.05E-08	TG(10:0_18:2_18:3)	TG	TG	-8.77E-01	4.39E-04
LPE(24:1)	LPE	PL	-9.84E-01	2.38E-08	DG(16:0_18:1)	DG	DG	-8.76E-01	4.01E-04
PE(16:0_16:0)	PE	PL	-9.84E-01	4.51E-08	TG(43:9)	TG	TG	-8.76E-01	4.02E-04
DG(20:1_20:1)	DG	DG	-9.83E-01	2.42E-07	DG(24:1_18:2)	DG	DG	-8.74E-01	5.53E-04
WE(19:0_17:4)	WE	WE	-9.81E-01	2.96E-07	PA(16:1_18:3)	PA	PL	-8.74E-01	4.10E-04
DG(18:4_16:1)	DG	DG	-9.80E-01	5.54E-07	TG(18:3_18:2_22:3)	TG	TG	-8.74E-01	5.53E-04
DGDG(18:1_18:3)	DGDG	GL	-9.80E-01	8.30E-07	Cer(d18:2_25:0+O)	Cer	Cer	-8.73E-01	6.30E-04
LPE(22:0)	LPE	PL	-9.80E-01	6.17E-07	PE(18:2_23:0)	PE	PL	-8.73E-01	2.78E-04
LPC(14:0)	LPC	PL	-9.78E-01	7.46E-07	Cer(d18:1+hO_27:0)	Cer	Cer	-8.71E-01	7.51E-04
dMePE(32:2)	dMePE	PL	-9.76E-01	4.26E-07	PE(24:0_18:2)	PE	PL	-8.69E-01	2.96E-04
LPE(16:0)	LPE	PL	-9.76E-01	3.95E-07	TG(18:4_16:1_18:3)	TG	TG	-8.69E-01	6.28E-04
SQDG(16:0_18:3)	SQDG	GL	-9.72E-01	1.74E-06	Cer(d18:0+pO_22:0)	Cer	Cer	-8.68E-01	8.37E-04
dMePE(18:1_18:2)	dMePE	PL	-9.71E-01	1.60E-06	DG(18:2_23:1)	DG	DG	-8.67E-01	6.90E-04
LPE(18:1)	LPE	PL	-9.71E-01	6.43E-07	CerG1(d18:1+hO_26:0+O)	CerG1	Cer	-8.66E-01	6.30E-04
PE(20:1_18:2)	PE	PL	-9.71E-01	1.61E-06	Cer(d18:0+pO_26:0)	Cer	Cer	-8.65E-01	7.73E-04
PG(16:0_16:0)	PG	PL	-9.71E-01	2.72E-06	Cer(d18:1+hO_26:0+O)	Cer	Cer	-8.57E-01	1.18E-03
So(d18:1+hO)	So	So	-9.70E-01	3.64E-06	CerG1(d18:1+hO_24:0+O)	CerG1	Cer	-8.56E-01	7.97E-04
DG(14:0_18:3)	DG	DG	-9.69E-01	3.10E-06	AGlcSiE(18:1)	AGlcSiE	AGlcSiE	-8.54E-01	1.04E-03
DG(18:2_23:0)	DG	DG	-9.68E-01	3.01E-06	DGDG(18:3_18:3)	DGDG	GL	-8.47E-01	1.39E-03
Cer(d38:3)	Cer	Cer	-9.67E-01	3.81E-06	Cer(d18:1+hO_28:0+O)	Cer	Cer	-8.42E-01	1.48E-03
DGDG(18:0_18:2)	DGDG	GL	-9.66E-01	6.23E-06	Cer(d18:2_26:0+O)	Cer	Cer	-8.42E-01	1.46E-03
LPG(18:2)	LPG	PL	-9.65E-01	4.88E-06	PI(20:3_18:2)	PI	PL	-8.38E-01	8.20E-04
DG(15:0_18:1)	DG	DG	-9.64E-01	3.04E-06	PC(27:1_11:4)	PC	PL	-8.30E-01	1.40E-03
LPC(16:0)	LPC	PL	-9.63E-01	3.99E-06	PA(18:3_18:3)	PA	PL	-8.29E-01	1.35E-03
DG(17:1_18:2)	DG	DG	-9.61E-01	2.95E-06	TG(18:3_20:3_22:3)	TG	TG	-8.29E-01	1.56E-03
DG(22:1_18:2)	DG	DG	-9.61E-01	5.88E-06	PE(25:0_18:2)	PE	PL	-8.24E-01	1.03E-03
PG(16:0_16:1)	PG	PL	-9.60E-01	5.54E-06	DG(18:0_18:1)	DG	DG	-8.23E-01	1.72E-03
PI(20:2_18:2)	PI	PL	-9.60E-01	2.38E-06	DG(17:0_18:2)	DG	DG	-8.14E-01	1.93E-03
Cer(d18:2_24:0+O)	Cer	Cer	-9.59E-01	7.48E-06	DG(18:1_18:3)	DG	DG	-8.14E-01	2.18E-03
DG(15:0_18:3)	DG	DG	-9.57E-01	8.17E-06	MGMG(18:3)	MGMG	GL	-8.14E-01	2.68E-03
MGDG(18:1_18:2)	MGDG	GL	-9.57E-01	1.05E-05	DG(18:1_18:1)	DG	DG	-8.13E-01	1.95E-03
DG(20:1_18:1)	DG	DG	-9.56E-01	7.83E-06	PI(34:6)	PI	PL	-8.10E-01	1.97E-03
LPG(16:0)	LPG	PL	-9.55E-01	9.37E-06	Cer(d18:1+hO_26:0)	Cer	Cer	-8.06E-01	3.26E-03
DG(20:1_18:2)	DG	DG	-9.53E-01	1.01E-05	TG(16:0_14:0_18:2)	TG	TG	-8.02E-01	2.84E-03
DGDG(16:0_18:2)	DGDG	GL	-9.50E-01	2.61E-05	PC(42:4)	PC	PL	-7.96E-01	2.56E-03
DG(16:1_18:3)	DG	DG	-9.49E-01	1.65E-05	DG(16:0_16:0)	DG	DG	-7.90E-01	3.38E-03
StE(24:7)	StE	Sterols	-9.49E-01	1.18E-05	DG(17:0_18:1)	DG	DG	-7.89E-01	2.94E-03
DG(16:0_16:1)	DG	DG	-9.48E-01	1.57E-05	TG(18:4_17:1_18:3)	TG	TG	-7.81E-01	4.04E-03
AGlcSiE(18:2)	AGlcSiE	AGlcSiE	-9.46E-01	2.14E-05	DG(19:1_18:3)	DG	DG	-7.60E-01	4.95E-03
DGDG(16:1_18:3)	DGDG	GL	-9.43E-01	3.28E-05	So(d18:0+pO)	So	So	-7.57E-01	7.34E-03
MGDG(16:2_18:2)	MGDG	GL	-9.38E-01	4.57E-05	TG(18:3_14:1_18:3)	TG	TG	-7.44E-01	7.63E-03
DG(17:1_18:3)	DG	DG	-9.36E-01	2.48E-05	PC(34:6)	PC	PL	-7.38E-01	6.42E-03
DG(18:3_20:2)	DG	DG	-9.32E-01	4.16E-05	LPI(16:0)	LPI	PL	-7.35E-01	7.43E-03
MGDG(18:2_18:2)	MGDG	GL	-9.29E-01	7.66E-05	TG(18:1_18:2_18:3)	TG	TG	-7.29E-01	9.04E-03
PI(20:1_18:2)	PI	PL	-9.27E-01	3.40E-05	TG(12:0_18:2_18:3)	TG	TG	-7.25E-01	9.57E-03
DG(20:1_18:3)	DG	DG	-9.24E-01	6.64E-05	LPI(18:2)	LPI	PL	-7.22E-01	8.67E-03
WE(3:0_18:1)	WE	WE	-9.18E-01	1.05E-04	TG(16:0_12:0_18:2)	TG	TG	-7.17E-01	1.06E-02
PC(42:2)	PC	PL	-9.11E-01	8.62E-05	PI(14:0_18:3)	PI	PL	-7.11E-01	1.25E-02
PE(20:1_18:3)	PE	PL	-9.11E-01	1.40E-04	PC(37:3)	PC	PL	-7.08E-01	9.69E-03
LPC(18:1)	LPC	PL	-9.08E-01	1.03E-04	PE(15:0_18:2)	PE	PL	-7.03E-01	1.45E-02
PC(40:3)	PC	PL	-9.07E-01	1.13E-04	TG(18:3_17:1_18:3)	TG	TG	-7.01E-01	1.24E-02
LPC(16:1)	LPC	PL	-9.04E-01	1.84E-04	LdMePE(16:0)	LdMePE	PL	-6.80E-01	1.48E-02
DG(16:1_16:1)	DG	DG	-9.02E-01	1.52E-04	AGlcSiE(16:1)	AGlcSiE	AGlcSiE	-6.79E-01	1.49E-02
					DG(16:0_14:0)	DG	DG	-6.79E-01	1.61E-02
					TG(18:3_18:2_20:3)	TG	TG	-6.79E-01	1.66E-02
					TG(16:1_18:3_18:3)	TG	TG	-6.70E-01	1.89E-02
					TG(16:0_18:1_18:2)	TG	TG	-6.62E-01	2.02E-02
					PI(15:0_18:2)	PI	PL	-6.61E-01	1.81E-02
					CerG1(d18:1+hO_23:0+O)	CerG1	Cer	-6.60E-01	2.00E-02

PC(30:0)	PC	PL	-6.45E-01	2.04E-02	PS(22:0_18:3)	PS	PL	4.49E-01	1.13E-01
LPE(18:0)	LPE	PL	-6.20E-01	2.41E-02	PC(18:3_18:3)	PC	PL	4.72E-01	8.50E-02
Cer(d18:0+pO_23:0)	Cer	Cer	-6.01E-01	3.81E-02	PI(16:1_18:3)	PI	PL	4.79E-01	7.34E-02
DGDG(18:2_18:3)	DGDG	GL	-5.80E-01	3.90E-02	PS(18:3_18:2)	PS	PL	4.95E-01	8.43E-02
LPS(18:2)	LPS	PL	-5.79E-01	3.58E-02	PG(18:3_18:3)	PG	PL	5.00E-01	5.87E-02
AGlcSIE(19:1)	AGlcSIE	AGlcSIE	-5.73E-01	4.21E-02	TG(4:0_16:0_18:3)	TG	TG	5.28E-01	6.26E-02
SQDG(18:2_18:3)	SQDG	GL	-5.73E-01	3.59E-02	PS(22:0_18:2)	PS	PL	5.30E-01	6.84E-02
PI(20:0_18:2)	PI	PL	-5.63E-01	3.65E-02	LPC(18:0)	LPC	PL	5.34E-01	5.57E-02
DG(16:1_18:2)	DG	DG	-5.62E-01	4.94E-02	LPI(18:0)	LPI	PL	5.56E-01	5.37E-02
PG(15:0_18:3)	PG	PL	-5.61E-01	5.35E-02	MG(24:1)	MG	MG	5.66E-01	3.46E-02
LPC(18:3)	LPC	PL	-5.56E-01	5.07E-02	PE(18:2_18:2)	PE	PL	5.74E-01	3.45E-02
Cer(d18:1+hO_24:0+O)	Cer	Cer	-5.52E-01	5.75E-02	PI(16:0_18:2)	PI	PL	5.82E-01	4.61E-02
TG(18:3_18:2_18:3)	TG	TG	-5.49E-01	5.47E-02	TG(18:3_18:3_20:3)	TG	TG	5.86E-01	3.60E-02
PC(33:2)	PC	PL	-5.40E-01	5.86E-02	PE(16:0_16:1)	PE	PL	6.31E-01	2.07E-02
MG(20:0)	MG	MG	-5.36E-01	5.13E-02	PE(16:1_18:3)	PE	PL	6.51E-01	1.69E-02
TG(19:0_18:3_18:3)	TG	TG	-5.29E-01	5.84E-02	TG(18:3_18:3_22:3)	TG	TG	6.60E-01	1.84E-02
LPI(18:1)	LPI	PL	-5.27E-01	5.18E-02	TG(19:1_18:3_18:3)	TG	TG	6.94E-01	1.29E-02
TG(14:0_18:2_18:3)	TG	TG	-5.25E-01	6.36E-02	TG(15:0_18:3_18:3)	TG	TG	6.99E-01	1.09E-02
MG(16:0)	MG	MG	-5.20E-01	5.84E-02	PS(24:1_18:2)	PS	PL	7.08E-01	1.47E-02
DG(24:1_18:3)	DG	DG	-5.11E-01	6.87E-02	PC(37:4)	PC	PL	7.46E-01	6.99E-03
PG(16:1_18:2)	PG	PL	-5.08E-01	8.10E-02	PE(16:0_18:2)	PE	PL	7.79E-01	2.91E-03
BisMePE(16:0_18:2)	BisMePE	PL	-4.92E-01	7.53E-02	PI(15:0_18:3)	PI	PL	8.02E-01	2.85E-03
LPC(15:0)	LPC	PL	-4.72E-01	9.79E-02	AGlcSIE(18:3)	AGlcSIE	AGlcSIE	8.18E-01	1.66E-03
PA(18:1_18:2)	PA	PL	-4.71E-01	8.07E-02	PI(18:0_20:1)	PI	PL	8.23E-01	2.48E-03
dMePE(18:3_18:2)	dMePE	PL	-4.61E-01	1.03E-01	PS(20:1_18:3)	PS	PL	8.28E-01	2.32E-03
Cer(d18:0+pO_25:0)	Cer	Cer	-4.44E-01	1.14E-01	PE(18:3_22:1)	PE	PL	8.29E-01	1.29E-03
PC(16:0_18:2)	PC	PL	-4.35E-01	1.07E-01	TG(16:0_18:3_18:3)	TG	TG	8.39E-01	1.03E-03
PC(38:6)	PC	PL	-4.33E-01	1.01E-01	PI(18:2_23:1)	PI	PL	8.50E-01	1.34E-03
AGlcSIE(16:0)	AGlcSIE	AGlcSIE	-4.28E-01	1.14E-01	PS(18:3_22:1)	PS	PL	8.52E-01	1.31E-03
PS(18:1_18:2)	PS	PL	-4.26E-01	9.17E-02	PI(14:0_18:2)	PI	PL	8.59E-01	5.55E-04
PC(35:4)	PC	PL	-4.15E-01	1.03E-01	TG(18:4_15:0_18:3)	TG	TG	8.62E-01	5.84E-04
TG(18:1_12:0_18:2)	TG	TG	-3.84E-01	1.42E-01	PS(18:0_18:2)	PS	PL	8.72E-01	3.20E-04
PC(16:0_18:1)	PC	PL	-3.72E-01	1.43E-01	So(d18:0)	So	So	8.74E-01	3.96E-04
LPE(18:3)	LPE	PL	-3.68E-01	1.54E-01	PI(17:0_18:2)	PI	PL	8.77E-01	6.97E-04
WE(5:0_17:3)	WE	WE	-3.45E-01	1.79E-01	PI(18:3_18:2)	PI	PL	8.92E-01	3.17E-04
So(d22:0+pO)	So	So	-3.15E-01	1.93E-01	PG(18:3_18:2)	PG	PL	9.00E-01	9.29E-05
MG(18:0)	MG	MG	-2.84E-01	2.12E-01	PE(16:0_20:1)	PE	PL	9.11E-01	2.26E-04
PI(18:2_23:0)	PI	PL	-2.74E-01	1.97E-01	PI(18:0_18:2)	PI	PL	9.20E-01	1.32E-04
Cer(d18:1+hO_25:0+O)	Cer	Cer	-2.44E-01	2.69E-01	dMePE(16:1_18:1)	dMePE	PL	9.21E-01	7.74E-05
DG(18:0_18:0)	DG	DG	-2.33E-01	2.64E-01	PE(18:1_18:1)	PE	PL	9.29E-01	5.10E-05
PA(18:1_18:1)	PA	PL	-2.33E-01	2.42E-01	PS(24:1_18:3)	PS	PL	9.30E-01	9.31E-05
So(d20:0+pO)	So	So	-2.06E-01	2.95E-01	Cer(d16:0_19:0)	Cer	Cer	9.33E-01	4.42E-05
TG(12:0_18:3_18:3)	TG	TG	-1.78E-01	3.17E-01	PE(18:3_18:2)	PE	PL	9.33E-01	2.00E-05
TG(10:0_18:3_18:3)	TG	TG	-1.71E-01	3.17E-01	MGMG(16:3)	MGMG	GL	9.34E-01	5.16E-05
TG(18:3_18:3_18:3)	TG	TG	-1.26E-01	3.76E-01	PI(18:0_18:1)	PI	PL	9.36E-01	6.87E-05
PG(18:2_18:2)	PG	PL	-1.08E-01	4.09E-01	PE(24:1_18:2)	PE	PL	9.39E-01	4.56E-05
DG(18:0_16:0)	DG	DG	-7.22E-02	4.24E-01	TG(10:0_10:1_18:1)	TG	TG	9.39E-01	2.92E-05
PG(16:1_18:1)	PG	PL	-6.57E-02	4.63E-01	DGDG(16:3_18:3)	DGDG	GL	9.44E-01	1.10E-05
PC(35:3)	PC	PL	-2.05E-02	4.65E-01	AGlcSIE(17:0)	AGlcSIE	AGlcSIE	9.45E-01	1.72E-05
PA(20:1_18:2)	PA	PL	2.48E-03	4.79E-01	PS(16:0_18:3)	PS	PL	9.48E-01	3.03E-05
dMePE(16:0_18:3)	dMePE	PL	1.06E-02	4.69E-01	Cer(d18:1_15:0)	Cer	Cer	9.74E-01	7.32E-07
PE(18:1_18:2)	PE	PL	1.58E-02	4.63E-01	PE(18:3_18:3)	PE	PL	9.76E-01	2.74E-07
PG(15:0_18:2)	PG	PL	2.85E-02	4.42E-01	PI(18:2_18:2)	PI	PL	9.76E-01	2.36E-06
PE(17:0_18:2)	PE	PL	3.43E-02	4.39E-01	PE(16:0_18:1)	PE	PL	9.77E-01	1.06E-06
MGDG(16:3_18:3)	MGDG	GL	3.82E-02	4.37E-01	PS(18:3_18:3)	PS	PL	9.79E-01	1.15E-06
PC(34:4)	PC	PL	4.25E-02	4.70E-01	PI(17:0_18:3)	PI	PL	9.82E-01	9.32E-07
DG(20:0_22:0)	DG	DG	4.96E-02	4.26E-01	PI(18:3_18:3)	PI	PL	9.85E-01	1.10E-07
PA(18:2_18:2)	PA	PL	5.24E-02	4.48E-01	PI(16:0_18:3)	PI	PL	9.89E-01	5.09E-08
PC(16:0_20:1)	PC	PL	6.52E-02	4.50E-01	LPI(17:0)	LPI	PL	9.91E-01	4.24E-08
Cer(d18:0_16:0)	Cer	Cer	9.06E-02	3.72E-01	dMePE(16:1_18:3)	dMePE	PL	9.92E-01	6.38E-10
PC(17:1_13:0)	PC	PL	1.36E-01	3.79E-01	DGDG(17:0_18:2)	DGDG	GL	9.93E-01	7.84E-10
AGlcSIE(17:1)	AGlcSIE	AGlcSIE	1.38E-01	3.56E-01	LPC(17:0)	LPC	PL	9.93E-01	1.90E-09
TG(15:0_18:2_18:3)	TG	TG	1.76E-01	3.00E-01					
AGlcSIE(15:0)	AGlcSIE	AGlcSIE	1.96E-01	2.83E-01					
PI(18:0_18:3)	PI	PL	2.35E-01	2.93E-01					
DG(18:3_18:3)	DG	DG	2.93E-01	1.98E-01					
PS(20:0_18:2)	PS	PL	3.14E-01	2.09E-01					
PC(34:3)	PC	PL	3.16E-01	1.88E-01					
PC(35:2)	PC	PL	3.23E-01	1.86E-01					
PS(16:0_18:2)	PS	PL	3.53E-01	1.83E-01					
TG(16:0_18:2_18:3)	TG	TG	3.86E-01	1.27E-01					
TG(17:0_18:3_18:3)	TG	TG	4.00E-01	1.23E-01					
TG(20:1_18:3_18:3)	TG	TG	4.35E-01	9.89E-02					

**Table S5** : List of  $p_{\text{corr}}$  from OPLS-DA and  $P$ -value from Welsch T-test of *Arabidopsis thaliana* seed samples *ndufs8* vs *col0*

ID	family	cat	pcorr	pvalue					
AGlcSiE(15:0)	AGlcSiE	AGlcSiE	-2.20E-01	2.67E-01	DGDG(16:0_18:3)	DGDG	GL	-2.85E-01	2.17E-01
AGlcSiE(16:0)	AGlcSiE	AGlcSiE	-5.74E-01	4.06E-02	DGDG(16:1_18:3)	DGDG	GL	9.20E-01	4.51E-05
AGlcSiE(16:1)	AGlcSiE	AGlcSiE	-4.06E-01	1.22E-01	DGDG(16:3_18:3)	DGDG	GL	4.14E-01	1.10E-01
AGlcSiE(17:0)	AGlcSiE	AGlcSiE	6.86E-01	1.45E-02	DGDG(17:0_18:2)	DGDG	GL	9.94E-01	1.25E-10
AGlcSiE(17:1)	AGlcSiE	AGlcSiE	-7.69E-01	4.13E-03	DGDG(18:0_18:2)	DGDG	GL	2.96E-01	1.90E-01
AGlcSiE(18:1)	AGlcSiE	AGlcSiE	-9.38E-01	2.89E-05	DGDG(18:1_18:3)	DGDG	GL	-8.56E-01	9.75E-04
AGlcSiE(18:2)	AGlcSiE	AGlcSiE	-9.47E-01	1.52E-05	DGDG(18:2_18:3)	DGDG	GL	3.59E-01	1.48E-01
AGlcSiE(18:3)	AGlcSiE	AGlcSiE	1.29E-01	3.63E-01	DGDG(18:2_20:1)	DGDG	GL	-7.65E-01	7.28E-03
AGlcSiE(19:1)	AGlcSiE	AGlcSiE	-8.83E-01	3.55E-04	DGDG(18:3_18:3)	DGDG	GL	8.26E-01	1.16E-03
BisMePE(16:0_18:2)	BisMePE	PL	-9.01E-01	1.79E-04	DGDG(18:3_20:2)	DGDG	GL	3.98E-01	1.13E-01
Cer(d16:0_19:0)	Cer	Cer	8.97E-01	2.25E-04	DGDG(18:3_20:3)	DGDG	GL	-9.42E-01	2.94E-05
Cer(d18:0_16:0)	Cer	Cer	-6.66E-01	2.10E-02	DGMG(18:2)	DGMG	GL	-8.56E-01	1.16E-03
Cer(d18:0+pO_22:0)	Cer	Cer	-9.35E-01	5.27E-05	DGMG(18:3)	DGMG	GL	-6.86E-01	1.69E-02
Cer(d18:0+pO_23:0)	Cer	Cer	-8.90E-01	3.31E-04	dMePE(16:0_18:3)	dMePE	PL	-7.30E-02	4.35E-01
Cer(d18:0+pO_24:0)	Cer	Cer	-9.32E-01	5.80E-05	dMePE(16:1_18:1)	dMePE	PL	9.86E-01	1.01E-07
Cer(d18:0+pO_25:0)	Cer	Cer	-8.91E-01	3.29E-04	dMePE(16:1_18:3)	dMePE	PL	9.68E-01	8.39E-07
Cer(d18:0+pO_26:0)	Cer	Cer	-9.35E-01	4.76E-05	dMePE(18:1_18:2)	dMePE	PL	-9.48E-01	1.76E-05
Cer(d18:1_15:0)	Cer	Cer	8.63E-01	4.23E-04	dMePE(18:3_18:2)	dMePE	PL	-4.36E-01	1.15E-01
Cer(d18:1+hO_24:0+O)	Cer	Cer	-6.79E-01	1.70E-02	dMePE(32:2)	dMePE	PL	-9.72E-01	2.22E-06
Cer(d18:1+hO_25:0+O)	Cer	Cer	-7.17E-01	1.08E-02	LdMePE(16:0)	LdMePE	PL	-7.65E-01	5.18E-03
Cer(d18:1+hO_26:0)	Cer	Cer	-8.78E-01	4.69E-04	LPC(14:0)	LPC	PL	-9.55E-01	1.68E-05
Cer(d18:1+hO_26:0+O)	Cer	Cer	-8.06E-01	2.47E-03	LPC(15:0)	LPC	PL	-8.19E-01	2.73E-03
Cer(d18:1+hO_27:0)	Cer	Cer	-9.35E-01	5.23E-05	LPC(16:0)	LPC	PL	-6.40E-01	2.75E-02
Cer(d18:1+hO_28:0+O)	Cer	Cer	-8.87E-01	3.97E-04	LPC(16:1)	LPC	PL	-9.04E-01	2.64E-04
Cer(d18:2_24:0+O)	Cer	Cer	-9.74E-01	1.30E-06	LPC(17:0)	LPC	PL	9.79E-01	1.89E-07
Cer(d18:2_25:0+O)	Cer	Cer	-9.45E-01	2.41E-05	LPC(18:0)	LPC	PL	9.72E-01	8.61E-07
Cer(d18:2_26:0+O)	Cer	Cer	-9.05E-01	1.93E-04	LPC(18:1)	LPC	PL	7.98E-01	2.79E-03
Cer(d38:3)	Cer	Cer	-8.47E-01	1.10E-03	LPC(18:2)	LPC	PL	-8.89E-01	4.45E-04
CerG1(d18:1+hO_23:0+O)	CerG1	Cer	-8.44E-01	1.04E-03	LPC(18:3)	LPC	PL	4.11E-01	1.05E-01
CerG1(d18:1+hO_24:0+O)	CerG1	Cer	-9.18E-01	8.82E-05	LPC(20:1)	LPC	PL	4.43E-01	9.98E-02
CerG1(d18:1+hO_26:0+O)	CerG1	Cer	-9.21E-01	6.60E-05	LPC(20:2)	LPC	PL	-9.77E-01	8.60E-07
DG(14:0_18:3)	DG	DG	-9.76E-01	1.30E-06	LPC(20:3)	LPC	PL	-2.08E-01	2.76E-01
DG(15:0_18:1)	DG	DG	-9.35E-01	3.88E-05	LPE(16:0)	LPE	PL	-5.33E-01	6.02E-02
DG(15:0_18:3)	DG	DG	-9.72E-01	1.21E-06	LPE(16:1)	LPE	PL	-9.15E-01	1.61E-04
DG(16:0_14:0)	DG	DG	-6.54E-01	2.35E-02	LPE(18:0)	LPE	PL	8.83E-01	3.76E-04
DG(16:0_16:0)	DG	DG	-8.16E-01	2.39E-03	LPE(18:1)	LPE	PL	7.65E-01	5.39E-03
DG(16:0_16:1)	DG	DG	-9.33E-01	3.21E-05	LPE(18:2)	LPE	PL	-9.25E-01	8.25E-05
DG(16:0_18:1)	DG	DG	-5.43E-01	4.94E-02	LPE(18:3)	LPE	PL	8.36E-01	9.12E-04
DG(16:0_18:2)	DG	DG	-8.94E-01	2.27E-04	LPE(20:1)	LPE	PL	2.31E-01	2.69E-01
DG(16:1_16:1)	DG	DG	-3.24E-01	1.79E-01	LPE(22:0)	LPE	PL	-9.70E-01	3.43E-06
DG(16:1_18:2)	DG	DG	2.92E-01	2.06E-01	LPE(24:0)	LPE	PL	-9.14E-01	1.57E-04
DG(16:1_18:3)	DG	DG	4.10E-01	1.27E-01	LPE(24:1)	LPE	PL	-9.34E-01	4.31E-05
DG(17:0_18:1)	DG	DG	4.60E-01	9.11E-02	LPG(16:0)	LPG	PL	-9.85E-01	2.75E-07
DG(17:0_18:2)	DG	DG	7.08E-01	1.06E-02	LPG(18:2)	LPG	PL	-9.90E-01	8.64E-08
DG(17:1_18:2)	DG	DG	1.35E-01	3.71E-01	LPI(16:0)	LPI	PL	-8.43E-01	1.51E-03
DG(17:1_18:3)	DG	DG	-8.51E-02	4.25E-01	LPI(17:0)	LPI	PL	9.93E-01	4.62E-09
DG(18:0_16:0)	DG	DG	-5.37E-01	5.91E-02	LPI(18:0)	LPI	PL	9.04E-01	1.77E-04
DG(18:0_18:0)	DG	DG	-5.97E-01	3.64E-02	LPI(18:1)	LPI	PL	9.72E-01	1.38E-06
DG(18:0_18:1)	DG	DG	-4.33E-01	1.02E-01	LPI(18:2)	LPI	PL	-9.29E-01	7.28E-05
DG(18:1_18:1)	DG	DG	5.96E-01	3.82E-02	LPS(18:2)	LPS	PL	-6.47E-01	2.08E-02
DG(18:1_18:2)	DG	DG	9.63E-02	4.36E-01	MG(16:0)	MG	MG	-2.57E-01	2.52E-01
DG(18:1_18:3)	DG	DG	-6.19E-01	2.57E-02	MG(18:0)	MG	MG	-2.22E-01	2.74E-01
DG(18:2_23:0)	DG	DG	-9.62E-01	3.84E-06	MG(20:0)	MG	MG	-5.81E-01	3.99E-02
DG(18:2_23:1)	DG	DG	-9.59E-01	4.54E-06	MG(24:1)	MG	MG	6.06E-01	2.34E-02
DG(18:3_18:3)	DG	DG	9.91E-01	1.80E-08	MGDG(16:2_18:2)	MGDG	GL	8.06E-01	2.08E-03
DG(18:3_20:2)	DG	DG	-9.26E-01	3.96E-05	MGDG(16:3_18:3)	MGDG	GL	1.14E-01	3.65E-01
DG(18:4_16:1)	DG	DG	-8.82E-01	3.04E-04	MGDG(18:1_18:2)	MGDG	GL	-7.59E-01	6.84E-03
DG(19:1_18:3)	DG	DG	1.75E-01	3.32E-01	MGDG(18:2_18:2)	MGDG	GL	-8.52E-01	1.15E-03
DG(20:0_22:0)	DG	DG	-9.40E-01	3.10E-05	MGMG(16:3)	MGMG	GL	-8.42E-01	9.02E-04
DG(20:1_18:1)	DG	DG	-8.91E-01	2.25E-04	MGMG(18:3)	MGMG	GL	3.01E-01	1.93E-01
DG(20:1_18:2)	DG	DG	-9.05E-01	1.21E-04	PA(16:1_18:3)	PA	PL	-9.23E-01	6.22E-05
DG(20:1_18:3)	DG	DG	-5.80E-01	3.50E-02	PA(18:1_18:1)	PA	PL	5.02E-02	4.59E-01
DG(20:1_20:1)	DG	DG	-9.60E-01	3.88E-06	PA(18:1_18:2)	PA	PL	-7.19E-01	8.54E-03
DG(22:1_18:2)	DG	DG	-9.01E-01	1.63E-04	PA(18:2_18:2)	PA	PL	-4.41E-01	9.64E-02
DG(24:1_18:2)	DG	DG	-7.82E-01	3.58E-03	PA(18:3_18:3)	PA	PL	-8.45E-01	8.64E-04
DG(24:1_18:3)	DG	DG	6.33E-01	2.58E-02	PA(20:1_18:2)	PA	PL	-1.88E-02	4.65E-01
DGDG(16:0_18:2)	DGDG	GL	-4.24E-01	1.18E-01	PC(16:0_18:1)	PC	PL	-4.84E-01	7.29E-02
					PC(16:0_18:2)	PC	PL	-6.62E-01	1.75E-02
					PC(16:0_20:1)	PC	PL	5.83E-01	4.32E-02
					PC(17:1_13:0)	PC	PL	5.47E-01	5.64E-02
					PC(18:3_18:3)	PC	PL	8.88E-01	3.45E-04
					PC(27:1_11:4)	PC	PL	-8.72E-01	4.21E-04
					PC(30:0)	PC	PL	-8.96E-01	2.02E-04

PC(33:2)	PC	PL	-9.08E-01	1.24E-04	PI(34:5)	PI	PL	-8.79E-01	2.71E-04
PC(34:3)	PC	PL	-1.99E-01	2.81E-01	PI(34:6)	PI	PL	-2.88E-01	2.00E-01
PC(34:4)	PC	PL	6.16E-01	3.23E-02	PS(16:0_18:2)	PS	PL	-2.99E-01	1.82E-01
PC(34:6)	PC	PL	-5.80E-01	3.48E-02	PS(16:0_18:3)	PS	PL	9.45E-01	3.16E-05
PC(35:2)	PC	PL	7.37E-01	8.12E-03	PS(18:0_18:2)	PS	PL	-2.27E-01	2.87E-01
PC(35:3)	PC	PL	9.16E-01	1.24E-04	PS(18:1_18:2)	PS	PL	2.61E-02	4.97E-01
PC(35:4)	PC	PL	5.93E-02	4.44E-01	PS(18:3_18:2)	PS	PL	7.53E-01	7.67E-03
PC(37:3)	PC	PL	-9.67E-02	3.80E-01	PS(18:3_18:3)	PS	PL	9.79E-01	8.92E-07
PC(37:4)	PC	PL	8.67E-01	6.40E-04	PS(18:3_22:1)	PS	PL	8.89E-01	3.98E-04
PC(38:6)	PC	PL	7.26E-01	1.02E-02	PS(20:0_18:2)	PS	PL	-4.81E-01	7.25E-02
PC(40:3)	PC	PL	-9.24E-01	4.65E-05	PS(20:1_18:3)	PS	PL	4.63E-01	1.01E-01
PC(40:4)	PC	PL	-7.50E-01	6.00E-03	PS(22:0_18:2)	PS	PL	-1.86E-01	2.94E-01
PC(42:2)	PC	PL	-9.39E-01	2.45E-05	PS(22:0_18:3)	PS	PL	1.03E-01	4.09E-01
PC(42:3)	PC	PL	-8.94E-01	2.11E-04	PS(24:1_18:2)	PS	PL	2.25E-01	2.80E-01
PC(42:4)	PC	PL	-9.21E-01	5.03E-05	PS(24:1_18:3)	PS	PL	8.66E-01	7.29E-04
PE(15:0_18:2)	PE	PL	-9.61E-01	9.18E-06	So(d18:0)	So	So	-7.42E-01	8.11E-03
PE(16:0_16:0)	PE	PL	-9.82E-01	1.54E-07	So(d18:0+pO)	So	So	-9.03E-01	2.33E-04
PE(16:0_16:1)	PE	PL	8.34E-01	9.47E-04	So(d18:1+hO)	So	So	-9.70E-01	2.05E-06
PE(16:0_18:1)	PE	PL	9.64E-01	4.59E-06	So(d20:0+pO)	So	So	-2.54E-01	2.58E-01
PE(16:0_18:2)	PE	PL	-8.68E-01	7.91E-04	So(d22:0+pO)	So	So	-2.90E-01	2.23E-01
PE(16:0_20:1)	PE	PL	9.63E-01	6.01E-06	SQDG(16:0_18:3)	SQDG	GL	9.78E-01	6.47E-07
PE(16:1_18:3)	PE	PL	7.83E-01	2.92E-03	SQDG(18:2_18:3)	SQDG	GL	-6.39E-01	2.28E-02
PE(17:0_18:2)	PE	PL	9.73E-01	7.04E-07	StE(24:7)	StE	Sterols	-9.63E-01	3.32E-06
PE(17:1_16:0)	PE	PL	-1.29E-01	3.71E-01	TG(10:0_10:1_18:1)	TG	TG	9.93E-01	9.44E-09
PE(18:1_18:1)	PE	PL	9.87E-01	8.32E-08	TG(10:0_18:2_18:3)	TG	TG	-8.65E-01	5.73E-04
PE(18:1_18:2)	PE	PL	-6.86E-02	4.40E-01	TG(10:0_18:3_18:3)	TG	TG	5.19E-01	6.50E-02
PE(18:2_18:2)	PE	PL	-7.23E-01	1.08E-02	TG(12:0_18:2_18:3)	TG	TG	-8.31E-01	1.40E-03
PE(18:2_23:0)	PE	PL	-9.41E-01	1.92E-05	TG(12:0_18:3_18:3)	TG	TG	2.55E-01	2.43E-01
PE(18:3_18:2)	PE	PL	7.91E-01	2.52E-03	TG(14:0_18:2_18:3)	TG	TG	-8.27E-01	1.49E-03
PE(18:3_18:3)	PE	PL	9.73E-01	3.87E-07	TG(15:0_18:2_18:3)	TG	TG	-6.70E-01	1.64E-02
PE(18:3_22:1)	PE	PL	-8.56E-01	1.00E-03	TG(15:0_18:3_18:3)	TG	TG	-5.66E-01	4.33E-02
PE(20:1_18:2)	PE	PL	-9.48E-01	1.74E-05	TG(16:0_12:0_18:2)	TG	TG	-6.04E-01	3.06E-02
PE(20:1_18:3)	PE	PL	-1.36E-01	3.64E-01	TG(16:0_14:0_18:2)	TG	TG	-7.89E-01	2.99E-03
PE(22:0_18:2)	PE	PL	-9.27E-01	5.48E-05	TG(16:0_18:1_18:2)	TG	TG	-6.09E-01	2.89E-02
PE(22:1_18:2)	PE	PL	-9.58E-01	4.55E-06	TG(16:0_18:2_18:3)	TG	TG	-8.59E-02	4.02E-01
PE(24:0_18:2)	PE	PL	-8.84E-01	3.25E-04	TG(16:0_18:3_18:3)	TG	TG	4.55E-01	9.45E-02
PE(24:1_18:2)	PE	PL	-8.58E-01	6.93E-04	TG(16:1_18:3_18:3)	TG	TG	-8.85E-01	3.23E-04
PE(25:0_18:2)	PE	PL	-8.88E-01	2.81E-04	TG(17:0_18:3_18:3)	TG	TG	-3.04E-01	1.94E-01
PG(15:0_18:2)	PG	PL	-8.65E-01	8.17E-04	TG(18:1_12:0_18:2)	TG	TG	-6.45E-01	2.13E-02
PG(15:0_18:3)	PG	PL	-7.84E-01	5.20E-03	TG(18:1_18:2_18:3)	TG	TG	-6.35E-01	2.29E-02
PG(16:0_16:0)	PG	PL	-9.92E-01	9.11E-09	TG(18:3_14:1_18:3)	TG	TG	-8.66E-01	5.96E-04
PG(16:0_16:1)	PG	PL	2.22E-01	2.69E-01	TG(18:3_17:1_18:3)	TG	TG	-9.01E-01	1.73E-04
PG(16:0_18:1)	PG	PL	9.71E-01	2.44E-06	TG(18:3_18:2_18:3)	TG	TG	-8.40E-01	1.13E-03
PG(16:0_20:1)	PG	PL	-9.54E-01	9.49E-06	TG(18:3_18:2_20:3)	TG	TG	-5.43E-01	5.19E-02
PG(16:1_18:1)	PG	PL	-8.99E-01	2.67E-04	TG(18:3_18:2_22:3)	TG	TG	-7.92E-01	3.05E-03
PG(16:1_18:2)	PG	PL	-9.27E-01	8.18E-05	TG(18:3_18:3_18:3)	TG	TG	-8.36E-01	1.25E-03
PG(16:1_20:2)	PG	PL	-8.88E-01	3.26E-04	TG(18:3_18:3_20:3)	TG	TG	7.21E-01	9.59E-03
PG(18:2_18:2)	PG	PL	-9.44E-01	2.83E-05	TG(18:3_18:3_22:3)	TG	TG	7.94E-01	3.01E-03
PG(18:3_18:2)	PG	PL	-8.79E-01	5.72E-04	TG(18:3_20:3_22:3)	TG	TG	6.44E-02	4.40E-01
PG(18:3_18:3)	PG	PL	4.84E-01	6.53E-02	TG(18:4_15:0_18:3)	TG	TG	1.28E-01	3.64E-01
PG(20:1_18:2)	PG	PL	-9.25E-01	7.51E-05	TG(18:4_16:1_18:3)	TG	TG	-9.41E-01	2.42E-05
PI(14:0_18:2)	PI	PL	9.41E-01	1.93E-05	TG(18:4_17:1_18:3)	TG	TG	-9.29E-01	5.22E-05
PI(14:0_18:3)	PI	PL	-9.88E-01	3.40E-08	TG(19:0_18:3_18:3)	TG	TG	-4.10E-01	1.15E-01
PI(15:0_18:2)	PI	PL	-9.32E-01	3.14E-05	TG(19:1_18:3_18:3)	TG	TG	1.91E-01	3.04E-01
PI(15:0_18:3)	PI	PL	5.22E-01	6.95E-02	TG(20:1_18:3_18:3)	TG	TG	5.59E-01	4.77E-02
PI(16:0_18:2)	PI	PL	-8.87E-01	1.38E-04	TG(4:0_16:0_18:3)	TG	TG	9.89E-01	6.73E-08
PI(16:0_18:3)	PI	PL	8.89E-01	4.53E-04	TG(43:9)	TG	TG	-9.31E-01	3.71E-05
PI(16:1_18:3)	PI	PL	9.39E-01	2.11E-05	WE(19:0_17:4)	WE	WE	-9.45E-01	1.16E-05
PI(17:0_18:2)	PI	PL	9.51E-01	2.07E-05	WE(3:0_18:1)	WE	WE	-9.83E-01	6.63E-08
PI(17:0_18:3)	PI	PL	9.59E-01	1.24E-05	WE(3:0_20:3)	WE	WE	-9.86E-01	6.88E-08
PI(18:0_18:1)	PI	PL	9.74E-01	2.12E-06	WE(3:0_20:4)	WE	WE	-9.80E-01	2.27E-07
PI(18:0_18:2)	PI	PL	9.54E-01	1.98E-05	WE(5:0_17:3)	WE	WE	1.15E-02	4.61E-01
PI(18:0_18:3)	PI	PL	9.83E-01	8.59E-07					
PI(18:0_20:1)	PI	PL	8.87E-01	4.11E-04					
PI(18:2_18:2)	PI	PL	9.68E-01	5.20E-06					
PI(18:2_23:0)	PI	PL	-7.66E-01	4.52E-03					
PI(18:2_23:1)	PI	PL	-7.87E-01	2.65E-03					
PI(18:3_18:2)	PI	PL	7.96E-01	3.74E-03					
PI(18:3_18:3)	PI	PL	9.94E-01	1.11E-08					
PI(20:0_18:2)	PI	PL	9.03E-01	2.85E-04					
PI(20:1_18:2)	PI	PL	5.85E-01	4.45E-02					
PI(20:2_18:2)	PI	PL	-8.27E-01	9.43E-04					
PI(20:3_18:2)	PI	PL	-6.58E-01	1.50E-02					

**Table S6** : List of  $p_{\text{corr}}$  from OPLS-DA and  $P$ -value from Welsch T-test of *Nicotiana sylvestris* seed samples CMSII vs WT

ID	family	cat	pcorr	pvalue					
PI(18:1_18:2)	PI	PL	-0.996364	3.62E-20	PMe(18:1_18:2)	PMe	PL	-0.81869	1.19E-05
PE(16:0_18:1)_11.38	PE	PL	-0.994034	2.38E-22	Hex1Cer(d34:3)	Hex1Cer	Cer	-0.818064	1.31E-05
PE(16:0_18:1)_13.40	PE	PL	-0.994034	2.38E-22	PS(16:0_18:2)	PS	PL	-0.815784	1.97E-05
PI(20:2_18:2)	PI	PL	-0.993624	1.79E-17	PI(16:0_16:0)	PI	PL	-0.807947	1.77E-05
PG(16:0_17:0)	PG	PL	-0.992158	7.1E-20	Hex2Cer(d42:2+O)	Hex2Cer	Cer	-0.801831	2.48E-05
PE(18:1_18:2)_10.29	PE	PL	-0.991432	3.52E-20	DG(18:0_18:1)	DG	DG	-0.796143	3.28E-05
PE(18:1_18:2)_12.60	PE	PL	-0.991432	3.52E-20	DG(34:5)	DG	DG	-0.79001	3.46E-05
PI(20:0_18:2)	PI	PL	-0.991039	1.49E-17	PMe(18:0_18:1)	PMe	PL	-0.781976	6.14E-05
PC(16:0_18:1)	PC	PL	-0.990653	8.14E-20	DG(17:0_18:1)	DG	DG	-0.781219	5.63E-05
PE(18:0_18:1)	PE	PL	-0.989073	3.08E-18	DG(17:1_16:0)	DG	DG	-0.78115	4.58E-05
PI(18:2_18:2)	PI	PL	-0.98774	1.25E-15	Hex1Cer(d18:2_21:0+O)	Hex1Cer	Cer	-0.779218	5.69E-05
PC(17:0_18:1)	PC	PL	-0.987249	2.69E-17	Hex1Cer(d18:2_25:0+O)	Hex1Cer	Cer	-0.77299	7.02E-05
PE(20:0_18:2)_13.12	PE	PL	-0.986992	6.77E-17	DG(20:1_18:2)	DG	DG	-0.770431	8.13E-05
PE(20:0_18:2)_14.89	PE	PL	-0.986992	6.77E-17	DG(18:1_18:2)_14.41	DG	DG	-0.764497	8.98E-05
PI(16:0_18:1)	PI	PL	-0.986385	3.04E-15	PI(16:0_18:2)	PI	PL	-0.761912	0.00016
PC(18:1_18:2)	PC	PL	-0.982547	6.68E-16	Hex1Cer(d18:2_15:0+O)	Hex1Cer	Cer	-0.74556	0.000174
LPE(18:1)	LPE	PL	-0.981359	4.91E-15	TG(18:4_16:1_18:3)	TG	TG	-0.729513	0.000312
MGDG(18:1_18:2)	MGDG	GL	-0.980285	1.77E-15	CL(72:4)	CL	PL	-0.726811	0.0003
PC(16:1_18:3)	PC	PL	-0.980233	3.01E-15	Hex1Cer(d18:2_23:0+O)	Hex1Cer	Cer	-0.716019	0.000382
PE(18:1_20:2)	PE	PL	-0.978868	6.82E-15	SPH(t18:1)	SPH	SPH	-0.71473	0.000355
PI(18:0_18:1)	PI	PL	-0.9737	7.68E-13	PS(16:1_20:3)	PS	PL	-0.710599	0.000598
PE(20:2_18:2)	PE	PL	-0.973586	8.21E-15	DG(20:1_18:1)	DG	DG	-0.70974	0.000498
PC(17:1_18:2)	PC	PL	-0.96751	1.1E-11	AcHexSiE(18:0)	AcHexSiE	Sterols	-0.704235	0.000618
LPE(16:0)	LPE	PL	-0.966928	1.27E-12	DG(42:2e)	DG	DG	-0.689342	0.000878
LPI(16:0)	LPI	PL	-0.963655	4.61E-11	SM(t18:1_19:1)	SM	SM	-0.687375	0.000907
PI(18:3_18:2)	PI	PL	-0.963501	1.21E-11	AcHexSiE(16:0)	AcHexSiE	Sterols	-0.658831	0.001625
PI(17:0_18:1)	PI	PL	-0.963041	2.88E-11	PS(18:0_22:4)	PS	PL	-0.644109	0.002848
MGDG(16:0_18:2)	MGDG	GL	-0.959608	2.69E-12	PE(16:0_18:3)	PE	PL	-0.633213	0.00303
LPC(18:1)	LPC	PL	-0.956615	1.48E-10	CL(76:4)	CL	PL	-0.629394	0.002985
LPC(16:0)	LPC	PL	-0.956551	1.47E-10	AcHexSiE(15:0)	AcHexSiE	Sterols	-0.595529	0.005947
PG(16:0_16:1)	PG	PL	-0.948541	1.2E-10	DG(19:0_18:2)	DG	DG	-0.590104	0.00641
PE(15:0_18:2)	PE	PL	-0.946606	6.01E-11	AcHexCmE(18:2)	AcHexCmE	Sterols	-0.589315	0.006677
PC(18:0_18:1)	PC	PL	-0.945881	1.1E-10	DG(19:1_18:2)	DG	DG	-0.580824	0.006163
PS(18:2_21:0)	PS	PL	-0.944763	1.68E-09	DG(16:0_16:0)	DG	DG	-0.574152	0.007023
PC(20:1_18:2)	PC	PL	-0.941119	1.68E-10	PMe(20:2_18:2)	PMe	PL	-0.573359	0.008509
LPC(16:1)	LPC	PL	-0.936103	2.98E-09	CL(70:1)	CL	PL	-0.558406	0.011433
AcHexCmE(20:0)	AcHexCmE	Sterols	-0.935524	4.14E-09	DG(14:0_18:2)	DG	DG	-0.526216	0.015865
LPC(20:2)	LPC	PL	-0.933888	2.87E-09	Hex1Cer(d18:2_22:0+O)	Hex1Cer	Cer	-0.525482	0.017915
CL(74:5)	CL	PL	-0.930298	4.81E-09	CmE(20:4)	CmE	Sterols	-0.507338	0.022551
PC(16:0_16:1)	PC	PL	-0.930034	1.83E-09	DG(18:2_21:0)	DG	DG	-0.488885	0.028694
PC(17:1_16:0)	PC	PL	-0.919913	1.49E-09	TG(14:0_18:2_18:2)	TG	TG	-0.488244	0.032035
PI(18:0_18:2)	PI	PL	-0.913975	4.29E-08	AEA(18:1)	AEA	AEA	-0.472299	0.036967
PS(20:0_18:2)	PS	PL	-0.912336	6.94E-08	CL(70:3)	CL	PL	-0.465545	0.038543
SM(t38:2)	SM	SM	-0.909714	4.92E-08	AcHexStE(18:1)	AcHexStE	Sterols	-0.458098	0.043192
PS(20:0_18:3)	PS	PL	-0.905216	1.14E-07	DG(17:1_18:2)	DG	DG	-0.456392	0.042645
LPC(17:0)	LPC	PL	-0.901234	9.61E-08	DG(15:0_18:3)	DG	DG	-0.454396	0.043211
DG(25:0_18:2)	DG	DG	-0.899892	1.3E-07	Hex1Cer(d18:2_24:0+O)	Hex1Cer	Cer	-0.422759	0.062443
DG(16:0_18:1)	DG	DG	-0.898359	1.04E-07	Hex1Cer(t18:1_23:0+O)	Hex1Cer	Cer	-0.407636	0.074951
PS(22:0_18:2)	PS	PL	-0.896809	2.75E-07	TG(12:0_18:2_18:2)	TG	TG	-0.390538	0.095864
AcHexZyE(17:0)	AcHexZyE	Sterols	-0.892733	2.45E-07	TG(16:1_18:3_18:3)	TG	TG	-0.390447	0.092437
PI(15:0_18:2)	PI	PL	-0.892632	2.06E-07	PMe(16:0_18:2)	PMe	PL	-0.373937	0.103238
AcHexStE(18:0)	AcHexStE	Sterols	-0.892397	2.18E-07	CL(72:6)	CL	PL	-0.360714	0.116245
LPI(18:2)	LPI	PL	-0.891187	3.25E-07	Cer(t17:1_21:0+O)	Cer	Cer	-0.334106	0.146517
LPC(18:0)	LPC	PL	-0.889691	1.99E-07	Hex1Cer(d18:2_20:0+O)	Hex1Cer	Cer	-0.302133	0.192366
LPC(18:2)	LPC	PL	-0.886421	2.46E-07	DG(33:0)	DG	DG	-0.279289	0.204662
Hex1Cer(d42:3+O)	Hex1Cer	Cer	-0.883823	3.1E-07	DG(39:3e)	DG	DG	-0.276497	0.227424
AcHexStE(17:0)	AcHexStE	Sterols	-0.870549	9.1E-07	PMe(18:2_18:2)	PMe	PL	-0.24749	0.282841
PI(16:0_18:3)	PI	PL	-0.865564	1.37E-06	AcHexSiE(20:2)	AcHexSiE	Sterols	-0.244435	0.297474
PMe(16:0_18:1)	PMe	PL	-0.864535	1.25E-06	DG(18:0_16:0)	DG	DG	-0.225279	0.301792
LPE(18:2)	LPE	PL	-0.861753	6.44E-07	DG(15:0_18:2)	DG	DG	-0.18223	0.423259
MePC(38:1)_12.971	MePC	PL	-0.853082	2.13E-06	PC(20:0_18:2)	PC	PL	-0.180241	0.395276
PS(36:3)	PS	PL	-0.85299	3.68E-06	DG(20:2_18:2)	DG	DG	-0.1311	0.563772
DG(16:1_18:3)	DG	DG	-0.847399	2.85E-06	DG(18:2_18:2)	DG	DG	-0.0739082	0.736049
PS(18:0_18:2)	PS	PL	-0.844658	6.08E-06	DG(16:0_18:2)_15.16	DG	DG	-0.0325751	0.868578
SM(t34:2)	SM	SM	-0.830041	7.9E-06	MePC(34:5)	MePC	PL	0.00683912	0.995414
AcHexSiE(17:0)	AcHexSiE	Sterols	-0.8287	9.7E-06	Hex1Cer(d18:2_26:0+O)	Hex1Cer	Cer	0.00764691	0.982836
Cer(t40:2)	Cer	Cer	-0.818696	9.34E-06	DG(31:3e)	DG	DG	0.0484939	0.853009
					TG(15:0_18:3_18:3)	TG	TG	0.0565007	0.808194
					PE(14:0_18:2)	PE	PL	0.0636328	0.93321
					Hex1Cer(d18:1_16:0+O)	Hex1Cer	Cer	0.0663336	0.795894
					Hex2Cer(t41:0)	Hex2Cer	Cer	0.0791029	0.736032
					TG(18:1_10:1_10:1)	TG	TG	0.0791808	0.761153
					TG(16:0_18:3_18:3)	TG	TG	0.0982274	0.674028

TG(10:0_18:2_18:2)	TG	TG	0.211888	0.365136	PG(18:3_18:2)	PG	PL	0.990535	4.73E-17
PI(17:0_18:2)	PI	PL	0.251843	0.237561	PG(16:0_18:3)	PG	PL	0.990624	1.44E-17
CL(78:6)	CL	PL	0.260716	0.278081	PE(24:0_18:2)	PE	PL	0.990903	4.98E-17
Hex1Cer(d18:2_16:0)	Hex1Cer	Cer	0.291579	0.21457	dMePE(20:2_18:2)	dMePE	PL	0.991321	3.83E-17
CL(74:9)	CL	PL	0.296811	0.206055	PE(22:2_18:2)	PE	PL	0.991321	3.83E-17
Hex1Cer(t18:1_24:0+O)	Hex1Cer	Cer	0.317943	0.17872	PG(16:0_18:2)	PG	PL	0.99359	1.42E-20
Hex1Cer(t18:1_22:0+O)	Hex1Cer	Cer	0.318051	0.174493	PC(18:3_18:2)	PC	PL	0.99539	1.39E-20
LPC(24:0)	LPC	PL	0.335405	0.156656	PC(24:0_18:2)	PC	PL	0.995712	1.11E-20
PG(16:0_18:1)	PG	PL	0.362375	0.118446	PC(22:2_18:2)	PC	PL	0.995846	4.38E-21
ChE(20:0)	ChE	Sterols	0.381983	0.094397	PC(17:0_18:2)	PC	PL	0.996529	3.81E-22
SPH(t18:0)	SPH	SPH	0.395776	0.098388	PC(18:0_18:2)	PC	PL	0.99655	5.52E-21
Hex1Cer(t18:1_26:0+O)	Hex1Cer	Cer	0.416465	0.07132	PC(22:0_18:2)	PC	PL	0.997316	4.29E-22
LPC(22:0)	LPC	PL	0.43865	0.059181					
DG(22:0_18:2)	DG	DG	0.465079	0.042046					
DG(18:0_18:2)	DG	DG	0.466592	0.040752					
DG(17:1_18:3)	DG	DG	0.488531	0.033332					
DG(18:3_18:2)	DG	DG	0.528228	0.018864					
DG(14:0_18:3)	DG	DG	0.545648	0.015543					
DG(19:1_18:3)	DG	DG	0.612537	0.00473					
Cer(t16:0_18:1)	Cer	Cer	0.657439	0.00222					
PE(24:0_18:3)	PE	PL	0.663196	0.00121					
PE(16:0_18:2)	PE	PL	0.673056	0.001598					
DG(17:0_18:2)	DG	DG	0.676388	0.0013					
PE(18:3_18:3)	PE	PL	0.71774	0.000495					
TG(18:2_10:1_10:1)	TG	TG	0.755582	0.000159					
DG(22:2_18:2)	DG	DG	0.76522	0.000117					
TG(19:1_18:2_18:3)	TG	TG	0.766583	9.4E-05					
AcHexSIE(20:0)	AcHexSIE	Sterols	0.772029	8.55E-05					
CL(82:6)	CL	PL	0.776125	7.86E-05					
DG(18:3_18:3)	DG	DG	0.776271	8.11E-05					
TG(18:3_18:2_18:3)	TG	TG	0.7907	3.66E-05					
TG(18:3_10:1_10:1)	TG	TG	0.81561	1.87E-05					
PG(18:0_18:1)	PG	PL	0.840787	3.27E-06					
Hex1Cer(d18:2_18:0)	Hex1Cer	Cer	0.854257	3.04E-06					
DG(41:5e)	DG	DG	0.856103	2.08E-06					
MGDG(18:3_18:3)	MGDG	GL	0.863149	7.81E-07					
TG(19:1_18:3_18:3)	TG	TG	0.878311	4.54E-07					
PG(16:0_16:0)	PG	PL	0.892081	1.14E-07					
TG(18:3_17:1_18:3)	TG	TG	0.892174	1.69E-07					
DG(18:3_22:2)	DG	DG	0.895797	1.94E-07					
PC(19:0_18:2)	PC	PL	0.896794	6.34E-08					
PG(18:1_18:2)	PG	PL	0.914099	1.73E-08					
PC(16:0_18:3)	PC	PL	0.921893	1.55E-09					
PG(18:0_16:0)	PG	PL	0.925176	4.9E-09					
Cer(t17:1_22:0+O)	Cer	Cer	0.929561	1.64E-09					
Cer(d34:0+O)	Cer	Cer	0.932114	2.65E-09					
Cer(t18:0_16:0)	Cer	Cer	0.932114	2.65E-09					
PE(18:2_18:2)	PE	PL	0.933781	3.56E-09					
Cer(t17:1_24:0+O)	Cer	Cer	0.93451	1.68E-09					
PC(15:0_18:2)	PC	PL	0.937231	2.62E-09					
Cer(t18:0_20:0)	Cer	Cer	0.942159	1.83E-10					
TG(18:3_18:3_18:3)	TG	TG	0.946114	8.07E-10					
PC(16:0_16:0)	PC	PL	0.949636	3.67E-10					
PE(18:0_18:2)	PE	PL	0.953264	8.12E-10					
PC(18:0_16:0)	PC	PL	0.955167	1.29E-10					
PE(18:3_18:2)	PE	PL	0.960422	5.84E-11					
Cer(t17:1_23:0+O)	Cer	Cer	0.961162	1.09E-11					
Cer(d18:2_16:0+O)	Cer	Cer	0.966188	2.15E-11					
PE(18:1_22:0)	PE	PL	0.969088	3.72E-12					
MePC(41:5)	MePC	PL	0.974373	4.92E-12					
MGDG(18:2_18:2)	MGDG	GL	0.979972	1.47E-13					
PC(18:2_18:2)	PC	PL	0.980402	1.21E-14					
Cer(t44:1+O)	Cer	Cer	0.981062	1.06E-14					
Cer(t18:0_24:0)	Cer	Cer	0.981169	4.25E-15					
Cer(t17:1_25:0+O)	Cer	Cer	0.981941	4.26E-15					
Cer(t18:0_21:0)	Cer	Cer	0.982218	1.02E-15					
Cer(t18:0_23:0)	Cer	Cer	0.983275	7.58E-16					
PC(16:0_18:2)	PC	PL	0.983955	3.48E-14					
PC(20:2_18:2)	PC	PL	0.983959	5.23E-14					
Cer(t18:0_22:0)	Cer	Cer	0.984241	5.11E-16					
PC(18:3_18:3)	PC	PL	0.984762	4.71E-15					
PG(18:2_18:2)	PG	PL	0.98504	1.2E-15					
PE(22:0_18:2)	PE	PL	0.98826	4.27E-16					



**Table S7** List of  $p_{\text{corr}}$  from OPLS-DA and  $P$ -value from Welsch T-test of *Nicotiana sylvestris* pollen samples CMSII vs WT

Primary ID	family	cat	pcorr	pvalue					
cPA(18:2)	cPA	PL	-0.99888	1.55E-06	ChE(18:3)	ChE	Sterols	0.554787	0.126033
TG(18:3_18:3_18:3)	TG	TG	-0.99775	9.36E-08	PI(18:3_18:3)	PI	PL	0.623243	0.058693
TG(25:0_18:3_18:3)	TG	TG	-0.99745	2.50E-06	TG(18:0_18:0_18:0)	TG	TG	0.774719	0.02645
DG(18:1_18:1)	DG	DG	-0.99744	3.41E-06	TG(18:3_18:2_20:3)	TG	TG	0.800346	0.016719
PC(40:3)	PC	PL	-0.99626	1.40E-08	DG(20:2_18:2)	DG	DG	0.819169	0.003636
DG(17:1_18:3)	DG	DG	-0.9958	2.10E-05	PC(36:6p)	PC	PL	0.908296	0.001053
TG(22:0_18:2_18:3)	TG	TG	-0.9958	1.08E-08	TG(18:3_18:3_22:3)	TG	TG	0.908535	0.001841
PC(38:1)	PC	PL	-0.99564	1.11E-06	TG(18:3_18:2_20:2)	TG	TG	0.917667	0.002114
TG(24:0_18:3_18:3)	TG	TG	-0.99545	1.00E-05	AcCa(18:3)	AcCa	AcCa	0.924536	0.00021
DG(18:1_18:2)	DG	DG	-0.99539	1.27E-05	PC(32:2)	PC	PL	0.924793	0.000915
TG(24:0_18:2_18:3)	TG	TG	-0.99538	5.36E-07	PI(18:3_18:2)	PI	PL	0.938754	0.00016
DG(18:3_18:3)	DG	DG	-0.99524	2.31E-05	WE(5:0_26:1)	WE	WE	0.939134	0.000302
TG(17:0_18:3_18:3)	TG	TG	-0.99502	2.14E-05	WE(3:0_20:2)	WE	WE	0.940534	0.00052
TG(16:1_18:2_18:3)	TG	TG	-0.99492	6.78E-09	SQDG(43:6)	SQDG	GL	0.946801	0.000762
TG(18:3_18:2_21:0)	TG	TG	-0.99425	8.86E-07	TG(18:0_18:2_18:3)	TG	TG	0.953322	0.000173
cPA(18:3)	cPA	PL	-0.99362	8.25E-06	PC(31:0)	PC	PL	0.958304	2.26E-05
TG(25:0_18:2_18:3)	TG	TG	-0.99348	1.63E-05	TG(18:3_18:2_22:3)	TG	TG	0.960741	0.000245
Cer(d18:2_16:0+O)	Cer	Cer	-0.99301	1.28E-05	TG(4:0_18:1_24:0)	TG	TG	0.961916	0.000505
PC(42:3)	PC	PL	-0.9923	1.11E-05	TG(22:3_18:2_18:2)	TG	TG	0.962445	0.000397
DG(18:2_23:0)	DG	DG	-0.99194	3.51E-05	WE(5:0_24:0)	WE	WE	0.96656	0.000112
DG(16:0_16:0)	DG	DG	-0.9913	3.85E-06	WE(5:0_26:2)	WE	WE	0.971626	0.000123
DG(18:3_23:0)	DG	DG	-0.99077	6.27E-05	TG(24:1_18:3_18:3)	TG	TG	0.972573	4.96E-06
TG(24:0_18:2_18:2)	TG	TG	-0.99021	1.69E-07	TG(45:3e)	TG	TG	0.980581	6.22E-05
TG(16:0_18:2_22:0)	TG	TG	-0.99019	1.33E-06	PC(33:2)	PC	PL	0.980973	5.86E-07
TG(17:0_18:2_18:3)	TG	TG	-0.99019	3.93E-05	PG(18:2_18:2)	PG	PL	0.984116	2.11E-07
PG(18:1_18:2)	PG	PL	-0.98946	3.11E-05	PC(32:0)	PC	PL	0.984612	2.71E-07
TG(18:4_17:1_18:3)	TG	TG	-0.98919	7.32E-05	TG(4:0_18:2_22:0)	TG	TG	0.985399	6.39E-05
DG(15:0_18:2)	DG	DG	-0.98814	7.20E-07	TG(6:0_16:1_22:1)	TG	TG	0.985411	6.37E-05
DG(16:0_16:1)	DG	DG	-0.98808	2.50E-07	MG(26:0)	MG	PL	0.988323	2.05E-05
PC(38:0)	PC	PL	-0.98678	1.29E-06	cPA(16:0)	cPA	PL	0.989615	6.41E-08
TG(22:2_18:2_18:2)	TG	TG	-0.98624	1.85E-07	PC(34:0)	PC	PL	0.993883	2.76E-06
PE(24:0_18:2)	PE	PL	-0.98574	6.63E-07	PC(33:1)	PC	PL	0.995444	1.01E-07
PC(36:1)	PC	PL	-0.9856	0.000111					
PC(44:2)	PC	PL	-0.9848	0.000116					
LPC(18:1)	LPC	PL	-0.98441	5.79E-05					
TG(22:0_18:2_18:2)	TG	TG	-0.98415	1.64E-07					
PE(25:0_18:2)	PE	PL	-0.98398	1.24E-06					
TG(18:1_18:2_21:0)	TG	TG	-0.98392	9.83E-05					
DG(18:2_18:2)	DG	DG	-0.98347	0.000192					
PG(18:3_18:2)	PG	PL	-0.98313	8.32E-05					
TG(16:1_18:3_18:3)	TG	TG	-0.98126	0.000196					
PE(26:0_18:3)	PE	PL	-0.98086	1.66E-06					
CerG1(d18:2_26:0+O)	CerG1	Cer	-0.98067	0.000215					
TG(18:3_17:1_18:3)	TG	TG	-0.97808	0.000231					
TG(20:1_18:1_18:2)	TG	TG	-0.9771	6.65E-06					
DG(14:0_18:3)	DG	DG	-0.97664	1.26E-06					
PC(40:2)	PC	PL	-0.97634	0.000314					
CerG1(d18:2_17:0+O)	CerG1	Cer	-0.97052	2.95E-06					
LPC(18:2)	LPC	PL	-0.96355	0.000655					
LPC(16:1)	LPC	PL	-0.96346	0.000497					
TG(18:1_18:2_24:0)	TG	TG	-0.95985	0.000264					
DG(17:0_18:3)	DG	DG	-0.95904	2.71E-05					
LPC(15:0)	LPC	PL	-0.95563	0.000844					
TG(26:0_16:0_18:2)	TG	TG	-0.94744	0.000888					
PC(36:2)	PC	PL	-0.94432	0.000338					
PC(33:3)	PC	PL	-0.92453	0.000894					
TG(22:0_18:2_22:0)	TG	TG	-0.89117	0.004361					
PC(32:1)	PC	PL	-0.88623	0.003511					
LPC(17:0)	LPC	PL	-0.8714	0.001216					
TG(18:3_18:2_18:2)	TG	TG	-0.86855	0.001386					
CerG1(d18:2_16:0+O)	CerG1	Cer	-0.86575	0.001081					
PC(33:4)	PC	PL	-0.81559	0.004614					
PE(16:0_16:0)	PE	PL	-0.64633	0.043411					
PE(18:0_18:1)	PE	PL	-0.59372	0.078046					
LPC(16:0)	LPC	PL	-0.45529	0.209559					
PE(17:0_18:3)	PE	PL	-0.1558	0.675082					
Cer(d36:3)	Cer	Cer	0.199213	0.600423					