**Methods and Materials.**

Non-targeted global metabolomics was performed by Metabolon, Inc. (Durham, NC) and employed two independent platforms: ultrahigh performance liquid chromatography/tandem mass spectrometry (UHPLC-MS/MS) optimized for basic or acidic species, and gas chromatography/mass spectrometry (GC/MS) (1,2).

For each serum sample, 100 µL was used for analyses.

Using an automated liquid handler (Hamilton LabStar, Salt Lake City, UT), protein was precipitated with methanol that contained four standards to report on extraction efficiency. The resulting supernatant was split into equal aliquots for analysis on two platforms. Aliquots, dried under nitrogen and vacuum-desiccated, were subsequently either reconstituted in 50 µL 0.1% formic acid in water (acidic conditions) or in 50 µL 6.5 mM ammonium bicarbonate in water, pH 8 (basic conditions) for the two UHPLC-MS/MS analyses or derivatized to a final volume of 50 µL for GC/MS analysis using equal parts bistrimethyl-silyl-trifluoroacetamide and solvent mixture acetonitrile: dichloromethane: cyclohexane (5:4:1) with 5% triethylamine at 60°C for 1 hour. In addition, three types of controls were analyzed in concert with the experimental samples: aliquots of a well-characterized human plasma pool served as technical replicates throughout the data set, extracted water samples served as process blanks, and a cocktail of standards spiked into every analyzed sample allowed instrument performance monitoring. Experimental samples and controls were randomized across platform run days.

UHLC-MS/MS samples were separated using a Waters Acquity UPLC (Waters, Millford, MA) instrument with separate acid/base-dedicated 2.1 mm × 100 mm Waters BEH C18 1.7 µm particle columns heated to 40°C and analyzed using an LTQ mass spectrometer (Thermo Fisher Scientific, Inc., Waltham, MA) which consisted of an electrospray ionization (ESI) source and linear ion-trap (LIT) mass analyzer (1). Extracts reconstituted in formic acid were gradient eluted at 350 µL/min using (A) 0.1% formic acid in water and (B) 0.1% formic acid in methanol (0% B to 70% B in 4 min, 70-98% B in 0.5 min, 98% B for 0.9 min), whereas extracts reconstituted in ammonium bicarbonate used (A) 6.5 mM ammonium bicarbonate in water, pH 8, and (B) 6.5 mM ammonium bicarbonate in 95/5 methanol/water (same gradient profile as above) at 350 µL/min. The MS instrument scanned 99-1000 m/z and alternated between MS and MS2 scans

using dynamic exclusion with approximately 6 scans per second. Derivatized samples for GC/MS were separated on a 5% diphenyl/ 95% dimethyl polysiloxane fused silica column with helium as the carrier gas and a temperature ramp from 60°C to 340°C and then analyzed on a Thermo-Finnigan Trace DSQ MS (Thermo Fisher Scientific, Inc.) operated at unit mass resolving power with electron impact ionization and a 50-750 atomic mass unit scan range (2).

Metabolites were identified by automated comparison of the ion features in the experimental samples to a reference library of chemical standard entries that included retention time, molecular weight (m/z), preferred adducts, and in-source fragments as well as associated MS spectra, and were curated by visual inspection for quality control using software (3). For statistical analyses and data display purposes, any missing values were assumed to be below the limits of detection and these values were imputed with the compound minimum. Statistical analysis of log-transformed data was performed using "R" (http://cran.r-project.org/), which is a freely available, open-source software package. Repeated measures 2-way ANOVA with post-test contrasts was performed to compare data between experimental groups and across study time points. Multiple comparisons were accounted for by estimating the false discovery rate using q-values (4).

**References.**

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3. DeHaven C.D., Evans A.M., Dai H., Lawton K.A. Organization of GC/MS and LC/MS Metabolomics data into Chemical Libraries. J. Cheminform 2010; 2(1):9.

4. Storey J.D., Tibshirani R. Statistical significance for genomewide studies. Proc. Natl. Acad. Sci. USA 2003; 100:9440-9445.

**Table A1. A Global Metabolomic Study: Statistical data associated with all 476 compounds detected.**

* Green and red shaded cells indicate p≤0.05 (green indicates that the mean values are significantly higher for that comparison; red - values significantly lower). Light green and light red shaded cells indicate 0.05<p<0.10 (light green indicates that the mean values trend higher for that comparison; light red - values trend lower.

| Biochemical Name | Heat map of statistically significant biochemicals* | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| | Fold Change and ANOVA Contrasts | | | | | | | | |
| | Pre-Op to BL Comparison | | | Post-Op to BL Comparison | | | Post-Op to Pre-Op Comparison | | |
| | SG Non-T2D | SG T2D | GB T2D | SG Non-T2D | SG T2D | GB T2D | SG Non-T2D | SG T2D | GB T2D |
| glycine | 1 | 0.78 | 0.64 | 1.57 | 2.19 | 1.16 | 1.57 | 2.83 | 1.81 |
| N-acetylglycine | 1.8 | 4.79 | 1.44 | 1.64 | 1.55 | 1.83 | 0.91 | 0.32 | 1.27 |
| dimethylglycine | 0.73 | 0.84 | 0.96 | 0.57 | 0.61 | 0.71 | 0.78 | 0.73 | 0.74 |
| betaine | 0.76 | 0.82 | 0.77 | 0.96 | 0.97 | 0.94 | 1.25 | 1.17 | 1.22 |
| serine | 1.1 | 0.7 | 0.79 | 2.44 | 4.03 | 2.43 | 2.22 | 5.79 | 3.07 |
| N-acetylserine | 1 | 0.82 | 1.08 | 4.09 | 6.57 | 8.6 | 4.1 | 7.97 | 8 |
| beta-hydroxypyruvate | 1.17 | 1.02 | 1.13 | 0.93 | 0.69 | 0.65 | 0.79 | 0.67 | 0.57 |
| threonine | 0.86 | 0.73 | 0.8 | 1.34 | 1.45 | 1.65 | 1.57 | 1.99 | 2.05 |
| N-acetylthreonine | 0.87 | 0.72 | 1.29 | 1.3 | 1.1 | 1.59 | 1.49 | 1.54 | 1.23 |
| homoserine | 1.4 | 0.42 | 0.91 | 0.62 | 0.59 | 0.48 | 0.44 | 1.42 | 0.52 |
| alanine | 0.69 | 0.47 | 0.71 | 0.63 | 0.8 | 0.52 | 0.91 | 1.7 | 0.73 |
| N-acetylalanine | 1.03 | 0.85 | 0.94 | 0.94 | 1.07 | 1.01 | 0.91 | 1.26 | 1.07 |
| aspartate | 0.91 | 0.72 | 0.67 | 2.01 | 3.58 | 1.37 | 2.22 | 4.94 | 2.03 |
| asparagine | 0.92 | 0.94 | 0.53 | 0.92 | 1.58 | 0.72 | 1.01 | 1.68 | 1.35 |
| glutamate | 0.89 | 0.81 | 0.81 | 1.85 | 2.48 | 1.96 | 2.09 | 3.05 | 2.41 |
| glutamine | 0.88 | 0.81 | 0.78 | 0.88 | 0.75 | 0.91 | 1.01 | 0.93 | 1.17 |
| pyroglutamine* | 1.16 | 0.82 | 0.98 | 2.17 | 1.71 | 1.34 | 1.87 | 2.09 | 1.36 |
| histidine | 0.75 | 0.7 | 1.03 | 1.26 | 1.64 | 1.82 | 1.68 | 2.34 | 1.76 |
| 1-methylhistidine | 0.81 | 0.73 | 1.02 | 1.4 | 2.08 | 3.91 | 1.73 | 2.87 | 3.83 |
| 3-methylhistidine | 2.26 | 6.83 | 0.45 | 0.78 | 1.66 | 0.38 | 0.34 | 0.24 | 0.84 |
| trans-urocanate | 0.92 | 1.83 | 1.33 | 103.87 | 268.09 | 353.71 | 113.05 | 146.41 | 266.35 |
| cis-urocanate | 0.77 | 1.44 | 1.26 | 76.94 | 329.32 | 543.33 | 99.74 | 229.09 | 431.96 |
| imidazole propionate | 0.8 | 1.14 | 0.76 | 2.07 | 30.7 | 6.51 | 2.59 | 27.03 | 8.56 |
| lysine | 0.91 | 0.76 | 0.71 | 1.43 | 1.15 | 1.27 | 1.57 | 1.52 | 1.79 |
| glutarylcarnitine (C5) | 0.89 | 0.75 | 0.96 | 0.83 | 0.67 | 0.79 | 0.92 | 0.89 | 0.83 |
| pipecolate | 1.26 | 0.87 | 0.49 | 0.9 | 0.79 | 0.63 | 0.72 | 0.91 | 1.3 |
| N-acetyl-cadaverine | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 |
| phenylalanine | 0.85 | 0.77 | 0.69 | 1.15 | 1.21 | 1 | 1.36 | 1.57 | 1.45 |
| N-acetylphenylalanine | 0.64 | 0.62 | 0.88 | 1.16 | 1.51 | 1.39 | 1.82 | 2.43 | 1.58 |
| phenyllactate (PLA) | 0.79 | 0.8 | 0.65 | 0.72 | 0.98 | 0.71 | 0.91 | 1.22 | 1.09 |
| phenylacetate | 1.03 | 0.6 | 0.91 | 0.61 | 1.17 | 0.93 | 0.6 | 1.94 | 1.02 |

| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| 4-hydroxyphenylacetate | 0.65 | 0.78 | 0.79 | 0.69 | 0.94 | 1.07 | 1.07 | 1.19 | 1.35 |
| phenylacetylglutamine | 1.35 | 0.69 | 0.8 | 0.51 | 0.7 | 1.09 | 0.38 | 1.01 | 1.35 |
| tyrosine | 0.81 | **0.62** | **0.62** | 1.18 | 0.96 | 1.12 | **1.46** | **1.53** | **1.8** |
| N-acetyltyrosine | 0.86 | 0.7 | 0.67 | **9.33** | 1.56 | 1.5 | **10.91** | 2.23 | 2.23 |
| tyramine | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 |
| 3-(4-hydroxyphenyl)lactate | 0.81 | **0.64** | **0.66** | **0.65** | **0.66** | **0.65** | 0.8 | 1.03 | 1 |
| phenol sulfate | 0.66 | 0.73 | 0.66 | 1.34 | 1.07 | 1.19 | **2.01** | 1.47 | 1.81 |
| p-cresol sulfate | 0.91 | 0.65 | 0.76 | 0.61 | 0.81 | 0.83 | 0.68 | 1.23 | 1.08 |
| o-cresol sulfate | **3.32** | 1.02 | 1.15 | 1.07 | 1.02 | 0.4 | **0.32** | 1 | **0.35** |
| 3-methoxytyrosine | 1.31 | 0.77 | 0.83 | 1.03 | 0.92 | 1.02 | 0.79 | 1.2 | 1.23 |
| 3-(3-hydroxyphenyl)propionate | 0.79 | 0.89 | **0.54** | 0.86 | 1.26 | **0.48** | 1.08 | 1.42 | 0.89 |
| tryptophan | **0.72** | **0.63** | 0.75 | 0.87 | 0.79 | 0.82 | 1.21 | 1.26 | 1.09 |
| indolelactate | **0.72** | **0.59** | **0.61** | **0.63** | **0.56** | **0.5** | 0.88 | 0.94 | 0.82 |
| indoleacetate | 1.07 | 0.75 | **0.51** | 1.09 | 0.95 | **0.63** | 1.02 | 1.27 | 1.23 |
| indolepropionate | 0.73 | **0.59** | **0.38** | **0.65** | 0.65 | **0.29** | 0.89 | 1.1 | 0.75 |
| 3-indoxyl sulfate | **0.51** | **0.51** | **0.59** | **0.6** | **0.74** | **0.64** | 1.17 | **1.46** | 1.09 |
| kynurenine | **0.77** | **0.64** | **0.69** | **0.71** | **0.62** | **0.58** | 0.92 | 0.97 | 0.84 |
| kynurenate | 1.38 | 0.87 | 1.22 | 0.93 | 0.86 | 0.83 | 0.68 | 0.98 | 0.68 |
| serotonin (5HT) | 0.71 | 0.62 | **0.54** | **0.41** | **0.3** | **0.31** | 0.58 | **0.48** | **0.56** |
| tryptophan betaine | 1.03 | 0.72 | **0.84** | **0.59** | **0.65** | **0.69** | **0.57** | 0.9 | 0.82 |
| C-glycosyltryptophan | 1.06 | 0.89 | 1.09 | 0.94 | 0.95 | 0.99 | 0.88 | 1.06 | 0.91 |
| leucine | 1.09 | 0.78 | 0.78 | 1.23 | 0.85 | 0.8 | 1.14 | 1.09 | 1.02 |
| 4-methyl-2-oxopentanoate | 1.14 | 0.73 | 0.96 | 1.01 | **0.6** | **0.67** | 0.89 | 0.82 | **0.7** |
| isovalerate | 1.37 | 0.66 | 1.22 | 1.58 | 0.85 | 1.33 | 1.15 | 1.29 | 1.09 |
| isovalerylcarnitine | 0.83 | 0.75 | 1.02 | **1.89** | 1.73 | **4.12** | **2.27** | **2.32** | **4.06** |
| beta-hydroxyisovalerate | 1.9 | 0.73 | 1.52 | **20.74** | 0.54 | 0.51 | 10.91 | 0.74 | **0.34** |
| beta-hydroxyisovaleroylcarnitine | 1.1 | 0.9 | 1.7 | 0.96 | 1.02 | 1.37 | 0.87 | 1.13 | 0.81 |
| 3-methylglutarylcarnitine (C6) | 0.68 | 0.79 | 1.18 | 0.75 | 0.51 | 0.6 | 1.1 | 0.65 | 0.51 |
| alpha-hydroxyisovalerate | 0.99 | 0.82 | 0.98 | 1.24 | 0.76 | 0.97 | 1.25 | 0.93 | 0.99 |
| isoleucine | 1.04 | 0.75 | 0.79 | 1.22 | 0.91 | 0.92 | 1.18 | 1.22 | 1.17 |
| 3-methyl-2-oxovalerate | 1.21 | 0.77 | 0.95 | 1.05 | **0.69** | 0.67 | 0.87 | 0.9 | 0.71 |
| 2-methylbutyrylcarnitine (C5) | 0.84 | **0.65** | 0.79 | 1.08 | **0.62** | 0.85 | **1.29** | 0.96 | 1.07 |
| tiglyl carnitine | 1.41 | 0.89 | 2.58 | 0.72 | **0.41** | 0.64 | **0.51** | 0.46 | **0.25** |
| 2-hydroxy-3-methylvalerate | 1.22 | 0.69 | 0.7 | 1.06 | 0.78 | 0.82 | 0.87 | 1.13 | 1.18 |
| 3-hydroxy-2-ethylpropionate | 1.49 | 1.23 | **1.53** | 0.99 | 1.02 | 1.02 | 0.66 | 0.83 | 0.67 |
| valine | 1.07 | 0.81 | 0.85 | 1.1 | **0.78** | **0.79** | 1.03 | 0.97 | 0.93 |
| 3-methyl-2-oxobutyrate | 1.26 | 1.09 | 1.28 | 0.78 | **0.67** | 0.88 | **0.62** | **0.62** | **0.69** |
| isobutyrylcarnitine | 0.82 | **0.62** | 1.39 | 1.04 | 0.75 | 0.8 | 1.27 | 1.2 | 0.58 |
| 3-hydroxyisobutyrate | 1.03 | 0.76 | 1.13 | 1.14 | **0.75** | **0.66** | 1.11 | 0.98 | **0.59** |
| alpha-hydroxyisocaproate | 1.43 | 1.3 | 1.09 | 1.1 | 1.07 | 1.81 | 0.77 | 0.82 | 1.67 |
| methionine | 0.92 | 0.82 | **0.75** | 1.02 | 0.81 | 0.79 | 1.11 | 0.99 | 1.06 |

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|---|---|---|---|---|---|---|---|---|---|
| N-acetylmethionine | 0.86 | 1.09 | 0.81 | 1.02 | **1.92** | 1.02 | 1.18 | 1.76 | 1.26 |
| N-formylmethionine | 0.97 | 0.78 | 0.84 | **0.57** | **0.56** | **0.65** | **0.58** | 0.72 | 0.77 |
| homocysteine | 1 | 1 | 1 | 1.75 | **2.23** | **2.39** | 1.75 | **2.23** | **2.39** |
| alpha-ketobutyrate | **2.32** | 0.88 | **2.48** | 0.54 | **0.1** | 1.24 | **0.23** | **0.12** | **0.5** |
| 2-aminobutyrate | **2.21** | 1.16 | **1.73** | **1.45** | 0.82 | **1.49** | **0.65** | **0.7** | 0.86 |
| 2-hydroxybutyrate (AHB) | **2.68** | 1.21 | **2.79** | 1.27 | **0.65** | **1.54** | **0.47** | **0.54** | **0.55** |
| cysteine | 1.18 | **0.63** | 1.08 | 1.21 | 1.59 | **1.87** | 1.02 | **2.52** | **1.73** |
| cystine | 0.6 | 0.45 | 0.66 | 0.95 | **1.73** | 1.24 | 1.58 | **3.85** | 1.88 |
| S-methylcysteine | 1.24 | 0.85 | 0.95 | 1.36 | 0.81 | 1 | 1.1 | 0.96 | 1.06 |
| 4-amino-2-hydroxybutyrate | 1.11 | **0.7** | **1.52** | 0.81 | **0.66** | **0.76** | 0.72 | 0.94 | **0.5** |
| arginine | 0.93 | 0.79 | 0.77 | 0.78 | **0.69** | **0.7** | 0.84 | 0.88 | 0.91 |
| urea | 0.94 | **0.61** | 2.03 | 0.9 | 0.71 | 0.67 | 0.96 | 1.17 | **0.33** |
| ornithine | 0.59 | 0.69 | 0.93 | **6.39** | **17.59** | **23.2** | **10.81** | **25.39** | **24.82** |
| proline | 0.81 | **0.68** | **0.63** | 1.07 | 0.91 | 0.83 | 1.32 | 1.34 | 1.32 |
| citrulline | 0.9 | 1.1 | 1.36 | 0.86 | 1.55 | 1.83 | 0.95 | 1.41 | 1.35 |
| homocitrulline | 1.19 | 0.91 | 1.23 | 1.1 | **0.68** | 0.82 | 0.92 | 0.75 | 0.66 |
| dimethylarginine (SDMA + ADMA) | 1.07 | 1.1 | 1.07 | 0.84 | 0.82 | **0.72** | 0.78 | 0.75 | **0.68** |
| N-delta-acetylornithine* | 0.6 | **0.42** | 1.03 | 0.94 | 0.85 | 0.77 | 1.57 | **2.01** | 0.75 |
| trans-4-hydroxyproline | 1.08 | **0.43** | 0.55 | 2.93 | 0.68 | 0.54 | 2.71 | 1.59 | 0.99 |
| pro-hydroxy-pro | 1.25 | 0.7 | 0.76 | **4.58** | 0.96 | 1.28 | **3.67** | 1.38 | 1.68 |
| creatine | 0.76 | **0.59** | 0.92 | 1.22 | 0.91 | 1.49 | **1.61** | **1.54** | **1.61** |
| creatinine | 1.16 | 0.91 | 1.01 | 0.93 | 0.94 | 1 | **0.8** | 1.03 | 0.98 |
| acisoga | 0.98 | 1 | 0.86 | 0.93 | 0.72 | 0.98 | 0.95 | 0.72 | 1.13 |
| N-acetylputrescine | 0.79 | 1.01 | 1.16 | 0.93 | 2.11 | 1.07 | 1.17 | 2.09 | 0.92 |
| 4-acetamidobutanoate | 1.24 | 0.78 | 0.96 | 1.3 | 0.86 | **0.78** | 1.04 | 1.1 | 0.81 |
| 4-guanidinobutanoate | 0.72 | **0.5** | 0.67 | 0.9 | 3.03 | 1.4 | 1.25 | **6.06** | 2.1 |
| glutathione, oxidized (GSSG) | 1.01 | 1.18 | 0.66 | 26.34 | **23.63** | **101.52** | 26.11 | **20.03** | **154.42** |
| cysteine-glutathione disulfide | 0.95 | 1.38 | 1.28 | **5.62** | **4.86** | **10.46** | **5.91** | **3.51** | **8.19** |
| cys-gly, oxidized | 0.68 | 0.7 | 1.16 | 1.17 | 1.19 | **3.63** | 1.72 | **1.71** | **3.12** |
| 5-oxoproline | 0.8 | **0.66** | 0.71 | **4.01** | **7.95** | **8.08** | **4.98** | **12.04** | **11.32** |
| ophthalmate | 0.91 | 1.69 | 2.58 | 2.79 | 3.63 | **8.81** | **3.08** | 2.15 | **3.41** |
| gamma-glutamylalanine | **0.58** | **0.64** | 0.77 | **0.45** | **0.5** | **0.33** | 0.77 | 0.77 | **0.43** |
| gamma-glutamylglutamate | 1.24 | 0.8 | 0.92 | **3.99** | **5.21** | **6.96** | **3.23** | **6.48** | **7.58** |
| gamma-glutamylglutamine | 0.82 | 0.72 | 1 | 0.77 | **0.49** | **0.56** | 0.93 | **0.68** | **0.56** |
| gamma-glutamylisoleucine* | 0.85 | **0.56** | 0.72 | **2.52** | 1.71 | 2.09 | **2.95** | **3.06** | **2.91** |
| gamma-glutamylleucine | 0.86 | **0.59** | 0.75 | **1.75** | 1.07 | 1.29 | **2.02** | **1.82** | **1.71** |
| gamma-glutamylmethionine | 0.97 | 0.71 | 0.91 | 0.77 | **0.48** | **0.47** | 0.79 | **0.67** | **0.52** |
| gamma-glutamylphenylalanine | 0.84 | 0.82 | 0.73 | **1.68** | **1.64** | 1.69 | **1.99** | **2.01** | **2.31** |
| gamma-glutamylthreonine* | 0.88 | **0.56** | 0.94 | **2.24** | **1.81** | **2.31** | **2.55** | **3.22** | **2.46** |
| gamma-glutamyltyrosine | 0.89 | **0.57** | **0.62** | **1.76** | 1.34 | 1.59 | **1.97** | **2.35** | **2.56** |
| gamma-glutamylvaline | 1.23 | **0.6** | 1.14 | **1.81** | 1.21 | 1.64 | 1.48 | **2.02** | 1.44 |

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|---|---|---|---|---|---|---|---|---|---|
| N-acetylcarnosine | 1.06 | 0.72 | 0.79 | 0.93 | 0.78 | 0.68 | 0.88 | 1.08 | 0.85 |
| alpha-glutamylglutamate | 0.61 | 1.32 | 0.25 | 1.49 | 6.03 | 1.55 | 2.45 | 4.57 | 6.09 |
| alpha-glutamyltyrosine | 0.84 | 0.94 | 1.16 | 0.42 | 0.46 | 0.98 | 0.5 | 0.48 | 0.85 |
| aspartylleucine | 0.67 | 0.66 | 0.91 | 0.72 | 2.8 | 1.19 | 1.08 | 4.21 | 1.32 |
| aspartylphenylalanine | 0.55 | 0.67 | 0.98 | 0.32 | 1.22 | 0.37 | 0.58 | 1.81 | 0.38 |
| cyclo(glu-glu) | 0.64 | 1.02 | 0.63 | 2.79 | 5.63 | 4.98 | 4.36 | 5.52 | 7.93 |
| cyclo(leu-pro) | 0.57 | 1.11 | 0.46 | 0.81 | 0.76 | 0.38 | 1.42 | 0.69 | 0.83 |
| glycylglycine | 0.78 | 1 | 0.61 | 1.09 | 1.92 | 1.32 | 1.4 | 1.93 | 2.16 |
| glycylphenylalanine | 0.86 | 1.35 | 0.95 | 0.78 | 1.96 | 0.89 | 0.9 | 1.45 | 0.94 |
| glycylvaline | 0.9 | 0.47 | 0.37 | 0.41 | 1.88 | 0.42 | 0.46 | 4.01 | 1.14 |
| histidyltryptophan | 1.4 | 1.65 | 0.99 | 1.37 | 2.6 | 0.85 | 0.99 | 1.58 | 0.87 |
| isoleucylvaline | 1.42 | 0.73 | 1.01 | 0.31 | 0.28 | 0.3 | 0.22 | 0.39 | 0.3 |
| leucylalanine | 0.77 | 0.68 | 1.47 | 0.26 | 0.64 | 0.39 | 0.34 | 0.94 | 0.26 |
| phenylalanylglutamate | 0.62 | 1.24 | 1.37 | 4.45 | 10.76 | 4.01 | 7.16 | 8.67 | 2.93 |
| phenylalanylleucine | 0.49 | 0.48 | 1.44 | 0.53 | 1.79 | 0.65 | 1.06 | 3.74 | 0.45 |
| phenylalanylphenylalanine | 0.58 | 0.88 | 0.95 | 0.34 | 0.76 | 0.38 | 0.59 | 0.86 | 0.4 |
| phenylalanylserine | 0.6 | 1.1 | 1.3 | 0.23 | 0.66 | 0.6 | 0.38 | 0.61 | 0.46 |
| phenylalanyltryptophan | 0.71 | 0.68 | 1.25 | 0.36 | 0.44 | 0.48 | 0.51 | 0.65 | 0.38 |
| prolylglycine | 0.82 | 0.73 | 0.8 | 4.23 | 3.09 | 7.75 | 5.18 | 4.23 | 9.68 |
| pyroglutamylglycine | 0.68 | 0.7 | 0.53 | 0.91 | 1.74 | 0.58 | 1.33 | 2.5 | 1.1 |
| pyroglutamylvaline | 0.95 | 0.74 | 0.8 | 81.09 | 111.34 | 180.96 | 84.99 | 150.6 | 226.67 |
| seryltyrosine | 1.19 | 1.99 | 1.74 | 1.54 | 1.35 | 1.16 | 1.29 | 0.68 | 0.67 |
| threonylphenylalanine | 1 | 1.06 | 0.91 | 0.61 | 0.62 | 0.49 | 0.61 | 0.59 | 0.53 |
| tryptophylglutamate | 1.52 | 1.13 | 0.5 | 4.43 | 12.82 | 2.1 | 2.92 | 11.31 | 4.25 |
| tyrosylglutamate | 1.05 | 1.3 | 1.23 | 2.55 | 7.02 | 5.44 | 2.44 | 5.39 | 4.42 |
| valylarginine | 0.79 | 0.73 | 1.4 | 0.25 | 0.4 | 0.36 | 0.32 | 0.54 | 0.26 |
| bradykinin, des-arg(9) | 1.72 | 1.6 | 2.35 | 1 | 1.11 | 1 | 0.58 | 0.69 | 0.43 |
| HWESASXX* | 2.74 | 0.65 | 1.05 | 1.18 | 0.94 | 0.87 | 0.43 | 1.45 | 0.83 |
| ADSGEGDFXAEGGGVR* | 1.05 | 7.36 | 0.96 | 1.1 | 0.6 | 0.96 | 1.05 | 0.08 | 1.01 |
| DSGEGDFXAEGGGVR* | 2.51 | 1.23 | 0.88 | 1.2 | 0.2 | 0.76 | 0.48 | 0.16 | 0.87 |
| ADpSGEGDFXAEGGGVR* | 2.86 | 2.27 | 0.7 | 3.54 | 2.09 | 3.38 | 1.24 | 0.92 | 4.8 |
| 1,5-anhydroglucitol (1,5-AG) | 0.94 | 0.86 | 0.93 | 0.73 | 0.81 | 0.63 | 0.77 | 0.94 | 0.68 |
| glucose | 1.07 | 0.8 | 1.18 | 0.76 | 0.53 | 0.76 | 0.71 | 0.67 | 0.64 |
| 2,3-diphosphoglycerate | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 |
| 3-phosphoglycerate | 1.03 | 1.01 | 0.93 | 8.83 | 17.11 | 37.08 | 8.55 | 16.99 | 39.97 |
| pyruvate | 1.05 | 0.89 | 1.24 | 0.44 | 0.3 | 0.53 | 0.42 | 0.34 | 0.43 |
| lactate | 1.06 | 1.54 | 1.51 | 1.09 | 2.44 | 1 | 1.03 | 1.59 | 0.66 |
| glycerate | 0.99 | 0.68 | 0.69 | 1.77 | 2.74 | 1.07 | 1.78 | 4.01 | 1.55 |
| ribulose/xylulose 5-phosphate | 0.87 | 1 | 1.91 | 9.26 | 9.94 | 16.01 | 10.7 | 9.94 | 8.37 |
| ribulose | 1.56 | 0.94 | 1.09 | 11.87 | 7.51 | 5.14 | 7.6 | 8.01 | 4.71 |
| ribose | 0.81 | 1.05 | 1.19 | 3.98 | 3.07 | 1.77 | 4.89 | 2.92 | 1.49 |

| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| ribitol | 1.01 | 0.76 | 0.84 | 0.8 | **2.37** | 0.77 | 0.8 | **3.11** | 0.92 |
| xylulose | 1.41 | 3.37 | 1.97 | **8.38** | **16.31** | **10.84** | **5.95** | **4.84** | **5.51** |
| xylonate | 0.74 | **0.28** | **0.6** | 1.4 | **0.47** | 0.84 | 1.9 | 1.72 | 1.39 |
| xylose | 1.05 | **0.69** | 0.82 | 0.83 | 1.12 | 0.74 | 0.79 | **1.63** | 0.91 |
| xylitol | 2.23 | 1.17 | 1.1 | 1.14 | 1.29 | 2.17 | 0.51 | 1.1 | 1.98 |
| arabinose | 0.73 | 0.97 | 0.92 | **0.4** | **0.49** | 0.62 | **0.55** | **0.5** | 0.67 |
| threitol | 0.96 | **0.62** | 0.93 | 0.75 | 0.89 | **0.68** | 0.79 | 1.43 | 0.73 |
| arabitol | 0.81 | **0.55** | 1.42 | 0.7 | 0.67 | 0.84 | 0.87 | 1.21 | 0.59 |
| fucose | 1.23 | 0.78 | 0.95 | **0.41** | 0.75 | **0.59** | **0.33** | 0.97 | **0.62** |
| maltotriose | 0.53 | 0.77 | 1.71 | **1.97** | **6.28** | **4.64** | **3.74** | **8.2** | **2.71** |
| sucrose | **0.27** | 0.4 | **0.14** | **2.7** | **35.83** | **6.45** | **9.85** | **89.85** | **44.52** |
| fructose | 1.48 | 0.61 | 0.88 | 0.56 | 0.48 | **0.31** | **0.38** | 0.78 | **0.35** |
| sorbitol | 0.56 | 0.53 | 0.75 | **6.39** | **4.52** | **5.64** | **11.31** | **8.49** | **7.56** |
| mannose | 1.59 | 0.96 | 1.52 | 0.79 | **0.51** | **0.69** | **0.5** | **0.53** | **0.46** |
| mannitol | **0.16** | 0.63 | 1.17 | 0.38 | 1.04 | 0.36 | 2.46 | 1.65 | 0.31 |
| glucuronate | 0.66 | **0.34** | 1.1 | **0.47** | **0.12** | **0.33** | 0.71 | **0.36** | **0.3** |
| N-acetylneuraminate | 1.03 | 0.75 | 1.33 | 1.05 | 1.76 | 1.54 | 1.02 | **2.34** | 1.16 |
| erythronate* | 0.88 | **0.6** | 1.02 | **0.74** | 0.84 | 0.87 | 0.84 | **1.42** | 0.85 |
| citrate | **1.51** | 1.12 | 1.27 | 1.16 | **1.56** | 1.39 | 0.77 | 1.38 | 1.09 |
| alpha-ketoglutarate | 0.87 | 0.54 | 0.87 | 0.66 | 0.61 | 0.49 | 0.77 | 1.12 | 0.57 |
| succinylcarnitine | 0.91 | 0.95 | 1.09 | 1.43 | 1.41 | **2.56** | **1.57** | 1.48 | **2.36** |
| fumarate | 1.2 | 0.82 | 0.82 | 1.55 | **2.71** | **2.04** | 1.29 | **3.31** | **2.48** |
| malate | 0.79 | 0.78 | 0.68 | **2.29** | **4.24** | **3.03** | **2.91** | **5.42** | **4.43** |
| acetylphosphate | 1.07 | **0.7** | 0.89 | 0.94 | 0.75 | 0.93 | 0.88 | 1.07 | 1.05 |
| pyrophosphate (PPi) | 2.2 | 0.88 | 0.95 | 2.41 | 0.67 | 0.94 | 1.09 | 0.75 | 0.98 |
| phosphate | 0.89 | 0.78 | 0.91 | 0.91 | 0.99 | 1.22 | 1.03 | 1.27 | **1.35** |
| caproate (6:0) | 1.12 | 0.96 | 0.91 | 0.8 | 1.08 | 0.91 | **0.72** | 1.12 | 1.01 |
| heptanoate (7:0) | 0.96 | 1.05 | 1.24 | **17.47** | 0.99 | 1.22 | **18.13** | 0.94 | 0.99 |
| caprylate (8:0) | 0.94 | 1.01 | 0.75 | 1.22 | **1.6** | 1.45 | 1.3 | **1.58** | **1.92** |
| pelargonate (9:0) | 0.78 | **0.68** | 0.91 | **0.59** | **0.48** | **0.51** | 0.76 | **0.7** | **0.56** |
| caprate (10:0) | 0.65 | 1.02 | 0.74 | 0.69 | 1.3 | 1.04 | 1.07 | 1.27 | 1.41 |
| 10-undecenoate (11:1n1) | 1.09 | **0.53** | 1.1 | 0.9 | **0.63** | 1.07 | 0.82 | 1.19 | 0.97 |
| laurate (12:0) | 1.16 | 1.58 | 2.31 | 1.56 | **3.65** | **2.19** | 1.34 | **2.31** | 0.95 |
| 5-dodecenoate (12:1n7) | 1.26 | 1.19 | 1.39 | 0.92 | 1.17 | 1.31 | 0.73 | 0.98 | 0.95 |
| myristate (14:0) | 1.52 | 1.49 | 2.01 | 1.34 | 2.18 | **3.84** | 0.88 | 1.46 | 1.92 |
| myristoleate (14:1n5) | 1.97 | **1.99** | **2.16** | 1.61 | **3.12** | **2.52** | 0.82 | 1.57 | 1.17 |
| pentadecanoate (15:0) | 1.69 | 1.18 | 1.13 | **3.02** | **3.36** | **2.44** | 1.79 | 2.84 | **2.15** |
| palmitate (16:0) | **1.53** | 1.31 | **1.62** | 1.04 | 1.08 | 1.51 | **0.68** | 0.82 | 0.93 |
| palmitoleate (16:1n7) | **2.4** | **1.79** | **2.68** | 1.54 | 1.7 | **2.23** | 0.64 | 0.95 | 0.83 |
| margarate (17:0) | **1.83** | 1.36 | **1.8** | 1.32 | 1.27 | **2.21** | 0.72 | 0.93 | 1.23 |
| 10-heptadecenoate (17:1n7) | 1.9 | 1.5 | 1.93 | 2.29 | **3.8** | **2.94** | 1.21 | 2.53 | 1.52 |

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|---|---|---|---|---|---|---|---|---|---|
| stearate (18:0) | 1.39 | 1.22 | 1.39 | 0.97 | 1.05 | 1.41 | **0.7** | 0.86 | 1.01 |
| oleate (18:1n9) | **2.84** | **1.74** | **3.11** | 1.57 | 1.12 | **2.18** | **0.55** | 0.64 | 0.7 |
| cis-vaccenate (18:1n7) | **2.18** | **1.52** | **2.07** | 1.39 | 1.13 | **1.63** | **0.64** | 0.75 | 0.79 |
| nonadecanoate (19:0) | 1.35 | 1.13 | 1.09 | 1.51 | 1.6 | **2.6** | 1.12 | 1.42 | **2.39** |
| 10-nonadecenoate (19:1n9) | **2.53** | 1.72 | **2.08** | 1.71 | 2.09 | **2.41** | 0.68 | 1.21 | 1.16 |
| eicosenoate (20:1n9 or 11) | **2.8** | **1.87** | **2.62** | 1.7 | 1.61 | **2.91** | 0.61 | 0.86 | 1.11 |
| stearidonate (18:4n3) | 1.46 | 1.4 | **2.82** | 1 | 1.01 | 1.32 | 0.68 | 0.72 | **0.47** |
| eicosapentaenoate (EPA; 20:5n3) | 1.14 | 1.19 | 1.39 | **0.63** | **0.66** | 1.15 | **0.55** | **0.56** | 0.82 |
| docosapentaenoate (n3 DPA; 22:5n3) | **1.72** | 1.59 | **2.36** | 0.96 | 0.84 | **1.97** | **0.56** | **0.53** | 0.83 |
| docosahexaenoate (DHA; 22:6n3) | 1.26 | 1.06 | 1.2 | **0.73** | 0.71 | 1.24 | **0.58** | 0.67 | 1.03 |
| linoleate (18:2n6) | **1.93** | **1.46** | **2.09** | 0.98 | 0.91 | **1.56** | **0.51** | **0.62** | 0.74 |
| linolenate [alpha or gamma; (18:3n3 or 6)] | **2.81** | **1.6** | **2.67** | 0.84 | 0.75 | 1.4 | **0.3** | **0.47** | **0.53** |
| dihomo-linolenate (20:3n3 or n6) | 1.24 | 1.09 | **1.62** | 0.76 | 0.75 | 1.22 | **0.61** | 0.69 | 0.75 |
| arachidonate (20:4n6) | 1.16 | 0.93 | 0.96 | 0.84 | 1.08 | 1.2 | 0.72 | 1.16 | 1.25 |
| adrenate (22:4n6) | 0.96 | 1.12 | 0.65 | **0.53** | 0.75 | **0.55** | **0.56** | 0.67 | 0.85 |
| docosapentaenoate (n6 DPA; 22:5n6) | 1.54 | 1.08 | 1.22 | 0.85 | 0.8 | 1.13 | **0.55** | 0.74 | 0.93 |
| docosadienoate (22:2n6) | 1.84 | 1.68 | 1.76 | 2.33 | **3.17** | **3.28** | 1.27 | 1.88 | 1.86 |
| dihomo-linoleate (20:2n6) | **2.33** | **1.77** | **2.64** | 1.43 | 1.57 | **2.8** | 0.61 | 0.89 | 1.06 |
| 13-methylmyristic acid | 1.05 | 0.93 | 1.28 | 1.05 | 1.06 | 2.15 | 1 | 1.13 | 1.68 |
| 15-methylpalmitate (isobar with 2-methylpalmitate) | 1.58 | 1.29 | 1.33 | 2.12 | **4.94** | **2.26** | 1.34 | 3.84 | 1.7 |
| 17-methylstearate | **1.92** | 1.38 | 1.17 | 1.71 | **2.36** | **2.23** | 0.89 | 1.71 | 1.92 |
| 2-hydroxyglutarate | **0.74** | 1.09 | **0.63** | 1.04 | **1.77** | 1.1 | **1.4** | **1.62** | **1.74** |
| azelate (nonanedioate) | **3.4** | **4.6** | 1.43 | **3.96** | **6** | **21.88** | 1.16 | 1.31 | **15.32** |
| sebacate (decanedioate) | **2.39** | 1.73 | 0.94 | **5.28** | **3.68** | **6.45** | 2.21 | 2.13 | **6.88** |
| undecanedioate | 1.34 | **0.55** | 0.61 | **3.02** | **2.92** | **3.61** | **2.25** | **5.35** | **5.93** |
| 1,11-undecanedicarboxylate | 0.9 | 0.83 | 0.64 | **4.51** | **8.2** | **26.79** | **4.99** | **9.82** | **41.8** |
| dodecanedioate | 1.76 | 1.17 | 0.96 | 1.76 | 1.93 | 1.42 | 1 | 1.64 | 1.48 |
| tetradecanedioate | **1.89** | 1.48 | 1.15 | 1.1 | 0.9 | 0.8 | **0.58** | 0.6 | 0.7 |
| hexadecanedioate | **1.76** | 1.64 | 1.24 | 1.17 | 1.13 | 1.18 | 0.66 | 0.69 | 0.96 |
| octadecanedioate | **2.09** | 1.56 | 1.29 | 1.51 | 1.22 | 1.42 | **0.72** | 0.78 | 1.1 |
| 3-carboxy-4-methyl-5-propyl-2-furanpropanoate (CMPF) | 1.14 | **0.64** | 0.85 | **0.43** | **0.44** | 0.64 | **0.38** | 0.7 | 0.75 |
| palmitate, methyl ester | 0.97 | **0.52** | 0.92 | **0.42** | **0.35** | **0.61** | **0.44** | 0.67 | **0.66** |
| n-Butyl Oleate | 0.92 | 1.4 | 1.26 | 0.88 | 1.3 | 1.23 | 0.95 | 0.92 | 0.98 |
| 2-aminoheptanoate | 0.71 | **0.59** | **0.41** | 0.72 | 0.61 | **0.56** | 1.01 | 1.04 | 1.35 |
| 2-aminooctanoate | 0.82 | **0.62** | **0.54** | 0.79 | 0.74 | **0.59** | 0.97 | 1.18 | 1.09 |
| butyrylcarnitine | 0.79 | **0.64** | 0.75 | 1.07 | 0.81 | 0.82 | 1.35 | 1.26 | 1.09 |
| propionylcarnitine | **0.58** | **0.52** | 0.93 | 1.13 | 0.8 | 1.2 | **1.92** | **1.54** | **1.29** |
| acetylcarnitine | **1.74** | 1.29 | **1.63** | **1.71** | 1.16 | **1.55** | 0.98 | 0.9 | 0.95 |
| hydroxybutyrylcarnitine* | **8.65** | **3.87** | **6.95** | **5.99** | **2.83** | **4.89** | **0.69** | 0.73 | 0.7 |
| hexanoylcarnitine | 0.87 | 0.91 | 1.12 | 1.17 | 0.88 | 1.6 | 1.34 | 0.97 | 1.42 |
| octanoylcarnitine | **0.53** | **0.54** | 0.8 | 0.9 | **0.41** | 1.43 | **1.68** | 0.76 | **1.79** |

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|---|---|---|---|---|---|---|---|---|---|
| decanoylcarnitine | **0.48** | **0.57** | 0.68 | 0.93 | 0.7 | 1.27 | **1.95** | 1.24 | **1.88** |
| cis-4-decenoyl carnitine | **0.57** | **0.59** | **0.61** | 0.78 | **0.67** | 1.19 | 1.37 | 1.15 | **1.94** |
| laurylcarnitine | 0.79 | **0.43** | 0.97 | 0.9 | 0.53 | 1 | 1.14 | 1.23 | 1.03 |
| palmitoylcarnitine | 1.25 | 0.91 | 1.36 | 0.9 | 0.87 | 1.5 | 0.72 | 0.96 | 1.1 |
| stearoylcarnitine | 1.09 | 1.26 | 1.09 | 0.8 | 0.8 | 1.31 | 0.73 | 0.63 | 1.2 |
| oleoylcarnitine | 1.2 | 0.71 | 1.19 | 0.81 | 0.92 | 1.73 | 0.68 | 1.29 | 1.45 |
| deoxycarnitine | 0.93 | **0.7** | 0.95 | 1.03 | 0.96 | **1.28** | 1.11 | **1.36** | **1.34** |
| carnitine | 1.03 | 0.99 | 1.11 | 0.99 | 0.86 | 0.9 | 0.95 | 0.88 | **0.81** |
| 3-dehydrocarnitine | 0.94 | **0.81** | 1.05 | 1.02 | **0.73** | 1.03 | 1.08 | 0.9 | 0.98 |
| acetoacetate | **13.88** | **5.66** | **8.71** | 2.06 | **0.46** | 3.58 | **0.15** | **0.08** | **0.41** |
| 3-hydroxybutyrate (BHBA) | **18.77** | **5.79** | **11.25** | **9.44** | 2.5 | **5.87** | **0.5** | **0.43** | 0.52 |
| 2-hydroxydecanoate | 0.81 | **0.36** | **0.52** | 0.61 | 0.61 | 1.46 | 0.75 | **1.69** | **2.81** |
| 2-hydroxypalmitate | 1.08 | 0.93 | 0.95 | 0.76 | 0.97 | 1.53 | 0.7 | 1.04 | 1.61 |
| 2-hydroxystearate | 0.87 | 0.73 | 0.76 | 0.64 | 1.01 | 1.35 | 0.73 | 1.38 | 1.77 |
| 3-hydroxypropanoate | 1.07 | 0.86 | 0.9 | 1.21 | 0.9 | 0.95 | 1.14 | 1.04 | 1.05 |
| 3-hydroxyoctanoate | 1.43 | 0.76 | 0.39 | 0.93 | 0.61 | 0.59 | 0.65 | 0.81 | 1.49 |
| 3-hydroxydecanoate | 1.22 | 0.69 | 0.46 | 0.96 | 0.72 | 0.77 | 0.78 | 1.04 | 1.68 |
| 13-HODE + 9-HODE | **4.57** | **2.46** | **2.32** | 1.34 | **2.49** | **3.74** | **0.29** | 1.01 | 1.61 |
| prostaglandin E2 | 1 | 1 | 1 | 1 | 1.26 | **1.53** | 1 | 1.26 | **1.53** |
| 12-HETE | 0.78 | 1.26 | 0.86 | 1.39 | **13.96** | 2.22 | 1.79 | **11.06** | 2.58 |
| myo-inositol | 0.99 | 0.69 | 1.44 | 0.95 | 0.88 | 1.28 | 0.95 | 1.27 | 0.89 |
| chiro-inositol | 1.1 | 1.49 | 0.58 | 0.49 | 0.7 | 3.1 | 0.45 | 0.47 | 5.39 |
| scyllo-inositol | 0.93 | **0.65** | 2.03 | 0.95 | 0.7 | 1.76 | 1.02 | 1.08 | 0.87 |
| inositol 1-phosphate (I1P) | 0.76 | 0.65 | **0.8** | 0.75 | **0.59** | 0.78 | 0.99 | 0.91 | 0.97 |
| choline | **0.69** | **0.69** | **0.68** | 1.01 | 1.07 | 0.95 | **1.47** | **1.55** | 1.39 |
| glycerophosphorylcholine (GPC) | 0.87 | 1.04 | 0.8 | 0.96 | **1.77** | **2.05** | 1.11 | **1.71** | **2.58** |
| 1-myristoylglycerophosphocholine (14:0) | **0.33** | **0.32** | 0.82 | **0.27** | **0.31** | **0.28** | 0.81 | 0.99 | **0.34** |
| 2-myristoylglycerophosphocholine* | **0.23** | **0.49** | **0.71** | **0.21** | **0.66** | **0.33** | 0.93 | 1.36 | 0.47 |
| 1-pentadecanoylglycerophosphocholine (15:0)* | 0.8 | **0.37** | 0.9 | 0.61 | **0.42** | 0.7 | 0.76 | 1.13 | 0.78 |
| 1-palmitoylglycerophosphocholine (16:0) | 0.79 | 0.63 | 0.8 | **0.55** | 0.61 | **0.6** | 0.7 | 0.98 | **0.74** |
| 2-palmitoylglycerophosphocholine* | 0.77 | **0.44** | 0.75 | **0.45** | **0.43** | **0.53** | 0.58 | 0.98 | **0.71** |
| 1-palmitoleoylglycerophosphocholine (16:1)* | **0.6** | **0.44** | **0.67** | **0.37** | **0.39** | **0.4** | **0.61** | 0.89 | **0.6** |
| 1-margaroylglycerophosphocholine (17:0) | 0.71 | **0.36** | 0.68 | **0.43** | **0.44** | **0.7** | 0.61 | 1.21 | 1.03 |
| 1-stearoylglycerophosphocholine (18:0) | 0.48 | 0.61 | 0.74 | **0.33** | 0.59 | **0.46** | 0.7 | 0.97 | **0.62** |
| 2-stearoylglycerophosphocholine* | **0.29** | **0.57** | 0.68 | **0.32** | 0.61 | **0.45** | 1.11 | 1.06 | 0.66 |
| 1-oleoylglycerophosphocholine (18:1) | 0.78 | 0.55 | 0.75 | **0.37** | **0.42** | **0.51** | **0.47** | 0.76 | **0.68** |
| 2-oleoylglycerophosphocholine* | 0.89 | 0.68 | 0.9 | **0.53** | **0.55** | 0.75 | **0.6** | 0.81 | 0.83 |
| 1-linoleoylglycerophosphocholine (18:2n6) | 0.65 | **0.5** | 0.65 | **0.31** | **0.3** | **0.39** | **0.47** | 0.59 | **0.61** |
| 2-linoleoylglycerophosphocholine* | 0.69 | **0.4** | **0.58** | **0.36** | **0.31** | **0.39** | **0.53** | 0.76 | **0.66** |
| 1-linolenoylglycerophosphocholine (18:3n3)* | **0.4** | **0.51** | **0.81** | **0.18** | **0.32** | **0.34** | **0.46** | 0.63 | 0.41 |
| 1-dihomo-linoleoylglycerophosphocholine (20:2n6)* | **0.48** | **0.5** | 0.65 | **0.31** | **0.34** | **0.44** | 0.64 | 0.68 | 0.67 |

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|---|---|---|---|---|---|---|---|---|---|
| 1-eicosatrienoylglycerophosphocholine (20:3)* | 0.57 | 0.35 | 0.78 | 0.2 | 0.16 | 0.32 | 0.35 | 0.47 | 0.41 |
| 1-arachidonoylglycerophosphocholine (20:4n6)* | 1.37 | 0.64 | 0.92 | 0.46 | 0.37 | 0.49 | 0.33 | 0.58 | 0.53 |
| 2-arachidonoylglycerophosphocholine* | 1.21 | 0.75 | 1.04 | 0.67 | 0.75 | 0.61 | 0.55 | 1.01 | 0.59 |
| 1-eicosapentaenoylglycerophosphocholine (20:5n3)* | 0.62 | 0.5 | 1.13 | 0.15 | 0.2 | 0.5 | 0.24 | 0.4 | 0.45 |
| 1-docosapentaenoylglycerophosphocholine (22:5n3)* | 1.02 | 0.84 | 0.93 | 0.54 | 0.45 | 0.77 | 0.53 | 0.54 | 0.83 |
| 1-docosahexaenoylglycerophosphocholine (22:6n3)* | 1.36 | 0.83 | 1.04 | 0.53 | 0.49 | 0.89 | 0.39 | 0.58 | 0.85 |
| 1-palmitoylplasmenylethanolamine* | 0.41 | 0.55 | 0.69 | 0.72 | 2.02 | 1.15 | 1.77 | 3.68 | 1.66 |
| 1-stearoylplasmenylethanolamine* | 0.97 | 0.94 | 0.43 | 1.54 | 3 | 0.49 | 1.58 | 3.2 | 1.16 |
| 1-palmitoylglycerophosphoethanolamine | 0.77 | 0.71 | 1.01 | 0.74 | 0.97 | 0.97 | 0.96 | 1.36 | 0.96 |
| 2-palmitoylglycerophosphoethanolamine* | 0.79 | 0.84 | 1.14 | 0.73 | 1.3 | 1.03 | 0.92 | 1.54 | 0.9 |
| 1-stearoylglycerophosphoethanolamine | 0.69 | 0.78 | 0.91 | 0.72 | 1.26 | 0.72 | 1.04 | 1.62 | 0.79 |
| 1-oleoylglycerophosphoethanolamine | 0.69 | 0.62 | 0.81 | 0.45 | 0.68 | 0.56 | 0.66 | 1.09 | 0.69 |
| 2-oleoylglycerophosphoethanolamine* | 0.72 | 0.57 | 0.87 | 0.46 | 0.7 | 0.64 | 0.63 | 1.24 | 0.73 |
| 1-linoleoylglycerophosphoethanolamine* | 0.51 | 0.52 | 0.6 | 0.39 | 0.46 | 0.41 | 0.76 | 0.88 | 0.68 |
| 2-linoleoylglycerophosphoethanolamine* | 0.48 | 0.59 | 0.63 | 0.4 | 0.61 | 0.52 | 0.83 | 1.04 | 0.82 |
| 1-arachidonoylglycerophosphoethanolamine* | 0.92 | 0.81 | 0.87 | 0.74 | 0.76 | 0.78 | 0.81 | 0.93 | 0.9 |
| 2-arachidonoylglycerophosphoethanolamine* | 0.9 | 0.99 | 0.93 | 0.82 | 1.01 | 0.93 | 0.91 | 1.02 | 1 |
| 2-docosahexaenoylglycerophosphoethanolamine* | 1.1 | 0.72 | 0.59 | 1.26 | 0.73 | 0.59 | 1.14 | 1 | 0.99 |
| 1-docosahexaenoylglycerophosphoethanolamine* | 1.11 | 1.05 | 1.13 | 0.88 | 0.99 | 1.2 | 0.8 | 0.94 | 1.06 |
| 1-palmitoylglycerophosphoinositol* | 0.52 | 0.53 | 0.9 | 0.3 | 0.39 | 0.54 | 0.58 | 0.73 | 0.6 |
| 1-stearoylglycerophosphoinositol | 0.65 | 0.66 | 0.71 | 0.29 | 0.38 | 0.57 | 0.44 | 0.58 | 0.8 |
| 2-stearoylglycerophosphoinositol* | 0.68 | 0.69 | 0.77 | 0.49 | 0.26 | 0.55 | 0.72 | 0.38 | 0.71 |
| 1-arachidonoylglycerophosphoinositol* | 1.03 | 0.72 | 1.12 | 0.47 | 0.44 | 0.69 | 0.45 | 0.61 | 0.61 |
| 1-palmitoylglycerophosphate | 1.07 | 0.6 | 0.67 | 0.81 | 1.22 | 1.02 | 0.76 | 2.02 | 1.51 |
| 1-arachidonoylglyercophosphate | 1.07 | 0.55 | 0.89 | 0.63 | 1 | 0.89 | 0.59 | 1.83 | 1 |
| glycerol | 1.98 | 1.99 | 1.85 | 3.25 | 8.37 | 3.51 | 1.64 | 4.21 | 1.9 |
| glycerol 3-phosphate (G3P) | 0.67 | 0.56 | 0.71 | 0.61 | 1.27 | 0.97 | 0.91 | 2.27 | 1.37 |
| 1-myristoylglycerol (1-monomyristin) | 1.16 | 1.4 | 4.99 | 0.59 | 0.61 | 0.42 | 0.51 | 0.44 | 0.08 |
| 1-palmitoylglycerol (1-monopalmitin) | 1.78 | 1.77 | 2.72 | 1.22 | 1.61 | 0.8 | 0.68 | 0.91 | 0.29 |
| 2-palmitoylglycerol (2-monopalmitin) | 0.91 | 1.06 | 1.34 | 1 | 1.04 | 1.02 | 1.1 | 0.98 | 0.76 |
| 1-stearoylglycerol (1-monostearin) | 0.71 | 0.84 | 1.16 | 0.69 | 0.98 | 0.88 | 0.98 | 1.16 | 0.76 |
| 1-oleoylglycerol (1-monoolein) | 7.26 | 3.84 | 5.8 | 2.05 | 0.94 | 0.76 | 0.28 | 0.25 | 0.13 |
| 1-linoleoylglycerol (1-monolinolein) | 6.48 | 4.75 | 5.77 | 1.87 | 1.15 | 0.73 | 0.29 | 0.24 | 0.13 |
| 1-linolenoylglycerol | 9.97 | 7.16 | 7.06 | 0.93 | 0.67 | 0.38 | 0.09 | 0.09 | 0.05 |
| 1,2-dipalmitoylglycerol | 1.07 | 0.44 | 2.17 | 0.36 | 1.25 | 1.05 | 0.33 | 2.85 | 0.49 |
| palmitoyl sphingomyelin | 0.87 | 0.67 | 0.84 | 0.82 | 0.96 | 1.02 | 0.94 | 1.43 | 1.21 |
| stearoyl sphingomyelin | 1.49 | 0.98 | 1.18 | 1.64 | 1.51 | 2.14 | 1.1 | 1.54 | 1.8 |
| sphingosine 1-phosphate | 0.73 | 0.49 | 0.75 | 0.63 | 0.47 | 0.61 | 0.86 | 0.95 | 0.82 |
| sphingosine | 0.88 | 0.76 | 0.21 | 1.08 | 0.96 | 0.24 | 1.22 | 1.26 | 1.16 |
| lathosterol | 0.77 | 0.82 | 1.25 | 1.09 | 1.33 | 1.87 | 1.42 | 1.63 | 1.49 |
| cholesterol | 0.81 | 0.66 | 0.93 | 0.79 | 0.86 | 1.02 | 0.98 | 1.3 | 1.1 |

| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| 7-beta-hydroxycholesterol | **0.48** | 0.86 | 0.6 | 0.78 | 1.15 | 1.02 | 1.63 | 1.33 | 1.71 |
| 7-alpha-hydroxy-3-oxo-4-cholestenoate (7-Hoca) | **0.65** | **0.67** | 0.97 | **0.63** | 0.82 | 0.94 | 0.96 | 1.23 | 0.97 |
| cholestanol | 0.77 | 1.04 | 1.14 | 0.8 | 1.23 | 0.96 | 1.04 | 1.18 | 0.84 |
| beta-sitosterol | **0.54** | **0.59** | 1 | **0.54** | **0.59** | 1.06 | 1 | 1 | 1.06 |
| campesterol | **0.61** | **0.43** | 0.72 | 0.69 | 0.65 | **0.4** | 1.13 | 1.51 | 0.56 |
| pregnenolone sulfate | 0.75 | 0.75 | **0.64** | 0.79 | 0.84 | **0.61** | 1.05 | 1.12 | 0.94 |
| 21-hydroxypregnenolone disulfate | 1.5 | 1.06 | 0.74 | 1.5 | 0.78 | 0.97 | 1 | 0.74 | 1.32 |
| 5alpha-pregnan-3beta,20alpha-diol disulfate | 1.06 | 2.09 | 0.91 | 0.66 | 2.57 | 0.95 | 0.63 | 1.23 | 1.04 |
| 5alpha-pregnan-3alpha,20beta-diol disulfate 1* | 0.63 | 2.56 | 0.88 | 0.58 | 2.99 | 1.01 | 0.92 | 1.17 | 1.14 |
| pregnen-diol disulfate* | 1.42 | 1.04 | 1.08 | **1.53** | 0.93 | 1.45 | 1.08 | 0.89 | 1.34 |
| pregn steroid monosulfate* | 0.98 | 0.75 | 0.72 | 0.98 | 0.92 | 0.84 | 1 | 1.24 | 1.18 |
| pregnanediol-3-glucuronide | 0.68 | 1.75 | 0.94 | 0.44 | 1.09 | 0.85 | 0.64 | 0.62 | 0.9 |
| cortisol | 1.11 | 1.14 | 0.74 | 1.46 | 7.27 | 0.72 | 1.32 | 6.4 | 0.97 |
| cortisone | 0.97 | 0.74 | 0.67 | 1.2 | 0.74 | 1.14 | 1.23 | 1.01 | **1.71** |
| dehydroisoandrosterone sulfate (DHEA-S) | 1.04 | 0.69 | 0.62 | 0.9 | **0.79** | 0.71 | 0.86 | 1.14 | 1.14 |
| epiandrosterone sulfate | 0.95 | 0.63 | 0.59 | 0.74 | **0.69** | **0.79** | 0.78 | 1.09 | 1.34 |
| androsterone sulfate | 1.4 | 0.79 | 0.69 | 1 | **0.78** | 0.94 | 0.71 | 0.99 | 1.36 |
| 4-androsten-3beta,17beta-diol disulfate (1)* | 1.1 | 0.69 | 0.76 | 0.95 | **0.61** | 1.46 | 0.87 | 0.88 | 1.92 |
| 4-androsten-3beta,17beta-diol disulfate (2)* | 1.39 | 0.85 | 0.83 | 1.16 | 0.76 | 1 | 0.83 | 0.9 | 1.22 |
| 5alpha-androstan-3beta,17beta-diol disulfate | 1.08 | 0.71 | 0.73 | 0.88 | **0.63** | 1.14 | 0.81 | 0.89 | 1.55 |
| andro steroid monosulfate 2* | **1.64** | 1.05 | 0.84 | **1.4** | 0.93 | 0.92 | 0.85 | 0.88 | **1.1** |
| cholate | **0.04** | **0.34** | 0.44 | 0.15 | 0.98 | 0.74 | **3.47** | 2.93 | 1.67 |
| glycocholate | 0.4 | **0.17** | **0.4** | 0.7 | 0.67 | 1.78 | 1.76 | **3.84** | 4.41 |
| taurocholate | 0.82 | **0.17** | 0.31 | 1.08 | 0.36 | 3.64 | 1.31 | 2.05 | **11.78** |
| glycochenodeoxycholate | 0.63 | **0.29** | **0.2** | 0.87 | 0.47 | 1.18 | 1.39 | 1.59 | **6.06** |
| taurochenodeoxycholate | 1.71 | 0.32 | 0.45 | 1.15 | 0.3 | 2.77 | 0.67 | 0.94 | 6.19 |
| glycodeoxycholate | 1.41 | **0.34** | **0.29** | 0.76 | 0.87 | **0.6** | 0.54 | **2.56** | 2.1 |
| taurodeoxycholate | 1.65 | 0.2 | **0.29** | 1.13 | 0.3 | 1.53 | 0.68 | 1.53 | 5.23 |
| glycolithocholate sulfate* | **2.96** | 0.71 | **0.23** | **3.56** | 1.7 | 0.76 | 1.2 | 2.38 | **3.29** |
| taurolithocholate 3-sulfate | **4.28** | 0.33 | 0.73 | **3.56** | 0.56 | 1.2 | 0.83 | 1.72 | 1.64 |
| glycoursodeoxycholate | 1.27 | **0.3** | **0.42** | 0.7 | 0.61 | **0.61** | 0.55 | 2.03 | 1.45 |
| hyocholate | 0.71 | **0.5** | 0.79 | 0.71 | **0.57** | **0.56** | 1.01 | 1.13 | 0.7 |
| glycohyocholate | 1.13 | **0.37** | 0.74 | 1.55 | 0.59 | 1.4 | 1.38 | 1.58 | **1.9** |
| glycocholenate sulfate* | 1.06 | 0.9 | **0.57** | 1.35 | 0.86 | 0.98 | 1.28 | 0.95 | **1.7** |
| taurocholenate sulfate* | **2.69** | 0.85 | 1.42 | **2.06** | 0.68 | **2.05** | 0.77 | 0.8 | 1.44 |
| inosine | 0.86 | 1.51 | **1.72** | **3.04** | **3.52** | **2.3** | **3.53** | 2.34 | 1.34 |
| hypoxanthine | 0.74 | 0.94 | 0.7 | **3.03** | **7.25** | **2.07** | **4.09** | **7.73** | **2.97** |
| xanthine | 0.79 | 0.84 | 0.87 | 1.24 | **1.49** | 1.11 | **1.57** | **1.77** | 1.28 |
| xanthosine | 1.32 | 1.43 | 1.19 | 1.22 | **2.3** | **2.53** | 0.92 | 1.61 | **2.13** |
| 2'-deoxyinosine | 1.78 | 5.3 | 1 | 1.83 | **4.2** | **8.54** | 1.03 | 0.79 | **8.54** |
| urate | 1.12 | 0.92 | 0.94 | 0.91 | 0.76 | **0.72** | 0.81 | 0.82 | **0.77** |

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|---|---|---|---|---|---|---|---|---|---|
| allantoin | **0.43** | **0.38** | **0.31** | **9.42** | **21.79** | **10.08** | **21.79** | **57.52** | **32.06** |
| adenosine 5'-monophosphate (AMP) | 1 | 21.91 | 1 | 26.36 | **32.11** | 80.16 | 26.36 | 1.47 | 80.16 |
| adenosine | 1.21 | 17.92 | 1.12 | 3.14 | 2.05 | 1.76 | 2.6 | 0.11 | 1.57 |
| N1-methyladenosine | 1 | 0.89 | 0.91 | **0.64** | **0.53** | **0.48** | **0.64** | **0.59** | **0.53** |
| N6-carbamoylthreonyladenosine | 0.99 | 1.02 | 1.03 | 1.08 | 1.08 | 1.24 | 1.09 | 1.06 | 1.21 |
| guanosine | 1.11 | 0.94 | 1.32 | 0.68 | 0.41 | 0.58 | 0.61 | 0.43 | 0.44 |
| 7-methylguanine | 0.7 | 0.9 | 0.87 | 1.01 | 0.88 | 0.75 | 1.45 | 0.98 | 0.87 |
| N1-methylguanosine | 1.73 | 2.07 | 0.55 | 1.28 | 1.54 | 1.06 | 0.74 | 0.74 | **1.94** |
| N2,N2-dimethylguanosine | 1.02 | 1.31 | 1.24 | 0.96 | 0.88 | 1.02 | 0.94 | 0.67 | 0.82 |
| uridine | 0.87 | **0.81** | 1.02 | 0.94 | 1.04 | 0.83 | 1.08 | **1.29** | 0.81 |
| pseudouridine | 1.04 | **0.79** | 1.09 | 0.96 | 0.78 | 0.81 | 0.92 | 0.99 | **0.75** |
| 5-methyluridine (ribothymidine) | 0.89 | 0.79 | 1.03 | 0.82 | 0.75 | 1.02 | 0.92 | 0.95 | 0.99 |
| beta-alanine | 0.56 | **0.37** | 0.68 | 0.61 | 0.98 | **0.45** | 1.1 | **2.62** | 0.66 |
| N-acetyl-beta-alanine | 0.81 | 0.69 | 0.76 | 1.37 | 1.15 | 1.42 | **1.68** | **1.67** | **1.86** |
| methylphosphate | 0.84 | **0.73** | **0.72** | 0.84 | 0.93 | 0.98 | 0.99 | 1.26 | **1.37** |
| nicotinamide | 0.67 | 1.72 | 1.32 | **7.51** | **7.69** | **6.9** | **11.29** | **4.47** | **5.24** |
| N1-Methyl-2-pyridone-5-carboxamide | 2.13 | 0.84 | **1.98** | 1.05 | **0.52** | **0.46** | **0.49** | 0.61 | **0.23** |
| riboflavin (Vitamin B2) | 1.45 | 0.7 | 0.9 | 1.06 | **0.55** | **0.57** | 0.73 | 0.78 | 0.63 |
| pantothenate | **2.53** | **1.67** | 1.26 | **1.52** | 1.11 | 1.32 | **0.6** | 0.67 | 1.04 |
| gulono-1,4-lactone | 1.16 | 0.77 | 0.85 | **1.82** | **2.66** | 1.56 | 1.57 | **3.47** | **1.84** |
| ascorbate (Vitamin C) | 1.72 | 0.42 | 1.1 | **0.08** | **0.02** | **0.07** | **0.05** | **0.05** | **0.06** |
| threonate | **1.4** | 0.66 | 1.47 | 0.81 | 0.69 | 0.85 | **0.58** | 1.05 | **0.58** |
| arabonate | 1 | 0.69 | 1.2 | 0.93 | 0.67 | 1.08 | 0.94 | 0.97 | 0.9 |
| oxalate (ethanedioate) | **1.62** | 0.76 | **1.83** | 0.99 | 0.56 | 1.08 | **0.61** | 0.73 | 0.59 |
| alpha-tocopherol | 0.84 | **0.64** | 1.08 | **0.52** | **0.6** | **0.58** | **0.62** | 0.93 | **0.54** |
| beta-tocopherol | **0.46** | 0.71 | 1.02 | **0.42** | 0.8 | **0.43** | 0.91 | 1.14 | **0.43** |
| gamma-tocopherol | **0.23** | **0.6** | 0.69 | **0.39** | 0.64 | **0.61** | **1.71** | 1.07 | 0.88 |
| gamma-CEHC | **0.63** | **0.45** | **0.38** | **0.38** | **0.24** | **0.17** | 0.6 | **0.54** | **0.45** |
| gamma-CEHC glucuronide* | **0.54** | **0.45** | **0.36** | **0.39** | **0.28** | **0.28** | 0.71 | 0.62 | 0.8 |
| alpha-CEHC glucuronide* | 0.88 | 1.18 | 1.3 | 0.58 | 0.63 | 0.64 | 0.66 | **0.53** | **0.49** |
| heme | 2.15 | 5.17 | 3.85 | **108.58** | **94.24** | **104.2** | **50.62** | **18.24** | **27.04** |
| bilirubin (Z,Z) | 0.73 | 0.73 | 1.01 | **0.29** | **0.1** | **0.3** | **0.4** | **0.14** | **0.3** |
| bilirubin (E,E)* | 1.31 | 0.62 | 1.8 | **0.37** | **0.18** | **0.44** | **0.28** | **0.29** | **0.24** |
| bilirubin (E,Z or Z,E)* | 1.06 | 1.29 | 1.66 | 1.03 | 2.36 | 3.56 | 0.97 | 1.83 | 2.15 |
| biliverdin | **2.3** | 1.07 | **2.32** | **3.03** | 2.43 | **5.87** | 1.32 | 2.26 | **2.53** |
| I-urobilinogen | 1.61 | 0.62 | 0.7 | 1.71 | 0.58 | 1.4 | 1.06 | 0.93 | 2 |
| L-urobilin | 0.66 | 2.09 | 0.44 | 0.63 | 0.54 | 1.59 | 0.94 | **0.26** | **3.59** |
| pyridoxate | 2.04 | 0.88 | 0.88 | 1.6 | 0.49 | 0.57 | 0.79 | 0.55 | 0.64 |
| hippurate | 0.53 | **0.4** | **0.3** | 0.83 | 0.69 | 1.3 | 1.58 | 1.73 | **4.29** |
| 2-hydroxyhippurate (salicylurate) | 0.17 | 1.5 | **0.1** | 0.14 | 0.82 | **0.03** | 0.81 | 0.55 | 0.32 |
| 3-hydroxyhippurate | **0.18** | **0.3** | **0.27** | **0.28** | **0.28** | 0.64 | 1.56 | 0.92 | **2.32** |

| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| 4-hydroxyhippurate | 1.15 | 0.66 | **0.41** | **0.54** | 0.82 | 0.64 | 0.47 | 1.24 | 1.56 |
| benzoate | 0.82 | **0.78** | 0.91 | **0.67** | **0.67** | **0.66** | 0.81 | 0.86 | **0.72** |
| catechol sulfate | **0.59** | 0.93 | **0.69** | **0.59** | **0.34** | **0.49** | 1.01 | **0.37** | 0.72 |
| O-methylcatechol sulfate | 0.48 | 0.71 | 0.62 | 0.52 | **0.2** | **0.87** | 1.09 | 0.29 | 1.4 |
| 3-methyl catechol sulfate (1) | **0.15** | **0.21** | **0.02** | **0.48** | **0.12** | **0.14** | 3.09 | 0.58 | **5.77** |
| 3-methyl catechol sulfate (2) | 0.84 | 1 | **0.32** | 0.93 | 1 | **0.33** | 1.11 | 1 | 1.02 |
| 4-methylcatechol sulfate | 0.9 | 0.57 | 0.75 | 0.66 | 0.95 | 0.97 | 0.73 | 1.65 | 1.29 |
| 3-ethylphenylsulfate* | 1 | 0.62 | **0.45** | 1 | 0.62 | **0.45** | 1 | 1 | 1 |
| 4-ethylphenylsulfate | 1.54 | **0.38** | 1.39 | 0.48 | **0.24** | 0.38 | 0.32 | 0.64 | 0.27 |
| 4-vinylphenol sulfate | **0.2** | **0.11** | **0.13** | **0.16** | 1.03 | **0.5** | 0.8 | **9.22** | 3.8 |
| caffeine | 0.43 | 0.29 | 0.12 | 0.44 | **0.1** | 0.13 | 1.02 | 0.36 | 1.1 |
| paraxanthine | 0.88 | 0.47 | 0.27 | 0.43 | **0.17** | 0.24 | 0.49 | **0.36** | 0.91 |
| theobromine | **1.28** | **0.23** | 1.82 | 1.13 | **0.25** | 0.72 | 0.88 | 1.12 | 0.39 |
| theophylline | 0.96 | **0.32** | 0.4 | 0.7 | **0.19** | 0.36 | 0.72 | 0.6 | 0.9 |
| 7-methylurate | 1.59 | 0.41 | 0.81 | **0.61** | **0.24** | 0.44 | 0.38 | 0.59 | 0.55 |
| 1,3-dimethylurate | 1.24 | 0.46 | 0.58 | 0.6 | **0.32** | **0.47** | 0.49 | 0.69 | 0.81 |
| 1,7-dimethylurate | 1.41 | **0.24** | 0.69 | **0.36** | **0.08** | 0.95 | 0.25 | 0.32 | 1.38 |
| 1,3,7-trimethylurate | 0.37 | 0.36 | 0.14 | 0.4 | **0.19** | 0.19 | 1.07 | 0.53 | 1.37 |
| 1-methylxanthine | 0.93 | 0.71 | 0.55 | 0.62 | 0.67 | 0.52 | 0.66 | 0.94 | 0.96 |
| 3-methylxanthine | 1.81 | 0.83 | 1.28 | 0.88 | **0.45** | 0.64 | 0.49 | 0.54 | 0.5 |
| 7-methylxanthine | 1.85 | 0.67 | 1.24 | 0.77 | 0.53 | 0.71 | 0.42 | 0.79 | 0.57 |
| 5-acetylamino-6-amino-3-methyluracil | 1.6 | 0.63 | 0.82 | 0.78 | **0.4** | 0.66 | 0.48 | 0.63 | 0.81 |
| cotinine | 1 | 1 | **0.83** | 1 | 1 | **0.83** | 1 | 1 | 1 |
| 2-piperidinone | **0.24** | 0.28 | 1.12 | 1.32 | 0.59 | 1.27 | 5.59 | 2.11 | 1.14 |
| 1,6-anhydroglucose | 0.9 | 0.92 | 1.58 | 1.12 | 0.54 | 0.76 | 1.25 | 0.59 | 0.48 |
| gluconate | 0.81 | **0.54** | 1.17 | 0.83 | 1.25 | 1.5 | 1.02 | **2.31** | 1.28 |
| ergothioneine | 0.73 | 0.84 | 1.01 | 1.17 | 1.55 | **3.41** | 1.61 | **1.84** | **3.39** |
| erythritol | 0.92 | 0.69 | 0.85 | 0.83 | 1.21 | 0.77 | 0.9 | 1.77 | 0.91 |
| homostachydrine* | 0.71 | 0.8 | 0.95 | **0.67** | **0.3** | **0.49** | 0.95 | **0.38** | **0.51** |
| N-(2-furoyl)glycine | 0.19 | 1 | **0.64** | 1 | 1 | **0.08** | 5.25 | 1 | 0.13 |
| piperine | **0.15** | **0.09** | **0.36** | **0.29** | **0.2** | **0.44** | **1.88** | 2.07 | 1.24 |
| 2-furoic acid | 0.58 | 0.65 | **0.21** | 0.79 | 0.49 | 0.27 | 1.36 | 0.76 | 1.28 |
| quinate | **0.25** | 0.22 | **0.04** | 0.5 | 0.66 | 0.28 | 2.04 | 3.07 | **6.86** |
| saccharin | 2.3 | 1.65 | 0.09 | **8.01** | **6.92** | **1.17** | **3.48** | **4.19** | **12.65** |
| stachydrine | 0.62 | 0.36 | 0.57 | 0.21 | **0.05** | 1.43 | 0.34 | 0.14 | 2.53 |
| thymol sulfate | **0.6** | **0.09** | 0.68 | **0.67** | 0.59 | **0.25** | 1.11 | **6.67** | **0.36** |
| tribuloside | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 |
| 2-hydroxyacetaminophen sulfate* | 0.49 | 1 | 0.4 | 0.67 | 8.1 | 0.33 | 1.36 | 8.1 | 0.84 |
| 2-methoxyacetaminophen sulfate* | 0.48 | 1 | 0.42 | 0.62 | 3.88 | 0.95 | 1.31 | 3.88 | 2.27 |
| 3-(cystein-S-yl)acetaminophen* | 0.75 | 1 | 0.69 | 0.75 | 1.38 | 0.99 | 1 | 1.38 | 1.43 |
| 3-(N-acetyl-L-cystein-S-yl) acetaminophen* | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 |

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|---|---|---|---|---|---|---|---|---|---|
| 4-acetaminophen sulfate | 0.9 | 1.3 | 0.31 | 0.79 | 21.59 | 0.14 | 0.88 | 16.55 | 0.46 |
| 4-acetamidophenol | 0.55 | 1 | 0.43 | 0.66 | 4.33 | 0.79 | 1.2 | 4.33 | 1.81 |
| 4-acetamidophenylglucuronide | 0.21 | 1.21 | 0.37 | 0.6 | 7.41 | 0.6 | 2.83 | 6.14 | 1.61 |
| ibuprofen acyl glucuronide | 1 | **0.9** | 1 | 1 | **0.9** | 1 | 1 | 1 | 1 |
| ibuprofen | **0.83** | 0.91 | 1 | **0.83** | 0.91 | 1 | 1 | 1 | 1 |
| 2-hydroxyibuprofen | 1 | **0.8** | 1 | 1 | **0.8** | 1 | 1 | 1 | 1 |
| carboxyibuprofen | **0.9** | 0.95 | 1 | **0.9** | 0.95 | 1 | 1 | 1 | 1 |
| atenolol | 1 | 1 | 0.75 | 1 | 1.44 | 0.72 | 1 | 1.44 | 0.96 |
| desmethylnaproxen sulfate* | 0.97 | **0.75** | 1 | 0.97 | 0.88 | 1 | 1 | 1.17 | 1 |
| O-desmethylvenlafaxine | **0.94** | 1 | 1 | **0.94** | 1 | 1 | 1 | 1 | 1 |
| escitalopram | **0.85** | 1 | 1 | **0.85** | 1 | 1 | 1 | 1 | 1 |
| fluoxetine | **1.18** | 1 | 1 | 0.98 | 1 | 1 | **0.83** | 1 | 1 |
| gabapentin | 1 | 1 | **0.48** | 1 | 1 | 0.54 | 1 | 1 | 1.12 |
| hydrochlorothiazide | 1.05 | 1 | 0.94 | 0.96 | 1 | **0.8** | 0.91 | 1 | 0.85 |
| hydroquinone sulfate | 1 | 1 | 0.91 | 1 | 1 | 1.06 | 1 | 1 | **1.17** |
| hydroxypioglitazone (M-IV) | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 |
| ketopioglitazone | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 |
| lidocaine | **8.5** | **18.75** | **12.61** | 1 | 1 | 1 | **0.12** | **0.05** | **0.08** |
| metformin | 1 | **0.21** | **0.23** | 1 | **0.29** | **0.33** | 1 | 1.37 | 1.43 |
| metoprolol | 0.97 | 1 | 1 | **0.88** | 1 | 1 | **0.91** | 1 | 1 |
| metoprolol acid metabolite* | **1.11** | 1 | 1 | **1.08** | 1 | 1 | 0.98 | 1 | 1 |
| naproxen | 0.49 | 0.33 | 0.86 | **0.03** | 1.25 | 0.86 | 0.07 | 3.82 | 1 |
| norfluoxetine | **1.09** | 1 | 1 | 1.02 | 1 | 1 | 0.94 | 1 | 1 |
| omeprazole | 1 | **1.13** | 1 | 1 | 1 | 1 | 1 | **0.89** | 1 |
| pantoprazole | 0.1 | 0.52 | 11.84 | **6.24** | 2.6 | **50.56** | **64.39** | 5.02 | 4.27 |
| pioglitazone* | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 |
| salicylate | 0.39 | 1.37 | 0.1 | 0.24 | 1.68 | 0.13 | 0.63 | 1.23 | 1.33 |
| 1,2-propanediol | 1.7 | 3.17 | 0.81 | **6.4** | **4.06** | 2.52 | **3.77** | 1.28 | **3.09** |
| 2-aminophenol sulfate | **0.16** | **0.18** | 1.06 | **0.3** | 0.34 | **0.25** | 1.83 | 1.87 | 0.23 |
| bisphenol A monosulfate | 1.35 | 1.62 | 0.98 | 1.67 | **2.94** | 2.67 | 1.24 | 1.81 | 2.71 |
| 2-ethylhexanoate | 0.76 | **0.53** | 0.98 | **0.41** | **0.32** | **0.48** | **0.54** | 0.6 | **0.49** |
| 2-hydroxyisobutyrate | 1.41 | 0.54 | 7.86 | 0.88 | 9.48 | 0.69 | 0.62 | 17.58 | **0.09** |
| dexpanthenol | 1 | 1 | 1 | 1 | **4.61** | 1 | 1 | **4.61** | 1 |
| glycerol 2-phosphate | 0.92 | 0.78 | **0.68** | 0.8 | **1.58** | 0.99 | 0.88 | **2.03** | **1.45** |
| glycolate (hydroxyacetate) | 1.24 | 0.74 | 0.79 | 1.59 | 1.26 | 1 | 1.28 | **1.71** | 1.27 |

* Green and red shaded cells indicate $p \leq 0.05$ (green indicates that the mean values are significantly higher for that comparison; red - values significantly lower). Light green and light red shaded cells indicate $0.05 < p < 0.10$ (light green indicates that the mean values trend higher for that comparison; light red - values trend lower).

**Table A2. A Global Metabolomic Study: Analytical Technique of Detection (Platform) and The Percentage of Detection in a Given Group or Time Point (% filled values) for all 476 compounds detected.**

| Biochemical Name | Platform | % Filled Values | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | | GB T2D BL | GB T2D Pre-Op | GB T2D Post-Op | SG T2D BL | SG T2D Pre-Op | SG T2D Post-Op | SG Non-T2D BL | SG Non-T2D Pre-Op | SG Non-T2D Post-Op |
| glycine | GC/MS | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 |
| N-acetylglycine | GC/MS | 100 | 100 | 100 | 80 | 100 | 100 | 100 | 100 | 100 |
| dimethylglycine | GC/MS | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 |
| betaine | LC/MS pos | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 |
| serine | GC/MS | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 |
| N-acetylserine | GC/MS | 100 | 100 | 100 | 100 | 80 | 100 | 100 | 100 | 100 |
| beta-hydroxypyruvate | GC/MS | 60 | 80 | 40 | 80 | 60 | 40 | 60 | 80 | 60 |
| threonine | LC/MS pos | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 |
| N-acetylthreonine | LC/MS neg | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 |
| homoserine | GC/MS | 60 | 40 | 20 | 60 | 40 | 20 | 20 | 60 | 0 |
| alanine | GC/MS | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 |
| N-acetylalanine | LC/MS neg | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 |
| aspartate | GC/MS | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 |
| asparagine | GC/MS | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 |
| glutamate | LC/MS pos | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 |
| glutamine | LC/MS pos | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 |
| pyroglutamine* | LC/MS pos | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 |
| histidine | LC/MS neg | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 |
| 1-methylhistidine | GC/MS | 60 | 40 | 60 | 20 | 0 | 60 | 40 | 40 | 60 |
| 3-methylhistidine | LC/MS neg | 100 | 100 | 100 | 100 | 60 | 100 | 100 | 100 | 100 |
| trans-urocanate | LC/MS pos | 100 | 100 | 100 | 80 | 100 | 100 | 100 | 100 | 100 |
| cis-urocanate | LC/MS neg | 0 | 20 | 100 | 0 | 40 | 100 | 40 | 60 | 100 |
| imidazole propionate | LC/MS pos | 40 | 20 | 100 | 20 | 20 | 100 | 20 | 0 | 80 |
| lysine | LC/MS pos | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 |
| glutarylcarnitine (C5) | LC/MS pos | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 |
| pipecolate | LC/MS pos | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 |
| N-acetyl-cadaverine | LC/MS pos | 0 | 0 | 0 | 0 | 0 | 20 | 0 | 0 | 0 |
| phenylalanine | LC/MS pos | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 |
| N-acetylphenylalanine | LC/MS neg | 100 | 80 | 80 | 100 | 80 | 100 | 100 | 40 | 80 |
| phenyllactate (PLA) | LC/MS neg | 100 | 100 | 100 | 100 | 80 | 60 | 100 | 80 | 100 |

| | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| phenylacetate | GC/MS | 40 | 60 | 80 | 60 | 20 | 80 | 60 | 60 | 20 |
| 4-hydroxyphenylacetate | GC/MS | 80 | 60 | 40 | 60 | 40 | 60 | 60 | 40 | 60 |
| phenylacetylglutamine | LC/MS pos | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 |
| tyrosine | LC/MS pos | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 |
| N-acetyltyrosine | LC/MS neg | 20 | 0 | 60 | 60 | 0 | 20 | 60 | 40 | 80 |
| tyramine | LC/MS pos | 0 | 0 | 0 | 0 | 0 | 20 | 0 | 0 | 0 |
| 3-(4-hydroxyphenyl)lactate | LC/MS neg | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 |
| phenol sulfate | LC/MS neg | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 |
| p-cresol sulfate | LC/MS neg | 100 | 100 | 100 | 100 | 80 | 100 | 100 | 100 | 100 |
| o-cresol sulfate | LC/MS neg | 80 | 80 | 60 | 0 | 20 | 20 | 20 | 80 | 20 |
| 3-methoxytyrosine | LC/MS pos | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 |
| 3-(3-hydroxyphenyl)propionate | LC/MS neg | 60 | 20 | 0 | 20 | 0 | 20 | 40 | 0 | 40 |
| tryptophan | LC/MS pos | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 |
| indolelactate | GC/MS | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 |
| indoleacetate | LC/MS pos | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 |
| indolepropionate | LC/MS neg | 100 | 60 | 80 | 100 | 60 | 80 | 100 | 100 | 100 |
| 3-indoxyl sulfate | LC/MS neg | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 |
| kynurenine | LC/MS pos | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 |
| kynurenate | LC/MS neg | 100 | 100 | 100 | 100 | 80 | 100 | 100 | 100 | 100 |
| serotonin (5HT) | LC/MS pos | 100 | 100 | 80 | 100 | 100 | 80 | 100 | 80 | 80 |
| tryptophan betaine | LC/MS pos | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 |
| C-glycosyltryptophan | LC/MS pos | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 |
| leucine | LC/MS pos | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 |
| 4-methyl-2-oxopentanoate | LC/MS neg | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 |
| isovalerate | LC/MS neg | 80 | 100 | 80 | 100 | 100 | 100 | 80 | 80 | 100 |
| isovalerylcarnitine | LC/MS pos | 100 | 100 | 100 | 100 | 80 | 100 | 100 | 100 | 100 |
| beta-hydroxyisovalerate | LC/MS neg | 100 | 100 | 60 | 100 | 100 | 100 | 100 | 100 | 100 |
| beta-hydroxyisovaleroylcarnitine | LC/MS pos | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 |
| 3-methylglutarylcarnitine (C6) | LC/MS pos | 100 | 100 | 80 | 100 | 100 | 80 | 100 | 100 | 100 |
| alpha-hydroxyisovalerate | LC/MS neg | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 |
| isoleucine | LC/MS pos | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 |
| 3-methyl-2-oxovalerate | LC/MS neg | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 |
| 2-methylbutyrylcarnitine (C5) | LC/MS pos | 100 | 100 | 100 | 100 | 80 | 100 | 100 | 100 | 100 |
| tiglyl carnitine | LC/MS pos | 100 | 80 | 80 | 100 | 60 | 60 | 100 | 100 | 100 |
| 2-hydroxy-3-methylvalerate | LC/MS | 60 | 60 | 40 | 80 | 60 | 60 | 80 | 60 | 60 |

| | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | neg | | | | | | | | | |
| 3-hydroxy-2-ethylpropionate | GC/MS | 80 | 100 | 100 | 80 | 100 | 80 | 100 | 100 | 100 |
| valine | LC/MS pos | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 |
| 3-methyl-2-oxobutyrate | LC/MS neg | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 |
| isobutyrylcarnitine | LC/MS pos | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 |
| 3-hydroxyisobutyrate | GC/MS | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 |
| alpha-hydroxyisocaproate | GC/MS | 20 | 20 | 40 | 20 | 60 | 40 | 60 | 60 | 60 |
| methionine | LC/MS pos | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 |
| N-acetylmethionine | LC/MS neg | 100 | 100 | 100 | 100 | 80 | 100 | 100 | 100 | 100 |
| N-formylmethionine | LC/MS neg | 100 | 100 | 100 | 100 | 100 | 80 | 100 | 100 | 80 |
| homocysteine | GC/MS | 20 | 0 | 60 | 0 | 0 | 40 | 0 | 0 | 20 |
| alpha-ketobutyrate | GC/MS | 40 | 100 | 60 | 100 | 100 | 40 | 80 | 100 | 60 |
| 2-aminobutyrate | LC/MS pos | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 |
| 2-hydroxybutyrate (AHB) | GC/MS | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 |
| cysteine | GC/MS | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 |
| cystine | GC/MS | 100 | 100 | 100 | 100 | 40 | 100 | 100 | 60 | 100 |
| S-methylcysteine | LC/MS pos | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 |
| 4-amino-2-hydroxybutyrate | GC/MS | 100 | 100 | 100 | 100 | 80 | 100 | 100 | 100 | 100 |
| arginine | LC/MS pos | 100 | 100 | 80 | 100 | 100 | 100 | 100 | 100 | 100 |
| urea | GC/MS | 100 | 100 | 100 | 100 | 80 | 100 | 100 | 100 | 100 |
| ornithine | GC/MS | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 |
| proline | LC/MS pos | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 |
| citrulline | LC/MS pos | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 |
| homocitrulline | LC/MS pos | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 |
| dimethylarginine (SDMA + ADMA) | LC/MS pos | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 |
| N-delta-acetylornithine* | LC/MS pos | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 |
| trans-4-hydroxyproline | GC/MS | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 |
| pro-hydroxy-pro | LC/MS pos | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 |
| creatine | LC/MS pos | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 |
| creatinine | LC/MS pos | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 |
| acisoga | LC/MS pos | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 |
| N-acetylputrescine | LC/MS pos | 80 | 80 | 80 | 80 | 80 | 60 | 80 | 60 | 80 |
| 4-acetamidobutanoate | LC/MS pos | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 |
| 4-guanidinobutanoate | LC/MS pos | 80 | 40 | 100 | 100 | 40 | 80 | 60 | 20 | 60 |
| glutathione, oxidized (GSSG) | LC/MS pos | 100 | 60 | 80 | 60 | 60 | 80 | 80 | 60 | 60 |
| cysteine-glutathione disulfide | LC/MS pos | 80 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 |

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|---|---|---|---|---|---|---|---|---|---|---|
| cys-gly, oxidized | LC/MS neg | 60 | 80 | 100 | 100 | 80 | 100 | 100 | 80 | 100 |
| 5-oxoproline | LC/MS neg | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 |
| ophthalmate | LC/MS pos | 0 | 40 | 100 | 20 | 60 | 60 | 40 | 20 | 60 |
| gamma-glutamylalanine | LC/MS pos | 100 | 100 | 100 | 100 | 100 | 80 | 100 | 100 | 100 |
| gamma-glutamylglutamate | LC/MS pos | 100 | 80 | 100 | 100 | 80 | 100 | 100 | 100 | 100 |
| gamma-glutamylglutamine | LC/MS pos | 100 | 100 | 80 | 100 | 100 | 100 | 100 | 100 | 100 |
| gamma-glutamylisoleucine* | LC/MS pos | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 80 | 100 |
| gamma-glutamylleucine | LC/MS pos | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 |
| gamma-glutamylmethionine | LC/MS pos | 100 | 100 | 60 | 100 | 100 | 60 | 100 | 100 | 100 |
| gamma-glutamylphenylalanine | LC/MS pos | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 |
| gamma-glutamylthreonine* | LC/MS pos | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 |
| gamma-glutamyltyrosine | LC/MS pos | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 |
| gamma-glutamylvaline | LC/MS pos | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 |
| N-acetylcarnosine | LC/MS pos | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 |
| alpha-glutamylglutamate | LC/MS pos | 40 | 0 | 80 | 0 | 20 | 100 | 20 | 0 | 40 |
| alpha-glutamyltyrosine | LC/MS pos | 40 | 60 | 40 | 100 | 80 | 40 | 100 | 100 | 80 |
| aspartylleucine | LC/MS pos | 80 | 80 | 80 | 80 | 40 | 80 | 100 | 80 | 100 |
| aspartylphenylalanine | LC/MS pos | 100 | 100 | 100 | 100 | 80 | 100 | 100 | 100 | 100 |
| cyclo(glu-glu) | LC/MS pos | 60 | 20 | 100 | 40 | 20 | 100 | 60 | 0 | 100 |
| cyclo(leu-pro) | LC/MS pos | 80 | 40 | 40 | 60 | 40 | 40 | 40 | 40 | 60 |
| glycylglycine | GC/MS | 100 | 100 | 100 | 60 | 60 | 80 | 100 | 80 | 100 |
| glycylphenylalanine | LC/MS neg | 100 | 80 | 60 | 20 | 40 | 80 | 100 | 100 | 80 |
| glycylvaline | LC/MS pos | 100 | 80 | 100 | 100 | 100 | 100 | 100 | 100 | 100 |
| histidyltryptophan | LC/MS pos | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 |
| isoleucylvaline | LC/MS pos | 60 | 80 | 20 | 100 | 100 | 40 | 80 | 80 | 20 |
| leucylalanine | LC/MS pos | 100 | 100 | 80 | 100 | 80 | 100 | 100 | 100 | 100 |
| phenylalanylglutamate | LC/MS pos | 80 | 60 | 100 | 60 | 40 | 100 | 100 | 60 | 100 |
| phenylalanylleucine | LC/MS neg | 100 | 80 | 80 | 100 | 100 | 100 | 100 | 100 | 100 |
| phenylalanylphenylalanine | LC/MS pos | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 |
| phenylalanylserine | LC/MS pos | 60 | 80 | 80 | 80 | 80 | 60 | 100 | 100 | 100 |
| phenylalanyltryptophan | LC/MS pos | 100 | 80 | 80 | 100 | 100 | 60 | 100 | 100 | 100 |
| prolylglycine | LC/MS pos | 80 | 100 | 100 | 80 | 40 | 100 | 80 | 20 | 100 |
| pyroglutamylglycine | LC/MS neg | 80 | 60 | 100 | 100 | 60 | 100 | 100 | 100 | 100 |
| pyroglutamylvaline | LC/MS neg | 20 | 20 | 100 | 60 | 0 | 100 | 20 | 20 | 100 |

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|---|---|---|---|---|---|---|---|---|---|---|
| seryltyrosine | LC/MS pos | 80 | 100 | 80 | 100 | 80 | 60 | 100 | 100 | 100 |
| threonylphenylalanine | LC/MS pos | 100 | 80 | 60 | 80 | 80 | 20 | 100 | 100 | 60 |
| tryptophylglutamate | LC/MS pos | 80 | 60 | 100 | 20 | 40 | 100 | 60 | 100 | 100 |
| tyrosylglutamate | LC/MS pos | 40 | 60 | 60 | 0 | 20 | 100 | 60 | 60 | 100 |
| valylarginine | LC/MS neg | 80 | 80 | 60 | 100 | 80 | 40 | 100 | 100 | 80 |
| bradykinin, des-arg(9) | LC/MS neg | 0 | 40 | 0 | 20 | 60 | 20 | 0 | 60 | 0 |
| HWESASXX* | LC/MS pos | 100 | 100 | 80 | 100 | 100 | 100 | 100 | 100 | 80 |
| ADSGEGDFXAEGGGVR* | LC/MS pos | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 |
| DSGEGDFXAEGGGVR* | LC/MS pos | 100 | 100 | 100 | 100 | 100 | 100 | 80 | 100 | 80 |
| ADpSGEGDFXAEGGGVR* | LC/MS pos | 40 | 60 | 100 | 100 | 100 | 80 | 80 | 100 | 100 |
| 1,5-anhydroglucitol (1,5-AG) | GC/MS | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 |
| glucose | GC/MS | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 |
| 2,3-diphosphoglycerate | LC/MS neg | 0 | 0 | 20 | 0 | 0 | 0 | 0 | 0 | 0 |
| 3-phosphoglycerate | GC/MS | 40 | 20 | 80 | 0 | 20 | 80 | 20 | 20 | 60 |
| pyruvate | GC/MS | 100 | 100 | 80 | 100 | 100 | 80 | 100 | 100 | 100 |
| lactate | GC/MS | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 |
| glycerate | GC/MS | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 |
| ribulose/xylulose 5-phosphate | GC/MS | 0 | 20 | 80 | 0 | 20 | 60 | 20 | 20 | 60 |
| ribulose | GC/MS | 80 | 80 | 80 | 40 | 60 | 80 | 20 | 60 | 100 |
| ribose | GC/MS | 100 | 100 | 100 | 100 | 60 | 80 | 100 | 100 | 100 |
| ribitol | GC/MS | 100 | 100 | 80 | 100 | 80 | 100 | 100 | 100 | 100 |
| xylulose | GC/MS | 20 | 60 | 80 | 20 | 80 | 80 | 60 | 60 | 100 |
| xylonate | GC/MS | 100 | 80 | 100 | 80 | 20 | 80 | 80 | 40 | 100 |
| xylose | GC/MS | 100 | 100 | 100 | 80 | 60 | 100 | 80 | 80 | 80 |
| xylitol | GC/MS | 80 | 100 | 80 | 60 | 60 | 60 | 60 | 80 | 60 |
| arabinose | GC/MS | 60 | 100 | 60 | 100 | 100 | 40 | 80 | 80 | 60 |
| threitol | GC/MS | 100 | 100 | 80 | 100 | 100 | 100 | 100 | 100 | 100 |
| arabitol | GC/MS | 80 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 |
| fucose | GC/MS | 100 | 100 | 100 | 100 | 80 | 80 | 100 | 100 | 60 |
| maltotriose | GC/MS | 40 | 60 | 100 | 80 | 40 | 80 | 80 | 40 | 100 |
| sucrose | LC/MS neg | 80 | 40 | 100 | 80 | 20 | 100 | 80 | 20 | 100 |
| fructose | GC/MS | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 |
| sorbitol | GC/MS | 80 | 80 | 100 | 100 | 80 | 100 | 60 | 60 | 100 |
| mannose | GC/MS | 100 | 100 | 100 | 100 | 100 | 80 | 100 | 100 | 100 |
| mannitol | GC/MS | 100 | 100 | 100 | 100 | 80 | 100 | 80 | 80 | 100 |
| glucuronate | GC/MS | 100 | 100 | 80 | 100 | 80 | 60 | 100 | 80 | 80 |
| N-acetylneuraminate | GC/MS | 100 | 100 | 100 | 100 | 80 | 100 | 100 | 100 | 80 |
| erythronate* | GC/MS | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 |
| citrate | GC/MS | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 |

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|---|---|---|---|---|---|---|---|---|---|---|
| alpha-ketoglutarate | GC/MS | 80 | 80 | 80 | 80 | 80 | 80 | 100 | 100 | 80 |
| succinylcarnitine | LC/MS pos | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 |
| fumarate | GC/MS | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 |
| malate | GC/MS | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 |
| acetylphosphate | GC/MS | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 |
| pyrophosphate (PPi) | GC/MS | 100 | 100 | 100 | 100 | 80 | 100 | 80 | 100 | 100 |
| phosphate | GC/MS | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 |
| caproate (6:0) | LC/MS neg | 100 | 100 | 100 | 100 | 80 | 100 | 100 | 100 | 100 |
| heptanoate (7:0) | LC/MS neg | 80 | 80 | 80 | 80 | 80 | 100 | 80 | 60 | 80 |
| caprylate (8:0) | LC/MS neg | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 |
| pelargonate (9:0) | GC/MS | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 |
| caprate (10:0) | LC/MS neg | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 |
| 10-undecenoate (11:1n1) | LC/MS neg | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 |
| laurate (12:0) | LC/MS neg | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 |
| 5-dodecenoate (12:1n7) | LC/MS neg | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 |
| myristate (14:0) | LC/MS neg | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 |
| myristoleate (14:1n5) | LC/MS neg | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 |
| pentadecanoate (15:0) | GC/MS | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 |
| palmitate (16:0) | LC/MS neg | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 |
| palmitoleate (16:1n7) | LC/MS neg | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 |
| margarate (17:0) | LC/MS neg | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 |
| 10-heptadecenoate (17:1n7) | LC/MS neg | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 |
| stearate (18:0) | LC/MS neg | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 |
| oleate (18:1n9) | GC/MS | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 |
| cis-vaccenate (18:1n7) | GC/MS | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 |
| nonadecanoate (19:0) | LC/MS neg | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 |
| 10-nonadecenoate (19:1n9) | LC/MS neg | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 |
| eicosenoate (20:1n9 or 11) | LC/MS neg | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 |
| stearidonate (18:4n3) | LC/MS neg | 100 | 100 | 80 | 100 | 100 | 100 | 100 | 100 | 80 |
| eicosapentaenoate (EPA; 20:5n3) | LC/MS neg | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 |
| docosapentaenoate (n3 DPA; 22:5n3) | LC/MS neg | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 |
| docosahexaenoate (DHA; 22:6n3) | LC/MS neg | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 |
| linoleate (18:2n6) | LC/MS neg | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 |
| linolenate [alpha or gamma; (18:3n3 or 6)] | LC/MS neg | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 |
| dihomo-linolenate (20:3n3 or n6) | LC/MS neg | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 |
| arachidonate (20:4n6) | LC/MS neg | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 |

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|---|---|---|---|---|---|---|---|---|---|---|
| adrenate (22:4n6) | LC/MS neg | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 |
| docosapentaenoate (n6 DPA; 22:5n6) | LC/MS neg | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 |
| docosadienoate (22:2n6) | LC/MS neg | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 |
| dihomo-linoleate (20:2n6) | LC/MS neg | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 |
| 13-methylmyristic acid | GC/MS | 20 | 20 | 20 | 20 | 40 | 60 | 20 | 20 | 40 |
| 15-methylpalmitate (isobar with 2-methylpalmitate) | LC/MS neg | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 |
| 17-methylstearate | LC/MS neg | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 |
| 2-hydroxyglutarate | GC/MS | 100 | 100 | 100 | 80 | 60 | 100 | 100 | 40 | 100 |
| azelate (nonanedioate) | LC/MS neg | 80 | 100 | 100 | 60 | 100 | 100 | 100 | 100 | 100 |
| sebacate (decanedioate) | LC/MS neg | 60 | 100 | 100 | 40 | 60 | 100 | 20 | 100 | 80 |
| undecanedioate | LC/MS neg | 60 | 60 | 100 | 60 | 0 | 100 | 0 | 40 | 100 |
| 1,11-undecanedicarboxylate | LC/MS neg | 80 | 60 | 100 | 40 | 40 | 100 | 100 | 80 | 100 |
| dodecanedioate | LC/MS neg | 100 | 100 | 100 | 100 | 80 | 100 | 100 | 100 | 100 |
| tetradecanedioate | LC/MS neg | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 |
| hexadecanedioate | LC/MS neg | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 |
| octadecanedioate | LC/MS neg | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 |
| 3-carboxy-4-methyl-5-propyl-2-furanpropanoate (CMPF) | LC/MS neg | 100 | 100 | 100 | 100 | 80 | 100 | 100 | 100 | 100 |
| palmitate, methyl ester | GC/MS | 100 | 100 | 80 | 100 | 100 | 100 | 100 | 100 | 100 |
| n-Butyl Oleate | GC/MS | 20 | 40 | 20 | 20 | 40 | 40 | 60 | 40 | 20 |
| 2-aminoheptanoate | LC/MS pos | 100 | 80 | 80 | 100 | 100 | 100 | 100 | 100 | 80 |
| 2-aminooctanoate | LC/MS pos | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 |
| butyrylcarnitine | LC/MS pos | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 |
| propionylcarnitine | LC/MS pos | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 |
| acetylcarnitine | LC/MS pos | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 |
| hydroxybutyrylcarnitine* | LC/MS pos | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 |
| hexanoylcarnitine | LC/MS pos | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 |
| octanoylcarnitine | LC/MS pos | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 |
| decanoylcarnitine | LC/MS pos | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 |
| cis-4-decenoyl carnitine | LC/MS pos | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 |
| laurylcarnitine | LC/MS pos | 80 | 100 | 60 | 100 | 100 | 100 | 60 | 60 | 100 |
| palmitoylcarnitine | LC/MS pos | 100 | 100 | 80 | 100 | 100 | 100 | 100 | 100 | 100 |
| stearoylcarnitine | LC/MS pos | 100 | 80 | 100 | 80 | 100 | 100 | 100 | 80 | 80 |
| oleoylcarnitine | LC/MS pos | 100 | 100 | 80 | 100 | 100 | 100 | 100 | 100 | 100 |
| deoxycarnitine | LC/MS pos | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 |
| carnitine | LC/MS pos | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 |

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|---|---|---|---|---|---|---|---|---|---|---|
| 3-dehydrocarnitine | LC/MS pos | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 |
| acetoacetate | GC/MS | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 |
| 3-hydroxybutyrate (BHBA) | GC/MS | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 |
| 2-hydroxydecanoate | LC/MS neg | 100 | 100 | 100 | 100 | 80 | 100 | 100 | 100 | 100 |
| 2-hydroxypalmitate | LC/MS neg | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 |
| 2-hydroxystearate | LC/MS neg | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 |
| 3-hydroxypropanoate | GC/MS | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 |
| 3-hydroxyoctanoate | LC/MS neg | 80 | 100 | 80 | 100 | 80 | 100 | 100 | 100 | 100 |
| 3-hydroxydecanoate | LC/MS neg | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 |
| 13-HODE + 9-HODE | LC/MS neg | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 |
| prostaglandin E2 | LC/MS neg | 0 | 0 | 20 | 0 | 0 | 40 | 0 | 0 | 0 |
| 12-HETE | LC/MS neg | 100 | 80 | 100 | 80 | 100 | 100 | 100 | 100 | 100 |
| myo-inositol | GC/MS | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 |
| chiro-inositol | GC/MS | 40 | 40 | 40 | 40 | 60 | 60 | 60 | 20 | 0 |
| scyllo-inositol | GC/MS | 100 | 100 | 80 | 100 | 80 | 100 | 100 | 100 | 100 |
| inositol 1-phosphate (I1P) | GC/MS | 100 | 100 | 100 | 100 | 100 | 80 | 100 | 100 | 100 |
| choline | LC/MS pos | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 |
| glycerophosphorylcholine (GPC) | LC/MS pos | 80 | 80 | 100 | 100 | 80 | 100 | 100 | 100 | 100 |
| 1-myristoylglycerophosphocholine (14:0) | LC/MS pos | 100 | 100 | 60 | 100 | 80 | 80 | 100 | 80 | 100 |
| 2-myristoylglycerophosphocholine* | LC/MS neg | 100 | 40 | 40 | 80 | 40 | 80 | 100 | 80 | 60 |
| 1-pentadecanoylglycerophosphocholine (15:0)* | LC/MS pos | 100 | 100 | 80 | 100 | 40 | 60 | 100 | 100 | 100 |
| 1-palmitoylglycerophosphocholine (16:0) | LC/MS pos | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 |
| 2-palmitoylglycerophosphocholine* | LC/MS pos | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 |
| 1-palmitoleoylglycerophosphocholine (16:1)* | LC/MS pos | 100 | 100 | 60 | 100 | 100 | 100 | 100 | 100 | 100 |
| 1-margaroylglycerophosphocholine (17:0) | LC/MS pos | 100 | 100 | 40 | 100 | 60 | 100 | 100 | 100 | 80 |
| 1-stearoylglycerophosphocholine (18:0) | LC/MS pos | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 |
| 2-stearoylglycerophosphocholine* | LC/MS pos | 100 | 100 | 80 | 100 | 100 | 100 | 100 | 100 | 100 |
| 1-oleoylglycerophosphocholine (18:1) | LC/MS pos | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 |
| 2-oleoylglycerophosphocholine* | LC/MS pos | 100 | 100 | 60 | 100 | 100 | 80 | 100 | 100 | 100 |
| 1-linoleoylglycerophosphocholine (18:2n6) | LC/MS pos | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 |
| 2-linoleoylglycerophosphocholine* | LC/MS pos | 100 | 100 | 80 | 100 | 100 | 100 | 100 | 100 | 100 |
| 1-linolenoylglycerophosphocholine (18:3n3)* | LC/MS pos | 80 | 40 | 40 | 80 | 40 | 0 | 80 | 60 | 0 |
| 1-dihomo-linoleoylglycerophosphocholine (20:2n6)* | LC/MS pos | 100 | 40 | 20 | 100 | 40 | 40 | 100 | 80 | 40 |
| 1-eicosatrienoylglycerophosphocholine (20:3)* | LC/MS pos | 100 | 100 | 60 | 100 | 100 | 100 | 100 | 100 | 100 |
| 1-arachidonoylglycerophosphocholine (20:4n6)* | LC/MS pos | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 |

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|---|---|---|---|---|---|---|---|---|---|---|
| 2-arachidonoylglycerophosphocholine* | LC/MS pos | 100 | 100 | 80 | 60 | 100 | 100 | 80 | 100 | 80 |
| 1-eicosapentaenoylglycerophosphocholine (20:5n3)* | LC/MS pos | 100 | 100 | 60 | 100 | 60 | 20 | 100 | 80 | 40 |
| 1-docosapentaenoylglycerophosphocholine (22:5n3)* | LC/MS pos | 100 | 100 | 80 | 80 | 80 | 80 | 100 | 80 | 100 |
| 1-docosahexaenoylglycerophosphocholine (22:6n3)* | LC/MS pos | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 |
| 1-palmitoylplasmenylethanolamine* | LC/MS neg | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 |
| 1-stearoylplasmenylethanolamine* | LC/MS neg | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 |
| 1-palmitoylglycerophosphoethanolamine | LC/MS neg | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 |
| 2-palmitoylglycerophosphoethanolamine* | LC/MS neg | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 |
| 1-stearoylglycerophosphoethanolamine | LC/MS neg | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 |
| 1-oleoylglycerophosphoethanolamine | LC/MS neg | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 |
| 2-oleoylglycerophosphoethanolamine* | LC/MS neg | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 |
| 1-linoleoylglycerophosphoethanolamine* | LC/MS neg | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 |
| 2-linoleoylglycerophosphoethanolamine* | LC/MS neg | 100 | 100 | 100 | 100 | 80 | 100 | 100 | 100 | 100 |
| 1-arachidonoylglycerophosphoethanolamine* | LC/MS neg | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 |
| 2-arachidonoylglycerophosphoethanolamine* | LC/MS neg | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 |
| 2-docosahexaenoylglycerophosphoethanolamine* | LC/MS pos | 100 | 80 | 80 | 60 | 20 | 80 | 60 | 80 | 100 |
| 1-docosahexaenoylglycerophosphoethanolamine* | LC/MS neg | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 |
| 1-palmitoylglycerophosphoinositol* | LC/MS neg | 100 | 80 | 80 | 100 | 80 | 100 | 100 | 100 | 100 |
| 1-stearoylglycerophosphoinositol | LC/MS neg | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 |
| 2-stearoylglycerophosphoinositol* | LC/MS neg | 100 | 100 | 80 | 80 | 80 | 40 | 80 | 80 | 80 |
| 1-arachidonoylglycerophosphoinositol* | LC/MS neg | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 |
| 1-palmitoylglycerophosphate | LC/MS neg | 100 | 100 | 80 | 100 | 100 | 100 | 100 | 100 | 100 |
| 1-arachidonoylglyercophosphate | LC/MS neg | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 |
| glycerol | GC/MS | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 |
| glycerol 3-phosphate (G3P) | GC/MS | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 |
| 1-myristoylglycerol (1-monomyristin) | LC/MS neg | 100 | 100 | 60 | 100 | 80 | 60 | 100 | 100 | 60 |
| 1-palmitoylglycerol (1-monopalmitin) | GC/MS | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 |
| 2-palmitoylglycerol (2-monopalmitin) | GC/MS | 0 | 20 | 20 | 20 | 80 | 40 | 20 | 20 | 40 |
| 1-stearoylglycerol (1-monostearin) | GC/MS | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 |
| 1-oleoylglycerol (1-monoolein) | GC/MS | 100 | 100 | 80 | 60 | 80 | 80 | 100 | 100 | 100 |
| 1-linoleoylglycerol (1-monolinolein) | LC/MS neg | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 |
| 1-linolenoylglycerol | LC/MS neg | 100 | 100 | 60 | 60 | 100 | 60 | 100 | 100 | 60 |
| 1,2-dipalmitoylglycerol | GC/MS | 20 | 60 | 60 | 80 | 40 | 100 | 80 | 60 | 60 |
| palmitoyl sphingomyelin | GC/MS | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 |
| stearoyl sphingomyelin | GC/MS | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 |
| sphingosine 1-phosphate | LC/MS | 100 | 100 | 60 | 100 | 100 | 80 | 100 | 100 | 60 |

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|---|---|---|---|---|---|---|---|---|---|---|
| | pos | | | | | | | | | |
| sphingosine | LC/MS pos | 100 | 60 | 80 | 60 | 40 | 80 | 60 | 20 | 80 |
| lathosterol | GC/MS | 80 | 80 | 100 | 60 | 40 | 60 | 100 | 60 | 100 |
| cholesterol | GC/MS | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 |
| 7-beta-hydroxycholesterol | GC/MS | 100 | 80 | 80 | 60 | 100 | 100 | 100 | 60 | 100 |
| 7-alpha-hydroxy-3-oxo-4-cholestenoate (7-Hoca) | LC/MS neg | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 |
| cholestanol | GC/MS | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 |
| beta-sitosterol | GC/MS | 0 | 0 | 20 | 60 | 0 | 0 | 80 | 20 | 0 |
| campesterol | GC/MS | 80 | 60 | 20 | 60 | 20 | 40 | 80 | 40 | 80 |
| pregnenolone sulfate | LC/MS neg | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 |
| 21-hydroxypregnenolone disulfate | LC/MS neg | 100 | 100 | 100 | 100 | 80 | 100 | 100 | 100 | 100 |
| 5alpha-pregnan-3beta,20alpha-diol disulfate | LC/MS neg | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 |
| 5alpha-pregnan-3alpha,20beta-diol disulfate 1* | LC/MS neg | 40 | 60 | 80 | 40 | 40 | 60 | 40 | 60 | 60 |
| pregnen-diol disulfate* | LC/MS neg | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 |
| pregn steroid monosulfate* | LC/MS neg | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 |
| pregnanediol-3-glucuronide | LC/MS neg | 80 | 100 | 100 | 100 | 80 | 100 | 100 | 100 | 80 |
| cortisol | LC/MS pos | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 |
| cortisone | LC/MS pos | 100 | 100 | 100 | 100 | 100 | 80 | 100 | 100 | 100 |
| dehydroisoandrosterone sulfate (DHEA-S) | LC/MS neg | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 |
| epiandrosterone sulfate | LC/MS neg | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 |
| androsterone sulfate | LC/MS neg | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 |
| 4-androsten-3beta,17beta-diol disulfate (1)* | LC/MS neg | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 |
| 4-androsten-3beta,17beta-diol disulfate (2)* | LC/MS neg | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 |
| 5alpha-androstan-3beta,17beta-diol disulfate | LC/MS neg | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 |
| andro steroid monosulfate 2* | LC/MS neg | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 |
| cholate | LC/MS neg | 100 | 100 | 100 | 100 | 80 | 80 | 80 | 40 | 100 |
| glycocholate | LC/MS neg | 100 | 60 | 80 | 100 | 40 | 100 | 80 | 40 | 60 |
| taurocholate | LC/MS neg | 100 | 100 | 100 | 100 | 80 | 100 | 80 | 60 | 80 |
| glycochenodeoxycholate | LC/MS neg | 100 | 80 | 100 | 100 | 100 | 100 | 100 | 100 | 100 |
| taurochenodeoxycholate | LC/MS neg | 100 | 100 | 100 | 100 | 80 | 80 | 80 | 100 | 100 |
| glycodeoxycholate | LC/MS neg | 100 | 80 | 100 | 100 | 60 | 100 | 100 | 100 | 100 |
| taurodeoxycholate | LC/MS neg | 100 | 80 | 100 | 100 | 80 | 100 | 100 | 100 | 100 |
| glycolithocholate sulfate* | LC/MS neg | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 |
| taurolithocholate 3-sulfate | LC/MS neg | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 |
| glycoursodeoxycholate | LC/MS neg | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 80 | 100 |

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|---|---|---|---|---|---|---|---|---|---|---|
| hyocholate | LC/MS neg | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 |
| glycohyocholate | LC/MS neg | 100 | 80 | 100 | 80 | 40 | 60 | 100 | 80 | 100 |
| glycocholenate sulfate* | LC/MS neg | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 80 | 100 |
| taurocholenate sulfate* | LC/MS neg | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 |
| inosine | LC/MS neg | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 |
| hypoxanthine | LC/MS neg | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 |
| xanthine | LC/MS pos | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 |
| xanthosine | LC/MS pos | 0 | 40 | 60 | 0 | 60 | 80 | 20 | 20 | 60 |
| 2'-deoxyinosine | LC/MS neg | 0 | 0 | 80 | 0 | 20 | 80 | 0 | 40 | 60 |
| urate | LC/MS neg | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 |
| allantoin | GC/MS | 100 | 80 | 100 | 100 | 40 | 100 | 100 | 80 | 100 |
| adenosine 5'-monophosphate (AMP) | LC/MS pos | 20 | 0 | 20 | 0 | 40 | 40 | 0 | 0 | 20 |
| adenosine | LC/MS pos | 40 | 60 | 80 | 40 | 40 | 60 | 60 | 40 | 60 |
| N1-methyladenosine | LC/MS pos | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 |
| N6-carbamoylthreonyladenosine | LC/MS pos | 100 | 100 | 80 | 100 | 100 | 80 | 100 | 80 | 100 |
| guanosine | LC/MS neg | 80 | 100 | 80 | 100 | 100 | 100 | 80 | 80 | 80 |
| 7-methylguanine | LC/MS pos | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 |
| N1-methylguanosine | LC/MS pos | 100 | 60 | 100 | 80 | 80 | 100 | 20 | 60 | 40 |
| N2,N2-dimethylguanosine | LC/MS pos | 100 | 100 | 80 | 100 | 100 | 80 | 100 | 80 | 100 |
| uridine | LC/MS neg | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 |
| pseudouridine | LC/MS neg | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 |
| 5-methyluridine (ribothymidine) | LC/MS neg | 80 | 100 | 100 | 100 | 80 | 80 | 100 | 100 | 100 |
| beta-alanine | GC/MS | 100 | 100 | 80 | 100 | 60 | 100 | 100 | 100 | 100 |
| N-acetyl-beta-alanine | LC/MS pos | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 80 | 100 |
| methylphosphate | GC/MS | 100 | 80 | 100 | 100 | 100 | 100 | 100 | 100 | 100 |
| nicotinamide | LC/MS pos | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 |
| N1-Methyl-2-pyridone-5-carboxamide | LC/MS pos | 100 | 100 | 60 | 100 | 100 | 100 | 100 | 100 | 100 |
| riboflavin (Vitamin B2) | LC/MS pos | 80 | 80 | 40 | 80 | 60 | 40 | 60 | 60 | 40 |
| pantothenate | LC/MS pos | 100 | 100 | 80 | 100 | 100 | 100 | 100 | 100 | 100 |
| gulono-1,4-lactone | GC/MS | 100 | 100 | 100 | 100 | 100 | 100 | 80 | 100 | 100 |
| ascorbate (Vitamin C) | GC/MS | 100 | 80 | 60 | 100 | 100 | 40 | 100 | 100 | 80 |
| threonate | GC/MS | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 |
| arabonate | GC/MS | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 |
| oxalate (ethanedioate) | GC/MS | 100 | 80 | 100 | 100 | 100 | 100 | 100 | 100 | 100 |
| alpha-tocopherol | GC/MS | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 |
| beta-tocopherol | GC/MS | 80 | 60 | 0 | 80 | 80 | 60 | 100 | 100 | 80 |

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|---|---|---|---|---|---|---|---|---|---|---|
| gamma-tocopherol | GC/MS | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 |
| gamma-CEHC | LC/MS neg | 100 | 100 | 80 | 100 | 80 | 80 | 100 | 100 | 80 |
| gamma-CEHC glucuronide* | LC/MS neg | 100 | 60 | 60 | 80 | 80 | 20 | 100 | 20 | 0 |
| alpha-CEHC glucuronide* | LC/MS neg | 60 | 80 | 0 | 60 | 60 | 0 | 20 | 60 | 0 |
| heme | LC/MS pos | 100 | 100 | 100 | 100 | 80 | 100 | 100 | 80 | 100 |
| bilirubin (Z,Z) | LC/MS neg | 100 | 100 | 80 | 100 | 100 | 60 | 100 | 100 | 80 |
| bilirubin (E,E)* | LC/MS pos | 100 | 100 | 80 | 100 | 80 | 100 | 100 | 100 | 100 |
| bilirubin (E,Z or Z,E)* | LC/MS pos | 80 | 80 | 40 | 60 | 60 | 40 | 80 | 80 | 60 |
| biliverdin | LC/MS neg | 80 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 |
| I-urobilinogen | LC/MS neg | 80 | 100 | 80 | 100 | 80 | 40 | 80 | 80 | 100 |
| L-urobilin | LC/MS pos | 60 | 60 | 80 | 80 | 60 | 40 | 60 | 40 | 40 |
| pyridoxate | LC/MS neg | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 |
| hippurate | LC/MS neg | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 |
| 2-hydroxyhippurate (salicylurate) | LC/MS neg | 100 | 60 | 80 | 60 | 60 | 80 | 60 | 80 | 80 |
| 3-hydroxyhippurate | LC/MS neg | 100 | 20 | 80 | 60 | 20 | 40 | 100 | 0 | 60 |
| 4-hydroxyhippurate | LC/MS neg | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 80 | 80 |
| benzoate | GC/MS | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 |
| catechol sulfate | LC/MS neg | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 |
| O-methylcatechol sulfate | LC/MS neg | 100 | 80 | 80 | 100 | 80 | 100 | 80 | 100 | 80 |
| 3-methyl catechol sulfate (1) | LC/MS neg | 100 | 40 | 40 | 100 | 20 | 40 | 100 | 40 | 60 |
| 3-methyl catechol sulfate (2) | LC/MS neg | 60 | 0 | 20 | 0 | 0 | 0 | 40 | 0 | 20 |
| 4-methylcatechol sulfate | LC/MS neg | 100 | 100 | 100 | 100 | 80 | 100 | 100 | 100 | 100 |
| 3-ethylphenylsulfate* | LC/MS neg | 20 | 0 | 20 | 20 | 0 | 0 | 0 | 0 | 0 |
| 4-ethylphenylsulfate | LC/MS neg | 100 | 100 | 100 | 100 | 60 | 60 | 100 | 80 | 60 |
| 4-vinylphenol sulfate | LC/MS neg | 100 | 80 | 80 | 100 | 40 | 80 | 100 | 100 | 100 |
| caffeine | LC/MS pos | 80 | 80 | 100 | 100 | 100 | 100 | 100 | 100 | 100 |
| paraxanthine | LC/MS pos | 80 | 60 | 100 | 60 | 100 | 20 | 100 | 80 | 80 |
| theobromine | LC/MS pos | 80 | 80 | 100 | 100 | 100 | 100 | 100 | 100 | 100 |
| theophylline | LC/MS neg | 80 | 60 | 100 | 80 | 80 | 60 | 80 | 80 | 60 |
| 7-methylurate | LC/MS neg | 100 | 80 | 100 | 100 | 100 | 80 | 100 | 80 | 80 |
| 1,3-dimethylurate | LC/MS neg | 60 | 60 | 20 | 60 | 40 | 0 | 60 | 20 | 40 |
| 1,7-dimethylurate | LC/MS neg | 80 | 60 | 100 | 80 | 60 | 40 | 80 | 80 | 60 |
| 1,3,7-trimethylurate | LC/MS neg | 60 | 60 | 100 | 80 | 60 | 40 | 80 | 40 | 60 |
| 1-methylxanthine | LC/MS pos | 60 | 60 | 80 | 60 | 60 | 60 | 80 | 80 | 60 |

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|---|---|---|---|---|---|---|---|---|---|---|
| 3-methylxanthine | LC/MS pos | 40 | 40 | 20 | 80 | 80 | 60 | 100 | 80 | 40 |
| 7-methylxanthine | LC/MS pos | 40 | 40 | 40 | 80 | 80 | 80 | 80 | 80 | 60 |
| 5-acetylamino-6-amino-3-methyluracil | LC/MS neg | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 |
| cotinine | LC/MS pos | 20 | 0 | 20 | 0 | 0 | 0 | 0 | 0 | 0 |
| 2-piperidinone | GC/MS | 60 | 60 | 40 | 60 | 80 | 60 | 100 | 20 | 60 |
| 1,6-anhydroglucose | GC/MS | 100 | 80 | 100 | 60 | 80 | 80 | 100 | 80 | 100 |
| gluconate | GC/MS | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 |
| ergothioneine | LC/MS pos | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 80 |
| erythritol | GC/MS | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 |
| homostachydrine* | LC/MS pos | 80 | 80 | 80 | 100 | 80 | 0 | 80 | 60 | 60 |
| N-(2-furoyl)glycine | LC/MS pos | 80 | 20 | 60 | 0 | 0 | 0 | 20 | 0 | 20 |
| piperine | LC/MS pos | 100 | 80 | 80 | 100 | 60 | 80 | 100 | 40 | 100 |
| 2-furoic acid | GC/MS | 80 | 80 | 80 | 60 | 40 | 40 | 60 | 20 | 40 |
| quinate | GC/MS | 60 | 40 | 80 | 40 | 0 | 40 | 80 | 40 | 60 |
| saccharin | LC/MS neg | 20 | 0 | 100 | 40 | 60 | 100 | 60 | 100 | 100 |
| stachydrine | LC/MS pos | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 80 | 100 |
| thymol sulfate | LC/MS neg | 100 | 100 | 60 | 100 | 80 | 100 | 100 | 60 | 40 |
| tribuloside | LC/MS neg | 0 | 0 | 0 | 0 | 20 | 0 | 0 | 0 | 0 |
| 2-hydroxyacetaminophen sulfate* | LC/MS neg | 40 | 20 | 40 | 0 | 0 | 20 | 20 | 20 | 20 |
| 2-methoxyacetaminophen sulfate* | LC/MS neg | 20 | 20 | 20 | 0 | 0 | 20 | 20 | 20 | 20 |
| 3-(cystein-S-yl)acetaminophen* | LC/MS pos | 20 | 20 | 20 | 0 | 0 | 20 | 20 | 0 | 0 |
| 3-(N-acetyl-L-cystein-S-yl) acetaminophen* | LC/MS pos | 20 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 4-acetaminophen sulfate | LC/MS neg | 40 | 40 | 60 | 0 | 40 | 20 | 20 | 20 | 20 |
| 4-acetamidophenol | LC/MS pos | 20 | 20 | 40 | 0 | 0 | 20 | 20 | 0 | 20 |
| 4-acetamidophenylglucuronide | LC/MS neg | 20 | 20 | 20 | 0 | 20 | 20 | 20 | 20 | 20 |
| ibuprofen acyl glucuronide | LC/MS neg | 0 | 0 | 0 | 20 | 0 | 0 | 20 | 0 | 0 |
| ibuprofen | LC/MS neg | 0 | 0 | 0 | 40 | 0 | 0 | 20 | 0 | 0 |
| 2-hydroxyibuprofen | LC/MS pos | 0 | 0 | 0 | 40 | 0 | 0 | 20 | 0 | 0 |
| carboxyibuprofen | LC/MS neg | 0 | 0 | 0 | 40 | 0 | 0 | 20 | 0 | 0 |
| atenolol | LC/MS pos | 20 | 20 | 0 | 0 | 20 | 20 | 0 | 0 | 0 |
| desmethylnaproxen sulfate* | LC/MS neg | 0 | 0 | 0 | 20 | 20 | 20 | 20 | 0 | 0 |
| O-desmethylvenlafaxine | LC/MS pos | 0 | 0 | 0 | 0 | 0 | 0 | 20 | 0 | 20 |
| escitalopram | LC/MS pos | 0 | 0 | 0 | 0 | 0 | 0 | 20 | 20 | 20 |
| fluoxetine | LC/MS pos | 0 | 0 | 0 | 0 | 0 | 0 | 20 | 20 | 20 |
| gabapentin | LC/MS neg | 20 | 20 | 20 | 0 | 0 | 0 | 0 | 0 | 0 |

| | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| hydrochlorothiazide | LC/MS neg | 40 | 40 | 0 | 0 | 0 | 0 | 20 | 20 | 0 |
| hydroquinone sulfate | LC/MS neg | 20 | 20 | 20 | 0 | 0 | 0 | 0 | 0 | 0 |
| hydroxypioglitazone (M-IV) | LC/MS neg | 0 | 0 | 0 | 20 | 0 | 0 | 0 | 0 | 0 |
| ketopioglitazone | LC/MS neg | 0 | 0 | 0 | 20 | 0 | 0 | 0 | 0 | 0 |
| lidocaine | LC/MS pos | 0 | 80 | 20 | 0 | 80 | 0 | 0 | 80 | 0 |
| metformin | LC/MS pos | 60 | 40 | 20 | 100 | 20 | 20 | 0 | 0 | 0 |
| metoprolol | LC/MS pos | 0 | 0 | 0 | 0 | 0 | 0 | 20 | 20 | 20 |
| metoprolol acid metabolite* | LC/MS pos | 0 | 0 | 0 | 0 | 0 | 0 | 20 | 20 | 20 |
| naproxen | LC/MS neg | 40 | 0 | 0 | 20 | 20 | 20 | 40 | 20 | 0 |
| norfluoxetine | LC/MS pos | 0 | 0 | 0 | 0 | 0 | 0 | 20 | 20 | 20 |
| omeprazole | LC/MS neg | 0 | 0 | 0 | 0 | 20 | 20 | 0 | 0 | 0 |
| pantoprazole | LC/MS neg | 0 | 20 | 60 | 40 | 40 | 60 | 20 | 0 | 60 |
| pioglitazone* | LC/MS pos | 0 | 0 | 0 | 20 | 0 | 0 | 0 | 0 | 0 |
| salicylate | LC/MS neg | 40 | 20 | 40 | 0 | 20 | 40 | 20 | 60 | 40 |
| 1,2-propanediol | GC/MS | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 |
| 2-aminophenol sulfate | LC/MS neg | 100 | 40 | 80 | 80 | 0 | 40 | 100 | 0 | 60 |
| bisphenol A monosulfate | LC/MS neg | 60 | 80 | 60 | 60 | 80 | 100 | 80 | 80 | 100 |
| 2-ethylhexanoate | GC/MS | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 |
| 2-hydroxyisobutyrate | GC/MS | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 |
| dexpanthenol | LC/MS pos | 0 | 0 | 0 | 0 | 0 | 40 | 0 | 0 | 0 |
| glycerol 2-phosphate | GC/MS | 100 | 100 | 100 | 80 | 80 | 100 | 100 | 100 | 100 |
| glycolate (hydroxyacetate) | GC/MS | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 100 |

| Table A3. Conserved Pre-Operation Diet (Pre-op) to Baseline (BL) Changes, p<0.05, q<0.05. | | | | |
|---|---|---|---|---|
| **Pathway** | **Biochemical Name** | **Fold-Change** | | |
| | | **SG NonT2D** | **SG T2D** | **GB T2D** |
| Amino Acid | 3-indoxyl sulfate | 0.51 | 0.51 | 0.59 |
| Lipid | oleate (18:1n9) | 2.84 | 1.74 | 3.11 |
| Lipid | cis-vaccenate (18:1n7) | 2.18 | 1.52 | 2.07 |
| Lipid | hydroxybutyrylcarnitine* | 8.65 | 3.87 | 6.95 |
| Lipid | acetoacetate | 13.88 | 5.66 | 8.71 |
| Lipid | 3-hydroxybutyrate (BHBA) | 18.77 | 5.79 | 11.25 |
| Lipid | 2-myristoylglycerophosphocholine | 0.23 | 0.49 | 0.71 |
| Lipid | 1-linoleoylglycerophosphoethanolamine | 0.51 | 0.52 | 0.6 |
| Lipid | 2-linoleoylglycerophosphoethanolamine | 0.48 | 0.59 | 0.63 |
| Lipid | 1-oleoylglycerol (1-monoolein) | 7.26 | 3.84 | 5.8 |
| Lipid | 1-linoleoylglycerol (1-monolinolein) | 6.48 | 4.75 | 5.77 |
| Lipid | 1-linolenoylglycerol | 9.97 | 7.16 | 7.06 |
| Xenobiotics | 3-methyl catechol sulfate (1) | 0.15 | 0.21 | 0.02 |
| Xenobiotics | piperine | 0.15 | 0.09 | 0.36 |

| Table A4. Conserved Post- Metabolic Surgery (Post-op) to Baseline (BL) Changes, p<0.05, q<0.05. | | | | |
|---|---|---|---|---|
| Pathway | Biochemical Name | Fold-Change | | |
| | | SG NonT2D | SG T2D | GB T2D |
| Amino Acid | serine | 2.44 | 4.03 | 2.43 |
| Amino Acid | N-acetylserine | 4.09 | 6.57 | 8.6 |
| Amino Acid | glutamate | 1.85 | 2.48 | 1.96 |
| Amino Acid | pyroglutamine | 2.17 | 1.71 | 1.34 |
| Amino Acid | trans-urocanate | 103.87 | 268.09 | 353.71 |
| Amino Acid | cis-urocanate | 76.94 | 329.32 | 543.33 |
| Amino Acid | 3-(4-hydroxyphenyl)lactate | 0.65 | 0.66 | 0.65 |
| Amino Acid | indolelactate | 0.63 | 0.56 | 0.5 |
| Amino Acid | kynurenine | 0.71 | 0.62 | 0.58 |
| Amino Acid | ornithine | 6.39 | 17.59 | 23.2 |
| Amino Acid | cysteine-glutathione disulfide | 5.62 | 4.86 | 10.46 |
| Amino Acid | 5-oxoproline | 4.01 | 7.95 | 8.08 |
| Peptide | gamma-glutamylalanine | 0.45 | 0.5 | 0.33 |
| Peptide | gamma-glutamylglutamate | 3.99 | 5.21 | 6.96 |
| Peptide | gamma-glutamylthreonine | 2.24 | 1.81 | 2.31 |
| Peptide | cyclo(glu-glu) | 2.79 | 5.63 | 4.98 |
| Peptide | isoleucylvaline | 0.31 | 0.28 | 0.3 |
| Peptide | phenylalanylglutamate | 4.45 | 10.76 | 4.01 |
| Peptide | prolylglycine | 4.23 | 3.09 | 7.75 |
| Peptide | pyroglutamylvaline | 81.09 | 111.34 | 180.96 |
| Peptide | tyrosylglutamate | 2.55 | 7.02 | 5.44 |
| Peptide | valylarginine | 0.25 | 0.4 | 0.36 |
| Carbohydrate | 3-phosphoglycerate | 8.83 | 17.11 | 37.08 |
| Carbohydrate | ribulose/xylulose 5-phosphate | 9.26 | 9.94 | 16.01 |
| Carbohydrate | ribulose | 11.87 | 7.51 | 5.14 |
| Carbohydrate | ribose | 3.98 | 3.07 | 1.77 |
| Carbohydrate | ribitol | 0.8 | 2.37 | 0.77 |
| Carbohydrate | xylulose | 8.38 | 16.31 | 10.84 |
| Energy | malate | 2.29 | 4.24 | 3.03 |
| Lipid | pelargonate (9:0) | 0.59 | 0.48 | 0.51 |
| Lipid | sebacate (decanedioate) | 5.28 | 3.68 | 6.45 |
| Lipid | undecanedioate | 3.02 | 2.92 | 3.61 |
| Lipid | 1,11-undecanedicarboxylate | 4.51 | 8.2 | 26.79 |
| Lipid | palmitate, methyl ester | 0.42 | 0.35 | 0.61 |
| Lipid | 1-myristoylglycerophosphocholine | 0.27 | 0.31 | 0.28 |
| Lipid | 1-palmitoleoylglycerophosphocholine | 0.37 | 0.39 | 0.4 |
| Lipid | 1-oleoylglycerophosphocholine | 0.37 | 0.42 | 0.51 |
| Lipid | 1-linoleoylglycerophosphocholine | 0.31 | 0.3 | 0.39 |
| Lipid | 2-linoleoylglycerophosphocholine | 0.36 | 0.31 | 0.39 |

| | | | | |
|---|---|---|---|---|
| Lipid | 1-linolenoylglycerophosphocholine | 0.18 | 0.32 | 0.34 |
| Lipid | 1-dihomo-linoleoylglycerophosphocholine | 0.31 | 0.34 | 0.44 |
| Lipid | 1-eicosatrienoylglycerophosphocholine | 0.2 | 0.16 | 0.32 |
| Lipid | 1-arachidonoylglycerophosphocholine | 0.46 | 0.37 | 0.49 |
| Lipid | 1-eicosapentaenoylglycerophosphocholine | 0.15 | 0.2 | 0.5 |
| Lipid | 1-oleoylglycerophosphoethanolamine | 0.45 | 0.68 | 0.56 |
| Lipid | 2-oleoylglycerophosphoethanolamine | 0.46 | 0.7 | 0.64 |
| Lipid | 1-linoleoylglycerophosphoethanolamine | 0.39 | 0.46 | 0.41 |
| Lipid | 2-linoleoylglycerophosphoethanolamine | 0.4 | 0.61 | 0.52 |
| Lipid | 1-stearoylglycerophosphoinositol | 0.29 | 0.38 | 0.57 |
| Lipid | glycerol | 3.25 | 8.37 | 3.51 |
| Nucleotide | inosine | 3.04 | 3.52 | 2.3 |
| Nucleotide | allantoin | 9.42 | 21.79 | 10.08 |
| Nucleotide | N1-methyladenosine | 0.64 | 0.53 | 0.48 |
| Cofactors & Vitamins | nicotinamide | 7.51 | 7.69 | 6.9 |
| Cofactors & Vitamins | ascorbate (Vitamin C) | 0.08 | 0.02 | 0.07 |
| Cofactors & Vitamins | gamma-CEHC | 0.38 | 0.24 | 0.17 |
| Cofactors & Vitamins | gamma-CEHC glucuronide | 0.39 | 0.28 | 0.28 |
| Cofactors & Vitamins | heme | 108.58 | 94.24 | 104.2 |
| Cofactors & Vitamins | bilirubin (Z,Z) | 0.29 | 0.1 | 0.3 |
| Cofactors & Vitamins | bilirubin (E,E) | 0.37 | 0.18 | 0.44 |
| Xenobiotics | benzoate | 0.67 | 0.67 | 0.66 |
| Xenobiotics | catechol sulfate | 0.59 | 0.34 | 0.49 |
| Xenobiotics | piperine | 0.29 | 0.2 | 0.44 |
| Xenobiotics | saccharin | 8.01 | 6.92 | 1.17 |

| Table A5. Conserved Post- Metabolic Surgery (Post-op) to Pre-Operation Diet (Pre-op) Changes, p<0.05, q<0.05. | | | | |
|---|---|---|---|---|
| **Pathway** | **Biochemical Name** | **Fold-Change** | | |
| | | **SG NonT2D** | **SG T2D** | **GB T2D** |
| Amino Acid | N-acetylserine | 4.1 | 7.97 | 8 |
| Amino Acid | aspartate | 2.22 | 4.94 | 2.03 |
| Amino Acid | glutamate | 2.09 | 3.05 | 2.41 |
| Amino Acid | trans-urocanate | 113.05 | 146.41 | 266.35 |
| Amino Acid | cis-urocanate | 99.74 | 229.09 | 431.96 |
| Amino Acid | 3-methyl-2-oxobutyrate | 0.62 | 0.62 | 0.69 |
| Amino Acid | alpha-ketobutyrate | 0.23 | 0.12 | 0.5 |
| Amino Acid | 2-hydroxybutyrate (AHB) | 0.47 | 0.54 | 0.55 |
| Amino Acid | ornithine | 10.81 | 25.39 | 24.82 |
| Amino Acid | 5-oxoproline | 4.98 | 12.04 | 11.32 |
| Peptide | gamma-glutamylglutamate | 3.23 | 6.48 | 7.58 |
| Peptide | gamma-glutamylisoleucine | 2.95 | 3.06 | 2.91 |
| Peptide | gamma-glutamylthreonine | 2.55 | 3.22 | 2.46 |
| Peptide | gamma-glutamyltyrosine | 1.97 | 2.35 | 2.56 |
| Peptide | cyclo(glu-glu) | 4.36 | 5.52 | 7.93 |
| Peptide | phenylalanylglutamate | 7.16 | 8.67 | 2.93 |
| Peptide | prolylglycine | 5.18 | 4.23 | 9.68 |
| Peptide | pyroglutamylvaline | 84.99 | 150.6 | 226.67 |
| Peptide | tyrosylglutamate | 2.44 | 5.39 | 4.42 |
| Carbohydrate | 3-phosphoglycerate | 8.55 | 16.99 | 39.97 |
| Carbohydrate | pyruvate | 0.42 | 0.34 | 0.43 |
| Carbohydrate | ribulose/xylulose 5-phosphate | 10.7 | 9.94 | 8.37 |
| Carbohydrate | ribulose | 7.6 | 8.01 | 4.71 |
| Carbohydrate | maltotriose | 3.74 | 8.2 | 2.71 |
| Carbohydrate | sucrose | 9.85 | 89.85 | 44.52 |
| Carbohydrate | fructose | 0.38 | 0.78 | 0.35 |
| Carbohydrate | sorbitol | 11.31 | 8.49 | 7.56 |
| Carbohydrate | mannose | 0.5 | 0.53 | 0.46 |
| Energy | malate | 2.91 | 5.42 | 4.43 |
| Lipid | linolenate [alpha or gamma] | 0.3 | 0.47 | 0.53 |
| Lipid | 2-hydroxyglutarate | 1.4 | 1.62 | 1.74 |
| Lipid | undecanedioate | 2.25 | 5.35 | 5.93 |
| Lipid | 1,11-undecanedicarboxylate | 4.99 | 9.82 | 41.8 |
| Lipid | acetoacetate | 0.15 | 0.08 | 0.41 |
| Lipid | 1-eicosatrienoylglycerophosphocholine | 0.35 | 0.47 | 0.41 |
| Lipid | 1-eicosapentaenoylglycerophosphocholine | 0.24 | 0.4 | 0.45 |
| Lipid | 1-oleoylglycerol (1-monoolein) | 0.28 | 0.25 | 0.13 |
| Lipid | 1-linoleoylglycerol (1-monolinolein) | 0.29 | 0.24 | 0.13 |
| Lipid | 1-linolenoylglycerol | 0.09 | 0.09 | 0.05 |

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|---|---|---|---|---|
| Nucleotide | hypoxanthine | 4.09 | 7.73 | 2.97 |
| Nucleotide | allantoin | 21.79 | 57.52 | 32.06 |
| Nucleotide | N1-methyladenosine | 0.64 | 0.59 | 0.53 |
| Cofactors & Vitamins | nicotinamide | 11.29 | 4.47 | 5.24 |
| Cofactors & Vitamins | ascorbate (Vitamin C) | 0.05 | 0.05 | 0.06 |
| Cofactors & Vitamins | heme | 50.62 | 18.24 | 27.04 |
| Cofactors & Vitamins | bilirubin (Z,Z) | 0.4 | 0.14 | 0.3 |
| Cofactors & Vitamins | bilirubin (E,E) | 0.28 | 0.29 | 0.24 |
| Xenobiotics | saccharin | 3.48 | 4.19 | 12.65 |