

Worksheet	Description
MetaboliteNames	Numbers for metabolites in U-system model arbitrarily given. X_i represent metabolites.
Fluxes	Fluxes for U-system model. V_j represent fluxes.
ODE	Ordinary differential equations (ODE) for the modified U-system model. F_i represent ODE of metabolite i . For the original model, a_0, a_1, a_2, a_3 are 1.0. For the Monte-Carlo simulations, the value of a_3 was varied while other parameters a in the original model were kept to be 1.0. For the modified model, $a_0=0.05, a_1=0.01, a_2=0.1$ and $a_3=1.0$.
CorrelationAnalysis	Correlation coefficient and p-values for the comparisons of experimental data and U-system simulation. CorrMetabolomeSimulation and pValMetabolomeSimulation refer to correlation coefficients and p-values between relative concentrations from metabolome analysis and U-system concentrations. CorrAminoAcidSimulation and pValAminoAcidSimulation refer to correlation coefficients and p-values between relative concentrations from amino acid analysis and U-system concentrations. CorrMetabolomeAminoAcid and pValMetabolomeAminoAcid refer to correlation coefficients and p-values between relative concentrations from metabolome analysis and those from amino acid analysis. Columns for Simulation, AminoAcidAnalysis and MetabolomeAnalysis represents metabolic names for each analysis system.

The correlation coefficients, testing for the significance of the correlation coefficients, and student's t continuous random variable based on a survival function were calculated for comparing model simulations with experimental data.

$$r = \frac{\sum xy - n\bar{x}\bar{y}}{\sqrt{(\sum x^2 - n\bar{x}^2)(\sum y^2 - n\bar{y}^2)}}$$

$$t = \frac{r}{\sqrt{\frac{1-r^2}{N-2}}}$$

$$F(t) = 1 - S(t)$$

$$p = P(T \geq t) = 1 - F(t)$$

where r represents correlation coefficient while x and y represent experimental and simulated data; t is testing for the significance of the correlation coefficients while p is p-value which is calculated using survival function,

X_1	=	sucrose
X_2	=	glucose-6P
X_3	=	fructose-6P
X_4	=	fructose-1,6-bis-P
X_5	=	glyceraldehyde-3-P
X_6	=	dihydroxyacetone-P
X_7	=	1,3-diPglycerate
X_8	=	3-phosphoglycerate
X_9	=	2-phosphoglycerate
X_{10}	=	phosphoenolpyruvate
X_{11}	=	pyruvate
X_{12}	=	2-acetolactate
X_{13}	=	2,3-dihydroxyisovalerate
X_{14}	=	2-ketoisovalerate
X_{15}	=	2-isopropylmalate
X_{16}	=	isopropylmaleate
X_{17}	=	3-isopropylmalate
X_{18}	=	2-isopropyl-3-oxosuccinate
X_{19}	=	2-ketoisocaproate
X_{20}	=	leucine
X_{21}	=	3-phosphohydroxypyruvate
X_{22}	=	3-phosphoserine
X_{23}	=	L-serine
X_{24}	=	D-serine
X_{25}	=	glycine
X_{26}	=	threonine
X_{27}	=	2-oxobutanoate
X_{28}	=	2-aceto-2-hydroxybutyrate
X_{29}	=	2,3-dihydroxy-3-methylvalerate
X_{30}	=	2-keto-3-methylvalerate
X_{31}	=	isoleucine
X_{32}	=	S-2-methylbutyryl-CoA
X_{33}	=	tigloylCoA
X_{34}	=	2-methyl-3-hydroxybutyryl-CoA
X_{35}	=	2-methylacetoacetyl-CoA
X_{36}	=	acetylCoA
X_{37}	=	glutamate
X_{38}	=	N-acetyl-L-glutamate
X_{39}	=	N-acetylglutamyl-P
X_{40}	=	N-acetyl-L-glutamate-5-semialdehyde
X_{41}	=	N-acetyl-L-ornithine
X_{42}	=	ornithine
X_{43}	=	carbamoyl-P
X_{44}	=	glutamine
X_{45}	=	citrulline
X_{46}	=	argininosuccinate
X_{47}	=	arginine
X_{48}	=	glutamate-gamma-semialdehyde
X_{49}	=	S-1-pyrroline-5-carboxylate

X_{50}	=	proline
X_{51}	=	O-acetyl-L-serine
X_{52}	=	5-phosphoribosyl-1-pyrophosphate
X_{53}	=	phosphoribosylATP
X_{54}	=	phosphoribosylAMP
X_{55}	=	phosphoribosylformiminoAICARP
X_{56}	=	phosphoribulosylformiminoAICARP
X_{57}	=	AICAR
X_{58}	=	D-erythroimidazoleglycerol-P
X_{59}	=	imidazoleacetol-P
X_{60}	=	histidinolP
X_{61}	=	histidinol
X_{62}	=	histidinal
X_{63}	=	histidine
X_{64}	=	citrate
X_{65}	=	cisaconitate
X_{66}	=	isocitrate
X_{67}	=	ketoglutarate
X_{68}	=	succinyl-CoA
X_{69}	=	succinate
X_{70}	=	fumarate
X_{71}	=	malate
X_{72}	=	oxaloacetate
X_{73}	=	alanine
X_{74}	=	cysteine
X_{75}	=	4-aminobutyrate
X_{76}	=	succinatesemialdehyde
X_{77}	=	asparagine
X_{78}	=	aspartate
X_{79}	=	aspartate-4P
X_{80}	=	aspartatesemialdehyde
X_{81}	=	homoserine
X_{82}	=	O-phospho-L-homoserine
X_{83}	=	cystathionine
X_{84}	=	homocysteine
X_{85}	=	methionine
X_{86}	=	S-adenosyl-L-methionine
X_{87}	=	S-adenosyl-L-homocysteine
X_{88}	=	adenosine
X_{89}	=	L-2,3-dihydrodipicolinate
X_{90}	=	tetrahydrodipicolinate
X_{91}	=	L,L-diamionopimelate
X_{92}	=	mesodiaminopimelate
X_{93}	=	lysine
X_{94}	=	S-methyl-5-thioadenosine
X_{95}	=	5-methylthioribose
X_{96}	=	5-methylthioribose-1P
X_{97}	=	5-methylthioribulose-1P
X_{98}	=	5-methylthio-2,3-dioxopentyl-P

X_{99}	=	2-hydroxy-3-keto-5-methylthio-1-phosphopentene
X_{100}	=	1,2-dihydroxy-3-keto-5-methylthiopentene
X_{101}	=	2-oxo-4-methylthiobutanoate
X_{102}	=	3-deoxyDarabinoheptulosonate-7P
X_{103}	=	3-dehydroquinate
X_{104}	=	3-dehydroshikimate
X_{105}	=	shikimate
X_{106}	=	shikimate-3P
X_{107}	=	5-enolpyruvylshikimate-3P
X_{108}	=	prephenate
X_{109}	=	arogenate
X_{110}	=	phenylalanine
X_{111}	=	phenylpyruvate
X_{112}	=	phenylacetaldehyde
X_{113}	=	tyrosine
X_{114}	=	phydroxyphenylpyruvate
X_{115}	=	homogentisate
X_{116}	=	maleylacetoacetate
X_{117}	=	4-fumarylacetoacetate
X_{118}	=	anthranilate
X_{119}	=	N-5-phosphoribosylanthranilate
X_{120}	=	1-O-carboxyphenylamino-1-deoxyribulose-5P
X_{121}	=	indole3glycerolP
X_{122}	=	indole
X_{123}	=	tryptophan
X_{124}	=	valine
X_{125}	=	glyoxylate
X_{126}	=	SmethylLmethionine
X_{127}	=	chorismate
X_{128}	=	glutamylcysteine
X_{129}	=	glutathione
X_{130}	=	2-methylmalate
X_{131}	=	methylmaleate
X_{132}	=	3-methylmalate
X_{133}	=	hydroxylysine
X_{134}	=	acetylhydroxylysine
X_{135}	=	D-lysine
X_{136}	=	diaminohexanoate
X_{137}	=	N-acetyllysine
X_{138}	=	acetamidooxohexanoate
X_{139}	=	aminooxohexanoate
X_{140}	=	piperideine-2-carboxylate
X_{141}	=	pipecolate
X_{142}	=	piperideine-6-carboxylate
X_{143}	=	aminoadipatesemialdehyde
X_{144}	=	saccharopine
X_{145}	=	cadaverine
X_{146}	=	piperideine
X_{147}	=	aminopentanamide

X_{148}	=	aminopentanoate
X_{149}	=	acetyllysine
X_{150}	=	acetamidopentanoate
X_{151}	=	glutaratesemialdehyde
X_{152}	=	glutarate
X_{153}	=	aminoadipate
X_{154}	=	oxoadipate
X_{155}	=	glutaryl dihydroliipoamide
X_{156}	=	glutaryl-CoA
X_{157}	=	crotonoyl-CoA
X_{158}	=	hydroxybutanoyl-CoA
X_{159}	=	acetoacetyl-CoA
X_{160}	=	2,2-methylthioethylmalate
X_{161}	=	3,2-methylthioethylmalate
X_{162}	=	2-oxo-5-methylthiopentanoic acid
X_{163}	=	2,3-methylthiopropylmalate
X_{164}	=	3,3-methylthiopropylmalate
X_{165}	=	2-oxo-6-methylthiohexanoate
X_{166}	=	2,4-methylthiobutylmalate
X_{167}	=	3,4-methylthiobutylmalate
X_{168}	=	2-oxo-7-methylthioheptanoate
X_{169}	=	2,5-methylthiopentylmalate
X_{170}	=	3,5-methylthiobutylmalate
X_{171}	=	2-oxo-8-methyloctanoate
X_{172}	=	2,6-methylthiohexylmalate
X_{173}	=	3,6-methylthiohexylmalate
X_{174}	=	2-oxo-9-methylononanoate
X_{175}	=	2,7-methylthioheptylmalate
X_{176}	=	3,7-methylthioheptylmalate
X_{177}	=	2-oxo-1,0-methylthiodecanoate
X_{178}	=	homomethionine
X_{179}	=	methylthiobutanaldoxime
X_{180}	=	methylthiobutanonitrileoxide
X_{181}	=	methylthiobutylhydroximoylglutathione
X_{182}	=	methylthiobutylhydroximoylcysteinylglycine
X_{183}	=	methylthiobutylhydroximate
X_{184}	=	methylthiopropyl desulfoglucosinolate
X_{185}	=	methylthiopropylglucosinolate
X_{186}	=	methylsulfinylpropylglucosinolate
X_{187}	=	propenylglucosinolate
X_{188}	=	hydroxypropylglucosinolate
X_{189}	=	benzoyloxypropylglucosinolate
X_{190}	=	sinapoyloxypropylglucosinolate
X_{191}	=	dihomomethionine
X_{192}	=	methylthiopentanaloxime
X_{193}	=	methylthiopentanonitrileoxide
X_{194}	=	methylthiopentylhydroximoylglutathione
X_{195}	=	methylthiopentylhydroximoylcysteinylglycine
X_{196}	=	methylthiopentylhydroximate

X_{197}	=	methylthiobutylsulfoglucosinolate
X_{198}	=	methylthiobutylglucosinolate
X_{199}	=	methylsulfinylbutylglucosinolate
X_{200}	=	butenylglucosinolate
X_{201}	=	hydroxy-3-butenylglucosinolate
X_{202}	=	benzoyloxy-3-butenylglucosinolate
X_{203}	=	sinapoyloxy-3-butenylglucosinolate
X_{204}	=	hydroxybutylglucosinolate
X_{205}	=	benzoyloxybutylglucosinolate
X_{206}	=	sinapoyloxybutylglucosinolate
X_{207}	=	trihomomethionine
X_{208}	=	methylthiohexanaldoxime
X_{209}	=	methylthiohexanonitrileoxide
X_{210}	=	methylthiohexylhydroximoylglutathione
X_{211}	=	methylthiohexylhydroximoylcysteinylglycine
X_{212}	=	methylthiohexylhydroximate
X_{213}	=	methylthiopentylsulfoglucosinolate
X_{214}	=	methylthiopentylglucosinolate
X_{215}	=	methylsulfinylpentylglucosinolate
X_{216}	=	pentenylglucosinolate
X_{217}	=	tetrahomomethionine
X_{218}	=	methylthioheptanaldoxime
X_{219}	=	methylthioheptanonitrileoxide
X_{220}	=	methylthioheptylhydroximoylglutathione
X_{221}	=	methylthioheptylhydroximoylcysteinylglycine
X_{222}	=	methylthioheptylhydroximate
X_{223}	=	methylthiohexylsulfoglucosinolate
X_{224}	=	methylthiohexylglucosinolate
X_{225}	=	methylsulfinylhexylglucosinolate
X_{226}	=	pentahomomethionine
X_{227}	=	methylthiooctanaldoxime
X_{228}	=	methylthiooctanonitrileoxide
X_{229}	=	methylthiooctylhydroximoylglutathione
X_{230}	=	methylthiooctylhydroximoylcysteinylglycine
X_{231}	=	methylthiooctylhydroximate
X_{232}	=	methylthioheptylsulfoglucosinolate
X_{233}	=	methylthioheptylglucosinolate
X_{234}	=	methylsulfinylheptylglucosinolate
X_{235}	=	hexahomomethionine
X_{236}	=	methylthiononanaldoxime
X_{237}	=	methylthiononanitrileoxide
X_{238}	=	methylthiononylhydroximoylglutathione
X_{239}	=	methylthiononylhydroximoylcysteinylglycine
X_{240}	=	methylthiononylhydroximate
X_{241}	=	methylthiooctylsulfoglucosinolate
X_{242}	=	methylthiooctylglucosinolate
X_{243}	=	methylsulfinyloctylglucosinolate
X_{244}	=	phenylacetaldoxime
X_{245}	=	phenylacetoneitrileoxide

<i>X</i> ₂₄₆	=	phenylacetohydroximoylglutathione
<i>X</i> ₂₄₇	=	phenylacetohydroximoylcysteinylglycine
<i>X</i> ₂₄₈	=	phenylacetothiohydroximate
<i>X</i> ₂₄₉	=	benzyldesulfoglucosinolate
<i>X</i> ₂₅₀	=	benzylglucosinolate
<i>X</i> ₂₅₁	=	indole-3-acetaldoxime
<i>X</i> ₂₅₂	=	indole-3-acetonitrileoxide
<i>X</i> ₂₅₃	=	indole-3-acetohydroximoylglutathione
<i>X</i> ₂₅₄	=	indole-3-acetohydroximoylcysteinylglycine
<i>X</i> ₂₅₅	=	indolylmethylthiohydroximate
<i>X</i> ₂₅₆	=	indolylmethylsulfoglucosinolate
<i>X</i> ₂₅₇	=	indol-3-ylmethylglucosinolate
<i>X</i> ₂₅₈	=	1-hydroxy-3-indolylmethylglucosinolate
<i>X</i> ₂₅₉	=	1-methoxy-3-indolylmethylglucosinolate
<i>X</i> ₂₆₀	=	4-hydroxy-3-indolylmethylglucosinolate
<i>X</i> ₂₆₁	=	4-methoxy-3-indolylmethylglucosinolate
<i>X</i> ₂₆₂	=	histamine
<i>X</i> ₂₆₃	=	imidazoleacetaldehyde
<i>X</i> ₂₆₄	=	imidazole4acetate
<i>X</i> ₂₆₅	=	imidazoloneacetate
<i>X</i> ₂₆₆	=	NformiminoLaspartate
<i>X</i> ₂₆₇	=	NformylLaspartate
<i>X</i> ₂₆₈	=	D-glucono-1,5-lactone-6P
<i>X</i> ₂₆₉	=	6-phospho-D-gluconate
<i>X</i> ₂₇₀	=	D-ribulose-5P
<i>X</i> ₂₇₁	=	D-ribose-5P
<i>X</i> ₂₇₂	=	D-ribose
<i>X</i> ₂₇₃	=	D-ribose-1P
<i>X</i> ₂₇₄	=	D-ribose-1,5P
<i>X</i> ₂₇₅	=	D-xylulose-5P
<i>X</i> ₂₇₆	=	D-erythrose-4P
<i>X</i> ₂₇₇	=	D-sedoheptulose-7P
<i>X</i> ₂₇₈	=	D-gluconate
<i>X</i> ₂₇₉	=	D-glucono-1,5-lactone
<i>X</i> ₂₈₀	=	2-dehydro-D-gluconate
<i>X</i> ₂₈₁	=	2-dehydrogluconate-6P
<i>X</i> ₂₈₂	=	5-phospho-B-D-ribosylamine
<i>X</i> ₂₈₃	=	5-phosphoribosylglycineamine
<i>X</i> ₂₈₄	=	5-phosphoribosyl-N-formylglycineamide
<i>X</i> ₂₈₅	=	5-phosphoribosyl-N-formylglycineamidine
<i>X</i> ₂₈₆	=	5-aminoimidazoleribonucleotide
<i>X</i> ₂₈₇	=	4-carboxyaminoimidazoleribonucleotide
<i>X</i> ₂₈₈	=	5-phosphoribosyl-4-N-succinocarboxamide-5-aminoimidazole
<i>X</i> ₂₈₉	=	phosphoribosylformamidocarboxamide
<i>X</i> ₂₉₀	=	inosine-5-phosphate
<i>X</i> ₂₉₁	=	adenylosuccinate
<i>X</i> ₂₉₂	=	xanthosine-5-phosphate
<i>X</i> ₂₉₃	=	AMP
<i>X</i> ₂₉₄	=	GMP

X_{295}	=	inosine
X_{296}	=	hypoxanthine
X_{297}	=	xanthosine
X_{298}	=	guanine
X_{299}	=	xanthine
X_{300}	=	urate
X_{301}	=	5-hydroxyisourate
X_{302}	=	5-hydroxy-2-oxo-4-ureido-2,5-dihydro-1H-imidazole-5-carboxylate
X_{303}	=	S-allantoin
X_{304}	=	allantoate
X_{305}	=	ureidoglycine
X_{306}	=	ureidoglycolate
X_{307}	=	urea
X_{308}	=	GDP
X_{309}	=	GTP
X_{310}	=	dGDP
X_{311}	=	dGTP
X_{312}	=	ADP
X_{313}	=	dADP
X_{314}	=	ATP
X_{315}	=	dATP
X_{316}	=	dAMP
X_{317}	=	deoxyadenosine
X_{318}	=	deoxyinosine
X_{319}	=	adenine
X_{320}	=	guanosine
X_{321}	=	NcarbamoylLAspartate
X_{322}	=	dihydroorotate
X_{323}	=	orotate
X_{324}	=	orotidine-5P
X_{325}	=	UMP
X_{326}	=	UDP
X_{327}	=	UTP
X_{328}	=	CTP
X_{329}	=	CMP
X_{330}	=	CDP
X_{331}	=	dCDP
X_{332}	=	dCTP
X_{333}	=	dihydrouracil
X_{334}	=	dUDP
X_{335}	=	uracil
X_{336}	=	dUTP
X_{337}	=	dUMP
X_{338}	=	dTMP
X_{339}	=	dTDP
X_{340}	=	dTTP
X_{341}	=	dCMP
X_{342}	=	deoxycytidine
X_{343}	=	deoxyuridine

X_{344}	=	3-ureidopropionate
X_{345}	=	thymidine
X_{346}	=	thymine
X_{347}	=	dihydrothymine
X_{348}	=	3-ureidoisobutyrate
X_{349}	=	3-aminoisobutanoate
X_{350}	=	cytidine
X_{351}	=	uridine
X_{352}	=	Supplementation of threonine in medium
X_{353}	=	Supplementation of lysine in medium
X_{354}	=	Transporation of threonine to cells
X_{355}	=	Transporation of lysine to cells

V_1 = sucrose*2
 V_2 = glucose6P - fructose6P
 V_3 = fructose6P
 V_4 = fructose16bisP
 V_5 = fructose16bisP - glyceraldehyde3P
 V_6 = fructose16bisP - dihydroxyacetoneP
 V_7 = dihydroxyacetoneP - glyceraldehyde3P
 V_8 = glyceraldehyde3P - 13diPglycerate
 V_9 = 13diPglycerate - 3phosphoglycerate
 V_{10} = 3phosphoglycerate - 2phosphoglycerate
 V_{11} = 2phosphoglycerate - phosphoenolpyruvate
 V_{12} = phosphoenolpyruvate * 6phosphoDgluconate**0.5 / glutamate**0.5
 V_{13} = pyruvate
 V_{14} = 3phosphoglycerate - 3phosphohydroxypyruvate
 V_{15} = 3phosphohydroxypyruvate**0.5*glutamate**0.5
 V_{16} = 3phosphoserine
 V_{17} = Lserine
 V_{18} = Dserine
 V_{19} = Lserine - glycine
 V_{20} = glyoxylate**0.5*glutamate**0.5
 V_{21} = glyoxylate**0.5*Lserine**0.5
 V_{22} = threonine - glycine
 V_{23} = threonine*valine**0.5/isleucine**0.5
 V_{24} = 2oxobutanoate*pyruvate
 V_{25} = 2aceto2hydroxybutyrate
 V_{26} = 23dihydroxy3methylvalerate
 V_{27} = 2keto3methylvalerate**0.5*glutamate**0.5 - isoleucine**0.5*ketoglutarate**0.5
 V_{28} = 2keto3methylvalerate
 V_{29} = S2methylbutyrylCoA
 V_{30} = tigloylCoA
 V_{31} = 2methyl3hydroxybutyrylCoA
 V_{32} = 2methylacetoacetylCoA
 V_{33} = acetylCoA
 V_{34} = pyruvate / isoleucine**0.5 / leucine**0.5 / valine**0.5
 V_{35} = 2acetolactate
 V_{36} = 23dihydroxyisovalerate
 V_{37} = 2ketoisovalerate**0.5*glutamate**0.5 - valine**0.5*ketoglutarate**0.5
 V_{38} = 2ketoisovalerate**0.5*acetylCoA**0.5/leucine**0.5
 V_{39} = 2isopropylmalate
 V_{40} = isopropylmaleate
 V_{41} = 3isopropylmalate
 V_{42} = 2isopropyl3oxosuccinate
 V_{43} = 2ketoisocaproate**0.5*glutamate**0.5 - leucine**0.5*ketoglutarate**0.5
 V_{44} = glutamate
 V_{45} = NacetylLglutamate
 V_{46} = NacetylglutamylP
 V_{47} = NacetylLglutamate5semialdehyde
 V_{48} = NacetylLornithine
 V_{49} = ornithine - citrulline
 V_{50} = carbamoylP - citrulline
 V_{51} = ornithine - carbamoylP
 V_{52} = citrulline
 V_{53} = argininosuccinate/argininosuccinate**0.5
 V_{54} = glutamine
 V_{55} = arginine
 V_{56} = ornithine - glutamateGsemialdehyde
 V_{57} = glutamateGsemialdehyde
 V_{58} = S1pyrroline5carboxylate
 V_{59} = S1pyrroline5carboxylate
 V_{60} = arginine
 V_{61} = citrulline
 V_{62} = citrulline - ornithine**0.5*carbamoylP**0.5
 V_{63} = glutamate
 V_{64} = succinatesemialdehyde
 V_{65} = aspartate**0.5 * ketoglutarate**0.5
 V_{66} = Lserine / cysteine**0.5
 V_{67} = OacetylLserine
 V_{68} = 5phosphoribosyl1pyrophosphate/histidine**0.5
 V_{69} = phosphoribosylATP
 V_{70} = phosphoribosylAMP
 V_{71} = phosphoribosylformiminoAICARP
 V_{72} = phosphoribulosylformiminoAICARP**0.5*glutamine**0.5
 V_{73} = DerythroimidazoleglycerolP
 V_{74} = imidazoleacetolP**0.5*glutamate**0.5
 V_{75} = histidinolP
 V_{76} = histidinol
 V_{77} = histidinal

V_{78} = cysteine
 V_{79} = pyruvate**0.5*glutamate**0.5 – alanine**0.5*ketoglutarate**0.5
 V_{80} = glutamine
 V_{81} = glutamate
 V_{82} = glutamate
 V_{83} = 4aminobutyrate**0.5*pyruvate**0.5
 V_{84} = 4aminobutyrate**0.5*ketoglutarate**0.5
 V_{85} = pyruvate
 V_{86} = citrate
 V_{87} = acetylCoA**0.5 * oxaloacetate**0.5
 V_{88} = citrate
 V_{89} = cisaconitate
 V_{90} = isocitrate
 V_{91} = isocitrate
 V_{92} = ketoglutarate
 V_{93} = glyoxylate
 V_{94} = succinylCoA
 V_{95} = succinate/oxaloacetate**0.5
 V_{96} = fumarate
 V_{97} = malate
 V_{98} = oxaloacetate
 V_{99} = oxaloacetate**0.5*glutamate**0.5
 V_{100} = asparagine
 V_{101} = aspartate**0.5*glutamate**0.5
 V_{102} = aspartate * alanine**0.5 * cysteine**0.5 * isoleucine**0.5 * valine**0.5 * leucine**0.5 * Lserine**0.5 / lysine**0.5 / threonine**0.5 / SadenosylMethionine**0.5
 V_{103} = aspartate4P
 V_{104} = aspartatesemialdehyde / cysteine**0.5 / threonine**0.5
 V_{105} = homoserine
 V_{106} = OphosphoLhomoserine * SadenosylMethionine**0.5
 V_{107} = OphosphoLhomoserine**0.5 * cysteine**0.5 / SadenosylMethionine**0.5
 V_{108} = cystathionine
 V_{109} = aspartatesemialdehyde**0.5 * pyruvate**0.5 / lysine**0.5
 V_{110} = L23dihydrodipicolinate
 V_{111} = tetrahydrodipicolinate**0.5 * glutamate**0.5
 V_{112} = Lldiamionopimelate
 V_{113} = mesodiamionopimelate
 V_{114} = SmethylMethionine**0.5 * homocysteine**0.5
 V_{115} = methionine**0.5 * SadenosylMethionine**0.5
 V_{116} = methionine / SadenosylMethionine**0.5
 V_{117} = SadenosylMethionine
 V_{118} = SadenosylLhomocysteine
 V_{119} = homocysteine
 V_{120} = methionine
 V_{121} = SadenosylMethionine
 V_{122} = Smethyl5thioadenosine
 V_{123} = 5methylthioribose / SadenosylLhomocysteine**0.5
 V_{124} = 5methylthioribose1P
 V_{125} = 5methioribulose1P
 V_{126} = 5methylthio23dioxopentylP
 V_{127} = 2hydroxy3keto5methylthio1phosphopentene
 V_{128} = 12dihydroxy3keto5methylthiopentene
 V_{129} = 2oxo4methylthiobutanoate – methionine
 V_{130} = Derythrose4P**0.5 * phosphoenolpyruvate**0.5
 V_{131} = 3deoxyDarabinoheptulosonate7P
 V_{132} = 3dehydroquininate
 V_{133} = 3dehydroshikimate
 V_{134} = shikimate
 V_{135} = shikimate3P**0.5 * phosphoenolpyruvate**0.5
 V_{136} = 5enolpyruvylshikimate3P
 V_{137} = chorismate * tryptophan**0.5 / phenylalanine**0.5 / tyrosine**0.5
 V_{138} = prephenate**0.5 * glutamate**0.5
 V_{139} = arogenate
 V_{140} = arogenate / tyrosine**0.5
 V_{141} = phenylalanine**0.5 * ketoglutarate**0.5
 V_{142} = phenylalanine**0.5 * pyruvate**0.5
 V_{143} = phenylpyruvate
 V_{144} = phenylacetaldehyde
 V_{145} = tyrosine**0.5 * ketoglutarate**0.5
 V_{146} = phydroxyphenylpyruvate
 V_{147} = homogentisate
 V_{148} = maleylacetoacetate
 V_{149} = 4fumarylacetoacetate
 V_{150} = 4fumarylacetoacetate
 V_{151} = chorismate**0.5 * glutamine**0.5 / tryptophan**0.5
 V_{152} = anthranilate**0.5 * 5phosphoribosyl1pyrophosphate**0.5
 V_{153} = N5phosphoribosylanthranilate
 V_{154} = 1Ocarboxyphenylamino1 deoxyribulose5P

V_{155} = indole3glycerolP
 V_{156} = indole**0.5 * Lserine**0.5
 V_{157} = glutamate**0.5 * cysteine**0.5 / glutathione**0.5
 V_{158} = glutamylcysteine / glutathione**0.5
 V_{159} = pyruvate
 V_{160} = 2methylmalate
 V_{161} = methylmaleate
 V_{162} = 3methylmalate
 V_{163} = lysine - Dlysine
 V_{164} = Dlysine
 V_{165} = diaminohexanoate
 V_{166} = lysine
 V_{167} = hydroxylysine
 V_{168} = acetylhydroxylysine
 V_{169} = lysine - acetyllysine
 V_{170} = lysine
 V_{171} = cadaverine
 V_{172} = piperideine
 V_{173} = lysine
 V_{174} = aminopentanamide - aminopentanoate
 V_{175} = acetamidopentanoate - aminopentanoate
 V_{176} = acetamidooxohexanoate - acetamidopentanoate
 V_{177} = acetyllysine - acetamidooxohexanoate
 V_{178} = aminopentanoate - glutaratesemialdehyde
 V_{179} = glutaratesemialdehyde - glutarate
 V_{180} = glutarate
 V_{181} = lysine
 V_{182} = Nacetyllysine
 V_{183} = lysine
 V_{184} = Nacetyllysine - acetamidooxohexanoate
 V_{185} = acetamidooxohexanoate
 V_{186} = Dlysine
 V_{187} = aminooxohexanoate
 V_{188} = piperideine2carboxylate
 V_{189} = pipecolate
 V_{190} = lysine**0.5 * ketoglutarate**0.5
 V_{191} = saccharopine - aminoadipatesemialdehyde
 V_{192} = piperideine6carboxylate - aminoadipatesemialdehyde
 V_{193} = aminoadipatesemialdehyde
 V_{194} = aminoadipate - oxoadipate
 V_{195} = oxoadipate
 V_{196} = glutaryl dihydrolipoamide - glutarylCoA
 V_{197} = glutarylCoA
 V_{198} = crotonoylCoA
 V_{199} = hydroxybutanoylCoA
 V_{200} = acetoacetylCoA
 V_{201} = 2oxo4methylthiobutanoate
 V_{202} = 22methylthioethylmalate
 V_{203} = 32methylthioethylmalate
 V_{204} = 2oxo5methylthiopentanoicacid
 V_{205} = 23methylthiopropylmalate
 V_{206} = 33methylthiopropylmalate
 V_{207} = 2oxo6methylthiohexanoate
 V_{208} = 24methylthiobutylmalate
 V_{209} = 34methylthiobutylmalate
 V_{210} = 2oxo7methylthioheptanoate
 V_{211} = 25methylthiopentylmalate
 V_{212} = 35methylthiobutylmalate
 V_{213} = 2oxo8methyloctanoate
 V_{214} = 26methylthiohexylmalate
 V_{215} = 36methylthiohexylmalate
 V_{216} = 2oxo9methylnonanoate
 V_{217} = 27methylthioheptylmalate
 V_{218} = 37methylthioheptylmalate
 V_{219} = 2oxo5methylthiopentanoicacid - homomethionine
 V_{220} = homomethionine
 V_{221} = methylthiobutanaldoxime
 V_{222} = methylthiobutanonitrileoxide
 V_{223} = methylthiobutylhydroximoylglutathione
 V_{224} = methylthiobutylhydroximoylcysteinylglycine
 V_{225} = methylthiobutylhydroximate
 V_{226} = methylthiopropyl desulfoglucosinolate
 V_{227} = methylthiopropylglucosinolate
 V_{228} = methylsulfinylpropylglucosinolate
 V_{229} = methylsulfinylpropylglucosinolate
 V_{230} = hydroxypropylglucosinolate
 V_{231} = hydroxypropylglucosinolate

V₂₃₂ = 2oxo6methylthiohexanoate – dihomomethionine
V₂₃₃ = dihomomethionine
V₂₃₄ = methylthiopentanaloxime
V₂₃₅ = methylthiopentanitrileoxide
V₂₃₆ = methylthiopentylhydroximoylglutathione
V₂₃₇ = methylthiopentylhydroximoylcysteinylglycine
V₂₃₈ = methylthiopentylhydroximate
V₂₃₉ = methylthiobutylsulfoglucosinolate
V₂₄₀ = methylthiobutylglucosinolate
V₂₄₁ = methylsulfinylbutylglucosinolate
V₂₄₂ = butenylglucosinolate
V₂₄₃ = hydroxy3butenylglucosinolate
V₂₄₄ = hydroxy3butenylglucosinolate
V₂₄₅ = methylsulfinylbutylglucosinolate
V₂₄₆ = hydroxybutylglucosinolate
V₂₄₇ = hydroxybutylglucosinolate
V₂₄₈ = 2oxo7methylthioheptanoate – trihomomethionine
V₂₄₉ = trihomomethionine
V₂₅₀ = methylthiohexanaloxime
V₂₅₁ = methylthiohexanitrildoxide
V₂₅₂ = methylthiohexylhydroximoylglutathione
V₂₅₃ = methylthiohexylhydroximoylcysteinylglycine
V₂₅₄ = methylthiohexylhydroximate
V₂₅₅ = methylthiopentylsulfoglucosinolate
V₂₅₆ = methylthiopentylglucosinolate
V₂₅₇ = methylsulfinylpentylglucosinolate
V₂₅₈ = 2oxo8methyloctanoate – tetrahomomethionine
V₂₅₉ = tetrahomomethionine
V₂₆₀ = methylthioheptanaloxime
V₂₆₁ = methylthioheptanitrileoxide
V₂₆₂ = methylthioheptylhydroximoylglutathione
V₂₆₃ = methylthioheptylhydroximoylcysteinylglycine
V₂₆₄ = methylthioheptylhydroximate
V₂₆₅ = methylthiohexylsulfoglucosinolate
V₂₆₆ = methylthiohexylglucosinolate
V₂₆₇ = 2oxo9methylononanoate – pentahomomethionine
V₂₆₈ = pentahomomethionine
V₂₆₉ = methylthiooctanaloxime
V₂₇₀ = methylthiooctanitrileoxide
V₂₇₁ = methylthiooctylhydroximoylglutathione
V₂₇₂ = methylthiooctylhydroximoylcysteinylglycine
V₂₇₃ = methylthiooctylhydroximate
V₂₇₄ = methylthioheptylsulfoglucosinolate
V₂₇₅ = methylthioheptylglucosinolate
V₂₇₆ = 2oxo10methylthiodecanoate – hexahomomethionine
V₂₇₇ = hexahomomethionine
V₂₇₈ = methylthiononanaloxime
V₂₇₉ = methylthiononanitrileoxide
V₂₈₀ = methylthiononylhydroximoylglutathione
V₂₈₁ = methylthiononylhydroximoylcysteinylglycine
V₂₈₂ = methylthiononylhydroximate
V₂₈₃ = methylthiooctylsulfoglucosinolate
V₂₈₄ = methylthiooctylglucosinolate
V₂₈₅ = phenylalanine
V₂₈₆ = phenylacetaloxime
V₂₈₇ = phenylacetoneitrileoxide
V₂₈₈ = phenylacetohydroximoylglutathione
V₂₈₉ = phenylacetohydroximoylcysteinylglycine
V₂₉₀ = phenylacetothiohydroximate
V₂₉₁ = benzylsulfoglucosinolate
V₂₉₂ = tryptophan
V₂₉₃ = indole3acetaloxime
V₂₉₄ = indole3acetoneitrileoxide
V₂₉₅ = indole3acetohydroximoylglutathione
V₂₉₆ = indole3acetohydroximoylcysteinylglycine
V₂₉₇ = indolylmethylthiohydroximate
V₂₉₈ = indolylmethylsulfoglucosinolate
V₂₉₉ = indol3ylmethylglucosinolate
V₃₀₀ = 1hydroxy3indolylmethylglucosinolate
V₃₀₁ = indol3ylmethylglucosinolate
V₃₀₂ = 4hydroxy3indolylmethylglucosinolate
V₃₀₃ = histidine
V₃₀₄ = histamine
V₃₀₅ = imidazoleacetaldehyde
V₃₀₆ = imidazole4acetate
V₃₀₇ = imidazoloneacetate
V₃₀₈ = NformiminoLaspertate

V₃₀₉ = NformylLAspartate
V₃₁₀ = glucose6P
V₃₁₁ = Dglucono15lactone6P
V₃₁₂ = glucose6P
V₃₁₃ = 6phosphoDgluconate
V₃₁₄ = Dribose5P – Dribulose5P
V₃₁₅ = Dribose – Dribose5P
V₃₁₆ = Dribose5P – Dribose1P
V₃₁₇ = Dribose1P
V₃₁₈ = Dribose15P
V₃₁₉ = Dribose5P – x5phosphoribosyl1pyrophosphate
V₃₂₀ = Dxylulose5P**0.5 * Dribose5P**0.5 – Dsedoheptulose7P**0.5 * glyceraldehyde3P**0.5
V₃₂₁ = Dsedoheptulose7P**0.5 * glyceraldehyde3P**0.5 – fructose6P**0.5 * Derythrose4P**0.5
V₃₂₂ = Dgluconate
V₃₂₃ = 2dehydroDgluconate – Dgluconate
V₃₂₄ = Dgluconate
V₃₂₅ = 2dehydroDgluconate
V₃₂₆ = 2dehydrogluconate6P
V₃₂₇ = Dglucono15lactone
V₃₂₈ = glucose6P
V₃₂₉ = Dribulose5P
V₃₃₀ = Dxylulose5P**0.5 * Derythrose4P**0.5 – fructose6P**0.5 * glyceraldehyde3P**0.5
V₃₃₁ = cystathionine
V₃₃₂ = homocysteine**0.5 * Lserine**0.5
V₃₃₃ = homocysteine**0.5 * SadenosylLmethionine**0.5
V₃₃₄ = 5phosphoribosyl1pyrophosphate**0.5 * glutamine**0.5
V₃₃₅ = 5phosphoBDribosylamine**0.5 * glycine**0.5
V₃₃₆ = 5phosphoribosylglycineamine
V₃₃₇ = 5phosphoribosylNformylglycineamide**0.5 * glutamine**0.5
V₃₃₈ = 5phosphoribosylNformylglycineamidine
V₃₃₉ = 5aminoimidazoleribonucleotide
V₃₄₀ = 4carboxyaminoimidazoleribonucleotide**0.5 * aspartate**0.5
V₃₄₁ = 5phosphoribosyl4Nsuccinocarboxamide5aminoimidazole
V₃₄₂ = AICAR
V₃₄₃ = phosphoribosylformamidocarboxamide
V₃₄₄ = inosine5phosphate**0.5 * aspartate**0.5
V₃₄₅ = inosine5phosphate
V₃₄₆ = adenylosuccinate
V₃₄₇ = xanthosine5phosphate**0.5 * glutamine**0.5
V₃₄₈ = AMP
V₃₄₉ = inosine5phosphate / adenosine**0.5
V₃₅₀ = inosine
V₃₅₁ = hypoxanthine
V₃₅₂ = inosine5phosphate
V₃₅₃ = xanthosine5phosphate
V₃₅₄ = xanthosine
V₃₅₅ = GMP / adenosine**0.5
V₃₅₆ = guanosine
V₃₅₇ = guanosine
V₃₅₈ = guanine
V₃₅₉ = xanthine
V₃₆₀ = urate
V₃₆₁ = 5hydroxyisourate
V₃₆₂ = 5hydroxy2oxo4ureido25dihydro1Himidazole5carboxylate
V₃₆₃ = Sallantoin
V₃₆₄ = allantoate
V₃₆₅ = ureidoglycine
V₃₆₆ = ureidoglycolate
V₃₆₇ = allantoate
V₃₆₈ = urea
V₃₆₉ = guanosine
V₃₇₀ = guanine**0.5 * 5phosphoribosyl1pyrophosphate**0.5
V₃₇₁ = adenine**0.5 * 5phosphoribosyl1pyrophosphate**0.5
V₃₇₂ = adenosine / adenine**0.5
V₃₇₃ = adenosine
V₃₇₄ = AMP
V₃₇₅ = GMP
V₃₇₆ = GDP
V₃₇₇ = GDP
V₃₇₈ = GTP
V₃₇₉ = dGDP
V₃₈₀ = AMP
V₃₈₁ = ADP
V₃₈₂ = ADP
V₃₈₃ = dADP
V₃₈₄ = ATP
V₃₈₅ = dATP

V₃₈₆ = dAMP
V₃₈₇ = deoxyadenosine
V₃₈₈ = deoxyinosine
V₃₈₉ = dGTP
V₃₉₀ = glutamine
V₃₉₁ = carbamoylP
V₃₉₂ = NcarbamoylLAspartate
V₃₉₃ = dihydroorotate
V₃₉₄ = $\text{orotate}^{**0.5} * 5\text{phosphoribosyl}1\text{pyrophosphate}^{**0.5}$
V₃₉₅ = orotidine5P
V₃₉₆ = UMP
V₃₉₇ = UDP
V₃₉₈ = UDP
V₃₉₉ = UTP
V₄₀₀ = UTP
V₄₀₁ = UTP
V₄₀₂ = CTP
V₄₀₃ = CTP
V₄₀₄ = CDP
V₄₀₅ = CMP
V₄₀₆ = CDP
V₄₀₇ = dCDP - dCTP
V₄₀₈ = CTP
V₄₀₉ = UDP
V₄₁₀ = dCTP
V₄₁₁ = UTP
V₄₁₂ = dUDP
V₄₁₃ = dUTP
V₄₁₄ = dUMP
V₄₁₅ = dTMP
V₄₁₆ = dTDP
V₄₁₇ = dTTP
V₄₁₈ = dCMP
V₄₁₉ = dCDP
V₄₂₀ = dCMP
V₄₂₁ = dCMP
V₄₂₂ = deoxycytidine
V₄₂₃ = deoxyuridine
V₄₂₄ = dUMP
V₄₂₅ = dTMP
V₄₂₆ = thymidine
V₄₂₇ = thymidine
V₄₂₈ = thymine
V₄₂₉ = dihydrothymine
V₄₃₀ = 3ureidoisobutyrate
V₄₃₁ = 3aminoisobutanoate
V₄₃₂ = CMP
V₄₃₃ = cytidine
V₄₃₄ = uridine
V₄₃₅ = $\text{uracil}^{**0.5} * 5\text{phosphoribosyl}1\text{pyrophosphate}^{**0.5}$
V₄₃₆ = UMP
V₄₃₇ = $\text{uridine}^{**0.5} * \text{GTP}^{**0.5}$
V₄₃₈ = uracil
V₄₃₉ = dihydrouracil
V₄₄₀ = 3ureidopropionate
V₄₄₁ = methionine

$$\begin{aligned}
f_1 &= a2*(0) \\
f_2 &= a2*(V_1 - V_2 - V_{310} - V_{312} - V_{328}) \\
f_3 &= a2*(V_2 + V_4 - V_3 + V_{330} + V_{321}) \\
f_4 &= a2*(V_3 - V_4 - V_5 - V_6) \\
f_5 &= a2*(V_5 + V_7 - V_8 + V_{320} - V_{321} + V_{330}) \\
f_6 &= a2*(V_6 - V_7) \\
f_7 &= a2*(V_8 - V_9) \\
f_8 &= a2*(V_9 - V_{10} - V_{14}) \\
f_9 &= a2*(V_{10} - V_{11}) \\
f_{10} &= a2*(V_{11} + V_{13} - V_{12}) \\
f_{11} &= a2*(V_{12} - V_{13} - V_{34} + V_{18} - V_{79} - V_{85} - V_{159} - \text{pyruvate}) \\
f_{12} &= a2*(V_{34} - V_{35}) \\
f_{13} &= a2*(V_{35} - V_{36}) \\
f_{14} &= a2*(V_{36} - V_{37} - V_{38}) \\
f_{15} &= a2*(V_{38} - V_{39}) \\
f_{16} &= a2*(V_{39} - V_{40}) \\
f_{17} &= a2*(V_{40} - V_{41}) \\
f_{18} &= a2*(V_{41} - V_{42}) \\
f_{19} &= a2*(V_{42} - V_{43}) \\
f_{20} &= a2*(V_{43} - \text{leucine}) \\
f_{21} &= a2*(V_{14} - V_{15}) \\
f_{22} &= a2*(V_{15} - V_{16}) \\
f_{23} &= a1*(V_{16} - V_{17} - V_{66} - V_{19} - \text{Lserine}) \\
f_{24} &= a1*(V_{17} - V_{18}) \\
f_{25} &= a2*(V_{19} + V_{20} + V_{21} + V_{22} - \text{glycine}) \\
f_{26} &= a2*(V_{106} - V_{22} - V_{23} - \text{threonine}) + 0.04*X353 \\
f_{27} &= a2*(V_{23} - V_{24} + V_{162} + V_{441}) \\
f_{28} &= a2*(V_{24} - V_{25}) \\
f_{29} &= a2*(V_{25} - V_{26}) \\
f_{30} &= a2*(V_{26} - V_{27} - V_{28}) \\
f_{31} &= a2*(V_{27} - \text{isoleucine}) \\
f_{32} &= a2*(V_{28} - V_{29}) \\
f_{33} &= a2*(V_{29} - V_{30}) \\
f_{34} &= a2*(V_{30} - V_{31}) \\
f_{35} &= a2*(V_{31} - V_{32}) \\
f_{36} &= a2*(V_{32} - V_{33} + V_{85} + V_{86} + V_{200}) \\
f_{37} &= a2*(V_{80} - V_{44} - V_{81} - V_{82} - V_{63} + V_{58} + V_{65}/2 - V_{157}/2 - V_{74}/2 - \text{glutamate}) \\
f_{38} &= a2*(V_{44} - V_{45}) \\
f_{39} &= a2*(V_{45} - V_{46}) \\
f_{40} &= a2*(V_{46} - V_{47}) \\
f_{41} &= a2*(V_{47} - V_{48}) \\
f_{42} &= a3*(V_{48} - V_{49} - V_{51} + V_{55} - V_{56} + V_{61} + V_{62}) \\
f_{43} &= a2*(V_{51} + V_{54} - V_{50} - V_{391}) \\
f_{44} &= a2*(V_{63} - V_{54} - V_{80} + \text{constant} - \text{glutamine} - V_{72}/2) \\
f_{45} &= a2*(V_{49} + V_{50} - V_{52} + V_{60} - V_{61} - V_{62}) \\
f_{46} &= a2*(V_{52} - V_{53}) \\
f_{47} &= a2*(V_{53} - V_{55} - V_{60} - \text{arginine}) \\
f_{48} &= a3*(V_{56} - V_{57}) \\
f_{49} &= a3*(V_{57} - V_{58} - V_{59}) \\
f_{50} &= a3*(V_{59} - \text{proline}) \\
f_{51} &= a2*(V_{66} - V_{67}) \\
f_{52} &= a2*(V_{319} + V_{318} - V_{68} - V_{334} - V_{370}/2 - V_{371}/2 - V_{394}/2) \\
f_{53} &= a2*(V_{68} - V_{69}) \\
f_{54} &= a2*(V_{69} - V_{70}) \\
f_{55} &= a2*(V_{70} - V_{71}) \\
f_{56} &= a2*(V_{71} - V_{72}/2) \\
f_{57} &= a2*(V_{341} - V_{342} + V_{72}/2) \\
f_{58} &= a2*(V_{72}/2 - V_{73}) \\
f_{59} &= a2*(V_{73} - V_{74}/2) \\
f_{60} &= a2*(V_{74} - V_{75}) \\
f_{61} &= a2*(V_{75} - V_{76}) \\
f_{62} &= a2*(V_{76} - V_{77})
\end{aligned}$$

f_{63}	=	$a2*(V_{77} - \text{histidine} - V_{303}$)	
f_{64}	=	$a2*(V_{87} - V_{88} - V_{86}$)	
f_{65}	=	$a2*(V_{88} - V_{89}$)	
f_{66}	=	$a2*(V_{89} - V_{90} - V_{91}$)	
f_{67}	=	$a2*(V_{90} - V_{92} + V_{81} - V_{65}/2 - V_{190}/2$)	
f_{68}	=	$a2*(V_{92} - V_{94}$)	
f_{69}	=	$a2*(V_{94} - V_{95} + V_{64}$)	
f_{70}	=	$a2*(V_{95} - V_{96} + V_{150}$)	
f_{71}	=	$a2*(V_{96} + V_{93} - V_{97}$)	
f_{72}	=	$a2*(V_{97} - V_{87} + V_{65}/2$)	
f_{73}	=	$a0*(V_{79} + V_{78} + V_{440} - \text{alanine}$)	
f_{74}	=	$a2*(V_{67} - V_{78} - V_{157}/2 - \text{cysteine}$)	
f_{75}	=	$a2*(V_{82} - V_{83} - V_{84}$)	
f_{76}	=	$a2*(V_{83} + V_{84} - V_{64}$)	
f_{77}	=	$a2*(V_{101} - V_{100} - \text{asparagine}$)	
f_{78}	=	$a2*(V_{100} - V_{101} - V_{102} - V_{65}/2 + V_{309} - \text{aspartate}$)	
f_{79}	=	$a2*(V_{102} - V_{103}$)	
f_{80}	=	$a2*(V_{103} - V_{104} - V_{109}$)	
f_{81}	=	$a2*(V_{104} - V_{105}$)	
f_{82}	=	$a2*(V_{105} - V_{106} - V_{107}$)	
f_{83}	=	$a3*(V_{107} - V_{108} + V_{332}$)	
f_{84}	=	$a3*(V_{118}/2 - V_{119} + V_{108} - V_{114}/2 - V_{332} - V_{333}/2$)	
f_{85}	=	$a3*(V_{129} - V_{120} + V_{119} - V_{116} + V_{114} - V_{115}/2 - \text{methionine} + V_{333}/2 + V_{441}$)	
f_{86}	=	$a3*(V_{120} - V_{121} + V_{116} - V_{117} - V_{115}/2 - V_{333}/2$)	
f_{87}	=	$a3*(V_{117} - V_{118} + V_{115}/2 + V_{333}/2$)	
f_{88}	=	$a3*(V_{374} - V_{373} - V_{372} + V_{118}/2$)	
f_{89}	=	$a2*(V_{109} - V_{110}$)	
f_{90}	=	$a2*(V_{110} - V_{111}$)	
f_{91}	=	$a2*(V_{111} - V_{112}$)	
f_{92}	=	$a2*(V_{112} - V_{113}$)	
f_{93}	=	$a2*(V_{113} - \text{lysine} + V_{182} - V_{181} - V_{163} - V_{166} - V_{169} - V_{173} - V_{170} - V_{190}/2 - V_{183}$) +	0.011*X355
f_{94}	=	$a2*(V_{121} - V_{122}$)	
f_{95}	=	$a2*(V_{122} - V_{123}$)	
f_{96}	=	$a2*(V_{123} - V_{124}$)	
f_{97}	=	$a2*(V_{124} - V_{125}$)	
f_{98}	=	$a2*(V_{125} - V_{126}$)	
f_{99}	=	$a2*(V_{126} - V_{127}$)	
f_{100}	=	$a2*(V_{127} - V_{128}$)	
f_{101}	=	$a2*(V_{128} - V_{129} - V_{201}$)	
f_{102}	=	$a2*(V_{130} - V_{131}$)	
f_{103}	=	$a2*(V_{131} - V_{132}$)	
f_{104}	=	$a2*(V_{132} - V_{133}$)	
f_{105}	=	$a2*(V_{133} - V_{134}$)	
f_{106}	=	$a2*(V_{134} - V_{135}$)	
f_{107}	=	$a2*(V_{135} - V_{136}$)	
f_{108}	=	$a2*(V_{137} - V_{138}$)	
f_{109}	=	$a2*(V_{138} - V_{139} - V_{140}$)	
f_{110}	=	$a2*(V_{139} - V_{141} - V_{142} - V_{285} - \text{phenylalanine}$)	
f_{111}	=	$a2*(V_{141} + V_{142} - V_{143}$)	
f_{112}	=	$a2*(V_{143} - V_{144}$)	
f_{113}	=	$a2*(V_{140} - V_{145} - \text{tyrosine}$)	
f_{114}	=	$a2*(V_{145} - V_{146}$)	
f_{115}	=	$a2*(V_{146} - V_{147}$)	
f_{116}	=	$a2*(V_{147} - V_{148}$)	
f_{117}	=	$a2*(V_{148} - V_{149} - V_{150}$)	
f_{118}	=	$a2*(V_{151} - V_{152}$)	
f_{119}	=	$a2*(V_{152} - V_{153}$)	
f_{120}	=	$a2*(V_{153} - V_{154}$)	
f_{121}	=	$a2*(V_{154} - V_{155}$)	
f_{122}	=	$a2*(V_{155} - V_{156}$)	
f_{123}	=	$a2*(V_{156} - V_{292} - \text{tryptophan}$)	
f_{124}	=	$a2*(V_{37} - \text{valine}$)	

$$\begin{aligned}
f_{125} &= a2*(V_{91} - V_{93} - V_{20} - V_{21}) &&) \\
f_{126} &= a3*(V_{115}/2 - V_{114}/2) &&) \\
f_{127} &= a2*(V_{136} - V_{137} - V_{151}) &&) \\
f_{128} &= a2*(V_{157} - V_{158}) &&) \\
f_{129} &= a2*(V_{158} - \text{glutathione}) &&) \\
f_{130} &= a2*(V_{159} - V_{160}) &&) \\
f_{131} &= a2*(V_{160} - V_{161}) &&) \\
f_{132} &= a2*(V_{161} - V_{162}) &&) \\
f_{133} &= a3*(V_{166} - V_{167}) &&) \\
f_{134} &= a3*(V_{167} - V_{168}) &&) \\
f_{135} &= a3*(V_{163} - V_{164} - V_{186}) &&) \\
f_{136} &= a3*(V_{164} - V_{165}) &&) \\
f_{137} &= a3*(V_{181} - V_{182} - V_{184}) &&) \\
f_{138} &= a3*(V_{184} - V_{185} + V_{177} - V_{176}) &&) \\
f_{139} &= a3*(V_{183} + V_{185} + V_{186} - V_{187}) &&) \\
f_{140} &= a3*(V_{187} - V_{188}) &&) \\
f_{141} &= a3*(V_{188} - V_{189}) &&) \\
f_{142} &= a3*(V_{189} - V_{192}) &&) \\
f_{143} &= a3*(V_{192} + V_{191} - V_{193}) &&) \\
f_{144} &= a3*(V_{190} - V_{191}) &&) \\
f_{145} &= a3*(V_{170} - V_{171}) &&) \\
f_{146} &= a3*(V_{171} - V_{172}) &&) \\
f_{147} &= a3*(V_{173} - V_{174}) &&) \\
f_{148} &= a3*(V_{172} + V_{174} + V_{175} - V_{178}) &&) \\
f_{149} &= a3*(V_{169} - V_{177}) &&) \\
f_{150} &= a3*(V_{176} - V_{175}) &&) \\
f_{151} &= a3*(V_{178} - V_{179}) &&) \\
f_{152} &= a3*(V_{179} - V_{180}) &&) \\
f_{153} &= a3*(V_{193} - V_{194}) &&) \\
f_{154} &= a3*(V_{194} - V_{195}) &&) \\
f_{155} &= a3*(V_{195} - V_{196}) &&) \\
f_{156} &= a3*(V_{196} + V_{180} - V_{197}) &&) \\
f_{157} &= a3*(V_{197} - V_{198}) &&) \\
f_{158} &= a3*(V_{198} - V_{199}) &&) \\
f_{159} &= a3*(V_{199} - V_{200}) &&) \\
f_{160} &= a2*(V_{201} - V_{202}) &&) \\
f_{161} &= a2*(V_{202} - V_{203}) &&) \\
f_{162} &= a2*(V_{203} - V_{204} - V_{219}) &&) \\
f_{163} &= a2*(V_{204} - V_{205}) &&) \\
f_{164} &= a2*(V_{205} - V_{206}) &&) \\
f_{165} &= a2*(V_{206} - V_{207} - V_{232}) &&) \\
f_{166} &= a2*(V_{207} - V_{208}) &&) \\
f_{167} &= a2*(V_{208} - V_{209}) &&) \\
f_{168} &= a2*(V_{209} - V_{210} - V_{248}) &&) \\
f_{169} &= a2*(V_{210} - V_{211}) &&) \\
f_{170} &= a2*(V_{211} - V_{212}) &&) \\
f_{171} &= a2*(V_{212} - V_{213} - V_{258}) &&) \\
f_{172} &= a2*(V_{213} - V_{214}) &&) \\
f_{173} &= a2*(V_{214} - V_{215}) &&) \\
f_{174} &= a2*(V_{215} - V_{216} - V_{267}) &&) \\
f_{175} &= a2*(V_{216} - V_{217}) &&) \\
f_{176} &= a2*(V_{217} - V_{218}) &&) \\
f_{177} &= a2*(V_{218} - V_{276}) &&) \\
f_{178} &= a2*(V_{219} - V_{220}) &&) \\
f_{179} &= a2*(V_{220} - V_{221}) &&) \\
f_{180} &= a2*(V_{221} - V_{222}) &&) \\
f_{181} &= a2*(V_{222} - V_{223}) &&) \\
f_{182} &= a2*(V_{223} - V_{224}) &&) \\
f_{183} &= a2*(V_{224} - V_{225}) &&) \\
f_{184} &= a2*(V_{225} - V_{226}) &&) \\
f_{185} &= a2*(V_{226} - V_{227}) &&) \\
f_{186} &= a2*(V_{227} - V_{228} - V_{229}) &&)
\end{aligned}$$

$$\begin{aligned}
f_{187} &= a2*(V_{228} - X_{187}) &&) \\
f_{188} &= a2*(V_{229} - V_{230} - V_{231}) &&) \\
f_{189} &= a2*(V_{230} - X_{189}) &&) \\
f_{190} &= a2*(V_{231} - X_{190}) &&) \\
f_{191} &= a2*(V_{232} - V_{233}) &&) \\
f_{192} &= a2*(V_{233} - V_{234}) &&) \\
f_{193} &= a2*(V_{234} - V_{235}) &&) \\
f_{194} &= a2*(V_{235} - V_{236}) &&) \\
f_{195} &= a2*(V_{236} - V_{237}) &&) \\
f_{196} &= a2*(V_{237} - V_{238}) &&) \\
f_{197} &= a2*(V_{238} - V_{239}) &&) \\
f_{198} &= a2*(V_{239} - V_{240}) &&) \\
f_{199} &= a2*(V_{240} - V_{241} - V_{245}) &&) \\
f_{200} &= a2*(V_{241} - V_{242}) &&) \\
f_{201} &= a2*(V_{242} - V_{243} - V_{244}) &&) \\
f_{202} &= a2*(V_{243} - X_{202}) &&) \\
f_{203} &= a2*(V_{244} - X_{203}) &&) \\
f_{204} &= a2*(V_{245} - V_{246} - V_{247}) &&) \\
f_{205} &= a2*(V_{246} - X_{205}) &&) \\
f_{206} &= a2*(V_{247} - X_{206}) &&) \\
f_{207} &= a2*(V_{248} - V_{249}) &&) \\
f_{208} &= a2*(V_{249} - V_{250}) &&) \\
f_{209} &= a2*(V_{250} - V_{251}) &&) \\
f_{210} &= a2*(V_{251} - V_{252}) &&) \\
f_{211} &= a2*(V_{252} - V_{253}) &&) \\
f_{212} &= a2*(V_{253} - V_{254}) &&) \\
f_{213} &= a2*(V_{254} - V_{255}) &&) \\
f_{214} &= a2*(V_{255} - V_{256}) &&) \\
f_{215} &= a2*(V_{256} - V_{257}) &&) \\
f_{216} &= a2*(V_{257} - X_{216}) &&) \\
f_{217} &= a2*(V_{258} - V_{259}) &&) \\
f_{218} &= a2*(V_{259} - V_{260}) &&) \\
f_{219} &= a2*(V_{260} - V_{261}) &&) \\
f_{220} &= a2*(V_{261} - V_{262}) &&) \\
f_{221} &= a2*(V_{262} - V_{263}) &&) \\
f_{222} &= a2*(V_{263} - V_{264}) &&) \\
f_{223} &= a2*(V_{264} - V_{265}) &&) \\
f_{224} &= a2*(V_{265} - V_{266}) &&) \\
f_{225} &= a2*(V_{266} - X_{225}) &&) \\
f_{226} &= a2*(V_{267} - V_{268}) &&) \\
f_{227} &= a2*(V_{268} - V_{269}) &&) \\
f_{228} &= a2*(V_{269} - V_{270}) &&) \\
f_{229} &= a2*(V_{270} - V_{271}) &&) \\
f_{230} &= a2*(V_{271} - V_{272}) &&) \\
f_{231} &= a2*(V_{272} - V_{273}) &&) \\
f_{232} &= a2*(V_{273} - V_{274}) &&) \\
f_{233} &= a2*(V_{274} - V_{275}) &&) \\
f_{234} &= a2*(V_{275} - X_{234}) &&) \\
f_{235} &= a2*(V_{276} - V_{277}) &&) \\
f_{236} &= a2*(V_{277} - V_{278}) &&) \\
f_{237} &= a2*(V_{278} - V_{279}) &&) \\
f_{238} &= a2*(V_{279} - V_{280}) &&) \\
f_{239} &= a2*(V_{280} - V_{281}) &&) \\
f_{240} &= a2*(V_{281} - V_{282}) &&) \\
f_{241} &= a2*(V_{282} - V_{283}) &&) \\
f_{242} &= a2*(V_{283} - V_{284}) &&) \\
f_{243} &= a2*(V_{284} - X_{243}) &&) \\
f_{244} &= a2*(V_{285} - V_{286}) &&) \\
f_{245} &= a2*(V_{286} - V_{287}) &&) \\
f_{246} &= a2*(V_{287} - V_{288}) &&) \\
f_{247} &= a2*(V_{288} - V_{289}) &&) \\
f_{248} &= a2*(V_{289} - V_{290}) &&)
\end{aligned}$$

$$\begin{aligned}
f_{249} &= a2*(V_{290} - V_{291}) \\
f_{250} &= a2*(V_{291} - X_{250}) \\
f_{251} &= a2*(V_{292} - V_{293}) \\
f_{252} &= a2*(V_{293} - V_{294}) \\
f_{253} &= a2*(V_{294} - V_{295}) \\
f_{254} &= a2*(V_{295} - V_{296}) \\
f_{255} &= a2*(V_{296} - V_{297}) \\
f_{256} &= a2*(V_{297} - V_{298}) \\
f_{257} &= a2*(V_{298} - V_{299} - V_{301}) \\
f_{258} &= a2*(V_{299} - V_{300}) \\
f_{259} &= a2*(V_{300} - X_{259}) \\
f_{260} &= a2*(V_{301} - V_{302}) \\
f_{261} &= a2*(V_{302} - X_{261}) \\
f_{262} &= a2*(V_{303} - V_{304}) \\
f_{263} &= a2*(V_{304} - V_{305}) \\
f_{264} &= a2*(V_{305} - V_{306}) \\
f_{265} &= a2*(V_{306} - V_{307}) \\
f_{266} &= a2*(V_{307} - V_{308}) \\
f_{267} &= a2*(V_{308} - V_{309}) \\
f_{268} &= a2*(V_{310} - V_{311}) \\
f_{269} &= a2*(V_{311} + V_{312} + V_{322} + V_{326} - V_{313}) \\
f_{270} &= a2*(V_{313} + V_{314} - V_{329}) \\
f_{271} &= a2*(- V_{314} - V_{316} - V_{319} - V_{320}) \\
f_{272} &= a2*(0) \\
f_{273} &= a2*(V_{316} - V_{317}) \\
f_{274} &= a2*(V_{317} - V_{318}) \\
f_{275} &= a2*(V_{329} - V_{330} - V_{320}) \\
f_{276} &= a2*(V_{321} - V_{330} - V_{130}) \\
f_{277} &= a2*(V_{320} - V_{321}) \\
f_{278} &= a2*(V_{327} - V_{324} + V_{323} - V_{322}) \\
f_{279} &= a2*(V_{328} - V_{327}) \\
f_{280} &= a2*(V_{324} - V_{323} - V_{325}) \\
f_{281} &= a2*(V_{325} - V_{326}) \\
f_{282} &= a2*(V_{334} - V_{335}) \\
f_{283} &= a2*(V_{335} - V_{336}) \\
f_{284} &= a2*(V_{336} - V_{337}) \\
f_{285} &= a2*(V_{337} - V_{338}) \\
f_{286} &= a2*(V_{338} - V_{339}) \\
f_{287} &= a2*(V_{339} - V_{340}) \\
f_{288} &= a2*(V_{340} - V_{341}) \\
f_{289} &= a2*(V_{342} - V_{343}) \\
f_{290} &= a2*(V_{343} - V_{344} - V_{345} + V_{348} - V_{349} - V_{352}) \\
f_{291} &= a2*(V_{344} - V_{346}) \\
f_{292} &= a2*(V_{345} - V_{347} + V_{352} - V_{353}) \\
f_{293} &= a2*(V_{346} - V_{374} + V_{373} + V_{371} - V_{348} - V_{380}) \\
f_{294} &= a2*(V_{347} - V_{355} + V_{369} + V_{370} - V_{375}) \\
f_{295} &= a2*(V_{349} - V_{350}) \\
f_{296} &= a2*(V_{350} - V_{351} + V_{388}) \\
f_{297} &= a2*(V_{353} + V_{356} - V_{354}) \\
f_{298} &= a2*(V_{357} - V_{358} - V_{370}/2) \\
f_{299} &= a2*(V_{351} + V_{354} + V_{358} - V_{359}) \\
f_{300} &= a2*(V_{359} - V_{360}) \\
f_{301} &= a2*(V_{360} - V_{361}) \\
f_{302} &= a2*(V_{361} - V_{362}) \\
f_{303} &= a2*(V_{362} - V_{363}) \\
f_{304} &= a2*(V_{363} - V_{364} - V_{367}) \\
f_{305} &= a2*(V_{364} - V_{365}) \\
f_{306} &= a2*(V_{365} - V_{366}) \\
f_{307} &= a2*(V_{366} + V_{367} - V_{368}) \\
f_{308} &= a2*(V_{375} - V_{376} - V_{377}) \\
f_{309} &= a2*(V_{377} - V_{378}) \\
f_{310} &= a2*(V_{376} - V_{379})
\end{aligned}$$

$$\begin{aligned}
f_{311} &= a2*(V_{378} + V_{379} - V_{389}) \\
f_{312} &= a2*(V_{380} - V_{381} - V_{382}) \\
f_{313} &= a2*(V_{381} - V_{383}) \\
f_{314} &= a2*(V_{382} - V_{384}) \\
f_{315} &= a2*(V_{383} + V_{384} - V_{385}) \\
f_{316} &= a2*(V_{385} - V_{386}) \\
f_{317} &= a2*(V_{386} - V_{387}) \\
f_{318} &= a2*(V_{387} - V_{388}) \\
f_{319} &= a2*(V_{372} - V_{371}/2) \\
f_{320} &= a2*(V_{355} - V_{357} - V_{369} - V_{356}) \\
f_{321} &= a2*(V_{391} - V_{392}) \\
f_{322} &= a2*(V_{392} - V_{393}) \\
f_{323} &= a2*(V_{393} - V_{394}/2) \\
f_{324} &= a2*(V_{394} - V_{395}) \\
f_{325} &= a2*(V_{395} + V_{397} + V_{400} - V_{396} + V_{437} - V_{436} + V_{435}) \\
f_{326} &= a2*(V_{396} + V_{399} - V_{398} - V_{397} - V_{409}) \\
f_{327} &= a2*(V_{398} - V_{399} - V_{400} - V_{401} - V_{411}) \\
f_{328} &= a2*(V_{401} - V_{402} - V_{403} - V_{408}) \\
f_{329} &= a2*(V_{402} + V_{404} - V_{405} - V_{432}) \\
f_{330} &= a2*(V_{403} - V_{404} + V_{405} - V_{406}) \\
f_{331} &= a2*(V_{406} - V_{407} + V_{418} - V_{419}) \\
f_{332} &= a2*(V_{407} + V_{408} - V_{410}) \\
f_{333} &= a2*(V_{438} - V_{439}) \\
f_{334} &= a2*(V_{409} - V_{412}) \\
f_{335} &= a2*(V_{434} - V_{435} - V_{438}) \\
f_{336} &= a2*(V_{410} + V_{411} + V_{412} - V_{413}) \\
f_{337} &= a2*(V_{413} - V_{414} + V_{420} + V_{423}) \\
f_{338} &= a2*(V_{414} - V_{415} - V_{425} + V_{426}) \\
f_{339} &= a2*(V_{415} - V_{416}) \\
f_{340} &= a2*(V_{416} - V_{417}) \\
f_{341} &= a2*(V_{419} - V_{418} - V_{421} - V_{420}) \\
f_{342} &= a2*(V_{421} - V_{422}) \\
f_{343} &= a2*(V_{422} - V_{423}) \\
f_{344} &= a2*(V_{439} - V_{440}) \\
f_{345} &= a2*(V_{425} - V_{426} - V_{427}) \\
f_{346} &= a2*(V_{427} - V_{428}) \\
f_{347} &= a2*(V_{428} - V_{429}) \\
f_{348} &= a2*(V_{429} - V_{430}) \\
f_{349} &= a2*(V_{430} - V_{431}) \\
f_{350} &= a2*(V_{432} - V_{433}) \\
f_{351} &= a2*(V_{433} + V_{436} - V_{437} - V_{434})
\end{aligned}$$

#Supplementation

$$\begin{aligned}
f_{352} &= -0.04*X_{352} \\
f_{353} &= 0.04*X_{352} - 0.04*X_{353} \\
f_{354} &= -0.011*X_{354} \\
f_{355} &= 0.011*X_{354} + 0.011*X_{355}
\end{aligned}$$

No.	Simulation	AminoAcidAnalysis	MetabolomeAnalysis	CorrMetabolomeSimulation	CorrAminoAcidSimulation	CorrMetabolomeAminoAcid	pValMetabolomeSimulation	pValAminoAcidSimulation	pValMetabolomeAminoAcid
X ₁	sucrose			0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₂	glucose-6P			0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₃	fructose-6P		4i_D-Fructose-6-phosphate disodium salt	0.755	0.000	0.000	5.417E-03	0.000E+00	0.000E+00
X ₄	fructose-1,6-bis-P			0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₅	glyceraldehyde-3-P			0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₆	dihydroxyacetone-P			0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₇	1,3-diPglycerate			0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₈	3-phosphoglycerate			0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₉	2-phosphoglycerate			0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₁₀	phosphoenolpyruvate			0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₁₁	pyruvate			0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₁₂	2-acetolactate			0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₁₃	2,3-dihydroxyisovalerate			0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₁₄	2-ketoisovalerate			0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₁₅	2-isopropylmalate			0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₁₆	isopropylmaleate			0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₁₇	3-isopropylmalate			0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₁₈	2-isopropyl-3-oxosuccinate			0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₁₉	2-ketoisocaproate			0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₂₀	leucine	Leu	L-Leucine- (Cell Culture Reagent- Cry	-0.678	-0.751	0.654	1.982E+00	1.989E+00	1.982E+00
X ₂₁	3-phosphohydroxypyruvate			0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₂₂	3-phosphoserine		o-Phospho-L-serine	-0.079	0.000	0.000	1.184E+00	0.000E+00	0.000E+00
X ₂₃	Lserine	Ser	L-Serine	0.816	0.807	0.887	1.396E-03	1.624E-03	1.396E-03
X ₂₄	Dserine			0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₂₅	glycine	Gly	Glycine	0.118	0.739	-0.073	7.275E-01	6.090E-01	7.275E-01
X ₂₆	threonine	Thr	L-allo-threonine	0.811	0.871	0.955	1.573E-03	4.364E-04	1.573E-03
X ₂₇	2-oxobutanoate			0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₂₈	2-aceto-2-hydroxybutyrate			0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₂₉	2,3-dihydroxy-3-methylvalerate			0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₃₀	2-keto-3-methylvalerate			0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₃₁	isoleucine	Ile	L-Isoleucine	-0.811	-0.889	0.784	1.998E+00	2.000E+00	1.998E+00
X ₃₂	S-2-methylbutyryl-CoA			0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₃₃	tigloylCoA			0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₃₄	2-methyl-3-hydroxybutyryl-CoA			0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₃₅	2-methylacetoacetyl-CoA			0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₃₆	acetylCoA			0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₃₇	glutamate	Glu	L-Glutamic acid	0.594	-0.226	0.148	4.855E-02	9.432E-02	4.855E-02
X ₃₈	N-acetyl-L-glutamate		N-Acetyl-DL-glutamic acid	0.317	0.000	0.000	3.368E-01	0.000E+00	0.000E+00
X ₃₉	N-acetylglutamyl-P			0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₄₀	N-acetyl-L-glutamate-5-semialdehyde			0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₄₁	N-acetyl-L-ornithine			0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₄₂	ornithine		L-Ornithine monohydrochloride	0.550	0.000	0.000	7.409E-02	0.000E+00	0.000E+00
X ₄₃	carbamoyl-P			0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₄₄	glutamine	Gln	L-Glutamine	0.736	0.427	0.464	7.632E-03	3.279E-02	7.632E-03
X ₄₅	citrulline			0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₄₆	argininosuccinate			0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₄₇	arginine			0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₄₈	glutamate-gamma-semialdehyde			0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₄₉	S-1-pyrroline-5-carboxylate			0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₅₀	proline	Pro	L-Proline	0.921	0.869	0.988	2.005E-05	1.631E-04	2.005E-05
X ₅₁	O-acetyl-L-serine		O-acetyl-L-serine hydrochloride	-0.735	0.000	0.000	1.992E+00	0.000E+00	0.000E+00
X ₅₂	5-phosphoribosyl-1-pyrophosphate			0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₅₃	phosphoribosylATP			0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₅₄	phosphoribosylAMP			0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₅₅	phosphoribosylformiminoAICARP			0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₅₆	phosphoribuloylformiminoAICARP			0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₅₇	AICAR			0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₅₈	D-erythroimidazoleglycerol-P			0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₅₉	imidazoleacetol-P			0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₆₀	histidinolP			0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00

X ₆₁	histidinol			0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₆₂	histidinal			0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₆₃	histidine		L-Histidine	0.854	0.000	0.000	4.545E-04	0.000E+00	0.000E+00
X ₆₄	citrate		Citric acid-Anhydrous	0.199	0.000	0.000	5.546E-01	0.000E+00	0.000E+00
X ₆₅	cisaconitate		cis-Aconitic Acid	-0.367	0.000	0.000	1.739E+00	0.000E+00	0.000E+00
X ₆₆	isocitrate		DL-Isocitric acid trisodium salt	0.095	0.000	0.000	7.810E-01	0.000E+00	0.000E+00
X ₆₇	ketoglutarate			0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₆₈	succinyl-CoA			0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₆₉	succinate			0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₇₀	fumarate		Fumaric acid	-0.253	0.000	0.000	1.551E+00	0.000E+00	0.000E+00
X ₇₁	malate		DL-Malic acid	0.810	0.000	0.000	1.650E-03	0.000E+00	0.000E+00
X ₇₂	oxaloacetate			0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₇₃	alanine	Ala	2i_L-Alanine_Sarcosine	0.908	0.704	0.911	4.314E-05	2.768E-03	4.314E-05
X ₇₄	cysteine		DL-Cysteine	0.772	0.000	0.000	3.842E-03	0.000E+00	0.000E+00
X ₇₅	4-aminobutyrate		3i_L-2-Aminobutyric acid_N-N-Dimethy	-0.469	0.000	0.000	1.860E+00	0.000E+00	0.000E+00
X ₇₆	succinatesemialdehyde			0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₇₇	asparagine	Asn	L-Asparagine	0.390	0.412	0.021	2.302E-01	2.256E-01	2.302E-01
X ₇₈	aspartate	Asp	L-Aspartic acid	0.287	-0.690	-0.474	3.886E-01	2.601E-01	3.886E-01
X ₇₉	aspartate-4P			0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₈₀	aspartatesemialdehyde			0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₈₁	homoserine			0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₈₂	O-phospho-L-homoserine			0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₈₃	cystathionine		Cystathionine	0.732	0.000	0.000	8.053E-03	0.000E+00	0.000E+00
X ₈₄	homocysteine		DL-homocysteine	0.919	0.000	0.000	2.288E-05	0.000E+00	0.000E+00
X ₈₅	methionine		L-Methionine	0.702	0.000	0.000	1.310E-02	0.000E+00	0.000E+00
X ₈₆	S-adenosyl-L-methionine		S-(5'-Adenosyl)-L-methionine chloride	0.884	0.000	0.000	1.432E-04	0.000E+00	0.000E+00
X ₈₇	S-adenosyl-L-homocysteine		S-Adenosyl-L-homocysteine	0.484	0.000	0.000	1.250E-01	0.000E+00	0.000E+00
X ₈₈	adenosine		Adenosine	0.284	0.000	0.000	3.934E-01	0.000E+00	0.000E+00
X ₈₉	L-2,3-dihydrodipicolinate			0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₉₀	tetrahydrodipicolinate			0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₉₁	L,L-diamionopimelate			0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₉₂	mesodiamionopimelate			0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₉₃	lysine	Lys	L-Lysine	0.881	0.991	0.902	1.633E-04	6.690E-10	1.633E-04
X ₉₄	S-methyl-5-thioadenosine		5'-Deoxy-5'-Methylthioadenosine	0.704	0.000	0.000	1.271E-02	0.000E+00	0.000E+00
X ₉₅	5-methylthioribose			0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₉₆	5-methylthioribose-1P			0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₉₇	5-methioribulose-1P			0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₉₈	5-methylthio-2,3-dioxopentyl-P			0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₉₉	2-hydroxy-3-keto-5-methylthio-1-phosphopentene			0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₁₀₀	1,2-dihydroxy-3-keto-5-methylthiopentene			0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₁₀₁	2-oxo-4-methylthiobutanoate			0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₁₀₂	3-deoxyDarabinoheptulosonate-7P			0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₁₀₃	3-dehydroquinate			0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₁₀₄	3-dehydroshikimate			0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₁₀₅	shikimate		(-)-Shikimic acid	0.955	0.000	0.000	1.069E-06	0.000E+00	0.000E+00
X ₁₀₆	shikimate-3P			0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₁₀₇	5-enolpyruvylshikimate-3P			0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₁₀₈	prephenate			0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₁₀₉	arogenate			0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₁₁₀	phenylalanine		L(-)-Phenylalanine	-0.810	0.000	0.000	1.998E+00	0.000E+00	0.000E+00
X ₁₁₁	phenylpyruvate		Sodium phenylpyruvate	-0.792	0.000	0.000	1.998E+00	0.000E+00	0.000E+00
X ₁₁₂	phenylacetaldehyde			0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₁₁₃	tyrosine	Tyr	L-Tyrosine	-0.175	-0.608	0.102	1.395E+00	1.477E+00	1.395E+00
X ₁₁₄	phydroxyphenylpyruvate			0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₁₁₅	homogentisate			0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₁₁₆	maleylacetoacetate			0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₁₁₇	4-fumarylacetoacetate			0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₁₁₈	anthranilate			0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₁₁₉	N-5-phosphoribosylanthranilate			0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₁₂₀	1-O-carboxyphenylamino-1-deoxyribulose-5P			0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₁₂₁	indole3glycerolP			0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00

X ₁₂₂	indole			0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₁₂₃	tryptophan	Tryp	L-Tryptophane	-0.619	0.326	-0.084	1.963E+00	1.925E+00	1.963E+00
X ₁₂₄	valine	Val	2i_L-Norvaline_L-Valine	-0.055	0.430	0.066	1.128E+00	1.141E+00	1.128E+00
X ₁₂₅	glyoxylate			0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₁₂₆	S-methylmethionine		S-Methylmethionine	0.663	0.000	0.000	2.236E-02	0.000E+00	0.000E+00
X ₁₂₇	chorismate			0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₁₂₈	glutamylcysteine			0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₁₂₉	glutathione	GSH	Glutathione (oxidized form)	0.668	-0.193	0.055	2.081E-02	6.571E-02	2.081E-02
X ₁₃₀	2-methylmalate			0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₁₃₁	methylmaleate			0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₁₃₂	3-methylmalate			0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₁₃₃	hydroxylysine			0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₁₃₄	acetylhydroxylysine			0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₁₃₅	D-lysine			0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₁₃₆	diaminohexanoate			0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₁₃₇	N-acetyllysine			0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₁₃₈	acetamidooxohexanoate			0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₁₃₉	aminooxohexanoate			0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₁₄₀	piperidine-2-carboxylate			0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₁₄₁	pipicolate		DL-Pipecolic acid	0.971	0.000	0.000	9.817E-08	0.000E+00	0.000E+00
X ₁₄₂	piperidine-6-carboxylate			0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₁₄₃	aminoadipatesemialdehyde			0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₁₄₄	saccharopine		L-saccharopine	0.939	0.000	0.000	5.139E-06	0.000E+00	0.000E+00
X ₁₄₅	cadaverine			0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₁₄₆	piperidine			0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₁₄₇	aminopentanamide			0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₁₄₈	aminopentanoate			0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₁₄₉	acetyllysine			0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₁₅₀	acetamidopentanoate			0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₁₅₁	glutaratesemialdehyde			0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₁₅₂	glutarate		3i_Ethylmalonic acid_Glutaric acid_Meth	0.979	0.000	0.000	1.819E-08	0.000E+00	0.000E+00
X ₁₅₃	aminoadipate		DL-2-Aminoadipic Acid	0.945	0.000	0.000	3.105E-06	0.000E+00	0.000E+00
X ₁₅₄	oxoadipate			0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₁₅₅	glutaryl-dihydroipoamide			0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₁₅₆	glutaryl-CoA			0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₁₅₇	crotonoyl-CoA			0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₁₅₈	hydroxybutanoyl-CoA			0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₁₅₉	acetoacetyl-CoA			0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₁₆₀	2,2-methylthioethylmalate			0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₁₆₁	3,2-methylthioethylmalate			0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₁₆₂	2-oxo-5-methylthiopentanoic acid			0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₁₆₃	2,3-methylthiopropylmalate			0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₁₆₄	3,3-methylthiopropylmalate			0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₁₆₅	2-oxo-6-methylthiohexanoate			0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₁₆₆	2,4-methylthiobutylmalate			0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₁₆₇	3,4-methylthiobutylmalate			0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₁₆₈	2-oxo-7-methylthioheptanoate			0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₁₆₉	2,5-methylthiopentylmalate			0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₁₇₀	3,5-methylthiobutylmalate			0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₁₇₁	2-oxo-8-methyloctanoate			0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₁₇₂	2,6-methylthiohexylmalate			0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₁₇₃	3,6-methylthiohexylmalate			0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₁₇₄	2-oxo-9-methylononanoate			0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₁₇₅	2,7-methylthioheptylmalate			0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₁₇₆	3,7-methylthioheptylmalate			0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₁₇₇	2-oxo-1,0-methylthiodecanoate			0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₁₇₈	homomethionine		L-beta-homomethionine-HCl	-0.180	0.000	0.000	1.407E+00	0.000E+00	0.000E+00
X ₁₇₉	methylthiobutanaldoxime			0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₁₈₀	methylthiobutanonitrile oxide			0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₁₈₁	methylthiobutylhydroximoylglutathione			0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₁₈₂	methylthiobutylhydroximoylcysteinylglycine			0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00

X ₁₈₃	methylthiobutylhydroximate		0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₁₈₄	methylthiopropylsulfoglucosinolate		0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₁₈₅	methylthiopropylglucosinolate	3-Methylthio-n-propyl-glucosinolate	0.093	0.000	0.000	7.853E-01	0.000E+00	0.000E+00
X ₁₈₆	methylsulfanylpropylglucosinolate	3-Methylsulfanyl-n-propyl-glucosinolate	0.196	0.000	0.000	5.618E-01	0.000E+00	0.000E+00
X ₁₈₇	propenylglucosinolate		0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₁₈₈	hydroxypropylglucosinolate		0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₁₈₉	benzoyloxypropylglucosinolate	3-Benzoyloxy-n-propyl-glucosinolate	0.008	0.000	0.000	9.806E-01	0.000E+00	0.000E+00
X ₁₉₀	sinapoyloxypropylglucosinolate		0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₁₉₁	dihomomethionine		0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₁₉₂	methylthiopentanaloxime		0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₁₉₃	methylthiopentanitrileoxide		0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₁₉₄	methylthiopentylhydroximoylglutathione		0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₁₉₅	methylthiopentylhydroximoylcysteinylglycine		0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₁₉₆	methylthiopentylhydroximate		0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₁₉₇	methylthiobutylsulfoglucosinolate		0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₁₉₈	methylthiobutylglucosinolate	4-Methylthio-n-butyl-glucosinolate	0.021	0.000	0.000	9.502E-01	0.000E+00	0.000E+00
X ₁₉₉	methylsulfanylbutylglucosinolate	4-Methylsulfanyl-n-butyl-glucosinolate	-0.035	0.000	0.000	1.081E+00	0.000E+00	0.000E+00
X ₂₀₀	butenylglucosinolate		0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₂₀₁	hydroxy-3-butenylglucosinolate		0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₂₀₂	benzoyloxy-3-butenylglucosinolate		0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₂₀₃	sinapoyloxy-3-butenylglucosinolate		0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₂₀₄	hydroxybutylglucosinolate		0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₂₀₅	benzoyloxybutylglucosinolate		0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₂₀₆	sinapoyloxybutylglucosinolate		0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₂₀₇	trihomomethionine		0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₂₀₈	methylthiohexanaloxime		0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₂₀₉	methylthiohexanitrildioxide		0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₂₁₀	methylthiohexylhydroximoylglutathione		0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₂₁₁	methylthiohexylhydroximoylcysteinylglycine		0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₂₁₂	methylthiohexylhydroximate		0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₂₁₃	methylthiopentylsulfoglucosinolate		0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₂₁₄	methylthiopentylglucosinolate	5-Methylthio-n-pentyl-glucosinolate	-0.060	0.000	0.000	1.139E+00	0.000E+00	0.000E+00
X ₂₁₅	methylsulfanylpentylglucosinolate	5-Methylsulfanyl-n-pentyl-glucosinolate	0.125	0.000	0.000	7.136E-01	0.000E+00	0.000E+00
X ₂₁₆	pentenylglucosinolate		0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₂₁₇	tetrahomomethionine		0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₂₁₈	methylthioheptanaloxime		0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₂₁₉	methylthioheptanitrileoxide		0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₂₂₀	methylthioheptylhydroximoylglutathione		0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₂₂₁	methylthioheptylhydroximoylcysteinylglycine		0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₂₂₂	methylthioheptylhydroximate		0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₂₂₃	methylthiohexylsulfoglucosinolate		0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₂₂₄	methylthiohexylglucosinolate	6-Methylthio-n-hexyl-glucosinolate	-0.058	0.000	0.000	1.136E+00	0.000E+00	0.000E+00
X ₂₂₅	methylsulfanylhexylglucosinolate	6-Methylsulfanyl-n-hexyl-glucosinolate	0.001	0.000	0.000	9.972E-01	0.000E+00	0.000E+00
X ₂₂₆	pentahomomethionine		0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₂₂₇	methylthiooctanaloxime		0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₂₂₈	methylthiooctanitrileoxide		0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₂₂₉	methylthiooctylhydroximoylglutathione		0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₂₃₀	methylthiooctylhydroximoylcysteinylglycine		0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₂₃₁	methylthiooctylhydroximate		0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₂₃₂	methylthioheptylsulfoglucosinolate		0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₂₃₃	methylthioheptylglucosinolate	7-Methylthio-n-heptyl-glucosinolate	-0.051	0.000	0.000	1.119E+00	0.000E+00	0.000E+00
X ₂₃₄	methylsulfanylheptylglucosinolate	7-Methylsulfanyl-n-heptyl-glucosinolate	0.306	0.000	0.000	3.553E-01	0.000E+00	0.000E+00
X ₂₃₅	hexahomomethionine		0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₂₃₆	methylthiononananaloxime		0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₂₃₇	methylthiononanitrileoxide		0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₂₃₈	methylthiononylhydroximoylglutathione		0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₂₃₉	methylthiononylhydroximoylcysteinylglycine		0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₂₄₀	methylthiononylhydroximate		0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₂₄₁	methylthiooctylsulfoglucosinolate		0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₂₄₂	methylthiooctylglucosinolate	8-Methylthio-n-octyl-glucosinolate	-0.061	0.000	0.000	1.143E+00	0.000E+00	0.000E+00
X ₂₄₃	methylsulfanyloctylglucosinolate	8-Methylsulfanyl-n-octyl-glucosinolate	0.409	0.000	0.000	2.058E-01	0.000E+00	0.000E+00

X ₂₄₄	phenylacetaldoxime		0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₂₄₅	phenylacetoneitrileoxide		0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₂₄₆	phenylacetohydroximoylglutathione		0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₂₄₇	phenylacetohydroximoylcysteinylglycine		0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₂₄₈	phenylacetothiohydroximate		0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₂₄₉	benzylsulfoglucosinolate		0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₂₅₀	benzylglucosinolate		0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₂₅₁	indole-3-acetaldoxime		0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₂₅₂	indole-3-acetonitrileoxide		0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₂₅₃	indole-3-acetohydroximoylglutathione		0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₂₅₄	indole-3-acetohydroximoylcysteinylglycine		0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₂₅₅	indolylmethylthiohydroximate		0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₂₅₆	indolylmethylsulfoglucosinolate		0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₂₅₇	indol-3-ylmethylglucosinolate	Indol-3-ylmethyl-glucosinolate	-0.615	0.000	0.000	1.961E+00	0.000E+00	0.000E+00
X ₂₅₈	1-hydroxy-3-indolylmethylglucosinolate		0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₂₅₉	1-methoxy-3-indolylmethylglucosinolate	1-Methoxyindole-glucosinolate	-0.112	0.000	0.000	1.259E+00	0.000E+00	0.000E+00
X ₂₆₀	4-hydroxy-3-indolylmethylglucosinolate		0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₂₆₁	4-methoxy-3-indolylmethylglucosinolate	4-Methoxyindole-glucosinolate	0.852	0.000	0.000	4.842E-04	0.000E+00	0.000E+00
X ₂₆₂	histamine		0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₂₆₃	imidazoleacetaldehyde		0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₂₆₄	imidazole4acetate		0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₂₆₅	imidazoloneacetate		0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₂₆₆	NformiminoLaspertate		0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₂₆₇	NformylLaspertate		0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₂₆₈	D-glucono-1,5-lactone-6P		0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₂₆₉	6-phospho-D-gluconate		0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₂₇₀	D-ribose-5P		0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₂₇₁	D-ribose-5P	D-Ribose-5-phosphate disodium salt hy	0.341	0.000	0.000	2.994E-01	0.000E+00	0.000E+00
X ₂₇₂	D-ribose		0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₂₇₃	D-ribose-1P		0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₂₇₄	D-ribose-1,5P		0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₂₇₅	D-xylulose-5P		0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₂₇₆	D-erythrose-4P	D-Erythrose-4-phosphate sodium salt	0.717	0.000	0.000	1.035E-02	0.000E+00	0.000E+00
X ₂₇₇	D-sedoheptulose-7P		0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₂₇₈	D-gluconate		0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₂₇₉	D-glucono-1,5-lactone		0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₂₈₀	2-dehydro-D-gluconate		0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₂₈₁	2-dehydrogluconate-6P		0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₂₈₂	5-phospho-B-D-ribosylamine		0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₂₈₃	5-phosphoribosylglycineamine		0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₂₈₄	5-phosphoribosyl-N-formylglycineamide		0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₂₈₅	5-phosphoribosyl-N-formylglycineamidine		0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₂₈₆	5-aminoimidazole-ribose nucleotide		0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₂₈₇	4-carboxyaminoimidazole-ribose nucleotide		0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₂₈₈	5-phosphoribosyl-4-N-succinocarboxamide-5-aminoimidazole		0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₂₈₉	phosphoribosylformamidocarboxamide		0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₂₉₀	inosine-5-phosphate	Inosine-5'-monophosphate	0.517	0.000	0.000	9.751E-02	0.000E+00	0.000E+00
X ₂₉₁	adenylosuccinate		0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₂₉₂	xanthosine-5-phosphate		0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₂₉₃	AMP	Adenosine-5'-monophosphate sodium s	0.596	0.000	0.000	4.763E-02	0.000E+00	0.000E+00
X ₂₉₄	GMP	Guanosine-3'-5'-cyclic monophosphate	-0.259	0.000	0.000	1.561E+00	0.000E+00	0.000E+00
X ₂₉₅	inosine	Inosine	0.242	0.000	0.000	4.706E-01	0.000E+00	0.000E+00
X ₂₉₆	hypoxanthine	Hypoxanthine	0.048	0.000	0.000	8.882E-01	0.000E+00	0.000E+00
X ₂₉₇	xanthosine		0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₂₉₈	guanine	Guanine	0.797	0.000	0.000	2.242E-03	0.000E+00	0.000E+00
X ₂₉₉	xanthine	Xanthine	0.895	0.000	0.000	8.825E-05	0.000E+00	0.000E+00
X ₃₀₀	urate		0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₃₀₁	5-hydroxyisourate		0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₃₀₂	5-hydroxy-2-oxo-4-ureido-2,5-dihydro-1H-imidazole-5-carboxylate		0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₃₀₃	S-allantoin	Allantoin	0.737	0.000	0.000	7.461E-03	0.000E+00	0.000E+00
X ₃₀₄	allantoate	Allantoic acid	0.060	0.000	0.000	8.611E-01	0.000E+00	0.000E+00

X ₃₀₅	ureidoglycine		0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₃₀₆	ureidoglycolate		0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₃₀₇	urea		0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₃₀₈	GDP		0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₃₀₉	GTP		0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₃₁₀	dGDP		0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₃₁₁	dGTP		0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₃₁₂	ADP		0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₃₁₃	dADP		0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₃₁₄	ATP		0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₃₁₅	dATP		0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₃₁₆	dAMP	2'-Deoxyadenosine-5'-monophosphate	0.089	0.000	0.000	7.943E-01	0.000E+00	0.000E+00
X ₃₁₇	deoxyadenosine	2'-Deoxyadenosine monohydrate	0.250	0.000	0.000	4.548E-01	0.000E+00	0.000E+00
X ₃₁₈	deoxyinosine		0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₃₁₉	adenine	Adenine	0.183	0.000	0.000	5.879E-01	0.000E+00	0.000E+00
X ₃₂₀	guanosine	Guanosine	-0.126	0.000	0.000	1.290E+00	0.000E+00	0.000E+00
X ₃₂₁	NcarbamoylLaspartate	Carbamoyl-DL-aspartic acid	-0.583	0.000	0.000	1.946E+00	0.000E+00	0.000E+00
X ₃₂₂	dihydroorotate		0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₃₂₃	orotate		0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₃₂₄	orotidine-5P		0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₃₂₅	UMP	Uridine-5'-monophosphate	0.218	0.000	0.000	5.166E-01	0.000E+00	0.000E+00
X ₃₂₆	UDP		0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₃₂₇	UTP		0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₃₂₈	CTP		0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₃₂₉	CMP	Cytidine-3'-monophosphate	0.346	0.000	0.000	2.926E-01	0.000E+00	0.000E+00
X ₃₃₀	CDP		0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₃₃₁	dCDP		0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₃₃₂	dCTP		0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₃₃₃	dihydrouracil	5-6-Dihydrouracil	0.924	0.000	0.000	1.676E-05	0.000E+00	0.000E+00
X ₃₃₄	dUDP		0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₃₃₅	uracil		0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₃₃₆	dUTP		0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₃₃₇	dUMP		0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₃₃₈	dTMP		0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₃₃₉	dTDP		0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₃₄₀	dTTP		0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₃₄₁	dCMP		0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₃₄₂	deoxycytidine	2'-Deoxycytidine	0.215	0.000	0.000	5.234E-01	0.000E+00	0.000E+00
X ₃₄₃	deoxyuridine	(+)-2'-Deoxyuridine	0.698	0.000	0.000	1.374E-02	0.000E+00	0.000E+00
X ₃₄₄	3-ureidopropionate	3-ureidopropionic acid	0.824	0.000	0.000	1.140E-03	0.000E+00	0.000E+00
X ₃₄₅	thymidine	Thymidine	0.815	0.000	0.000	1.447E-03	0.000E+00	0.000E+00
X ₃₄₆	thymine		0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₃₄₇	dihydrothymine		0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₃₄₈	3-ureidoisobutyrate		0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₃₄₉	3-aminoisobutanoate		0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₃₅₀	cytidine	Cytidine-cell culture tested	-0.232	0.000	0.000	1.512E+00	0.000E+00	0.000E+00
X ₃₅₁	uridine	Uridine	-0.715	0.000	0.000	1.989E+00	0.000E+00	0.000E+00
X ₃₅₂		(-)-Norepinephrine	0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₃₅₃		(-)-Riboflavin	0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₃₅₄		(+)-Jasmonic acid	0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₃₅₅		(2R)-2-Hydroxy-2-phenethylglucosinola	0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₃₅₆		10-camphorsulfonic acid	0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₃₅₇		1-1-Dimethylbiguanide hydrochloride	0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₃₅₈		1i.D(-)-Fructose_D-(+)-Galactose_D-	0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₃₅₉		1-Amino-1-cyclopentanecarboxylic acid	0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₃₆₀		1-Aminocyclopropane-1-carboxylic acid	0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₃₆₁		1-Isothiocyanato-6-(methylsulfonyl)-hex	0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₃₆₂		1-Isothiocyanato-6-(methylsulfonyl)-he	0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₃₆₃		1-Methylguanidine hydrochloride	0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₃₆₄		1-Methylhistamine dihydrochloride	0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₃₆₅		1-O-b-D-glucopyranosyl sinapate	0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00

X ₃₆₆		2-Aminoethylphosphonic acid	0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₃₆₇		2-Deoxyguanosine monohydrate	0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₃₆₈		2-Deoxyribose-5-phosphate sodium salt	0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₃₆₉		2i_1-3-Diaminopropane dihydrochloride	0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₃₇₀		2i_Adipic acid_2-Methylglutaric Acid	0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₃₇₁		2i_alpha-Ketoglutaric acid disodium salt	0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₃₇₂		2i_alpha-Lipoamide_DL-Thioctamide	0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₃₇₃		2i_cyanidin-3-5-di-O-glucoside chloride	0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₃₇₄		2i_D(-)-Ribose_D-Xylulose	0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₃₇₅		2i_D(+)-Cellobiose_Lactulose	0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₃₇₆		2i_D(+)-Cellobiose_Lactulose	0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₃₇₇		2i_D(+)-Melezitose monohydrate_1-Kes	0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₃₇₈		2i_D-Mannose-6-phosphate barium salt	0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₃₇₉		2i_eriodictyol-7-O-glucoside_Marein	0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₃₈₀		2i_Ideain chloride_cyanidin-3-glucoside c	0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₃₈₁		2i_Indole-3-carboxyaldehyde_Indole-3-a	0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₃₈₂		2i_Kaempferol-3-Glucoside-2-Rhamnos	0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₃₈₃		2i_L-Norleucine_D-Alloisoleucine	0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₃₈₄		2i_Maritimein_luteolin-7-O-glucoside	0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₃₈₅		2i_Nicotinic Acid_Isonicotinic acid	0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₃₈₆		2i_Quercitrin_Quercetin-7-O-rhamnosid	0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₃₈₇		2i_Rutin_Quercetin-3-O-b-glucopyrano	0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₃₈₈		2i_Sarsapogenine_Smilagenin	0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₃₈₉		2i_Theophylline-anhydrous_1-7-Dimethy	0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₃₉₀		2i_Uridine-5'-diphospho-N-acetylgalact	0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₃₉₁		2-Isopropylmalic acid	0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₃₉₂		3-5-Dimethoxycinnamic acid (predomina	0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₃₉₃		3-Chloro-L-tyrosine hydrochloride	0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₃₉₄		3-cyanopyridine	0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₃₉₅		3-Dephosphocoenzyme A	0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₃₉₆		3-hydroxy-3-methylbutanoic acid	0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₃₉₇		3-Hydroxy-3-methylglutarate	0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₃₉₈		3i_Glycolaldehyde dimer-mixture of ster	0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₃₉₉		3i_Isorhamnetin-3-Glucoside-6-Rhamnd	0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₄₀₀		3i_L-Iditol_D-Sorbitol_D(-)-Mannitol	0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₄₀₁		3i_L-Threonine_-Methyl-DL-serine_L-H	0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₄₀₂		3i_Sodium pantothenate_D-Pantothenic	0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₄₀₃		3i_Uridine-5'-diphosphogalactose disodi	0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₄₀₄		3-Methyl-L-histidine	0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₄₀₅		4-(Methylsulfinyl)but-3-enylglucosinol	0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₄₀₆		4-Hydroxybenzoate	0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₄₀₇		4i_Kaempferol-3-Rhamnoside-7-Rhamn	0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₄₀₈		4i_L(+)-ArginineJHCl_Nalpha-Acetyl-L-c	0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₄₀₉		4-Methyl-5-thiazoleethanol	0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₄₁₀		4-Nitrophenol	0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₄₁₁		4-Pyridoxate	0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₄₁₂		5-Aminovaleric acid	0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₄₁₃		5-Hydroxyindole-3-acetate (5-HIAA)	0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₄₁₄		5-Methylcytosine hydrochloride	0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₄₁₅		6-Aminohexanoic acid	0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₄₁₆		6i_Melibiose hydrate_D(+)-Turanose_Isc	0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₄₁₇		7i_kaempferol-3-O-rutinoside	0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₄₁₈		Acetaminophen	0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₄₁₉		Acetylcholine chloride	0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₄₂₀		Adenosine 3'-monophosphate From Yea	0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₄₂₁		Adenosine-5'-phosphosulfate sodium sa	0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₄₂₂		Agmatine sulfate salt	0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₄₂₃		alpha-Lactose monohydrate	0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₄₂₄		alpha-Methyl-DL-histidine dihydrochlor	0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₄₂₅		alpha-Tocotrienol	0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₄₂₆		Amantadine hydrochloride	0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00

X ₄₂₇		Benzylglucosinolate	0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₄₂₈		Betaine	0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₄₂₉		beta-Nicotinamide adenine dinucleotide	0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₄₃₀		beta-Nicotinamide mononucleotide	0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₄₃₁		Callistephin Chloride	0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₄₃₂		Choline chloride	0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₄₃₃		cis or trans-Cinnamyl alcohol	0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₄₃₄		Citramalic acid	0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₄₃₅		Creatinine-anhydrous	0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₄₃₆		Cyanidin-3-O-(2-O-beta-xylopyranosyl	0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₄₃₇		Cyanidin-3-O-(2-O-beta-xylopyranosyl	0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₄₃₈		cyanidin-3-O-rhamnoside chloride	0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₄₃₉		cysteinylglycine	0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₄₄₀		Cytidine-5'-diphosphocholine sodium sa	0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₄₄₁		Cytidine-5'-monophosphate disodium sa	0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₄₄₂		D-(-)-Quinic acid	0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₄₄₃		D-(+)-Raffinose pentahydrate	0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₄₄₄		D-Ala-D-ala	0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₄₄₅		Daphnetin	0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₄₄₆		Delphinidin-3-O-(6-O-alpha-rhamnopyr	0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₄₄₇		D-Glucoheptose	0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₄₄₈		Diethanolamine	0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₄₄₉		DL-2-3-Diaminopropionic acid monohyd	0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₄₅₀		DL-beta-Hydroxybutyric acid	0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₄₅₁		DL-Glyceric Acid calcium Salt	0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₄₅₂		DL-homocystine	0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₄₅₃		DL-threo-beta-Methylaspartic acid	0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₄₅₄		D-Panose	0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₄₅₅		dUDP	0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₄₅₆		gamma-Amino-n-butyric acid	0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₄₅₇		Gluconasturtiin	0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₄₅₈		Glycocyanine	0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₄₅₉		Glycyl-L-proline	0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₄₆₀		Guanosine-5'-diphospho-beta-L-fucose	0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₄₆₁		Guanosine-5'-diphosphoglucose sodium	0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₄₆₂		Guanosine-5'-monophosphate Jdisodium	0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₄₆₃		Hesperetin	0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₄₆₄		Hesperidin	0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₄₆₅		Isoguvacine hydrochloride	0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₄₆₆		isorhamnetin-3-O-glucoside	0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₄₆₇		Itaconic acid	0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₄₆₈		Kaempferol-3-Galactoside-6-Rhamnosi	0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₄₆₉		Kaempferol-7-O-alpha-L-rhamnoside	0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₄₇₀		Keracyanin Chloride	0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₄₇₁		L-Anserine nitrate salt	0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₄₇₂		L-beta-homoglutamine-HCl	0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₄₇₃		L-beta-homoleucine-HCl	0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₄₇₄		L-beta-homolysine-2HCl	0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₄₇₅		L-beta-homoproline-HCl	0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₄₇₆		L-beta-homothreonine	0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₄₇₇		L-Carnosine	0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₄₇₈		L-Cystine	0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₄₇₉		L-Glutathione (reduced form)	0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₄₈₀		Lidocain	0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₄₈₁		Lignoceric Acid	0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₄₈₂		L-Kynurenine	0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₄₈₃		L-Pyrogutamic acid	0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₄₈₄		L-Threonic acid hemicalcium salt	0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₄₈₅		luteolin-4'-O-glucoside	0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₄₈₆		Maleic acid	0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₄₈₇		Maltitol	0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00

X ₄₈₈		Methionine sulfoxide	0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₄₈₉		Methylmalonic acid	0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₄₉₀		m-Hydroxycinnamic acid	0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₄₉₁		mucic acid	0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₄₉₂		N-6-(delta-2-Isopentenyl)adenosine	0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₄₉₃		N-acetyl putrescine hydrochloride	0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₄₉₄		N-Acetyl-DL-aspartic acid	0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₄₉₅		N-acetyl-DL-serine	0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₄₉₆		N-acetyl-D-mannosamine	0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₄₉₇		N-Acetylglycine	0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₄₉₈		N-acetylneuraminic acid-Type IV-S-Sy	0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₄₉₉		naringenin-7-O-glucoside	0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₅₀₀		Neofericitrin	0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₅₀₁		Neohesperidin	0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₅₀₂		Nicotinic acid mono nucleotide	0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₅₀₃		Nystose Trihydrate	0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₅₀₄		O-Acetyl-L-homoserine hydrochloride	0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₅₀₅		o-Anisic Acid	0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₅₀₆		O-Phosphocholine	0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₅₀₇		O-Succinyl-L-homoserine	0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₅₀₈		Pimelic acid	0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₅₀₉		Puerarin	0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₅₁₀		pyridoxal hydrochloride	0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₅₁₁		pyridoxal-5'-phosphate hydrate	0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₅₁₂		Pyridoxamine dihydrochloride	0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₅₁₃		Pyridoxine	0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₅₁₄		Quercetin-3-7-O-alpha-L-dirhamnopyr	0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₅₁₅		Quercetin-3-O-alpha-L-rhamnopyranos	0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₅₁₆		Robinin	0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₅₁₇		Safranin	0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₅₁₈		Salicylic Acid	0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₅₁₉		Sinapic acid	0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₅₂₀		Sinapine	0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₅₂₁		Sinapoyl malate	0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₅₂₂		S-Methyl-L-cysteine	0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₅₂₃		sn-Glycero-3-phosphocholine 1:1 cadm	0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₅₂₄		Suberic acid	0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₅₂₅		Sucrose	0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₅₂₆		Thiamine hydrochloride	0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₅₂₇		Thioglycolic acid solution	0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₅₂₈		trans-Zeatin-riboside	0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₅₂₉		Trimethylamine N-oxide dihydrate	0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₅₃₀		UDP-beta-L-rhamnose	0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₅₃₁		UDP-xylose	0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₅₃₂		Vanillin	0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00
X ₅₃₃		Zeatin-9-glucoside	0.000	0.000	0.000	0.000E+00	0.000E+00	0.000E+00