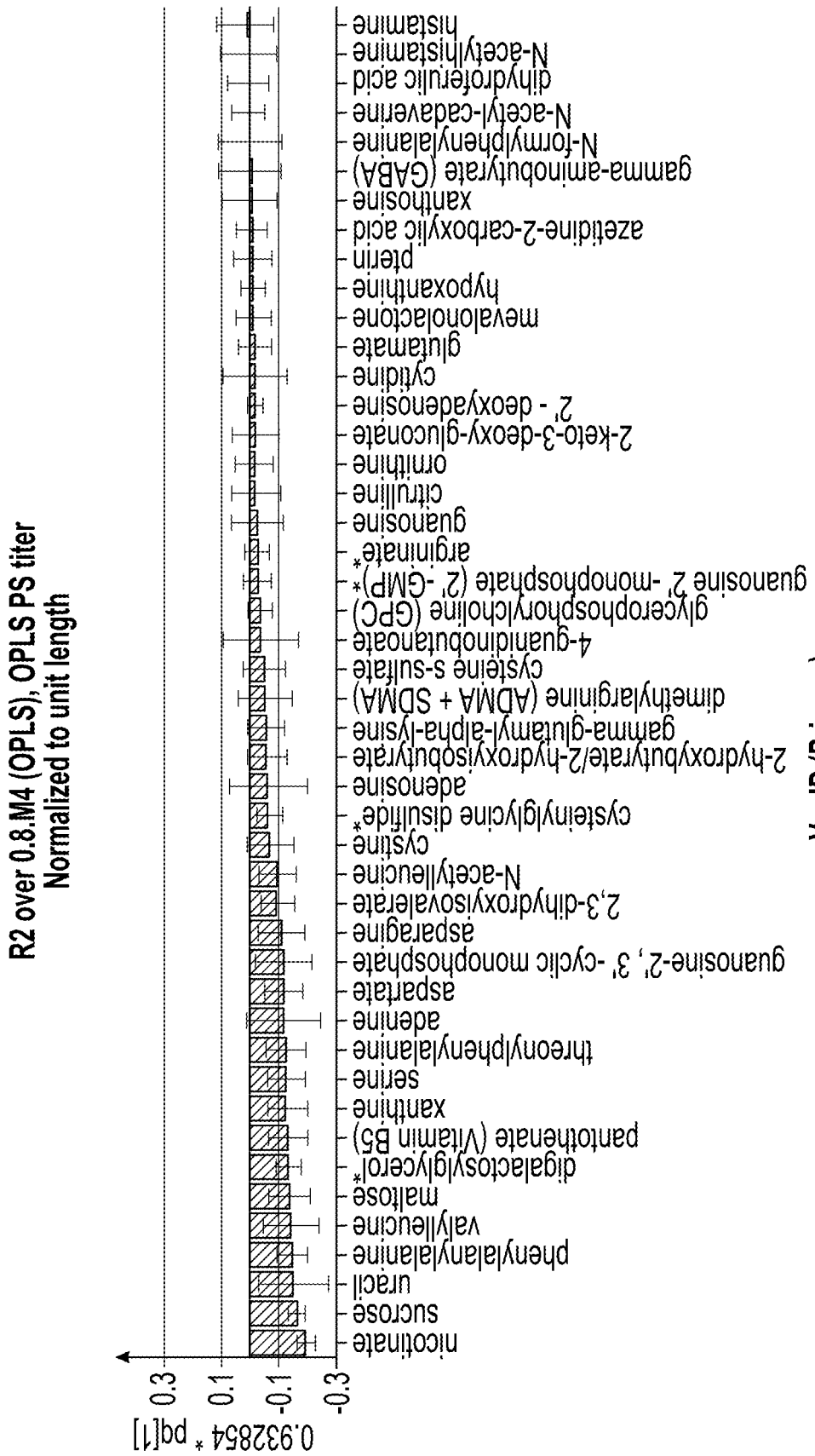
R2 over 0.8.M4 (OPLS), OPLS PS titer
Normalized to unit length
0.932854 * pq[1]
0.3
0.1
-0.1
-0.3
nicotinate
sucrose
uracil
phenylalanylalanine
valylleucine
maltose
digalactosylglycerol*
pantothenate (Vitamin B5)
xanthine
serine
threonylphenylalanine
adenine
aspartate
guanosine-2', 3'-cyclic monophosphate
asparagine
2,3-dihydroxyisovalerate
N-acetylleucine
cystine
cysteinylglycine disulfide*
adenosine
2-hydroxybutyrate/2-hydroxyisobutyrate
gamma-glutamyl-alpha-lysine
dimethylarginine (ADMA + SDMA)
cysteine s-sulfate
4-guanidinobutanoate
glycerophosphorylcholine (GPC)
guanosine 2'-monophosphate (2'-GMP)*
arginine*
guanosine
citrulline
ornithine
2-keto-3-deoxy-gluconate
2' - deoxyadenosine
cytidine
glutamate
mevalonolactone
hypoxanthine
pterin
azetidine-2-carboxylic acid
xanthosine
gamma-aminobutyrate (GABA)
N-formylphenylalanine
N-acetyl-cadaverine
dihydroferulic acid
N-acetylhistamine
histamine
Var ID (Primary)
R2X[1] = 0.159

FIG. 1