Unraveling the lipidome and antioxidant activity of native *Bifurcaria bifurcata* and invasive *Sargassum muticum* seaweeds: A lipid perspective on how systemic intrusion may present an opportunity

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Figure S1. LC–MS/MS spectra of SQDG (34:1), namely of the [M − H]− ion at m/z 819.5 (a) and [M + NH4]+ ion at m/z 838.5 (b). The SQDG (34:1), was identified as SQDG (16:0/18:1) species. Typical fragmentation of SQDG species observed in LC-MS/MS spectrum of [M − H]− ions at m/z 819.5 showed the characteristic ion at m/z 225.0, corresponding to the dehydrlosulfoglycosyl anion ([C$_{6}$H$_{9}$O$_{7}$S]$^{-}$) of the polar head group that confirms the sulfoglycolipid class (a). The neutral loss of 261 Da, corresponding to the loss of sulfoglycosyl group (C$_{6}$H$_{12}$O$_{8}$S) and ammonia (NH$_{3}$) observed in LC-MS/MS spectrum of [M + NH$_{4}$]$^{+}$ ion, confirms the sulfonoglycolipid identity. The fatty acyl chains can be confirmed in positive mode due to the presence of the acylium ion of fatty acyl chain plus 74 ([RCO + 74]$^{+}$ ions). These ions can be seen at m/z 313.3 and m/z 339.3 in the LC-MS/MS spectrum of [M + NH$_{4}$]$^{+}$ ion of SQDG (16:0/18:1), corresponding to 16:0 and 18:1 fatty acids, confirming the SQDG (16:0/18:1) species (c). The representative structure of SQDG is depicted (c).
Figure S2. LC–MS/MS spectra of [M + NH₄]⁺ ions of MGDG (36:2), at m/z 800.5 corresponding to MGDG (16:0/20:2), (18:0/18:2), (18:1/18:1) and (16:1/20:1) species, (a) and of [M + NH₄]⁺ ion of MGMG (16:1) at m/z 508.3 (b). The LC-MS/MS spectrum of the [M + NH₄]⁺ ion of MGDG (36:2) at m/z 800.5 (a) showed a typical combined loss of NH₃ plus loss of galactosyl unit (-197 Da), a typical fragmentation of MGDG species with formation of the product ion at m/z 603.5 [1,2]. The product ions [RCO + 74]⁺ seen at m/z 311.3, m/z 313.3, m/z 339.3, m/z 341.3 and m/z 365.3, corresponding to the fatty acids 16:1, 16:0, 18:1, 18:0 and 20:2, respectively, allowed to pinpoint fatty acyl composition and to propose the contribution of the lipid molecular species MGDG (16:0/20:2), (18:1/18:1), (18:0/18:2) and (16:1/20:1) for the MGDG (36:2) (Table S1). The LC-MS/MS spectrum of [M+NH₄]⁺ of MGMG (16:1) at m/z 508.3 (b) showed the typical neutral loss of 197 Da, due to the combined loss of NH₃ and galactosyl residue (-179 Da), with the formation of the product ion at m/z 311.3. For the MGMG class, the fatty acyl chain composition can be observed as [RCO]⁺ and [RCO + 74]⁺ product ions, seen at m/z 237.2 and m/z 311.3, respectively, which correspond to the fatty acid 16:1 confirming the presence of the MGMG (16:1) (b). The representative structure of MGDG (c) and MGMG (d) are depicted in the figure.
Figure S3. LC–MS/MS spectrum of [M + NH₄]⁺ ion of DGDG (32:2) at m/z 906.7 corresponding to the DGDG (14:0/18:2) species (a). The typical fragmentation of this class of GL, namely neutral loss of the carbohydrate moiety (loss of 180 + 162 Da) combined with loss of NH₃ (-17 Da) is seen as a total neutral loss of (-359 Da) with formation of the product ion at m/z 547.5. The [RCO + 74]⁺ product ions allow to confirm the fatty acyl composition and are seen at m/z 285.2 and m/z 337.3, corresponding to the fatty acids 14:0 and 18:2, respectively, confirming the presence of the DGDG (14:0/18:2). The representative structure of DGDG is depicted in the figure.
Figure S4. LC–MS/MS spectra of [M + H]$^+$ ion at m/z 736.6 of DGTS (34:2), corresponding to the DGTS (16:0/18:2) species (a) and the DGTA (34:2), namely DGTA (16:0/18:2) species, at m/z 736.6 (b). These two isomeric betaine classes eluted at different retention times: DGTS at RT = 4.2 and DGTA at RT = 9.4. LC-MS/MS spectra of DGTS (34:2) (a) and DGTA (34:2) (b) show the typical reported product ions of these classes at m/z 144.1, corresponding to loss of both fatty acyl groups as keto derivatives (R$_1$CO + R$_2$CO) plus glycerol, and at m/z 236.1 corresponding to the loss of both fatty acyl chains as keto derivatives (R$_1$CO + R$_2$CO) [3–5]. These characteristic product ions at m/z 144.1 and m/z 236.1 can be used to conduct the qualitative characterization of DGTS and DGTA classes as positive [M + H]$^+$ ions, but it can’t be used to differentiate DGTS from DGTA, since both ions can be present in DGTA and DGTS spectra [6]. In these cases, the DGTA and DGTS differentiation can only be made by the specific retention time of each class, as mentioned before [6]. The fatty acyl composition can be assigned by the losses of fatty acyl chains as acid (-RCOOH) and ketene (-R=CO) derivatives. In the spectrum of DGTS (16:0/18:2) (a), the ion at m/z 474.4 corresponds to the loss of 18:2 fatty acyl chain as keto derivative (-262 Da) and the at m/z 456.4 corresponds to 18:2 as RCOOH (-280 Da), confirming the presence of the fatty acid 18:2. In the LC-MS/MS spectrum of DGTA (16:0/18:2) (b), the ions at m/z 498.4 and 474.4 corresponding to the loss of fatty acyl chains as keto derivatives (-238 and -262 Da), match to 16:0 and 18:2 fatty acids, respectively. Moreover, the ions at m/z 480.4 and 456.4 confirmed the presence of the fatty acids 16:0 and 18:2, respectively, since they correspond to the loss of RCOOH (-256 and -280 Da). The representative structures of DGTS (c) and DGTA (d) are depicted in the figure.
Figure S5. LC-MS/MS spectra of [M − H]⁻ ions of PG (34:4) at m/z 741.5, corresponding to the PG (18:3/16:1) species (a), LPG (16:0) at m/z 483.3 (b), and PI (34:2) at m/z 833.5 corresponding to the PI (18:2/16:0) species (c). PG (a) and LPG (b) species were identified by the presence of the product ion at m/z 153.1, corresponding to glycerol phosphate minus one water molecule, and m/z 227.1 corresponding to \([\text{C}_6\text{H}_{12}\text{O}_7\text{P}]^-\) anion corresponding to glycerophosphate glycerol minus one water molecule [3]. The PI class (c) was identified in the MS/MS spectra through the characteristic product ion at m/z 241.0 that corresponds to the inositol-1,2-cyclic phosphate anion \((\text{C}_6\text{H}_{12}\text{O}_5\text{PO}_3^-)\) of the polar head of PI [1]. The carboxylate anions \((\text{R}_1\text{COO}^-\text{ and } \text{R}_2\text{COO}^-)\) allowed the identification of fatty acyl chains in PG, its lyso form, and PI [7]. The representative structures of PG (d), LPG (e), and PI (f) are depicted in the figure.
Figure S6. LC-MS/MS spectra of the [M + H]+ ion of LPE (20:4) at m/z 502.3 (a), [M − H]− ion of LPE (20:4) at m/z 500.3 (b); [M + H]+ ion of PE (40:8) at m/z 788.5, corresponding to the PE (20:4/20:4) and PE (20:3/20:5) species (d); [M − H]− ion of PE (40:8) at m/z 786.5 corresponding to the PE (20:4/20:4) and PE (20:3/20:5) species (e); [M + H]+ ion at m/z 522.6 of LPC (18:1) (g); and [M+H]+ ion at m/z 758.6 of PC (34:2) (i). Typical loss of 141 Da was observed in the LC-MS/MS spectra of [M + H]+ ions of LPE (a) and PE (d), while the carboxylate anions (RCOO−) of the fatty acyl chains were identified in the LC-MS/MS spectra of [M − H]− ions of LPE (b) and PE (e). The LC-MS/MS spectra of [M + H]+ ions of LPC (g) and PC (i) showed the typical product ion of the polar head at m/z 184.0. The representative structures of LPE (c), PE (f), LPC (h), and PC (j) are depicted in the figure.
Tandem mass spectrometry analysis was based on the following literature:

1. Lopes, D.; Moreira, A. S. P.; Rey, F.; da Costa, E.; Melo, T.; Maciel, E.; Rego, A.; Abreu, M. H.; Domingues, P.; Calado, R.; Lillebø, A. I.; Rosário Domingues, M. Lipidomic signature of the green macroalgae *Ulva rigida* farmed in a sustainable integrated multi-trophic aquaculture. *J. Appl. Phycol.* 2018.

2. Da Costa, E.; Domingues, P.; Melo, T.; Coelho, E.; Pereira, R.; Calado, R.; Abreu, M. H.; Domingues, M. R. Lipidomic signatures reveal seasonal shifts on the relative abundance of high-valued lipids from the brown algae *Fucus vesiculosus*. *Mar. Drugs* 2019.

3. Melo, T.; Alves, E.; Azevedo, V.; Martins, A. S.; Neves, B.; Domingues, P.; Calado, R.; Abreu, M. H.; Domingues, M. R. Lipidomics as a new approach for the bioprospecting of marine macroalgae — Unraveling the polar lipid and fatty acid composition of *Chondrus crispus*. *Algal Res.* 2015.

4. Da Costa, E.; Melo, T.; Moreira, A. S. P. A.; Bernardo, C.; Helguero, L.; Ferreira, I.; Cruz, M. T. M.; Rego, A. M. A.; Domingues, P.; Calado, R.; Abreu, M. M. H.; Domingues, M. Valorization of lipids from *Gracilaria* sp. through lipidomics and decoding of antiproliferative and anti-inflammatory Activity. *Mar. Drugs* 2017.

5. Roche, S. A.; Leblond, J. D. Betaine lipids in chlorarachniophytes. *Phycol. Res.* 2010.

6. Li, Y.; Lou, Y.; Mu, T.; Xu, J.; Zhou, C.; Yan, X. Simultaneous structural identification of diacylglyceryl-N-trimethylhomoserine (DGTS) and diacylglycerylhydroxymethyl-N,N,N-trimethyl-β-alanine (DGTA) in microalgae using dual Li+/H+ adduct ion mode by ultra-performance liquid chromatography/quadrupole ti. *Rapid Commun. Mass Spectrom.* 2017.

7. Murphy, R. C. *Tandem Mass Spectrometry of Lipids*; Ron M A Heeren Mitsutoshi Setou, R. C. M., Ed.; Royal Soci.; THomas Graham House, Science Park, Milton Road, 2014; ISBN 9781849738279.
Table S1. Molecular species identified by HILIC-MS in *B. bifurcata*. Identification of different polar lipid classes and fatty acyl composition was confirmed by the analysis of the LC-MS/MS spectra of each ion. C represents the total number of carbon atoms and N the total number of double bonds on the fatty acyl chains. The most abundant species are marked in bold.

| Lipid species (C:N) | Observed m/z | Delta (ppm) | Retention time | Fatty acyl chains (C:N) | Formula |
|---------------------|-------------|-------------|----------------|--------------------------|---------|
| MGDG identified as [M + NH4]+ |             |             |                |                          |         |
| MGDG(30:4) | 712.5000 | 0.0000 | 2.05 | (14:0/16:4) | C39H70NO10 |
| MGDG(30:1) | 718.5477 | 1.8092 | 2.16 | (14:0/16:1) | C39H76NO10 |
| MGDG(32:4) | 740.5307 | 0.0000 | 2.08 | (16:0/16:4) and (14:1/18:3) | C41H74NO10 |
| MGDG(32:3) | 742.5487 | 3.0974 | 2.32 | (18:3/14:0) and (16:1/16:2) | C41H76NO10 |
| MGDG(32:2) | 744.5618 | -1.0745 | 2.13 | (16:1/16:1) and (18:2/14:0) | C41H78NO10 |
| MGDG(32:1) | 746.5775 | -0.2679 | 2.13 | (16:0/16:1) and (18:1/14:0) | C41H80NO10 |
| MGDG(34:4) | 768.5627 | 0.1301 | 2.08 | (18:4/16:0), (18:3/16:1) and (14:0/20:4) | C43H78NO10 |
| MGDG(34:3) | 770.5771 | -1.4586 | 2.13 | (16:0/18:3) and (18:2/16:1) | C43H80NO10 |
| MGDG(34:2) | 772.5932 | -0.1294 | 2.13 | (16:0/18:2) | C43H82NO10 |
| MGDG(34:1) | 774.6092 | 0.2582 | 2.16 | (16:0/18:1) | C43H84NO10 |
| MGDG(36:8) | 788.5308 | -0.596 | 2.21 | (18:4/18:4) and (20:4/16:4) | C45H74NO10 |
| MGDG(36:7) | 790.5469 | 0.0000 | 2.16 | (18:3/18:4) | C45H78NO10 |
| MGDG(36:6) | 792.5616 | -1.1356 | 2.18 | (18:3/18:3) and (18:4/18:2) | C45H80NO10 |
| MGDG(36:5) | 794.5788 | 0.7551 | 2.13 | (18:3/18:2), (20:4/16:1) and (20:5/16:0) | C45H82NO10 |
| MGDG(36:4) | 796.5942 | 1.1298 | 2.16 | (18:3/18:1), (18:2/18:2) and (20:4/16:0) | C45H84NO10 |
| MGDG(36:3) | 798.6082 | -1.6529 | 2.16 | (16:1/20:2), (18:2/18:1) and (16:0/20:3) | C45H86NO10 |
| MGDG(36:2) | 800.6249 | -0.3422 | 2.18 | (18:1/18:1) and (16:0/20:2) | C45H88NO10 |
| MGDG(38:10) | 812.5319 | 0.7754 | 2.02 | * | C47H74NO10 |
| MGDG(38:9) | 814.5463 | -0.7661 | 2.13 | (20:5/18:4) | C47H76NO10 |
| MGDG(38:8) | 816.5617 | -1.0654 | 2.13 | (20:4/18:4) and (20:5/18:3) | C47H78NO10 |
| MGDG(38:7) | 818.5761 | -2.5947 | 2.18 | (18:3/20:4) | C47H80NO10 |
| MGDG(38:6) | 820.5934 | -0.6093 | 2.16 | (18:1/20:5) | C47H82NO10 |
| MGDG(38:5) | 822.6093 | -0.2674 | 2.08 | (18:1/20:4), (20:3/18:2), (18:3/20:2) and (18:4/20:1) | C47H84NO10 |
| MGDG(40:10) | 840.5645 | 2.2961 | 1.77 | (20:5/20:5) | C49H78NO10 |
| MGDG(40:9) | 842.5782 | 0.0000 | 2.13 | (20:5/20:4) | C49H80NO10 |
| MGDG(40:8) | 844.5933 | -0.6749 | 2.13 | (20:4/20:4) | C49H82NO10 |

DGDG identified as [M + NH4]+

| Lipid species (C:N) | Observed m/z | Delta (ppm) | Retention time | Fatty acyl chains (C:N) | Formula |
|---------------------|-------------|-------------|----------------|--------------------------|---------|
| DGDG(28:0) | 854.582 | -2.4573 | 2.74 | * | C43H84O15N |
| DGDG(32:3) | 904.5995 | -0.2211 | 2.32 | (14:0/18:3) | C47H86O15N |
| DGDG(32:2) | 906.6154 | 0.0000 | 2.35 | (18:2/14:0) and (16:1/16:1) | C47H88O15N |
| DGDG(32:1) | 908.6310 | 0.0000 | 2.33 | (16:0/16:1) and (14:0/18:1) | C47H90O15N |
| DGDG(34:4) | 930.6154 | 0.0000 | 2.30 | (18:3/16:1) and (16:0/18:4) | C49H88O15N |
| DGDG(34:3) | 932.6308 | -0.2144 | 2.33 | (18:3/16:0) | C49H90O15N |
| DGDG(34:2) | 934.6457 | -1.0699 | 2.44 | (16:0/18:2) and (18:1/16:1) | C49H92O15N |
| DGDG(34:1) | 936.6619 | -0.427 | 2.32 | (16:0/18:1) | C49H94O15N |
| Molecule     | Mass      | PPM       | m/z       | Precursor Ion | Molecular Formula |
|--------------|-----------|-----------|-----------|---------------|-------------------|
| DGDG(36:7)   | 952.6001  | 0.4199    | 2.39      | (18:4/18:3)   | C51H86O15N        |
| DGDG(36:6)   | 954.6152  | -0.2095   | 2.32      | (18:3/18:3)   | C51H88O15N        |
| DGDG(36:5)   | 956.6299  | -1.1499   | 2.33      | (20:5/16:0), (18:3/18:2) and (16:1/20:4) | C51H90O15N |
| DGDG(36:4)   | 958.6467  | 0.0000    | 2.39      | *             | C51H92O15N        |
| DGDG(38:9)   | 976.5997  | 0.0000    | 2.46      | (18:4/20:5)   | C53H86O15N        |
| DGDG(38:8)   | 978.6155  | 0.1022    | 2.45      | *             | C53H88O15N        |

**SQDG identified as [M – H]**

| Molecule     | Mass      | PPM       | m/z       | Precursor Ion | Molecular Formula |
|--------------|-----------|-----------|-----------|---------------|-------------------|
| SQDG(30:1)   | 763.4667  | 0.0956    | 1.69      | (14:0/16:1)   | C39H71O12S        |
| SQDG(30:0)   | 765.4823  | 0.0300    | 1.82      | (16:0/14:0)   | C39H73O12S        |
| SQDG(32:3)   | 787.4667  | 0.9927    | 1.86      | (14:0/18:3)   | C41H71O12S        |
| SQDG(32:2)   | 789.4823  | 0.0291    | 1.75      | (16:0/16:1)   | C41H73O12S        |
| SQDG(32:1)   | 791.4988  | 1.1030    | 1.80      | (16:1/16:0) and (18:1/14:0) | C41H75O12S |
| SQDG(32:0)   | 793.5135  | -0.0958   | 1.69      | *             | C41H77O12S        |
| SQDG(34:4)   | 813.4839  | 1.9951    | 1.75      | (18:4/16:0)   | C43H73O12S        |
| SQDG(34:3)   | 815.4996  | 2.0515    | 1.82      | (18:3/16:0) and (18:2/16:1) | C43H75O12S |
| SQDG(34:2)   | 817.5143  | 0.8856    | 1.72      | (18:1/16:1)   | C43H77O12S        |
| SQDG(34:1)   | 819.5295  | 0.3331    | 1.75      | (14:0/20:1), (16:0/18:1) and (16:1/18:0) | C43H79O12S |
| SQDG(34:0)   | 821.5449  | 0.0280    | 1.8       | (16:0/18:0)   | C43H81O12S        |
| SQDG(36:7)   | 863.4979  | -0.0313   | 1.82      | (20:5/18:2)   | C47H75O12S        |
| SQDG(36:6)   | 865.5136  | 0.0277    | 1.75      | *             | C47H77O12S        |
| SQDG(36:5)   | 867.5305  | 1.4674    | 1.82      | (18:1/20:4)   | C47H90O12S        |
| SQDG(38:6)   | 869.5455  | 0.7165    | 2.18      | **             | C47H91O12S        |
| SQDG(38:5)   | 871.5675  | 0.0226    | 1.75      | **             | C47H92O12S        |
| SQDG(38:4)   | 873.5835  | -0.0854   | 1.86      | *             | C49H90O12S        |
| SQDG(38:3)   | 875.5991  | 0.0819    | 1.87      | *             | C49H92O12S        |
| SQDG(38:2)   | 877.6151  | -0.0850   | 1.82      | **             | C49H93O12S        |

**PC identified as [M + H]**

| Molecule     | Mass      | PPM       | m/z       | Precursor Ion | Molecular Formula |
|--------------|-----------|-----------|-----------|---------------|-------------------|
| PC(30:3)     | 700.4913  | -0.6167   | 12.15     | *             | C38H71NO8P        |
| PC(34:2)     | 758.5700  | 0.0237    | 11.88     | **            | C42H81NO8P        |
| PC(38:6)     | 806.5700  | 0.0223    | 11.28     | *             | C46H81NO8P        |

**PE identified as [M + H]**

| Molecule     | Mass      | PPM       | m/z       | Precursor Ion | Molecular Formula |
|--------------|-----------|-----------|-----------|---------------|-------------------|
| PE(30:3)     | 658.4426  | -3.3139   | 4.57      | **            | C35H65NO8P        |
| PE(34:4)     | 712.4924  | 0.9376    | 4.05      | (14:0/20:4)   | C39H71NO8P        |
| PE(34:2)     | 716.5234  | 0.5136    | 4.19      | *             | C39H75NO8P        |
| PE(34:1) | 718.5387 | 0.0251 | 4.05 | (14:0/20:1) | C39H77NO8P |
| PE(36:5) | 738.5078 | 0.5660 | 4.10 | (16:1/20:4) and (16:0/20:5) | C41H73O8NP |
| PE(36:4) | 740.5226 | -0.8384 | 4.05 | ** | C41H75NO8P |
| PE(36:3) | 742.5383 | -0.5145 | 4.20 | ** | C41H77NO8P |
| PE(36:2) | 744.5557 | 1.8387 | 4.09 | (16:1/20:1) | C41H79O8NP |
| PE(38:8) | 760.4889 | -3.7229 | 4.01 | ** | C43H79O8NP |
| PE(39:7) | 762.5059 | -1.9463 | 3.99 | ** | C43H73O8NP |
| PE(38:6) | 764.5227 | -0.4343 | 4.05 | (16:1/20:5) and (20:4/18:2) | C43H75O8NP |
| PE(38:5) | 766.5369 | -2.3247 | 4.05 | (20:4/18:1) and (20:5/18:0) | C43H77NO8P |
| PE(38:4) | 768.553 | -1.7318 | 4.05 | ** | C43H79O8NP |
| PE(40:10) | 784.4918 | 0.0867 | 4.05 | * | C45H71NO8P |
| PE(40:9) | 786.5071 | -0.3885 | 3.92 | (20:4/20:5) | C45H73O8NP |
| PE(40:8) | 788.5228 | -0.2942 | 3.92 | (20:4/20:4) | C45H75O8NP |
| PE(40:7) | 790.5389 | 0.2758 | 3.78 | * | C45H77NO8P |
| PE(40:6) | 792.5543 | -0.0391 | 3.92 | (20:4/20:2) and (20:3/20:3) | C45H79O8NP |
| PE(40:5) | 794.5700 | 0.0227 | 3.92 | (16:0/24:5) | C45H81O8NP |
| PE(40:4) | 796.5869 | 1.5918 | 3.86 | (20:0/20:4) | C45H83O8NP |
| PE(42:11) | 810.5045 | -3.5558 | 3.85 | ** | C47H73O8NP |
| PE(42:5) | 822.6013 | 0.0219 | 3.92 | (20:4/22:1) and (20:5/22:0) | C47H85O8NP |
| PE(42:4) | 824.6169 | -0.0388 | 3.92 | (22:0/20:4) | C47H87O8NP |
| PE(44:4) | 852.6482 | -0.3735 | 3.92 | (20:4/24:0) | C49H91O8NP |

**PG identified as [M – H]**

| PG(32:1) | 719.4863 | 0.0000 | 1.97 | (16:1/16:0) and (16:1/14:0) | C39H72O10P |
| PG(34:4) | 741.4706 | -0.1349 | 1.97 | (14:0/20:4) and (16:1/18:3) | C40H70O10P |
| PG(34:3) | 743.4863 | 0.0000 | 1.97 | (18:3/16:0) and (16:1/18:2) | C40H72O10P |
| PG(34:2) | 745.5032 | 1.6097 | 1.92 | (14:0/20:2) | C40H74O10P |
| PG(34:1) | 747.5201 | 3.3444 | 1.95 | (16:0/18:1) and (14:0/20:1) | C40H76O10P |
| PG(34:0) | 749.5336 | 0.4002 | 1.95 | * | C40H78O10P |
| PG(36:5) | 767.4863 | 0.0000 | 1.86 | * | C42H72O10P |
| PG(36:4) | 769.502 | 0.0000 | 1.92 | (20:4/16:0), (18:3/18:1) and (18:2/18:2) | C42H74O10P |
| PG(36:3) | 771.5176 | 0.0000 | 1.98 | (16:1/20:2), (16:0/20:3) and (18:2/18:1) | C42H76O10P |
| PG(36:2) | 773.5333 | 0.0000 | 1.92 | (18:1/18:1) and (16:0/20:2) | C42H78O10P |

**PI identified as [M – H]**

| PI(30:2) | 777.4554 | 0.0000 | 1.62 | * | C39H70O13P |
| PI(34:1) | 835.5337 | 0.0000 | 1.97 | (18:1/16:0) | C43H80O13P |
| PI(36:8) | 849.4554 | -0.0094 | 1.82 | * | C45H70O13P |
| PI(38:8) | 877.4878 | 1.2536 | 1.75 | * | C47H74O13P |
| PI(40:6) | 909.5528 | 3.8481 | 1.82 | * | C49H80O13P |
| PI(40:5) | 911.5664 | 1.5358 | 1.87 | * | C49H84O13P |
| PI(46:3) | 999.6912 | 1.0423 | 2.03 | * | C55H100O13P |

**DGTS identified as [M + H]**

| DGTS(32:1) | 710.5935 | 0.0000 | 4.10 | * | C42H80O7N |
| DGTS(32:2) | 708.5779 | 0.1411 | 4.10 | * | C42H78O7N |
| DGTS(34:2) | 736.6097 | 0.8145 | 4.16 | * | C44H82O7N |
| DGTS(34:1) | 738.6244 | -0.5415 | 4.36 | * | C44H84O7N |
| DGTS(36:4) | 760.6091 | 0.0000 | 4.37 | * | C46H82O7N |

DGTA identified as \([M + H]^+\):

| DGTA(30:1) | 682.5622 | 0.0000 | 10.14 | * | C40H76O7N |
| DGTA(32:4) | 704.5465 | 0.0000 | 9.46 | ** | C42H74O7N |
| DGTA(32:3) | 706.5615 | -0.9907 | 9.87 | * | C42H76O7N |
| DGTA(32:2) | 708.5782 | 0.5645 | 9.66 | * | C42H78O7N |
| DGTA(32:1) | 710.5933 | -0.2815 | 9.73 | * | C42H80O7N |
| DGTA(34:5) | 730.5619 | -0.4106 | 9.76 | ** | C44H76O7N |
| DGTA(34:4) | 732.5782 | 0.5460 | 9.87 | (14:0/20:4) | C44H78O7N |
| DGTA(34:3) | 734.5913 | -2.9949 | 9.87 | * | C44H80O7N |
| DGTA(34:2) | 736.6100 | 1.2218 | 9.24 | (18:2/16:0) | C44H82O7N |
| DGTA(34:1) | 738.6242 | -0.8123 | 9.87 | (16:1/18:0) and (16:0/18:1) | C44H84O7N |
| DGTA(36:7) | 754.5622 | 0.0000 | 9.67 | ** | C46H76O7N |
| DGTA(36:6) | 756.5763 | -1.9826 | 9.87 | ** | C46H78O7N |
| DGTA(36:5) | 758.5927 | -1.0546 | 9.87 | (20:5/16:0) and (20:4/16:1) | C46H80O7N |
| DGTA(36:4) | 760.6080 | -1.4462 | 9.87 | (16:0/20:4) and (18:0/18:4) | C46H82O7N |
| DGTA(36:3) | 762.6229 | -2.4914 | 10.14 | (16:0/20:3) | C46H84O7N |
| DGTA(36:2) | 764.6387 | -2.2233 | 9.87 | * | C46H86O7N |
| DGTA(38:8) | 780.5778 | 0.0000 | 9.19 | ** | C48H78O7N |
| DGTA(38:7) | 782.5929 | -0.7667 | 9.00 | ** | C48H80O7N |
| DGTA(38:6) | 784.6082 | -1.1471 | 9.87 | (18:2/20:4) | C48H82O7N |
| DGTA(38:5) | 786.6231 | -2.1611 | 9.42 | (18:1/20:4) | C48H84O7N |
| DGTA(40:9) | 806.5935 | 0.0000 | 9.00 | (20:5/20:4) | C50H80O7N |
| DGTA(40:8) | 808.6087 | -0.4947 | 9.00 | (20:4/20:4) | C50H82O7N |
| DGTA(40:7) | 810.6225 | -2.8373 | 9.00 | (20:3/20:4) | C50H84O7N |
| DGTA(40:6) | 812.6387 | -2.0919 | 9.81 | * | C50H86O7N |
| DGTA(42:11) | 830.5902 | -3.9478 | 9.00 | **, # | C52H80O7N |
| DGTA(42:8) | 836.6403 | -0.1542 | 9.05 | * | C52H86O7N |

*: Molecular species identified by retention time and mass accuracy;

**: Molecular species identified by retention time, mass accuracy, and polar head product ion;

#: Contribution of sodiated adduct ion
Table S2. Molecular species identified by HILIC-MS and MS/MS in *S. muticum*. The identification of different polar lipid classes and fatty acyl composition was confirmed by mass accuracy, retention time and the analysis of the LC-MS/MS spectra of each ion. C represents the total number of carbon atoms and N the total number of double bonds on the fatty acyl chains. The most abundant species are marked in bold.

| Lipid species (C:N) | Observed m/z | Delta (ppm) | Retention time | Fatty acyl chains (C:N) | Formula |
|---------------------|--------------|-------------|----------------|------------------------|---------|
| MGDG(30:1)          | 718.5464     | 0.0000      | 2.40           | (14:1/16:0) and (16:1/14:0) | C39H76NO10 |
| MGDG(30:0)          | 720.5616     | -1.2490     | 2.31           | (16:0/14:0)            | C39H78NO10 |
| MGDG(32:8)          | 732.4683     | -0.5461     | 2.14           | *                      | C41H66NO10 |
| MGDG(32:5)          | 738.5156     | -0.0325     | 2.25           | *                      | C41H72NO10 |
| MGDG(32:4)          | 740.5307     | 0.0000      | 2.22           | (14:0/18:4) and (16:1/16:3) | C41H74NO10 |
| MGDG(32:3)          | 742.5463     | -0.1347     | 2.31           | (18:3/14:0), (18:2/14:1) and (16:0/16:3) | C41H76NO10 |
| MGDG(32:2)          | 744.562      | -0.8058     | 2.31           | (16:1/16:1), (16:0/16:2) and (18:2/14:0) | C41H78NO10 |
| MGDG(32:1)          | 746.5775     | -0.2679     | 2.2            | (18:1/14:0) and (16:0/16:1) | C41H80NO10 |
| MGDG(34:7)          | 762.5163     | 0.8865      | 1.87           | (16:3/18:4)            | C43H72NO10 |
| MGDG(34:6)          | 764.5314     | 0.1661      | 2.04           | (18:4/16:2) and (18:3/16:3) | C43H74NO10 |
| MGDG(34:5)          | 766.5469     | -0.0313     | 2.20           | (16:1/18:4), (16:2/18:3) and (16:3/18:2) | C43H76NO10 |
| MGDG(34:4)          | 768.563      | 0.5205      | 2.31           | (16:1/18:3)            | C43H78NO10 |
| MGDG(34:3)          | 770.5781     | -0.1609     | 2.20           | (18:3/16:0) and (16:1/18:2) | C43H80NO10 |
| MGDG(34:2)          | 772.5933     | 0.0000      | 2.20           | (16:0/18:2) and (18:1/16:1) | C43H82NO10 |
| MGDG(34:1)          | 774.6086     | -0.5164     | 2.20           | (18:1/16:0)            | C43H84NO10 |
| MGDG(36:9)          | 786.5158     | 0.2543      | 2.32           | (20:5/16:4)            | C45H72NO10 |
| MGDG(36:8)          | 788.5308     | -0.5960     | 2.20           | (18:4/18:4)            | C45H74NO10 |
| MGDG(36:7)          | 790.5465     | -0.5060     | 2.20           | (18:3/18:4)            | C45H76NO10 |
| MGDG(36:6)          | 792.5625     | 0.0000      | 2.19           | (20:5/16:1) and (18:3/18:3) | C45H78NO10 |
| MGDG(36:5)          | 794.5777     | -0.6293     | 2.19           | (18:3/18:2), (20:4/16:1), (20:5/16:0) and (18:4/18:1) | C45H80NO10 |
| MGDG(36:4)          | 796.5928     | -0.6277     | 2.19           | (18:2/18:2), (18:3/18:1) and (20:4/16:0) | C45H82NO10 |
| MGDG(36:3)          | 798.6071     | -3.0303     | 2.12           | (18:2/18:1), (18:3/18:0), (16:0/20:3) and (16:1/20:2) | C45H84NO10 |
| MGDG(36:2)          | 800.6249     | -0.3422     | 2.31           | (20:2/16:0), (18:0/18:2), (18:1/18:1) and (16:1/20:1) | C45H86NO10 |
| MGDG(36:1)          | 802.6408     | -0.0299     | 2.18           | (20:1/16:0) and (18:0/18:1) | C45H88NO10 |
| MGDG(38:9)          | 814.5466     | -0.3978     | 2.20           | (20:5/18:4)            | C47H76NO10 |
| MGDG(38:8)          | 816.5597     | -3.5147     | 2.31           | (20:4/18:4) and (20:5/18:3) | C47H78NO10 |
| MGDG(38:7)          | 818.5759     | -2.8391     | 2.31           | (18:3/20:4) and (18:2/20:5) | C47H80NO10 |
| MGDG(38:6)          | 820.5939     | 0.0000      | 2.20           | (18:1/20:5)            | C47H82NO10 |
| MGDG(38:5)          | 822.6095     | -0.0243     | 2.31           | (18:2/20:3), (20:4/18:1), (20:2/18:3) and (20:1/18:4) | C47H84NO10 |
| MGDG(38:4)          | 824.6251     | 0.0000      | 2.20           | *                      | C47H86NO10 |
| MGDG(40:10)         | 840.5637     | 1.3443      | 2.12           | (20:5/20:5)            | C49H78NO10 |
| MGDG(40:9)          | 842.5781     | -0.1187     | 2.20           | (20:5/20:4)            | C49H80NO10 |
| MGDG(40:8)          | 844.5925     | -1.6221     | 2.31           | (20:4/20:4)            | C49H82NO10 |
| MGDG(40:6)          | 846.6252     | 0.0306      | 2.27           | *                      | C49H86NO10 |
### MGDG identified as [M + NH₄]⁺

| MGDG(42:9) | 870.6088 | -0.8316 | 1.67 | * | C51H84NO10 |

| MGDG(16:4) | 502.3016 | -0.0179 | 2.31 | (16:4) | C25H44NO9 |
| MGDG(16:1) | 508.3485 | -0.1161 | 2.31 | (16:1) | C25H50NO9 |
| MGDG(16:0) | 510.3642 | 0.0000 | 2.36 | (16:0) | C25H52NO9 |
| MGDG(18:4) | 530.3326 | -0.5827 | 2.38 | (18:4) | C27H48NO9 |
| MGDG(16:3) | 504.3733 | 0.0813 | 2.36 | (16:3) | C27H52NO9 |
| MGDG(16:2) | 506.3890 | 0.0000 | 2.40 | (16:2) | C27H54NO9 |
| MGDG(16:1) | 508.3947 | 0.0813 | 2.36 | (16:1) | C27H56NO9 |
| MGDG(16:0) | 510.3994 | 0.0000 | 2.40 | (16:0) | C27H58NO9 |
| MGDG(18:3) | 532.3487 | 0.2649 | 2.36 | * | C27H54NO9 |
| MGDG(18:2) | 534.3642 | -0.0204 | 2.36 | * | C27H56NO9 |
| MGDG(18:1) | 536.3799 | 0.0764 | 2.31 | (18:1) | C27H58NO9 |
| MGDG(20:5) | 556.3487 | 0.2625 | 2.36 | * | C29H50NO9 |
| MGDG(20:4) | 558.3642 | -0.0161 | 2.31 | (20:4) | C29H52NO9 |

### DGDG identified as [M + NH₄]⁺

| DGDG(28:0) | 854.5827 | -1.6382 | 2.12 | (16:0/12:0) | C43H84O15N |
| DGDG(32:3) | 906.6154 | 0.0000 | 2.36 | (14:0/18:2) | C47H88O15N |
| DGDG(32:2) | 908.6310 | 0.0000 | 2.31 | (18:1/14:0) and (16:0/16:1) | C47H90O15N |
| DGDG(32:1) | 928.5997 | 0.0000 | 2.36 | * | C49H86O15N |
| DGDG(32:0) | 930.6154 | 0.0000 | 2.38 | (18:3/16:1) and (16:0/18:4) | C49H88O15N |
| DGDG(34:5) | 932.6310 | 0.0000 | 2.38 | (18:3/16:0) and (16:1/18:2) | C49H90O15N |
| DGDG(34:4) | 934.6447 | -2.1398 | 2.31 | (18:2/16:0) | C49H92O15N |
| DGDG(34:3) | 936.6608 | -1.6014 | 2.43 | (18:1/16:0) | C49H94O15N |
| DGDG(34:2) | 938.6764 | 0.0000 | 2.36 | * | C51H82O15N |
| DGDG(34:1) | 940.6920 | 0.3156 | 2.38 | (18:4/18:4) | C51H84O15N |
| DGDG(36:1) | 942.6920 | 0.3156 | 2.38 | (18:4/18:4) and (20:5/16:2) | C51H86O15N |
| DGDG(36:0) | 944.7076 | -0.3136 | 2.38 | (18:3/16:1) and (20:5/16:0) | C51H88O15N |
| DGDG(36:3) | 946.7232 | 2.1137 | 1.83 | (16:0/18:0) and (14:0/16:0) | C51H90O15N |
| DGDG(36:2) | 948.7388 | 0.7633 | 1.71 | (18:2/16:1) and (16:0/18:4) | C51H92O15N |
| DGDG(36:1) | 950.7544 | 0.7633 | 1.71 | (18:1/16:0) and (20:5/18:2) | C51H94O15N |
| DGDG(38:9) | 952.7700 | 0.7633 | 1.71 | (20:5/18:4) | C53H86O15N |

### SQDG identified as [M − H]⁻

| SQDG(28:0) | 737.4517 | 0.8048 | 1.84 | ** | C37H69O12S |
| SQDG(30:1) | 763.4666 | -0.0354 | 1.76 | (14:0/16:1) | C39H71O12S |
| SQDG(30:0) | 765.4817 | -0.7538 | 1.71 | (14:0/16:0) | C39H73O12S |
| SQDG(30:1) | 785.4509 | -0.0980 | 1.72 | * | C41H69O12S |
| SQDG(30:3) | 787.4685 | -1.0520 | 1.76 | ** | C41H71O12S |
| SQDG(32:2) | 789.4819 | -0.4775 | 1.64 | (14:0/18:2), (16:1/16:1) and (16:0/16:2) | C41H73O12S |
| SQDG(32:1) | 791.4966 | 2.1137 | 1.83 | (16:1/16:0) and (14:0/18:1) | C41H75O12S |
| SQDG(32:0) | 793.5146 | 1.2905 | 1.83 | (16:0/16:0) | C41H77O12S |
| SQDG(34:5) | 811.4666 | -0.0333 | 1.71 | * | C43H71O12S |
| SQDG(34:4) | 813.4832 | 1.1346 | 1.74 | (16:1/18:3) and (16:0/18:4) | C43H73O12S |
| SQDG(34:3) | 815.4999 | 2.1944 | 1.64 | (18:2/16:1) and (16:0/18:3) | C43H75O12S |
| SQDG(34:2) | 817.5142 | 0.7633 | 1.71 | (16:0/18:2) and (18:1/16:1) | C43H77O12S |
| SQDG(34:1) | 819.5292 | -0.0329 | 1.76 | (16:0/18:1) | C43H79O12S |
| SQDG(36:7) | 835.4669 | 0.3268 | 1.72 | ** | C45H81O12S |
| SQDG(36:6) | 837.4821 | -0.2113 | 1.76 | (18:3/18:3) | C45H73O12S |
| SQDG(36:5) | 839.4995 | 1.8737 | 1.64 | (20:5/16:0), (20:4/16:1) and (18:3/18:2) | C45H75O12S |
| SQDG(36:4) | 841.5121 | -1.7540 | 1.76 | (20:4/16:0) and (18:4/18:0) | C45H77O12S |
| SQDG(36:3) | 843.5291 | -0.1506 | 1.74 | * | C45H79O12S |
| SQDG(36:2) | 845.5428 | -2.4564 | 1.76 | (20:2/16:0) | C45H81O12S |
| SQDG(36:1) | 847.5624 | 2.2099 | 1.83 | ** | C45H83O12S |
| SQDG(38:9) | 859.4667 | 0.0849 | 1.74 | ** | C47H71O12S |
| SQDG(38:8) | 861.4819 | -0.4376 | 1.73 | ** | C47H73O12S |
| SQDG(38:7) | 863.4980 | 0.7758 | 1.70 | ** | C47H75O12S |
| SQDG(38:6) | 865.5121 | -1.7053 | 1.70 | ** | C47H77O12S |
| SQDG(38:5) | 867.5299 | 0.7758 | 1.70 | ** | C47H79O12S |
| SQDG(38:4) | 873.5769 | 0.8276 | 1.83 | ** | C47H81O12S |
| SQDG(38:3) | 875.5903 | -1.7440 | 1.71 | (22:1/16:0) | C49H83O12S |
| SQDG(38:2) | 877.6070 | -0.5435 | 1.71 | (22:0/16:0) | C49H85O12S |
| SQDG(38:1) | 889.5137 | 0.1394 | 1.73 | (20:4/20:4) | C49H77O12S |
| SQDG(38:0) | 893.5448 | -0.0862 | 1.71 | * | C49H81O12S |
| SQDG(40:8) | 903.6245 | 1.5194 | 1.74 | ** | C49H91O12S |
| SQDG(40:0) | 905.6388 | 0.0254 | 1.71 | * | C49H93O12S |

**LPC identified as [M + H]+**

| LPC(16:0) | 496.3403 | -0.0322 | 15.07 | ** | C24H51NO7P |
| LPC(18:1) | 522.3560 | 0.0632 | 15.07 | ** | C26H53NO7P |
| LPC(18:0) | 524.3716 | -0.0324 | 14.92 | * | C26H55NO7P |

**PC identified as [M + H]+**

| PC(30:3) | 700.4896 | -3.0436 | 11.73 | * | C38H71NO8P |
| PC(34:2) | 758.5685 | -1.9357 | 12.19 | ** | C42H81NO8P |
| PC(34:1) | 760.5848 | -1.0939 | 12.33 | ** | C42H83NO8P |
| PC(36:5) | 780.5541 | -0.2959 | 11.89 | * | C44H79NO8P |
| PC(36:4) | 782.5709 | 1.1731 | 10.98 | ** | C44H81NO8P |
| PC(36:2) | 786.6012 | -0.1042 | 11.84 | * | C44H83NO8P |
| PC(36:1) | 788.6165 | -0.5478 | 11.34 | * | C44H87NO8P |
| PC(38:7) | 804.5543 | -0.0385 | 10.88 | * | C46H79NO8P |
| PC(38:6) | 806.5696 | -0.4736 | 11.10 | ** | C46H81NO8P |
| PC(40:10) | 826.5385 | -0.2202 | 10.88 | * | C48H77NO8P |

**LPE identified as [M + H]+**

| LPE(20:5) | 500.2778 | 0.1659 | 5.95 | ** | C25H43NO7P |
| LPE(20:4) | 502.2926 | -1.5270 | 5.76 | ** | C25H45NO7P |

**PE identified as [M + H]+**

| PE(30:3) | 658.4425 | -3.4657 | 4.60 | ** | C35H65NO8P |
| PE(30:1) | 662.4761 | 0.0272 | 4.41 | * | C35H69NO8P |
| PE(32:2) | 688.4927 | 1.4060 | 4.33 | * | C37H71NO8P |
| PE(32:1) | 690.5068 | -0.8429 | 4.41 | (16:1/16:0) | C37H73NO8P |
| PE(34:5)    | 710.4758  | -0.3969 | 4.04     | *       | C39H69NO8P |
| PE(34:4)    | 712.4918  | 0.0954  | 4.10     |         | C39H71NO8P |
| PE(34:3)    | 714.5074  | 0.0252  | 4.04     | *       | C39H73O8NP |
| PE(34:2)    | 716.5230  | -0.0447 | 4.10     | **      | C39H75NO8P |
| PE(34:1)    | 718.5385  | -0.2533 | 4.08     | (14:0/20:1) | C39H77NO8P |
| PE(36:7)    | 734.4758  | -0.3839 | 4.08     | **      | C41H69NO8P |
| PE(36:6)    | 736.4922  | 0.6354  | 4.04     | **      | C41H71NO8P |
| PE(36:5)    | 738.5068  | -0.7881 | 4.10     |         | C41H73O8NP |
| PE(36:4)    | 740.5230  | -0.0432 | 4.32     | **      | C41H75NO8P |
| PE(38:9)    | 758.4744  | -2.2176 | 4.13     |         | C43H69NO8P |
| PE(38:8)    | 760.4890  | -3.5924 | 3.97     |         | C43H71NO8P |
| PE(38:7)    | 762.5063  | -1.4190 | 3.97     | (18:2/20:5) and (20:4/18:3) | C43H73NO8P |
| PE(38:6)    | 764.5227  | -0.4343 | 4.13     | (20:4/18:2) | C43H75NO8P |
| PE(38:5)    | 766.5370  | -2.1943 | 3.97     | (20:4/18:1) and (20:5/18:0) | C43H77NO8P |
| PE(38:4)    | 768.5536  | -0.9511 | 3.97     | **      | C43H79O8NP |
| PE(38:3)    | 770.5700  | 0.0234  | 3.97     | **      | C43H81NO8P |
| PE(40:10)   | 784.4921  | 0.4691  | 3.97     |         | C45H71NO8P |
| PE(40:9)    | 786.5071  | -0.3585 | 3.73     |         | C45H73O8NP |
| PE(40:8)    | 788.5226  | -0.5479 | 3.73     | (20:4/20:4) and (20:3/20:5) | C45H75O8NP |
| PE(40:7)    | 790.5395  | 1.0347  | 3.93     | (20:5/20:2) and (20:4/20:3) | C45H79O8NP |
| PE(40:6)    | 792.5547  | 0.4656  | 3.93     | (20:4/20:2) and (20:1/20:5) | C45H81O8NP |
| PE(40:5)    | 794.5705  | 0.6519  | 3.73     | (20:5/20:0), (20:4/20:1) and (20:2/20:3) | C45H83O8NP |
| PE(40:4)    | 796.5858  | 0.2109  | 4.07     | (20:4/20:0) | C45H85NO8P |
| PE(42:11)   | 810.5053  | -2.5688 | 4.13     | **      | C47H73NO8P |
| PE(42:7)    | 818.5700  | 0.0220  | 3.93     | **      | C47H81O8NP |
| PE(42:6)    | 820.5873  | 2.0327  | 4.07     | (20:5/22:1) and (20:4/22:2) | C47H83NO8P |
| PE(42:5)    | 822.6011  | -0.2212 | 3.81     | (20:4/22:1) and (20:5/22:0) | C47H85O8NP |
| PE(42:4)    | 824.6169  | -0.0388 | 3.81     | **      | C47H87O8NP |
| PE(44:7)    | 846.6012  | -0.0969 | 4.07     | (20:4/24:3) | C49H85NO8P |
| PE(44:4)    | 852.6482  | -0.0375 | 3.87     | **      | C49H91NO8P |
| LPG identified as [M – H]^− |
| LPG(16:0)   | 483.2733  | 2.0734  | 2.16     | (16:0)  | C22H44O9P |
| PG identified as [M – H]^− |
| PG(30:0)    | 693.4733  | 3.7493  | 2.14     | *       | C36H7010P |
| PG(32:2)    | 717.4707  | 0.0000  | 1.93     | (16:1/16:1) and (16:0/16:2) | C38H7010P |
| PG(32:1)    | 719.4867  | 0.5560  | 1.90     | (16:1/16:0) | C38H7210P |
| PG(32:0)    | 721.5020  | 0.0000  | 2.02     | (16:0/16:0) | C38H7410P |
| PG(34:5)    | 739.4550  | 0.0000  | 1.91     | (18:4/16:1) and (16:0/18:5) | C40H6810P |
| PG(34:4)    | 741.4710  | 0.4046  | 1.90     | (18:3/16:1) | C40H7010P |
| PG(34:3)    | 743.4863  | 0.0000  | 1.95     | (16:0/18:3) and (18:2/18:1) | C40H7210P |
| PG(34:2)    | 745.5016  | -0.5366 | 1.93     | (14:0/20:2), (16:1/18:1) and (16:0/18:2) | C40H7410P |
| PG(34:1)    | 747.5179  | 0.4013  | 1.91     | (14:0/20:1), (16:1/18:0) and (18:1/16:0) | C40H7610P |
| PG(36:4)    | 769.5020  | 0.0000  | 1.91     | (20:4/16:0), (18:2/18:2) and (18:3/18:1) | C42H7410P |
| Molecule       | Mass         | Charge | Isotope | Description                                    |
|---------------|--------------|--------|---------|-----------------------------------------------|
| PG(36:3)      | 771.5176     | 0.0000 | 1.98    | (18:2/18:1), (16:1/20:2) and (16:0/20:3) C42H76O10P |
| PG(36:2)      | 773.5333     | 0.0000 | 1.91    | (20:1/16:1), (16:0/20:2) and (18:1/18:1) C42H78O10P |
| PG(38:5)      | 795.5176     | 0.0000 | 1.71    | (20:4/18:1) and (20:0/18:5) C44H76O10P          |
| PG(40:6)      | 821.5357     | 2.9214 | 1.73    | *                                              |
| PG(42:6)      | 849.5670     | 2.8250 | 1.71    | (20:4/22:2), (18:4/24:2), (18:3/24:3) and (20:5/22:1) C48H82O10P |
| PI(28:2)      | 749.4241     | 0.0000 | 2.24    | *                                              |
| PI(28:1)      | 751.4398     | 0.0000 | 2.18    | *                                              |
| PI(34:2)      | 833.5180     | 0.0000 | 2.12    | (18:2/16:0) C43H78O13P                         |
| PI(34:1)      | 835.5337     | 0.0000 | 2.07    | (16:0/18:1) C43H80O13P                         |
| PI(38:10)     | 873.4554     | -0.0092| 1.72    | *                                              |
| PI(38:8)      | 877.4867     | 0.0000 | 1.84    | *                                              |
| PI(42:11)     | 927.5047     | 2.4798 | 2.10    | *                                              |
| PI(42:8)      | 933.5493     | 0.0000 | 1.77    | *                                              |
| DGTS(30:1)    | 682.5620     | -0.2930| 4.34    | *                                              |
| DGTS(32:2)    | 708.5779     | 0.1411 | 4.30    | (18:2/14:0) C42H78O7N                         |
| DGTS(32:1)    | 710.5913     | -3.0960| 4.34    | (16:1/16:0) C42H80O7N                         |
| DGTS(34:5)    | 730.5622     | 0.0000 | 4.38    | *                                              |
| DGTS(34:4)    | 732.5760     | -2.4571| 4.33    | *                                              |
| DGTS(34:3)    | 734.5915     | -2.7226| 4.30    | *                                              |
| DGTS(34:2)    | 736.6100     | 1.2218 | 4.30    | (16:0/18:2) C44H80O7N                         |
| DGTS(34:1)    | 738.6245     | -0.4062| 4.08    | (16:0/18:1) C44H84O7N                         |
| DGTS(36:7)    | 754.5622     | 0.0000 | 4.10    | *                                              |
| DGTS(36:6)    | 756.5769     | -1.1896| 4.10    | *                                              |
| DGTS(36:5)    | 758.5932     | -0.3955| 4.17    | *                                              |
| DGTS(36:4)    | 760.6083     | -1.0518| 4.13    | *                                              |
| DGTS(36:3)    | 762.6241     | -0.8899| 4.32    | (18:1/20:4) C48H84O7N                         |
| DGTA(28:1)    | 654.5309     | 0.0000 | 9.55    | *                                              |
| DGTA(28:0)    | 656.5466     | 0.1523 | 10.29   | *                                              |
| DGTA(30:3)    | 678.5309     | 0.0000 | 9.95    | *                                              |
| DGTA(30:2)    | 680.5444     | -3.0858| 10.29   | *                                              |
| DGTA(30:1)    | 682.5610     | -1.7581| 10.43   | *                                              |
| DGTA(30:0)    | 684.5778     | 0.0000 | 10.29   | *                                              |
| DGTA(32:4)    | 704.5446     | -2.6968| 10.06   | (16:3/16:1) C42H74O7N                         |
| DGTA(32:3)    | 706.5618     | -0.5661| 10.52   | (14:0/18:3) C42H76O7N                         |
| DGTA(32:2)    | 708.5780     | 0.2823 | 10.70   | (16:0/16:2) and (18:2/14:0) C42H78O7N         |
| DGTA(32:1)    | 710.5916     | -2.6738| 10.41   | (16:1/16:0) C42H80O7N                         |
| DGTA(34:6)    | 728.5443     | -3.0197| 10.09   | *                                              |
| DGTA(34:5)    | 730.5622     | 0.0000 | 9.70    | *                                              |
| DGTA(34:4)    | 732.5757     | -2.8666| 9.35    | (20:4/14:0) C44H80O7N                         |
| DGTA(34:3)    | 734.5916     | -2.5865| 9.70    | (16:0/18:3) C44H80O7N                         |
| DGTA (molecular species) | m/z value | Retention time | Mass accuracy | Identified by: |
|-------------------------|-----------|---------------|--------------|---------------|
| DGTA(34:2)              | 736.6071  | -2.7151       | 9.43         | (18:2/16:0) C44H80O7N |
| DGTA(34:1)              | 738.6248  | 0.0000        | 9.70         | (16:0/18:1) C44H84O7N |
| DGTA(36:8)              | 752.5461  | -0.5581       | 9.70         | *             C46H74O7N |
| DGTA(36:7)              | 754.5621  | -0.1325       | 9.70         | **            C46H76O7N |
| DGTA(36:6)              | 756.5762  | -2.1148       | 9.70         | *             C46H78O7N |
| DGTA(36:5)              | 758.5930  | -0.6591       | 9.70         | (18:2/18:3), (20:5/16:0), and (20:4/16:1) C46H80O7N |
| **DGTA(36:4)            | 760.6084  | -0.9203       | 9.29         | (16:0/20:4) C46H82O7N |
| DGTA(36:2)              | 764.6391  | -1.7001       | 9.70         | (20:2/16:0) C46H86O7N |
| DGTA(36:1)              | 766.6561  | 0.0000        | 9.34         | (16:0/20:1) C46H88O7N |
| DGTA(38:8)              | 780.5751  | -3.4590       | 9.29         | *             C48H80O7N |
| DGTA(38:7)              | 782.5914  | -2.6834       | 9.34         | (18:3/20:4) C48H80O7N |
| DGTA(38:6)              | 784.6084  | -0.8922       | 9.29         | (18:2/20:4) C48H82O7N |
| DGTA(38:5)              | 786.6235  | -1.6526       | 9.70         | (20:4/18:1) C48H84O7N |
| DGTA(38:4)              | 788.6402  | -0.2536       | 9.34         | *             C48H86O7N |
| DGTA(40:10)             | 804.5759  | -2.3615       | 9.29         | *             C50H80O7N |
| DGTA(40:9)              | 806.5915  | -2.4796       | 9.70         | (20:4/20:5) C50H80O7N |
| DGTA(40:8)              | 808.6091  | 0.0000        | 9.34         | (20:4/20:4) C50H82O7N |
| DGTA(40:6)              | 812.6392  | -1.4767       | 9.36         | (20:2/20:4) C50H86O7N |
| DGTA(40:5)              | 814.6561  | 0.0000        | 9.34         | (20:1/20:4) C50H88O7N |
| DGTA(42:11)             | 830.5935  | 0.0253        | 9.34         | *             C52H80O7N |
| DGTA(42:9)              | 834.6220  | -3.3296       | 9.29         | *             C52H84O7N |
| DGTA(42:6)              | 840.6731  | 1.6308        | 8.88         | *             C52H90O7N |
| DGTA(42:5)              | 842.6885  | 1.3303        | 8.58         | *             C52H92O7N |

*: Molecular species identified by retention time and mass accuracy;
**: Molecular species identified by retention time, mass accuracy, and polar head product ion;
#: Contribution of sodiated adduct ion
Table S3 List of common and unique lipid species in the lipidome of *B. bifurcata* and *S. muticum*.

| Unique lipid species | Common lipid species | Common lipid species |
|----------------------|----------------------|----------------------|
| Bifurcaria bifurcata | Sargassum muticum    | B. bifurcata | S. muticum |
| MGDG(30:4)           | MGDG(30:0)           | MGDG(30:1)         |
| MGDG(38:10)          | MGDG(32:5)           | MGDG(32:1)         |
| DGDG(36:4)           | MGDG(32:8)           | MGDG(32:2)         |
| DGDG(38:8)           | MGDG(34:5)           | MGDG(32:3)         |
| SQDG(34:0)           | MGDG(34:6)           | MGDG(32:4)         |
| SQDG(38:4)           | MGDG(34:7)           | MGDG(34:1)         |
| SQDG(40:7)           | MGDG(36:1)           | MGDG(34:2)         |
| PE(36:2)             | MGDG(36:9)           | MGDG(34:3)         |
| PE(36:3)             | MGDG(38:4)           | MGDG(34:4)         |
| PG(34:0)             | MGDG(40:6)           | MGDG(36:2)         |
| PG(36:5)             | MGDG(42:9)           | MGDG(36:3)         |
| PI(30:2)             | MGMG(16:0)           | MGDG(36:4)         |
| PI(36:8)             | MGMG(16:1)           | MGDG(36:5)         |
| PI(40:5)             | MGMG(16:3)           | MGDG(36:6)         |
| PI(40:6)             | MGMG(16:4)           | MGDG(36:7)         |
| PI(46:3)             | MGMG(18:1)           | MGDG(36:8)         |
| DGTA(36:3)           | MGMG(18:2)           | MGDG(38:5)         |
| DGTA(40:7)           | MGMG(18:3)           | MGDG(38:6)         |
| DGTA(42:8)           | MGMG(18:4)           | MGDG(38:7)         |
| MGMG(20:4)           | MGMG(20:5)           | MGMG(34:8)         |
| DGDG(34:5)           | MGDG(40:10)          | MGDG(40:8)         |
| DGDG(36:2)           | MGDG(40:9)           | MGDG(40:9)         |
| DGDG(36:3)           | DGDG(28:0)           | DGDG(28:0)         |
| DGDG(36:8)           | DGDG(32:1)           | DGDG(32:1)         |
| SQDG(28:0)           | DGDG(32:2)           | SQDG(30:0)         |
| SQDG(32:4)           | DGDG(34:1)           | SQDG(30:1)         |
| SQDG(36:1)           | DGDG(34:2)           | SQDG(30:2)         |
| SQDG(38:1)           | DGDG(34:3)           | SQDG(30:3)         |
| SQDG(38:2)           | DGDG(34:4)           | SQDG(30:4)         |
| SQDG(40:1)           | DGDG(34:5)           | SQDG(30:5)         |
| SQDG(40:6)           | DGTA(36:3)           | DGTA(36:3)         |
| LPC(16:0)            | DGTA(38:9)           | DGTA(38:9)         |
| LPC(18:0)            | LPC(18:1)            | LPC(18:1)          |
| LPC(34:1)            | SQDG(30:0)           | SQDG(30:1)         |
| PC(36:1)             | SQDG(30:2)           | SQDG(32:0)         |
| PC(36:2)             | SQDG(32:1)           | SQDG(32:1)         |
| PC(36:4)             | SQDG(32:2)           | SQDG(32:2)         |
| PC(36:5)             | SQDG(32:3)           | SQDG(32:3)         |
| PC(38:7)             | SQDG(32:4)           | SQDG(32:4)         |
| PC(40:10)            | SQDG(34:1)           | SQDG(34:1)         |
| LPE(20:4)            | SQDG(34:2)           | SQDG(34:2)         |
| LPE(20:5)            | SQDG(34:3)           | SQDG(34:3)         |
| PE(30:1)             | SQDG(34:4)           | SQDG(34:4)         |
| PE(32:1)             | SQDG(34:5)           | SQDG(34:5)         |
| PE(32:2)             | SQDG(36:2)           | SQDG(36:2)         |
| PE(34:3)             | SQDG(36:3)           | SQDG(36:3)         |
| PE(34:5)             | SQDG(36:4)           | SQDG(36:4)         |
| PE(36:6)             | SQDG(36:5)           | SQDG(36:5)         |
| PE(36:7)             | SQDG(36:6)           | SQDG(36:6)         |
| PE(38:3)             | SQDG(36:7)           | SQDG(36:7)         |
| PE(38:9)             | SQDG(38:0)           | SQDG(38:0)         |
| PE(42:6)             | SQDG(38:5)           | SQDG(38:5)         |
| PE(42:7) | SQDG(38:6) |
|----------|------------|
| PE(44:7) | SQDG(38:7) |
| LPG(16:0) | SQDG(38:8) |
| PG(30:0) | SQDG(38:9) |
| PG(32:0) | SQDG(40:0) |
| PG(32:2) | SQDG(40:8) |
| PG(34:5) | PC(30:3) |
| PG(38:5) | PC(34:2) |
| PG(40:6) | PC(38:6) |
| PG(42:6) | PE(30:3) |
| PI(28:1) | PE(34:1) |
| PI(28:2) | PE(34:2) |
| PI(34:2) | PE(34:4) |
| PI(38:10) | PE(36:4) |
| PI(42:11) | PE(36:5) |
| PI(42:8) | PE(38:4) |
| DGTS(30:1) | PE(38:5) |
| DGTS(34:3) | PE(38:6) |
| DGTS(34:4) | PE(38:7) |
| DGTS(34:5) | PE(38:8) |
| DGTS(36:5) | PE(40:10) |
| DGTS(36:6) | PE(40:4) |
| DGTS(36:7) | PE(40:5) |
| DGTS(38:5) | PE(40:6) |
| DGTA(28:0) | PE(40:7) |
| DGTA(28:1) | PE(40:8) |
| DGTA(30:0) | PE(40:9) |
| DGTA(30:2) | PE(42:11) |
| DGTA(30:3) | PE(42:4) |
| DGTA(34:6) | PE(42:5) |
| DGTA(36:1) | PE(44:4) |
| DGTA(36:8) | PG(32:1) |
| DGTA(38:4) | PG(34:1) |
| DGTA(40:10) | PG(34:2) |
| DGTA(40:5) | PG(34:3) |
| DGTA(42:5) | PG(34:4) |
| DGTA(42:6) | PG(36:2) |
| DGTA(42:9) | PG(36:3) |
| DGTA(32:1) | PG(36:4) |
| DGTA(32:2) | PI(34:1) |
| DGTA(32:3) | PI(38:8) |
| DGTS(32:1) | DGTS(32:2) |
| DGTS(32:2) | DGTS(34:2) |
| DGTS(34:1) | DGTS(34:4) |
| DGTS(36:4) | DGTA(30:1) |
| DGTA(32:1) | DGTA(32:2) |
| DGTA(32:3) | DGTA(32:4) |
| DGTA(34:1) | DGTA(34:2) |
| DGTA(34:3) | DGTA(34:4) |
| DGTA(34:5) | DGTA(34:5) |
| DGTA(36:2) | DGTA(36:4) |
| DGTA(36:5) | DGTA(36:6) |
| DGTA(36:7) | }
DGTA(38:5)
DGTA(38:6)
DGTA(38:7)
DGTA(38:8)
DGTA(40:6)
DGTA(40:8)
DGTA(40:9)
DGTA(42:11)