**Supplementary information**

**Improving the intestinal lipidome coverage in a gnotobiotic mouse model using UHPLC-MS-based approach through optimization of mobile phase modifiers and column selection**

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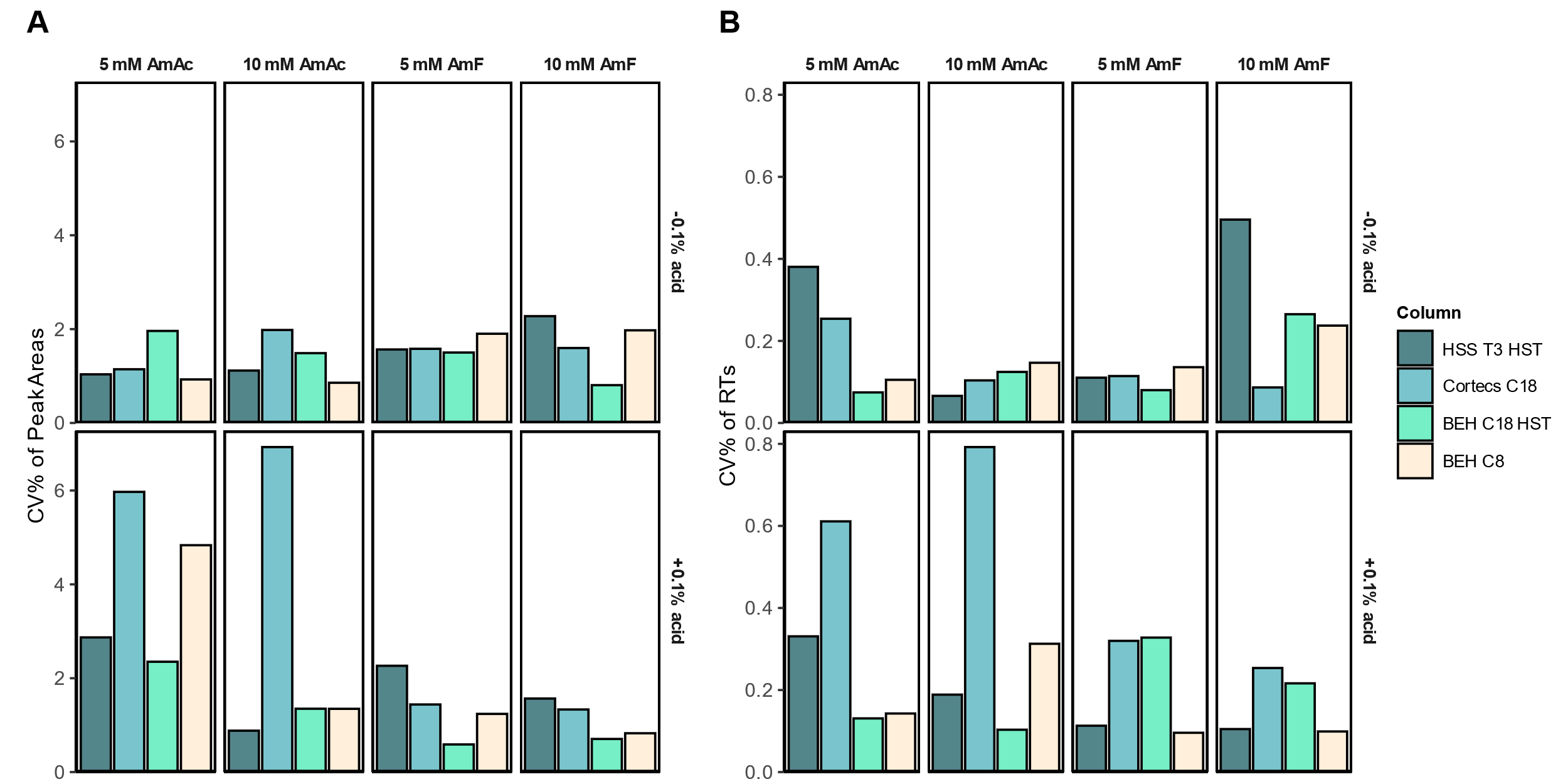
Department of Environmental Sciences

Analytical BioGeoChemistry

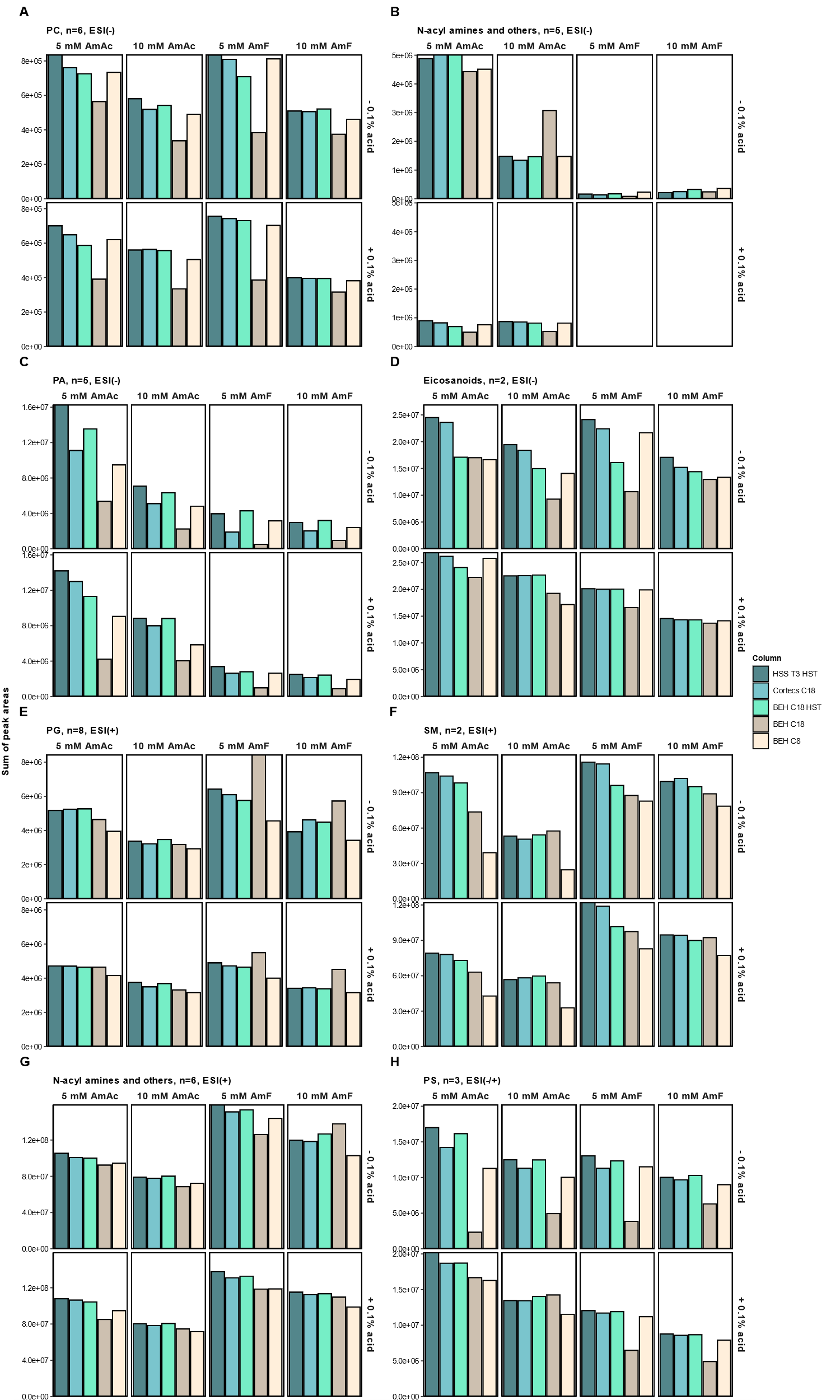
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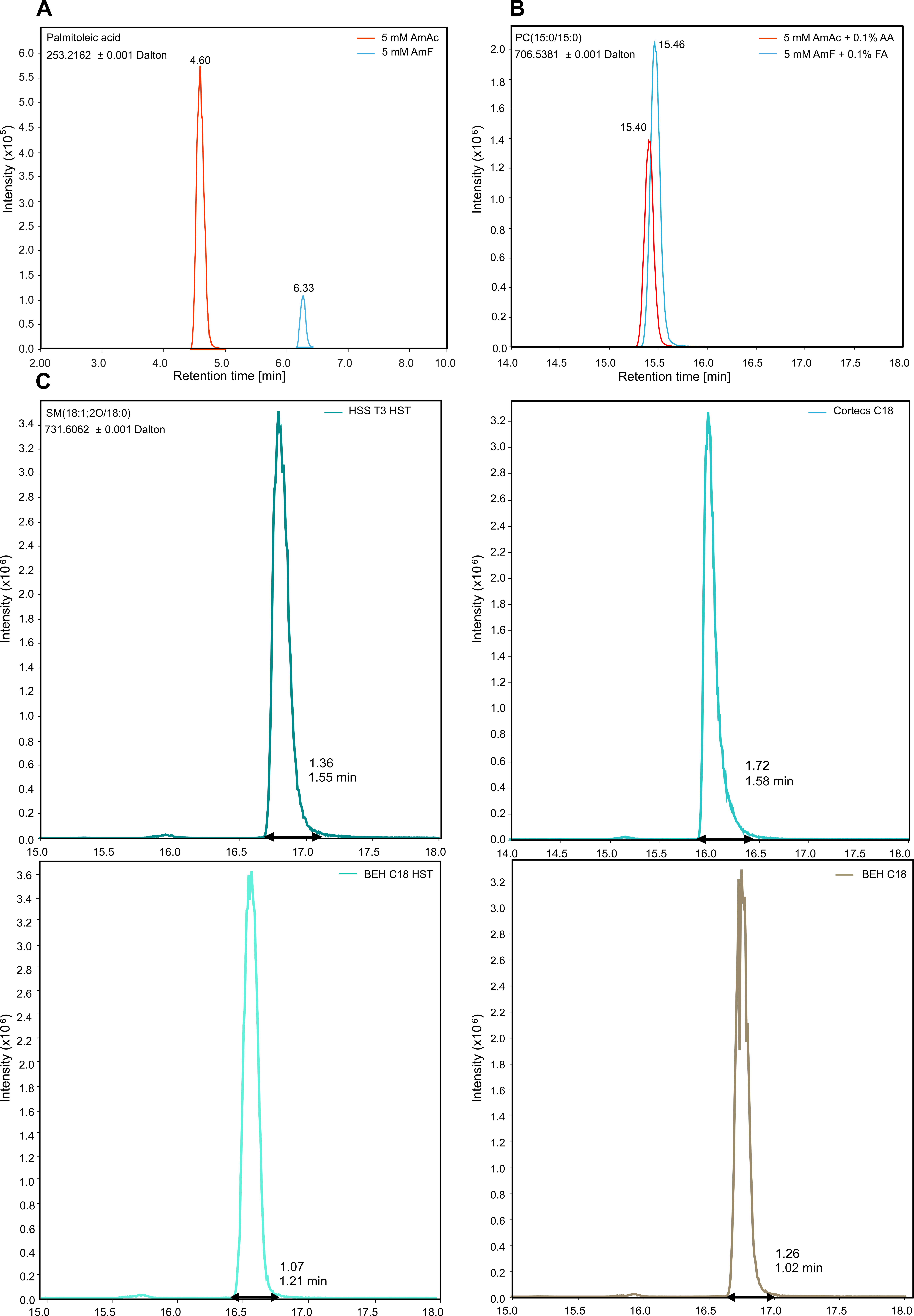
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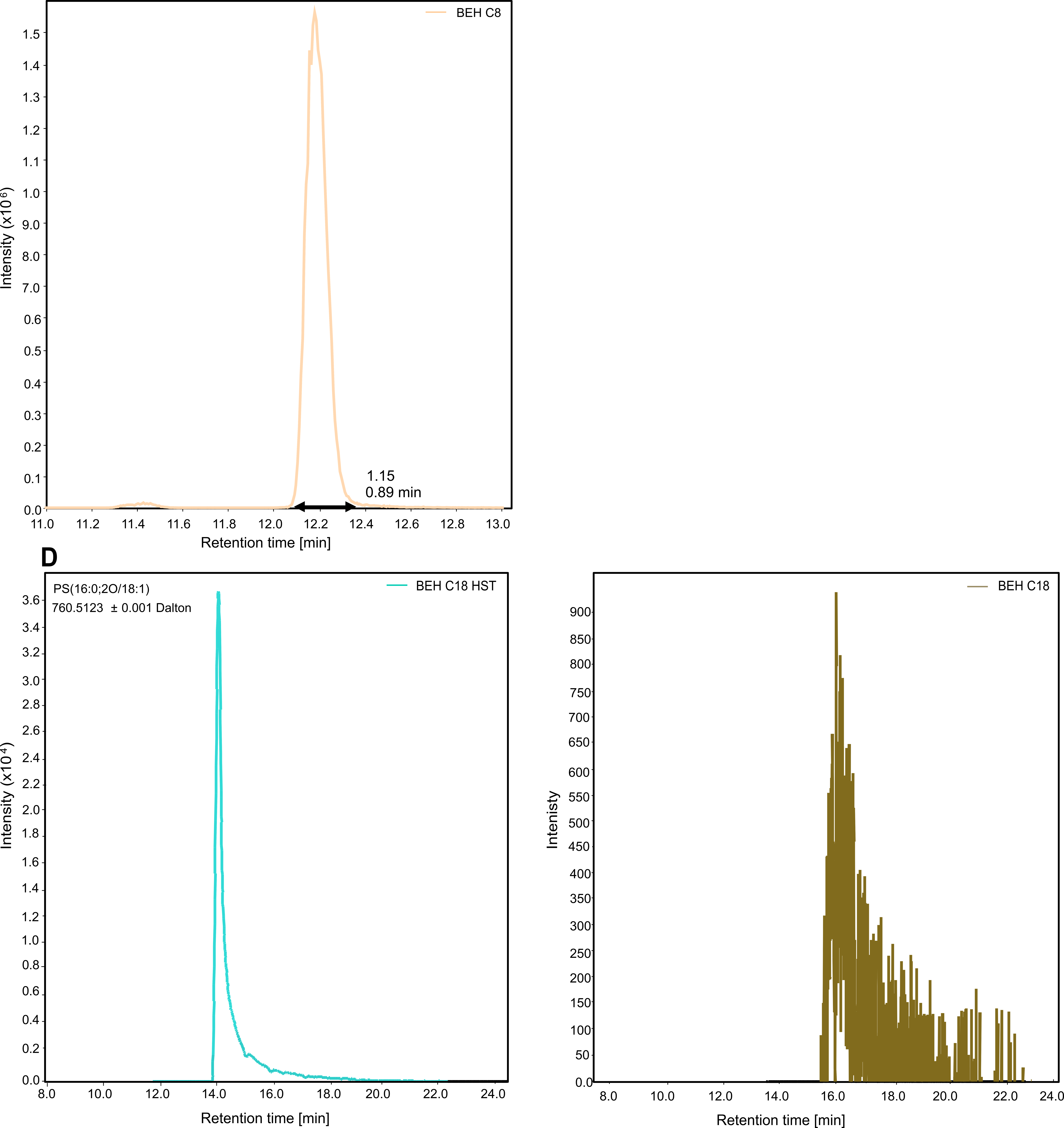
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**Fig. S1.** Precision of peak areas (A) and retention times (B) of four deuterated lipids (1-acetyl-d3-L-carnitine, decanoyl-L-carnitine-d3, 1-pentadecanoyl-2-oleoyl(d7)-sn-glycero-3 phosphocholine and 1-pentadecanoyl-2-oleoyl(d7)-sn-glycero-3-phosphoethanolamine) spiked in blanks and derived from replicate injections measured in ESI(+) RPLC-MS/MS, expressed as average of CV% and analyzed with four columns.

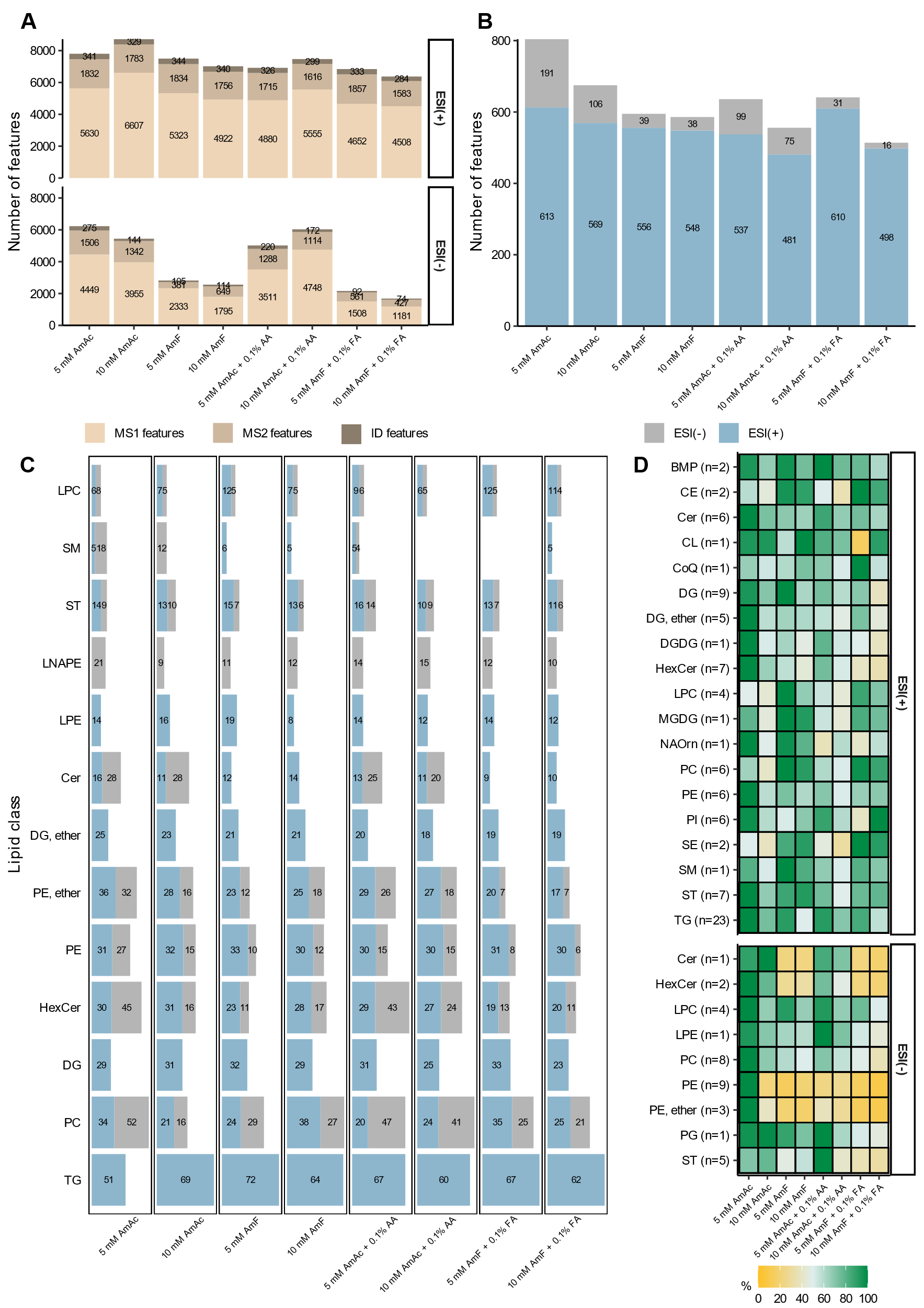


**Fig. S2.** The impact of two ammonium-based buffers (AmAc and AmF) at 5 and 10 mM and mobile phase acidification (+/-) 0.1% acid on ionization efficiency expressed by summed peak areas per condition of selected lipid standards. Lipid classes including PC (n=6), N-acyl amines and others (n=5), PA (n=5) and eicosanoids (n=2) in ESI(-) (**A-D**), PG (n=8), SM (n=2) and N-acyl amines and others (n=6) in ESI(+) (**E-G**) or PS (n=3) in both modes (ESI(-/+) (**H**) were analyzed with five columns. Legend: AmAc: ammonium acetate and AmF: ammonium formate. Acetic acid (0.1%) was added to 5 or 10 mM AmAc while formic acid (0.1%) was used with 5 or 10 mM AmF.





**Fig. S3.** Extracted ion chromatograms of lipid standards in both ESI(+/-). (**A**) Palmitoleic acid analyzed with the BEH C18 HST using 5 mM AmAc and AmF without acidification both in ESI(-) and (**B**) PC(15:0/15:0) with 5 mM AmAc and AmF with acidification in ESI(+). (**C**) SM(18:1;2O/18:0) analyzed with five different columns incorporating HST, conventional and core-shell technology, using 5 mM AmAc without acidification in ESI(+). Tailing factors and peak width values were displayed for each column. (**D**) PS(16:0;2O/18:1) analyzed with the BEH C18 HST and BEH C18 in ESI(-).



**Fig. S4.** The impact of various mobile phase modifiers on feature coverage, lipid classification and the ionization efficiency in a pooled ileum sample analyzed with LC-MS/MS in ESI(+/-). Intestinal lipids were separated using the BEH C18 HST column. (**A**) Bar plots showing the total number of detected features (MS1), features with MS2 and features annotated by the MS-DIAL library (ID). (**B**) Bar plots representing the total count of classified features (probability over 0.6) by CANOPUS. (**C**) Bar plots showing the individual count of common lipid classes among different buffer additives. (**D**) Heatmap showing the percentage of relative peak intensities, for lipid classes detected under all eight buffer conditions in ESI(+/-). The percentages of each lipid species were defined to the highest peak intensity set to 100%, observed for each common lipid species across the eight buffer conditions. Peak intensities of lipid classes were categorized as follows: moderate poor (<50%), sufficient (≥50%), and excellent (≥80%). Legend: AmAc: ammonium acetate; AmF: ammonium formate, AmAc + 0.1% AA: ammonium acetate and 0.1% acetic acid; AmF + 0.1% FA: ammonium formate and 0.1% formic acid.

**Table S1:** Detailed information on analyzed lipids

|  |  |  |  |
| --- | --- | --- | --- |
| **Name** | **Producer** | **Order Number** | **CAS** |
| [(3R)-3-Hydroxydodecanoyl]-L-carnitine | Sigma-Aldrich | 49853 | 1469900-99-9 |
| [(3R)-3-Hydroxyhexadecanoyl]-L-carnitine | Sigma-Aldrich | 52096 | 1469901-03-8 |
| 1,2-Diarachidoyl-sn-glycero-3-phosphocholine, powder | Cayman Chemical | 850368P | 61596-53-0 |
| 1,2-Dibehenoyl-sn-glycero-3-phosphocholine, powder | Avanti Polar Lipids | 850371P | 37070-48-7 |
| 1,2-Diheptadecanoyl-sn-glycero-3-phosphate (sodium salt) | Avanti Polar Lipids | 830856 | 154804-54-3 |
| 1,2-Diheptadecanoyl-sn-glycero-3-phospho-(1'-rac-glycerol) (sodium salt) | Avanti Polar Lipids | 830456 | 799268-52-3 |
| 1,2-Diheptadecanoyl-sn-glycero-3-phosphocholine, powder | Avanti Polar Lipids | 850360P | 70897-27-7 |
| 1,2-Diheptadecanoyl-sn-glycero-3-phosphoethanolamine | Avanti Polar Lipids | 830756 | 140219-78-9 |
| 1,2-Dimyristoyl-sn-glycero-3-phosphate (sodium salt) | Avanti Polar Lipids | 830845 | 80724-31-8 |
| 1,2-Dimyristoyl-sn-glycero-3-phospho-(1'-rac-glycerol) (sodium salt) | Avanti Polar Lipids | 840445 | 200880-40-6 |
| 1,2-Dimyristoyl-sn-glycero-3-phosphocholine | Avanti Polar Lipids | 850345 | 18194-24-6 |
| 1,2-Dimyristoyl-sn-glycero-3-phosphoethanolamine | Avanti Polar Lipids | 850745 | 998-07-2 |
| 1,2-Dipalmitoyl-sn-glycero-3-phosphate (sodium salt) | Avanti Polar Lipids | 830855 | 169051-60-9 |
| 1,2-Dipalmitoyl-sn-glycero-3-phospho-(1'-rac-glycerol) (sodium salt) | Avanti Polar Lipids | 840455 | 200880-41-7 |
| 1,2-Dipalmitoyl-sn-glycero-3-phosphoethanolamine | Avanti Polar Lipids | 850705 | 923-61-5 |
| 1,2-Dipalmitoyl-sn-glycero-3-phospho-L-serine (sodium salt) | Avanti Polar Lipids | 840037 | 145849-32-7 |
| 1,2-Dipentadecanoyl-sn-glycero-3-phospho-(1′-rac-glycerol) (sodium salt), powder | Avanti Polar Lipids | 840446P | 322647-32-5 |
| 1,2-Dipentadecanoyl-sn-glycero-3-phosphoethanolamine, powder | Avanti Polar Lipids | 850704P | 109032-52-2 |
| 1,2-Distearoyl-sn-glycero-3-phosphate (sodium salt) | Avanti Polar Lipids | 830865 | 108321-18-2 |
| 1,2-Distearoyl-sn-glycero-3-phospho-(1'-rac-glycerol) (sodium salt) | Avanti Polar Lipids | 840465 | 200880-42-8 |
| 1,2-Distearoyl-sn-glycero-3-phosphoethanolamine | Avanti Polar Lipids | 850715 | 1069-79-0 |
| 1,3-dipentadecanoyl-2-oleyol(d7)-glycerol | Avanti Polar Lipids | 791648 | 2097561-17-4 |
| 1.2-Didecanoyl-sn-glycero-3-phosphocholine | Avanti Polar Lipids | 850325 | 3436-44-0 |
| 1.2-Dilauroyl-sn-glycero-3-Phospho-L-Serine | Avanti Polar Lipids | 840038P | 208757-51-1 |
| 1.2-Dioleoyl-sn-glycero-3-phosphoethanolamine | Avanti Polar Lipids | 880130 | 474922-90-2 |
| 12-Methyltetradecanoic acid | Sigma-Aldrich | M3664 | 5502-94-3 |
| 13-Methylmyristic acid | Sigma-Aldrich | M7031 | 2485-71-4 |
| 1-Heptadecanoyl-2-hydroxy-sn-glycero-3-phosphocholine | Avanti Polar Lipids | 855676 | 50930-23-9 |
| 1-Myristoyl-2-hydroxy-sn-glycero-3-phosphocholine | Avanti Polar Lipids | 855575 | 20559-16-4 |
| 1-Oleoyl-2-hydroxy-sn-glycero-3-phosphoethanolamine | Avanti Polar Lipids | 846725 | 89576-29-4 |
| 1-Palmitoyl-2-arachidonoyl-sn-glycero-3-phospho-(1′-rac-glycerol) (sodium salt), chloroform | Avanti Polar Lipids | 840499C | 322647-47-2 |
| 1-Palmitoyl-2-arachidonoyl-sn-glycero-3-phosphocholine | Avanti Polar Lipids | 850459 | 35418-58-7 |
| 1-Palmitoyl-2-docosahexaenoyl-sn-glycero-3-phosphate (sodium salt) | Avanti Polar Lipids | 840860 | 474943-28-7 |
| 1-Palmitoyl-2-docosahexaenoyl-sn-glycero-3-phospho-(1′-rac-glycerol) (sodium salt), chloroform | Avanti Polar Lipids | 840500C | 384833-22-1 |
| 1-Palmitoyl-2-docosahexaenoyl-sn-glycero-3-phosphocholine | Avanti Polar Lipids | 850461 | 59403-54-2 |
| 1-Palmitoyl-2-docosahexaenoyl-sn-glycero-3-phosphoethanolamine | Avanti Polar Lipids | 850801 | 96998-00-4 |
| 1-Palmitoyl-2-glutaryl-sn-glycero-3-phosphocholine | Avanti Polar Lipids | 870602 | 89947-79-5 |
| 1-Palmitoyl-2-hydroxy-sn-glycero-3-phosphocholine | Avanti Polar Lipids | 855675 | 17364-16-8 |
| 1-Palmitoyl-2-linoleoyl-sn-glycero-3-phospho-(1′-rac-glycerol) (sodium salt), chloroform | Avanti Polar Lipids | 840497C | 322647-44-9 |
| 1-Palmitoyl-2-linoleoyl-sn-glycero-3-phosphocholine | Avanti Polar Lipids | 850458 | 159701-21-0 |
| 1-Palmitoyl-2-linoleoyl-sn-glycero-3-phosphoethanolamine | Avanti Polar Lipids | 850756 | 26662-95-3 |
| 1-Palmitoyl-2-linoleoyl-sn-glycero-3-phospho-L-serine (sodium salt) | Avanti Polar Lipids | 840060 | 384833-20-9 |
| 1-Palmitoyl-2-oleoyl-glycero-3-phosphocholine | Avanti Polar Lipids | 850457 | 26853-31-6 |
| 1-Palmitoyl-2-oleoyl-sn-glycero-3-phosphate (sodium salt) | Avanti Polar Lipids | 840857 | 169437-35-8 |
| 1-Palmitoyl-2-oleoyl-sn-glycero-3-phospho-(1'-rac-glycerol) (sodium salt) | Avanti Polar Lipids | 840457 | 268550-95-4 |
| 1-Palmitoyl-2-oleoyl-sn-glycero-3-phosphoethanolamine | Avanti Polar Lipids | 850757 | 26662-94-2 |
| 1-Palmitoyl-2-oleoyl-sn-glycero-3-phospho-L-serine (sodium salt) | Avanti Polar Lipids | 840034 | 321863-21-2 |
| 1-Palmitoyl-2-stearoyl-sn-glycero-3-phosphocholine | Avanti Polar Lipids | 850456 | 59403-51-9 |
| 1-Pentadecanoyl-2-hydroxy-sn-glycero-3-phosphocholine | Avanti Polar Lipids | 855576P | 108273-89-8 |
| 1-Stearoyl-2-arachidonoyl-sn-glycero-3-phosphocholine | Avanti Polar Lipids | 850469 | 35418-59-8 |
| 1-Stearoyl-2-arachidonoyl-sn-glycero-3-phosphoethanolamine | Avanti Polar Lipids | 850804 | 61216-62-4 |
| 1-Stearoyl-2-docosahexaenoyl-sn-glycero-3-phosphoethanolamine | Avanti Polar Lipids | 850806 | 96998-01-5 |
| 1-Stearoyl-2-hydroxy-sn-glycero-3-phosphocholine | Avanti Polar Lipids | 855775 | 19420-57-6 |
| 1-Stearoyl-2-hydroxy-sn-glycero-3-phosphoethanolamine | Avanti Polar Lipids | 856715 | 69747-55-3 |
| 1-Stearoyl-2-linoleoyl-sn-glycero-3-phosphocholine | Avanti Polar Lipids | 850468 | 27098-24-4 |
| 1-Stearoyl-2-linoleoyl-sn-glycero-3-phosphoethanolamine | Avanti Polar Lipids | 850802 | 7266-53-7 |
| 1-Stearoyl-2-oleoyl-sn-glycero-3-phosphoethanolamine | Avanti Polar Lipids | 850758 | 6418-95-7 |
| 1-Stearoyl-2-palmitoyl-sn-glycero-3-phosphocholine | Avanti Polar Lipids | 850465 | 59403-53-1 |
| 1-Tridecanoyl-2-hydroxy-sn-glycero-3-phosphocholine, powder | Avanti Polar Lipids | 855476P | 20559-17-5 |
| 2-Methylbutyryl-L-carnitine | Sigma-Aldrich | 50405 | 256928-75-3 |
| 3-Hydroxybutyrylcarnitine chloride | Sigma-Aldrich | 90941 | 918639-76-6 |
| 3-Methylglutaryl carnitine | Sigma-Aldrich | 738816 | 102673-95-0 |
| 3-sn-Lysophosphatidylethanolamine | Sigma-Aldrich | L4754 |  |
| Acetyl-d3-L-carnitine hydrochloride | Sigma-Aldrich | 617466 | 362049-62-5 |
| Acetyl-L-carnitine | Cayman Chemical | 16948 | 5080-50-2 |
| Adipoyl-L-carnitine | Sigma-Aldrich | 91926 | 102636-83-9 |
| Arachidonic acid, sodium salt | Cayman Chemical | 100006607 | 6610-25-9 |
| Arachidonoyl ethanolamide | Cayman Chemical | 10005765 | 94421-69-9 |
| Arachidonyl-L-carnitine | Sigma-Aldrich | 30172 | 36816-11-2 |
| Butyryl-L-carnitine | Sigma-Aldrich | 42623 | 25576-40-3 |
| C16 lactosyl(β) ceramides (d18:1/16:0) | Avanti Polar Lipids | 860576P | 4201-62-1 |
| C18 Glucosyl(ß) ceramide (d18:1/18:0) | Avanti Polar Lipids | 860547 | 95119-86-1 |
| Caprylic acid (C8:0) | Sigma-Aldrich | O3907 | 124-07-2 |
| Ceramide mixture | Cayman Chemical | 22853 | 100403-19-8 |
| Cholesterol | Sigma-Aldrich | C8667 | 57-88-5 |
| Cis, cis-9,12-octadecadienoyl-L-carnitine | Sigma-Aldrich | 76771 | 36816-10-1 |
| Decanoyl-L-carnitine | Sigma-Aldrich | 50637 | 3992-45-8 |
| Decanoyl-L-carnitine-d3 (chloride) | Cayman Chemical | 6568 | 2483831-87-2 |
| D-galactosyl-ß-1,1' N-palmitoyl-D-erythro-sphingosine | Avanti Polar Lipids | 860521P | 34324-89-5 |
| D-ribo-phytosphingosine | Avanti Polar Lipids | 860499 | 388566-94-7 |
| D-sphingosine | Avanti Polar Lipids | 860490 | 123-78-4 |
| Glutaryl-L-carnitine lithium salt | Sigma-Aldrich | 72715 | 102636-82-8 |
| Hexanoyl-L-carnitine | Sigma-Aldrich | 7439 | 22671-29-0 |
| Isobutyryl-L-carnitine | Sigma-Aldrich | 51085 | 25518-49-4 |
| Isovaleryl-L-carnitine | Sigma-Aldrich | 51371 | 31023-24-2 |
| Lauroyl-L-carnitine | Sigma-Aldrich | 91432 | 25518-54-1 |
| L-carnitine hydrochloride | Sigma-Aldrich | C0283 | 6645-46-1 |
| Malonyl-L-carnitine | Sigma-Aldrich | 92998 | 910825-21-7 |
| Methyl stearate | Sigma-Aldrich | S5376 | 112-61-8 |
| Myristoyl-L-carnitine | Sigma-Aldrich | 61367 | 25597-07-3 |
| N-(2-hydroxyethyl)-heptadecanamide | Cayman Chemical | 17567 | 5450-40-8 |
| N-heptadecanoyl-D-erythro-sphingosine | Avanti Polar Lipids | 860517 | 67492-16-4 |
| N-palmitoyl-D-erythro-sphingosylphosphorylcholine | Avanti Polar Lipids | 860584 | 6254-89-3 |
| N-stearoyl-D-erythro-sphingosine | Avanti Polar Lipids | 860518 | 2304-81-6 |
| N-stearoyl-D-erythro-sphingosylphosphorylcholine | Avanti Polar Lipids | 860586 | 58909-84-5 |
| N-stearoyl-Taurine | Cayman Chemical | 10005610 | 63155-80-6 |
| Octanoyl-L-carnitine | Sigma-Aldrich | 50892 | 25243-95-2 |
| Oleic acid | Sigma-Aldrich | O1008 | 112-80-1 |
| Oleoyl Ethanolamide | Sigma-Aldrich | O0383 | 111-58-0 |
| Oleoyl-L-carnitine | Sigma-Aldrich | 597562 | 31062-78-9 |
| O-succinyl-L-carnitine lithium salt | Sigma-Aldrich | 4609 |  |
| 1,2-dipentadecanoyl-sn-glycero-3-phosphocholine | Avanti Polar Lipids | 850350C | 3355-27-9 |
| Palmitoyl-L-carnitine | Sigma-Aldrich | 61251 | 2364-67-2 |
| Pentadecanoic acid | Sigma-Aldrich | P6125 | 1002-84-2 |
| Pentadecanoyl Ethanolamide | Cayman Chemical | 9001740 | 53832-58-9 |
| Propionyl-L-carnitine | Sigma-Aldrich | 52941 | 203806-01-3 |
| Prostaglandin E₂ | Sigma-Aldrich | P0409 | 363-24-6 |
| Prostaglandin F1α | Sigma-Aldrich | P5765 | 745-62-0 |
| Prostaglandin F2α | Avanti Polar Lipids | 900121O | 38562-01-5 |
| Stearoyl-L-carnitine | Sigma-Aldrich | 61229 | 25597-09-5 |
| Sulfatides | Avanti Polar Lipids | 131305 | 383906-24-9 |
| Tetradecanoyl-L-carnitine | Sigma-Aldrich | 730939 | 25597-07-3 |
| Tigloyl-L-carnitine | Sigma-Aldrich | 39588 | 64681-36-3 |
| Trans-2-Dodecenoyl-L-carnitine | Sigma-Aldrich | 74023 | 1631992-06-7 |
| Trans-2-Octenoyl-L-carnitine | Sigma-Aldrich | 55184 | 152064-94-3 |
| Trans-2-Tetradecenoyl-L-carnitine | Sigma-Aldrich | 40733 |  |
| Valeryl-L-carnitine | Sigma-Aldrich | 4265 | 40225-14-7 |
| α-linolenic acid | Cayman Chemical | 90210 | 463-40-1 |
| 1-pentadecanoyl-2-oleoyl(d7)-sn-glycero-3-phosphocholine | Avanti Polar Lipids | 791637 | 2097561-16-3 |
| 1-pentadecanoyl-2-oleoyl(d7)-sn-glycero-3-phosphoethanolamine | Avanti Polar Lipids | 791638 | 2097561-15-2 |
| Palmitoleic acid | Sigma-Aldrich | [76169](https://www.sigmaaldrich.com/DE/de/product/sial/76169) | [373-49-9](https://www.sigmaaldrich.com/DE/de/search/373-49-9?focus=products&page=1&perpage=30&sort=relevance&term=373-49-9&type=cas_number) |
| Palmitoleoyl Ethanolamide | Cayman Chemical | 10965 | 94421-67-7 |

**Table S2:** Mass spectrometric settings of lipidomics method

|  |  |  |
| --- | --- | --- |
| **Parameter** | **Value** | **Information** |
| Method duration | 25 min | Source and gas parameters |
| Total scan time | 0.412 s |
| Estimated cycles | 3643 |
| Ion source gas 1 | 45 psi |
| Ion source gas 2 | 45 psi |
| Curtain gas | 30 psi |
| CAD gas | 7 |
| Temperature | 500 °C |
| TOF start mass | 100 Da | TOF MS parameters |
| TOF stop mass | 1500 Da |
| Spray voltage | (+/-) 4500 V |
| Accumulation time | 0.1 s |
| Declustering potential | (+/-) 50 V |
| DP spread | 0 V |
| Collision energy | (+/-) 5 V |
| CE spread | 0 V |
| Maximum candidate ions | 10 |
| Intensity threshold exceeds | 1000 cps |
| TOF MS/MS start mass | 65 | TOF MS/MS parameters |
| TOF MS/MS stop mass | 1500 |
| Declustering potential | (+/-) 80 |
| Collision energy | (+/-) 35 V |
| CE spread | 15 V |
| DP spread | 0 |
| Accumulation time | 0.025 s |

|  |  |  |
| --- | --- | --- |
| **Table S3:** Lipid standards used for the RPLC targeted analysis | | |
| **ESI(+)** | | |
| **Lipid class** | **Lipid** | **Name** |
| PC | PC(15:0/15:0) | 1,2-dipentadecanoyl-sn-glycero-3-phosphocholine |
| PC | PC(10:0/10:0) | 1.2-Didecanoyl-sn-glycero-3-phosphocholine |
| PC | PC(18:0/20:4) | 1-Stearoyl-2-arachidonoyl-sn-glycero-3-phosphocholine |
| PC | PC(14:0/0:0) | 1-Myristoyl-2-hydroxy-sn-glycero-3-phosphocholine |
| PC | PC(16:0/18:1(9Z)) | 1-Palmitoyl-2-oleoyl-glycero-3-phosphocholine |
| PG | PG(14:0/14:0 | 1,2-Dimyristoyl-sn-glycero-3-phospho-(1'-rac-glycerol) |
| PG | PG(16:0/20:4) | 1-Palmitoyl-2-arachidonoyl-sn-glycero-3-phospho-(1′-rac-glycerol) |
| PG | PG(16:0/18:1) | 1-Palmitoyl-2-oleoyl-sn-glycero-3-phospho-(1'-rac-glycerol) |
| PG | PG(15:0/15:0) | 1,2-Dipentadecanoyl-sn-glycero-3-phospho-(1′-rac-glycerol) |
| PG | PG(16:0/16:0) | 1,2-Dipalmitoyl-sn-glycero-3-phospho-(1'-rac-glycerol) |
| PG | PG(17:0/17:0) | 1,2-Diheptadecanoyl-sn-glycero-3-phospho-(1'-rac-glycerol) |
| PG | PG(18:0/18:0) | 1,2-Distearoyl-sn-glycero-3-phospho-(1'-rac-glycerol) |
| PG | PG(16:0/18:2) | 1-Palmitoyl-2-linoleoyl-sn-glycero-3-phospho-(1′-rac-glycerol) |
| SM | SM(18:1;2O/16:0) | N-palmitoyl-D-erythro-sphingosylphosphorylcholine |
| SM | SM(18:1;2O/18:0) | N-stearoyl-D-erythro-sphingosylphosphorylcholine |
| N-acyl amines and others | Arachidoyl Ethanolamide | Arachidonoyl ethanolamide |
| N-acyl amines and others | D-Sphingosine | D-sphingosine |
| N-acyl amines and others | Heptadecanoyl Ethanolamide | N-(2-hydroxyethyl)-heptadecanamide |
| N-acyl amines and others | Oleoyl Ethanolamide | Oleoyl Ethanolamide |
| N-acyl amines and others | Palmitoleoyl Ethanolamide | Palmitoleoyl Ethanolamide |
| N-acyl amines and others | Pentadecanoyl Ethanolamide | Pentadecanoyl Ethanolamide |
| Fatty Acyls | Decanoyl-L-carnitine | Decanoyl-L-carnitine |
| Fatty Acyls | Hexanoyl-L-carnitine | Hexanoyl-L-carnitine |
| Fatty Acyls | Myristoyl-L-carnitine | Myristoyl-L-carnitine |
| Fatty Acyls | Octanoyl-L-carnitine | Octanoyl-L-carnitine |
| Fatty Acyls | Palmitoyl-L-carnitine | Palmitoyl-L-carnitine |
| Fatty Acyls | Stearoyl-L-carnitine | Stearoyl-L-carnitine |
| Fatty Acyls | Tetradecanoyl-L-carnitine | Tetradecanoyl-L-carnitine |
| **ESI(–)** | | |
| Eicosanoids | Prostaglandine E2 | Prostaglandin E₂ |
| Eicosanoids | Prostaglandine F2 alpha | Prostaglandin F2α |
| Fatty Acids | 12-Methyltetradecanoic acid | 12-Methyltetradecanoic acid |
| Fatty Acids | Arachidonic acid | Arachidonic acid, Porcine liver sodium salt |
| Fatty Acids | Oleic acid | Oleic acid |
| Fatty Acids | Palmitoleic acid | Palmitoleic acid |
| Fatty Acids | 13-Methylmyristic acid | 13-Methylmyristic acid |
| Fatty Acids | Pentadecanoic acid | Pentadecanoic acid |
| N-acyl amines and others | Oleoyl Ethanolamide | Oleoyl Ethanolamide |
| N-acyl amines and others | Palmitoleoyl Ethanolamide | Palmitoleoyl Ethanolamide |
| N-acyl amines and others | Heptadecanoyl Ethanolamide | N-(2-hydroxyethyl)-heptadecanamide |
| N-acyl amines and others | Pentadecanoyl Ethanolamide | Pentadecanoyl Ethanolamide |
| N-acyl amines and others | Arachidoyl Ethanolamide | Arachidonoyl ethanolamide |
| PA | PA(16:0/16:0) | 1,2-Dipalmitoyl-sn-glycero-3-phosphate |
| PA | PA(16:0/22:6) | 1-Palmitoyl-2-docosahexaenoyl-sn-glycero-3-phosphate |
| PA | PA(16:0/18:1(9Z)) | 1-Palmitoyl-2-oleoyl-sn-glycero-3-phosphate |
| PA | PA(17:0/17:0) | 1,2-Diheptadecanoyl-sn-glycero-3-phosphate |
| PA | PA(14:0/14:0) | 1,2-Dimyristoyl-sn-glycero-3-phosphate |
| PC | PC(18:0/20:4) | 1-Stearoyl-2-arachidonoyl-sn-glycero-3-phosphocholine |
| PC | PC(16:0/0:0) | 1-Palmitoyl-2-hydroxy-sn-glycero-3-phosphocholine |
| PC | PC(17:0/0:0) | 1-Heptadecanoyl-2-hydroxy-sn-glycero-3-phosphocholine |
| PC | PC(15:0/0:0) | 1-Pentadecanoyl-2-hydroxy-sn-glycero-3-phosphocholine |
| PC | PC(13:0/0:0) | 1-Tridecanoyl-2-hydroxy-sn-glycero-3-phosphocholine |
| PC | PGPC | 1-Palmitoyl-2-glutaryl-sn-glycero-3-phosphocholine |
| PG | PG(16:0/18:1) | 1-Palmitoyl-2-oleoyl-sn-glycero-3-phospho-(1'-rac-glycerol) |
| PG | PG(16:0/20:4) | 1-Palmitoyl-2-arachidonoyl-sn-glycero-3-phospho-(1′-rac-glycerol) |
| PG | PG(17:0/17:0) | 1,2-Diheptadecanoyl-sn-glycero-3-phospho-(1'-rac-glycerol) |
| PG | PG(18:0/18:0) | 1,2-Distearoyl-sn-glycero-3-phospho-(1'-rac-glycerol) |
| PG | PG(16:0/16:0) | 1,2-Dipalmitoyl-sn-glycero-3-phospho-(1'-rac-glycerol) |
| PG | PG(16:0/18:2) | 1-Palmitoyl-2-linoleoyl-sn-glycero-3-phospho-(1′-rac-glycerol) |
| PG | PG(16:0/22:6) | 1-Palmitoyl-2-docosahexaenoyl-sn-glycero-3-phospho-(1′-rac-glycerol) |
| PG | PG(14:0/14:0) | 1,2-Dimyristoyl-sn-glycero-3-phospho-(1'-rac-glycerol) |
| **ESI(–/+)** | | |
| Ceramides | C16 lactosyl(beta) Ceramides (d18:1/16:0) | C16 lactosyl(β) ceramides (d18:1/16:0) |
| Ceramides | Cer(d18:1/25:1) | Ceramide mixture |
| Ceramides | C18 Glucosyl(beta) Ceramide (d18:1/18:0) | C18 Glucosyl(ß) ceramide (d18:1/18:0) |
| Ceramides | Cer(d18:1/26:1) | Ceramide mixture |
| Ceramides | Cer(d18:1/16:0(2OH)) | Ceramide mixture |
| Ceramides | Cer(d18:1/17:0) | Ceramide mixture |
| Ceramides | Cer(d18:1/18:0(2OH)) | Ceramide mixture |
| Ceramides | Cer(d18:1/18:0) | Ceramide mixture |
| Ceramides | Cer(d18:1/22:0(2OH)) | Ceramide mixture |
| Ceramides | Cer(d18:1/22:0) | Ceramide mixture |
| Ceramides | Cer(d18:1/23:0(2OH)) | Ceramide mixture |
| Ceramides | Cer(d18:1/24:0(2OH)) | Ceramide mixture |
| Ceramides | Cer(d18:1/24:0) | Ceramide mixture |
| Ceramides | Cer(d18:1/24:1) | Ceramide mixture |
| Ceramides | Galactosylceramide (d18:1/16:0) | Ceramide mixture |
| Ceramides | Cer(d18:1/20:0) | Ceramide mixture |
| Ceramides | Cer(d18:1/25:0(2OH)) | Ceramide mixture |
| Ceramides | Cer(d18:1/25:0) | Ceramide mixture |
| Ceramides | Cer(d18:1/26:0) | Ceramide mixture |
| Ceramides | Cer(d18:1/27:1) | Ceramide mixture |
| PE | PE(18:0/0:0) | 1-Stearoyl-2-hydroxy-sn-glycero-3-phosphoethanolamine |
| PE | PE(18:1/0:0) | 1-Oleoyl-2-hydroxy-sn-glycero-3-phosphoethanolamine |
| PE | PE(14:0/14:0) | 1,2-Dimyristoyl-sn-glycero-3-phosphoethanolamine |
| PE | PE(15:0/15:0) | 1,2-Dipentadecanoyl-sn-glycero-3-phosphoethanolamine, powder |
| PE | PE(15:0/18:1)-d7 | 1-pentadecanoyl-2-oleoyl(d7)-sn-glycero-3-phosphoethanolamine |
| PE | PE(16:0/16:0) | 1,2-Dipalmitoyl-sn-glycero-3-phosphoethanolamine |
| PE | PE(16:0/18:1) | 1-Palmitoyl-2-oleoyl-sn-glycero-3-phosphoethanolamine |
| PE | PE(16:0/18:2) | 1-Palmitoyl-2-linoleoyl-sn-glycero-3-phosphoethanolamine |
| PE | PE(16:0/22:6) | 1-Palmitoyl-2-docosahexaenoyl-sn-glycero-3-phosphoethanolamine |
| PE | PE(17:0/17:0) | 1,2-Diheptadecanoyl-sn-glycero-3-phosphoethanolamine |
| PE | PE(18:0/18:0) | 1,2-Distearoyl-sn-glycero-3-phosphoethanolamine |
| PE | PE(18:0/18:1) | 1-Stearoyl-2-oleoyl-sn-glycero-3-phosphoethanolamine |
| PE | PE(18:0/18:2) | 1-Stearoyl-2-linoleoyl-sn-glycero-3-phosphoethanolamine |
| PE | PE(18:0/20:4) | 1-Stearoyl-2-arachidonoyl-sn-glycero-3-phosphoethanolamine |
| PE | PE(18:0/22:6) | 1-Stearoyl-2-docosahexaenoyl-sn-glycero-3-phosphoethanolamine |
| PE | PE(18:1/18:1) | 1.2-Dioleoyl-sn-glycero-3-phosphoethanolamine |
| PS | PS(16:0/18:1) | 1-Palmitoyl-2-oleoyl-sn-glycero-3-phospho-L-serine |
| PS | PS(12:0/12:0) | 1.2-Dilauroyl-sn-glycero-3-Phospho-L-Serine |
| PS | PS(16:0/16:0) | 1,2-Dipalmitoyl-sn-glycero-3-phospho-L-serine |