Electronic Supplementary Information for

Metabolic Transformation of Microalgae Due to Light Acclimation and Genetic Modifications Followed by Laser Ablation Electrospray Ionization Mass Spectrometry with Ion Mobility Separation

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Table S1. Identification of membrane lipids detected in positive ion mode by LAESI-IMS-MS. Identifications were based on accurate mass measurements, isotope distribution patterns, tandem MS, TAP measurements, and database searches. Species marked by * were verified using tandem MS and are represented by their acyl chains in the (sn-1/sn-2) positions.

Identification	Formula	Measured mass *m/z*	Calculated mass *m/z*	Δm (mDa)	DT (ms)
DGTS(32:5)	$C_{42}H_{72}O_7N^+$	702.533	702.5309	2	160.8
DGTS (16:4/16:0)*	$C_{42}H_{74}O_7N^+$	704.547	704.5465	1	159.7
DGTS (16:3/16:0)*	$C_{42}H_{76}O_7N^+$	706.564	706.5622	2	155.0
DGTS (16:2/16:0)*	$C_{42}H_{78}O_7N^+$	708.585	708.5778	7	157.4
DGTS (16:1/16:0)*	$C_{42}H_{80}O_7N^+$	710.597	710.5934	3	159.7
DGTS(32:0)	$C_{42}H_{82}O_7N^+$	712.599	712.6091	10	157.4
DGTS(32:4)	$C_{42}H_{73}O_7NNa^+$	726.533	726.5284	5	155.0
DGTS(16:3/16:0)*	$C_{42}H_{75}O_7NNa^+$	728.546	728.5441	2	155.0
DGTS(32:2)	$C_{42}H_{77}O_7NNa^+$	730.562	730.5598	3	157.4
DGTS(18:4/16:0)*	$C_{44}H_{78}O_7N^+$	732.581	732.5778	4	159.7
DGTS(18:3/16:0)*	$C_{44}H_{80}O_7N^+$	734.591	734.5934	2	163.1
DGTS(34:2)	$C_{44}H_{82}O_7N^+$	736.604	736.6091	5	165.5
DGTS(34:1)	$C_{44}H_{84}O_7N^+$	738.619	738.6248	6	167.8
DGTS(18:3/16:0)*	$C_{44}H_{79}O_7NNa^+$	756.581	756.5753	6	162.0
DGTS(34:2)	$C_{44}H_{81}O_7NNa^+$	758.599	758.5910	9	164.3
DGTS(18:1/16:0)*	$C_{44}H_{83}O_7NNa^+$	760.609	760.6091	0	167.8
DGTS(18:0/16:0)*	$C_{44}H_{85}O_7NNa^+$	762.620	762.6223	2	168.9
MGDG(18:3/16:4)*	$C_{43}H_{68}O_{10}Na^+$	767.474	767.4710	3	152.7
MGDG(34:6)	$C_{43}H_{70}O_{10}Na^+$	769.487	769.4827	4	153.9
MGDG(34:5)	$C_{43}H_{72}O_{10}Na^+$	771.494	771.5023	8	156.2
DGDG(18:3/16:3)*	$C_{49}H_{80}O_{15}Na^+$	931.539	931.5436	4	184.0
DGDG(18:2/16:3)*	$C_{49}H_{82}O_{15}Na^+$	933.557	933.5551	1	187.4
DGDG(18:4/16:0)*	$C_{49}H_{84}O_{15}Na^+$	935.571	935.5707	0	188.6
DGDG(18:3/16:0)*	$C_{49}H_{86}O_{15}Na^+$	937.589	937.5864	2	192.1
DGDG(34:2)	$C_{49}H_{88}O_{15}Na^+$	939.595	939.6021	7	195.5
DGDG (34:1)	$C_{49}H_{90}O_{15}Na^+$	941.616	941.6177	2	196.7

Table S2. Neutral storage lipids detected in positive ion mode by LAESI-IMS-MS. Identifications were based on accurate mass measurements, isotope distribution patterns, tandem MS, TAP measurements, and database searches.

Identification	Formula	Measured mass *m/z*	Calculated mass *m/z*	Δm (mDa)	DT (ms)
TAG(50:5)	$C_{53}H_{92}O_6H^+$	825.699	825.6967	2	184.0
TAG(50:4)	$C_{53}H_{94}O_6H^+$	827.707	827.7123	5	186.3
TAG(50:3)	$C_{53}H_{96}O_6H^+$	829.718	829.7237	6	193.2
TAG(50:2)	$C_{53}H_{98}O_6H^+$	831.732	831.7441	13	197.8
TAG(50:1)	$C_{53}H_{100}O_6H^+$	833.722	833.7297	8	197.8
TAG(50:10)	$C_{53}H_{84}O_6NH_4^+$	834.658	834.6611	3	177.0
TAG(50:0)	$C_{53}H_{102}O_6H^+$	835.774	835.7754	2	178.2
TAG(50:9)	$C_{53}H_{86}O_6NH_4^+$	836.674	836.6768	3	179.3
TAG(50:8)	$C_{53}H_{88}O_6NH_4^+$	838.683	838.6924	9	188.6
TAG(50:7)	$C_{53}H_{90}O_6NH_4^+$	840.707	840.7081	1	190.9
TAG(50:6)	$C_{53}H_{92}O_6NH_4^+$	842.721	842.7238	3	192.1
TAG(50:5)	$C_{53}H_{94}O_6NH_4^+$	844.737	844.7394	3	196.7
TAG(50:4)	$C_{53}H_{96}O_6NH_4^+$	846.755	846.7551	0	199.0
TAG(50:3)	$C_{53}H_{98}O_6NH_4^+$	848.763	848.7708	7	201.3
TAG(50:2)	$C_{53}H_{100}O_6NH_4^+$	850.786	850.7865	0	205.9
TAG(50:1)	$C_{53}H_{102}O_6NH_4^+$	852.786	852.8021	16	205.9
TAG(50:3)	$C_{53}H_{96}O_6Na^+$	851.701	851.7099	9	204.8
TAG(52:8)	$C_{55}H_{90}O_6NH_4^+$	864.701	864.7081	2	193.2
TAG(52:7)	$C_{55}H_{92}O_6NH_4^+$	866.714	866.7238	10	196.7
TAG(52:6)	$C_{55}H_{94}O_6NH_4^+$	868.730	868.7395	9	199.0
TAG(52:5)	$C_{55}H_{96}O_6NH_4^+$	870.751	870.7551	4	200.2
TAG(52:4)	$C_{55}H_{98}O_6NH_4^+$	872.762	872.7708	9	204.8
TAG(52:3)	$C_{55}H_{100}O_6NH_4^+$	874.778	874.7865	9	207.1
TAG(52:2)	$C_{55}H_{102}O_6NH_4^+$	876.790	876.8022	12	208.3
TAG(52:1)	$C_{55}H_{104}O_6NH_4^+$	878.808	878.8179	10	210.6
TAG(54:9)	$C_{57}H_{92}O_6NH_4^+$	890.714	890.7237	10	199.0
TAG(54:8)	$C_{57}H_{94}O_6NH_4^+$	892.734	892.7394	5	200.2
TAG(54:7)	$C_{57}H_{96}O_6NH_4^+$	894.744	894.7550	11	204.8

TAG(54:6)	$C_{57}H_{98}O_6NH_4^+$	896.756	896.7707	15	207.1
TAG(54:5)	$C_{57}H_{100}O_6NH_4^+$	898.769	898.7863	16	208.3
TAG(54:4)	$C_{57}H_{102}O_6NH_4^+$	900.799	900.8020	3	212.9
TAG(54:3)	$C_{57}H_{104}O_6NH_4^+$	902.805	902.8176	13	216.4
TAG(54:2)	$C_{57}H_{106}O_6NH_4^+$	904.826	904.8333	7	216.4

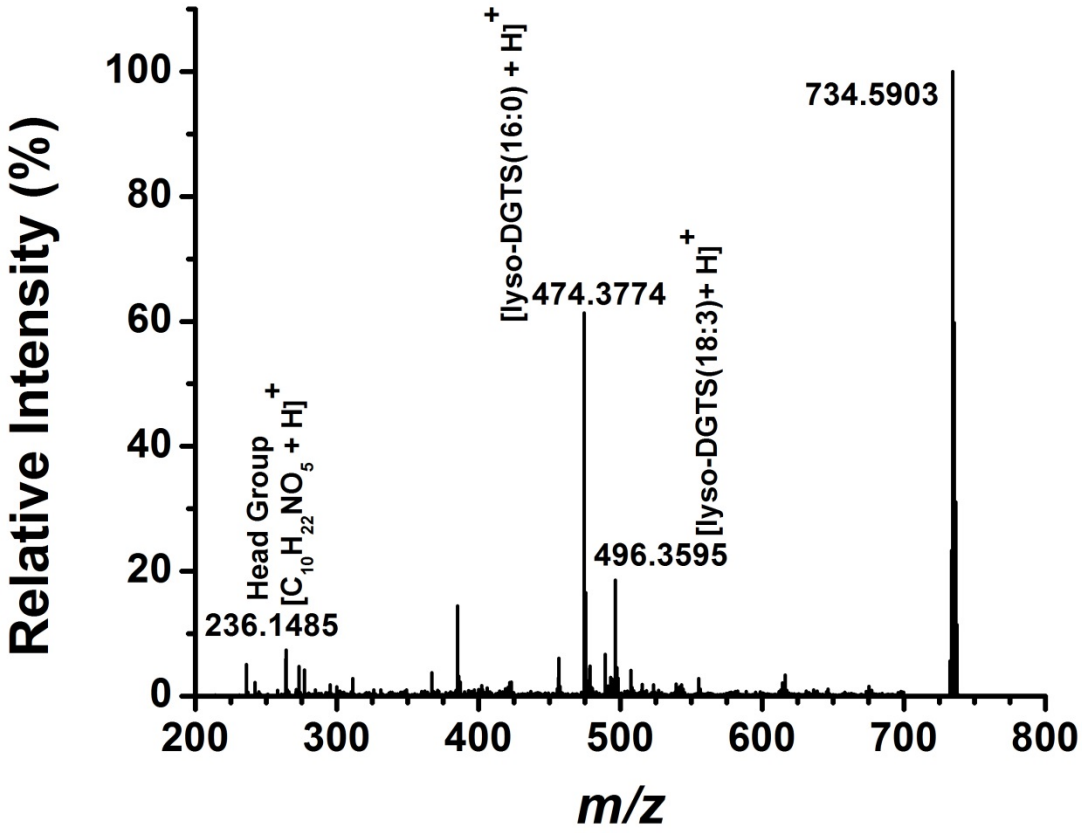

Figure S1. Tandem mass spectrum of protonated DGTS(18:3/16:0) produced by LAESI.

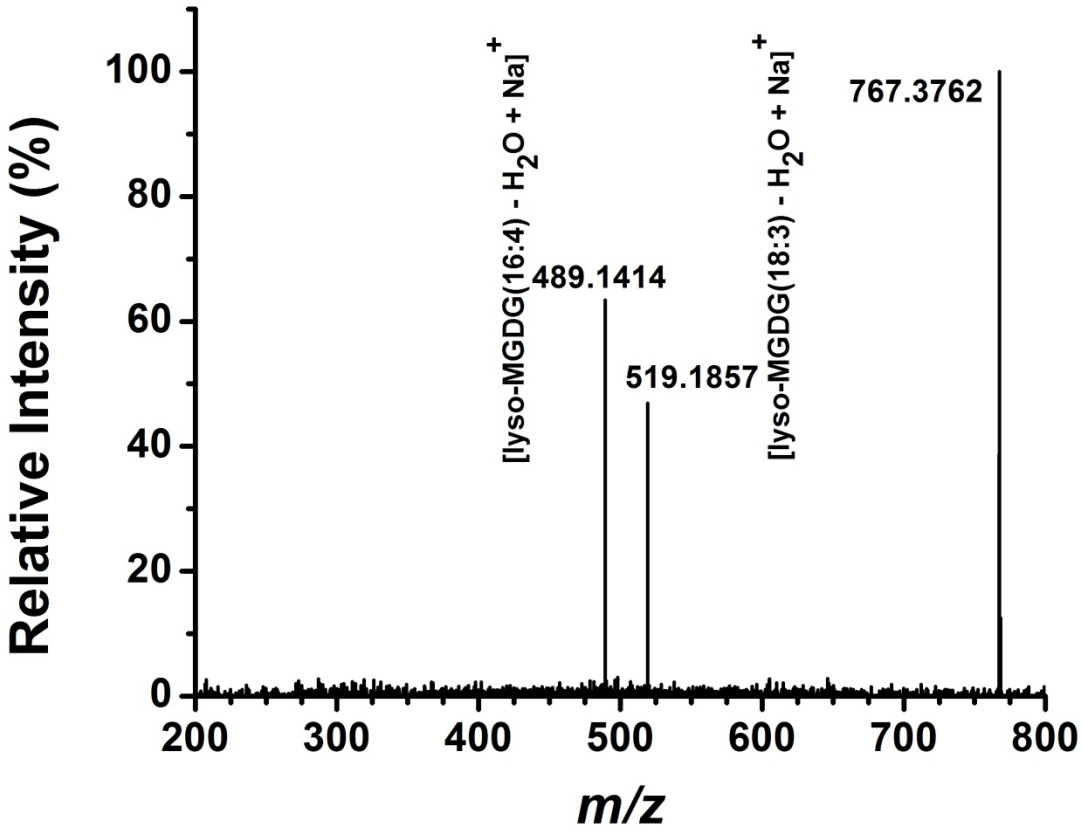

Figure S2. Tandem mass spectrum of sodiated MGDG(18:3/16:4) produced by LAESI.

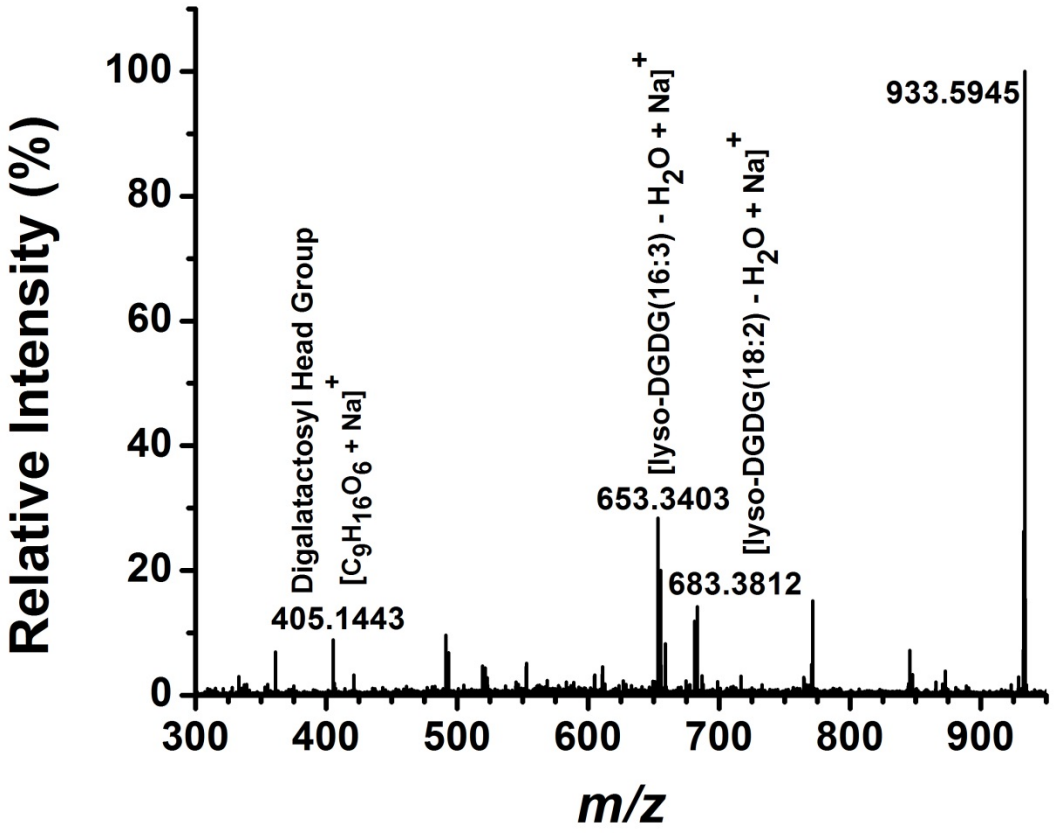

Figure S3. Tandem mass spectrum of sodiated DGDG(18:2/16:3) produced by LAESI.

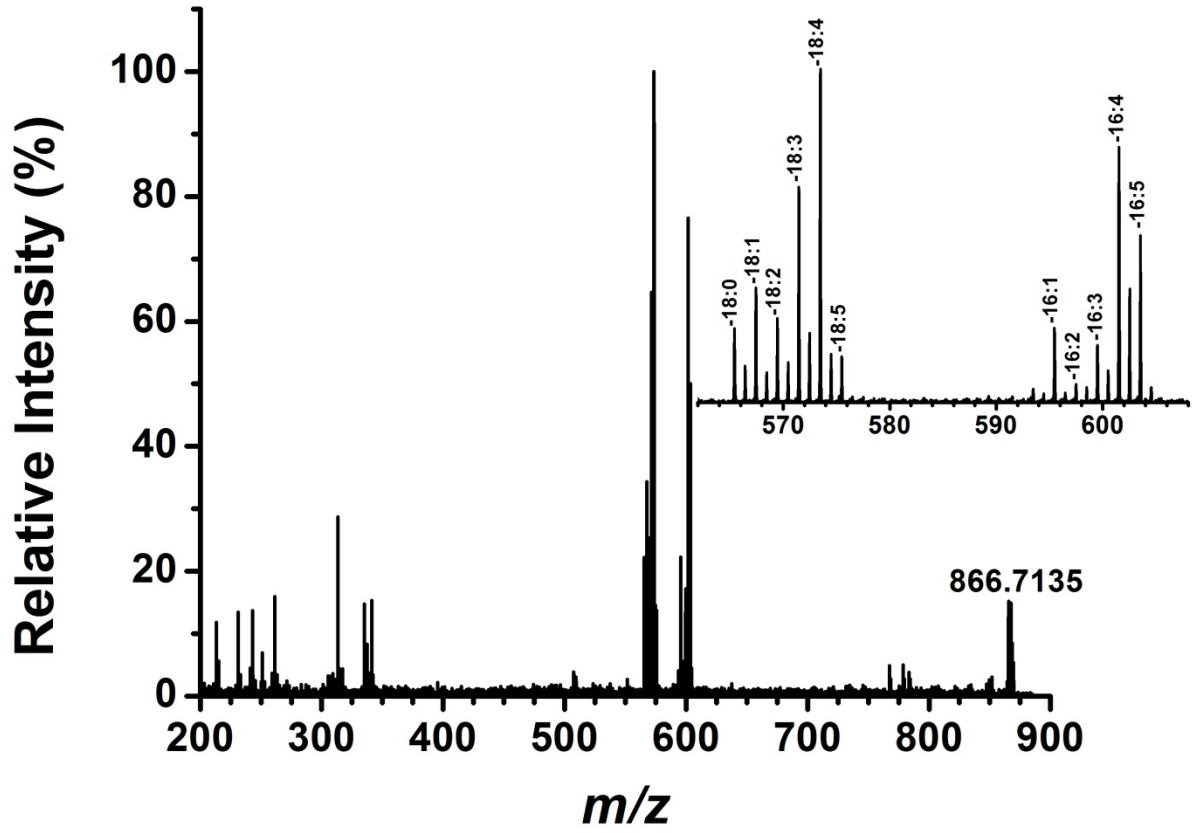

Figure S4. Tandem mass spectrum of cationized TAG(52:7) produced by LAESI-MS. Zoomed version of the fatty acid fragment region is shown in the inset.