**Table S1**

Molecular species of lipids in fresh untreated buckwheat

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
| Lipid | m/z | Ion mode | Retention time | Class | Formula | Relative abundance/% | SD |
| Cer(d18:1/16:0+O) | 554.514 | pos | 8.27 | Cer | C34 H68 O4 N1 | 0.04 | 0.01 |
| Cer(d25:0/18:1+O) | 680.655 | pos | 12.74 | Cer | C43 H86 O4 N1 | 0.02 | 0.00 |
| Cer(d38:7) | 582.488 | pos | 8.14 | Cer | C38 H64 O3 N1 | 0.02 | 0.00 |
| Cer(d24:0/16:1) | 622.613 | pos | 12.95 | Cer | C40 H80 O3 N1 | 0.03 | 0.00 |
| Cer(d16:0/18:0) | 540.535 | pos | 9.74 | Cer | C34 H70 O3 N1 | 0.02 | 0.00 |
| Cer(d18:0) | 316.285 | pos | 1.79 | Cer | C18 H38 O3 N1 | 0.03 | 0.01 |
| Cer(d18:1/20:5) | 584.504 | pos | 9.48 | Cer | C38 H66 O3 N1 | 0.02 | 0.00 |
| Cer(d18:1/18:4) | 558.488 | pos | 9.28 | Cer | C36 H64 O3 N1 | 0.03 | 0.01 |
| Cer(d32:0) | 512.504 | pos | 7.97 | Cer | C32 H66 O3 N1 | 0.03 | 0.00 |
| Cer(d18:2/18:1+O) | 578.514 | pos | 7.46 | Cer | C36 H68 O4 N1 | 0.05 | 0.01 |
| Cer(d24:0/18:0+O) | 668.655 | pos | 12.75 | Cer | C42 H86 O4 N1 | 0.04 | 0.01 |
| Cer(d18:2/18:0+O) | 580.530 | pos | 8.58 | Cer | C36 H70 O4 N1 | 0.04 | 0.01 |
| Cer(d18:2/18:2) | 560.504 | pos | 8.14 | Cer | C36 H66 O3 N1 | 0.08 | 0.01 |
| Cer(d24:0/18:1+O) | 666.639 | pos | 12.55 | Cer | C42 H84 O4 N1 | 0.06 | 0.01 |
| Cer(d18:2/16:0) | 536.504 | pos | 9.29 | Cer | C34 H66 O3 N1 | 0.10 | 0.02 |
| Cer(d22:1) | 368.317 | neg | 4.81 | Cer | C22 H42 O3 N1 | 0.04 | 0.01 |
| Cer(d24:2) | 394.333 | neg | 4.91 | Cer | C24 H44 O3 N1 | 0.05 | 0.01 |
| Cer(d20:2) | 338.270 | neg | 3.92 | Cer | C20 H36 O3 N1 | 0.06 | 0.01 |
| Cer(d20:2/2:0) | 366.301 | neg | 4.33 | Cer | C22 H40 O3 N1 | 0.10 | 0.02 |
| CL(71:1) | 723.526 | neg | 8.12 | CL | C80 H152 O17 P2 | 0.02 | 0.00 |
| CL(83:7) | 801.573 | neg | 11.65 | CL | C92 H164 O17 P2 | 0.02 | 0.00 |
| CL(87:9) | 827.588 | neg | 11.65 | CL | C96 H168 O17 P2 | 0.02 | 0.00 |
| CL(18:2/18:1/18:1/24:1) | 768.549 | neg | 9.01 | CL | C87 H158 O17 P2 | 0.03 | 0.01 |
| CL(87:11) | 825.573 | neg | 10.21 | CL | C96 H164 O17 P2 | 0.02 | 0.00 |
| CL(18:2/18:1/18:1/22:4) | 1504.028 | neg | 9.42 | CL | C85 H149 O17 P2 | 0.03 | 0.01 |
| CL(18:2/18:2/18:2/22:4) | 1499.996 | neg | 8.09 | CL | C85 H145 O17 P2 | 0.02 | 0.00 |
| CL(18:2/18:1/18:2/18:2) | 1449.981 | neg | 13.46 | CL | C81 H143 O17 P2 | 0.03 | 0.01 |
| CL(18:2/18:2/18:2/18:2) | 1447.965 | neg | 13.22 | CL | C81 H141 O17 P2 | 0.03 | 0.00 |
| CL(87:13) | 823.557 | neg | 8.71 | CL | C96 H160 O17 P2 | 0.04 | 0.01 |
| DG(56:6) | 893.796 | pos | 13.62 | DG | C59 H105 O5 | 0.03 | 0.00 |
| DG(55:8) | 897.731 | pos | 14.71 | DG | C58 H98 O5 Na1 | 0.03 | 0.00 |
| DG(34:1p) | 601.517 | pos | 7.57 | DG | C37 H70 O4 Na1 | 0.02 | 0.00 |
| DG(58:7) | 919.811 | pos | 13.61 | DG | C61 H107 O5 | 0.04 | 0.01 |
| DG(18:2/18:2) | 639.496 | pos | 10.67 | DG | C39 H68 O5 Na1 | 0.03 | 0.00 |
| DG(38:3) | 664.587 | pos | 11.76 | DG | C41 H78 O5 N1 | 0.02 | 0.00 |
| DG(38:0e) | 661.611 | pos | 15.71 | DG | C41 H82 O4 Na1 | 0.02 | 0.00 |
| DG(38:2p) | 633.582 | pos | 15.36 | DG | C41 H77 O4 | 0.02 | 0.00 |
| DG(16:0/18:1) | 612.556 | pos | 12.09 | DG | C37 H74 O5 N1 | 0.02 | 0.00 |
| DG(36:1e) | 631.564 | pos | 14.96 | DG | C39 H76 O4 Na1 | 0.04 | 0.01 |
| DG(40:8) | 687.496 | pos | 8.38 | DG | C43 H68 O5 Na1 | 0.03 | 0.00 |
| DG(32:0p) | 575.501 | pos | 7.79 | DG | C35 H68 O4 Na1 | 0.07 | 0.01 |
| DG(41:4) | 704.619 | pos | 12.43 | DG | C44 H82 O5 N1 | 0.05 | 0.01 |
| DG(18:1/18:1) | 638.572 | pos | 12.10 | DG | C39 H76 O5 N1 | 0.06 | 0.01 |
| DG(42:10) | 711.496 | pos | 7.35 | DG | C45 H68 O5 Na1 | 0.03 | 0.00 |
| DG(42:8) | 715.527 | pos | 9.74 | DG | C45 H72 O5 Na1 | 0.02 | 0.00 |
| DG(16:0/18:2) | 610.541 | pos | 11.74 | DG | C37 H72 O5 N1 | 0.09 | 0.01 |
| DG(34:0p) | 603.532 | pos | 14.62 | DG | C37 H72 O4 Na1 | 0.14 | 0.02 |
| DG(42:9) | 713.512 | pos | 8.40 | DG | C45 H70 O5 Na1 | 0.07 | 0.01 |
| DGDG(18:1/18:2) | 987.626 | neg | 8.96 | DGDG | C52 H91 O17 | 0.03 | 0.00 |
| DGDG(16:0/18:2) | 961.611 | neg | 8.89 | DGDG | C50 H89 O17 | 0.03 | 0.00 |
| DGDG(18:3/18:3) | 981.579 | neg | 6.27 | DGDG | C52 H85 O17 | 0.02 | 0.00 |
| DGDG(18:2/18:3) | 983.595 | neg | 6.94 | DGDG | C52 H87 O17 | 0.08 | 0.01 |
| DGDG(18:2/18:2) | 985.611 | neg | 7.77 | DGDG | C52 H89 O17 | 0.16 | 0.03 |
| DGMG(18:3) | 721.365 | neg | 1.62 | DGMG | C34 H57 O16 | 0.02 | 0.00 |
| DGMG(18:1) | 725.397 | neg | 3.19 | DGMG | C34 H61 O16 | 0.05 | 0.01 |
| DGMG(18:2) | 723.381 | neg | 2.16 | DGMG | C34 H59 O16 | 0.12 | 0.02 |
| LPA(16:0) | 409.236 | neg | 2.74 | LPA | C19 H38 O7 N0 P1 | 0.03 | 0.00 |
| LPA(18:1) | 435.252 | neg | 3.08 | LPA | C21 H40 O7 N0 P1 | 0.17 | 0.03 |
| LPA(18:2) | 433.236 | neg | 2.16 | LPA | C21 H38 O7 N0 P1 | 0.19 | 0.03 |
| LPC(18:2) | 520.340 | pos | 2.38 | LPC | C26 H51 O7 N1 P1 | 0.19 | 0.03 |
| LPC(18:1) | 522.355 | pos | 3.29 | LPC | C26 H53 O7 N1 P1 | 0.17 | 0.03 |
| LPC(20:2) | 592.362 | neg | 3.60 | LPC | C29 H55 O9 N1 P1 | 0.02 | 0.00 |
| LPE(20:1) | 506.325 | neg | 4.42 | LPE | C25 H49 O7 N1 P1 | 0.03 | 0.00 |
| LPE(20:0) | 508.341 | neg | 5.05 | LPE | C25 H51 O7 N1 P1 | 0.04 | 0.01 |
| LPE(24:0) | 564.403 | neg | 6.83 | LPE | C29 H59 O7 N1 P1 | 0.02 | 0.00 |
| MGDG(34:2) | 753.552 | neg | 9.67 | MGDG | C43 H77 O10 | 0.02 | 0.00 |
| MGDG(16:0/18:1) | 801.573 | neg | 11.64 | MGDG | C44 H81 O12 | 0.02 | 0.00 |
| MGDG(18:1/18:1) | 827.589 | neg | 11.65 | MGDG | C46 H83 O12 | 0.02 | 0.00 |
| MGDG(18:1/18:2) | 825.573 | neg | 10.21 | MGDG | C46 H81 O12 | 0.02 | 0.00 |
| MGDG(18:2/18:2) | 823.558 | neg | 8.71 | MGDG | C46 H79 O12 | 0.04 | 0.01 |
| MGDG(47:12) | 961.605 | neg | 5.70 | MGDG | C57 H85 O12 | 0.17 | 0.03 |
| MGMG(18:2) | 561.328 | neg | 2.99 | MGMG | C28 H49 O11 | 0.10 | 0.02 |
| PA(16:0/18:1) | 673.481 | neg | 9.90 | PA | C37 H70 O8 N0 P1 | 0.35 | 0.06 |
| PA(16:0/18:2) | 671.466 | neg | 8.52 | PA | C37 H68 O8 N0 P1 | 0.34 | 0.06 |
| PA(18:1/18:1) | 699.497 | neg | 9.99 | PA | C39 H72 O8 N0 P1 | 0.79 | 0.13 |
| PA(18:2/18:2) | 695.466 | neg | 7.50 | PA | C39 H68 O8 N0 P1 | 0.67 | 0.11 |
| PA(18:1/18:2) | 697.481 | neg | 8.56 | PA | C39 H70 O8 N0 P1 | 1.04 | 0.17 |
| PC(18:3/18:2) | 802.536 | pos | 6.96 | PC | C44 H78 O8 N1 P1 Na1 | 0.03 | 0.00 |
| PC(33:2) | 744.554 | pos | 8.14 | PC | C41 H79 O8 N1 P1 | 0.03 | 0.00 |
| PC(33:1) | 746.569 | pos | 9.45 | PC | C41 H81 O8 N1 P1 | 0.03 | 0.00 |
| PC(26:1/8:0) | 760.585 | pos | 11.61 | PC | C42 H83 O8 N1 P1 | 0.03 | 0.00 |
| PC(15:1/18:1) | 744.554 | pos | 8.50 | PC | C41 H79 O8 N1 P1 | 0.02 | 0.00 |
| PC(34:3) | 756.554 | pos | 7.58 | PC | C42 H79 O8 N1 P1 | 0.13 | 0.02 |
| PC(32:1) | 732.554 | pos | 8.60 | PC | C40 H79 O8 N1 P1 | 0.06 | 0.01 |
| PC(38:3) | 812.616 | pos | 10.88 | PC | C46 H87 O8 N1 P1 | 0.11 | 0.02 |
| PC(36:1) | 788.616 | pos | 11.81 | PC | C44 H87 O8 N1 P1 | 0.10 | 0.02 |
| PC(38:2) | 814.632 | pos | 11.79 | PC | C46 H89 O8 N1 P1 | 0.12 | 0.02 |
| PC(36:5) | 780.554 | pos | 6.96 | PC | C44 H79 O8 N1 P1 | 0.24 | 0.04 |
| PC(16:0/18:1) | 782.567 | pos | 10.47 | PC | C42 H82 O8 N1 P1 Na1 | 0.10 | 0.02 |
| PC(32:2) | 730.538 | pos | 7.45 | PC | C40 H77 O8 N1 P1 | 0.03 | 0.01 |
| PC(16:0/18:2) | 780.551 | pos | 8.90 | PC | C42 H80 O8 N1 P1 Na1 | 0.12 | 0.02 |
| PC(18:2/18:2) | 804.551 | pos | 7.78 | PC | C44 H80 O8 N1 P1 Na1 | 0.18 | 0.03 |
| PC(18:1/18:2) | 806.567 | pos | 9.02 | PC | C44 H82 O8 N1 P1 Na1 | 0.24 | 0.04 |
| PC(18:1/18:1) | 808.583 | pos | 10.61 | PC | C44 H84 O8 N1 P1 Na1 | 0.28 | 0.05 |
| PC(34:1) | 760.585 | pos | 10.49 | PC | C42 H83 O8 N1 P1 | 2.54 | 0.42 |
| PC(16:1/18:1) | 758.569 | pos | 8.41 | PC | C42 H81 O8 N1 P1 | 0.77 | 0.13 |
| PC(34:2) | 758.569 | pos | 8.91 | PC | C42 H81 O8 N1 P1 | 3.64 | 0.60 |
| PC(36:4) | 782.569 | pos | 7.79 | PC | C44 H81 O8 N1 P1 | 6.50 | 1.07 |
| PC(36:2) | 786.601 | pos | 10.58 | PC | C44 H85 O8 N1 P1 | 7.75 | 1.28 |
| PC(36:3) | 784.585 | pos | 8.99 | PC | C44 H83 O8 N1 P1 | 11.18 | 1.85 |
| PC(22:0/18:2) | 886.654 | neg | 12.26 | PC | C49 H93 O10 N1 P1 | 0.02 | 0.00 |
| PC(17:1/18:1) | 816.576 | neg | 9.58 | PC | C44 H83 O10 N1 P1 | 0.02 | 0.00 |
| PC(18:1/14:0) | 776.545 | neg | 8.61 | PC | C41 H79 O10 N1 P1 | 0.03 | 0.01 |
| PE(34:3) | 714.507 | pos | 7.48 | PE | C39 H73 O8 N1 P1 | 0.03 | 0.00 |
| PE(34:2) | 716.522 | pos | 8.59 | PE | C39 H75 O8 N1 P1 | 0.03 | 0.01 |
| PE(16:1/18:1) | 716.522 | pos | 8.87 | PE | C39 H75 O8 N1 P1 | 0.02 | 0.00 |
| PE(18:3/18:2) | 738.507 | pos | 7.18 | PE | C41 H73 O8 N1 P1 | 0.02 | 0.00 |
| PE(22:0/18:2) | 800.616 | pos | 12.32 | PE | C45 H87 O8 N1 P1 | 0.02 | 0.00 |
| PE(47:11) | 880.585 | pos | 7.50 | PE | C52 H83 O8 N1 P1 | 0.03 | 0.01 |
| PE(34:1) | 740.520 | pos | 10.98 | PE | C39 H76 O8 N1 P1 Na1 | 0.03 | 0.01 |
| PE(36:0) | 748.585 | pos | 10.57 | PE | C41 H83 O8 N1 P1 | 0.02 | 0.00 |
| PE(38:0) | 776.616 | pos | 11.79 | PE | C43 H87 O8 N1 P1 | 0.04 | 0.01 |
| PE(36:3) | 764.520 | pos | 9.39 | PE | C41 H76 O8 N1 P1 Na1 | 0.05 | 0.01 |
| PE(39:1) | 788.616 | pos | 8.31 | PE | C44 H87 O8 N1 P1 | 0.07 | 0.01 |
| PE(44:2p) | 840.684 | pos | 12.85 | PE | C49 H95 O7 N1 P1 | 0.12 | 0.02 |
| PE(39:0) | 790.632 | pos | 9.68 | PE | C44 H89 O8 N1 P1 | 0.06 | 0.01 |
| PE(41:3) | 812.616 | pos | 7.34 | PE | C46 H87 O8 N1 P1 | 0.12 | 0.02 |
| PE(41:1) | 816.648 | pos | 9.77 | PE | C46 H91 O8 N1 P1 | 0.15 | 0.02 |
| PE(41:2) | 814.632 | pos | 8.41 | PE | C46 H89 O8 N1 P1 | 0.18 | 0.03 |
| PE(33:0) | 706.538 | pos | 9.66 | PE | C38 H77 O8 N1 P1 | 0.14 | 0.02 |
| PE(35:0) | 734.569 | pos | 9.68 | PE | C40 H81 O8 N1 P1 | 0.19 | 0.03 |
| PE(33:1) | 704.522 | pos | 8.33 | PE | C38 H75 O8 N1 P1 | 0.35 | 0.06 |
| PE(37:3) | 756.554 | pos | 7.40 | PE | C42 H79 O8 N1 P1 | 0.38 | 0.06 |
| PE(37:1) | 760.585 | pos | 9.77 | PE | C42 H83 O8 N1 P1 | 0.45 | 0.07 |
| PE(35:3) | 728.522 | pos | 7.35 | PE | C40 H75 O8 N1 P1 | 0.41 | 0.07 |
| PE(35:1) | 732.554 | pos | 9.75 | PE | C40 H79 O8 N1 P1 | 0.42 | 0.07 |
| PE(37:2) | 758.569 | pos | 8.41 | PE | C42 H81 O8 N1 P1 | 0.77 | 0.13 |
| PE(35:2) | 730.538 | pos | 8.39 | PE | C40 H77 O8 N1 P1 | 1.13 | 0.19 |
| PG(46:0) | 919.736 | pos | 13.04 | PG | C52 H104 O10 N0 P1 | 0.03 | 0.01 |
| PG(42:1) | 861.658 | pos | 12.76 | PG | C48 H94 O10 N0 P1 | 0.03 | 0.00 |
| PG(42:0) | 863.674 | pos | 13.06 | PG | C48 H96 O10 N0 P1 | 0.03 | 0.00 |
| PG(16:0/18:1) | 766.559 | pos | 8.95 | PG | C40 H81 O10 N1 P1 | 0.09 | 0.01 |
| PG(37:2) | 787.549 | neg | 4.59 | PG | C43 H80 O10 N0 P1 | 0.04 | 0.01 |
| PG(18:0/18:2) | 773.534 | neg | 9.30 | PG | C42 H78 O10 N0 P1 | 0.02 | 0.00 |
| PG(36:7) | 763.456 | neg | 7.53 | PG | C42 H68 O10 N0 P1 | 0.06 | 0.01 |
| PG(33:0) | 735.518 | neg | 4.58 | PG | C39 H76 O10 N0 P1 | 0.38 | 0.06 |
| PG(35:1) | 761.534 | neg | 4.58 | PG | C41 H78 O10 N0 P1 | 0.20 | 0.03 |
| PG(36:6) | 765.471 | neg | 8.54 | PG | C42 H70 O10 N0 P1 | 0.16 | 0.03 |
| PI(18:2/18:2) | 876.560 | pos | 6.70 | PI | C45 H83 O13 N1 P1 | 0.02 | 0.00 |
| PI(16:0/18:2) | 852.560 | pos | 7.49 | PI | C43 H83 O13 N1 P1 | 0.18 | 0.03 |
| PI(16:0/18:1) | 854.575 | pos | 8.61 | PI | C43 H85 O13 N1 P1 | 0.16 | 0.03 |
| PI(52:6) | 1077.738 | neg | 12.74 | PI | C61 H106 O13 N0 P1 | 0.02 | 0.00 |
| PI(15:0/18:1) | 821.519 | neg | 7.87 | PI | C42 H78 O13 N0 P1 | 0.02 | 0.00 |
| PI(15:0/18:2) | 819.503 | neg | 6.93 | PI | C42 H76 O13 N0 P1 | 0.02 | 0.00 |
| PI(18:1/18:1) | 861.550 | neg | 8.70 | PI | C45 H82 O13 N0 P1 | 0.77 | 0.13 |
| PIP(54:5) | 1187.751 | neg | 12.08 | PIP | C63 H113 O16 N0 P2 | 0.03 | 0.00 |
| PIP(54:6) | 1185.735 | neg | 11.83 | PIP | C63 H111 O16 N0 P2 | 0.03 | 0.00 |
| PIP(42:8p) | 997.521 | neg | 8.70 | PIP | C51 H83 O15 N0 P2 | 0.05 | 0.01 |
| PIP(42:9p) | 995.506 | neg | 7.57 | PIP | C51 H81 O15 N0 P2 | 0.06 | 0.01 |
| PIP(40:8p) | 969.490 | neg | 7.49 | PIP | C49 H79 O15 N0 P2 | 0.16 | 0.03 |
| PIP(40:7p) | 971.506 | neg | 8.59 | PIP | C49 H81 O15 N0 P2 | 0.16 | 0.03 |
| PIP3(18:1/24:6) | 1175.465 | neg | 8.64 | PIP3 | C51 H87 O22 N0 P4 | 0.02 | 0.00 |
| PS(33:4/14:1) | 958.651 | pos | 7.76 | PS | C53 H94 O10 N1 P1 Na1 | 0.07 | 0.01 |
| PS(38:4) | 810.529 | neg | 7.71 | PS | C44 H77 O10 N1 P1 | 0.03 | 0.01 |
| PS(34:1p) | 744.518 | neg | 10.63 | PS | C40 H75 O9 N1 P1 | 0.02 | 0.00 |
| PS(38:6) | 806.498 | neg | 6.19 | PS | C44 H73 O10 N1 P1 | 0.04 | 0.01 |
| PS(38:1) | 816.576 | neg | 9.58 | PS | C44 H83 O10 N1 P1 | 0.03 | 0.00 |
| PS(38:7) | 804.482 | neg | 7.18 | PS | C44 H71 O10 N1 P1 | 0.02 | 0.00 |
| PS(41:2) | 856.607 | neg | 10.88 | PS | C47 H87 O10 N1 P1 | 0.15 | 0.02 |
| PS(36:3) | 784.513 | neg | 11.00 | PS | C42 H75 O10 N1 P1 | 0.28 | 0.05 |
| PS(39:4) | 824.545 | neg | 6.97 | PS | C45 H79 O10 N1 P1 | 0.26 | 0.04 |
| PS(39:3) | 826.560 | neg | 7.82 | PS | C45 H81 O10 N1 P1 | 3.75 | 0.62 |
| PS(39:1) | 830.592 | neg | 10.59 | PS | C45 H85 O10 N1 P1 | 7.64 | 1.26 |
| So(d22:0) | 358.368 | pos | 4.29 | So | C22 H48 O2 N1 | 0.03 | 0.01 |
| So(d20:0) | 330.337 | pos | 3.23 | So | C20 H44 O2 N1 | 0.05 | 0.01 |
| So(d16:1) | 272.258 | pos | 1.47 | So | C16 H34 O2 N1 | 0.04 | 0.01 |
| So(d14:0) | 246.243 | pos | 0.85 | So | C14 H32 O2 N1 | 0.07 | 0.01 |
| So(d16:0) | 274.274 | pos | 1.20 | So | C16 H36 O2 N1 | 7.76 | 1.28 |
| SQDG(41:6) | 953.567 | neg | 2.35 | SQDG | C51 H85 O14 S1 | 0.02 | 0.00 |
| SQDG(40:2) | 947.614 | neg | 2.98 | SQDG | C50 H91 O14 S1 | 0.03 | 0.00 |
| SQDG(44:4) | 999.645 | neg | 3.30 | SQDG | C54 H95 O14 S1 | 0.10 | 0.02 |
| SQDG(44:6) | 995.614 | neg | 2.37 | SQDG | C54 H91 O14 S1 | 0.12 | 0.02 |
| SQDG(18:2/18:2) | 841.514 | neg | 6.59 | SQDG | C45 H77 O12 S1 | 0.03 | 0.00 |
| SQDG(40:7) | 937.535 | neg | 11.03 | SQDG | C50 H81 O14 S1 | 0.02 | 0.00 |
| SQDG(16:0/18:2) | 817.514 | neg | 7.33 | SQDG | C43 H77 O12 S1 | 0.04 | 0.01 |
| TG(20:1/9:0/9:0) | 682.598 | pos | 9.39 | TG | C41 H80 O6 N1 | 0.02 | 0.00 |
| TG(15:0/18:2/18:3) | 861.694 | pos | 13.53 | TG | C54 H94 O6 Na1 | 0.02 | 0.00 |
| TG(54:9p) | 879.684 | pos | 13.81 | TG | C57 H92 O5 Na1 | 0.02 | 0.00 |
| TG(63:15) | 1004.770 | pos | 12.41 | TG | C66 H102 O6 N1 | 0.02 | 0.00 |
| TG(57:5) | 940.833 | pos | 14.13 | TG | C60 H110 O6 N1 | 0.02 | 0.00 |
| TG(24:0/18:2/18:3) | 987.835 | pos | 15.13 | TG | C63 H112 O6 Na1 | 0.02 | 0.00 |
| TG(16:0/14:0/18:1) | 822.755 | pos | 14.28 | TG | C51 H100 O6 N1 | 0.02 | 0.00 |
| TG(18:3/18:2/23:0) | 968.864 | pos | 14.93 | TG | C62 H114 O6 N1 | 0.02 | 0.00 |
| TG(14:0/18:2/18:2) | 849.694 | pos | 13.63 | TG | C53 H94 O6 Na1 | 0.02 | 0.00 |
| TG(57:9e) | 923.746 | pos | 14.57 | TG | C60 H100 O5 Na1 | 0.02 | 0.00 |
| TG(18:0/17:0/18:1) | 892.833 | pos | 15.21 | TG | C56 H110 O6 N1 | 0.02 | 0.00 |
| TG(57:10p) | 919.715 | pos | 13.93 | TG | C60 H96 O5 Na1 | 0.02 | 0.00 |
| TG(4:0/16:2/18:2) | 676.551 | pos | 11.63 | TG | C41 H74 O6 N1 | 0.02 | 0.00 |
| TG(18:0/18:1/24:0) | 990.942 | pos | 16.42 | TG | C63 H124 O6 N1 | 0.02 | 0.00 |
| TG(4:0/18:2/18:2) | 687.556 | pos | 8.28 | TG | C43 H75 O6 | 0.02 | 0.00 |
| TG(37:0p) | 654.603 | pos | 12.05 | TG | C40 H80 O5 N1 | 0.02 | 0.00 |
| TG(18:2/18:2/23:0) | 975.835 | pos | 15.23 | TG | C62 H112 O6 Na1 | 0.03 | 0.00 |
| TG(55:10p) | 891.684 | pos | 13.72 | TG | C58 H92 O5 Na1 | 0.03 | 0.01 |
| TG(18:1/18:2/23:0) | 977.851 | pos | 15.56 | TG | C62 H114 O6 Na1 | 0.03 | 0.00 |
| TG(20:1/18:1/24:0) | 1016.958 | pos | 16.39 | TG | C65 H126 O6 N1 | 0.03 | 0.01 |
| TG(22:0/18:3/18:3) | 952.833 | pos | 14.36 | TG | C61 H110 O6 N1 | 0.03 | 0.00 |
| TG(16:0/18:1/21:0) | 920.864 | pos | 15.56 | TG | C58 H114 O6 N1 | 0.03 | 0.01 |
| TG(18:1/18:2/20:5) | 920.770 | pos | 13.11 | TG | C59 H102 O6 N1 | 0.03 | 0.01 |
| TG(18:1/18:2/22:4) | 933.791 | pos | 14.59 | TG | C61 H105 O6 | 0.04 | 0.01 |
| TG(19:1/18:3/21:1) | 954.848 | pos | 14.27 | TG | C61 H112 O6 N1 | 0.05 | 0.01 |
| TG(18:3/18:3/18:3) | 873.697 | pos | 13.43 | TG | C57 H93 O6 | 0.04 | 0.01 |
| TG(24:1/18:2/18:2) | 982.880 | pos | 14.93 | TG | C63 H116 O6 N1 | 0.07 | 0.01 |
| TG(19:1/18:1/18:3) | 912.801 | pos | 13.81 | TG | C58 H106 O6 N1 | 0.04 | 0.01 |
| TG(18:1/18:2/21:1) | 942.848 | pos | 14.46 | TG | C60 H112 O6 N1 | 0.03 | 0.01 |
| TG(55:9p) | 893.699 | pos | 14.05 | TG | C58 H94 O5 Na1 | 0.05 | 0.01 |
| TG(18:1/17:1/18:2) | 891.741 | pos | 14.17 | TG | C56 H100 O6 Na1 | 0.04 | 0.01 |
| TG(25:0/13:1/23:0) | 1004.958 | pos | 15.36 | TG | C64 H126 O6 N1 | 0.02 | 0.00 |
| TG(16:0/18:1/23:0) | 948.895 | pos | 15.91 | TG | C60 H118 O6 N1 | 0.05 | 0.01 |
| TG(18:1/14:0/18:2) | 846.755 | pos | 13.63 | TG | C53 H100 O6 N1 | 0.05 | 0.01 |
| TG(16:0/16:0/18:2) | 853.726 | pos | 14.36 | TG | C53 H98 O6 Na1 | 0.05 | 0.01 |
| TG(26:0/18:2/18:2) | 1012.927 | pos | 15.76 | TG | C65 H122 O6 N1 | 0.06 | 0.01 |
| TG(14:0/18:2/18:3) | 842.723 | pos | 13.35 | TG | C53 H96 O6 N1 | 0.05 | 0.01 |
| TG(61:2) | 1002.942 | pos | 15.89 | TG | C64 H124 O6 N1 | 0.05 | 0.01 |
| TG(15:0/18:2/18:2) | 863.710 | pos | 13.81 | TG | C54 H96 O6 Na1 | 0.05 | 0.01 |
| TG(59:7) | 964.833 | pos | 13.38 | TG | C62 H110 O6 N1 | 0.06 | 0.01 |
| TG(15:0/18:1/18:2) | 865.726 | pos | 14.14 | TG | C54 H98 O6 Na1 | 0.05 | 0.01 |
| TG(18:3/18:2/20:2) | 922.786 | pos | 13.72 | TG | C59 H104 O6 N1 | 0.06 | 0.01 |
| TG(19:0/19:0/23:4) | 998.911 | pos | 15.23 | TG | C64 H120 O6 N1 | 0.06 | 0.01 |
| TG(18:1/18:1/21:1) | 944.864 | pos | 14.86 | TG | C60 H114 O6 N1 | 0.06 | 0.01 |
| TG(16:0/14:0/18:2) | 820.739 | pos | 13.95 | TG | C51 H98 O6 N1 | 0.06 | 0.01 |
| TG(15:0/16:0/18:1) | 836.770 | pos | 14.48 | TG | C52 H102 O6 N1 | 0.07 | 0.01 |
| TG(6:0/14:1/18:2) | 678.567 | pos | 12.01 | TG | C41 H76 O6 N1 | 0.05 | 0.01 |
| TG(18:1/20:4/24:0) | 993.884 | pos | 16.05 | TG | C65 H117 O6 | 0.07 | 0.01 |
| TG(25:1/18:1/18:1) | 1000.927 | pos | 15.56 | TG | C64 H122 O6 N1 | 0.07 | 0.01 |
| TG(6:0/14:1/18:1) | 680.582 | pos | 12.32 | TG | C41 H78 O6 N1 | 0.06 | 0.01 |
| TG(66:2) | 1073.021 | pos | 16.05 | TG | C69 H134 O6 N1 | 0.08 | 0.01 |
| TG(16:0/18:2/21:0) | 918.848 | pos | 15.22 | TG | C58 H112 O6 N1 | 0.11 | 0.02 |
| TG(41:0p) | 710.666 | pos | 12.77 | TG | C44 H88 O5 N1 | 0.10 | 0.02 |
| TG(18:3/18:2/18:2) | 899.710 | pos | 13.38 | TG | C57 H96 O6 Na1 | 0.11 | 0.02 |
| TG(26:0/18:1/18:2) | 1014.942 | pos | 16.07 | TG | C65 H124 O6 N1 | 0.10 | 0.02 |
| TG(18:1/18:1/20:4) | 907.775 | pos | 14.58 | TG | C59 H103 O6 | 0.11 | 0.02 |
| TG(18:1/18:1/24:1) | 986.911 | pos | 15.37 | TG | C63 H120 O6 N1 | 0.63 | 0.10 |
| TG(18:0/17:2/18:2) | 886.786 | pos | 13.81 | TG | C56 H104 O6 N1 | 0.14 | 0.02 |
| TG(18:2/18:2/21:0) | 942.848 | pos | 14.87 | TG | C60 H112 O6 N1 | 0.15 | 0.02 |
| TG(18:1/18:2/20:4) | 905.759 | pos | 14.25 | TG | C59 H101 O6 | 0.11 | 0.02 |
| TG(18:1/18:1/23:0) | 974.911 | pos | 15.89 | TG | C62 H120 O6 N1 | 0.15 | 0.02 |
| TG(22:1/18:2/18:2) | 954.848 | pos | 14.64 | TG | C61 H112 O6 N1 | 0.15 | 0.02 |
| TG(18:1/18:2/22:1) | 956.864 | pos | 14.60 | TG | C61 H114 O6 N1 | 0.13 | 0.02 |
| TG(19:1/18:1/18:1) | 916.833 | pos | 14.81 | TG | C58 H110 O6 N1 | 0.15 | 0.03 |
| TG(18:1/18:1/21:0) | 946.880 | pos | 15.56 | TG | C60 H116 O6 N1 | 0.18 | 0.03 |
| TG(59:3) | 972.895 | pos | 14.58 | TG | C62 H118 O6 N1 | 0.12 | 0.02 |
| TG(25:1/18:2/19:0) | 1014.942 | pos | 15.73 | TG | C65 H124 O6 N1 | 0.19 | 0.03 |
| TG(62:2) | 1016.958 | pos | 16.05 | TG | C65 H126 O6 N1 | 0.17 | 0.03 |
| TG(16:1/18:2/18:3) | 868.739 | pos | 13.42 | TG | C55 H98 O6 N1 | 0.23 | 0.04 |
| TG(20:5/18:2/18:2) | 901.728 | pos | 13.66 | TG | C59 H97 O6 | 0.26 | 0.04 |
| TG(19:1/16:0/18:1) | 890.817 | pos | 14.82 | TG | C56 H108 O6 N1 | 0.24 | 0.04 |
| TG(17:4/17:3/22:0) | 922.786 | pos | 13.38 | TG | C59 H104 O6 N1 | 0.29 | 0.05 |
| TG(15:0/18:1/18:1) | 862.786 | pos | 14.47 | TG | C54 H104 O6 N1 | 0.31 | 0.05 |
| TG(18:1/18:2/24:1) | 984.895 | pos | 15.07 | TG | C63 H118 O6 N1 | 0.38 | 0.06 |
| TG(16:0/18:1/24:0) | 962.911 | pos | 16.08 | TG | C61 H120 O6 N1 | 0.36 | 0.06 |
| TG(18:1/17:1/18:1) | 888.801 | pos | 14.45 | TG | C56 H106 O6 N1 | 0.39 | 0.06 |
| TG(20:1/18:2/18:3) | 924.801 | pos | 14.02 | TG | C59 H106 O6 N1 | 0.44 | 0.07 |
| TG(16:0/18:1/22:0) | 934.880 | pos | 15.74 | TG | C59 H116 O6 N1 | 0.53 | 0.09 |
| TG(18:0/16:0/18:1) | 878.817 | pos | 15.03 | TG | C55 H108 O6 N1 | 0.62 | 0.10 |
| TG(20:1/18:1/18:1) | 930.848 | pos | 14.59 | TG | C59 H112 O6 N1 | 0.98 | 0.16 |
| TG(18:1/18:1/24:0) | 988.927 | pos | 16.05 | TG | C63 H122 O6 N1 | 0.89 | 0.15 |
| TG(18:1/18:3/24:0) | 984.895 | pos | 15.41 | TG | C63 H118 O6 N1 | 1.29 | 0.21 |
| TG(18:1/18:2/24:0) | 986.911 | pos | 15.73 | TG | C63 H120 O6 N1 | 1.30 | 0.21 |
| TG(20:1/18:2/18:2) | 926.817 | pos | 14.30 | TG | C59 H108 O6 N1 | 1.26 | 0.21 |
| TG(16:0/16:0/18:1) | 850.786 | pos | 14.67 | TG | C53 H104 O6 N1 | 1.50 | 0.25 |
| TG(22:0/18:2/18:2) | 956.864 | pos | 15.04 | TG | C61 H114 O6 N1 | 2.23 | 0.37 |
| TG(18:1/18:1/22:0) | 960.895 | pos | 15.71 | TG | C61 H118 O6 N1 | 2.00 | 0.33 |
| TG(20:0/18:2/18:2) | 928.833 | pos | 14.62 | TG | C59 H110 O6 N1 | 2.11 | 0.35 |
| TG(18:1/18:2/22:0) | 958.880 | pos | 15.38 | TG | C61 H116 O6 N1 | 2.64 | 0.44 |
| TG(20:0/18:1/18:1) | 932.864 | pos | 15.36 | TG | C59 H114 O6 N1 | 2.55 | 0.42 |

**Table S2**

Molecular species of lipids in fresh SS-treated buckwheat

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
| Lipid | m/z | Ion mode | Retention time | Class | Formula | Relative abundance/% | SD |
| Cer(d38:3) | 590.551 | pos | 11.83 | Cer | C38 H72 O3 N1 | 0.05 | 0.01 |
| Cer(d20:2/18:2) | 588.535 | pos | 11.03 | Cer | C38 H70 O3 N1 | 0.05 | 0.01 |
| Cer(d18:1/16:0+O) | 554.514 | pos | 8.27 | Cer | C34 H68 O4 N1 | 0.08 | 0.01 |
| Cer(d16:0/18:0) | 540.535 | pos | 9.74 | Cer | C34 H70 O3 N1 | 0.02 | 0.00 |
| Cer(d18:0) | 316.285 | pos | 1.79 | Cer | C18 H38 O3 N1 | 0.07 | 0.01 |
| Cer(d18:1/20:5) | 584.504 | pos | 9.48 | Cer | C38 H66 O3 N1 | 0.02 | 0.00 |
| Cer(d32:0) | 512.504 | pos | 7.97 | Cer | C32 H66 O3 N1 | 0.04 | 0.00 |
| Cer(d18:2/18:1+O) | 578.514 | pos | 7.46 | Cer | C36 H68 O4 N1 | 0.06 | 0.01 |
| Cer(d18:2/18:0+O) | 580.530 | pos | 8.58 | Cer | C36 H70 O4 N1 | 0.08 | 0.01 |
| Cer(d18:2/18:2) | 560.504 | pos | 8.14 | Cer | C36 H66 O3 N1 | 0.06 | 0.01 |
| Cer(d24:0/18:1+O) | 666.639 | pos | 12.55 | Cer | C42 H84 O4 N1 | 0.03 | 0.00 |
| Cer(d18:2/16:0) | 536.504 | pos | 9.29 | Cer | C34 H66 O3 N1 | 0.05 | 0.01 |
| Cer(d22:1) | 368.317 | neg | 4.81 | Cer | C22 H42 O3 N1 | 0.06 | 0.01 |
| Cer(d24:2) | 394.333 | neg | 4.91 | Cer | C24 H44 O3 N1 | 0.08 | 0.01 |
| Cer(d20:2) | 338.270 | neg | 3.92 | Cer | C20 H36 O3 N1 | 0.09 | 0.01 |
| Cer(d20:2/2:0) | 366.301 | neg | 4.33 | Cer | C22 H40 O3 N1 | 0.14 | 0.02 |
| CL(71:1) | 723.526 | neg | 8.12 | CL | C80 H152 O17 P2 | 0.03 | 0.00 |
| CL(18:2/18:1/18:1/18:2) | 1451.996 | neg | 13.72 | CL | C81 H145 O17 P2 | 0.02 | 0.00 |
| CL(83:7) | 801.573 | neg | 11.65 | CL | C92 H164 O17 P2 | 0.03 | 0.00 |
| CL(87:9) | 827.588 | neg | 11.65 | CL | C96 H168 O17 P2 | 0.03 | 0.00 |
| CL(83:15) | 793.510 | neg | 8.24 | CL | C92 H148 O17 P2 | 0.02 | 0.00 |
| CL(18:2/18:1/18:1/24:1) | 768.549 | neg | 9.01 | CL | C87 H158 O17 P2 | 0.05 | 0.01 |
| CL(87:11) | 825.573 | neg | 10.21 | CL | C96 H164 O17 P2 | 0.03 | 0.00 |
| CL(18:2/18:1/18:1/22:4) | 1504.028 | neg | 9.42 | CL | C85 H149 O17 P2 | 0.05 | 0.01 |
| CL(18:2/18:2/18:2/22:4) | 1499.996 | neg | 8.09 | CL | C85 H145 O17 P2 | 0.03 | 0.00 |
| CL(18:2/18:1/18:2/18:2) | 1449.981 | neg | 13.46 | CL | C81 H143 O17 P2 | 0.05 | 0.01 |
| CL(18:2/18:2/18:2/18:2) | 1447.965 | neg | 13.22 | CL | C81 H141 O17 P2 | 0.04 | 0.01 |
| CL(87:13) | 823.557 | neg | 8.71 | CL | C96 H160 O17 P2 | 0.06 | 0.01 |
| DG(18:1/18:2) | 619.530 | pos | 9.38 | DG | C39 H71 O5 | 0.02 | 0.00 |
| DG(18:3/18:2) | 615.498 | pos | 7.21 | DG | C39 H67 O5 | 0.02 | 0.00 |
| DG(58:6) | 921.827 | pos | 13.93 | DG | C61 H109 O5 | 0.26 | 0.04 |
| DG(60:6) | 949.858 | pos | 14.28 | DG | C63 H113 O5 | 0.14 | 0.02 |
| DG(56:3) | 921.825 | pos | 13.93 | DG | C59 H110 O5 Na1 | 0.28 | 0.04 |
| DG(58:3) | 949.856 | pos | 14.28 | DG | C61 H114 O5 Na1 | 0.14 | 0.02 |
| DG(20:1/18:1) | 666.603 | pos | 12.45 | DG | C41 H80 O5 N1 | 0.05 | 0.01 |
| DG(24:0/18:2) | 722.666 | pos | 13.22 | DG | C45 H88 O5 N1 | 0.03 | 0.00 |
| DG(22:0/18:2) | 694.634 | pos | 12.87 | DG | C43 H84 O5 N1 | 0.04 | 0.01 |
| DG(34:1e) | 603.532 | pos | 12.10 | DG | C37 H72 O4 Na1 | 0.24 | 0.03 |
| DG(20:1/18:2) | 664.587 | pos | 12.14 | DG | C41 H78 O5 N1 | 0.15 | 0.02 |
| DG(38:2) | 666.603 | pos | 12.11 | DG | C41 H80 O5 N1 | 0.04 | 0.00 |
| DG(56:6) | 893.796 | pos | 13.62 | DG | C59 H105 O5 | 1.17 | 0.16 |
| DG(40:0e) | 689.642 | pos | 16.06 | DG | C43 H86 O4 Na1 | 0.02 | 0.00 |
| DG(58:7) | 919.811 | pos | 13.61 | DG | C61 H107 O5 | 2.01 | 0.27 |
| DG(18:2/18:2) | 639.496 | pos | 10.67 | DG | C39 H68 O5 Na1 | 0.93 | 0.12 |
| DG(38:3) | 664.587 | pos | 11.76 | DG | C41 H78 O5 N1 | 0.07 | 0.01 |
| DG(38:0e) | 661.611 | pos | 15.71 | DG | C41 H82 O4 Na1 | 0.03 | 0.00 |
| DG(38:2p) | 633.582 | pos | 15.36 | DG | C41 H77 O4 | 0.03 | 0.00 |
| DG(16:0/18:1) | 612.556 | pos | 12.09 | DG | C37 H74 O5 N1 | 0.27 | 0.04 |
| DG(36:1e) | 631.564 | pos | 14.96 | DG | C39 H76 O4 Na1 | 0.06 | 0.01 |
| DG(41:4) | 704.619 | pos | 12.43 | DG | C44 H82 O5 N1 | 0.02 | 0.00 |
| DG(18:1/18:1) | 638.572 | pos | 12.10 | DG | C39 H76 O5 N1 | 1.15 | 0.15 |
| DG(16:0/18:2) | 610.541 | pos | 11.74 | DG | C37 H72 O5 N1 | 0.69 | 0.09 |
| DG(34:0p) | 603.532 | pos | 14.62 | DG | C37 H72 O4 Na1 | 0.16 | 0.02 |
| DGDG(18:1/18:1) | 989.642 | neg | 10.54 | DGDG | C52 H93 O17 | 0.03 | 0.00 |
| DGDG(18:1/18:2) | 987.626 | neg | 8.96 | DGDG | C52 H91 O17 | 0.04 | 0.01 |
| DGDG(16:0/18:2) | 961.611 | neg | 8.89 | DGDG | C50 H89 O17 | 0.04 | 0.01 |
| DGDG(18:3/18:3) | 981.579 | neg | 6.27 | DGDG | C52 H85 O17 | 0.04 | 0.00 |
| DGDG(18:2/18:3) | 983.595 | neg | 6.94 | DGDG | C52 H87 O17 | 0.11 | 0.01 |
| DGDG(18:2/18:2) | 985.611 | neg | 7.77 | DGDG | C52 H89 O17 | 0.23 | 0.03 |
| DGMG(18:3) | 721.365 | neg | 1.62 | DGMG | C34 H57 O16 | 0.03 | 0.00 |
| DGMG(18:1) | 725.397 | neg | 3.19 | DGMG | C34 H61 O16 | 0.07 | 0.01 |
| DGMG(18:2) | 723.381 | neg | 2.16 | DGMG | C34 H59 O16 | 0.17 | 0.02 |
| LPA(16:0) | 409.236 | neg | 2.74 | LPA | C19 H38 O7 N0 P1 | 0.04 | 0.01 |
| LPA(18:1) | 435.252 | neg | 3.08 | LPA | C21 H40 O7 N0 P1 | 0.24 | 0.03 |
| LPA(18:2) | 433.236 | neg | 2.16 | LPA | C21 H38 O7 N0 P1 | 0.27 | 0.04 |
| LPC(18:2) | 520.340 | pos | 2.38 | LPC | C26 H51 O7 N1 P1 | 0.04 | 0.01 |
| LPC(18:1) | 522.355 | pos | 3.29 | LPC | C26 H53 O7 N1 P1 | 0.05 | 0.01 |
| LPC(20:2) | 592.362 | neg | 3.60 | LPC | C29 H55 O9 N1 P1 | 0.03 | 0.00 |
| LPE(20:1) | 506.325 | neg | 4.42 | LPE | C25 H49 O7 N1 P1 | 0.04 | 0.01 |
| LPE(20:0) | 508.341 | neg | 5.05 | LPE | C25 H51 O7 N1 P1 | 0.06 | 0.01 |
| LPE(24:0) | 564.403 | neg | 6.83 | LPE | C29 H59 O7 N1 P1 | 0.03 | 0.00 |
| MG(36:4) | 603.535 | pos | 12.10 | MG | C39 H71 O4 | 0.25 | 0.03 |
| MG(36:5) | 601.519 | pos | 11.75 | MG | C39 H69 O4 | 0.36 | 0.05 |
| MGDG(34:2) | 753.552 | neg | 9.67 | MGDG | C43 H77 O10 | 0.03 | 0.00 |
| MGDG(31:2) | 711.505 | neg | 4.99 | MGDG | C40 H71 O10 | 0.02 | 0.00 |
| MGDG(16:0/18:1) | 801.573 | neg | 11.64 | MGDG | C44 H81 O12 | 0.03 | 0.00 |
| MGDG(18:1/18:1) | 827.589 | neg | 11.65 | MGDG | C46 H83 O12 | 0.03 | 0.00 |
| MGDG(18:1/18:2) | 825.573 | neg | 10.21 | MGDG | C46 H81 O12 | 0.03 | 0.00 |
| MGDG(18:2/18:2) | 823.558 | neg | 8.71 | MGDG | C46 H79 O12 | 0.06 | 0.01 |
| MGDG(47:12) | 961.605 | neg | 5.70 | MGDG | C57 H85 O12 | 0.25 | 0.03 |
| MGMG(18:2) | 561.328 | neg | 2.99 | MGMG | C28 H49 O11 | 0.15 | 0.02 |
| PA(16:0/18:1) | 673.481 | neg | 9.90 | PA | C37 H70 O8 N0 P1 | 0.51 | 0.07 |
| PA(16:0/18:2) | 671.466 | neg | 8.52 | PA | C37 H68 O8 N0 P1 | 0.49 | 0.07 |
| PA(18:1/18:1) | 699.497 | neg | 9.99 | PA | C39 H72 O8 N0 P1 | 1.15 | 0.15 |
| PA(18:2/18:2) | 695.466 | neg | 7.50 | PA | C39 H68 O8 N0 P1 | 0.97 | 0.13 |
| PA(18:1/18:2) | 697.481 | neg | 8.56 | PA | C39 H70 O8 N0 P1 | 1.51 | 0.20 |
| PC(34:1) | 760.585 | pos | 10.49 | PC | C42 H83 O8 N1 P1 | 0.04 | 0.01 |
| PC(34:2) | 758.569 | pos | 8.91 | PC | C42 H81 O8 N1 P1 | 0.21 | 0.03 |
| PC(36:4) | 782.569 | pos | 7.79 | PC | C44 H81 O8 N1 P1 | 0.06 | 0.01 |
| PC(36:2) | 786.601 | pos | 10.58 | PC | C44 H85 O8 N1 P1 | 0.14 | 0.02 |
| PC(36:3) | 784.585 | pos | 8.99 | PC | C44 H83 O8 N1 P1 | 0.22 | 0.03 |
| PC(22:0/18:2) | 886.654 | neg | 12.26 | PC | C49 H93 O10 N1 P1 | 0.03 | 0.00 |
| PC(17:1/18:1) | 816.576 | neg | 9.58 | PC | C44 H83 O10 N1 P1 | 0.03 | 0.00 |
| PC(18:1/14:0) | 776.545 | neg | 8.61 | PC | C41 H79 O10 N1 P1 | 0.05 | 0.01 |
| PE(34:2) | 716.522 | pos | 8.59 | PE | C39 H75 O8 N1 P1 | 0.06 | 0.01 |
| PE(16:0/16:1) | 690.507 | pos | 8.89 | PE | C37 H73 O8 N1 P1 | 0.03 | 0.00 |
| PE(16:1/18:1) | 716.522 | pos | 8.87 | PE | C39 H75 O8 N1 P1 | 0.09 | 0.01 |
| PE(42:2p) | 812.653 | pos | 12.80 | PE | C47 H91 O7 N1 P1 | 0.03 | 0.00 |
| PE(44:2p) | 840.684 | pos | 12.85 | PE | C49 H95 O7 N1 P1 | 0.06 | 0.01 |
| PG(47:4) | 925.689 | pos | 12.34 | PG | C53 H98 O10 N0 P1 | 0.02 | 0.00 |
| PG(49:5) | 951.705 | pos | 12.31 | PG | C55 H100 O10 N0 P1 | 0.02 | 0.00 |
| PG(48:1) | 945.752 | pos | 13.17 | PG | C54 H106 O10 N0 P1 | 0.03 | 0.00 |
| PG(28:0/18:2) | 915.705 | pos | 12.60 | PG | C52 H100 O10 N0 P1 | 0.04 | 0.00 |
| PG(28:0/18:1) | 917.721 | pos | 12.84 | PG | C52 H102 O10 N0 P1 | 0.19 | 0.03 |
| PG(46:0) | 919.736 | pos | 13.04 | PG | C52 H104 O10 N0 P1 | 0.40 | 0.05 |
| PG(18:0/18:1) | 775.549 | neg | 10.95 | PG | C42 H80 O10 N0 P1 | 0.02 | 0.00 |
| PG(37:2) | 787.549 | neg | 4.59 | PG | C43 H80 O10 N0 P1 | 0.07 | 0.01 |
| PG(18:0/18:2) | 773.534 | neg | 9.30 | PG | C42 H78 O10 N0 P1 | 0.03 | 0.00 |
| PG(36:7) | 763.456 | neg | 7.53 | PG | C42 H68 O10 N0 P1 | 0.09 | 0.01 |
| PG(33:0) | 735.518 | neg | 4.58 | PG | C39 H76 O10 N0 P1 | 0.55 | 0.07 |
| PG(35:1) | 761.534 | neg | 4.58 | PG | C41 H78 O10 N0 P1 | 0.29 | 0.04 |
| PG(36:6) | 765.471 | neg | 8.54 | PG | C42 H70 O10 N0 P1 | 0.23 | 0.03 |
| PG(37:6) | 779.487 | neg | 8.44 | PG | C43 H72 O10 N0 P1 | 0.02 | 0.00 |
| PI(16:0/18:2) | 852.560 | pos | 7.49 | PI | C43 H83 O13 N1 P1 | 0.03 | 0.00 |
| PI(16:0/18:1) | 854.575 | pos | 8.61 | PI | C43 H85 O13 N1 P1 | 0.05 | 0.01 |
| PI(52:5) | 1079.753 | neg | 12.99 | PI | C61 H108 O13 N0 P1 | 0.02 | 0.00 |
| PI(52:7) | 1075.722 | neg | 12.51 | PI | C61 H104 O13 N0 P1 | 0.02 | 0.00 |
| PI(17:0/18:1) | 849.550 | neg | 9.46 | PI | C44 H82 O13 N0 P1 | 0.02 | 0.00 |
| PI(52:6) | 1077.738 | neg | 12.74 | PI | C61 H106 O13 N0 P1 | 0.03 | 0.00 |
| PI(17:0/18:2) | 847.534 | neg | 8.16 | PI | C44 H80 O13 N0 P1 | 0.02 | 0.00 |
| PI(18:1/14:0) | 807.503 | neg | 7.24 | PI | C41 H76 O13 N0 P1 | 0.02 | 0.00 |
| PI(15:0/18:1) | 821.519 | neg | 7.87 | PI | C42 H78 O13 N0 P1 | 0.03 | 0.00 |
| PI(15:0/18:2) | 819.503 | neg | 6.93 | PI | C42 H76 O13 N0 P1 | 0.03 | 0.00 |
| PI(18:1/18:1) | 861.550 | neg | 8.70 | PI | C45 H82 O13 N0 P1 | 1.12 | 0.15 |
| PIP(56:8) | 1209.735 | neg | 12.08 | PIP | C65 H111 O16 N0 P2 | 0.02 | 0.00 |
| PIP(54:4) | 1189.767 | neg | 12.36 | PIP | C63 H115 O16 N0 P2 | 0.03 | 0.00 |
| PIP(54:5) | 1187.751 | neg | 12.08 | PIP | C63 H113 O16 N0 P2 | 0.04 | 0.01 |
| PIP(54:6) | 1185.735 | neg | 11.83 | PIP | C63 H111 O16 N0 P2 | 0.04 | 0.00 |
| PIP(16:0/22:6) | 961.485 | neg | 8.60 | PIP | C47 H79 O16 N0 P2 | 0.02 | 0.00 |
| PIP(42:8p) | 997.521 | neg | 8.70 | PIP | C51 H83 O15 N0 P2 | 0.08 | 0.01 |
| PIP(42:9p) | 995.506 | neg | 7.57 | PIP | C51 H81 O15 N0 P2 | 0.09 | 0.01 |
| PIP(40:8p) | 969.490 | neg | 7.49 | PIP | C49 H79 O15 N0 P2 | 0.24 | 0.03 |
| PIP(40:7p) | 971.506 | neg | 8.59 | PIP | C49 H81 O15 N0 P2 | 0.24 | 0.03 |
| PIP3(18:1/24:6) | 1175.465 | neg | 8.64 | PIP3 | C51 H87 O22 N0 P4 | 0.03 | 0.00 |
| PS(47:4) | 960.666 | pos | 8.95 | PS | C53 H96 O10 N1 P1 Na1 | 0.05 | 0.01 |
| PS(33:4/14:1) | 958.651 | pos | 7.76 | PS | C53 H94 O10 N1 P1 Na1 | 0.04 | 0.01 |
| PS(38:4) | 810.529 | neg | 7.71 | PS | C44 H77 O10 N1 P1 | 0.04 | 0.01 |
| PS(38:5) | 808.513 | neg | 6.76 | PS | C44 H75 O10 N1 P1 | 0.02 | 0.00 |
| PS(34:1p) | 744.518 | neg | 10.63 | PS | C40 H75 O9 N1 P1 | 0.03 | 0.00 |
| PS(38:6) | 806.498 | neg | 6.19 | PS | C44 H73 O10 N1 P1 | 0.07 | 0.01 |
| PS(38:2) | 814.560 | neg | 8.25 | PS | C44 H81 O10 N1 P1 | 0.02 | 0.00 |
| PS(38:1) | 816.576 | neg | 9.58 | PS | C44 H83 O10 N1 P1 | 0.04 | 0.00 |
| PS(36:1) | 788.545 | neg | 8.15 | PS | C42 H79 O10 N1 P1 | 0.02 | 0.00 |
| PS(38:7) | 804.482 | neg | 7.18 | PS | C44 H71 O10 N1 P1 | 0.03 | 0.00 |
| PS(41:2) | 856.607 | neg | 10.88 | PS | C47 H87 O10 N1 P1 | 0.22 | 0.03 |
| PS(39:2) | 828.576 | neg | 9.49 | PS | C45 H83 O10 N1 P1 | 0.03 | 0.00 |
| PS(36:3) | 784.513 | neg | 11.00 | PS | C42 H75 O10 N1 P1 | 0.41 | 0.05 |
| PS(39:4) | 824.545 | neg | 6.97 | PS | C45 H79 O10 N1 P1 | 0.38 | 0.05 |
| PS(39:3) | 826.560 | neg | 7.82 | PS | C45 H81 O10 N1 P1 | 5.47 | 0.73 |
| PS(39:1) | 830.592 | neg | 10.59 | PS | C45 H85 O10 N1 P1 | 11.12 | 1.48 |
| So(d18:2) | 298.274 | pos | 1.99 | So | C18 H36 O2 N1 | 0.05 | 0.01 |
| So(d22:0) | 358.368 | pos | 4.29 | So | C22 H48 O2 N1 | 0.04 | 0.01 |
| So(d20:0) | 330.337 | pos | 3.23 | So | C20 H44 O2 N1 | 0.05 | 0.01 |
| So(d16:1) | 272.258 | pos | 1.47 | So | C16 H34 O2 N1 | 0.06 | 0.01 |
| So(d14:0) | 246.243 | pos | 0.85 | So | C14 H32 O2 N1 | 0.07 | 0.01 |
| So(d16:0) | 274.274 | pos | 1.20 | So | C16 H36 O2 N1 | 9.58 | 1.28 |
| SQDG(41:6) | 953.567 | neg | 2.35 | SQDG | C51 H85 O14 S1 | 0.03 | 0.00 |
| SQDG(40:2) | 947.614 | neg | 2.98 | SQDG | C50 H91 O14 S1 | 0.04 | 0.01 |
| SQDG(44:4) | 999.645 | neg | 3.30 | SQDG | C54 H95 O14 S1 | 0.15 | 0.02 |
| SQDG(44:6) | 995.614 | neg | 2.37 | SQDG | C54 H91 O14 S1 | 0.18 | 0.02 |
| SQDG(16:0/16:0) | 793.514 | neg | 8.24 | SQDG | C41 H77 O12 S1 | 0.02 | 0.00 |
| SQDG(36:3) | 843.530 | neg | 7.40 | SQDG | C45 H79 O12 S1 | 0.02 | 0.00 |
| SQDG(18:2/18:2) | 841.514 | neg | 6.59 | SQDG | C45 H77 O12 S1 | 0.04 | 0.01 |
| SQDG(40:7) | 937.535 | neg | 11.03 | SQDG | C50 H81 O14 S1 | 0.03 | 0.00 |
| SQDG(16:0/18:2) | 817.514 | neg | 7.33 | SQDG | C43 H77 O12 S1 | 0.06 | 0.01 |
| TG(38:1) | 682.598 | pos | 9.00 | TG | C41 H80 O6 N1 | 0.04 | 0.01 |
| TG(40:2) | 708.614 | pos | 9.79 | TG | C43 H82 O6 N1 | 0.02 | 0.00 |
| TG(38:2) | 680.582 | pos | 7.81 | TG | C41 H78 O6 N1 | 0.05 | 0.01 |
| TG(10:0/10:0/18:2) | 680.582 | pos | 9.28 | TG | C41 H78 O6 N1 | 0.02 | 0.00 |
| TG(6:0/12:0/18:1) | 637.540 | pos | 9.38 | TG | C39 H73 O6 | 0.04 | 0.01 |
| TG(20:1/10:0/10:0) | 710.629 | pos | 11.38 | TG | C43 H84 O6 N1 | 0.03 | 0.00 |
| TG(8:0/10:0/18:1) | 654.567 | pos | 8.91 | TG | C39 H76 O6 N1 | 0.02 | 0.00 |
| TG(6:0/16:0/18:1) | 710.629 | pos | 12.08 | TG | C43 H84 O6 N1 | 0.03 | 0.00 |
| TG(6:0/11:0/17:2) | 624.520 | pos | 7.33 | TG | C37 H70 O6 N1 | 0.02 | 0.00 |
| TG(6:0/12:0/18:2) | 635.525 | pos | 8.08 | TG | C39 H71 O6 | 0.03 | 0.00 |
| TG(20:0/9:0/9:0) | 684.614 | pos | 11.39 | TG | C41 H82 O6 N1 | 0.02 | 0.00 |
| TG(6:0/13:1/17:2) | 650.535 | pos | 7.55 | TG | C39 H72 O6 N1 | 0.02 | 0.00 |
| TG(6:0/15:2/15:2) | 648.520 | pos | 6.58 | TG | C39 H70 O6 N1 | 0.06 | 0.01 |
| TG(36:1) | 654.567 | pos | 8.33 | TG | C39 H76 O6 N1 | 0.39 | 0.05 |
| TG(59:9p) | 927.780 | pos | 12.85 | TG | C62 H103 O5 | 0.04 | 0.00 |
| TG(64:8p) | 999.874 | pos | 14.16 | TG | C67 H115 O5 | 0.07 | 0.01 |
| TG(6:0/14:1/18:3) | 676.551 | pos | 6.59 | TG | C41 H74 O6 N1 | 0.10 | 0.01 |
| TG(36:3) | 633.509 | pos | 9.27 | TG | C39 H69 O6 | 0.20 | 0.03 |
| TG(38:3) | 678.567 | pos | 7.21 | TG | C41 H76 O6 N1 | 0.48 | 0.06 |
| TG(4:0/14:1/16:0) | 631.491 | pos | 8.13 | TG | C37 H68 O6 Na1 | 0.10 | 0.01 |
| TG(4:0/16:0/16:2) | 652.551 | pos | 7.31 | TG | C39 H74 O6 N1 | 0.06 | 0.01 |
| TG(4:0/16:0/16:0) | 656.582 | pos | 9.29 | TG | C39 H78 O6 N1 | 0.42 | 0.06 |
| TG(20:1/9:0/9:0) | 682.598 | pos | 9.39 | TG | C41 H80 O6 N1 | 0.95 | 0.13 |
| TG(55:7) | 913.726 | pos | 13.62 | TG | C58 H98 O6 Na1 | 0.03 | 0.00 |
| TG(59:7e) | 933.827 | pos | 13.62 | TG | C62 H109 O5 | 0.05 | 0.01 |
| TG(6:0/14:0/18:2) | 680.582 | pos | 8.11 | TG | C41 H78 O6 N1 | 1.66 | 0.22 |
| TG(18:4/15:2/24:7) | 907.681 | pos | 12.85 | TG | C60 H91 O6 | 0.04 | 0.01 |
| TG(19:5/18:2/18:3) | 907.679 | pos | 12.85 | TG | C58 H92 O6 Na1 | 0.04 | 0.01 |
| TG(18:1/18:3/22:4) | 931.775 | pos | 12.33 | TG | C61 H103 O6 | 0.14 | 0.02 |
| TG(18:3/18:2/21:6) | 933.694 | pos | 12.83 | TG | C60 H94 O6 Na1 | 0.04 | 0.01 |
| TG(15:2/22:6/22:6) | 933.697 | pos | 12.84 | TG | C62 H93 O6 | 0.04 | 0.01 |
| TG(62:5p) | 977.890 | pos | 14.68 | TG | C65 H117 O5 | 0.13 | 0.02 |
| TG(59:11) | 939.744 | pos | 13.60 | TG | C62 H99 O6 | 0.05 | 0.01 |
| TG(62:4e) | 1003.903 | pos | 14.40 | TG | C65 H120 O5 Na1 | 0.08 | 0.01 |
| TG(60:6p) | 947.843 | pos | 13.93 | TG | C63 H111 O5 | 0.62 | 0.08 |
| TG(18:1/18:3/21:6) | 935.710 | pos | 13.07 | TG | C60 H96 O6 Na1 | 0.07 | 0.01 |
| TG(59:8e) | 931.811 | pos | 13.32 | TG | C62 H107 O5 | 0.08 | 0.01 |
| TG(64:9e) | 999.874 | pos | 13.87 | TG | C67 H115 O5 | 0.05 | 0.01 |
| TG(18:3/18:3/21:5) | 911.712 | pos | 13.34 | TG | C60 H95 O6 | 0.08 | 0.01 |
| TG(55:8) | 911.710 | pos | 13.33 | TG | C58 H96 O6 Na1 | 0.09 | 0.01 |
| TG(12:0p/8:0/16:2) | 619.530 | pos | 11.76 | TG | C39 H71 O5 | 0.09 | 0.01 |
| TG(18:1/18:3/21:5) | 937.726 | pos | 13.31 | TG | C60 H98 O6 Na1 | 0.08 | 0.01 |
| TG(59:8p) | 929.796 | pos | 13.08 | TG | C62 H105 O5 | 0.07 | 0.01 |
| TG(59:9e) | 929.796 | pos | 13.08 | TG | C62 H105 O5 | 0.07 | 0.01 |
| TG(18:1/18:3/19:5) | 909.694 | pos | 13.12 | TG | C58 H94 O6 Na1 | 0.07 | 0.01 |
| TG(64:8e) | 1001.890 | pos | 14.08 | TG | C67 H117 O5 | 0.14 | 0.02 |
| TG(38:1p) | 666.603 | pos | 12.11 | TG | C41 H80 O5 N1 | 0.04 | 0.00 |
| TG(16:0/18:2/18:3) | 853.728 | pos | 12.73 | TG | C55 H97 O6 | 0.03 | 0.00 |
| TG(62:6p) | 975.874 | pos | 14.36 | TG | C65 H115 O5 | 0.24 | 0.03 |
| TG(25:0/18:1/18:1) | 1002.942 | pos | 16.23 | TG | C64 H124 O6 N1 | 0.04 | 0.00 |
| TG(62:9e) | 971.843 | pos | 13.72 | TG | C65 H111 O5 | 0.07 | 0.01 |
| TG(62:8e) | 973.858 | pos | 14.07 | TG | C65 H113 O5 | 0.27 | 0.04 |
| TG(25:3/19:0/19:0) | 1028.958 | pos | 15.90 | TG | C66 H126 O6 N1 | 0.03 | 0.00 |
| TG(20:0/16:0/18:1) | 911.804 | pos | 15.39 | TG | C57 H108 O6 Na1 | 0.02 | 0.00 |
| TG(57:5) | 940.833 | pos | 14.13 | TG | C60 H110 O6 N1 | 0.02 | 0.00 |
| TG(24:0/18:2/18:3) | 987.835 | pos | 15.13 | TG | C63 H112 O6 Na1 | 0.03 | 0.00 |
| TG(16:0/14:0/18:1) | 822.755 | pos | 14.28 | TG | C51 H100 O6 N1 | 0.03 | 0.00 |
| TG(18:3/18:2/23:0) | 968.864 | pos | 14.93 | TG | C62 H114 O6 N1 | 0.02 | 0.00 |
| TG(64:3) | 1042.974 | pos | 16.06 | TG | C67 H128 O6 N1 | 0.03 | 0.00 |
| TG(57:9e) | 923.746 | pos | 14.57 | TG | C60 H100 O5 Na1 | 0.02 | 0.00 |
| TG(18:1/18:2/21:0) | 949.819 | pos | 15.20 | TG | C60 H110 O6 Na1 | 0.03 | 0.00 |
| TG(18:0/17:0/18:1) | 892.833 | pos | 15.21 | TG | C56 H110 O6 N1 | 0.02 | 0.00 |
| TG(4:0/16:2/18:2) | 676.551 | pos | 11.63 | TG | C41 H74 O6 N1 | 0.02 | 0.00 |
| TG(18:0/18:1/24:0) | 990.942 | pos | 16.42 | TG | C63 H124 O6 N1 | 0.06 | 0.01 |
| TG(4:0/18:2/18:2) | 687.556 | pos | 8.28 | TG | C43 H75 O6 | 0.03 | 0.00 |
| TG(37:0p) | 654.603 | pos | 12.05 | TG | C40 H80 O5 N1 | 0.02 | 0.00 |
| TG(18:2/18:2/23:0) | 975.835 | pos | 15.23 | TG | C62 H112 O6 Na1 | 0.04 | 0.01 |
| TG(18:1/18:2/23:0) | 977.851 | pos | 15.56 | TG | C62 H114 O6 Na1 | 0.05 | 0.01 |
| TG(20:1/18:1/24:0) | 1016.958 | pos | 16.39 | TG | C65 H126 O6 N1 | 0.08 | 0.01 |
| TG(22:0/18:3/18:3) | 952.833 | pos | 14.36 | TG | C61 H110 O6 N1 | 0.03 | 0.00 |
| TG(16:0/18:1/21:0) | 920.864 | pos | 15.56 | TG | C58 H114 O6 N1 | 0.05 | 0.01 |
| TG(18:1/18:2/22:4) | 933.791 | pos | 14.59 | TG | C61 H105 O6 | 0.05 | 0.01 |
| TG(19:1/18:3/21:1) | 954.848 | pos | 14.27 | TG | C61 H112 O6 N1 | 0.08 | 0.01 |
| TG(22:2/18:2/18:2) | 952.833 | pos | 14.10 | TG | C61 H110 O6 N1 | 0.02 | 0.00 |
| TG(24:1/18:2/18:2) | 982.880 | pos | 14.93 | TG | C63 H116 O6 N1 | 0.05 | 0.01 |
| TG(18:1/18:2/21:1) | 942.848 | pos | 14.46 | TG | C60 H112 O6 N1 | 0.04 | 0.01 |
| TG(55:9p) | 893.699 | pos | 14.05 | TG | C58 H94 O5 Na1 | 0.04 | 0.01 |
| TG(18:1/17:1/18:2) | 891.741 | pos | 14.17 | TG | C56 H100 O6 Na1 | 0.03 | 0.00 |
| TG(25:0/13:1/23:0) | 1004.958 | pos | 15.36 | TG | C64 H126 O6 N1 | 0.03 | 0.00 |
| TG(16:0/18:1/23:0) | 948.895 | pos | 15.91 | TG | C60 H118 O6 N1 | 0.10 | 0.01 |
| TG(18:1/14:0/18:2) | 846.755 | pos | 13.63 | TG | C53 H100 O6 N1 | 0.02 | 0.00 |
| TG(16:0/16:0/18:2) | 853.726 | pos | 14.36 | TG | C53 H98 O6 Na1 | 0.07 | 0.01 |
| TG(26:0/18:2/18:2) | 1012.927 | pos | 15.76 | TG | C65 H122 O6 N1 | 0.10 | 0.01 |
| TG(14:0/18:2/18:3) | 842.723 | pos | 13.35 | TG | C53 H96 O6 N1 | 0.03 | 0.00 |
| TG(61:2) | 1002.942 | pos | 15.89 | TG | C64 H124 O6 N1 | 0.09 | 0.01 |
| TG(15:0/18:2/18:2) | 863.710 | pos | 13.81 | TG | C54 H96 O6 Na1 | 0.02 | 0.00 |
| TG(15:0/18:1/18:2) | 865.726 | pos | 14.14 | TG | C54 H98 O6 Na1 | 0.04 | 0.01 |
| TG(18:3/18:2/20:2) | 922.786 | pos | 13.72 | TG | C59 H104 O6 N1 | 0.05 | 0.01 |
| TG(19:0/19:0/23:4) | 998.911 | pos | 15.23 | TG | C64 H120 O6 N1 | 0.09 | 0.01 |
| TG(18:1/18:1/21:1) | 944.864 | pos | 14.86 | TG | C60 H114 O6 N1 | 0.06 | 0.01 |
| TG(16:0/14:0/18:2) | 820.739 | pos | 13.95 | TG | C51 H98 O6 N1 | 0.06 | 0.01 |
| TG(15:0/16:0/18:1) | 836.770 | pos | 14.48 | TG | C52 H102 O6 N1 | 0.08 | 0.01 |
| TG(6:0/14:1/18:2) | 678.567 | pos | 12.01 | TG | C41 H76 O6 N1 | 0.06 | 0.01 |
| TG(18:1/20:4/24:0) | 993.884 | pos | 16.05 | TG | C65 H117 O6 | 0.10 | 0.01 |
| TG(25:1/18:1/18:1) | 1000.927 | pos | 15.56 | TG | C64 H122 O6 N1 | 0.12 | 0.02 |
| TG(6:0/14:1/18:1) | 680.582 | pos | 12.32 | TG | C41 H78 O6 N1 | 0.07 | 0.01 |
| TG(66:2) | 1073.021 | pos | 16.05 | TG | C69 H134 O6 N1 | 0.12 | 0.02 |
| TG(16:0/18:2/21:0) | 918.848 | pos | 15.22 | TG | C58 H112 O6 N1 | 0.12 | 0.02 |
| TG(41:0p) | 710.666 | pos | 12.77 | TG | C44 H88 O5 N1 | 0.03 | 0.00 |
| TG(26:0/18:1/18:2) | 1014.942 | pos | 16.07 | TG | C65 H124 O6 N1 | 0.19 | 0.03 |
| TG(18:1/18:1/20:4) | 907.775 | pos | 14.58 | TG | C59 H103 O6 | 0.15 | 0.02 |
| TG(18:1/18:1/24:1) | 986.911 | pos | 15.37 | TG | C63 H120 O6 N1 | 0.90 | 0.12 |
| TG(18:0/17:2/18:2) | 886.786 | pos | 13.81 | TG | C56 H104 O6 N1 | 0.07 | 0.01 |
| TG(18:2/18:2/21:0) | 942.848 | pos | 14.87 | TG | C60 H112 O6 N1 | 0.17 | 0.02 |
| TG(18:1/18:2/20:4) | 905.759 | pos | 14.25 | TG | C59 H101 O6 | 0.13 | 0.02 |
| TG(18:1/18:1/23:0) | 974.911 | pos | 15.89 | TG | C62 H120 O6 N1 | 0.31 | 0.04 |
| TG(22:1/18:2/18:2) | 954.848 | pos | 14.64 | TG | C61 H112 O6 N1 | 0.18 | 0.02 |
| TG(18:1/18:2/22:1) | 956.864 | pos | 14.60 | TG | C61 H114 O6 N1 | 0.19 | 0.03 |
| TG(19:1/18:1/18:1) | 916.833 | pos | 14.81 | TG | C58 H110 O6 N1 | 0.15 | 0.02 |
| TG(18:1/18:1/21:0) | 946.880 | pos | 15.56 | TG | C60 H116 O6 N1 | 0.27 | 0.04 |
| TG(59:3) | 972.895 | pos | 14.58 | TG | C62 H118 O6 N1 | 0.27 | 0.04 |
| TG(25:1/18:2/19:0) | 1014.942 | pos | 15.73 | TG | C65 H124 O6 N1 | 0.31 | 0.04 |
| TG(62:2) | 1016.958 | pos | 16.05 | TG | C65 H126 O6 N1 | 0.30 | 0.04 |
| TG(16:1/18:2/18:3) | 868.739 | pos | 13.42 | TG | C55 H98 O6 N1 | 0.10 | 0.01 |
| TG(20:5/18:2/18:2) | 901.728 | pos | 13.66 | TG | C59 H97 O6 | 0.11 | 0.01 |
| TG(19:1/16:0/18:1) | 890.817 | pos | 14.82 | TG | C56 H108 O6 N1 | 0.22 | 0.03 |
| TG(17:4/17:3/22:0) | 922.786 | pos | 13.38 | TG | C59 H104 O6 N1 | 0.03 | 0.00 |
| TG(15:0/18:1/18:1) | 862.786 | pos | 14.47 | TG | C54 H104 O6 N1 | 0.31 | 0.04 |
| TG(18:1/18:2/24:1) | 984.895 | pos | 15.07 | TG | C63 H118 O6 N1 | 0.40 | 0.05 |
| TG(16:0/18:1/24:0) | 962.911 | pos | 16.08 | TG | C61 H120 O6 N1 | 0.70 | 0.09 |
| TG(18:1/17:1/18:1) | 888.801 | pos | 14.45 | TG | C56 H106 O6 N1 | 0.35 | 0.05 |
| TG(20:1/18:2/18:3) | 924.801 | pos | 14.02 | TG | C59 H106 O6 N1 | 0.48 | 0.06 |
| TG(16:0/18:1/22:0) | 934.880 | pos | 15.74 | TG | C59 H116 O6 N1 | 0.84 | 0.11 |
| TG(18:0/16:0/18:1) | 878.817 | pos | 15.03 | TG | C55 H108 O6 N1 | 0.74 | 0.10 |
| TG(20:1/18:1/18:1) | 930.848 | pos | 14.59 | TG | C59 H112 O6 N1 | 0.98 | 0.13 |
| TG(18:1/18:1/24:0) | 988.927 | pos | 16.05 | TG | C63 H122 O6 N1 | 1.89 | 0.25 |
| TG(18:1/18:3/24:0) | 984.895 | pos | 15.41 | TG | C63 H118 O6 N1 | 1.89 | 0.25 |
| TG(18:1/18:2/24:0) | 986.911 | pos | 15.73 | TG | C63 H120 O6 N1 | 2.23 | 0.30 |
| TG(20:1/18:2/18:2) | 926.817 | pos | 14.30 | TG | C59 H108 O6 N1 | 1.79 | 0.24 |
| TG(16:0/16:0/18:1) | 850.786 | pos | 14.67 | TG | C53 H104 O6 N1 | 1.85 | 0.25 |
| TG(22:0/18:2/18:2) | 956.864 | pos | 15.04 | TG | C61 H114 O6 N1 | 2.76 | 0.37 |
| TG(18:1/18:1/22:0) | 960.895 | pos | 15.71 | TG | C61 H118 O6 N1 | 3.38 | 0.45 |
| TG(20:0/18:2/18:2) | 928.833 | pos | 14.62 | TG | C59 H110 O6 N1 | 3.86 | 0.51 |
| TG(18:1/18:2/22:0) | 958.880 | pos | 15.38 | TG | C61 H116 O6 N1 | 3.74 | 0.50 |
| TG(20:0/18:1/18:1) | 932.864 | pos | 15.36 | TG | C59 H114 O6 N1 | 3.38 | 0.45 |

**Table S3**

Molecular species of lipids in stored untreated buckwheat

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
| Lipid | m/z | Ion mode | Retention time | Class | Formula | Relative abundance/% | SD |
| Cer(d42:1) | 650.645 | pos | 13.35 | Cer | C42 H84 O3 N1 | 0.02 | 0.00 |
| Cer(d25:0/18:1+O) | 680.655 | pos | 12.74 | Cer | C43 H86 O4 N1 | 0.02 | 0.00 |
| Cer(d38:7) | 582.488 | pos | 8.14 | Cer | C38 H64 O3 N1 | 0.02 | 0.00 |
| Cer(d24:0/16:1) | 622.613 | pos | 12.95 | Cer | C40 H80 O3 N1 | 0.02 | 0.00 |
| Cer(d16:0/18:0) | 540.535 | pos | 9.74 | Cer | C34 H70 O3 N1 | 0.03 | 0.00 |
| Cer(d18:0) | 316.285 | pos | 1.79 | Cer | C18 H38 O3 N1 | 0.03 | 0.00 |
| Cer(d18:1/20:5) | 584.504 | pos | 9.48 | Cer | C38 H66 O3 N1 | 0.03 | 0.01 |
| Cer(d18:1/18:4) | 558.488 | pos | 9.28 | Cer | C36 H64 O3 N1 | 0.03 | 0.01 |
| Cer(d32:0) | 512.504 | pos | 7.97 | Cer | C32 H66 O3 N1 | 0.04 | 0.01 |
| Cer(d18:2/18:1+O) | 578.514 | pos | 7.46 | Cer | C36 H68 O4 N1 | 0.04 | 0.01 |
| Cer(d24:0/18:0+O) | 668.655 | pos | 12.75 | Cer | C42 H86 O4 N1 | 0.04 | 0.01 |
| Cer(d18:2/18:0+O) | 580.530 | pos | 8.58 | Cer | C36 H70 O4 N1 | 0.05 | 0.01 |
| Cer(d18:2/18:2) | 560.504 | pos | 8.14 | Cer | C36 H66 O3 N1 | 0.07 | 0.01 |
| Cer(d24:0/18:1+O) | 666.639 | pos | 12.55 | Cer | C42 H84 O4 N1 | 0.07 | 0.01 |
| Cer(d18:2/16:0) | 536.504 | pos | 9.29 | Cer | C34 H66 O3 N1 | 0.08 | 0.01 |
| CL(24:0/18:1/18:1/18:1) | 770.565 | neg | 10.60 | CL | C87 H162 O17 P2 | 0.02 | 0.00 |
| CL(22:3/16:0/16:0/18:1) | 1456.028 | neg | 10.98 | CL | C81 H149 O17 P2 | 0.02 | 0.00 |
| CL(18:2/16:0/18:1/22:4) | 1478.012 | neg | 9.35 | CL | C83 H147 O17 P2 | 0.02 | 0.00 |
| CL(20:5/18:2/18:1/18:2) | 1471.965 | neg | 13.47 | CL | C83 H141 O17 P2 | 0.02 | 0.00 |
| CL(18:2/16:0/16:0/22:4) | 1451.996 | neg | 9.29 | CL | C81 H145 O17 P2 | 0.02 | 0.00 |
| CL(20:5/18:2/18:2/18:2) | 1469.949 | neg | 13.22 | CL | C83 H139 O17 P2 | 0.03 | 0.00 |
| CL(18:2/18:1/18:1/18:2) | 1451.996 | neg | 13.72 | CL | C81 H145 O17 P2 | 0.03 | 0.00 |
| CL(83:7) | 801.573 | neg | 11.65 | CL | C92 H164 O17 P2 | 0.03 | 0.01 |
| CL(87:9) | 827.588 | neg | 11.65 | CL | C96 H168 O17 P2 | 0.03 | 0.01 |
| CL(83:15) | 793.510 | neg | 8.24 | CL | C92 H148 O17 P2 | 0.03 | 0.01 |
| CL(83:9) | 799.557 | neg | 10.17 | CL | C92 H160 O17 P2 | 0.04 | 0.01 |
| CL(18:2/18:1/18:1/24:1) | 768.549 | neg | 9.01 | CL | C87 H158 O17 P2 | 0.04 | 0.01 |
| CL(87:11) | 825.573 | neg | 10.21 | CL | C96 H164 O17 P2 | 0.04 | 0.01 |
| CL(18:2/18:1/18:1/22:4) | 1504.028 | neg | 9.42 | CL | C85 H149 O17 P2 | 0.05 | 0.01 |
| CL(18:2/18:2/18:2/22:4) | 1499.996 | neg | 8.09 | CL | C85 H145 O17 P2 | 0.05 | 0.01 |
| CL(18:2/18:1/18:2/18:2) | 1449.981 | neg | 13.46 | CL | C81 H143 O17 P2 | 0.06 | 0.01 |
| CL(18:2/18:2/18:2/18:2) | 1447.965 | neg | 13.22 | CL | C81 H141 O17 P2 | 0.07 | 0.01 |
| CL(87:13) | 823.557 | neg | 8.71 | CL | C96 H160 O17 P2 | 0.09 | 0.02 |
| DG(34:1p) | 601.517 | pos | 7.57 | DG | C37 H70 O4 Na1 | 0.02 | 0.00 |
| DG(58:7) | 919.811 | pos | 13.61 | DG | C61 H107 O5 | 0.02 | 0.00 |
| DG(18:2/18:2) | 639.496 | pos | 10.67 | DG | C39 H68 O5 Na1 | 0.02 | 0.00 |
| DG(38:3) | 664.587 | pos | 11.76 | DG | C41 H78 O5 N1 | 0.02 | 0.00 |
| DG(36:3p) | 603.535 | pos | 8.67 | DG | C39 H71 O4 | 0.02 | 0.00 |
| DG(38:0e) | 661.611 | pos | 15.71 | DG | C41 H82 O4 Na1 | 0.02 | 0.00 |
| DG(38:2p) | 633.582 | pos | 15.36 | DG | C41 H77 O4 | 0.02 | 0.00 |
| DG(16:0/18:1) | 612.556 | pos | 12.09 | DG | C37 H74 O5 N1 | 0.02 | 0.00 |
| DG(40:7) | 689.512 | pos | 9.67 | DG | C43 H70 O5 Na1 | 0.03 | 0.01 |
| DG(36:1e) | 631.564 | pos | 14.96 | DG | C39 H76 O4 Na1 | 0.04 | 0.01 |
| DG(40:8) | 687.496 | pos | 8.38 | DG | C43 H68 O5 Na1 | 0.05 | 0.01 |
| DG(32:0p) | 575.501 | pos | 7.79 | DG | C35 H68 O4 Na1 | 0.06 | 0.01 |
| DG(41:4) | 704.619 | pos | 12.43 | DG | C44 H82 O5 N1 | 0.06 | 0.01 |
| DG(18:1/18:1) | 638.572 | pos | 12.10 | DG | C39 H76 O5 N1 | 0.06 | 0.01 |
| DG(42:10) | 711.496 | pos | 7.35 | DG | C45 H68 O5 Na1 | 0.07 | 0.01 |
| DG(42:8) | 715.527 | pos | 9.74 | DG | C45 H72 O5 Na1 | 0.08 | 0.02 |
| DG(16:0/18:2) | 610.541 | pos | 11.74 | DG | C37 H72 O5 N1 | 0.08 | 0.02 |
| DG(34:0p) | 603.532 | pos | 14.62 | DG | C37 H72 O4 Na1 | 0.14 | 0.02 |
| DG(42:9) | 713.512 | pos | 8.40 | DG | C45 H70 O5 Na1 | 0.17 | 0.03 |
| DGDG(16:0/18:1) | 963.626 | neg | 10.42 | DGDG | C50 H91 O17 | 0.03 | 0.00 |
| DGDG(18:1/18:1) | 989.642 | neg | 10.54 | DGDG | C52 H93 O17 | 0.03 | 0.00 |
| DGDG(18:1/18:2) | 987.626 | neg | 8.96 | DGDG | C52 H91 O17 | 0.04 | 0.01 |
| DGDG(16:0/18:2) | 961.611 | neg | 8.89 | DGDG | C50 H89 O17 | 0.04 | 0.01 |
| DGDG(18:3/18:3) | 981.579 | neg | 6.27 | DGDG | C52 H85 O17 | 0.06 | 0.01 |
| DGDG(18:2/18:3) | 983.595 | neg | 6.94 | DGDG | C52 H87 O17 | 0.17 | 0.03 |
| DGDG(18:2/18:2) | 985.611 | neg | 7.77 | DGDG | C52 H89 O17 | 0.24 | 0.04 |
| DGMG(18:2) | 723.381 | neg | 2.16 | DGMG | C34 H59 O16 | 0.03 | 0.00 |
| LPC(18:2) | 520.340 | pos | 2.38 | LPC | C26 H51 O7 N1 P1 | 0.10 | 0.02 |
| LPC(18:1) | 522.355 | pos | 3.29 | LPC | C26 H53 O7 N1 P1 | 0.11 | 0.02 |
| MGDG(16:0/18:1) | 801.573 | neg | 11.64 | MGDG | C44 H81 O12 | 0.03 | 0.01 |
| MGDG(18:1/18:1) | 827.589 | neg | 11.65 | MGDG | C46 H83 O12 | 0.03 | 0.01 |
| MGDG(16:0/18:2) | 799.558 | neg | 10.17 | MGDG | C44 H79 O12 | 0.04 | 0.01 |
| MGDG(18:1/18:2) | 825.573 | neg | 10.21 | MGDG | C46 H81 O12 | 0.04 | 0.01 |
| MGDG(18:2/18:2) | 823.558 | neg | 8.71 | MGDG | C46 H79 O12 | 0.09 | 0.02 |
| MGDG(47:12) | 961.605 | neg | 5.70 | MGDG | C57 H85 O12 | 0.12 | 0.02 |
| MGMG(18:1) | 563.344 | neg | 3.81 | MGMG | C28 H51 O11 | 0.03 | 0.01 |
| MGMG(18:2) | 561.328 | neg | 2.99 | MGMG | C28 H49 O11 | 0.06 | 0.01 |
| PA(37:1) | 715.528 | neg | 11.58 | PA | C40 H76 O8 N0 P1 | 0.13 | 0.02 |
| PA(16:0/18:1) | 673.481 | neg | 9.90 | PA | C37 H70 O8 N0 P1 | 0.26 | 0.05 |
| PA(16:0/18:2) | 671.466 | neg | 8.52 | PA | C37 H68 O8 N0 P1 | 0.29 | 0.05 |
| PA(18:1/18:1) | 699.497 | neg | 9.99 | PA | C39 H72 O8 N0 P1 | 0.52 | 0.09 |
| PA(18:2/18:2) | 695.466 | neg | 7.50 | PA | C39 H68 O8 N0 P1 | 0.56 | 0.10 |
| PA(18:1/18:2) | 697.481 | neg | 8.56 | PA | C39 H70 O8 N0 P1 | 0.87 | 0.16 |
| PC(39:7p) | 824.556 | pos | 10.62 | PC | C47 H80 O7 N1 P1 Na1 | 0.02 | 0.00 |
| PC(34:3) | 756.554 | pos | 7.58 | PC | C42 H79 O8 N1 P1 | 0.03 | 0.00 |
| PC(32:1) | 732.554 | pos | 8.60 | PC | C40 H79 O8 N1 P1 | 0.04 | 0.01 |
| PC(38:3) | 812.616 | pos | 10.88 | PC | C46 H87 O8 N1 P1 | 0.05 | 0.01 |
| PC(16:2/18:2) | 754.538 | pos | 6.74 | PC | C42 H77 O8 N1 P1 | 0.05 | 0.01 |
| PC(36:1) | 788.616 | pos | 11.81 | PC | C44 H87 O8 N1 P1 | 0.05 | 0.01 |
| PC(38:2) | 814.632 | pos | 11.79 | PC | C46 H89 O8 N1 P1 | 0.06 | 0.01 |
| PC(36:5) | 780.554 | pos | 6.96 | PC | C44 H79 O8 N1 P1 | 0.06 | 0.01 |
| PC(16:0/18:1) | 782.567 | pos | 10.47 | PC | C42 H82 O8 N1 P1 Na1 | 0.06 | 0.01 |
| PC(32:2) | 730.538 | pos | 7.45 | PC | C40 H77 O8 N1 P1 | 0.07 | 0.01 |
| PC(16:0/18:2) | 780.551 | pos | 8.90 | PC | C42 H80 O8 N1 P1 Na1 | 0.08 | 0.01 |
| PC(18:2/18:2) | 804.551 | pos | 7.78 | PC | C44 H80 O8 N1 P1 Na1 | 0.13 | 0.02 |
| PC(18:1/18:2) | 806.567 | pos | 9.02 | PC | C44 H82 O8 N1 P1 Na1 | 0.22 | 0.04 |
| PC(18:1/18:1) | 808.583 | pos | 10.61 | PC | C44 H84 O8 N1 P1 Na1 | 0.27 | 0.05 |
| PC(34:1) | 760.585 | pos | 10.49 | PC | C42 H83 O8 N1 P1 | 1.26 | 0.23 |
| PC(16:1/18:1) | 758.569 | pos | 8.41 | PC | C42 H81 O8 N1 P1 | 1.46 | 0.26 |
| PC(34:2) | 758.569 | pos | 8.91 | PC | C42 H81 O8 N1 P1 | 1.99 | 0.36 |
| PC(36:4) | 782.569 | pos | 7.79 | PC | C44 H81 O8 N1 P1 | 2.35 | 0.42 |
| PC(36:2) | 786.601 | pos | 10.58 | PC | C44 H85 O8 N1 P1 | 5.11 | 0.92 |
| PC(36:3) | 784.585 | pos | 8.99 | PC | C44 H83 O8 N1 P1 | 6.50 | 1.17 |
| PC(16:0/16:0) | 778.560 | neg | 10.35 | PC | C41 H81 O10 N1 P1 | 0.02 | 0.00 |
| PC(24:0/18:2) | 914.686 | neg | 12.59 | PC | C51 H97 O10 N1 P1 | 0.03 | 0.01 |
| PC(22:0/18:2) | 886.654 | neg | 12.26 | PC | C49 H93 O10 N1 P1 | 0.04 | 0.01 |
| PC(17:1/18:1) | 816.576 | neg | 9.58 | PC | C44 H83 O10 N1 P1 | 0.04 | 0.01 |
| PC(18:1/14:0) | 776.545 | neg | 8.61 | PC | C41 H79 O10 N1 P1 | 0.06 | 0.01 |
| PE(42:9p) | 820.525 | pos | 7.78 | PE | C47 H76 O7 N1 P1 Na1 | 0.02 | 0.00 |
| PE(47:11) | 880.585 | pos | 7.50 | PE | C52 H83 O8 N1 P1 | 0.02 | 0.00 |
| PE(18:1/18:1) | 744.554 | pos | 7.65 | PE | C41 H79 O8 N1 P1 | 0.02 | 0.00 |
| PE(34:1) | 740.520 | pos | 10.98 | PE | C39 H76 O8 N1 P1 Na1 | 0.02 | 0.00 |
| PE(36:0) | 748.585 | pos | 10.57 | PE | C41 H83 O8 N1 P1 | 0.03 | 0.00 |
| PE(38:0) | 776.616 | pos | 11.79 | PE | C43 H87 O8 N1 P1 | 0.04 | 0.01 |
| PE(36:3) | 764.520 | pos | 9.39 | PE | C41 H76 O8 N1 P1 Na1 | 0.04 | 0.01 |
| PE(37:4) | 754.538 | pos | 6.66 | PE | C42 H77 O8 N1 P1 | 0.05 | 0.01 |
| PE(39:1) | 788.616 | pos | 8.31 | PE | C44 H87 O8 N1 P1 | 0.09 | 0.02 |
| PE(44:2p) | 840.684 | pos | 12.85 | PE | C49 H95 O7 N1 P1 | 0.10 | 0.02 |
| PE(39:0) | 790.632 | pos | 9.68 | PE | C44 H89 O8 N1 P1 | 0.12 | 0.02 |
| PE(41:3) | 812.616 | pos | 7.34 | PE | C46 H87 O8 N1 P1 | 0.20 | 0.04 |
| PE(41:1) | 816.648 | pos | 9.77 | PE | C46 H91 O8 N1 P1 | 0.26 | 0.05 |
| PE(41:2) | 814.632 | pos | 8.41 | PE | C46 H89 O8 N1 P1 | 0.26 | 0.05 |
| PE(33:0) | 706.538 | pos | 9.66 | PE | C38 H77 O8 N1 P1 | 0.47 | 0.09 |
| PE(35:0) | 734.569 | pos | 9.68 | PE | C40 H81 O8 N1 P1 | 0.50 | 0.09 |
| PE(33:1) | 704.522 | pos | 8.33 | PE | C38 H75 O8 N1 P1 | 0.65 | 0.12 |
| PE(37:3) | 756.554 | pos | 7.40 | PE | C42 H79 O8 N1 P1 | 0.75 | 0.13 |
| PE(37:1) | 760.585 | pos | 9.77 | PE | C42 H83 O8 N1 P1 | 1.03 | 0.19 |
| PE(35:3) | 728.522 | pos | 7.35 | PE | C40 H75 O8 N1 P1 | 1.06 | 0.19 |
| PE(35:1) | 732.554 | pos | 9.75 | PE | C40 H79 O8 N1 P1 | 1.45 | 0.26 |
| PE(37:2) | 758.569 | pos | 8.41 | PE | C42 H81 O8 N1 P1 | 1.46 | 0.26 |
| PE(35:2) | 730.538 | pos | 8.39 | PE | C40 H77 O8 N1 P1 | 2.82 | 0.51 |
| PG(42:1) | 861.658 | pos | 12.76 | PG | C48 H94 O10 N0 P1 | 0.02 | 0.00 |
| PG(42:0) | 863.674 | pos | 13.06 | PG | C48 H96 O10 N0 P1 | 0.03 | 0.00 |
| PG(16:0/18:1) | 766.559 | pos | 8.95 | PG | C40 H81 O10 N1 P1 | 0.11 | 0.02 |
| PG(39:6) | 807.518 | neg | 10.02 | PG | C45 H76 O10 N0 P1 | 0.02 | 0.00 |
| PG(15:0/18:2) | 731.487 | neg | 7.19 | PG | C39 H72 O10 N0 P1 | 0.02 | 0.00 |
| PG(18:0/18:1) | 775.549 | neg | 10.95 | PG | C42 H80 O10 N0 P1 | 0.02 | 0.00 |
| PG(39:5) | 809.534 | neg | 11.57 | PG | C45 H78 O10 N0 P1 | 0.02 | 0.00 |
| PG(37:4) | 783.518 | neg | 11.58 | PG | C43 H76 O10 N0 P1 | 0.02 | 0.00 |
| PG(37:2) | 787.549 | neg | 4.59 | PG | C43 H80 O10 N0 P1 | 0.04 | 0.01 |
| PG(18:0/18:2) | 773.534 | neg | 9.30 | PG | C42 H78 O10 N0 P1 | 0.06 | 0.01 |
| PG(37:8) | 775.456 | neg | 6.63 | PG | C43 H68 O10 N0 P1 | 0.06 | 0.01 |
| PG(36:7) | 763.456 | neg | 7.53 | PG | C42 H68 O10 N0 P1 | 0.06 | 0.01 |
| PG(33:0) | 735.518 | neg | 4.58 | PG | C39 H76 O10 N0 P1 | 0.09 | 0.02 |
| PG(35:1) | 761.534 | neg | 4.58 | PG | C41 H78 O10 N0 P1 | 0.09 | 0.02 |
| PG(36:6) | 765.471 | neg | 8.54 | PG | C42 H70 O10 N0 P1 | 0.11 | 0.02 |
| PG(35:5) | 753.471 | neg | 8.31 | PG | C41 H70 O10 N0 P1 | 0.30 | 0.05 |
| PG(35:4) | 755.487 | neg | 9.66 | PG | C41 H72 O10 N0 P1 | 0.33 | 0.06 |
| PG(37:7) | 777.471 | neg | 7.38 | PG | C43 H70 O10 N0 P1 | 0.55 | 0.10 |
| PG(37:6) | 779.487 | neg | 8.44 | PG | C43 H72 O10 N0 P1 | 0.69 | 0.13 |
| PG(37:5) | 781.503 | neg | 9.81 | PG | C43 H74 O10 N0 P1 | 0.75 | 0.14 |
| PI(16:0/18:2) | 852.560 | pos | 7.49 | PI | C43 H83 O13 N1 P1 | 0.11 | 0.02 |
| PI(16:0/18:1) | 854.575 | pos | 8.61 | PI | C43 H85 O13 N1 P1 | 0.13 | 0.02 |
| PI(52:6) | 1077.738 | neg | 12.74 | PI | C61 H106 O13 N0 P1 | 0.02 | 0.00 |
| PI(17:0/18:2) | 847.534 | neg | 8.16 | PI | C44 H80 O13 N0 P1 | 0.02 | 0.00 |
| PI(18:1/14:0) | 807.503 | neg | 7.24 | PI | C41 H76 O13 N0 P1 | 0.02 | 0.00 |
| PI(14:0/18:2) | 805.487 | neg | 6.43 | PI | C41 H74 O13 N0 P1 | 0.02 | 0.00 |
| PI(15:0/18:1) | 821.519 | neg | 7.87 | PI | C42 H78 O13 N0 P1 | 0.03 | 0.01 |
| PI(15:0/18:2) | 819.503 | neg | 6.93 | PI | C42 H76 O13 N0 P1 | 0.06 | 0.01 |
| PI(18:1/18:1) | 861.550 | neg | 8.70 | PI | C45 H82 O13 N0 P1 | 0.91 | 0.17 |
| PIP(30:2e) | 843.443 | neg | 6.62 | PIP | C39 H73 O15 N0 P2 | 0.04 | 0.01 |
| PIP(42:8p) | 997.521 | neg | 8.70 | PIP | C51 H83 O15 N0 P2 | 0.05 | 0.01 |
| PIP(42:9p) | 995.506 | neg | 7.57 | PIP | C51 H81 O15 N0 P2 | 0.06 | 0.01 |
| PIP(40:8p) | 969.490 | neg | 7.49 | PIP | C49 H79 O15 N0 P2 | 0.13 | 0.02 |
| PIP(40:7p) | 971.506 | neg | 8.59 | PIP | C49 H81 O15 N0 P2 | 0.16 | 0.03 |
| PIP2(37:6) | 1027.436 | neg | 9.65 | PIP2 | C46 H78 O19 N0 P3 | 0.02 | 0.00 |
| PIP2(39:7) | 1053.451 | neg | 9.86 | PIP2 | C48 H80 O19 N0 P3 | 0.04 | 0.01 |
| PIP3(18:1/24:6) | 1175.465 | neg | 8.64 | PIP3 | C51 H87 O22 N0 P4 | 0.02 | 0.00 |
| PS(47:4) | 960.666 | pos | 8.95 | PS | C53 H96 O10 N1 P1 Na1 | 0.03 | 0.00 |
| PS(33:4/14:1) | 958.651 | pos | 7.76 | PS | C53 H94 O10 N1 P1 Na1 | 0.05 | 0.01 |
| PS(40:2) | 842.592 | neg | 9.92 | PS | C46 H85 O10 N1 P1 | 0.02 | 0.00 |
| PS(44:4) | 894.623 | neg | 12.66 | PS | C50 H89 O10 N1 P1 | 0.02 | 0.00 |
| PS(22:0/18:2) | 842.592 | neg | 12.36 | PS | C46 H85 O10 N1 P1 | 0.03 | 0.00 |
| PS(42:4) | 866.592 | neg | 12.32 | PS | C48 H85 O10 N1 P1 | 0.03 | 0.01 |
| PS(38:2) | 814.560 | neg | 8.25 | PS | C44 H81 O10 N1 P1 | 0.03 | 0.01 |
| PS(38:1) | 816.576 | neg | 9.58 | PS | C44 H83 O10 N1 P1 | 0.04 | 0.01 |
| PS(39:5) | 822.529 | neg | 6.29 | PS | C45 H77 O10 N1 P1 | 0.04 | 0.01 |
| PS(36:1) | 788.545 | neg | 8.15 | PS | C42 H79 O10 N1 P1 | 0.06 | 0.01 |
| PS(38:7) | 804.482 | neg | 7.18 | PS | C44 H71 O10 N1 P1 | 0.07 | 0.01 |
| PS(41:2) | 856.607 | neg | 10.88 | PS | C47 H87 O10 N1 P1 | 0.28 | 0.05 |
| PS(39:2) | 828.576 | neg | 9.49 | PS | C45 H83 O10 N1 P1 | 0.30 | 0.05 |
| PS(36:3) | 784.513 | neg | 11.00 | PS | C42 H75 O10 N1 P1 | 0.48 | 0.09 |
| PS(39:4) | 824.545 | neg | 6.97 | PS | C45 H79 O10 N1 P1 | 0.78 | 0.14 |
| PS(39:3) | 826.560 | neg | 7.82 | PS | C45 H81 O10 N1 P1 | 7.49 | 1.35 |
| PS(39:1) | 830.592 | neg | 10.59 | PS | C45 H85 O10 N1 P1 | 10.60 | 1.91 |
| So(d12:0) | 218.211 | pos | 0.71 | So | C12 H28 O2 N1 | 0.02 | 0.00 |
| So(d18:2) | 298.274 | pos | 1.99 | So | C18 H36 O2 N1 | 0.03 | 0.00 |
| So(d22:0) | 358.368 | pos | 4.29 | So | C22 H48 O2 N1 | 0.03 | 0.01 |
| So(d20:0) | 330.337 | pos | 3.23 | So | C20 H44 O2 N1 | 0.04 | 0.01 |
| So(d16:1) | 272.258 | pos | 1.47 | So | C16 H34 O2 N1 | 0.04 | 0.01 |
| So(d14:0) | 246.243 | pos | 0.85 | So | C14 H32 O2 N1 | 0.08 | 0.01 |
| So(d16:0) | 274.274 | pos | 1.20 | So | C16 H36 O2 N1 | 7.64 | 1.38 |
| SQDG(30:2) | 807.457 | neg | 7.35 | SQDG | C40 H71 O14 S1 | 0.02 | 0.00 |
| SQDG(39:13) | 911.426 | neg | 6.62 | SQDG | C49 H67 O14 S1 | 0.02 | 0.00 |
| SQDG(17:5/23:2) | 937.535 | neg | 11.63 | SQDG | C50 H81 O14 S1 | 0.02 | 0.00 |
| SQDG(16:0/16:0) | 793.514 | neg | 8.24 | SQDG | C41 H77 O12 S1 | 0.03 | 0.01 |
| SQDG(34:1) | 819.530 | neg | 8.35 | SQDG | C43 H79 O12 S1 | 0.03 | 0.01 |
| SQDG(30:1) | 809.473 | neg | 8.39 | SQDG | C40 H73 O14 S1 | 0.04 | 0.01 |
| SQDG(36:3) | 843.530 | neg | 7.40 | SQDG | C45 H79 O12 S1 | 0.05 | 0.01 |
| SQDG(18:2/18:2) | 841.514 | neg | 6.59 | SQDG | C45 H77 O12 S1 | 0.06 | 0.01 |
| SQDG(40:7) | 937.535 | neg | 11.03 | SQDG | C50 H81 O14 S1 | 0.06 | 0.01 |
| SQDG(16:0/18:2) | 817.514 | neg | 7.33 | SQDG | C43 H77 O12 S1 | 0.09 | 0.02 |
| SQDG(39:12) | 913.441 | neg | 7.36 | SQDG | C49 H69 O14 S1 | 0.09 | 0.02 |
| SQDG(39:11) | 915.457 | neg | 8.47 | SQDG | C49 H71 O14 S1 | 0.10 | 0.02 |
| SQDG(39:10) | 917.473 | neg | 9.82 | SQDG | C49 H73 O14 S1 | 0.16 | 0.03 |
| SQDG(37:7) | 849.483 | neg | 9.80 | SQDG | C46 H73 O12 S1 | 0.33 | 0.06 |
| TG(20:0/16:0/18:1) | 911.804 | pos | 15.39 | TG | C57 H108 O6 Na1 | 0.02 | 0.00 |
| TG(63:15) | 1004.770 | pos | 12.41 | TG | C66 H102 O6 N1 | 0.02 | 0.00 |
| TG(57:5) | 940.833 | pos | 14.13 | TG | C60 H110 O6 N1 | 0.02 | 0.00 |
| TG(24:0/18:2/18:3) | 987.835 | pos | 15.13 | TG | C63 H112 O6 Na1 | 0.02 | 0.00 |
| TG(19:1/18:1/18:2) | 919.773 | pos | 14.46 | TG | C58 H104 O6 Na1 | 0.02 | 0.00 |
| TG(16:0/14:0/18:1) | 822.755 | pos | 14.28 | TG | C51 H100 O6 N1 | 0.02 | 0.00 |
| TG(18:3/18:2/23:0) | 968.864 | pos | 14.93 | TG | C62 H114 O6 N1 | 0.02 | 0.00 |
| TG(14:0/18:2/18:2) | 849.694 | pos | 13.63 | TG | C53 H94 O6 Na1 | 0.02 | 0.00 |
| TG(64:3) | 1042.974 | pos | 16.06 | TG | C67 H128 O6 N1 | 0.02 | 0.00 |
| TG(57:9e) | 923.746 | pos | 14.57 | TG | C60 H100 O5 Na1 | 0.02 | 0.00 |
| TG(26:0/8:0/18:1) | 883.773 | pos | 14.27 | TG | C55 H104 O6 Na1 | 0.02 | 0.00 |
| TG(18:1/18:2/21:0) | 949.819 | pos | 15.20 | TG | C60 H110 O6 Na1 | 0.02 | 0.00 |
| TG(18:0/17:0/18:1) | 892.833 | pos | 15.21 | TG | C56 H110 O6 N1 | 0.02 | 0.00 |
| TG(57:10p) | 919.715 | pos | 13.93 | TG | C60 H96 O5 Na1 | 0.02 | 0.00 |
| TG(4:0/16:2/18:2) | 676.551 | pos | 11.63 | TG | C41 H74 O6 N1 | 0.02 | 0.00 |
| TG(18:0/18:1/24:0) | 990.942 | pos | 16.42 | TG | C63 H124 O6 N1 | 0.02 | 0.00 |
| TG(4:0/18:2/18:2) | 687.556 | pos | 8.28 | TG | C43 H75 O6 | 0.02 | 0.00 |
| TG(40:0p) | 696.650 | pos | 12.60 | TG | C43 H86 O5 N1 | 0.02 | 0.00 |
| TG(37:0p) | 654.603 | pos | 12.05 | TG | C40 H80 O5 N1 | 0.03 | 0.00 |
| TG(18:2/18:2/23:0) | 975.835 | pos | 15.23 | TG | C62 H112 O6 Na1 | 0.03 | 0.00 |
| TG(55:10p) | 891.684 | pos | 13.72 | TG | C58 H92 O5 Na1 | 0.03 | 0.01 |
| TG(18:1/18:2/23:0) | 977.851 | pos | 15.56 | TG | C62 H114 O6 Na1 | 0.03 | 0.01 |
| TG(20:1/18:1/24:0) | 1016.958 | pos | 16.39 | TG | C65 H126 O6 N1 | 0.03 | 0.01 |
| TG(22:0/18:3/18:3) | 952.833 | pos | 14.36 | TG | C61 H110 O6 N1 | 0.03 | 0.01 |
| TG(18:1/12:0/18:2) | 818.723 | pos | 13.60 | TG | C51 H96 O6 N1 | 0.03 | 0.01 |
| TG(16:0/18:1/21:0) | 920.864 | pos | 15.56 | TG | C58 H114 O6 N1 | 0.03 | 0.01 |
| TG(18:1/18:2/20:5) | 920.770 | pos | 13.11 | TG | C59 H102 O6 N1 | 0.03 | 0.01 |
| TG(18:1/18:2/22:4) | 933.791 | pos | 14.59 | TG | C61 H105 O6 | 0.03 | 0.01 |
| TG(19:1/18:3/21:1) | 954.848 | pos | 14.27 | TG | C61 H112 O6 N1 | 0.03 | 0.01 |
| TG(18:3/18:3/18:3) | 873.697 | pos | 13.43 | TG | C57 H93 O6 | 0.04 | 0.01 |
| TG(22:2/18:2/18:2) | 952.833 | pos | 14.10 | TG | C61 H110 O6 N1 | 0.04 | 0.01 |
| TG(24:1/18:2/18:2) | 982.880 | pos | 14.93 | TG | C63 H116 O6 N1 | 0.04 | 0.01 |
| TG(19:1/18:1/18:3) | 912.801 | pos | 13.81 | TG | C58 H106 O6 N1 | 0.04 | 0.01 |
| TG(18:1/18:2/21:1) | 942.848 | pos | 14.46 | TG | C60 H112 O6 N1 | 0.04 | 0.01 |
| TG(55:9p) | 893.699 | pos | 14.05 | TG | C58 H94 O5 Na1 | 0.04 | 0.01 |
| TG(18:1/17:1/18:2) | 891.741 | pos | 14.17 | TG | C56 H100 O6 Na1 | 0.04 | 0.01 |
| TG(25:0/13:1/23:0) | 1004.958 | pos | 15.36 | TG | C64 H126 O6 N1 | 0.04 | 0.01 |
| TG(16:0/18:1/23:0) | 948.895 | pos | 15.91 | TG | C60 H118 O6 N1 | 0.04 | 0.01 |
| TG(18:1/14:0/18:2) | 846.755 | pos | 13.63 | TG | C53 H100 O6 N1 | 0.04 | 0.01 |
| TG(16:0/16:0/18:2) | 853.726 | pos | 14.36 | TG | C53 H98 O6 Na1 | 0.04 | 0.01 |
| TG(26:0/18:2/18:2) | 1012.927 | pos | 15.76 | TG | C65 H122 O6 N1 | 0.04 | 0.01 |
| TG(14:0/18:2/18:3) | 842.723 | pos | 13.35 | TG | C53 H96 O6 N1 | 0.05 | 0.01 |
| TG(61:2) | 1002.942 | pos | 15.89 | TG | C64 H124 O6 N1 | 0.05 | 0.01 |
| TG(15:0/18:2/18:2) | 863.710 | pos | 13.81 | TG | C54 H96 O6 Na1 | 0.05 | 0.01 |
| TG(59:7) | 964.833 | pos | 13.38 | TG | C62 H110 O6 N1 | 0.05 | 0.01 |
| TG(15:0/18:1/18:2) | 865.726 | pos | 14.14 | TG | C54 H98 O6 Na1 | 0.05 | 0.01 |
| TG(18:3/18:2/20:2) | 922.786 | pos | 13.72 | TG | C59 H104 O6 N1 | 0.06 | 0.01 |
| TG(19:0/19:0/23:4) | 998.911 | pos | 15.23 | TG | C64 H120 O6 N1 | 0.06 | 0.01 |
| TG(18:1/18:1/21:1) | 944.864 | pos | 14.86 | TG | C60 H114 O6 N1 | 0.06 | 0.01 |
| TG(16:0/14:0/18:2) | 820.739 | pos | 13.95 | TG | C51 H98 O6 N1 | 0.06 | 0.01 |
| TG(15:0/16:0/18:1) | 836.770 | pos | 14.48 | TG | C52 H102 O6 N1 | 0.06 | 0.01 |
| TG(6:0/14:1/18:2) | 678.567 | pos | 12.01 | TG | C41 H76 O6 N1 | 0.06 | 0.01 |
| TG(18:1/20:4/24:0) | 993.884 | pos | 16.05 | TG | C65 H117 O6 | 0.06 | 0.01 |
| TG(25:1/18:1/18:1) | 1000.927 | pos | 15.56 | TG | C64 H122 O6 N1 | 0.07 | 0.01 |
| TG(6:0/14:1/18:1) | 680.582 | pos | 12.32 | TG | C41 H78 O6 N1 | 0.07 | 0.01 |
| TG(66:2) | 1073.021 | pos | 16.05 | TG | C69 H134 O6 N1 | 0.08 | 0.01 |
| TG(16:0/18:2/21:0) | 918.848 | pos | 15.22 | TG | C58 H112 O6 N1 | 0.09 | 0.02 |
| TG(41:0p) | 710.666 | pos | 12.77 | TG | C44 H88 O5 N1 | 0.09 | 0.02 |
| TG(18:3/18:2/18:2) | 899.710 | pos | 13.38 | TG | C57 H96 O6 Na1 | 0.09 | 0.02 |
| TG(26:0/18:1/18:2) | 1014.942 | pos | 16.07 | TG | C65 H124 O6 N1 | 0.09 | 0.02 |
| TG(18:1/18:1/20:4) | 907.775 | pos | 14.58 | TG | C59 H103 O6 | 0.10 | 0.02 |
| TG(18:1/18:1/24:1) | 986.911 | pos | 15.37 | TG | C63 H120 O6 N1 | 0.10 | 0.02 |
| TG(18:0/17:2/18:2) | 886.786 | pos | 13.81 | TG | C56 H104 O6 N1 | 0.11 | 0.02 |
| TG(18:2/18:2/21:0) | 942.848 | pos | 14.87 | TG | C60 H112 O6 N1 | 0.12 | 0.02 |
| TG(18:1/18:2/20:4) | 905.759 | pos | 14.25 | TG | C59 H101 O6 | 0.12 | 0.02 |
| TG(18:1/18:1/23:0) | 974.911 | pos | 15.89 | TG | C62 H120 O6 N1 | 0.13 | 0.02 |
| TG(22:1/18:2/18:2) | 954.848 | pos | 14.64 | TG | C61 H112 O6 N1 | 0.13 | 0.02 |
| TG(18:1/18:2/22:1) | 956.864 | pos | 14.60 | TG | C61 H114 O6 N1 | 0.15 | 0.03 |
| TG(19:1/18:1/18:1) | 916.833 | pos | 14.81 | TG | C58 H110 O6 N1 | 0.15 | 0.03 |
| TG(18:1/18:1/21:0) | 946.880 | pos | 15.56 | TG | C60 H116 O6 N1 | 0.16 | 0.03 |
| TG(59:3) | 972.895 | pos | 14.58 | TG | C62 H118 O6 N1 | 0.17 | 0.03 |
| TG(25:1/18:2/19:0) | 1014.942 | pos | 15.73 | TG | C65 H124 O6 N1 | 0.18 | 0.03 |
| TG(62:2) | 1016.958 | pos | 16.05 | TG | C65 H126 O6 N1 | 0.19 | 0.03 |
| TG(16:1/18:2/18:3) | 868.739 | pos | 13.42 | TG | C55 H98 O6 N1 | 0.21 | 0.04 |
| TG(20:5/18:2/18:2) | 901.728 | pos | 13.66 | TG | C59 H97 O6 | 0.24 | 0.04 |
| TG(19:1/16:0/18:1) | 890.817 | pos | 14.82 | TG | C56 H108 O6 N1 | 0.24 | 0.04 |
| TG(17:4/17:3/22:0) | 922.786 | pos | 13.38 | TG | C59 H104 O6 N1 | 0.25 | 0.05 |
| TG(15:0/18:1/18:1) | 862.786 | pos | 14.47 | TG | C54 H104 O6 N1 | 0.29 | 0.05 |
| TG(18:1/18:2/24:1) | 984.895 | pos | 15.07 | TG | C63 H118 O6 N1 | 0.32 | 0.06 |
| TG(16:0/18:1/24:0) | 962.911 | pos | 16.08 | TG | C61 H120 O6 N1 | 0.38 | 0.07 |
| TG(18:1/17:1/18:1) | 888.801 | pos | 14.45 | TG | C56 H106 O6 N1 | 0.38 | 0.07 |
| TG(20:1/18:2/18:3) | 924.801 | pos | 14.02 | TG | C59 H106 O6 N1 | 0.42 | 0.08 |
| TG(16:0/18:1/22:0) | 934.880 | pos | 15.74 | TG | C59 H116 O6 N1 | 0.56 | 0.10 |
| TG(18:0/16:0/18:1) | 878.817 | pos | 15.03 | TG | C55 H108 O6 N1 | 0.67 | 0.12 |
| TG(20:1/18:1/18:1) | 930.848 | pos | 14.59 | TG | C59 H112 O6 N1 | 0.82 | 0.15 |
| TG(18:1/18:1/24:0) | 988.927 | pos | 16.05 | TG | C63 H122 O6 N1 | 0.95 | 0.17 |
| TG(18:1/18:3/24:0) | 984.895 | pos | 15.41 | TG | C63 H118 O6 N1 | 1.10 | 0.20 |
| TG(18:1/18:2/24:0) | 986.911 | pos | 15.73 | TG | C63 H120 O6 N1 | 1.23 | 0.22 |
| TG(20:1/18:2/18:2) | 926.817 | pos | 14.30 | TG | C59 H108 O6 N1 | 1.29 | 0.23 |
| TG(16:0/16:0/18:1) | 850.786 | pos | 14.67 | TG | C53 H104 O6 N1 | 1.35 | 0.24 |
| TG(22:0/18:2/18:2) | 956.864 | pos | 15.04 | TG | C61 H114 O6 N1 | 1.92 | 0.35 |
| TG(18:1/18:1/22:0) | 960.895 | pos | 15.71 | TG | C61 H118 O6 N1 | 2.10 | 0.38 |
| TG(20:0/18:2/18:2) | 928.833 | pos | 14.62 | TG | C59 H110 O6 N1 | 2.22 | 0.40 |
| TG(18:1/18:2/22:0) | 958.880 | pos | 15.38 | TG | C61 H116 O6 N1 | 2.46 | 0.44 |
| TG(20:0/18:1/18:1) | 932.864 | pos | 15.36 | TG | C59 H114 O6 N1 | 2.59 | 0.47 |

**Table S4**

Molecular species of lipids in stored SS-treated buckwheat

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
| Lipid | m/z | Ion mode | Retention time | Class | Formula | Relative abundance/% | SD |
| Cer(d20:2/18:2) | 588.535 | pos | 11.03 | Cer | C38 H70 O3 N1 | 0.01 | 0.00 |
| Cer(d38:7) | 582.488 | pos | 8.14 | Cer | C38 H64 O3 N1 | 0.01 | 0.01 |
| Cer(d16:0/18:0) | 540.535 | pos | 9.74 | Cer | C34 H70 O3 N1 | 0.01 | 0.01 |
| Cer(d18:0) | 316.285 | pos | 1.79 | Cer | C18 H38 O3 N1 | 0.02 | 0.01 |
| Cer(d18:1/20:5) | 584.504 | pos | 9.48 | Cer | C38 H66 O3 N1 | 0.02 | 0.01 |
| Cer(d18:1/18:4) | 558.488 | pos | 9.28 | Cer | C36 H64 O3 N1 | 0.02 | 0.01 |
| Cer(d32:0) | 512.504 | pos | 7.97 | Cer | C32 H66 O3 N1 | 0.03 | 0.01 |
| Cer(d18:2/18:1+O) | 578.514 | pos | 7.46 | Cer | C36 H68 O4 N1 | 0.04 | 0.02 |
| Cer(d24:0/18:0+O) | 668.655 | pos | 12.75 | Cer | C42 H86 O4 N1 | 0.01 | 0.00 |
| Cer(d18:2/18:0+O) | 580.530 | pos | 8.58 | Cer | C36 H70 O4 N1 | 0.05 | 0.02 |
| Cer(d18:2/18:2) | 560.504 | pos | 8.14 | Cer | C36 H66 O3 N1 | 0.04 | 0.02 |
| Cer(d24:0/18:1+O) | 666.639 | pos | 12.55 | Cer | C42 H84 O4 N1 | 0.02 | 0.01 |
| Cer(d18:2/16:0) | 536.504 | pos | 9.29 | Cer | C34 H66 O3 N1 | 0.04 | 0.02 |
| Cer(d22:1) | 368.317 | neg | 4.81 | Cer | C22 H42 O3 N1 | 0.48 | 0.20 |
| Cer(d24:2) | 394.333 | neg | 4.91 | Cer | C24 H44 O3 N1 | 0.62 | 0.26 |
| Cer(d20:2) | 338.270 | neg | 3.92 | Cer | C20 H36 O3 N1 | 0.95 | 0.39 |
| Cer(d20:2/2:0) | 366.301 | neg | 4.33 | Cer | C22 H40 O3 N1 | 0.32 | 0.13 |
| CL(71:1) | 723.526 | neg | 8.12 | CL | C80 H152 O17 P2 | 0.97 | 0.40 |
| CL(71:3) | 721.510 | neg | 7.22 | CL | C80 H148 O17 P2 | 0.51 | 0.21 |
| CL(53:3) | 1191.746 | neg | 12.71 | CL | C62 H113 O17 P2 | 0.02 | 0.01 |
| CL(51:2) | 1165.730 | neg | 12.71 | CL | C60 H111 O17 P2 | 0.03 | 0.01 |
| CL(87:15) | 821.541 | neg | 7.68 | CL | C96 H156 O17 P2 | 0.03 | 0.01 |
| CL(18:2/20:4/18:1/18:2) | 1473.981 | neg | 13.71 | CL | C83 H143 O17 P2 | 0.02 | 0.01 |
| CL(20:5/18:2/18:1/18:2) | 1471.965 | neg | 13.47 | CL | C83 H141 O17 P2 | 0.03 | 0.01 |
| CL(20:5/18:2/18:2/18:2) | 1469.949 | neg | 13.22 | CL | C83 H139 O17 P2 | 0.02 | 0.01 |
| CL(18:2/18:1/18:1/18:2) | 1451.996 | neg | 13.72 | CL | C81 H145 O17 P2 | 0.05 | 0.02 |
| CL(83:7) | 801.573 | neg | 11.65 | CL | C92 H164 O17 P2 | 0.05 | 0.02 |
| CL(87:9) | 827.588 | neg | 11.65 | CL | C96 H168 O17 P2 | 0.10 | 0.04 |
| CL(83:15) | 793.510 | neg | 8.24 | CL | C92 H148 O17 P2 | 0.11 | 0.05 |
| CL(83:9) | 799.557 | neg | 10.17 | CL | C92 H160 O17 P2 | 0.06 | 0.03 |
| CL(87:11) | 825.573 | neg | 10.21 | CL | C96 H164 O17 P2 | 0.12 | 0.05 |
| CL(18:2/18:1/18:2/18:2) | 1449.981 | neg | 13.46 | CL | C81 H143 O17 P2 | 0.09 | 0.04 |
| CL(18:2/18:2/18:2/18:2) | 1447.965 | neg | 13.22 | CL | C81 H141 O17 P2 | 0.06 | 0.02 |
| CL(87:13) | 823.557 | neg | 8.71 | CL | C96 H160 O17 P2 | 0.19 | 0.08 |
| DG(58:6) | 921.827 | pos | 13.93 | DG | C61 H109 O5 | 0.08 | 0.03 |
| DG(60:6) | 949.858 | pos | 14.28 | DG | C63 H113 O5 | 0.05 | 0.02 |
| DG(56:3) | 921.825 | pos | 13.93 | DG | C59 H110 O5 Na1 | 0.08 | 0.03 |
| DG(58:3) | 949.856 | pos | 14.28 | DG | C61 H114 O5 Na1 | 0.04 | 0.02 |
| DG(20:1/18:1) | 666.603 | pos | 12.45 | DG | C41 H80 O5 N1 | 0.02 | 0.01 |
| DG(22:0/18:2) | 694.634 | pos | 12.87 | DG | C43 H84 O5 N1 | 0.02 | 0.01 |
| DG(34:1e) | 603.532 | pos | 12.10 | DG | C37 H72 O4 Na1 | 0.03 | 0.01 |
| DG(20:1/18:2) | 664.587 | pos | 12.14 | DG | C41 H78 O5 N1 | 0.04 | 0.01 |
| DG(56:6) | 893.796 | pos | 13.62 | DG | C59 H105 O5 | 0.41 | 0.17 |
| DG(55:8) | 897.731 | pos | 14.71 | DG | C58 H98 O5 Na1 | 0.01 | 0.01 |
| DG(34:1p) | 601.517 | pos | 7.57 | DG | C37 H70 O4 Na1 | 0.01 | 0.00 |
| DG(58:7) | 919.811 | pos | 13.61 | DG | C61 H107 O5 | 0.62 | 0.26 |
| DG(18:2/18:2) | 639.496 | pos | 10.67 | DG | C39 H68 O5 Na1 | 0.06 | 0.02 |
| DG(38:3) | 664.587 | pos | 11.76 | DG | C41 H78 O5 N1 | 0.02 | 0.01 |
| DG(36:3p) | 603.535 | pos | 8.67 | DG | C39 H71 O4 | 0.01 | 0.00 |
| DG(38:0e) | 661.611 | pos | 15.71 | DG | C41 H82 O4 Na1 | 0.01 | 0.00 |
| DG(38:2p) | 633.582 | pos | 15.36 | DG | C41 H77 O4 | 0.01 | 0.00 |
| DG(16:0/18:1) | 612.556 | pos | 12.09 | DG | C37 H74 O5 N1 | 0.04 | 0.02 |
| DG(36:1e) | 631.564 | pos | 14.96 | DG | C39 H76 O4 Na1 | 0.02 | 0.01 |
| DG(32:0p) | 575.501 | pos | 7.79 | DG | C35 H68 O4 Na1 | 0.02 | 0.01 |
| DG(41:4) | 704.619 | pos | 12.43 | DG | C44 H82 O5 N1 | 0.02 | 0.01 |
| DG(18:1/18:1) | 638.572 | pos | 12.10 | DG | C39 H76 O5 N1 | 0.16 | 0.07 |
| DG(16:0/18:2) | 610.541 | pos | 11.74 | DG | C37 H72 O5 N1 | 0.14 | 0.06 |
| DG(34:0p) | 603.532 | pos | 14.62 | DG | C37 H72 O4 Na1 | 0.09 | 0.04 |
| DGDG(16:0/18:0) | 965.642 | neg | 11.75 | DGDG | C50 H93 O17 | 0.01 | 0.00 |
| DGDG(18:0/18:2) | 989.642 | neg | 10.88 | DGDG | C52 H93 O17 | 0.03 | 0.01 |
| DGDG(16:0/16:0) | 937.611 | neg | 10.32 | DGDG | C48 H89 O17 | 0.02 | 0.01 |
| DGDG(16:0/18:1) | 963.626 | neg | 10.42 | DGDG | C50 H91 O17 | 0.10 | 0.04 |
| DGDG(18:1/18:1) | 989.642 | neg | 10.54 | DGDG | C52 H93 O17 | 0.18 | 0.08 |
| DGDG(18:1/18:2) | 987.626 | neg | 8.96 | DGDG | C52 H91 O17 | 0.33 | 0.14 |
| DGDG(16:0/18:2) | 961.611 | neg | 8.89 | DGDG | C50 H89 O17 | 0.20 | 0.08 |
| DGDG(18:3/18:3) | 981.579 | neg | 6.27 | DGDG | C52 H85 O17 | 0.12 | 0.05 |
| DGDG(18:2/18:3) | 983.595 | neg | 6.94 | DGDG | C52 H87 O17 | 0.31 | 0.13 |
| DGDG(18:2/18:2) | 985.611 | neg | 7.77 | DGDG | C52 H89 O17 | 0.88 | 0.36 |
| DGMG(18:3) | 721.365 | neg | 1.62 | DGMG | C34 H57 O16 | 0.04 | 0.02 |
| DGMG(18:1) | 725.397 | neg | 3.19 | DGMG | C34 H61 O16 | 0.26 | 0.11 |
| DGMG(18:2) | 723.381 | neg | 2.16 | DGMG | C34 H59 O16 | 0.32 | 0.13 |
| LPA(16:0) | 409.236 | neg | 2.74 | LPA | C19 H38 O7 N0 P1 | 0.04 | 0.02 |
| LPA(18:1) | 435.252 | neg | 3.08 | LPA | C21 H40 O7 N0 P1 | 0.29 | 0.12 |
| LPA(18:2) | 433.236 | neg | 2.16 | LPA | C21 H38 O7 N0 P1 | 0.24 | 0.10 |
| LPC(16:1) | 494.324 | pos | 2.01 | LPC | C24 H49 O7 N1 P1 | 0.01 | 0.01 |
| LPC(20:1) | 550.387 | pos | 4.37 | LPC | C28 H57 O7 N1 P1 | 0.03 | 0.01 |
| LPC(16:0) | 496.340 | pos | 2.70 | LPC | C24 H51 O7 N1 P1 | 0.06 | 0.02 |
| LPC(18:0) | 524.371 | pos | 4.25 | LPC | C26 H55 O7 N1 P1 | 0.03 | 0.01 |
| LPC(20:5) | 542.324 | pos | 2.37 | LPC | C28 H49 O7 N1 P1 | 0.08 | 0.03 |
| LPC(20:4) | 544.340 | pos | 3.28 | LPC | C28 H51 O7 N1 P1 | 0.09 | 0.04 |
| LPC(18:2) | 520.340 | pos | 2.38 | LPC | C26 H51 O7 N1 P1 | 2.54 | 1.05 |
| LPC(18:1) | 522.355 | pos | 3.29 | LPC | C26 H53 O7 N1 P1 | 3.20 | 1.32 |
| LPE(20:0) | 508.341 | neg | 5.05 | LPE | C25 H51 O7 N1 P1 | 0.03 | 0.01 |
| MG(36:4) | 603.535 | pos | 12.10 | MG | C39 H71 O4 | 0.03 | 0.01 |
| MG(36:5) | 601.519 | pos | 11.75 | MG | C39 H69 O4 | 0.05 | 0.02 |
| MGDG(45:5) | 901.677 | neg | 4.10 | MGDG | C54 H93 O10 | 0.10 | 0.04 |
| MGDG(34:2) | 753.552 | neg | 9.67 | MGDG | C43 H77 O10 | 0.14 | 0.06 |
| MGDG(34:3) | 751.537 | neg | 8.26 | MGDG | C43 H75 O10 | 0.11 | 0.05 |
| MGDG(31:2) | 711.505 | neg | 4.99 | MGDG | C40 H71 O10 | 0.20 | 0.08 |
| MGDG(18:3/18:3) | 819.526 | neg | 6.87 | MGDG | C46 H75 O12 | 0.02 | 0.01 |
| MGDG(29:0) | 687.505 | neg | 5.34 | MGDG | C38 H71 O10 | 0.05 | 0.02 |
| MGDG(18:2/18:3) | 821.542 | neg | 7.68 | MGDG | C46 H77 O12 | 0.03 | 0.01 |
| MGDG(16:0/18:1) | 801.573 | neg | 11.64 | MGDG | C44 H81 O12 | 0.03 | 0.01 |
| MGDG(18:1/18:1) | 827.589 | neg | 11.65 | MGDG | C46 H83 O12 | 0.10 | 0.04 |
| MGDG(16:0/18:2) | 799.558 | neg | 10.17 | MGDG | C44 H79 O12 | 0.06 | 0.03 |
| MGDG(18:1/18:2) | 825.573 | neg | 10.21 | MGDG | C46 H81 O12 | 0.12 | 0.05 |
| MGDG(18:2/18:2) | 823.558 | neg | 8.71 | MGDG | C46 H79 O12 | 0.19 | 0.08 |
| MGDG(47:12) | 961.605 | neg | 5.70 | MGDG | C57 H85 O12 | 0.94 | 0.39 |
| MGMG(18:3) | 559.312 | neg | 2.23 | MGMG | C28 H47 O11 | 0.04 | 0.02 |
| MGMG(18:1) | 563.344 | neg | 3.81 | MGMG | C28 H51 O11 | 0.32 | 0.13 |
| MGMG(18:2) | 561.328 | neg | 2.99 | MGMG | C28 H49 O11 | 0.52 | 0.21 |
| PA(31:5/18:2) | 871.622 | neg | 12.47 | PA | C52 H88 O8 N0 P1 | 0.05 | 0.02 |
| PA(16:0/18:1) | 673.481 | neg | 9.90 | PA | C37 H70 O8 N0 P1 | 2.24 | 0.93 |
| PA(16:0/18:2) | 671.466 | neg | 8.52 | PA | C37 H68 O8 N0 P1 | 1.60 | 0.66 |
| PA(18:1/18:1) | 699.497 | neg | 9.99 | PA | C39 H72 O8 N0 P1 | 4.56 | 1.89 |
| PA(18:2/18:2) | 695.466 | neg | 7.50 | PA | C39 H68 O8 N0 P1 | 2.29 | 0.95 |
| PA(18:1/18:2) | 697.481 | neg | 8.56 | PA | C39 H70 O8 N0 P1 | 6.06 | 2.51 |
| PC(39:8p) | 822.541 | pos | 8.98 | PC | C47 H78 O7 N1 P1 Na1 | 0.01 | 0.01 |
| PC(39:7p) | 824.556 | pos | 10.62 | PC | C47 H80 O7 N1 P1 Na1 | 0.02 | 0.01 |
| PC(34:3) | 756.554 | pos | 7.58 | PC | C42 H79 O8 N1 P1 | 0.01 | 0.00 |
| PC(32:1) | 732.554 | pos | 8.60 | PC | C40 H79 O8 N1 P1 | 0.01 | 0.00 |
| PC(38:3) | 812.616 | pos | 10.88 | PC | C46 H87 O8 N1 P1 | 0.04 | 0.01 |
| PC(36:1) | 788.616 | pos | 11.81 | PC | C44 H87 O8 N1 P1 | 0.03 | 0.01 |
| PC(38:2) | 814.632 | pos | 11.79 | PC | C46 H89 O8 N1 P1 | 0.05 | 0.02 |
| PC(36:5) | 780.554 | pos | 6.96 | PC | C44 H79 O8 N1 P1 | 0.05 | 0.02 |
| PC(16:0/18:1) | 782.567 | pos | 10.47 | PC | C42 H82 O8 N1 P1 Na1 | 0.05 | 0.02 |
| PC(16:0/18:2) | 780.551 | pos | 8.90 | PC | C42 H80 O8 N1 P1 Na1 | 0.06 | 0.03 |
| PC(18:2/18:2) | 804.551 | pos | 7.78 | PC | C44 H80 O8 N1 P1 Na1 | 0.09 | 0.04 |
| PC(18:1/18:2) | 806.567 | pos | 9.02 | PC | C44 H82 O8 N1 P1 Na1 | 0.17 | 0.07 |
| PC(18:1/18:1) | 808.583 | pos | 10.61 | PC | C44 H84 O8 N1 P1 Na1 | 0.24 | 0.10 |
| PC(34:1) | 760.585 | pos | 10.49 | PC | C42 H83 O8 N1 P1 | 0.87 | 0.36 |
| PC(16:1/18:1) | 758.569 | pos | 8.41 | PC | C42 H81 O8 N1 P1 | 0.02 | 0.01 |
| PC(34:2) | 758.569 | pos | 8.91 | PC | C42 H81 O8 N1 P1 | 1.54 | 0.64 |
| PC(36:4) | 782.569 | pos | 7.79 | PC | C44 H81 O8 N1 P1 | 1.78 | 0.74 |
| PC(36:2) | 786.601 | pos | 10.58 | PC | C44 H85 O8 N1 P1 | 3.51 | 1.45 |
| PC(36:3) | 784.585 | pos | 8.99 | PC | C44 H83 O8 N1 P1 | 4.53 | 1.88 |
| PE(27:4e) | 622.384 | pos | 2.54 | PE | C32 H58 O7 N1 P1 Na1 | 0.01 | 0.00 |
| PE(32:1) | 690.507 | pos | 8.45 | PE | C37 H73 O8 N1 P1 | 0.01 | 0.00 |
| PE(18:0p) | 480.308 | pos | 3.03 | PE | C23 H47 O7 N1 P1 | 0.01 | 0.01 |
| PE(34:3) | 714.507 | pos | 7.48 | PE | C39 H73 O8 N1 P1 | 0.01 | 0.01 |
| PE(34:2) | 716.522 | pos | 8.59 | PE | C39 H75 O8 N1 P1 | 0.04 | 0.02 |
| PE(16:1/18:1) | 716.522 | pos | 8.87 | PE | C39 H75 O8 N1 P1 | 0.03 | 0.01 |
| PE(42:2p) | 812.653 | pos | 12.80 | PE | C47 H91 O7 N1 P1 | 0.08 | 0.03 |
| PE(42:9p) | 820.525 | pos | 7.78 | PE | C47 H76 O7 N1 P1 Na1 | 0.01 | 0.01 |
| PE(47:11) | 880.585 | pos | 7.50 | PE | C52 H83 O8 N1 P1 | 0.01 | 0.01 |
| PE(34:1) | 740.520 | pos | 10.98 | PE | C39 H76 O8 N1 P1 Na1 | 0.01 | 0.01 |
| PE(36:3) | 764.520 | pos | 9.39 | PE | C41 H76 O8 N1 P1 Na1 | 0.03 | 0.01 |
| PE(37:2) | 758.569 | pos | 8.41 | PE | C42 H81 O8 N1 P1 | 0.02 | 0.01 |
| PE(35:2) | 730.538 | pos | 8.39 | PE | C40 H77 O8 N1 P1 | 0.01 | 0.00 |
| PG(28:0/18:2) | 915.705 | pos | 12.60 | PG | C52 H100 O10 N0 P1 | 0.01 | 0.01 |
| PG(28:0/16:0) | 891.705 | pos | 12.55 | PG | C50 H100 O10 N0 P1 | 0.01 | 0.00 |
| PG(28:0/18:1) | 917.721 | pos | 12.84 | PG | C52 H102 O10 N0 P1 | 0.07 | 0.03 |
| PG(46:0) | 919.736 | pos | 13.04 | PG | C52 H104 O10 N0 P1 | 0.16 | 0.07 |
| PG(42:1) | 861.658 | pos | 12.76 | PG | C48 H94 O10 N0 P1 | 0.01 | 0.01 |
| PG(16:0/18:1) | 766.559 | pos | 8.95 | PG | C40 H81 O10 N1 P1 | 0.04 | 0.02 |
| PG(37:2) | 787.549 | neg | 4.59 | PG | C43 H80 O10 N0 P1 | 0.44 | 0.18 |
| PG(36:7) | 763.456 | neg | 7.53 | PG | C42 H68 O10 N0 P1 | 0.27 | 0.11 |
| PG(33:0) | 735.518 | neg | 4.58 | PG | C39 H76 O10 N0 P1 | 2.11 | 0.87 |
| PG(35:1) | 761.534 | neg | 4.58 | PG | C41 H78 O10 N0 P1 | 1.32 | 0.54 |
| PG(36:6) | 765.471 | neg | 8.54 | PG | C42 H70 O10 N0 P1 | 1.03 | 0.43 |
| PI(16:0/18:2) | 852.560 | pos | 7.49 | PI | C43 H83 O13 N1 P1 | 0.06 | 0.02 |
| PI(16:0/18:1) | 854.575 | pos | 8.61 | PI | C43 H85 O13 N1 P1 | 0.08 | 0.03 |
| PI(52:5) | 1079.753 | neg | 12.99 | PI | C61 H108 O13 N0 P1 | 0.02 | 0.01 |
| PI(52:7) | 1075.722 | neg | 12.51 | PI | C61 H104 O13 N0 P1 | 0.01 | 0.01 |
| PI(17:0/18:1) | 849.550 | neg | 9.46 | PI | C44 H82 O13 N0 P1 | 0.01 | 0.00 |
| PI(52:6) | 1077.738 | neg | 12.74 | PI | C61 H106 O13 N0 P1 | 0.04 | 0.02 |
| PI(17:0/18:2) | 847.534 | neg | 8.16 | PI | C44 H80 O13 N0 P1 | 0.01 | 0.01 |
| PI(18:1/14:0) | 807.503 | neg | 7.24 | PI | C41 H76 O13 N0 P1 | 0.02 | 0.01 |
| PI(14:0/18:2) | 805.487 | neg | 6.43 | PI | C41 H74 O13 N0 P1 | 0.02 | 0.01 |
| PI(15:0/18:1) | 821.519 | neg | 7.87 | PI | C42 H78 O13 N0 P1 | 0.03 | 0.01 |
| PI(15:0/18:2) | 819.503 | neg | 6.93 | PI | C42 H76 O13 N0 P1 | 0.03 | 0.01 |
| PI(18:1/18:1) | 861.550 | neg | 8.70 | PI | C45 H82 O13 N0 P1 | 1.43 | 0.59 |
| PIP(56:8) | 1209.735 | neg | 12.08 | PIP | C65 H111 O16 N0 P2 | 0.04 | 0.01 |
| PIP(54:4) | 1189.767 | neg | 12.36 | PIP | C63 H115 O16 N0 P2 | 0.05 | 0.02 |
| PIP(54:5) | 1187.751 | neg | 12.08 | PIP | C63 H113 O16 N0 P2 | 0.05 | 0.02 |
| PIP(54:6) | 1185.735 | neg | 11.83 | PIP | C63 H111 O16 N0 P2 | 0.07 | 0.03 |
| PIP(16:0/22:6) | 961.485 | neg | 8.60 | PIP | C47 H79 O16 N0 P2 | 0.03 | 0.01 |
| PIP(42:8p) | 997.521 | neg | 8.70 | PIP | C51 H83 O15 N0 P2 | 0.10 | 0.04 |
| PIP(42:9p) | 995.506 | neg | 7.57 | PIP | C51 H81 O15 N0 P2 | 0.14 | 0.06 |
| PIP(40:8p) | 969.490 | neg | 7.49 | PIP | C49 H79 O15 N0 P2 | 0.34 | 0.14 |
| PIP(40:7p) | 971.506 | neg | 8.59 | PIP | C49 H81 O15 N0 P2 | 0.35 | 0.14 |
| PIP3(18:1/24:6) | 1175.465 | neg | 8.64 | PIP3 | C51 H87 O22 N0 P4 | 0.10 | 0.04 |
| PS(47:4) | 960.666 | pos | 8.95 | PS | C53 H96 O10 N1 P1 Na1 | 0.01 | 0.00 |
| PS(33:4/14:1) | 958.651 | pos | 7.76 | PS | C53 H94 O10 N1 P1 Na1 | 0.03 | 0.01 |
| PS(53:5) | 1018.748 | neg | 11.72 | PS | C59 H105 O10 N1 P1 | 0.15 | 0.06 |
| PS(38:4) | 810.529 | neg | 7.71 | PS | C44 H77 O10 N1 P1 | 0.22 | 0.09 |
| PS(38:5) | 808.513 | neg | 6.76 | PS | C44 H75 O10 N1 P1 | 0.04 | 0.02 |
| PS(34:1p) | 744.518 | neg | 10.63 | PS | C40 H75 O9 N1 P1 | 0.08 | 0.03 |
| PS(37:3) | 798.529 | neg | 6.78 | PS | C43 H77 O10 N1 P1 | 0.01 | 0.00 |
| PS(38:6) | 806.498 | neg | 6.19 | PS | C44 H73 O10 N1 P1 | 0.10 | 0.04 |
| PS(39:2) | 828.576 | neg | 9.49 | PS | C45 H83 O10 N1 P1 | 0.02 | 0.01 |
| PS(36:3) | 784.513 | neg | 11.00 | PS | C42 H75 O10 N1 P1 | 0.05 | 0.02 |
| PS(39:4) | 824.545 | neg | 6.97 | PS | C45 H79 O10 N1 P1 | 0.04 | 0.02 |
| PS(39:3) | 826.560 | neg | 7.82 | PS | C45 H81 O10 N1 P1 | 0.49 | 0.20 |
| PS(39:1) | 830.592 | neg | 10.59 | PS | C45 H85 O10 N1 P1 | 1.39 | 0.58 |
| So(d15:0) | 260.258 | pos | 0.99 | So | C15 H34 O2 N1 | 0.01 | 0.00 |
| So(d12:0) | 218.211 | pos | 0.71 | So | C12 H28 O2 N1 | 0.01 | 0.01 |
| So(d18:2) | 298.274 | pos | 1.99 | So | C18 H36 O2 N1 | 0.01 | 0.01 |
| So(d22:0) | 358.368 | pos | 4.29 | So | C22 H48 O2 N1 | 0.02 | 0.01 |
| So(d20:0) | 330.337 | pos | 3.23 | So | C20 H44 O2 N1 | 0.03 | 0.01 |
| So(d16:1) | 272.258 | pos | 1.47 | So | C16 H34 O2 N1 | 0.03 | 0.01 |
| So(d14:0) | 246.243 | pos | 0.85 | So | C14 H32 O2 N1 | 0.05 | 0.02 |
| So(d16:0) | 274.274 | pos | 1.20 | So | C16 H36 O2 N1 | 5.90 | 2.44 |
| SQDG(34:3) | 815.498 | neg | 6.61 | SQDG | C43 H75 O12 S1 | 0.03 | 0.01 |
| SQDG(16:0/16:0) | 793.514 | neg | 8.24 | SQDG | C41 H77 O12 S1 | 0.12 | 0.05 |
| SQDG(34:1) | 819.530 | neg | 8.35 | SQDG | C43 H79 O12 S1 | 0.05 | 0.02 |
| SQDG(36:3) | 843.530 | neg | 7.40 | SQDG | C45 H79 O12 S1 | 0.05 | 0.02 |
| SQDG(18:2/18:2) | 841.514 | neg | 6.59 | SQDG | C45 H77 O12 S1 | 0.07 | 0.03 |
| SQDG(40:7) | 937.535 | neg | 11.03 | SQDG | C50 H81 O14 S1 | 0.05 | 0.02 |
| SQDG(16:0/18:2) | 817.514 | neg | 7.33 | SQDG | C43 H77 O12 S1 | 0.10 | 0.04 |
| TG(36:1) | 654.567 | pos | 8.33 | TG | C39 H76 O6 N1 | 0.05 | 0.02 |
| TG(59:9p) | 927.780 | pos | 12.85 | TG | C62 H103 O5 | 0.01 | 0.01 |
| TG(6:0/14:1/18:3) | 676.551 | pos | 6.59 | TG | C41 H74 O6 N1 | 0.01 | 0.00 |
| TG(36:3) | 633.509 | pos | 9.27 | TG | C39 H69 O6 | 0.03 | 0.01 |
| TG(38:3) | 678.567 | pos | 7.21 | TG | C41 H76 O6 N1 | 0.04 | 0.01 |
| TG(4:0/14:1/16:0) | 631.491 | pos | 8.13 | TG | C37 H68 O6 Na1 | 0.01 | 0.01 |
| TG(4:0/16:0/16:0) | 656.582 | pos | 9.29 | TG | C39 H78 O6 N1 | 0.05 | 0.02 |
| TG(20:1/9:0/9:0) | 682.598 | pos | 9.39 | TG | C41 H80 O6 N1 | 0.14 | 0.06 |
| TG(55:7) | 913.726 | pos | 13.62 | TG | C58 H98 O6 Na1 | 0.02 | 0.01 |
| TG(59:7e) | 933.827 | pos | 13.62 | TG | C62 H109 O5 | 0.03 | 0.01 |
| TG(6:0/14:0/18:2) | 680.582 | pos | 8.11 | TG | C41 H78 O6 N1 | 0.10 | 0.04 |
| TG(18:4/15:2/24:7) | 907.681 | pos | 12.85 | TG | C60 H91 O6 | 0.02 | 0.01 |
| TG(19:5/18:2/18:3) | 907.679 | pos | 12.85 | TG | C58 H92 O6 Na1 | 0.02 | 0.01 |
| TG(18:1/18:3/22:4) | 931.775 | pos | 12.33 | TG | C61 H103 O6 | 0.02 | 0.01 |
| TG(18:3/18:2/21:6) | 933.694 | pos | 12.83 | TG | C60 H94 O6 Na1 | 0.02 | 0.01 |
| TG(15:2/22:6/22:6) | 933.697 | pos | 12.84 | TG | C62 H93 O6 | 0.02 | 0.01 |
| TG(62:5p) | 977.890 | pos | 14.68 | TG | C65 H117 O5 | 0.03 | 0.01 |
| TG(59:11) | 939.744 | pos | 13.60 | TG | C62 H99 O6 | 0.02 | 0.01 |
| TG(62:4e) | 1003.903 | pos | 14.40 | TG | C65 H120 O5 Na1 | 0.03 | 0.01 |
| TG(60:6p) | 947.843 | pos | 13.93 | TG | C63 H111 O5 | 0.13 | 0.05 |
| TG(18:1/18:3/21:6) | 935.710 | pos | 13.07 | TG | C60 H96 O6 Na1 | 0.04 | 0.02 |
| TG(59:8e) | 931.811 | pos | 13.32 | TG | C62 H107 O5 | 0.03 | 0.01 |
| TG(16:0/18:1/18:3) | 855.744 | pos | 12.97 | TG | C55 H99 O6 | 0.01 | 0.00 |
| TG(64:9e) | 999.874 | pos | 13.87 | TG | C67 H115 O5 | 0.01 | 0.01 |
| TG(18:3/18:3/21:5) | 911.712 | pos | 13.34 | TG | C60 H95 O6 | 0.04 | 0.02 |
| TG(55:8) | 911.710 | pos | 13.33 | TG | C58 H96 O6 Na1 | 0.04 | 0.02 |
| TG(12:0p/8:0/16:2) | 619.530 | pos | 11.76 | TG | C39 H71 O5 | 0.01 | 0.01 |
| TG(18:1/18:3/21:5) | 937.726 | pos | 13.31 | TG | C60 H98 O6 Na1 | 0.04 | 0.01 |
| TG(59:8p) | 929.796 | pos | 13.08 | TG | C62 H105 O5 | 0.02 | 0.01 |
| TG(59:9e) | 929.796 | pos | 13.08 | TG | C62 H105 O5 | 0.02 | 0.01 |
| TG(18:1/18:2/18:3) | 879.744 | pos | 12.73 | TG | C57 H99 O6 | 0.01 | 0.00 |
| TG(18:1/18:3/19:5) | 909.694 | pos | 13.12 | TG | C58 H94 O6 Na1 | 0.03 | 0.01 |
| TG(64:8e) | 1001.890 | pos | 14.08 | TG | C67 H117 O5 | 0.04 | 0.02 |
| TG(16:0/18:2/18:3) | 853.728 | pos | 12.73 | TG | C55 H97 O6 | 0.01 | 0.01 |
| TG(62:6p) | 975.874 | pos | 14.36 | TG | C65 H115 O5 | 0.08 | 0.03 |
| TG(62:9e) | 971.843 | pos | 13.72 | TG | C65 H111 O5 | 0.03 | 0.01 |
| TG(61:13) | 980.770 | pos | 12.64 | TG | C64 H102 O6 N1 | 0.01 | 0.01 |
| TG(63:14) | 1006.786 | pos | 12.64 | TG | C66 H104 O6 N1 | 0.02 | 0.01 |
| TG(16:0/16:0/18:3) | 851.710 | pos | 14.05 | TG | C53 H96 O6 Na1 | 0.01 | 0.00 |
| TG(62:8e) | 973.858 | pos | 14.07 | TG | C65 H113 O5 | 0.07 | 0.03 |
| TG(20:0/16:0/18:1) | 911.804 | pos | 15.39 | TG | C57 H108 O6 Na1 | 0.01 | 0.00 |
| TG(63:15) | 1004.770 | pos | 12.41 | TG | C66 H102 O6 N1 | 0.02 | 0.01 |
| TG(24:0/18:2/18:3) | 987.835 | pos | 15.13 | TG | C63 H112 O6 Na1 | 0.01 | 0.00 |
| TG(16:0/14:0/18:1) | 822.755 | pos | 14.28 | TG | C51 H100 O6 N1 | 0.02 | 0.01 |
| TG(57:9e) | 923.746 | pos | 14.57 | TG | C60 H100 O5 Na1 | 0.01 | 0.01 |
| TG(18:1/18:2/21:0) | 949.819 | pos | 15.20 | TG | C60 H110 O6 Na1 | 0.01 | 0.00 |
| TG(18:0/17:0/18:1) | 892.833 | pos | 15.21 | TG | C56 H110 O6 N1 | 0.01 | 0.00 |
| TG(57:10p) | 919.715 | pos | 13.93 | TG | C60 H96 O5 Na1 | 0.01 | 0.01 |
| TG(4:0/16:2/18:2) | 676.551 | pos | 11.63 | TG | C41 H74 O6 N1 | 0.01 | 0.01 |
| TG(18:0/18:1/24:0) | 990.942 | pos | 16.42 | TG | C63 H124 O6 N1 | 0.01 | 0.00 |
| TG(4:0/18:2/18:2) | 687.556 | pos | 8.28 | TG | C43 H75 O6 | 0.02 | 0.01 |
| TG(18:2/18:2/23:0) | 975.835 | pos | 15.23 | TG | C62 H112 O6 Na1 | 0.02 | 0.01 |
| TG(55:10p) | 891.684 | pos | 13.72 | TG | C58 H92 O5 Na1 | 0.02 | 0.01 |
| TG(18:1/18:2/23:0) | 977.851 | pos | 15.56 | TG | C62 H114 O6 Na1 | 0.02 | 0.01 |
| TG(20:1/18:1/24:0) | 1016.958 | pos | 16.39 | TG | C65 H126 O6 N1 | 0.01 | 0.01 |
| TG(22:0/18:3/18:3) | 952.833 | pos | 14.36 | TG | C61 H110 O6 N1 | 0.01 | 0.00 |
| TG(16:0/18:1/21:0) | 920.864 | pos | 15.56 | TG | C58 H114 O6 N1 | 0.02 | 0.01 |
| TG(18:1/18:2/22:4) | 933.791 | pos | 14.59 | TG | C61 H105 O6 | 0.03 | 0.01 |
| TG(19:1/18:3/21:1) | 954.848 | pos | 14.27 | TG | C61 H112 O6 N1 | 0.05 | 0.02 |
| TG(22:2/18:2/18:2) | 952.833 | pos | 14.10 | TG | C61 H110 O6 N1 | 0.01 | 0.01 |
| TG(24:1/18:2/18:2) | 982.880 | pos | 14.93 | TG | C63 H116 O6 N1 | 0.02 | 0.01 |
| TG(19:1/18:1/18:3) | 912.801 | pos | 13.81 | TG | C58 H106 O6 N1 | 0.01 | 0.00 |
| TG(18:1/18:2/21:1) | 942.848 | pos | 14.46 | TG | C60 H112 O6 N1 | 0.02 | 0.01 |
| TG(55:9p) | 893.699 | pos | 14.05 | TG | C58 H94 O5 Na1 | 0.03 | 0.01 |
| TG(18:1/17:1/18:2) | 891.741 | pos | 14.17 | TG | C56 H100 O6 Na1 | 0.02 | 0.01 |
| TG(25:0/13:1/23:0) | 1004.958 | pos | 15.36 | TG | C64 H126 O6 N1 | 0.02 | 0.01 |
| TG(16:0/18:1/23:0) | 948.895 | pos | 15.91 | TG | C60 H118 O6 N1 | 0.03 | 0.01 |
| TG(18:1/14:0/18:2) | 846.755 | pos | 13.63 | TG | C53 H100 O6 N1 | 0.02 | 0.01 |
| TG(16:0/16:0/18:2) | 853.726 | pos | 14.36 | TG | C53 H98 O6 Na1 | 0.05 | 0.02 |
| TG(26:0/18:2/18:2) | 1012.927 | pos | 15.76 | TG | C65 H122 O6 N1 | 0.03 | 0.01 |
| TG(14:0/18:2/18:3) | 842.723 | pos | 13.35 | TG | C53 H96 O6 N1 | 0.01 | 0.01 |
| TG(61:2) | 1002.942 | pos | 15.89 | TG | C64 H124 O6 N1 | 0.03 | 0.01 |
| TG(15:0/18:2/18:2) | 863.710 | pos | 13.81 | TG | C54 H96 O6 Na1 | 0.02 | 0.01 |
| TG(59:7) | 964.833 | pos | 13.38 | TG | C62 H110 O6 N1 | 0.01 | 0.00 |
| TG(15:0/18:1/18:2) | 865.726 | pos | 14.14 | TG | C54 H98 O6 Na1 | 0.02 | 0.01 |
| TG(18:3/18:2/20:2) | 922.786 | pos | 13.72 | TG | C59 H104 O6 N1 | 0.02 | 0.01 |
| TG(19:0/19:0/23:4) | 998.911 | pos | 15.23 | TG | C64 H120 O6 N1 | 0.03 | 0.01 |
| TG(18:1/18:1/21:1) | 944.864 | pos | 14.86 | TG | C60 H114 O6 N1 | 0.03 | 0.01 |
| TG(16:0/14:0/18:2) | 820.739 | pos | 13.95 | TG | C51 H98 O6 N1 | 0.04 | 0.02 |
| TG(15:0/16:0/18:1) | 836.770 | pos | 14.48 | TG | C52 H102 O6 N1 | 0.04 | 0.02 |
| TG(6:0/14:1/18:2) | 678.567 | pos | 12.01 | TG | C41 H76 O6 N1 | 0.04 | 0.02 |
| TG(18:1/20:4/24:0) | 993.884 | pos | 16.05 | TG | C65 H117 O6 | 0.04 | 0.02 |
| TG(25:1/18:1/18:1) | 1000.927 | pos | 15.56 | TG | C64 H122 O6 N1 | 0.04 | 0.02 |
| TG(6:0/14:1/18:1) | 680.582 | pos | 12.32 | TG | C41 H78 O6 N1 | 0.04 | 0.02 |
| TG(66:2) | 1073.021 | pos | 16.05 | TG | C69 H134 O6 N1 | 0.04 | 0.02 |
| TG(16:0/18:2/21:0) | 918.848 | pos | 15.22 | TG | C58 H112 O6 N1 | 0.05 | 0.02 |
| TG(41:0p) | 710.666 | pos | 12.77 | TG | C44 H88 O5 N1 | 0.03 | 0.01 |
| TG(18:3/18:2/18:2) | 899.710 | pos | 13.38 | TG | C57 H96 O6 Na1 | 0.01 | 0.00 |
| TG(26:0/18:1/18:2) | 1014.942 | pos | 16.07 | TG | C65 H124 O6 N1 | 0.04 | 0.02 |
| TG(18:1/18:1/20:4) | 907.775 | pos | 14.58 | TG | C59 H103 O6 | 0.08 | 0.03 |
| TG(18:1/18:1/24:1) | 986.911 | pos | 15.37 | TG | C63 H120 O6 N1 | 0.34 | 0.14 |
| TG(18:0/17:2/18:2) | 886.786 | pos | 13.81 | TG | C56 H104 O6 N1 | 0.05 | 0.02 |
| TG(18:2/18:2/21:0) | 942.848 | pos | 14.87 | TG | C60 H112 O6 N1 | 0.07 | 0.03 |
| TG(18:1/18:2/20:4) | 905.759 | pos | 14.25 | TG | C59 H101 O6 | 0.09 | 0.04 |
| TG(18:1/18:1/23:0) | 974.911 | pos | 15.89 | TG | C62 H120 O6 N1 | 0.07 | 0.03 |
| TG(22:1/18:2/18:2) | 954.848 | pos | 14.64 | TG | C61 H112 O6 N1 | 0.07 | 0.03 |
| TG(18:1/18:2/22:1) | 956.864 | pos | 14.60 | TG | C61 H114 O6 N1 | 0.07 | 0.03 |
| TG(19:1/18:1/18:1) | 916.833 | pos | 14.81 | TG | C58 H110 O6 N1 | 0.08 | 0.03 |
| TG(18:1/18:1/21:0) | 946.880 | pos | 15.56 | TG | C60 H116 O6 N1 | 0.08 | 0.03 |
| TG(59:3) | 972.895 | pos | 14.58 | TG | C62 H118 O6 N1 | 0.14 | 0.06 |
| TG(25:1/18:2/19:0) | 1014.942 | pos | 15.73 | TG | C65 H124 O6 N1 | 0.10 | 0.04 |
| TG(62:2) | 1016.958 | pos | 16.05 | TG | C65 H126 O6 N1 | 0.11 | 0.04 |
| TG(16:1/18:2/18:3) | 868.739 | pos | 13.42 | TG | C55 H98 O6 N1 | 0.06 | 0.03 |
| TG(20:5/18:2/18:2) | 901.728 | pos | 13.66 | TG | C59 H97 O6 | 0.08 | 0.03 |
| TG(19:1/16:0/18:1) | 890.817 | pos | 14.82 | TG | C56 H108 O6 N1 | 0.13 | 0.05 |
| TG(17:4/17:3/22:0) | 922.786 | pos | 13.38 | TG | C59 H104 O6 N1 | 0.03 | 0.01 |
| TG(15:0/18:1/18:1) | 862.786 | pos | 14.47 | TG | C54 H104 O6 N1 | 0.17 | 0.07 |
| TG(18:1/18:2/24:1) | 984.895 | pos | 15.07 | TG | C63 H118 O6 N1 | 0.18 | 0.07 |
| TG(16:0/18:1/24:0) | 962.911 | pos | 16.08 | TG | C61 H120 O6 N1 | 0.21 | 0.09 |
| TG(20:1/18:2/18:3) | 924.801 | pos | 14.02 | TG | C59 H106 O6 N1 | 0.22 | 0.09 |
| TG(16:0/18:1/22:0) | 934.880 | pos | 15.74 | TG | C59 H116 O6 N1 | 0.36 | 0.15 |
| TG(18:0/16:0/18:1) | 878.817 | pos | 15.03 | TG | C55 H108 O6 N1 | 0.41 | 0.17 |
| TG(20:1/18:1/18:1) | 930.848 | pos | 14.59 | TG | C59 H112 O6 N1 | 0.49 | 0.20 |
| TG(18:1/18:1/24:0) | 988.927 | pos | 16.05 | TG | C63 H122 O6 N1 | 0.50 | 0.21 |
| TG(18:1/18:3/24:0) | 984.895 | pos | 15.41 | TG | C63 H118 O6 N1 | 0.67 | 0.28 |
| TG(18:1/18:2/24:0) | 986.911 | pos | 15.73 | TG | C63 H120 O6 N1 | 0.70 | 0.29 |
| TG(20:1/18:2/18:2) | 926.817 | pos | 14.30 | TG | C59 H108 O6 N1 | 0.81 | 0.34 |
| TG(16:0/16:0/18:1) | 850.786 | pos | 14.67 | TG | C53 H104 O6 N1 | 0.98 | 0.41 |
| TG(22:0/18:2/18:2) | 956.864 | pos | 15.04 | TG | C61 H114 O6 N1 | 0.20 | 0.08 |
| TG(18:1/18:1/22:0) | 960.895 | pos | 15.71 | TG | C61 H118 O6 N1 | 1.20 | 0.50 |
| TG(20:0/18:2/18:2) | 928.833 | pos | 14.62 | TG | C59 H110 O6 N1 | 1.40 | 0.58 |
| TG(18:1/18:2/22:0) | 958.880 | pos | 15.38 | TG | C61 H116 O6 N1 | 1.44 | 0.59 |
| TG(20:0/18:1/18:1) | 932.864 | pos | 15.36 | TG | C59 H114 O6 N1 | 1.50 | 0.62 |