

Supplement 1. List of Metabolites Analyzed

Amino Acids

Alanine, Lysine, Arginine, Methionine, Asparagine, Ornithine, Aspartate, Phenylalanine, Citrulline, Proline, Glutamate, Serine, Glutamine, Threonine, Glycine, Tryptophan, Histidine, Tyrosine, Isoleucine, Valine

Biogenic Amines

Acetylornithine, Nitrotyrosine, Asymmetric dimethylarginine, Phenylethylamine, alpha-Aminoadipic acid, Putrescine, Carnosine, Sarcosine, cis-4-Hydroxyproline, Symmetric dimethylarginine, Creatinine, Serotonin, Dihydroxyphenylalanine, Spermidine, Dopamine, Spermine, Histamine, Taurine, Kynurenine, trans-4-Hydroxyproline, Methionine sulfoxide

Monosaccharides

Hexoses (including glucose)

Acylcarnitines

Carnitine, Fumaryl carnitine, Acetyl carnitine, Valeryl carnitine, Propionyl carnitine, Glutaryl carnitine, Malonyl carnitine, Hydroxyvaleryl carnitine, Hydroxypropionyl carnitine, Tiglyl carnitine, Propenoyl carnitine, Glutaconyl carnitine, Butyryl carnitine, Hexanoyl carnitine, Methylmalonyl carnitine, Adipoyl carnitine, Hydroxybutyryl carnitine, Hydroxyhexanoyl carnitine, Butenyl carnitine, Hexenoyl carnitine, Heptanoyl carnitine, Carboxytridecenoyl carnitine, Pimeloyl carnitine, Hydroxytetradecenoyl carnitine, Octanoyl carnitine, Tetradecadienoyl carnitine, Octenoyl carnitine, Hydroxytetradecadienoyl carnitine, Hydroxyoctenoyl carnitine, Pentadecanoyl carnitine, Nonayl carnitine, Hexadecanoyl carnitine, Decanoyl carnitine, Hydroxyhexadecanoyl carnitine, Decenoyl carnitine, Hexadecenoyl carnitine, Decadienoyl carnitine, Hydroxyhexadecenoyl carnitine, Decatrienoyl carnitine, Hexadecadienoyl carnitine, Dimethylnonanoyl carnitine, Hydroxyhexadecadienoyl carnitine, Dodecanoyl carnitine, Heptadecanoyl carnitine, Dodecanedioyl carnitine, Octadecanoyl carnitine, Dodecenoyl carnitine, Octadecenoyl carnitine, Tridecanoyl carnitine, Hydroxyoctadecenoyl carnitine, Tetradecanoyl carnitine, Octadecadienyl carnitine, Hydroxymyristoyl carnitine, Nonadecanoyl carnitine, Tetradecenoyl carnitine

Diglycerides

DG(32:1), DG(36:3), DG(41:1), DG-O(32:2), DG(32:2), DG(36:4), DG(42:0), DG-O(34:1), DG(34:1), DG(38:0), DG(42:1), DG-O(36:4), DG(34:3), DG(38:5), DG(42:2), DG(36:2), DG(39:0), DG(44:3)

Triglycerides

TG(44:1), TG(50:3), TG(52:6), TG(54:7), TG(44:2), TG(50:4), TG(52:7), TG(55:6), TG(44:4), TG(51:1), TG(53:3), TG(55:7), TG(46:2), TG(51:2), TG(53:4), TG(55:8), TG(48:1), TG(51:3), TG(53:5), TG(55:9), TG(48:2), TG(51:4), TG(53:6), TG(56:6), TG(48:3), TG(51:5), TG(54:2), TG(56:7), TG(49:1), TG(52:2), TG(54:3), TG(56:8), TG(49:2), TG(52:3), TG(54:4), TG(56:9), TG(50:1), TG(52:4), TG(54:5), TG(50:2), TG(52:5), TG(54:6)

Lysophosphatidylcholines

LPC(12:0), LPC(17:1), LPC(20:2), LPC(24:1), LPC(14:0), LPC(18:0), LPC(20:3), LPC-O(16:1), LPC(15:0),

LPC(18:1), LPC(20:4), LPC-O(17:1), LPC(16:0), LPC(18:2), LPC(22:5), LPC-O(18:0), LPC(16:1), LPC(20:0), LPC(22:6), LPC-O(18:1), LPC(17:0), LPC(20:1), LPC(24:0), LPC-O(18:2)

Phosphatidylcholines

PC(24:0), PC(36:1), PC(41:5), PC-O(34:0), PC(25:0), PC(36:2), PC(41:8), PC-O(34:1), PC(26:0), PC(36:3), PC(42:0), PC-O(34:2), PC(27:0), PC(36:4), PC(42:1), PC-O(34:3), PC(27:1), PC(36:5), PC(42:2), PC-O(34:4), PC(28:1), PC(36:6), PC(42:3), PC-O(35:3), PC(29:0), PC(37:0), PC(42:4), PC-O(35:4), PC(29:1), PC(37:1), PC(42:5), PC-O(36:0), PC(29:2), PC(37:2), PC(42:6), PC-O(36:1), PC(30:0), PC(37:3), PC(42:7), PC-O(36:2), PC(30:1), PC(37:4), PC(42:10), PC-O(36:3), PC(30:2), PC(37:5), PC(43:2), PC-O(36:4), PC(30:3), PC(37:6), PC(43:6), PC-O(36:5), PC(31:0), PC(37:7), PC(44:1), PC-O(36:6), PC(31:1), PC(38:0), PC(44:3), PC-O(37:6), PC(31:2), PC(38:1), PC(44:5), PC-O(37:7), PC(31:3), PC(38:2), PC(44:6), PC-O(38:0), PC(32:0), PC(38:3), PC(44:7), PC-O(38:1), PC(32:1), PC(38:4), PC(44:10), PC-O(38:2), PC(32:2), PC(38:5), PC(44:12), PC-O(38:3), PC(32:3), PC(38:6), PC(46:1), PC-O(38:4), PC(32:4), PC(38:7), PC(46:2), PC-O(38:5), PC(32:5), PC(39:0), PC-O(26:0), PC-O(38:6), PC(32:6), PC(39:1), PC-O(26:1), PC-O(40:0), PC(33:0), PC(39:2), PC-O(28:0), PC-O(40:1), PC(33:1), PC(39:3), PC-O(28:1), PC-O(40:2), PC(33:2), PC(39:4), PC-O(29:0), PC-O(40:3), PC(33:3), PC(39:5), PC-O(30:0), PC-O(40:4), PC(33:4), PC(39:6), PC-O(30:1), PC-O(40:5), PC(33:5), PC(39:7), PC-O(30:2), PC-O(40:6), PC(34:0), PC(40:1), PC-O(31:0), PC-O(40:7), PC(34:1), PC(40:2), PC-O(31:1), PC-O(40:8), PC(34:2), PC(40:3), PC-O(31:3), PC-O(42:0), PC(34:3), PC(40:4), PC-O(32:0), PC-O(42:1), PC(34:4), PC(40:5), PC-O(32:1), PC-O(42:2), PC(34:5), PC(40:6), PC-O(32:2), PC-O(42:3), PC(35:0), PC(40:7), PC-O(32:3), PC-O(42:4), PC(35:1), PC(40:8), PC-O(33:0), PC-O(42:5), PC(35:2), PC(40:9), PC-O(33:1), PC-O(42:6), PC(35:3), PC(41:1), PC-O(33:2), PC-O(44:3), PC(35:4), PC(41:2), PC-O(33:3), PC-O(44:4), PC(35:5), PC(41:3), PC-O(33:4), PC-O(44:5), PC(36:0), PC(41:4), PC-O(33:6), PC-O(44:6)

Sphingomyelins

SM(30:1), SM(34:2), SM(38:3), SM(42:1), SM(31:0), SM(35:1), SM(39:1), SM(42:2), SM(31:1), SM(36:0), SM(39:2), SM(42:3), SM(32:1), SM(36:1), SM(40:1), SM(43:1), SM(32:2), SM(36:2), SM(40:2), SM(43:2), SM(33:1), SM(37:1), SM(40:4), SM(44:1), SM(33:2), SM(38:1), SM(41:1), SM(44:2), SM(34:1), SM(38:2), SM(41:2)

Ceramides

Cer(34:0), Cer(40:1), Cer(42:2), Cer(34:1), Cer(41:1), Cer(43:1), Cer(38:1), Cer(42:1), Cer(44:0)

Cholesteryl Esters

CE(16:0), CE(17:2), CE(19:2), CE(22:5), CE(16:1), CE(18:1), CE(19:3), CE(22:6), CE(17:0), CE(18:2), CE(20:4), CE(17:1), CE(18:3), CE(20:5)