In [1]:
```
import mfapy
%matplotlib inline
import numpy as np
import scipy.integrate
from matplotlib import pyplot as plt
```

In [2]:
```
# User input code goes here:

simulation_model = input("Enter the name of the metabolic model .txt file: ")

simulation_csv = input("Enter the name of the .csv file containing the parame

MDV_data = input("Enter the name of the MDV .txt file: ")
```

```
Enter the name of the metabolic model .txt file: Elim2_model.txt
Enter the name of the .csv file containing the parameters: Elim2_status.csv
Enter the name of the MDV .txt file: Elim2_mdv.txt
```

In [3]:
```
#Sets up model variables using simulation model.txt file
reactions, reversible, metabolites, target_fragments = mfapy.mfapyio.load_met
model = mfapy.metabolicmodel.MetabolicModel(reactions, reversible, metabolite

#loads states and values from .csv file
flux = model.load_states(simulation_csv, format = 'csv')
model.set_constraints_from_state_dict(flux)
model.update()
```

```
Caution: Formate was not used in the metabolid network
```

Out[3]:
```
True
```

In [4]:
```
# Generation of CarbonSource instance
cs1 = model.generate_carbon_source_template()
cs1.set_each_isotopomer('SubsCO2',{'#0': 0.01, '#1': 0.99}, correction = 'yes
cs1.set_each_isotopomer('Subsmeoh',{'#0': 1.0, '#1': 0.0}, correction = 'yes'
```

Out[4]:
```
True
```

In [5]:
```
# Load MDV data
mdv1 = model.load_mdv_data(MDV_data) #string variable from user input

#include more if there are more data files
```

In [6]:
```
# Flux estimation Step 1: Setting experimments
model.set_experiment('ex1', mdv1, cs1)
#include more for more data sets
```

Out[6]:
```
True
```

In [7]:
```
# Flux estimation step 2: Generation of intical flux vectors
initialstate, flux_initial = model.generate_initial_states(50, 4, method ="nc
```

In [8]:
```
# Flux estimation step 3: Fitting model

#GN_CRS2_LM
initialstate, RSS, flux_opt_GN_CRS2_LM = model.fitting_flux(method = "GN_CRS2

#SLSQP
initialstate, RSS, flux_opt_SLSQP = model.fitting_flux(method = "SLSQP", flux

#LN_SBPLX
initialstate, RSS, flux_opt_LN_SBPLX = model.fitting_flux(method = "LN_SBPLX"
```

In [9]:
```
#Print results of each method onto the console
model.show_results([("GN_CRS2_LM", flux_opt_GN_CRS2_LM[0])])
```

```
1.0   0.01000.0 ABCDE-->ABCDE
r62             E4P+PEP+PEP-->Phe        (kegg:Biom    10.0 pseudo     1.0
1.0   0.01000.0 ABCD+EFG+HIJ-->EFGIJABCD
r63             E4P+PEP+PEP-->Tyr        (kegg:Biom    10.0 pseudo     1.0
1.0   0.01000.0 ABCD+EFG+HIJ-->EFGIJABCD
r64             Oxa+Pyr-->Ile            (kegg:R015    10.0 pseudo     1.0
1.0   0.01000.0 ABCD+EFG-->ABFGCD
r65             AcCOA+Pyr+Pyr-->Leu      (kegg:Biom    10.0 pseudo     1.0
1.0   0.01000.0 AB+CDE+FGH-->ABDEGH
r66             Pyr+Pyr-->Val            (kegg:Biom    10.0 pseudo     1.0
1.0   0.01000.0 ABC+DEF-->ABECF
r67             PGA-->Ser                (kegg:Biom     4.3 free       1.0
1.0   0.01000.0 ABC-->ABC
r68             Ser-->Gly+MEETHF         (kegg:Glu2   773.8 free       1.0
1.0   0.01000.0 ABC-->AB+C
r69             Gly+MEETHF-->Ser         (kegg:Biom   771.1 free       1.0
1.0   0.01000.0 AB+C-->ABC
r72             G6P-->Biomass            (kegg:Biom     1.0 fixed      1.0
1.0   0.01000.0 nd
```

In [10]:
```
model.show_results([("SLSQP", flux_opt_SLSQP[0])])
```

```
Id              Reaction                 External i   SLSQP
RSS                                                462854.64
Thres                                                 38.89
p_value                                                0.00
Id              Reaction                 External i   SLSQP Type     Value
Stdev    lb     ub Atom_mapping
r1              SubsGlc-->G6P            (kegg:R028     0.0 fixed      0.0
1.0   0.01000.0 ABCDEF-->ABCDEF
r2              G6P-->F6P                (kegg:R007   259.6 free       1.0
1.0   0.01000.0 ABCDEF-->ABCDEF
r3              F6P-->G6P                (kegg:R007   272.1 free       1.0
1.0   0.01000.0 ABCDEF-->ABCDEF
r4              F6P-->FBP                (kegg:R007   791.7 free       1.0
1.0   0.01000.0 ABCDEF-->ABCDEF
r5              FBP-->F6P                (kegg:R010   800.3 free       1.0
1.0   0.01000.0 ABCDEF-->ABCDEF
r6              FBP-->DHAP+GAP           (kegg:R010   567.2 free       1.0
1.0   0.01000.0 ABCDEF-->CBA+DEF
r7              DHAP+GAP-->FBP           (kegg:R010   575.7 free       1.0
```

In [11]:
```
model.show_results([("LN_SBPLX", flux_opt_LN_SBPLX[0])])
```

```
Id              Reaction                 External i LN_SBPL
RSS                                               56894.39
Thres                                                38.89
p_value                                               0.00
Id              Reaction                 External i LN_SBPL Type     Value
Stdev    lb     ub Atom_mapping
r1              SubsGlc-->G6P            (kegg:R028     0.0 fixed      0.0
1.0   0.01000.0 ABCDEF-->ABCDEF
r2              G6P-->F6P                (kegg:R007   544.0 free       1.0
1.0   0.01000.0 ABCDEF-->ABCDEF
r3              F6P-->G6P                (kegg:R007   551.0 free       1.0
1.0   0.01000.0 ABCDEF-->ABCDEF
r4              F6P-->FBP                (kegg:R007   991.5 free       1.0
1.0   0.01000.0 ABCDEF-->ABCDEF
r5              FBP-->F6P                (kegg:R010  1000.0 free       1.0
1.0   0.01000.0 ABCDEF-->ABCDEF
r6              FBP-->DHAP+GAP           (kegg:R010   991.5 free       1.0
1.0   0.01000.0 ABCDEF-->CBA+DEF
r7              DHAP+GAP-->FBP           (kegg:R010  1000.0 free       1.0
```

In [12]:
```
# Output fitted metabolic flux into CSV file

model.show_results([("GN_CRS2_LM", flux_opt_GN_CRS2_LM[0])], filename = "Elim

model.show_results([("SLSQP", flux_opt_SLSQP[0])], filename = "Elim2_output_S

model.show_results([("LN_SBPLX", flux_opt_LN_SBPLX[0])], filename = "Elim2_ou
```

```
#----------------------------------------------------------------------------
# Name:       Adapted E. limosum Model
#           Model definition file for E. limosum of mfapy
#
# Author:     Katie Hoyt Christian Byrd Fumio_Matsuda
#
# Created:    12/06/2018, revised December 2022
# Copyright:  (c) Fumio_Matsuda 2021
# Licence:    MIT license
#----------------------------------------------------------------------------
//Reactions
r1          SubsGlc --> ( SubsGlc --> ( ABCDEF --> A (kegg:R0284  0       1000
r2          G6P --> F6P   G6P --> F6P   ABCDEF --> A (kegg:R0077  0       1000
r3          F6P --> G6P   F6P --> G6P   ABCDEF --> A (kegg:R0077  0       1000
r4          F6P --> FBP   F6P --> FBP   ABCDEF --> A (kegg:R0075  0       1000
r5          FBP --> F6P   FBP --> F6P   ABCDEF --> A (kegg:R0106  0       1000
r6          FBP --> DHAI FBP --> DHAI ABCDEF --> ( (kegg:R0106  0       1000
r7          DHAP + GAP  DHAP + GAP  CBA + DEF -- (kegg:R0101  0       1000
r8          DHAP --> GA DHAP --> GA ABC --> ABC (kegg:R0101  0       1000
r9          GAP --> DHA GAP --> DHA ABC --> ABC (kegg:R0106  0       1000
r10         GAP --> PGA GAP --> PGA ABC --> ABC (kegg:R0106  0       1000
r11         PGA --> GAP PGA --> GAP ABC --> ABC (kegg:R0151  0       1000
r12         PGA --> PEP  PGA --> PEP  ABC --> ABC (kegg:R0151  0       1000
r13         PEP --> PGA  PEP --> PGA  ABC --> ABC (kegg:R0020  0       1000
r14         PEP --> Pyr  PEP --> Pyr  ABC --> ABC (kegg:R0119  0       1000
r15         Pyr --> PEP  Pyr --> PEP  ABC --> ABC (kegg:R0035  0       1000
r16         Pyr --> AcCO, Pyr --> AcCO, ABC --> BC + (kegg:R0070  0       1000
r17         AcCOA + Oxa AcCOA + Oxa AB + CDEF -- (kegg:R0070  0       1000
r18         IsoCit --> aK( IsoCit --> aK( ABCDEF --> A (kegg:R0119  0       1000
r19         aKG --> Suc - aKG --> Suc - ABCDE --> B( (kegg:R0216  0       1000
r20         Suc --> Fum  Suc --> Fum  ABCD --> AB( (kegg:R0216  0       1000
r21         Fum --> Suc  Fum --> Suc  ABCD --> AB( (kegg:R0108  0       1000
r22         Fum --> Mal  Fum --> Mal  ABCD --> AB( (kegg:R0108  0       1000
r23         Mal --> Fum  Mal --> Fum  ABCD --> AB( (kegg:R0034  0       1000
r24         Mal --> Oxa  Mal --> Oxa  ABCD --> AB( (kegg:R0034  0       1000
r25         Oxa --> Mal  Oxa --> Mal  ABCD --> AB( (kegg:R0034  0       1000
r26         IsoCit + AcCC IsoCit + AcCC ABCDEF + GH (kegg:R0021  0       1000
r27         G6P --> m6P G6P --> m6P ABCDEF --> A (kegg:R0083  0       1000
r28         m6PG --> Ru m6PG --> Ru ABCDEF --> E (kegg:R0152  0       1000
r29         Ru5P --> R5F Ru5P --> R5F ABCDE --> AI (kegg:R0105  0       1000
r30         R5P --> Ru5F R5P --> Ru5F ABCDE --> AI (kegg:R0105  0       1000
r31         Ru5P --> Xu5 Ru5P --> Xu5 ABCDE --> AI (kegg:R0152  0       1000
r32         Xu5P --> Ru5 Xu5P --> Ru5 ABCDE --> AI (kegg:R0152  0       1000
r33         R5P + Xu5P - R5P + Xu5P - ABCDE + FGH (kegg:R0164  0       1000
```

r34	GAP + S7P --	GAP + S7P --	HIJ + FGABCI	(kegg:R0164	0	1000
r35	GAP + S7P --	GAP + S7P --	ABC + DEFGI	(kegg:R0857	0	1000
r36	E4P + F6P -->	E4P + F6P -->	GHIJ + DEFAI	(kegg:R0857	0	1000
r37	E4P + Xu5P --	E4P + Xu5P --	ABCD + EFGI	(kegg:R0106	0	1000
r38	GAP + F6P --	GAP + F6P --	GHI + EFABC	(kegg:R0106	0	1000
r39	m6PG --> Py	m6PG --> Py	ABCDEF --> A	(kegg:R0070	0	1000
r40	PEP + CO2in	PEP + CO2in	ABC + D --> A	(kegg:Lacex)	0	1000
r41	Oxa --> PEP -	Oxa --> PEP -	ABCD --> AB	(kegg:SubsGl	0	1000
r42	Mal --> Pyr +	Mal --> Pyr +	ABCD --> AB	(kegg:R0025	0	1000
r49	AcCOA --> Ac	AcCOA --> Ac	AB --> AB	(kegg:Aspex)	0	1000
r50	Acetate --> A	nd	nd	(kegg:R0048	0	1000
r56	SubsCO2 -->	SubsCO2 -->	A --> A	(kegg:SubsVa	0	1000
r57	CO2in --> CO	nd	nd	(kegg:Glu)	0	1000
r58	Pyr --> Ala	Pyr --> Ala	ABC --> ABC	(kegg:Arg)	0	1000
r59	Oxa --> Asp	Oxa --> Asp	ABCD --> AB	(kegg:R0035	0	1000
r60	Oxa --> Thr	Oxa --> Thr	ABCD --> AB	(kegg:Bioma	0	1000
r61	aKG --> Glu	aKG --> Glu	ABCDE --> AI	(kegg:Bioma	0	1000
r62	E4P + PEP + I	E4P + PEP + I	ABCD + EFG	(kegg:Bioma	0	1000
r63	E4P + PEP + I	E4P + PEP + I	ABCD + EFG	(kegg:Bioma	0	1000
r64	Oxa + Pyr -->	Oxa + Pyr -->	ABCD + EFG	(kegg:R0151	0	1000
r65	AcCOA + Pyr	AcCOA + Pyr	AB + CDE + F	(kegg:Bioma	0	1000
r66	Pyr + Pyr -->	Pyr + Pyr -->	ABC + DEF --	(kegg:Bioma	0	1000
r67	PGA --> Ser	PGA --> Ser	ABC --> ABC	(kegg:Bioma	0	1000
r68	Ser --> Gly +	Ser --> Gly +	ABC --> AB +	(kegg:Glu2)	0	1000
r69	Gly + MEETH	Gly + MEETH	AB + C --> AI	(kegg:Bioma	0	1000
r72	G6P --> Biom	nd	nd	(kegg:Bioma	0	1000
r73	F6P --> Biom	nd	nd	(kegg:Bioma	0	1000
r74	DHAP --> Bio	nd	nd	(kegg:Bioma	0	1000
r75	PGA --> Biom	nd	nd	(kegg:CO2ex	0	1000
r76	Ser --> Biom	nd	nd	(kegg:SubsC(	0	1000
r77	Gly --> Biom	nd	nd	(keggPGAex)	0	1000
r78	MEETHF --> I	nd	nd	(kegg:FAex)	0	1000
r79	PEP --> Biom	nd	nd	(kegg:MAL_c	0	1000
r80	Pyr --> Biom	nd	nd	(kegg:MAL_c	0	1000
r81	AcCOA --> Bi	nd	nd	(kegg:OXA_c	0	1000
r82	aKG --> Biom	nd	nd	(kegg:OXA_c	0	1000
r83	Oxa --> Biom	nd	nd	(kegg:ATP)	0	1000
r84	R5P --> Biom	nd	nd	(kegg:NADH)	0	1000
r85	E4P --> Biom	nd	nd	(kegg:NADPH	0	1000
r86	Ala --> Alaex	nd	nd	(kegg:Arg)	0	1000
r87	Asp --> Aspe	nd	nd	(kegg:R0035	0	1000
r88	Thr --> Threx	nd	nd	(kegg:Bioma	0	1000
r89	Glu --> Glue	nd	nd	(kegg:Bioma	0	1000
r90	Phe --> Phee	nd	nd	(kegg:Bioma	0	1000

r91	Tyr --> Tyrex	nd	nd	(kegg:Bioma	0	1000
r92	Ile --> Ileex	nd	nd	(kegg:R0151	0	1000
r93	Leu --> Leuex	nd	nd	(kegg:Bioma	0	1000
r94	Val --> Valex	nd	nd	(kegg:Bioma	0	1000
r104	Subsmeoh --	Subsmeoh --	A --> A	(kegg:MTI/M	0	1000
r105	meoh --> ME	meoh --> ME	A --> A	(kegg:TBD)	0	1000
r106	METHF --> M	METHF --> M	A --> A	(kegg:TBD)	0	1000
r107	MEETHF -->	MEETHF -->	A --> A	(kegg:TBD)	0	1000
r108	CO2in + MET	CO2in + MET	A + B --> AB	(kegg:TBD)	0	1000
r109	AcCOA + CO2	AcCOA + CO2	BC + A --> AE	(kegg:R0070	0	1000

//Reversible_reactions

PGI	r2	r3	(kegg:R0077	-1000	1000
FBA	r4	r5	(kegg:R0106	-1000	1000
TPI	r8	r9	(kegg:R0101	-1000	1000
GAPDH	r10	r11	(kegg:R0106	-1000	1000
PEPH	r12	r13	(kegg:R0151	-1000	1000
SDH	r20	r21	(kegg:R0216	-1000	1000
MDH	r24	r25	(kegg:R0034	-1000	1000
RPI	r29	r30	(kegg:R0105	-1000	1000
RBE	r31	r32	(kegg:R0152	-1000	1000
TKT1	r33	r34	(kegg:R0164	-1000	1000
TAL	r35	r36	(kegg:R0857	-1000	1000
TKT2	r37	r38	(kegg:R0106	-1000	1000
FH	r22	r23	(kegg:R0108	-1000	1000
THF	r106	r107	(kegg:TBD)	-1000	1000
PFOR	r16	r109	(kegg:R0070	-1000	1000

#

#Name_ofintermediate{\t}carbon_number

#

//Metabolites

m6PG	6	no	no	no	(kegg:C00345	0	300
AcCOA	2	no	no	no	(kegg:C00024	0	300
Acetate	2	no	no	no	(dummy)	0	300
Acetateex	2	no	no	excreted	(dummy)	0	300
aKG	5	no	no	no	(kegg:C00026	0	300
Ala	3	no	no	no	(kegg:C00041	0	300
Asp	4	no	no	no	(kegg:C00049	0	300
Biomass	1	no	no	excreted	(dummy)	0	300
CO2ex	1	no	no	excreted	(dummy)	0	300
CO2in	1	no	no	no	(dummy)	0	300
DHAP	3	no	no	no	(kegg:C00111	0	300
E4P	4	no	no	no	(kegg:C00279	0	300
F6P	6	no	no	no	(kegg:C00085	0	300
FBP	6	no	no	no	(kegg:C00354	0	300

Formate	1	no	no	no	(dummy)	0	300
G6P	6	no	no	no	(kegg:C0009	0	300
GAP	3	no	no	no	(kegg:C0011	0	300
Glu	5	no	no	no	(kegg:C0002	0	300
Gly	2	no	no	no	(kegg:C0003	0	300
Ile	6	no	no	no	(kegg:C0040	0	300
IsoCit	6	no	no	no	(dummy)	0	300
Leu	6	no	no	no	(kegg:C0012	0	300
Mal	4	no	no	no	(kegg:C0014	0	300
MEETHF	1	no	no	no	(dummy)	0	300
METHF	1	no	no	no	(dummy)	0	300
Subsmeoh	1	no	carbonsource	no	(dummy)	0	300
meoh	1	no	no	no	(dummy)	0	300
Oxa	4	no	no	no	(kegg:C0003	0	300
PEP	3	no	no	no	(kegg:C0007	0	300
PGA	3	no	no	no	(kegg:C0063	0	300
Phe	9	no	no	no	(dummy)	0	300
Pyr	3	no	no	no	(kegg:C0002	0	300
R5P	5	no	no	no	(kegg:C0011	0	300
Ru5P	5	no	no	no	(kegg:C0019	0	300
S7P	7	no	no	no	(kegg:C0538	0	300
Ser	3	no	no	no	(kegg:C0006	0	300
SubsCO2	1	no	carbonsource	no	(dummy)	0	300
SubsGlc	6	no	carbonsource	no	(dummy)	0	300
Fum	4	symmetry	no	no	(kegg:C0012	0	300
Suc	4	symmetry	no	no	(kegg:C0004	0	300
Thr	4	no	no	no	(dummy)	0	300
Tyr	9	no	no	no	(dummy)	0	300
Val	5	no	no	no	(kegg:C0018	0	300
Xu5P	5	no	no	no	(kegg:C0023	0	300
Alaex	3	no	no	excreted	(dummy)	0	300
Aspex	4	no	no	excreted	(dummy)	0	300
Threx	4	no	no	excreted	(dummy)	0	300
Gluex	5	no	no	excreted	(dummy)	0	300
Pheex	9	no	no	excreted	(dummy)	0	300
Tyrex	9	no	no	excreted	(dummy)	0	300
Ileex	6	no	no	excreted	(dummy)	0	300
Leuex	6	no	no	excreted	(dummy)	0	300
Valex	5	no	no	excreted	(dummy)	0	300

//Target_fragments

AlaMes	intermediate	Ala_1:2:3	use	C3H7NO2
AspMes	intermediate	Asp_1:2:3:4	use	C4H7NO4
GluMes	intermediate	Glu_1:2:3:4:5	use	C5H9NO4
PheMes	intermediate	Phe_1:2:3:4:5	use	C9H11NO2
GlyMes	intermediate	Gly_1:2	use	C2H5NO2
IleMes	intermediate	Ile_1:2:3:4:5:	use	C6H13NO2
SerMes	intermediate	Ser_1:2:3	use	C3H7NO3
ValMes	intermediate	Val_1:2:3:4:5	use	C5H11NO2
TyrMes	intermediate	Tyr_1:2:3:4:5	use	C9H11NO3
ThrMes	intermediate	Thr_1:2:3:4	use	C4H9NO3

State	Id	type	flux_calue	flux_std	lb	ub	
reaction	r1	fixed	0	1	0.0001	1000	SubsGlc --> G6P
reaction	r2	free	1	1	0.0001	1000	G6P --> F6P
reaction	r3	free	1	1	0.0001	1000	F6P --> G6P
reaction	r4	free	1	1	0.0001	1000	F6P --> FBP
reaction	r5	free	1	1	0.0001	1000	FBP --> F6P
reaction	r6	free	1	1	0.0001	1000	FBP --> DHAP + GAP
reaction	r7	free	1	1	0.0001	1000	DHAP + GAP --> FBP
reaction	r8	free	1	1	0.0001	1000	DHAP --> GAP
reaction	r9	free	1	1	0.0001	1000	GAP --> DHAP
reaction	r10	free	1	1	0.0001	1000	GAP --> PGA
reaction	r11	free	1	1	0.0001	1000	PGA --> GAP
reaction	r12	free	1	1	0.0001	1000	PGA --> PEP
reaction	r13	free	1	1	0.0001	1000	PEP --> PGA
reaction	r14	free	1	1	0.0001	1000	PEP --> Pyr
reaction	r15	free	1	1	0.0001	1000	Pyr --> PEP
reaction	r16	free	1	1	0.0001	1000	Pyr --> AcCOA + CO2in
reaction	r17	free	1	1	0.0001	1000	AcCOA + Oxa --> IsoCit
reaction	r18	free	1	1	0.0001	1000	IsoCit --> aKG + CO2in
reaction	r19	free	1	1	0.0001	1000	aKG --> Suc + CO2in
reaction	r20	free	1	1	0.0001	1000	Suc --> Fum
reaction	r21	free	1	1	0.0001	1000	Fum --> Suc
reaction	r22	free	1	1	0.0001	1000	Fum --> Mal
reaction	r23	free	1	1	0.0001	1000	Mal --> Fum
reaction	r24	free	1	1	0.0001	1000	Mal --> Oxa
reaction	r25	free	1	1	0.0001	1000	Oxa --> Mal
reaction	r26	free	1	1	0.0001	1000	IsoCit + AcCOA --> Mal + S
reaction	r27	free	1	1	0.0001	1000	G6P --> m6PG
reaction	r28	free	1	1	0.0001	1000	m6PG --> Ru5P + CO2in
reaction	r29	free	1	1	0.0001	1000	Ru5P --> R5P
reaction	r30	free	1	1	0.0001	1000	R5P --> Ru5P
reaction	r31	free	1	1	0.0001	1000	Ru5P --> Xu5P
reaction	r32	free	1	1	0.0001	1000	Xu5P --> Ru5P
reaction	r33	free	1	1	0.0001	1000	R5P + Xu5P --> S7P + GAP
reaction	r34	free	1	1	0.0001	1000	GAP + S7P --> Xu5P + R5P
reaction	r35	free	1	1	0.0001	1000	GAP + S7P --> F6P + E4P
reaction	r36	free	1	1	0.0001	1000	E4P + F6P --> S7P + GAP
reaction	r37	free	1	1	0.0001	1000	E4P + Xu5P --> F6P + GAP
reaction	r38	free	1	1	0.0001	1000	GAP + F6P --> Xu5P + E4P
reaction	r39	free	1	1	0.0001	1000	m6PG --> Pyr + GAP
reaction	r40	free	1	1	0.0001	1000	PEP + CO2in --> Oxa
reaction	r41	free	1	1	0.0001	1000	Oxa --> PEP + CO2in
reaction	r42	free	1	1	0.0001	1000	Mal --> Pyr + CO2in
reaction	r49	free	1	1	0.0001	1000	AcCOA --> Acetate
reaction	r50	fitting	36.8120029	2.81761854	0.0001	1000	Acetate --> Acetateex
reaction	r56	free	1	1	0.0001	1000	SubsCO2 --> CO2in
reaction	r57	free	1	1	0.0001	1000	CO2in --> CO2ex
reaction	r58	pseudo	1	1	0.0001	1000	Pyr --> Ala
reaction	r59	pseudo	1	1	0.0001	1000	Oxa --> Asp
reaction	r60	pseudo	1	1	0.0001	1000	Oxa --> Thr
reaction	r61	pseudo	1	1	0.0001	1000	aKG --> Glu
reaction	r62	pseudo	1	1	0.0001	1000	E4P + PEP + PEP --> Phe
reaction	r63	pseudo	1	1	0.0001	1000	E4P + PEP + PEP --> Tyr
reaction	r64	pseudo	1	1	0.0001	1000	Oxa + Pyr --> Ile
reaction	r65	pseudo	1	1	0.0001	1000	AcCOA + Pyr + Pyr --> Leu
reaction	r66	pseudo	1	1	0.0001	1000	Pyr + Pyr --> Val

reaction	r67	free	1	1	0.0001	1000	PGA --> Ser
reaction	r68	free	1	1	0.0001	1000	Ser --> Gly + MEETHF
reaction	r69	free	1	1	0.0001	1000	Gly + MEETHF --> Ser
reaction	r72	fixed	0.95021467	1	0.0001	1000	G6P --> Biomass
reaction	r73	fixed	0.32863522	1	0.0001	1000	F6P --> Biomass
reaction	r74	fixed	0.59793996	1	0.0001	1000	DHAP --> Biomass
reaction	r75	fixed	2.61888434	1	0.0001	1000	PGA --> Biomass
reaction	r76	fixed	1.60377696	1	0.0001	1000	Ser --> Biomass
reaction	r77	fixed	2.69768263	1	0.0001	1000	Gly --> Biomass
reaction	r78	fixed	3.1472964	1	0.0001	1000	MEETHF --> Biomass
reaction	r79	fixed	3.33316766	1	0.0001	1000	PEP --> Biomass
reaction	r80	fixed	13.1315032	1	0.0001	1000	Pyr --> Biomass
reaction	r81	fixed	13.5718466	1	0.0001	1000	AcCOA --> Biomass
reaction	r82	fixed	5.00091029	1	0.0001	1000	aKG --> Biomass
reaction	r83	fixed	8.28170026	1	0.0001	1000	Oxa --> Biomass
reaction	r84	fixed	4.16101322	1	0.0001	1000	R5P --> Biomass
reaction	r85	fixed	1.67330486	1	0.0001	1000	E4P --> Biomass
reaction	r86	fixed	10	1	0.0001	1000	Ala --> Alaex
reaction	r87	fixed	10	1	0.0001	1000	Asp --> Aspex
reaction	r88	fixed	10	1	0.0001	1000	Thr --> Threx
reaction	r89	fixed	10	1	0.0001	1000	Glu --> Gluex
reaction	r90	fixed	10	1	0.0001	1000	Phe --> Pheex
reaction	r91	fixed	10	1	0.0001	1000	Tyr --> Tyrex
reaction	r92	fixed	10	1	0.0001	1000	Ile --> Ileex
reaction	r93	fixed	10	1	0.0001	1000	Leu --> Leuex
reaction	r94	fixed	10	1	0.0001	1000	Val --> Valex
reaction	r104	fixed	100	1	0.0001	1000	Subsmeoh --> meoh
reaction	r105	free	1	1	0.0001	1000	meoh --> METHF
reaction	r106	free	1	1	0.0001	1000	METHF --> MEETHF
reaction	r107	free	1	1	0.0001	1000	MEETHF --> METHF
reaction	r108	free	1	1	0.0001	1000	CO2in + METHF --> AcCOA
reaction	r109	free	1	1	0.0001	1000	AcCOA + CO2in --> Pyr
reversible	PGI	free	1	1	-300	300	
reversible	FBA	free	1	1	-300	300	
reversible	TPI	free	1	1	-300	300	
reversible	GAPDH	free	1	1	-300	300	
reversible	PEPH	free	1	1	-300	300	
reversible	SDH	free	1	1	-300	300	
reversible	MDH	free	1	1	-300	300	
reversible	RPI	free	1	1	-300	300	
reversible	RBE	free	1	1	-300	300	
reversible	TKT1	free	1	1	-300	300	
reversible	TAL	free	1	1	-300	300	
reversible	TKT2	free	1	1	-300	300	
reversible	FH	free	1	1	-300	300	
reversible	THF	free	1	1	-300	300	
reversible	PFOR	free	1	1	-300	300	
metabolite	m6PG	fixed	10	1	0.001	100	
metabolite	AcCOA	fixed	10	1	0.001	100	
metabolite	Acetate	fixed	10	1	0.001	100	
metabolite	Acetateex	fixed	10	1	0.001	100	
metabolite	aKG	fixed	10	1	0.001	100	
metabolite	Ala	fixed	10	1	0.001	100	
metabolite	Asp	fixed	10	1	0.001	100	
metabolite	Biomass	fixed	10	1	0.001	100	
metabolite	CO2ex	fixed	10	1	0.001	100	

metabolite	CO2in	fixed	10	1	0.001	100
metabolite	DHAP	fixed	10	1	0.001	100
metabolite	E4P	fixed	10	1	0.001	100
metabolite	F6P	fixed	10	1	0.001	100
metabolite	FBP	fixed	10	1	0.001	100
metabolite	Formate	fixed	10	1	0.001	100
metabolite	G6P	fixed	10	1	0.001	100
metabolite	GAP	fixed	10	1	0.001	100
metabolite	Glu	fixed	10	1	0.001	100
metabolite	Gly	fixed	10	1	0.001	100
metabolite	Ile	fixed	10	1	0.001	100
metabolite	IsoCit	fixed	10	1	0.001	100
metabolite	Leu	fixed	10	1	0.001	100
metabolite	Mal	fixed	10	1	0.001	100
metabolite	MEETHF	fixed	10	1	0.001	100
metabolite	METHF	fixed	10	1	0.001	100
metabolite	Subsmeoh	fixed	10	1	0.001	100
metabolite	meoh	fixed	10	1	0.001	100
metabolite	Oxa	fixed	10	1	0.001	100
metabolite	PEP	fixed	10	1	0.001	100
metabolite	PGA	fixed	10	1	0.001	100
metabolite	Phe	fixed	10	1	0.001	100
metabolite	Pyr	fixed	10	1	0.001	100
metabolite	R5P	fixed	10	1	0.001	100
metabolite	Ru5P	fixed	10	1	0.001	100
metabolite	S7P	fixed	10	1	0.001	100
metabolite	Ser	fixed	10	1	0.001	100
metabolite	SubsCO2	fixed	10	1	0.001	100
metabolite	SubsGlc	fixed	10	1	0.001	100
metabolite	Fum	fixed	10	1	0.001	100
metabolite	Suc	fixed	10	1	0.001	100
metabolite	Thr	fixed	10	1	0.001	100
metabolite	Tyr	fixed	10	1	0.001	100
metabolite	Val	fixed	10	1	0.001	100
metabolite	Xu5P	fixed	10	1	0.001	100

E. limosum MDV Data

Name	Spectrum	Select	MDV	Std
AlaMes	0	1	0.17114061	0.00394227
AlaMes	1	1	0.36655829	0.00409504
AlaMes	2	1	0.39550499	0.00346101
AlaMes	3	1	0.06679612	0.00192223
AspMes	0	1	0.04914449	0.00150066
AspMes	1	1	0.22826684	0.00126331
AspMes	2	1	0.39034445	0.0047016
AspMes	3	1	0.2898729	0.00491101
AspMes	4	1	0.04237139	0.00075246
GluMes	0	1	0.02805793	0.00130279
GluMes	1	1	0.15216688	0.0095609
GluMes	2	1	0.43438327	0.00347245
GluMes	3	1	0.30825694	0.00426113
GluMes	4	1	0.07044202	0.00291386
GluMes	5	1	0.00669295	0.00035686
PheMes	0	1	0.00684417	0.01185445
PheMes	1	1	0.04785495	0.00311974
PheMes	2	1	0.1278987	0.00327924
PheMes	3	1	0.22363331	0.0027905
PheMes	4	1	0.27565234	0.00316041
PheMes	5	1	0.20542865	0.00308032
PheMes	6	1	0.0891477	0.00158648
PheMes	7	1	0.02049608	0.00076243
PheMes	8	1	0.00279879	0.00021621
PheMes	9	1	0.00024535	4.19E-05
GlyMes	0	1	0.20787736	0.02461689
GlyMes	1	1	0.43055291	0.02852062
GlyMes	2	1	0.36156692	0.01336146
IleMes	0	1	0.04136346	0.00074437
IleMes	1	1	0.22092766	0.00329951
IleMes	2	1	0.35356635	0.00207376
IleMes	3	1	0.27468045	0.00312924
IleMes	4	1	0.09319801	0.00026546
IleMes	5	1	0.01499805	0.00045037
IleMes	6	1	0.00126607	4.41E-05
SerMes	0	1	0.19444841	0.00556176
SerMes	1	1	0.39087055	0.00831015
SerMes	2	1	0.35548474	0.0032906
SerMes	3	1	0.05919655	0.00092983
ValMes	0	1	0.13016281	0.00185205
ValMes	1	1	0.26218626	0.00255883
ValMes	2	1	0.33951318	0.00309477

ValMes	3	1	0.21669176	0.00280704
ValMes	4	1	0.0473229	0.00164188
ValMes	5	1	0.0041231	0.00016117
TyrMes	0	1	0.02019424	0.0019056
TyrMes	1	1	0.0456291	0.00125604
TyrMes	2	1	0.12545546	0.00289849
TyrMes	3	1	0.21522188	0.00475372
TyrMes	4	1	0.26154935	0.00377846
TyrMes	5	1	0.20866449	0.00273764
TyrMes	6	1	0.09360523	0.00127952
TyrMes	7	1	0.02545485	0.00094753
TyrMes	8	1	0.00387081	0.00024769
TyrMes	9	1	0.00035456	0.00031265
ThrMes	0	1	0.05167582	0.00155364
ThrMes	1	1	0.24602017	0.00132254
ThrMes	2	1	0.38594425	0.00328518
ThrMes	3	1	0.28174731	0.00328829
ThrMes	4	1	0.03461259	0.00291231