3 2 1 Samples GFP MCAT OXSM MECR - 4-HYDROXYBENZOATE 2-DEOXY-D-GLUCOSE RHAMNOSE - PHENYLETHANOLAMINE - ALLOTHREONINE - HOMOSERINE O-SUCCINYL-HOMOSERINE-2 - METHIONINE SULFOXIDE - ANSERINE - CYSTINE - PYRAZOLE - GLUTAMINE - GALACTITOL - MANNITOL - THREONINE 1-AMINOCYCLOPROPANECARBOXYLATE - O-ACETYLSERINE GLYCINE - UREA - GLYOXYLATE - 6-PHOSPHOGLUCONATE - GLUCURONATE GALACTURONATE N,N,N-TRIMETHYLLYSINE - HISTIDINE · CITRULLINE - ASPARAGINE - ETHANOLAMINE PHOSPHATE O-PHOSPHOETHANOLAMINE **BETA-ALANINE** SARCOSINE **SERINE** PHOSPHOSERINE **PHOSPHORYLCHOLINE** - ASPARTATE D-ALANINE · L-ALANINE CYSTEINE **GALACTARATE** SACCHARATE **GLUCOSAMINE 6-PHOSPHATE GLUCONATE** - SEDOHEPTULOSE-7-PHOSPHATE MANNOSE 6-PHOSPHATE GLUCOSE 6-PHOSPHATE **GLUCOSE 1-PHOSPHATE** FRUCTOSE 6-PHOSPHATE - GLYCOLATE **ERYTHROSE-4-PHOSPHATE** HYPOTAURINE TAURINE - 6-Phosphonoglucono-D-lactone Fructose 1,6-bisphosphate DEOXYCYTIDINE MONOPHOSPHATE-1 D-RIBOSE 5-PHOSPHATE Ribose-5-phosphate Xylulose-5-phosphate RIBULOSE-5-PHOSPHATE DIMETHYLGLYCINE **GAMMA-AMINOBUTYRATE** SORBITOL PHENYLACETATE HEXOSE CARNOSINE DEOXYCARNITINE N-ACETYLMETHIONINE - N-ACETYLALANINE - MALATE FUMARATE - MALEATE N-FORMYL-L-METHIONINE · 2-HYDROXY-4-(METHYLTHIO)BUTANOATE Hydroxyphenyllactic acid - 3,4-Dihydroxyhydrocinnamic acid HYDROXYPHENYLLACTATE - PHENYLLACTATE - 3-(2-HYDROXYPHENYL)PROPANOATE - Glyceraldehyde 3-phosphate - DIHYDROXYACETONEPHOSPHATE PHOSPHOCREATINE - GLUTAMATE N-METHYLASPARTATE - DEOXYCYTIDINE-DIPHOSPHATE - LEUCINE - URIDINE MONOPHOSPHATE - CYTIDINE MONOPHOSPHATE - DEOXYINOSINE - OXIDIZED GLUTATHIONE - AMINOADIPATE - DIETHANOLAMINE - SPERMIDINE - NICOTINAMIDE MONONUCLEOTIDE - THYMIDINE-MONOPHOSPHATE - DEOXYGUANOSINE-MONOPHOSPHATE - ADENOSINE-MONOPHOSPHATE GUANOSINE MONOPHOSPHATE - HYPOXANTHINE - INOSINE DL-2-AMINOCTANOATE - P-HYDROXYPHENYLACETATE - 2-HYDROXYPHENYLACETATE - MANDELATE - 6-HYDROXYDOPAMINE - AICAR - SPERMINE - 7-HYDROXYOCTANOATE DIMER BETA-GLYCEROPHOSPHATE GLYCEROL 3-PHOSPHATE 4-HYDROXY-3-METHOXYPHENYLGLYCOL - GLUTATHIONE REDUCED OXOGLUTARATE - SALICYLATE - TRIMETHYLAMINE - THYMIDINE OXOADIPATE - 2-HYDROXYGLUTARIC - PROPIONYLCHOLINE N-METHYLGLUTAMATE - CREATINE Dodecanoic acid - PALMITATE Octanoate DEOXYGUANOSINE - ACETOIN 3-Hydroxysebacic acid GLUTARATE - ADIPATE 2-METHYLGLUTARATE MONOMETHYLGLUTARATE METHYGLUTARATE 7-HYDROXYOCTANOATE Azelaic acid - AZELATE - 2-ETHYLOCTANEDIOATE SEBACATE - SUBERATE Dimethyl adipate undecanedioic acid - 6-CARBOXYHEXANOATE · URIDINE 5'-DIPHOSPHATE · URIDINE octanoylcarnitine - HYDROXYISOCAPROIC - GLYCERALDEHYDE - LACTATE BETAINE ALDEHYDE - L-CARNITINE hexanoylcarnitine Butyrylcarnitine MEVALONATE PYRUVATE PORPHOBILINOGEN-1 - KYNURENATE - ARGININE **RAFFINOSE** - VALINE STACHYOSE · 1-METHYL-L-HISTIDINE - L-ORNITHINE - D-ORNITHINE - 2-HYDROXYBUTYRATE - PIPECOLATE - LPC(18:1) - KYNURENINE - OXOPROLINE - URATE-2 - URATE-1 · TRIGONELLINE SALSOLINOL-2 SALSOLINOL-1 3-HYDROXYMETHYLGLUTARATE - 4-GUANIDINOBUTANOATE - METHYLTHIOADENOSINE 2-HYDROXYPYRIDINE GLYCERATE - SUCCINATE URACIL-1 - N-ACETYLNEURAMINATE - 2-KETOHEXANOIC - 3-METHYL-2-OXOVALERATE - KETOLEUCINE - LPC(16:0) - GLYCEROPHOSPHOCHOLINE - CYTIDINE 5-HYDROXYTRYPTOPHAN - DEOXYCYTIDINE-1 - N,N-DIMETHYLARGININE BENZYLAMINE - METHYL 4-AMINOBUTYRATE - PYRIDOXINE-1 - PYRIDOXINE-2 Isovalerylcarnitine - NICOTINAMIDE-1 - BUTANOATE N-ACETYLLEUCINE N-ACETYLPHENYLALANINE - URACIL-2 - ETHYLMALONATE - ISOLEUCINE - LYSINE - PANTOTHENATE - TRYPTOPHAN - TYROSINE METHIONINE-2 - RIBOFLAVIN - NICOTINAMIDE-2 - GLUTARYLCARNITINE PROPIONYLCARNITINE - ALLANTOIN - XANTHINE-2 - PHENYLALANINE METHIONINE-1 - FOLATE - GLYCOCHENODEOXYCHOLATE - 4-ACETAMIDOBUTANOATE - GLYCOCHOLATE - HIPPURATE - 4-PYRIDOXATE - CREATININE - XANTHOSINE N-ALPHA-ACETYLLYSINE - CITRAMALATE - S-ADENOSYLMETHIONINE - 2-AMINOPHENOL-2 - N-ACETYLASPARAGINE BETAINE 4-HYDROXYBENZALDEHYDE 4-HYDROXYPHENYLPYRUVATE - PYROGLUTAMATE - NAD+ - 4-GUANIDINOBUTANOATE-2 - 3-(3,4,5-Trimethoxyphenyl)propanoic acid NICOTINATE-1 · 2-METHYLMALEATE - ITACONATE URIDINE DIPHOSPHATE-N-ACETYLGALACTOSAMINE - URIDINE DIPHOSPHATE-N-ACETYLGLUCOSAMINE UDPgalactose - URIDINE DIPHOSPHATE GLUCOSE - N-ACETYLGLYCINE N-ACETYLPUTRESCINE GUANIDINOACETATE O-ACETYLCARNITINE PROLINE O-ACETYLCARNITINE-2 cis-ACONITATE-1 · CITRATE OPHTHALMATE-2 N-ACETYLASPARTATE 02-9 -Oh- B Me3-8 -Oh- B Me3-8 -Oh- C GFP9 -Oh- A GFP9 -Oh- B GFP9 -Oh- B M3-12 -Oh- A M3-12 -Oh- B M3-12 -Oh- C 02-9 -Oh- A 02-9 -Oh- C Me3-8 -Oh- A