Table S2. List of automatically identified lipid species from the mouse kidney tissue

Lipid class assignments are done so according to the nomenclature of the LIPIDMAPS database and showing only one match per m/z.

Notes:

1. For sterols many isomeric species are possible and thus identifications are assigned to the general “sterols” class.

2. 1-alkyl and 1-(1Z-alkenyl) chains cannot be distinguished. These lipids should be interpreted as belonging to a general ether sub-class (e.g., PC-O and PE-O) lipids. Note for 1-(1Z-alkenyl) chains the alkenyl double bond is not included in the number of unsaturated sites contained within the sum-composition formula. E.g., the plasmalogen PE(P-40:6) should instead be interpreted as PE(O-40:7).

3. For glycosphingolipids, the order and identity of the sugar groups is unknown and should just be interpreted as hexose (Hex) substituent. E.g., Hex2Cer(d42:1) instead of LacCer(d42:1).

4. In general identifications are tentative are based on accurate mass alone. The presence of isomeric and isobaric (within the achievable mass resolution) species cannot be excluded.

| m/z       | Formula     | LIPIDMAPS Lipid Class | Sub-Class Abbreviation | Common Name (sphingomyelins) | Neutral Mass | Mass delta ppm | Adduct           | Normalized Intensity (0-100%) | Chaos score |
|-----------|-------------|-----------------------|------------------------|-----------------------------|--------------|----------------|------------------|-----------------------------|-------------|
| 367.3363  | C27H44O     | Sterols               |                        |                             | 384.3392     | 1              | [M+H-H2O]+       | 6.1                         | 98.9        |
| 369.3517  | C27H46O     | Sterols               |                        |                             | 386.3549     | 0.4            | [M+H-H2O]+       | 32.7                        | 98.48       |
| 502.2936  | C25H44NO7P  | Monoacylglycerophosphoethanolamines | PE                   | LPE(20:4)                   | 501.2855     | 1.6            | [M+H]+           | 0.2                         | 77.83       |
| 526.2933  | C27H44NO7P  | Monoacylglycerophosphoethanolamines | PE                   | LPE(22:6)                   | 525.2855     | 1              | [M+H]+           | 0.2                         | 84.32       |
| 689.5605  | C38H77N2O6P | Ceramide phosphoethanolamines | PE-Cer               | PE-Cer(d36:1)               | 688.5519     | 1.9            | [M+H]+           | 0.1                         | 74.33       |
| 701.5602  | C39H77N2O6P | Ceramide phosphocholines | SM-M(D34:1)           | 700.5519                    | 1.5          | [M+H]+         | 0.1              | 71.02                       |
| 702.5441  | C39H76N2O7P | 1-alkyl,2-acylglycerophosphoethanolamines | PE                   | PE(O-34:2)                  | 701.5359     | 1.2            | [M+H]+           | 0.2                         | 79.65       |
| 703.575   | C39H79N2O6P | Ceramide phosphocholines | SM-M(D34:1)           | 702.5676                    | 0.3          | [M+H]+         | 1.3              | 96.09                       |
| 716.5235  | C39H74NO8P  | Diacylglycerophosphoethanolamines | PE                   | PE(34:2)                    | 715.5152     | 1.4            | [M+H]+           | 0.6                         | 93.34       |
| 718.5393  | C39H76N08P  | Diacylglycerophosphoethanolamines | PE                   | PE(34:1)                    | 717.5309     | 1.7            | [M+H]+           | 0.5                         | 90.88       |
| 720.555   | C39H78N08P  | Diacylglycerophosphoethanolamines | PE                   | PE(34:0)                    | 719.5465     | 1.7            | [M+H]+           | 1.5                         | 97.05       |
| 724.5287  | C41H74N07P  | 1-alkyl,2-acylglycerophosphoethanolamines | PE                   | PE(O-36:5)                  | 723.5203     | 1.5            | [M+H]+           | 5.0                         | 97.98       |
| 726.5445  | C41H76N07P  | 1-alkyl,2-acylglycerophosphoethanolamines | PE                   | PE(O-36:4)                  | 725.5359     | 1.8            | [M+H]+           | 0.1                         | 80.23       |
| 734.5702  | C40H80N08P  | Diacylglycerophosphocholines | PC                   | PC(32:0)                    | 733.5622     | 1.1            | [M+H]+           | 7.2                         | 98.47       |
| 738.5055  | C41H72N08P  | Diacylglycerophosphoethanolamines | PE                   | PE(36:5)                    | 737.4996     | 1.7            | [M+H]+           | 0.2                         | 78.47       |
| 738.5078  | C41H72N08P  | Diacylglycerophosphoethanolamines | PE                   | PE(36:5)                    | 737.4996     | 1.3            | [M+H]+           | 0.5                         | 92.07       |
| 740.5233  | C41H74N08P  | Diacylglycerophosphoethanolamines | PE                   | PE(36:4)                    | 739.5152     | 1.1            | [M+H]+           | 10.3                        | 98.65       |
| 742.539   | C41H76N08P  | Diacylglycerophosphoethanolamines | PE                   | PE(36:3)                    | 741.5309     | 1.2            | [M+H]+           | 0.7                         | 93.5        |
| C41H78NO8P | Diacylglycerophosphoethanolamines | PE | PE(O-36:2) | 743.5465 | 1.8 | [M+H]+ | 3.5 | 98.7 |
| C41H80NO8P | Diacylglycerophosphoethanolamines | PE | PE(O-36:1) | 745.5622 | 1.8 | [M+H]+ | 1.3 | 96.98 |
| C43H74NO7P | 1-(1Z-alkenyl),2-acylglycerophosphoethanolamines | PE | PE(O-38:7) | 747.5203 | 1 | [M+H]+ | 2.5 | 98.17 |
| C40H77O10P | Diacylglycerophosphoglycerols | PG | PG(34:1) | 748.5254 | 0.9 | [M+H]+ | 0.4 | 93.45 |
| C43H76NO7P | 1-alkyl,2-acylglycerophosphoethanolamines | PE | PE(O-36:6) | 749.5359 | 1.2 | [M+H]+ | 1.0 | 95.66 |
| C40H79O10P | Diacylglycerophosphoglycerols | PG | PG(34:0) | 750.5411 | 1.3 | [M+H]+ | 0.4 | 80.56 |
| C43H78NO7P | 1-alkyl,2-acylglycerophosphoethanolamines | PE | PE(O-38:5) | 751.5516 | 1.1 | [M+H]+ | 3.9 | 98.21 |
| C42H76NO8P | Diacylglycerophosphocholines | PC | PC(34:4) | 753.5309 | 1.1 | [M+H]+ | 0.4 | 74.19 |
| C43H80NO7P | 1-alkyl,2-acylglycerophosphoethanolamines | PE | PE(O-38:4) | 753.5672 | 1.6 | [M+H]+ | 0.2 | 85.74 |
| C44H78NO6P | Diacylglycerophosphocholines | PC | PC(34:3) | 755.5465 | 1.9 | [M+H]+ | 6.3 | 98.81 |
| C44H86NO6P | Ceramide 1-phosphates | C1P | C1P(d44:2) | 755.6193 | 0.5 | [M+H]+ | 0.1 | 71.11 |
| C42H80NO8P | Diacylglycerophosphocholines | PC | PC(O-34:2) | 757.5622 | 1.5 | [M+H]+ | 3.9 | 98.17 |
| C42H82NO8P | Diacylglycerophosphocholines | PC | PC(34:1) | 759.5778 | 1.1 | [M+H]+ | 4.5 | 98.14 |
| C43H72NO8P | Diacylglycerophosphoethanolamines | PE | PE(O-38:7) | 761.4996 | 1.6 | [M+H]+ | 0.4 | 85.57 |
| C43H74NO8P | Diacylglycerophosphoethanolamines | PE | PE(O-38:6) | 763.5152 | 0.9 | [M+H]+ | 5.2 | 98.71 |
| C43H76NO8P | Diacylglycerophosphoethanolamines | PE | PE(O-38:5) | 765.5309 | 1 | [M+H]+ | 11.3 | 98.49 |
| C43H78NO8P | Diacylglycerophosphoethanolamines | PE | PE(O-38:4) | 767.5465 | 0 | [M+H]+ | 49.3 | 98.81 |
| C44H82NO7P | 1-alkyl,2-acylglycerophosphocholines | PC | PC(O-36:4) | 767.5829 | 0 | [M+H]+ | 0.2 | 72.75 |
| C43H82NO8P | Diacylglycerophosphocholines | PE | PE(O-38:2) | 771.5778 | 0.6 | [M+H]+ | 0.4 | 74.58 |
| C43H76NO7P | 1-(1Z-alkenyl),2-acylglycerophosphoethanolamines | PE | PE(O-40:8) | 773.5359 | 0.3 | [M+H]+ | 1.5 | 97.98 |
| C45H78NO7P | 1-(1Z-alkenyl),2-acylglycerophosphoethanolamines | PE | PE(O-40:7) | 775.5516 | 1.5 | [M+H]+ | 1.5 | 98.06 |
| C45H80NO7P | 1-alkyl,2-acylglycerophosphoethanolamines | PE | PE(O-40:6) | 777.5672 | 0.1 | [M+H]+ | 0.7 | 95.74 |
| C44H78NO8P | Diacylglycerophosphocholines | PC | PC(36:5) | 779.5465 | 1.3 | [M+H]+ | 3.3 | 98.68 |
| C45H82NO7P | 1-alkyl,2-acylglycerophosphoethanolamines | PE | PE(O-40:5) | 779.5829 | 0.2 | [M+H]+ | 0.1 | 89.1 |
| C44H80NO8P | Diacylglycerophosphocholines | PC | PC(36:4) | 781.5622 | 0.5 | [M+H]+ | 6.6 | 98.73 |
| C44H82NO8P | Diacylglycerophosphocholines | PC | PC(36:3) | 783.5778 | 0.2 | [M+H]+ | 0.7 | 85.77 |
| C45H84NO8P | Diacylglycerophosphocholines | PC | PC(36:2) | 785.5935 | 1.2 | [M+H]+ | 2.0 | 97.44 |
| C45H91N2O6P | Ceramide phosphocholines (sphingomyelins) | SM | SM(d40:1) | 786.615 | 1.3 | [M+H]+ | 0.3 | 86.79 |
| C45H74NO8P | Diacylglycerophosphoethanolamines | PE | PE(O-40:8) | 787.5152 | 1.3 | [M+H]+ | 0.4 | 90.48 |
| C44H86NO8P | Diacylglycerophosphocholines | PC | PC(36:1) | 787.6091 | 1.6 | [M+H]+ | 0.6 | 94.47 |
| C45H76NO8P | Diacylglycerophosphoethanolamines | PE | PE(O-40:7) | 789.5309 | 0.6 | [M+H]+ | 3.4 | 96.21 |
| C42H80NO10P | Diacylglycerophosphoserines | PS | PS(36:1) | 789.552 | 1.3 | [M+H]+ | 0.2 | 76.13 |
| M/Z               | Formula                  | Description                                         | Retention Time | Area     | [M+H]+    | Relative Abundance |
|-------------------|--------------------------|-----------------------------------------------------|----------------|----------|-----------|-------------------|
| 790.5738          | C46H80NO7P               | 1-(1Z-alkenyl),2-acylglycerophosphocholines          | PC             | 0.9      | [M+H]+    | 0.3               |
| 792.5525          | C45H78NO8P               | Diacylglycerophosphoethanolamines                    | PE             | 1.6      | [M+H]+    | 0.2               |
| 792.5525          | C45H78NO8P               | Diacylglycerophosphoethanolamines                    | PE             | 1.8      | [M+H]+    | 4.4               |
| 792.5909          | C46H82NO7P               | 1-alkyl,2-acylglycerophosphocholines                 | PC             | 1        | [M+H]+    | 3.7               |
| 794.5701          | C45H80NO8P               | Diacylglycerophosphoethanolamines                    | PE             | 0.9      | [M+H]+    | 0.7               |
| 796.586           | C45H82NO8P               | Diacylglycerophosphoethanolamines                    | PE             | 1.1      | [M+H]+    | 1.5               |
| 804.5525          | C46H78NO8P               | Diacylglycerophospholipids                           | PC             | 1.6      | [M+H]+    | 2.8               |
| 806.5702          | C46H80NO8P               | Diacylglycerophospholipids                           | PC             | 1        | [M+H]+    | 6.7               |
| 808.5845          | C46H82NO8P               | Diacylglycerophospholipids                           | PC             | 0.7      | [M+H]+    | 2.4               |
| 810.6022          | C46H84NO8P               | Diacylglycerophospholipids                           | PE             | 1.1      | [M+H]+    | 2.3               |
| 812.5445          | C44H76NO10P              | Diacylglycerophospholipids                           | PS             | 1        | [M+H]+    | 1.8               |
| 813.6851          | C47H93N2O6P              | Ceramide phosphocholines (sphingomyelins)            | SM             | 0.9      | [M+H]+    | 0.4               |
| 814.5368          | C47H76NO8P               | Diacylglycerophosphoethanolamines                    | PE             | 1.6      | [M+H]+    | 0.2               |
| 815.7008          | C47H95N2O6P              | Ceramide phosphocholines (sphingomyelins)            | SM             | 0.9      | [M+H]+    | 0.2               |
| 818.5691          | C47H80NO8P               | Diacylglycerophosphoethanolamines                    | PE             | 0.5      | [M+H]+    | 0.1               |
| 818.6056          | C48H84NO7P               | 1-(1Z-alkenyl),2-acylglycerophosphocholines          | PC             | 0.3      | [M+H]+    | 0.2               |
| 820.585           | C47H82NO8P               | Diacylglycerophosphoethanolamines                    | PE             | 0.1      | [M+H]+    | 0.4               |
| 830.5682          | C48H80NO8P               | Diacylglycerophosphoethanolamines                    | PE             | 1.5      | [M+H]+    | 0.4               |
| 832.5835          | C48H82NO8P               | Diacylglycerophospholipids                           | PC             | 1.9      | [M+H]+    | 2.3               |
| 834.6002          | C48H84NO8P               | Diacylglycerophospholipids                           | PC             | 0.7      | [M+H]+    | 0.9               |
| 836.5447          | C46H78NO10P              | Diacylglycerophosphoethanolamines                    | PS             | 1.3      | [M+H]+    | 0.2               |
| 856.5842          | C50H82NO8P               | Diacylglycerophospholipids                           | PC             | 1.1      | [M+H]+    | 0.5               |
| 972.734           | C54H101NO13              | Simple Glc series                                    | Hex2Cer        | 0.6      | [M+H]+    | 0.1               |