```
(* Pseudomonas putida (P. putida) -- Null space analysis *)
In[496]:= (* List of metabolite identifiers *)
    metaboliteIds = {"2dda7p_c", "2ddg6p_c", "2dhg1cn_c", "34dhbz_c", "3dhq_c",
       "3dhsk_c", "3pg_c", "6p2dhglcn_c", "6pgc_c", "ac_c", "acald_c", "accoa_c",
       "acon c", "actp c", "adp c", "akg c", "amp c", "atp c", "catechol c",
       "ccmuac_c", "cit_c", "co2_c", "coa_c", "dhap_c", "e4p_c", "etoh_c", "f6p_c",
       "fdp_c", "fum_c", "g3p_c", "g6p_c", "g1c__D_c", "g1cn_c", "g1n__L_c",
       "glu__L_c", "glx_c", "glyc3p_c", "glyc_c", "h2o_c", "h_c", "hco3_c", "icit_c",
       "lac D c", "mal L c", "nad c", "nadh c", "nadp c", "nadph c", "nh4 c",
       "o2_c", "oaa_c", "pep_c", "pi_c", "pyr_c", "q8_c", "q8h2_c", "r5p_c",
       "ru5p__D_c", "s7p_c", "succ_c", "xu5p__D_c", "ac_e", "acald_e", "akg_e",
       "co2_e", "fum_e", "glc__D_e", "gln__L_e", "glu__L_e", "glyc_e", "h2o_e", "h_e",
       "lac__D_e", "mal__L_e", "nh4_e", "o2_e", "pi_e", "pyr_e", "succ_e", "toh_e"};
    (* List of reaction identifiers *)
    reactionIds = {"3-DEHYDROQUINATE-DEHYDRATASE-RXN$r", "ACALD$r", "ACALDt$r",
       "ACKr$r", "ACONTa$r", "ACONTb$r", "ALCD2x$r", "ATPS4r$r", "CO2t$r",
       "CS$r", "DAHPSYN-RXN$r", "ENO$r", "ETOHt2r$r", "EX co2 e$r", "EX qlc e$r",
       "EX_h2o_e$r", "EX_h_e$r", "EX_nh4_e$r", "EX_o2_e$r", "EX_pi_e$r",
       "FBA$r", "FRD7$r", "FUM$r", "GAPD$r", "GLUDy$r", "GLYCT$r", "H2Ot$r",
       "HCO3E$r", "ICDHyr$r", "ICL$r", "MDH$r", "NADTRHD$r", "NH4t$r", "O2t$r",
       "PDH$r", "PGI$r", "PGLCNDH$r", "PROTOCATECHUATE-DECARBOXYLASE-RXN$r",
       "PTAr$r", "PYRt2$r", "RPE$r", "RPI$r", "TALA$r", "TKT1$r", "TKT2$r",
       "TPI$r", "XYLA$r", "2DHGLCK$f", "3-DEHYDROQUINATE-DEHYDRATASE-RXN$f",
       "3-DEHYDROQUINATE-SYNTHASE-RXN$f", "ACALD$f", "ACALDt$f", "ACKr$f", "ACONTa$f",
       "ACONTb$f", "ACt2r$f", "ADK1$f", "AKGDH$f", "AKGt2r$f", "ALCD2x$f", "ATPM$f",
       "ATPS4r$f", "Biomass_Ecoli_core_w_GAM$f", "CATECHOL-12-DIOXYGENASE-RXN$f",
       "CO2t$f", "CS$f", "CYTBD$f", "DAHPSYN-RXN$f", "DHSHIKIMATE-DEHYDRO-RXN$f",
       "D_LACt2$f", "ENO$f", "ETOHt2r$f", "EX_ac_e$f", "EX_acald_e$f", "EX_akg_e$f",
       "EX_co2_e$f", "EX_etoh_e$f", "EX_fum_e$f", "EX_glc_e$f", "EX_gln__L_e$f",
       "EX_glu__L_e$f", "EX_glyc_e$f", "EX_h2o_e$f", "EX_h_e$f", "EX_lac__D_e$f",
       "EX mal L e$f", "EX nh4 e$f", "EX o2 e$f", "EX pi e$f", "EX pyr e$f",
       "EX_succ_e$f", "EX_xyl_e$f", "FBA$f", "FBP$f", "FRD7$f", "FUM$f", "FUMt2_2$f",
       "G3PD$f", "G6PDH2r$f", "GADktpp$f", "GAPD$f", "GLCDpp$f", "GLCabcpp$f",
       "GLNS$f", "GLNabc$f", "GLUDy$f", "GLUN$f", "GLUSy$f", "GLUt2r$f", "GLYCT$f",
       "GLYK$f", "GND$f", "GNK$f", "H2Ot$f", "HCO3E$f", "HEX1$f", "ICDHyr$f",
       "ICL$f", "KDPGALDOL$f", "LDH_D$f", "MALS$f", "MALt2_2$f", "MDH$f", "ME1$f",
       "ME2$f", "NADH16$f", "NADTRHD$f", "NH4t$f", "O2t$f", "PC$f", "PDH$f",
       "PGI$f", "PGL$f", "PGLCNDH$f", "PGLUCONDEHYDRAT$f", "PIt2r$f", "PPC$f",
       "PPCK$f", "PROTOCATECHUATE-DECARBOXYLASE-RXN$f", "PTAr$f", "PYK$f",
       "PYRt2$f", "RPE$f", "RPI$f", "SUCCt2_2$f", "SUCCt3$f", "TALA$f", "THD2$f",
       "TKT1$f", "TKT2$f", "TPI$f", "XYLA$f", "XYL_ABC$f", "muconate_sink$f"};
    (* Matrix of stoichiometric coefficients
     (Rows=Metabolites; Columns=Reactions) *)
```

0, 0, 0, 0, 0, 0, 0, 0, 0, 0, -1.496, 0, 0, 0, 0, 0, 0, 0, -1, 0, 0, 0, 0, 0, 00, 0, 0, 0, 0, 0, 0, 0, 0, 0, 1, 0, 0, 0, 0, 0, 0, 0, 0, 0, 1, 0, 0, 0,

0, 0, 0, 0, 0, 0, 0, 0, -1, 0, 0, 0, 1, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 1, 0,0, 0, 0, 0, 0, 0, 0, 0, 0, 0, -3.7478, 0, 0, -1, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 00, 1, 0, 0, 0, 0, 0, 0, 0, 1, 0, 0, -1, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 1, 00, 0, 0, 1, 0, -1, 0, 0, 0, 0, 0, 0, 0, 1, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, -1, 0, 0, 0, 0, 0, 0, 0, -1, 0, 0, 1, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, -1, 0},

```
0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 1, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0,
```

0, 1, -1, 0, 0, 0, 0, 0, -1, -1, -59.81, 0, 0, -1, 1, -1, 1, 0, 1, 0, 0, 0, 0, 0 $\{0, -1, 0, 0, 0, 0, -1, 3, 0, -1, 0, 0, -1, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, -1,$ -1, 0, 0, 1, 0, 0, -1, 0, 0, 0, 0, 0, 0, -2, 1, 0, -1, 0, 0, 0, 0, 0, 0, 0, -2, 0, 0, 1, 0, 0, 0, 0, 1, 0, 0, 1, 1, 1, -3, 59.81, 2, 0, 1, -2, 0, 0, 1, 0, 1, 0, 0,1, 1, 1, 1, 0, -1, 2, 0, 1, 0, 1, 0, -1, 1, 0, 0, 0, -1, 1, 2, 1, 0, 0, -4, 0, 0,0, 1, 0, 0, 1, 2, 0, 1, 0, 0, -1, 0, -1, 1, 0, 0, 2, 1, 0, 1, 0, 0, 0, 0, 1, 00, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, -1, -1, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 01, 0, 0, 0, 0, 0, 1, 0, 1, 0, 0, 3.547, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, -1, 0, 1, 0, 0, 0, -1, 0, 0, 0, 0, -1, 0, 0, 0, 0, 0, 0, 0, -1, 0, 1, 0,0, 0, 0, 0, 0, 1, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, -1, 0, 0, 0, 0, 0, 0

0, 0, 0, 1, 0, -1, 0, 0, 0, 1, 0, 0, 0, 0, 1, 0, 0, 0, 0, 0, 0, 0, 1, 0, -1, 0,0, 0, 0, 0, 0, -1, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 1, 0, 0, 0, 0, 0, 00, 0, 0, 0, 0, 0, 0, 0, 0, 0, -1.7867, 0, 0, -1, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 00, 0, 0, 0, 0, 0, 0, 0, 0, -0.5191, 0, 0, 0, 0, -1, 0, 0, 1, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 1, 0, 0, 0, 0, 0, 0, 0, 0, 0, 1, 0, 0, 0, 0, 0, 0, 0, -1, 0, 0, 1, 1, 59.81, 0, 0, 0, 0, 1, 0, 0, 0, 0, 0, 0, 0, 0, 0, 00, 1, 0, 0, 0, 0, 0, 1, 1, 0, 0, -1, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 1, 0

0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, -1, 1, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 00, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 1, 0, 0, 0, 0, 0, 1, -1, 0, 0, 0, 00, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, -1, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, -1, 0,

0, 0, -1, 0, 0, -1, 0, 0, 4, 0, 0, 0, 0, 2, 0, 0, -1, 0, -1, 0, 0, 0, 0, 0, 0, 00, 0, 0, 0, 0, -1, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, -2, 0, 0, 0, 1, 0, 0,0, 0, 0, 0, -2, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, -2, 0, 0, 0, 3, 0, 0, 0, 0, 00, 0, 0, 0, 0, -1, 0, 0, 0, 0, 0, -1, 0, 0, -2, -1, 0, -1, 0, 0, 0, 0, 0, 0, 0

```
0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 1, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0,
 (* Numerical tolerance, viz., the neighborhood of zero with
respect to the matrix of stoichiometric coefficients. *)
tolerance = Times[Max[Dimensions[stoichiometryMatrix]],
 $MachineEpsilon, Norm[stoichiometryMatrix, Infinity]];
(* Extracellular metabolites are denoted by the "_e" suffix. *)
extracellularMetaboliteIds = Select[metaboliteIds,
Function[string, Last[StringSplit[string, "_"]] == "e"]]; (* not used *)
(* Intracellular metabolites are denoted by the "_c" suffix. *)
intracellularMetaboliteIds =
Select[metaboliteIds, Function[string, Last[StringSplit[string, "_"]] == "c"]];
(* The block of the matrix of stoichiometric
coefficients for extracellular metabolites only. *)
extracellularStoichiometryMatrix =
Drop[stoichiometryMatrix, Length[intracellularMetaboliteIds]]; (* not used *)
(* The block of the matrix of stoichiometric
coefficients for intracellular metabolites only. *)
intracellularStoichiometryMatrix =
Take[stoichiometryMatrix, Length[intracellularMetaboliteIds]];
(* The "null space" of the block of the matrix of stoichiometric
coefficients for intracellular metabolites only. *)
intracellularNullspaceMatrix = Transpose[
 RowReduce[NullSpace[intracellularStoichiometryMatrix], Tolerance → tolerance];
(* Print the matrix of stoichiometric coefficients. *)
```

Dimensions[stoichiometryMatrix] ${\tt MatrixForm[stoichiometryMatrix, Table Headings} \rightarrow \{{\tt metaboliteIds, reactionIds}\}]$

 $\mathsf{Out}[\mathsf{503}] = \; \left\{\, \mathsf{80} \; \mathsf{,} \; \; \mathsf{154} \, \right\}$

Out[504]//MatrixForm=

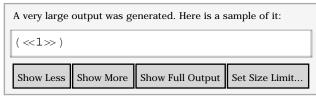
trixForm=					
	3-DEHYDROQUINATE-DEHYDRATASE-RXN\$r	ACALD\$r	ACALDt\$r	ACKr\$r	ACONTa\$r 1
2dda7p_c	0	0	0	0	0
2ddg6p_c	0	0	0	0	0
2dhglcn_c	0	0	0	0	0
34dhbz_c	0	0	0	0	0
3dhq_c	1	0	0	0	0
3dhsk_c	-1	0	0	0	0
3pg_c	0	0	0	0	0
6p2dhglcn_c	0	0	0	0	0
брдс_с	0	0	0	0	0
ac_c	0	0	0	1	0
acald_c	0	1	- 1	0	0
accoa_c	0	- 1	0	0	0
acon_c	0	0	0	0	- 1
actp_c	0	0	0	- 1	0
adp_c	0	0	0	- 1	0
akg_c	0	0	0	0	0
amp_c	0	0	0	0	0
atp_c	0	0	0	1	0
catechol_c	0	0	0	0	0
ccmuac_c	0	0	0	0	0
cit_c	0	0	0	0	1
co2_c	0	0	0	0	0
coa_c	0	1	0	0	0
dhap_c	0	0	0	0	0
e4p_c	0	0	0	0	0
etoh_c	0	0	0	0	0
f6p_c	0	0	0	0	0
fdp_c	0	0	0	0	0
fum_c	0	0	0	0	0
g3p_c	0	0	0	0	0
дбр_с	0	0	0	0	0
glcD_c	0	0	0	0	0
glcn_c	0	0	0	0	0
glnL_c	0	0	0	0	0
gluL_c	0	0	0	0	0
glx_c	0	0	0	0	0
glyc3p_c	0	0	0	0	0
glyc_c	0	0	0	0	0
h2o_c	-1	0	0	0	- 1
h_c	0	- 1	0	0	0
hco3_c	0	0	0	0	0
icit_c	0	0	0	0	0
lacD_c	0	0	0	0	0
malL_c	0	0	0	0	0
nad_c	0	1	0	0	0
ļ					

nadh_c	0	- 1	0	0	0
nadp_c	0	0	0	0	0
nadph_c	0	0	0	0	0
nh4_c	0	0	0	0	0
o2_c	0	0	0	0	0
oaa_c	0	0	0	0	0
pep_c	0	0	0	0	0
pi_c	0	0	0	0	0
pyr_c	0	0	0	0	0
q8_c	0	0	0	0	0
q8h2_c	0	0	0	0	0
r5p_c	0	0	0	0	0
ru5pD_c	0	0	0	0	0
s7p_c	0	0	0	0	0
succ_c	0	0	0	0	0
xu5pD_c	0	0	0	0	0
ac_e	0	0	0	0	0
acald_e	0	0	1	0	0
akg_e	0	0	0	0	0
co2_e	0	0	0	0	0
fum_e	0	0	0	0	0
glcD_e	0	0	0	0	0
glnL_e	0	0	0	0	0
gluL_e	0	0	0	0	0
glyc_e	0	0	0	0	0
h2o_e	0	0	0	0	0
h_e	0	0	0	0	0
lacD_e	0	0	0	0	0
malL_e	0	0	0	0	0
nh4_e	0	0	0	0	0
o2_e	0	0	0	0	0
pi_e	0	0	0	0	0
pyr_e	0	0	0	0	0
succ_e	0	0	0	0	0
toh_e	0	0	0	0	0

In[505]:= (* Print the "null space", then replace values in the neighborhood of zero with zero. *) Dimensions[intracellularNullspaceMatrix] MatrixForm[intracellularNullspaceMatrix, TableHeadings → {reactionIds}] TableHeadings → {reactionIds}]

Out[505]= $\{154, 98\}$

Out[506]//MatrixForm=



3-DEHYDROQUINATE-DEHYDRATASE-RXN\$r	1	0	0	0	0	0
ACALD\$r	0	1	0	0	0	0
ACALDt\$r	0	0	1	0	0	0
ACKr\$r	0	0	0	1	0	0
ACONTa\$r	0	0	0	0	1	0
ACONTb\$r	0	0	0	0	0	1
ALCD2x\$r	0	0	0	0	0	0
ATPS4r\$r	0	0	0	0	0	0
CO2t\$r	0	0	0	0	0	0
CS\$r	0	0	0	0	0	0
DAHPSYN-RXN\$r	0	0	0	0	0	0
ENO\$r	0	0	0	0	0	0
ETOHt2r\$r	0	0	0	0	0	0
EX_co2_e\$r	0	0	0	0	0	0
EX_glc_e\$r	0	0	0	0	0	0
EX_h2o_e\$r	0	0	0	0	0	0
EX_h_e\$r	0	0	0	0	0	0
EX_nh4_e\$r	0	0	0	0	0	0
EX_o2_e\$r	0	0	0	0	0	0
EX_pi_e\$r	0	0	0	0	0	0
FBA\$r	0	0	0	0	0	0
FRD7\$r	0	0	0	0	0	0
FUM\$r	0	0	0	0	0	0
GAPD\$r	0	0	0	0	0	0
GLUDy\$r	0	0	0	0	0	0
GLYCT\$r H2Ot\$r	0	0	0	0	0	0
HZOUŞI HCO3E\$r	0		0	0 0	0 0	0
· ·	0	0	0	0	0	0
ICDHyr\$r ICL\$r	0	0	0	0	0	0
MDH\$r	0	0	0	0	0	0
MDH31 NADTRHD\$r	0	0	0	0	0	0
NADIRADŞI NH4t\$r	0	0	0	0	0	0
O2t\$r	0	0	0	0	0	0
PDH\$r	0	0	0	0	0	0
PGI\$r	0	0	0	0	0	0
PG131 PGLCNDH\$r	0	0	0	0	0	0
PROTOCATECHUATE-DECARBOXYLASE-RXN\$r	0	0	0	0	0	0
PTAr\$r	0	0	0	0	0	0
PYRt2\$r	0	0	0	0	0	0
RPE\$r	0	0	0	0	0	0
RPI\$r	0	0	0	0	0	0
TALA\$r	0	0	0	0	0	0
TKT1\$r	0	0	0	0	0	0
TKT151	0	0	0	0	0	0
TPI\$r	0	0	0	0	0	0
XYLA\$r	0	0	0	0	0	0
2DHGLCK\$f	0	0	0	0	0	0
3-DEHYDROQUINATE-DEHYDRATASE-RXN\$f	0	0	0	0	0	0
3-DEHYDROQUINATE-SYNTHASE-RXN\$f	-1.	0	0	0	0	0
		^	^	2	^	^

ACALDŞİ	I U	U	U	U	U	U
ACALDt\$f	0	0	0	0	0	0
ACKr\$f	0	0	0	0	0	0
ACONTa\$f	0	0	0	0	0	0
ACONTb\$f	0	0	0	0	-1.	1.
ACt2r\$f	0	0	0	-1.	0	0
ADK1\$f	0	0	0	0	0	0
AKGDH\$f	0	0	0	0	0	0
AKGt2r\$f	0	0	0	0	0	0
ALCD2x\$f	0	-1.	1.	0	0	0
ATPM\$f	0	0	0	0	0	0
ATPS4r\$f	0	0	0	0	0	0
Biomass_Ecoli_core_w_GAM\$f	0	0	0	0	0	0
CATECHOL-12-DIOXYGENASE-RXN\$f	-1.	0	0	0	0	0
CO2t\$f	0	0	0	0	0	0
CS\$f	0	0	0	0	-1.	0
CYTBD\$f	0	0	0	0	0	0
DAHPSYN-RXN\$f	-1.	0	0	0	0	0
DHSHIKIMATE-DEHYDRO-RXN\$f	-1.	0	0	0	0	0
D_LACt2\$f	0	0	0	0	0	0
ENO\$f	0	0	0	0	0	0
ETOHt2r\$f	0	-1.	1.	0	0	0
EX_ac_e\$f	0	0	0	0	0	0
EX_acald_e\$f	0	0	0	0	0	0
EX_akg_e\$f	0	0	0	0	0	0
EX_co2_e\$f	0	0	0	0	0	0
EX_etoh_e\$f	0	0	0	0	0	0
EX_fum_e\$f	0	0	0	0	0	0
EX_glc_e\$f	0	0	0	0	0	0
EX_glnL_e\$f	0	0	0	0	0	0
EX_gluL_e\$f	0	0	0	0	0	0
EX_glyc_e\$f	0	0	0	0	0	0
EX_h2o_e\$f	0	0	0	0	0	0
EX_h_e\$f	0	0	0	0	0	0
EX_lacD_e\$f	0	0	0	0	0	0
EX_malL_e\$f	0	0	0	0	0	0
EX_nh4_e\$f	0	0	0	0	0	0
EX_o2_e\$f	0	0	0	0	0	0
EX_pi_e\$f	0	0	0	0	0	0
EX_pyr_e\$f	0	0	0	0	0	0
EX_succ_e\$f	0	0	0	0	0	0
					0	
EX_xyl_e\$f	0	0	0	0		0
FBA\$f	0	0	0	0	0	0
FBP\$f	0	0	0	0	0	0
FRD7\$f	0	0	0	0	0	0
FUM\$f	0	0	0	0	0 0	0
FUMt2_2\$f		0				0
G3PD\$f G6PDH2r\$f	0	0	0	0	0 0	0
GOPDHZTŞI CADk+nncf	0	0	0	0	0	0
: :::::::::::::::::::::::::::::::::::::	• •			* *		

GAUKTPPŞI	I U	U	U	U	U	U
GAPD\$f	0	0	0	0	0	0
GLCDpp\$f	0	0	0	0	0	0
GLCabcpp\$f	0	0	0	0	0	0
GLNS\$f	0	0	0	0	0	0
GLNabc\$f	0	0	0	0	0	0
GLUDy\$f	0	0	0	0	0	0
GLUN\$f	-1.	2.	-1.	0	1.	0
GLUSy\$f	1.	-2.	1.	0	-1.	0
GLUt2r\$f	-1.	2.	-1.	0	1.	0
GLYCT\$f	0	0	0	0	0	0
GLYK\$f	0	0	0	0	0	0
GND\$f	-0.5	0	0	0	0	0
GNK\$f	0	0	0	0	0	0
H2Ot\$f	-0.5	4.	-2.	1.	0	0
HCO3E\$f	0	0	0	0	0	0
HEX1\$f	0	0	0	0	0	0
ICDHyr\$f	1.	-2.	1.	0	-1.	0
ICL\$f	-1.	2.	-1.	0	0	0
KDPGALDOL\$f	-0.5	0	0	0	0	0
LDH_D\$f	0	0	0	0	0	0
MALS\$f	-1.	2.	-1.	0	0	0
MALt2_2\$f	2.5	∠. -3.	1.	-1.	1.	0
MDH\$f	0	0	0	0	0	0
ME1\$f	0	0	0	0	0	0
ME1\$1 ME2\$f			0		1.	0
MEZŞI NADH16\$f	1.5 0	-1. 0		-1. O	0	
			0			0
NADTRHD\$f	0	0	0	0	0	0
NH4t\$f	1.	-2.	1.	0	-1.	0
02t\$f	-1. 0	0	0	0	0	0
PC\$f		0	0	•	0	0
PDH\$f	-1.	3.	-1.	1.	-1.	0
PGI\$f	0	0	0	0	0	0
PGL\$f	-1.	0	0	0	0	0
PGLCNDH\$f	0	0	0	0		0
PGLUCONDEHYDRAT\$f	-0.5	0	0	0	0	0
PIt2r\$f	1. 0	0	0	0	0	0
PPC\$f	0	0	0	0	-	0
PPCK\$f	1	0	0	0	1. 0	0
PROTOCATECHUATE-DECARBOXYLASE-RXN\$f	-1. 0	0	0	•	-	0
PTAr\$f		0	0	1. 0	0	0
PYK\$f	1.	0	0		1.	0
PYRt2\$f	-3.	4.	-1.	2.	-3.	0
RPE\$f	0	0	0	0	0	0
RPI\$f	0.5	0	0	0	0	0
SUCCt2_2\$f	1.66667	-2.		-0.333333		0
SUCCt3\$f	0.666667	0		-0.333333		0
TALA\$f	-0.5	0	0	0	0	0
THD2\$f	-1.	1.	0	1.	-1.	0
TKT1\$f	0.5	0	0	0	0	0
TKT2\$f	0.5	0	0	0	0	0

```
TPI$f
                                    0
                                             0
                                                      0
                                                                   0
                                                                                      0
     XYLA$f
                                    0
                                             0
                                                      0
                                                                   0
                                                                                      0
                                                                               Ω
                                                      0
                                                                  1.
                                                                                      0
   XYL_ABC$f
                                    1.
                                             0
                                                                               0
                                                                                      0
muconate_sink$f
                                             0
                                                                   0
                                   - 1 .
```

IN[508]:= (* Print the application of the "null space" to the "whole" matrix, then replace values in the neighborhood of zero with zero. *) (* By definition, all elements of the block for intracellular metabolites are in the neighborhood of zero. *) Dimensions[stoichiometryMatrix.intracellularNullspaceMatrix] MatrixForm[stoichiometryMatrix.intracellularNullspaceMatrix, TableHeadings → {metaboliteIds}] MatrixForm[stoichiometryMatrix.intracellularNullspaceMatrix/. $x_{-}/;$ (Abs[x] \le tolerance) \rightarrow 0, TableHeadings \rightarrow {metaboliteIds}]

 $Out[508] = \{80, 98\}$

Out[509]//MatrixForm=

```
2dda7p_c
                    1.9984 \times 10^{-15}
                                          -4.11206 \times 10^{-16}
                                                                    2.6786 \times 10^{-16}
                                                                                            7.8217 \times 10^{-17}
                                                                                                                   -5.16358
                   -1.22125 \times 10^{-15}
                                           1.55769 \times 10^{-15}
                                                                  -4.09496 \times 10^{-16}
                                                                                            1.06699 \times 10^{-15}
                                                                                                                   -5.20446
  2ddq6p_c
                   -5.18696 \times 10^{-16} -1.87398 \times 10^{-16} -3.65368 \times 10^{-16}
                                                                                            6.26584 \times 10^{-17}
 2dhglcn_c
                                                                                                                   -2.16686
                   -1.11022 \times 10^{-16}
                                          -1.08677 \times 10^{-15}
                                                                    7.8208 \times 10^{-16}
                                                                                            8.37876 \times 10^{-16}
                                                                                                                    -8.4968
  34dhbz_c
                                            -5.1384 \times 10^{-17}
                                                                  -9.84386 \times 10^{-17} -3.93248 \times 10^{-17} -2.56873
                            0.
   3dhq_c
                                                                   -1.54999 \times 10^{-16} -6.00843 \times 10^{-17}
  3dhsk_c
                                            2.20899 \times 10^{-16}
                                                                                                                     3.7753:
                                                                    4.15646 \times 10^{-16}
                    6.56802 \times 10^{-17}
                                           -9.77234 \times 10^{-16}
                                                                                           -1.97016 \times 10^{-19}
                                                                                                                    3.50899
    3pg_c
                    6.5236 \times 10^{-16}
                                           -2.12981 \times 10^{-16}
                                                                    3.28551 \times 10^{-16}
                                                                                           -9.37632 \times 10^{-17}
6p2dhglcn_c
                                                                                                                    4.67058
                    1.22125 \times 10^{-15}
                                            1.08812 \times 10^{-16}
                                                                    2.79236 \times 10^{-16}
                                                                                           -7.35375 \times 10^{-16} - 8.85166
   брдс_с
                   -7.51485 \times 10^{-17}
                                            3.3709 \times 10^{-16}
                                                                   -1.80935 \times 10^{-16} -2.22045 \times 10^{-16}
                                                                                                                    1.91545
     ac_c
                                                                   -7.77156 \times 10^{-16} -5.51852 \times 10^{-16}
  acald_c
                    7.67209 \times 10^{-16}
                                                    0.
                                                                                                                    2.12045
                                            2.06614 \times 10^{-15}
                   -2.24927 \times 10^{-15}
                                                                   -1.08166 \times 10^{-15} 1.11022 \times 10^{-15}
                                                                                                                   -1.07796
  accoa_c
                   -2.49228 \times 10^{-16}
                                           -6.57715 \times 10^{-16}
                                                                    6.6446 \times 10^{-16}
                                                                                            2.35949 \times 10^{-16}
                                                                                                                   -1.11022
   acon_c
                   -5.26283 \times 10^{-16}
                                            1.54303 \times 10^{-16}
                                                                    3.04506 \times 10^{-16}
                                                                                            6.66134 \times 10^{-16}
                                                                                                                   -1.36453
   actp_c
                                                                   -1.30624 \times 10^{-14} -1.66533 \times 10^{-15}
                   -1.22125 \times 10^{-15}
                                            2.13996 \times 10^{-14}
                                                                                                                    1.70981
    adp_c
                   -6.66134 \times 10^{-16}
                                                                   -2.22045 \times 10^{-16} -4.84286 \times 10^{-16}
    akg_c
                                                    0.
                                                                                                                    -1.9984
                                          -1.24449 \times 10^{-15}
                   -2.05662 \times 10^{-16}
                                                                    3.34072 \times 10^{-16} -5.42262 \times 10^{-16} -4.15022
    amp_c
                   1.44329 \times 10^{-15}
                                           -2.01551 \times 10^{-14}
                                                                    1.27284 \times 10^{-14}
                                                                                            2.10942 \times 10^{-15}
    atp_c
                                                                                                                   -1.66541
                    3.33067 \times 10^{-16}
                                            6.95499 \times 10^{-16}
                                                                   -7.68698 \times 10^{-16} -5.40677 \times 10^{-16}
                                                                                                                   1.55725
catechol_c
                   -3.33067 \times 10^{-16}
                                            1.02776 \times 10^{-16}
                                                                     4.2365 \times 10^{-16}
                                                                                            5.45329 \times 10^{-16}
                                                                                                                   -1.43541
  ccmuac_c
                   -1.65232 \times 10^{-16}
                                            1.62972 \times 10^{-16}
                                                                   -3.64328 \times 10^{-16} -2.29411 \times 10^{-16}
                                                                                                                    2.22045
    cit_c
                   -3.55271 \times 10^{-15}
                                            4.49792 \times 10^{-15}
                                                                   -2.27357 \times 10^{-15}
                                                                                            1.01076 \times 10^{-15}
                                                                                                                   -2.19239
    co2_c
                    2.24927 \times 10^{-15}
                                           -2.06614 \times 10^{-15}
                                                                    1.08166 \times 10^{-15}
                                                                                           -1.11022 \times 10^{-15}
                                                                                                                   1.07796
    coa_c
                   -1.65942 \times 10^{-15}
                                            2.12708 \times 10^{-15}
                                                                   -9.92501 \times 10^{-16}
                                                                                            4.15736 \times 10^{-16}
                                                                                                                   -1.47519
   dhap_c
                   -1.44329 \times 10^{-15}
                                            5.64058 \times 10^{-16}
                                                                  -2.77219 \times 10^{-16} - 4.82228 \times 10^{-16}
                                                                                                                    1.36935
    e4p_c
                                                                    3.33067 \times 10^{-16}
                                                                                            8.28166 \times 10^{-16}
   etoh_c
                   -2.75392 \times 10^{-16}
                                                    0.
                                                                                                                   -6.88041
                   -8.88178 \times 10^{-16} -9.05573 \times 10^{-16}
                                                                    2.55881 \times 10^{-16}
                                                                                            6.54574 \times 10^{-16}
                                                                                                                    4.32663
    f6p_c
                    8.30761 \times 10^{-16} -6.57715 \times 10^{-16}
                                                                    1.47658 \times 10^{-16}
                                                                                           -7.86496 \times 10^{-16} -6.32302
    fdp_c
                                             4 11070 10-16
                                                                                            D 06406 10-17
```

```
rum_c
                   1.0UU51 × 1U --
                                          -4.11U/2×1U **
                                                                  -2.46U96 × 1U -~
                                                                                           - /.86496 × 1U -
                                                                                                                     1.24485
                   4.38174 \times 10^{-16}
                                          -1.53486 \times 10^{-15}
                                                                    3.15094 \times 10^{-16}
                                                                                            -2.3974 \times 10^{-16}
  g3p_c
                                                                                                                    -6.29738
                   8.79931 \times 10^{-16}
                                          -5.42866 \times 10^{-16}
                                                                   -1.11497 \times 10^{-16}
                                                                                            -3.5449 \times 10^{-17}
  дбр_с
                                                                                                                     2.42854
                  -6.89416 \times 10^{-16}
                                            1.9616 \times 10^{-17}
                                                                    2.82043 \times 10^{-16}
                                                                                            2.59081 \times 10^{-16}
                                                                                                                    -9.91685
glc__D_c
                  1.11863 \times 10^{-16}
                                          -\,3.52174\times 10^{-16}
                                                                    9.68155 \times 10^{-17}
                                                                                           -\,3.19568\times 10^{-16}
                                                                                                                     6.40186
  glcn_c
                  1.33227 \times 10^{-15}
                                          -1.77636 \times 10^{-15}
                                                                    5.55112 \times 10^{-16}
                                                                                           -\,4.71897\times 10^{-16}
gln__L_c
                                                                                                                              0.
                  1.11022 \times 10^{-16}
                                                                                             4.96617 \times 10^{-16}
                                           8.88178 \times 10^{-16}
                                                                            0.
                                                                                                                    -4.44089
glu__L_c
                  -7.77156 \times 10^{-16}
                                           4.44089 \times 10^{-16}
                                                                   -3.33067 \times 10^{-16}
                                                                                           -4.40024 \times 10^{-17}
                                                                                                                     2.97505
  glx_c
                   8.96662 \times 10^{-16}
                                           -5.70334 \times 10^{-16}
                                                                    3.54564 \times 10^{-16}
                                                                                           -5.44785 \times 10^{-16}
                                                                                                                    -1.11361
glyc3p_c
                  -5.24277 \times 10^{-16}
                                           7.05381 \times 10^{-16}
                                                                   -4.22114 \times 10^{-16}
                                                                                            5.89322 \times 10^{-16}
                                                                                                                     1,22893
  glyc_c
                  -4.77396 \times 10^{-15}
                                           -1.82826 \times 10^{-14}
                                                                    1.14018 \times 10^{-14}
                                                                                             4.10783 \times 10^{-15}
                                                                                                                    -1.65473
  h2o_c
                  -7.66054 \times 10^{-15}
                                                                   -1.26674 \times 10^{-14}
                                                                                           -4.32987 \times 10^{-15}
                                           2.28361 \times 10^{-14}
    h_c
                                                                                                                     9.43761
                                                                                            3.34261 \times 10^{-16}
                  -1.66152 \times 10^{-16}
                                           8.22144 \times 10^{-17}
                                                                    2.70706 \times 10^{-16}
                                                                                                                    -6.32302
  hco3_c
                   2.88658 \times 10^{-15}
                                          -1.55431 \times 10^{-15}
                                                                                           -6.63862 \times 10^{-16}
                                                                    3.33067 \times 10^{-16}
  icit_c
                                                                                                                     1.20119
                   9.08673 \times 10^{-17}
                                          -2.53594 \times 10^{-16}
                                                                     1.464 \times 10^{-16}
                                                                                            6.72415 \times 10^{-17}
                                                                                                                     -3.0875
 lac__D_c
                   2.22045 \times 10^{-16}
                                           8.88178 \times 10^{-16}
                                                                    2.19813 \times 10^{-16}
                                                                                            4.44089 \times 10^{-16}
                                                                                                                    -1.33227
mal__L_c
                   3.10862 \times 10^{-15}
                                           -5.21805 \times 10^{-15}
                                                                    2.44156 \times 10^{-15}
                                                                                           -5.55112 \times 10^{-16}
                                                                                                                    -1.11022
  nad_c
                  -3.10862 \times 10^{-15}
                                           5.21805 \times 10^{-15}
                                                                   -2.44156 \times 10^{-15}
                                                                                            5.55112 \times 10^{-16}
                                                                                                                     1.11022
  nadh_c
                  -1.11022 \times 10^{-15}
                                           6.32827 \times 10^{-15}
                                                                   -3.66052 \times 10^{-15}
                                                                                            7.77156 \times 10^{-16}
                                                                                                                      3.9968:
  nadp_c
                   1.11022 \times 10^{-15}
                                           -6.32827 \times 10^{-15}
                                                                    3.66052 \times 10^{-15}
                                                                                           -7.77156 \times 10^{-16}
                                                                                                                     -3.9968
 nadph_c
                   2.22045 \times 10^{-16}
                                           -8.88178 \times 10^{-16}
                                                                                            -2.08202 \times 10^{-16}
  nh4_c
                                                                            Ω
                                                                                                                    -6.66134
                                           1.60959 \times 10^{-15}
                                                                   -9.74478 \times 10^{-16}
                                                                                           -5.78918 \times 10^{-16}
                                                                                                                     1.06674
   o2_c
                  -6.24194 \times 10^{-16}
                                           1.00774 \times 10^{-15}
                                                                   -3.62505 \times 10^{-17}
                                                                                            8.82159 \times 10^{-16}
                                                                                                                    -2.22045
  oaa c
                  -6.66134 \times 10^{-16}
                                           -3.10756 \times 10^{-16}
                                                                   -1.62598 \times 10^{-16}
                                                                                           -6.96556 \times 10^{-16}
                                                                                                                     8.88178
  pep_c
                                                                                           -3.88578 \times 10^{-15}
                  -2.10942 \times 10^{-15}
                                           1.91294 \times 10^{-14}
                                                                   -1.23155 \times 10^{-14}
                                                                                                                     1.63753
   pi_c
                  -4.44089 \times 10^{-16}
                                          -3.55271 \times 10^{-15}
                                                                    2.44249 \times 10^{-15}
                                                                                           -1.33227 \times 10^{-15}
                                                                                                                    -8.88178
  pyr_c
                  -1.1049 \times 10^{-15}
                                           3.63586 \times 10^{-16}
                                                                     6.1929 \times 10^{-16}
                                                                                            1.02957 \times 10^{-15}
   q8_c
                                                                                                                    -6.71445
                   1.1049 \times 10^{-15}
                                                                                           -1.02957 \times 10^{-15}
                                           -3.63586 \times 10^{-16}
                                                                    -6.1929 \times 10^{-16}
  q8h2_c
                                                                                                                     6.71445
                   5.55112 \times 10^{-16}
                                          -1.17261 \times 10^{-15}
                                                                    4.17771 \times 10^{-16}
                                                                                           -1.34434 \times 10^{-16}
                                                                                                                    -1.66931
  r5p_c
                                           1.69655 \times 10^{-15}
                  -1.11022 \times 10^{-16}
                                                                   -6.26305 \times 10^{-16}
                                                                                            4.86794 \times 10^{-16}
ru5p__D_c
                                                                                                                    -2.63944
                                                                    5.2225 \times 10^{-17}
                  -3.33067 \times 10^{-16}
                                           2.33192 \times 10^{-16}
                                                                                            1.34611 \times 10^{-16}
  s7p_c
                                                                                                                    -4.92594
                   \textbf{4.44089} \times \textbf{10}^{-16}
                                                                                           -5.55112 \times 10^{-17}
                                          -1.47225 \times 10^{-15}
                                                                    1.94289 \times 10^{-15}
                                                                                                                     7.21645
  succ c
                   \textbf{4.44089} \times \textbf{10}^{-16}
                                                                    1.66808 \times 10^{-16}
                                                                                           -1.69908 \times 10^{-16}
                                          -4.47098 \times 10^{-17}
                                                                                                                       6.195 \times
xu5p__D_c
                   7.51485 \times 10^{-17}
                                           -3.3709 \times 10^{-16}
                                                                    1.80935 \times 10^{-16}
                                                                                                                    -1.91545
    ac_e
                                                                                                     1.
                           0.
                                                    0.
 acald_e
                                                                             1.
                                                                                                     0.
                                                                                                                              0.
                           0.
                                                    0.
                                                                             0.
                                                                                                                              0.
   akg_e
                                                                                                     0.
                           0.
                                                    0.
                                                                             Ο.
                                                                                                     0.
                                                                                                                              0.
  co2_e
                                                                    2.46096 \times 10^{-16}
                                                                                             7.86496 \times 10^{-17}
                  -1.60051 \times 10^{-15}
                                           4.11072 \times 10^{-16}
   fum e
                                                                                                                    -1.24485
glc__D_e
                           0.
                                                    0.
                                                                             0.
                                                                                                     0.
                                                                                                                              0.
                                                    0.
                                                                             0.
                                                                                                     0.
                                                                                                                              0.
gln__L_e
                           0.
                                                                                            3.33755 \times 10^{-15}
                                                   - 2. .
 glu__L_e
                           1.
                                                                             1.
                                                                                                                             _ 1
                  -3.72385 \times 10^{-16} -1.35047 \times 10^{-16} 6.75507 \times 10^{-17}
                                                                                           -4.45367 \times 10^{-17} -1.15314
  glyc_e
  h20 0
                                                                                                                      2 5664:
```

ĺ	1120_6	Ī	U.J			-	.					۷.					- . .			- 4			
	h_e	-4.					2.			-1.							1.			- 1			
	lacD_e	0.				(0.			0.						0.					0.		
	malL_e	-2.5					3.					- 1					1.			- 1			
	nh4_e		-1.				2.					- 1				2 68	 3217	× 1 (1-15		1.		
					1	779		. 1 (n-15	0	2.0		· ×10	-16			033:			1			
	o2_e		1.																	1.83575			
	pi_e		-1.		5.	9437	11 ×	10	-10	- 8	.07	781	4×1	.0 ⁻¹⁶	2	.35	488		-13	1.	30489		
	pyr_e		3.			-	4.					1	•				-2.			3.			
	succ_e		-1.			:	2.					- 1			- 3	2.38	8698	× 10)-15	1.66533			
	toh_e	-4.9	1817 ×	10-16		:	1.					- 1			- :	2.76	314	× 10)-16	4.	75996		
Out[510]//Matri	ixForm=																						
	2dda7p_c	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0		
	2ddg6p_c	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0		
	2dhglcn_c	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0		
	34dhbz_c	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0		
	3dhq_c	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0		
	3dhsk_c	0	0	0	0	0	0		0	0	0	0	0	0	0	0	0	0	0	0	0		
	3pg_c	0	0	0	0	0	0		0	0	0	0	0	0	0	0	0	0	0	0	0		
	6p2dhglcn_c	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0		
	брдс_с	0	0	0	0	0	0		0	0	0	0	0	0	0	0	0	0	0	0	0		
	ac_c	0	0	0	0	0	0		0	0	0	0	0	0	0	0	0	0	0	0	0		
	acald_c	0	0	0	0	0	0		0	0	0	0	0	0	0	0	0	0	0	0	0		
	accoa_c	0	0	0	0	0	0		0	0	0	0	0	0	0	0	0	0	0	0	0		
	acon_c	0	0	0	0	0	0		0	0	0	0	0	0	0	0	0	0	0	0	0		
	actp_c -	0	0	0	0	0	0		0	0	0	0	0	0	0	0	0	0	0	0	0		
	adp_c	0	0	0	0	0	0		0	0	0	0	0	0	0	0	0	0	0	0	0		
	akg_c	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0		
	amp_c	0	0	0	0	0	0		0	0	0	0	0	0	0	0	0	0	0	0	0		
	atp_c	0	0	0	0	0	0		0	0	0	0	0	0	0	0	0	0	0	0	0		
	catechol_c	0	0	0 0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0		
	ccmuac_c						0			0										0			
	cit_c	0	0	0	0	0	0		0	0	0	0	0	0	0	0	0	0	0	0	0		
	co2_c coa_c	0	0	0 0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0		
	dhap_c	0	0	0	0	0	0		0	0	0	0	0	0	0	0	0	0	0	0	0		
	e4p_c	0	0	0	0	0	0	0		0	0	0	0	0	0	0	0	0	0	0	0		
	etoh_c	0	0	0	0	0	0		0	0	0	0	0	0	0	0	0	0	0	0	0		
	f6p_c	0	0	0	0	0	0		0	0	0	0	0	0	0	0	0	0	0	0	0		
	fdp_c	0	0	0	0	0	0		0	0	0	0	0	0	0	0	0	0	0	0	0		
	fum_c	0	0	0	0	0	0		0	0	0	0	0	0	0	0	0	0	0	0	0		
	g3p_c	0	0	0	0	0	0		0	0	0	0	0	0	0	0	0	0	0	0	0		
	g6p_c	0	0	0	0	0	0		0	0	0	0	0	0	0	0	0	0	0	0	0		
	glcD_c	0	0	0	0	0	0		0	0	0	0	0	0	0	0	0	0	0	0	0		
	glcn_c	0	0	0	0	0	0	0		0	0	0	0	0	0	0	0	0	0	0	0		
	glnL_c	0	0	0	0	0	0		0	0	0	0	0	0	0	0	0	0	0	0	0		
	gluL_c	0	0	0	0	0	0		0	0	0	0	0	0	0	0	0	0	0	0	0		
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|n[512]:= Dimensions[extracellularStoichiometryMatrix.intracellularNullspaceMatrix] MatrixForm[extracellularStoichiometryMatrix.intracellularNullspaceMatrix, TableHeadings → {extracellularMetaboliteIds}] MatrixForm[extracellularStoichiometryMatrix.intracellularNullspaceMatrix /. $x_{-}/; (Abs[x] \le tolerance) \rightarrow 0, TableHeadings \rightarrow \{extracellularMetaboliteIds\}$ Out[512]= $\{19, 98\}$

Out[513]//MatrixForm=

Out[513]//Mat	/	l 7 E1	40E v	10-17	-	270	0	1 0	-16	1.80935×10^{-16} 1.									_1				
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Out[514]//Mat	rixForm=																						
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	akg_e	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	
	co2_e	0	0	0	0	0	0	0	0	1.	0	0	0	0	1.	0	0	0	0	0	0	0	
	fum_e	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	
	glcD_e	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1.	0	0	0	0	0	0	
	glnL_e	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	
	gluL_e	1.	-2.	1.	0	-1.	0	0	0	1.	0	0	-1.	0	0	0	0	0	0	0	0	0	
	glyc_e	0	0	0	0	0	0	0	0	0	0	0	0 -1.	0	0	0	0	0	0	0	0	0	
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