Supplementary Materials: Variability of Lipids in Human Milk

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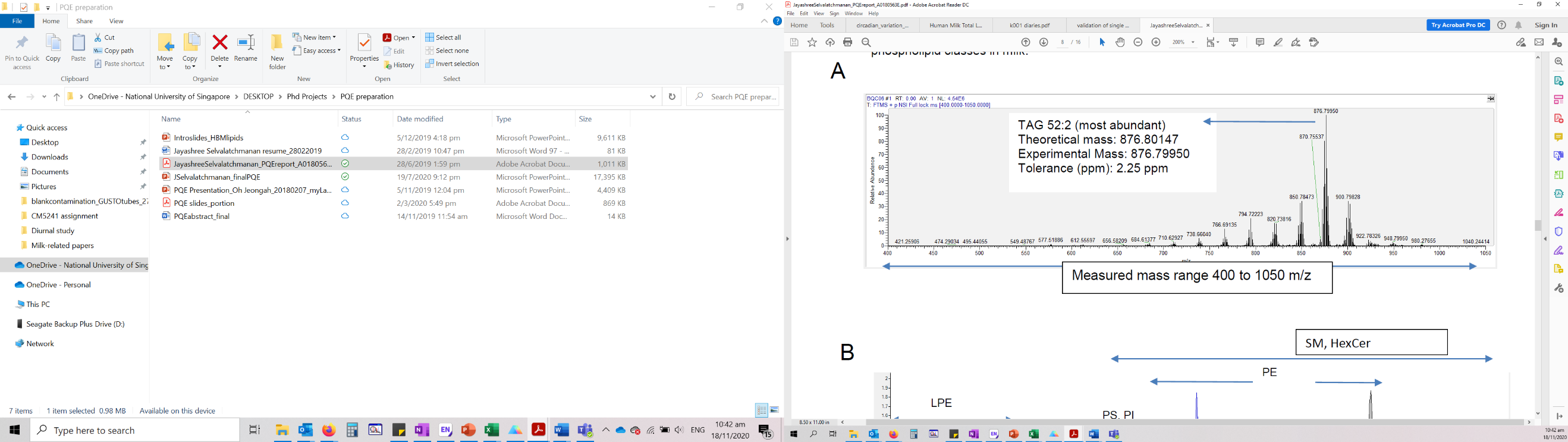
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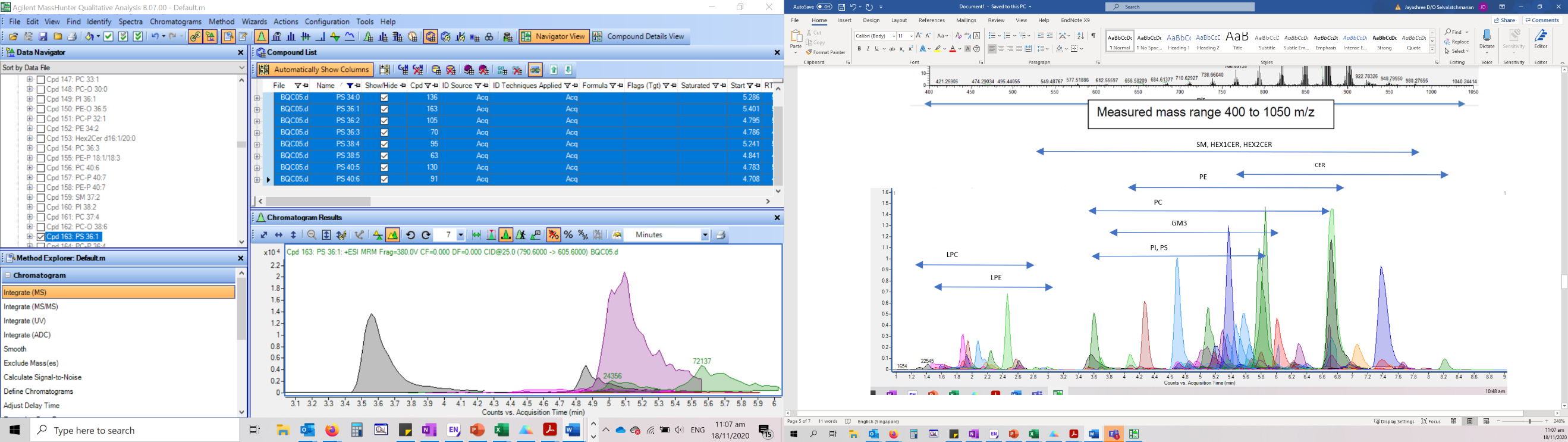
**Figures S1 (a) and (b)** Linearity curves for TAG 52:2 and DAG 34:1 extracted via 2-phase MTBE/MeOH method using 4-16 µL of human milk (analysed using Thermo QExactive plus quadruple-orbitrap mass spectrometer)

**Figures S1 (c) –(f):** Linearity curves for PE 38:1, PI 36:2, SM 40:1 and PC 36:1 extracted via 2-phase MTBE/MeOH method using 4-16 µL of human milk (analysed using Agilent 6495A QQQ)

**Figures S2 (a)-(f):** Linearity curve for GM3 d18:1/20:0, Hex1Cer d18:2/24:0, Hex2cer d18:1/16:0, LPC 18:1, LPE 18:1, Cer d18:1/24: extracted via 2-phase MTBE/MeOH method using 4-16 µL of human milk (analysed using Agilent 6495A QQQ)



**Figure S3.** Representative spectrum of TAGs and DAGs in human milk via direct-infusion mass spectrometry. Full scan of precursors shown measuring from 400 to 1050 m/z.



**Figure S4.** Representative chromatogram separating the various PL and SP classes via RP-LCMSMS (using dMRM)

**Chart, bubble chart

Description automatically generated**

**Figure S5.** PCA plot of participants who provided a milk sample before (0) and after (1) dinner.

Table S1: Evening/Morning Concentration (Median) values for every PL and SL measured

|  |  |  |  |
| --- | --- | --- | --- |
| Lipid | Evening/Morning concentration (median) | Lipid | Evening/Morning concentration (median) |
| GM3 d18:1/16:0 | 1.17 | PC 32:1 | 1.21 |
| GM3 d18:1/18:0 | 1.19 | PC 32:2 | 1.10 |
| GM3 d18:1/20:0 | 1.41 | PC 33:0 | 1.18 |
| GM3 d18:1/22:0 | 1.15 | PC 33:1 | 1.36 |
| GM3 d18:1/24:0 | 1.08 | PC 34:0 | 1.11 |
| Cer d18:1/18:0 | 1.17 | PC 34:1 | 1.12 |
| Cer d18:1/20:0 | 1.21 | PC 34:2 | 1.18 |
| Cer d18:1/22:0 | 1.15 | PC 34:3 | 1.26 |
| Cer d18:1/23:0 | 1.24 | PC 35:2 | 1.26 |
| Cer d18:1/24:0 | 1.08 | PC 36:1 | 1.22 |
| Cer d18:1/24:1 | 1.10 | PC 36:2 | 1.23 |
| Cer d18:2/22:0 | 1.17 | PC 36:3 | 1.30 |
| Cer d18:2/24:0 | 1.09 | PC 36:4 | 1.19 |
| Hex1Cer d18:2/22:0 | 1.18 | PC 38:3 | 1.18 |
| Hex1Cer d18:2/24:0 | 1.09 | PC 38:4 | 1.12 |
| Hex2Cer d18:1/16:0 | 1.13 | PC 38:5 | 1.12 |
| Hex2Cer d18:1/20:0 | 1.20 | PC 38:6 | 1.09 |
| Hex2Cer d18:1/22:0 | 1.15 | PC 40:6 | 1.17 |
| Hex2Cer d18:1/24:0 | 1.16 | PC 40:8 | 1.32 |
| LPC 14:0 | 1.00 | PS 36:1 | 1.08 |
| LPC 18:1 | 1.14 | PS 36:2 | 1.12 |
| LPC 20:1 | 1.13 | PS 36:3 | 1.18 |
| LPC 20:3 | 1.07 | PS 38:4 | 1.11 |
| LPC 22:5 | 1.01 | PS 40:6 | 1.09 |
| LPC 22:6 | 0.97 | SM 30:1 | 0.99 |
| LPE 16:0 | 1.01 | SM 31:1 | 1.03 |
| LPE 18:0 | 1.24 | SM 32:0 | 1.02 |
| LPE 18:1 | 1.09 | SM 32:1 | 1.07 |
| LPE 20:1 | 1.10 | SM 33:1 | 1.07 |
| LPE 22:1 | 1.11 | SM 34:0 | 1.05 |
| LPE 22:5 | 1.10 | SM 34:1 | 1.06 |
| PE 32:0 | 1.35 | SM 34:2 | 1.02 |
| PE 34:0 | 1.25 | SM 35:1 | 1.16 |
| PE 34:1 | 1.32 | SM 36:0 | 1.14 |
| PE 36:1 | 1.39 | SM 36:1 | 1.07 |
| PE 36:2 | 1.30 | SM 36:2 | 1.14 |
| PE 36:4 | 1.48 | SM 37:1 | 1.07 |
| PE 38:1 | 1.23 | SM 38:0 | 1.08 |
| PE 38:2 | 1.36 | SM 38:1 | 1.09 |
| PE 38:3 | 1.35 | SM 38:2 | 1.01 |
| PE 38:4 | 1.33 | SM 39:1 | 1.05 |
| PE 38:6 | 1.50 | SM 40:0 | 1.07 |
| PE 40:2 | 1.32 | SM 40:1 | 1.08 |
| PE 40:7 | 1.34 | SM 40:2 | 1.02 |
| PI 34:1 | 1.18 | SM 40:3 | 1.02 |
| PI 34:2 | 1.10 | SM 41:1 | 1.09 |
| PI 36:1 | 1.21 | SM 42:0 | 1.05 |
| PI 36:2 | 1.08 | SM 42:1 | 1.04 |
| PI 36:3 | 1.13 | SM 42:2 | 1.05 |
| PI 38:3 | 1.13 | SM 42:3 | 0.99 |
| PI 38:4 | 1.21 | SM 43:1 | 1.13 |
| PI 38:5 | 1.22 | SM 43:2 | 1.02 |
| PC 30:0 | 1.12 | SM 44:1 | 1.03 |
| PC 31:0 | 1.24 | SM 44:2 | 1.11 |
| PC 32:0 | 1.08 |  |  |

Table S2: Evening/Morning Concentration (Median) values for every TAG and DAG measured

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| Lipid | Evening/Morning concentration (median) | Lipid | Evening/Morning concentration (median) | Lipid | Evening/Morning concentration (median) |
| DAG 32:0 | 1.20 | TAG 47:4 | 1.15 | TAG 56:5 | 1.36 |
| DAG 34:2 | 1.09 | TAG 47:3 | 1.36 | TAG 56:4 | 1.32 |
| DAG 34:1 | 1.06 | TAG 47:2 | 1.39 | TAG 56:3 | 1.42 |
| DAG 34:0 | 1.17 | TAG 47:1 | 1.47 | TAG 56:2 | 1.50 |
| DAG 36:4 | 1.11 | TAG 48:7 | 1.37 | TAG 56:1 | 1.29 |
| DAG 36:3 | 1.12 | TAG 47:0 | 1.76 | TAG 58:10 | 1.17 |
| DAG 36:2 | 1.03 | TAG 48:6 | 1.26 | TAG 58:9 | 1.36 |
| DAG 36:1 | 0.95 | TAG 48:5 | 1.09 | TAG 58:8 | 1.31 |
| DAG 38:6 | 0.96 | TAG 48:4 | 1.10 | TAG 58:7 | 1.37 |
| DAG 44:10 | 1.25 | TAG 48:3 | 1.14 | TAG 58:6 | 1.36 |
| TAG 32:0 | 1.20 | TAG 48:2 | 1.12 | TAG 58:5 | 1.24 |
| TAG 34:1 | 1.64 | TAG 48:1 | 1.41 | TAG 58:4 | 1.24 |
| TAG 34:0 | 1.37 | TAG 49:4 | 1.53 |  |  |
| TAG 36:2 | 1.80 | TAG 49:3 | 1.43 |  |  |
| TAG 36:1 | 1.55 | TAG 49:2 | 1.53 |  |  |
| TAG 36:0 | 1.42 | TAG 50:8 | 1.22 |  |  |
| TAG 37:0 | 1.55 | TAG 49:1 | 1.88 |  |  |
| TAG 38:3 | 1.22 | TAG 50:7 | 1.15 |  |  |
| TAG 38:2 | 1.37 | TAG 50:6 | 1.25 |  |  |
| TAG 38:1 | 1.46 | TAG 50:5 | 1.25 |  |  |
| TAG 38:0 | 1.42 | TAG 50:4 | 1.22 |  |  |
| TAG 39:1 | 1.54 | TAG 50:3 | 1.28 |  |  |
| TAG 39:0 | 1.55 | TAG 50:2 | 1.27 |  |  |
| TAG 40:4 | 1.33 | TAG 50:1 | 1.34 |  |  |
| TAG 40:3 | 1.22 | TAG 51:4 | 1.61 |  |  |
| TAG 40:2 | 1.16 | TAG 51:3 | 1.60 |  |  |
| TAG 40:1 | 1.16 | TAG 51:2 | 1.66 |  |  |
| TAG 40:0 | 1.25 | TAG 52:8 | 1.09 |  |  |
| TAG 41:1 | 1.54 | TAG 51:1 | 1.68 |  |  |
| TAG 41:0 | 1.48 | TAG 52:7 | 1.12 |  |  |
| TAG 42:5 | 1.57 | TAG 52:6 | 1.30 |  |  |
| TAG 42:4 | 1.20 | TAG 52:5 | 1.42 |  |  |
| TAG 42:3 | 1.14 | TAG 52:4 | 1.41 |  |  |
| TAG 42:2 | 1.13 | TAG 52:3 | 1.36 |  |  |
| TAG 42:1 | 1.18 | TAG 52:2 | 1.39 |  |  |
| TAG 42:0 | 1.22 | TAG 53:5 | 1.48 |  |  |
| TAG 43:2 | 1.53 | TAG 53:4 | 1.45 |  |  |
| TAG 43:1 | 1.48 | TAG 53:3 | 1.52 |  |  |
| TAG 43:0 | 1.36 | TAG 53:2 | 1.65 |  |  |
| TAG 44:6 | 1.45 | TAG 54:8 | 1.37 |  |  |
| TAG 44:5 | 1.46 | TAG 53:1 | 1.60 |  |  |
| TAG 44:4 | 1.21 | TAG 54:7 | 1.54 |  |  |
| TAG 44:3 | 1.20 | TAG 54:6 | 1.48 |  |  |
| TAG 44:2 | 1.25 | TAG 54:5 | 1.34 |  |  |
| TAG 44:1 | 1.30 | TAG 54:4 | 1.39 |  |  |
| TAG 44:0 | 1.11 | TAG 54:3 | 1.35 |  |  |
| TAG 45:3 | 1.42 | TAG 54:2 | 1.37 |  |  |
| TAG 45:2 | 1.36 | TAG 55:6 | 1.78 |  |  |
| TAG 45:1 | 1.39 | TAG 55:5 | 1.62 |  |  |
| TAG 45:0 | 1.49 | TAG 55:4 | 1.50 |  |  |
| TAG 46:6 | 1.25 | TAG 55:3 | 1.62 |  |  |
| TAG 46:5 | 1.35 | TAG 56:9 | 1.28 |  |  |
| TAG 46:4 | 1.21 | TAG 55:2 | 1.78 |  |  |
| TAG 46:3 | 1.16 | TAG 56:8 | 1.35 |  |  |
| TAG 46:2 | 1.24 | TAG 56:7 | 1.31 |  |  |
| TAG 46:1 | 1.30 | TAG 56:6 | 1.34 |  |  |

Table S3: List of class-specific internal standards (ISTDs) made up in extraction solvent (MTBE/MeOH 7:2) and their final concentrations in the measured extract. DAG was normalised to TAG standard.

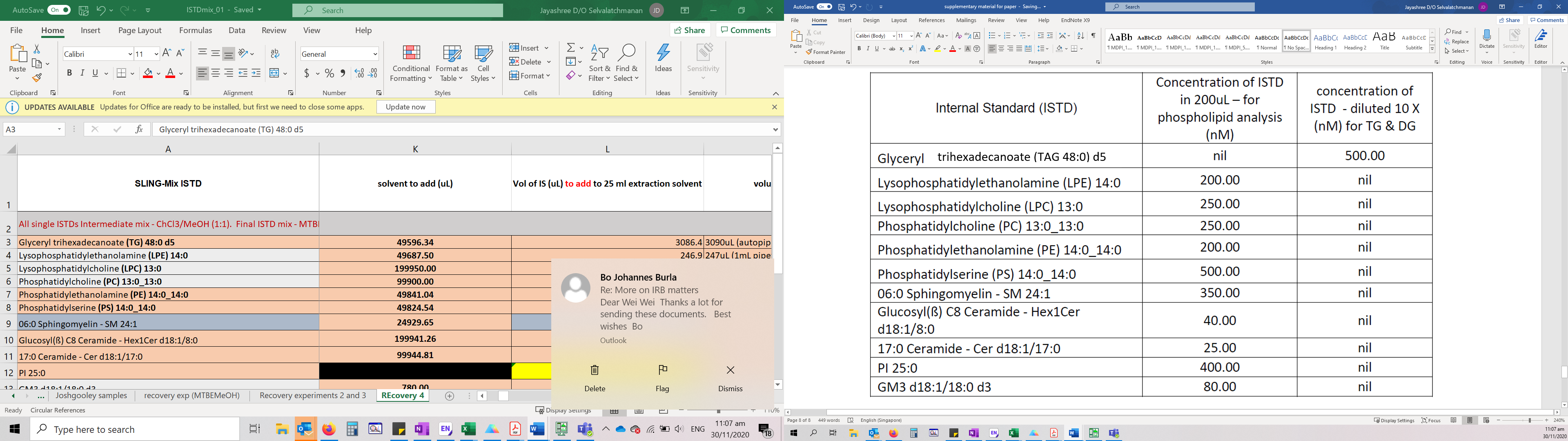


Table S4: Variance components analysis of individual lipids. Z: Wald Z-test value, p: p-value (significance set to 0.05), ICC: Intra-class correlation coefficient, F: F-test value.

|  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **Number** | **Analyte name** | **Variance analysis** | | | **Time of day** | | **Order of study visit** | |
| **Z** | **p** | **ICC** | **F** | **p** | **F** | **p** |
| 1 | PE\_34\_1 | 2.73 | 0.00 | 0.80 | 20.29 | 0.00 | 2.39 | 0.14 |
| 2 | PE\_32\_0 | 2.80 | 0.00 | 0.84 | 17.37 | 0.00 | 8.26 | 0.01 |
| 3 | PE\_38\_3 | 2.44 | 0.01 | 0.68 | 16.26 | 0.00 | 2.74 | 0.12 |
| 4 | PE\_38\_2 | 2.79 | 0.00 | 0.83 | 15.75 | 0.00 | 3.46 | 0.08 |
| 5 | PE\_36\_1 | 2.38 | 0.01 | 0.65 | 14.20 | 0.00 | 3.85 | 0.07 |
| 6 | LPE\_18\_0 | 2.40 | 0.01 | 0.66 | 13.40 | 0.00 | 0.77 | 0.39 |
| 7 | PE\_40\_7 | 2.39 | 0.01 | 0.66 | 12.92 | 0.00 | 2.31 | 0.15 |
| 8 | PE\_36\_2 | 2.01 | 0.02 | 0.52 | 11.81 | 0.00 | 1.07 | 0.31 |
| 9 | PE\_38\_6 | 2.42 | 0.01 | 0.67 | 11.79 | 0.00 | 1.52 | 0.23 |
| 10 | PE\_38\_4 | 1.24 | 0.11 | 0.30 | 11.08 | 0.00 | 0.01 | 0.91 |
| 11 | PE\_36\_4 | 2.42 | 0.01 | 0.67 | 10.97 | 0.00 | 0.60 | 0.45 |
| 12 | TG\_50\_1 | 1.73 | 0.04 | 0.43 | 9.69 | 0.01 | 1.34 | 0.26 |
| 13 | TG\_52\_3 | 1.89 | 0.03 | 0.48 | 8.61 | 0.01 | 0.35 | 0.56 |
| 14 | TG\_44\_5 | 2.28 | 0.01 | 0.62 | 8.45 | 0.01 | 1.11 | 0.31 |
| 15 | TG\_56\_8 | 2.06 | 0.02 | 0.54 | 8.44 | 0.01 | 1.23 | 0.28 |
| 16 | TG\_46\_5 | 2.25 | 0.01 | 0.60 | 8.04 | 0.01 | 0.70 | 0.41 |
| 17 | TG\_50\_2 | 1.90 | 0.03 | 0.49 | 7.97 | 0.01 | 1.13 | 0.30 |
| 18 | TG\_52\_4 | 2.24 | 0.01 | 0.60 | 7.92 | 0.01 | 0.16 | 0.70 |
| 19 | TG\_44\_4 | 2.21 | 0.01 | 0.59 | 7.91 | 0.01 | 0.64 | 0.43 |
| 20 | TG\_40\_4 | 2.26 | 0.01 | 0.61 | 7.90 | 0.01 | 0.06 | 0.80 |
| 21 | TG\_42\_4 | 1.92 | 0.03 | 0.49 | 7.76 | 0.01 | 0.34 | 0.57 |
| 22 | SM\_36\_0 | 2.33 | 0.01 | 0.63 | 7.74 | 0.01 | 0.29 | 0.60 |
| 23 | TG\_56\_7 | 1.71 | 0.04 | 0.43 | 7.58 | 0.01 | 1.06 | 0.32 |
| 24 | TG\_43\_2 | 2.00 | 0.02 | 0.52 | 7.51 | 0.01 | 1.92 | 0.18 |
| 25 | PE\_40\_2 | 2.84 | 0.00 | 0.86 | 7.49 | 0.01 | 4.46 | 0.05 |
| 26 | TG\_56\_6 | 1.52 | 0.06 | 0.38 | 7.36 | 0.01 | 0.69 | 0.42 |
| 27 | TG\_52\_6 | 2.18 | 0.01 | 0.58 | 7.33 | 0.01 | 1.79 | 0.20 |
| 28 | TG\_48\_6 | 2.21 | 0.01 | 0.59 | 7.27 | 0.01 | 2.29 | 0.15 |
| 29 | TG\_50\_3 | 2.11 | 0.02 | 0.56 | 7.20 | 0.02 | 1.29 | 0.27 |
| 30 | TG\_42\_5 | 2.11 | 0.02 | 0.55 | 7.18 | 0.02 | 0.24 | 0.63 |
| 31 | TG\_49\_4 | 2.19 | 0.01 | 0.58 | 7.05 | 0.02 | 1.75 | 0.20 |
| 32 | PE\_34\_0 | 2.68 | 0.00 | 0.78 | 7.00 | 0.02 | 9.48 | 0.01 |
| 33 | TG\_44\_3 | 2.19 | 0.01 | 0.58 | 6.95 | 0.02 | 1.26 | 0.28 |
| 34 | TG\_52\_5 | 2.30 | 0.01 | 0.62 | 6.94 | 0.02 | 0.28 | 0.60 |
| 35 | TG\_50\_5 | 2.33 | 0.01 | 0.63 | 6.93 | 0.02 | 1.30 | 0.27 |
| 36 | TG\_46\_4 | 2.17 | 0.01 | 0.58 | 6.91 | 0.02 | 0.59 | 0.45 |
| 37 | TG\_51\_3 | 1.85 | 0.03 | 0.47 | 6.91 | 0.02 | 0.72 | 0.41 |
| 38 | TG\_48\_1 | 2.17 | 0.02 | 0.58 | 6.84 | 0.02 | 3.11 | 0.09 |
| 39 | TG\_50\_4 | 2.37 | 0.01 | 0.65 | 6.78 | 0.02 | 1.17 | 0.29 |
| 40 | TG\_49\_3 | 2.07 | 0.02 | 0.54 | 6.76 | 0.02 | 1.33 | 0.26 |
| 41 | TG\_51\_4 | 1.83 | 0.03 | 0.47 | 6.76 | 0.02 | 0.27 | 0.61 |
| 42 | TG\_47\_3 | 2.28 | 0.01 | 0.62 | 6.74 | 0.02 | 2.48 | 0.13 |
| 43 | TG\_49\_2 | 2.06 | 0.02 | 0.54 | 6.73 | 0.02 | 1.67 | 0.21 |
| 44 | TG\_38\_2 | 2.15 | 0.02 | 0.57 | 6.73 | 0.02 | 0.22 | 0.64 |
| 45 | TG\_54\_8 | 2.28 | 0.01 | 0.62 | 6.68 | 0.02 | 0.69 | 0.42 |
| 46 | TG\_54\_6 | 2.36 | 0.01 | 0.64 | 6.66 | 0.02 | 0.06 | 0.81 |
| 47 | TG\_44\_2 | 2.10 | 0.02 | 0.55 | 6.60 | 0.02 | 1.56 | 0.23 |
| 48 | TG\_54\_5 | 2.25 | 0.01 | 0.60 | 6.57 | 0.02 | 0.15 | 0.70 |
| 49 | TG\_58\_9 | 2.06 | 0.02 | 0.54 | 6.56 | 0.02 | 1.05 | 0.32 |
| 50 | TG\_50\_6 | 2.26 | 0.01 | 0.61 | 6.54 | 0.02 | 2.68 | 0.12 |
| 51 | PC\_36\_1 | 2.42 | 0.01 | 0.67 | 6.51 | 0.02 | 1.67 | 0.21 |
| 52 | PI\_38\_3 | 2.13 | 0.02 | 0.56 | 6.46 | 0.02 | 2.28 | 0.15 |
| 53 | TG\_54\_7 | 2.29 | 0.01 | 0.62 | 6.43 | 0.02 | 0.18 | 0.68 |
| 54 | TG\_45\_2 | 2.11 | 0.02 | 0.55 | 6.35 | 0.02 | 2.15 | 0.16 |
| 55 | TG\_38\_3 | 2.21 | 0.01 | 0.59 | 6.35 | 0.02 | 0.41 | 0.53 |
| 56 | GM3\_d18\_1\_18\_0 | 2.35 | 0.01 | 0.64 | 6.34 | 0.02 | 2.15 | 0.16 |
| 57 | TG\_46\_6 | 2.02 | 0.02 | 0.53 | 6.33 | 0.02 | 1.37 | 0.26 |
| 58 | TG\_40\_3 | 2.07 | 0.02 | 0.54 | 6.28 | 0.02 | 0.44 | 0.52 |
| 59 | TG\_36\_2 | 2.24 | 0.01 | 0.60 | 6.28 | 0.02 | 0.62 | 0.44 |
| 60 | TG\_43\_1 | 2.09 | 0.02 | 0.55 | 6.27 | 0.02 | 2.62 | 0.12 |
| 61 | TG\_45\_3 | 2.05 | 0.02 | 0.54 | 6.25 | 0.02 | 1.81 | 0.19 |
| 62 | TG\_48\_7 | 1.93 | 0.03 | 0.50 | 6.24 | 0.02 | 1.27 | 0.27 |
| 63 | GM3\_d18\_1\_22\_0 | 1.62 | 0.05 | 0.40 | 6.22 | 0.02 | 2.48 | 0.13 |
| 64 | PE\_38\_1 | 2.82 | 0.00 | 0.85 | 6.21 | 0.02 | 4.65 | 0.04 |
| 65 | PC\_40\_6 | 2.21 | 0.01 | 0.59 | 6.13 | 0.02 | 3.06 | 0.10 |
| 66 | TG\_44\_1 | 2.09 | 0.02 | 0.55 | 6.10 | 0.02 | 2.25 | 0.15 |
| 67 | TG\_50\_8 | 2.46 | 0.01 | 0.69 | 6.07 | 0.02 | 2.55 | 0.13 |
| 68 | TG\_42\_3 | 2.15 | 0.02 | 0.57 | 6.02 | 0.02 | 1.22 | 0.28 |
| 69 | DAG\_44\_10 | 2.13 | 0.02 | 0.56 | 6.01 | 0.02 | 0.80 | 0.38 |
| 70 | TG\_44\_6 | 1.92 | 0.03 | 0.49 | 5.93 | 0.03 | 0.85 | 0.37 |
| 71 | TG\_56\_5 | 1.62 | 0.05 | 0.40 | 5.83 | 0.03 | 0.93 | 0.35 |
| 72 | TG\_46\_3 | 2.18 | 0.01 | 0.58 | 5.80 | 0.03 | 1.57 | 0.23 |
| 73 | TG\_56\_9 | 2.23 | 0.01 | 0.60 | 5.80 | 0.03 | 1.38 | 0.25 |
| 74 | PS\_38\_4 | 0.69 | 0.24 | 0.16 | 5.76 | 0.03 | 0.39 | 0.54 |
| 75 | TG\_49\_1 | 2.00 | 0.02 | 0.52 | 5.75 | 0.03 | 2.15 | 0.16 |
| 76 | PC\_36\_3 | 2.05 | 0.02 | 0.53 | 5.68 | 0.03 | 2.00 | 0.17 |
| 77 | TG\_48\_5 | 2.54 | 0.01 | 0.72 | 5.64 | 0.03 | 2.67 | 0.12 |
| 78 | TG\_37\_0 | 1.57 | 0.06 | 0.39 | 5.54 | 0.03 | 2.32 | 0.15 |
| 79 | TG\_54\_4 | 1.84 | 0.03 | 0.47 | 5.53 | 0.03 | 0.44 | 0.52 |
| 80 | TG\_39\_0 | 2.16 | 0.02 | 0.57 | 5.53 | 0.03 | 4.44 | 0.05 |
| 81 | TG\_46\_1 | 2.21 | 0.01 | 0.59 | 5.50 | 0.03 | 2.84 | 0.11 |
| 82 | TG\_53\_5 | 1.86 | 0.03 | 0.47 | 5.50 | 0.03 | 0.35 | 0.56 |
| 83 | TG\_41\_1 | 1.86 | 0.03 | 0.47 | 5.44 | 0.03 | 1.94 | 0.18 |
| 84 | TG\_50\_7 | 2.22 | 0.01 | 0.59 | 5.42 | 0.03 | 1.72 | 0.21 |
| 85 | TG\_47\_2 | 2.21 | 0.01 | 0.59 | 5.42 | 0.03 | 2.84 | 0.11 |
| 86 | PI\_36\_1 | 2.23 | 0.01 | 0.60 | 5.39 | 0.03 | 3.45 | 0.08 |
| 87 | TG\_40\_2 | 2.02 | 0.02 | 0.52 | 5.39 | 0.03 | 0.65 | 0.43 |
| 88 | TG\_51\_2 | 1.76 | 0.04 | 0.44 | 5.38 | 0.03 | 1.09 | 0.31 |
| 89 | SM\_40\_0 | 2.15 | 0.02 | 0.57 | 5.28 | 0.03 | 0.73 | 0.40 |
| 90 | TG\_55\_5 | 1.39 | 0.08 | 0.34 | 5.28 | 0.03 | 0.86 | 0.37 |
| 91 | PI\_36\_3 | 2.46 | 0.01 | 0.68 | 5.22 | 0.03 | 0.35 | 0.56 |
| 92 | TG\_58\_8 | 1.70 | 0.04 | 0.43 | 5.21 | 0.03 | 0.81 | 0.38 |
| 93 | TG\_53\_4 | 1.74 | 0.04 | 0.44 | 5.18 | 0.04 | 0.45 | 0.51 |
| 94 | TG\_52\_7 | 2.28 | 0.01 | 0.61 | 5.18 | 0.04 | 2.70 | 0.12 |
| 95 | PS\_36\_3 | 2.46 | 0.01 | 0.68 | 5.17 | 0.04 | 1.57 | 0.23 |
| 96 | PI\_36\_2 | 2.28 | 0.01 | 0.62 | 5.13 | 0.04 | 0.49 | 0.49 |
| 97 | PC\_32\_0 | 2.32 | 0.01 | 0.63 | 5.12 | 0.04 | 2.29 | 0.15 |
| 98 | TG\_45\_1 | 2.19 | 0.01 | 0.58 | 5.11 | 0.04 | 2.99 | 0.10 |
| 99 | TG\_48\_2 | 2.18 | 0.01 | 0.58 | 5.09 | 0.04 | 2.66 | 0.12 |
| 100 | TG\_38\_1 | 1.75 | 0.04 | 0.44 | 5.08 | 0.04 | 0.25 | 0.62 |
| 101 | PI\_34\_2 | 2.28 | 0.01 | 0.62 | 5.06 | 0.04 | 0.87 | 0.36 |
| 102 | Hex2Cer\_d18\_1\_24\_0 | 2.35 | 0.01 | 0.64 | 4.98 | 0.04 | 0.42 | 0.52 |
| 103 | TG\_46\_2 | 2.21 | 0.01 | 0.59 | 4.94 | 0.04 | 2.32 | 0.15 |
| 104 | TG\_42\_0 | 2.11 | 0.02 | 0.56 | 4.93 | 0.04 | 4.05 | 0.06 |
| 105 | TG\_55\_6 | 1.55 | 0.06 | 0.38 | 4.93 | 0.04 | 1.40 | 0.25 |
| 106 | PC\_35\_2 | 2.32 | 0.01 | 0.63 | 4.84 | 0.04 | 1.09 | 0.31 |
| 107 | TG\_58\_10 | 2.32 | 0.01 | 0.63 | 4.84 | 0.04 | 0.65 | 0.43 |
| 108 | TG\_47\_0 | 2.33 | 0.01 | 0.64 | 4.83 | 0.04 | 2.75 | 0.11 |
| 109 | TG\_47\_1 | 2.24 | 0.01 | 0.60 | 4.78 | 0.04 | 3.45 | 0.08 |
| 110 | TG\_36\_0 | 1.90 | 0.03 | 0.48 | 4.74 | 0.04 | 1.54 | 0.23 |
| 111 | TG\_41\_0 | 2.26 | 0.01 | 0.61 | 4.73 | 0.04 | 4.22 | 0.05 |
| 112 | TG\_58\_7 | 1.30 | 0.10 | 0.32 | 4.66 | 0.04 | 0.73 | 0.41 |
| 113 | TG\_40\_1 | 1.90 | 0.03 | 0.49 | 4.62 | 0.05 | 0.91 | 0.35 |
| 114 | TG\_51\_1 | 1.67 | 0.05 | 0.42 | 4.52 | 0.05 | 1.25 | 0.28 |
| 115 | TG\_34\_0 | 2.00 | 0.02 | 0.52 | 4.46 | 0.05 | 1.60 | 0.22 |
| 116 | Hex1Cer\_d18\_2\_22\_0 | 2.22 | 0.01 | 0.59 | 4.44 | 0.05 | 0.07 | 0.79 |
| 117 | PC\_36\_4 | 2.54 | 0.01 | 0.72 | 4.44 | 0.05 | 1.38 | 0.26 |
| 118 | TG\_38\_0 | 1.94 | 0.03 | 0.50 | 4.42 | 0.05 | 2.32 | 0.15 |
| 119 | TG\_32\_0 | 2.02 | 0.02 | 0.53 | 4.42 | 0.05 | 1.27 | 0.27 |
| 120 | PI\_34\_1 | 2.32 | 0.01 | 0.63 | 4.38 | 0.05 | 0.52 | 0.48 |
| 121 | PS\_36\_1 | 2.47 | 0.01 | 0.69 | 4.38 | 0.05 | 0.29 | 0.60 |
| 122 | TG\_45\_0 | 2.35 | 0.01 | 0.64 | 4.36 | 0.05 | 3.69 | 0.07 |
| 123 | PC\_40\_8 | 2.62 | 0.00 | 0.75 | 4.36 | 0.05 | 1.57 | 0.23 |
| 124 | TG\_42\_2 | 2.15 | 0.02 | 0.57 | 4.30 | 0.05 | 1.55 | 0.23 |
| 125 | TG\_36\_1 | 1.75 | 0.04 | 0.44 | 4.28 | 0.05 | 0.70 | 0.41 |
| 126 | PC\_36\_2 | 2.21 | 0.01 | 0.59 | 4.27 | 0.05 | 1.72 | 0.21 |
| 127 | TG\_43\_0 | 2.24 | 0.01 | 0.60 | 4.26 | 0.05 | 3.56 | 0.08 |
| 128 | GM3\_d18\_1\_16\_0 | 2.46 | 0.01 | 0.69 | 4.15 | 0.06 | 3.94 | 0.06 |
| 129 | TG\_55\_4 | 1.57 | 0.06 | 0.39 | 4.14 | 0.06 | 1.01 | 0.33 |
| 130 | PC\_38\_3 | 2.26 | 0.01 | 0.61 | 4.13 | 0.06 | 0.76 | 0.39 |
| 131 | TG\_58\_6 | 1.11 | 0.13 | 0.27 | 4.07 | 0.06 | 0.60 | 0.45 |
| 132 | GM3\_d18\_1\_20\_0 | 0.93 | 0.18 | 0.22 | 4.01 | 0.06 | 1.46 | 0.24 |
| 133 | PC\_33\_1 | 2.51 | 0.01 | 0.71 | 3.98 | 0.06 | 1.05 | 0.32 |
| 134 | PI\_38\_4 | 1.75 | 0.04 | 0.44 | 3.97 | 0.06 | 1.23 | 0.28 |
| 135 | SM\_42\_0 | 2.45 | 0.01 | 0.68 | 3.95 | 0.06 | 0.39 | 0.54 |
| 136 | TG\_44\_0 | 2.11 | 0.02 | 0.55 | 3.91 | 0.06 | 3.61 | 0.07 |
| 137 | TG\_52\_8 | 2.33 | 0.01 | 0.63 | 3.91 | 0.06 | 2.68 | 0.12 |
| 138 | TG\_42\_1 | 1.97 | 0.02 | 0.51 | 3.89 | 0.06 | 1.58 | 0.22 |
| 139 | TG\_48\_3 | 2.27 | 0.01 | 0.61 | 3.87 | 0.06 | 2.00 | 0.17 |
| 140 | TG\_53\_3 | 1.48 | 0.07 | 0.36 | 3.85 | 0.07 | 0.68 | 0.42 |
| 141 | TG\_39\_1 | 1.39 | 0.08 | 0.34 | 3.83 | 0.07 | 0.84 | 0.37 |
| 142 | PC\_38\_4 | 1.30 | 0.10 | 0.31 | 3.81 | 0.07 | 0.87 | 0.36 |
| 143 | Cer\_d18\_2\_22\_0 | 2.18 | 0.01 | 0.58 | 3.75 | 0.07 | 0.15 | 0.71 |
| 144 | Hex2Cer\_d18\_1\_22\_0 | 2.20 | 0.01 | 0.59 | 3.70 | 0.07 | 0.09 | 0.77 |
| 145 | TG\_40\_0 | 2.02 | 0.02 | 0.52 | 3.64 | 0.07 | 3.39 | 0.08 |
| 146 | PS\_36\_2 | 1.83 | 0.03 | 0.47 | 3.64 | 0.07 | 0.93 | 0.35 |
| 147 | PC\_34\_3 | 2.53 | 0.01 | 0.71 | 3.54 | 0.08 | 1.35 | 0.26 |
| 148 | SM\_44\_2 | 2.87 | 0.00 | 0.88 | 3.54 | 0.08 | 1.72 | 0.21 |
| 149 | SM\_36\_2 | 1.83 | 0.03 | 0.47 | 3.49 | 0.08 | 0.03 | 0.85 |
| 150 | TG\_55\_2 | 1.59 | 0.06 | 0.39 | 3.47 | 0.08 | 2.69 | 0.12 |
| 151 | TG\_34\_1 | 1.79 | 0.04 | 0.45 | 3.44 | 0.08 | 1.00 | 0.33 |
| 152 | SM\_38\_1 | 1.65 | 0.05 | 0.41 | 3.43 | 0.08 | 1.20 | 0.29 |
| 153 | TG\_53\_1 | 1.67 | 0.05 | 0.42 | 3.32 | 0.08 | 1.96 | 0.18 |
| 154 | TG\_48\_4 | 2.51 | 0.01 | 0.70 | 3.26 | 0.09 | 2.08 | 0.17 |
| 155 | PC\_34\_2 | 1.81 | 0.03 | 0.46 | 3.26 | 0.09 | 0.29 | 0.60 |
| 156 | PI\_38\_5 | 2.52 | 0.01 | 0.71 | 3.23 | 0.09 | 2.59 | 0.12 |
| 157 | TG\_47\_4 | 1.99 | 0.02 | 0.52 | 3.19 | 0.09 | 0.05 | 0.83 |
| 158 | SM\_38\_0 | 1.79 | 0.04 | 0.45 | 3.11 | 0.09 | 0.52 | 0.48 |
| 159 | PC\_33\_0 | 2.66 | 0.00 | 0.77 | 3.03 | 0.10 | 2.99 | 0.10 |
| 160 | LPE\_22\_5 | 2.57 | 0.01 | 0.73 | 3.03 | 0.10 | 0.29 | 0.60 |
| 161 | TG\_58\_5 | 1.23 | 0.11 | 0.30 | 2.99 | 0.10 | 0.94 | 0.35 |
| 162 | SM\_34\_0 | 2.34 | 0.01 | 0.64 | 2.97 | 0.10 | 0.20 | 0.66 |
| 163 | TG\_55\_3 | 1.43 | 0.08 | 0.35 | 2.96 | 0.10 | 1.37 | 0.26 |
| 164 | PC\_34\_1 | 2.33 | 0.01 | 0.64 | 2.84 | 0.11 | 1.68 | 0.21 |
| 165 | TG\_54\_3 | 1.39 | 0.08 | 0.34 | 2.82 | 0.11 | 0.85 | 0.37 |
| 166 | SM\_36\_1 | 1.91 | 0.03 | 0.49 | 2.79 | 0.11 | 0.06 | 0.82 |
| 167 | Hex1Cer\_d18\_2\_24\_0 | 2.57 | 0.01 | 0.73 | 2.75 | 0.11 | 1.73 | 0.21 |
| 168 | GM3\_d18\_1\_24\_0 | 1.97 | 0.02 | 0.51 | 2.70 | 0.12 | 0.46 | 0.50 |
| 169 | TG\_58\_1 | 2.19 | 0.01 | 0.58 | 2.69 | 0.12 | 3.01 | 0.10 |
| 170 | TG\_56\_1 | 1.55 | 0.06 | 0.38 | 2.67 | 0.12 | 2.24 | 0.15 |
| 171 | SM\_39\_1 | 1.99 | 0.02 | 0.51 | 2.67 | 0.12 | 0.01 | 0.91 |
| 172 | Hex2Cer\_d18\_1\_20\_0 | 2.51 | 0.01 | 0.70 | 2.64 | 0.12 | 1.94 | 0.18 |
| 173 | Cer\_d18\_1\_22\_0 | 2.16 | 0.02 | 0.57 | 2.61 | 0.12 | 1.17 | 0.29 |
| 174 | LPE\_22\_1 | 2.99 | 0.00 | 0.94 | 2.47 | 0.13 | 3.05 | 0.10 |
| 175 | LPE\_20\_1 | 2.77 | 0.00 | 0.82 | 2.45 | 0.13 | 1.37 | 0.26 |
| 176 | PC\_38\_6 | 2.41 | 0.01 | 0.67 | 2.42 | 0.14 | 0.00 | 1.00 |
| 177 | TG\_53\_2 | 1.43 | 0.08 | 0.35 | 2.40 | 0.14 | 0.94 | 0.35 |
| 178 | Cer\_d18\_1\_24\_0 | 2.48 | 0.01 | 0.69 | 2.33 | 0.14 | 1.30 | 0.27 |
| 179 | PS\_40\_6 | 2.45 | 0.01 | 0.68 | 2.33 | 0.14 | 0.58 | 0.46 |
| 180 | LPE\_18\_1 | 2.50 | 0.01 | 0.70 | 2.31 | 0.15 | 0.25 | 0.62 |
| 181 | TG\_56\_4 | 1.59 | 0.06 | 0.39 | 2.28 | 0.15 | 1.89 | 0.19 |
| 182 | SM\_40\_1 | 1.76 | 0.04 | 0.44 | 2.26 | 0.15 | 0.68 | 0.42 |
| 183 | SM\_42\_2 | 2.71 | 0.00 | 0.79 | 2.26 | 0.15 | 1.21 | 0.29 |
| 184 | SM\_43\_1 | 2.44 | 0.01 | 0.68 | 2.22 | 0.15 | 0.78 | 0.39 |
| 185 | LPC\_20\_1 | 2.79 | 0.00 | 0.83 | 2.16 | 0.16 | 1.55 | 0.23 |
| 186 | TG\_58\_2 | 1.56 | 0.06 | 0.39 | 2.16 | 0.16 | 3.39 | 0.08 |
| 187 | SM\_37\_1 | 1.48 | 0.07 | 0.36 | 2.14 | 0.16 | 0.12 | 0.74 |
| 188 | DAG\_32\_0 | 2.34 | 0.01 | 0.64 | 2.12 | 0.16 | 1.44 | 0.25 |
| 189 | SM\_42\_1 | 2.17 | 0.02 | 0.57 | 1.88 | 0.19 | 1.12 | 0.30 |
| 190 | LPC\_18\_1 | 2.53 | 0.01 | 0.71 | 1.84 | 0.19 | 0.23 | 0.64 |
| 191 | PC\_32\_1 | 2.38 | 0.01 | 0.65 | 1.74 | 0.20 | 2.20 | 0.15 |
| 192 | Cer\_d18\_1\_20\_0 | 1.85 | 0.03 | 0.47 | 1.70 | 0.21 | 0.55 | 0.47 |
| 193 | SM\_38\_2 | 1.58 | 0.06 | 0.39 | 1.67 | 0.21 | 0.36 | 0.56 |
| 194 | PC\_31\_0 | 2.62 | 0.00 | 0.75 | 1.66 | 0.21 | 0.36 | 0.55 |
| 195 | TG\_58\_3 | 1.54 | 0.06 | 0.38 | 1.63 | 0.22 | 4.46 | 0.05 |
| 196 | PC\_34\_0 | 2.11 | 0.02 | 0.55 | 1.61 | 0.22 | 2.70 | 0.12 |
| 197 | SM\_35\_1 | 2.15 | 0.02 | 0.57 | 1.60 | 0.22 | 0.56 | 0.46 |
| 198 | Cer\_d18\_1\_23\_0 | 2.19 | 0.01 | 0.58 | 1.55 | 0.23 | 0.89 | 0.36 |
| 199 | DAG\_34\_1 | 2.53 | 0.01 | 0.71 | 1.50 | 0.24 | 1.55 | 0.23 |
| 200 | SM\_41\_1 | 1.98 | 0.02 | 0.51 | 1.49 | 0.24 | 0.26 | 0.62 |
| 201 | SM\_43\_2 | 2.83 | 0.00 | 0.85 | 1.37 | 0.26 | 0.47 | 0.50 |
| 202 | DAG\_34\_0 | 2.53 | 0.01 | 0.71 | 1.36 | 0.26 | 1.49 | 0.24 |
| 203 | TG\_60\_3 | 1.50 | 0.07 | 0.37 | 1.30 | 0.27 | 4.09 | 0.06 |
| 204 | TG\_58\_4 | 1.90 | 0.03 | 0.49 | 1.29 | 0.27 | 2.96 | 0.10 |
| 205 | TG\_56\_3 | 1.23 | 0.11 | 0.30 | 1.27 | 0.27 | 2.90 | 0.11 |
| 206 | TG\_56\_2 | 1.36 | 0.09 | 0.33 | 1.26 | 0.28 | 4.35 | 0.05 |
| 207 | SM\_31\_1 | 2.61 | 0.00 | 0.75 | 1.21 | 0.29 | 0.63 | 0.44 |
| 208 | Cer\_d18\_2\_24\_0 | 2.46 | 0.01 | 0.69 | 1.18 | 0.29 | 1.73 | 0.21 |
| 209 | Hex2Cer\_d18\_1\_16\_0 | 0.27 | 0.39 | 0.06 | 1.18 | 0.29 | 0.85 | 0.37 |
| 210 | SM\_40\_2 | 2.32 | 0.01 | 0.63 | 1.14 | 0.30 | 0.09 | 0.77 |
| 211 | DAG\_34\_2 | 2.62 | 0.00 | 0.75 | 1.12 | 0.30 | 1.35 | 0.26 |
| 212 | SM\_32\_1 | 2.51 | 0.01 | 0.70 | 1.10 | 0.31 | 0.86 | 0.36 |
| 213 | SM\_44\_1 | 2.47 | 0.01 | 0.69 | 1.07 | 0.31 | 0.57 | 0.46 |
| 214 | PC\_38\_5 | 2.21 | 0.01 | 0.59 | 1.04 | 0.32 | 0.98 | 0.33 |
| 215 | DAG\_38\_6 | 2.61 | 0.00 | 0.75 | 1.03 | 0.32 | 2.53 | 0.13 |
| 216 | PC\_32\_2 | 2.17 | 0.02 | 0.58 | 0.92 | 0.35 | 3.45 | 0.08 |
| 217 | SM\_34\_1 | 2.24 | 0.01 | 0.60 | 0.89 | 0.36 | 0.00 | 0.95 |
| 218 | SM\_32\_0 | 2.46 | 0.01 | 0.68 | 0.87 | 0.36 | 0.85 | 0.37 |
| 219 | DAG\_36\_1 | 2.54 | 0.01 | 0.72 | 0.82 | 0.38 | 1.94 | 0.18 |
| 220 | Cer\_d18\_1\_18\_0 | 2.19 | 0.01 | 0.58 | 0.78 | 0.39 | 1.17 | 0.29 |
| 221 | SM\_42\_3 | 2.37 | 0.01 | 0.65 | 0.77 | 0.39 | 0.18 | 0.68 |
| 222 | SM\_33\_1 | 2.51 | 0.01 | 0.71 | 0.65 | 0.43 | 1.12 | 0.30 |
| 223 | DAG\_36\_2 | 2.74 | 0.00 | 0.81 | 0.52 | 0.48 | 1.25 | 0.28 |
| 224 | TG\_54\_2 | 1.03 | 0.15 | 0.25 | 0.49 | 0.49 | 1.93 | 0.18 |
| 225 | PC\_30\_0 | 2.23 | 0.01 | 0.60 | 0.47 | 0.50 | 2.59 | 0.12 |
| 226 | LPC\_20\_3 | 2.48 | 0.01 | 0.69 | 0.45 | 0.51 | 0.38 | 0.55 |
| 227 | SM\_34\_2 | 2.45 | 0.01 | 0.68 | 0.40 | 0.53 | 0.02 | 0.88 |
| 228 | SM\_40\_3 | 2.06 | 0.02 | 0.54 | 0.40 | 0.53 | 0.20 | 0.66 |
| 229 | Cer\_d18\_1\_24\_1 | 2.46 | 0.01 | 0.68 | 0.38 | 0.54 | 1.90 | 0.18 |
| 230 | SM\_30\_1 | 2.31 | 0.01 | 0.63 | 0.28 | 0.60 | 0.51 | 0.48 |
| 231 | DAG\_36\_3 | 2.78 | 0.00 | 0.83 | 0.19 | 0.67 | 0.81 | 0.38 |
| 232 | LPE\_16\_0 | 2.82 | 0.00 | 0.85 | 0.17 | 0.69 | 1.27 | 0.27 |
| 233 | LPC\_22\_6 | 2.66 | 0.00 | 0.77 | 0.14 | 0.71 | 0.41 | 0.53 |
| 234 | LPC\_14\_0 | 2.46 | 0.01 | 0.69 | 0.03 | 0.87 | 1.27 | 0.28 |
| 235 | DAG\_36\_4 | 2.68 | 0.00 | 0.78 | 0.01 | 0.92 | 0.24 | 0.63 |
| 236 | LPC\_22\_5 | 2.42 | 0.01 | 0.67 | 0.01 | 0.93 | 0.15 | 0.71 |
| 237 | TG\_52\_2 | 1.82 | 0.03 | 0.49 | NaN | NaN | 0.49 | 0.49 |