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The future of research and health

# MxP<sup>®</sup> Quant 1000 kit

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List of metabolites

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## MxP® Quant 1000 kit – List of metabolites

### Transform medicine with metabolomics

The MxP® Quant 1000 kit delivers the largest combination of lipids and small molecules for quantitative metabolic profiling in a single kit. Powered by biocrates' standardized, quality-controlled, and reproducible metabolomics technology, the kit covers 1,233 metabolites across 49 biochemical classes from over 100 metabolic pathways to study microbiome-host interactions, metabolic health, and disease metabolism.

| Analyte class (number of metabolites) |                              | Analytical method |
|---------------------------------------|------------------------------|-------------------|
| Small molecules (327)                 | Alkaloids (2)                | LC-MS/MS          |
|                                       | Amine oxides (1)             |                   |
|                                       | Amino acids (20)             |                   |
|                                       | Amino acid-related (77)      |                   |
|                                       | Bile acids (24)              |                   |
|                                       | Biogenic amines (10)         |                   |
|                                       | Carboxylic acids (8)         |                   |
|                                       | Catechols (3)                |                   |
|                                       | Cresols (2)                  |                   |
|                                       | Dicarboxylic acids (25)      |                   |
|                                       | Fatty acids (39)             |                   |
|                                       | Hormones and related (5)     |                   |
|                                       | Indoles and derivatives (18) |                   |
|                                       | Nucleobases (5)              |                   |
|                                       | Nucleobase-related (14)      |                   |
|                                       | Nucleotides (2)              |                   |
|                                       | Organic acids (16)           |                   |
|                                       | Phenolic acids (22)          |                   |
|                                       | Phenoxy compounds (2)        |                   |
|                                       | Polyamines (7)               |                   |
|                                       | Pyridinecarboxylic acids (6) |                   |
|                                       | Sugars (7)                   |                   |
|                                       | Tricarboxylic acids (3)      |                   |
|                                       | Vitamins and cofactors (9)   |                   |

| Analyte class (number of metabolites) |                                            | Analytical method |
|---------------------------------------|--------------------------------------------|-------------------|
| Lipids<br>(906)                       | Acylcarnitines (40)                        | FIA-MS/MS         |
|                                       | Ceramides (29)                             |                   |
|                                       | Cholesteryl esters (22)                    |                   |
|                                       | Diglycerides (41)                          |                   |
|                                       | Dihexosylceramides (9)                     |                   |
|                                       | Dihydroceramides (8)                       |                   |
|                                       | Hexosylceramides (20)                      |                   |
|                                       | Lysophosphatidic acids (8)                 |                   |
|                                       | Lysophosphatidylcholines (12)              |                   |
|                                       | Lysophosphatidylethanolamines (43)         |                   |
|                                       | Lysophosphatidylglycerols (10)             |                   |
|                                       | Lysophosphatidylinositols (15)             |                   |
|                                       | Lysophosphatidylserines (12)               |                   |
|                                       | Monoglycerides (12)                        |                   |
|                                       | Phosphatidic acids (41)                    |                   |
|                                       | Phosphatidylcholines (76)                  |                   |
|                                       | Phosphatidylethanolamines (95)             |                   |
|                                       | Phosphatidylglycerols (64)                 |                   |
|                                       | Phosphatidylinositols (53)                 |                   |
|                                       | Phosphatidylserines (18)                   |                   |
|                                       | Sphinganine and sphingosines (8)           |                   |
|                                       | Sphinganine and sphingosine phosphates (8) |                   |
|                                       | Sphingomyelins (14)                        |                   |
|                                       | Triglycerides (242)                        |                   |
|                                       | Trihexosylceramide (6)                     |                   |

| Alkaloids (2) |          |              |              |
|---------------|----------|--------------|--------------|
| Nicotine      | Nicotine | Trigonelline | Trigonelline |

| Amine oxides (1) |                        |  |  |
|------------------|------------------------|--|--|
| TMAO             | Trimethylamine N-oxide |  |  |

| Amino acids (20) |               |     |               |
|------------------|---------------|-----|---------------|
| Ala              | Alanine       | Leu | Leucine       |
| Arg              | Arginine      | Lys | Lysine        |
| Asn              | Asparagine    | Met | Methionine    |
| Asp              | Aspartic acid | Phe | Phenylalanine |
| Cys              | Cysteine      | Pro | Proline       |
| Gln              | Glutamine     | Ser | Serine        |
| Glu              | Glutamic acid | Thr | Threonine     |
| Gly              | Glycine       | Trp | Tryptophan    |
| His              | Histidine     | Tyr | Tyrosine      |
| Ile              | Isoleucine    | Val | Valine        |

| Amino acid-related (77)   |                             |                          |                         |
|---------------------------|-----------------------------|--------------------------|-------------------------|
| 1-Met-His                 | 1-Methylhistidine           | Hypotaurine              | Hypotaurine             |
| 3-Met-2-oxovaleric acid   | 3-Methyl-2-oxovaleric acid  | Imidazole-propionic acid | Imidazolepropionic acid |
| 3-Met-His                 | 3-Methylhistidine           | Kynurenine               | Kynurenine              |
| 3-OH-Anthranilic acid     | 3-Hydroxyanthranilic acid   | Met-SO                   | Methionine sulfoxide    |
| 3-OH-Kynurenine           | 3-Hydroxykynurenine         | N2-Ac-Lys                | N2-Acetyllysine         |
| 4-Guanidino-butanoic acid | 4-Guanidinobutanoic acid    | N6-Ac-Lys                | N6-Acetyllysine         |
| 4-Met-2-oxovaleric acid   | 2-Oxoisocaproic acid        | N-Ac-Ala                 | N-Acetylalanine         |
| 5-Amino-4-oxovaleric acid | 5-Amino-4-oxovaleric acid   | N-Ac-Arg                 | N-Acetylarginine        |
| 5-AVA                     | 5-Aminovaleric acid         | N-Ac-Asn                 | N-Acetylaspargine       |
| 5-OH-Trp                  | 5-Hydroxytryptophan         | N-Ac-Asp                 | N-Acetylaspartic acid   |
| 5-Oxo-Pro                 | 5-Oxoproline                | N-Ac-Gln                 | N-Acetylglutamine       |
| AABA                      | $\alpha$ -Aminobutyric acid | N-Ac-Glu                 | N-Acetylglutamic acid   |
| Ac-Orn                    | Acetylornithine             | N-Ac-Gly                 | N-Acetyl glycine        |

| Amino acid-related (77) continued |                               |                        |                                |
|-----------------------------------|-------------------------------|------------------------|--------------------------------|
| ADMA                              | Asymmetric dimethylarginine   | N-Ac-His               | N-Acetylhistidine              |
| Agmatine                          | Agmatine                      | N-Ac-Ile               | N-Acetylisoleucine             |
| $\alpha$ -Ketoiso-valeric acid    | $\alpha$ -Ketoisovaleric acid | N-Ac-Leu               | N-Acetylleucine                |
| alpha-AAA                         | $\alpha$ -Aminoadipic acid    | N-Ac-Met               | N-Acetylmethionine             |
| Anserine                          | Anserine                      | N-Ac-Phe               | N-Acetylphenylalanine          |
| Anthranilic - acid                | Anthranilic acid              | N-Ac-Pro               | N-Acetylproline                |
| Arginino-Suc                      | Argininosuccinic acid         | N-Ac-Ser               | N-Acetylserine                 |
| BABA                              | $\beta$ -Aminobutyric acid    | N-Ac-Trp               | N-Acetyltryptophan             |
| BAIBA                             | 3-Aminoisobutyric acid        | N-Ac-Tyr               | N-Acetyltyrosine               |
| Betaine                           | Betaine                       | N-Ac-Val               | N-Acetylvaline                 |
| c4-OH-Pro                         | <i>cis</i> -4-Hydroxyproline  | Nitro-Tyr              | Nitrotyrosine                  |
| Carbamoyl-PO4                     | Carbamoylphosphate            | N-Met-Asp              | N-Methylaspartic acid          |
| Carnosine                         | Carnosine                     | N-Nitroso-Pro          | N-Nitrosoproline               |
| Cinnamoyl-Gly                     | Cinnamoylglycine              | Orn                    | Ornithine                      |
| Cit                               | Citrulline                    | PAG                    | Phenylacetylglutamine          |
| Creatine                          | Creatine                      | PheAlaBetaine          | Phenylalanine betaine          |
| Creatinine                        | Creatinine                    | Phenylacetyl-glutamine | Phenylacetylglutamine          |
| Cystine                           | Cystine                       | ProBetaine             | Proline betaine                |
| DMG                               | Dimethylglycine               | Sarcosine              | Sarcosine                      |
| DOPA                              | Dihydroxyphenylalanine        | SDMA                   | Symmetric dimethylarginine     |
| Furoyl-Gly                        | Furoylglycine                 | t4-OH-Pro              | <i>trans</i> -4-Hydroxyproline |
| Guanidino-acetic acid             | Guanidinoacetic acid          | Taurine                | Taurine                        |
| HArg                              | Homoarginine                  | TrpBetaine             | Tryptophan betaine             |
| HCit                              | Homocitrulline                | Tryptamine             | Tryptamine                     |
| HCys                              | Homocysteine                  | Tyramine               | Tyramine                       |
| HSer                              | Homoserine                    |                        |                                |

| Bile acids (24) |                            |         |                            |
|-----------------|----------------------------|---------|----------------------------|
| 12-KetoDCA      | 12-Ketodeoxycholic acid    | IsoLCA  | Isolithocholic acid        |
| 3-EpiDCA        | 3-Epideoxycholic acid      | IsoUDCA | Isoursodeoxycholic acid    |
| 7-KetoDCA       | 7-Ketodeoxycholic acid     | LCA     | Lithocholic acid           |
| CA              | Cholic acid                | NorDCA  | Nordeoxycholic acid        |
| CDCA            | Chenodeoxycholic acid      | TCA     | Taurocholic acid           |
| DCA             | Deoxycholic acid           | TCDCa   | Taurochenodeoxycholic acid |
| GCA             | Glycocholic acid           | TDCA    | Taurodeoxycholic acid      |
| GCDCA           | Glycochenodeoxycholic acid | THDCA   | Taurohyodeoxycholic acid   |

### Bile acids (24) continued

|       |                               |       |                           |
|-------|-------------------------------|-------|---------------------------|
| GDCA  | Glycodeoxycholic acid         | TLCA  | Taurolithocholic acid     |
| GLCA  | Glycolithocholic acid         | TMCA  | Tauromuricholic acids     |
| GLCAS | Glycolithocholic acid sulfate | TUDCA | Tauroursodeoxycholic acid |
| GUDCA | Glycoursodeoxycholic acid     | UDCA  | Ursodeoxycholic acid      |

### Biogenic amines (10)

|           |                             |            |            |
|-----------|-----------------------------|------------|------------|
| beta-Ala  | $\beta$ -Alanine            | Putrescine | Putrescine |
| GABA      | $\gamma$ -Aminobutyric acid | Serotonin  | Serotonin  |
| Dopamine  | Dopamine                    | Spermidine | Spermidine |
| Histamine | Histamine                   | Spermine   | Spermine   |
| PEA       | Phenylethylamine            | Urea       | Urea       |

### Carboxylic acids (8)

|                   |                       |                |                |
|-------------------|-----------------------|----------------|----------------|
| 2-OH-Butyric acid | 2-Hydroxybutyric acid | HipAcid        | Hippuric acid  |
| 3-OH-Butyric acid | 3-Hydroxybutyric acid | Lac            | Lactic acid    |
| Glycolic acid     | Glycolic acid         | Mevalonic acid | Mevalonic acid |
| Glyoxylic acid    | Glyoxylic acid        | Pyruvic acid   | Pyruvic acid   |

### Catechols (3)

|                       |                           |                |                |
|-----------------------|---------------------------|----------------|----------------|
| 3,4-DiOH-Benzaldehyde | 3,4-Dihydroxybenzaldehyde | Norepinephrine | Norepinephrine |
| Epinephrine           | Epinephrine               |                |                |

### Cresols (2)

|                              |                              |                                  |                          |
|------------------------------|------------------------------|----------------------------------|--------------------------|
| <i>p</i> -Cresol glucuronide | <i>p</i> -Cresol glucuronide | <i>p</i> -Cresol-SO <sub>4</sub> | <i>p</i> -Cresol sulfate |
|------------------------------|------------------------------|----------------------------------|--------------------------|

### Dicarboxylic acids (25)

|                    |                              |               |               |
|--------------------|------------------------------|---------------|---------------|
| 2-OH-Glutaric acid | 2-Hydroxyglutaric acid       | Fumaric acid  | Fumaric acid  |
| 3-HMGA             | 3-Hydroxymethylglutaric acid | Glutaric acid | Glutaric acid |
| 3-Met-adipic acid  | 3-Methyladipic acid          | Itaconic acid | Itaconic acid |

| Dicarboxylic acids (25) continued |                             |                         |                           |
|-----------------------------------|-----------------------------|-------------------------|---------------------------|
| 3-Met-glutaric acid               | 3-Methylglutaric acid       | Maleic acid             | Maleic acid               |
| 3-OH-Glutaric acid                | 3-Hydroxyglutaric acid      | Malic acid              | Malic acid                |
| 3-OH-Sebacic acid                 | 3-Hydroxysebacic acid       | Malonic acid            | Malonic acid              |
| Adipic acid                       | Adipic acid                 | Methylmalonic acid      | Methylmalonic acid        |
| $\alpha$ -Ketoglutaric acid       | $\alpha$ -Ketoglutaric acid | Oxalic acid             | Oxalic acid               |
| Citramalic acid                   | Citramalic acid             | Oxaloacetic acid        | Oxaloacetic acid          |
| DiCA 12:0                         | Dodecanedioic acid          | Suberic acid            | Suberic acid              |
| DiCA 14:0                         | Tetradecanedioic acid       | Suc                     | Succinic acid             |
| E-3-Met-glutaconic acid           | E-3-Methylglutaconic acid   | Z-3-Met-glutaconic acid | Z-3-Methylglutaconic acid |
| Ethylmalonic acid                 | Ethylmalonic acid           |                         |                           |

| Fatty acids (39) |                      |                  |                                                |
|------------------|----------------------|------------------|------------------------------------------------|
| FA 2:0           | Acetic acid          | FA 16:1          | Palmitoleic acid                               |
| FA 3:0           | Propanoic acid       | FA 18:0          | Stearic acid                                   |
| FA 3:0-2M        | Isobutyric acid      | FA 18:1          | Oleic acid                                     |
| FA 4:0           | Butyric acid         | FA 18:2          | Linoleic acid                                  |
| FA 4:0-2M        | 2-Methylbutyric acid | FA 18:3          | Octadecatrienoic acid                          |
| FA 4:0-3M        | Isovaleric acid      | FA 20:0          | Arachidic acid                                 |
| FA 5:0           | Valeric acid         | FA 20:1n-9       | Gondoic acid                                   |
| FA 5:0-3M        | 3-Methylvaleric acid | FA 20:2          | Eicosadienoic acid                             |
| FA 5:0-4M        | Isocaproic acid      | FA 20:3n-6       | Dihomo- $\gamma$ -linolenic acid ( $\omega$ 6) |
| FA 6:0           | Caproic acid         | FA 20:3n-9       | Mead acid                                      |
| FA 7:0           | Heptanoic acid       | FA 20:4n-6 (AA)  | Arachidonic acid (AA; $\omega$ 6)              |
| FA 8:0           | Caprylic acid        | FA 20:5n-3 (EPA) | Eicosapentaenoic acid (EPA; $\omega$ 3)        |
| FA 9:0           | Nonanoic acid        | FA 22:0          | Behenic acid                                   |
| FA 10:0          | Capric acid          | FA 22:4n-6       | Docosatetraenoic acid ( $\omega$ 6)            |
| FA 11:0          | Undecanoic acid      | FA 22:5n-3 (DPA) | Docosapentaenoic acid (DPA, $\omega$ 3)        |
| FA 12:0          | Lauric acid          | FA 22:6n-3 (DHA) | Docosahexaenoic acid (DHA; $\omega$ 3)         |
| FA 14:0          | Myristic acid        | FA 24:0          | Lignoceric acid                                |

| Fatty acids (39) continued |                    |            |                               |
|----------------------------|--------------------|------------|-------------------------------|
| FA 14:1n-5                 | Myristoleic acid   | FA 24:1n-9 | Nervonic acid                 |
| FA 15:0                    | Pentadecanoic acid | FA 24:4n-6 | Tetracosatetraenoic acid (ω6) |
| FA 16:0                    | Palmitic acid      |            |                               |

| Hormones and related (5) |                                |    |                              |
|--------------------------|--------------------------------|----|------------------------------|
| Cortisol                 | Cortisol                       | T3 | 3,3',5-Triiodothyronine (T3) |
| Cortisone                | Cortisone                      | T4 | Thyroxine (T4)               |
| DHEAS                    | Dehydroepiandrosterone sulfate |    |                              |

| Indoles and derivatives (18) |                            |                     |                               |
|------------------------------|----------------------------|---------------------|-------------------------------|
| 3-IAA                        | 3-Indoleacetic acid        | Indoleacrylic acid  | Indoleacrylic acid            |
| 3-IPA                        | 3-Indolepropionic acid     | Indolealdehyde      | Indolealdehyde                |
| 5-HIAA                       | 5-Hydroxyindoleacetic acid | Indole-Lac          | Indolelactic acid             |
| IAG                          | Indolylacryloylglycine     | Indolepyruvic acid  | Indolepyruvic acid            |
| Indole-3-acetamide           | Indole-3-acetamide         | Indoxyl glucuronide | Indoxyl glucuronide           |
| Indole-3-carboxylic acid     | Indole-3-carboxylic acid   | Ind-SO4             | Indoxyl sulfate               |
| Indole-3-ethanol             | Indole-3-ethanol           | Melatonin           | Melatonin                     |
| Indole-3-methanol            | Indole-3-methanol          | Met-IAA             | Methylindole-3-acetic acid    |
| Indoleacet-aldehyde          | Indoleacetaldehyde         | Met-IPA             | Methylindole-3-propionic acid |

| Nucleobases (5) |          |         |         |
|-----------------|----------|---------|---------|
| Adenine         | Adenine  | Thymine | Thymine |
| Cytosine        | Cytosine | Uracil  | Uracil  |
| Guanine         | Guanine  |         |         |

| Nucleobase-related (14) |                        |               |                   |
|-------------------------|------------------------|---------------|-------------------|
| Adenosine               | Adenosine              | Inosine       | Inosine           |
| AHCys                   | S-Adenosylhomocysteine | N-Ac-Cytidine | N4-Acetylcytidine |
| Cytidine                | Cytidine               | Orotic acid   | Orotic acid       |



| Nucleobase-related (14) continued |                |           |           |
|-----------------------------------|----------------|-----------|-----------|
| Deoxycytidine                     | Deoxycytidine  | Thymidine | Thymidine |
| Deoxyguanosine                    | Deoxyguanosine | Uric acid | Uric acid |
| Guanosine                         | Guanosine      | Uridine   | Uridine   |
| Hypoxanthine                      | Hypoxanthine   | Xanthine  | Xanthine  |

| Nucleotides (2) |                                        |      |                                        |
|-----------------|----------------------------------------|------|----------------------------------------|
| cAMP            | Adenosine monophosphate, cyclic (cAMP) | cGMP | Guanosine monophosphate, cyclic (cGMP) |

| Organic acids (16)          |                                |                             |                                                   |
|-----------------------------|--------------------------------|-----------------------------|---------------------------------------------------|
| 2,5-Furandi-carboxylic acid | Furan-2,5-dicarboxylic acid    | 4-Quinoline-carboxylic acid | 4-Quinolinecarboxylic acid                        |
| 2-Met-HipAcid               | 2-Methylhippuric acid          | Abscisic acid               | Abscisic acid                                     |
| 2-OH-2-Met-butyric acid     | 2-Hydroxy-2-methylbutyric acid | Argininic acid              | Argininic acid                                    |
| 2-OH-Isobutyric acid        | 2-Hydroxyisobutyric acid       | Bilirubin                   | Bilirubin                                         |
| 3-Guanidino-propionic acid  | 3-Guanidinopropionic acid      | Biliverdin                  | Biliverdin                                        |
| 3-OH-HipAcid                | 3-Hydroxyhippuric acid         | CMPE                        | 3-Carboxy-4-methyl-5-propyl-2-furanpropionic acid |
| 3-OH-Isobutyric acid        | 3-Hydroxyisobutyric acid       | Glyceric acid               | Glyceric acid                                     |
| 4-OH-HipAcid                | 4-Hydroxyhippuric acid         | Nicotinuric acid            | Nicotinuric acid                                  |

| Phenolic acids (22)            |                                   |                   |                                             |
|--------------------------------|-----------------------------------|-------------------|---------------------------------------------|
| 2-OH-Benzoic acid              | 2-Hydroxybenzoic acid             | DOPAC             | 3,4-Dihydroxyphenylacetic acid              |
| 2-OH-Phenylacetic acid         | 2-Hydroxyphenylacetic acid        | Homovanillic acid | Homovanillic acid                           |
| 3-(3-OH-Phenyl)-propanoic acid | 3-(3-Hydroxyphenyl)propanoic acid | HPHPA             | 3-(3-Hydroxyphenyl)-3-hydroxypropanoic acid |

| Phenolic acids (22) continued |                             |                       |                          |
|-------------------------------|-----------------------------|-----------------------|--------------------------|
| 3,5-DiOH-Benzoic acid         | 3,5-Dihydroxybenzoic acid   | OH-Phenyl-Lac         | Hydroxyphenyllactic acid |
| 3-OH-Phenylacetic acid        | 3-Hydroxyphenylacetic acid  | Phenylacetic acid     | Phenylacetic acid        |
| 3-OH-Phenylpyruvic acid       | 3-Hydroxyphenylpyruvic acid | Phenyl-Lac            | Phenyllactic acid        |
| 4-OH-Benzoic acid             | 4-Hydroxybenzoic acid       | Phenylpyruvic acid    | Phenylpyruvic acid       |
| 4-OH-Phenylacetic acid        | 4-Hydroxyphenylacetic acid  | t-p-Coumaric acid     | trans-p-Coumaric acid    |
| 4-OH-Phenylpyruvic acid       | 4-Hydroxyphenylpyruvic acid | Vanillactic acid      | Vanillactic acid         |
| Benzoic acid                  | Benzoic acid                | Vanillic acid         | Vanillic acid            |
| Desamino-Tyr                  | Desaminotyrosine            | Vanillylmandelic acid | Vanillylmandelic acid    |

| Phenoxy compounds (2) |                       |                   |                   |
|-----------------------|-----------------------|-------------------|-------------------|
| 4-EPS                 | 4-Ethylphenyl sulfate | Phenylglucuronide | Phenylglucuronide |

| Polyamines (7)         |                          |                  |                     |
|------------------------|--------------------------|------------------|---------------------|
| Cadaverine             | Cadaverine               | N1-Ac-Spermine   | N1-Acetylspermine   |
| N1,N8-Di-Ac-Spermidine | N1,N8-Diacetylspermidine | N8-Ac-Spermidine | N8-Acetylspermidine |
| N1,N12-Di-Ac-Spermine  | N1,N12-Diacetylspermine  | N-Ac-Putrescine  | N-Acetylputrescine  |
| N1-Ac-Spermidine       | N1-Acetylspermidine      |                  |                     |

| Pyridinecarboxylic acids (6) |                   |                  |                  |
|------------------------------|-------------------|------------------|------------------|
| Isonicotinic acid            | Isonicotinic acid | Quinaldic acid   | Quinaldic acid   |
| Kynurenic acid               | Kynurenic acid    | Quinolinic acid  | Quinolinic acid  |
| Picolinic acid               | Picolinic acid    | Xanthurenic acid | Xanthurenic acid |

| Sugars (7)        |                  |               |                       |
|-------------------|------------------|---------------|-----------------------|
| 3-Deoxy-glucosone | 3-Deoxyglucosone | NeuAc         | Acetylneuraminic acid |
| Fructose          | Fructose         | Ribose        | Ribose                |
| Glucose           | Glucose          | Threonic acid | Threonic acid         |
| Mannose           | Mannose          |               |                       |

| Tricarboxylic acids (3) |               |                |                |
|-------------------------|---------------|----------------|----------------|
| AconAcid                | Aconitic acid | Isocitric acid | Isocitric acid |
| Citric acid             | Citric acid   |                |                |

| Vitamins and cofactors (9) |                     |                       |                           |
|----------------------------|---------------------|-----------------------|---------------------------|
| Biotin (B7)                | Biotin (B7)         | Pantothenic acid (B5) | Pantothenic acid (B5)     |
| Choline                    | Choline             | PMP                   | Pyridoxamine 5'-phosphate |
| Folic acid (B9)            | Folic acid (B9)     | Pyridoxine (B6)       | Pyridoxine (B6)           |
| Nicotinamide (B3)          | Nicotinamide (B3)   | Riboflavin (B2)       | Riboflavin (B2)           |
| Nicotinic acid (B3)        | Nicotinic acid (B3) |                       |                           |

| Acylcarnitines (40) |                                                   |          |                                   |
|---------------------|---------------------------------------------------|----------|-----------------------------------|
| C0                  | Carnitine                                         | C10:1    | Decenoylcarnitine                 |
| C2                  | Acetylcarnitine                                   | C10:2    | Decadienoylcarnitine              |
| C3                  | Propionylcarnitine                                | C12      | Dodecanoylcarnitine               |
| C3-DC (C4-OH)       | Malonylcarnitine (Hydroxybutyrylcarnitine)        | C12-DC   | Dodecanedioylcarnitine            |
| C3-OH               | Hydroxypropionylcarnitine                         | C12:1    | Dodecenoylcarnitine               |
| C3:1                | Propenoylcarnitine                                | C14      | Tetradecanoylcarnitine            |
| C4                  | Butyrylcarnitine                                  | C14:1    | Tetradecenoylcarnitine            |
| C4:1                | Butenylcarnitine                                  | C14:1-OH | Hydroxytetradecenoylcarnitine     |
| C5                  | Valeryl carnitine                                 | C14:2    | Tetradecadienoylcarnitine         |
| C5-DC (C6-OH)       | Glutaryl carnitine (Hydroxyhexanoylcarnitine)     | C14:2-OH | Hydroxytetradecadienoyl carnitine |
| C5-M-DC             | Methylglutaryl carnitine                          | C16      | Hexadecanoylcarnitine             |
| C5-OH (C3-DC-M)     | Hydroxyvaleryl carnitine (Methylmalonylcarnitine) | C16-OH   | Hydroxyhexadecanoylcarnitine      |
| C5:1                | Tiglylcarnitine                                   | C16:1    | Hexadecenoylcarnitine             |
| C5:1-DC             | Glutaconyl carnitine                              | C16:1-OH | Hydroxyhexadecenoylcarnitine      |

| Acylcarnitines (40) continued |                                       |          |                                  |
|-------------------------------|---------------------------------------|----------|----------------------------------|
| C6 (C4:1-DC)                  | Hexanoylcarnitine (Fumaryl carnitine) | C16:2    | Hexadecadienoylcarnitine         |
| C6:1                          | Hexenoylcarnitine                     | C16:2-OH | Hydroxyhexadecadienoyl carnitine |
| C7-DC                         | Pimeloylcarnitine                     | C18      | Octadecanoylcarnitine            |
| C8                            | Octanoylcarnitine                     | C18:1    | Octadecenoylcarnitine            |
| C9                            | Nonanoylcarnitine                     | C18:1-OH | Hydroxyoctadecenoylcarnitine     |
| C10                           | Decanoylcarnitine                     | C18:2    | Octadecadienoylcarnitine         |

| Ceramides (29)    |                   |                |                 |
|-------------------|-------------------|----------------|-----------------|
| Cer d16:1/18:0    | Cer d18:1/18:0    | Cer d18:1/25:0 | Cer d18:2/22:0  |
| Cer d16:1/20:0    | Cer d18:1/18:1    | Cer d18:1/26:0 | Cer d18:2/23:0  |
| Cer d16:1/22:0    | Cer d18:1/20:0-OH | Cer d18:1/26:1 | Cer d18:2/24:0  |
| Cer d16:1/23:0    | Cer d18:1/20:0    | Cer d18:2/14:0 | Cer d18:2/24:1  |
| Cer d16:1/24:0    | Cer d18:1/22:0    | Cer d18:2/16:0 | CerP d18:1/16:0 |
| Cer d18:1/14:0    | Cer d18:1/23:0    | Cer d18:2/18:0 |                 |
| Cer d18:1/16:0    | Cer d18:1/24:0    | Cer d18:2/18:1 |                 |
| Cer d18:1/18:0-OH | Cer d18:1/24:1    | Cer d18:2/20:0 |                 |

| Cholesteryl esters (22) |         |         |         |
|-------------------------|---------|---------|---------|
| CE 14:0                 | CE 17:0 | CE 20:0 | CE 22:1 |
| CE 14:1                 | CE 17:1 | CE 20:1 | CE 22:2 |
| CE 15:0                 | CE 18:0 | CE 20:3 | CE 22:5 |
| CE 15:1                 | CE 18:1 | CE 20:4 | CE 22:6 |
| CE 16:0                 | CE 18:2 | CE 20:5 |         |
| CE 16:1                 | CE 18:3 | CE 22:0 |         |

| Diglycerides (41) |              |              |                |
|-------------------|--------------|--------------|----------------|
| DG 14:0_14:0      | DG 16:0_20:4 | DG 18:1_20:1 | DG 18:3_20:2   |
| DG 14:0_18:1      | DG 16:1_18:0 | DG 18:1_20:2 | DG 21:0_22:6   |
| DG 14:0_18:2      | DG 16:1_18:1 | DG 18:1_20:3 | DG 22:1_22:2   |
| DG 14:0_20:0      | DG 16:1_18:2 | DG 18:1_20:4 | DG O-14:0_18:2 |
| DG 14:1_18:1      | DG 16:1_20:0 | DG 18:1_22:5 | DG O-16:0_18:1 |
| DG 14:1_20:2      | DG 17:0_18:1 | DG 18:1_22:6 | DG O-18:2_18:2 |
| DG 16:0_16:0      | DG 18:0_20:4 | DG 18:2_18:2 |                |
| DG 16:0_16:1      | DG 18:1_18:1 | DG 18:2_18:3 |                |
| DG 16:0_18:1      | DG 18:1_18:2 | DG 18:2_18:4 |                |
| DG 16:0_18:2      | DG 18:1_18:3 | DG 18:2_20:0 |                |

| Diglycerides (41) continued |              |              |  |
|-----------------------------|--------------|--------------|--|
| DG 16:0_20:0                | DG 18:1_18:4 | DG 18:2_20:4 |  |
| DG 16:0_20:3                | DG 18:1_20:0 | DG 18:3_18:3 |  |

| Dihexosylceramides (9) |                    |                    |  |
|------------------------|--------------------|--------------------|--|
| Hex2Cer d18:1/14:0     | Hex2Cer d18:1/20:0 | Hex2Cer d18:1/24:1 |  |
| Hex2Cer d18:1/16:0     | Hex2Cer d18:1/22:0 | Hex2Cer d18:1/26:0 |  |
| Hex2Cer d18:1/18:0     | Hex2Cer d18:1/24:0 | Hex2Cer d18:1/26:1 |  |

| Dihydroceramides (8) |                |                |                   |
|----------------------|----------------|----------------|-------------------|
| Cer d18:0/18:0-OH    | Cer d18:0/20:0 | Cer d18:0/24:0 | Cer d18:0/26:1-OH |
| Cer d18:0/18:0       | Cer d18:0/22:0 | Cer d18:0/24:1 | Cer d18:0/26:1    |

| Hexosylceramides (20) |                    |                    |                    |
|-----------------------|--------------------|--------------------|--------------------|
| Hex-Cer d16:1/20:0    | Hex-Cer d18:1/18:0 | Hex-Cer d18:1/24:0 | Hex-Cer d18:2/18:0 |
| Hex-Cer d16:1/22:0    | Hex-Cer d18:1/18:1 | Hex-Cer d18:1/24:1 | Hex-Cer d18:2/20:0 |
| Hex-Cer d16:1/24:0    | Hex-Cer d18:1/20:0 | Hex-Cer d18:1/26:0 | Hex-Cer d18:2/22:0 |
| Hex-Cer d18:1/14:0    | Hex-Cer d18:1/22:0 | Hex-Cer d18:1/26:1 | Hex-Cer d18:2/23:0 |
| Hex-Cer d18:1/16:0    | Hex-Cer d18:1/23:0 | Hex-Cer d18:2/16:0 | Hex-Cer d18:2/24:0 |

| Lysophosphatidic acids (8) |          |          |          |
|----------------------------|----------|----------|----------|
| LPA 14:0                   | LPA 15:0 | LPA 18:1 | LPA 22:3 |
| LPA 14:1                   | LPA 16:0 | LPA 18:2 | LPA 22:4 |

| Lysophosphatidylcholines (12) |          |          |          |
|-------------------------------|----------|----------|----------|
| LPC 14:0                      | LPC 17:0 | LPC 18:2 | LPC 24:0 |
| LPC 16:0                      | LPC 18:0 | LPC 20:3 | LPC 26:0 |
| LPC 16:1                      | LPC 18:1 | LPC 20:4 | LPC 26:1 |

| Lysophosphatidylethanolamines (43) |          |            |            |
|------------------------------------|----------|------------|------------|
| LPE 12:0                           | LPE 18:3 | LPE 22:1   | LPE P-18:2 |
| LPE 14:0                           | LPE 19:0 | LPE 22:4   | LPE P-20:0 |
| LPE 14:1                           | LPE 19:1 | LPE 22:5   | LPE P-20:1 |
| LPE 15:0                           | LPE 19:2 | LPE 22:6   | LPE P-20:4 |
| LPE 16:0                           | LPE 20:0 | LPE 24:0   | LPE P-20:5 |
| LPE 16:1                           | LPE 20:1 | LPE P-14:0 | LPE P-22:0 |
| LPE 17:0                           | LPE 20:2 | LPE P-15:0 | LPE P-22:1 |
| LPE 17:1                           | LPE 20:3 | LPE P-16:0 | LPE P-22:4 |

| Lysophosphatidylethanolamines (43) continued |          |            |            |
|----------------------------------------------|----------|------------|------------|
| LPE 18:0                                     | LPE 20:4 | LPE P-17:0 | LPE P-22:5 |
| LPE 18:1                                     | LPE 20:5 | LPE P-18:0 | LPE P-22:6 |
| LPE 18:2                                     | LPE 22:0 | LPE P-18:1 |            |

| Lysophosphatidylglycerols (10) |          |          |          |
|--------------------------------|----------|----------|----------|
| LPG 14:0                       | LPG 16:1 | LPG 18:0 | LPG 20:1 |
| LPG 14:1                       | LPG 17:0 | LPG 18:1 |          |
| LPG 16:0                       | LPG 17:1 | LPG 18:2 |          |

| Lysophosphatidylinositols (15) |          |          |          |
|--------------------------------|----------|----------|----------|
| LPI 14:0                       | LPI 17:0 | LPI 18:2 | LPI 20:4 |
| LPI 14:1                       | LPI 17:1 | LPI 18:3 | LPI 22:0 |
| LPI 16:0                       | LPI 18:0 | LPI 19:0 | LPI 22:1 |
| LPI 16:1                       | LPI 18:1 | LPI 20:1 |          |

| Lysophosphatidylserines (12) |          |          |          |
|------------------------------|----------|----------|----------|
| LPS 16:0                     | LPS 18:1 | LPS 20:0 | LPS 20:5 |
| LPS 16:1                     | LPS 18:2 | LPS 20:1 | LPS 22:0 |
| LPS 18:0                     | LPS 18:3 | LPS 20:4 | LPS 22:6 |

| Monoglycerides (12) |         |         |         |
|---------------------|---------|---------|---------|
| MG 16:1             | MG 18:3 | MG 20:4 | MG 22:2 |
| MG 18:1             | MG 20:1 | MG 20:5 | MG 22:4 |
| MG 18:2             | MG 20:3 | MG 22:1 | MG 22:6 |

| Phosphatidic acids (41) |              |              |              |
|-------------------------|--------------|--------------|--------------|
| PA 14:0_14:1            | PA 17:0_18:3 | PA 18:1_20:0 | PA 18:2_20:1 |
| PA 16:0_18:1            | PA 17:1_18:1 | PA 18:1_20:1 | PA 18:2_20:2 |
| PA 16:0_18:2            | PA 17:1_18:2 | PA 18:1_20:2 | PA 18:2_22:0 |
| PA 16:0_18:3            | PA 17:2_18:1 | PA 18:1_20:3 | PA 18:2_22:1 |
| PA 16:0_19:2            | PA 18:0_18:1 | PA 18:1_22:0 | PA 18:2_22:3 |
| PA 16:1_18:1            | PA 18:0_18:2 | PA 18:1_22:1 | PA 18:2_22:4 |
| PA 16:1_18:2            | PA 18:0_18:3 | PA 18:1_22:2 | PA 18:3_18:3 |
| PA 16:1_22:0            | PA 18:1_18:1 | PA 18:1_22:3 | PA 20:0_20:4 |
| PA 16:2_18:1            | PA 18:1_18:2 | PA 18:2_18:2 |              |
| PA 17:0_18:1            | PA 18:1_18:3 | PA 18:2_18:3 |              |
| PA 17:0_18:2            | PA 18:1_18:4 | PA 18:2_20:0 |              |

| Phosphatidylcholines (76) |           |           |           |
|---------------------------|-----------|-----------|-----------|
| PC 24:0                   | PC 38:3   | PC O-30:2 | PC O-40:1 |
| PC 26:0                   | PC 38:4   | PC O-32:1 | PC O-40:2 |
| PC 28:1                   | PC 38:5   | PC O-32:2 | PC O-40:3 |
| PC 30:0                   | PC 38:6   | PC O-34:0 | PC O-40:4 |
| PC 32:0                   | PC 40:1   | PC O-34:1 | PC O-40:5 |
| PC 32:1                   | PC 40:2   | PC O-34:2 | PC O-40:6 |
| PC 32:2                   | PC 40:3   | PC O-34:3 | PC O-42:0 |
| PC 32:3                   | PC 40:4   | PC O-36:0 | PC O-42:1 |
| PC 34:1                   | PC 40:5   | PC O-36:1 | PC O-42:2 |
| PC 34:2                   | PC 40:6   | PC O-36:2 | PC O-42:3 |
| PC 34:3                   | PC 42:0   | PC O-36:3 | PC O-42:4 |
| PC 34:4                   | PC 42:1   | PC O-36:4 | PC O-42:5 |
| PC 36:0                   | PC 42:2   | PC O-36:5 | PC O-44:3 |
| PC 36:1                   | PC 42:4   | PC O-38:0 | PC O-44:4 |
| PC 36:2                   | PC 42:5   | PC O-38:1 | PC O-44:5 |
| PC 36:3                   | PC 42:6   | PC O-38:2 | PC O-44:6 |
| PC 36:4                   | PC O-28:0 | PC O-38:3 |           |
| PC 36:5                   | PC O-28:1 | PC O-38:4 |           |
| PC 36:6                   | PC O-30:0 | PC O-38:5 |           |
| PC 38:0                   | PC O-30:1 | PC O-38:6 |           |

| Phosphatidylethanolamines (95) |         |                |                |
|--------------------------------|---------|----------------|----------------|
| PE 20:0                        | PE 36:4 | PE P-16:0/14:0 | PE P-18:0/20:3 |
| PE 28:0                        | PE 36:5 | PE P-16:0/15:0 | PE P-18:0/20:4 |
| PE 28:1                        | PE 36:6 | PE P-16:0/16:0 | PE P-18:0/20:5 |
| PE 30:0                        | PE 38:0 | PE P-16:0/16:1 | PE P-18:0/22:1 |
| PE 30:1                        | PE 38:1 | PE P-16:0/18:1 | PE P-18:0/22:2 |
| PE 31:0                        | PE 38:2 | PE P-16:0/18:2 | PE P-18:0/22:3 |
| PE 32:0                        | PE 38:3 | PE P-16:0/18:3 | PE P-18:0/22:4 |
| PE 32:1                        | PE 38:4 | PE P-16:0/20:3 | PE P-18:0/22:5 |
| PE 32:2                        | PE 38:5 | PE P-16:0/20:4 | PE P-18:0/22:6 |
| PE 33:0                        | PE 38:6 | PE P-16:0/20:5 | PE P-18:1/18:1 |
| PE 33:1                        | PE 38:7 | PE P-16:0/22:4 | PE P-18:1/18:2 |
| PE 33:2                        | PE 40:1 | PE P-16:0/22:5 | PE P-18:1/20:4 |
| PE 34:0                        | PE 40:3 | PE P-16:0/22:6 | PE P-18:1/20:5 |
| PE 34:1                        | PE 40:4 | PE P-18:0/14:0 | PE P-18:1/22:6 |
| PE 34:2                        | PE 40:5 | PE P-18:0/16:0 | PE P-20:0/14:0 |
| PE 34:3                        | PE 40:6 | PE P-18:0/16:1 | PE P-20:0/16:0 |
| PE 34:4                        | PE 40:7 | PE P-18:0/17:1 | PE P-20:0/16:1 |
| PE 35:1                        | PE 40:8 | PE P-18:0/18:0 | PE P-20:0/17:1 |
| PE 35:2                        | PE 42:7 | PE P-18:0/18:1 | PE P-20:0/18:1 |

### Phosphatidylethanolamines (95) continued

|         |          |                |                |
|---------|----------|----------------|----------------|
| PE 35:3 | PE 42:8  | PE P-18:0/18:2 | PE P-20:0/18:2 |
| PE 36:0 | PE 44:11 | PE P-18:0/18:3 | PE P-20:0/20:0 |
| PE 36:1 | PE 44:12 | PE-P-18:0/19:1 | PE P-20:0/20:4 |
| PE 36:2 | PE 44:6  | PE P-18:0/20:1 | PE P-20:0/20:5 |
| PE 36:3 | PE 44:7  | PE P-18:0/20:2 |                |

### Phosphatidylglycerols (64)

|              |              |              |              |
|--------------|--------------|--------------|--------------|
| PG 14:0_16:0 | PG 16:1_18:2 | PG 18:1_20:0 | PG 18:2_20:2 |
| PG 15:0_18:1 | PG 16:1_20:4 | PG 18:1_20:1 | PG 18:2_20:3 |
| PG 16:0_16:0 | PG 16:1_22:1 | PG 18:1_20:2 | PG 18:2_20:4 |
| PG 16:0_16:1 | PG 16:2_18:1 | PG 18:1_20:3 | PG 18:2_20:5 |
| PG 16:0_18:1 | PG 16:2_18:2 | PG 18:1_20:4 | PG 18:2_22:0 |
| PG 16:0_18:2 | PG 16:3_18:1 | PG 18:1_20:5 | PG 18:2_22:1 |
| PG 16:0_18:3 | PG 17:0_18:1 | PG 18:1_22:0 | PG 18:2_22:3 |
| PG 16:0_19:1 | PG 17:0_18:2 | PG 18:1_22:1 | PG 18:2_22:4 |
| PG 16:0_20:3 | PG 17:1_18:1 | PG 18:1_22:2 | PG 20:3_20:4 |
| PG 16:0_20:4 | PG 18:0_18:1 | PG 18:1_22:3 | PG 20:4_20:4 |
| PG 16:0_20:5 | PG 18:0_18:2 | PG 18:1_22:4 | PG 20:4_22:1 |
| PG 16:0_22:1 | PG 18:0_18:3 | PG 18:1_22:5 | PG 20:4_22:3 |
| PG 16:0_22:2 | PG 18:0_22:1 | PG 18:2_18:2 | PG 20:4_22:4 |
| PG 16:1_16:1 | PG 18:1_18:1 | PG 18:2_18:3 | PG 22:4_22:6 |
| PG 16:1_18:0 | PG 18:1_18:2 | PG 18:2_18:4 | PG 22:5_22:6 |
| PG 16:1_18:1 | PG 18:1_18:3 | PG 18:2_20:0 | PG 22:6_22:6 |

### Phosphatidylinositols (53)

|              |              |              |              |
|--------------|--------------|--------------|--------------|
| PI 14:0_18:1 | PI 16:0_22:1 | PI 18:0_22:0 | PI 18:1_22:4 |
| PI 14:0_18:2 | PI 16:1_18:0 | PI 18:1_18:1 | PI 18:1_22:5 |
| PI 15:0_16:0 | PI 16:1_18:1 | PI 18:1_18:2 | PI 18:1_22:6 |
| PI 15:1_16:0 | PI 16:1_18:2 | PI 18:1_18:3 | PI 18:2_18:3 |
| PI 16:0_16:0 | PI 17:0_18:1 | PI 18:1_20:0 | PI 18:2_20:0 |
| PI 16:0_17:0 | PI 17:1_18:1 | PI 18:1_20:1 | PI 18:2_20:1 |
| PI 16:0_17:1 | PI 17:1_18:2 | PI 18:1_20:2 | PI 18:2_20:4 |
| PI 16:0_17:2 | PI 18:0_18:0 | PI 18:1_20:3 | PI 18:2_20:5 |
| PI 16:0_18:1 | PI 18:0_18:1 | PI 18:1_20:4 | PI 18:2_22:0 |
| PI 16:0_18:2 | PI 18:0_18:2 | PI 18:1_20:5 | PI 18:2_22:1 |
| PI 16:0_18:3 | PI 18:0_18:3 | PI 18:1_22:0 | PI 18:2_22:6 |
| PI 16:0_20:0 | PI 18:0_20:0 | PI 18:1_22:1 |              |
| PI 16:0_20:3 | PI 18:0_20:3 | PI 18:1_22:2 |              |
| PI 16:0_20:4 | PI 18:0_20:4 | PI 18:1_22:3 |              |



| Phosphatidylserines (18) |         |         |         |
|--------------------------|---------|---------|---------|
| PS 30:0                  | PS 36:2 | PS 38:5 | PS 40:6 |
| PS 32:0                  | PS 36:3 | PS 38:6 | PS 40:7 |
| PS 34:1                  | PS 36:4 | PS 38:7 | PS 40:8 |
| PS 34:2                  | PS 36:5 | PS 40:4 |         |
| PS 36:1                  | PS 38:4 | PS 40:5 |         |

| Sphinganine and sphingosines (8) |           |           |           |
|----------------------------------|-----------|-----------|-----------|
| SPB d14:0                        | SPB d16:0 | SPB d17:0 | SPB d18:0 |
| SPB d14:1                        | SPB d16:1 | SPB d17:1 | SPB d18:1 |

| Sphinganine and sphingosine phosphates (8) |            |            |            |
|--------------------------------------------|------------|------------|------------|
| SPBP d14:0                                 | SPBP d16:0 | SPBP d17:0 | SPBP d18:0 |
| SPBP d14:1                                 | SPBP d16:1 | SPBP d17:1 | SPBP d18:1 |

| Sphingomyelins (14) |         |         |         |
|---------------------|---------|---------|---------|
| SM 33:1             | SM 36:1 | SM 41:2 | SM 44:1 |
| SM 34:1             | SM 36:2 | SM 42:1 | SM 44:2 |
| SM 34:2             | SM 38:3 | SM 42:2 |         |
| SM 35:1             | SM 41:1 | SM 43:1 |         |

| Triglycerides (242) |              |              |              |
|---------------------|--------------|--------------|--------------|
| TG 14:0_32:2        | TG 16:0_34:1 | TG 16:1_32:0 | TG 17:1_34:3 |
| TG 14:0_34:0        | TG 16:0_34:2 | TG 16:1_32:1 | TG 17:1_36:3 |
| TG 14:0_34:1        | TG 16:0_34:3 | TG 16:1_32:2 | TG 17:1_36:4 |
| TG 14:0_34:2        | TG 16:0_34:4 | TG 16:1_33:1 | TG 17:1_36:5 |
| TG 14:0_34:3        | TG 16:0_35:1 | TG 16:1_34:0 | TG 17:1_38:5 |
| TG 14:0_35:1        | TG 16:0_35:2 | TG 16:1_34:1 | TG 17:1_38:6 |
| TG 14:0_35:2        | TG 16:0_35:3 | TG 16:1_34:2 | TG 17:1_38:7 |
| TG 14:0_36:1        | TG 16:0_36:2 | TG 16:1_34:3 | TG 17:2_34:2 |
| TG 14:0_36:2        | TG 16:0_36:3 | TG 16:1_36:1 | TG 17:2_34:3 |
| TG 14:0_36:3        | TG 16:0_36:4 | TG 16:1_36:2 | TG 17:2_36:2 |
| TG 14:0_36:4        | TG 16:0_36:5 | TG 16:1_36:3 | TG 17:2_36:3 |
| TG 14:0_38:4        | TG 16:0_36:6 | TG 16:1_36:4 | TG 17:2_36:4 |
| TG 14:0_38:5        | TG 16:0_37:3 | TG 16:1_36:5 | TG 17:2_38:5 |
| TG 14:0_39:3        | TG 16:0_38:1 | TG 16:1_38:3 | TG 17:2_38:6 |
| TG 14:0_40:5        | TG 16:0_38:2 | TG 16:1_38:4 | TG 17:2_38:7 |
| TG 16:0_28:1        | TG 16:0_38:3 | TG 16:1_38:5 | TG 18:0_30:0 |
| TG 16:0_28:2        | TG 16:0_38:4 | TG 17:0_32:1 | TG 18:0_30:1 |
| TG 16:0_30:2        | TG 16:0_38:5 | TG 17:0_34:1 | TG 18:0_32:0 |

| Triglycerides (242) continued |              |              |              |
|-------------------------------|--------------|--------------|--------------|
| TG 16:0_32:0                  | TG 16:0_38:6 | TG 17:0_34:3 | TG 18:0_34:2 |
| TG 16:0_32:1                  | TG 16:0_38:7 | TG 17:0_36:3 | TG 18:0_34:3 |
| TG 16:0_32:2                  | TG 16:0_40:6 | TG 17:0_36:4 | TG 18:0_36:1 |
| TG 16:0_32:3                  | TG 16:0_40:7 | TG 17:1_32:1 | TG 18:0_36:2 |
| TG 16:0_33:1                  | TG 16:0_40:8 | TG 17:1_34:1 | TG 18:0_36:3 |
| TG 16:0_33:2                  | TG 16:1_28:0 | TG 17:1_34:2 | TG 20:4_30:0 |
| TG 16:0_34:0                  | TG 16:1_30:1 | TG 18:3_36:3 | TG 20:4_32:0 |
| TG 18:0_36:4                  | TG 18:2_30:1 | TG 18:3_36:4 | TG 20:4_32:1 |
| TG 18:0_36:5                  | TG 18:2_31:0 | TG 18:3_38:5 | TG 20:4_32:2 |
| TG 18:0_38:6                  | TG 18:2_32:0 | TG 18:3_38:6 | TG 20:4_33:2 |
| TG 18:0_38:7                  | TG 18:2_32:1 | TG 20:0_32:3 | TG 20:4_34:0 |
| TG 18:1_26:0                  | TG 18:2_32:2 | TG 20:0_32:4 | TG 20:4_34:1 |
| TG 18:1_28:1                  | TG 18:2_33:0 | TG 20:0_34:1 | TG 20:4_34:2 |
| TG 18:1_30:0                  | TG 18:2_33:1 | TG 20:1_26:1 | TG 20:4_34:3 |
| TG 18:1_30:1                  | TG 18:2_33:2 | TG 20:1_30:1 | TG 20:4_35:3 |
| TG 18:1_30:2                  | TG 18:2_34:1 | TG 20:1_31:0 | TG 20:4_36:2 |
| TG 18:1_31:0                  | TG 18:2_34:2 | TG 20:1_32:0 | TG 20:4_36:3 |
| TG 18:1_32:0                  | TG 18:2_34:3 | TG 20:1_32:1 | TG 20:4_36:4 |
| TG 18:1_32:1                  | TG 18:2_34:4 | TG 20:1_32:2 | TG 20:4_36:5 |
| TG 18:1_32:2                  | TG 18:2_35:1 | TG 20:1_32:3 | TG 20:5_34:0 |
| TG 18:1_32:3                  | TG 18:2_35:2 | TG 20:1_34:0 | TG 20:5_34:1 |
| TG 18:1_33:0                  | TG 18:2_35:3 | TG 20:1_34:1 | TG 20:5_34:2 |
| TG 18:1_33:1                  | TG 18:2_36:0 | TG 20:1_34:2 | TG 20:5_36:2 |
| TG 18:1_33:2                  | TG 18:2_36:1 | TG 20:1_34:3 | TG 20:5_36:3 |
| TG 18:1_33:3                  | TG 18:2_36:2 | TG 20:2_32:0 | TG 22:0_32:4 |
| TG 18:1_34:1                  | TG 18:2_36:3 | TG 20:2_32:1 | TG 22:1_32:5 |
| TG 18:1_34:2                  | TG 18:2_36:4 | TG 20:2_34:1 | TG 22:2_32:4 |
| TG 18:1_34:3                  | TG 18:2_36:5 | TG 20:2_34:2 | TG 22:3_30:2 |
| TG 18:1_34:4                  | TG 18:2_38:4 | TG 20:2_34:3 | TG 22:4_32:0 |
| TG 18:1_35:2                  | TG 18:2_38:5 | TG 20:2_34:4 | TG 22:4_32:2 |
| TG 18:1_35:3                  | TG 18:2_38:6 | TG 20:2_36:5 | TG 22:4_34:2 |
| TG 18:1_36:0                  | TG 18:3_30:0 | TG 20:3_32:0 | TG 22:5_32:0 |
| TG 18:1_36:1                  | TG 18:3_32:0 | TG 20:3_32:1 | TG 22:5_32:1 |
| TG 18:1_36:2                  | TG 18:3_32:1 | TG 20:3_32:2 | TG 22:5_34:1 |
| TG 18:1_36:3                  | TG 18:3_33:2 | TG 20:3_34:0 | TG 22:5_34:2 |
| TG 18:1_36:4                  | TG 18:3_34:0 | TG 20:3_34:1 | TG 22:5_34:3 |
| TG 18:1_36:5                  | TG 18:3_34:1 | TG 20:3_34:2 | TG 22:6_32:0 |
| TG 18:1_36:6                  | TG 18:3_34:2 | TG 20:3_34:3 | TG 22:6_32:1 |
| TG 18:1_38:5                  | TG 18:3_34:3 | TG 20:3_36:3 | TG 22:6_34:1 |
| TG 18:1_38:6                  | TG 18:3_35:2 | TG 20:3_36:4 | TG 22:6_34:2 |
| TG 18:1_38:7                  | TG 18:3_36:1 | TG 20:3_36:5 | TG 22:6_34:3 |
| TG 18:2_28:0                  | TG 18:3_36:2 | TG 18:0_32:1 |              |
| TG 18:2_30:0                  | TG 17:0_34:2 | TG 18:0_32:2 |              |

| Trihexosylceramides (6) |                    |                    |  |
|-------------------------|--------------------|--------------------|--|
| Hex3Cer d18:1/16:0      | Hex3Cer d18:1/20:0 | Hex3Cer d18:1/24:1 |  |
| Hex3Cer d18:1/18:0      | Hex3Cer d18:1/22:0 | Hex3Cer d18:1/26:1 |  |

## Ordering

|                     |                                                                   |
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