Model S1: **Metabolic model *i*HD922 of *C. difficile* 630Δ*erm***

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#########################################################################################################################################################################
#Biomass
Protein_via_tRNA                                                : 0.59772 |Charged-GLY-tRNAs| + 0.63120 |Charged-ALA-tRNAs| + 0.44284 |Charged-VAL-tRNAs| + 0.62167 |Charged-LEU-
tRNAs| + 0.37755 |Charged-ILE-tRNAs| + 0.43067 |Charged-SER-tRNAs| + 0.44035 |Charged-THR-tRNAs| + 0.26329 |Charged-PHE-tRNAs| + 0.21261 |Charged-TYR-tRNAs| + 0.06332 |Charged-
TRP-tRNAs| + 0.09966 |Charged-CYS-tRNAs| + 0.07019 |Charged-MET-tRNAs| + 0.65890 |Charged-LYS-tRNAs| + 0.27429 |Charged-ARG-tRNAs| + 0.10099 |Charged-HIS-tRNAs| + 0.47959 |
Charged-ASP-tRNAs| + 0.88041 |Charged-GLT-tRNAs| + 0.47953 |Charged-ASN-tRNAs| + 0.29371 |Charged-GLN-tRNAs| + 0.36118 |Charged-PRO-tRNAs| + 0.00094 |Charged-SEC-tRNAs| --> 1.0
Protein + 0.59772 |GLY-tRNAs| + 0.63120 |ALA-tRNAs| + 0.44284 |VAL-tRNAs| + 0.62167 |LEU-tRNAs| + 0.37755 |ILE-tRNAs| + 0.43067 |SER-tRNAs| + 0.44035 |THR-tRNAs| + 0.26329 |PHE-
tRNAs| + 0.21261 |TYR-tRNAs| + 0.06332 |TRP-tRNAs| + 0.09966 |CYS-tRNAs| + 0.07019 |MET-tRNAs| + 0.65890 |LYS-tRNAs| + 0.27429 |ARG-tRNAs| + 0.10099 |HIS-tRNAs| + 0.47959 |ASP-
tRNAs| + 0.88041 |GLT-tRNAs| + 0.47953 |ASN-tRNAs| + 0.29371 |GLN-tRNAs| + 0.36118 |PRO-tRNAs| + 0.00094 |SEC-tRNAs| + 15.56122 H+

RNA-Biosyn                                                      : 0.83394 ATP + 0.69615 UTP + 0.66708 GTP + 0.90005 CTP + 0.02785 S-adenosyl-L-methionine + 0.00657 NADPH -->
0.02128 H+ + 3.09722 diphosphate + 1.0 RNA + 0.02785 S-adenosyl-L-homocysteine + 0.00657 NADP+

DNA-Biosyn                                                      : 1.15183 dATP + 1.15183 dTTP + 0.47233 dGTP + 0.47233 dCTP + 0.00303 S-adenosyl-L-methionine --> 0.00303 H+ + 1.0
DNA + 0.00303 S-adenosyl-L-homocysteine + 3.24832 diphosphate

Lipid-Biosyn                                                    : 0.69236 Phosphatidylglycerol + 0.36976 a_cardiolipin --> 1.0 Lipid

L-CWG-Biosyn                                                    : 2.59231 UDP-N-acetyl-alpha-D-glucosamine + 1.29615 2-phospho-D-glycerate + 0.76635 UDP-alpha-D-glucose + 0.25545
|diacyl-3-Glc-16-Glc-16-Glc-glycerol| + 1.29615 ATP + 0.05676 H2O -->  1.0 L-CWG + 3.35866 UDP + 0.31221 acetate + 1.295615 ADP + 1.29615 phosphate + 3.67087 H+  # H+ = NAcGlu +
Gluc + DeAc + ATP - 2PG; H2O = 12DG + 2PG -DeAc -ATP

Peptidoglycan-Biosyn                                            : 1.17591 a_peptidoglycan --> 1.0 Peptidoglycan

P-CWG-Biosyn                                                    : 1.76376 UDP-N-acetyl-alpha-D-galactosamine + 0.88188 GDP-alpha-D-mannose + 2.64564 UDP-alpha-D-glucose --> 1.0
P-CWG + 0.88188 GMP + 4.40940 UDP + 5.29128 H+

Glycogen-Biosyn                                                 : 6.16732 |Glycogens| --> 1.0 Glycogen

Ion-Biosyn                                                      : 20.96743 K+ + 1.87732 Mg2+ + 0.14628 Fe3+ + 0.09752 Ca2+ + 1.04837 phosphate + 0.12190 diphosphate + 0.02438 Na+
+ 0.02438 Fe2+ + 0.02438 Ni2+ + 0.02438 Cd2+ + 0.02438 Zn2+ --> 1.0 Ion

Metabolite-Biosyn                                               : 0.33818 ATP + 0.08481 ADP + 0.03094 AMP + 0.17332 acetyl-CoA + 0.06667 FAD + 0.16617 NAD+ + 0.03514 NADH +
0.00043 NADP+ + 0.02501 NADPH + 0.06667 ppGpp + 0.06667 tetrahydropteroyl_tri-L-glutamate + 0.06667 di-trans,octa-cis-undecaprenyl_diphosphate + 0.06667 thiamine_diphosphate +
0.06667 adenosylcobalamin + 0.06667 Mg-protoporphyrin + 0.06667 MoO2-molybdopterin_cofactor + 0.06667 |Carboxybiotin-BCCP| + 0.06667 Me-Thr-P-GluNAc-FliC + 0.06667 pyridoxine_5'-
phosphate + 0.06667 L-threonylcarbamoyladenylate --> 1.0 Metabolites + 0.13334 |BCCP-monomers|

Protease                                                        : 1.0 Protein + 7.78061 H2O --> 0.59772 glycine + 0.63120 L-alanine + 0.44284 L-valine + 0.62167 L-leucine +
0.37755 L-isoleucine + 0.43067 L-serine + 0.44035 L-threonine + 0.26329 L-phenylalanine + 0.21261 L-tyrosine + 0.06332 L-tryptophan + 0.09966 L-cysteine + 0.07019 L-methionine +
0.65890 L-lysine + 0.27429 L-arginine + 0.10099 L-histidine + 0.47959 L-aspartate + 0.88041 L-glutamate + 0.47953 L-asparagine + 0.29371 L-glutamine + 0.36118 L-proline + 0.0094
L-selenocysteine

RNAase                                                          : 1.0 RNA + 0.02858 S-adenosyl-L-homocysteine + 0.00695 NAD+ + 3.13828 H2O --> 0.83394 AMP + 0.69615 UMP + 0.66708
GMP + 0.90005 CMP + 0.02858 S-adenosyl-L-methionine + 0.00695 NADH + 3.11665 H+

DNAase                                                          : 1.0 DNA + 0.00303 S-adenosyl-L-homocysteine + 3.24832 H2O --> 1.15220 dAMP + 1.15220 dTMP + 0.47195 dGMP +
0.47195 dCMP + 0.00303 S-adenosyl-L-methionine + 3.24529 H+

Biomass                                                         : 0.508 Protein + 0.091 RNA + 0.043 DNA + 0.060 Lipid + 0.024 L-CWG + 0.145 Peptidoglycan + 0.097 P-CWG + 0.005
Glycogen + 0.022 Ion + 0.005 Metabolites + 45 ATP + 45 H2O --> 45 ADP + 45 phosphate + 45 H+

NGAM                                                            : 1.0 H2O + 1.0 ATP --> 1.0 ADP + 1.0 phosphate + 1.0 H+

#########################################################################################################################################################################
#EXCHANGE
###################
H+_exchange                             : 1.0 H+[ex] <=>
H2O_exchange                            : 1.0 H2O[ex] <=>
H2_exchange                             : 1.0 H2[ex] <=>
H2S_exchange                            : 1.0 hydrogen_sulfide[ex] <=>
CO2_exchange                            : 1.0 CO2[ex] <=>
CO_exchange                             : 1.0 carbon_monoxide[ex] <=>
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ammonium_exchange                              : 1.0 ammonium[ex] <=>
sulfite_exchange                               : 1.0 sulfite[ex] <=>

phosphate_exchange                             : 1.0 phosphate[ex] <=>
selenide_exchange                              : 1.0 selenide[ex] <=>

Co2+_exchange                                  : 1.0 Co2+[ex] <=>
Na+_exchange                                   : 1.0 Na+[ex] <=>
K+_exchange                                    : 1.0 K+[ex] <=>
Mg2+_exchange                                  : 1.0 Mg2+[ex] <=>
Fe2+_exchange                                  : 1.0 Fe2+[ex] <=>
Fe3+_exchange                                  : 1.0 Fe3+[ex] <=>
Ca2+_exchange                                  : 1.0 Ca2+[ex] <=>
Ni2+_exchange                                  : 1.0 Ni2+[ex] <=>
Cd2+_exchange                                  : 1.0 Cd2+[ex] <=>
Zn2+_exchange                                  : 1.0 Zn2+[ex] <=>
molybdate_exchange                             : 1.0 molybdate[ex] <=>

D-Glucose_exchange                            : 1.0 D-glucose[ex] <=>
urea_exchange                                  : 1.0 urea[ex] <=>
methanethiol_exchange                          : 1.0 methanethiol[ex] <=>

ethanol_exchange                              : 1.0 ethanol[ex] <=>
propanol_exchange                             : 1.0 n-propanol[ex] <=>
butanol_exchange                              : 1.0 n-butanol[ex] <=>
isobutanol_exchange                           : 1.0 isobutanol[ex] <=>
4-methylphenol_exchange                       : 1.0 4-methylphenol[ex] <=>
acetone_exchange                              : 1.0 acetone[ex] <=>

(R)-pantothenate_exchange                      : 1.0 (R)-pantothenate[ex] <=>
biotin_exchange                                : 1.0 biotin[ex] <=>
pyridoxine_exchange                            : 1.0 pyridoxine[ex] <=>

2-aminobutanoate_exchange                      : 1.0 (S)-2-aminobutanoate[ex] <=>
S-methyl-5-thio-D-ribose_exchange              : 1.0 S-methyl-5-thio-D-ribose[ex] <=>
5-aminopentanoate_exchange                     : 1.0 5-aminopentanoate[ex] <=>
THMF_exchange                                  : 1.0 (2R,4S)-2-methyl-2,3,3,4-tetrahydroxytetrahydrofuran[ex] <=>
5-deoxy-D-ribose_exchange                      : 1.0 5-deoxy-D-ribose[ex] <=>
beta-alanine_exchange                          : 1.0 beta-alanine[ex] <=>
3-amino-2-methylpropanoate_exchange            : 1.0 (R)-3-amino-2-methylpropanoate[ex] <=>
aminoaceton_exchange                           : 1.0 aminoacetone[ex] <=>
glycolaldehyde_exchange                        : 1.0 glycolaldehyde[ex] <=>
S-methyl-5-thio-alpha-D-ribose_1-phosphate_exchange      : 1.0 S-methyl-5-thio-alpha-D-ribose_1-phosphate[ex] <=>



valine_exchange                             : 1.0 L-valine[ex] <=>
leucine_exchange                            : 1.0 L-leucine[ex] <=>
isoleucine_exchange                         : 1.0 L-isoleucine[ex] <=>
tryptophan_exchange                         : 1.0 L-tryptophan[ex] <=>
cysteine_exchange                           : 1.0 L-cysteine[ex] <=>
methionine_exchange                         : 1.0 L-methionine[ex] <=>
proline_exchange                            : 1.0 L-proline[ex] <=>

glycine_exchange                            : 1.0 glycine[ex] <=>
alanine_exchange                            : 1.0 L-alanine[ex] <=>
aspartate_exchange                          : 1.0 L-aspartate[ex] <=>
glutamate_exchange                          : 1.0 L-glutamate[ex] <=>
serine_exchange                             : 1.0 L-serine[ex] <=>
threonine_exchange                          : 1.0 L-threonine[ex] <=>
tyrosine_exchange                           : 1.0 L-tyrosine[ex] <=>
phenylalanine_exchange                      : 1.0 L-phenylalanine[ex] <=>
arginine_exchange                           : 1.0 L-arginine[ex] <=>
histidine_exchange                          : 1.0 L-histidine[ex] <=>
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lysine_exchange                           : 1.0 L-lysine[ex] <=>


formate_exchange                            : 1.0 formate[ex] <=>
acetate_exchange                            : 1.0 acetate[ex] <=>
propanoate_exchange                         : 1.0 propanoate[ex] <=>
butanoate_exchange                          : 1.0 butanoate[ex] <=>
valerate_exchange                           : 1.0 pentanoate[ex] <=>
hexanoate_exchange                          : 1.0 hexanoate[ex] <=>
(S)-lactate_exchange                        : 1.0 (S)-lactate[ex] <=>
(R)-lactate_exchange                        : 1.0 (R)-lactate[ex] <=>
isocaproate_exchange                        : 1.0 isocaproate[ex] <=>
(R)-3-hydroxybutanoate_exchange             : 1.0 (R)-3-hydroxybutanoate[ex] <=>

indole-3-acetate_exchange                   : 1.0 indole-3-acetate[ex] <=>
4-hydroxyphenylacetate_exchange             : 1.0 4-hydroxyphenylacetate[ex] <=>
phenylacetate_exchange                      : 1.0 phenylacetate[ex] <=>
4-imidazoleacetate_exchange                 : 1.0 4-imidazoleacetate[ex] <=>

3-phenylpropanoate_exchange                 : 1.0 3-phenylpropanoate[ex] <=>
3-(4-hydroxyphenyl)propanoate_exchange      : 1.0 3-(4-hydroxyphenyl)propanoate[ex] <=>

isobutyrate_exchange                        : 1.0 isobutyrate[ex] <=>
isovalerate_exchange                        : 1.0 isovalerate[ex] <=>
2-methylbutanoate_exchange                  : 1.0 2-methylbutanoate[ex] <=>
##############################################################################################################################################################################
#TRANSPORT
###################
#Diffusion

H2O_transport                                : 1.0 H2O <=> 1.0 H2O[ex]
H2_transport                                 : 1.0 H2 <=> 1.0 H2[ex]
CO2_transport                                : 1.0 CO2 <=> 1.0 CO2[ex]
CO_transport                                 : 1.0 carbon_monoxide <=> 1.0 carbon_monoxide[ex]
H2S_transport                                : 1.0 hydrogen_sulfide <=> hydrogen_sulfide[ex]
methanethiol_transport                       : 1.0 methanethiol <=> 1.0 methanethiol[ex]

#No ammonium transporter (amtB/nrgA)
#Ammonium can diffuse with the gradient across the membrane (Kleiner 1985)
#Usually no import necessary due to amino acid degradation
spontaneous_no-pathway_RXN-11811             : 1.0 ammonia + 1.0 H+ <=> 1.0 ammonium  # metacyc
ammonia_transport                            : 1.0 ammonia <=> 1.0 ammonia[ex]
spontaneous_no-pathway_RXN-11811[ex]         : 1.0 ammonia[ex] + 1.0 H+[ex] <=> 1.0 ammonium[ex]  # metacyc

#Diffusion as uncharged molecule assumed
spontaneous_sulfite_dissotiation             : 1.0 sulfite + 2.0 H+ <=> 1.0 SO2 + H2O
sulfite_transport                            : 1.0 SO2 <=> 1.0 SO2[ex]
spontaneous_sulfite_dissotiation[ex]         : 1.0 sulfite[ex] + 2.0 H+[ex] <=> 1.0 SO2[ex] + H2O[ex]

#Diffusion as uncharged molecule assumed
spontaneous_selenide_dissotiation            : 1.0 hydrogen_selenide <=> 2.0 H+ + 1.0 selenide
selenide_transport                           : 1.0 hydrogen_selenide <=> 1.0 hydrogen_selenide[ex]
spontaneous_selenide_dissotiation[ex]        : 1.0 hydrogen_selenide[ex] <=> 2.0 H+[ex] + 1.0 selenide[ex]

#products
ethanol_transport                            : 1.0 ethanol <=> 1.0 ethanol[ex]
propanol_transport                           : 1.0 n-propanol <=> 1.0 n-propanol[ex]
butanol_transport                            : 1.0 n-butanol <=> 1.0 n-butanol[ex]
isobutanol_transport                         : 1.0 isobutanol <=> 1.0 isobutanol[ex]
4-methylphenol_transport                     : 1.0 4-methylphenol <=> 1.0 4-methylphenol[ex]
acetone_transport                            : 1.0 acetone <=> 1.0 acetone[ex]

#small-quantity products/deadends
aminoaceton_transport                        : 1.0 aminoacetone <=> 1.0 aminoacetone[ex]
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urea_transport                                  : 1.0 urea <=> 1.0 urea[ex]
THMF_transport                                  : 1.0 (2R,4S)-2-methyl-2,3,3,4-tetrahydroxytetrahydrofuran <=> 1.0 (2R,4S)-2-methyl-2,3,3,4-tetrahydroxytetrahydrofuran[ex]
S-methyl-5-thio-D-ribose_transport                        : 1.0 S-methyl-5-thio-D-ribose <=> 1.0 S-methyl-5-thio-D-ribose[ex]
S-methyl-5-thio-alpha-D-ribose_1-phosphate_transport      : 1.0 S-methyl-5-thio-alpha-D-ribose_1-phosphate <=> 1.0 S-methyl-5-thio-alpha-D-ribose_1-phosphate[ex]
5-deoxy-D-ribose_transport                                : 1.0 5-deoxy-D-ribose <=> 1.0 5-deoxy-D-ribose[ex]
glycolaldehyde_transport                                  : 1.0 glycolaldehyde <=> 1.0 glycolaldehyde[ex]
####################
#Weak acids

##CDIF630erm_03708,CDIF630erm_02463
formate_transport                               : 1.0 H+ + 1.0 formate <=> 1.0 formate[ex] + 1.0 H+[ex]
acetate_transport                               : 1.0 H+ + 1.0 acetate <=> 1.0 acetate[ex] + 1.0 H+[ex]
propanoate_transport                            : 1.0 H+ + 1.0 propanoate <=> 1.0 propanoate[ex] + 1.0 H+[ex]
n-butanoate_transport                           : 1.0 H+ + 1.0 butanoate <=> 1.0 butanoate[ex] + 1.0 H+[ex]
pentanoate_transport                            : 1.0 H+ + 1.0 pentanoate <=> 1.0 pentanoate[ex] + 1.0 H+[ex]
hexanoate_transport                             : 1.0 H+ + 1.0 hexanoate <=> 1.0 hexanoate[ex] + 1.0 H+[ex]
(R)-3-hydroxybutanoate_transport                : 1.0 H+ + 1.0 (R)-3-hydroxybutanoate <=> 1.0 (R)-3-hydroxybutanoate[ex] + 1.0 H+[ex]
##CDIF630erm_00920
(S)-lactate_transport                           : 1.0 Na+ + 1.0 (S)-lactate <=> 1.0 (S)-lactate[ex] + 1.0 Na+[ex]
(R)-lactate_transport                           : 1.0 Na+ + 1.0 (R)-lactate <=> 1.0 (R)-lactate[ex] + 1.0 Na+[ex]

indole-3-acetate_transport                      : 1.0 H+ + 1.0 indole-3-acetate <=> 1.0 indole-3-acetate[ex] + 1.0 H+[ex]
4-hydroxyphenylacetate_transport                : 1.0 H+ + 1.0 4-hydroxyphenylacetate <=> 1.0 4-hydroxyphenylacetate[ex] + 1.0 H+[ex]
phenylacetate_transport                         : 1.0 H+ + 1.0 phenylacetate <=> 1.0 phenylacetate[ex] + 1.0 H+[ex]
4-imidazoleacetate_transport                    : 1.0 H+ + 1.0 4-imidazoleacetate <=> 1.0 4-imidazoleacetate[ex] + 1.0 H+[ex]

3-phenylpropanoate_transport                    : 1.0 H+ + 1.0 3-phenylpropanoate <=> 3-phenylpropanoate[ex] + 1.0 H+[ex]
3-(4-hydroxyphenyl)propanoate_transport         : 1.0 H+ + 1.0 3-(4-hydroxyphenyl)propanoate <=> 3-(4-hydroxyphenyl)propanoate[ex] + 1.0 H+[ex]

isobutyrate_transport                           : 1.0 H+ + 1.0 isobutyrate <=> 1.0 isobutyrate[ex] + 1.0 H+[ex]
isovalerate_transport                           : 1.0 H+ + 1.0 isovalerate <=> 1.0 isovalerate[ex] + 1.0 H+[ex]
2-methylbutanoate_transport                     : 1.0 H+ + 1.0 2-methylbutanoate <=> 1.0 2-methylbutanoate[ex] + 1.0 H+[ex]
isocaproate_transport                           : 1.0 H+ + 1.0 isocaproate <=> 1.0 isocaproate[ex] + 1.0 H+[ex]
####################
#Amino acids

##CDIF630erm_02711; CDIF630erm_01724
threonine_antiport                              : 1.0 L-serine[ex] + 1.0 L-threonine <=> 1.0 L-serine + 1.0 L-threonine[ex]

##CDIF630erm_02948
serine_transport                                : 1.0 Na+ + 1.0 L-serine <=> 1.0 Na+[ex] + 1.0 L-serine[ex]
threonine_transport                             : 1.0 Na+ + 1.0 L-threonine <=> 1.0 Na+[ex] + 1.0 L-threonine[ex]

##CDIF630erm_02511, CDIF630erm_02664
alanine_transport                               : 1.0 Na+ + 1.0 L-alanine <=> 1.0 Na+[ex] + 1.0 L-alanine[ex]
#glycine similar to alanine
glycine_transport                               : 1.0 Na+ + 1.0 glycine <=> 1.0 Na+[ex] + 1.0 glycine[ex]

##CDIF630erm_02521, CDIF630erm_02522; CDIF630erm_02958; CDIF630erm_01412; CDIF630erm_01413; CDIF630erm_00949
valine_transport                                : 1.0 Na+ + 1.0 L-valine <=> 1.0 Na+[ex] + 1.0 L-valine[ex]
leucine_transport                               : 1.0 Na+ + 1.0 L-leucine <=> 1.0 Na+[ex] + 1.0 L-leucine[ex]
isoleucine_transport                            : 1.0 Na+ + 1.0 L-isoleucine <=> 1.0 Na+[ex] + 1.0 L-isoleucine[ex]

##CDIF630erm_02197
tryptophan_transport                            : 1.0 Na+ + 1.0 L-tryptophan <=> 1.0 Na+[ex] + 1.0 L-tryptophan[ex]

##CDIF630erm_00949? Used by the Leu-Operon; CDIF630erm_02197? Similar to trp
tyrosine_transport                              : 1.0 Na+ + 1.0 L-tyrosine <=> 1.0 Na+[ex] + 1.0 L-tyrosine[ex]
phenylalanine_transport                         : 1.0 Na+ + 1.0 L-phenylalanine <=> 1.0 Na+[ex] + 1.0 L-phenylalanine[ex]

##CDIF630erm_01940
glutamate_transport                             : 1.0 Na+ + 1.0 L-glutamate <=> 1.0 L-glutamate[ex] + 1.0 Na+[ex]

#Transport unknown, Na+ symport as a guess
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```
proline_transport                              : 1.0 Na+ + 1.0 L-proline <=> 1.0 Na+[ex] + 1.0 L-proline[ex]
cysteine_transport                             : 1.0 Na+ + 1.0 L-cysteine <=> 1.0 Na+[ex] + 1.0 L-cysteine[ex]
lysine_transport                               : 1.0 Na+ + 1.0 L-lysine <=> 1.0 Na+[ex] + 1.0 L-lysine[ex]
5-aminopentanoate_transport                    : 1.0 Na+ + 1.0 5-aminopentanoate <=> 1.0 Na+[ex] + 1.0 5-aminopentanoate[ex]
2-aminobutanoate_transport                     : 1.0 Na+ + 1.0 (S)-2-aminobutanoate <=> 1.0 Na+[ex] + 1.0 (S)-2-aminobutanoate[ex]
beta-alanine_transport                         : 1.0 Na+ + 1.0 beta-alanine <=> 1.0 Na+[ex] + 1.0 beta-alanine[ex]
(R)-pantothenate_transport                     : 1.0 Na+ + 1.0 (R)-pantothenate <=> 1.0 Na+[ex] + 1.0 (R)-pantothenate[ex]
(R)-3-amino-2-methylpropanoate_transport       : 1.0 Na+ + 1.0 (R)-3-amino-2-methylpropanoate[ex] <=> 1.0 Na+[ex] + 1.0 (R)-3-amino-2-methylpropanoate

#CDIF630erm_00868-CDIF630erm_00870
arginine_3.6.3.-_transport                     : 1.0 H2O + 1.0 ATP + 1.0 L-arginine[ex] --> 1.0 H+ + 1.0 phosphate + 1.0 ADP + 1.0 L-arginine

##CDIF630erm_01654-CDIF630erm_01656
methionine_transport                           : 1.0 L-methionine[ex] + 1.0 H2O + 1.0 ATP --> 1.0 ADP + 1.0 L-methionine + 1.0 phosphate + 1.0 H+

#unknown, ABC-transporter is a guess
##CDIF630erm_01972-CDIF630erm_01974?; CDIF630erm_00868-CDIF630erm_00870?
aspartate_transport                            : 1.0 H2O + 1.0 L-aspartate[ex] + 1.0 ATP --> 1.0 L-aspartate + 1.0 ADP + 1.0 phosphate + 1.0 H+
histidine_transport                            : 1.0 H2O + 1.0 ATP + 1.0 L-histidine[ex] --> 1.0 H+ + 1.0 phosphate + 1.0 ADP + 1.0 L-histidine
pyridoxine_transport                           : 1.0 H2O + 1.0 ATP + 1.0 pyridoxine[ex] --> 1.0 H+ + 1.0 phosphate + 1.0 ADP + 1.0 pyridoxine
####################
#ABC-Transport

phosphate_transport                            : 1.0 H2O + 1.0 ATP + 1.0 phosphate[ex] --> 1.0 ADP + 2.0 phosphate + 1.0 H+

Ni2+_transport                                 : 1.0 H2O + 1.0 ATP + 1.0 Ni2+[ex] --> 1.0 Ni2+ + 1.0 ADP + 1.0 phosphate + 1.0 H+
#CDIF630erm_00452-CDIF630erm_00455
Co2+_transport_3.6.3.2_3.6.3.5                 : 1.0 H2O + 1.0 Co2+[ex] + 1.0 ATP --> 1.0 phosphate + 1.0 ADP + 1.0 Co2+ + 1.0 H+
Mg2+_transport_3.6.3.2_                        : 1.0 H2O + 1.0 Mg2+[ex] + 1.0 ATP --> 1.0 Mg2+ + 1.0 phosphate + 1.0 ADP + 1.0 H+
Fe3+_transport_3.6.3.30                        : 1.0 ATP + 1.0 Fe3+[ex] + 1.0 H2O --> 1.0 ADP + 1.0 Fe3+ + 1.0 phosphate + 1.0 H+
K+_transport_3.6.3.12                          : 1.0 H2O + 1.0 K+[ex] + 1.0 ATP --> 1.0 K+ + 1.0 phosphate + 1.0 ADP + 1.0 H+
Ca2+_transport_3.6.3.8                         : 1.0 ATP + 1.0 H2O + 1.0 Ca2+[ex] --> 1.0 phosphate + 1.0 ADP + 1.0 Ca2+ + 1.0 H+
##CDIF630erm_00989-CDIF630erm_00991
molybdate_transport_3.6.3.29                   : 1.0 H2O + 1.0 ATP + 1.0 molybdate[ex] --> 1.0 phosphate + 1.0 ADP + 1.0 molybdate + 1.0 H+
##CDIF630erm_01641 - CDIF630erm_01643; CDIF630erm_01684, CDIF630erm_01685; CDIF630erm_01939; CDIF630erm_03573, CDIF630erm_03574
Fe2+_transport                                 : 1.0 GTP + 1.0 H2O + 1.0 Fe2+[ex] --> 1.0 phosphate + 1.0 H+ + 1.0 GDP  + 1.0 Fe2+
Cd2+_transport_3.6.3.3                         : 1.0 H2O + 1.0 ATP + 1.0 Cd2+[ex] <=> 1.0 Cd2+ + 1.0 ADP + 1.0 phosphate + 1.0 H+
Zn2+_transport_3.6.3.5                         : 1.0 Zn2+[ex] + 1.0 ATP + 1.0 H2O --> 1.0 Zn2+ + 1.0 phosphate + 1.0 ADP + 1.0 H+

####################
#Other

##CDIF630erm_03256
biotin_transport                               : 1.0 biotin[ex] <=> 1.0 biotin

##CDIF630erm_02351
Mg2+_transport                                 : 1.0 Mg2+[ex] <-- 1.0 Mg2+

##CDIF630erm_01919
PO4/Na_transport                               : 1.0 Na+[ex] + 1.0 phosphate[ex] <=> 1.0 Na+ + 1.0 phosphate

##CDIF630erm_02923; CDIF630erm_02325; CDIF630erm_03939
potassium_transport                            : 1.0 K+[ex] + 1.0 H+ <=> 1.0 K+ + 1.0 H+[ex]


####################
#Proton and Na+ transport

#10 c-subunits (9-12 normal?) in E.coli (Jiang et al., 2001) --> 3.3 H+/ATP
#F-type-ATPase_transport_3.6.3.14_mod_ATPSYN-RXN                        : 1.0 H2O + 1.0 ATP + 2.33333 H+ <=> 1.0 phosphate + 1.0 ADP + 3.33333 H+[ex]
#F-type-ATPase_transport_3.6.3.14_mod_ATPSYN-RXN                        : 1.0 H2O + 1.0 ATP + 2.66667 H+ <=> 1.0 phosphate + 1.0 ADP + 3.66667 H+[ex]
#F-type-ATPase_transport_3.6.3.14_mod_ATPSYN-RXN                        : 1.0 H2O + 1.0 ATP + 3 H+ <=> 1.0 phosphate + 1.0 ADP + 4 H+[ex]
F-type-ATPase_transport_3.6.3.14_mod_ATPSYN-RXN                       : 1.0 H2O + 1.0 ATP + 3.33333 H+ <=> 1.0 phosphate + 1.0 ADP + 4.33333 H+[ex]
```

```
#Subunit K is highly similar to E. hirae; E. hirae has 10 K-subunits per ATPase (Murata et al., 2005) --> 3.3 Na+/ATP
#V-type-ATPase_transport_3.6.3.15_mod_3.6.3.15-RXN                      : 1.0 H2O + 1.0 ATP + 3.33333 Na+ <=> 1.0 phosphate + 1.0 ADP + 3.33333 Na+[ex] + 1.0 H+
#V-type-ATPase_transport_3.6.3.15_mod_3.6.3.15-RXN                      : 1.0 H2O + 1.0 ATP + 3.66667 Na+ <=> 1.0 phosphate + 1.0 ADP + 3.66667 Na+[ex] + 1.0 H+
#V-type-ATPase_transport_3.6.3.15_mod_3.6.3.15-RXN                      : 1.0 H2O + 1.0 ATP + 4 Na+ <=> 1.0 phosphate + 1.0 ADP + 4 Na+[ex] + 1.0 H+
V-type-ATPase_transport_3.6.3.15_mod_3.6.3.15-RXN                      : 1.0 H2O + 1.0 ATP + 4.33333 Na+ <=> 1.0 phosphate + 1.0 ADP + 4.33333 Na+[ex] + 1.0 H+

##CDIF630erm_01284-CDIF630erm_01289
#Proton dependence assumed because the Rnf-complex of C. ljungdahlii is proton dependent (Tremblay et al., 2013)
#Reversible in vitro in A. woodii (Hess et al., 2013)
rnfABCDEG_transport                                                    : 2.0 |Reduced-ferredoxins| + 1.0 NAD+ + 3.0 H+ <=> 2.0 |Oxidized-ferredoxins| + 1.0 NADH + 2.0 H+[ex]

##CDIF630erm_00770; CDIF630erm_02996; CDIF630erm_02923
sodium_transport                                                       : 1.0 Na+[ex] + 1.0 H+ <=> 1.0 Na+ + 1.0 H+[ex]

#############Glucose PTS-system#############
PTS-system_2.7.3.9_2.7.3.9-RXN                          : 1.0 phosphoenolpyruvate + 1.0 |PTS-I-Histidines| --> 1.0 pyruvate + 1.0 |PTS-I-pi-phospho-L-histidines|  # source:
MetaCyc (queried 2.7.3.9)
glucose_transport_2.7.1.199                             : 1.0 |PTS-I-pi-phospho-L-histidines| + 1.0 D-glucose[ex] --> 1.0 |PTS-I-Histidines| + 1.0 D-glucose_6-phosphate
#########################################################################################################################################################################
#glycolysis I:

glycolysis-I/1_5.3.1.9_PGLUCISOM-RXN                    : 1.0 D-glucose_6-phosphate <=> 1.0 beta-D-fructofuranose_6-phosphate  # source: MetaCyc, BRENDA, KEGG (queried
5.3.1.9)
glycolysis-I/2b_3.1.3.11_F16BDEPHOS-RXN                 : 1.0 fructose_1,6-bisphosphate + 1.0 H2O --> 1.0 beta-D-fructofuranose_6-phosphate + 1.0 phosphate  # source: MetaCyc,
BRENDA, KEGG (queried 3.1.3.11)
glycolysis-I/2a_2.7.1.11_6PFRUCTPHOS-RXN                : 1.0 beta-D-fructofuranose_6-phosphate + 1.0 ATP --> 1.0 fructose_1,6-bisphosphate + 1.0 H+ + 1.0 ADP  # source:
MetaCyc, BRENDA, KEGG (queried 2.7.1.11)
glycolysis-I/3_4.1.2.13_F16ALDOLASE-RXN                 : 1.0 fructose_1,6-bisphosphate <=> 1.0 D-glyceraldehyde_3-phosphate + 1.0 glycerone_phosphate  # source: MetaCyc,
BRENDA, KEGG (queried 4.1.2.13)
glycolysis-I/p4_5.3.1.1_TRIOSEPISOMERIZATION-RXN        : 1.0 D-glyceraldehyde_3-phosphate <=> 1.0 glycerone_phosphate  # source: MetaCyc, BRENDA, KEGG (queried 5.3.1.1)
glycolysis-I/4_1.2.1.12_GAPDHSYNEC-RXN_WOP              : 1.0 D-glyceraldehyde_3-phosphate + 1.0 phosphate + 1.0 NAD+ <=> 1.0 1,3-bisphospho-D-glycerate + 1.0 NADH + 1.0 H+  #
ource: MetaCyc, BRENDA, KEGG (queried 1.2.1.12) // other EC numbers for this reaction: 1.2.1.13, 1.2.1.59
glycolysis-I/5_2.7.2.3_PHOSGLYPHOS-RXN                  : 1.0 3-phospho-D-glycerate + 1.0 ATP <=> 1.0 ADP + 1.0 1,3-bisphospho-D-glycerate  # source: MetaCyc, BRENDA, KEGG
(queried 2.7.2.3)
glycolysis-I/6_5.4.2.12_3PGAREARR-RXN                   : 1.0 2-phospho-D-glycerate <=> 1.0 3-phospho-D-glycerate  # source: MetaCyc, BRENDA, KEGG (queried 5.4.2.12) // other
EC numbers for this reaction: 5.4.2.11
glycolysis-I/7_4.2.1.11_2PGADEHYDRAT-RXN                : 1.0 2-phospho-D-glycerate <=> 1.0 H2O + 1.0 phosphoenolpyruvate  # source: MetaCyc, BRENDA, KEGG (queried 4.2.1.11)
glycolysis-I/8_2.7.1.40_PEPDEPHOS-RXN                   : 1.0 ATP + 1.0 pyruvate <=> 1.0 phosphoenolpyruvate + 1.0 ADP + 1.0 H+  # source: MetaCyc, BRENDA, KEGG (queried
2.7.1.40)

#glycolysis IV
glycolysis-IV/2c_2.7.1.90_2.7.1.90-RXN                  : 1.0 diphosphate + 1.0 beta-D-fructofuranose_6-phosphate <=> 1.0 fructose_1,6-bisphosphate + 1.0 phosphate + 1.0 H+  #
source: MetaCyc, BRENDA, KEGG (queried 2.7.1.90)
glycolysis-IV/4b_1.2.1.9_1.2.1.9-RXN                    : 1.0 NADP+ + 1.0 H2O + 1.0 D-glyceraldehyde_3-phosphate --> 1.0 3-phospho-D-glycerate + 2.0 H+ + 1.0 NADPH  # source:
MetaCyc, BRENDA, KEGG (queried 1.2.1.9) // other EC numbers for this reaction: 1.2.1.90
#
glycolysis-C/8b_2.7.9.1_PYRUVATEORTHOPHOSPHATE-DIKINASE-RXN : 1.0 phosphate + 1.0 ATP + 1.0 pyruvate --> 1.0 diphosphate + 1.0 phosphoenolpyruvate + 1.0 H+ + 1.0 AMP  # source:
MetaCyc, BRENDA, KEGG (queried 2.7.9.1)
#########################################################################################################################################################################
#methylglyoxal-degradation-I
#S-lactoyl-glutathione not found in all tested Clostridia (Fahey et al., 1978) and no 6.3.2.2/3 found in Cdiff; probably other coenzyme

methylglyoxal-degradation-I/p1_4.2.3.3_METHGLYSYN-RXN   : 1.0 glycerone_phosphate --> 1.0 methylglyoxal + 1.0 phosphate  # source: MetaCyc, BRENDA, KEGG (queried 4.2.3.3)
methylglyoxal-degradation-I/1_4.4.1.5_GLYOXI-RXN        : 1.0 (R)-S-lactoylglutathione <=> 1.0 methylglyoxal + 1.0 glutathione  # source: MetaCyc, BRENDA, KEGG (queried
4.4.1.5)
methylglyoxal-degradation-I/2_3.1.2.6_GLYOXII-RXN       : 1.0 H2O + 1.0 (R)-S-lactoylglutathione --> 1.0 glutathione + 1.0 (R)-lactate + 1.0 H+  # source: MetaCyc, BRENDA,
KEGG (queried 3.1.2.6)
#########################################################################################################################################################################
#Wood-Ljungdahl
#Pathway can act in the reverse direction (Spormann and Thauer, 1988, Schauder et al., 1988)

#Reversible in C. cylindrosporum (Curthoys and Rabinowitz, 1972)
Wood-Ljungdahl/1_moddir_6.3.4.3_FORMATETHFLIG-RXN        : 1.0 formate + 1.0 ATP + 1.0 tetrahydropteroyl_tri-L-glutamate <=> 1.0 ADP + 1.0 10-formyltetrahydrofolate + 1.0
phosphate  # source: MetaCyc (queried 6.3.4.3)
```

```
Wood-Ljungdahl/2_moddir_3.5.4.9_METHENYLTHFCYCLOHYDRO-RXN   : 1.0 5,10-methenyltetrahydrofolate + 1.0 H2O <=> 1.0 H+ + 1.0 10-formyltetrahydrofolate  # source: MetaCyc, BRENDA,
KEGG (queried 3.5.4.9)
Wood-Ljungdahl/3_1.5.1.5_METHYLENETHFDEHYDROG-NADP-RXN      : 1.0 5,10-methylene-tetrahydrofolate + 1.0 NADP+ <=> 1.0 5,10-methenyltetrahydrofolate + 1.0 NADPH  # source: MetaCyc,
BRENDA, KEGG (queried 1.5.1.5)
#Bifurcating methylene-tetrahydrofolate reductase as proposed C. ljungdahlii and C. autoethanogenum (Köpke et al. 2010, Nagarajan et al. 2013, Mock et al. 2015)
Wood-Ljungdahl/4_manual_1.5.-_HD-MetFV                      : 1.0 N5-methyl-tetrahydrofolate  + 2.0 |Reduced-ferredoxins| + 2.0 NAD+ <-- 1.0 5,10-methylene-tetrahydrofolate + 2.0
NADH + 2.0 |Oxidized-ferredoxins|
Wood-Ljungdahl/5_2.1.1.258_METHCOCLTH-RXN                   : 1.0 |Methylated-corrinoid-Fe-S-Proteins| + 1.0 tetrahydropteroyl_tri-L-glutamate <=> 1.0 H+ + 1.0 |CoI-Corrinoid-Fe-
S-proteins| + 1.0 N5-methyl-tetrahydrofolate  # source: MetaCyc (queried 2.1.1.258)
#CDIF630erm_00832: 1.2.7.4 in Wood-Ljungdahl-Operon; production of CO with Ferredoxins used; only <-- because of CO degradation (see below)
Wood-Ljungdahl/p6_moddir_1.2.7.4_1.2.7.4-RXN                : 1.0 H2O + 1.0 carbon_monoxide + 2.0 |Oxidized-ferredoxins| <-- 2.0 H+ + 1.0 CO2 + 2.0 |Reduced-ferredoxins|  #
source: MetaCyc, KEGG (queried 1.2.7.4) // other EC numbers for this reaction: 1.2.99.2
Wood-Ljungdahl/6_2.3.1.169_ACETYLSYNCLTH-RXN                : 1.0 H+ + 1.0 acetyl-CoA + 1.0 |CoI-Corrinoid-Fe-S-proteins| <=> 1.0 |Methylated-corrinoid-Fe-S-Proteins| + 1.0
coenzyme_A + 1.0 carbon_monoxide  # source: MetaCyc, BRENDA (queried 2.3.1.169)
##########################################################################################################################################################################
#CO degradation C (CDIF630erm_00296-CDIF630erm_00298)
CO-drgradation-C_manual_HD-CO-DEHYD                         : 1.0 carbon_monoxide + 1.0 H2O + 1.0 NAD+ --> 1.0 CO2 + 1.0 NADH + 1.0 H+
##########################################################################################################################################################################
#Dihydrogen
dihydrogen-production-A_moddir_1.12.7.2_HYDROG-RXN                : 2.0 |Oxidized-ferredoxins| + 1.0 H2 <-- 2.0 H+ + 2.0 |Reduced-ferredoxins|  # source: MetaCyc, KEGG (queried
1.12.7.2) // other EC numbers for this reaction: 1.12.99
#Homolog to the bifurcating hydrogenase of T. maritima (Schut and Adams, 2009)
dihydrogen-production-B_manual_1.12.1.-_HD-Bifur-Hyd              : 2.0 |Oxidized-ferredoxins| + 2.0 H2 + 1.0 NADP+ <=> 3.0 H+ + 1.0 NADPH + 2.0 |Reduced-ferredoxins|
#CDIF630erm_03614-CDIF630erm_03619 (Calusinska et al. 2010)
dihydrogen-production-C_manual_1.1.99.33_1.12.1.3_HD-Form-Hyd     : 1.0 H+ + 1.0 formate --> 1.0 CO2 + 1.0 H2
##########################################################################################################################################################################
#ppp non-ox
ppp-non-ox/1a_5.3.1.6_RIB5PISOM-RXN                         : 1.0 D-ribose_5-phosphate <=> 1.0 D-ribulose_5-phosphate  # source: MetaCyc, BRENDA, KEGG (queried 5.3.1.6)
ppp-non-ox/1b_5.1.3.1_RIBULP3EPIM-RXN                       : 1.0 D-ribulose_5-phosphate <=> 1.0 D-xylulose_5-phosphate  # source: MetaCyc, BRENDA, KEGG (queried 5.1.3.1)
ppp-non-ox/2_2.2.1.1_R06863                                 : 1.0 thiamine_diphosphate + 1.0 D-sedoheptulose_7-phosphate <=> 1.0 D-ribose_5-phosphate + 1.0 alpha,beta-
Dihydroxyethyl-TPP  # source: KEGG (queried 2.2.1.1)
ppp-non-ox/3_2.2.1.1_R06861                                 : 1.0 D-xylulose_5-phosphate + 1.0 thiamine_diphosphate <=> 1.0 D-glyceraldehyde_3-phosphate + 1.0 alpha,beta-
Dihydroxyethyl-TPP  # source: KEGG (queried 2.2.1.1) // other EC numbers for this reaction: 2.2.1.3
ppp-non-ox/4_2.2.1.2_TRANSALDOL-RXN                         : 1.0 D-glyceraldehyde_3-phosphate + 1.0 D-sedoheptulose_7-phosphate <=> 1.0 beta-D-fructofuranose_6-phosphate + 1.0 D-
erythrose_4-phosphate  # source: MetaCyc, BRENDA, KEGG (queried 2.2.1.2)
ppp-non-ox/5_2.2.1.1_2TRANSKETO-RXN                         : 1.0 D-xylulose_5-phosphate + 1.0 D-erythrose_4-phosphate <=> 1.0 D-glyceraldehyde_3-phosphate + 1.0 beta-D-
fructofuranose_6-phosphate  # source: MetaCyc, BRENDA, KEGG (queried 2.2.1.1) // other EC numbers for this reaction: 2.2.1.3

PRPP-biosynthesis-I_2.7.6.1_PRPPSYN-RXN                     : 1.0 D-ribose_5-phosphate + 1.0 ATP <=> 1.0 H+ + 1.0 AMP + 1.0 5-phospho-alpha-D-ribose_1-diphosphate  # source:
MetaCyc, BRENDA, KEGG (queried 2.7.6.1)

#side reactions
sedoheptulose-bisphosphate-bypass_2.7.1.11_RXN0-6541                      : 1.0 D-sedoheptulose_7-phosphate + 1.0 ATP --> 1.0 ADP + 1.0 D-sedoheptulose-1,7-bisphosphate + 1.0 H+
# source: MetaCyc, KEGG (queried 2.7.1.11) // other EC numbers for this reaction: 2.7.1
sedoheptulose-bisphosphate-bypass_4.1.2.13_SEDOBISALDOL-RXN               : 1.0 glycerone_phosphate + 1.0 D-erythrose_4-phosphate <=> 1.0 D-sedoheptulose-1,7-bisphosphate  #
source: MetaCyc, BRENDA, KEGG (queried 4.1.2.13) // other EC numbers for this reaction: 4.1.2
Calvin-Benson-Bassham-cycle_3.1.3.11_SEDOHEPTULOSE-BISPHOSPHATASE-RXN      : 1.0 H2O + 1.0 D-sedoheptulose-1,7-bisphosphate --> 1.0 D-sedoheptulose_7-phosphate + 1.0 phosphate  #
source: MetaCyc, BRENDA, KEGG (queried 3.1.3.11) // other EC numbers for this reaction: 3.1.3.37
##########################################################################################################################################################################
#TCA
TCA-cycle/1_4.2.1.1_CARBODEHYDRAT-RXN                       : 1.0 hydrogen_carbonate <=> 1.0 CO2 + 1.0 H2O  # source: MetaCyc, BRENDA, KEGG (queried 4.2.1.1)
TCA-cycle/2_6.4.1.1_PYRUVATE-CARBOXYLASE-RXN                : 1.0 hydrogen_carbonate + 1.0 ATP + 1.0 pyruvate --> 1.0 phosphate + 1.0 oxaloacetate + 1.0 ADP + 1.0 H+  # source:
MetaCyc, BRENDA, KEGG (queried 6.4.1.1)
TCA-cycle/3_2.3.3.3_CITSYN-RXN                              : 1.0 H2O + 1.0 acetyl-CoA + 1.0 oxaloacetate --> 1.0 H+ + 1.0 coenzyme_A + 1.0 citrate  # source: MetaCyc, BRENDA,
KEGG (queried 2.3.3.3) // other EC numbers for this reaction: 2.3.3.16, 2.3.3.1
TCA-cycle/4_4.2.1.3_ACONITATEDEHYDR-RXN                     : 1.0 citrate <=> 1.0 H2O + 1.0 cis-aconitate  # source: MetaCyc, BRENDA, KEGG (queried 4.2.1.3)
TCA-cycle/5_4.2.1.3_ACONITATEHYDR-RXN                       : 1.0 cis-aconitate + 1.0 H2O <=> 1.0 D-threo-isocitrate  # source: MetaCyc, BRENDA, KEGG (queried 4.2.1.3)
TCA-cycle/6_1.1.1.41_ISOCITRATE-DEHYDROGENASE-NAD+-RXN      : 1.0 D-threo-isocitrate + 1.0 NAD+ --> 1.0 NADH + 1.0 2-oxoglutarate + 1.0 CO2  # source: MetaCyc, BRENDA, KEGG
(queried 1.1.1.41) // other EC numbers for this reaction: 1.1.1.286

TCA-cycle/7_4.2.1.2_FUMHYDR-RXN                             : 1.0 (S)-malate <=> 1.0 H2O + 1.0 fumarate  # source: MetaCyc, BRENDA, KEGG (queried 4.2.1.2)
TCA-cycle/8_1.1.1.38_1.1.1.39-RXN                           : 1.0 (S)-malate + 1.0 NAD+ --> 1.0 NADH + 1.0 CO2 + 1.0 pyruvate  # source: MetaCyc, BRENDA, KEGG (queried
1.1.1.38) // other EC numbers for this reaction: 1.1.1.39, 1.3.1.7
TCA-cycle/9_1.1.1.38_OXALODECARB-RXN                        : 1.0 H+ + 1.0 oxaloacetate --> 1.0 CO2 + 1.0 pyruvate  # source: MetaCyc, BRENDA, KEGG (queried 1.1.1.38) // other EC
```

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numbers for this reaction: 1.1.1.40, 4.1.1.3
#################################################################################################################################################################################
#Fatty acids I

#C. kluyveri complex characterized (Wang et al., 2010)
NADP-reduction_manual_HD-NfnAB                                  : 2.0 |Reduced-ferredoxins| + 1.0 NADH + 2.0 NADP+ + 1.0 H+ <=> 2.0 |Oxidized-ferredoxins| + 1.0 NAD+ + 2.0 NADPH

fatty-acid-I/1_6.4.1.2_ACETYL-COA-CARBOXYLTRANSFER-RXN      : 1.0 hydrogen_carbonate + 1.0 ATP + 1.0 acetyl-CoA --> 1.0 ADP + 1.0 H+ + 1.0 phosphate + 1.0 malonyl-CoA  # source:
MetaCyc, BRENDA, KEGG (queried 6.4.1.2)
fatty-acid-I/2_2.3.1.39_MALONYL-COA-ACP-TRANSACYL-RXN       : 1.0 malonyl-CoA + 1.0 Acyl-carrier_protein <=> 1.0 coenzyme_A + 1.0 Malonyl-[acyl-carrier_protein]  # source:
MetaCyc, BRENDA, KEGG (queried 2.3.1.39) // other EC numbers for this reaction: 2.3.1, 2.3.1.86, 2.3.1.85

#chain lenght: 16.246
#unsaturated: 0.164
#from C. difficile NCIB 10666 (Elsden et al., 1980)
#2.3.1.41/179/180/n2_1.1.1.100_1.3.1.9_4.2.1.59
fatty-acid-I/3a_manual_HD-acet                                  : 1.0 acetyl_phosphate + 7.123 Malonyl-[acyl-carrier_protein] + 21.205 H+ + 14.082 NADPH --> 1.0 Acyl-[acyl-
carrier_protein] + 6.123 Acyl-carrier_protein + 7.123 H2O + 7.123 CO2 + 14.082 NADP+ + 1.0 phosphate
fatty-acid-I/3b_manual_HD-prop                                  : 1.0 propanoyl_phosphate + 6.623 Malonyl-[acyl-carrier_protein] + 19.705 H+ + 13.082 NADPH --> 1.0 Acyl-[acyl-
carrier_protein] + 5.623 Acyl-carrier_protein + 6.623 H2O + 6.623 CO2 + 13.082 NADP+ + 1.0 phosphate
fatty-acid-I/3c_manual_HD-buta                                  : 1.0 butanoyl_phosphate + 6.123 Malonyl-[acyl-carrier_protein] + 18.205 H+ + 12.082 NADPH --> 1.0 Acyl-[acyl-
carrier_protein] + 5.123 Acyl-carrier_protein + 6.123 H2O + 6.123 CO2 + 12.082 NADP+ + 1.0 phosphate
fatty-acid-I/3d_manual_HD-ibut                                  : 1.0 isobutyryl_phosphate + 6.123 Malonyl-[acyl-carrier_protein] + 18.205 H+ + 12.082 NADPH --> 1.0 Acyl-[acyl-
carrier_protein] + 5.123 Acyl-carrier_protein + 6.123 H2O + 6.123 CO2 + 12.082 NADP+ + 1.0 phosphate
fatty-acid-I/3e_manual_HD-vale                                  : 1.0 pentanoyl_phosphate + 5.623 Malonyl-[acyl-carrier_protein] + 16.705 H+ + 11.082 NADPH --> 1.0 Acyl-[acyl-
carrier_protein] + 4.623 Acyl-carrier_protein + 5.623 H2O + 5.623 CO2 + 11.082 NADP+ + 1.0 phosphate
fatty-acid-I/3f_manual_HD-ival                                  : 1.0 isovaleryl_phosphate + 5.623 Malonyl-[acyl-carrier_protein] + 16.705 H+ + 11.082 NADPH --> 1.0 Acyl-[acyl-
carrier_protein] + 4.623 Acyl-carrier_protein + 5.623 H2O + 5.623 CO2 + 11.082 NADP+ + 1.0 phosphate
fatty-acid-I/3g_manual_HD-aval                                  : 1.0 2-methylbutanoyl_phosphate + 5.623 Malonyl-[acyl-carrier_protein] + 16.705 H+ + 11.082 NADPH --> 1.0 Acyl-[acyl-
carrier_protein] + 4.623 Acyl-carrier_protein + 5.623 H2O + 5.623 CO2 + 11.082 NADP+ + 1.0 phosphate
fatty-acid-I/3h_manual_HD-icap                                  : 1.0 isocaproyl_phosphate + 5.123 Malonyl-[acyl-carrier_protein] + 15.205 H+ + 10.082 NADPH --> 1.0 Acyl-[acyl-
carrier_protein] + 4.123 Acyl-carrier_protein + 5.123 H2O + 5.123 CO2 + 10.082 NADP+ + 1.0 phosphate
fatty-acid-I/3i_manual_HD-hexa                                  : 1.0 hexanoyl_phosphate + 5.123 Malonyl-[acyl-carrier_protein] + 15.205 H+ + 10.082 NADPH --> 1.0 Acyl-[acyl-
carrier_protein] + 4.123 Acyl-carrier_protein + 5.123 H2O + 5.123 CO2 + 10.082 NADP+ + 1.0 phosphate

fatty-acid-I/4_manual_2.3.1.n2_HD-2.3.1.n2                      : 1.0 Acyl-[acyl-carrier_protein] + 1.0 phosphate <=> 1.0 fatty_acid_phosphate + 1.0 Acyl-carrier_protein
#################################################################################################################################################################################
#CDP-diacylglycerol-biosyn-I

CDP-diacylglycerol-biosyn-I/1_modnames_1.1.1.94_1.1.1.261-RXN        : 1.0 sn-glycerol_3-phosphate + 1.0 NADP+ <-- 1.0 H+ + 1.0 glycerone_phosphate + 1.0 NADPH  # source: MetaCyc,
BRENDA, KEGG (queried 1.1.1.94) // other EC numbers for this reaction: 1.1.1.261
CDP-diacylglycerol-biosyn-I/2_manual_2.3.1.n3_HD-2.3.1.n3            : 1.0 fatty_acid_phosphate + 1.0 sn-glycerol_3-phosphate <=> 1.0 1-acyl-sn-glycerol_3-phosphate + 1.0
phosphate
CDP-diacylglycerol-biosyn-I/3_2.3.1.51_BS321039                      : 1.0 Acyl-[acyl-carrier_protein] + 1.0 1-acyl-sn-glycerol_3-phosphate <=> 1.0 1,2-diacyl-sn-glycerol_3-
phosphate + 1.0 Acyl-carrier_protein  # source: MetaCyc, BRENDA, KEGG (queried 2.3.1.51)
CDP-diacylglycerol-biosyn-I/4_2.7.7.41_CDPDIGLYSYN-RXN               : 1.0 1,2-diacyl-sn-glycerol_3-phosphate + 1.0 CTP + 1.0 H+ --> 1.0 diphosphate + 1.0 CDP-1,2-diacyl-sn-
glycerol  # source: MetaCyc, BRENDA, KEGG (queried 2.7.7.41)
#################################################################################################################################################################################
#cardiolipin biosynthesis I
cardiolipin-biosyn-I/1_2.7.8.5_PHOSPHAGLYPSYN-RXN                    : 1.0 CDP-1,2-diacyl-sn-glycerol + 1.0 sn-glycerol_3-phosphate <=> 1.0 H+ + 1.0 CMP + 1.0
Phosphatidylglycerophosphate  # source: MetaCyc, BRENDA, KEGG (queried 2.7.8.5)
cardiolipin-biosyn-I/2_3.1.3.27_PGPPHOSPHA-RXN                       : 1.0 Phosphatidylglycerophosphate + 1.0 H2O --> 1.0 phosphate + 1.0 Phosphatidylglycerol  # source: MetaCyc,
BRENDA, KEGG (queried 3.1.3.27)
cardiolipin-biosyn-I/3_2.7.8.-_CARDIOLIPSYN-RXN                      : 2.0 Phosphatidylglycerol --> 1.0 a_cardiolipin + 1.0 glycerol  # source: MetaCyc, BRENDA, KEGG (queried
2.7.8.-) // other EC numbers for this reaction: 2.7.8.B10, 2.7.8
#################################################################################################################################################################################
#glycerol degradation I

glycerol-degradation-I_2.7.1.30_GLYCEROL-KIN-RXN                     : 1.0 glycerol + 1.0 ATP --> 1.0 ADP + 1.0 sn-glycerol_3-phosphate + 1.0 H+  # source: MetaCyc, BRENDA, KEGG
(queried 2.7.1.30)
#################################################################################################################################################################################
#UDP-N-acetyl-D-glucosamine biosynthesis I

UDP-N-acetyl-D-glucosamine-biosyn-I/1_2.6.1.16_L-GLN-FRUCT-6-P-AMINOTRANS-RXN     : 1.0 L-glutamine + 1.0 beta-D-fructofuranose_6-phosphate <=> 1.0 D-glucosamine_6-phosphate + 1.0
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L-glutamate  # source: MetaCyc, BRENDA, KEGG (queried 2.6.1.16)
UDP-N-acetyl-D-glucosamine-biosyn-I/2_5.4.2.10_5.4.2.10-RXN                    : 1.0 D-glucosamine_6-phosphate <=> 1.0 D-glucosamine_1-phosphate  # source: MetaCyc, BRENDA,
KEGG (queried 5.4.2.10)
UDP-N-acetyl-D-glucosamine-biosyn-I/3_2.3.1.157_2.3.1.157-RXN                  : 1.0 acetyl-CoA + 1.0 D-glucosamine_1-phosphate --> 1.0 N-acetyl-alpha-D-glucosamine_1-phosphate
+ 1.0 coenzyme_A + 1.0 H+  # source: MetaCyc, BRENDA, KEGG (queried 2.3.1.157)
UDP-N-acetyl-D-glucosamine-biosyn-I/4_2.7.7.23_NAG1P-URIDYLTRANS-RXN            : 1.0 H+ + 1.0 UTP + 1.0 N-acetyl-alpha-D-glucosamine_1-phosphate --> 1.0 UDP-N-acetyl-alpha-D-
glucosamine + 1.0 diphosphate  # source: MetaCyc, BRENDA, KEGG (queried 2.7.7.23)
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#UDP-N-acetyl-D-galactosamine biosynthesis I
UDP-N-acetyl-D-galactosamine-biosyn-I_5.1.3.2_UDP-N-ACETYLGLUCOSAMINE-4-EPIMERASE-RXN      : 1.0 UDP-N-acetyl-alpha-D-glucosamine <=> 1.0 UDP-N-acetyl-alpha-D-galactosamine  #
source: MetaCyc, BRENDA, KEGG (queried 5.1.3.2) // other EC numbers for this reaction: 5.1.3.7
#########################################################################################################################################################
#GDP-mannose biosyn

GDP-mannose-biosyn/1_5.3.1.8_MANNPISOM-RXN                                     : 1.0 D-mannopyranose_6-phosphate <=> 1.0 beta-D-fructofuranose_6-phosphate  # source: MetaCyc
(queried 5.3.1.8)
GDP-mannose-biosyn/2_5.4.2.8_PHOSMANMUT-RXN                                    : 1.0 alpha-D-mannose_1-phosphate <=> 1.0 D-mannopyranose_6-phosphate  # source: MetaCyc
(queried 5.4.2.8)
GDP-mannose-biosyn/3_2.7.7.13_2.7.7.13-RXN                                     : 1.0 alpha-D-mannose_1-phosphate + 1.0 H+ + 1.0 GTP --> 1.0 GDP-alpha-D-mannose + 1.0
diphosphate  # source: MetaCyc, BRENDA, KEGG (queried 2.7.7.13) // other EC numbers for this reaction: 2.7.7.34, 2.7.7.30
#########################################################################################################################################################
#UDP-glucose biosyn
UDP-glucose-biosyn/1_5.4.2.2_5.4.2.8_PHOSPHOGLUCMUT-RXN                        : 1.0 alpha-D-glucopyranose_1-phosphate <=> 1.0 D-glucose_6-phosphate  # source: MetaCyc,
BRENDA, KEGG (queried 5.4.2.2, 5.4.2.8) // other EC numbers for this reaction: 5.4.2.5
UDP-glucose-biosyn/2_2.7.7.9_GLUC1PURIDYLTRANS-RXN                             : 1.0 UTP + 1.0 alpha-D-glucopyranose_1-phosphate + 1.0 H+ <=> 1.0 UDP-alpha-D-glucose + 1.0
diphosphate  # source: MetaCyc, BRENDA, KEGG (queried 2.7.7.9) // other EC numbers for this reaction: 2.7.7.64
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#peptidoglycan biosynthesis I (meso-diaminopimelate containing)

peptidoglycan-biosyn-I/1_2.5.1.7_UDPNACETYLGLUCOSAMENOLPYRTRANS-RXN            : 1.0 UDP-N-acetyl-alpha-D-glucosamine + 1.0 phosphoenolpyruvate --> 1.0 phosphate + 1.0 UDP-N-
acetyl-alpha-D-glucosamine-enolpyruvate  # source: MetaCyc, BRENDA, KEGG (queried 2.5.1.7)
peptidoglycan-biosyn-I/2_1.3.1.98_UDPNACETYLMURAMATEDEHYDROG-RXN               : 1.0 NADP+ + 1.0 UDP-N-acetyl-alpha-D-muramate <-- 1.0 H+ + 1.0 NADPH + 1.0 UDP-N-acetyl-alpha-
D-glucosamine-enolpyruvate  # source: MetaCyc, BRENDA, KEGG (queried 1.3.1.98)
peptidoglycan-biosyn-I/3_6.3.2.8_UDP-NACMUR-ALA-LIG-RXN                        : 1.0 L-alanine + 1.0 ATP + 1.0 UDP-N-acetyl-alpha-D-muramate --> 1.0 phosphate + 1.0 UDP-N-
acetyl-alpha-D-muramoyl-L-alanine + 1.0 ADP + 1.0 H+  # source: MetaCyc, BRENDA, KEGG (queried 6.3.2.8)

D-glutamate_5.1.1.3_GLUTRACE-RXN                                               : 1.0 L-glutamate <=> 1.0 D-glutamate  # source: MetaCyc, BRENDA, KEGG (queried 5.1.1.3)

peptidoglycan-biosyn-I/4_6.3.2.9_UDP-NACMURALA-GLU-LIG-RXN                     : 1.0 D-glutamate + 1.0 UDP-N-acetyl-alpha-D-muramoyl-L-alanine + 1.0 ATP --> 1.0 phosphate +
1.0 ADP + 1.0 UDP-N-acetyl-alpha-D-muramoyl-L-alanyl-D-glutamate + 1.0 H+  # source: MetaCyc, BRENDA, KEGG (queried 6.3.2.9)
peptidoglycan-biosyn-I/5_6.3.2.13_UDP-NACMURALGLDAPLIG-RXN                     : 1.0 UDP-N-acetyl-alpha-D-muramoyl-L-alanyl-D-glutamate + 1.0 meso-diaminopimelate + 1.0 ATP
--> 1.0 UDP-N-acetyl-alpha-D-muramoyl-L-alanyl-gamma-D-glutamyl-meso-2,6-diaminopimelate + 1.0 H+ + 1.0 phosphate + 1.0 ADP  # source: MetaCyc, BRENDA, KEGG (queried 6.3.2.13)

D-alanyl-D-alanine/1_5.1.1.1_ALARACECAT-RXN                                    : 1.0 L-alanine <=> 1.0 D-alanine  # source: MetaCyc, BRENDA, KEGG (queried 5.1.1.1)
D-alanyl-D-alanine/2_6.3.2.4_DALADALALIG-RXN                                   : 2.0 D-alanine + 1.0 ATP --> 1.0 phosphate + 1.0 D-alanyl-D-alanine + 1.0 ADP + 1.0 H+  #
source: MetaCyc, BRENDA, KEGG (queried 6.3.2.4)

peptidoglycan-biosyn-I/6_6.3.2.10_UDP-NACMURALGLDAPAALIG-RXN                   : 1.0 UDP-N-acetyl-alpha-D-muramoyl-L-alanyl-gamma-D-glutamyl-meso-2,6-diaminopimelate + 1.0 D-
alanyl-D-alanine + 1.0 ATP --> 1.0 H+ + 1.0 phosphate + 1.0 UDP-N-acetyl-alpha-D-muramoyl-L-alanyl-gamma-D-glutamyl-meso-2,6-diaminopimeloyl-D-alanyl-D-alanine + 1.0 ADP  #
source: MetaCyc, KEGG (queried 6.3.2.10)
peptidoglycan-biosyn-I/p7_3.6.1.27_UNDECAPRENYL-DIPHOSPHATASE-RXN              : 1.0 H2O + 1.0 di-trans,octa-cis-undecaprenyl_diphosphate --> 1.0 H+ + 1.0 di-trans,octa-cis-
undecaprenyl_phosphate + 1.0 phosphate  # source: MetaCyc, BRENDA, KEGG (queried 3.6.1.27)
peptidoglycan-biosyn-I/7_2.7.8.13_PHOSNACMURPENTATRANS-RXN                     : 1.0 di-trans,octa-cis-undecaprenyl_phosphate + 1.0 UDP-N-acetyl-alpha-D-muramoyl-L-alanyl-
gamma-D-glutamyl-meso-2,6-diaminopimeloyl-D-alanyl-D-alanine --> 1.0 undecaprenyldiphospho-N-acetylmuramoyl-L-alanyl-gamma-D-glutamyl-meso-2,6-diaminopimeloyl-D-alanyl-D-alanine +
1.0 UMP  # source: MetaCyc, KEGG (queried 2.7.8.13)
peptidoglycan-biosyn-I/8_2.4.1.227_NACGLCTRANS-RXN                             : 1.0 undecaprenyldiphospho-N-acetylmuramoyl-L-alanyl-gamma-D-glutamyl-meso-2,6-diaminopimeloyl-
D-alanyl-D-alanine + 1.0 UDP-N-acetyl-alpha-D-glucosamine <=> 1.0 ditrans,octacis-undecaprenyldiphospho-N-acetyl-(N-acetylglucosaminyl)muramoyl-L-alanyl-gamma-D-glutamyl-meso-2,6-
diaminopimeloyl-D-alanyl-D-alanine + 1.0 H+ + 1.0 UDP  # source: MetaCyc, KEGG (queried 2.4.1.227)

#Based on HPLC-MS-studies (Peltier et al., 2011)
#Gly: -0.0453
#meso-DAP: +0.0035
#D-Ala: 2-0.6109 = +1.3891
#Cross: 0.3107
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#deAc: 0.9278
#H2O: -deAc -meso-DAP -D-Ala + Cross - Gly = -1.9644
peptidoglycan-biosyn-I/10_manual_3.4.16.4_3.5.1.104_HD-murein-mods                : 1.0 ditrans,octacis-undecaprenyldiphospho-N-acetyl-(N-acetylglucosaminyl)muramoyl-L-alanyl-
gamma-D-glutamyl-meso-2,6-diaminopimeloyl-D-alanyl-D-alanine + 1.9644 H2O + 0.0453 glycine + 1.3891 D-alanine --> 0.9278 acetate + 0.0035 meso-diaminopimelate + 1.0 di-trans,octa-
cis-undecaprenyl_diphosphate + 1.0 H+ + 1.0 a_peptidoglycan
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#peptidoglycan degradation
#H2O: 2 - Anh - acetate + 1 + glycine = 2.114
#1x ABC transport (appABCF)
peptidoglycan-degr/1_manual_3.5.1.28_3.2.1.96_3.5.1.104_HD-appABCF                : 1.0 a_peptidoglycan + 0.9278 acetate + 3.114 H2O + 1.0 ATP --> 0.0035 1,6-anhydro-N-acetyl-
beta-muramate + 0.9965 N-acetylmuramate + 1.0 N-acetyl-beta-D-glucosamine + 0.6109 L-alanyl-gamma-D-glutamyl-meso-2,6-diaminopimeloyl-D-alanine + 0.3856 L-alanyl-gamma-D-glutamyl-
meso-diaminopimelate + 0.0035 L-alanyl-D-glutamate + 0.0453 glycine + 1.0 ADP + 1.0 H+ + 1.0 phosphate
peptidoglycan-degr/2a_2.7.1.170_RXN0-4621                                         : 1.0 1,6-anhydro-N-acetyl-beta-muramate + 1.0 ATP + 1.0 H2O --> 1.0 H+ + 1.0 N-acetyl-beta-
muramate_6-phosphate + 1.0 ADP  # source: MetaCyc, BRENDA, KEGG (queried 2.7.1.170)
#Additional reaction of EC 2.7.1.59 shown for C. acetobutylicum (Reith et al., 2011)
peptidoglycan-degr/2b_manual_2.7.1.59_HD-2.7.1.59                                 : 1.0 N-acetylmuramate + 1.0 ATP --> 1.0 ADP + 1.0 H+ + 1.0 N-acetyl-beta-muramate_6-phosphate
peptidoglycan-degr/3_4.2.1.126_RXN0-4641                                          : 1.0 H2O + 1.0 N-acetyl-beta-muramate_6-phosphate <=> 1.0 N-acetyl-D-glucosamine_6-phosphate +
1.0 (R)-lactate  # source: MetaCyc (queried 4.2.1.126)
peptidoglycan-degr/4_2.7.1.59_N-ACETYLGLUCOSAMINE-KINASE-RXN                      : 1.0 N-acetyl-beta-D-glucosamine + 1.0 ATP --> 1.0 ADP + 1.0 H+ + 1.0 N-acetyl-D-glucosamine_6-
phosphate  # source: MetaCyc, BRENDA, KEGG (queried 2.7.1.59)

#N-acetylglucosamine degradation I
N-acetylglucosamine-degr-I/1_3.5.1.25_NAG6PDEACET-RXN                             : 1.0 H2O + 1.0 N-acetyl-D-glucosamine_6-phosphate --> 1.0 acetate + 1.0 D-glucosamine_6-
phosphate  # source: MetaCyc, BRENDA, KEGG (queried 3.5.1.25)
N-acetylglucosamine-degr-I/2_3.5.99.6_BS363214                                    : 1.0 H2O + 1.0 D-glucosamine_6-phosphate --> 1.0 ammonia + 1.0 beta-D-fructofuranose_6-
phosphate  # source: BRENDA, KEGG (queried 3.5.99.6)

#muropeptide degradation
muropeptide-degr/1_3.4.17.13_RXN0-5227                                            : 1.0 H2O + 1.0 L-alanyl-gamma-D-glutamyl-meso-2,6-diaminopimeloyl-D-alanine --> 1.0 L-alanyl-
gamma-D-glutamyl-meso-diaminopimelate + 1.0 D-alanine  # source: MetaCyc (queried 3.4.17.13)
muropeptide-degr/2_RXN0-961                                                       : 1.0 L-alanyl-gamma-D-glutamyl-meso-diaminopimelate + 1.0 H2O --> 1.0 L-alanyl-D-glutamate
muropeptide-degr/3_5.1.1.20_RXN0-5228                                             : 1.0 L-alanyl-D-glutamate <=> 1.0 L-alanyl-L-glutamate  # source: MetaCyc, BRENDA, KEGG
(queried 5.1.1.20)
muropeptide-degr/4_3.4.13.18_RXN0-6981                                            : 1.0 H2O + 1.0 L-alanyl-L-glutamate --> 1.0 L-glutamate + 1.0 L-alanine  # source: MetaCyc,
BRENDA (queried 3.4.13.18) // other EC numbers for this reaction: 3.4.11.14
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#L-CWG biosynthesis
L-CWG-biosyn/1a_3.1.3.4_PHOSPHATIDATE-PHOSPHATASE-RXN                           : 1.0 1,2-diacyl-sn-glycerol_3-phosphate + 1.0 H2O --> 1.0 1,2-diacyl-sn-glycerol + 1.0 phosphate
# source: MetaCyc, BRENDA, KEGG (queried 3.1.3.4) // other EC numbers for this reaction: 3.1.3.81
L-CWG-biosyn/1b_2.7.1.107_DIACYLGLYKIN-RXN                                      : 1.0 ATP + 1.0 1,2-diacyl-sn-glycerol --> 1.0 H+ + 1.0 ADP + 1.0 1,2-diacyl-sn-glycerol_3-
phosphate  # source: MetaCyc, BRENDA, KEGG (queried 2.7.1.107)
L-CWG-biosyn/2_2.4.1.315_2.4.1.337_2.4.1.157-RXN                                : 1.0 1,2-diacyl-sn-glycerol + 1.0 UDP-alpha-D-glucose --> 1.0 3-D-Glucosyl-1,2-diacylglycerol +
1.0 H+ + 1.0 UDP  # source: MetaCyc, BRENDA, KEGG (queried 2.4.1.315, 2.4.1.337) // other EC numbers for this reaction: 2.4.1.336, 2.4.1.157, 2.4.1.cp
L-CWG-biosyn/3_2.4.1.315_RXN-15117                                              : 1.0 3-D-Glucosyl-1,2-diacylglycerol + 1.0 UDP-alpha-D-glucose <=> 1.0 |diacyl-3-O-glucl-1-6-gluc-
sn-glycerol| + 1.0 UDP + 1.0 H+  # source: MetaCyc (queried 2.4.1.315)
L-CWG-biosyn/4_2.4.1.315_RXN-15118                                              : 1.0 |diacyl-3-O-glucl-1-6-gluc-sn-glycerol| + 1.0 UDP-alpha-D-glucose <=> 1.0 H+ + 1.0 |diacyl-3-
Glc-16-Glc-16-Glc-glycerol| + 1.0 UDP  # source: MetaCyc (queried 2.4.1.315)
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#Flagellin modification (Faulds-Pain et al. 2014)
flagellin-modification/1_manual_2.4.-_HD-fla1                                   : 1.0 UDP-N-acetyl-alpha-D-glucosamine --> 1.0 UDP + 1.0 H+ + 1.0 GluNAc-FliC
flagellin-modification/p1_manual_3.1.3.-_HD-fla2                                : 1.0 L-threonine + 1.0 phosphate <=> 1.0 H2O + 1.0 3-phospho-L-threonine
flagellin-modification/2_manual_3.1.4.-_HD-fla3                                 : 1.0 GluNAc-FliC + 1.0 3-phospho-L-threonine + 1.0 H+ --> 1.0 H2O + 1.0 Thr-P-GluNAc-FliC
flagellin-modification/3_manual_2.1.1.-_HD-fla4                                 : 1.0 Thr-P-GluNAc-FliC + 1.0 S-adenosyl-L-methionine --> 1.0 Me-Thr-P-GluNAc-FliC + 2.0 H+ + 1.0
S-adenosyl-L-homocysteine
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#glycogen biosynthesis I + degradation

glycogen-biosyn-I/1_2.7.7.27_GLUC1PADENYLTRANS-RXN                              : 1.0 H+ + 1.0 alpha-D-glucopyranose_1-phosphate + 1.0 ATP --> 1.0 diphosphate + 1.0 ADP-alpha-D-
glucose  # source: MetaCyc, BRENDA, KEGG (queried 2.7.7.27)
glycogen-biosyn-I/2_manual_2.4.1.21_HD-2.4.1.21                                 : 1.0 ADP-alpha-D-glucose --> 1.0 ADP + 1.0 |1-4-alpha-D-Glucan| + 1.0 H+
glycogen-biosyn-I/3_2.4.1.18_3.2.1.54_3.2.1.41_3.2.1.1_GLYCOGEN-BRANCH-RXN      : 1.0 |1-4-alpha-D-Glucan| --> 1.0 |Glycogens|  # source: MetaCyc, BRENDA (queried 2.4.1.18,
3.2.1.54, 3.2.1.41, 3.2.1.1) // other EC numbers for this reaction: 2.4.1.25, 3.2.1.68, 3.2.1.116

glycogen-degr_manual_3.2.1.54_3.2.1.41_3.2.1.1_HD-Glycogen                      : 3.0 |Glycogens| + 1.0 H2O --> 1.0 |Maltodextrins|  # source: MetaCyc, BRENDA (queried 2.4.1.18,
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3.2.1.54, 3.2.1.41, 3.2.1.1) // other EC numbers for this reaction: 2.4.1.25, 3.2.1.68, 3.2.1.116
glycogen-degr_3.2.1.133_3.2.1.1_RXN-12188                                    : 1.0 |Maltodextrins| + 1.0 H2O --> 1.0 D-glucose + 1.0 alpha,alpha-trehalose  # source: MetaCyc,
BRENDA (queried 3.2.1.133, 3.2.1.1) // there are 4 more EC numbers for this reaction
glycogen-degr_2.4.1.64_2.4.1.8_ALPHAALPHA-TREHALOSE-PHOSPHORYLASE-RXN         : 1.0 phosphate + 1.0 alpha,alpha-trehalose <=> 1.0 beta-D-glucose_1-phosphate + 1.0 D-glucose  #
source: MetaCyc, BRENDA, KEGG (queried 2.4.1.64, 2.4.1.8)
glycogen-degr_3.2.1.10_RXN-15910                                             : 1.0 alpha,alpha-trehalose + 1.0 H2O --> 2.0 D-glucose  # source: MetaCyc, BRENDA (queried
3.2.1.10) // other EC numbers for this reaction: 3.2.1.20

glucose-degr/1_2.7.1.2_GLUCOKIN-RXN                                          : 1.0 D-glucose + 1.0 ATP --> 1.0 D-glucose_6-phosphate + 1.0 H+ + 1.0 ADP  # source: MetaCyc,
BRENDA, KEGG (queried 2.7.1.2) // other EC numbers for this reaction: 2.7.1.1
glucose-degr/2_5.4.2.6_BETA-PHOSPHOGLUCOMUTASE-RXN                           : 1.0 beta-D-glucose_1-phosphate <=> 1.0 beta-D-glucose_6-phosphate  # source: MetaCyc, BRENDA,
KEGG (queried 5.4.2.6)
glucose-degr/3_5.3.1.9_R03321                                                : 1.0 beta-D-glucose_6-phosphate <=> 1.0 beta-D-fructofuranose_6-phosphate  # source: KEGG (queried
5.3.1.9)
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#polymer biosynthesis
exopolysaccharide-biosynthesis/1_manual_2.4.1.12_HD-2.4.1.12                 : 1.0 UDP-alpha-D-glucose --> 1.0 UDP + 1.0 cellulose + 1.0 H+
#1 ATP per glucose subunit
exopolysaccharide-biosynthesis/2_transport                                   : 1.0 cellulose + 1.0 ATP + 1.0 H2O --> 1.0 cellulose[ex] + 1.0 ADP + 1.0 phosphate + 1.0 H+
#CDIF630erm_02795; 50 % acetylation
exopolysaccharide-biosynthesis/3_manual_2.3.1.-_HD-PSac                      : 1.0 cellulose[ex] + 0.5 acetyl-CoA <=> 0.5 coenzyme_A + 1.0 acetyl-cellulose[ex]
#trimming; chain-length: 100
exopolysaccharide-biosynthesis/4_manual_3.2.1.4_HD-3.2.1.4                   : 1.0 acetyl-cellulose[ex] + 0.01 H2O --> 1.0 exopolysaccharide[ex]

exopolysaccharide_exchange                                                   : exopolysaccharide[ex] -->
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#glutamate/mine
glutamate_6.3.1.2_GLUTAMINESYN-RXN                                           : 1.0 ammonium + 1.0 L-glutamate + 1.0 ATP --> 1.0 L-glutamine + 1.0 ADP + 1.0 H+ + 1.0 phosphate
# source: MetaCyc, BRENDA, KEGG (queried 6.3.1.2)
glutamate_3.5.1.2_6.3.5.2_6.3.5.5_6.3.5.4_GLUTAMIN-RXN                       : 1.0 H2O + 1.0 L-glutamine --> 1.0 ammonium + 1.0 L-glutamate  # source: MetaCyc, BRENDA, KEGG
(queried 3.5.1.2, 6.3.5.2, 6.3.5.5, 6.3.5.4) // there are 6 more EC numbers for this reaction
glutamate_1.4.1.2_GLUTAMATE-DEHYDROGENASE-NADP+-RXN_WOP                       : 1.0 NAD+ + 1.0 H2O + 1.0 L-glutamate <=> 1.0 H+ + 1.0 NADH + 1.0 2-oxoglutarate + 1.0 ammonium  #
source: MetaCyc, BRENDA, KEGG (queried 1.4.1.2) // other EC numbers for this reaction: 1.4.1.3
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#asp biosyn,asn biosyn I+II,asn degr. I
aspartate_2.6.1.1_ASPAMINOTRANS-RXN                                          : 1.0 2-oxoglutarate + 1.0 L-aspartate <=> 1.0 L-glutamate + 1.0 oxaloacetate  # source: MetaCyc,
BRENDA, KEGG (queried 2.6.1.1) // other EC numbers for this reaction: 2.6.1.39
aspartate_6.3.5.4_ASNSYNB-RXN                                                : 1.0 L-glutamine + 1.0 ATP + 1.0 H2O + 1.0 L-aspartate --> 1.0 L-asparagine + 1.0 AMP + 1.0 H+ +
1.0 diphosphate + 1.0 L-glutamate  # source: MetaCyc, BRENDA, KEGG (queried 6.3.5.4)
aspartate_6.3.1.1_6.3.5.4_ASNSYNA-RXN                                        : 1.0 ATP + 1.0 ammonium + 1.0 L-aspartate --> 1.0 L-asparagine + 1.0 AMP + 1.0 H+ + 1.0
diphosphate  # source: MetaCyc, BRENDA, KEGG (queried 6.3.1.1, 6.3.5.4)
aspartate_3.5.5.4_3.5.1.1_ASPARAGHYD-RXN                                     : 1.0 H2O + 1.0 L-asparagine --> 1.0 ammonium + 1.0 L-aspartate  # source: MetaCyc, BRENDA, KEGG
(queried 3.5.5.4, 3.5.1.1) // other EC numbers for this reaction: 3.5.1.38
#########################################################################################################################################################################
#lys biosyn II
lysine-biosyn-II/1_2.7.2.4_ASPARTATEKIN-RXN                                  : 1.0 ATP + 1.0 L-aspartate --> 1.0 ADP + 1.0 L-aspartyl-4-phosphate  # source: MetaCyc, BRENDA,
KEGG (queried 2.7.2.4)
lysine-biosyn-II/2_1.2.1.11_ASPARTATE-SEMIALDEHYDE-DEHYDROGENASE-RXN         : 1.0 NADP+ + 1.0 L-aspartate-semialdehyde + 1.0 phosphate <=> 1.0 L-aspartyl-4-phosphate + 1.0 H+
+ 1.0 NADPH  # source: MetaCyc, BRENDA, KEGG (queried 1.2.1.11)
lysine-biosyn-II/3_4.3.3.7_DIHYDRODIPICSYN-RXN                               : 1.0 pyruvate + 1.0 L-aspartate-semialdehyde --> 1.0 (2S,4S)-4-hydroxy-2,3,4,5-
tetrahydrodipicolinate + 1.0 H+ + 1.0 H2O  # source: MetaCyc, BRENDA, KEGG (queried 4.3.3.7)
lysine-biosyn-II/4_1.17.1.8_RXN-14014                                        : 1.0 (S)-2,3,4,5-tetrahydrodipicolinate + 1.0 H2O + 1.0 NADP+ <-- 1.0 H+ + 1.0 NADPH + 1.0
(2S,4S)-4-hydroxy-2,3,4,5-tetrahydrodipicolinate  # source: MetaCyc, BRENDA, KEGG (queried 1.17.1.8)
lysine-biosyn-II/5_2.3.1.89_2.3.1.89-RXN                                     : 1.0 H2O + 1.0 (S)-2,3,4,5-tetrahydrodipicolinate + 1.0 acetyl-CoA --> 1.0 coenzyme_A + 1.0 L-2-
acetamido-6-oxoheptanedioate  # source: MetaCyc, BRENDA, KEGG (queried 2.3.1.89) // other EC numbers for this reaction: 2.3.1
lysine-biosyn-II/6_2.6.1.-_RXN-4822                                          : 1.0 L-2-acetamido-6-oxoheptanedioate + 1.0 L-glutamate --> 1.0 2-oxoglutarate + 1.0 N-acetyl-L,L-
2,6-diaminopimelate  # source: MetaCyc, KEGG (queried 2.6.1.-) // other EC numbers for this reaction: 2.6.1
lysine-biosyn-II/7_3.5.1.47_N-ACETYLDIAMINOPIMELATE-DEACETYLASE-RXN          : 1.0 N-acetyl-L,L-2,6-diaminopimelate + 1.0 H2O --> 1.0 acetate + 1.0 L,L-diaminopimelate  #
source: MetaCyc, BRENDA, KEGG (queried 3.5.1.47)
lysine-biosyn-II/8_5.1.1.7_DIAMINOPIMEPIM-RXN                                : 1.0 L,L-diaminopimelate <=> 1.0 meso-diaminopimelate  # source: MetaCyc, BRENDA, KEGG (queried
5.1.1.7)
lysine-biosyn-II/9_4.1.1.20_DIAMINOPIMDECARB-RXN                             : 1.0 H+ + 1.0 meso-diaminopimelate --> 1.0 CO2 + 1.0 L-lysine  # source: MetaCyc, BRENDA, KEGG
(queried 4.1.1.20)
#########################################################################################################################################################################
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#arginine biosyn II
arginine-biosyn-II/1_2.3.1.1_N-ACETYLTRANSFER-RXN                                : 1.0 L-glutamate + 1.0 acetyl-CoA <=> 1.0 N-acetyl-L-glutamate + 1.0 coenzyme_A + 1.0 H+  #
source: MetaCyc, BRENDA, KEGG (queried 2.3.1.1)
arginine-biosyn-II/2_2.7.2.8_ACETYLGLUTKIN-RXN                                   : 1.0 ATP + 1.0 N-acetyl-L-glutamate --> 1.0 N-acetylglutamyl-phosphate + 1.0 ADP  # source:
MetaCyc, BRENDA, KEGG (queried 2.7.2.8)
arginine-biosyn-II/3_1.2.1.38_N-ACETYLGLUTPREDUCT-RXN                            : 1.0 phosphate + 1.0 NADP+ + 1.0 N-acetyl-L-glutamate_5-semialdehyde <=> 1.0 N-acetylglutamyl-
phosphate + 1.0 H+ + 1.0 NADPH  # source: MetaCyc, BRENDA, KEGG (queried 1.2.1.38)
arginine-biosyn-II/4_2.6.1.11_ACETYLORNTRANSAM-RXN                               : 1.0 N-acetyl-L-ornithine + 1.0 2-oxoglutarate <=> 1.0 N-acetyl-L-glutamate_5-semialdehyde + 1.0
L-glutamate  # source: MetaCyc, BRENDA, KEGG (queried 2.6.1.11)
arginine-biosyn-II/5_2.3.1.35_GLUTAMATE-N-ACETYLTRANSFERASE-RXN                  : 1.0 N-acetyl-L-ornithine + 1.0 L-glutamate --> 1.0 N-acetyl-L-glutamate + 1.0 L-ornithine  #
source: MetaCyc, BRENDA, KEGG (queried 2.3.1.35)
arginine-biosyn-II/p6_6.3.5.5_CARBPSYN-RXN                                       : 2.0 ATP + 1.0 H2O + 1.0 L-glutamine + 1.0 hydrogen_carbonate --> 2.0 ADP + 1.0 phosphate + 1.0 L-
glutamate + 1.0 carbamoyl_phosphate + 2.0 H+  # source: MetaCyc, BRENDA, KEGG (queried 6.3.5.5)
arginine-biosyn-II/6_2.1.3.3_ORNCARBAMTRANSFER-RXN                               : 1.0 carbamoyl_phosphate + 1.0 L-ornithine <=> 1.0 phosphate + 1.0 L-citrulline + 1.0 H+  #
source: MetaCyc, BRENDA, KEGG (queried 2.1.3.3) // other EC numbers for this reaction: 3.5.3.12
arginine-biosyn-II/7_6.3.4.5_ARGSUCCINSYN-RXN                                    : 1.0 L-citrulline + 1.0 L-aspartate + 1.0 ATP --> 1.0 diphosphate + 1.0 L-arginino-succinate + 1.0
AMP + 1.0 H+  # source: MetaCyc, BRENDA, KEGG (queried 6.3.4.5)
arginine-biosyn-II/8_4.3.2.1_ARGSUCCINLYA-RXN                                    : 1.0 L-arginino-succinate <=> 1.0 fumarate + 1.0 L-arginine  # source: MetaCyc, BRENDA, KEGG
(queried 4.3.2.1)
#################################################################################################################################################################
#arginine degr
arginine-degradation/1_3.5.3.6_ARGININE-DEIMINASE-RXN                            : 1.0 L-arginine + 1.0 H2O --> 1.0 ammonium + 1.0 L-citrulline  # source: MetaCyc, BRENDA, KEGG
(queried 3.5.3.6) // other EC numbers for this reaction: 3.5.3.15
#3.5.1.87 assumed to use citrulline as substrate
arginine-degradation/2_3.5.1.87_CITRULLINASE-RXN                                 : 2.0 H+ + 1.0 L-citrulline + 1.0 H2O --> 1.0 CO2 + 1.0 ammonium + 1.0 L-ornithine
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#putrescine/spermidine biosyn

putrescine-biosyn-I/1_4.1.1.19_ARGDECARBOX-RXN                                   : 1.0 H+ + 1.0 L-arginine --> 1.0 CO2 + 1.0 agmatine  # source: MetaCyc, BRENDA, KEGG (queried
4.1.1.19)
putrescine-biosyn-I/2_3.5.3.11_AGMATIN-RXN                                       : 1.0 H2O + 1.0 agmatine --> 1.0 putrescine + 1.0 urea  # source: MetaCyc, BRENDA, KEGG (queried
3.5.3.11)
spermidine-biosyn-I/1_4.1.1.50_SAMDECARB-RXN                                     : 1.0 S-adenosyl-L-methionine + 1.0 H+ --> 1.0 S-adenosyl_3-(methylthio)propylamine + 1.0 CO2  #
source: MetaCyc, BRENDA, KEGG (queried 4.1.1.50)
spermidine-biosyn-I/2_2.5.1.16_SPERMIDINESYN-RXN                                 : 1.0 putrescine + 1.0 S-adenosyl_3-(methylthio)propylamine <=> 1.0 H+ + 1.0 S-methyl-5'-
thioadenosine + 1.0 spermidine  # source: MetaCyc, BRENDA, KEGG (queried 2.5.1.16)

#possible side reaction
spermine-biosynthesis_2.5.1.16_SPERMINE-SYNTHASE-RXN                             : 1.0 spermidine + 1.0 S-adenosyl_3-(methylthio)propylamine --> 1.0 H+ + 1.0 S-methyl-5'-
thioadenosine + 1.0 spermine  # source: MetaCyc, BRENDA, KEGG (queried 2.5.1.16) // other EC numbers for this reaction: 2.5.1.22

N-acetylputrescine-biosyn_2.3.1.57_RXN-0                                         : 1.0 putrescine + 1.0 acetyl-CoA --> 1.0 coenzyme_A + 1.0 N-acetylputrescine + 1.0 H+  # source:
MetaCyc, BRENDA, KEGG (queried 2.3.1.57)
N-acetylspermidine-biosyn_2.3.1.57_SPERMACTRAN-RXN                               : 1.0 acetyl-CoA + 1.0 spermidine --> 1.0 coenzyme_A + 1.0 N1-acetylspermidine + 1.0 H+  # source:
MetaCyc, BRENDA (queried 2.3.1.57)
N-acetylspermine-biosyn_2.3.1.57_RXN-9939                                        : 1.0 spermine + 1.0 acetyl-CoA --> 1.0 coenzyme_A + 1.0 N1-acetylspermine + 1.0 H+  # source:
MetaCyc (queried 2.3.1.57)
N-diacetylspermine-biosyn_2.3.1.57_BS321087                                      : 1.0 acetyl-CoA + 1.0 N1-acetylspermine --> 1.0 N1,N12-diacetylspermine + 1.0 coenzyme_A  #
source: BRENDA (queried 2.3.1.57)
#################################################################################################################################################################
#S-methyl-5'-thioadenosine degradation
S-methyl-5'-thioadenosine-degr_3.2.2.16_3.2.2.9_METHYLTHIOADENOSINE-NUCLEOSIDASE-RXN        : 1.0 H2O + 1.0 S-methyl-5'-thioadenosine --> 1.0 adenine + 1.0 S-methyl-5-thio-D-
ribose  # source: MetaCyc, BRENDA, KEGG (queried 3.2.2.16, 3.2.2.9)
S-methyl-5'-thioadenosine-degr_3.2.2.9_5-METHYLTHIOADENOSINE-PHOSPHORYLASE-RXN             : 1.0 S-methyl-5'-thioadenosine + 1.0 phosphate --> 1.0 adenine + 1.0 S-methyl-5-thio-
alpha-D-ribose_1-phosphate  # source: MetaCyc, BRENDA, KEGG (queried 3.2.2.9) // other EC numbers for this reaction: 2.4.2.28
#################################################################################################################################################################
#S-adenosyl-L-methionine cycle I

S-adenosyl-L-methionine-cycle-I/1_3.2.2.9_ADENOSYLHOMOCYSTEINE-NUCLEOSIDASE-RXN             : 1.0 S-adenosyl-L-homocysteine + 1.0 H2O --> 1.0 adenine + 1.0 S-ribosyl-L-
homocysteine  # source: MetaCyc, BRENDA, KEGG (queried 3.2.2.9)
S-adenosyl-L-methionine-cycle-I/2_4.4.1.21_RIBOSYLHOMOCYSTEINASE-RXN                     : 1.0 S-ribosyl-L-homocysteine --> 1.0 autoinducer_2 + 1.0 L-homocysteine  # source:
MetaCyc, BRENDA, KEGG (queried 4.4.1.21)
S-adenosyl-L-methionine-cycle-I/3_2.1.1.13_HOMOCYSMETB12-RXN                     : 1.0 N5-methyl-tetrahydrofolate + 1.0 L-homocysteine --> 1.0 tetrahydropteroyl_tri-
L-glutamate + 1.0 L-methionine  # source: MetaCyc (queried 2.1.1.13)
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S-adenosyl-L-methionine-cycle-I/4_2.5.1.6_S-ADENMETSYN-RXN                                  : 1.0 L-methionine + 1.0 ATP + 1.0 H2O --> 1.0 diphosphate + 1.0 S-adenosyl-L-
methionine + 1.0 phosphate  # source: MetaCyc, BRENDA, KEGG (queried 2.5.1.6)
#GAP: 2.1.1.; mostly DNA or t/rRNA
#auto-inducer
autoinducer-AI-2-biosyn/1_spontaneous_RXN-10015                                             : 1.0 autoinducer_2 --> 1.0 (2R,4S)-2-methyl-2,4-dihydroxydihydrofuran-3-one  #
source: MetaCyc
autoinducer-AI-2-biosyn/2_spontaneous_RXN-10017                                             : 1.0 H2O + 1.0 (2R,4S)-2-methyl-2,4-dihydroxydihydrofuran-3-one --> 1.0 (2R,4S)-2-
methyl-2,3,3,4-tetrahydroxytetrahydrofuran  # source: MetaCyc
#########################################################################################################################################################
#met biosyn C
methionine-biosyn/1_2.3.1.46_HOMSUCTRAN-RXN                                 : 1.0 succinyl-CoA + 1.0 L-homoserine --> 1.0 coenzyme_A + 1.0 O-succinyl-L-homoserine  # source:
MetaCyc, BRENDA, KEGG (queried 2.3.1.46)
methionine-biosyn/2_2.5.1.49_RXN-9384                                       : 1.0 O-succinyl-L-homoserine + 1.0 hydrogen_sulfide <=> 1.0 L-homocysteine + 1.0 H+ + 1.0
succinate  # source: MetaCyc, BRENDA, KEGG (queried 2.5.1.49) // other EC numbers for this reaction: 2.5.1.48, 2.5.1
#########################################################################################################################################################
#met degr II
methionine-degr-II_4.4.1.11_RXN-14301                                       : 1.0 L-methionine --> 1.0 H+ + 1.0 (2Z)-2-aminobut-2-enoate + 1.0 methanethiol  # source:
MetaCyc, KEGG (queried 4.4.1.11)
#########################################################################################################################################################
#2-amino-2-enoate degradation
2-aminobut-2-enoate-degr/1_spontaneous_4.4.1.1_4.3.1.19_3.5.99.7_4.4.1.2_RXN-15121                      : 1.0 (2Z)-2-aminobut-2-enoate --> 1.0 2-iminobutanoate  # source:
MetaCyc, BRENDA, KEGG (queried 4.4.1.1, 4.3.1.19, 3.5.99.7, 4.4.1.2)
2-aminobut-2-enoate-degr/2_spontaneous_3.5.99.7_3.5.99.10_4.4.1.1_4.3.1.19_4.4.1.2_3.5.99.-_RXN-15123         : 1.0 H2O + 1.0 H+ + 1.0 2-iminobutanoate --> 1.0 2-oxobutanoate +
1.0 ammonium  # source: MetaCyc, BRENDA, KEGG (queried 3.5.99.7, 3.5.99.10, 4.4.1.1, 4.3.1.19, 4.4.1.2, 3.5.99.-) // other EC numbers for this reaction: 3.5.99

2-aminoprop-2-enoate-degr/1_spontaneous_4.4.1.8_4.4.1.13_4.4.1.25_4.3.1.17_4.4.1.28_RXN-15124              : 1.0 2-aminoprop-2-enoate --> 1.0 2-iminopropanoate  # source:
MetaCyc, BRENDA, KEGG (queried 4.4.1.8, 4.4.1.13, 4.4.1.25, 4.3.1.17, 4.4.1.28)
2-aminoprop-2-enoate-degr/2_spontaneous_4.4.1.8_4.4.1.13_4.3.1.17_4.4.1.28_3.5.99.10_4.4.1.25_RXN-15127       : 1.0 H2O + 1.0 2-iminopropanoate + 1.0 H+ --> 1.0 ammonium + 1.0
pyruvate  # source: MetaCyc, BRENDA, KEGG (queried 4.4.1.8, 4.4.1.13, 4.3.1.17, 4.4.1.28, 3.5.99.10, 4.4.1.25)
#########################################################################################################################################################
#2-aminobutanoate
2-aminobutanoate_2.6.1.42_BS356546                                          : 1.0 (S)-2-aminobutanoate + 1.0 2-oxoglutarate <-- 1.0 2-oxobutanoate + 1.0 L-glutamate  #
source: BRENDA, KEGG (queried 2.6.1.42)
#########################################################################################################################################################
#threonine biosyn
threonine-from-homoserine/0_1.1.1.3_HOMOSERDEHYDROG-RXN                     : 1.0 NADP+ + 1.0 L-homoserine <-- 1.0 H+ + 1.0 L-aspartate-semialdehyde + 1.0 NADPH  # source:
MetaCyc, BRENDA, KEGG (queried 1.1.1.3)
threonine-from-homoserine/1_2.7.1.39_HOMOSERKIN-RXN                         : 1.0 L-homoserine + 1.0 ATP --> 1.0 H+ + 1.0 ADP + 1.0 O-phospho-L-homoserine  # source:
MetaCyc, BRENDA, KEGG (queried 2.7.1.39)
threonine-from-homoserine/2_4.2.3.1_THRESYN-RXN                             : 1.0 H2O + 1.0 O-phospho-L-homoserine --> 1.0 phosphate + 1.0 L-threonine  # source: MetaCyc,
BRENDA, KEGG (queried 4.2.3.1)
#########################################################################################################################################################
#threonine degr
threonine-degr-IV_4.1.2.5_THREONINE-ALDOLASE-RXN                            : 1.0 L-threonine --> 1.0 glycine + 1.0 acetaldehyde  # source: MetaCyc, BRENDA, KEGG (queried
4.1.2.5) // other EC numbers for this reaction: 4.1.2.48

threonine-degr-V_4.3.1.19_RXN-15122                                         : 1.0 L-threonine --> 1.0 (2Z)-2-aminobut-2-enoate + 1.0 H+ + 1.0 H2O  # source: MetaCyc,
BRENDA (queried 4.3.1.19)

threonine-degr-II/1_1.1.1.103_THREODEHYD-RXN                                : 1.0 L-threonine + 1.0 NAD+ --> 1.0 L-2-amino-3-oxobutanoate + 1.0 NADH + 1.0 H+  # source:
MetaCyc, BRENDA, KEGG (queried 1.1.1.103)
threonine-degr-II/2_spontaneous_THREOSPON-RXN                               : 1.0 L-2-amino-3-oxobutanoate + 1.0 H+ --> 1.0 aminoacetone + 1.0 CO2
#########################################################################################################################################################
#homoserine degr
#C. sporogenes (Kreis and Hession, 1973) enzyme homolog
homoserine-degr_4.4.1.1_4.3.1.19_4.4.1.11_HOMOSERDEAM-RXN                   : 1.0 L-homoserine --> 1.0 2-oxobutanoate + 1.0 ammonium  # source: MetaCyc, BRENDA (queried
4.4.1.1, 4.3.1.19, 4.4.1.11)
#########################################################################################################################################################
#serine biosyn
serine-biosyn_2.1.2.1_GLYOHMETRANS-RXN                                      : 1.0 tetrahydropteroyl_tri-L-glutamate + 1.0 L-serine <=> 1.0 glycine + 1.0 H2O + 1.0 5,10-
methylene-tetrahydrofolate  # source: MetaCyc (queried 2.1.2.1)
#########################################################################################################################################################
#serine degr
serine-degr-A_4.3.1.17_RXN-15125                                            : 1.0 L-serine --> 1.0 H2O + 1.0 2-aminoprop-2-enoate + 1.0 H+  # source: MetaCyc, BRENDA, KEGG
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(queried 4.3.1.17)

serine-degr-B/1a_2.6.1.51_SERINE--PYRUVATE-AMINOTRANSFERASE-RXN                    : 1.0 L-serine + 1.0 pyruvate <=> 1.0 hydroxypyruvate + 1.0 L-alanine  # source: MetaCyc,
BRENDA, KEGG (queried 2.6.1.51)
serine-degr-B/1b_2.6.1.2_RXN-974                                                  : 1.0 L-serine + 1.0 2-oxoglutarate <=> 1.0 L-glutamate + 1.0 hydroxypyruvate  # source:
MetaCyc, BRENDA (queried 2.6.1.2)
serine-degr-B/2a_1.1.1.81_1.1.1.60_GLYCERATE-DEHYDROGENASE-RXN                    : 1.0 NAD+ + 1.0 D-glycerate <-- 1.0 NADH + 1.0 hydroxypyruvate + 1.0 H+  # source: MetaCyc,
BRENDA, KEGG (queried 1.1.1.81, 1.1.1.60) // other EC numbers for this reaction: 1.1.1.29, 1.1.1.26, 1.1.1.79
serine-degr-B/2b_1.1.1.81_RXN0-300                                                : 1.0 D-glycerate + 1.0 NADP+ <-- 1.0 hydroxypyruvate + 1.0 NADPH + 1.0 H+  # source: MetaCyc,
BRENDA, KEGG (queried 1.1.1.81) // other EC numbers for this reaction: 1.1.1, 1.1.1.215, 1.1.1.79
serine-degr-B/3_2.7.1.31_GLY3KIN-RXN                                              : 1.0 ATP + 1.0 D-glycerate --> 1.0 ADP + 1.0 3-phospho-D-glycerate + 1.0 H+  # source:
MetaCyc, BRENDA, KEGG (queried 2.7.1.31)
#####################################################################################################################################################################
#sec biosyn I
selenocysteine-biosyn-I/1_2.7.9.3_2.7.9.3-RXN                                     : 1.0 H2O + 1.0 selenide + 1.0 ATP --> 1.0 selenophosphate + 1.0 phosphate + 1.0 AMP  # source:
MetaCyc, BRENDA, KEGG (queried 2.7.9.3)
selenocysteine-biosyn-I/2_2.9.1.1_2.9.1.1-RXN                                     : 1.0 selenophosphate + 1.0 |L-seryl-SEC-tRNAs| --> 1.0 phosphate + 1.0 |Charged-SEC-tRNAs|  #
source: MetaCyc (queried 2.9.1.1)

seleno-amino-acid-biosynthesis_2.5.1.47_RXN-12726                                 : 1.0 O-acetyl-L-serine + 1.0 hydrogen_selenide --> 1.0 acetate + 1.0 L-selenocysteine + 1.0 H+
# source: MetaCyc, BRENDA, KEGG (queried 2.5.1.47)
#####################################################################################################################################################################
#sec degr C
#NADH as a guess
selenocysteine-degr_mod_4.4.1.16_mod_SELENOCYSTEINE-LYASE-RXN                     : 1.0 NADPH + 1.0 L-selenocysteine --> 1.0 selenide + 1.0 NADP+ + 1.0 L-alanine + 1.0 H+ #
source: MetaCyc, BRENDA, KEGG (queried 4.4.1.16)
#####################################################################################################################################################################
#cys biosyn I
cysteine-biosyn-I/1_2.5.1.47_ACSERLY-RXN                                          : 1.0 hydrogen_sulfide + 1.0 O-acetyl-L-serine <=> 1.0 acetate + 1.0 L-cysteine + 1.0 H+  #
source: MetaCyc, BRENDA, KEGG (queried 2.5.1.47) // other EC numbers for this reaction: 2.5.1.65
cysteine-biosyn-I/2_2.3.1.30_SERINE-O-ACETTRAN-RXN                                : 1.0 L-serine + 1.0 acetyl-CoA --> 1.0 O-acetyl-L-serine + 1.0 coenzyme_A  # source: MetaCyc,
BRENDA, KEGG (queried 2.3.1.30)
#####################################################################################################################################################################
#cys degr II
cysteine-degr-II_4.4.1.8_4.4.1.1_LCYSDESULF-RXN                                   : 1.0 H2O + 1.0 L-cysteine --> 1.0 pyruvate + 1.0 hydrogen_sulfide + 1.0 ammonium  # source:
MetaCyc, BRENDA, KEGG (queried 4.4.1.8, 4.4.1.1) // other EC numbers for this reaction: 4.4.1.28
#####################################################################################################################################################################
#sulfite degr
sulfite-degr_manual_1.8.1.-_HD-sulf                                               : 1.0 sulfite + 3.0 NADH + 5.0 H+ <=> 3.0 H2O + 1.0 hydrogen_sulfide + 3.0 NAD+
#####################################################################################################################################################################
#histidine biosyn
histidine-biosyn/1_2.4.2.17_ATPPHOSPHORIBOSYLTRANS-RXN                            : 1.0 diphosphate + 1.0 1-(5-phospho-beta-D-ribosyl)-ATP <=> 1.0 H+ + 1.0 ATP + 1.0 5-phospho-
alpha-D-ribose_1-diphosphate  # source: MetaCyc, BRENDA, KEGG (queried 2.4.2.17)
histidine-biosyn/2_3.6.1.31_HISTPRATPHYD-RXN                                      : 1.0 H2O + 1.0 1-(5-phospho-beta-D-ribosyl)-ATP --> 1.0 1-(5-phospho-beta-D-ribosyl)-AMP + 2.0
H+ + 1.0 diphosphate  # source: MetaCyc, BRENDA, KEGG (queried 3.6.1.31)
histidine-biosyn/3_3.5.4.19_HISTCYCLOHYD-RXN                                      : 1.0 1-(5-phospho-beta-D-ribosyl)-AMP + 1.0 H2O --> 1.0 1-(5-phospho-beta-D-ribosyl)-5-[(5-
phosphoribosylamino)methylideneamino]imidazole-4-carboxamide  # source: MetaCyc, BRENDA, KEGG (queried 3.5.4.19)
histidine-biosyn/4_5.3.1.16_PRIBFAICARPISOM-RXN                                   : 1.0 1-(5-phospho-beta-D-ribosyl)-5-[(5-phosphoribosylamino)methylideneamino]imidazole-4-
carboxamide --> 1.0 phosphoribulosylformimino-AICAR-P  # source: MetaCyc, BRENDA, KEGG (queried 5.3.1.16)
histidine-biosyn/5_4.1.3.-_2.4.2.-_GLUTAMIDOTRANS-RXN                             : 1.0 phosphoribulosylformimino-AICAR-P + 1.0 L-glutamine --> 1.0 D-erythro-imidazole-glycerol-
phosphate + 1.0 H+ + 1.0 5-amino-1-(5-phospho-D-ribosyl)imidazole-4-carboxamide + 1.0 L-glutamate  # source: MetaCyc, BRENDA, KEGG (queried 4.1.3.-, 2.4.2.-) // other EC numbers
for this reaction: 2.4.2, 4.3.1.B2, 4.1.3
histidine-biosyn/6_4.2.1.19_IMIDPHOSDEHYD-RXN                                     : 1.0 D-erythro-imidazole-glycerol-phosphate --> 1.0 imidazole_acetol-phosphate + 1.0 H2O  #
source: MetaCyc, BRENDA, KEGG (queried 4.2.1.19)
histidine-biosyn/7_2.6.1.9_HISTAMINOTRANS-RXN                                     : 1.0 L-glutamate + 1.0 imidazole_acetol-phosphate --> 1.0 2-oxoglutarate + 1.0 L-histidinol-
phosphate  # source: MetaCyc, BRENDA, KEGG (queried 2.6.1.9)
histidine-biosyn/8_3.1.3.15_HISTIDPHOS-RXN                                        : 1.0 H2O + 1.0 L-histidinol-phosphate --> 1.0 histidinol + 1.0 phosphate  # source: MetaCyc,
BRENDA, KEGG (queried 3.1.3.15)
histidine-biosyn/9_1.1.1.23_HISTOLDEHYD-RXN                                       : 1.0 histidinol + 1.0 NAD+ --> 1.0 NADH + 1.0 histidinal + 1.0 H+  # source: MetaCyc, BRENDA,
KEGG (queried 1.1.1.23)
histidine-biosyn/10_1.1.1.23_HISTALDEHYD-RXN                                      : 1.0 histidinal + 1.0 H2O + 1.0 NAD+ --> 2.0 H+ + 1.0 NADH + 1.0 L-histidine  # source:
MetaCyc, BRENDA, KEGG (queried 1.1.1.23)
#####################################################################################################################################################################
#alanine biosyn
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alanine-biosyn_4.1.1.12_ASPARTATE-4-DECARBOXYLASE-RXN                                : 1.0 H+ + 1.0 L-aspartate --> 1.0 CO2 + 1.0 L-alanine  # source: MetaCyc, BRENDA, KEGG
(queried 4.1.1.12)
alanine-biosyn_2.6.1.2_ALANINE-AMINOTRANSFERASE-RXN                                  : 1.0 L-alanine + 1.0 2-oxoglutarate <=> 1.0 pyruvate + 1.0 L-glutamate  # source: MetaCyc,
BRENDA, KEGG (queried 2.6.1.2)
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#ornithine degr. II
ornithine-degr-II/1_5.1.1.12_ORNITHINE-RACEMASE-RXN                                  : 1.0 L-ornithine <=> 1.0 D-ornithine  # source: MetaCyc, BRENDA, KEGG (queried 5.1.1.12) //
other EC numbers for this reaction: 5.1.1.9, 5.1.1.10
ornithine-degr-II/2_5.4.3.5_ORNMUTST-RXN                                             : 1.0 D-ornithine <=> 1.0 (2R,4S)-2,_4-diaminopentanoate  # source: MetaCyc, BRENDA, KEGG
(queried 5.4.3.5)
ornithine-degr-II/3_1.4.1.12_24-DIAMINOPENTANOATE-DEHYDROGENASE-RXN_WOP              : 1.0 (2R,4S)-2,_4-diaminopentanoate + 1.0 H2O + 1.0 NAD+ <=> 1.0 ammonium + 1.0 NADH + 1.0 H+
+ 1.0 2-amino-4-oxopentanoate  # source: MetaCyc, BRENDA, KEGG (queried 1.4.1.12)
ornithine-degr-II/4_2.3.1.B10_AKPTHIOL-RXN                                           : 1.0 2-amino-4-oxopentanoate + 1.0 coenzyme_A <=> 1.0 acetyl-CoA + 1.0 D-alanine  # source:
MetaCyc, BRENDA, KEGG (queried 2.3.1.B10) // other EC numbers for this reaction: 2.3.1
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#pro degr
proline-degr/1_5.1.1.4_PROLINE-RACEMASE-RXN                                          : 1.0 L-proline <=> 1.0 D-proline  # source: MetaCyc, BRENDA, KEGG (queried 5.1.1.4)
proline-degr/2_1.21.4.1_BS370299                                                     : 1.0 H+ + 1.0 D-proline + 1.0 NADH <=> 1.0 5-aminopentanoate + 1.0 NAD+  # source: BRENDA
(queried 1.21.4.1) // balanced // contains implicit reactant(s): H+, H2O
#######################################################################################################################################################################
#glycine degr.
glycine-cleavage/1_moddir_1.4.4.2_GCVP-RXN                                           : 1.0 glycine + 1.0 lipoamide + 1.0 H+ <=> 1.0 [glycine-cleavage_complex_H_protein]_N6-
aminomethyldihydrolipoyl-L-lysine + 1.0 CO2  # source: MetaCyc (queried 1.4.4.2)
glycine-cleavage/2_2.1.2.10_GCVT-RXN                                                 : 1.0 tetrahydropteroyl_tri-L-glutamate + 1.0 [glycine-cleavage_complex_H_protein]_N6-
aminomethyldihydrolipoyl-L-lysine <=> 1.0 dihydrolipoamide + 1.0 5,10-methylene-tetrahydrofolate + 1.0 ammonium  # source: MetaCyc (queried 2.1.2.10)
glycine-cleavage/3_1.8.1.4_RXN-7719                                                  : 1.0 NAD+ + 1.0 dihydrolipoamide <=> 1.0 lipoamide + 1.0 NADH + 1.0 H+  # source: MetaCyc
(queried 1.8.1.4)

glycine-degr/1_1.21.4.2_RXN-7566                                                     : 1.0 |Ox-Thioredoxin| + 1.0 H2O + 1.0 ammonium + 1.0 acetyl_phosphate <-- 1.0 |Red-
Thioredoxin| + 1.0 H+ + 1.0 phosphate + 1.0 glycine  # source: MetaCyc, KEGG (queried 1.21.4.2)
glycine-degr/2_1.8.1.9_THIOREDOXIN-REDUCT-NADPH-RXN                                  : 1.0 NADP+ + 1.0 |Red-Thioredoxin| <-- 1.0 NADPH + 1.0 H+ + 1.0 |Ox-Thioredoxin|  # source:
MetaCyc, KEGG (queried 1.8.1.9)
#######################################################################################################################################################################
#chorismate biosyn I
chorismate-biosyn-I/1_2.5.1.54_DAHPSYN-RXN                                           : 1.0 H2O + 1.0 phosphoenolpyruvate + 1.0 D-erythrose_4-phosphate <=> 1.0 phosphate + 1.0 3-
deoxy-D-arabino-heptulosonate-7-phosphate  # source: MetaCyc, BRENDA, KEGG (queried 2.5.1.54)
chorismate-biosyn-I/2_4.2.3.4_3-DEHYDROQUINATE-SYNTHASE-RXN                          : 1.0 3-deoxy-D-arabino-heptulosonate-7-phosphate --> 1.0 phosphate + 1.0 3-dehydroquinate  #
source: MetaCyc, BRENDA, KEGG (queried 4.2.3.4)
chorismate-biosyn-I/3_4.2.1.10_3-DEHYDROQUINATE-DEHYDRATASE-RXN                      : 1.0 3-dehydroquinate <=> 1.0 H2O + 1.0 3-dehydroshikimate  # source: MetaCyc, BRENDA, KEGG
(queried 4.2.1.10)
chorismate-biosyn-I/4_1.1.1.25_RXN-7968                                              : 1.0 shikimate + 1.0 NADP+ <-- 1.0 3-dehydroshikimate + 1.0 H+ + 1.0 NADPH  # source: MetaCyc,
BRENDA, KEGG (queried 1.1.1.25) // other EC numbers for this reaction: 1.1.1.282, 1.1.1.24
chorismate-biosyn-I/5_2.7.1.71_SHIKIMATE-KINASE-RXN                                  : 1.0 ATP + 1.0 shikimate --> 1.0 H+ + 1.0 ADP + 1.0 shikimate_3-phosphate  # source: MetaCyc,
BRENDA, KEGG (queried 2.7.1.71)
chorismate-biosyn-I/6_2.5.1.19_2.5.1.19-RXN                                          : 1.0 phosphoenolpyruvate + 1.0 shikimate_3-phosphate <=> 1.0 5-enolpyruvyl-shikimate_3-
phosphate + 1.0 phosphate  # source: MetaCyc, BRENDA, KEGG (queried 2.5.1.19)
chorismate-biosyn-I/7_4.2.3.5_CHORISMATE-SYNTHASE-RXN                                : 1.0 5-enolpyruvyl-shikimate_3-phosphate --> 1.0 phosphate + 1.0 chorismate  # source:
MetaCyc, BRENDA, KEGG (queried 4.2.3.5)
#######################################################################################################################################################################
#tyr/phe biosyn

tyr/phe-biosyn_5.4.99.5_CHORISMATEMUT-RXN                                            : 1.0 chorismate <=> 1.0 prephenate  # source: MetaCyc, BRENDA, KEGG (queried 5.4.99.5)

tyrosine-biosyn_I/1_1.3.1.12_PREPHENATEDEHYDROG-RXN                                  : 1.0 prephenate + 1.0 NAD+ --> 1.0 4-hydroxyphenylpyruvate + 1.0 CO2 + 1.0 NADH  # source:
MetaCyc, BRENDA, KEGG (queried 1.3.1.12)
tyrosine-biosyn_I/2a_2.6.1.9_2.6.1.1_2.6.1.57_TYROSINE-AMINOTRANSFERASE-RXN          : 1.0 L-tyrosine + 1.0 2-oxoglutarate <=> 1.0 4-hydroxyphenylpyruvate + 1.0 L-glutamate  #
source: MetaCyc, BRENDA, KEGG (queried 2.6.1.9, 2.6.1.1, 2.6.1.57) // other EC numbers for this reaction: 2.6.1.5
tyrosine-biosyn_I/2b_2.6.1.51_RXN3O-4157                                             : 1.0 L-tyrosine + 1.0 pyruvate <=> 1.0 L-alanine + 1.0 4-hydroxyphenylpyruvate  # source:
MetaCyc, BRENDA, KEGG (queried 2.6.1.51) // other EC numbers for this reaction: 2.6.1.44, 2.6.1.58

phenylalanine-biosyn-I/1_4.2.1.51_PREPHENATEDEHYDRAT-RXN                             : 1.0 prephenate + 1.0 H+ --> 1.0 2-oxo-3-phenylpropanoate + 1.0 CO2 + 1.0 H2O  # source:
MetaCyc, BRENDA, KEGG (queried 4.2.1.51) // other EC numbers for this reaction: 4.2.1.91
phenylalanine-biosyn-I/2a_2.6.1.57_2.6.1.9_2.6.1.1_2.6.1.42_PHEAMINOTRANS-RXN       : 1.0 L-glutamate + 1.0 2-oxo-3-phenylpropanoate <=> 1.0 2-oxoglutarate + 1.0 L-phenylalanine
# source: MetaCyc, BRENDA, KEGG (queried 2.6.1.57, 2.6.1.9, 2.6.1.1, 2.6.1.42) // there are 5 more EC numbers for this reaction
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phenylalanine-biosyn-I/2b_2.6.1.57_RXN-7708                                    : 1.0 2-oxo-3-phenylpropanoate + 1.0 L-methionine <=> 1.0 2-oxo-4-methylthiobutanoate + 1.0 L-
phenylalanine  # source: MetaCyc, BRENDA (queried 2.6.1.57) // other EC numbers for this reaction: 2.6.1.28

#side reactions
phenylalanine-biosyn-II/1_2.6.1.57_PREPHENATE-ASP-TRANSAMINE-RXN               : 1.0 oxaloacetate + 1.0 L-arogenate <=> 1.0 L-aspartate + 1.0 prephenate  # source: MetaCyc,
BRENDA, KEGG (queried 2.6.1.57) // other EC numbers for this reaction: 2.6.1.78
phenylalanine-biosyn-II/2_4.2.1.51_CARBOXYCYCLOHEXADIENYL-DEHYDRATASE-RXN      : 1.0 H+ + 1.0 L-arogenate --> 1.0 L-phenylalanine + 1.0 CO2 + 1.0 H2O  # source: MetaCyc,
BRENDA, KEGG (queried 4.2.1.51) // other EC numbers for this reaction: 4.2.1.91

methionine-from-2-oxo-4-methylthiobutanoate_2.6.1.57_RXN-14147                 : 1.0 2-oxoglutarate + 1.0 L-methionine <=> 1.0 2-oxo-4-methylthiobutanoate + 1.0 L-glutamate
# source: MetaCyc, BRENDA, KEGG (queried 2.6.1.57) // other EC numbers for this reaction: 2.6.1.5, 2.6.1.7
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#trp/tyr/phe/his degr

tryptophan-degr_2.6.1.27_TRYPTOPHAN-AMINOTRANSFERASE-RXN                       : 1.0 L-tryptophan + 1.0 2-oxoglutarate <=> 1.0 L-glutamate + 1.0 indole-3-pyruvate  # source:
MetaCyc, BRENDA, KEGG (queried 2.6.1.27)
tryptophan-degr_2.6.1.57_RXN-14685                                             : 1.0 indole-3-pyruvate + 1.0 L-methionine <=> 1.0 2-oxo-4-methylthiobutanoate + 1.0 L-
tryptophan  # source: MetaCyc, BRENDA (queried 2.6.1.57)
histidine-degr_2.6.1.38_HISTTRANSAM-RXN                                        : 1.0 L-histidine + 1.0 2-oxoglutarate <=> 1.0 imidazole-pyruvate + 1.0 L-glutamate  # source:
MetaCyc, BRENDA, KEGG (queried 2.6.1.38)

tryptophan-ox/1_1.2.7.8_1.2.7.8-RXN                                            : 1.0 coenzyme_A + 2.0 |Oxidized-ferredoxins| + 1.0 indole-3-pyruvate --> 2.0 |Reduced-
ferredoxins| + 1.0 S-2-(indol-3_yl)acetyl-CoA + 1.0 H+ + 1.0 CO2  # source: MetaCyc, KEGG (queried 1.2.7.8)
tyrosine-ox/1_manual_1.2.7.8_HD-1.2.7.8-tyr                                    : 1.0 4-hydroxyphenylpyruvate + 2.0 |Oxidized-ferredoxins| + 1.0 coenzyme_A --> 1.0 CO2 + 2.0 |
Reduced-ferredoxins| + 1.0 4-hydroxyphenylacetyl-CoA  + 1.0 H+
phenylalanine-ox/1_manual_1.2.7.8_HD-1.2.7.8-phe                               : 1.0 2-oxo-3-phenylpropanoate + 2.0 |Oxidized-ferredoxins| + 1.0 coenzyme_A --> 1.0 CO2 + 2.0
|Reduced-ferredoxins| + 1.0 phenylacetyl-CoA
histidine-ox/1_manual_1.2.7.8_HD-1.2.7.8-his                                   : 1.0 imidazole-pyruvate + 2.0 |Oxidized-ferredoxins| + 1.0 coenzyme_A --> 1.0 CO2 + 2.0 |
Reduced-ferredoxins| + 1.0 imidazolylacetyl-CoA

tryptophan-ox/2_manual_2.3.1.-_HD-2.3.1.-trp                                   : 1.0 S-2-(indol-3_yl)acetyl-CoA + 1.0 phosphate --> 1.0 indole-3-acetyl_phosphate + 1.0
coenzyme_A
tyrosine-ox/2_2.3.1.-_manual_HD-2.3.1.-tyr                                     : 1.0 4-hydroxyphenylacetyl-CoA + 1.0 phosphate --> 1.0 4-hydroxyphenylacetyl_phosphate + 1.0
coenzyme_A
phenylalanine-ox/2_2.3.1.-_manual_HD-2.3.1.-phe                                : 1.0 phenylacetyl-CoA + 1.0 phosphate --> 1.0 phenylacetyl_phosphate + 1.0 coenzyme_A
histidine-ox/2_2.3.1.-_manual_HD-2.3.1.-his                                    : 1.0 imidazolylacetyl-CoA + 1.0 phosphate --> 1.0 imidazolylacetyl_phosphate + 1.0 coenzyme_A

tryptophan-ox/3_manual_2.7.2.-_HD-2.7.2.-trp                                   : 1.0 indole-3-acetyl_phosphate + 1.0 ADP --> 1.0 indole-3-acetate + 1.0 ATP
tyrosine-ox/3_manual_2.7.2.-_HD-2.7.2.-tyr                                     : 1.0 4-hydroxyphenylacetyl_phosphate + 1.0 ADP --> 1.0 4-hydroxyphenylacetate + 1.0 ATP
phenylalanine-ox/3_manual_2.7.2.-_HD-2.7.2.-phe                                : 1.0 phenylacetyl_phosphate + 1.0 ADP --> 1.0 phenylacetate + 1.0 ATP
histidine-ox/3_manual_2.7.2.-_HD-2.7.2.-his                                    : 1.0 imidazolylacetyl_phosphate + 1.0 ADP --> 1.0 4-imidazoleacetate + 1.0 ATP

tyrosine-ox/4_4.1.1.83_4.1.1.83-RXN                                            : 1.0 H+ + 1.0 4-hydroxyphenylacetate --> 1.0 CO2 + 1.0 4-methylphenol  # source: MetaCyc,
BRENDA, KEGG (queried 4.1.1.83)
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#arom red
phe-red/1_1.1.1.222_BS186998                                                   : 1.0 (R)-phenyllactate + 1.0 NAD+ <-- 1.0 H+ + 1.0 NADH + 1.0 2-oxo-3-phenylpropanoate  #
source: BRENDA, KEGG (queried 1.1.1.222) // other EC numbers for this reaction: 1.1.1.110, 1.1.1.237 // balanced // contains implicit reactant(s): H+, H2O
phe-red/2_manual_2.8.3.-_HD-2.8.3.-phe                                         : 1.0 (R)-phenyllactoyl-CoA + 1.0 3-phenylpropanoate <=> 1.0 3-phenylpropanoyl-CoA + 1.0 (R)-
phenyllactate
phe-red/3_manual_4.2.1.-_HD-4.2.1.-phe                                         : 1.0 (R)-phenyllactoyl-CoA --> 1.0 3-phenylacryloyl-CoA + 1.0 H2O
phe-red/4_manual_1.3.98.-_HD-1.3.98.-phe                                       : 1.0 3-phenylacryloyl-CoA + 2.0 NADH + 2.0 |Oxidized-ferredoxins| <=> 1.0 3-phenylpropanoyl-
CoA + 2.0 |Reduced-ferredoxins| + 2.0 NAD+

tyr-red/1_1.1.1.222_1.1.1.222-RXN_WOP                                          : 1.0 NADH + 1.0 4-hydroxyphenylpyruvate + 1.0 H+ <=> 1.0 (R)-3-(4-hydroxyphenyl)lactate + 1.0
NAD+  # source: MetaCyc, BRENDA, KEGG (queried 1.1.1.222)
tyr-red/2_manual_2.8.3.-_HD-2.8.3.-tyr                                         : 1.0 (R)-(4-hydroxyphenyl)lactoyl-CoA + 1.0 3-(4-hydroxyphenyl)propanoate <=> 1.0 3-(4-
hydroxyphenyl)propanoyl-CoA + 1.0 (R)-3-(4-hydroxyphenyl)lactate
tyr-red/3_manual_4.2.1.-_HD-4.2.1.-tyr                                         : 1.0 (R)-(4-hydroxyphenyl)lactoyl-CoA --> 1.0 3-(4-hydroxyphenyl)acryloyl-CoA + 1.0 H2O
tyr-red/4_manual_1.3.98.-_HD-1.3.98.-tyr                                       : 1.0 3-(4-hydroxyphenyl)acryloyl-CoA + 2.0 NADH + 2.0 |Oxidized-ferredoxins| <=> 1.0 3-(4-
hydroxyphenyl)propanoyl-CoA + 2.0 |Reduced-ferredoxins| + 2.0 NAD+
#########################################################################################################################################################
#valine biosyn
valine-biosyn/1_2.2.1.6_RXN-12583                                              : 1.0 thiamine_diphosphate + 1.0 pyruvate + 1.0 H+ --> 1.0 2-(alpha-
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hydroxyethyl)thiamine_diphosphate + 1.0 CO2  # source: MetaCyc, KEGG (queried 2.2.1.6) // other EC numbers for this reaction: 4.1.1.1, 1.2.4.1
valine-biosyn/2_2.2.1.6_RXN-14037                                                : 1.0 (S)-2-acetolactate + 1.0 thiamine_diphosphate <=> 1.0 2-(alpha-
hydroxyethyl)thiamine_diphosphate + 1.0 pyruvate  # source: MetaCyc, KEGG (queried 2.2.1.6)
valine-biosyn/3_1.1.1.86_RXN-16061                                               : 1.0 NADP+ + 1.0 (2R)-2,3-dihydroxy-3-methylbutanoate <=> 1.0 H+ + 1.0 (S)-2-acetolactate +
1.0 NADPH  # source: MetaCyc, BRENDA, KEGG (queried 1.1.1.86) // other EC numbers for this reaction: 1.1.1.383
valine-biosyn/4_4.2.1.9_DIHYDROXYISOVALDEHYDRAT-RXN                              : 1.0 (2R)-2,3-dihydroxy-3-methylbutanoate --> 1.0 H2O + 1.0 3-methyl-2-oxobutanoate  # source:
MetaCyc, KEGG (queried 4.2.1.9)

valine-biosyn/5_2.6.1.42_BRANCHED-CHAINAMINOTRANSFERVAL-RXN                      : 1.0 2-oxoglutarate + 1.0 L-valine <=> 1.0 3-methyl-2-oxobutanoate + 1.0 L-glutamate  #
source: MetaCyc, BRENDA, KEGG (queried 2.6.1.42) // other EC numbers for this reaction: 2.6.1.6
################################################################################################################################################################
#leucine biosyn
leucine-biosyn/1_2.3.3.13_2-ISOPROPYLMALATESYN-RXN                               : 1.0 H2O + 1.0 acetyl-CoA + 1.0 3-methyl-2-oxobutanoate --> 1.0 H+ + 1.0 coenzyme_A + 1.0
(2S)-2-isopropylmalate  # source: MetaCyc, BRENDA, KEGG (queried 2.3.3.13)
leucine-biosyn/2_4.2.1.33_RXN-13163                                              : 1.0 (2R,3S)-3-isopropylmalate <=> 1.0 (2S)-2-isopropylmalate  # source: MetaCyc, BRENDA, KEGG
(queried 4.2.1.33)
leucine-biosyn/3_1.1.1.85_3-ISOPROPYLMALDEHYDROG-RXN                             : 1.0 NAD+ + 1.0 (2R,3S)-3-isopropylmalate <=> 1.0 H+ + 1.0 NADH + 1.0 (2S)-2-isopropyl-3-
oxosuccinate  # source: MetaCyc, BRENDA, KEGG (queried 1.1.1.85)
leucine-biosyn/4_spontaneous_1.1.1.85_RXN-7800                                   : 1.0 (2S)-2-isopropyl-3-oxosuccinate + 1.0 H+ --> 1.0 4-methyl-2-oxopentanoate + 1.0 CO2  #
source: MetaCyc, KEGG (queried 1.1.1.85)

leucine-biosyn/5_2.6.1.42_BRANCHED-CHAINAMINOTRANSFERLEU-RXN                     : 1.0 L-leucine + 1.0 2-oxoglutarate <=> 1.0 4-methyl-2-oxopentanoate + 1.0 L-glutamate  #
source: MetaCyc, BRENDA, KEGG (queried 2.6.1.42) // other EC numbers for this reaction: 2.6.1.67, 2.6.1.6
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#isoleucine biosyn

isoleucine-biosyn-II/1_2.3.1.182_RXN-7743                                        : 1.0 pyruvate + 1.0 acetyl-CoA + 1.0 H2O --> 1.0 H+ + 1.0 (R)-citramalate + 1.0 coenzyme_A  #
source: MetaCyc, BRENDA, KEGG (queried 2.3.1.182)
isoleucine-biosyn-II/2_4.2.1.35_R-2-METHYLMALATE-DEHYDRATASE-RXN                 : 1.0 (R)-citramalate <=> 1.0 H2O + 1.0 citraconate  # source: MetaCyc, BRENDA, KEGG (queried
4.2.1.35)
isoleucine-biosyn-II/3_4.2.1.35_RXN-7744                                         : 1.0 citraconate + 1.0 H2O --> 1.0 (2R,3S)-3-methylmalate  # source: MetaCyc, KEGG (queried
4.2.1.35)
isoleucine-biosyn-II/4_1.1.1.85_RXN-7745                                         : 1.0 NAD+ + 1.0 (2R,3S)-3-methylmalate --> 1.0 CO2 + 1.0 2-oxobutanoate + 1.0 NADH  # source:
MetaCyc, KEGG (queried 1.1.1.85) // other EC numbers for this reaction: 1.1.1
isoleucine-biosyn-II/5_2.2.1.6_R04673                                            : 1.0 2-oxobutanoate + 1.0 2-(alpha-hydroxyethyl)thiamine_diphosphate <=> 1.0
thiamine_diphosphate + 1.0 (S)-2-aceto-2-hydroxybutanoate  # source: KEGG (queried 2.2.1.6)
isoleucine-biosyn-II/6_1.1.1.86_ACETOOHBUTREDUCTOISOM-RXN                        : 1.0 (R)-2,3-dihydroxy-3-methylpentanoate + 1.0 NADP+ <-- 1.0 NADPH + 1.0 (S)-2-aceto-2-
hydroxybutanoate + 1.0 H+  # source: MetaCyc (queried 1.1.1.86)
isoleucine-biosyn-II/7_4.2.1.9_DIHYDROXYMETVALDEHYDRAT-RXN                       : 1.0 (R)-2,3-dihydroxy-3-methylpentanoate --> 1.0 H2O + 1.0 (S)-3-methyl-2-oxopentanoate  #
source: MetaCyc, KEGG (queried 4.2.1.9)
isoleucine-biosyn-II/8_2.6.1.42_BRANCHED-CHAINAMINOTRANSFERILEU-RXN              : 1.0 L-isoleucine + 1.0 2-oxoglutarate <=> 1.0 (S)-3-methyl-2-oxopentanoate + 1.0 L-glutamate
# source: MetaCyc, BRENDA, KEGG (queried 2.6.1.42) // other EC numbers for this reaction: 2.6.1.67
################################################################################################################################################################
#val/leu/ile degr ox

valine-ox/1_1.2.7.7_1.2.7.7-RXN                                                  : 1.0 coenzyme_A + 1.0 3-methyl-2-oxobutanoate + 2.0 |Oxidized-ferredoxins| --> 1.0 CO2 + 2.0 |
Reduced-ferredoxins| + 1.0 H+ + 1.0 isobutanoyl-CoA  # source: MetaCyc, KEGG (queried 1.2.7.7)
leucine-ox/1_manual_1.2.7.7_HD-1.2.7.7-leu                                       : 1.0 4-methyl-2-oxopentanoate + 2.0 |Oxidized-ferredoxins| + 1.0 coenzyme_A --> 1.0
isovaleryl-CoA + 1.0 CO2 + 2.0 |Reduced-ferredoxins| + 1.0 H+
isoleucine-ox/1_manual_1.2.7.7_HD-1.2.7.7-ile                                    : 1.0 (S)-3-methyl-2-oxopentanoate + 2.0 |Oxidized-ferredoxins| + 1.0 coenzyme_A --> 1.0 2-
methylbutanoyl-CoA + 1.0 CO2 + 2.0 |Reduced-ferredoxins| + 1.0 H+

valine-ox/2_manual_2.3.1.-_HD-2.3.1.-val                                         : 1.0 isobutanoyl-CoA + 1.0 phosphate --> 1.0 isobutyryl_phosphate + 1.0 coenzyme_A
leucine-ox/2_manual_2.3.1.-_HD-2.3.1.-leu                                        : 1.0 isovaleryl-CoA + 1.0 phosphate --> 1.0 isovaleryl_phosphate + 1.0 coenzyme_A
isoleucine-ox/2_manual_2.3.1.-_HD-2.3.1.-ile                                     : 1.0 2-methylbutanoyl-CoA + 1.0 phosphate --> 1.0 2-methylbutanoyl_phosphate + 1.0 coenzyme_A

valine-ox/3_manual_2.7.2.-_HD-2.7.2.-val                                         : 1.0 isobutyryl_phosphate + 1.0 ADP --> 1.0 isobutyrate + 1.0 ATP
leucine-ox/3_manual_2.7.2.-_HD-.7.2.-leu                                         : 1.0 isovaleryl_phosphate + 1.0 ADP --> 1.0 isovalerate + 1.0 ATP
isoleucine-ox/3_manual_2.7.2.-_HD-2.7.2.-ile                                     : 1.0 2-methylbutanoyl_phosphate + 1.0 ADP --> 1.0 2-methylbutanoate + 1.0 ATP
################################################################################################################################################################
#leu degr red
leu-red/1_manual_1.1.1.345_HD-1.1.1.345                                          : 1.0 D-2-hydroxyisocaproate + 1.0 NAD+ <-- 1.0 4-methyl-2-oxopentanoate + 1.0 H+ + 1.0 NADH
leu-red/2a_manual_2.8.3.-_HD-2.8.3.-leu-A                                        : 1.0 D-2-hydroxyisocaproyl-CoA + 1.0 isocaproate <=> 1.0 isocaproyl-CoA + 1.0 D-2-
hydroxyisocaproate
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leu-red/3_manual_4.2.1.-_HD-4.2.1.-leu                                                    : 1.0 D-2-hydroxyisocaproyl-CoA --> 1.0 2-isocaprenoyl-CoA + 1.0 H2O
leu-red/4_manual_1.3.98.-_HD-1.3.98.-leu                                                  : 1.0 2-isocaprenoyl-CoA + 2.0 NADH + 2.0 |Oxidized-ferredoxins| <=> 1.0 isocaproyl-CoA + 2.0 |
Reduced-ferredoxins| + 2.0 NAD+ # Li et al. 2007: Coupled Ferredoxin and Crotonyl ...; Blast and position
#for the fatty acids
leu-red/2b_manual_2.8.3.-_HD-2.8.3.-leu-B                                                 : 1.0 D-2-hydroxyisocaproyl-CoA + 1.0 acetate <=> 1.0 acetyl-CoA + 1.0 D-2-hydroxyisocaproate
leu-red/5_manual_2.3.1.-_HD-2.3.1.-leu-red                                                : 1.0 isocaproyl-CoA + 1.0 phosphate --> 1.0 isocaproyl_phosphate + 1.0 coenzyme_A
#########################################################################################################################################################################
#pyruvate decarbox.
formate_2.3.1.54_PYRUVFORMLY-RXN                                                          : 1.0 formate + 1.0 acetyl-CoA <=> 1.0 coenzyme_A + 1.0 pyruvate  # source: MetaCyc, BRENDA,
KEGG (queried 2.3.1.54)
formate_2.3.1.54_KETOBUTFORMLY-RXN                                                        : 1.0 coenzyme_A + 1.0 2-oxobutanoate --> 1.0 formate + 1.0 propanoyl-CoA  # source: MetaCyc,
BRENDA, KEGG (queried 2.3.1.54) // other EC numbers for this reaction: 2.3.1
#########################################################################################################################################################################
#ferm. EtOH/PropOH/ButOH:
ferm-EtOH/1_1.2.1.10_ACETALD-DEHYDROG-RXN                                                 : 1.0 NAD+ + 1.0 coenzyme_A + 1.0 acetaldehyde <=> 1.0 acetyl-CoA + 1.0 H+ + 1.0 NADH  #
source: MetaCyc, BRENDA, KEGG (queried 1.2.1.10)
ferm-EtOH/2_1.1.1.1_ALCOHOL-DEHYDROGENASE-NADP+-RXN_WOP                                   : 1.0 ethanol + 1.0 NAD+ <=> 1.0 H+ + 1.0 NADH + 1.0 acetaldehyde  # source: MetaCyc, BRENDA,
KEGG (queried 1.1.1.1) // other EC numbers for this reaction: 1.1.1.71

ferm-PropOH/1_1.2.1.87_RXN-12736                                                          : 1.0 coenzyme_A + 1.0 NAD+ + 1.0 propanal <=> 1.0 NADH + 1.0 H+ + 1.0 propanoyl-CoA  # source:
MetaCyc, BRENDA, KEGG (queried 1.2.1.87)
ferm-PropOH/2_1.1.1.1_RXN-13198                                                           : 1.0 n-propanol + 1.0 NAD+ <=> 1.0 H+ + 1.0 propanal + 1.0 NADH  # source: MetaCyc, BRENDA,
KEGG (queried 1.1.1.1) // other EC numbers for this reaction: 1.1.1.202, 1.1.1.265

ferm-ButOH/1_1.2.1.10_1.2.1.87_BUTANAL-DEHYDROGENASE-RXN_WOP                              : 1.0 butanal + 1.0 coenzyme_A + 1.0 NAD+ <=> 1.0 butanoyl-CoA + 1.0 NADH + 1.0 H+  # source:
MetaCyc, BRENDA, KEGG (queried 1.2.1.10, 1.2.1.87) // other EC numbers for this reaction: 1.2.1.57
ferm-ButOH/2_1.1.1.-_RXN-161                                                              : 1.0 n-butanol + 1.0 NAD+ <-- 1.0 NADH + 1.0 butanal + 1.0 H+  # source: MetaCyc, BRENDA, KEGG
(queried 1.1.1.-) // other EC numbers for this reaction: 1.1.1, 1.1.1.265

ferm-IbutOH/1_1.2.1.10_RXN-13671                                                          : 1.0 NAD+ + 1.0 coenzyme_A + 1.0 isobutanal <=> 1.0 H+ + 1.0 NADH + 1.0 isobutanoyl-CoA  #
source: MetaCyc, BRENDA (queried 1.2.1.10)
ferm-IbutOH/2_1.1.1.1_RXN-7657                                                            : 1.0 NAD+ + 1.0 isobutanol <=> 1.0 NADH + 1.0 isobutanal + 1.0 H+  # source: MetaCyc, BRENDA
(queried 1.1.1.1)
#########################################################################################################################################################################
#ferm acetate/propanoate
ferm-acetate/1_1.2.7.1_PYRUFLAVREDUCT-RXN                                                 : 1.0 coenzyme_A + 1.0 pyruvate + 2.0 |Oxidized-ferredoxins| <=> 1.0 acetyl-CoA + 2.0 |Reduced-
ferredoxins| + 1.0 H+ + 1.0 CO2  # source: MetaCyc, KEGG (queried 1.2.7.1) // other EC numbers for this reaction: 1.2.7.11
ferm-acetate/2_2.3.1.8_PHOSACETYLTRANS-RXN                                                : 1.0 acetyl-CoA + 1.0 phosphate <=> 1.0 acetyl_phosphate + 1.0 coenzyme_A  # source: MetaCyc,
BRENDA, KEGG (queried 2.3.1.8)
ferm-acetate/3_2.7.2.1_moddir_ACETATEKIN-RXN                                              : 1.0 ATP + 1.0 acetate <=> 1.0 acetyl_phosphate + 1.0 ADP  # source: MetaCyc, BRENDA, KEGG
(queried 2.7.2.1) // other EC numbers for this reaction: 2.7.2.15

ferm-propanoate/1_1.2.7.1_2-OXOBUTYRATE-SYNTHASE-RXN                                      : 1.0 2-oxobutanoate + 1.0 coenzyme_A + 2.0 |Oxidized-ferredoxins| <=> 1.0 H+ + 1.0 propanoyl-
CoA + 1.0 CO2 + 2.0 |Reduced-ferredoxins|  # source: MetaCyc, KEGG (queried 1.2.7.1) // other EC numbers for this reaction: 1.2.7
ferm-propanoate/2_2.3.1.222_2.3.1.8_PTAALT-RXN                                            : 1.0 phosphate + 1.0 propanoyl-CoA <=> 1.0 coenzyme_A + 1.0 propanoyl_phosphate  # source:
MetaCyc, BRENDA, KEGG (queried 2.3.1.222, 2.3.1.8)
ferm-propanoate/3_2.7.2.1_moddir_PROPKIN-RXN                                              : 1.0 propanoate + 1.0 ATP <=> 1.0 ADP + 1.0 propanoyl_phosphate  # source: MetaCyc, BRENDA,
KEGG (queried 2.7.2.1) // other EC numbers for this reaction: 2.7.2.15
#########################################################################################################################################################################
#6.2.1.13
#Homolog to priviously characterized Isoenzyme I of Archaeoglobus fulgidus (Musfeldt and Schönheit, 2002)
acetyl-CoA-to-acid_6.2.1.13_ACETATE--COA-LIGASE-ADP-FORMING-RXN                           : 1.0 ATP + 1.0 coenzyme_A + 1.0 acetate <=> 1.0 ADP + 1.0 acetyl-CoA + 1.0 phosphate  #
source: MetaCyc, BRENDA, KEGG (queried 6.2.1.13)
propanoyl-CoA-to-acid_6.2.1.13_PROPANOATECOA-LIGASE-RXN                                   : 1.0 propanoate + 1.0 coenzyme_A + 1.0 ATP <=> 1.0 propanoyl-CoA + 1.0 phosphate + 1.0 ADP  #
source: MetaCyc, BRENDA, KEGG (queried 6.2.1.13)
butanoyl-CoA-to-acid_manual_6.2.1.13_HD-6.2.1.13                                          : 1.0 ATP + 1.0 coenzyme_A + 1.0 butanoate <=> 1.0 ADP + 1.0 butanoyl-CoA + 1.0 phosphate
#########################################################################################################################################################################
#fermentation to propanoate C (stickland-reductive-like)
propanoate-ferm/1a_2.8.3.-_PROPIONLACT-RXN                                                    : 1.0 propanoyl-CoA + 1.0 (S)-lactate <=> 1.0 (S)-lactoyl-CoA + 1.0 propanoate  #
source: MetaCyc, KEGG (queried 2.8.3.-) // other EC numbers for this reaction: 2.8.3.1, 2.8.3
propanoate-ferm/2a_4.2.1.54_RXN-781                                                           : 1.0 (S)-lactoyl-CoA <=> 1.0 H2O + 1.0 acryloyl-CoA  # source: MetaCyc, BRENDA, KEGG
(queried 4.2.1.54) // other EC numbers for this reaction: 4.2.1
propanoate-ferm/1b_2.8.3.-_LACCOA-RXN                                                         : 1.0 propanoyl-CoA + 1.0 (R)-lactate <=> 1.0 (R)-lactoyl-CoA + 1.0 propanoate  #
source: MetaCyc, BRENDA (queried 2.8.3.-) // other EC numbers for this reaction: 2.8.3.1, 2.8.3
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propanoate-ferm/2b_4.2.1.54_LACTOYL-COA-DEHYDRATASE-RXN                                    : 1.0 (R)-lactoyl-CoA <=> 1.0 acryloyl-CoA + 1.0 H2O  # source: MetaCyc, BRENDA
(queried 4.2.1.54)
propanoate-ferm/3_manual_1.3.98.-_HD-1.3.98.-prop                                          : 1.0 acryloyl-CoA + 2.0 NADH + 2.0 |Oxidized-ferredoxins| --> 1.0 propanoyl-CoA +
2.0 |Reduced-ferredoxins| + 2.0 NAD+ # Bifurcating like Li et al. 2007: Coupled Ferredoxin and Crotonyl ...
#propanoate-ferm/3_1.3.1.95_RXN-8568                                                       : 1.0 acryloyl-CoA + 1.0 NADH + 1.0 H+ --> 1.0 propanoyl-CoA + 1.0 NAD+  # source:
MetaCyc, BRENDA, KEGG (queried 1.3.1.95)
#############################################################################################################################################################
#lactate metabolism
#Both lactate dehydrogenases irreversible to prevent cycles
pyruvate-ferm-to-lactate_moddir_1.1.1.27_L-LACTATE-DEHYDROGENASE-RXN                        : 1.0 (S)-lactate + 1.0 NAD+ <-- 1.0 H+ + 1.0 NADH + 1.0 pyruvate  # source: MetaCyc,
BRENDA, KEGG (queried 1.1.1.27)
lactate-recemation_5.1.2.1_LACTATE-RACEMASE-RXN                                            : 1.0 (S)-lactate <=> 1.0 (R)-lactate  # source: MetaCyc, BRENDA, KEGG (queried
5.1.2.1)
lactate-oxidation_manual_1.1.98.-_HD-1.1.98.-pyr                                           : 1.0 pyruvate + 2.0 NADH + 2.0 |Oxidized-ferredoxins| <-- 1.0 (R)-lactate + 2.0 |
Reduced-ferredoxins| + 2.0 NAD+
#############################################################################################################################################################
#ferm. butanoate/butyrate
succinate-to-butyrate/1_2.8.3.18_RXN-8807                                                  : 1.0 acetate + 1.0 succinyl-CoA <=> 1.0 acetyl-CoA + 1.0 succinate  # source:
MetaCyc, BRENDA, KEGG (queried 2.8.3.18)
succinate-to-butyrate/2_1.2.1.76_RXN-8891                                                  : 1.0 succinate_semialdehyde + 1.0 NADP+ + 1.0 coenzyme_A <-- 1.0 succinyl-CoA + 1.0
H+ + 1.0 NADPH  # source: MetaCyc, BRENDA, KEGG (queried 1.2.1.76)
succinate-to-butyrate/3_1.1.1.61_RXN-6903_WOP                                              : 1.0 NAD+ + 1.0 4-hydroxybutanoate <=> 1.0 H+ + 1.0 NADH + 1.0
succinate_semialdehyde  # source: MetaCyc, BRENDA, KEGG (queried 1.1.1.61) // other EC numbers for this reaction: 1.1.1
succinate-to-butyrate/4a_2.8.3.-_RXN-8889                                                  : 1.0 acetyl-CoA + 1.0 4-hydroxybutanoate --> 1.0 4-hydroxybutanoyl-CoA + 1.0 acetate
# source: MetaCyc, BRENDA, KEGG (queried 2.8.3.-) // other EC numbers for this reaction: 2.8.3.1, 2.8.3
succinate-to-butyrate/4b_manual_2.8.3.-_HD-4hbut                                           : 1.0 4-hydroxybutanoate + 1.0 butanoyl-CoA --> 1.0 4-hydroxybutanoyl-CoA + 1.0
butanoate
succinate-to-butyrate/5a_4.2.1.120_RXN-8890                                                : 1.0 4-hydroxybutanoyl-CoA <=> 1.0 H2O + 1.0 crotonyl-CoA  # source: MetaCyc,
BRENDA, KEGG (queried 4.2.1.120)
succinate-to-butyrate/5b_moddir_4.2.1.120_BS403853                                         : 1.0 4-hydroxybutanoyl-CoA <=> 1.0 vinylacetyl-CoA + 1.0 H2O  # source: BRENDA, KEGG
(queried 4.2.1.120)
succinate-to-butyrate/6_5.3.3.3_VINYLACETYL-COA-DELTA-ISOMERASE-RXN                        : 1.0 vinylacetyl-CoA <=> 1.0 crotonyl-CoA  # source: MetaCyc, BRENDA, KEGG (queried
5.3.3.3)

acetyl-CoA-to-butyrate-II/1_2.3.1.9_ACETYL-COA-ACETYLTRANSFER-RXN                          : 2.0 acetyl-CoA <=> 1.0 acetoacetyl-CoA + 1.0 coenzyme_A  # source: MetaCyc, BRENDA,
KEGG (queried 2.3.1.9)
#The enzyme of C. difficile uses NADH (Aboulnaga et al., 2013)
acetyl-CoA-to-butyrate-II/2_1.1.1.35_HD-1.1.1.35                                           : 1.0 (S)-3-hydroxybutanoyl-CoA + 1.0 NAD+ <-- 1.0 acetoacetyl-CoA + 1.0 NADH + 1.0
H+
acetyl-CoA-to-butyrate-II/3_4.2.1.150_RXN-11667                                            : 1.0 (S)-3-hydroxybutanoyl-CoA <=> 1.0 crotonyl-CoA + 1.0 H2O  # source: MetaCyc,
BRENDA, KEGG (queried 4.2.1.150) // other EC numbers for this reaction: 4.2.1.17

crotonyl-CoA-to-butanoate/1_manual_1.3.98.-_HD-1.3.98.-but                                 : 1.0 crotonyl-CoA + 2.0 NADH + 2.0 |Oxidized-ferredoxins| <=> 1.0 butanoyl-CoA + 2.0
|Reduced-ferredoxins| + 2.0 NAD+
crotonyl-CoA-to-butanoate/2_2.3.1.19_PHOSPHATE-BUTYRYLTRANSFERASE-RXN                      : 1.0 phosphate + 1.0 butanoyl-CoA <=> 1.0 coenzyme_A + 1.0 butanoyl_phosphate  #
source: MetaCyc, BRENDA, KEGG (queried 2.3.1.19)
crotonyl-CoA-to-butanoate/3_moddir_2.7.2.7_BUTYRATE-KINASE-RXN                             : 1.0 butanoate + 1.0 ATP <=> 1.0 ADP + 1.0 butanoyl_phosphate  # source: MetaCyc,
BRENDA, KEGG (queried 2.7.2.7)

(R)-3-hydroxybutanoate-ferm/1a_2.8.3.9_2.8.3.9-RXN                                         : 1.0 acetoacetate + 1.0 butanoyl-CoA <=> 1.0 acetoacetyl-CoA + 1.0 butanoate  #
source: MetaCyc, BRENDA, KEGG (queried 2.8.3.9)
(R)-3-hydroxybutanoate-ferm/1b_2.8.3.9_ACETOACETYL-COA-TRANSFER-RXN                        : 1.0 acetyl-CoA + 1.0 acetoacetate <=> 1.0 acetoacetyl-CoA + 1.0 acetate  # source:
MetaCyc, BRENDA, KEGG (queried 2.8.3.9) // other EC numbers for this reaction: 2.8.3.8, 2.8.3
(R)-3-hydroxybutanoate-ferm/2_1.1.1.30_3-HYDROXYBUTYRATE-DEHYDROGENASE-RXN                 : 1.0 (R)-3-hydroxybutanoate + 1.0 NAD+ <=> 1.0 NADH + 1.0 acetoacetate + 1.0 H+  #
source: MetaCyc, BRENDA, KEGG (queried 1.1.1.30)

#spontaneous (Han et al. 2011)
acetone-fermentation_spontaneous_ACETOACETATE-DECARBOXYLASE-RXN                             : 1.0 acetoacetate + 1.0 H+ --> 1.0 acetone + 1.0 CO2  # source: MetaCyc, BRENDA,
KEGG
acetone-fermentation-ex_spontaneous_ACETOACETATE-DECARBOXYLASE-RXN                          : 1.0 acetoacetate[ex] + 1.0 H+[ex] --> 1.0 acetone[ex] + 1.0 CO2[ex]  # source:
MetaCyc, BRENDA, KEGG
#############################################################################################################################################################
#ferm. pentanoate
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pentanoate-ferm/1_2.3.1.9_RXN-12561 : 1.0 acetyl-CoA + 1.0 propanoyl-CoA <=> 1.0 coenzyme_A + 1.0 beta-ketovaleryl-CoA  # source: MetaCyc, BRENDA (queried 2.3.1.9) // other EC numbers for this reaction: 2.3.1.16
pentanoate-ferm/2_manual_1.1.1.157_HD-1.1.1.157-pent : 1.0 (R)-3-hydroxypentanoyl-CoA + 1.0 NAD+ <-- 1.0 H+ + 1.0 NADH + 1.0 beta-ketovaleryl-CoA
pentanoate-ferm/3_manual_4.2.1.150_HD-4.2.1.150-pent : 1.0 (R)-3-hydroxypentanoyl-CoA --> 1.0 2-pentenoyl-CoA + 1.0 H2O
pentanoate-ferm/4_manual_1.3.98.-_HD-1.3.98.-pent : 1.0 2-pentenoyl-CoA + 2.0 NADH + 2.0 |Oxidized-ferredoxins| <=> 1.0 pentanoyl-CoA + 2.0 |Reduced-ferredoxins| + 2.0 NAD+
pentanoate-ferm/5_manual_2.3.1.19_HD-2.3.1.19-pent : 1.0 pentanoyl-CoA + 1.0 phosphate --> 1.0 pentanoyl_phosphate + 1.0 coenzyme_A
pentanoate-ferm/6_manual_2.7.2.7_HD-2.7.2.7-pent : 1.0 pentanoyl_phosphate + 1.0 ADP --> 1.0 pentanoate + 1.0 ATP
########################################################################################################################################################################
#ferm. hexanoate
hexanoate-ferm/1_2.3.1.9_RXN-12565 : 1.0 acetyl-CoA + 1.0 butanoyl-CoA --> 1.0 coenzyme_A + 1.0 3-oxohexanoyl-CoA  # source: MetaCyc, BRENDA, KEGG (queried 2.3.1.9) // other EC numbers for this reaction: 2.3.1.16, 2.3.1.155
hexanoate-ferm/2_manual_1.1.1.157_HD-1.1.1.157-hex : 1.0 (R)-3-hydroxyhexanoyl-CoA + 1.0 NAD+ <-- 1.0 H+ + 1.0 NADH + 1.0 3-oxohexanoyl-CoA
hexanoate-ferm/3_manual_4.2.1.150_HD-4.2.1.150-hex : 1.0 (R)-3-hydroxyhexanoyl-CoA --> 1.0 2-hexenoyl-CoA + 1.0 H2O
hexanoate-ferm/4_manual_1.3.98.-_HD-1.3.98.-hex : 1.0 2-hexenoyl-CoA + 2.0 NADH + 2.0 |Oxidized-ferredoxins| <=> 1.0 hexanoyl-CoA + 2.0 |Reduced-ferredoxins| + 2.0 NAD+
hexanoate-ferm/5_manual_2.3.1.19_HD-2.3.1.19-hex : 1.0 hexanoyl-CoA + 1.0 phosphate --> 1.0 hexanoyl_phosphate + 1.0 coenzyme_A
hexanoate-ferm/6_manual_2.7.2.7_HD-2.7.2.7-hex : 1.0 hexanoyl_phosphate + 1.0 ADP --> 1.0 hexanoate + 1.0 ATP
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#5-aminoimidazole ribonucleotide biosynthesis II
5-aminoimidazole-ribonucleotide-biosyn-II/1_2.4.2.14_PRPPAMIDOTRANS-RXN : 1.0 diphosphate + 1.0 L-glutamate + 1.0 5-phospho-beta-D-ribosylamine <=> 1.0 L-glutamine + 1.0 H2O + 1.0 5-phospho-alpha-D-ribose_1-diphosphate  # source: MetaCyc, BRENDA, KEGG (queried 2.4.2.14)
5-aminoimidazole-ribonucleotide-biosyn-II/2_6.3.4.13_GLYRIBONUCSYN-RXN : 1.0 glycine + 1.0 ATP + 1.0 5-phospho-beta-D-ribosylamine --> 1.0 H+ + 1.0 phosphate + 1.0 ADP + 1.0 N1-(5-phospho-beta-D-ribosyl)glycinamide  # source: MetaCyc, BRENDA, KEGG (queried 6.3.4.13)
5-aminoimidazole-ribonucleotide-biosyn-II/3_2.1.2.2_GART-RXN : 1.0 10-formyltetrahydrofolate + 1.0 N1-(5-phospho-beta-D-ribosyl)glycinamide <=> 1.0 tetrahydropteroyl_tri-L-glutamate + 1.0 N2-formyl-N1-(5-phospho-beta-D-ribosyl)glycinamide + 1.0 H+  # source: MetaCyc (queried 2.1.2.2)
5-aminoimidazole-ribonucleotide-biosyn-II/4_6.3.5.3_FGAMSYN-RXN : 1.0 H2O + 1.0 L-glutamine + 1.0 ATP + 1.0 N2-formyl-N1-(5-phospho-beta-D-ribosyl)glycinamide --> 1.0 ADP + 1.0 2-(formamido)-N1-(5-phospho-beta-D-ribosyl)acetamidine + 1.0 H+ + 1.0 phosphate + 1.0 L-glutamate  # source: MetaCyc, BRENDA, KEGG (queried 6.3.5.3)
5-aminoimidazole-ribonucleotide-biosyn-II/5_6.3.3.1_AIRS-RXN : 1.0 2-(formamido)-N1-(5-phospho-beta-D-ribosyl)acetamidine + 1.0 ATP --> 1.0 phosphate + 1.0 ADP + 1.0 5-amino-1-(5-phospho-beta-D-ribosyl)imidazole + 1.0 H+  # source: MetaCyc, BRENDA, KEGG (queried 6.3.3.1)
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#inosine-5'-phosphate biosynthesis
#E. coli class I 5.4.99.18 (PurE) without 6.3.4.18 (PurK) sufficient in vitro under high bicarbonate concentrations (Meyer et al., 1992).
#Overexpression of purE complements purK deletion in E. coli (Patrick et al., 2007).
#Several archea with class I 5.4.99.18 (PurE) and missing purK found (Brown et al., 2011)
inosine-5'-phosphate-biosyn/1_manual_spontaneous_5.4.99.18_HD-5.4.99.18 : 1.0 hydrogen_carbonate + 1.0 5-amino-1-(5-phospho-beta-D-ribosyl)imidazole --> 1.0 H+ + 1.0 N5-carboxyaminoimidazole_ribonucleotide  # metacyc
inosine-5'-phosphate-biosyn/2_5.4.99.18_RXN0-743 : 1.0 N5-carboxyaminoimidazole_ribonucleotide --> 1.0 5-amino-1-(5-phospho-D-ribosyl)imidazole-4-carboxylate  # source: MetaCyc, BRENDA, KEGG (queried 5.4.99.18)
inosine-5'-phosphate-biosyn/3_6.3.2.6_SAICARSYN-RXN : 1.0 5-amino-1-(5-phospho-D-ribosyl)imidazole-4-carboxylate + 1.0 L-aspartate + 1.0 ATP --> 1.0 5'-phosphoribosyl-4-(N-succinocarboxamide)-5-aminoimidazole + 1.0 ADP + 1.0 H+ + 1.0 phosphate  # source: MetaCyc, BRENDA, KEGG (queried 6.3.2.6)
inosine-5'-phosphate-biosyn/4_4.3.2.2_AICARSYN-RXN : 1.0 5'-phosphoribosyl-4-(N-succinocarboxamide)-5-aminoimidazole <=> 1.0 5-amino-1-(5-phospho-D-ribosyl)imidazole-4-carboxamide + 1.0 fumarate  # source: MetaCyc, BRENDA, KEGG (queried 4.3.2.2)
inosine-5'-phosphate-biosyn/5_2.1.2.3_AICARTRANSFORM-RXN : 1.0 10-formyltetrahydrofolate + 1.0 5-amino-1-(5-phospho-D-ribosyl)imidazole-4-carboxamide <=> 1.0 tetrahydropteroyl_tri-L-glutamate + 1.0 5-formamido-1-(5-phospho-D-ribosyl)-imidazole-4-carboxamide  # source: MetaCyc (queried 2.1.2.3)
inosine-5'-phosphate-biosyn/6_moddir_3.5.4.10_2.1.2.3_IMPCYCLOHYDROLASE-RXN : 1.0 H2O + 1.0 IMP <=> 1.0 5-formamido-1-(5-phospho-D-ribosyl)-imidazole-4-carboxamide  # source: MetaCyc, BRENDA, KEGG (queried 3.5.4.10, 2.1.2.3)
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#tRNA
tRNA-charging_6.1.1.10_METHIONINE--TRNA-LIGASE-RXN : 1.0 ATP + 1.0 |MET-tRNAs| + 1.0 H+ + 1.0 L-methionine --> 1.0 |Charged-MET-tRNAs| + 1.0 diphosphate + 1.0 AMP  # source: MetaCyc, KEGG (queried 6.1.1.10)
tRNA-charging_6.1.1.11_SERINE--TRNA-LIGASE-RXN : 1.0 H+ + 1.0 ATP + 1.0 |SER-tRNAs| + 1.0 L-serine --> 1.0 |Charged-SER-tRNAs| + 1.0 diphosphate + 1.0 AMP  # source: MetaCyc, KEGG (queried 6.1.1.11)
tRNA-charging_6.1.1.12_ASPARTATE--TRNA-LIGASE-RXN : 1.0 |ASP-tRNAs| + 1.0 H+ + 1.0 L-aspartate + 1.0 ATP --> 1.0 |Charged-ASP-tRNAs| + 1.0 diphosphate + 1.0 AMP  # source: MetaCyc, KEGG (queried 6.1.1.12) // other EC numbers for this reaction: 6.1.1.23
tRNA-charging_6.1.1.14_GLYCINE--TRNA-LIGASE-RXN : 1.0 |GLY-tRNAs| + 1.0 H+ + 1.0 glycine + 1.0 ATP --> 1.0 |Charged-GLY-tRNAs| + 1.0 diphosphate + 1.0 AMP  # source: MetaCyc, KEGG (queried 6.1.1.14)
tRNA-charging_6.1.1.15_PROLINE--TRNA-LIGASE-RXN : 1.0 ATP + 1.0 L-proline + 1.0 |PRO-tRNAs| + 1.0 H+ --> 1.0 |Charged-PRO-tRNAs| + 1.0 diphosphate + 1.0 AMP  # source: MetaCyc, KEGG (queried 6.1.1.15)
tRNA-charging_6.1.1.16_CYSTEINE--TRNA-LIGASE-RXN : 1.0 |CYS-tRNAs| + 1.0 H+ + 1.0 L-cysteine + 1.0 ATP --> 1.0 AMP + 1.0 |Charged-CYS-tRNAs| + 1.0 diphosphate  # source: MetaCyc, KEGG (queried 6.1.1.16)
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tRNA-charging_6.1.1.17_GLURS-RXN                                    : 1.0 |GLT-tRNAs| + 1.0 H+ + 1.0 L-glutamate + 1.0 ATP --> 1.0 |Charged-GLT-tRNAs| + 1.0 AMP + 1.0
diphosphate  # source: MetaCyc, KEGG (queried 6.1.1.17)
tRNA-charging_6.1.1.18_GLUTAMINE--TRNA-LIGASE-RXN                   : 1.0 H+ + 1.0 L-glutamine + 1.0 ATP + 1.0 |GLN-tRNAs| --> 1.0 |Charged-GLN-tRNAs| + 1.0 diphosphate + 1.0
AMP  # source: MetaCyc, KEGG (queried 6.1.1.18)
tRNA-charging_6.1.1.19_ARGININE--TRNA-LIGASE-RXN                    : 1.0 L-arginine + 1.0 |ARG-tRNAs| + 1.0 H+ + 1.0 ATP --> 1.0 |Charged-ARG-tRNAs| + 1.0 diphosphate + 1.0
AMP  # source: MetaCyc, KEGG (queried 6.1.1.19)
tRNA-charging_6.1.1.1_TYROSINE--TRNA-LIGASE-RXN                     : 1.0 ATP + 1.0 |TYR-tRNAs| + 1.0 L-tyrosine + 1.0 H+ --> 1.0 |Charged-TYR-tRNAs| + 1.0 diphosphate + 1.0
AMP  # source: MetaCyc, KEGG (queried 6.1.1.1)
tRNA-charging_6.1.1.20_PHENYLALANINE--TRNA-LIGASE-RXN               : 1.0 H+ + 1.0 L-phenylalanine + 1.0 ATP + 1.0 |PHE-tRNAs| --> 1.0 |Charged-PHE-tRNAs| + 1.0 AMP + 1.0
diphosphate  # source: MetaCyc, KEGG (queried 6.1.1.20)
tRNA-charging_6.1.1.21_HISTIDINE--TRNA-LIGASE-RXN                   : 1.0 |HIS-tRNAs| + 1.0 H+ + 1.0 L-histidine + 1.0 ATP --> 1.0 |Charged-HIS-tRNAs| + 1.0 diphosphate + 1.0
AMP  # source: MetaCyc, KEGG (queried 6.1.1.21)
tRNA-charging_6.1.1.22_ASPARAGINE--TRNA-LIGASE-RXN                  : 1.0 |ASN-tRNAs| + 1.0 H+ + 1.0 ATP + 1.0 L-asparagine --> 1.0 |Charged-ASN-tRNAs| + 1.0 diphosphate + 1.0
AMP  # source: MetaCyc, KEGG (queried 6.1.1.22)
tRNA-charging_6.1.1.2_TRYPTOPHAN--TRNA-LIGASE-RXN                   : 1.0 ATP + 1.0 |TRP-tRNAs| + 1.0 L-tryptophan + 1.0 H+ --> 1.0 |Charged-TRP-tRNAs| + 1.0 diphosphate + 1.0
AMP  # source: MetaCyc, KEGG (queried 6.1.1.2)
tRNA-charging_6.1.1.3_THREONINE--TRNA-LIGASE-RXN                    : 1.0 |THR-tRNAs| + 1.0 L-threonine + 1.0 H+ + 1.0 ATP --> 1.0 |Charged-THR-tRNAs| + 1.0 diphosphate + 1.0
AMP  # source: MetaCyc, KEGG (queried 6.1.1.3)
tRNA-charging_6.1.1.4_LEUCINE--TRNA-LIGASE-RXN                      : 1.0 ATP + 1.0 |LEU-tRNAs| + 1.0 H+ + 1.0 L-leucine --> 1.0 |Charged-LEU-tRNAs| + 1.0 diphosphate + 1.0
AMP  # source: MetaCyc, KEGG (queried 6.1.1.4)
tRNA-charging_6.1.1.5_ISOLEUCINE--TRNA-LIGASE-RXN                   : 1.0 ATP + 1.0 |ILE-tRNAs| + 1.0 H+ + 1.0 L-isoleucine --> 1.0 |Charged-ILE-tRNAs| + 1.0 AMP + 1.0
diphosphate  # source: MetaCyc, KEGG (queried 6.1.1.5)
tRNA-charging_6.1.1.6_LYSINE--TRNA-LIGASE-RXN                       : 1.0 ATP + 1.0 |LYS-tRNAs| + 1.0 H+ + 1.0 L-lysine --> 1.0 |Charged-LYS-tRNAs| + 1.0 diphosphate + 1.0 AMP
# source: MetaCyc, KEGG (queried 6.1.1.6)
tRNA-charging_6.1.1.7_ALANINE--TRNA-LIGASE-RXN                      : 1.0 H+ + 1.0 |ALA-tRNAs| + 1.0 L-alanine + 1.0 ATP --> 1.0 AMP + 1.0 |Charged-ALA-tRNAs| + 1.0
diphosphate  # source: MetaCyc, KEGG (queried 6.1.1.7)
tRNA-charging_6.1.1.9_VALINE--TRNA-LIGASE-RXN                       : 1.0 H+ + 1.0 ATP + 1.0 |VAL-tRNAs| + 1.0 L-valine --> 1.0 |Charged-VAL-tRNAs| + 1.0 diphosphate + 1.0 AMP
# source: MetaCyc, KEGG (queried 6.1.1.9)
selenocysteine-biosynthesis_6.1.1.11_RXN0-2161                      : 1.0 |SEC-tRNAs| + 1.0 L-serine + 1.0 H+ + 1.0 ATP --> 1.0 AMP + 1.0 |L-seryl-SEC-tRNAs| + 1.0 diphosphate
# source: MetaCyc, KEGG (queried 6.1.1.11)
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#NAD biosyn I/NADP
NAD-biosyn-I/1a_1.4.3.16_L-ASPARTATE-OXID-RXN                       : 1.0 oxygen + 1.0 L-aspartate --> 1.0 2-iminosuccinate + 1.0 hydrogen_peroxide + 1.0 H+  # source:
MetaCyc, BRENDA, KEGG (queried 1.4.3.16)
NAD-biosyn-I/1b_1.4.3.16_RXN-9772                                   : 1.0 L-aspartate + 1.0 fumarate --> 1.0 2-iminosuccinate + 1.0 H+ + 1.0 succinate  # source: MetaCyc,
BRENDA (queried 1.4.3.16) // other EC numbers for this reaction: 1.5.99
NAD-biosyn-I/2_2.5.1.72_QUINOLINATE-SYNTHA-RXN                      : 1.0 2-iminosuccinate + 1.0 glycerone_phosphate --> 1.0 quinolinate + 1.0 phosphate + 2.0 H2O  # source:
MetaCyc, BRENDA, KEGG (queried 2.5.1.72)
NAD-biosyn-I/3_2.4.2.19_QUINOPRIBOTRANS-RXN                         : 1.0 diphosphate + 1.0 beta-nicotinate_D-ribonucleotide + 1.0 CO2 <-- 1.0 5-phospho-alpha-D-ribose_1-
diphosphate + 2.0 H+ + 1.0 quinolinate  # source: MetaCyc, BRENDA, KEGG (queried 2.4.2.19)
NAD-biosyn-I/4_2.7.7.18_NICONUCADENYLYLTRAN-RXN                     : 1.0 beta-nicotinate_D-ribonucleotide + 1.0 H+ + 1.0 ATP --> 1.0 nicotinate_adenine_dinucleotide + 1.0
diphosphate  # source: MetaCyc, BRENDA, KEGG (queried 2.7.7.18) // other EC numbers for this reaction: 2.7.7.1
NAD-biosyn-I/5_6.3.1.5_NAD-SYNTH-NH3-RXN                            : 1.0 ATP + 1.0 ammonium + 1.0 nicotinate_adenine_dinucleotide --> 1.0 NAD+ + 1.0 AMP + 1.0 H+ + 1.0
diphosphate  # source: MetaCyc, BRENDA, KEGG (queried 6.3.1.5) // other EC numbers for this reaction: 6.3.5.1
NADP-biosyn_2.7.1.23_NAD-KIN-RXN                                    : 1.0 NAD+ + 1.0 ATP --> 1.0 ADP + 1.0 NADP+ + 1.0 H+  # source: MetaCyc, BRENDA, KEGG (queried 2.7.1.23)
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#NADH repair
NADH-repair_spontaneous_RXN-12753                                   : 1.0 NADH + 1.0 H2O --> 1.0 (S)-NADHX  # source: MetaCyc
NADH-repair_spontaneous_RXN-12754                                   : 1.0 H2O + 1.0 NADH --> 1.0 (R)-NADHX  # source: MetaCyc
NADH-repair_5.1.99.6_RXN-12752                                      : 1.0 (R)-NADHX --> 1.0 (S)-NADHX  # source: MetaCyc, BRENDA, KEGG (queried 5.1.99.6)
NADH-repair_4.2.1.136_RXN0-6727                                     : 1.0 (S)-NADHX + 1.0 ADP --> 1.0 H+ + 1.0 phosphate + 1.0 NADH + 1.0 AMP  # source: MetaCyc, BRENDA, KEGG
(queried 4.2.1.136)

NADPH-repair_manual_spontaneous_HD-(S)-NADPHX                       : 1.0 NADPH + 1.0 H2O --> 1.0 (S)-NADPHX
NADPH-repair_manual_spontaneous_HD-(R)-NADPHX                       : 1.0 H2O + 1.0 NADPH --> 1.0 (R)-NADPHX
NADPH-repair_5.1.99.6_RXN-13142                                     : 1.0 (R)-NADPHX <=> 1.0 (S)-NADPHX  # source: MetaCyc, BRENDA, KEGG (queried 5.1.99.6)
NADPH-repair_4.2.1.136_RXN-13141                                    : 1.0 (S)-NADPHX + 1.0 ADP --> 1.0 NADPH + 1.0 AMP + 1.0 H+ + 1.0 phosphate  # source: MetaCyc, BRENDA,
KEGG (queried 4.2.1.136)
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#nicotine transitions
nicotine-transitions-A/1_3.1.3.5_RXN-14227                          : 1.0 beta-nicotinate_D-ribonucleotide + 1.0 H2O --> 1.0 beta-D-ribosylnicotinate + 1.0 phosphate  #
source: MetaCyc, KEGG (queried 3.1.3.5) // other EC numbers for this reaction: 3.1.3
nicotine-transitions-A/2_2.4.2.1_R02295                             : 1.0 phosphate + 1.0 beta-D-ribosylnicotinate <=> 1.0 alpha-D-ribose-1-phosphate + 1.0 nicotinate  #
source: KEGG (queried 2.4.2.1) // balanced // contains implicit reactant(s): H+, H2O
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nicotine-transitions-B_3.6.1.9_BS165396                                 : 1.0 nicotinate_adenine_dinucleotide + 1.0 H2O --> 1.0 AMP + 1.0 beta-nicotinate_D-ribonucleotide  #
source: BRENDA, KEGG (queried 3.6.1.9) // other EC numbers for this reaction: 3.6.1.22

nicotine-transitions-C/1_3.6.1.9_NADPYROPHOSPHAT-RXN                    : 1.0 H2O + 1.0 NAD+ --> 2.0 H+ + 1.0 beta-nicotinamide_D-ribonucleotide + 1.0 AMP  # source: MetaCyc,
BRENDA, KEGG (queried 3.6.1.9) // other EC numbers for this reaction: 3.6.1.22
nicotine-transitions-C/2_3.1.3.5_3.1.3.2_RXN-5841                       : 1.0 H2O + 1.0 beta-nicotinamide_D-ribonucleotide --> 1.0 1-(beta-D_ribofuranosyl)nicotinamide + 1.0
phosphate  # source: MetaCyc, BRENDA, KEGG (queried 3.1.3.5, 3.1.3.2) // other EC numbers for this reaction: 3.1.3
nicotine-transitions-C/3_3.2.2.1_BS94861                                : 1.0 1-(beta-D_ribofuranosyl)nicotinamide + 1.0 H2O --> 1.0 nicotinamide + 1.0 beta-D-ribopyranose  #
source: BRENDA, KEGG (queried 3.2.2.1) // other EC numbers for this reaction: 3.2.2.3, 3.2.2.8
nicotine-transitions-C/4a_3.5.1.19_NICOTINAMID-RXN                      : 1.0 H2O + 1.0 nicotinamide --> 1.0 ammonium + 1.0 nicotinate  # source: MetaCyc, BRENDA, KEGG (queried
3.5.1.19)
nicotine-transitions-C/4b_2.4.2.1_RXN0-7092                             : 1.0 alpha-D-ribose-1-phosphate + 1.0 H+ + 1.0 nicotinamide <=> 1.0 phosphate + 1.0 1-(beta-
D_ribofuranosyl)nicotinamide  # source: MetaCyc, BRENDA, KEGG (queried 2.4.2.1) // other EC numbers for this reaction: 2.4.2
nicotine-transitions-C/5_2.7.7.18_2.7.7.1-RXN                           : 1.0 H+ + 1.0 beta-nicotinamide_D-ribonucleotide + 1.0 ATP --> 1.0 diphosphate + 1.0 NAD+  # source:
MetaCyc, BRENDA, KEGG (queried 2.7.7.18) // other EC numbers for this reaction: 2.7.7.1
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#FAD biosyn I
flavin-biosyn-I/1_3.5.4.25_GTP-CYCLOHYDRO-II-RXN                                : 3.0 H2O + 1.0 GTP --> 1.0 diphosphate + 1.0 formate + 1.0 2,5-diamino-6-(5-phospho-D-
ribosylamino)pyrimidin-4(3H)-one + 2.0 H+  # source: MetaCyc, BRENDA, KEGG (queried 3.5.4.25)
flavin-biosyn-I/2_3.5.4.26_RIBOFLAVINSYNDEAM-RXN                                : 1.0 H2O + 1.0 H+ + 1.0 2,5-diamino-6-(5-phospho-D-ribosylamino)pyrimidin-4(3H)-one --> 1.0
ammonium + 1.0 5-amino-6-(5-phospho-D-ribosylamino)uracil  # source: MetaCyc, BRENDA, KEGG (queried 3.5.4.26)
flavin-biosyn-I/3_1.1.1.193_RIBOFLAVINSYNREDUC-RXN                              : 1.0 NADP+ + 1.0 5-amino-6-(5-phospho-D-ribitylamino)uracil <-- 1.0 H+ + 1.0 5-amino-6-(5-
phospho-D-ribosylamino)uracil + 1.0 NADPH  # source: MetaCyc, BRENDA, KEGG (queried 1.1.1.193)
flavin-biosyn-I/4_3.1.3.-_RIBOPHOSPHAT-RXN                                      : 1.0 H2O + 1.0 5-amino-6-(5-phospho-D-ribitylamino)uracil --> 1.0 5-amino-6-(D-
ribitylamino)uracil + 1.0 phosphate  # source: MetaCyc, KEGG (queried 3.1.3.-) // other EC numbers for this reaction: 3.1.3
flavin-biosyn-I/5_4.1.99.12_DIOHBUTANONEPSYN-RXN                                : 1.0 D-ribulose_5-phosphate --> 1.0 H+ + 1.0 1-deoxy-L-glycero-tetrulose_4-phosphate + 1.0
formate  # source: MetaCyc, BRENDA, KEGG (queried 4.1.99.12)
flavin-biosyn-I/6_2.5.1.78_LUMAZINESYN-RXN                                      : 1.0 1-deoxy-L-glycero-tetrulose_4-phosphate + 1.0 5-amino-6-(D-ribitylamino)uracil --> 1.0
H+ + 1.0 phosphate + 1.0 6,7-dimethyl-8-(1-D-ribityl)lumazine + 2.0 H2O  # source: MetaCyc, BRENDA, KEGG (queried 2.5.1.78)
flavin-biosyn-I/7_2.5.1.9_RIBOFLAVIN-SYN-RXN                                    : 1.0 H+ + 2.0 6,7-dimethyl-8-(1-D-ribityl)lumazine --> 1.0 5-amino-6-(D-ribitylamino)uracil
+ 1.0 riboflavin  # source: MetaCyc, BRENDA, KEGG (queried 2.5.1.9)
flavin-biosyn-I/8_2.7.1.26_RIBOFLAVINKIN-RXN                                    : 1.0 riboflavin + 1.0 ATP --> 1.0 FMN + 1.0 ADP + 1.0 H+  # source: MetaCyc, BRENDA, KEGG
(queried 2.7.1.26)
flavin-biosyn-I/9_2.7.7.2_FADSYN-RXN                                            : 1.0 H+ + 1.0 FMN + 1.0 ATP --> 1.0 FAD + 1.0 diphosphate  # source: MetaCyc, BRENDA, KEGG
(queried 2.7.7.2)
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#phosphopantothenate biosynthesis I
phosphopantothenate-biosyn-I/1_2.1.2.11_3-CH3-2-OXOBUTANOATE-OH-CH3-XFER-RXN    : 1.0 5,10-methylene-tetrahydrofolate + 1.0 H2O + 1.0 3-methyl-2-oxobutanoate <=> 1.0 2-
dehydropantoate + 1.0 tetrahydropteroyl_tri-L-glutamate  # source: MetaCyc (queried 2.1.2.11)
phosphopantothenate-biosyn-I/2_1.1.1.169_2-DEHYDROPANTOATE-REDUCT-RXN           : 1.0 (R)-pantoate + 1.0 NADP+ <-- 1.0 NADPH + 1.0 2-dehydropantoate + 1.0 H+  # source:
MetaCyc, BRENDA, KEGG (queried 1.1.1.169)
phosphopantothenate-biosyn-I/3_6.3.2.1_PANTOATE-BETA-ALANINE-LIG-RXN            : 1.0 (R)-pantoate + 1.0 beta-alanine + 1.0 ATP --> 1.0 diphosphate + 1.0 (R)-pantothenate +
1.0 AMP + 1.0 H+  # source: MetaCyc, BRENDA, KEGG (queried 6.3.2.1)
phosphopantothenate-biosyn-I/4_2.7.1.33_PANTOTHENATE-KIN-RXN                    : 1.0 (R)-pantothenate + 1.0 ATP --> 1.0 (R)-4'-phosphopantothenate + 1.0 H+ + 1.0 ADP  #
source: MetaCyc, BRENDA, KEGG (queried 2.7.1.33)
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#coenzyme A biosyn
coenzyme-A-biosyn/1_6.3.2.5_P-PANTOCYSLIG-RXN                                   : 1.0 L-cysteine + 1.0 CTP + 1.0 (R)-4'-phosphopantothenate --> 1.0 diphosphate + 1.0 CMP +
1.0 R-4'-phosphopantothenoyl-L-cysteine + 1.0 H+  # source: MetaCyc, BRENDA, KEGG (queried 6.3.2.5)
coenzyme-A-biosyn/2_4.1.1.36_P-PANTOCYSDECARB-RXN                               : 1.0 R-4'-phosphopantothenoyl-L-cysteine + 1.0 H+ --> 1.0 CO2 + 1.0 4'-phosphopantetheine  #
source: MetaCyc, BRENDA, KEGG (queried 4.1.1.36)
coenzyme-A-biosyn/3_2.7.7.3_PANTEPADENYLYLTRAN-RXN                              : 1.0 H+ + 1.0 4'-phosphopantetheine + 1.0 ATP --> 1.0 diphosphate + 1.0 3'-dephospho-CoA  #
source: MetaCyc, BRENDA, KEGG (queried 2.7.7.3)
coenzyme-A-biosyn/4_2.7.1.24_DEPHOSPHOCOAKIN-RXN                                : 1.0 ATP + 1.0 3'-dephospho-CoA --> 1.0 ADP + 1.0 coenzyme_A + 1.0 H+  # source: MetaCyc,
BRENDA, KEGG (queried 2.7.1.24)
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#4-aminobenzoate biosynthesis
4-aminobenzoate-biosyn/1_2.6.1.85_PABASYN-RXN                                   : 1.0 chorismate + 1.0 L-glutamine <=> 1.0 4-amino-4-deoxychorismate + 1.0 L-glutamate  #
source: MetaCyc, BRENDA, KEGG (queried 2.6.1.85)
4-aminobenzoate-biosyn/2_4.1.3.38_ADCLY-RXN                                     : 1.0 4-amino-4-deoxychorismate <=> 1.0 4-aminobenzoate + 1.0 pyruvate + 1.0 H+  # source:
MetaCyc, BRENDA, KEGG (queried 4.1.3.38)
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#6-hydroxymethyl-dihydropterin diphosphate biosynthesis I
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6-hydroxymethyl-dihydropterin-PP-biosyn-I/1_3.5.4.16_R00428                                  : 1.0 GTP + 1.0 H2O --> 1.0 Formamidopyrimidine_nucleoside_triphosphate  # source: KEGG
(queried 3.5.4.16)
6-hydroxymethyl-dihydropterin-PP-biosyn-I/2_3.5.4.16_R05046                                  : 1.0 Formamidopyrimidine_nucleoside_triphosphate + 1.0 H2O --> 1.0 formate + 1.0 N-
(2,5-diamino-6-oxo-1,6-dihydropyrimidin-4-yl)-beta-D-ribofuranosylamine_5'-triphosphate  # source: KEGG (queried 3.5.4.16)
6-hydroxymethyl-dihydropterin-PP-biosyn-I/3_3.5.4.16_R05048                                  : 1.0 N-(2,5-diamino-6-oxo-1,6-dihydropyrimidin-4-yl)-beta-D-ribofuranosylamine_5'-
triphosphate <=> 1.0 2,5-Diamino-6-(5'-triphosphoryl-3,4'-trihydroxy-2'-oxopentyl)-amino-4-oxopyrimidine  # source: KEGG (queried 3.5.4.16)
6-hydroxymethyl-dihydropterin-PP-biosyn-I/4_moddir_3.5.4.16_R04639                           : 1.0 7,8-dihydroneopterin_3'-triphosphate + 1.0 H2O <=> 1.0 2,5-Diamino-6-(5'-
triphosphoryl-3,4'-trihydroxy-2'-oxopentyl)-amino-4-oxopyrimidine  # source: KEGG (queried 3.5.4.16)
6-hydroxymethyl-dihydropterin-PP-biosyn-I/5_3.6.1.67_H2NEOPTERINP3PYROPHOSPHOHYDRO-RXN      : 1.0 H2O + 1.0 7,8-dihydroneopterin_3'-triphosphate --> 1.0 diphosphate + 1.0 7,8-
dihydroneopterin_3'-phosphate + 1.0 H+  # source: MetaCyc, BRENDA, KEGG (queried 3.6.1.67) // other EC numbers for this reaction: 3.6.1.B15
6-hydroxymethyl-dihydropterin-PP-biosyn-I/6_3.6.1.-_DIHYDRONEOPTERIN-MONO-P-DEPHOS-RXN      : 1.0 H2O + 1.0 7,8-dihydroneopterin_3'-phosphate --> 1.0 7,8-dihydroneopterin + 1.0
phosphate  # source: MetaCyc, KEGG (queried 3.6.1.-) // other EC numbers for this reaction: 3.6.1
6-hydroxymethyl-dihydropterin-PP-biosyn-I/7_4.1.2.25_H2NEOPTERINALDOL-RXN                    : 1.0 7,8-dihydroneopterin <=> 1.0 glycolaldehyde + 1.0 6-hydroxymethyl-7,8-
dihydropterin  # source: MetaCyc, BRENDA, KEGG (queried 4.1.2.25)
6-hydroxymethyl-dihydropterin-PP-biosyn-I/8_2.7.6.3_H2PTERIDINEPYROPHOSPHOKIN-RXN           : 1.0 6-hydroxymethyl-7,8-dihydropterin + 1.0 ATP --> 1.0 6-hydroxymethyl-7,8-
dihydropterin_diphosphate + 1.0 AMP + 1.0 H+  # source: MetaCyc, BRENDA, KEGG (queried 2.7.6.3)
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#THF biosyn
tetrahydrofolate-biosynthesis_2.5.1.15_H2PTEROATESYNTH-RXN                                   : 1.0 4-aminobenzoate + 1.0 6-hydroxymethyl-7,8-dihydropterin_diphosphate --> 1.0 7,8-
dihydropteroate + 1.0 diphosphate  # source: MetaCyc, BRENDA, KEGG (queried 2.5.1.15)
tetrahydrofolate-biosynthesis_6.3.2.17_DIHYDROFOLATESYNTH-RXN                                : 1.0 L-glutamate + 1.0 ATP + 1.0 7,8-dihydropteroate --> 1.0 ADP + 1.0 H+ + 1.0
phosphate + 1.0 7,8-dihydrofolate_monoglutamate  # source: MetaCyc, BRENDA, KEGG (queried 6.3.2.17) // other EC numbers for this reaction: 6.3.2.12
tetrahydrofolate-biosyn/3_manual_1.5.1.3_HD-1.5.1.3                                          : 1.0 NADP+ + 1.0 tetrahydropteroyl_mono-L-glutamate <-- 1.0 H+ + 1.0 NADPH + 1.0 7,8-
dihydrofolate_monoglutamate
#primary triglutamyl in Clostridium acidi-urici (Curthoys et al. 1972)
tetrahydrofolate-biosyn/4_manual_6.3.2.17_HD-6.3.2.17                                        : 1.0 tetrahydropteroyl_mono-L-glutamate + 2.0 L-glutamate + 2.0 ATP --> 1.0
tetrahydropteroyl_tri-L-glutamate + 2.0 ADP + 2.0 phosphate
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#folate transformations
folate-transformations/1_3.5.4.9_2.1.2.10_RXN-6321                                           : 1.0 5,10-methenyltetrahydrofolate + 1.0 H2O --> 1.0 H+ + 1.0 |N5-Formyl-THF-Glu-N|  #
source: MetaCyc, BRENDA, KEGG (queried 3.5.4.9, 2.1.2.10)
folate-transformations/2_6.3.3.2_5-FORMYL-THF-CYCLO-LIGASE-RXN                               : 1.0 ATP + 1.0 |N5-Formyl-THF-Glu-N| --> 1.0 ADP + 1.0 phosphate + 1.0 5,10-
methenyltetrahydrofolate  # source: MetaCyc, BRENDA, KEGG (queried 6.3.3.2)
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#methylerythr path
methylerythritol-phosphate-pathway/1_2.2.1.7_DXS-RXN                                         : 1.0 pyruvate + 1.0 H+ + 1.0 D-glyceraldehyde_3-phosphate --> 1.0 CO2 + 1.0 1-deoxy-D-
xylulose_5-phosphate  # source: MetaCyc, BRENDA, KEGG (queried 2.2.1.7)
methylerythritol-phosphate-pathway/2_1.1.1.267_DXPREDISOM-RXN                                : 1.0 2-C-methyl-D-erythritol_4-phosphate + 1.0 NADP+ <=> 1.0 NADPH + 1.0 1-deoxy-D-
xylulose_5-phosphate + 1.0 H+  # source: MetaCyc, BRENDA, KEGG (queried 1.1.1.267)
methylerythritol-phosphate-pathway/3_2.7.7.60_2.7.7.60-RXN                                   : 1.0 H+ + 1.0 2-C-methyl-D-erythritol_4-phosphate + 1.0 CTP --> 1.0 diphosphate + 1.0
4-(cytidine_5'-diphospho)-2-C-methyl-D-erythritol  # source: MetaCyc, BRENDA, KEGG (queried 2.7.7.60)
methylerythritol-phosphate-pathway/4_2.7.1.148_2.7.1.148-RXN                                 : 1.0 ATP + 1.0 4-(cytidine_5'-diphospho)-2-C-methyl-D-erythritol --> 1.0 ADP + 1.0 2-
phospho-4-(cytidine_5'-diphospho)-2-C-methyl-D-erythritol + 1.0 H+  # source: MetaCyc, BRENDA, KEGG (queried 2.7.1.148)
methylerythritol-phosphate-pathway/5_4.6.1.12_RXN0-302                                       : 1.0 2-phospho-4-(cytidine_5'-diphospho)-2-C-methyl-D-erythritol --> 1.0 2-C-methyl-D-
erythritol-2,4-cyclodiphosphate + 1.0 CMP  # source: MetaCyc, BRENDA, KEGG (queried 4.6.1.12)
methylerythritol-phosphate-pathway/6_1.17.7.1_RXN0-882                                       : 2.0 |Oxidized-ferredoxins| + 1.0 H2O + 1.0 1-hydroxy-2-methyl-2-(E)-butenyl_4-
diphosphate <-- 2.0 |Reduced-ferredoxins| + 1.0 H+ + 1.0 2-C-methyl-D-erythritol-2,4-cyclodiphosphate  # source: MetaCyc, KEGG (queried 1.17.7.1)
methylerythritol-phosphate-pathway/7a_1.17.7.4_ISPH2-RXN                                     : 1.0 isopentenyl_diphosphate + 2.0 |Oxidized-ferredoxins| + 1.0 H2O <-- 2.0 H+ + 1.0
1-hydroxy-2-methyl-2-(E)-butenyl_4-diphosphate + 2.0 |Reduced-ferredoxins|  # source: MetaCyc, KEGG (queried 1.17.7.4) // other EC numbers for this reaction: 1.17.7.c
methylerythritol-phosphate-pathway/7b_1.17.7.4_RXN0-884                                      : 2.0 |Oxidized-ferredoxins| + 1.0 H2O + 1.0 dimethylallyl_diphosphate <-- 1.0 1-
hydroxy-2-methyl-2-(E)-butenyl_4-diphosphate + 2.0 |Reduced-ferredoxins| + 2.0 H+  # source: MetaCyc, KEGG (queried 1.17.7.4) // other EC numbers for this reaction: 1.17.7.c
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#farnesyl PP biosyn
farnesyl-PP-biosyn/1_2.5.1.1_GPPSYN-RXN                                                      : 1.0 dimethylallyl_diphosphate + 1.0 isopentenyl_diphosphate <=> 1.0
geranyl_diphosphate + 1.0 diphosphate  # source: MetaCyc, BRENDA, KEGG (queried 2.5.1.1)
farnesyl-PP-biosyn/2a_2.5.1.10_FPPSYN-RXN                                                    : 1.0 geranyl_diphosphate + 1.0 isopentenyl_diphosphate <=> 1.0 (2E,6E)-
farnesyl_diphosphate + 1.0 diphosphate  # source: MetaCyc, BRENDA, KEGG (queried 2.5.1.10)
farnesyl-PP-biosyn/2b_2.5.1.10_BS421953                                                      : 1.0 dimethylallyl_diphosphate + 1.0 geranyl_diphosphate <=> 1.0 diphosphate + 1.0
(2E,6E)-farnesyl_diphosphate  # source: BRENDA (queried 2.5.1.10)
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#undecaprenyl PP biosyn
undecaprenyl-PP-biosyn_2.5.1.31_RXN-8999                                                     : 1.0 (2E,6E)-farnesyl_diphosphate + 8.0 isopentenyl_diphosphate --> 8.0 diphosphate +
1.0 di-trans,octa-cis-undecaprenyl_diphosphate  # source: MetaCyc, BRENDA, KEGG (queried 2.5.1.31)
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#4-amino-2-methyl-5-diphosphomethylpyrimidine biosynthesis
4-amino-2-methyl-5-diphosphomethylpyrimidine-biosyn/1_4.1.99.17_PYRIMSYN1-RXN              : 1.0 S-adenosyl-L-methionine + 1.0 5-amino-1-(5-phospho-beta-D-ribosyl)imidazole -->
1.0 4-amino-2-methyl-5-phosphomethylpyrimidine + 3.0 H+ + 1.0 L-methionine + 1.0 carbon_monoxide + 1.0 formate + 1.0 5'-deoxyadenosine  # source: MetaCyc, BRENDA, KEGG (queried
4.1.99.17)
4-amino-2-methyl-5-diphosphomethylpyrimidine-biosyn/2_2.7.4.7_PYRIMSYN3-RXN               : 1.0 4-amino-2-methyl-5-phosphomethylpyrimidine + 1.0 ATP --> 1.0 ADP + 1.0 4-amino-2-
methyl-5-diphosphomethylpyrimidine  # source: MetaCyc, BRENDA, KEGG (queried 2.7.4.7)
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#5'-deoxyadenosine degradation
5'-deoxyadenosine-degr_3.2.2.16_3.2.2.1_3.2.2.9_RXN0-6550                                  : 1.0 H2O + 1.0 5'-deoxyadenosine --> 1.0 adenine + 1.0 5-deoxy-D-ribose  # source:
MetaCyc, BRENDA (queried 3.2.2.16, 3.2.2.1, 3.2.2.9)
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#molybdenum cofactor biosynthesis
molybdenum-cofactor-biosynthesis/1_2.8.1.7_RXN0-308                                        : 1.0 |Cysteine-Desulfurase-L-cysteine| + 1.0 L-cysteine --> 1.0 L-alanine + 1.0 |L-
Cysteine-Desulfurase-persulfide|  # source: MetaCyc (queried 2.8.1.7)
molybdenum-cofactor-biosynthesis/2_2.7.7.80_RXN-11361                                      : 1.0 ATP + 1.0 |MPT-Synthases| + 1.0 H+ --> 1.0 diphosphate + 1.0 |Carboxyadenylated-
MPT-synthases|  # source: MetaCyc (queried 2.7.7.80)
molybdenum-cofactor-biosynthesis/3_mod_2.8.1.11_RXN-12473                                  : 2.0 |Reduced-ferredoxins| + 1.0 H+ + 1.0 |Carboxyadenylated-MPT-synthases| + 1.0 |L-
Cysteine-Desulfurase-persulfide| --> 1.0 |Cysteine-Desulfurase-L-cysteine| + 1.0 AMP + 1.0 |Thiocarboxylated-MPT-synthases| + 2.0 |Oxidized-ferredoxins|  # source: MetaCyc
(queried 2.8.1.11)
molybdenum-cofactor-biosynthesis/4_4.1.99.18_RXN-8340                                      : 1.0 GTP --> 1.0 cyclic_pyranopterin_phosphate + 1.0 diphosphate  # source: MetaCyc,
BRENDA, KEGG (queried 4.1.99.18)
molybdenum-cofactor-biosynthesis/5_2.8.1.12_RXN-8342                                       : 1.0 cyclic_pyranopterin_phosphate + 2.0 |Thiocarboxylated-MPT-synthases| + 1.0 H2O
--> 1.0 molybdopterin + 2.0 |MPT-Synthases| + 4.0 H+  # source: MetaCyc (queried 2.8.1.12)
molybdenum-cofactor-biosynthesis/6_2.7.7.75_RXN-8344                                       : 1.0 ATP + 1.0 H+ + 1.0 molybdopterin --> 1.0 molybdopterin_adenine_dinucleotide + 1.0
diphosphate  # source: MetaCyc, BRENDA, KEGG (queried 2.7.7.75)
molybdenum-cofactor-biosynthesis/7_2.10.1.1_RXN-8348                                       : 1.0 molybdopterin_adenine_dinucleotide + 1.0 molybdate + 1.0 H+ --> 1.0 MoO2-
molybdopterin_cofactor + 1.0 AMP + 1.0 H2O  # source: MetaCyc, BRENDA, KEGG (queried 2.10.1.1)
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#thiazole biosynthesis
thiazole-biosynthesis/1_2.8.1.7_RXN-9787                                                   : 1.0 |Sulfur-Carrier-Proteins-ThiI| + 1.0 L-cysteine <=> 1.0 L-alanine + 1.0 |
Sulfurylated-ThiI|  # source: MetaCyc (queried 2.8.1.7)
thiazole-biosynthesis/2_2.7.7.73_RXN-9789                                                  : 1.0 H+ + 1.0 |Thi-S| + 1.0 ATP --> 1.0 |Adenylated-ThiS-Proteins| + 1.0 diphosphate
# source: MetaCyc, BRENDA (queried 2.7.7.73)
thiazole-biosynthesis/3_2.8.1.-_RXN-9788                                                   : 2.0 |Reduced-ferredoxins| + 1.0 |Adenylated-ThiS-Proteins| + 1.0 |Sulfurylated-ThiI|
--> 1.0 |Thiocarboxyadenylated-ThiS-Proteins| + 1.0 |Sulfur-Carrier-Proteins-ThiI| + 2.0 |Oxidized-ferredoxins| + 1.0 AMP  # source: MetaCyc (queried 2.8.1.-) // other EC numbers
for this reaction: 2.8.1
thiazole-biosynthesis/p4_4.1.99.19_RXN-11319                                               : 1.0 S-adenosyl-L-methionine + 1.0 NADPH + 1.0 L-tyrosine --> 1.0 5'-deoxyadenosine +
1.0 H+ + 1.0 NADP+ + 1.0 L-methionine + 1.0 2-iminoacetate + 1.0 4-methylphenol  # source: MetaCyc, BRENDA (queried 4.1.99.19)
thiazole-biosynthesis/4_2.8.1.10_THIAZOLSYN2-RXN                                           : 1.0 1-deoxy-D-xylulose_5-phosphate + 1.0 |Thiocarboxyadenylated-ThiS-Proteins| + 1.0
2-iminoacetate --> 2.0 H2O + 1.0 |Thi-S| + 1.0 2-[(2R,5Z)-2-carboxy-4-methylthiazol-5(2H)-ylidene]ethyl_phosphate  # source: MetaCyc (queried 2.8.1.10)
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#thiamin diphosphate biosynthesis III (Staphylococcus)
thiamin-diphosphate-biosyn-III/1_2.5.1.3_RXN-12611                                         : 2.0 H+ + 1.0 2-[(2R,5Z)-2-carboxy-4-methylthiazol-5(2H)-ylidene]ethyl_phosphate + 1.0
4-amino-2-methyl-5-diphosphomethylpyrimidine --> 1.0 thiamine_phosphate + 1.0 diphosphate + 1.0 CO2  # source: MetaCyc, BRENDA (queried 2.5.1.3)
thiamin-diphosphate-biosyn-III/2_3.1.3.2_RXNQT-4191                                        : 1.0 thiamine_phosphate + 1.0 H2O --> 1.0 phosphate + 1.0 thiamine  # source: MetaCyc,
BRENDA, KEGG (queried 3.1.3.2) // other EC numbers for this reaction: 3.1.3, 3.1.3.w
thiamin-diphosphate-biosyn-III/3_2.7.6.2_THIAMIN-PYROPHOSPHOKINASE-RXN                     : 1.0 thiamine + 1.0 ATP --> 1.0 H+ + 1.0 AMP + 1.0 thiamine_diphosphate  # source:
MetaCyc, BRENDA, KEGG (queried 2.7.6.2)
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#thiamin salvage
thiamin-salvage/1_3.5.99.2_THIAMINASE-RXN                                                  : 1.0 thiamine + 1.0 H2O --> 1.0 H+ + 1.0 4-amino-2-methyl-5-pyrimidinemethanol + 1.0
5-(2-hydroxyethyl)-4-methylthiazole  # source: MetaCyc, BRENDA, KEGG (queried 3.5.99.2)
thiamin-salvage/2_2.7.1.50_THIAZOLSYN3-RXN                                                 : 1.0 ATP + 1.0 5-(2-hydroxyethyl)-4-methylthiazole --> 1.0 H+ + 1.0 ADP + 1.0 4-
methyl-5-(2-phosphonooxyethyl)thiazole  # source: MetaCyc, BRENDA, KEGG (queried 2.7.1.50)
thiamin-salvage/p3_2.7.1.49_OHMETPYRKIN-RXN                                                : 1.0 ATP + 1.0 4-amino-2-methyl-5-pyrimidinemethanol --> 1.0 ADP + 1.0 4-amino-2-
methyl-5-phosphomethylpyrimidine + 1.0 H+  # source: MetaCyc, BRENDA, KEGG (queried 2.7.1.49)
thiamin-salvage/4_2.5.1.3_THI-P-SYN-RXN                                                    : 1.0 4-methyl-5-(2-phosphonooxyethyl)thiazole + 1.0 4-amino-2-methyl-5-
diphosphomethylpyrimidine + 1.0 H+ --> 1.0 diphosphate + 1.0 thiamine_phosphate  # source: MetaCyc, BRENDA, KEGG (queried 2.5.1.3)
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#tetrapyrrole biosynthesis I
tetrapyrrole-biosynthesis/1_1.2.1.70_GLUTRNAREDUCT-RXN                                     : 1.0 |GLT-tRNAs| + 1.0 NADP+ + 1.0 (S)-4-amino-5-oxopentanoate <-- 1.0 |Charged-GLT-
tRNAs| + 1.0 NADPH  # source: MetaCyc (queried 1.2.1.70)
tetrapyrrole-biosynthesis/2_5.4.3.8_GSAAMINOTRANS-RXN                                      : 1.0 (S)-4-amino-5-oxopentanoate --> 1.0 5-aminolevulinate  # source: MetaCyc, BRENDA,
KEGG (queried 5.4.3.8)
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tetrapyrrole-biosynthesis/3_4.2.1.24_PORPHOBILSYNTH-RXN                                    : 2.0 5-aminolevulinate --> 1.0 H+ + 1.0 porphobilinogen + 2.0 H2O  # source: MetaCyc,
BRENDA, KEGG (queried 4.2.1.24)
tetrapyrrole-biosynthesis/4_2.5.1.61_OHMETHYLBILANESYN-RXN                                 : 4.0 porphobilinogen + 1.0 H2O --> 4.0 ammonium + 1.0 preuroporphyrinogen  # source:
MetaCyc, BRENDA, KEGG (queried 2.5.1.61)
tetrapyrrole-biosynthesis/5_4.2.1.75_UROGENIIISYN-RXN                                      : 1.0 preuroporphyrinogen --> 1.0 H2O + 1.0 uroporphyrinogen-III  # source: MetaCyc,
BRENDA, KEGG (queried 4.2.1.75)
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#cobyrinate biosyn I
cobyrinate-biosyn-I/1_2.1.1.107_UROPORIIIMETHYLTRANSA-RXN                : 1.0 uroporphyrinogen-III + 1.0 S-adenosyl-L-methionine --> 1.0 precorrin-1 + 1.0 S-adenosyl-L-
homocysteine + 1.0 H+  # source: MetaCyc, BRENDA, KEGG (queried 2.1.1.107)
cobyrinate-biosyn-I/2_2.1.1.107_RXN-8675                                 : 1.0 S-adenosyl-L-methionine + 1.0 precorrin-1 --> 1.0 S-adenosyl-L-homocysteine + 1.0 precorrin-2  #
source: MetaCyc, BRENDA, KEGG (queried 2.1.1.107)
cobyrinate-biosyn-I/3_1.3.1.76_DIMETHUROPORDEHYDROG-RXN                  : 1.0 NAD+ + 1.0 precorrin-2 <=> 2.0 H+ + 1.0 NADH + 1.0 sirohydrochlorin  # source: MetaCyc, BRENDA, KEGG
(queried 1.3.1.76)
cobyrinate-biosyn-I/4_4.99.1.3_4.99.1.3-RXN                              : 1.0 sirohydrochlorin + 1.0 Co2+ --> 1.0 cobalt-sirohydrochlorin + 2.0 H+  # source: MetaCyc, BRENDA, KEGG
(queried 4.99.1.3)
cobyrinate-biosyn-I/5_2.1.1.151_2.1.1.151-RXN                            : 1.0 cobalt-sirohydrochlorin + 1.0 S-adenosyl-L-methionine --> 1.0 cobalt-factor_III + 1.0 S-adenosyl-L-
homocysteine + 1.0 H+  # source: MetaCyc, BRENDA, KEGG (queried 2.1.1.151)
#Electron donor may be thioredoxin (Moore et al. 2013)
cobyrinate-biosyn-I/6_mod_2.1.1.272_RXN-14314                            : 1.0 |Red-Thioredoxin| + 1.0 cobalt-factor_III + 1.0 S-adenosyl-L-methionine --> 1.0 cobalt-precorrin-4 +
1.0 |Ox-Thioredoxin| + 1.0 S-adenosyl-L-homocysteine  # source: MetaCyc, BRENDA (queried 2.1.1.272)
cobyrinate-biosyn-I/7_2.1.1.271_RXN-8762                                 : 1.0 cobalt-precorrin-4 + 1.0 S-adenosyl-L-methionine --> 1.0 S-adenosyl-L-homocysteine + 1.0 cobalt-
precorrin-5A + 1.0 H+  # source: MetaCyc, BRENDA, KEGG (queried 2.1.1.271)
cobyrinate-biosyn-I/8_3.7.1.12_RXN-8763                                  : 1.0 cobalt-precorrin-5A + 1.0 H2O --> 1.0 acetaldehyde + 1.0 cobalt-precorrin-5B + 1.0 H+  # source:
MetaCyc, BRENDA, KEGG (queried 3.7.1.12)
cobyrinate-biosyn-I/9_2.1.1.195_RXN-8764                                 : 1.0 cobalt-precorrin-5B + 1.0 S-adenosyl-L-methionine --> 1.0 S-adenosyl-L-homocysteine + 1.0 cobalt-
precorrin-6A  # source: MetaCyc, BRENDA, KEGG (queried 2.1.1.195)
cobyrinate-biosyn-I/10_1.3.1.106_RXN-8765                                : 1.0 cobalt-precorrin-6B + 1.0 NAD+ <-- 1.0 cobalt-precorrin-6A + 1.0 NADH  # source: MetaCyc, BRENDA,
KEGG (queried 1.3.1.106)
cobyrinate-biosyn-I/11_2.1.1.196_RXN-8766                                : 1.0 cobalt-precorrin-6B + 1.0 S-adenosyl-L-methionine + 1.0 H+ --> 1.0 cobalt-precorrin-7 + 1.0 CO2 + 1.0
S-adenosyl-L-homocysteine  # source: MetaCyc, BRENDA, KEGG (queried 2.1.1.196)
cobyrinate-biosyn-I/12_2.1.1.289_RXN-8767                                : 1.0 S-adenosyl-L-methionine + 1.0 cobalt-precorrin-7 --> 1.0 S-adenosyl-L-homocysteine + 1.0 cobalt-
precorrin-8  # source: MetaCyc, BRENDA, KEGG (queried 2.1.1.289)
cobyrinate-biosyn-I/13_5.4.99.60_RXN-8768                                : 1.0 cobalt-precorrin-8 --> 1.0 H+ + 1.0 cobyrinate  # source: MetaCyc, BRENDA, KEGG (queried 5.4.99.60)
cobyrinate-biosyn-I/14_6.3.5.11_RXN-14256                                : 1.0 H2O + 1.0 L-glutamine + 1.0 cobyrinate + 1.0 ATP --> 1.0 cob(II)yrinate_c-monoamide + 1.0 ADP + 1.0
H+ + 1.0 L-glutamate + 1.0 phosphate  # source: MetaCyc, BRENDA, KEGG (queried 6.3.5.11)
cobyrinate-biosyn-I/15_6.3.5.11_RXN-14257                                : 1.0 L-glutamine + 1.0 cob(II)yrinate_c-monoamide + 1.0 ATP + 1.0 H2O --> 1.0 L-glutamate + 1.0
cob(II)yrinate_a,c-diamide + 1.0 ADP + 1.0 H+ + 1.0 phosphate  # source: MetaCyc, BRENDA, KEGG (queried 6.3.5.11)
#########################################################################################################################################################
#5,6-dimethylbenzimidazole biosyn II
#4.1.99.M1: Ferredoxins as a guess
5,6-dimethylbenzimidazole-biosyn-II/1_4.1.99.M1_RXN-17122                          : 1.0 5-amino-1-(5-phospho-beta-D-ribosyl)imidazole + 1.0 S-adenosyl-L-methionine + 2.0 |
Reduced-ferredoxins| --> 1.0 5-hydroxy-benzimidazole + 1.0 ammonium + 1.0 formate + 1.0 5'-deoxyadenosine + 1.0 L-methionine + 1.0 phosphate + 2.0 |Oxidized-ferredoxins|
5,6-dimethylbenzimidazole-biosyn-II/2_2.1.1.M9_RXN-17123                           : 1.0 5-hydroxy-benzimidazole + 1.0 S-adenosyl-L-methionine --> 1.0 5-methoxy-
benzimidazole + 1.0 S-adenosyl-L-homocysteine + 1.0 H+
5,6-dimethylbenzimidazole-biosyn-II/3_2.1.1.M10_RXN-17124                          : 1.0 5-methoxy-benzimidazole + 1.0 S-adenosyl-L-methionine --> 1.0 5-methoxy-6-
methylbenzimidazole + 1.0 S-adenosyl-L-homocysteine + 1.0 H+
#mechanism completely unclear
5,6-dimethylbenzimidazole-biosyn-II/4_unknown_RXN-17125                            : 1.0 5-methoxy-6-methylbenzimidazole --> 5,6-dimethylbenzimidazole
#########################################################################################################################################################
#adenosylcobalamin biosyn I
#1.16.8.1: NADH as a guess
adenosylcobalamin-biosynthesis-I/1_mod_1.16.8.1_R343-RXN                           : 2.0 H+ + 1.0 NAD+ + 2.0 cob(I)yrinate_a,c-diamide <-- 2.0 cob(II)yrinate_a,c-diamide +
1.0 NADH  # source: MetaCyc, BRENDA, KEGG (queried 1.16.8.1)
adenosylcobalamin-biosynthesis-I/2_2.5.1.17_R344-RXN                               : 1.0 cob(I)yrinate_a,c-diamide + 1.0 ATP --> 1.0 adenosyl-cobyrinate_a,c-diamide + 1.0
PPPi  # source: MetaCyc, BRENDA, KEGG (queried 2.5.1.17)
adenosylcobalamin-biosynthesis-I/3_6.3.5.10_R345-RXN                               : 4.0 L-glutamine + 1.0 adenosyl-cobyrinate_a,c-diamide + 4.0 ATP + 4.0 H2O --> 4.0 ADP +
4.0 H+ + 4.0 L-glutamate + 4.0 phosphate + 1.0 adenosylcobyrate  # source: MetaCyc, BRENDA, KEGG (queried 6.3.5.10)
adenosylcobalamin-biosynthesis-I/pp4_2.7.1.177_RXN-8626                            : 1.0 L-threonine + 1.0 ATP --> 1.0 L-threonine_3-O-phosphate + 1.0 ADP + 1.0 H+  #
source: MetaCyc, BRENDA, KEGG (queried 2.7.1.177)
adenosylcobalamin-biosynthesis-I/p4_4.1.1.81_4.1.1.81-RXN                          : 1.0 L-threonine_3-O-phosphate + 1.0 H+ --> 1.0 CO2 + 1.0 (R)-1-amino-2-propanol_O-2-
phosphate  # source: MetaCyc, BRENDA, KEGG (queried 4.1.1.81)
adenosylcobalamin-biosynthesis-I/4_6.3.1.10_RXN-6261                               : 1.0 ATP + 1.0 (R)-1-amino-2-propanol_O-2-phosphate + 1.0 adenosylcobyrate --> 1.0
phosphate + 1.0 ADP + 1.0 adenosyl-cobinamide_phosphate + 1.0 H+  # source: MetaCyc, BRENDA, KEGG (queried 6.3.1.10)
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adenosylcobalamin-biosynthesis-I/5_2.7.7.62_COBINPGUANYLYLTRANS-RXN                    : 1.0 H+ + 1.0 GTP + 1.0 adenosyl-cobinamide_phosphate <=> 1.0 diphosphate + 1.0
adenosylcobinamide-GDP  # source: MetaCyc, BRENDA, KEGG (queried 2.7.7.62)
adenosylcobalamin-biosynthesis-I/pp6_6.3.4.21_NICOTINATEPRIBOSYLTRANS-RXN              : 1.0 ATP + 1.0 H2O + 1.0 5-phospho-alpha-D-ribose_1-diphosphate + 1.0 nicotinate --> 1.0
beta-nicotinate_D-ribonucleotide + 1.0 phosphate + 1.0 ADP + 1.0 diphosphate  # source: MetaCyc, BRENDA, KEGG (queried 6.3.4.21)
adenosylcobalamin-biosynthesis-I/p6_2.4.2.21_DMBPPRIBOSYLTRANS-RXN                    : 1.0 beta-nicotinate_D-ribonucleotide + 1.0 5,6-dimethylbenzimidazole --> 1.0 nicotinate
+ 1.0 alpha-ribazole_5'-phosphate + 1.0 H+  # source: MetaCyc, BRENDA, KEGG (queried 2.4.2.21)
adenosylcobalamin-biosynthesis-I/6a_2.7.8.26_COBALAMIN5PSYN-RXN                       : 1.0 alpha-ribazole_5'-phosphate + 1.0 adenosylcobinamide-GDP --> 1.0
adenosylcobalamin_5'-phosphate + 1.0 H+ + 1.0 GMP  # source: MetaCyc, BRENDA (queried 2.7.8.26)
adenosylcobalamin-biosynthesis-I/7a_3.1.3.73_RXN-8770                                 : 1.0 adenosylcobalamin_5'-phosphate + 1.0 H2O --> 1.0 adenosylcobalamin + 1.0 phosphate
# source: MetaCyc, BRENDA (queried 3.1.3.73)
adenosylcobalamin-biosynthesis-I/6b_3.1.3.73_RIBAZOLEPHOSPHAT-RXN                     : 1.0 alpha-ribazole_5'-phosphate + 1.0 H2O --> 1.0 alpha-ribazole + 1.0 phosphate  #
source: MetaCyc, BRENDA, KEGG (queried 3.1.3.73)
adenosylcobalamin-biosynthesis-I/7b_2.7.8.26_COBALAMINSYN-RXN                         : 1.0 alpha-ribazole + 1.0 adenosylcobinamide-GDP <=> 1.0 adenosylcobalamin + 1.0 GMP +
1.0 H+  # source: MetaCyc, BRENDA, KEGG (queried 2.7.8.26)
#########################################################################################################################################################
#protoporphyrin biosynthesis
protoporphyrin-biosyn/1_4.1.1.37_UROGENDECARBOX-RXN                                   : 1.0 uroporphyrinogen-III + 4.0 H+ --> 4.0 CO2 + 1.0 coproporphyrinogen_III  # source:
MetaCyc, BRENDA, KEGG (queried 4.1.1.37)
protoporphyrin-biosyn/2_modnames_1.3.99.22_HEMN-RXN                                   : 1.0 coproporphyrinogen_III + 2.0 S-adenosyl-L-methionine --> 1.0 protoporphyrin_IX + 2.0
L-methionine + 2.0 5'-deoxyadenosine + 2.0 CO2  # source: MetaCyc, BRENDA, KEGG (queried 1.3.99.22)
protoporphyrin-biosyn/3_6.6.1.1_RXN1F-20                                              : 1.0 ATP + 1.0 H2O + 1.0 protoporphyrin_IX + 1.0 Mg2+ --> 1.0 phosphate + 1.0 Mg-
protoporphyrin + 1.0 ADP + 3.0 H+  # source: MetaCyc, BRENDA, KEGG (queried 6.6.1.1)
#########################################################################################################################################################
#biotin carboxyl carrier protein assembly
biotin-carboxyl-carrier-protein-assembly/1_6.3.4.15_BIOTINLIG-RXN                     : 1.0 biotin + 1.0 ATP + 1.0 |BCCP-monomers| --> 1.0 H+ + 1.0 diphosphate + 1.0 AMP + 1.0
|BCCP-biotin-monomers|  # source: MetaCyc (queried 6.3.4.15)
biotin-carboxyl-carrier-protein-assembly/2_spontaneous_RXN-7101                       : 2.0 |BCCP-biotin-monomers| --> 1.0 |BCCP-dimers|  # source: MetaCyc
biotin-carboxyl-carrier-protein-assembly/3_6.3.4.14_BIOTIN-CARBOXYL-RXN               : 1.0 ATP + 1.0 |BCCP-dimers| + 1.0 hydrogen_carbonate --> 1.0 H+ + 1.0 phosphate + 1.0
ADP + 1.0 |Carboxybiotin-BCCP|  # source: MetaCyc (queried 6.3.4.14)
#########################################################################################################################################################
#pyridoxal
PLP-biosyn_2.7.1.49_PNKIN-RXN                                                         : 1.0 ATP + 1.0 pyridoxine --> 1.0 ADP + 1.0 pyridoxine_5'-phosphate + 1.0 H+  # source:
MetaCyc, BRENDA, KEGG (queried 2.7.1.49) // other EC numbers for this reaction: 2.7.1.35
#########################################################################################################################################################
#L-threonylcarbamoyladenylate
L-threonylcarbamoyladenylate_2.7.7.87_RXN-14569                                       : 1.0 hydrogen_carbonate + 1.0 L-threonine + 1.0 ATP <=> 1.0 diphosphate + 1.0 L-
threonylcarbamoyladenylate + 1.0 H2O  # source: MetaCyc, BRENDA, KEGG (queried 2.7.7.87)
#########################################################################################################################################################
#NXP de novo biosyn
diphosphate_3.6.1.1_INORGPYROPHOSPHAT-RXN                                             : 1.0 H2O + 1.0 diphosphate --> 2.0 phosphate + 1.0 H+  # source: MetaCyc, BRENDA, KEGG
(queried 3.6.1.1) // other EC numbers for this reaction: 2.7.99.1
triphosphate_3.6.1.1_modb_BS383385                                                    : 2.0 H2O + 1.0 PPPi --> 3.0 phosphate + 1.0 H+  # source: BRENDA (queried 3.6.1.1) //
balanced // contains implicit reactant(s): H+, H2O

diphosphate_2.7.11.32_RXN-13757                                                       : 1.0 ADP + 1.0 |pyruvate-phosphate-dikinase| --> 1.0 H+ + 1.0 AMP + 1.0 |pyruvate-
phosphate-dikinase-phosphate|  # source: MetaCyc, BRENDA (queried 2.7.11.32)
diphosphate_2.7.4.27_RXN-13756                                                        : 1.0 |pyruvate-phosphate-dikinase-phosphate| + 1.0 H+ + 1.0 phosphate <=> 1.0 diphosphate
+ 1.0 |pyruvate-phosphate-dikinase|  # source: MetaCyc, BRENDA (queried 2.7.4.27)


#AMP
adenosine-ribonucleotides-de-novo-biosyn/1_6.3.4.4_ADENYLOSUCCINATE-SYNTHASE-RXN      : 1.0 L-aspartate + 1.0 IMP + 1.0 GTP --> 1.0 GDP + 1.0 adenylo-succinate + 2.0 H+ + 1.0
phosphate  # source: MetaCyc, BRENDA, KEGG (queried 6.3.4.4)
adenosine-ribonucleotides-de-novo-biosyn/2_4.3.2.2_AMPSYN-RXN                         : 1.0 adenylo-succinate <=> 1.0 fumarate + 1.0 AMP  # source: MetaCyc, BRENDA, KEGG
(queried 4.3.2.2)

#GMP
guanosine-ribonucleotides-de-novo-biosyn/1_1.1.1.205_IMP-DEHYDROG-RXN                 : 1.0 H2O + 1.0 NAD+ + 1.0 IMP <=> 1.0 NADH + 1.0 XMP + 1.0 H+  # source: MetaCyc, BRENDA,
KEGG (queried 1.1.1.205)
guanosine-ribonucleotides-de-novo-biosyn/2_6.3.5.2_GMP-SYN-GLUT-RXN                   : 1.0 L-glutamine + 1.0 ATP + 1.0 XMP + 1.0 H2O --> 1.0 AMP + 1.0 diphosphate + 2.0 H+ +
1.0 GMP + 1.0 L-glutamate  # source: MetaCyc, BRENDA, KEGG (queried 6.3.5.2)

#UMP
UMP-biosyn/1_2.1.3.2_ASPCARBTRANS-RXN                                                 : 1.0 carbamoyl_phosphate + 1.0 L-aspartate <=> 1.0 N-carbamoyl-L-aspartate + 1.0
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phosphate + 1.0 H+  # source: MetaCyc, BRENDA, KEGG (queried 2.1.3.2)
UMP-biosyn/2_moddir_3.5.2.3_DIHYDROOROT-RXN                                    : 1.0 H2O + 1.0 (S)-dihydroorotate <=> 1.0 N-carbamoyl-L-aspartate + 1.0 H+  # source:
MetaCyc, BRENDA, KEGG (queried 3.5.2.3)
UMP-biosyn/3_1.3.1.14_OROTATE-REDUCTASE-NADH-RXN                               : 1.0 NAD+ + 1.0 (S)-dihydroorotate <=> 1.0 orotate + 1.0 H+ + 1.0 NADH  # source:
MetaCyc, BRENDA, KEGG (queried 1.3.1.14)
UMP-biosyn/4_2.4.2.10_OROPRIBTRANS-RXN                                         : 1.0 diphosphate + 1.0 orotidine_5'-phosphate <=> 1.0 orotate + 1.0 5-phospho-alpha-D-
ribose_1-diphosphate  # source: MetaCyc, BRENDA, KEGG (queried 2.4.2.10)
UMP-biosyn/5_4.1.1.23_OROTPDECARB-RXN                                          : 1.0 orotidine_5'-phosphate + 1.0 H+ --> 1.0 CO2 + 1.0 UMP  # source: MetaCyc, BRENDA,
KEGG (queried 4.1.1.23)

#CTP
CTP-biosy2_6.3.4.2_CTPSYN-RXN                                                  : 1.0 L-glutamine + 1.0 H2O + 1.0 UTP + 1.0 ATP --> 1.0 CTP + 1.0 ADP + 2.0 H+ + 1.0
phosphate + 1.0 L-glutamate  # source: MetaCyc, BRENDA, KEGG (queried 6.3.4.2)

#UTP
UTP-biosyn_3.5.4.5_RXN-14118                                                   : 1.0 H2O + 1.0 H+ + 1.0 CTP --> 1.0 ammonium + 1.0 UTP  # source: MetaCyc, BRENDA, KEGG
(queried 3.5.4.5) // other EC numbers for this reaction: 3.5.4.13

#XDP -> dXDP
deoxyribonucleotides-biosyn_1.17.4.1_ADPREDUCT-RXN                             : 1.0 dADP + 1.0 |Ox-Thioredoxin| + 1.0 H2O <=> 1.0 ADP + 1.0 |Red-Thioredoxin|  # source:
MetaCyc, KEGG (queried 1.17.4.1)
deoxyribonucleotides-biosyn_1.17.4.1_GDPREDUCT-RXN                             : 1.0 |Ox-Thioredoxin| + 1.0 H2O + 1.0 dGDP <-- 1.0 GDP + 1.0 |Red-Thioredoxin|  # source:
MetaCyc, KEGG (queried 1.17.4.1)
deoxyribonucleotides-biosyn_1.17.4.1_CDPREDUCT-RXN                             : 1.0 H2O + 1.0 |Ox-Thioredoxin| + 1.0 dCDP <-- 1.0 |Red-Thioredoxin| + 1.0 CDP  # source:
MetaCyc, KEGG (queried 1.17.4.1)
deoxyribonucleotides-biosyn_1.17.4.1_UDPREDUCT-RXN                             : 1.0 |Ox-Thioredoxin| + 1.0 H2O + 1.0 dUDP <-- 1.0 |Red-Thioredoxin| + 1.0 UDP  # source:
MetaCyc, KEGG (queried 1.17.4.1)

#|Oxidized-flavodoxins| --> |Ox-Thioredoxin| because of BRENDA 1.17.4.2 and Clostridium sp.
deoxyribonucleotides-biosyn_mod_1.17.4.2_RXN0-723                              : 1.0 |Ox-Thioredoxin| + 1.0 dCTP + 1.0 H2O <-- 1.0 CTP + 1.0 |Red-Thioredoxin|  # source:
MetaCyc (queried 1.17.4.2)
deoxyribonucleotides-biosyn_mod_1.17.4.2_RXN0-724                              : 1.0 H2O + 1.0 |Ox-Thioredoxin| + 1.0 dUTP <-- 1.0 UTP + 1.0 |Red-Thioredoxin|  # source:
MetaCyc (queried 1.17.4.2)
deoxyribonucleotides-biosyn_mod_1.17.4.2_RXN0-745                              : 1.0 |Ox-Thioredoxin| + 1.0 dATP + 1.0 H2O <-- 1.0 |Red-Thioredoxin| + 1.0 ATP  # source:
MetaCyc (queried 1.17.4.2)
deoxyribonucleotides-biosyn_mod_1.17.4.2_RXN0-746                              : 1.0 |Ox-Thioredoxin| + 1.0 H2O + 1.0 dGTP <-- 1.0 GTP + 1.0 |Red-Thioredoxin|  # source:
MetaCyc (queried 1.17.4.2)

#dTTP
dTTP-biosyn/1_3.6.1.23_DUTP-PYROP-RXN                                          : 1.0 H2O + 1.0 dUTP --> 1.0 diphosphate + 1.0 dUMP + 1.0 H+  # source: MetaCyc, BRENDA,
KEGG (queried 3.6.1.23) // other EC numbers for this reaction: 3.6.1.19
dTTP-biosyn/2_2.1.1.148_RXN-8850                                               : 1.0 NADPH + 1.0 5,10-methylene-tetrahydrofolate + 1.0 H+ + 1.0 dUMP --> 1.0
tetrahydropteroyl_tri-L-glutamate + 1.0 dTMP + 1.0 NADP+  # source: MetaCyc (queried 2.1.1.148)
#########################################################################################################################################################################
##(d)NMP degradation

#RNA-Abbau
#CMP
CMP-salvage/1_3.1.3.5_RXN-14026                                                : 1.0 H2O + 1.0 CMP --> 1.0 cytidine + 1.0 phosphate  # source: MetaCyc, BRENDA, KEGG
(queried 3.1.3.5) // other EC numbers for this reaction: 3.1.3.91
CMP-salvage/2a_2.7.1.48_CYTIKIN-RXN                                            : 1.0 cytidine + 1.0 ATP --> 1.0 ADP + 1.0 H+ + 1.0 CMP  # source: MetaCyc, BRENDA, KEGG
(queried 2.7.1.48) // other EC numbers for this reaction: 2.7.1.B24
CMP-salvage/2b_3.5.4.5_CYTIDEAM2-RXN                                           : 1.0 H2O + 1.0 H+ + 1.0 cytidine --> 1.0 ammonium + 1.0 uridine  # source: MetaCyc,
BRENDA, KEGG (queried 3.5.4.5)
CMP-salvage/2c_2.4.2.2_BS355365                                                : 1.0 cytidine + 1.0 phosphate <=> 1.0 cytosine + 1.0 alpha-D-ribose-1-phosphate  #
source: BRENDA, KEGG (queried 2.4.2.2) // other EC numbers for this reaction: 2.4.2.3
#UMP
UMP-salvage/1_3.1.3.5_3.1.3.2_RXN-14025                                        : 1.0 H2O + 1.0 UMP --> 1.0 uridine + 1.0 phosphate  # source: MetaCyc, BRENDA, KEGG
(queried 3.1.3.5, 3.1.3.2)
UMP-salvage/2a_2.7.1.48_URIDINEKIN-RXN                                         : 1.0 ATP + 1.0 uridine --> 1.0 H+ + 1.0 ADP + 1.0 UMP  # source: MetaCyc, BRENDA, KEGG
(queried 2.7.1.48)
UMP-salvage/2b_2.4.2.2_URPHOS-RXN                                              : 1.0 phosphate + 1.0 uridine <=> 1.0 alpha-D-ribose-1-phosphate + 1.0 uracil  # source:
MetaCyc, BRENDA, KEGG (queried 2.4.2.2) // other EC numbers for this reaction: 2.4.2.3
UMP-salvage/3_2.4.2.9_URACIL-PRIBOSYLTRANS-RXN                                 : 1.0 UMP + 1.0 diphosphate <-- 1.0 5-phospho-alpha-D-ribose_1-diphosphate + 1.0 uracil  #
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source: MetaCyc, BRENDA, KEGG (queried 2.4.2.9)
#AMP
AMP-salvage/1_3.1.3.5_3.1.3.2_AMP-DEPHOSPHORYLATION-RXN                                    : 1.0 H2O + 1.0 AMP --> 1.0 phosphate + 1.0 adenosine  # source: MetaCyc, BRENDA, KEGG
(queried 3.1.3.5, 3.1.3.2)
AMP-salvage/2_2.4.2.1_ADENPHOSPHOR-RXN                                                    : 1.0 adenosine + 1.0 phosphate <=> 1.0 adenine + 1.0 alpha-D-ribose-1-phosphate  #
source: MetaCyc, BRENDA, KEGG (queried 2.4.2.1) // other EC numbers for this reaction: 2.4.2.44
AMP-salvage/3_2.4.2.8_2.4.2.7_ADENPRIBOSYLTRAN-RXN                                        : 1.0 AMP + 1.0 diphosphate <-- 1.0 adenine + 1.0 5-phospho-alpha-D-ribose_1-diphosphate
# source: MetaCyc, BRENDA, KEGG (queried 2.4.2.8, 2.4.2.7)
#GMP
GMP-salvage/1_3.1.3.5_3.1.3.2_RXN-7609                                                    : 1.0 H2O + 1.0 GMP --> 1.0 guanosine + 1.0 phosphate  # source: MetaCyc, BRENDA, KEGG
(queried 3.1.3.5, 3.1.3.2)
GMP-salvage/2_2.4.2.1_RXN0-5199                                                           : 1.0 guanosine + 1.0 phosphate <=> 1.0 guanine + 1.0 alpha-D-ribose-1-phosphate  #
source: MetaCyc, BRENDA, KEGG (queried 2.4.2.1) // other EC numbers for this reaction: 2.4.2.15
GMP-salvage/3_3.5.4.3_GUANINE-DEAMINASE-RXN                                               : 1.0 H2O + 1.0 H+ + 1.0 guanine --> 1.0 ammonium + 1.0 xanthine  # source: MetaCyc,
BRENDA, KEGG (queried 3.5.4.3)
GMP-salvage/4_2.4.2.8_2.4.2.22_XANPRIBOSYLTRAN-RXN                                        : 1.0 XMP + 1.0 diphosphate <-- 1.0 xanthine + 1.0 5-phospho-alpha-D-ribose_1-diphosphate
# source: MetaCyc, BRENDA, KEGG (queried 2.4.2.8, 2.4.2.22)
#XMP
XMP-salvage/1_3.1.3.5_XMPXAN-RXN                                                          : 1.0 XMP + 1.0 H2O --> 1.0 phosphate + 1.0 xanthosine  # source: MetaCyc, BRENDA, KEGG
(queried 3.1.3.5)
XMP-salvage/2_2.4.2.1_XANTHOSINEPHOSPHORY-RXN                                             : 1.0 phosphate + 1.0 xanthosine --> 1.0 alpha-D-ribose-1-phosphate + 1.0 xanthine  #
source: MetaCyc, BRENDA, KEGG (queried 2.4.2.1) // other EC numbers for this reaction: 2.4.2
#IMP
IMP-salvage_3.1.3.5_RXN-7607                                                              : 1.0 IMP + 1.0 H2O --> 1.0 inosine + 1.0 phosphate  # source: MetaCyc, BRENDA, KEGG
(queried 3.1.3.5) // other EC numbers for this reaction: 3.1.3.v

#adenosine salvage
adenosine-salvage/pa1_3.1.3.5_3.1.3.2_BS73811                                             : 2.0 H2O + 1.0 ADP --> 2.0 phosphate + 1.0 adenosine  # source: BRENDA (queried 3.1.3.5,
3.1.3.2) // other EC numbers for this reaction: 3.6.1.5
adenosine-salvage/pb1_3.1.3.5_BS73810                                                     : 1.0 H2O + 1.0 ADP --> 1.0 diphosphate + 1.0 adenosine  # source: BRENDA (queried
3.1.3.5) // other EC numbers for this reaction: 3.1.3.31, 3.6.1.19
adenosine-salvage/1_3.5.4.4_ADENODEAMIN-RXN                                               : 1.0 H2O + 1.0 adenosine + 1.0 H+ --> 1.0 ammonium + 1.0 inosine  # source: MetaCyc,
BRENDA, KEGG (queried 3.5.4.4)
adenosine-salvage/2_2.4.2.1_INOPHOSPHOR-RXN                                               : 1.0 phosphate + 1.0 inosine <=> 1.0 alpha-D-ribose-1-phosphate + 1.0 hypoxanthine  #
source: MetaCyc, BRENDA, KEGG (queried 2.4.2.1) // other EC numbers for this reaction: 2.4.2.15, 2.4.2.3, 2.4.2.44
adenosine-salvage/3_1.17.1.4_RXN-7682                                                     : 1.0 H2O + 1.0 NAD+ + 1.0 hypoxanthine --> 1.0 xanthine + 1.0 H+ + 1.0 NADH  # source:
MetaCyc, BRENDA, KEGG (queried 1.17.1.4) // other EC numbers for this reaction: 1.17.3.2

#DNA-Abbau
#dCMP
dCMP-salvage/1a_3.1.3.5_RXN0-5292                                                         : 1.0 dCMP + 1.0 H2O --> 1.0 2'-deoxycytidine + 1.0 phosphate  # source: MetaCyc, BRENDA,
KEGG (queried 3.1.3.5) // other EC numbers for this reaction: 3.1.3.89
dCMP-salvage/2_3.5.4.5_CYTIDEAM-RXN                                                       : 1.0 H+ + 1.0 H2O + 1.0 2'-deoxycytidine --> 1.0 2'-deoxyuridine + 1.0 ammonium  #
source: MetaCyc, BRENDA, KEGG (queried 3.5.4.5)
dCMP-salvage/11b_3.5.4.12_DCMP-DEAMINASE-RXN                                              : 1.0 H2O + 1.0 H+ + 1.0 dCMP --> 1.0 dUMP + 1.0 ammonium  # source: MetaCyc, BRENDA, KEGG
(queried 3.5.4.12)
#dUMP
dUMP-salvage/1_3.1.3.5_RXN-14143                                                          : 1.0 H2O + 1.0 dUMP --> 1.0 phosphate + 1.0 2'-deoxyuridine  # source: MetaCyc, BRENDA,
KEGG (queried 3.1.3.5) // other EC numbers for this reaction: 3.1.3.89, 3.1.3.34
dUMP-salvage/2_2.4.2.1_2.4.2.2_URA-PHOSPH-RXN                                             : 1.0 phosphate + 1.0 2'-deoxyuridine <=> 1.0 uracil + 1.0 2-deoxy-alpha-D-ribose_1-
phosphate  # source: MetaCyc, BRENDA, KEGG (queried 2.4.2.1, 2.4.2.2) // other EC numbers for this reaction: 2.4.2.3, 2.4.2.4
#dAMP
dAMP-salvage/1_3.1.3.5_3.1.3.2_RXN-14161                                                  : 1.0 H2O + 1.0 dAMP --> 1.0 2'-deoxyadenosine + 1.0 phosphate  # source: MetaCyc, BRENDA,
KEGG (queried 3.1.3.5, 3.1.3.2) // other EC numbers for this reaction: 3.1.3.89
dAMP-salvage/2a_2.4.2.1_DEOXYADENPHOSPHOR-RXN                                             : 1.0 phosphate + 1.0 2'-deoxyadenosine <=> 1.0 adenine + 1.0 2-deoxy-alpha-D-ribose_1-
phosphate  # source: MetaCyc, BRENDA, KEGG (queried 2.4.2.1)
dAMP-salvage/2b_3.5.4.4_ADDALT-RXN                                                        : 1.0 H+ + 1.0 H2O + 1.0 2'-deoxyadenosine --> 1.0 ammonium + 1.0 2'-deoxyinosine  #
source: MetaCyc, BRENDA, KEGG (queried 3.5.4.4) // other EC numbers for this reaction: 3.5.4.17
dAMP-salvage/3_2.4.2.1_DEOXYINOPHOSPHOR-RXN                                               : 1.0 phosphate + 1.0 2'-deoxyinosine <=> 1.0 hypoxanthine + 1.0 2-deoxy-alpha-D-ribose_1-
phosphate  # source: MetaCyc, BRENDA, KEGG (queried 2.4.2.1) // other EC numbers for this reaction: 2.4.2.4
#dGMP
dGMP-salvage/1_3.1.3.5_3.1.3.2_RXN-14142                                                  : 1.0 H2O + 1.0 dGMP --> 1.0 phosphate + 1.0 2'-deoxyguanosine  # source: MetaCyc, BRENDA,
KEGG (queried 3.1.3.5, 3.1.3.2) // there are 4 more EC numbers for this reaction
dGMP-salvage/2_2.4.2.1_DEOXYGUANPHOSPHOR-RXN                                              : 1.0 phosphate + 1.0 2'-deoxyguanosine <=> 1.0 2-deoxy-alpha-D-ribose_1-phosphate + 1.0
```

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guanine  # source: MetaCyc, BRENDA, KEGG (queried 2.4.2.1) // other EC numbers for this reaction: 2.4.2.15, 2.4.2.4
#dTMP
dTMP-salvage/1_3.1.3.5_THYMIDYLATE-5-PHOSPHATASE-RXN                                    : 1.0 H2O + 1.0 dTMP --> 1.0 phosphate + 1.0 thymidine  # source: MetaCyc, BRENDA, KEGG
(queried 3.1.3.5) // other EC numbers for this reaction: 3.1.3.89, 3.1.3.35
dTMP-salvage/2_2.4.2.2_THYM-PHOSPH-RXN                                                  : 1.0 thymidine + 1.0 phosphate <=> 1.0 thymine + 1.0 2-deoxy-alpha-D-ribose_1-phosphate
# source: MetaCyc, BRENDA, KEGG (queried 2.4.2.2) // other EC numbers for this reaction: 2.4.2.4

#Salvage - like guanine and guanosine salvage II
#adenosine
adenosine-salvage/1_3.2.2.1_BR16044                                                     : 1.0 adenosine + 1.0 H2O --> 1.0 beta-D-ribopyranose + 1.0 adenine  # source: BRENDA,
KEGG (queried 3.2.2.1) // other EC numbers for this reaction: 3.2.2.8, 3.2.2.7
adenosine-salvage/2_3.5.4.2_ADENINE-DEAMINASE-RXN                                       : 1.0 H2O + 1.0 H+ + 1.0 adenine --> 1.0 hypoxanthine + 1.0 ammonium  # source: MetaCyc,
BRENDA, KEGG (queried 3.5.4.2)
#guanosine
guanosine-salvage/1_3.2.2.1_RXN0-366                                                    : 1.0 H2O + 1.0 guanosine --> 1.0 beta-D-ribopyranose + 1.0 guanine  # source: MetaCyc
(queried 3.2.2.1)
guanosine-salvage/2_2.4.2.8_2.4.2.7_2.4.2.22_GUANPRIBOSYLTRAN-RXN                       : 1.0 GMP + 1.0 diphosphate <=> 1.0 guanine + 1.0 5-phospho-alpha-D-ribose_1-diphosphate
# source: MetaCyc, BRENDA, KEGG (queried 2.4.2.8, 2.4.2.7, 2.4.2.22)
#inosine
inosine-salvage/1_3.2.2.1_BR16042                                                       : 1.0 inosine + 1.0 H2O --> 1.0 hypoxanthine + 1.0 beta-D-ribopyranose  # source: BRENDA,
KEGG (queried 3.2.2.1) // other EC numbers for this reaction: 3.2.2.2, 3.2.2.8
inosine-salvage/2_2.4.2.8_HYPOXANPRIBOSYLTRAN-RXN                                       : 1.0 diphosphate + 1.0 IMP <=> 1.0 hypoxanthine + 1.0 5-phospho-alpha-D-ribose_1-
diphosphate  # source: MetaCyc, BRENDA, KEGG (queried 2.4.2.8)
#xanthosine
xanthosine-salvage_3.2.2.1_RXN0-363                                                     : 1.0 xanthosine + 1.0 H2O --> 1.0 beta-D-ribopyranose + 1.0 xanthine  # source: MetaCyc
(queried 3.2.2.1)
#cytidine
cytidine-salvage_3.2.2.1_BS214504                                                                                  : 1.0 cytidine + 1.0 H2O --> 1.0 cytosine + 1.0 beta-D-
ribopyranose  # source: BRENDA, KEGG (queried 3.2.2.1) // other EC numbers for this reaction: 3.2.2.3, 3.2.2.8
#################################################################################################################################################################################
#2'-deoxy-α-D-ribose 1-phosphate degradation

2'-deoxy-alpha-D-ribose-1-phosphate-degr/1_5.4.2.7_D-PPENTOMUT-RXN                      : 1.0 2-deoxy-alpha-D-ribose_1-phosphate <=> 1.0 2-deoxy-D-ribose_5-phosphate  # source:
MetaCyc, BRENDA, KEGG (queried 5.4.2.7)
2'-deoxy-alpha-D-ribose-1-phosphate-degr/2_4.1.2.4_DEOXYRIBOSE-P-ALD-RXN                : 1.0 2-deoxy-D-ribose_5-phosphate <=> 1.0 D-glyceraldehyde_3-phosphate + 1.0 acetaldehyde
# source: MetaCyc, BRENDA, KEGG (queried 4.1.2.4)

acetaldehyde-degradation_1.2.1.3_1.17.1.4_RXN66-3                                       : 1.0 H2O + 1.0 NAD+ + 1.0 acetaldehyde --> 1.0 acetate + 2.0 H+ + 1.0 NADH  # source:
MetaCyc, BRENDA, KEGG (queried 1.2.1.3, 1.17.1.4) // there are 20 more EC numbers for this reaction

#alpha-D-ribose-1-phosphate degradation
PRPP-biosynthesis-II_5.4.2.2_5.4.2.7_PPENTOMUT-RXN                                      : 1.0 alpha-D-ribose-1-phosphate <=> 1.0 D-ribose_5-phosphate  # source: MetaCyc, BRENDA,
KEGG (queried 5.4.2.2, 5.4.2.7)

#beta-D-ribopyranose degradation
beta-D-ribopyranose-degradation_modb_2.7.1.15_BR47755                                   : 1.0 ATP + 1.0 beta-D-ribopyranose --> 1.0 D-ribose_5-phosphate + 1.0 ADP + 1.0 H+ #
source: BRENDA, KEGG (queried 2.7.1.15)
#################################################################################################################################################################################
#(d)NXP-transitions (2.7.4.25,2.7.4.3,2.7.4.22,2.7.4.8,2.7.4.9 + not sequence based: 2.7.4.6)

NXP-transitions_2.7.4.3_RXN-14074                                   : 1.0 GTP + 1.0 AMP --> 1.0 ADP + 1.0 GDP  # source: MetaCyc, BRENDA (queried 2.7.4.3) // other EC numbers
for this reaction: 2.7.4.4, 2.7.4.10
NXP-transitions_2.7.4.8_GUANYL-KIN-RXN                              : 1.0 ATP + 1.0 GMP --> 1.0 ADP + 1.0 GDP  # source: MetaCyc, BRENDA, KEGG (queried 2.7.4.8)
NXP-transitions_2.7.4.6_GDPKIN-RXN                                  : 1.0 ATP + 1.0 GDP --> 1.0 ADP + 1.0 GTP  # source: MetaCyc, BRENDA, KEGG (queried 2.7.4.6)

NXP-transitions_2.7.4.22_RXN-12002                                  : 1.0 UMP + 1.0 ATP --> 1.0 ADP + 1.0 UDP  # source: MetaCyc, BRENDA, KEGG (queried 2.7.4.22) // other EC
numbers for this reaction: 2.7.4.4, 2.7.4.14
NXP-transitions_2.7.4.3_BS358186                                    : 1.0 UTP + 1.0 AMP <-- 1.0 ADP + 1.0 UDP  # source: BRENDA, KEGG (queried 2.7.4.3) // other EC numbers for
this reaction: 2.7.4.10

NXP-transitions_2.7.4.25_2.7.4.3_RXN-11832                          : 1.0 CMP + 1.0 ATP --> 1.0 ADP + 1.0 CDP  # source: MetaCyc, BRENDA, KEGG (queried 2.7.4.25, 2.7.4.3) //
other EC numbers for this reaction: 2.7.4.14
NXP-transitions_2.7.4.3_CDPKIN-RXN                                  : 1.0 ATP + 1.0 CDP --> 1.0 ADP + 1.0 CTP  # source: MetaCyc, BRENDA, KEGG (queried 2.7.4.3) // other EC
numbers for this reaction: 2.7.4.6
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```
NXP-transitions_2.7.4.3_ADENYL-KIN-RXN                                  : 1.0 ATP + 1.0 AMP --> 2.0 ADP  # source: MetaCyc, BRENDA, KEGG (queried 2.7.4.3)

NXP-transitions_2.7.4.3_DEOXYADENYLATE-KINASE-RXN                       : 1.0 dAMP + 1.0 ATP --> 1.0 ADP + 1.0 dADP  # source: MetaCyc, BRENDA, KEGG (queried 2.7.4.3) // other EC
numbers for this reaction: 2.7.4.13, 2.7.4.11
NXP-transitions_2.7.4.8_GMKALT-RXN                                      : 1.0 dGMP + 1.0 ATP --> 1.0 ADP + 1.0 dGDP  # source: MetaCyc, BRENDA, KEGG (queried 2.7.4.8) // other EC
numbers for this reaction: 2.7.4.12, 2.7.4.13
NXP-transitions_2.7.4.25_RXN-7913                                       : 1.0 ATP + 1.0 dCMP --> 1.0 ADP + 1.0 dCDP  # source: MetaCyc, BRENDA, KEGG (queried 2.7.4.25) // other EC
numbers for this reaction: 2.7.4.14, 2.7.4.13
NXP-transitions_2.7.4.9_DTMPKI-RXN                                      : 1.0 dTMP + 1.0 ATP --> 1.0 dTDP + 1.0 ADP  # source: MetaCyc, BRENDA, KEGG (queried 2.7.4.9) // other EC
numbers for this reaction: 2.7.4.12, 2.7.4.13
NXP-transitions_2.7.4.9_RXN-17141                                       : 1.0 GTP + 1.0 dTMP --> 1.0 GDP + 1.0 dTDP  # source: MetaCyc, BRENDA (queried 2.7.4.9) // other EC numbers
for this reaction: 2.7.4.M1

NXP-transitions_2.7.4.6_DTDPKIN-RXN                                     : 1.0 dTDP + 1.0 ATP --> 1.0 ADP + 1.0 dTTP  # source: MetaCyc, BRENDA, KEGG (queried 2.7.4.6)

NXP-transitions_2.7.4.22_2.7.4.9_2.7.4.25_RXN-14122                     : 1.0 ATP + 1.0 dUMP --> 1.0 ADP + 1.0 dUDP  # source: MetaCyc, BRENDA, KEGG (queried 2.7.4.22, 2.7.4.9,
2.7.4.25) // there are 4 more EC numbers for this reaction

NXP-transitions_2.7.4.6_DADPKIN-RXN                                     : 1.0 dADP + 1.0 ATP --> 1.0 ADP + 1.0 dATP  # source: MetaCyc, BRENDA, KEGG (queried 2.7.4.6)
NXP-transitions_2.7.4.6_DGDPKIN-RXN                                     : 1.0 dGDP + 1.0 ATP --> 1.0 ADP + 1.0 dGTP  # source: MetaCyc, BRENDA, KEGG (queried 2.7.4.6)
NXP-transitions_2.7.4.6_DUDPKIN-RXN                                     : 1.0 ATP + 1.0 dUDP --> 1.0 ADP + 1.0 dUTP  # source: MetaCyc, BRENDA, KEGG (queried 2.7.4.6)
NXP-transitions_2.7.4.6_DCDPKIN-RXN                                     : 1.0 dCDP + 1.0 ATP --> 1.0 ADP + 1.0 dCTP  # source: MetaCyc, BRENDA, KEGG (queried 2.7.4.6)
##########################################################################################################################################################################
#ppGpp
ppGpp-biosynthesis_2.7.6.5_GDPPYPHOSKIN-RXN                             : 1.0 GDP + 1.0 ATP --> 1.0 AMP + 1.0 ppGpp  # source: MetaCyc, BRENDA (queried 2.7.6.5) // other EC numbers
for this reaction: 2.7.6.4
ppGpp-biosynthesis_2.7.6.5_GTPPYPHOSKIN-RXN                             : 1.0 GTP + 1.0 ATP --> 1.0 AMP + 1.0 pppGpp  # source: MetaCyc, BRENDA, KEGG (queried 2.7.6.5)
ppGpp-biosynthesis_3.6.1.40_PPPGPPHYDRO-RXN                             : 1.0 H2O + 1.0 pppGpp --> 1.0 ppGpp + 1.0 phosphate + 1.0 H+  # source: MetaCyc, BRENDA, KEGG (queried
3.6.1.40) // other EC numbers for this reaction: 3.6.1.11
##########################################################################################################################################################################
#uracil degr I
uracil-degr-I/1_1.3.1.1_DIHYDROURACIL-DEHYDROGENASE-NAD+-RXN             : 1.0 5,6-dihydrouracil + 1.0 NAD+ <=> 1.0 H+ + 1.0 NADH + 1.0 uracil  # source: MetaCyc, BRENDA, KEGG
(queried 1.3.1.1)
uracil-degr-I/2_3.5.2.2_DIHYDROPYRIMIDINASE-RXN                         : 1.0 5,6-dihydrouracil + 1.0 H2O --> 1.0 3-ureidopropanoate + 1.0 H+  # source: MetaCyc, BRENDA, KEGG
(queried 3.5.2.2)
uracil-degr-I/3_3.5.1.6_BETA-UREIDOPROPIONASE-RXN                       : 2.0 H+ + 1.0 3-ureidopropanoate + 1.0 H2O --> 1.0 ammonium + 1.0 CO2 + 1.0 beta-alanine  # source:
MetaCyc, BRENDA, KEGG (queried 3.5.1.6)

#thymine degr
thymine-degradation_1.3.1.1_RXN0-6565                                   : 1.0 NAD+ + 1.0 5,6-dihydrothymine <=> 1.0 thymine + 1.0 H+ + 1.0 NADH  # source: MetaCyc, BRENDA, KEGG
(queried 1.3.1.1)
thymine-degradation_3.5.2.2_RXN-11211                                   : 1.0 5,6-dihydrothymine + 1.0 H2O --> 1.0 (R)-3-ureido-isobutanoate + 1.0 H+  # source: MetaCyc, BRENDA
(queried 3.5.2.2)
thymine-degradation_3.5.1.6_RXN-11210                                   : 1.0 H2O + 2.0 H+ + 1.0 (R)-3-ureido-isobutanoate --> 1.0 (R)-3-amino-2-methylpropanoate + 1.0 CO2 + 1.0
ammonium  # source: MetaCyc, KEGG (queried 3.5.1.6)

##########################################################################################################################################################################
##########################################################################Non-MDM/CDMM substrates#########################################################################
##########################################################################################################################################################################
#cytosine
cytosine_exchange                           : 1.0 cytosine[ex] <=>
thymine_exchange                            : 1.0 thymine[ex] <=>

##CDIF630erm_01905; CDIF630erm_03001
cytosine_transport                          : 1.0 Na+ + 1.0 cytosine <=> 1.0 cytosine[ex] + 1.0 Na+[ex]
thymine_transport                           : 1.0 Na+ + 1.0 thymine <=> 1.0 thymine[ex] + 1.0 Na+[ex]
##########################################################################################################################################################################
#adenine/guanine/hypoxanthine
adenine_exchange                            : 1.0 adenine[ex] <=>
guanine_exchange                            : 1.0 guanine[ex] <=>
hypoxanthine_exchange                       : 1.0 hypoxanthine[ex] <=>

##CDIF630erm_02331; CDIF630erm_02961
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adenine_transport                              : 1.0 Na+ + 1.0 adenine <=> 1.0 adenine[ex] + 1.0 Na+[ex]
guanine_transport                              : 1.0 Na+ + 1.0 guanine <=> 1.0 guanine[ex] + 1.0 Na+[ex]
hypoxanthine_transport                         : 1.0 Na+ + 1.0 hypoxanthine <=> 1.0 hypoxanthine[ex] + 1.0 Na+[ex]
################################################################################################################################################################
#uracil
uracil_exchange                                : 1.0 uracil[ex] <=>

##CDIF630erm_02848
uracil_transport                               : 1.0 Na+ + 1.0 uracil <=> 1.0 uracil[ex] + 1.0 Na+[ex]
################################################################################################################################################################
#xanthine/urate
xanthine_exchange                              : 1.0 xanthine[ex] <=>
urate_exchange                                 : 1.0 urate[ex] <=>

##CDIF630erm_02298; CDIF630erm_02313; CDIF630erm_02314; CDIF630erm_03472
xanthine_transport                             : 1.0 Na+ + 1.0 xanthine <=> 1.0 xanthine[ex] + 1.0 Na+[ex]
urate_transport                                : 1.0 Na+ + 1.0 urate <=> 1.0 urate[ex] + 1.0 Na+[ex]

urate-degradation_1.17.1.4_RXN0-901            : 1.0 xanthine + 1.0 H2O + 1.0 NAD+ <=> 1.0 urate + 1.0 H+ + 1.0 NADH  # source: MetaCyc, BRENDA, KEGG (queried 1.17.1.4)

################################################################################################################################################################
asparagine_exchange                            : 1.0 L-asparagine[ex] <=>
glutamine_exchange                             : 1.0 L-glutamine[ex] <=>

#unknown, ABC-transporter is a guess
##CDIF630erm_01972-CDIF630erm_01974?; CDIF630erm_00868-CDIF630erm_00870?
glutamine_transport                            : 1.0 H2O + 1.0 ATP + 1.0 L-glutamine[ex] --> 1.0 L-glutamine + 1.0 ADP + 1.0 phosphate + 1.0 H+
asparagine_transport                           : 1.0 H2O + 1.0 ATP + 1.0 L-asparagine[ex] --> 1.0 H+ + 1.0 phosphate + 1.0 ADP + 1.0 L-asparagine
################################################################################################################################################################
#4-hydroxyproline
4-hydroxyproline_exchange                                          : 1.0 trans-4-hydroxy-L-proline[ex] <=>
4-hydroxyproline_transport                                         : 1.0 Na+ + 1.0 trans-4-hydroxy-L-proline <=> 1.0 Na+[ex] + 1.0 trans-4-hydroxy-L-proline[ex]
4-hydroxyproline-degr/1_manual_4.2.1.-_HD-Hyp                      : 1.0 trans-4-hydroxy-L-proline <=> 1.0 (S)-1-pyrroline-5-carboxylate + 1.0 H2O
4-hydroxyproline-degr/2_1.5.1.2_PYRROLINECARBREDUCT-RXN            : 1.0 NADP+ + 1.0 L-proline <-- 1.0 (S)-1-pyrroline-5-carboxylate + 1.0 NADPH + 2.0 H+  # source: MetaCyc,
BRENDA, KEGG (queried 1.5.1.2)
################################################################################################################################################################
#cystathionine
cystathionine_exchange                         : 1.0 L-cystathionine[ex] <=>

##CDIF630erm_02404-CDIF630erm_02406 vgl. Burguière et al., 2004
cystathionine_transport                        : 1.0 H2O + 1.0 ATP + 1.0 L-cystathionine[ex] --> 1.0 H+ + 1.0 phosphate + 1.0 ADP + 1.0 L-cystathionine

cystathionine-degr-A_4.4.1.8_RXN-15131         : 1.0 L-cystathionine --> 1.0 H+ + 1.0 2-aminoprop-2-enoate + 1.0 L-homocysteine  # source: MetaCyc, BRENDA (queried 4.4.1.8)
cystathionine-degr-B_4.4.1.1_RXN-14048         : 1.0 L-cystathionine --> 1.0 (2Z)-2-aminobut-2-enoate + 1.0 H+ + 1.0 L-cysteine  # source: MetaCyc, BRENDA, KEGG (queried 4.4.1.1)
################################################################################################################################################################
spermidine_exchange                            : 1.0 spermidine[ex] <=>
putrescine_exchange                            : 1.0 putrescine[ex] <=>

##CDIF630erm_01160-CDIF630erm_01163
putrescine_transport_3.6.3.31_modb_BS141431    : 1.0 ATP + 1.0 H2O + 1.0 putrescine[ex] --> 1.0 putrescine + 1.0 ADP + 1.0 phosphate + 1.0 H+   # ource: MetaCyc, BRENDA (queried
3.6.3.31)
spermidine_transport_3.6.3.31_modb_BS141432    : 1.0 ATP + 1.0 H2O + 1.0 spermidine[ex] --> 1.0 spermidine + 1.0 phosphate + 1.0 ADP + 1.0 H+  # source: MetaCyc, BRENDA (queried
3.6.3.31)
################################################################################################################################################################
#2,3-diaminopropanoate degradation
2,3-diaminopropanoate_exchange                                     : 1.0 |23-Diaminopropanoate|[ex] <=>
2,3-diaminopropanoate_transport                                    : 1.0 ATP + 1.0 |23-Diaminopropanoate|[ex] + 1.0 H2O --> 1.0 ADP + 1.0 phosphate + 1.0 |23-
Diaminopropanoate| + 1.0 H+
2,3-diaminopropanoate-degr_4.3.1.15_4.3.1.15-RXN                   : 1.0 |23-Diaminopropanoate| + 1.0 H2O --> 2.0 ammonium + 1.0 pyruvate  # source: MetaCyc, BRENDA, KEGG
(queried 4.3.1.15)

hydroxylamine_exchange                                             : 1.0 hydroxylamine[ex] <=>
hydroxylamine_transport                                            : 1.0 hydroxylamine[ex] <=> 1.0 hydroxylamine
hydroxylamine_1.7.99.1_HYDROXYLAMINE-REDUCTASE-NADH-RXN            : 1.0 H2O + 1.0 NAD+ + 1.0 ammonium <=> 2.0 H+ + 1.0 NADH + 1.0 hydroxylamine  # source: MetaCyc, BRENDA,
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KEGG (queried 1.7.99.1) // other EC numbers for this reaction: 1.7.1.10
#########################################################################################################################################################################
#ethanolamine utilization
#(Pitts et al., 2012)
ethanolamine_exchange                                                                                 : 1.0 ethanolamine[ex] <=>
##CDIF630erm_02128
ethanolamine_transport1                                                                               : 1.0 ethanolamine <=> 1.0 ethanolamine[ex]
##CDIF630erm_02119
ethanolamine_transport2                                                                               : 1.0 ethanolamine[BMC] <-- 1.0 ethanolamine

ethanolamine-utilization/1_4.3.1.7_ETHAMLY-RXN                                                        : 1.0 ethanolamine[BMC] --> 1.0 ammonium + 1.0 acetaldehyde[BMC]  # source: MetaCyc, BRENDA,
KEGG (queried 4.3.1.7)
ethanolamine-utilization/2_1.2.1.10_ACETALD-DEHYDROG-RXN                                              : 1.0 NAD+[BMC] + 1.0 coenzyme_A[BMC] + 1.0 acetaldehyde[BMC] <=> 1.0 NADH[BMC] + 1.0 acetyl-
CoA[BMC] + 1.0 H+  # source: MetaCyc, BRENDA, KEGG (queried 1.2.1.10)
ethanolamine-utilization/3_2.3.1.8_PHOSACETYLTRANS-RXN                                                : 1.0 acetyl-CoA[BMC] + 1.0 phosphate <=> 1.0 acetyl_phosphate + 1.0 coenzyme_A[BMC]  #
source: MetaCyc, BRENDA, KEGG (queried 2.3.1.8)
ethanolamine-utilization/4_1.1.1.1_ALCOHOL-DEHYDROGENASE-NADP+-RXN_WOP                                : 1.0 NAD+[BMC] + 1.0 ethanol <=> 1.0 NADH[BMC] + 1.0 acetaldehyde[BMC] + 1.0 H+  # source:
MetaCyc, BRENDA, KEGG (queried 1.1.1.1) // other EC numbers for this reaction: 1.1.1.71
#########################################################################################################################################################################
sn-glycerol-3-phosphate_exchange              : 1.0 sn-glycerol_3-phosphate[ex] <=>

##CDIF630erm_03719-CDIF630erm_03722
sn-glycerol-3-phosphate_transport             : 1.0 ATP + 1.0 sn-glycerol_3-phosphate[ex] + 1.0 H2O --> 1.0 ADP + 1.0 sn-glycerol_3-phosphate + 1.0 phosphate + 1.0 H+
#########################################################################################################################################################################
#methylphosphonate degr II
methylphosphonate_exchange                                                                          : 1.0 methylphosphonate[ex] <=>
##CDIF630erm_03847-CDIF630erm_03848
methylphosphonate_transport                                                                         : 1.0 methylphosphonate + 1.0 ADP + 1.0 H+ <-- 1.0 methylphosphonate[ex] + 1.0 ATP + 1.0 H2O
methane_transport                                                                                   : 1.0 methane <=> 1.0 methane[ex]
methane_exchange                                                                                    : 1.0 methane[ex] <=>

methylphosphonate-degr-II/1_2.7.8.37_RXN0-6732                                                      : 1.0 ATP + 1.0 methylphosphonate --> 1.0 adenine + 1.0 alpha-D-ribose-1-methylphosphonate-5-
triphosphate  # source: MetaCyc, BRENDA, KEGG (queried 2.7.8.37)
methylphosphonate-degr-II/2_3.6.1.63_RXN0-6733                                                      : 1.0 H2O + 1.0 alpha-D-ribose-1-methylphosphonate-5-triphosphate --> 1.0 H+ + 1.0 diphosphate
+ 1.0 alpha-D-ribose-1-methylphosphonate_5-phosphate  # source: MetaCyc, BRENDA, KEGG (queried 3.6.1.63)
methylphosphonate-degr-II/3_4.7.1.1_RXN0-6734                                                       : 1.0 alpha-D-ribose-1-methylphosphonate_5-phosphate --> 1.0 5-phospho-alpha-D-ribose_1,2-
cyclic_phosphate + 1.0 methane  # source: MetaCyc, BRENDA, KEGG (queried 4.7.1.1)
methylphosphonate-degr-II/4_3.1.4.57_RXN-14995                                                      : 1.0 H2O + 1.0 5-phospho-alpha-D-ribose_1,2-cyclic_phosphate --> 1.0 D-ribofuranose_2,5-
bisphosphate + 1.0 H+  # source: MetaCyc, BRENDA, KEGG (queried 3.1.4.57)
methylphosphonate-degr-II/5_3.1.4.57_RXN-14996                                                      : 1.0 D-ribofuranose_2,5-bisphosphate + 1.0 H2O --> 1.0 phosphate + 1.0 D-ribose_5-phosphate
# source: MetaCyc, BRENDA, KEGG (queried 3.1.4.57)
#########################################################################################################################################################################
#2-aminoethylP degr I
2-aminoethylphosphonate_exchange                                                                    : 1.0 (2-aminoethyl)phosphonate[ex] <=>
##CDIF630erm_03847-CDIF630erm_03848
2-aminoethylphosphonate_transport                                                                   : 1.0 2-aminoethylphosphonate + 1.0 ADP + 1.0 H+ <-- 1.0 (2-aminoethyl)phosphonate[ex] + 1.0
ATP + 1.0 H2O
2-aminoethylphosph-degr-I/1_2.6.1.37_2.6.1.37-RXN                                                   : 1.0 pyruvate + 1.0 (2-aminoethyl)phosphonate <=> 1.0 phosphonoacetaldehyde + 1.0 L-alanine
# source: MetaCyc, BRENDA, KEGG (queried 2.6.1.37)
2-aminoethylphosph-degr-I/2_3.11.1.1_PHOSPHONOACETALDEHYDE-HYDROLASE-RXN                            : 1.0 phosphonoacetaldehyde + 1.0 H2O --> 1.0 acetaldehyde + 1.0 phosphate + 1.0 H+  # source:
MetaCyc, BRENDA, KEGG (queried 3.11.1.1)
#########################################################################################################################################################################
#phosphonoacetate degradation
phosphonoacetate_exchange                                                                           : 1.0 phosphonoacetate[ex] <=>
##CDIF630erm_03847-CDIF630erm_03848
phosphonoacetate_transport                                                                          : 1.0 phosphonoacetate + 1.0 ADP + 1.0 H+ + 1.0 phosphate <-- 1.0 phosphonoacetate[ex] + 1.0
ATP + 1.0 H2O
phosphonoacetate-degradation_3.11.1.2_3.11.1.2-RXN                                                  : 1.0 H2O + 1.0 phosphonoacetate --> 1.0 acetate + 1.0 phosphate + 1.0 H+  # source: MetaCyc,
BRENDA, KEGG (queried 3.11.1.2)
#########################################################################################################################################################################
succinate_exchange                                                                                  : 1.0 succinate[ex] <=>
##CDIF630erm_02583
succinate_transport                                                                                 : 1.0 Na+ + 1.0 succinate <=> 1.0 succinate[ex] + 1.0 Na+[ex]
#########################################################################################################################################################################
```

```
#tartronate semialdehyde
tartronate-semialdehyde_exchange                                                    : 1.0 tartronate_semialdehyde[ex] <=>
tartronate-semialdehyde_transport                                                   : 1.0 tartronate_semialdehyde[ex] + 1.0 Na+[ex] <=> 1.0 tartronate_semialdehyde + 1.0 Na+

tartronate-semialdehyde-degr_1.1.1.60_TSA-REDUCT-RXN_WOP                            : 1.0 NAD+ + 1.0 D-glycerate <=> 1.0 NADH + 1.0 H+ + 1.0 tartronate_semialdehyde  # source:
MetaCyc, BRENDA, KEGG (queried 1.1.1.60) // other EC numbers for this reaction: 1.1.1
tartronate-semialdehyde-degr_1.1.1.60_TSA-REDUCT-RXN                                : 1.0 NADP+ + 1.0 D-glycerate <-- 1.0 tartronate_semialdehyde + 1.0 H+ + 1.0 NADPH  # source:
MetaCyc, BRENDA, KEGG (queried 1.1.1.60)
#####################################################################################################################################################################
#Acetoin degradation
acetoin_exchange                                                                    : 1.0 acetoin[ex] <=>
acetoin_transport                                                                   : 1.0 acetoin[ex] + 1.0 H+[ex] <=> 1.0 acetoin + 1.0 H+ # metacyc
acetoin-degradation_2.3.1.190_RXN-9718                                              : 1.0 acetoin + 1.0 NAD+ + 1.0 coenzyme_A --> 1.0 acetyl-CoA + 1.0 acetaldehyde + 1.0 H+ + 1.0
NADH  # source: MetaCyc, BRENDA, KEGG (queried 2.3.1.190)
#####################################################################################################################################################################
#3-hydroxy-3-methylglutarate
3-hydroxy-3-methylglutarate_exchange                                                : 1.0 3-hydroxy-3-methylglutarate[ex] <=>
##CDIF630erm_00917
3-hydroxy-3-methylglutarate_transport                                               : 1.0 H+ + 1.0 3-hydroxy-3-methylglutarate <=> 1.0 H+[ex] + 1.0 3-hydroxy-3-
methylglutarate[ex]
3-hydroxy-3-methylglutarate-degr/1_manual_2.8.3.-_HD-3MG                            : 1.0 acetyl-CoA + 1.0 3-hydroxy-3-methylglutarate --> 1.0 (S)-3-hydroxy-3-methylglutaryl-CoA
+ 1.0 acetate  # source: MetaCyc, BRENDA, KEGG (queried 2.8.3.-) // other EC numbers for this reaction: 2.8.3.1, 2.8.3
3-hydroxy-3-methylglutarate-degr/2_4.1.3.4_HYDROXYMETHYLGLUTARYL-COA-LYASE-RXN      : 1.0 (S)-3-hydroxy-3-methylglutaryl-CoA --> 1.0 acetyl-CoA + 1.0 acetoacetate  # source:
MetaCyc, BRENDA, KEGG (queried 4.1.3.4)
#####################################################################################################################################################################
#oxidized-GTP
hydroxyl-radical_exchange                                                           : 1.0 hydroxyl_radical[ex] <--
hydroxyl-radical_transport                                                          : 1.0 hydroxyl_radical[ex] --> 1.0 hydroxyl_radical
oxidized-GTP-and-dGTP-detoxification_spontaneous_RXN-11409                          : 1.0 GTP + 2.0 hydroxyl_radical --> 1.0 8-oxo-GTP + 1.0 H2O  # source: MetaCyc
oxidized-GTP-and-dGTP-detoxification_spontaneous_RXN-11410                          : 2.0 hydroxyl_radical + 1.0 dGTP --> 1.0 8-oxo-dGTP + 1.0 H2O  # source: MetaCyc
oxidized-GTP-and-dGTP-detoxification_3.6.1.55_RXN-11397                             : 1.0 H2O + 1.0 8-oxo-GTP --> 1.0 8-oxo-GMP + 1.0 diphosphate + 1.0 H+  # source: MetaCyc,
BRENDA (queried 3.6.1.55) // other EC numbers for this reaction: 3.6.1, 3.6.1.19, 3.6.1.56
oxidized-GTP-and-dGTP-detoxification_3.6.1.55_RXN-11396                             : 1.0 H2O + 1.0 8-oxo-dGTP --> 1.0 8-oxo-dGMP + 1.0 diphosphate + 1.0 H+  # source: MetaCyc,
BRENDA, KEGG (queried 3.6.1.55) // other EC numbers for this reaction: 3.6.1.65
8-oxo-GMP_transport                                                                 : 1.0 8-oxo-GMP[ex] <-- 1.0 8-oxo-GMP
8-oxo-dGMP_transport                                                                : 1.0 8-oxo-dGMP[ex] <-- 1.0 8-oxo-GMP
8-oxo-GMP_exchange                                                                  : 1.0 8-oxo-GMP[ex] -->
8-oxo-dGMP_exchange                                                                 : 1.0 8-oxo-dGMP[ex] -->
#####################################################################################################################################################################
#reactive oxygen detoxification
superoxide_exchange                                                 : 1.0 superoxide[ex] <--
hydrogen_peroxide_exchange                                          : 1.0 hydrogen_peroxide[ex] <--
oxygen_exchange                                                     : 1.0 oxygen[ex] <--
mathanol_exchange                                                   : 1.0 methanol[ex] <--
superoxide_transport                                                : 1.0 superoxide <=> 1.0 superoxide[ex]
hydrogen_peroxide_transport                                         : 1.0 hydrogen_peroxide <=> 1.0 hydrogen_peroxide[ex]
oxygen_transport                                                    : 1.0 oxygen <=> 1.0 oxygen[ex]
mathanol_transport                                                  : 1.0 methanol <=> 1.0 methanol[ex]


superoxide-radicals-degr-A/1_1.15.1.1_SUPEROX-DISMUT-RXN            : 2.0 H+ + 2.0 superoxide --> 1.0 hydrogen_peroxide + 1.0 oxygen  # source: MetaCyc, BRENDA, KEGG (queried
1.15.1.1)
superoxide-radicals-degr-A/2a_1.11.1.6_CATAL-RXN                    : 2.0 hydrogen_peroxide --> 2.0 H2O + 1.0 oxygen  # source: MetaCyc, BRENDA, KEGG (queried 1.11.1.6) //
other EC numbers for this reaction: 1.11.1.21
superoxide-radicals-degr-A/2b_1.11.1.6_RXN66-1                      : 1.0 ethanol + 1.0 hydrogen_peroxide --> 1.0 acetaldehyde + 2.0 H2O  # source: MetaCyc (queried 1.11.1.6)
superoxide-radicals-degr-A/2c_moddir_1.11.1.6_RXN-14189             : 1.0 methanol + 1.0 hydrogen_peroxide <=> 1.0 formaldehyde + 2.0 H2O  # source: MetaCyc, BRENDA, KEGG
(queried 1.11.1.6) // other EC numbers for this reaction: 1.11.1.7, 1.11.1.21

superoxide-radicals-degr-B/1_1.15.1.2_1.15.1.2-RXN                  : 1.0 superoxide + 1.0 |Reduced-Rubredoxins| + 2.0 H+ <=> 1.0 |Oxidized-Rubredoxins| + 1.0 hydrogen_peroxide
# source: MetaCyc, BRENDA, KEGG (queried 1.15.1.2)
superoxide-radicals-degr-B/2_manual_1.11.1.-_HD-1.11.1.-            : 1.0 |Reduced-Rubredoxins| + 2.0 H+ + 1.0 hydrogen_peroxide <=> 1.0 |Oxidized-Rubredoxins| + 2.0 H2O  #
source: MetaCyc, BRENDA, KEGG (queried 1.11.1.1)
superoxide-radicals-degr-B/3_manual_1.4.-_HD-1.4.-                  : 2.0 L-glutamate + 1.0 |Oxidized-Rubredoxins| --> 1.0 L-glutamine + 1.0 2-oxoglutarate + 1.0 |Reduced-
Rubredoxins| + 2.0 H+  # source: MetaCyc, KEGG (queried 1.4.7.1)
```

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oxygen-reduction-A_1.6.3.-_HD-1.6.3.-                                  : 2.0 |Reduced-Rubredoxins| + 4.0 H+ + 1.0 oxygen --> 2.0 |Oxidized-Rubredoxins| + 2.0 H2O

oxygen-reduction-B_1.6.3.4_RXN-14692                                   : 2.0 H+ + 2.0 NADH + 1.0 oxygen --> 2.0 NAD+ + 2.0 H2O  # source: MetaCyc, BRENDA, KEGG (queried
1.6.3.4) // other EC numbers for this reaction: 1.6.3.2
formaldehyde-assimilation_spontaneous_2.1.2.11_RXN-2881                : 1.0 formaldehyde + 1.0 tetrahydropteroyl_tri-L-glutamate --> 1.0 H2O + 1.0 5,10-methylene-tetrahydrofolate
# source: MetaCyc
#########################################################################################################################################################################
#cyanide detoxification I
cyanide_exchange                                                       : 1.0 hydrogen_cyanide[ex] <--
thiocyanate_exchange                                                   : 1.0 thiocyanate[ex] <--
cyanide_transport                                                      : 1.0 hydrogen_cyanide <=> 1.0 hydrogen_cyanide[ex]
thiocyanate_transport                                                  : 1.0 thiocyanate + 1.0 H+ <=> 1.0 thiocyanate[ex] + 1.0 H+[ex]

cyanide-detoxification-I/1_4.4.1.9_L-3-CYANOALANINE-SYNTHASE-RXN       : 1.0 hydrogen_cyanide + 1.0 L-cysteine <=> 1.0 3-cyano-L-alanine + 1.0 hydrogen_sulfide + 1.0 H+  #
source: MetaCyc, BRENDA, KEGG (queried 4.4.1.9)
cyanide-detoxification-I/2a_3.5.5.4_3.5.5.4-RXN                         : 2.0 H2O + 1.0 3-cyano-L-alanine + 1.0 H+ --> 1.0 ammonium + 1.0 L-aspartate  # source: MetaCyc,
BRENDA, KEGG (queried 3.5.5.4)
cyanide-detoxification-I/2b_4.2.1.65_3.5.5.4_3-CYANOALANINE-HYDRATASE-RXN  : 1.0 L-asparagine <-- 1.0 3-cyano-L-alanine + 1.0 H+ + 1.0 H2O  # source: MetaCyc, BRENDA, KEGG
(queried 4.2.1.65, 3.5.5.4)

#cyanide detoxification
cyanide-detoxification-III/1_2.8.1.2_R03105                             : 1.0 sulfite + 1.0 3-mercaptopyruvate <=> 1.0 pyruvate + 1.0 thiosulfate  # source: KEGG (queried
2.8.1.2)
cyanide-detoxification-III/2_2.8.1.1_THIOSULFATE-SULFURTRANSFERASE-RXN  : 1.0 thiosulfate + 1.0 hydrogen_cyanide --> 1.0 sulfite + 1.0 thiocyanate + 2.0 H+  # source: MetaCyc,
BRENDA, KEGG (queried 2.8.1.1)

#Cysteine degr III
L-cysteine-degradation-III/1_2.6.1.1_CYSTEINE-AMINOTRANSFERASE-RXN      : 1.0 L-cysteine + 1.0 2-oxoglutarate <=> 1.0 3-mercaptopyruvate + 1.0 L-glutamate  # source: MetaCyc,
BRENDA, KEGG (queried 2.6.1.1) // other EC numbers for this reaction: 2.6.1.3
L-cysteine-degradation-III/2_2.8.1.2_MERCAPYSTRANS-RXN                  : 1.0 hydrogen_cyanide + 1.0 3-mercaptopyruvate --> 1.0 thiocyanate + 1.0 H+ + 1.0 pyruvate  # source:
MetaCyc, BRENDA, KEGG (queried 2.8.1.2)
#########################################################################################################################################################################
#bile acids

taurochenodeoxycholate_exchange                                                : 1.0 taurochenodeoxycholate[ex] <=>
chenodeoxycholate_exchange                                                     : 1.0 chenodeoxycholate[ex] <=>
taurocholate_exchange                                                          : 1.0 taurocholate[ex] <=>
cholate_exchange                                                               : 1.0 cholate[ex] <=>

##DIF630erm_02170
taurochenodeoxycholate_transport                                               : 1.0 H+[ex] + 1.0 taurochenodeoxycholate[ex] <=> 1.0 H+ + 1.0 taurochenodeoxycholate
chenodeoxycholate_transport                                                    : 1.0 H+[ex] + 1.0 chenodeoxycholate[ex] <=> 1.0 H+ + 1.0 chenodeoxycholate
taurocholate_transport                                                         : 1.0 H+[ex] + 1.0 taurocholate[ex] <=> 1.0 H+ + 1.0 taurocholate
cholate_transport                                                              : 1.0 H+[ex] + 1.0 cholate[ex] <=> 1.0 H+ + 1.0 cholate

#C. difficile can degrade taurocholate and no glycocholate (Midtvedt and Norman, 1967)
# => no EC 3.5.1.24; No sequences for EC 3.5.1.74 known
#Highest similarity to mouse enzyme. Mouse enzyme is taurine-specific (Falany et al., 1997)
#Reverse biosynthesis pathway

taurochenodeoxycholate-degr/1_2.3.1.65_RXN-9852                                : 1.0 chenodeoxycholoyl-CoA + 1.0 taurine --> 1.0 taurochenodeoxycholate + 1.0 coenzyme_A +
1.0 H+  # source: MetaCyc, BRENDA, KEGG (queried 2.3.1.65)
taurochenodeoxycholate-degr/2_3.1.2.2_RXN-14289                                : 1.0 chenodeoxycholoyl-CoA + 1.0 H2O --> 1.0 coenzyme_A + 1.0 chenodeoxycholate + 1.0 H+  #
source: MetaCyc, BRENDA, KEGG (queried 3.1.2.2) // other EC numbers for this reaction: 3.1.2.27, 3.1.2.20
taurochenodeoxycholate-degr/3_manual_1.1.1.-_HD-ChChol                         : 1.0 chenodeoxycholate + 1.0 NADP+ --> 1.0 7-oxolithocholate + 1.0 NADPH + 1.0 H+

taurocholate-degr/1_moddir_2.3.1.65_RXN-9800                                   : 1.0 choloyl-CoA + 1.0 taurine <=> 1.0 coenzyme_A + 1.0 taurocholate + 1.0 H+  # source:
MetaCyc, BRENDA, KEGG (queried 2.3.1.65)
taurocholate-degr/2_manual_3.1.2.2_HD-3.1.2.2                                  : 1.0 choloyl-CoA + 1.0 H2O --> 1.0 coenzyme_A + 1.0 cholate + 1.0 H+
taurocholate-degr/3_manual_1.1.1.-_HD-Chol                                     : 1.0 cholate + 1.0 NADP+ --> 1.0 7-oxodeoxycholate + 1.0 NADPH + 1.0 H+

7-oxodeoxycholate_transport                                                    : 1.0 7-oxodeoxycholate + 1.0 H+ --> 1.0 7-oxodeoxycholate[ex] + H+[ex]
7-oxolithocholate_transport                                                    : 1.0 7-oxolithocholate + 1.0 H+ --> 1.0 7-oxolithocholate[ex] + H+[ex]
```

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taurine_transport                                                                                  : 1.0 taurine + 1.0 H+ --> 1.0 taurine[ex] + 1.0 H+[ex]

7-oxodeoxycholate_exchange                                                                         : 1.0 7-oxodeoxycholate[ex] -->
7-oxolithocholate_exchange                                                                         : 1.0 7-oxolithocholate[ex] -->
taurine_exchange                                                                                   : 1.0 taurine[ex] -->
##################################################################################################################################################################################
#choline degradation

choline_exchange                                                                                   : 1.0 choline[ex] <=>
choline_transport                                                                                  : 1.0 H+[ex] + 1.0 choline[ex] <=> 1.0 H+ + 1.0 choline
trimethylamine_exchange                                                                            : 1.0 trimethylamine[ex] <=>
trimethylamine_transport                                                                           : 1.0 H+[ex] + 1.0 trimethylamine[ex] <=> 1.0 H+ + 1.0 trimethylamine

choline-degradation-III_4.3.99.4_RXN-13946                                                         : 1.0 choline --> 1.0 trimethylamine + 1.0 acetaldehyde  # source: MetaCyc, BRENDA, KEGG
(queried 4.3.99.4)
##################################################################################################################################################################################
#D-arabinose degr
D-arabinose_exchange                                                                               : 1.0 D-arabinose[ex] <=>
##CDIF630erm_03311, CDIF630erm_03314; CDIF630erm_02563-CDIF630erm_02565
D-arabinose_transport_2.7.1.-                                                                      : 1.0 D-arabinose[ex] + 1.0 |PTS-I-pi-phospho-L-histidines| --> 1.0 |PTS-I-Histidines| + 1.0
aldehydo-D-arabinose_5-phosphate
D-arabinose-degr_5.3.1.13_DARAB5PISOM-RXN                                                          : 1.0 aldehydo-D-arabinose_5-phosphate <=> 1.0 D-ribulose_5-phosphate  # source: MetaCyc,
BRENDA, KEGG (queried 5.3.1.13)
##################################################################################################################################################################################
#xylose degr I/ xylan degr
#set ratio for chain length
xylan_exchange                                                                                     : 1.0 |Xylans|[ex] <=>
xylose_exchange                                                                                    : 1.0 alpha-D-xylopyranose[ex] <=>
##CDIF630erm_03350-CDIF630erm_03353
xylan_transport                                                                                    : 1.0 |Xylans| <=> 1.0 |Xylans|[ex]
xylose_transport_2.7.1.-                                                                           : 1.0 D-xylulose_5-phosphate + 1.0 |PTS-I-Histidines| <-- 1.0 alpha-D-xylopyranose[ex] + 1.0
|PTS-I-pi-phospho-L-histidines|

xylan-degradation_3.2.1.177_RXN0-5001                                                              : 1.0 |Xylans| + 1.0 H2O --> 1.0 alpha-D-xylopyranose  # source: MetaCyc (queried 3.2.1.177)
xylose-degradation-I/1_5.3.1.5_XYLISOM-RXN                                                         : 1.0 alpha-D-xylopyranose <=> 1.0 D-xylulose  # source: MetaCyc (queried 5.3.1.5)
xylose-degradation-I/2_2.7.1.17_XYLULOKIN-RXN                                                      : 1.0 ATP + 1.0 D-xylulose --> 1.0 ADP + 1.0 H+ + 1.0 D-xylulose_5-phosphate  # source:
MetaCyc, BRENDA, KEGG (queried 2.7.1.17)
##################################################################################################################################################################################
#galactose degradation I (Leloir-pathway)
galactose_exchange                                                                                 : 1.0 alpha-D-galactose[ex] <=>
##CDIF630erm_00408-CDIF630erm_00413; CDIF630erm_01218, CDIF630erm_01220-CDIF630erm_01222; CDIF630erm_03576-CDIF630erm_03579?
galactose_transport_2.7.1.-                                                                        : 1.0 alpha-D-galactose[ex] + 1.0 |PTS-I-pi-phospho-L-histidines| --> 1.0 |PTS-I-Histidines| +
1.0 alpha-D-galactose_1-phosphate

galactose-degr-I/1_2.7.7.12_GALACTURIDYLYLTRANS-RXN                                                : 1.0 alpha-D-galactose_1-phosphate + 1.0 UDP-alpha-D-glucose <=> 1.0 UDP-alpha-D-galactose +
1.0 alpha-D-glucopyranose_1-phosphate  # source: MetaCyc, BRENDA, KEGG (queried 2.7.7.12)
galactose-degr-I/2_5.1.3.2_UDPGLUCEPIM-RXN                                                         : 1.0 UDP-alpha-D-glucose <=> 1.0 UDP-alpha-D-galactose  # source: MetaCyc, BRENDA, KEGG
(queried 5.1.3.2)
galactose-degr-I/3_spontaneous_RXN-10639                                                           : 1.0 alpha-D-glucopyranose_1-phosphate <=> 1.0 beta-D-glucose_1-phosphate  # source: MetaCyc
##################################################################################################################################################################################
#xylitol degr A
xylitol_exchange                                                                                   : 1.0 xylitol[ex] <=>
#CDIF630erm_02563-CDIF630erm_02565
xylitol_transport                                                                                  : 1.0 |PTS-I-pi-phospho-L-histidines| + 1.0 xylitol[ex] --> 1.0 xylitol_5-phosphate + 1.0 |
PTS-I-Histidines|
xylitol-degr_manual_1.1.1.-_HD-xyl5                                                                : 1.0 NAD+ + 1.0 xylitol_5-phosphate <=> 1.0 D-xylulose_5-phosphate + 1.0 NADH + 1.0 H+

#xylitol degr B
##CDIF630erm_02515-CDIF630erm_02517
xylitol_transport_2.7.1.-                                                                          : 1.0 |PTS-I-pi-phospho-L-histidines| + 1.0 xylitol[ex] --> 1.0 xylitol_1-phosphate + 1.0 |
PTS-I-Histidines|
xylitol-degr_manual_1.1.1.-_HD-xyl1                                                                : 1.0 NAD+ + 1.0 xylitol_1-phosphate <=> 1.0 D-xylulose_5-phosphate + 1.0 NADH + 1.0 H+
xylulose-degradation/1_5.1.3.4_RIBULPEPIM-RXN                                                      : 1.0 L-ribulose_5-phosphate <=> 1.0 D-xylulose_5-phosphate  # source: MetaCyc, BRENDA, KEGG
(queried 5.1.3.4)
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#########################################################################################################################################################################################
#arabitol degr
#arabitol degr
arabitol_exchange                                                                                   : 1.0 D-arabitol[ex] <=>
##CDIF630erm_02563 - CDIF630erm_02565
arabitol_transport                                                                                  : 1.0 |PTS-I-pi-phospho-L-histidines| + 1.0 D-arabitol[ex] --> 1.0 D-arabitol_1-phosphate +
1.0 |PTS-I-Histidines|

arabitol-degr_1.1.1.301_RXN-11106                                                                   : 1.0 D-arabitol_1-phosphate + 1.0 NAD+ <=> 1.0 H+ + 1.0 NADH + 1.0 D-xylulose_5-phosphate  #
source: MetaCyc, BRENDA, KEGG (queried 1.1.1.301)
#########################################################################################################################################################################################
#ribitol degr
ribitol_exchange                                                                                    : 1.0 D-ribitol[ex] <=>
##CCDIF630erm_00620-CDIF630erm_00623
ribitol_transport_2.7.1.-                                                                           : 1.0 |PTS-I-pi-phospho-L-histidines| + 1.0 D-ribitol[ex] --> 1.0 D-ribitol_5-phosphate + 1.0
|PTS-I-Histidines|  # source: MetaCyc (queried 2.7.1.69)

ribitol-degr_1.1.1.137_RIBITOL-5-PHOSPHATE-2-DEHYDROGENASE-RXN_WOP                                  : 1.0 D-ribitol_5-phosphate + 1.0 NAD+ <=> 1.0 H+ + 1.0 D-ribulose_5-phosphate + 1.0 NADH  #
source: MetaCyc, BRENDA, KEGG (queried 1.1.1.137)
#########################################################################################################################################################################################
#D-sorbitol degradation II
D-sorbitol_exchange                                                                                 : 1.0 D-sorbitol[ex] <=>
##CDIF630erm_00882-CDIF630erm_00885
D-sorbitol_transport_2.7.1.198                                                                      : 1.0 D-sorbitol[ex] + 1.0 |PTS-I-pi-phospho-L-histidines| --> 1.0 D-sorbitol_6-phosphate +
1.0 |PTS-I-Histidines|

D-sorbitol-degradation-II_1.1.1.140_SORB6PDEHYDROG-RXN                                              : 1.0 NAD+ + 1.0 D-sorbitol_6-phosphate <=> 1.0 beta-D-fructofuranose_6-phosphate + 1.0 NADH +
1.0 H+  # source: MetaCyc, BRENDA, KEGG (queried 1.1.1.140)

sorbitol-biosyn_1.1.1.17_BS257116                                                                   : 1.0 NAD+ + 1.0 D-sorbitol_6-phosphate <-- 1.0 NADH + 1.0 H+ + 1.0 D-glucose_6-phosphate  #
source: BRENDA (queried 1.1.1.17)
#########################################################################################################################################################################################
#mannitol degradation I
D-mannitol_exchange                                                                                 : 1.0 D-mannitol[ex] <=>
##CDIF630erm_02571, CDIF630erm_02573
mannitol_transport_2.7.1.197                                                                        : 1.0 |PTS-I-pi-phospho-L-histidines| + 1.0 D-mannitol[ex] --> 1.0 D-mannitol_1-phosphate +
1.0 |PTS-I-Histidines|

mannitol-degradation-I_1.1.1.17_MANNPDEHYDROG-RXN                                                   : 1.0 NAD+ + 1.0 D-mannitol_1-phosphate <=> 1.0 NADH + 1.0 H+ + 1.0 beta-D-fructofuranose_6-
phosphate  # source: MetaCyc, BRENDA, KEGG (queried 1.1.1.17)
#########################################################################################################################################################################################
#D-ribofuranose and 2'-deoxyribose degr C
D-ribopyranose_exchange                                                                             : 1.0 beta-D-ribopyranose[ex] <=>
2'-deoxyribose_exchange                                                                             : 1.0 2'-deoxyribose[ex] <=>
##CDIF630erm_00425-CDIF630erm_00427
D-ribopyranose_transport                                                                            : 1.0 ATP + 1.0 H2O + 1.0 beta-D-ribopyranose[ex] --> 1.0 ADP + 1.0 phosphate + 1.0 H+ + 1.0
beta-D-ribopyranose
2'-deoxyribose_transport                                                                            : 1.0 ATP + 1.0 H2O + 1.0 2'-deoxyribose[ex] --> 1.0 ADP + 1.0 phosphate + 1.0 H+ + 1.0 2'-
deoxyribose

2'-deoxyribose-degradation_2.7.1.15_RXN-14223                                                       : 1.0 2'-deoxyribose + 1.0 ATP --> 1.0 H+ + 1.0 ADP + 1.0 2-deoxy-D-ribose_5-phosphate  #
source: MetaCyc, BRENDA, KEGG (queried 2.7.1.15)
#########################################################################################################################################################################################
#maltose degradation
maltose_exchange                                                                                    : 1.0 alpha-maltose[ex] <=>
##CDIF630erm_00981-CDIF630erm_00983;CDIF630erm_02759, CDIF630erm_02761; CDIF630erm_03341, CDIF630erm_03344
maltose_transport_2.7.1.208                                                                         : 1.0 alpha-maltose[ex] + 1.0 |PTS-I-pi-phospho-L-histidines| --> 1.0 alpha-maltose_6'-
phosphate + 1.0 |PTS-I-Histidines|

maltose-degr_3.2.1.122_MALTOSE-6-PHOSPHATE-GLUCOSIDASE-RXN                                          : 1.0 H2O + 1.0 alpha-maltose_6'-phosphate --> 1.0 D-glucose + 1.0 D-glucose_6-phosphate  #
source: MetaCyc, BRENDA, KEGG (queried 3.2.1.122)
#########################################################################################################################################################################################
#sucrose degradation I
sucrose_exchange                                                                                    : 1.0 sucrose[ex] <=>
```

```
##CDIF630erm_00597
sucrose_transport                                                                : 1.0 |PTS-I-pi-phospho-L-histidines| + 1.0 sucrose[ex] --> 1.0 sucrose_6-phosphate + 1.0 |
PTS-I-Histidines|

sucrose-degradation-I/1_3.2.1.B3_BR49793                                         : 1.0 sucrose_6-phosphate + 1.0 H2O --> 1.0 beta-D-fructofuranose + 1.0 alpha-D-glucose_6-
phosphate  # source: BRENDA, KEGG (queried 3.2.1.B3) // other EC numbers for this reaction: 3.2.1.26
sucrose-degradation-I/2a_2.7.1.4_FRUCTOKINASE-RXN                                : 1.0 ATP + 1.0 beta-D-fructofuranose --> 1.0 ADP + 1.0 beta-D-fructofuranose_6-phosphate +
1.0 H+  # source: MetaCyc, KEGG (queried 2.7.1.4) // other EC numbers for this reaction: 2.7.1.1
sucrose-degradation-I/2b_5.3.1.5_BS1055                                          : 1.0 D-glucose <-- 1.0 beta-D-fructofuranose  # source: BRENDA, KEGG (queried 5.3.1.5)

glucose-iso_5.3.1.9_R02740                                                       : 1.0 alpha-D-glucose_6-phosphate <=> 1.0 beta-D-fructofuranose_6-phosphate  # source: KEGG
(queried 5.3.1.9)
glucose-iso_5.1.3.15_5.3.1.9_spontaneous_GLUCOSE-6-PHOSPHATE-1-EPIMERASE-RXN     : 1.0 alpha-D-glucose_6-phosphate <=> 1.0 beta-D-glucose_6-phosphate  # source: MetaCyc,
BRENDA, KEGG (queried 5.1.3.15, 5.3.1.9)
################################################################################################################################################################
#D-tagatose degradation
D-tagatose_exchange                                                              : 1.0 D-tagatose[ex] <=>
##CDIF630erm_03358
D-tagatose_transport                                                             : 1.0 D-tagatose[ex] + 1.0 |PTS-I-pi-phospho-L-histidines| --> 1.0 |PTS-I-Histidines| + 1.0 D-
tagatose_1-phosphate
#CDIF630erm_03359
D-tagatose-degr/1_manual_2.7.1.-_HD-tag                                          : 1.0 D-tagatose_1-phosphate + 1.0 ATP --> 1.0 H+ + 1.0 ADP + 1.0 D-tagatofuranose_1,6-
bisphosphate
D-tagatose-degr/_4.1.2.40_TAGAALDOL-RXN                                          : 1.0 D-tagatofuranose_1,6-bisphosphate <=> 1.0 D-glyceraldehyde_3-phosphate + 1.0
glycerone_phosphate  # source: MetaCyc, BRENDA, KEGG (queried 4.1.2.40)
################################################################################################################################################################
#fructose degr
D-fructofuranose_exchange                                                        : 1.0 beta-D-fructofuranose[ex] <=>
##CDIF630erm_02503
fructose_transport_2.7.1.202                                                     : 1.0 |PTS-I-pi-phospho-L-histidines| + 1.0 beta-D-fructofuranose[ex] --> 1.0 beta-D-
fructofuranose_1-phosphate + 1.0 |PTS-I-Histidines|
fructose-degradation_2.7.1.56_1PFRUCTPHOSN-RXN                                   : 1.0 beta-D-fructofuranose_1-phosphate + 1.0 ATP --> 1.0 ADP + 1.0 fructose_1,6-bisphosphate
+ 1.0 H+  # source: MetaCyc, BRENDA (queried 2.7.1.56)
################################################################################################################################################################
#alternative 1-deoxy-D-xylulose_5-phosphate biosynthsis
1-deoxy-D-xylulose_5-phosphate-biosyn/1_4.1.2.13_RXN-8631                        : 1.0 beta-D-fructofuranose_1-phosphate --> 1.0 D-glyceraldehyde + 1.0 glycerone_phosphate  #
source: MetaCyc, BRENDA (queried 4.1.2.13)
1-deoxy-D-xylulose_5-phosphate-biosyn/2a_1.2.1.3_BS426217                        : 1.0 D-glyceraldehyde + 1.0 NAD+ + 1.0 H2O <=> 1.0 NADH + 1.0 D-glycerate + 1.0 H+  # source:
BRENDA, KEGG (queried 1.2.1.3)
1-deoxy-D-xylulose_5-phosphate-biosyn/2b_2.2.1.7_BS260855                        : 1.0 D-glyceraldehyde + 1.0 pyruvate --> 1.0 CO2 + 1.0 1-deoxy-D-xylulose  # source: BRENDA
(queried 2.2.1.7)
1-deoxy-D-xylulose_5-phosphate-biosyn/3_2.7.1.17_RXN0-382                        : 1.0 1-deoxy-D-xylulose + 1.0 ATP --> 1.0 ADP + 1.0 1-deoxy-D-xylulose_5-phosphate + 1.0 H+
# source: MetaCyc, BRENDA (queried 2.7.1.17) // other EC numbers for this reaction: 2.7.1
################################################################################################################################################################
#cellobiose degr C
D-cellobiose_exchange                                                            : 1.0 beta-D-cellobiose[ex] <=>
##CDIF630erm_03148; CDIF630erm_03151; CDIF630erm_03151
cellobiose_transport_2.7.1.205                                                   : 1.0 beta-D-cellobiose[ex] + 1.0 |PTS-I-pi-phospho-L-histidines| --> 1.0 6-phospho-beta-D-
glucosyl-(1,4)-D-glucose + 1.0 |PTS-I-Histidines|
cellobiose-degr_3.2.1.86_6-PHOSPHO-BETA-GLUCOSIDASE-RXN                          : 1.0 6-phospho-beta-D-glucosyl-(1,4)-D-glucose + 1.0 H2O --> 1.0 D-glucose + 1.0 D-glucose_6-
phosphate  # source: MetaCyc, BRENDA, KEGG (queried 3.2.1.86)
################################################################################################################################################################
#chitobiose degradation
chitobiose_exchange                                                              : 1.0 N,N'-diacetylchitobiose[ex] <=>
##CDIF630erm_03148; CDIF630erm_03151; CDIF630erm_03151
chitobiose_transport_2.7.1.196                                                   : 1.0 N,N'-diacetylchitobiose[ex] + 1.0 |PTS-I-pi-phospho-L-histidines| --> 1.0 |PTS-I-
Histidines| + 1.0 N,N'-diacetylchitobiose_6'-phosphate  # source: MetaCyc (queried 2.7.1.69)

chitobiose-degradation_3.5.1.105_RXN0-7001                                       : 1.0 H2O + 1.0 N,N'-diacetylchitobiose_6'-phosphate --> 1.0 acetate + 1.0 N-
monoacetylchitobiose_6'-phosphate  # source: MetaCyc (queried 3.5.1.105)
chitobiose-degradation_3.2.1.86_RXN0-7002                                        : 1.0 H2O + 1.0 N-monoacetylchitobiose_6'-phosphate --> 1.0 N-acetyl-D-glucosamine_6-phosphate
+ 1.0 D-glucosamine  # source: MetaCyc (queried 3.2.1.86)
#assumed to be side reaction of 2.7.1.59
chitobiose-degradation_2.7.1.59_GLUCOSAMINE-KINASE-RXN                           : 1.0 D-glucosamine + 1.0 ATP --> 1.0 D-glucosamine_6-phosphate + 1.0 ADP + 1.0 H+  # source:
```

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MetaCyc, BRENDA, KEGG (queried 2.7.1.8) // other EC numbers for this reaction: 2.7.1.1
#########################################################################################################################################################################
#trehalose degr I
trehalose_exchange                                                                    : 1.0 alpha,alpha-trehalose[ex] <=>
#CDIF630erm_03371-CDIF630erm_03372?
trehalose_transport                                                                   : 1.0 |PTS-I-pi-phospho-L-histidines| + 1.0 alpha,alpha-trehalose[ex] --> 1.0 |PTS-I-
Histidines| + 1.0 alpha,alpha-trehalose_6-phosphate

trehalose-degr-I_3.2.1.122_3.2.1.93_TRE6PHYDRO-RXN                                    : 1.0 alpha,alpha-trehalose_6-phosphate + 1.0 H2O --> 1.0 D-glucose_6-phosphate + 1.0 D-
glucose  # source: MetaCyc, BRENDA, KEGG (queried 3.2.1.122, 3.2.1.93)
#########################################################################################################################################################################
#sugars polymers

cyclodextrin_exchange                                                                 : 1.0 |Cyclodextrins|[ex] <=>
starch_exchange                                                                       : 1.0 |Starch|[ex] <=>
maltodextrin_exchange                                                                 : 1.0 |Maltodextrin|[ex] <=>
pullulan_exchange                                                                     : 1.0 |Pullulans|[ex] <=>
maltotriose_exchange                                                                  : 1.0 maltotriose[ex] <=>

cyclodextrin-degr_3.2.1.54_CYCLOMALTODEXTRINASE-RXN                                   : 1.0 H2O + 1.0 |Cyclodextrins|[ex] --> 1.0 |Maltodextrins|[ex]  # source: MetaCyc, BRENDA,
KEGG (queried 3.2.1.54) // other EC numbers for this reaction: 2.4.1.19
starch-degr_manual_2.4.1.18_3.2.1.41_3.2.1.1_HD-starch                                : 1.0 |Starch|[ex] + 1.0 H2O[ex] --> 1.0 |Maltodextrins|[ex]
maltodextrin-degr_3.2.1.133_3.2.1.1_RXN-12188                                         : 1.0 |Maltodextrins|[ex] + 1.0 H2O[ex] --> 1.0 D-glucose[ex] + 1.0 alpha,alpha-trehalose[ex]
# source: MetaCyc, BRENDA (queried 3.2.1.133, 3.2.1.1) // there are 4 more EC numbers for this reaction
pullulan-degr_3.2.1.54_3.2.1.41_RXN-12302                                             : 1.0 |Pullulans|[ex] + 1.0 H2O[ex] --> 2.0 maltotriose[ex]  # source: MetaCyc, BRENDA
(queried 3.2.1.54, 3.2.1.41) // other EC numbers for this reaction: 3.2.1.135
maltotriose-degr_modnames_3.2.1.10_R06199                                             : 2.0 H2O + 1.0 maltotriose[ex] --> 3.0 D-glucose[ex]  # source: KEGG (queried 3.2.1.10) //
other EC numbers for this reaction: 3.2.1.3
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#N-acetylneuraminate and N-acetylmannosamine degradation
N-acetylneuraminate_exchange                                                          : 1.0 N-acetylneuraminate[ex] <=>
##CDIF630erm_02472
N-acetylneuraminate_transport                                                         : 1.0 N-acetyl-beta-neuraminate + 1.0 Na+ <=> 1.0 N-acetylneuraminate[ex] + 1.0 Na+[ex]

N-acetylneur-degr/1_4.1.3.3_ACNEULY-RXN                                               : 1.0 N-acetyl-beta-neuraminate <=> 1.0 |N-acetyl-D-mannosamine| + 1.0 pyruvate  # source:
MetaCyc, BRENDA, KEGG (queried 4.1.3.3)
N-acetylneur-degr/2_2.7.1.59_NANK-RXN                                                 : 1.0 ATP + 1.0 |N-acetyl-D-mannosamine| --> 1.0 ADP + 1.0 N-acetyl-D-mannosamine_6-phosphate
+ 1.0 H+  # source: MetaCyc, BRENDA, KEGG (queried 2.7.1.59) // other EC numbers for this reaction: 2.7.1.60
N-acetylneur-degr/3_5.1.3.9_NANE-RXN                                                  : 1.0 N-acetyl-D-mannosamine_6-phosphate <=> 1.0 N-acetyl-D-glucosamine_6-phosphate  # source:
MetaCyc, BRENDA, KEGG (queried 5.1.3.9)
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#D-galactosamine and N-acetyl-D-galactosamine degradation
N-acetyl-D-galactosamine_exchange                                                     : 1.0 |N-acetyl-D-galactosamine|[ex]<=>
D-galactosamine_exchange                                                              : 1.0 D-galactosamine[ex] <=>
##CDIF630erm_00408-CDIF630erm_00413; CDIF630erm_01218, CDIF630erm_01220-CDIF630erm_01222; CDIF630erm_03576-CDIF630erm_03579?
N-acetyl-D-galactosamine_transport                                                    : 1.0 |PTS-I-pi-phospho-L-histidines| + 1.0 |N-acetyl-D-galactosamine| --> 1.0 |PTS-I-
Histidines| + 1.0 N-acetyl-D-galactosamine_6-phosphate
D-galactosamine_transport                                                             : 1.0 D-Galactosamine[ex] + 1.0 |PTS-I-pi-phospho-L-histidines| --> 1.0 D-galactosamine_6-
phosphate + 1.0 |PTS-I-Histidines|  # source: MetaCyc (queried 2.7.1.69)

(N-acetyl-)D-galactosamine-degr/1_3.5.1.25_3.5.1.80-RXN                               : 1.0 N-acetyl-D-galactosamine_6-phosphate + 1.0 H2O --> 1.0 acetate + 1.0 D-galactosamine_6-
phosphate  # source: MetaCyc, BRENDA, KEGG (queried 3.5.1.25)
(N-acetyl-)D-galactosamine-degr/2_5.3.1.-_RXN-13548                                   : 1.0 D-galactosamine_6-phosphate + 1.0 H2O --> 1.0 ammonium + 1.0 D-tagatofuranose_6-
phosphate  # source: MetaCyc, KEGG (queried 5.3.1.-) // other EC numbers for this reaction: 5.3.1, 3.5.99
(N-acetyl-)D-galactosamine-degr/3_2.7.1.11_2.7.1.144_2.7.1.56_TAGAKIN-RXN             : 1.0 D-tagatofuranose_6-phosphate + 1.0 ATP --> 1.0 ADP + 1.0 H+ + 1.0 D-tagatofuranose_1,6-
bisphosphate  # source: MetaCyc, BRENDA, KEGG (queried 2.7.1.11, 2.7.1.144, 2.7.1.56)
#########################################################################################################################################################################
#D-glucosaminate-degradation
D-glucosaminate_exchange                                                              : 1.0 D-glucosaminate[ex] <=>
##CDIF630erm_00408-CDIF630erm_00413; CDIF630erm_01218, CDIF630erm_01220-CDIF630erm_01222; CDIF630erm_03576-CDIF630erm_03579?
D-glucosaminate_transport                                                             : 1.0 |PTS-I-pi-phospho-L-histidines| + 1.0 D-glucosaminate[ex] --> 1.0 D-glucosaminate_6-
phosphate + 1.0 |PTS-I-Histidines|  # source: MetaCyc (queried 2.7.1.69)

D-glucosaminate-degr/1_4.3.1.29_RXN-14730                                             : 1.0 D-glucosaminate_6-phosphate --> 1.0 ammonium + 1.0 2-dehydro-3-deoxy-D-gluconate_6-
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phosphate  # source: MetaCyc, BRENDA, KEGG (queried 4.3.1.29)
D-glucosaminate-degr/2_2.7.1.45_DEOXYGLUCONOKIN-RXN                                    : 1.0 2-dehydro-3-deoxy-D-gluconate + 1.0 ATP --> 1.0 ADP + 1.0 2-dehydro-3-deoxy-D-
gluconate_6-phosphate + 1.0 H+  # source: MetaCyc, BRENDA, KEGG (queried 2.7.1.45) // other EC numbers for this reaction: 2.7.1.178
D-glucosaminate-degr/3_4.1.2.14_KDPGALDOL-RXN                                          : 1.0 2-dehydro-3-deoxy-D-gluconate_6-phosphate --> 1.0 pyruvate + 1.0 D-glyceraldehyde_3-
phosphate  # source: MetaCyc, BRENDA, KEGG (queried 4.1.2.14) // other EC numbers for this reaction: 4.1.2.20, 4.1.2.55
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#2-O-alpha-mannosyl-D-glycerate degradation C
2-O-alpha-mannosyl-D-glycerate_exchange                                                : 1.0 2-O-alpha-mannosyl-D-glycerate[ex] <=>
##CDIF630erm_03369; CDIF630erm_02819-CDIF630erm_02821
2-O-alpha-mannosyl-D-glycerate_transport_2.7.1.195                                     : 1.0 2-O-alpha-mannosyl-D-glycerate[ex] + 1.0 |PTS-I-pi-phospho-L-histidines| --> 1.0 2-O-(6-
phospho-alpha-D-mannosyl)-D-glycerate + 1.0 |PTS-I-Histidines|  # source: MetaCyc (queried 2.7.1.69)

2-O-alpha-mannosyl-D-glycerate-degr_3.2.1.170_RXN0-5216                                : 1.0 H2O + 1.0 2-O-(6-phospho-alpha-D-mannosyl)-D-glycerate --> 1.0 D-glycerate + 1.0 D-
mannopyranose_6-phosphate  # source: MetaCyc (queried 3.2.1.170)
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#altronate and 2-dehydro-3-deoxy-D-gluconate degradation
D-altronate_exchange                                                                   : 1.0 D-altronate <=>
2-dehydro-3-deoxy-D-gluconate_exchange                                                 : 1.0 2-dehydro-3-deoxy-D-gluconate <=>
##CDIF630erm_03138
2-dehydro-3-deoxy-D-gluconate_transport                                                : 1.0 2-dehydro-3-deoxy-D-gluconate + 1.0 Na+ <=> 1.0 2-dehydro-3-deoxy-D-gluconate[ex] + 1.0
Na+[ex]
D-altronate_transport                                                                  : 1.0 D-altronate + 1.0 Na+ <=> 1.0 D-altronate[ex] + 1.0 Na+[ex]
D-altronate-degr_4.2.1.7_ALTRODEHYDRAT-RXN                                             : 1.0 D-altronate --> 1.0 H2O + 1.0 2-dehydro-3-deoxy-D-gluconate  # source: MetaCyc, BRENDA,
KEGG (queried 4.2.1.7)
#########################################################################################################################################################
riboflavin_exchange                                                          : 1.0 riboflavin[ex] <=>
##CDIF630erm_00266
riboflavin_transport                                                         : 1.0 H2O + 1.0 ATP + 1.0 riboflavin[ex] --> 1.0 H+ + 1.0 phosphate + 1.0 ADP + 1.0 riboflavin
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#adenosylcobalamin salvage from cobinamide
cobinamide_exchange                                                          : 1.0 cobinamide[ex] <=>
coenzyme-B12_exchange                                                        : 1.0 adenosylcobalamin[ex] <=>

coenzyme-B12_transport_3.6.3.33                                              : 1.0 ATP + 1.0 adenosylcobalamin[ex] + 1.0 H2O --> 1.0 ADP + 1.0 phosphate + 1.0 adenosylcobalamin +
1.0 H+ # source: BRENDA (queried 3.6.3.33)
cobinamide_transport_3.6.3.33                                                : 1.0 ATP + 1.0 cobinamide[ex] + 1.0 H2O --> 1.0 ADP + 1.0 phosphate + 1.0 cobinamide + 1.0 H+ #
source: BRENDA (queried 3.6.3.33)

adenosylcobalamin-salvage-from-cobinamide/1_2.5.1.17_BTUR2-RXN               : 1.0 ATP + 1.0 cobinamide --> 1.0 adenosylcobinamide + 1.0 PPPi  # source: MetaCyc, BRENDA, KEGG
(queried 2.5.1.17)
adenosylcobalamin-salvage-from-cobinamide/2_2.7.1.156_COBINAMIDEKIN-RXN      : 1.0 adenosylcobinamide + 1.0 ATP --> 1.0 ADP + 1.0 adenosyl-cobinamide_phosphate + 1.0 H+  # source:
MetaCyc, BRENDA, KEGG (queried 2.7.1.156)
#########################################################################################################################################################
#dethiobiotin
dethiobiotin_exchange                                                  : 1.0 dethiobiotin[ex] <=>
##CDIF630erm_03256
dethiobiotin_transport                                                 : 1.0 ATP + 1.0 dethiobiotin[ex] + 1.0 H2O --> 1.0 ADP + 1.0 phosphate + 1.0 dethiobiotin + 1.0 H+ # source:
BRENDA (queried 3.6.3.33)

biotin-biosynthesis_2.8.1.7_RXN-12588                                  : 1.0 |Unsulfurated-Sulfur-Acceptors| + 1.0 L-cysteine --> 1.0 |Sulfurated-Sulfur-Acceptors| + 1.0 L-alanine
# source: MetaCyc (queried 2.8.1.7)
biotin-biosynthesis_modnames_2.8.1.6_2.8.1.6-RXN                       : 1.0 |Sulfurated-Sulfur-Acceptors| + 2.0 |Reduced-Ferredoxins| + 2.0 S-adenosyl-L-methionine + 1.0
dethiobiotin --> 2.0 L-methionine + 2.0 5'-deoxyadenosine + 1.0 biotin + 1.0 |Unsulfurated-Sulfur-Acceptors| + 2.0 |Oxidized-Ferredoxins|  # source: MetaCyc (queried 2.8.1.6)
#########################################################################################################################################################
#formylaminopyrimidine
formylaminopyrimidine_exchange                                         : 1.0 formylaminopyrimidine[ex] <=>
formylaminopyrimidine_transport                                        : 1.0 ATP + 1.0 formylaminopyrimidine[ex] + 1.0 H2O --> 1.0 ADP + 1.0 phosphate + 1.0 formylaminopyrimidine
+ 1.0 H+ # source: BRENDA (queried 3.6.3.33)

base-degraded-thiamine-salvage_3.5.1.-_RXN-12612                       : 1.0 formylaminopyrimidine + 1.0 H2O --> 1.0 aminomethylpyrimidine + 1.0 formate  # source: MetaCyc
(queried 3.5.1.-) // other EC numbers for this reaction: 3.5.1
base-degraded-thiamine-salvage_3.5.99.2_RXN-12613                      : 1.0 H2O + 1.0 aminomethylpyrimidine --> 1.0 4-amino-2-methyl-5-pyrimidinemethanol + 1.0 ammonium  #
source: MetaCyc, BRENDA, KEGG (queried 3.5.99.2)
#########################################################################################################################################################
```

```
#sulfolactate
sulfolactate_exchange                                                : 1.0 (2R)-3-sulfolactate <=>
##CDIF630erm_03289
sulfolactate_transport                                               : 1.0 (2R)-3-sulfolactate + 1.0 Na+ <=> 1.0 (2R)-3-sulfolactate[ex] + 1.0 Na+[ex]

sulfolactate-degr/1_4.4.1.24_RXN-11691                               : 1.0 (2R)-3-sulfolactate --> 1.0 H+ + 1.0 pyruvate + 1.0 sulfite  # source: MetaCyc, BRENDA (queried
4.4.1.24)
sulfolactate-degr/2_spontaneous_RXN-8315                             : 1.0 H+ + 1.0 sulfite <=> 1.0 hydrogen_sulfite  # source: MetaCyc
#######################################################################################################################################################################
#cyclic_di-3',5'-guanylate
cGDP_2.7.7.65_RXN0-5359                                              : 2.0 GTP --> 2.0 diphosphate + 1.0 cyclic_di-3',5'-guanylate  # source: MetaCyc, BRENDA, KEGG (queried
2.7.7.65)
cGDP_3.1.4.52_RXN0-4181                                              : 1.0 H2O + 1.0 cyclic_di-3',5'-guanylate --> 1.0 H+ + 1.0 linear_dimeric_GMP  # source: MetaCyc, BRENDA,
KEGG (queried 3.1.4.52)
#######################################################################################################################################################################


#Reactions without pathway
#############1.1.1.1#############
~no-pathway_1.1.1.1_RXN-6021                                                                         : 1.0 NAD+ + 1.0 choline --> 1.0 NADH + 1.0
betaine_aldehyde + 1.0 H+  # source: MetaCyc, KEGG (queried 1.1.1.1) // other EC numbers for this reaction: 1.1.1
~no-pathway_1.1.1.1_RXN-12582                                                                        : 1.0 choline + 1.0 NADP+ <=> 1.0 betaine_aldehyde + 1.0
NADPH + 1.0 H+  # source: MetaCyc, KEGG (queried 1.1.1.1) // other EC numbers for this reaction: 1.1.1
#############1.1.1.22#############
~no-pathway_1.1.1.22_UGD-RXN                                                                         : 2.0 NAD+ + 1.0 UDP-alpha-D-glucose + 1.0 H2O --> 1.0 UDP-
alpha-D-glucuronate + 3.0 H+ + 2.0 NADH  # source: MetaCyc, BRENDA, KEGG (queried 1.1.1.22)
#############1.2.1.3#############
~no-pathway_1.2.1.3_RXN-4142                                                                         : 1.0 H2O + 1.0 NAD+ + 1.0 |Fatty-Aldehydes| --> 1.0 |
Fatty-Acids| + 2.0 H+ + 1.0 NADH  # source: MetaCyc, BRENDA (queried 1.2.1.3) // other EC numbers for this reaction: 1.2.1.48
~no-pathway_1.2.1.3_AMINOBUTDEHYDROG-RXN                                                             : 1.0 NAD+ + 1.0 4-aminobutanal + 1.0 H2O --> 1.0 4-
aminobutanoate + 2.0 H+ + 1.0 NADH  # source: MetaCyc, BRENDA, KEGG (queried 1.2.1.3) // other EC numbers for this reaction: 1.2.1.19, 1.2.1
#############1.1.1.86#############
~no-pathway_1.1.1.86_R04440                                                                          : 1.0 (2R)-2,3-dihydroxy-3-methylbutanoate + 1.0 NADP+ <=>
1.0 NADPH + 1.0 H+ + 1.0 3-hydroxy-3-methyl-2-oxobutanoate  # source: KEGG (queried 1.1.1.86)
#############1.5.1.49#############
~no-pathway_1.5.1.49_PYRROLINE-2-CARBOXYLATE-REDUCTASE-RXN                                           : 1.0 L-proline + 1.0 NADP+ <-- 2.0 H+ + 1.0 1-pyrroline-2-
carboxylate + 1.0 NADPH  # source: MetaCyc, BRENDA, KEGG (queried 1.5.1.49) // other EC numbers for this reaction: 1.5.1.1, 1.5.1.21
~no-pathway_1.5.1.49_PYRROLINE-2-CARBOXYLATE-REDUCTASE-RXN_WOP                                       : 1.0 L-proline + 1.0 NAD+ <=> 2.0 H+ + 1.0 NADH + 1.0 1-
pyrroline-2-carboxylate  # source: MetaCyc, BRENDA, KEGG (queried 1.5.1.49) // other EC numbers for this reaction: 1.5.1.1
#############1.8.1.14#############
~no-pathway_1.8.1.14_COA-DISULFIDE-REDUCTASE-NADH-RXN                                                : 1.0 NADP+ + 2.0 coenzyme_A <=> 1.0 CoA-disulfide + 1.0 H+
+ 1.0 NADPH  # source: MetaCyc, BRENDA, KEGG (queried 1.8.1.14)
#############2.1.1.79#############
~no-pathway_2.1.1.79_2.1.1.79-RXN                                                                    : 1.0 S-adenosyl-L-methionine + 1.0 |Phospholipid-Olefinic-
Fatty-Acids| --> 1.0 H+ + 1.0 S-adenosyl-L-homocysteine + 1.0 |Phospholipid-Cyclopropane-Fatty-Acids|  # source: MetaCyc (queried 2.1.1.79)
#############2.3.1.181#############
~no-pathway_2.3.1.181_RXN0-947                                                                       : 1.0 |Octanoyl-ACPs| + 1.0 |Lipoyl-Protein-L-Lysine| -->
1.0 |Octanoylated-domains| + 1.0 Acyl-carrier_protein + 1.0 H+  # source: MetaCyc (queried 2.3.1.181)
#############2.3.1.79#############
~no-pathway_2.3.1.79_MALTACETYLTRAN-RXN                                                              : 1.0 acetyl-CoA + 1.0 alpha,alpha-trehalose <=> 1.0
coenzyme_A + 1.0 6-O-acetyl-alpha-D-glucopyranosyl-(1rarr4)-D-glucose  # source: MetaCyc, BRENDA, KEGG (queried 2.3.1.79)
#############2.5.1.17#############
~no-pathway_2.5.1.17_COBALADENOSYLTRANS-RXN                                                          : 1.0 cob(I)alamin + 1.0 ATP --> 1.0 adenosylcobalamin +
1.0 PPPi  # source: MetaCyc, BRENDA, KEGG (queried 2.5.1.17)
#############2.5.1.49#############
~no-pathway_2.5.1.49_O-ACETYLHOMOSERINE-THIOL-LYASE-RXN                                              : 1.0 methanethiol + 1.0 O-acetyl-L-homoserine --> 1.0
acetate + 1.0 L-methionine + 1.0 H+  # source: MetaCyc, BRENDA, KEGG (queried 2.5.1.49)
#############2.7.1.33#############
~no-pathway_2.7.1.33_PANTETHEINE-KINASE-RXN                                                          : 1.0 pantetheine + 1.0 ATP --> 1.0 ADP + 1.0 4'-
phosphopantetheine + 1.0 H+  # source: MetaCyc, BRENDA, KEGG (queried 2.7.1.33) // other EC numbers for this reaction: 2.7.1.34
~no-pathway_2.7.1.33_R04391                                                                          : 1.0 ATP + 1.0 N-[(R)-pantothenoyl]-L-cysteine --> 1.0 R-
4'-phosphopantothenoyl-L-cysteine + 1.0 ADP  # source: KEGG (queried 2.7.1.33)
#############2.7.1.49#############
~no-pathway_2.7.1.49_2.7.1.35_PYRAMKIN-RXN                                                           : 1.0 pyridoxamine + 1.0 ATP --> 1.0 H+ + 1.0 ADP + 1.0
```

```
pyridoxamine_5'-phosphate  # source: MetaCyc, BRENDA, KEGG (queried 2.7.1.49, 2.7.1.35)
~no-pathway_2.7.1.35_PYRIDOXKIN-RXN                                                                         : 1.0 pyridoxal + 1.0 ATP --> 1.0 H+ + 1.0 ADP + 1.0
pyridoxal_5'-phosphate  # source: MetaCyc, BRENDA, KEGG (queried 2.7.1.35)
#############2.7.1.66#############
~no-pathway_2.7.1.66_UNDECAPRENOL-KINASE-RXN                                                                : 1.0 di-trans,octa-cis-undecaprenol + 1.0 ATP --> 1.0 ADP
+ 1.0 di-trans,octa-cis-undecaprenyl_phosphate + 1.0 H+  # source: MetaCyc, BRENDA, KEGG (queried 2.7.1.66)
#############2.7.7.85#############
~no-pathway_2.7.7.85_RXN-14338                                                                              : 2.0 ATP <=> 1.0 cyclic_di-3',5'-adenylate + 2.0
diphosphate  # source: MetaCyc, BRENDA, KEGG (queried 2.7.7.85)
#############2.7.8.40#############
~no-pathway_2.7.8.40_RXN-14571                                                                              : 1.0 di-trans,octa-cis-undecaprenyl_phosphate + 1.0 UDP-N-
acetyl-alpha-D-galactosamine <=> 1.0 N-acetyl-alpha-D-galactosaminyl-diphospho-ditrans,octacis-undecaprenol + 1.0 UMP  # source: MetaCyc, BRENDA, KEGG (queried 2.7.8.40) // other
EC numbers for this reaction: 2.7.8.6
#############2.7.8.7#############
~no-pathway_2.7.8.7_HOLO-ACP-SYNTH-RXN                                                                      : 1.0 |apo-ACP| + 1.0 coenzyme_A --> 1.0 adenosine_3',5'-
bisphosphate + 1.0 Acyl-carrier_protein + 1.0 H+  # source: MetaCyc, KEGG (queried 2.7.8.7) // other EC numbers for this reaction: 2.7.8
#############3.1.3.18#############
photorespiration_3.1.3.18_GPH-RXN                                                                           : 1.0 H2O + 1.0 2-phosphoglycolate --> 1.0 glycolate + 1.0
phosphate  # source: MetaCyc, BRENDA, KEGG (queried 3.1.3.18)
#############3.1.4.46#############
~no-pathway_3.1.4.46_RXN-14073                                                                              : 1.0 glycerophosphoglycerol + 1.0 H2O --> 1.0 sn-
glycerol_3-phosphate + 1.0 glycerol + 1.0 H+  # source: MetaCyc, BRENDA (queried 3.1.4.46)
#############3.2.1.10#############
~no-pathway_3.2.1.10_3.2.1.10-RXN                                                                           : 1.0 beta-isomaltose + 1.0 H2O --> 2.0 D-glucose  #
source: MetaCyc (queried 3.2.1.10)
#############3.2.1.133#############
~no-pathway_3.2.1.133_3.2.1.133-RXN                                                                         : 1.0 H2O + 1.0 |Starch| --> 1.0 alpha-maltose  # source:
MetaCyc (queried 3.2.1.133)
#############3.2.1.37#############
~no-pathway_3.2.1.37_3.2.1.37-RXN                                                                           : 1.0 H2O + 1.0 |1-4-D-xylooligosaccharides| --> 1.0 beta-
D-xylopyranose  # source: MetaCyc (queried 3.2.1.37)
#############3.6.1.13#############
~no-pathway_3.6.1.13_RXN0-1441                                                                              : 1.0 H2O + 1.0 ADP-D-ribose --> 2.0 H+ + 1.0 AMP + 1.0 D-
ribose_5-phosphate  # source: MetaCyc, BRENDA, KEGG (queried 3.6.1.13) // other EC numbers for this reaction: 3.6.1, 3.6.1.53, 3.6.1.21
#############4.1.2.17#############
lactate-biosynthesis_fucose-degradation_4.1.2.17_FUCPALDOL-RXN                                              : 1.0 L-fuculose_1-phosphate <=> 1.0 (S)-lactaldehyde + 1.0
glycerone_phosphate  # source: MetaCyc, BRENDA, KEGG (queried 4.1.2.17)
#############4.1.3.16#############
~no-pathway_4.1.3.16_RXN-13990                                                                              : 1.0 (4S)-4-hydroxy-2-oxoglutarate <=> 1.0 glyoxylate +
1.0 pyruvate  # source: MetaCyc, BRENDA, KEGG (queried 4.1.3.16) // other EC numbers for this reaction: 4.1.3.42
#############5.1.1.13#############
~no-pathway_5.1.1.13_ASPARTATE-RACEMASE-RXN                                                                 : 1.0 L-aspartate <=> 1.0 D-aspartate  # source: MetaCyc,
BRENDA, KEGG (queried 5.1.1.13)
#############5.1.1.21#############
~no-pathway_5.1.1.21_RXN-16430                                                                              : 1.0 L-isoleucine <=> 1.0 D-allo-isoleucine  # source:
MetaCyc, BRENDA, KEGG (queried 5.1.1.21)
#############5.1.3.14#############
~metabolism-of-biosynthesis_5.1.3.14_UDPGLCNACEPIM-RXN                                                      : 1.0 UDP-N-acetyl-alpha-D-glucosamine <=> 1.0 UDP-N-
acetyl-alpha-D-mannosamine  # source: MetaCyc, BRENDA, KEGG (queried 5.1.3.14)
#############5.4.3.9#############
~no-pathway_5.4.3.9_RXN-13569                                                                               : 1.0 L-glutamate <=> 1.0 beta-glutamate  # source:
MetaCyc, BRENDA, KEGG (queried 5.4.3.9)
#############6.1.1.13#############
~no-pathway_6.1.1.13_6.1.1.13-RXN                                                                           : 1.0 ATP + 1.0 Poly(ribitol_phosphate) + 1.0 D-alanine -->
1.0 H+ + 1.0 diphosphate + 1.0 O-D-Alanyl-poly(ribitol_phosphate) + 1.0 AMP  # source: MetaCyc, BRENDA, KEGG (queried 6.1.1.13)
#################################################################################################################################################################################
#Genric
#############1.1.3.15#############
~no-pathway_1.1.3.15_S-2-HYDROXY-ACID-OXIDASE-RXN                                                           : 1.0 oxygen + 1.0 |S-2-Hydroxyacids| --> 1.0
hydrogen_peroxide + 1.0 |2-Oxo-carboxylates|  # source: MetaCyc, BRENDA, KEGG (queried 1.1.3.15)
#############1.11.1.15#############
~no-pathway_1.11.1.15_RXN0-5468                                                                             : 1.0 |Red-Thioredoxin| + 1.0 |Alkyl-Hydro-Peroxides| -->
1.0 |Alcohols| + 1.0 H2O + 1.0 |Ox-Thioredoxin|  # source: MetaCyc (queried 1.11.1.15)
#############1.2.1.3#############
```

~no-pathway_1.2.1.3_ALDHDEHYDROG-RXN : 1.0 |Aldehydes| + 1.0 H2O + 1.0 NAD+ --> 1.0 NADH + 1.0 |Carboxylates| + 2.0 H+ # source: MetaCyc, BRENDA, KEGG (queried 1.2.1.3) // other EC numbers for this reaction: 1.2.1.5
##############3.1.1.96##############
~no-pathway_3.1.1.96_RXN-15041 : 1.0 |D-aminoacyl-tRNAs| + 1.0 H2O --> 1.0 |tRNAs| + 2.0 H+ + 1.0 |D-Amino-Acids| # source: MetaCyc (queried 3.1.1.96)
##############3.5.1.3##############
~no-pathway_3.5.1.3_OMEGA-AMIDASE-RXN : 1.0 DICARBOXYLIC-ACID-MONOAMIDES + 1.0 H2O --> 1.0 ammonium + 1.0 |dicarboxylate| # source: MetaCyc (queried 3.5.1.3)
##############3.5.1.81##############
~no-pathway_3.5.1.81_3.5.1.81-RXN : 1.0 N-Acyl-D-amino_acid + 1.0 H2O --> 1.0 |Carboxylates| + 1.0 |D-Amino-Acids| # source: MetaCyc, BRENDA, KEGG (queried 3.5.1.81)
##############3.5.1.87##############
~no-pathway_3.5.1.87_3.5.1.87-RXN : 1.0 H2O + 2.0 H+ + 1.0 |N-Carbamoyl-L-Amino-Acids| --> 1.0 ammonium + 1.0 |L-Amino-Acids| + 1.0 CO2 # source: MetaCyc, BRENDA, KEGG (queried 3.5.1.87)
##############5.5.1.6##############
~no-pathway_5.5.1.6_CHALCONE-ISOMERASE-RXN : 1.0 |Chalcones| <=> 1.0 flavanone # source: MetaCyc, BRENDA, KEGG (queried 5.5.1.6)
##
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Scenario S1: **Exemplary scenario file (MDM, 3 h) for the metabolic model *i*HD922 of *C. difficile* 630Δ*erm***

```
LB    NGAM                                                    2
#to inhibit
fatty-acid-I/2_2.3.1.39_MALONYL-COA-ACP-TRANSACYL-RXN - 7.123 fatty-acid-
I/3a_manual_HD-acet = 0
acetyl-CoA-to-butyrate-II/1_2.3.1.9_ACETYL-COA-ACETYLTRANSFER-RXN - 20 hexanoate-
ferm/1_2.3.1.9_RXN-12565    >   0
acetyl-CoA-to-butyrate-II/1_2.3.1.9_ACETYL-COA-ACETYLTRANSFER-RXN - 3 pentanoate-
ferm/1_2.3.1.9_RXN-12561    >   0
#####Substrates/Products in MDM/CDMM#####
LB    glycine_exchange                                        0
LB    aspartate_exchange                                      0
LB    glutamate_exchange                                      0
LB    serine_exchange                                         0
LB    threonine_exchange                                      0
LB    tyrosine_exchange                                       0
LB    phenylalanine_exchange                                  0
LB    arginine_exchange                                       0
LB    histidine_exchange                                      0
LB    lysine_exchange                                         0
#Gases
LB    H2_exchange                                             0
LB    CO_exchange                                             0
UB    CO_exchange                                             0
LB    methanethiol_exchange                                   0
LB    sulfite_exchange                                        0
#Alcohols
LB    ethanol_exchange                                        0
LB    propanol_exchange                                       0
LB    butanol_exchange                                        0
LB    isobutanol_exchange                                     0
#Acids
LB    formate_exchange                                        0
LB    acetate_exchange                                        0
LB    propanoate_exchange                                     0
LB    butanoate_exchange                                      0
LB    valerate_exchange                                       0
LB    hexanoate_exchange                                      0
LB    (R)-3-hydroxybutanoate_exchange                         0
LB    isocaproate_exchange                                    0
LB    3-phenylpropanoate_exchange                             0
LB    3-(4-hydroxyphenyl)propanoate_exchange                  0
LB    (S)-lactate_exchange                                    0
LB    (R)-lactate_exchange                                    0
#Other
LB    S-methyl-5-thio-D-ribose_exchange                       0
LB    beta-alanine_exchange                                   0
LB    2-aminobutanoate_exchange                               0
#####Other Substrates/Products#####
#bases
LB    cytosine_exchange                                       0
LB    adenine_exchange                                        0
LB    guanine_exchange                                        0
LB    hypoxanthine_exchange                                   0
LB    uracil_exchange                                         0
LB    xanthine_exchange                                       0
LB    urate_exchange                                          0
LB    thymine_exchange                                        0
```

```
#amino acids and amines
LB    asparagine_exchange                                    0
LB    glutamine_exchange                                     0
LB    4-hydroxyproline_exchange                              0
LB    cystathionine_exchange                                 0
LB    spermidine_exchange                                    0
LB    putrescine_exchange                                    0
LB    2,3-diaminopropanoate_exchange                         0
LB    hydroxylamine_exchange                                 0
LB    ethanolamine_exchange                                  0
LB    4-hydroxyphenylacetate_exchange                        0
#with phosporous
LB    sn-glycerol-3-phosphate_exchange                       0
LB    methylphosphonate_exchange                             0
LB    2-aminoethylphosphonate_exchange                       0
LB    phosphonoacetate_exchange                              0
#non-sugar carbohydrates
LB    succinate_exchange                                     0
LB    tartronate-semialdehyde_exchange                       0
LB    acetoin_exchange                                       0
LB    3-hydroxy-3-methylglutarate_exchange                   0
#tox
LB    hydroxyl-radical_exchange                              0
LB    superoxide_exchange                                    0
LB    hydrogen_peroxide_exchange                             0
LB    oxygen_exchange                                        0
LB    mathanol_exchange                                      0
LB    cyanide_exchange                                       0
LB    thiocyanate_exchange                                   0
#bile acids
LB    taurochenodeoxycholate_exchange                        0
LB    chenodeoxycholate_exchange                             0
LB    taurocholate_exchange                                  0
LB    cholate_exchange                                       0
#sugars and sugar alcohols
LB    D-arabinose_exchange                                   0
LB    xylan_exchange                                         0
LB    xylose_exchange                                        0
LB    galactose_exchange                                     0
LB    xylitol_exchange                                       0
LB    arabitol_exchange                                      0
LB    ribitol_exchange                                       0
LB    D-sorbitol_exchange                                    0
LB    D-mannitol_exchange                                    0
LB    D-ribopyranose_exchange                                0
LB    2'-deoxyribose_exchange                                0
LB    maltose_exchange                                       0
LB    sucrose_exchange                                       0
LB    D-tagatose_exchange                                    0
LB    D-fructofuranose_exchange                              0
LB    D-cellobiose_exchange                                  0
LB    chitobiose_exchange                                    0
LB    trehalose_exchange                                     0
LB    cyclodextrin_exchange                                  0
LB    starch_exchange                                        0
LB    maltodextrin_exchange                                  0
LB    pullulan_exchange                                      0
LB    maltotriose_exchange                                   0
LB    N-acetylneuraminate_exchange                           0
```

```
LB    N-acetyl-D-galactosamine_exchange                    0
LB    D-galactosamine_exchange                             0
LB    D-glucosaminate_exchange                             0
LB    2-O-alpha-mannosyl-D-glycerate_exchange              0
LB    D-altronate_exchange                                 0
LB    2-dehydro-3-deoxy-D-gluconate_exchange               0
#other
LB    riboflavin_exchange                                  0
LB    cobinamide_exchange                                  0
LB    coenzyme-B12_exchange                                0
LB    dethiobiotin_exchange                                0
LB    sulfolactate_exchange                                0
LB    choline_exchange                                     0
LB    formylaminopyrimidine_exchange                       0
LB    D-Glucose_exchange                                   -47.3671043246
UB    D-Glucose_exchange                                   -47.3671043246
LB    cysteine_exchange                                    -73.4834483508
LB    methionine_exchange                                  -8.5664873159
LB    tryptophan_exchange                                  -1.0401670259
LB    isoleucine_exchange                                  -5.110423686
LB    leucine_exchange                                     -1.8333183353
LB    valine_exchange                                      -1.8581174684
LB    proline_exchange                                     -15.9071454768
LB    alanine_exchange                                     0
LB    Biomass                                              0.4139957168
OBJ max exopolysaccharide_exchange
```

Table S1: **Isotope labeling of glycolysis and glycolysis-related metabolites.** Intracellular metabolites analyzed by GC/MS of *C. difficile* 630Δ*erm* cultivated in MDM with full ^{13}C-labeled glucose and harvested at OD 0.22.

Metabolite	Derivative	Fragment	C/Si	Backbone	M+0	M+1	M+2	M+3	M+4	M+5
Glucose	1MeOX/5TMS	319	C13Si3	C2-C5	0.0	0.0	0.0	0.0	100.0	0.0
		205	C8Si2	C5+C6	0.0	0.0	100.0	0.0	0.0	0.0
		364	C14Si3	C1-C4	0.0	0.0	0.0	0.0	100.0	0.0
Glucose 6-phosphate	1MeOX/6TMS	387	C13Si3	C3-C6	36.9±2.2	0.0	0.0	0.0	63.1±4.9	0.0
		471	C16Si4	C2-C6	36.8±3.6	0.0	0.0	0.0	0.0	62.8±3.1
		160	C6Si1	C1+C2	35.9±3.7	0.0	64.1±2.0	0.0	0.0	0.0
Glycerate 3-phosphate	4TMS	387	C12Si3	C1-C3	89.5±7.5	0.0	0.0	10.5±1.5	0.0	0.0
		459	C14Si4	C1-C3	90.2±0.3	0.0	0.0	9.8±0.2	0.0	0.0
Pyruvate	2TMS	217	C8Si2	C1-C3	91.4±3.3	0.0	0.0	8.6±1.3	0.0	0.0
	1MeOX/1TMS	174	C6Si	C1-C3	91.0±3.0	0.0	0.0	9.0±0.6	0.0	0.0
		189	C7Si	C1-C3	90.9±3.4	0.0	0.0	9.1±0.4	0.0	0.0
Alanine	2TMS	116	C5Si	C2+C3	90.1±2.2	0.0	9.9±0.3	0.0	0.0	0.0
		190	C7Si2	2xC	90.1±0.1	0.0	8.9±0.0	0.0	0.0	0.0
Lactate	2TMS	219	C8Si2	C1-C3	91.2±6.3	0.0	0.0	8.8±1.5	0.0	0.0
		117	C5Si	C2+C3	93.0±1.9	0.0	7.0±1.1	0.0	0.0	0.0
Cysteine	3TMS	232	C9Si2	C1-C3	100.0	0.0	0.0	0.0	0.0	0.0

Table S2: **Biomass compostion used for the model *i*HD992**

Component	Cell composition					
Protein	0,508	0,508	±0.014	0,5284	0,4	0,55
RNA	0,091	0,091	±0.001	0,0655	0,12	0,205
DNA	0,043	0,043	±0.002	0,0260	0,03	0,031
Lipid	0,060	0,084	±0.002	0,076	0,04291	0,091
Lipoteichoic acid	0,024			0,0304	0,02709	0,034
Peptidoglycan	0,145			0,1009	0,1344	0,025
Polysaccharide II	0,097			0,1234	0,1056	
Glycogen	0,005			0,0000		0,025
Ions	0,022			0,0321	0,0944	0,01
Metabolites	0,005			0,0173	0,0456	0,029
Sum	1,000	0,726		1,0000	1,00000	1,000

Clostridium difficile NCTC 11223 (Poxton and Cartmill, 1982): Cell wall polysaccharide II 40% by weight of SDS-purified walls
Clostridium difficile 630Δ*erm* (this work)
Bacillus subtilis, dilution rate of 0.1/h (Dauner and Sauer, 2001)
Staphylococcus aureus (Heinemann et al., 2005)
Escherichia coli (Neidhard et al., 1990)

	Molecular weight [g/mol]
Water	18,015
Hydrogen	2,016
Glycerol-3-phosphate	170,06
Glycerol	92,094
Phosphate	95,979
Methane	16,043

Amino acid analysis of hydrolyzed cells

Amino acid	Mass [g]	standard deviation	Masses including assumptions [g]	Molecular weight [g/mol]	Molecular weight in protein [g/mol]	Demand per biomass [mmol]	Demand for peptidoglycan [mmol]	Demand for protein [g]
Glycine	0,0258760	0,0019797	0,0258760	75,07	57,05	0,34471	0,00655	0,01929
Alanine	0,0510480	0,0041868	0,0510480	89,09	71,08	0,57297	0,23278	0,02418
Valine	0,0263600	0,0021179	0,0263600	117,15	99,14	0,22501		0,02231
Leucine	0,0406434	0,0032087	0,0406434	131,17	113,16	0,30985		0,03506
Isoleucine	0,0246838	0,0020485	0,0246838	131,17	113,16	0,18818		0,02129
Serine	0,0234864	0,0017999	0,0234864	105,09	87,08	0,22349		0,01946
Threonine	0,0265723	0,0020727	0,0265723	119,12	101,11	0,22307		0,02255
Phenylalanine	0,0209894	0,0016538	0,0209894	165,19	147,18	0,12706		0,01870
Tyrosine	0,0183924	0,0011384	0,0183924	181,19	163,18	0,10151		0,01656
Tryptophan	not detected		0,0060981	204,23	186,22	0,02986		0,00556
Cysteine	not detected		0,0060981	121,15	103,14	0,05034		0,00519

Methionine	0,0051211	0,0002230	0,0051211	149,21	131,20	0,03432		0,00450
Lysine	0,0475186	0,0065515	0,0475186	147,20	129,19	0,32282		0,04170
Arginine	0,0230321	0,0026527	0,0230321	175,21	157,20	0,13145		0,02066
Histidine	0,0076227	0,0013264	0,0076227	155,16	137,15	0,04913		0,00674
Aspartate	0,0630830	0,0047067	0,0315415	132,10	114,09	0,23877		0,02724
Glutamate	0,1052600	0,0084886	0,0842080	146,12	128,11	0,57629	0,14451	0,05531
Asparagine	not detected		0,0315415	132,12	114,11	0,23873		0,02724
Glutamine	not detected		0,0210520	146,15	128,14	0,14404		0,01846
Proline	0,0211960	0,0024992	0,0211960	115,13	97,12	0,18411		0,01788
Selenocysteine	not detected		0,0000762	168,05	150,04	0,00045		0,00007
Diaminopimelate	0,0273905	0,0013085	0,0273905	190,20	172,19	0,14401	0,14401	0,00000
Sum	0,5582758		0,5705483					0,42997
Clostridium difficile 630Δ*erm* (this work)								

Peptidoglycan/Biomass based on corrected diaminopimelate concentration:	0,145035

Protein

Amino acid	Corrected demand for protein per biomass [g/g]	Demand [mmol/g Protein]
Glycine	0,02279	0,59772
L-alanine	0,02857	0,63120
L-valine	0,02635	0,44284
L-leucine	0,04142	0,62167
L-isoleucine	0,02516	0,37755
L-serine	0,02299	0,43067
L-threonine	0,02665	0,44035
L-phenylalanine	0,02209	0,26329
L-tyrosine	0,01957	0,21261
L-tryptophan	0,00657	0,06332
L-cysteine	0,00613	0,09966
L-methionine	0,00532	0,07019
L-lysine	0,04927	0,65890
L-arginine	0,02441	0,27429
L-histidine	0,00796	0,10099
L-aspartate	0,03218	0,47959
L-glutamate	0,06535	0,88041
L-asparagine	0,03218	0,47953

L-glutamine	0,02181	0,29371
L-proline	0,02112	0,36118
L-selenocysteine	0,00008	0,00094
Sum	0,50800	7,78062

RNA

	Weight per cell [fg]	χ
rRNA	48	0,81356
tRNA	8,6	0,14576
mRNA	2,4	0,04068

rRNA

	Count	χ	Molecular weight [g/mol]	Molecular weight (real) [g/mol]	Mass [g/mol monomer]	Demand [mmol/g RNA]
AMP (ATP)	14915	0,27661	345,21	328,20	90,78370	0,70362
GMP (GTP)	11726	0,21747	361,21	344,20	74,85255	0,55318
CMP (CTP)	15954	0,29588	321,18	304,17	89,99789	0,75264
UMP (UTP)	11326	0,21005	322,17	305,16	64,09889	0,53431
Methylation	360	0,00668	16,04	14,03	0,09365	0,01698
Hydrogenation	24	0,00045		2,02	0,00090	0,00113
	53921				319,82757	2,56186

tRNA

	Count	χ	Molecular weight [g/mol]	Molecular weight (real) [g/mol]	Mass [g/mol monomer]	Demand [mmol/g RNA]
AMP (ATP)	1409	0,19977	345,21	328,20	65,56615	0,08508
GMP (GTP)	1579	0,22388	361,21	344,20	77,05892	0,09535
CMP (CTP)	2134	0,30257	362,21	345,20	104,44679	0,12887
UMP (UTP)	1931	0,27378	363,21	346,20	94,78491	0,11661
Methylation	180	0,02552	16,04	14,03	0,35798	0,01087
Hydrogenation	90	0,01276		2,02	0,02573	0,00543
	7053				342,24047	0,44221

mRNA

	χ	Molecular weight [g/mol]	Molecular weight (real) [g/mol]	Mass [g/mol monomer]	Demand [mmol/g RNA]
AMP (ATP)	0,35459	345,21	328,20	116,37835	0,04524

GMP (GTP)	0,14541	361,21	344,20	50,04967	0,01855
CMP (CTP)	0,14541	321,18	304,17	44,22901	0,01855
UMP (UTP)	0,35459	322,17	305,16	108,20854	0,04524
Methylation	0,00000	16,04	14,03	0,00000	0,00000
Hydrogenation	0,00000		2,02	0,00000	0,00000
				318,86557	0,12757

Abundances of RNA types in *E. coli* (Neidhard *et al.*, 1990)

Methylation and hydrogenation based on Modomics database (Machnicka *et al.*, 2013)

23S rRNA: *E. coli*, 16S rRNA: *C. acetobutylicum*, tRNA: *B.subtilis*

GC contend of genome (unpublished work, Dannheim *et al.*, 2016)

	Demand [mmol/g RNA]
AMP (ATP)	0,83394
GMP (GTP)	0,66708
CMP (CTP)	0,90005
UMP (UTP)	0,69615
Metylation	0,02785
Hydrogenation	0,00657

DNA

	Count	χ	Molecular weight [g/mol]	Molecular weight (real) [g/mol]	Mass [g/mol monomer]	Demand [mmol/g DNA]
dAMP (dATP)	3044566	0,35459	329,21	312,20	110,70487	1,15183
dGMP (dGTP)	1248482	0,14541	345,21	328,20	47,72315	0,47233
dCMP (dCTP)	1248482	0,14541	305,18	288,17	41,90249	0,47233
dTMP (dTTP)	3044566	0,35459	320,20	303,19	107,50999	1,15183
Metylation	8000	0,00093	14,03	12,01	0,01119	0,00303
	8586096				307,85169	

Based on sequence (unpublished work, Dannheim *et al.*, 2016)

Estimated from literature (van Eijk *et al.*, 2015):

Lipid

	Molecular weight [g/mol]
Fatty acid	258,54
Glycerolphosphate	170,06
Glycerol	92,09

Fatty acids

chain length:	16,246
unsaturations:	0,164

	Molecular weight [g/mol]	χ	Demand [mmol/g Lipid]
phosphatidylglycerol	722,17	0,5	0,69236
cardiolipin	1352,24	0,5	0,36976

Fatty acids of *C. difficile* NCIB 10666 (Elsden *et al.*, 1980):

Only phosphatidylglycerol-analogs could be found in *C. difficile* isolates (Drucker *et al.*, 1996)

Lipoteichoic acid

	χ	Molecular weight [g/mol]	Molecular weight (real) [g/mol]	Mass [g/mol monomer]
N-Acetyl-D-Glucosamine	10,14804	221,21	203,20	2062,03
Deacetylation	1,22221	60,05	-42,04	-51,38
Glycerate	5,07402	105,07	87,06	441,72
Glucose	3,00000	180,16	162,15	486,44
1,2-diacyl-sn-glycerol	1,00000	575,16	575,16	575,16
Phosphate	5,07402	95,98	78,97	400,71
				3914,68

	Demand [mmol/g Lipoteichoic acid]
UDP-N-acetyl-D-Glucosamine	2,59231
Deacetylation	0,31221
2-phospho-D-glycerate	1,29615
UDP-Glucose	0,76635
1,2-diacyl-sn-glycerol	0,25545
ATP	1,29615

Composition and chain length in *C. difficile* 630 (Reid *et al.*, 2012)

Average chain length from integration of NMR data: 4,07

Peptidoglycan

	χ	Molecular weight [g/mol]	Molecular weight (real) [g/mol]	Mass [g/mol monomer]	Demand [mmol/g Peptidoglycan]
L-alanine	1,00000	89,09	71,08	71,08	1,17720
D-glutamate	1,00000	146,12	128,11	128,11	1,17720
Diaminopimelate	0,99654	190,20	172,19	171,59	1,17312
D-alanine	0,61085	89,09	71,08	43,42	0,71910
Glycine	0,04532	75,07	57,05	2,59	0,05335
Deacetylation	0,92783	59,04	-42,04	-39,00	1,09224

Other modifications	0,31933		-18,02	-5,75	0,37591
N-Acetyl-D-Glucosamine	1,00000	221,21	203,20	203,20	1,17720
N-Acetylmuramic acid	1,00000	292,27	274,26	274,26	1,17720
				849,47	

Peptidoglycan composition of *C. difficile* 630 (Peltier *et al.*, 2011)

Polysaccharide II

	χ	Molecular weight [g/mol]	Molecular weight (real) [g/mol]	Mass [g/mol monomer]	Demand [mmol/g Polysaccharide II]
N-Acetyl-D-Galactosamine	2	221,21	203,20	406,39	1,76376
Glucose	3	180,16	162,15	486,44	2,64564
Mannose	1	180,16	162,15	162,15	0,88188
Phosphate	1	95,98	78,97	78,97	0,88188
				1133,94	

Structure of polysaccharide II (Ganeshapillai *et al.*, 2008):
[→6)-β-D-Glcp-(1→3)-β-D-GalpNAc-(1→4)-α-D-Glcp-(1→4)-[β-D-Glcp-(1→]-β-D-GalpNAc-(1→3)-α-D-Manp-(1→P]

Glycogen

Demand [mmol/g Glycogen]
6,16732

Ions

	χ	Molecular weight [g/mol]	Mass [g/mol monomer]	mmol/g Ions
K	0,86	39,10	33,62	20,96743
Mg	0,077	24,31	1,87	1,87732
Fe(+3)	0,006	55,85	0,34	0,14628
Ca	0,004	40,08	0,16	0,09752
Phosphate	0,043	95,98	4,13	1,04837
Diphospate	0,005	174,95	0,87	0,12190
Na	0,001	22,99	0,02	0,02438
Fe(+2)	0,001	55,85	0,06	0,02438
Ni	0,001	58,70	0,06	0,02438
Cd	0,001	112,40	0,11	0,02438
Zn	0,001	65,38	0,07	0,02438
	1	745,58	41,02	

B. subtilis (Dauner and Sauer, 2001)

Metabolites

Mass [g/mol molecule]	Ratio	Molecular weight (real) [g/mol]	χ	Mass [g/mol Metabolite]	mmol/g Metabolite
ATP	3,2656	503,15	0,20446	102,87165	0,33818
ADP	0,8190	424,18	0,05128	21,75051	0,08481
AMP	0,2988	345,21	0,01871	6,45802	0,03094
Acetyl-CoA	1,6736	805,54	0,10478	84,40614	0,17332
FAD	0,6438	782,53	0,04031	31,54185	0,06667
NAD	1,6046	662,42	0,10046	66,54807	0,16617
NADH	0,3393	663,43	0,02124	14,09335	0,03514
NADP	0,0042	740,39	0,00026	0,19469	0,00043
NADPH	0,2415	741,39	0,01512	11,20983	0,02501
ppGpp	0,6438	598,12	0,04031	24,10874	0,06667
Tetrahydropteroyltriglutamate	0,6438	699,63	0,04031	28,20036	0,06667
Di-trans,octa-cis-undecaprenyl PP	0,6438	924,25	0,04031	37,25424	0,06667
Thiamin diphosphate	0,6438	422,29	0,04031	17,02147	0,06667
Adenosylcobalamin	0,6438	1579,60	0,04031	63,66978	0,06667
Mg-protoporphyrin	0,6438	582,94	0,04031	23,49687	0,06667
MoO2-molybdopterin	0,6438	519,25	0,04031	20,92969	0,06667
Biotin	0,6438	243,3	0,04031	9,80682	0,06667
Me-Thr-P-GluNAc-FliC	0,6438	279,94	0,04031	11,28379	0,06667
Pyridoxine 5'-phosphate	0,6438	247,14	0,04031	9,96160	0,06667
L-threonylcarbamoyladenylate	0,6438	490,32	0,04031	19,76359	0,06667
	15,9722	12255,02	1,00000	604,57108	

C. acetobutylicum in the acidogenic growth phase (Amador-Noguez *et al.*, 2011)

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Table S3: **Fits of the substrate concentrations and OD over time of MDM-cultures with *C. difficile* 630Δ*erm*.**

Function	Parameters		Range	R^2
$OD(t) = A_1 + \frac{A_2 - A_1}{(1+((t_0/t)^h)^s}$	$A_1 = 0.00500$ $t_0 = 9.09315$ $s = 0.10158$	$A_2 = 0.39989$ $h = 12.89192$	0.0 h to 12.0 h	0.99234
$Cys_{rel.}(t) = a + b_1 \cdot t + b_2 \cdot t^2 + b_3 \cdot t^3$	$a = 0.99488$ $b_2 = -0.01235$	$b_1 = -0.16893$ $b_3 = 0.00231$	0.0 h to 6.67 h	0.92454
$Ile_{rel.}(t) = A_1 + \frac{A_2 - A_1}{(1+e^{(t-t_0)/dt})}$	$A_1 = 0.99257$ $t_0 = 5.13433$ $span = 0.83222$	$A_2 = 0.14788$ $dt = 1.53344$ $EC_{50} = 169.75062$	0.0 h to 12.0 h	0.98845
$Leu_{rel.}(t) = a + b \cdot t$	$a = 0.96612$	$b = -0.02369$	0.0 h to 5.25 h	0.48804
$Leu_{rel.}(t) = A_1 \cdot e^{-t/x_1} + y_0$	$y_0 = 0.27023$ $x_1 = 1.20063$ $\tau = 0.83222$	$A_1 = 35.72743$ $k = 0.83289$	5.25 h to 12.0 h	0.87374
$Met_{rel.}(t) = a + b_1 \cdot t + b_2 \cdot t^2 + b_3 \cdot t^3$	$a = 1.01491$ $b_2 = -0.07927$	$b_1 = -0.07017$ $b_3 = 0.01041$	0.0 h to 4.67 h	0.87616
$Pro_{rel.}(t) = A_1 \cdot e^{-t/x_1} + y_0$	$y_0 = 1.31687$ $x_1 = -11.33440$ $\tau = -7.85641$	$A_1 = -0.32291$ $k = -0.08823$	0.0 h to 5.25 h	0.99559
$Pro_{rel.}(t) = A_1 \cdot e^{-t/x_1} + y_0$	$y_0 = 0.02347$ $x_1 = 1.07132$ $\tau = 0.74259$	$A_1 = 57.12713$ $k = 0.93342$	5.25 h to 12.0 h	0.95409
$Trp_{rel.}(t) = A_1 \cdot e^{-t/x_1} + y_0$	$y_0 = 1.34255$ $x_1 = -6.93747$ $\tau = -4.70769$	$A_1 = -0.37572$ $k = -0.14414$	0.0 h to 8.5 h	0.98919
$Val_{rel.}(t) = a + b \cdot t$	$a = 0.98328$	$b = -0.02910$	0.0 h to 5.25 h	0.84721
$Val_{rel.}(t) = A_1 \cdot e^{-t/x_1} + y_0$	$y_0 = 0.32975$ $x_1 = 0.88397$ $\tau = 0.61272$	$A_1 = 196.70196$ $k = 1.13126$	5.25 h to 12.0 h	0.97966

Table S3 – continued from previous page

Function	Parameters		Range	R^2
$Gluc_{rel.}(t) = a + b_1 \cdot t + b_2 \cdot t^2$	$a = 0.98356$ $b_2 = -0.01745$	$b_1 = -0.06647$	0.0 h to 5.25 h	0.99923
$Gluc_{rel.}(t) = A_1 + \frac{A_2 - A_1}{(1+((t_0/t)^h)^s}$	$A_1 = 0.05196$ $t_0 = 15.87124$ $s = 1225.95789$	$A_2 = 2.17470$ $h = -9.82418$	5.25 h to 12.0 h	0.99007

Table S4: **Fits of the substrate concentrations and OD over time of CDMM-cultures with *C. difficile* 630Δ*erm*.**

Function	Parameters		Range	R^2
$OD(t) = A_1 \cdot e^{-t/x_1} + y_0$	$y_0 = -0.04045$ $x_1 = -1.04652$ $\tau = 0.72539$	$A_1 = 0.04110$ $k = 0.955552$	0.0 h to 2.0 h	0.95351
$OD(t) = A_1 \cdot e^{-t/x_1} + y_0$	$y_0 = 0.00000$ $x_1 = -1.32201$ $\tau = 0.91635$	$A_1 = 0.04757$ $k = 0.75642$	1.0 h to 3.4 h	0.89764
$OD(t) = a + b \cdot t$	$a = -0.02090$	$b = 0.19075$	3.5 h to 8.0 h	0.86917
$Cys_{rel.}(t) = A_1 + \frac{A_2 - A_1}{(1+e^{(t-t_0)/dt})}$	$A_1 = 0.96740$ $t_0 = 2.03742$ $span = 0.86195$	$A_2 = 0.10545$ $dt = 0.34962$ $EC_{50} = 7.67078$	0.0 h to 3.5 h	0.99883
$Cys_{rel.}(t) = a + b \cdot t$	$a = 0.75591$	$b = -0.18272$	3.5 h to 4.0 h	0.99303
$Ile_{rel.}(t) = A_1 \cdot e^{-t/x_1} + y_0$	$y_0 = 1.12163$ $x_1 = -1.58509$ $\tau = -1.09870$	$A_1 = -0.10272$ $k = -0.63088$	0.0 h to 3.5 h	0.92790
$Ile_{rel.}(t) = a + b \cdot t$	$a = 0.58216$	$b = -0.12008$	3.5 h to 4.5 h	0.76521
$Leu_{rel.}(t) = a + b_1 \cdot t + b_2 \cdot t^2 + b_3 \cdot t^3$	$a = 0.99344$ $b_2 = 0.03270$	$b_1 = -0.10645$ $b_3 = -0.02375$	0.0 h to 3.5 h	0.96144
$Leu_{rel.}(t) = a + b \cdot t$	$a = 0.31681$	$b = -0.08192$	3.5 h to 3.75 h	-
$Met_{rel.}(t) = A_1 \cdot e^{-t/x_1} + y_0$	$y_0 = 0.94952$ $x_1 = -1.17058$ $\tau = -0.81139$	$A_1 = -0.03582$ $k = -0.85428$	0.0 h to 3.75 h	0.99105
$Pro_{rel.}(t) = A_1 + \frac{A_2 - A_1}{(1+e^{(t-t_0)/dt})}$	$A_1 = 1.31883$ $t_0 = 1.75619$ $span = 1.59886$	$A_2 = -0.28003$ $dt = 1.19337$ $EC_{50} = 5.79033$	0.0 h to 3.5 h	0.99472
$Trp_{rel.}(t) = A_1 \cdot e^{-t/x_1} + y_0$	$y_0 = 1.71645$ $x_1 = -9.26705$ $\tau = -6.42343$	$A_1 = -0.72456$ $k = -0.10791$	0.0 h to 5.25 h	0.99083

Table S4 – continued from previous page

Function	Parameters		Range	R^2
$Val_{rel.}(t) = A_1 \cdot e^{-t/x_1} + y_0$	$y_0 = 1.02750$ $x_1 = -2.33158$ $\tau = -1.61613$	$A_1 = -0.09812$ $k = -0.42889$	0.0 h to 5.25 h	0.99051
$Ala_{rel.}(t) = A_1 + \frac{A_2 - A_1}{(1+e^{(t-t_0)/dt})}$	$A_1 = 0.96241$ $t_0 = 2.44879$ $span = 0.63071$	$A_2 = 0.33169$ $dt = 0.41349$ $EC_{50} = 11.17042$	0.0 h to 3.5 h	0.96921
$Ala_{rel.}(t) = a + b_1 \cdot t + b_2 \cdot t^2$	$a = -1.07653$ $b_2 = -0.10834$	$b_1 = 0.80434$	3.5 h to 5.25 h	0.93296
$Arg_{rel.}(t) = A_1 + \frac{A_2 - A_1}{(1+e^{(t-t_0)/dt})}$	$A_1 = 1.05930$ $t_0 = 2.41832$ $span = 0.69836$	$A_2 = 0.36094$ $dt = 0.74592$ $EC_{50} = 11.22696$	0.0 h to 11.0 h	0.99115
$Asp_{rel.}(t) = A_1 + \frac{A_2 - A_1}{(1+e^{(t-t_0)/dt})}$	$A_1 = 0.99783$ $t_0 = 2.06163$ $span = 0.60847$	$A_2 = 0.38936$ $dt = 0.25586$ $EC_{50} = 7.85877$	0.0 h to 3.5 h	0.99395
$Asp_{rel.}(t) = A_1 \cdot e^{-t/x_1} + y_0$	$y_0 = 0.17968$ $x_1 = 0.43935$ $\tau = 0.30453$	$A_1 = 619.04429$ $k = 2.27611$	3.5 h to 5.25 h	0.97811
$Gly_{rel.}(t) = A_1 \cdot e^{-t/x_1} + y_0$	$y_0 = 1.34096$ $x_1 = -2.87096$ $\tau = -1.99000$	$A_1 = -0.32757$ $k = -0.34832$	3.5 h to 4.0 h	0.99942
$Phe_{rel.}(t) = A_1 \cdot e^{-t/x_1} + y_0$	$y_0 = 1.11495$ $x_1 = -1.62541$ $\tau = -1.12651$	$A_1 = -0.09174$ $k = -0.61530$	0.0 h to 4.0 h	0.99718
$Ser_{rel.}(t) = A_1 + \frac{A_2 - A_1}{(1+e^{(t-t_0)/dt})}$	$A_1 = 0.95887$ $t_0 = 2.83070$ $span = 0.99020$	$A_2 = -0.03133$ $dt = 0.23137$ $EC_{50} = 16.95729$	0.0 h to 3.5 h	0.99801
$Ser_{rel.}(t) = a + b \cdot t$	$a = 0.13832$	$b = -0.03361$	3.5 h to 3.75 h	-
$Thr_{rel.}(t) = A_1 \cdot e^{-t/x_1} + y_0$	$y_0 = 2.57581$ $x_1 = -9.94436$	$A_1 = -1.49028$ $k = -0.10056$	0.0 h to 5.25 h	0.96896

Table S4 – continued from previous page

Function	Parameters		Range	R^2
	$\tau = -6.89291$			
$Tyr_{rel.}(t) = A_1 \cdot e^{-t/x_1} + y_0$	$y_0 = 1.39161$	$A_1 = -0.39354$		
	$x_1 = -4.42492$	$k = -0.22599$	0.0 h to 4.5 h	0.96196
	$\tau = -3.06712$			
$His_{rel.}(t) = A_1 + \frac{A_2 - A_1}{(1+e^{(t-t_0)/dt})}$	$A_1 = 1.00560$	$A_2 = 0.23575$		
	$t_0 = 2.90486$	$dt = 0.75226$	0.0 h to 11.0 h	0.99096
	$span = 0.76985$	$EC_{50} = 18.26266$		
$Gluc_{rel.}(t) = a + b \cdot t$	$a = 0.99484$	$b = -0.02424$	0.0 h to 3.0 h	0.69519
$Gluc_{rel.}(t) = A_1 + \frac{A_2 - A_1}{(1+e^{(t-t_0)/dt})}$	$A_1 = 0.95438$	$A_2 = 0.09430$		
	$t_0 = 4.06080$	$dt = 0.35287$	1.5 h to 5.5 h	0.99589
	$span = 0.86008$	$EC_{50} = 58.02097$		