Appendices for Metabolic Pathway Analysis via Integer Linear Programming

by

Francisco J. Planes

May 2008

Contents

Appendix A: Biochemical Reactions

We give below full details of the set of biochemical reactions used in this dissertation. This set has been taken from the metabolic network of *E.Coli* presented by Reed *et al.*, 2003, which is available from http://systemsbiology.ucsd.edu/In_Silico_Organisms/E_coli/E_coli_reactions.

Please note that for some reactions listed below the reaction has not been reduced to its lowest form. For example:

R192 (100)h2o + (2) pa_EC --> (2) 12dgr_EC + (100) pi

can clearly be further reduced to

R192 (50)h2o + (1) pa_EC --> (1) 12dgr_EC + (50) pi

We automatically perform such reductions. Therefore any reference to a reaction in any discussion/pathway picture should be taken to refer to the reaction in its most reduced form.

1 R1a akg + ala-L → glu-L + pyr
2 R2a ala-L → ala-D
3 R3 asn-L + h2o → asp-L + nh4
4 R4 asp-L + atp + nh4 → amp + asn-L + h + ppi
5 R5 asp-L + atp + gln-L + h2o → amp + asn-L + glu-L + h + ppi
6 R6 asp-L → fum + nh4
7 R7a akg + asp-L → glu-L + oaa
8 R8 3mob + ala-L → pyr + val-L
9 R9 ala-D + fad + h2o → fadh2 + nh4 + pyr

10 R10 h2o + suc6p → fru + g6p

11 R11a ru5p-D → ara5p

12 R12a mmcoa-R → mmcoa-S

13 R13 2mcacn + h2o → micit

14 R14a glyald + h + nadh → glyc + nad

15 R15a tagdp-D → dhap + g3p

16 R16a h2o + lald-L + nad → (2) h + lac-L + nadh

17 R17 acald + h2o + nad → ac + (2) h + nadh

18 R18a arab-L → rbl-L

19 R19 atp + rbl-L → adp + h + ru5p-L

20 R20a ru5p-L → xu5p-D

21 R21 acac + accoa → aacoa + ac

22 R22 accoa + but → ac + btcoa

23 R23 arbt6p + h2o → g6p + hqn

24 R24a man1p → man6p

25 R25a 2dr1p → 2dr5p

26 R26a r1p → r5p

27 R27 2dr5p → acald + g3p

28 R28 galctn-D → 2dh3dgal + h2o

29 R29a 2dh3dgal6p → g3p + pyr

30 R30 2dh3dgal + atp → 2dh3dgal6p + adp + h

31 R31 dha + pep → dhap + pyr

32 R32 btcoa + fad + h2o + nad → aacoa + fadh2 + h + nadh

33 R33 h2o + nad + pacald → (2) h + nadh + pac

34 R34 atp + f1p → adp + fdp + h

35 R35a fc1p → dhap + lald-L

36 R36a fuc-L → fcl-L

37 R37 atp + fcl-L → adp + fc1p + h

38 R38a h + lald-L + nadh → 12ppd-S + nad

39 R39a udpg → udpgal

40 R40a atp + gal → adp + gal1p + h

41 R41a gal1p + udpg → g1p + udpgal

42 R42a g1p + h + utp → ppi + udpg

43 R43 galct-D → 5dh4dglc + h2o

44 R44a galt1p + nad → h + nadh + tag6p-D

45 R45 glyclt + q8 → glx + q8h2

46 R46 glyclt + mqn8 → glx + mql8

47 R47 2dmmq8 + glyclt → 2dmmql8 + glx

48 R48 glyc + nad → dha + h + nadh

49 R49 atp + glyc → adp + glyc3p + h

50 R50 2pglyc + h2o → glyclt + pi

51 R51a glyc3p + nadp → dhap + h + nadph

52 R52 5dh4dglc → 2h3oppan + pyr

53 R53 cechddd + nad → dhpppn + h + nadh

54 R54 cenchddd + nad → dhcinnm + h + nadh

55 R55 h + nadh + o2 + pppn → cechddd + nad

56 R56 cinnm + h + nadh + o2 → cenchddd + nad

57 R57a hpyr → 2h3oppan

58 R58a 5dglcn + h + nadh → idon-L + nad

59 R59 5dglcn + h + nadph → idon-L + nadp

60 R60 atp + glcn → 6pgc + adp + h

61 R61a 5dglcn + h + nadph → glcn + nadp

62 R62 2ddglcn + atp → 2ddg6p + adp + h

63 R63 h2o + lcts → gal + glc-D

64 R64a maltpt + pi → g1p + maltttr

65 R65a malthx + pi → g1p + maltpt

66 R66a malthp + pi → g1p + malthx

67 R67 malt + malttr → glc-D + maltttr

68 R68 malt + maltttr → glc-D + maltpt

69 R69 malt + maltpt → glc-D + malthx

70 R70 malt + malthx → glc-D + malthp

71 R71 h2o + malttr → glc-D + malt

72 R72 h2o + maltttr → glc-D + malttr

73 R73 h2o + maltpt → glc-D + maltttr

74 R74 h2o + malthx → glc-D + maltpt

75 R75 h2o + malthp → glc-D + malthx

76 R76a man6p → f6p

77 R77 h2o + melib → gal + glc-D

78 R78 3hcinnm + h + nadh + o2 → dhcinnm + h2o + nad

79 R79 3hpppn + h + nadh + o2 → dhpppn + h2o + nad

80 R80 dhcinnm + o2 → hkntd

81 R81 dhpppn + o2 → hkndd

82 R82 h2o + hkndd → (2) h + op4en + succ

83 R83 h2o + hkntd → fum + (2) h + op4en

84 R84 h2o + op4en → 4h2opntn

85 R85 4h2opntn → acald + pyr

86 R86 acald + coa + nad → accoa + h + nadh

87 R87a mnl1p + nad → f6p + h + nadh

88 R88 acgam6p + h2o → ac + gam6p

89 R89 gam6p + h2o → f6p + nh4

90 R90 acnam → acmana + pyr

91 R91 g6p + udpg → h + tre6p + udp

92 R92 h2o + tre6p → pi + tre

93 R93 atp + coa + pac → amp + phaccoa + ppi

94 R94 atp + tag6p-D → adp + h + tagdp-D

95 R95a g1p → g6p

96 R96a micit → pyr + succ

97 R97 h2o + oaa + ppcoa → 2mcit + coa + h

98 R98 2mcit → 2mcacn + h2o

99 R99 atp + coa + ppa → adp + pi + ppcoa

100 R100 pi + ppcoa → coa + ppap

101 R101 atp + rib-D → adp + h + r5p

102 R102a rmn → rml

103 R103 atp + rml → adp + h + rml1p

104 R104a rml1p → dhap + lald-L

105 R105 succoa → mmcoa-R

106 R106 3dgulnp + h → co2 + xu5p-L

107 R107 xu5p-L → ru5p-L

108 R108a nad + sbt6p → f6p + h + nadh

109 R109 akg + o2 + taur → aacald + co2 + h + so3 + succ

110 R110a adp + ppap → atp + ppa

111 R111 2obut + coa → for + ppcoa

113 R113 h2o + tre6p → g6p + glc-D
114 R114 tartr-L → h2o + oaa
115 R115 h2o + o2 + peamn → h2o2 + nh4 + pacald
116 R116 altrn → 2ddglcn + h2o
117 R117a altrn + nad → h + nadh + tagur
118 R118a glcur → fruur
119 R119a galur → tagur
120 R120 mana → 2ddglcn + h2o
121 R121a mana + nad → fruur + h + nadh
122 R122 fru → glc-D
123 R123a xyl-D → xylu-D
124 R124 atp + xylu-D → adp + h + xu5p-D
125 R125 25dkglcn + h + nadph → 2dhguln + nadp
126 R126 h + hpyr + nadh → glyc-R + nad
127 R127 h + hpyr + nadph → glyc-R + nadp
128 R128 glcr → 5dh4dglc + h2o
129 R129 h + mmcoa-S → co2 + ppcoa
130 R130 ppcoa + succ → ppa + succoa
131 R131 25dkglcn + h + nadph → 5dglcn + nadp
132 R132 2dhglcn + h + nadh → glcn + nad
133 R133 2dhglcn + h + nadph → glcn + nadp
134 R134 25dkglcn + h + nadh → 5dglcn + nad
135 R135 2dhguln + h + nadh → idon-L + nad
136 R136 2dhguln + h + nadph → idon-L + nadp
137 R137 23doguln + h + nadh → 3dhguln + nad
138 R138 icit → glx + succ
139 R139 accoa + glx + h2o → coa + h + mal-L
140 R140 mal-L + nadp → co2 + nadph + pyr
141 R141 atp + oaa → adp + co2 + pep
142 R142 h2o + ppi → h + (2) pi
143 R143 co2 + h2o + pep → h + oaa + pi
144 R144 mal-L + nad → co2 + nadh + pyr
145 R145 5mdru1p → dkmpp + h2o
146 R146 dkmpp + (3) h2o → 2kmb + for + (6) h + pi

147 R147 akg + ptrc → 4abutn + glu-L

148 R148 h2o + nad + sucsal → (2) h + nadh + succ

149 R149 4abutn + h2o + nad → 4abut + (2) h + nadh

150 R150 5mtr + atp → 5mdr1p + adp + h

151 R151a 5mdr1p → 5mdru1p

152 R152 dkmpp + h2o + o2 → 2kmb + for + (2) h + pi

153 R153 glu5sa → 1pyr5c + h + h2o

154 R154 2kmb + glu-L → akg + met-L

155 R155 accoa + glu-L → acglu + coa + h

156 R156 acglu + atp → acg5p + adp

157 R157a acg5sa + nadp + pi → acg5p + h + nadph

158 R158a acorn + akg → acg5sa + glu-L

159 R159 acg5sa + h2o → ac + glu5sa

160 R160 acorn + h2o → ac + orn

161 R161 asp-L + atp + citr-L → amp + argsuc + h + ppi

162 R162a argsuc → arg-L + fum

163 R163a cbp + orn → citr-L + h + pi

164 R164 arg-L + succoa → coa + h + sucarg

165 R165 akg + sucorn → glu-L + sucgsa

166 R166 (2) h + (2) h2o + sucarg → co2 + (2) nh4 + sucorn

167 R167 h2o + nad + sucgsa → (2) h + nadh + sucglu

168 R168 h2o + sucglu → glu-L + succ

169 R169 (2) atp + gln-L + h2o + hco3 → (2) adp + cbp + glu-L + (2) h + pi

170 R170 h2o + nadp + sucsal → (2) h + nadph + succ

171 R171 4abut + akg → glu-L + sucsal

172 R172 gtspmd + h2o → gthrd + spmd

173 R173 atp + gthrd + spmd → adp + gtspmd + h + pi

174 R174 5mta + h2o → 5mtr + ade

175 R175 glu5p + h + nadph → glu5sa + nadp + pi

176 R176 atp + glu-L → adp + glu5p

177 R177 1pyr5c + (2) h + nadph → nadp + pro-L

178 R178 1pyr5c + (2) h2o + nad → glu-L + h + nadh

179 R179 fad + pro-L → 1pyr5c + fadh2 + h

180 R180 arg-L + h → agm + co2

181 R181 agm + h2o → ptrc + urea

182 R182 h + orn → co2 + ptrc

183 R183a amet + h → ametam + co2

184 R184 ametam + ptrc → 5mta + h + spmd

185 R185 accoa + spmd → N1aspmd + coa + h

186 R186 accoa + spmd → coa + h + n8aspmd

187 R187 akg + orn → glu-L + glu5sa

188 R188 uaagmda → h + peptido_EC + udcpdp

189 R189 h2o + udcpdp → h + pi + udcpp

190 R190 h2o + kdo8p → kdo + pi

191 R191a (100) cmp + (100) h + (2) pe_EC → (2) 12dgr_EC + (100) cdpea

192 R192 (100)h2o + (2) pa_EC → (2) 12dgr_EC + (100) pi

193 R193 unagamuf → eca_EC + h + udcpdp

194 R194 ACP + atp + ttdca → amp + myrsACP + ppi

195 R195 ACP + atp + ttdcea → amp + ppi + tdeACP

196 R196 ACP + atp + hdca → amp + palmACP + ppi

197 R197 ACP + atp + hdcea → amp + hdeACP + ppi

198 R198 ACP + atp + ocdcea → amp + octeACP + ppi

199 R199a (2) ala-D + atp → adp + alaala + h + pi

200 R200 (2) 12dgr_EC + (100) atp → (100) adp + (100) h + (2) pa_EC

201 R201 etha → acald + nh4

202 R202 gdpddman → gdpofuc

203 R203 gdpofuc + h + nadph → gdpfuc + nadp

204 R204 udpgal → udpgalfur

205 R205 f6p + gln-L → gam6p + glu-L

206 R206 acgam1p + h + utp → ppi + uacgam

207 R207 accoa + gam1p → acgam1p + coa + h

208 R208 g3pc + h2o → chol + glyc3p + h

209 R209 g3pe + h2o → etha + glyc3p + h

210 R210 g3ps + h2o → glyc3p + h + ser-L

211 R211 g3pg + h2o → glyc + glyc3p + h

212 R212 g3pi + h2o → glyc3p + h + inost

213 R213 gdpmann → gdpddman + h2o

214 R214 s7p → gmhep7p

215 R215 gmhep17bp + h2o → gmhep1p + pi

216 R216 ara5p + h2o + pep → kdo8p + pi

217 R217 ctp + kdo → ckdo + ppi

218 R218 ckdo + lipidA → cmp + h + kdolipid4

219 R219 ckdo + kdolipid4 → cmp + h + kdo2lipid4

220 R220a 3hmrsACP + uacgam → ACP + u3aga

221 R221 lipidX + u23ga → h + lipidAds + udp

222 R222 h2o + u3aga → ac + u3hga

223 R223 3hmrsACP + u3hga → ACP + h + u23ga

224 R224 atp + lipidAds → adp + h + lipidA

225 R225 ddcaACP + kdo2lipid4 → ACP + kdo2lipid4L

226 R226 hdeACP + kdo2lipid4 → ACP + kdo2lipid4p

227 R227 gdp + h + man1p → gdpmann + pi

228 R228 udcpp + ugmda → uagmda + ump

229 R229a gam1p → gam6p

230 R230 kdo2lipid4p + myrsACP → ACP + lipa_cold

231 R231 kdo2lipid4L + myrsACP → ACP + lipa

232 R232 pep + uacgam → pi + uaccg

233 R233 h + nadph + uaccg → nadp + uamr

234 R234 ala-L + atp + uamr → adp + h + pi + uama

235 R235 atp + glu-D + uama → adp + h + pi + uamag

236 R236 26dap-M + atp + uamag → adp + h + pi + ugmd

237 R237 alaala + atp + ugmd → adp + h + pi + ugmda

238 R238 uacgam + uagmda → h + uaagmda + udp

239 R239a glu-D → glu-L

240 R240 (100) h2o + (2) pc_EC → (2) agpc_EC + (100) h + (36) hdca + (7) hdcea + (50) ocdcea + (2) ttdca + (5) ttdcea

241 R241 (100) h2o + (2) pg_EC → (2) agpg_EC + (100) h + (36) hdca + (7) hdcea + (50) ocdcea + (2) ttdca + (5) ttdcea

242 R242 (100) h2o + (2) pe_EC → (2) agpe_EC + (100) h + (36) hdca + (7) hdcea + (50) ocdcea + (2) ttdca + (5) ttdcea

243 R243 (2) agpg_EC + (100) h2o → (100) g3pg + (100) h + (36) hdca + (7) hdcea + (50) ocdcea + (2) ttdca + (5) ttdcea

244 R244 (2) agpe_EC + (100) h2o → (100) g3pe + (100) h + (36) hdca + (7) hdcea + (50) ocdcea + (2) ttdca + (5) ttdcea

245 R245 (2) agpc_EC + (100) h2o → (100) g3pc + (100) h + (36) hdca + (7) hdcea + (50) ocdcea + (2) ttdca + (5) ttdcea

246 R246 (2) agpe_EC + (2) pg_EC → (2) apg_EC + (100) g3pe

247 R247 (2) agpc_EC + (2) pg_EC → (2) apg_EC + (100) g3pc

248 R248 (2) agpg_EC + (2) pg_EC → (2) apg_EC + (100) g3pg

251 R251 atp + gmhep7p → adp + gmhep17bp + h

253 R253 dttp + g1p + h → dtdpglu + ppi

254 R254 dtdpglu → dtdp4d6dg + h2o

255 R255 dtdp4d6dg → dtdp4d6dm

256 R256 dtdp4d6dm + h + nadph → dtdprmn + nadp

257 R257 h2o + mi1p-D → inost + pi

258 R258 h2o + (2) nad + udpg → (3) h + (2) nadh + udpglcur

259 R259 h2o + u23ga → (2) h + lipidX + ump

260 R260 uacgam + udcpp → ump + unaga

261 R261 uacgam → uacmam

262 R262 h2o + (2) nad + uacmam → (3) h + (2) nadh + uacmamu

263 R263 accoa + dtdp4addg → coa + dtdp4aaddg + h

264 R264 dtdp4d6dg + glu-L → akg + dtdp4addg

265 R265 dtdp4aaddg + unagamu → dtdp + h + unagamuf

266 R266 uacmamu + unaga → h + udp + unagamu

267 R267a cit → icit

268 R268 cit → ac + oaa

269 R269 fum + mql8 → mqn8 + succ

270 R270 2dmmql8 + fum → 2dmmq8 + succ

271 R271a fum + h2o → mal-L

272 R272 accoa + h2o + oaa → cit + coa + h

273 R273a icit + nadp → akg + co2 + nadph

274 R274 akg + coa + nad → co2 + nadh + succoa

275 R275a mal-L + nad → h + nadh + oaa

276 R276 mal-L + q8 → oaa + q8h2

277 R277 mal-L + mqn8 → mql8 + oaa

278 R278 fad + succ → fadh2 + fum

279 R279a atp + coa + succ → adp + pi + succoa

280 R280 5aprbu + h2o → 4r5au + pi

281 R281 dhpmp + h2o → dhnpt + pi

282 R282 h2o + nadp → nad + pi

283 R283 h2o + nmn → h + ncam + r5p

285 R285 4ppcys + h → co2 + pan4p

286 R286 atp + dpcoa → adp + coa + h

287 R287 h2o + pyam5p → pi + pydam

288 R288 h2o + pydx5p → pi + pydx

289 R289 h2o + pdx5p → pi + pydxn

290 R290 h2o + nmn → nh4 + nicrnt

291 R291a atp + thm → adp + h + thmmp

292 R292 4ppan + ctp + cys-L → 4ppcys + cmp + h + ppi

293 R293 apoACP + coa → ACP + h + pap

294 R294a 8aonn + amet → amob + dann

295 R295a cys-L + dtbt → ala-L + btn + (2) h

296 R296a atp + co2 + dann → adp + dtbt + (3) h + pi

297 R297a ala-L + h + pmcoa → 8aonn + co2 + coa

298 R298 btnso + h + nadh → btn + h2o + nad

299 R299 btnso + h + nadph → btn + h2o + nadp

300 R300a atp + cbi + h2o → adocbi + pi + ppi

301 R301a atp + cbl1 + h2o → adocbl + pi + ppi

302 R302 atp + pnto-R → 4ppan + adp + h

303 R303 atp + h + pan4p → dpcoa + ppi

304 R304 agdpcbi + rdmbzi → adocbl + gmp + h

305 R305 dmbzid + nicrnt → 5prdmbz + h + nac

306 R306 adocbi + atp → adocbip + adp + h

307 R307 adocbip + gtp + h → agdpcbi + ppi

308 R308 frdp + h2o + pheme → hemeO + ppi

309 R309 nad + shcl → h + nadh + srch

310 R310 fe2 + srch → (3) h + sheme

311 R311 dxyl5p + h + nadph → 2me4p + nadp

312 R312 g3p + h + pyr → co2 + dxyl5p

313 R313a 23ddhb + nad → 23dhb + h + nadh

314 R314 h2o + ichor → 23ddhb + pyr

315 R315 (3) 23dhba + (3) seramp → (6) amp + enter + (6) h

316 R316a 23dhb + atp → 23dhba + ppi
317 R317a atp + h + ser-L → ppi + seramp
318 R318a e4p + h2o + nad → 4per + (2) h + nadh
319 R319a dhf + h + nadph → nadp + thf
320 R320 dhnpt → 6hmhpt + gcald
321 R321 atp + dhpt + glu-L → adp + dhf + pi
322 R322 gtp + h2o → ahdt + for
323 R323 6hmhpt + atp → 6hmhptpp + amp + h
324 R324 4abz + 6hmhptpp → dhpt + h + ppi
325 R325 2mecdp + h → h2mb4p + h2o
326 R326 atp + glu-L + trnaglu → amp + glutrna + ppi
327 R327 ala-D + pydx5p → pyam5p + pyr
328 R328 ala-L + pydx5p → pyam5p + pyr
329 R329a gthox + h + nadph → (2) gthrd + nadp
330 R330 atp + cys-L + glu-L → adp + glucys + h + pi
331 R331 atp + glucys + gly → adp + gthrd + h + pi
332 R332 glutrna + h + nadph → glu1sa + nadp + trnaglu
333 R333 (2) 5aop → h + (2) h2o + ppbng
334 R334 h2o + (4) ppbng → hmbil + (4) nh4
335 R335 hmbil → h2o + uppg3
336 R336 (4) h + uppg3 → (4) co2 + cpppg3
337 R337 cpppg3 + (2) h + o2 → (2) co2 + (2) h2o + pppg9
338 R338 (3) o2 + (2) pppg9 → (6) h2o + (2) ppp9
339 R339 fe2 + ppp9 → (2) h + pheme
340 R340 glu1sa → 5aop
341 R341 (2) amet + uppg3 → (2) ahcys + h + shcl
342 R342 ipdp → dmpp
343 R343 dmpp + ipdp → grdp + ppi
344 R344 grdp + ipdp → frdp + ppi
345 R345 frdp + (5) ipdp → octdp + (5) ppi
346 R346 2me4p + ctp + h → 4c2me + ppi
347 R347 4c2me + atp → 2p4c2me + adp + h
348 R348 2p4c2me → 2mecdp + cmp
349 R349 h + h2mb4p + nadh → dmpp + h2o + nad

350 R350 h + h2mb4p + nadh → h2o + ipdp + nad
351 R351 dhna + octdp → 2dmmq8 + co2 + h + ppi
352 R352 sbzcoa → coa + dhna
353 R353 2shchc → h2o + sucbz
354 R354 akg + h + thmpp → co2 + ssaltpp
355 R355 ichor + ssaltpp → 2shchc + pyr + thmpp
356 R356 atp + coa + sucbz → amp + ppi + sbzcoa
357 R357 chor → ichor
358 R358 2dmmq8 + amet → ahcys + h + mqn8
359 R359 dhap + iasp → h + (2) h2o + pi + quln
360 R360 asp-L + q8 → iasp + q8h2
361 R361 asp-L + mqn8 → iasp + mql8
362 R362 asp-L + fum → iasp + succ
363 R363 asp-L + o2 → h2o2 + iasp
364 R364 (2) h + prpp + quln → co2 + nicrnt + ppi
365 R365 atp + h + nicrnt → dnad + ppi
366 R366 atp + h + nmn → nad + ppi
367 R367 atp + dnad + nh4 → amp + h + nad + ppi
368 R368 ahdt + h2o → dhpmp + h + ppi
369 R369 chor + gln-L → 4adcho + glu-L
370 R370 4adcho → 4abz + h + pyr
371 R371 3mob + h2o + mlthf → 2dhp + thf
372 R372 ala-B + atp + pant-R → amp + h + pnto-R + ppi
373 R373 asp-L + h → ala-B + co2
374 R374 2dhp + h + nadph → nadp + pant-R
375 R375 dxyl5p + nad + phthr → co2 + h + (2) h2o + nadh + pdx5p + pi
376 R376a 4per + nad → h + nadh + ohpb
377 R377a o2 + pdx5p → h2o2 + pydx5p
378 R378 h2o + o2 + pyam5p → h2o2 + nh4 + pydx5p
379 R379 atp + pydxn → adp + h + pdx5p
380 R380 atp + pydam → adp + h + pyam5p
381 R381 atp + pydx → adp + h + pydx5p
382 R382 5prdmbz + h2o → pi + rdmbzi
383 R383 h2o + ncam → nac + nh4

384 R384 atp + h2o + nac + prpp → adp + nicrnt + pi + ppi

385 R385 gtp + (3) h2o → 25drapp + for + (2) h + ppi

386 R386 ru5p-D → db4p + for + h

387 R387 5apru + h + nadph → 5aprbu + nadp

388 R388 25drapp + h + h2o → 5apru + nh4

389 R389 4r5au + db4p → dmlz + (2) h2o + pi

390 R390 atp + ribflv → adp + fmn + h

391 R391 atp + fmn + h → fad + ppi

392 R392 (2) dmlz → 4r5au + ribflv

393 R393a glu-L + ohpb → akg + phthr

394 R394 air + h2o → 4ampm + (2) for + (4) h

395 R395 4ampm + atp → 2mahmp + adp

396 R396 4ahmmp + atp → 4ampm + adp + h

397 R397 2mahmp + 4mpetz + h → ppi + thmmp

398 R398a atp + thmmp → adp + thmpp

399 R399 4mhetz + atp → 4mpetz + adp + h

400 R400 atp + cys-L + dxyl5p + tyr-L → 4hba + 4mpetz + ala-L + amp + co2 + h + h2o + ppi

401 R401 h2o + phthr → 4hthr + pi

402 R402 4hbz + octdp → 3ophb + ppi

403 R403 (2) 2oph + (1) o2 → (2) 2ohph

404 R404 chor → 4hbz + pyr

405 R405 3ophb + h → 2oph + co2

406 R406 2ombzl + amet → 2ommbl + ahcys + h

407 R407 (2) 2ommbl + (1) o2 → (2) 2omhmbl

408 R408 2ohph + amet → 2omph + ahcys + h

409 R409 2omhmbl + amet → ahcys + h + q8h2

410 R410 (2) 2omph + (1) o2 → (2) 2ombzl

411 R411 frdp + (8) ipdp → (8) ppi + udcpdp

412 R412 atp + dxyl → adp + dxyl5p + h

413 R413 atp + nad → adp + h + nadp

414 R414 h2o + pap → amp + pi

415 R415 aps + atp → adp + h + paps

416 R416 atp + gtp + h2o + so4 → aps + gdp + pi + ppi

417 R417a accoa + ser-L → acser + coa

418 R418 paps + trdrd → (2) h + pap + so3 + trdox

419 R419a (3) h2o + h2s + (3) nadp → (5) h + (3) nadph + so3

420 R420 acser + h2s → ac + cys-L + h

421 R421 cys-L + h2o → h2s + nh4 + pyr

422 R422 gcald + h2o + nad → glyclt + (2) h + nadh

423 R423a h2o + methf → 10fthf

424 R424a mlthf + nadp → h + methf + nadph

425 R425 gly + nad + thf → co2 + mlthf + nadh + nh4

426 R426 h + mlthf + nadh → 5mthf + nad

427 R427 10fthf + h2o → for + h + thf

428 R428 glu-L + h → 4abut + co2

429 R429a glu-L + h2o + nadp → akg + h + nadph + nh4

430 R430 atp + glu-L + nh4 → adp + gln-L + h + pi

431 R431 akg + gln-L + h + nadph → (2) glu-L + nadp

432 R432 gln-L + h2o → glu-L + nh4

433 R433 ser-D → nh4 + pyr

434 R434 ser-L + thf → gly + h2o + mlthf

435 R435 2aobut + coa → accoa + gly

436 R436 3pg + nad → 3php + h + nadh

437 R437 h2o + pser-L → pi + ser-L

438 R438 3php + glu-L → akg + pser-L

439 R439 ser-L → nh4 + pyr

440 R440 nad + thr-L → 2aobut + h + nadh

441 R441 coa + nad + pyr → accoa + co2 + nadh

442 R442 g1p + h2o → glc-D + pi

443 R443a 2pg → h2o + pep

444 R444a fdp → dhap + g3p

445 R445 fdp + h2o → f6p + pi

446 R446a f6p → dha + g3p

447 R447a g3p + nad + pi → 13dpg + h + nadh

448 R448 adpglc → adp + glycogen + h

449 R449 atp + g1p + h → adpglc + ppi

450 R450 glycogen + pi → g1p

451 R451 atp + glc-D → adp + g6p + h

452 R452a 2pg → 3pg

453 R453 atp + f6p → adp + fdp + h

454 R454a g6p → f6p

455 R455a 3pg + atp → 13dpg + adp

456 R456 atp + h2o + pyr → amp + (2) h + pep + pi

457 R457 adp + h + pep → atp + pyr

458 R458a dhap → g3p

459 R459 2h3oppan + h + nadh → glyc-R + nad

460 R460 (2) glx + h → 2h3oppan + co2

461 R461 atp + glyc-R → 3pg + adp + h

462 R462 glx + h + nadph → glyclt + nadp

463 R463 glx + h + nadh → glyclt + nad

464 R464 prfp → prlp

465 R465 eig3p → h2o + imacp

466 R466 h2o + hisp → histd + pi

467 R467 glu-L + imacp → akg + hisp

468 R468 h2o + histd + (2) nad → (3) h + his-L + (2) nadh

469 R469 gln-L + prlp → aicar + eig3p + glu-L + h

470 R470 atp + prpp → ppi + prbatp

471 R471 h2o + prbatp → h + ppi + prbamp

472 R472 h2o + prbamp → prfp

473 R473a atp + r5p → amp + h + prpp

474 R474a accoa + atp + hco3 → adp + h + malcoa + pi

475 R475a (2) accoa → aacoa + coa

476 R476 (2) cdpdag1 + (100) h2o → (100) cmp + (200) h + (2) pa_EC

477 R477a (100) ctp + (100) h + (2) pa_EC → (2) cdpdag1 + (100) ppi

478 R478a (4) pg_EC → (2) clpn_EC + (100) glyc

479 R479 actACP + (17) h + (5) malACP + (12) nadph → (5) ACP + (5) co2 + (6) h2o + myrsACP + (12) nadp

480 R480 actACP + (14) h + (4) malACP + (10) nadph → (4) ACP + (4) co2 + ddcaACP + (5) h2o + (10) nadp

481 R481 h + malACP → acACP + co2

482 R482 acACP + h + malACP → ACP + actACP + co2

483 R483a ACP + malcoa → coa + malACP

484 R484 actACP + (20) h + (6) malACP + (14) nadph → (6) ACP + (6) co2 + (7) h2o + (14) nadp + palmACP

485 R485 ddcaACP + (2) h + malACP + nadph → 3hmrsACP + ACP + co2 + nadp

486 R486 actACP + (22) h + (7) malACP + (15) nadph → (7) ACP + (7) co2 + (8) h2o + (15) nadp + octeACP

487 R487 actACP + (16) h + (5) malACP + (11) nadph → (5) ACP + (5) co2 + (6) h2o + (11) nadp + tdeACP

488 R488 accoa + h + malACP → actACP + co2 + coa

489 R489a ACP + accoa → acACP + coa

490 R490 actACP + (19) h + (6) malACP + (13) nadph → (6) ACP + (6) co2 + (7) h2o + hdeACP + (13) nadp

491 R491 atp + (8) coa + (7) fad + (7) h2o + hdca + (7) nad → (8) accoa + amp + (7) fadh2 + (7) h + (7) nadh + ppi

492 R492 atp + (7) coa + (6) fad + (6) h2o + (6) nad + ttdca → (7) accoa + amp + (6) fadh2 + (6) h + (6) nadh + ppi

493 R493 atp + (9) coa + (8) fad + (8) h2o + (8) nad + ocdca → (9) accoa + amp + (8) fadh2 + (8) h + (8) nadh + ppi

494 R494 (100) h2o + (2) pgp_EC → (2) pg_EC + (100) pi

495 R495a (2) cdpdag1 + (100) glyc3p → (100) cmp + (100) h + (2) pgp_EC

496 R496 (100) glyc3p + (14) hdeACP + (4) myrsACP + (100) octeACP + (72) palmACP + (10) tdeACP → (200) ACP + (2) pa_EC

497 R497 (100) h + (2) ps_EC → (100) co2 + (2) pe_EC

498 R498a (2) cdpdag1 + (100) ser-L → (100) cmp + (100) h + (2) ps_EC

499 R499a ahcys + h2o → adn + hcys-L

500 R500 dhptd → h2o + hmfurn

501 R501 rhcys → dhptd + hcys-L

502 R502 hom-L + succoa → coa + suchms

503 R503 cys-L + suchms → cyst-L + h + succ

504 R504 cyst-L + h2o → hcys-L + nh4 + pyr

505 R505 5mthf + hcys-L → met-L + thf

506 R506 atp + h2o + met-L → amet + pi + ppi

507 R507 ahcys + h2o → ade + rhcys

508 R508 gthrd + mthgxl → lgt-S

509 R509 h2o + lgt-S → gthrd + h + lac-D

510 R510 dhap → mthgxl + pi

511 R511 (2) h + h2o + urdglyc → co2 + glx + (2) nh4

512 R512 alltn + h2o → alltt + h

513 R513 alltt + h2o → urdglyc + urea

514 R514 cynt + (3) h + hco3 → (2) co2 + nh4

515 R515 cmp + h2o → csn + r5p

516 R516 adn + h + h2o → ins + nh4

517 R517 dad-2 + h + h2o → din + nh4

518 R518 adn + atp → adp + amp + h

519 R519a amp + atp → (2) adp

520 R520a atp + damp → adp + dadp

521 R521a amp + itp → adp + idp

522 R522a amp + gtp → adp + gdp

523 R523 amp + h2o → ade + r5p

524 R524 ap4a + h2o → (2) adp + (2) h

525 R525 gp4g + h2o → (2) gdp + (2) h

526 R526 ap5a + h2o → adp + atp + (2) h

527 R527 ade + prpp → amp + ppi

528 R528 cytd + h + h2o → nh4 + uri

529 R529 dcyt + h + h2o → duri + nh4

530 R530a atp + dcmp → adp + dcdp

531 R531a atp + cmp → adp + cdp

532 R532a atp + ump → adp + udp

533 R533 csn + h + h2o → nh4 + ura

534 R534 atp → camp + ppi

535 R535 dctp + h + h2o → dutp + nh4

536 R536a pi + thymd → 2dr1p + thym

537 R537a duri + pi → 2dr1p + ura

538 R538 dgtp + h2o → dgsn + pppi

539 R539 gtp + h2o → gsn + pppi

540 R540 dutp + h2o → dump + h + ppi

541 R541a atp + gmp → adp + gdp

542 R542a atp + dgmp → adp + dgdp

543 R543 prpp + xan → ppi + xmp

544 R544 hxan + prpp → imp + ppi
545 R545 gua + prpp → gmp + ppi
546 R546 atp + ins → adp + h + imp
547 R547 atp + gsn → adp + gmp + h
548 R548 dctp + h2o → dcmp + h + ppi
549 R549 ctp + h2o → cmp + h + ppi
550 R550 datp + h2o → damp + h + ppi
551 R551 atp + h2o → amp + h + ppi
552 R552 dttp + h2o → dtmp + h + ppi
553 R553 h2o + utp → h + ppi + ump
554 R554 dgtp + h2o → dgmp + h + ppi
555 R555 gtp + h2o → gmp + h + ppi
556 R556a atp + gdp → adp + gtp
557 R557a atp + udp → adp + utp
558 R558a atp + cdp → adp + ctp
559 R559a atp + dgdp → adp + dgtp
560 R560a atp + dudp → adp + dutp
561 R561a atp + dcdp → adp + dctp
562 R562a atp + dadp → adp + datp
563 R563a atp + dtdp → adp + dttp
564 R564 adp + trdrd → dadp + h2o + trdox
565 R565 gdp + trdrd → dgdp + h2o + trdox
566 R566 trdrd + udp → dudp + h2o + trdox
567 R567 cdp + trdrd → dcdp + h2o + trdox
568 R568 atp + trdrd → datp + h2o + trdox
569 R569 gtp + trdrd → dgtp + h2o + trdox
570 R570 ctp + trdrd → dctp + h2o + trdox
571 R571 trdrd + utp → dutp + h2o + trdox
572 R572a atp + dump → adp + dudp
573 R573 atp + duri → adp + dump + h
574 R574 atp + thymd → adp + dtmp + h
575 R575 dump + mlthf → dhf + dtmp
576 R576a atp + dtmp → adp + dtdp

577 R577 gtp + uri → gdp + h + ump
578 R578 cytd + gtp → cmp + gdp + h
579 R579a pi + uri → r1p + ura
580 R580 prpp + ura → ppi + ump
581 R581 dump + h2o → duri + pi
582 R582 dtmp + h2o → pi + thymd
583 R583 damp + h2o → dad-2 + pi
584 R584 dgmp + h2o → dgsn + pi
585 R585 dcmp + h2o → dcyt + pi
586 R586 cmp + h2o → cytd + pi
587 R587 amp + h2o → adn + pi
588 R588 gmp + h2o → gsn + pi
589 R589 h2o + imp → ins + pi
590 R590 h2o + xmp → pi + xtsn
591 R591 h2o + ump → pi + uri
592 R592a din + pi → 2dr1p + hxan
593 R593a ins + pi → hxan + r1p
594 R594a dad-2 + pi → 2dr1p + ade
595 R595a dgsn + pi → 2dr1p + gua
596 R596a adn + pi → ade + r1p
597 R597a gsn + pi → gua + r1p
598 R598a pi + xtsn → r1p + xan
599 R599 gua + h + h2o → nh4 + xan
600 R600 ade + h + h2o → hxan + nh4
601 R601 lac-L + q8 → pyr + q8h2
602 R602 lac-L + mqn8 → mql8 + pyr
604 R604a bbtcoa + crn → crncoa + gbbtn
605 R605a crn + ctbtcoa → crncoa + ctbt
606 R606a crncoa → ctbtcoa + h2o
609 R609 lac-D + q8 → pyr + q8h2
617 R617 2dmmq8 + glyc3p → 2dmmql8 + dhap
618 R618 glyc3p + mqn8 → dhap + mql8
619 R619 glyc3p + q8 → dhap + q8h2
625 R625 h + nadh + q8 → nad + q8h2

626 R626 2dmmq8 + h + nadh → 2dmmql8 + nad

627 R627 h + mqn8 + nadh → mql8 + nad

628 R628 (5) h + (3) nadh + no2 → (2) h2o + (3) nad + nh4

633 R633 h2o + pyr + q8 → ac + co2 + q8h2

634 R634a fadh2 + q8 → fad + q8h2

635 R635 nad + nadph → nadh + nadp

636 R636 h + nadph + trdox → nadp + trdrd

637 R637 6pgl + h2o → 6pgc + h

638 R638 2ddg6p → g3p + pyr

639 R639 6pgc → 2ddg6p + h2o

640 R640 6pgc + nadp → co2 + nadph + ru5p-D

641 R641a ru5p-D → xu5p-D

642 R642a r5p → ru5p-D

643 R643a g3p + s7p → e4p + f6p

644 R644a r5p + xu5p-D → g3p + s7p

645 R645a e4p + xu5p-D → f6p + g3p

646 R646a g6p + nadp → 6pgl + h + nadph

647 R647 atp + gln-L + h2o + xmp → amp + glu-L + gmp + (2) h + ppi

648 R648 h2o + imp + nad → h + nadh + xmp

649 R649 gmp + (2) h + nadph → imp + nadp + nh4

650 R650 asp-L + gtp + imp → dcamp + gdp + (2) h + pi

651 R651a 25aics → aicar + fum

652 R652a dcamp → amp + fum

653 R653a 5aizc + asp-L + atp → 25aics + adp + h + pi

654 R654a atp + gly + pram → adp + gar + h + pi

655 R655a 5aizc → 5caiz

656 R656 gln-L + h2o + prpp → glu-L + ppi + pram

657 R657a 10fthf + aicar → fprica + thf

658 R658a h2o + imp → fprica

659 R659 air + atp + hco3 → 5caiz + adp + h + pi

660 R660 atp + fgam + gln-L + h2o → adp + fpram + glu-L + h + pi

661 R661 atp + fpram → adp + air + (2) h + pi

662 R662a 10fthf + gar → fgam + h + thf

663 R663 atp + for + gar → adp + fgam + h + pi

664 R664 asp-L + cbp → cbasp + h + pi

665 R665a dhor-S + h2o → cbasp + h

666 R666 dhor-S + q8 → orot + q8h2

667 R667 dhor-S + mqn8 → mql8 + orot

668 R668a orot5p + ppi → orot + prpp

669 R669 h + orot5p → co2 + ump

670 R670 atp + gln-L + h2o + utp → adp + ctp + glu-L + (2) h + pi

671 R671 atp + co2 + nh4 → adp + cbp + (2) h

672 R672 acmanap → acgam6p

673 R673 acmana + atp → acmanap + adp + h

674 R674a ac + atp → actp + adp

675 R675 ac + atp + coa → accoa + amp + ppi

676 R676a accoa + (2) h + (2) nadh → coa + etoh + (2) nad

677 R677a lac-D + nad → h + nadh + pyr

678 R678 for + h → co2 + h2

679 R679a accoa + pi → actp + coa

680 R680 coa + pyr → accoa + for

681 R681a akg + sl26da → glu-L + sl2a6o

682 R682a aspsa + nadp + pi → 4pasp + h + nadph

683 R683 aspsa + pyr → 23dhdp + h + (2) h2o

684 R684 23dhdp + h + nadph → nadp + thdp

685 R685 h2o + succoa + thdp → coa + sl2a6o

686 R686 h2o + sl26da → 26dap-LL + succ

687 R687a 26dap-LL → 26dap-M

688 R688 h + lys-L → 15dap + co2

689 R689a thr-L → acald + gly

690 R690 26dap-M + h → co2 + lys-L

691 R691a hom-L + nadp → aspsa + h + nadph

692 R692a asp-L + atp → 4pasp + adp

693 R693 atp + hom-L → adp + h + phom

694 R694 h2o + phom → pi + thr-L

695 R695 2dda7p → 3dhq + pi

696 R696 3psme → chor + pi

697 R697a 3dhq → 3dhsk + h2o

698 R698a 3dhsk + h + nadph → nadp + skm

699 R699 e4p + h2o + pep → 2dda7p + pi

700 R700 atp + skm → adp + h + skm5p

701 R701 h + pphn → co2 + h2o + phpyr

702 R702 chor → pphn

703 R703a h2o + trp-L → indole + nh4 + pyr

704 R704 indole + ser-L → h2o + trp-L

705 R705 3ig3p → g3p + indole

706 R706 3ig3p + ser-L → g3p + h2o + trp-L

707 R707 pran → 2cpr5p

708 R708 2cpr5p + h → 3ig3p + co2 + h2o

709 R709 chor + gln-L → anth + glu-L + h + pyr

710 R710 anth + prpp → ppi + pran

711 R711 nad + pphn → 34hpp + co2 + nadh

712 R712a akg + tyr-L → 34hpp + glu-L

713 R713a akg + phe-L → glu-L + phpyr

714 R714 atp + h2o → adp + h + pi

715 R715 betald + h2o + nad → glyb + (2) h + nadh

716 R716 betald + h2o + nadp → glyb + (2) h + nadph

717 R717a co2 + h2o → h + hco3

718 R718 cyan + tsul → h + so3 + tcynt

719 R719 (2) h2o2 → (2) h2o + o2

720 R720 atp + h2o + seln → amp + pi + selnp

721 R721 (2) h + (2) o2- → h2o2 + o2

722 R722 acon-T + amet → aconm + ahcys

723 R723 thr-L → 2obut + nh4

724 R724 2obut + h + pyr → 2ahbut + co2

725 R725 h + (2) pyr → alac-S + co2

726 R726 2ahbut + h + nadph → 23dhmp + nadp

727 R727 alac-S + h + nadph → 23dhmb + nadp

728 R728 23dhmp → 3mop + h2o

729 R729 23dhmb → 3mob + h2o

730 R730a akg + ile-L → 3mop + glu-L

731 R731a akg + val-L → 3mob + glu-L

732 R732 4mop + glu-L → akg + leu-L

733 R733 3mob + accoa + h2o → 3c3hmp + coa + h

734 R734 3c2hmp + nad → 3c4mop + h + nadh

735 R735 3c4mop + h → 4mop + co2

736 R736a 3c2hmp → 2ippm + h2o

737 R737a 2ippm + h2o → 3c3hmp

738 R1b glu-L + pyr → akg + ala-L

739 R2b ala-D → ala-L

740 R7b glu-L + oaa → akg + asp-L

741 R11b ara5p → ru5p-D

742 R12b mmcoa-S → mmcoa-R

743 R14b glyc + nad → glyald + h + nadh

744 R15b dhap + g3p → tagdp-D

745 R16b (2) h + lac-L + nadh → h2o + lald-L + nad

746 R18b rbl-L → arab-L

747 R20b xu5p-D → ru5p-L

748 R24b man6p → man1p

749 R25b 2dr5p → 2dr1p

750 R26b r5p → r1p

751 R29b g3p + pyr → 2dh3dgal6p

752 R35b dhap + lald-L → fc1p

753 R36b fcl-L → fuc-L

754 R38b 12ppd-S + nad → h + lald-L + nadh

755 R39b udpgal → udpg

756 R40b adp + gal1p + h → atp + gal

757 R41b g1p + udpgal → gal1p + udpg

758 R42b ppi + udpg → g1p + h + utp

759 R44b h + nadh + tag6p-D → galt1p + nad

760 R51b dhap + h + nadph → glyc3p + nadp

761 R57b 2h3oppan → hpyr

762 R58b idon-L + nad → 5dglcn + h + nadh

763 R61b glcn + nadp → 5dglcn + h + nadph

764 R64b g1p + maltttr → maltpt + pi

765 R65b g1p + maltpt → malthx + pi

766 R66b g1p + malthx → malthp + pi

767 R76b f6p → man6p

768 R87b f6p + h + nadh → mnl1p + nad

769 R95b g6p → g1p

770 R96b pyr + succ → micit

771 R102b rml → rmn

772 R104b dhap + lald-L → rml1p

773 R108b f6p + h + nadh → nad + sbt6p

774 R110b atp + ppa → adp + ppap

775 R117b h + nadh + tagur → altrn + nad

776 R118b fruur → glcur

777 R119b tagur → galur

778 R121b fruur + h + nadh → mana + nad

779 R123b xylu-D → xyl-D

780 R151b 5mdru1p → 5mdr1p

781 R157b acg5p + h + nadph → acg5sa + nadp + pi

782 R158b acg5sa + glu-L → acorn + akg

783 R162b arg-L + fum → argsuc

784 R163b citr-L + h + pi → cbp + orn

785 R183b ametam + co2 → amet + h

786 R191b (2) 12dgr_EC + (100) cdpea → (100) cmp + (100) h + (2) pe_EC

787 R199b adp + alaala + h + pi → (2) ala-D + atp

788 R220b ACP + u3aga → 3hmrsACP + uacgam

789 R229b gam6p → gam1p

790 R239b glu-L → glu-D

791 R267b icit → cit

792 R271b mal-L → fum + h2o

793 R273b akg + co2 + nadph → icit + nadp

794 R275b h + nadh + oaa → mal-L + nad

795 R279b adp + pi + succoa → atp + coa + succ

796 R291b adp + h + thmmp → atp + thm

797 R294b amob + dann → 8aonn + amet

798 R295b ala-L + btn + (2) h → cys-L + dtbt

799 R296b adp + dtbt + (3) h + pi → atp + co2 + dann

800 R297b 8aonn + co2 + coa → ala-L + h + pmcoa
801 R300b adocbi + pi + ppi → atp + cbi + h2o
802 R301b adocbl + pi + ppi → atp + cbl1 + h2o
803 R313b 23dhb + h + nadh → 23ddhb + nad
804 R316b 23dhba + ppi → 23dhb + atp
805 R317b ppi + seramp → atp + h + ser-L
806 R318b 4per + (2) h + nadh → e4p + h2o + nad
807 R319b nadp + thf → dhf + h + nadph
808 R329b (2) gthrd + nadp → gthox + h + nadph
809 R376b h + nadh + ohpb → 4per + nad
810 R377b h2o2 + pydx5p → o2 + pdx5p
811 R393b akg + phthr → glu-L + ohpb
812 R398b adp + thmpp → atp + thmmp
813 R417b acser + coa → accoa + ser-L
814 R419b (5) h + (3) nadph + so3 → (3) h2o + h2s + (3) nadp
815 R423b 10fthf → h2o + methf
816 R424b h + methf + nadph → mlthf + nadp
817 R429b akg + h + nadph + nh4 → glu-L + h2o + nadp
818 R443b h2o + pep → 2pg
819 R444b dhap + g3p → fdp
820 R446b dha + g3p → f6p
821 R447b 13dpg + h + nadh → g3p + nad + pi
822 R452b 3pg → 2pg
823 R454b f6p → g6p
824 R455b 13dpg + adp → 3pg + atp
825 R458b g3p → dhap
826 R473b amp + h + prpp → atp + r5p
827 R474b adp + h + malcoa + pi → accoa + atp + hco3
828 R475b aacoa + coa → (2) accoa
829 R477b (2) cdpdag1 + (100) ppi → (100) ctp + (100) h + (2) pa_EC
830 R478b (2) clpn_EC + (100) glyc → (4) pg_EC
831 R483b coa + malACP → ACP + malcoa
832 R489b acACP + coa → ACP + accoa
833 R495b (100) cmp + (100) h + (2) pgp_EC → (2) cdpdag1 + (100) glyc3p

834 R498b (100) cmp + (100) h + (2) ps_EC → (2) cdpdag1 + (100) ser-L
835 R499b adn + hcys-L → ahcys + h2o
836 R519b (2) adp → amp + atp
837 R520b adp + dadp → atp + damp
838 R521b adp + idp → amp + itp
839 R522b adp + gdp → amp + gtp
840 R530b adp + dcdp → atp + dcmp
841 R531b adp + cdp → atp + cmp
842 R532b adp + udp → atp + ump
843 R536b 2dr1p + thym → pi + thymd
844 R537b 2dr1p + ura → duri + pi
845 R541b adp + gdp → atp + gmp
846 R542b adp + dgdp → atp + dgmp
847 R556b adp + gtp → atp + gdp
848 R557b adp + utp → atp + udp
849 R558b adp + ctp → atp + cdp
850 R559b adp + dgtp → atp + dgdp
851 R560b adp + dutp → atp + dudp
852 R561b adp + dctp → atp + dcdp
853 R562b adp + datp → atp + dadp
854 R563b adp + dttp → atp + dtdp
855 R572b adp + dudp → atp + dump
856 R576b adp + dtdp → atp + dtmp
857 R579b r1p + ura → pi + uri
858 R592b 2dr1p + hxan → din + pi
859 R593b hxan + r1p → ins + pi
860 R594b 2dr1p + ade → dad-2 + pi
861 R595b 2dr1p + gua → dgsn + pi
862 R596b ade + r1p → adn + pi
863 R597b gua + r1p → gsn + pi
864 R598b r1p + xan → pi + xtsn
866 R604b crncoa + gbbtn → bbtcoa + crn
867 R605b crncoa + ctbt → crn + ctbtcoa
868 R606b ctbtcoa + h2o → crncoa

869 R634b fad + q8h2 → fadh2 + q8
870 R641b xu5p-D → ru5p-D
871 R642b ru5p-D → r5p
872 R643b e4p + f6p → g3p + s7p
873 R644b g3p + s7p → r5p + xu5p-D
874 R645b f6p + g3p → e4p + xu5p-D
875 R646b 6pgl + h + nadph → g6p + nadp
876 R651b aicar + fum → 25aics
877 R652b amp + fum → dcamp
878 R653b 25aics + adp + h + pi → 5aizc + asp-L + atp
879 R654b adp + gar + h + pi → atp + gly + pram
880 R655b 5caiz → 5aizc
881 R657b fprica + thf → 10fthf + aicar
882 R658b fprica → h2o + imp
883 R662b fgam + h + thf → 10fthf + gar
884 R665b cbasp + h → dhor-S + h2o
885 R668b orot + prpp → orot5p + ppi
886 R674b actp + adp → ac + atp
887 R676b coa + etoh + (2) nad → accoa + (2) h + (2) nadh
888 R677b h + nadh + pyr → lac-D + nad
889 R679b actp + coa → accoa + pi
890 R681b glu-L + sl2a6o → akg + sl26da
891 R682b 4pasp + h + nadph → aspsa + nadp + pi
892 R687b 26dap-M → 26dap-LL
893 R689b acald + gly → thr-L
894 R691b aspsa + h + nadph → hom-L + nadp
895 R692b 4pasp + adp → asp-L + atp
896 R697b 3dhsk + h2o → 3dhq
897 R698b nadp + skm → 3dhsk + h + nadph
898 R703b indole + nh4 + pyr → h2o + trp-L
899 R712b 34hpp + glu-L → akg + tyr-L
900 R713b glu-L + phpyr → akg + phe-L
901 R717b h + hco3 → co2 + h2o
902 R730b 3mop + glu-L → akg + ile-L

903 R731b 3mob + glu-L → akg + val-L

904 R736b 2ippm + h2o → 3c2hmp

905 R737b 3c3hmp → 2ippm + h2o

Appendix B: Biochemical compounds

We give below full details of the set of biochemical compounds used in this dissertation. As noted above, this set has been taken from the metabolic network of *E.Coli* presented by Reed *et al.*, 2003, which is available from http://systemsbiology.ucsd.edu/In_Silico_Organisms/E_coli/E_coli_reactions.

10fthf 10-Formyltetrahydrofolate

12dgr_EC 1,2-Diacylglycerol

12ppd-S (S)-Propane-1,2-diol

13dpg 3-Phospho-D-glyceroyl phosphate

15dap 1,5-Diaminopentane

1pyr5c 1-Pyrroline-5-carboxylate

23ddhb 2,3-Dihydro-2,3-dihydroxybenzoate

23dhb 2,3-Dihydroxybenzoate

23dhba (2,3-Dihydroxybenzoyl)adenylate

23dhdp 2,3-Dihydrodipicolinate

23dhmb (R)-2,3-Dihydroxy-3-methylbutanoate

23dhmp (R)-2,3-Dihydroxy-3-methylpentanoate

23doguln 2,3-Dioxo-L-gulonate

25aics (S)-2-[5-Amino-1-(5-phospho-D-ribosyl)imidazole-4-carboxamido]succinate

25dkglcn 2,5-diketo-D-gluconate

25drapp 2,5-Diamino-6-(ribosylamino)-4-(3H)-pyrimidinone 5'-phosphate

26dap-LL LL-2,6-Diaminoheptanedioate

26dap-M meso-2,6-Diaminoheptanedioate

2ahbut (S)-2-Aceto-2-hydroxybutanoate

2aobut L-2-Amino-3-oxobutanoate

2cpr5p 1-(2-Carboxyphenylamino)-1-deoxy-D-ribulose 5-phosphate

2dda7p 2-Dehydro-3-deoxy-D-arabino-heptonate 7-phosphate

2ddg6p 2-Dehydro-3-deoxy-D-gluconate 6-phosphate

2ddglcn 2-Dehydro-3-deoxy-D-gluconate
2dh3dgal 2-Dehydro-3-deoxy-D-galactonate
2dh3dgal6p 2-Dehydro-3-deoxy-D-galactonate 6-phosphate
2dhglcn 2-Dehydro-D-gluconate
2dhguln 2-Dehydro-L-gulonate
2dhp 2-Dehydropantoate
2dmmq8 2-Demethylmenaquinone 8
2dmmql8 2-Demethylmenaquinol 8
2dr1p 2-Deoxy-D-ribose 1-phosphate
2dr5p 2-Deoxy-D-ribose 5-phosphate
2h3oppan 2-Hydroxy-3-oxopropanoate
2ippm 2-Isopropylmaleate
2kmb 2-keto-4-methylthiobutyrate
2mahmp 2-Methyl-4-amino-5-hydroxymethylpyrimidine diphosphate
2mcacn cis-2-Methylaconitate
2mcit 2-Methylcitrate
2me4p 2-C-methyl-D-erythritol 4-phosphate
2mecdp 2-C-methyl-D-erythritol "2,4-cyclodiphosphate"
2obut 2-Oxobutanoate
2ohph 2-Octaprenyl-6-hydroxyphenol
2ombzl "2-Octaprenyl-6-methoxy-1,4-benzoquinol"
2omhmbl "2-Octaprenyl-3-methyl-5-hydroxy-6-methoxy-1,4-benzoquinol"
2ommbl 2-Octaprenyl-3-methyl-6-methoxy- "1,4-benzoquinol"
2omph 2-Octaprenyl-6-methoxyphenol
2oph 2-Octaprenylphenol
2p4c2me 2-phospho-4-(cytidine 5'-diphospho)-2-C-methyl-D-erythritol
2pg D-Glycerate 2-phosphate
2pglyc 2-Phosphoglycolate
2shchc 2-Succinyl-6-hydroxy-2,4-cyclohexadiene-1-carboxylate
34hpp 3-(4-Hydroxyphenyl)pyruvate
3c2hmp 3-Carboxy-2-hydroxy-4-methylpentanoate
3c3hmp 3-Carboxy-3-hydroxy-4-methylpentanoate
3c4mop 3-Carboxy-4-methyl-2-oxopentanoate
3dgulnp 3-keto-L-gulonate-6-phosphate

3dhguln 3-Dehydro-L-gulonate

3dhq 3-Dehydroquinate

3dhsk 3-Dehydroshikimate

3hcinnm 3-hydroxycinnamic acid

3hmrsACP R-3-hydroxy-myristoyl-ACP

3hpppn 3-(3-hydroxy-phenyl)propionate

3ig3p C'-(3-Indolyl)-glycerol 3-phosphate

3mob 3-Methyl-2-oxobutanoate

3mop (S)-3-Methyl-2-oxopentanoate

3ophb 3-Octaprenyl-4-hydroxybenzoate

3pg 3-Phospho-D-glycerate

3php 3-Phosphohydroxypyruvate

3psme 5-O-(1-Carboxyvinyl)-3-phosphoshikimate

4abut 4-Aminobutanoate

4abutn 4-Aminobutanal

4abz 4-Aminobenzoate

4adcho 4-amino-4-deoxychorismate

4ahmmp 4-Amino-5-hydroxymethyl-2-methylpyrimidine

4ampm 4-Amino-2-methyl-5-phosphomethylpyrimidine

4c2me 4-(cytidine 5'-diphospho)-2-C-methyl-D-erythritol

4h2opntn 4-Hydroxy-2-oxopentanoate

4hba 4-Hydroxy-benzyl alcohol

4hbz 4-Hydroxybenzoate

4hthr 4-Hydroxy-L-threonine

4mhetz 4-Methyl-5-(2-hydroxyethyl)-thiazole

4mop 4-Methyl-2-oxopentanoate

4mpetz 4-Methyl-5-(2-phosphoethyl)-thiazole

4pasp 4-Phospho-L-aspartate

4per 4-Phospho-D-erythronate

4ppan D-4'-Phosphopantothenate

4ppcys N-((R)-4-Phosphopantothenoyl)-L-cysteine

4r5au 4-(1-D-Ribitylamino)-5-aminouracil

5aizc 5-amino-1-(5-phospho-D-ribosyl)imidazole-4-carboxylate

5aop 5-Amino-4-oxopentanoate

5aprbu 5-Amino-6-(5'-phosphoribitylamino)uracil
5apru 5-Amino-6-(5'-phosphoribosylamino)uracil
5caiz 5-phosphoribosyl-5-carboxyaminoimidazole
5dglcn 5-Dehydro-D-gluconate
5dh4dglc 5-Dehydro-4-deoxy-D-glucarate
5mdr1p 5-Methylthio-5-deoxy-D-ribose 1-phosphate
5mdru1p 5-Methylthio-5-deoxy-D-ribulose 1-phosphate
5mta 5-Methylthioadenosine
5mthf 5-Methyltetrahydrofolate
5mtr 5-Methylthio-D-ribose
5prdmbz "N1-(5-Phospho-alpha-D-ribosyl)-5,6-dimethylbenzimidazole"
6hmhpt 6-hydroxymethyl dihydropterin
6hmhptpp 6-hydroxymethyl-dihydropterin pyrophosphate
6pgc 6-Phospho-D-gluconate
6pgl "6-phospho-D-glucono-1,5-lactone"
8aonn 8-Amino-7-oxononanoate
aacald Aminoacetaldehyde
aacoa Acetoacetyl-CoA
ac Acetate
acac Acetoacetate
acACP Acetyl-ACP
acald Acetaldehyde
accoa Acetyl-CoA
acg5p N-Acetyl-L-glutamyl 5-phosphate
acg5sa N-Acetyl-L-glutamate 5-semialdehyde
acgam1p N-Acetyl-D-glucosamine 1-phosphate
acgam6p N-Acetyl-D-glucosamine 6-phosphate
acglu N-Acetyl-L-glutamate
acmana N-Acetyl-D-mannosamine
acmanap N-Acetyl-D-mannosamine 6-phosphate
acnam N-Acetylneuraminate
aconm E-3-carboxy-2-pentenedioate 6-methyl ester
acon-T trans-Aconitate
acorn N2-Acetyl-L-ornithine

ACP acyl carrier protein

acser O-Acetyl-L-serine

actACP Acetoacetyl-ACP

actp Acetyl phosphate

ade Adenine

adn Adenosine

adocbi Adenosyl cobinamide

adocbip Adenosyl cobinamide phosphate

adocbl Adenosylcobalamin

adp ADP

adpglc ADPglucose

agdpcbi Adenosine-GDP-cobinamide

agm Agmatine

agpc_EC acyl-glycerophosphocholine

agpe_EC acyl-glycerophosphoethanolamine

agpg_EC acyl-glycerophosphoglycerol

ahcys S-Adenosyl-L-homocysteine

ahdt "2-Amino-4-hydroxy-6-(erythro-1,2,3-trihydroxypropyl)dihydropteridine" triphosphate

aicar 5-Amino-1-(5-Phospho-D-ribosyl)imidazole-4-carboxamide

air 5-amino-1-(5-phospho-D-ribosyl)imidazole

akg 2-Oxoglutarate

alaala D-Alanyl-D-alanine

ala-B beta-Alanine

alac-S (S)-2-Acetolactate

ala-D D-Alanine

ala-L L-Alanine

altrn D-Altronate

alltn Allantoin

alltt Allantoate

amet S-Adenosyl-L-methionine

ametam S-Adenosylmethioninamine

amob S-Adenosyl-4-methylthio-2-oxobutanoate

amp AMP

anth Anthranilate
ap4a P1,P4-Bis(5'-adenosyl) tetraphosphate
ap5a P1,P5-Bis(5'-adenosyl) pentaphosphate
apg_EC acyl phosphatidylglycerol
apoACP apoprotein [acyl carrier protein]
aps Adenosine 5'-phosphosulfate
ara5p D-Arabinose 5-phosphate
arab-L L-Arabinose
arbt6p Arbutin 6-phosphate
arg-L L-Arginine
argsuc N(omega)-(L-Arginino)succinate
asn-L L-Asparagine
asp-L L-Aspartate
aspsa L-Aspartate 4-semialdehyde
atp ATP
bbtcoa gamma-butyrobetainyl-CoA
betald Betaine aldehyde
btcoa Butanoyl-CoA
btn Biotin
btnso d-biotin d-sulfoxide
but Butyrate (n-C4:0)
camp cAMP
cbasp N-Carbamoyl-L-aspartate
cbi Cobinamide
cbl1 Cob(I)alamin
cbp Carbamoyl phosphate
cdp CDP
cdpdag1 CDPdiacylglycerol
cdpea CDPethanolamine
cechddd cis-3-(3-carboxyethyl)-3,5-cyclohexadiene-1,2-diol
cenchddd cis-3-(3-carboxyethenyl)-3,5-cyclohexadiene-1,2-diol
cinnm trans-Cinnamate
cit Citrate
citr-L L-Citrulline

ckdo CMP-3-deoxy-D-manno-octulosonate
clpn_EC Cardiolipin
cmp CMP
co2 CO2
coa Coenzyme A
cpppg3 Coproporphyrinogen III
crn L-Carnitine
crncoa Carnitinyl-CoA
csn Cytosine
ctbt crotonobetaine
ctbtcoa crotonobetainyl-CoA
ctp CTP
cyan Cyanide
cynt Cyanate
cys-L L-Cysteine
cyst-L L-Cystathionine
cytd Cytidine
chol Choline
chor Chorismate
dad-2 Deoxyadenosine
dadp dADP
damp dAMP
dann 7,8-Diaminononanoate
datp dATP
db4p 3,4-dihydroxy-2-butanone 4-phosphate
dcamp N6-(1,2-Dicarboxyethyl)-AMP
dcdp dCDP
dcmp dCMP
dctp dCTP
dcyt Deoxycytidine
ddcaACP Dodecanoyl-ACP (n-C12:0ACP)
dgdp dGDP
dgmp dGMP
dgsn Deoxyguanosine

dgtp dGTP

dha Dihydroxyacetone

dhap Dihydroxyacetone phosphate

dhcinnm 2,3-dihydroxicinnamic acid

dhf 7,8-Dihydrofolate

dhna 1,4-Dihydroxy-2-naphthoate

dhnpt 2-Amino-4-hydroxy-6-(D-erythro-1,2,3-trihydroxypropyl)-7,8-dihydropteridine

dhor-S (S)-Dihydroorotate

dhpmp Dihydroneopterin monophosphate

dhpppn 3-(2,3-Dihydroxyphenyl)propanoate

dhpt Dihydropteroate

dhptd 4,5-dihydroxy-2,3-pentanedione

din Deoxyinosine

dkmpp 2,3-diketo-5-methylthio-1-phosphopentane

dmbzid 5,6-Dimethylbenzimidazole

dmlz 6,7-Dimethyl-8-(1-D-ribityl)lumazine

dmpp Dimethylallyl diphosphate

dms Dimethyl sulfide

dmso Dimethyl sulfoxide

dnad Deamino-NAD+

dpcoa Dephospho-CoA

dtbt Dethiobiotin

dtdp dTDP

dtdp4aaddg dTDP-4-acetamido-4,6-dideoxy-D-galactose

dtdp4addg dTDP-4-amino-4,6-dideoxy-D-glucose

dtdp4d6dg dTDP-4-dehydro-6-deoxy-D-glucose

dtdp4d6dm dTDP-4-dehydro-6-deoxy-L-mannose

dtdpglu dTDPglucose

dtdprmn dTDP-L-rhamnose

dtmp dTMP

dttp dTTP

dudp dUDP

dump dUMP

duri Deoxyuridine
dutp dUTP
dxyl 1-deoxy-D-xylulose
dxyl5p 1-deoxy-D-xylulose 5-phosphate
e4p D-Erythrose 4-phosphate
eca_EC Enterobacterial common antigen polysaccharide
eig3p D-erythro-1-(Imidazol-4-yl)glycerol 3-phosphate
enter Enterochelin
etha Ethanolamine
etoh Ethanol
f1p D-Fructose 1-phosphate
f6p D-Fructose 6-phosphate
fad FAD
fadh2 FADH2
fc1p L-Fuculose 1-phosphate
fcl-L L-fuculose
fdp D-Fructose 1,6-bisphosphate
fe2 Fe2+
fgam N2-Formyl-N1-(5-phospho-D-ribosyl)glycinamide
fmn FMN
for Formate
fpram 2-(Formamido)-N1-(5-phospho-D-ribosyl)acetamidine
fprica 5-Formamido-1-(5-phospho-D-ribosyl)imidazole-4-carboxamide
frdp Farnesyl diphosphate
fru D-Fructose
fruur D-Fructuronate
fuc-L L-Fucose
fum Fumarate
g1p D-Glucose 1-phosphate
g3p Glyceraldehyde 3-phosphate
g3pc sn-Glycero-3-phosphocholine
g3pe sn-Glycero-3-phosphoethanolamine
g3pg Glycerophosphoglycerol
g3pi sn-Glycero-3-phospho-1-inositol

g3ps Glycerophosphoserine
g6p D-Glucose 6-phosphate
gal D-Galactose
gal1p alpha-D-Galactose 1-phosphate
galct-D D-Galactarate
galctn-D D-Galactonate
galt1p Galactitol 1-phosphate
galur D-Galacturonate
gam1p D-Glucosamine 1-phosphate
gam6p D-Glucosamine 6-phosphate
gar N1-(5-Phospho-D-ribosyl)glycinamide
gbbtn gamma-butyrobetaine
gcald Glycolaldehyde
gdp GDP
gdpddman GDP-4-dehydro-6-deoxy-D-mannose
gdpfuc GDP-L-fucose
gdpmann GDP-D-mannose
gdpofuc GDP-4-oxo-L-fucose
glc-D D-Glucose
glcn D-Gluconate
glcr D-Glucarate
glcur D-Glucuronate
gln-L L-Glutamine
glu1sa L-Glutamate 1-semialdehyde
glu5p L-Glutamate 5-phosphate
glu5sa L-Glutamate 5-semialdehyde
glucys gamma-L-Glutamyl-L-cysteine
glu-D D-Glutamate
glu-L L-Glutamate
glutrna L-Glutamyl-tRNA(Glu)
glx Glyoxylate
gly Glycine
glyald D-Glyceraldehyde
glyb Glycine betaine

glyc Glycerol
glyc3p Glycerol 3-phosphate
glyclt Glycolate
glycogen glycogen
glyc-R (R)-Glycerate
gmhep17bp D-Glycero-D-manno-heptose 1,7-bisphosphate
gmhep1p D-Glycero-D-manno-heptose 1-phosphate
gmhep7p D-Glycero-D-manno-heptose 7-phosphate
gmp GMP
gp4g P1,P4-Bis(5'-guanosyl) tetraphosphate
grdp Geranyl diphosphate
gsn Guanosine
gthox Oxidized glutathione
gthrd Reduced glutathione
gtp GTP
gtspmd Glutathionylspermidine
gua Guanine
h H+
h2 H2
h2mb4p 1-hydroxy-2-methyl-2-(E)-butenyl 4-diphosphate
h2o H2O
h2o2 Hydrogen peroxide
h2s Hydrogen sulfide
hco3 Bicarbonate
hcys-L L-Homocysteine
hdca Hexadecanoate (n-C16:0)
hdcea hexadecenoate (n-C16:1)
hdeACP Hexadecenoyl-ACP (n-C16:1ACP)
hemeO Heme O
his-L L-Histidine
hisp L-Histidinol phosphate
histd L-Histidinol
hkndd 2-Hydroxy-6-oxonona-2,4-diene-1,9-dioate
hkntd 2-hydroxy-6-ketononatrienedioate

hmbil Hydroxymethylbilane
hmfurn 4-hydroxy-5-methyl-3(2H)-furanone
hom-L L-Homoserine
hpyr Hydroxypyruvate
hqn Hydroquinone
hxan Hypoxanthine
iasp Iminoaspartate
icit Isocitrate
ichor Isochorismate
idon-L L-Idonate
idp IDP
ile-L L-Isoleucine
imacp 3-(Imidazol-4-yl)-2-oxopropyl phosphate
imp IMP
indole Indole
inost myo-Inositol
ins Inosine
ipdp Isopentenyl diphosphate
itp ITP
kdo 3-Deoxy-D-manno-2-octulosonate
kdo2lipid4 KDO(2)-lipid IV(A)
kdo2lipid4L KDO(2)-lipid IV(A) with laurate
kdo2lipid4p KDO(2)-lipid IV(A) with palmitoleoyl
kdo8p 3-Deoxy-D-manno-octulosonate 8-phosphate
kdolipid4 KDO-lipid IV(A)
lac-D D-Lactate
lac-L L-Lactate
lald-L L-Lactaldehyde
lcts Lactose
leu-L L-Leucine
lgt-S (R)-S-Lactoylglutathione
lipa KDO(2)-lipid (A)
lipa_cold cold adapted KDO(2)-lipid (A)

lipidA 2,3,2'3'-Tetrakis(beta-hydroxymyristoyl)-D-glucosaminyl-1,6-beta-D-glucosamine 1,4'-bisphosphate

lipidAds Lipid A Disaccharide

lipidX 2,3-Bis(3-hydroxytetradecanoyl)-beta-D-glucosaminyl 1-phosphate

lps_EC lipopolysaccharide

lys-L L-Lysine

malACP Malonyl-[acyl-carrier protein]

malcoa Malonyl-CoA

mal-L L-Malate

malt Maltose

malthp Maltoheptaose

malthx Maltohexaose

maltpt Maltopentaose

malttr Maltotriose

maltttr Maltotetraose

man1p D-Mannose 1-phosphate

man6p D-Mannose 6-phosphate

mana D-Mannonate

melib Melibiose

methf 5,10-Methenyltetrahydrofolate

met-L L-Methionine

mi1p-D 1D-myo-Inositol 1-phosphate

micit methylisocitrate

mlthf 5,10-Methylenetetrahydrofolate

mmcoa-R (R)-Methylmalonyl-CoA

mmcoa-S (S)-Methylmalonyl-CoA

mnl1p D-Mannitol 1-phosphate

mql8 Menaquinol 8

mqn8 Menaquinone 8

mthgxl Methylglyoxal

myrsACP Myristoyl-ACP (n-C14:0ACP)

N1aspmd N1-Acetylspermidine

n8aspmd N8-Acetylspermidine

nac Nicotinate

nad Nicotinamide adenine dinucleotide
nadh Nicotinamide adenine dinucleotide - reduced
nadp Nicotinamide adenine dinucleotide phosphate
nadph Nicotinamide adenine dinucleotide phosphate - reduced
ncam Nicotinamide
nh4 ammonium
nicrnt Nicotinate D-ribonucleotide
nmn NMN
no2 Nitrite
no3 Nitrate
o2 O2
o2- Superoxide anion
oaa Oxaloacetate
ocdca octadecanoate (n-C18:0)
ocdcea octadecenoate (n-C18:1)
octdp all-trans-Octaprenyl diphosphate
octeACP Octadecenoyl-ACP (n-C18:1ACP)
ohpb 2-Oxo-3-hydroxy-4-phosphobutanoate
op4en 2-Oxopent-4-enoate
orn Ornithine
orot Orotate
orot5p Orotidine 5'-phosphate
pa_EC phosphatidate
pac Phenylacetic acid
pacald Phenylacetaldehyde
palmACP Palmitoyl-ACP (n-C16:0ACP)
pan4p Pantetheine 4'-phosphate
pant-R (R)-Pantoate
pap Adenosine 3',5'-bisphosphate
paps 3'-Phosphoadenylyl sulfate
pc_EC Phosphatidylcholine
pdx5p Pyridoxine 5'-phosphate
pe_EC Phosphatidylethanolamine
peamn Phenethylamine

pep Phosphoenolpyruvate

peptido_EC Peptidoglycan subunit of Escherichia coli

pg_EC Phosphatidylglycerol

pgp_EC Phosphatidylglycerophosphate

phaccoa Phenylacetyl-CoA

phe-L L-Phenylalanine

pheme Protoheme

phom O-Phospho-L-homoserine

phpyr Phenylpyruvate

phthr O-Phospho-4-hydroxy-L-threonine

pi Phosphate

pmcoa Pimeloyl-CoA

pnto-R (R)-Pantothenate

ppa Propionate

ppap Propanoyl phosphate

ppbng Porphobilinogen

ppcoa Propanoyl-CoA

pphn Prephenate

ppi Diphosphate

ppp9 Protoporphyrin

pppg9 Protoporphyrinogen IX

pppi Inorganic triphosphate

pppn Phenylpropanoate

pram 5-Phospho-beta-D-ribosylamine

pran N-(5-Phospho-D-ribosyl)anthranilate

prbamp 1-(5-Phosphoribosyl)-AMP

prbatp 1-(5-Phosphoribosyl)-ATP

prfp 1-(5-Phosphoribosyl)-5-[(5-phosphoribosylamino)methylideneamino]imidazole-4-carboxamide

prlp 5-[(5-phospho-1-deoxyribulos-1-ylamino)methylideneamino]-1-(5-phosphoribosyl)imidazole-4-carboxamide

pro-L L-Proline

prpp 5-Phospho-alpha-D-ribose 1-diphosphate

ps_EC phosphatidylserine

pser-L O-Phospho-L-serine
ptrc Putrescine
pyam5p Pyridoxamine 5'-phosphate
pydam Pyridoxamine
pydx Pyridoxal
pydx5p Pyridoxal 5'-phosphate
pydxn Pyridoxine
pyr Pyruvate
q8 Ubiquinone-8
q8h2 Ubiquinol-8
quln Quinolinate
r1p alpha-D-Ribose 1-phosphate
r5p alpha-D-Ribose 5-phosphate
rbl-L L-Ribulose
rdmbzi N1-(alpha-D-ribosyl)-5,6-dimethylbenzimidazole
rhcys S-Ribosyl-L-homocysteine
rib-D D-Ribose
ribflv Riboflavin
rml L-Rhamnulose
rml1p L-Rhamnulose 1-phosphate
rmn L-Rhamnose
ru5p-D D-Ribulose 5-phosphate
ru5p-L L-Ribulose 5-phosphate
s7p Sedoheptulose 7-phosphate
sbt6p D-Sorbitol 6-phosphate
sbzcoa O-Succinylbenzoyl-CoA
seln Selenide
selnp Selenophosphate
seramp L-seryl-AMP
ser-D D-Serine
ser-L L-Serine
shcl Sirohydrochlorin
sheme Siroheme
skm Shikimate

skm5p Shikimate 5-phosphate
sl26da N-Succinyl-LL-2,6-diaminoheptanedioate
sl2a6o N-Succinyl-2-L-amino-6-oxoheptanedioate
so3 Sulfite
so4 Sulfate
spmd Spermidine
srch Sirochlorin
ssaltpp Succinate semialdehyde-thiamin diphosphate anion
suc6p Sucrose 6-phosphate
sucarg N2-Succinyl-L-arginine
sucbz o-Succinylbenzoate
succ Succinate
succoa Succinyl-CoA
sucglu N2-Succinyl-L-glutamate
sucgsa N2-Succinyl-L-glutamate 5-semialdehyde
sucorn N2-Succinyl-L-ornithine
sucsal Succinic semialdehyde
suchms O-Succinyl-L-homoserine
tag6p-D D-Tagatose 6-phosphate
tagdp-D D-Tagatose 1,6-biphosphate
tagur D-Tagaturonate
tartr-L L-tartrate
taur Taurine
tcynt Thiocyanate
tdeACP Tetradecenoyl-ACP (n-C14:1ACP)
thdp 2,3,4,5-Tetrahydrodipicolinate
thf 5,6,7,8-Tetrahydrofolate
thm Thiamin
thmmp Thiamin monophosphate
thmpp Thiamine diphosphate
thr-L L-Threonine
thym Thymine
thymd Thymidine
tma Trimethylamine

tmao Trimethylamine N-oxide

trdox Oxidized thioredoxin

trdrd Reduced thioredoxin

tre Trehalose

tre6p alpha,alpha'-Trehalose 6-phosphate

trnaglu tRNA (Glu)

trp-L L-Tryptophan

tsul Thiosulfate

ttdca tetradecanoate (n-C14:0)

ttdcea tetradecenoate (n-C14:1)

tyr-L L-Tyrosine

u23ga UDP-2,3-bis(3-hydroxytetradecanoyl)glucosamine

u3aga UDP-3-O-(3-hydroxytetradecanoyl)-N-acetylglucosamine

u3hga UDP-3-O-(3-hydroxytetradecanoyl)-D-glucosamine

uaagmda Undecaprenyl-diphospho-N-acetylmuramoyl-(N-acetylglucosamine)-L-ala-D-glu-meso-2,6-diaminopimeloyl-D-ala-D-ala

uaccg UDP-N-acetyl-3-O-(1-carboxyvinyl)-D-glucosamine

uacgam UDP-N-acetyl-D-glucosamine

uacmam UDP-N-acetyl-D-mannosamine

uacmamu UDP-N-acetyl-D-mannosaminouronate

uagmda Undecaprenyl-diphospho-N-acetylmuramoyl-L-alanyl-D-glutamyl-meso-2,6-diaminopimeloyl-D-alanyl-D-alanine

uama UDP-N-acetylmuramoyl-L-alanine

uamag UDP-N-acetylmuramoyl-L-alanyl-D-glutamate

uamr UDP-N-acetylmuramate

udcpdp Undecaprenyl diphosphate

udcpp Undecaprenyl phosphate

udp UDP

udpg UDPglucose

udpgal UDPgalactose

udpgalfur UDP-D-galacto-1,4-furanose

udpglcur UDP-D-glucuronate

ugmd UDP-N-acetylmuramoyl-L-alanyl-D-gamma-glutamyl-meso-2,6-diaminopimelate

ugmda UDP-N-acetylmuramoyl-L-alanyl-D-glutamyl-meso-2,6-diaminopimeloyl-D-alanyl-D-alanine

ump UMP

unaga Undecaprenyl diphospho N-acetyl-glucosamine

unagamu Undecaprenyl-diphospho-N-acetylglucosamine-N-acetylmannosaminuronate

unagamuf Undecaprenyl-diphospho N-acetylglucosamine-N-acetylmannosaminuronate-N-acetamido-4,6-dideoxy-D-galactose

uppg3 Uroporphyrinogen III

ura Uracil

urdglyc (-)-Ureidoglycolate

urea Urea

uri Uridine

utp UTP

val-L L-Valine

xan Xanthine

xmp Xanthosine 5'-phosphate

xtsn Xanthosine

xu5p-D D-Xylulose 5-phosphate

xu5p-L L-Xylulose 5-phosphate

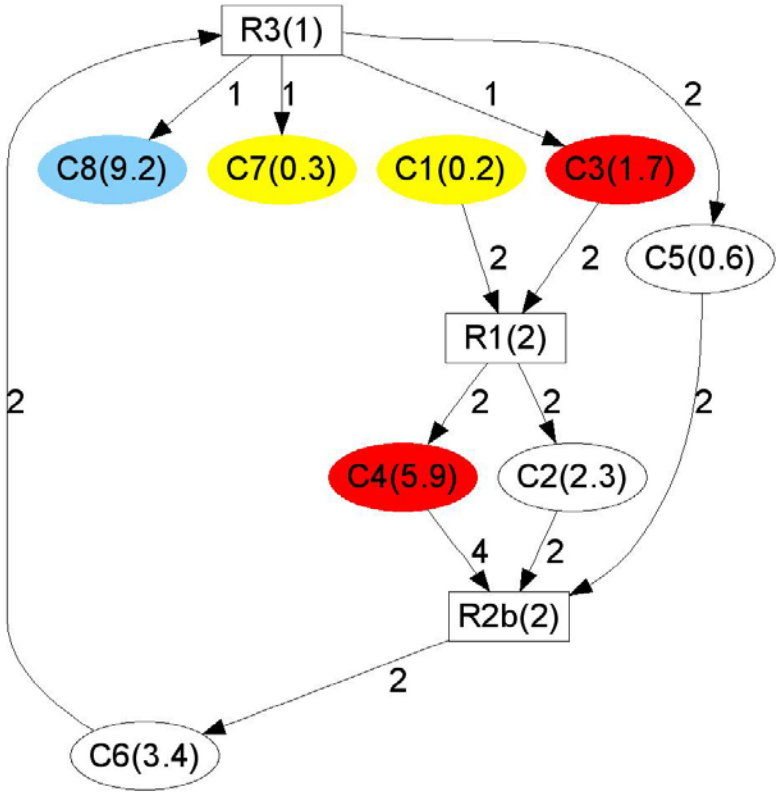
xyl-D D-Xylose

xylu-D D-Xylulose

Appendix C: Pathway details

For each of the metabolic pathways considered we give below a picture of the experimentally determined pathway that we used in this thesis. These pathways were drawn from the sources indicated below. The compound and reaction labelling/numbering is as listed in the data also provided in Appendices A and B.

To illustrate the notation we use the picture below shows an example metabolic pathway.



The reactions and the compounds (labelled R and C respectively) are the nodes in the above directed graph. The numbers associated with each arc are the number of molecules of each compound. For example reaction R3 takes two molecules of C6 and transforms them into one molecule of C3, C7 and C8 and two molecules of C5. The source and target compounds (C1 and C7 respectively) are coloured yellow and two

molecules of C1 are transformed into one molecule of C7. The numbers in brackets after each reaction label are the number of ticks, so for example reaction R1 ticks twice, each time converting one molecule of C1 and C3 into one molecule of C2 and C4. Compounds coloured blue are produced to excess (number of molecules needed is less than the number produced) whilst compounds coloured red are freely available (number of molecules needed is greater than the number produced). Compounds shown in white are balanced (number of molecules needed is equal to the number produced).

In our pathway pictures:

- for the compounds the number in brackets after the compound label is the percentage presence of the compound, δ_c defined using δ_c=100(number of reactions in which the compound appears)/(total number of reactions). So above, for example, C6 has a percentage presence of 3.4%.

- reversible reactions are split into two non-reversible reactions and (arbitrarily) labelled using an 'a' and a 'b' at the end of the reaction number. If a reaction is not reversible then no 'a' or 'b' is associated with it. So above, for example, R1 and R3 are not reversible, but R2b is a reversible reaction with the reverse of R2b being R2a.

The Beasley-Planes (BP) model distinguishes between compounds according to their percentage presence. Compounds for which percentage presence $\leq \Delta$ (where Δ is an input parameter) are called ***low presence*** compounds. Compounds for which $\delta_c > \Delta$ are called ***high presence*** compounds. In the computational results reported below we (as in Chapter 3) use Δ=4%. So above, for example, C6 is a low presence compound but C4 is a high presence compound.

In the notation of the BP model Q_S is the number of molecules of the source compound and Q_T is the number of molecules of the target compound. For those cases in which the BP model recovers the pathway structure (i.e. the reactions involved in the pathway and their appropriate ticks) we give below a table detailing, for each (Q_S,Q_T) pair $(Q_S,Q_T \leq 6)$, the number of reactions and excess ATP associated with the optimisation solution from the BP model. Situations where that optimisation model indicated that no feasible solution exists are indicated by a 'X'. In other words in these cases no values for the decision variables in the BP model exist which satisfy all the constraints of that model for the particular (Q_S,Q_T) pair examined. The purpose of this (Q_S,Q_T) analysis is to determine whether, in addition to recovering the pathway, we can also recover the (Q_S,Q_T) pair seen in the experimentally determined pathway. The BP model considers two possible objectives:

- objective (3.13), giving primary weight to minimising the total number of reactions and secondary weight to maximising excess ATP

- objective (3.14), giving primary weight to maximising excess ATP and secondary weight to minimising the total number of reactions.

Below we give details of the (Q_S,Q_T) analysis for those cases among the 40 experimentally determined pathways where the BP model achieved recovery.

With respect to the path finding approach presented in Chapter 5, we provide below the pictures of the metabolic path associated with the first ten experimentally determined metabolic pathways (as noted in Chapter 5) for both the R-R case and the C-C case. Given the set of reactions and compounds that comprise a particular metabolic pathway, the associated metabolic path is defined in this thesis as the shortest path (under the distance metric as described in Chapter 5) that links the initial compound

(reaction) and the final compound (reaction) of the pathway via balanced intermediate compounds. As noted above, balanced compounds (shown in white colouring) are those compounds where the number of molecules produced by reactions involved in the pathway is equal to the number of molecules consumed by reactions involved in the pathway. Note that for a given pathway (as discussed in Chapter 5) the metabolic path may not be uniquely defined. In addition, for each metabolic pathway considered the metabolic path (R-R and C-C case) and the computed shortest paths (for k=1,2,…,10) are systematically compared according to the correspondence criteria described in Chapter 5.

For the Improved Beasley Planes (IBP) model we, similarly to the BP model, give below details as to the (Q_S,Q_T) discussion. As noted in Chapter 6, the IBP model considers two different objectives:

- objective (6.26), giving primary weight to minimising the specificity (Ψ) and secondary weight to minimising the number of main compounds (W)

- objective (6.27), giving primary weight to minimising the length (L) and secondary weight to minimising the number of main compounds (W).

We have carried out the (Q_S,Q_T) discussion in those cases in which the IBP model achieved recovery of the pathway. We also include the (Q_S,Q_T) discussion for the cyclic pathways we recovered. In addition, we present the (Q_S,Q_T) discussion for Glycolysis (Pathway 3) when constraints related to atp production are included in the IBP model. Note that some cases take excessive computation time. This usually happens when the IBP model cannot find a biologically meaningful solution and outputs solutions containing cycles with an objective value far from the optimal value. In these

cases we applied a time limit of 30 minutes. This situation is indicated by a red colouring in the tables for (Q_S,Q_T) pairs below.

Pathway 1: Gluconeogenesis

Source compound	Pyruvate (pyr)
Target compound	D-Glucose 6-phosphate (g6p)
(Q_S,Q_T)	(2,1)
Low presence compounds that are not forced to be balanced	None
(Number of reactions, excess ATP)	(9,-4)
Number of unbalanced main compounds (W)	0
Specificity (Ψ)	8.57

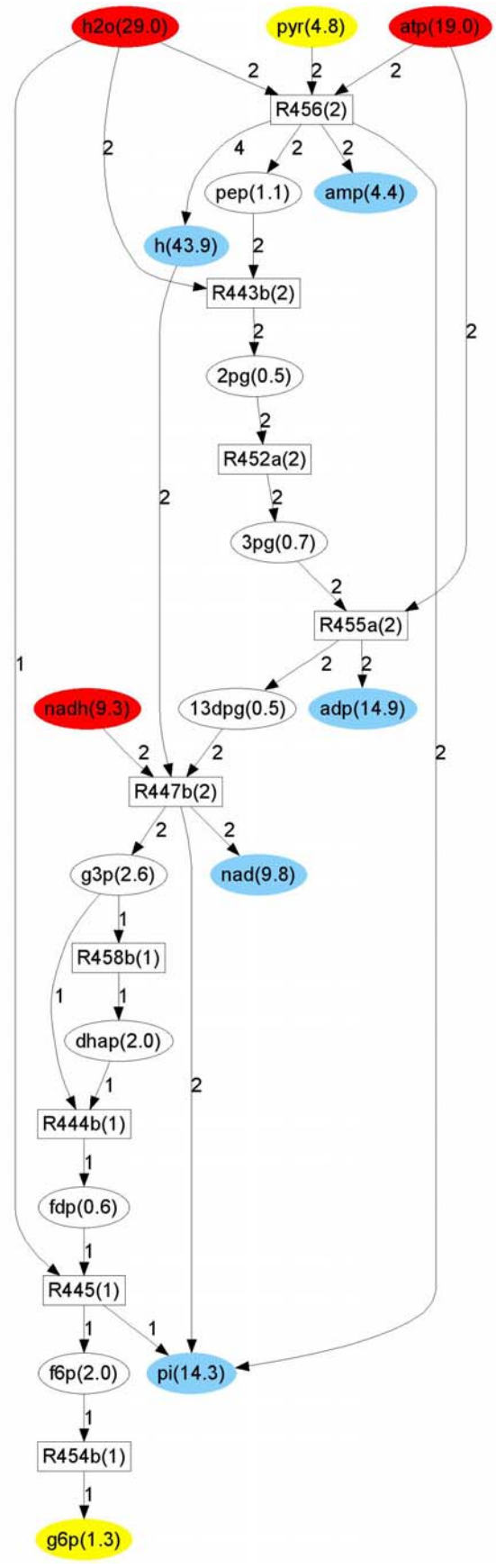
Note that the fourth and fifth rows of the above table relates to the BP model. Specifically, we give the low presence unbalanced compounds and the number of reactions and excess ATP of the pathway under study. The last two items relate to the IBP model, whose objective function involves the number of unbalanced main compounds and the specificity value. Note that the Ψ value shown above is for the maximum number of metabolic paths K=2.

Pathway description

This pathway has been taken from EcoCyc (http://biocyc.org/ECOLI/NEW-IMAGE?type=PATHWAY&object=GLUCONEO-PWY) and Lehninger (fourth edition) page 544.

In Lehninger the pathway is described as being from two molecules of pyruvate to one of glucose. However in EcoCyc it is described as being from malate to D-glucose-6-phosphate, without giving information about the number of molecules consumed or produced. Since the Lehninger description appears to be the more common one it is that which has informed the pathway picture seen below.

As shown below, the target compound is D-glucose-6-phosphate. According to our reaction database, a reaction to go from D-glucose-6-phosphate to glucose does not exist. This agrees with EcoCyc database. That is why the target compound is D-glucose-6-phosphate and not glucose.


h2o(29.0)
pyr(4.8)
atp(19.0)
R456(2)
pep(1.1)
amp(4.4)
h(43.9)
R443b(2)
2pg(0.5)
R452a(2)
3pg(0.7)
R455a(2)
nadh(9.3)
13dpg(0.5)
adp(14.9)
R447b(2)
g3p(2.6)
nad(9.8)
R458b(1)
dhap(2.0)
R444b(1)
fdp(0.6)
R445(1)
f6p(2.0)
pi(14.3)
R454b(1)
g6p(1.3)

(Q_S,Q_T) discussion for the BP model

This pathway was recovered with objective (3.13). Thus, the (Q_S,Q_T) discussion is carried out for objective (3.13). The table of pairs for objective (3.13) is shown below.

(number of reactions, excess ATP)		Number of molecules Q_T of target compound					
		1	2	3	4	5	6
Number of molecules Q_S of source compound	1	X	X	X	X	X	X
	2	(9,-4)*	X	X	X	X	X
	3	X	X	X	X	X	X
	4	X	(9,-8)	X	X	X	X
	5	X	X	X	X	X	X
	6	X	X	(9,-12)	X	X	X

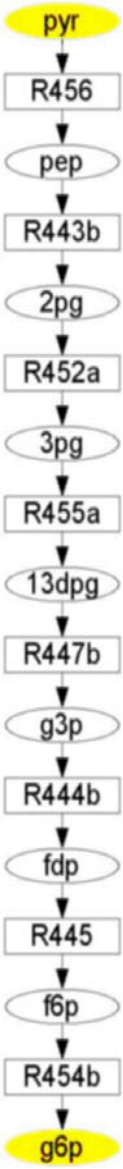
It can be seen that the majority of (Q_S,Q_T) pairs are infeasible. The three pairs seen are all repeats of each other, doubling and then tripling the number of source and target molecules (and excess ATP), whilst involving the same number of reactions. For this pathway the BP model indicates that the pair (Q_S,Q_T)=(2,1) dominates all other cases, since it involves fewer reactions and uses less ATP (and this is indicated by the * superscript on that entry in the above table). Hence in this case the BP model recovers the (Q_S,Q_T)=(2,1) pair observed in the experimentally determined pathway.

Metabolic path for the R-R case: correspondence values

k shortest path k	True positives (TP)	False positives (FP)	False negatives (FN)	Sensitivity (Sn)	Positive predictive value (PPV)	Accuracy (Ac)
1	5	2	8	0.385	0.714	0.549
2	10	1	3	0.769	0.909	0.839
3	10	1	3	0.769	0.909	0.839
4	3	4	10	0.231	0.429	0.330
5	3	4	10	0.231	0.429	0.330
6	13	0	0	1	1	1
7	2	13	11	0.154	0.133	0.144
8	2	13	11	0.154	0.133	0.144
9	2	13	11	0.154	0.133	0.144
10	10	3	3	0.769	0.769	0.769

For this pathway the metabolic path, from the first reaction R456 in the pathway, to the last reaction R454b in the pathway, is as shown above.

Metabolic path for the C-C case: correspondence values



k shortest path k	True positives (TP)	False positives (FP)	False negatives (FN)	Sensitivity (Sn)	Positive predictive value (PPV)	Accuracy (Ac)
1	2	15	13	0.133	0.118	0.125
2	7	2	8	0.467	0.778	0.622
3	0	21	15	0	0	0
4	0	27	15	0	0	0
5	2	23	13	0.133	0.080	0.107
6	2	21	13	0.133	0.087	0.110
7	0	18	15	0	0	0
8	0	23	15	0	0	0
9	2	23	13	0.133	0.080	0.107
10	0	20	15	0	0	0

For this pathway the metabolic path, from the source compound pyr in the pathway, to the target compound g6p in the pathway, is as shown above.

(Q_S,Q_T) discussion for the IBP model

This pathway was recovered with both objective (6.26) and objective (6.27). Thus, the (Q_S,Q_T) discussion is carried out for objective (6.26) and objective (6.27). The table of pairs for objective (6.26) is shown below.

(Ψ,W)		Number of molecules Q_T of target compound					
		1	2	3	4	5	6
Number of molecules Q_S of source compound	1	(8.13,1)*	(9.02,4)	(8.96,3)	(9.02,4)	(8.96,3)	(9.02,4)
	2	(8.57,0)	(8.13,1)	(9.02,4)	(8.96,3)	(9.02,4)	(9.06,2)
	3	(9.09,3)	(9.19,1)	(8.13,1)	(9.02,4)	(8.96,3)	(9.02,4)
	4	(9.09,3)	(8.57,0)	(9.19,1)	(8.13,1)	(9.02,4)	(8.96,3)
	5	(9.09,3)	(9.09,3)	(9.19,1)	(9.19,1)	(8.13,1)	(9.02,4)
	6	(9.09,3)	(9.09,3)	(8.57,0)	(9.19,1)	(9.19,1)	(8.13,1)

For this pathway the IBP model indicates that the pair (Q_S,Q_T)=(1,1) dominates all other cases. This is indicated by the * superscript on that entry in the above table. Hence in this case the IBP model does not recover the (Q_S,Q_T)=(2,1) pair observed in the experimentally determined pathway.

The results for objective (6.27) are shown below.

(L,W)		Number of molecules Q_T of target compound					
		1	2	3	4	5	6
Number of molecules Q_S of source compound	1	(7,1)*	(8,8)	(9,3)	(9,3)	(9,3)	(9,3)
	2	(9,0)	(7,1)	(9,3)	(8,8)	(9,3)	(9,3)
	3	(10,2)	(10,1)	(7,1)	(9,3)	(9,3)	(8,8)
	4	(10,2)	(9,0)	(10,1)	(7,1)	(9,3)	(9,3)
	5	(10,2)	(10,2)	(10,1)	(10,1)	(7,1)	(9,3)
	6	(10,2)	(10,2)	(9,0)	(10,1)	(10,1)	(7,1)

We obtain the same dominant pair as objective (6.26). Hence for this objective the IBP model does not recover the $(Q_S,Q_T)=(2,1)$ pair observed in the experimentally determined pathway.

Pathway 2: Glycogen

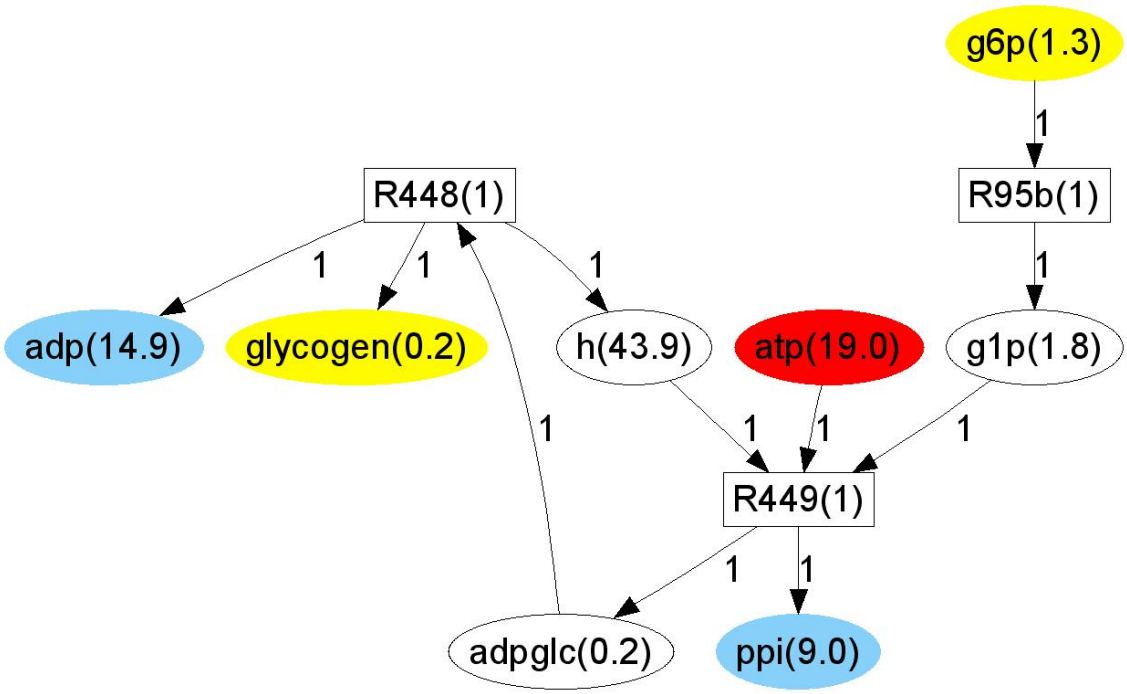
Source compound	D-Glucose 6-phosphate (g6p)
Target compound	Glycogen (glycogen)
(Q_S,Q_T)	(1,1)
Low presence compounds that are not forced to be balanced	None
(Number of reactions, excess ATP)	(3,-1)
Number of unbalanced main compounds (W)	0
Specificity (Ψ)	3

Pathway description

This pathway has been taken from EcoCyc (http://biocyc.org/ECOLI/NEW-IMAGE?type=PATHWAY&object=GLYCOGENSYNTH-PWY) and Lehninger (fourth edition) pages 568 and 596.

In Lehninger the pathway is described as being from one molecule of glucose-6-phosphate to elongated glycogen with n+1 residues. However in EcoCyc it is described as being from glucose-1-phosphate to elongated glycogen with n+1 residues. EcoCyc does not include the first reaction in Lehninger: D-Glucose-6-phosphate → D-Glucose-1-phosphate.

Since the Lehninger description appears to be the more general one and is consistent with our reaction database, it is that which has informed the pathway picture seen below.



Note here that we have one allowable c-cycle (see Chapter 3) in this pathway. More precisely the 2-cycle adpglc-R448-h-R449-adpglc which contains one high presence balanced compound (h).

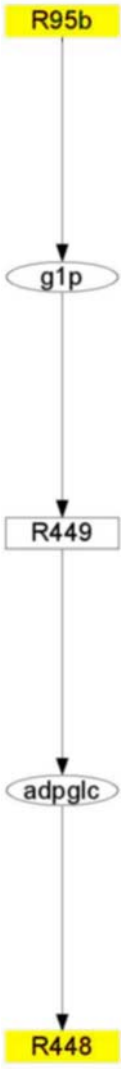
(Q_S,Q_T) discussion for the BP model

This pathway was recovered with objective (3.13). Thus, the (Q_S,Q_T) discussion is carried out for objective (3.13). The table of pairs for objective (3.13) is shown below.

(number of reactions, excess ATP)		Number of molecules Q_T of target compound					
		1	2	3	4	5	6
Number of molecules Q_S of source compound	1	(3,-1)*	X	X	X	X	X
	2	(15,0)	(3,-2)	X	X	X	X
	3	(15,0)	(13,0)	(3,-3)	X	X	X
	4	(15,1)	(15,0)	(13,0)	(3,-4)	X	X
	5	(15,2)	(15,0)	(15,0)	(13,0)	(3,-5)	X
	6	(15,3)	(15,1)	(15,0)	(13,0)	(13,0)	(3,-6)

Applying this procedure to the above table the dominant pair is (Q_S,Q_T)=(1,1). Hence in this case the BP model recovers the (Q_S,Q_T)=(1,1) pair observed in the experimentally determined pathway.

Metabolic path for the R-R case: correspondence values



k shortest path k	True positives (TP)	False positives (FP)	False negatives (FN)	Sensitivity (Sn)	Positive predictive value (PPV)	Accuracy (Ac)
1	3	0	0	1	1	1
2	3	4	0	1	0.429	0.714
3	3	12	0	1	0.200	0.600
4	3	6	0	1	0.333	0.667
5	3	6	0	1	0.333	0.667
6	3	6	0	1	0.333	0.667
7	3	8	0	1	0.273	0.636
8	3	6	0	1	0.333	0.667
9	3	6	0	1	0.333	0.667
10	3	6	0	1	0.333	0.667

Metabolic path for the C-C case: correspondence values

k shortest path k	True positives (TP)	False positives (FP)	False negatives (FN)	Sensitivity (Sn)	Positive predictive value (PPV)	Accuracy (Ac)
1	5	0	0	1	1	1
2	4	7	1	0.800	0.364	0.582
3	4	21	1	0.800	0.160	0.480
4	4	21	1	0.800	0.160	0.480
5	4	27	1	0.800	0.129	0.465
6	4	17	1	0.800	0.190	0.495
7	4	29	1	0.800	0.121	0.461
8	4	19	1	0.800	0.174	0.487
9	4	21	1	0.800	0.160	0.480
10	4	27	1	0.800	0.129	0.465

(Q_S,Q_T) discussion for the IBP model

This pathway was recovered with both objective (6.26) and objective (6.27). Thus, the (Q_S,Q_T) discussion is carried out for objective (6.26) and objective (6.27). The table of pairs for objective (6.26) is shown below.

(Ψ,W)		Number of molecules Q_T of target compound					
		1	2	3	4	5	6
Number of molecules Q_S of source compound	1	(3,0)*	X	X	X	X	X
	2	(8.63,3)	(3,0)	X	X	X	X
	3	(8.63,3)	(8.63,3)	(3,0)	X	X	X
	4	(8.63,3)	(8.63,3)	(8.63,3)	(3,0)	X	X
	5	(8.63,3)	(8.63,3)	(8.63,3)	(8.63,3)	(3,0)	X
	6	(8.63,3)	(8.63,3)	(8.63,3)	(8.63,3)	(8.63,3)	(3,0)

For this pathway the IBP model indicates that the pair (Q_S,Q_T)=(1,1) dominates all other cases. Hence in this case the IBP model recover the (Q_S,Q_T)=(1,1) pair observed in the experimentally determined pathway.

The results for objective (6.27) are shown below.

(L,W)		Number of molecules Q_T of target compound					
		1	2	3	4	5	6
Number of molecules Q_S of source compound	1	(3,0) *	X	X	X	X	X
	2	(12,5)	(3,0)	X	X	X	X
	3	(12,5)	(12,5)	(3,0)	X	X	X
	4	(12,5)	(12,5)	(12,5)	(3,0)	X	X
	5	(12,5)	(12,5)	(12,5)	(12,5)	(3,0)	X
	6	(12,5)	(12,5)	(12,5)	(12,5)	(12,5)	(3,0)

We obtain the same dominant pair as objective (6.26). Hence for this objective the IBP model also recovers the $(Q_S,Q_T)=(1,1)$ pair observed in the experimentally determined pathway.

Pathway 3: Glycolysis

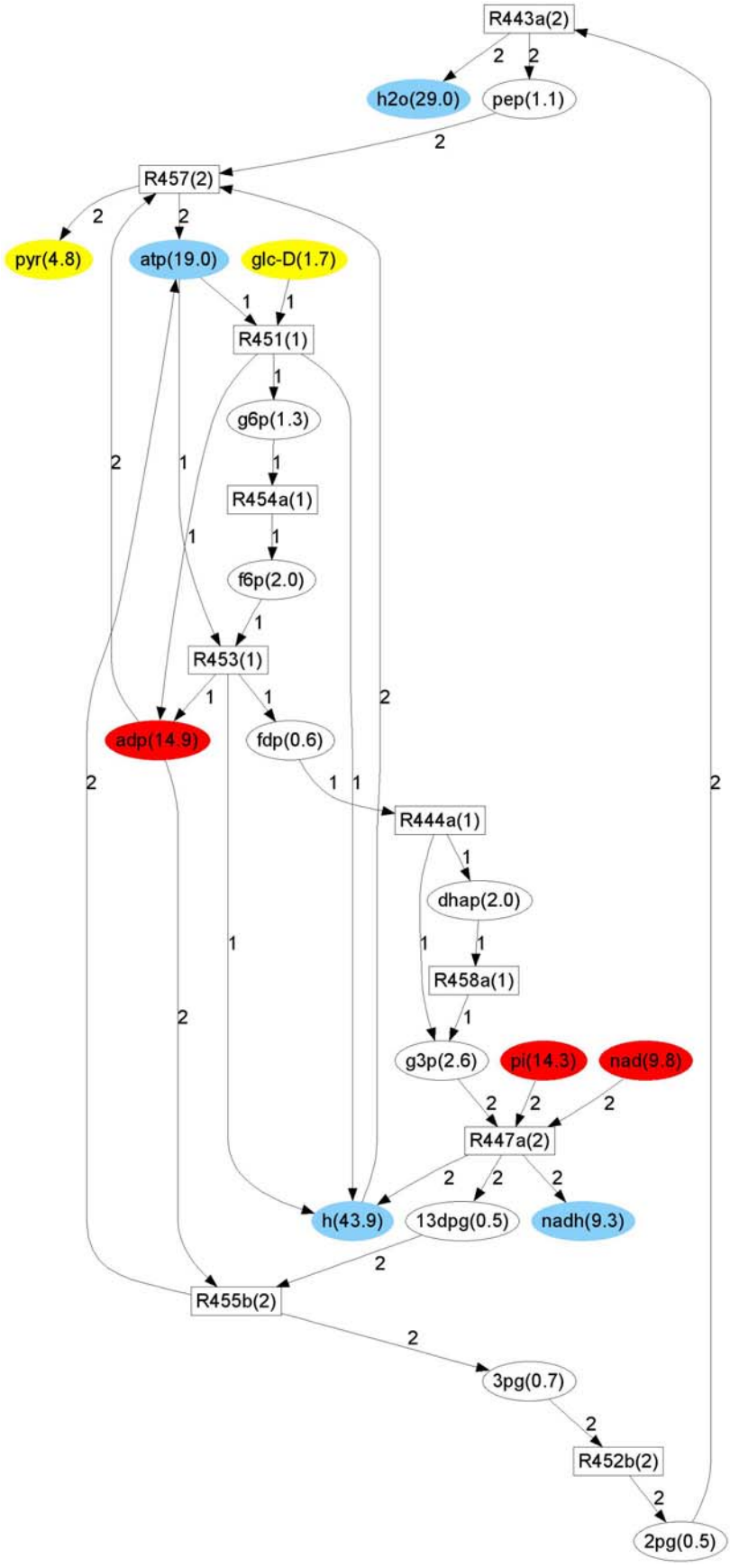
Source compound	D-Glucose (glc-D)
Target compound	Pyruvate (pyr)
(Q_S,Q_T)	(1,2)
Low presence compounds that are not forced to be balanced	None
(Number of reactions, excess ATP)	(10,2)
Number of unbalanced main compounds (W)	0
Specificity (Ψ)	9.57

Pathway description

This pathway has been taken from EcoCyc (http://biocyc.org/ECOLI/NEW-IMAGE?type=PATHWAY&object=GLYCOLYSIS) and Lehninger (fourth edition) page 524.

In Lehninger the pathway is described as being from one molecule of D-glucose to two molecules of pyruvate. However in EcoCyc it is described as being from one molecule of D-glucose-6-phosphate to two molecules of pyruvate. EcoCyc does not include first reaction in Lehninger: D-Glucose → D-Glucose-6-phosphate.

Since the Lehninger description appears to be the more general one and is consistent with our reaction database, it is that which has informed the pathway picture seen below.


R443a(2)
h2o(29.0)
pep(1.1)
R457(2)
pyr(4.8)
atp(19.0)
glc-D(1.7)
R451(1)
g6p(1.3)
R454a(1)
f6p(2.0)
R453(1)
adp(14.9)
fdp(0.6)
R444a(1)
dhap(2.0)
R458a(1)
g3p(2.6)
pi(14.3)
nad(9.8)
R447a(2)
h(43.9)
13dpg(0.5)
nadh(9.3)
R455b(2)
3pg(0.7)
R452b(2)
2pg(0.5)

(Q_S,Q_T) discussion for the BP model

This pathway was recovered with both objective (3.13) and objective (3.14). Thus, the (Q_S,Q_T) discussion is carried out for objective (3.13) and objective (3.14). The table of pairs for objective (3.13) is shown below.

(number of reactions, excess ATP)		Number of molecules Q_T of target compound					
		1	2	3	4	5	6
Number of molecules Q_S of source compound	1	X	(10,2)*	X	X	X	X
	2	X	X	X	(10,4)	X	X
	3	X	X	X	X	X	(10,6)
	4	X	X	X	X	X	X
	5	X	X	X	X	X	X
	6	X	X	X	X	X	X

It can be seen that the majority of (Q_S,Q_T) pairs are infeasible. The three pairs seen are all repeats of each other, doubling and then tripling the number of source and target molecules (and excess ATP). Hence in this case the BP model recovers the (Q_S,Q_T)=(1,2) pair observed in the experimentally determined pathway.

The results for objective (3.14) are shown below.

(number of reactions, excess ATP)		Number of molecules Q_T of target compound					
		1	2	3	4	5	6
Number of molecules Q_S of source compound	1	X	(10,2)*	X	X	X	X
	2	X	X	X	(10,4)	X	X
	3	X	X	X	X	X	(10,6)
	4	X	X	X	X	X	X
	5	X	X	X	X	X	X
	6	X	X	X	X	X	X

We get the same results as objective (3.13). Hence for this objective the BP model also recovers the $(Q_S,Q_T)=(1,2)$ pair observed in the experimentally determined pathway.

Metabolic path for the R-R case: correspondence values

k shortest path k	True positives (TP)	False positives (FP)	False negatives (FN)	Sensitivity (Sn)	Positive predictive value (PPV)	Accuracy (Ac)
1	10	7	5	0.667	0.588	0.627
2	2	9	13	0.133	0.182	0.158
3	12	1	3	0.800	0.923	0.862
4	12	1	3	0.800	0.923	0.862
5	15	0	0	1	1	1
6	10	9	5	0.667	0.526	0.596
7	10	9	5	0.667	0.526	0.596
8	12	3	3	0.800	0.800	0.800
9	2	21	13	0.133	0.087	0.110
10	4	5	11	0.267	0.444	0.356

Metabolic path for the C-C case: correspondence values

k shortest path k	True positives (TP)	False positives (FP)	False negatives (FN)	Sensitivity (Sn)	Positive predictive value (PPV)	Accuracy (Ac)
1	0	7	17	0	0	0
2	2	7	15	0.118	0.222	0.170
3	4	3	13	0.235	0.571	0.403
4	0	17	17	0	0	0
5	0	5	17	0	0	0
6	0	5	17	0	0	0
7	0	5	17	0	0	0
8	0	5	17	0	0	0
9	0	5	17	0	0	0
10	0	5	17	0	0	0

(Q_S,Q_T) discussion for the IBP model

This pathway was not recovered with either objective (6.26) or objective (6.27). However, when we include the constraints related to the production of atp as described in Chapter 6, we achieved recovery with objective (6.26). Thus, the (Q_S,Q_T) discussion is carried out for objective (6.26) under situation, i.e. atp forced to be produced. The table of pairs for objective (6.26) is shown below. Note here that we used K=1. The Ψ value of the pathway changes when K is modified. As seen below, the Ψ value for K=1 is precisely 10 for this pathway, whilst for K=2 the Ψ value is 9.57, as can be noted above.

(Ψ,W)		Number of molecules Q_T of target compound					
		1	2	3	4	5	6
Number of molecules Q_S of source compound	1	(10.39,1)	(10,0)*	(11.03,1)	(15.17,2)	(16.16,1)	(15.68,7)
	2	(17.46,4)	(10.5,0)	(15.13,2)	(10,0)	(16,1)	(11.03,1)
	3	(17.81,4)	(16.78,7)	(10.39,1)	(15.68,7)	(15.68,7)	(10,0)
	4	(18.05,7)	(17.46,4)	(16.68,8)	(10.39,1)	(15.68,7)	(15.13,2)
	5	(18.05,7)	(17.97,5)	(16.68,8)	(16.68,8)	(10.39,1)	(15.68,7)
	6	(18.15,6)	(17.81,4)	(17.46,4)	(16.68,8)	(16.68,8)	(10.39,1)

For this pathway the IBP model indicates that the pair (Q_S,Q_T)=(1,2) dominates all other cases. Hence in this case the IBP model recover the (Q_S,Q_T)=(1,2) pair observed in the experimentally determined pathway.

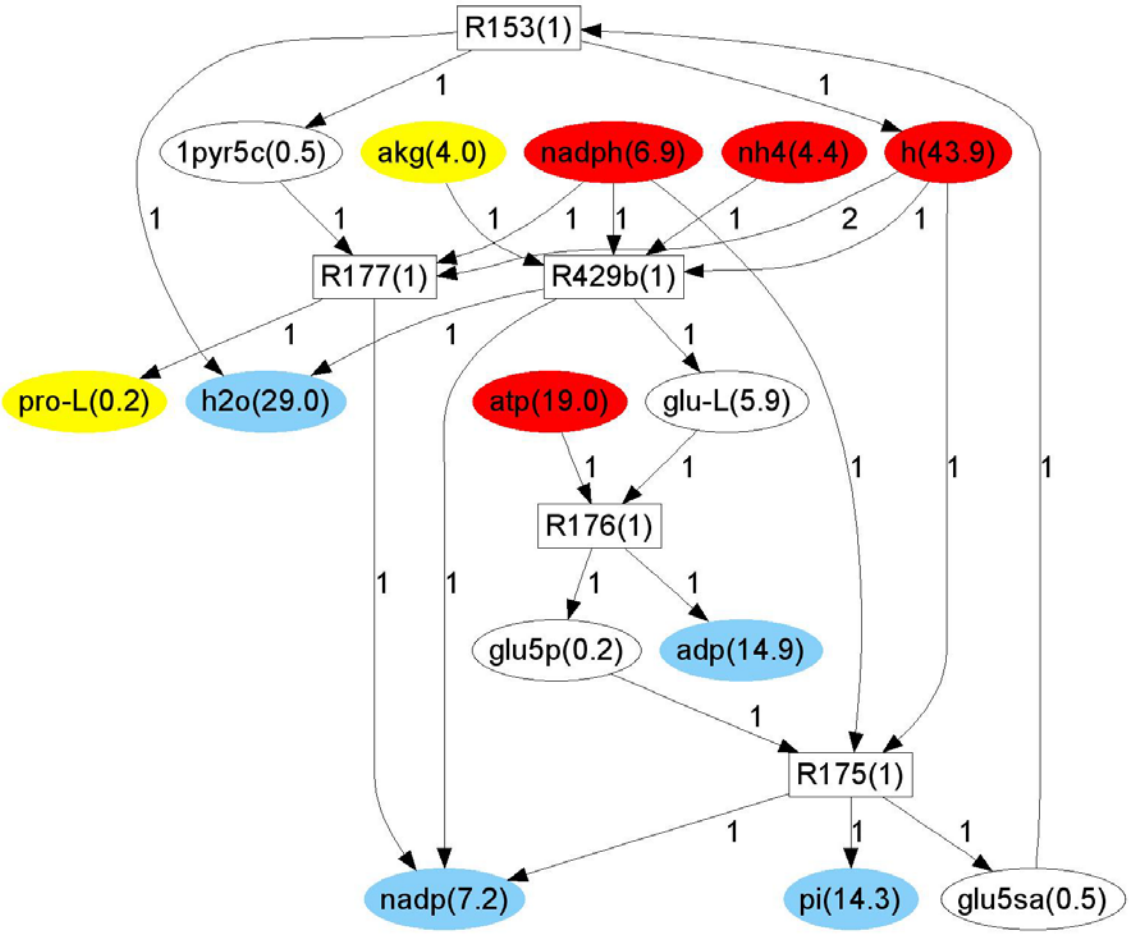
Pathway 4: Proline biosynthesis

Source compound	2-Oxoglutarate alpha-ketoglutarate (akg)
Target compound	L-Proline (pro-L)
(Q_S,Q_T)	(1,1)
Low presence compounds that are not forced to be balanced	None
(Number of reactions, excess ATP)	(5,-1)
Number of unbalanced main compounds (W)	0
Specificity (Ψ)	5

Pathway description

This pathway has been taken from EcoCyc (http://biocyc.org/ECOLI/NEW-IMAGE?type=PATHWAY&object=PROSYN-PWY&detail-level=3) and Lehninger (fourth edition) pages 842 and 843.

In Lehninger the pathway is described as being from one molecule of alpha-ketoglutarate to one molecule of proline. This pathway is described in the same way in EcoCyc.



(Q_S,Q_T) discussion for the BP model

This pathway was recovered with objective (3.13). Thus, the (Q_S,Q_T) discussion is carried out for objective (3.13). The table of pairs for objective (3.13) is shown below.

(number of reactions, excess ATP)		Number of molecules Q_T of target compound					
		1	2	3	4	5	6
Number of molecules Q_S of source compound	1	(5,-1)*	(7,-2)	(7,-3)	(7,-4)	(7,-5)	(7,-6)
	2	(7,-1)	(5,-2)	(7,-3)	(7,-4)	(7,-5)	(7,-6)
	3	(7,-1)	(7,-2)	(5,-3)	(7,-4)	(7,-5)	(7,-6)
	4	(7,-1)	(7,-2)	(7,-3)	(5,-4)	(7,-5)	(7,-6)
	5	(7,-1)	(7,-2)	(7,-3)	(7,-4)	(5,-5)	(7,-6)
	6	(7,-1)	(7,-2)	(7,-3)	(7,-4)	(7,-5)	(5,-6)

For this pathway the dominant pair is (Q_S,Q_T)=(1,1). Hence in this case the BP model recovers the (Q_S,Q_T)=(1,1) pair observed in the experimentally determined pathway.

Metabolic path for the R-R case: correspondence values

k shortest path k	True positives (TP)	False positives (FP)	False negatives (FN)	Sensitivity (Sn)	Positive predictive value (PPV)	Accuracy (Ac)
1	7	0	0	1	1	1
2	4	5	3	0.571	0.444	0.508
3	4	7	3	0.571	0.364	0.468
4	4	11	3	0.571	0.267	0.419
5	2	8	5	0.286	0.200	0.243
6	1	14	6	0.143	0.067	0.105
7	4	3	3	0.571	0.571	0.571
8	4	3	3	0.571	0.571	0.571
9	4	3	3	0.571	0.571	0.571
10	4	3	3	0.571	0.571	0.571

Metabolic path for the C-C case: correspondence values

k shortest path k	True positives (TP)	False positives (FP)	False negatives (FN)	Sensitivity (Sn)	Positive predictive value (PPV)	Accuracy (Ac)
1	4	1	5	0.444	0.800	0.622
2	4	3	5	0.444	0.571	0.508
3	2	7	7	0.222	0.222	0.222
4	2	9	7	0.222	0.182	0.202
5	2	9	7	0.222	0.182	0.202
6	2	11	7	0.222	0.154	0.188
7	2	9	7	0.222	0.182	0.202
8	2	13	7	0.222	0.133	0.178
9	2	9	7	0.222	0.182	0.202
10	2	13	7	0.222	0.133	0.178

(Q_S,Q_T) discussion for the IBP model

This pathway was recovered with objective (6.26). Thus, the (Q_S,Q_T) discussion is carried out for objective (6.26). The table of pairs for objective (6.26) is shown below.

(Ψ,W)		Number of molecules Q_T of target compound					
		1	2	3	4	5	6
Number of molecules Q_S of source compound	1	(5,0)*	(5.84,1)	X	X	X	X
	2	(9.6,0)	(5,0)	(5.42,1)	(5.84,1)	X	X
	3	(10.95,0)	(10.02,1)	(5,0)	(5.42,1)	(5.42,1)	(5.94,0)
	4	(10.95,0)	(9.6,0)	(11.36,8)	(5,0)	(5.42,1)	(5.42,1)
	5	(10.95,0)	(10.87,0)	(11.36,1)	(11.44,1)	(5,0)	(5.42,1)
	6	(10.95,0)	(10.95,0)	(9.6,0)	(10.02,1)	(9.95,4)	(5,0)

For this pathway the IBP model indicates that the pair (Q_S,Q_T)=(1,1) dominates all other cases. Hence in this case the IBP model recovers the (Q_S,Q_T)=(1,1) pair observed in the experimentally determined pathway.

Here the value in red (Q_S,Q_T)=(6,5) indicates that the result shown is not guaranteed to be optimal. Rather (9.95,4) is the best result obtained with objective (6.26) once our 30 minute time limit had been reached.

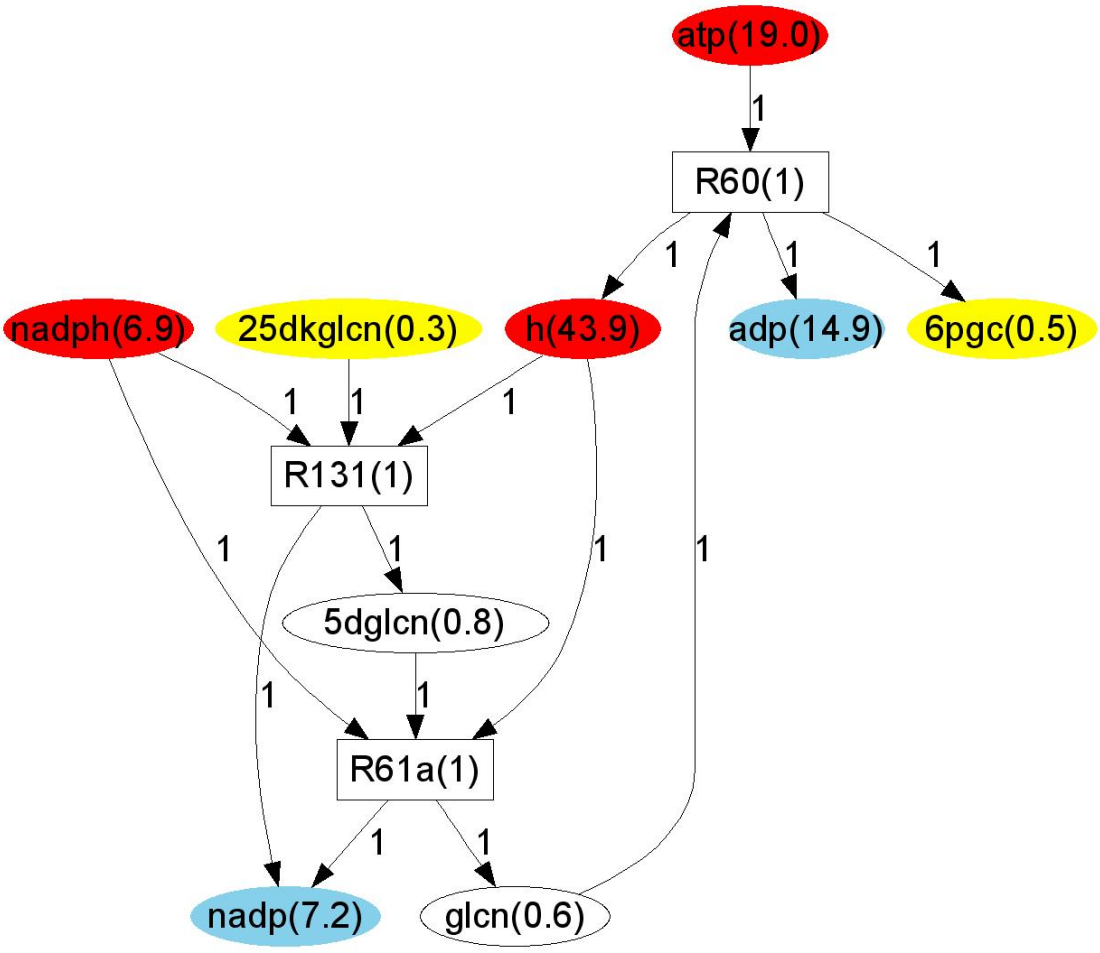
Pathway 5: Ketogluconate metabolism

Source compound	2,5-diketo-D-gluconate (25dkglcn)
Target compound	6-Phospho-D-gluconate (6pgc)
(Q_S,Q_T)	(1,1)
Low presence compounds that are not forced to be balanced	None
(Number of reactions, excess ATP)	(3,-1)
Number of unbalanced main compounds (W)	0
Specificity (Ψ)	3

Pathway description

This pathway has been taken from EcoCyc (http://biocyc.org/ECOLI/NEW-IMAGE?type=PATHWAY&object=KETOGLUCONMET-PWY).

In EcoCyc the pathway is described as being from 2,5-didehydro-D-gluconate to 6-Phospho-D-gluconate. However in our reaction database 2,5-didehydro-D-gluconate does not exist. Instead, 2,5-diketo-D-gluconate has been found and seems to fulfil the same function.



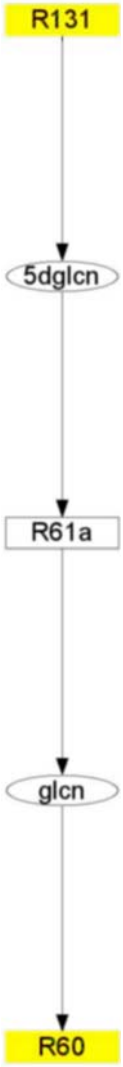
(Q_S,Q_T) discussion for the BP model

This pathway was recovered with objective (3.13). Thus, the (Q_S,Q_T) discussion is carried out for objective (3.13). The table of pairs for objective (3.13) is shown below.

(number of reactions, excess ATP)		Number of molecules Q_T of target compound					
		1	2	3	4	5	6
Number of molecules Q_S of source compound	1	(3,-1)*	(14,-5)	(14,-9)	(14,-13)	(14,-7)	(14,-21)
	2	X	(3,-2)	(14,-6)	(14,-10)	(14,-14)	(14,-18)
	3	X	X	(3,-3)	(14,-7)	(14,-11)	(14,-15)
	4	X	X	X	(3,-4)	(14,-8)	(14,-12)
	5	X	X	X	X	(3,-5)	(14,-9)
	6	X	X	X	X	X	(3,-6)

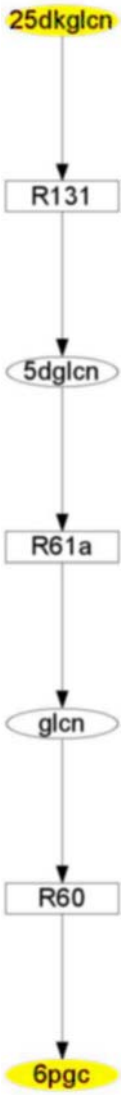
For this pathway the dominant pair is (Q_S,Q_T)=(1,1). Hence in this case the BP model recovers the (Q_S,Q_T)=(1,1) pair observed in the experimentally determined pathway.

Metabolic path for the R-R case: correspondence values



k shortest path k	True positives (TP)	False positives (FP)	False negatives (FN)	Sensitivity (Sn)	Positive predictive value (PPV)	Accuracy (Ac)
1	3	0	0	1	1	1
2	0	5	3	0	0	0
3	0	7	3	0	0	0
4	2	5	1	0.667	0.286	0.476
5	1	6	2	0.333	0.143	0.238
6	2	7	1	0.667	0.222	0.444
7	1	8	2	0.333	0.111	0.222
8	0	15	3	0	0	0
9	0	7	3	0	0	0
10	0	11	3	0	0	0

Metabolic path for the C-C case: correspondence values



k shortest path k	True positives (TP)	False positives (FP)	False negatives (FN)	Sensitivity (Sn)	Positive predictive value (PPV)	Accuracy (Ac)
1	5	0	0	1	1	1
2	4	1	1	0.800	0.800	0.800
3	4	5	1	0.800	0.444	0.622
4	4	5	1	0.800	0.444	0.622
5	1	4	4	0.200	0.200	0.200
6	0	5	5	0	0	0
7	0	7	5	0	0	0
8	2	5	3	0.400	0.286	0.343
9	3	4	2	0.600	0.429	0.514
10	1	6	4	0.200	0.143	0.171

(Q_S,Q_T) discussion for the IBP model

This pathway was recovered with both objective (6.26) and objective (6.27). Thus, the (Q_S,Q_T) discussion is carried out for objective (6.26) and objective (6.27). The table of pairs for objective (6.26) is shown below.

(Ψ,W)		Number of molecules Q_T of target compound					
		1	2	3	4	5	6
Number of molecules Q_S of source compound	1	(3,0)*	X	X	X	X	X
	2	X	(3,0)	X	X	X	X
	3	X	X	(3,0)	X	X	X
	4	X	X	X	(3,0)	X	X
	5	X	X	X	X	(3,0)	X
	6	X	X	X	X	X	(3,0)

For this pathway the IBP model indicates that the pair (Q_S,Q_T)=(1,1) dominates all other cases. Hence in this case the IBP model recovers the (Q_S,Q_T)=(1,1) pair observed in the experimentally determined pathway.

The results for objective (6.27) are shown below.

(L,W)		Number of molecules Q_T of target compound					
		1	2	3	4	5	6
Number	1	(3,0)	X	X	X	X	X
of	2	X	(3,0)	X	X	X	X
molecules	3	X	X	(3,0)	X	X	X
Q_S of	4	X	X	X	(3,0)	X	X
source	5	X	X	X	X	(3,0)	X
compound	6	X	X	X	X	X	(3,0)

We obtain the same dominant pair as objective (6.26). Hence for this objective the IBP model also recovers the $(Q_S,Q_T)=(1,1)$ pair observed in the experimentally determined pathway.

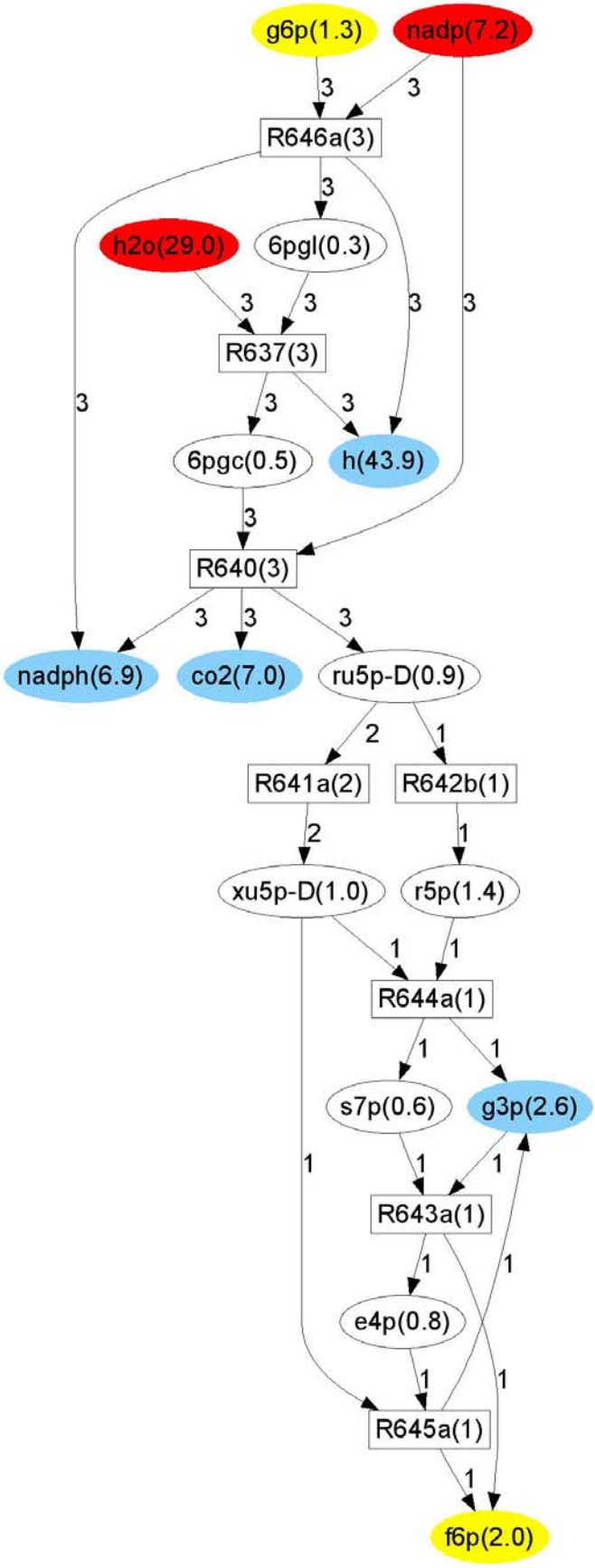
Pathway 6: Pentose phosphate

Source compound	D-Glucose 6-phosphate (g6p)
Target compound	D-Fructose 6-phosphate (f6p)
(Q_S,Q_T)	(3,2)
Low presence compounds that are not forced to be balanced	Glyceraldehyde 3-phosphate (g3p)
(Number of reactions, excess ATP)	(8,0)
Number of unbalanced main compounds (W)	1
Specificity (Ψ)	6.03

Pathway description

This pathway has been taken from EcoCyc (http://biocyc.org/ECOLI/NEW-IMAGE?type=PATHWAY&object=PENTOSE-P-PWY) and Lehninger (fourth edition) pages 549 to 553.

Both in Lehninger and EcoCyc, the pathway is described as being from three molecules of D-Glucose-6-phosphate to two molecules of D-Fructose 6-phosphate.


g6p(1.3)
nadp(7.2)
R646a(3)
h2o(29.0)
6pgl(0.3)
R637(3)
6pgc(0.5)
h(43.9)
R640(3)
nadph(6.9)
co2(7.0)
ru5p-D(0.9)
R641a(2)
R642b(1)
xu5p-D(1.0)
r5p(1.4)
R644a(1)
s7p(0.6)
g3p(2.6)
R643a(1)
e4p(0.8)
R645a(1)
f6p(2.0)

(Q_S,Q_T) discussion for the BP model

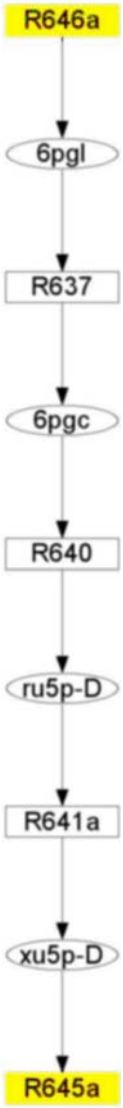
This pathway was recovered with objective (3.13). Thus, the (Q_S,Q_T) discussion is carried out for objective (3.13). The table of pairs for objective (3.13) is shown below.

(number of reactions, excess ATP)		Number of molecules Q_T of target compound					
		1	2	3	4	5	6
Number of molecules Q_S of source compound	1	(1,0)*	(4,0)	(4,0)	(4,0)	(4,0)	(4,0)
	2	(7,0)	(1,0)	(4,0)	(4,0)	(4,0)	(4,0)
	3	(13,1)	(8,0)	(1,0)	(4,0)	(4,0)	(4,0)
	4	(13,2)	(7,0)	(8,0)	(1,0)	(4,0)	(4,0)
	5	(13,3)	(13,2)	(8,0)	(8,0)	(1,0)	(4,0)
	6	(13,4)	(13,3)	(7,0)	(8,0)	(8,0)	(1,0)

Note the presence of a single reaction pathway involving no excess ATP as indicated down the diagonal of the above table. Technically, in the BP model, a single reaction pathway can be found if there exists a reaction converting the source compound into the target compound which also only involves (if at all) high presence compounds. Here there is a single reaction (R454a in our reaction database) associated with glucose-6-phosphate isomerase that directly converts D-Glucose 6-phosphate into D-Fructose 6-phosphate (and does not involve any other compounds).

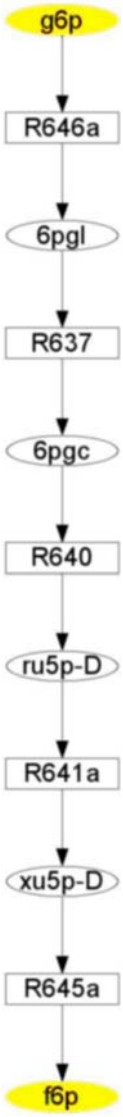
The dominant pair is (Q_S,Q_T)=(1,1). Hence in this case the BP model cannot recover the (Q_S,Q_T)=(3,2) pair associated with the experimentally determined pathway.

Metabolic path for the R-R case: correspondence values



k shortest path k	True positives (TP)	False positives (FP)	False negatives (FN)	Sensitivity (Sn)	Positive predictive value (PPV)	Accuracy (Ac)
1	7	0	0	1	1	1
2	7	4	0	1	0.636	0.818
3	5	6	2	0.714	0.455	0.584
4	3	6	4	0.429	0.333	0.381
5	4	5	3	0.571	0.444	0.508
6	7	4	0	1	0.636	0.818
7	5	6	2	0.714	0.455	0.584
8	6	7	1	0.857	0.462	0.659
9	4	9	3	0.571	0.308	0.440
10	5	16	2	0.714	0.238	0.476

Metabolic path for the C-C case: correspondence values



k shortest path k	True positives (TP)	False positives (FP)	False negatives (FN)	Sensitivity (Sn)	Positive predictive value (PPV)	Accuracy (Ac)
1	0	1	9	0	0	0
2	9	0	0	1	1	1
3	8	3	1	0.889	0.727	0.808
4	6	5	3	0.667	0.545	0.606
5	4	5	5	0.444	0.444	0.444
6	4	5	5	0.444	0.444	0.444
7	9	4	0	1	0.692	0.846
8	4	7	5	0.444	0.364	0.404
9	7	6	2	0.778	0.538	0.658
10	5	6	4	0.556	0.455	0.505

(Q_S,Q_T) discussion for the IBP model

This pathway was recovered with both objective (6.26) and objective (6.27). Thus, the (Q_S,Q_T) discussion is carried out for objective (6.26) and objective (6.27). The table of pairs for objective (6.26) is shown below.

(Ψ,W)		Number of molecules Q_T of target compound					
		1	2	3	4	5	6
Number of molecules Q_S of source compound	1	(5.13,2)*	(6.26,2)	(6.96,3)	(7.02,4)	(6.96,3)	(7.02,4)
	2	(6.56,0)	(5.13,2)	(5.63,2)	(6.26,2)	(7.02,4)	(6.96,3)
	3	(9.36,4)	(6.03,1)	(5.13,2)	(5.63,2)	(5.63,2)	(6.26,2)
	4	(9.53,0)	(6.56,0)	(6.16,0)	(5.13,2)	(5.63,2)	(5.63,2)
	5	(9.77,6)	(8.95,6)	(6.03,2)	(6.13,1)	(5.13,2)	(5.63,2)
	6	(9.77,6)	(8.95,6)	(6.56,0)	(6.03,1)	(6.06,1)	(5.13,2)

For this pathway the IBP model indicates that the pair (Q_S,Q_T)=(1,1) dominates all other cases. Hence in this case the IBP model does not recover the (Q_S,Q_T)=(3,2) pair observed in the experimentally determined pathway.

The results for objective (6.27) are shown below.

(Ψ,W)		Number of molecules Q_T of target compound					
		1	2	3	4	5	6
Number of molecules Q_S of source compound	1	(5,1)*	(6,1)	(7,3)	(7,3)	(7,3)	(7,3)
	2	(7,0)	(5,1)	(7,3)	(6,1)	(7,3)	(7,3)
	3	(8,7)	(8,1)	(5,1)	(7,3)	(7,3)	(6,1)
	4	(8,7)	(7,0)	(8,1)	(5,1)	(7,3)	(7,3)
	5	(8,7)	(8,7)	(8,1)	(8,1)	(5,1)	(7,3)
	6	(8,7)	(8,7)	(7,0)	(8,1)	(8,1)	(5,1)

We obtain the same dominant pair as objective (6.26). Hence for this objective the IBP model does not recover the $(Q_S,Q_T)=(3,2)$ pair observed in the experimentally determined pathway.

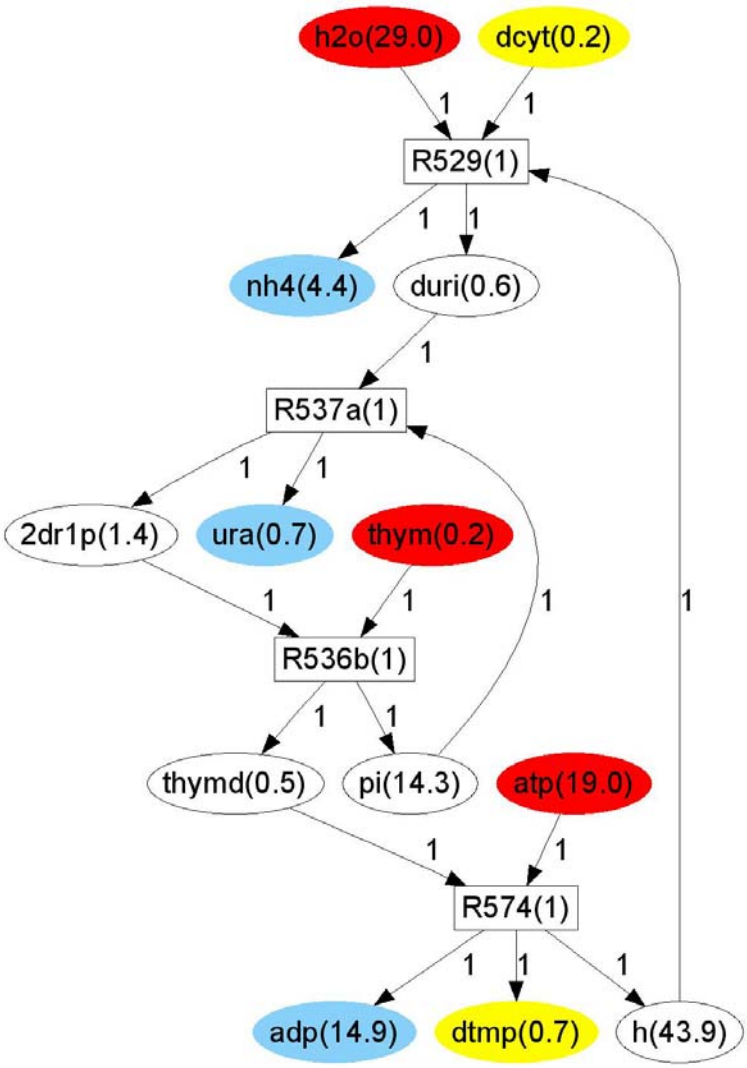
Pathway 7: Salvage pathway deoxythymidine phosphate

Source compound	Deoxycytidine (dcyt)
Target compound	dTMP (dtmp)
(Q_S,Q_T)	(1,1)
Low presence compounds that are not forced to be balanced	Uracil (ura) Thymine (thym)
(Number of reactions, excess ATP)	(4,-1)
Number of unbalanced main compounds (W)	2
Specificity (Ψ)	6.95

Pathway description

This pathway has been taken from EcoCyc (http://biocyc.org/ECOLI/NEW-IMAGE?type=PATHWAY&object=PWY0-181).

In EcoCyc the pathway is described as being from deoxycitidine to dTMP. The same set of reactions is present in our reaction database.



Note here that we have two allowable c-cycles in this pathway. More precisely:

- the 2-cycle 2dr1p-R536b-pi-R537a-2dr1p which contains one high presence balanced compound (pi).
- the 4-cycle 2dr1p-R536b-thymd-R574-h-R529-duri-R537a-2dr1p which contains one high presence balanced compound (h).

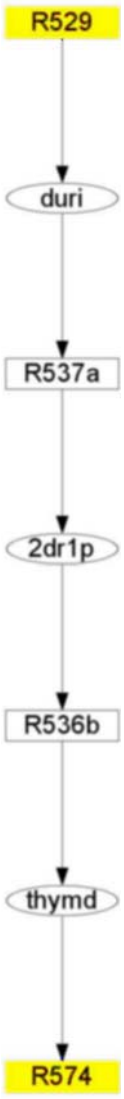
(Q_S,Q_T) discussion for the BP model

This pathway was recovered with objective (3.13). Thus, the (Q_S,Q_T) discussion is carried out for objective (3.13). The table of pairs for objective (3.13) is shown below.

(number of reactions, excess ATP)		Number of molecules Q_T of target compound					
		1	2	3	4	5	6
Number of molecules Q_S of source compound	1	(4,-1)*	X	X	X	X	X
	2	X	(4,-2)	X	X	X	X
	3	X	X	(4,-3)	X	X	X
	4	X	X	X	(4,-4)	X	X
	5	X	X	X	X	(4,-5)	X
	6	X	X	X	X	X	(4,-6)

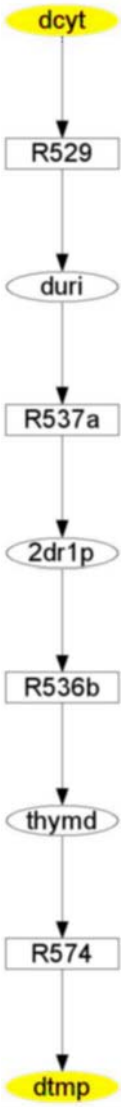
The pairs seen down the diagonal are all repeats of each other, doubling and then tripling, etc the number of source and target molecules (and excess ATP). The dominant pair is (Q_S,Q_T)=(1,1). Hence in this case the BP model recovers the (Q_S,Q_T)=(1,1) pair observed in the experimentally determined pathway.

Metabolic path for the R-R case: correspondence values



k shortest path k	True positives (TP)	False positives (FP)	False negatives (FN)	Sensitivity (Sn)	Positive predictive value (PPV)	Accuracy (Ac)
1	2	5	3	0.400	0.286	0.343
2	5	0	0	1	1	
3	3	12	2	0.600	0.200	0.400
4	3	14	2	0.600	0.176	0.388
5	3	14	2	0.600	0.176	0.388
6	5	12	0	1	0.294	0.647
7	5	12	0	1	0.294	0.647
8	4	15	1	0.800	0.211	0.505
9	3	14	2	0.600	0.176	0.388
10	3	16	2	0.600	0.158	0.379

Metabolic path for the C-C case: correspondence values



k shortest path k	True positives (TP)	False positives (FP)	False negatives (FN)	Sensitivity (Sn)	Positive predictive value (PPV)	Accuracy (Ac)
1	2	3	5	0.286	0.400	0.343
2	7	0	0	1	1	1
3	3	10	4	0.429	0.231	0.330
4	3	12	4	0.429	0.200	0.314
5	3	12	4	0.429	0.200	0.314
6	4	13	3	0.571	0.235	0.403
7	3	12	4	0.429	0.200	0.314
8	3	14	4	0.429	0.176	0.303
9	3	14	4	0.429	0.176	0.303
10	3	16	4	0.429	0.158	0.293

(Q_S,Q_T) discussion for the IBP model

This pathway was not recovered with either objective (6.26) or objective (6.27). For this reason (Q_S,Q_T) pairs discussion is omitted for this pathway.

Pathway 8: Tricarboxylic acid (citric acid, citrate, TCA, Krebs) cycle

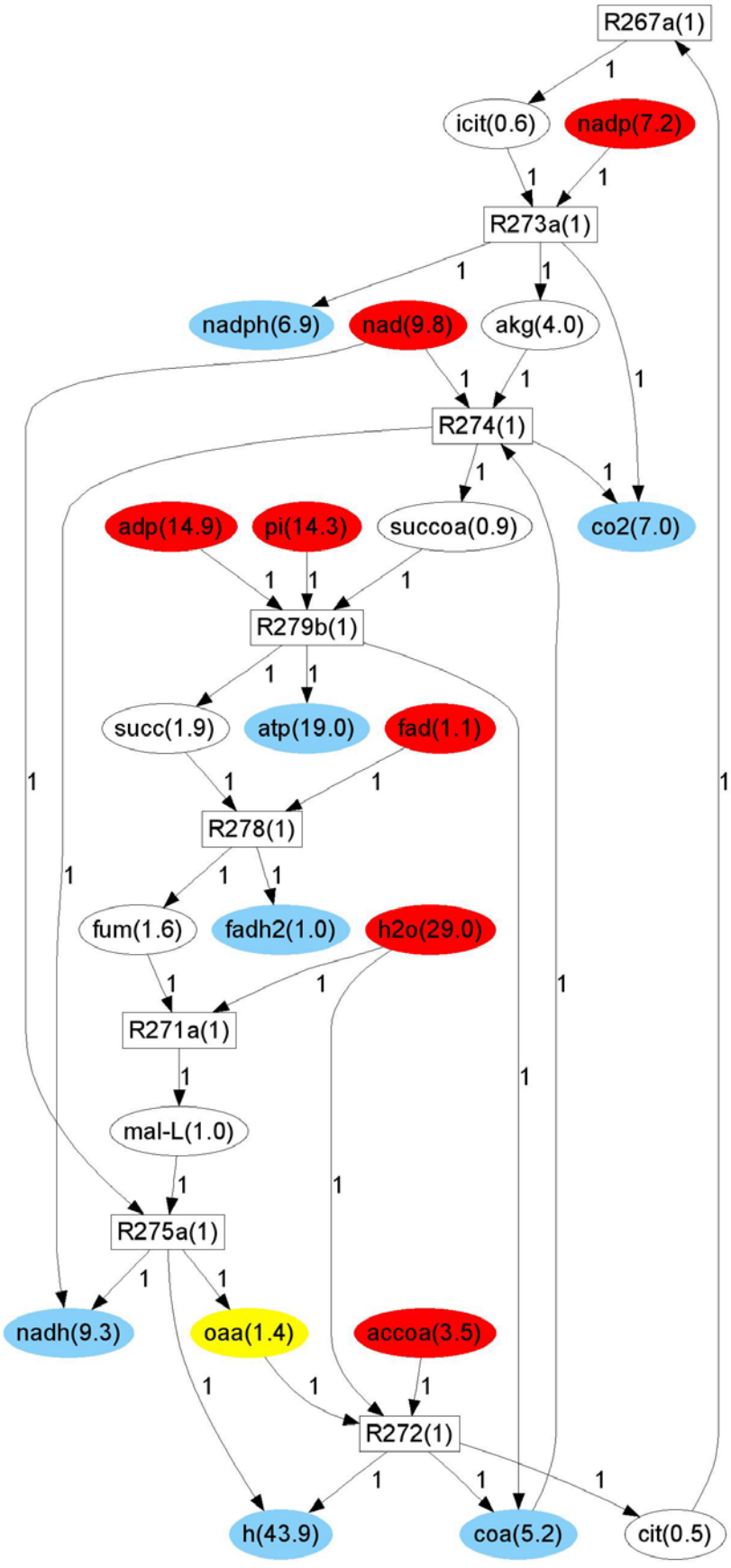
Source compound	Oxaloacetate (oaa)
Target compound	Oxaloacetate (oaa)
(Q_S,Q_T)	(1,1)
Low presence compounds that are not forced to be balanced	FAD (fad) FADH2 (fadh2) Acetyl-CoA (accoa)
(Number of reactions, excess ATP)	(8,1)
Number of unbalanced main compounds (W)	0
Specificity (Ψ)	8

Pathway description

This pathway has been taken from EcoCyc (http://biocyc.org/ECOLI/NEW-IMAGE?type=PATHWAY&object=TCA) and Lehninger (fourth edition) page 607.

Both in Lehninger and EcoCyc, the pathway is described as being a cycle starting and finishing at oxaloacetate with the same set of reactions involved.

The only difference is that EcoCyc produces ubiquinol and Lehninger produces fadh2 in the reaction in which succinate is converted to fumarate. Since our reaction database contains this reaction with fadh2, we have selected the Lehninger pathway.


R267a(1)
icit(0.6)
nadp(7.2)
R273a(1)
nadph(6.9)
nad(9.8)
akg(4.0)
R274(1)
adp(14.9)
pi(14.3)
succoa(0.9)
co2(7.0)
R279b(1)
succ(1.9)
atp(19.0)
fad(1.1)
R278(1)
fum(1.6)
fadh2(1.0)
h2o(29.0)
R271a(1)
mal-L(1.0)
R275a(1)
nadh(9.3)
oaa(1.4)
accoa(3.5)
R272(1)
h(43.9)
coa(5.2)
cit(0.5)

Note here that we have a number of allowable c-cycles in this pathway. There is an 8-cycle oaa-R272-cit-R267a-icit-R273a-akg-R274-succoa-R279b-succ-R278-fum-R271a-(mal-L)-R275a-oaa that starts and ends at the source/target compound (oaa). In terms of 2-cycles we have, for example, succoa-R279b-coa-R274-succoa that contains one high presence balanced compound (coa).

(Q_S,Q_T) discussion for the BP model

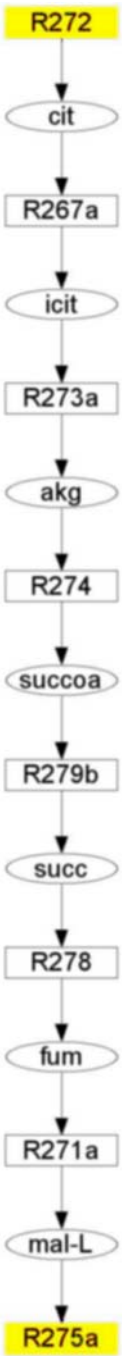
This pathway was recovered with objective (3.14). Thus, the (Q_S,Q_T) discussion is carried out for objective (3.14). The table of pairs for objective (3.14) is shown below.

(number of reactions, excess ATP)		Number of molecules Q_T of target compound					
		1	2	3	4	5	6
Number of molecules Q_S of source compound	1	(8,1)*	(9,2)	(9,3)	(9,4)	(9,5)	(9,6)
	2	(11,1)	(8,2)	(9,3)	(9,4)	(9,5)	(9,6)
	3	(11,1)	(11,2)	(8,3)	(9,4)	(9,5)	(9,6)
	4	(11,1)	(11,2)	(11,3)	(8,4)	(9,5)	(9,6)
	5	(11,1)	(11,2)	(11,3)	(11,4)	(8,5)	(9,6)
	6	(11,1)	(11,2)	(11,3)	(11,4)	(11,5)	(8,6)

In this pathway the source compound and the target compound are the same, moreover in the experimentally determined pathway the source/target compound is balanced (since Q_S=Q_T=1). It is therefore possible to interpret this pathway, a cycle, such that the only valid cases in the above (Q_S,Q_T) table of pairs are the diagonal entries (which are the only cases where the source/target compound is balanced).

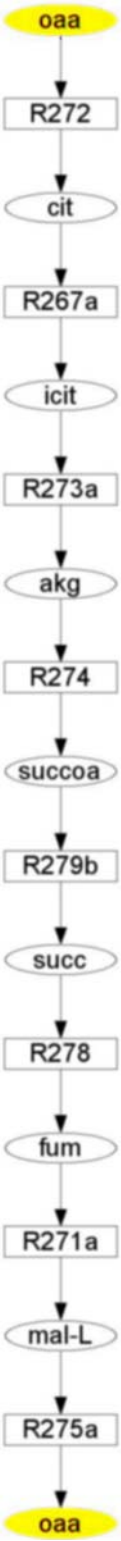
Adopting this interpretation the diagonal pairs. are all repeats of each other, doubling and then tripling, etc the number of source/target molecules. The dominant pair is (Q_S,Q_T)=(1,1). Hence in this case the BP model recovers the (Q_S,Q_T)=(1,1) pair observed in the experimentally determined pathway.

Metabolic path for the R-R case: correspondence values



k shortest path k	True positives (TP)	False positives (FP)	False negatives (FN)	Sensitivity (Sn)	Positive predictive value (PPV)	Accuracy (Ac)
1	4	3	9	0.308	0.571	0.440
2	8	1	5	0.615	0.889	0.752
3	4	5	9	0.308	0.444	0.376
4	2	5	11	0.154	0.286	0.220
5	4	7	9	0.308	0.364	0.336
6	4	7	9	0.308	0.364	0.336
7	4	7	9	0.308	0.364	0.336
8	2	7	11	0.154	0.222	0.188
9	6	9	7	0.462	0.400	0.431
10	7	6	6	0.538	0.538	0.538

Metabolic path for the C-C case: correspondence values



k shortest path k	True positives (TP)	False positives (FP)	False negatives (FN)	Sensitivity (Sn)	Positive predictive value (PPV)	Accuracy (Ac)
1	2	1	13	0.133	0.667	0.400
2	1	2	14	0.067	0.333	0.200
3	1	2	14	0.067	0.333	0.200
4	0	3	15	0	0	0
5	6	3	9	0.400	0.667	0.533
6	5	4	10	0.333	0.556	0.444
7	5	4	10	0.333	0.556	0.444
8	2	5	13	0.133	0.286	0.210
9	3	4	12	0.200	0.429	0.314
10	3	4	12	0.200	0.429	0.314

(Q_S,Q_T) discussion for the IBP model

This pathway was not recovered with either objective (6.26) or objective (6.27). However, as noted above, this pathway constitutes a cycle. When equations (6.28) and (6.29) related to cyclic pathways (as described in Chapter 6) were included in the IBP model, we achieved recovery for objective (6.26). The (Q_S,Q_T) discussion for objective (6.26) under this situation is shown below. As in the BP model, the only valid cases are those in the main diagonal. For this reason we neglected off-diagonal entries.

(Ψ,W)		Number of molecules Q_T of target compound					
		1	2	3	4	5	6
Number	1	(8,0)	-	-	-	-	-
of	2	-	(8,0)	-	-	-	-
molecules	3	-	-	(8,0)	-	-	-
Q_S of	4	-	-	-	(8,0)	-	-
source	5	-	-	-	-	(8,0)	-
compound	6	-	-	-	-	-	(8,0)

The IBP model indicates that the pair (Q_S,Q_T)=(1,1) dominates all other cases. Hence in this case the IBP model recovers the (Q_S,Q_T)=(1,1) pair observed in the experimentally determined pathway.

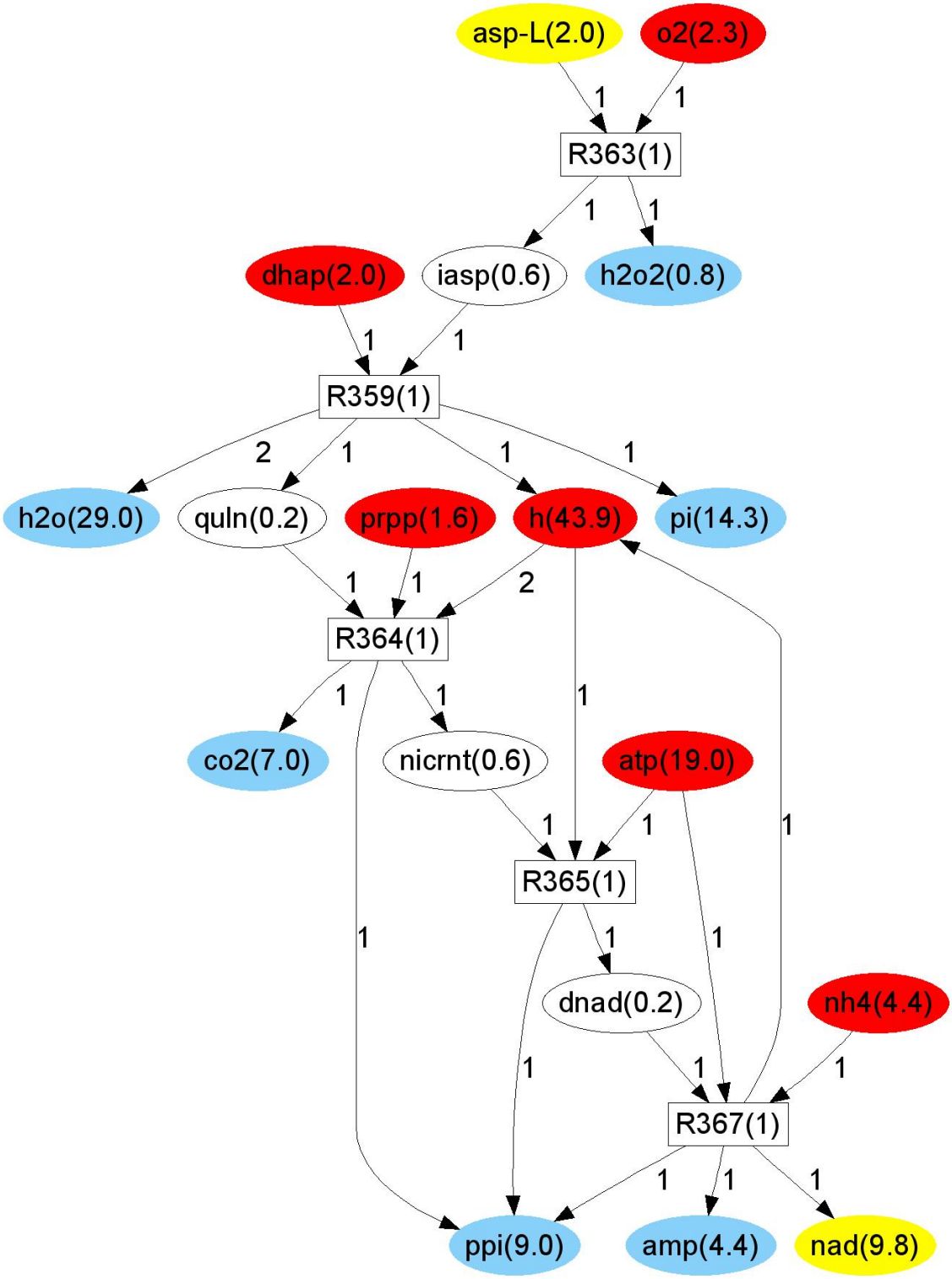
Pathway 9: NAD biosynthesis

Source compound	L-Aspartate (asp-L)
Target compound	Nicotinamide adenine dinucleotide (nad)
(Q_S,Q_T)	(1,1)
Low presence compounds that are not forced to be balanced	Dihydroxyacetone phosphate (dhap) Oxygen (o2) Hydrogen peroxide (h2o2) 5-Phospho-alpha-D-ribose 1-diphosphate (prpp)
(Number of reactions, excess ATP)	(5,-2)
Number of unbalanced main compounds (W)	2
Specificity (Ψ)	5.6

Pathway description

This pathway has been taken from EcoCyc (http://biocyc.org/ECOLI/NEW-IMAGE?type=PATHWAY&object=PYRIDNUCSYN-PWY).

In EcoCyc the pathway is described as being from L-Aspartate to NAD. The same set of reactions is found in our database, except that the last step can be carried out by two different reactions in EcoCyc. We only found one of these reactions in our reaction database.


asp-L(2.0)
o2(2.3)
R363(1)
dhap(2.0)
iasp(0.6)
h2o2(0.8)
R359(1)
h2o(29.0)
quln(0.2)
prpp(1.6)
h(43.9)
pi(14.3)
R364(1)
co2(7.0)
nicrnt(0.6)
atp(19.0)
R365(1)
dnad(0.2)
nh4(4.4)
R367(1)
ppi(9.0)
amp(4.4)
nad(9.8)

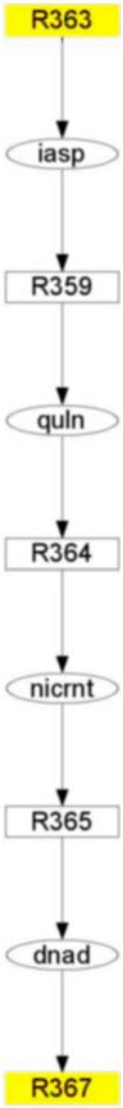
(Q_S,Q_T) discussion for the BP model

This pathway was recovered with objective (3.13). Thus, the (Q_S,Q_T) discussion is carried out for objective (3.13). The table of pairs for objective (3.13) is shown below.

(number of reactions, excess ATP)		Number of molecules Q_T of target compound					
		1	2	3	4	5	6
Number of molecules Q_S of source compound	1	(5,-2)*	(6,0)	(6,0)	(6,0)	(6,0)	(6,0)
	2	(6,0)	(5,-4)	(6,0)	(6,0)	(6,0)	(6,0)
	3	(6,0)	(6,0)	(5,-6)	(6,0)	(6,0)	(6,0)
	4	(6,0)	(6,0)	(6,0)	(5,-8)	(6,0)	(6,0)
	5	(6,0)	(6,0)	(6,0)	(6,0)	(5,-10)	(6,0)
	6	(6,0)	(6,0)	(6,0)	(6,0)	(6,0)	(5,-12)

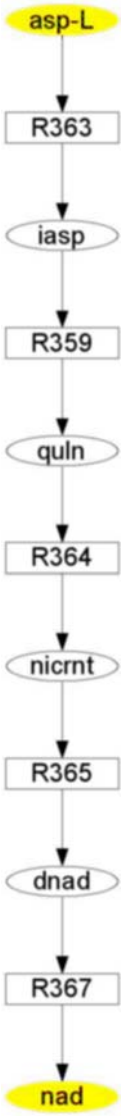
The pairs seen down the diagonal are all repeats of each other, doubling and then tripling, etc the number of source and target molecules (and excess ATP). The dominant pair is (Q_S,Q_T)=(1,1). Hence in this case the BP model recovers the (Q_S,Q_T)=(1,1) pair observed in the experimentally determined pathway.

Metabolic path for the R-R case: correspondence values



k shortest path k	True positives (TP)	False positives (FP)	False negatives (FN)	Sensitivity (Sn)	Positive predictive value (PPV)	Accuracy (Ac)
1	7	0	0	1	1	1
2	7	8	0	1	0.467	0.733
3	7	8	0	1	0.467	0.733
4	7	6	0	1	0.538	0.769
5	7	6	0	1	0.538	0.769
6	7	6	0	1	0.538	0.769
7	7	6	0	1	0.538	0.769
8	7	10	0	1	0.412	0.706
9	7	10	0	1	0.412	0.706
10	7	12	0	1	0.368	0.684

Metabolic path for the C-C case: correspondence values



k shortest path k	True positives (TP)	False positives (FP)	False negatives (FN)	Sensitivity (Sn)	Positive predictive value (PPV)	Accuracy (Ac)
1	0	3	9	0	0	0
2	8	1	1	0.889	0.889	0.889
3	8	1	1	0.889	0.889	0.889
4	8	1	1	0.889	0.889	0.889
5	9	0	0	1	1	1
6	0	5	9	0	0	0
7	0	5	9	0	0	0
8	0	5	9	0	0	0
9	0	9	9	0	0	0
10	0	5	9	0	0	0

(Q_S,Q_T) discussion for the IBP model

This pathway was recovered with objective (6.26). Thus, the (Q_S,Q_T) discussion is carried out for objective (6.26). The table of pairs for objective (6.26) is shown below.

(Ψ,W)		Number of molecules Q_T of target compound					
		1	2	3	4	5	6
Number of molecules Q_S of source compound	1	(5.6,2)*	(7.82,1)	(8.67,1)	(8.67,1)	(8.67,1)	(8.67,1)
	2	(6.17,3)	(5.6,2)	(7.67,1)	(7.67,1)	(7.67,1)	(7.67,1)
	3	(7.58,1)	(6.09,3)	(5.6,2)	(7.77,0)	(7.67,1)	(7.67,1)
	4	(7.58,1)	(6.26,2)	(6.09,3)	(5.6,2)	(7.67,1)	(7.67,1)
	5	(7.58,1)	(7.58,1)	(6.09,3)	(6.09,3)	(5.6,2)	(7.67,1)
	6	(7.58,1)	(7.58,1)	(6.17,3)	(6.09,3)	(6.09,3)	(5.6,2)

For this pathway the IBP model indicates that the pair (Q_S,Q_T)=(1,1) dominates all other cases. Hence in this case the IBP model recovers the (Q_S,Q_T)=(1,1) pair observed in the experimentally determined pathway.

Pathway 10: Arginine biosynthesis

Source compound	L-Glutamate (glu-L)
Target compound	L-Arginine (arg-L)
(Q_S,Q_T)	(2,1)
Low presence compounds that are not forced to be balanced	2-Oxoglutarate (akg) L-Aspartate (asp-L) Fumarate (fum) Acetate (ac) Acetyl-CoA (accoa) Carbamoyl phosphate (cbp)
(Number of reactions, excess ATP)	(8,-2)
Number of unbalanced main compounds (W)	4
Specificity (Ψ)	8.33

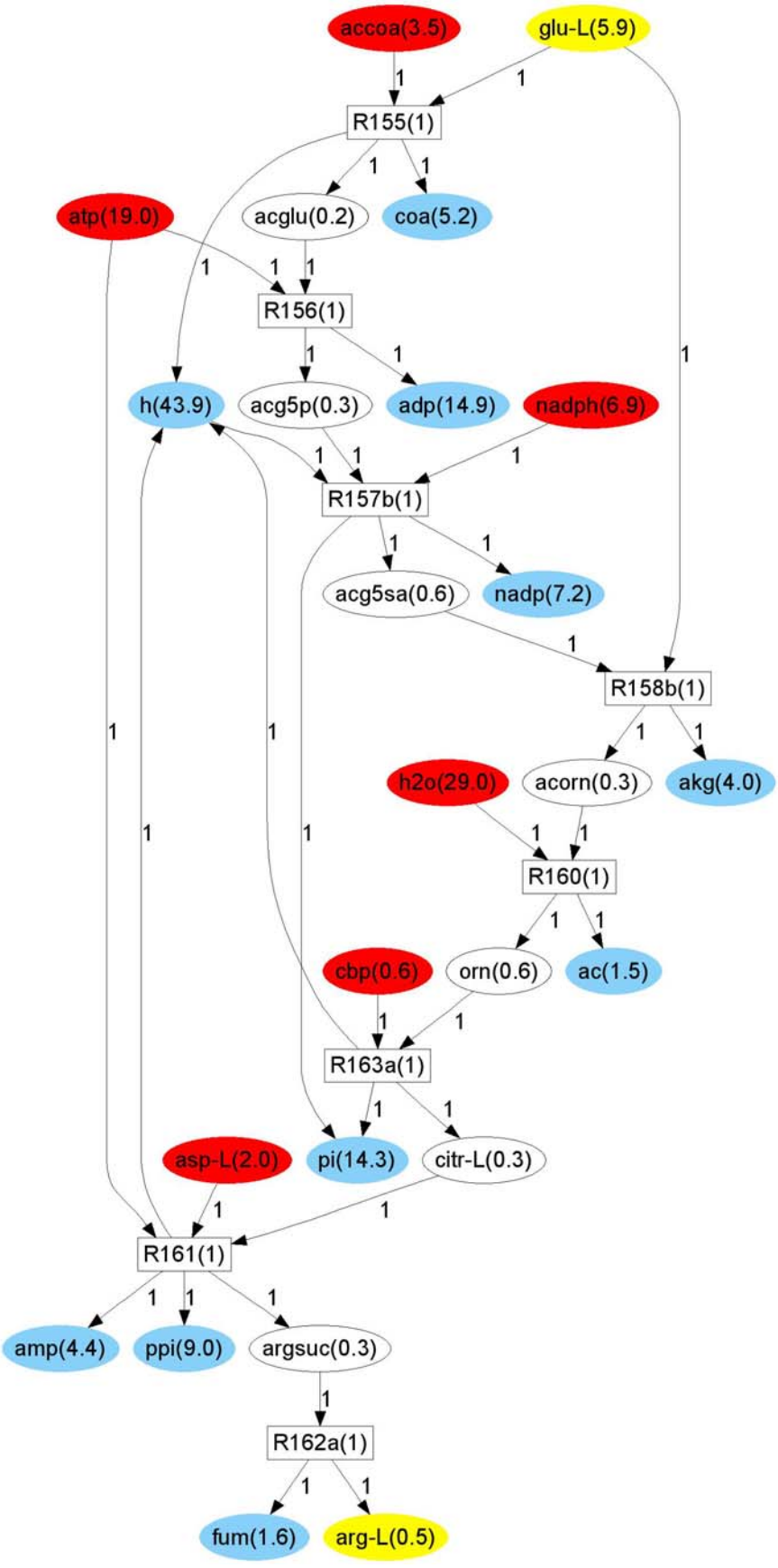
Pathway description

This pathway has been taken from EcoCyc (http://biocyc.org/ECOLI/NEW-IMAGE?type=PATHWAY&object=ARGSYN-PWY) and Lehninger (fourth edition) pages 842 and 843.

In Lehninger the pathway is described as being from two molecules of L-Glutamate to one molecule of L-Arginine. This pathway is described in the same way in EcoCyc with the same set of reactions, except that EcoCyc includes one additional reaction to produce carbamoyl phosphate (cbp).

Since the Lehninger description appears to be the clearer one it is that which has informed the pathway picture seen below.

Note that although 2-Oxoglutarate (akg) is shown below as having a percentage presence of 4.0 (which implies that it is a high presence compound) this is the result of rounding. The actual percentage presence value for this compound is 3.98% and so it is classed as a low presence compound.


accoa(3.5)
glu-L(5.9)
R155(1)
atp(19.0)
acglu(0.2)
coa(5.2)
R156(1)
h(43.9)
acg5p(0.3)
adp(14.9)
nadph(6.9)
R157b(1)
acg5sa(0.6)
nadp(7.2)
R158b(1)
h2o(29.0)
acorn(0.3)
akg(4.0)
R160(1)
cbp(0.6)
orn(0.6)
ac(1.5)
R163a(1)
asp-L(2.0)
pi(14.3)
citr-L(0.3)
R161(1)
amp(4.4)
ppi(9.0)
argsuc(0.3)
R162a(1)
fum(1.6)
arg-L(0.5)

(Q_S,Q_T) discussion for the BP model

This pathway was recovered with objective (3.13). Thus, the (Q_S,Q_T) discussion is carried out for objective (3.13). The table of pairs for objective (3.13) is shown below.

(number of reactions, excess ATP)		Number of molecules Q_T of target compound					
		1	2	3	4	5	6
Number of molecules Q_S of source compound	1	X	X	X	X	X	X
	2	(8,-2)*	X	X	X	X	X
	3	(11,-2)	X	X	X	X	X
	4	(12,-4)	(8,-4)	X	X	X	X
	5	(12,-5)	(11,-6)	X	X	X	X
	6	(12,-6)	(11,-4)	(8,-6)	X	X	X

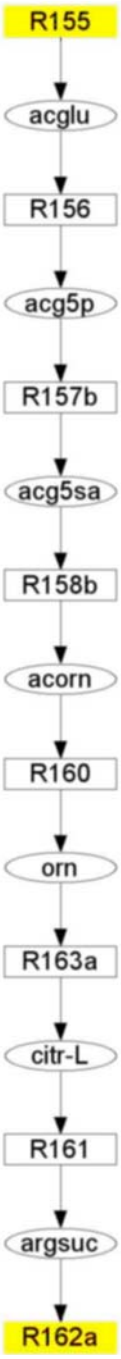
The dominant pair is (Q_S,Q_T)=(2,1). Hence in this case the BP model recovers the (Q_S,Q_T)=(2,1) pair observed in the experimentally determined pathway.

Metabolic path for the R-R case: correspondence values

For this pathway we have the source compound being involved in two reactions, R155 and R158b. Hence for the R-R case below we have two metabolic paths, one from R155 to R162a, the other from R158b to R162a.

k shortest path k	True positives (TP)	False positives (FP)	False negatives (FN)	Sensitivity (Sn)	Positive predictive value (PPV)	Accuracy (Ac)
1	7	0	0	1	1	1
2	5	18	2	0.714	0.217	0.466
3	7	10	0	1	0.412	0.706
4	5	16	2	0.714	0.238	0.476
5	5	20	2	0.714	0.200	0.457
6	5	16	2	0.714	0.238	0.476
7	5	16	2	0.714	0.238	0.476
8	2	9	5	0.286	0.182	0.234
9	7	12	0	1	0.368	0.684
10	5	20	2	0.714	0.200	0.457

Metabolic path for the R-R case: correspondence values



k shortest path k	True positives (TP)	False positives (FP)	False negatives (FN)	Sensitivity (Sn)	Positive predictive value (PPV)	Accuracy (Ac)
1	13	0	0	1	1	1
2	4	7	9	0.308	0.364	0.336
3	7	16	6	0.538	0.304	0.421
4	11	18	2	0.846	0.379	0.613
5	13	10	0	1	0.565	0.783
6	13	6	0	1	0.684	0.842
7	11	20	2	0.846	0.355	0.600
8	11	16	2	0.846	0.407	0.627
9	11	16	2	0.846	0.407	0.627
10	11	16	2	0.846	0.407	0.627

Metabolic path for the C-C case: correspondence values

k shortest path k	True positives (TP)	False positives (FP)	False negatives (FN)	Sensitivity (Sn)	Positive predictive value (PPV)	Accuracy (Ac)
1	9	0	0	1	1	1
2	3	2	6	0.333	0.600	0.467
3	5	4	4	0.556	0.556	0.556
4	9	6	0	1	0.600	0.800
5	3	6	6	0.333	0.333	0.333
6	3	8	6	0.333	0.273	0.303
7	3	10	6	0.333	0.231	0.282
8	5	4	4	0.556	0.556	0.556
9	5	12	4	0.556	0.294	0.425
10	3	10	6	0.333	0.231	0.282

(Q_S,Q_T) discussion for the IBP model

This pathway was recovered with objective (6.26). Thus, the (Q_S,Q_T) discussion is carried out for objective (6.26). The table of pairs for objective (6.26) is shown below.

(Ψ,W)		Number of molecules Q_T of target compound					
		1	2	3	4	5	6
Number of molecules Q_S of source compound	1	(7.17,3)*	(11.59,3)	(11.59,3)	(11.59,3)	(11.59,3)	(11.59,3)
	2	(8.33,4)	(7.17,3)	(11.06,4)	(11.16,3)	(11.06,4)	(11.06,4)
	3	(7.75,4)	(9.38,3)	(7.17,3)	(11.06,4)	(11.06,4)	(11.06,4)
	4	(9.38,3)	(8.33,4)	(9.38,3)	(7.17,3)	(11.06,4)	(11.16,3)
	5	(9.38,3)	(9.38,3)	(9.38,3)	(9.38,3)	(7.17,3)	(11.06,4)
	6	(9.38,3)	(7.75,4)	(8.33,4)	(9.38,3)	(9.38,3)	(7.17,3)

For this pathway the IBP model indicates that the pair (Q_S,Q_T)=(1,1) dominates all other cases. This is indicated by the * superscript. Hence in this case the IBP model does not recover the (Q_S,Q_T)=(2,1) pair observed in the experimentally determined pathway.

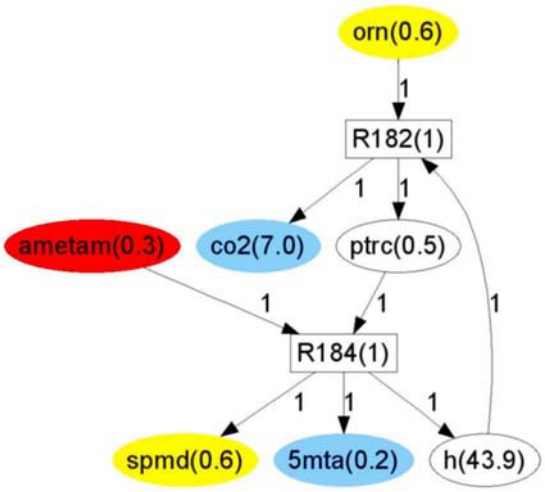
Pathway 11: Sperdimine biosynthesis

Source compound	Ornithine (orn)
Target compound	Spermidine (spmd)
(Q_S,Q_T)	(1,1)
Low presence compounds that are not forced to be balanced	5-Methylthioadenosine (5mta) S-Adenosylmethioninamine (ametam)
(Number of reactions, excess ATP)	(2,0)
Number of unbalanced main compounds (W)	2
Specificity (Ψ)	2.89

Pathway description

This pathway has been taken from EcoCyc (http://biocyc.org/ECOLI/NEW-IMAGE?type=PATHWAY&object=BSUBPOLYAMSYN-PWY) and Lehninger (fourth edition) pages 860 and 861.

In Lehninger the pathway is described as being from one molecule of Ornithine to one molecule of Spermidine. On the other hand, EcoCyc presents two different alternative pathways to synthesise sperdimine, one of them being identical to Lehninger. It is that which has informed the pathway picture seen below.



Note here that we have one allowable c-cycle (see Chapter 3) in this pathway. More precisely the 2-cycle ptrc-R184-h-R182-ptrc which contains one high presence balanced compound (h).

(Q_S,Q_T) discussion for the BP model

This pathway was recovered with both objective (3.13) and objective (3.14). Thus, the (Q_S,Q_T) discussion is carried out for objective (3.13) and objective (3.14). The table of pairs for objective (3.13) is shown below.

(number of reactions, excess ATP)		Number of molecules Q_T of target compound					
		1	2	3	4	5	6
Number of molecules Q_S of source compound	1	(2,0)*	X	X	X	X	X
	2	(11,-3)	(2,0)	X	X	X	X
	3	(11,-6)	(11,-3)	(2,0)	X	X	X
	4	(11,-9)	(11,-6)	(11,-3)	(2,0)	X	X
	5	(11,-12)	(11,-9)	(11,-6)	(11,-3)	(2,0)	X
	6	(11,-15)	(11,-12)	(11,-9)	(11,-6)	(11,-3)	(2,0)

The pairs seen down the diagonal are all repeats of each other, doubling and then tripling, etc the number of source and target molecules. The dominant pair is (Q_S,Q_T)=(1,1). Hence in this case the BP model recovers the (Q_S,Q_T)=(1,1) pair observed in the experimentally determined pathway.

The results for objective (3.14) are shown below.

(number of reactions, excess ATP)		Number of molecules Q_T of target compound					
		1	2	3	4	5	6
Number of molecules Q_S of source compound	1	(2,0)*	X	X	X	X	X
	2	(12,0)	(2,0)	X	X	X	X
	3	(12,0)	(12,0)	(2,0)	X	X	X
	4	(12,0)	(12,0)	(12,0)	(2,0)	X	X
	5	(12,0)	(12,0)	(12,0)	(12,0)	(2,0)	X
	6	(12,0)	(12,0)	(12,0)	(12,0)	(12,0)	(2,0)

The pairs seen down the diagonal are all repeats of each other, doubling and then tripling, etc the number of source and target molecules. The dominant pair is $(Q_S,Q_T)=(1,1)$. Hence in this case the BP model recovers the $(Q_S,Q_T)=(1,1)$ pair observed in the experimentally determined pathway.

(Q_S,Q_T) discussion for the IBP model

This pathway was recovered with both objective (6.26) and objective (6.27). Thus, the (Q_S,Q_T) discussion is carried out for objective (6.26) and objective (6.27). The table of pairs for objective (6.26) is shown below.

(Ψ,W)		Number of molecules Q_T of target compound					
		1	2	3	4	5	6
Number of molecules Q_S of source compound	1	(2.89,2)*	(12.22,6)	(13.63,10)	(13.89,9)	(14.72,9)	(14.72,9)
	2	(8.43,6)	(2.89,2)	(13.1,10)	(12.22,6)	(13.1,10)	(13.73,9)
	3	(10.83,4)	(7.55,5)	(2.89,2)	(12.03,7)	(13.1,10)	(12.22,6)
	4	(10.43,8)	(8.43,6)	(10.43,8)	(2.89,2)	(12.03,7)	(12.03,7)
	5	(10.43,8)	(10.53,7)	(10.43,8)	(10.43,8)	(2.89,2)	(12.03,7)
	6	(10.43,8)	(10.83,4)	(8.43,6)	(7.55,5)	(10.43,8)	(2.89,2)

For this pathway the IBP model indicates that the pair (Q_S,Q_T)=(1,1) dominates all other cases. Hence in this case the IBP model recovers the (Q_S,Q_T)=(1,1) pair observed in the experimentally determined pathway.

The results for objective (6.27) are shown below.

(L,W)		Number of molecules Q_T of target compound					
		1	2	3	4	5	6
Number of molecules Q_S of source compound	1	(2,2)*	(9,6)	(13,6)	(13,9)	(14,7)	(15,7)
	2	(12,8)	(2,2)	X	(9,6)	(14,8)	(14,6)
	3	(12,5)	(10,5)	(2,2)	(13,5)	X	(9,6)
	4	(11,5)	(12,5)	(12,5)	(2,2)	(13,6)	(13,5)
	5	(12,6)	(12,5)	(12,5)	(12,5)	(2,2)	(13,5)
	6	(12,6)	(12,5)	(12,3)	(10,5)	(12,6)	(2,2)

We obtain the same dominant pair as objective (6.26). Hence for this objective the IBP model recovers the $(Q_S,Q_T)=(1,1)$ pair observed in the experimentally determined pathway.

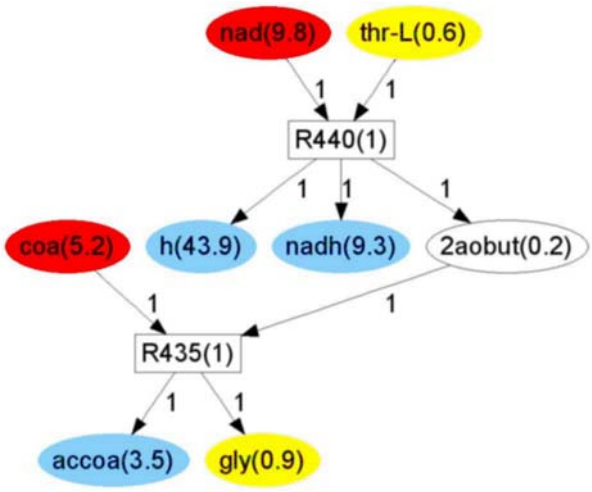
Pathway 12: Threonine degradation to synthesise glycine

Source compound	L-Threonine (thr-L)
Target compound	Glycine (gly)
(Q_S,Q_T)	(1,1)
Low presence compounds that are not forced to be balanced	Acetyl-Coa (accoa)
(Number of reactions, excess ATP)	(2,0)
Number of unbalanced main compounds (W)	0
Specificity (Ψ)	2

Pathway description

This pathway has been taken from EcoCyc (http://biocyc.org/ECOLI/NEW-IMAGE?type=PATHWAY&object=THREOCAT-PWY) and Lehninger (fourth edition) pages 675, 677 and 682.

In Lehninger the pathway is described as being from one molecule of L-Threonine to one molecule of Glycine. On the other hand, EcoCyc presents seven different alternative pathways to degrade L-Threonine, one of them being identical to Lehninger. It is that which has informed the pathway picture seen below.



(Q_S,Q_T) discussion for the BP model

This pathway was recovered with both objective (3.13) and objective (3.14). Thus, the (Q_S,Q_T) discussion is carried out for objective (3.13) and objective (3.14). The table of pairs for objective (3.13) is shown below.

(number of reactions, excess ATP)		Number of molecules Q_T of target compound					
		1	2	3	4	5	6
Number of molecules Q_S of source compound	1	(2,0)*	X	X	X	X	X
	2	X	(2,0)	X	X	X	X
	3	X	X	(2,0)	X	X	X
	4	X	X	X	(2,0)	X	X
	5	X	X	X	X	(2,0)	X
	6	X	X	X	X	X	(2,0)

The pairs seen down the diagonal are all repeats of each other, doubling and then tripling, etc the number of source and target molecules. The dominant pair is (Q_S,Q_T)=(1,1). Hence in this case the BP model recovers the (Q_S,Q_T)=(1,1) pair observed in the experimentally determined pathway.

The results for objective (3.14) are shown below.

(number of reactions, excess ATP)		Number of molecules Q_T of target compound					
		1	2	3	4	5	6
Number of molecules Q_S of source compound	1	(2,0)*	X	X	X	X	X
	2	X	(2,0)	X	X	X	X
	3	X	X	(2,0)	X	X	X
	4	X	X	X	(2,0)	X	X
	5	X	X	X	X	(2,0)	X
	6	X	X	X	X	X	(2,0)

The pairs seen down the diagonal are all repeats of each other, doubling and then tripling, etc the number of source and target molecules. The dominant pair is $(Q_S,Q_T)=(1,1)$. Hence in this case the BP model recovers the $(Q_S,Q_T)=(1,1)$ pair observed in the experimentally determined pathway.

(Q_S,Q_T) discussion for the IBP model

This pathway was recovered with both objective (6.26) and objective (6.27). Thus, the (Q_S,Q_T) discussion is carried out for objective (6.26) and objective (6.27). The table of pairs for objective (6.26) is shown below.

(Ψ,W)		Number of molecules Q_T of target compound					
		1	2	3	4	5	6
Number of molecules Q_S of source compound	1	(2,0)*	(8.81,4)	(8.81,4)	(8.81,4)	(8.81,4)	(8.81,4)
	2	(8.81,4)	(2,0)	(6.17,4)	(6.17,4)	(6.17,4)	(6.17,4)
	3	(8.81,4)	(6.17,4)	(2,0)	(6.17,4)	(6.17,4)	(6.17,4)
	4	(8.81,4)	(6.17,4)	(6.17,4)	(2,0)	(6.17,4)	(6.17,4)
	5	(8.81,4)	(6.17,4)	(6.17,4)	(6.17,4)	(2,0)	(6.17,4)
	6	(8.81,4)	(6.17,4)	(6.17,4)	(6.17,4)	(6.17,4)	(2,0)

For this pathway the IBP model indicates that the pair (Q_S,Q_T)=(1,1) dominates all other cases. Hence in this case the IBP model recovers the (Q_S,Q_T)=(1,1) pair observed in the experimentally determined pathway.

The results for objective (6.27) are shown below.

(L,W)		Number of molecules Q_T of target compound					
		1	2	3	4	5	6
Number	1	(2,0)*	(8,4)	(8,4)	(8,4)	(8,4)	(8,4)
of	2	(8,4)	(2,0)	(8,4)	(8,4)	(8,4)	(8,4)
molecules	3	(8,4)	(8,4)	(2,0)	(8,4)	(8,4)	(8,4)
Q_S of	4	(8,4)	(8,4)	(8,4)	(2,0)	(8,4)	(8,4)
source	5	(8,4)	(8,4)	(8,4)	(8,4)	(2,0)	(8,4)
compound	6	(8,4)	(8,4)	(8,4)	(8,4)	(8,4)	(2,0)

We obtain the same dominant pair as objective (6.26). Hence for this objective the IBP model recovers the $(Q_S,Q_T)=(1,1)$ pair observed in the experimentally determined pathway.

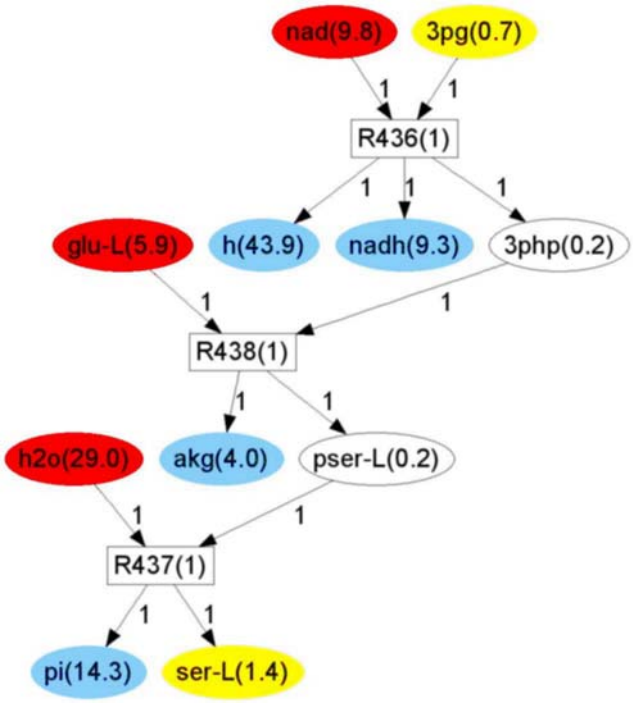
Pathway 13: Serine biosynthesis

Source compound	3-Phospho-D-glycerate (3pg)
Target compound	L-Serine (ser-L)
(Q_S,Q_T)	(1,1)
Low presence compounds that are not forced to be balanced	2-Oxoglutarate (akg)
(Number of reactions, excess ATP)	(3,0)
Number of unbalanced main compounds (W)	0
Specificity (Ψ)	3

Pathway description

This pathway has been taken from EcoCyc (http://biocyc.org/ECOLI/NEW-IMAGE?type=PATHWAY&object=SERSYN-PWY) and Lehninger (fourth edition) page 844.

Both in EcoCyc and Lehninger the pathway is described as being from one molecule of 3-Phospho-D-glycerate to one molecule of L-serine. The set of reactions is also the same in both EcoCyc and Lehninger.



(Q_S,Q_T) discussion for the BP model

This pathway was recovered with both objective (3.13) and objective (3.14). Thus, the (Q_S,Q_T) discussion is carried out for objective (3.13) and objective (3.14). The table of pairs for objective (3.13) is shown below.

(number of reactions, excess ATP)		Number of molecules Q_T of target compound					
		1	2	3	4	5	6
Number of molecules Q_S of source compound	1	(3,0)*	X	X	X	X	X
	2	(8,0)	(3,0)	X	X	X	X
	3	(8,0)	(8,0)	(3,0)	X	X	X
	4	(8,0)	(8,0)	(8,0)	(3,0)	X	X
	5	(8,0)	(8,0)	(8,0)	(8,0)	(3,0)	X
	6	(8,0)	(8,0)	(8,0)	(8,0)	(8,0)	(3,0)

The pairs seen down the diagonal are all repeats of each other, doubling and then tripling, etc the number of source and target molecules. The dominant pair is (Q_S,Q_T)=(1,1). Hence in this case the BP model recovers the (Q_S,Q_T)=(1,1) pair observed in the experimentally determined pathway.

The results for objective (3.14) are shown below.

(number of reactions, excess ATP)		Number of molecules Q_T of target compound					
		1	2	3	4	5	6
Number of molecules Q_S of source compound	1	(3,0)	X	X	X	X	X
	2	(8,0)	(3,0)	X	X	X	X
	3	(13,1)*	(8,0)	(3,0)	X	X	X
	4	(8,0)	(8,0)	(8,0)	(3,0)	X	X
	5	(17,1)	(8,0)	(8,0)	(8,0)	(3,0)	X
	6	(8,0)	(13,2)	(8,0)	(8,0)	(8,0)	(3,0)

The pairs seen down the diagonal are all repeats of each other, doubling and then tripling, etc the number of source and target molecules. The dominant pair is $(Q_S,Q_T)=(3,1)$. Hence in this case the BP model does not recover the $(Q_S,Q_T)=(1,1)$ pair observed in the experimentally determined pathway.

(Q_S,Q_T) discussion for the IBP model

This pathway was recovered with both objective (6.26) and objective (6.27). Thus, the (Q_S,Q_T) discussion is carried out for objective (6.26) and objective (6.27). The table of pairs for objective (6.26) is shown below.

(Ψ,W)		Number of molecules Q_T of target compound					
		1	2	3	4	5	6
Number of molecules Q_S of source compound	1	(3,0)*	X	X	X	X	X
	2	X	(3,0)	X	X	X	X
	3	X	X	(3,0)	X	X	X
	4	X	X	X	(3,0)	X	X
	5	X	X	X	X	(3,0)	X
	6	X	X	X	X	X	(3,0)

For this pathway the IBP model indicates that the pair (Q_S,Q_T)=(1,1) dominates all other cases. Hence in this case the IBP model recovers the (Q_S,Q_T)=(1,1) pair observed in the experimentally determined pathway.

The results for objective (6.27) are shown below.

(L,W)		Number of molecules Q_T of target compound					
		1	2	3	4	5	6
Number	1	(3,0)*	X	X	X	X	X
of	2	X	(3,0)	X	X	X	X
molecules	3	X	X	(3,0)	X	X	X
Q_S of	4	X	X	X	(3,0)	X	X
source	5	X	X	X	X	(3,0)	X
compound	6	X	X	X	X	X	(3,0)

We obtain the same dominant pair as objective (6.26). Hence for this objective the IBP model recovers the $(Q_S,Q_T)=(1,1)$ pair observed in the experimentally determined pathway.

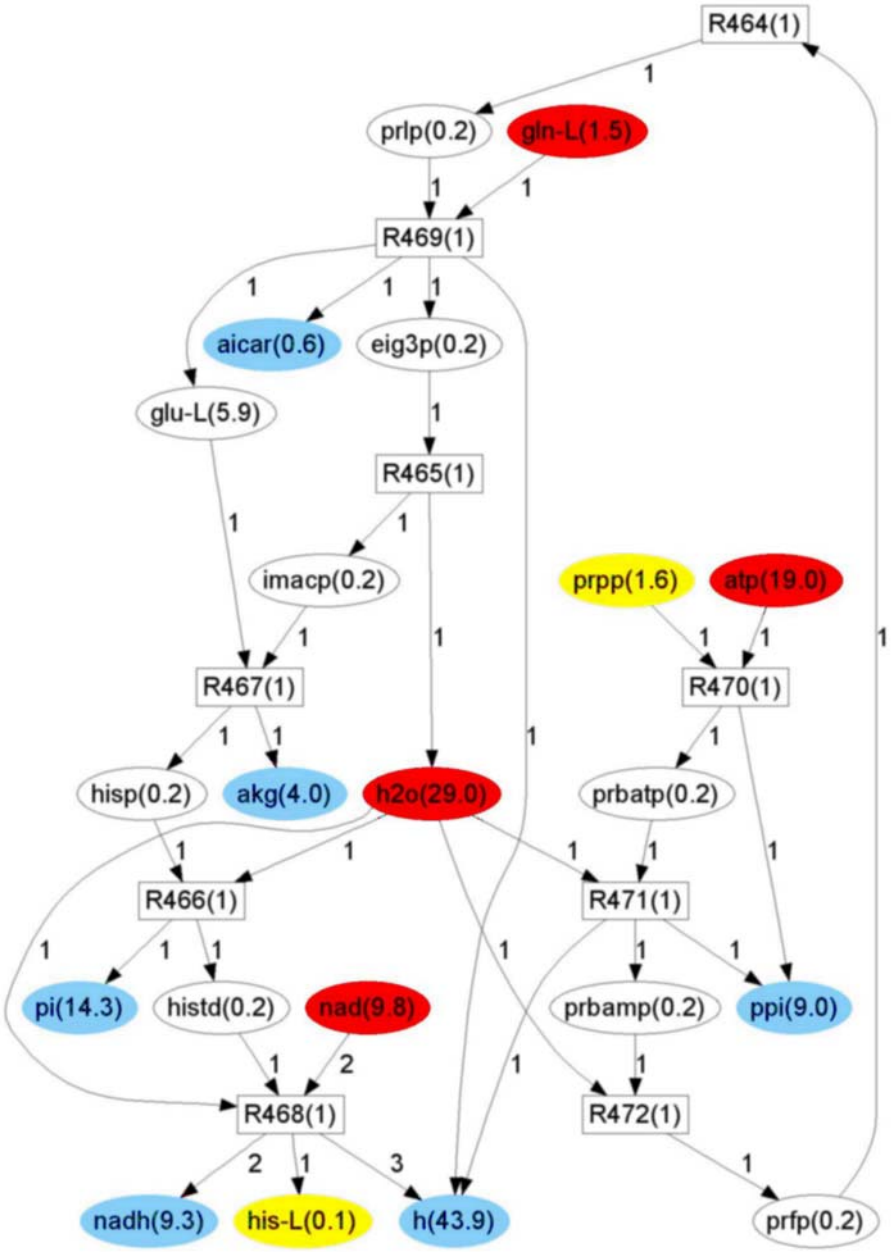
Pathway 14: Histidine biosynthesis

Source compound	5-Phospho-alpha-D-ribose 1-diphosphate (prpp)
Target compound	L-Histidine (his-L)
(Q_S,Q_T)	(1,1)
Low presence compounds that are not forced to be balanced	2-Oxoglutarate (akg) 5-Amino-1-(5-Phospho-D-ribosyl)imidazole-4-carboxamide (aicar) L-Glutamine (gln-L)
(Number of reactions, excess ATP)	(9,-1)
Number of unbalanced main compounds (W)	2
Specificity (Ψ)	9

Pathway description

This pathway has been taken from EcoCyc (http://biocyc.org/ECOLI/NEW-IMAGE?type=PATHWAY&object=HISTSYN-PWY) and Lehninger (fourth edition) page 852.

Both in EcoCyc and Lehninger the pathway is described as being from one molecule of 5-Phospho-alpha-D-ribose 1-diphosphate to one molecule of L-histidine. The set of reactions is also the same in both EcoCyc and Lehninger.


R464(1)
prlp(0.2)
gln-L(1.5)
R469(1)
aicar(0.6)
eig3p(0.2)
glu-L(5.9)
R465(1)
imacp(0.2)
prpp(1.6)
atp(19.0)
R467(1)
R470(1)
hisp(0.2)
akg(4.0)
h2o(29.0)
prbatp(0.2)
R466(1)
R471(1)
pi(14.3)
histd(0.2)
nad(9.8)
prbamp(0.2)
ppi(9.0)
R468(1)
R472(1)
nadh(9.3)
his-L(0.1)
h(43.9)
prfp(0.2)

(Q_S,Q_T) discussion for the BP model

This pathway was recovered with objective (3.13). Thus, the (Q_S,Q_T) discussion is carried out for objective (3.13). The table of pairs for objective (3.13) is shown below.

(number of reactions, excess ATP)		Number of molecules Q_T of target compound					
		1	2	3	4	5	6
Number of molecules Q_S of source compound	1	(9,-1)*	X	X	X	X	X
	2	X	(9,-2)	X	X	X	X
	3	X	X	(9,-3)	X	X	X
	4	X	X	X	(9,-4)	X	X
	5	X	X	X	X	(9,-5)	X
	6	X	X	X	X	X	(9,-6)

The pairs seen down the diagonal are all repeats of each other, doubling and then tripling, etc the number of source and target molecules (and ATP excess). The dominant pair is (Q_S,Q_T)=(1,1). Hence in this case the BP model recovers the (Q_S,Q_T)=(1,1) pair observed in the experimentally determined pathway.

(Q_S,Q_T) discussion for the IBP model

This pathway was recovered with both objective (6.26) and objective (6.27). Thus, the (Q_S,Q_T) discussion is carried out for objective (6.26) and objective (6.27). The table of pairs for objective (6.26) is shown below.

(Ψ,W)		Number of molecules Q_T of target compound					
		1	2	3	4	5	6
Number of molecules Q_S of source compound	1	(9,2)*	(17.5,7)	(17.6,6)	(17.5,7)	(17.5,7)	(17.6,6)
	2	(13.25,6)	(9,2)	(17.5,7)	(17.5,7)	(17.5,7)	(17.5,7)
	3	(13.25,6)	(13.25,6)	(9,2)	(17.5,7)	(17.6,6)	(17.5,7)
	4	(13.25,6)	(13.25,6)	(13.25,6)	(9,2)	(17.5,7)	(17.5,7)
	5	(13.25,6)	(13.25,6)	(13.25,6)	(13.35,5)	(9,2)	(17.5,7)
	6	(13.25,6)	(13.25,6)	(13.25,6)	(13.25,6)	(13.25,6)	(9,2)

For this pathway the IBP model indicates that the pair (Q_S,Q_T)=(1,1) dominates all other cases. Hence in this case the IBP model recovers the (Q_S,Q_T)=(1,1) pair observed in the experimentally determined pathway.

The results for objective (6.27) are shown below.

(L,W)		Number of molecules Q_T of target compound					
		1	2	3	4	5	6
Number of molecules Q_S of source compound	1	(9,2)*	(11,3)	(11,3)	(11,3)	(11,3)	(11,3)
	2	(11,3)	(9,2)	(11,3)	(11,3)	(11,3)	(11,3)
	3	(11,3)	(11,3)	(9,2)	(11,3)	(11,3)	(11,3)
	4	(11,3)	(11,3)	(11,3)	(9,2)	(11,3)	(11,3)
	5	(11,3)	(11,3)	(11,3)	(11,3)	(9,2)	(11,3)
	6	(11,3)	(11,3)	(11,3)	(11,3)	(11,3)	(9,2)

We obtain the same dominant pair as objective (6.26). Hence for this objective the IBP model recovers the $(Q_S,Q_T)=(1,1)$ pair observed in the experimentally determined pathway.

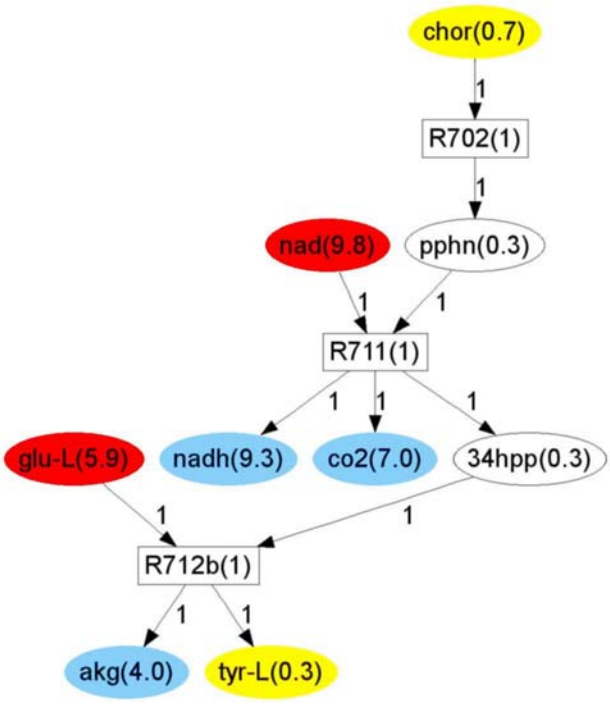
Pathway 15: Tirosine biosynthesis

Source compound	Chorismate (chor)
Target compound	L-Tyrosine (tyr-L)
(Q_S,Q_T)	(1,1)
Low presence compounds that are not forced to be balanced	2-Oxoglutarate (akg)
(Number of reactions, excess ATP)	(3,0)
Number of unbalanced main compounds (W)	0
Specificity (Ψ)	3

Pathway description

This pathway has been taken from EcoCyc (http://biocyc.org/ECOLI/NEW-IMAGE?type=PATHWAY&object=TYRSYN) and Lehninger (fourth edition) page 851.

Both in EcoCyc and Lehninger the pathway is described as being from one molecule of chorismate to one molecule of L-Tyrosine. The set of reactions is also the same in both EcoCyc and Lehninger.



(Q_S,Q_T) discussion for the BP model

This pathway was recovered with both objective (3.13) and objective (3.14). Thus, the (Q_S,Q_T) discussion is carried out for objective (3.13) and objective (3.14). The table of pairs for objective (3.13) is shown below.

(number of reactions, excess ATP)		Number of molecules Q_T of target compound					
		1	2	3	4	5	6
Number of molecules Q_S of source compound	1	(3,0)*	X	X	X	X	X
	2	X	(3,0)	X	X	X	X
	3	X	X	(3,0)	X	X	X
	4	X	X	X	(3,0)	X	X
	5	X	X	X	X	(3,0)	X
	6	X	X	X	X	X	(3,0)

The pairs seen down the diagonal are all repeats of each other, doubling and then tripling, etc the number of source and target molecules. The dominant pair is (Q_S,Q_T)=(1,1). Hence in this case the BP model recovers the (Q_S,Q_T)=(1,1) pair observed in the experimentally determined pathway.

The results for objective (3.14) are presented below.

(number of reactions, excess ATP)		Number of molecules Q_T of target compound					
		1	2	3	4	5	6
Number of molecules Q_S of source compound	1	(3,0)*	X	X	X	X	X
	2	X	(3,0)	X	X	X	X
	3	X	X	(3,0)	X	X	X
	4	X	X	X	(3,0)	X	X
	5	X	X	X	X	(3,0)	X
	6	X	X	X	X	X	(3,0)

The pairs seen down the diagonal are all repeats of each other, doubling and then tripling, etc the number of source and target molecules. The dominant pair is $(Q_S,Q_T)=(1,1)$. Hence in this case the BP model recovers the $(Q_S,Q_T)=(1,1)$ pair observed in the experimentally determined pathway.

(Q_S,Q_T) discussion for the IBP model

This pathway was recovered with both objective (6.26) and objective (6.27). Thus, the (Q_S,Q_T) discussion is carried out for objective (6.26) and objective (6.27). The table of pairs for objective (6.26) is shown below.

(Ψ,W)		Number of molecules Q_T of target compound					
		1	2	3	4	5	6
Number of molecules Q_S of source compound	1	(3,0)*	X	X	X	X	X
	2	X	(3,0)	X	X	X	X
	3	X	X	(3,0)	X	X	X
	4	X	X	(12.44,4)	(3,0)	X	X
	5	(15.03,5)	(12.55,3)	X	(12.44,4)	(3,0)	X
	6	X	(12.55,3)	(17.64,10)	(12.44,4)	(12.49,3)	(3,0)

For this pathway the IBP model indicates that the pair (Q_S,Q_T)=(1,1) dominates all other cases. Hence in this case the IBP model recovers the (Q_S,Q_T)=(1,1) pair observed in the experimentally determined pathway.

The results for objective (6.27) are shown below.

(L,W)		Number of molecules Q_T of target compound					
		1	2	3	4	5	6
Number of molecules Q_S of source compound	1	(3,0)*	X	X	X	X	X
	2	X	(3,0)	X	X	X	X
	3	X	X	(3,0)	X	X	X
	4	X	X	(17,2)	(3,0)	X	X
	5	(15,3)	(18,2)	(17,2)	(17,2)	(3,0)	X
	6	X	(15,3)	(16,3)	(17,2)	(15,3)	(3,0)

We obtain the same dominant pair as objective (6.26). Hence for this objective the IBP model recovers the $(Q_S,Q_T)=(1,1)$ pair observed in the experimentally determined pathway.

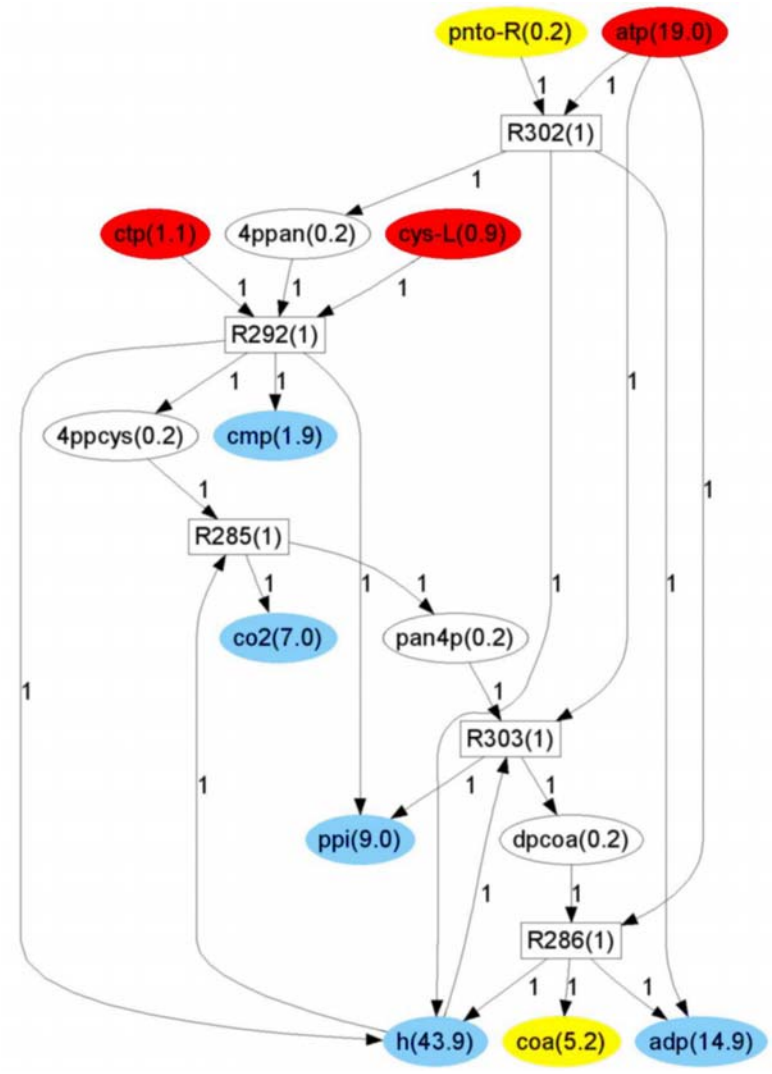
Pathway 16: Coenzyme A biosynthesis

Source compound	(R)-Pantothenate (pnto-R)
Target compound	Coenzyme A (coa)
(Q_S,Q_T)	(1,1)
Low presence compounds that are not forced to be balanced	CTP (ctp) CMP (cmp) L-Cysteine (cys-L)
(Number of reactions, excess ATP)	(5,-3)
Number of unbalanced main compounds (W)	3
Specificity (Ψ)	5

Pathway description

This pathway has been taken from EcoCyc (http://biocyc.org/ECOLI/NEW-IMAGE?type=PATHWAY&object=ARGSYN-PWY).

In EcoCyc the pathway is described as being from one molecule of (R)-Pantothenate to one molecule of Coenzyme A. The same set of reactions is present in our reaction database.



(Q_S,Q_T) discussion for the BP model

This pathway was recovered with objective (3.13). Thus, the (Q_S,Q_T) discussion is carried out for objective (3.13). The table of pairs for objective (3.13) is shown below.

(number of reactions, excess ATP)		Number of molecules Q_T of target compound					
		1	2	3	4	5	6
Number of molecules Q_S of source compound	1	(5,-3)*	X	X	X	X	X
	2	X	(5,-6)	X	X	X	X
	3	X	X	(5,-9)	X	X	X
	4	X	X	X	(5,-12)	X	X
	5	X	X	X	X	(5,-15)	X
	6	X	X	X	X	X	(5,-18)

The pairs seen down the diagonal are all repeats of each other, doubling and then tripling, etc the number of source and target molecules (and excess ATP). The dominant pair is (Q_S,Q_T)=(1,1). Hence in this case the BP model recovers the (Q_S,Q_T)=(1,1) pair observed in the experimentally determined pathway.

(Q_S,Q_T) discussion for the IBP model

This pathway was recovered with both objective (6.26) and objective (6.27). Thus, the (Q_S,Q_T) discussion is carried out for objective (6.26) and objective (6.27). The table of pairs for objective (6.26) is shown below.

(Ψ,W)		Number of molecules Q_T of target compound					
		1	2	3	4	5	6
Number of molecules Q_S of source compound	1	(5,3)*	(15.16,5)	(24.17,16)	X	X	(9.04,4)
	2	(18.39,7)	(5,3)	X	X	(9.06,4)	(9.53,4)
	3	(18.39,7)	(18.39,7)	(5,3)	X	(10.46,4)	X
	4	(18.39,7)	(18.39,7)	(18.29,8)	(5,3)	(8.96,6)	(20.39,11)
	5	(18.29,8)	(18.29,8)	(18.39,7)	(18.29,8)	(5,3)	X
	6	(18.39,7)	(18.39,7)	(18.39,7)	(18.29,8)	(18.39,7)	(5,3)

For this pathway the IBP model indicates that the pair (Q_S,Q_T)=(1,1) dominates all other cases. Hence in this case the IBP model recovers the (Q_S,Q_T)=(1,1) pair observed in the experimentally determined pathway.

The results for objective (6.27) are shown below.

(L,W)		Number of molecules Q_T of target compound					
		1	2	3	4	5	6
Number of molecules Q_S of source compound	1	(5,3)*	(8,7)	(8,7)	(8,7)	(8,7)	(8,7)
	2	(8,7)	(5,3)	(8,7)	(8,7)	(8,7)	(8,7)
	3	(8,7)	(8,7)	(5,3)	(8,7)	(8,7)	(8,7)
	4	(8,7)	(8,7)	(8,7)	(5,3)	(8,7)	(8,7)
	5	(8,7)	(8,7)	(8,7)	(8,7)	(5,3)	(8,7)
	6	(8,7)	(8,7)	(8,7)	(8,7)	(8,7)	(5,3)

We obtain the same dominant pair as objective (6.26). Hence for this objective the IBP model recovers the $(Q_S,Q_T)=(1,1)$ pair observed in the experimentally determined pathway.

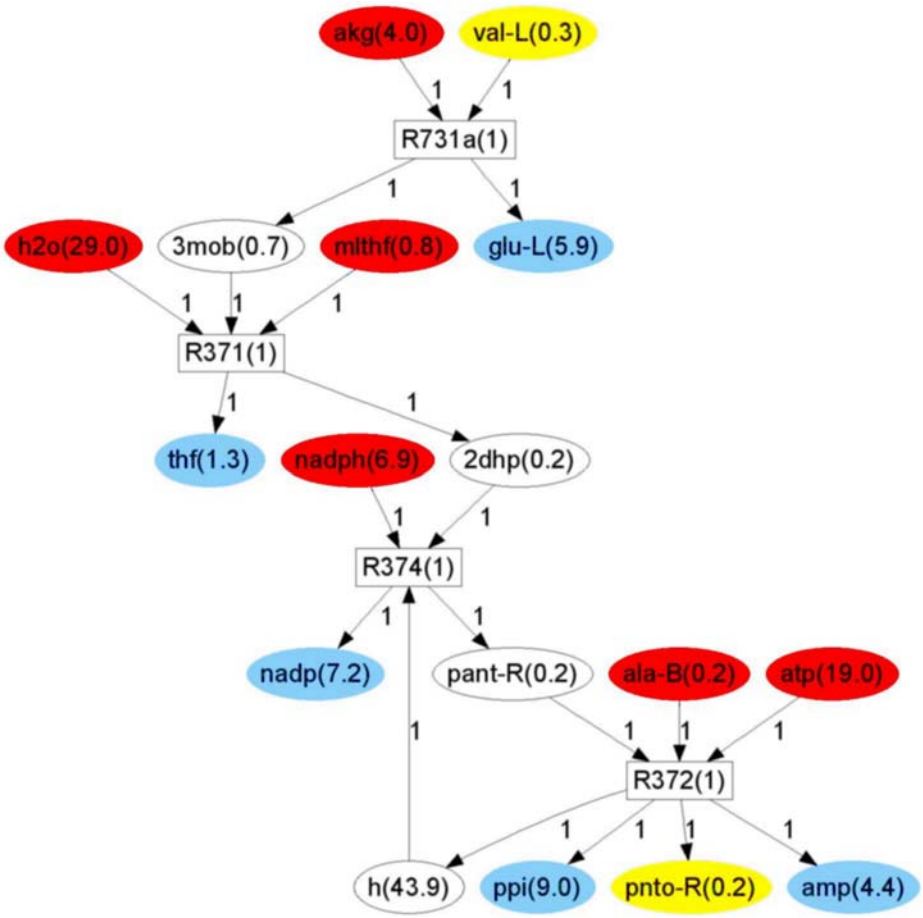
Pathway 17: Pantothenate biosynthesis

Source compound	L-Valine (val-L)
Target compound	(R)-Pantothenate (pnto-R)
(Q_S,Q_T)	(1,1)
Low presence compounds that are not forced to be balanced	2-Oxoglutarate (akg) 5,6,7,8-Tetrahydrofolate (thf) 5,10Methylenetetrahydrofolate (mlthf) beta-Alanine (ala-B)
(Number of reactions, excess ATP)	(4,-1)
Number of unbalanced main compounds (W)	3
Specificity (Ψ)	4

Pathway description

This pathway has been taken from EcoCyc (http://biocyc.org/ECOLI/NEW-IMAGE?type=PATHWAY&object=PANTO-PWY).

In EcoCyc the pathway is described as being from one molecule of L-Valine to one molecule of (R)-Pantothenate. The same set of reactions is present in our reaction database.



Note here that we have one allowable c-cycle in this pathway. More precisely the 2-cycle (pant-R)-R372-h-R374-(pant-R) which contains one high presence balanced compound (h).

(Q_S,Q_T) discussion for the BP model

This pathway was recovered with objective (3.13). Thus, the (Q_S,Q_T) discussion is carried out for objective (3.13). The table of pairs for objective (3.13) is shown below.

(number of reactions, excess ATP)		Number of molecules Q_T of target compound					
		1	2	3	4	5	6
Number of molecules Q_S of source compound	1	(4,-1)*	(7,-2)	(7,-3)	(7,-4)	(7,-5)	(7,-6)
	2	X	(4,-2)	(7,-3)	(7,-4)	(7,-5)	(7,-6)
	3	X	X	(4,-3)	(7,-4)	(7,-5)	(7,-6)
	4	X	X	X	(4,-4)	(7,-5)	(7,-6)
	5	X	X	X	X	(4,-5)	(7,-6)
	6	X	X	X	X	X	(4,-6)

The pairs seen down the diagonal are all repeats of each other, doubling and then tripling, etc the number of source and target molecules (and excess ATP). The dominant pair is (Q_S,Q_T)=(1,1). Hence in this case the BP model recovers the (Q_S,Q_T)=(1,1) pair observed in the experimentally determined pathway.

(Q_S,Q_T) discussion for the IBP model

This pathway was recovered with both objective (6.26) and objective (6.27). Thus, the (Q_S,Q_T) discussion is carried out for objective (6.26) and objective (6.27). The table of pairs for objective (6.26) is shown below.

(Ψ,W)		Number of molecules Q_T of target compound					
		1	2	3	4	5	6
Number of molecules Q_S of source compound	1	(4,3)*	(17.37,11)	(16.3,10)	X	X	X
	2	(16.25,10)	(4,3)	X	X	(16.3,10)	(17.17,10)
	3	(16.28,13)	(16.21,11)	(4,3)	X	X	X
	4	(16.52,13)	(16.25,10)	(16.42,9)	(4,3)	X	(18.19,10)
	5	(16.52,13)	(16.52,13)	(16.42,9)	(16.52,8)	(4,3)	X
	6	(16.62,12)	(17.17,10)	(16.25,10)	X	(16.52,8)	(4,3)

For this pathway the IBP model indicates that the pair (Q_S,Q_T)=(1,1) dominates all other cases. Hence in this case the IBP model recovers the (Q_S,Q_T)=(1,1) pair observed in the experimentally determined pathway.

The results for objective (6.27) are shown below.

(L,W)		Number of molecules Q_T of target compound					
		1	2	3	4	5	6
Number of molecules Q_S of source compound	1	(4,3)*	(15,8)	(15,8)	(15,8)	(15,8)	(15,8)
	2	(14,1)	(4,3)	(12,1)	(12,1)	X	X
	3	(24,6)	(14,1)	(4,3)	(12,1)	X	X
	4	(14,1)	(14,1)	(14,1)	(4,3)	(13,1)	X
	5	X	(14,1)	X	(14,1)	(4,3)	(13,1)
	6	(14,1)	X	X	(15,1)	(14,1)	(4,3)

We obtain the same dominant pair as objective (6.26). Hence for this objective the IBP model recovers the $(Q_S,Q_T)=(1,1)$ pair observed in the experimentally determined pathway.

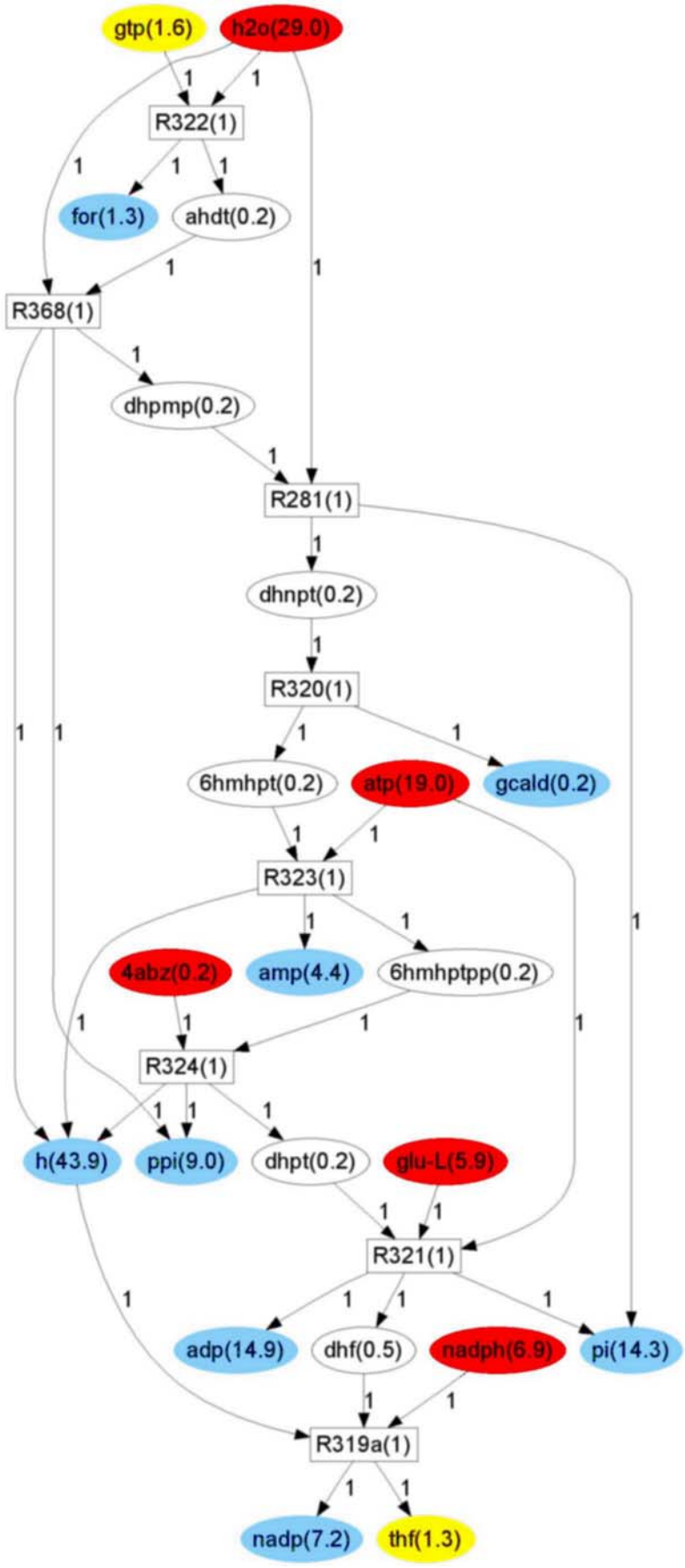
Pathway 18: Tetrahydrofolate biosynthesis

Source compound	GTP (gtp)
Target compound	5,6,7,8-Tetrahydrofolate (thf)
(Q_S,Q_T)	(1,1)
Low presence compounds that are not forced to be balanced	4-Aminobenzoate (4abz) Formate (for) Glycolaldehyde (gcald)
(Number of reactions, excess ATP)	(8,-2)
Number of unbalanced main compounds (W)	3
Specificity (Ψ)	8

Pathway description

This pathway has been taken from EcoCyc (http://biocyc.org/ECOLI/NEW-IMAGE?type=PATHWAY&object=FOLSYN-PWY) and Lehninger (fourth edition) pages 672 and 673.

In EcoCyc the pathway is described as being from one molecule of GTP to one molecule of 5,6,7,8-Tetrahydrofolate. The same set of reactions is present in our reaction database. Precursors of this pathway are explained in Lehninger.


gtp(1.6)
h2o(29.0)
R322(1)
for(1.3)
ahdt(0.2)
R368(1)
dhpmp(0.2)
R281(1)
dhnpt(0.2)
R320(1)
6hmhpt(0.2)
atp(19.0)
gcald(0.2)
R323(1)
4abz(0.2)
amp(4.4)
6hmhptpp(0.2)
R324(1)
h(43.9)
ppi(9.0)
dhpt(0.2)
glu-L(5.9)
R321(1)
adp(14.9)
dhf(0.5)
nadph(6.9)
pi(14.3)
R319a(1)
nadp(7.2)
thf(1.3)

(Q_S,Q_T) discussion for the BP model

This pathway was recovered with objective (3.13). Thus, the (Q_S,Q_T) discussion is carried out for objective (3.13). The table of pairs for objective (3.13) is shown below.

		Number of molecules Q_T of target compound					
		1	2	3	4	5	6
Number of molecules Q_S of source compound	1	(8,-2)*	X	X	X	X	X
	2	X	(8,-4)	X	X	X	X
	3	X	X	(8,-6)	X	X	X
	4	X	X	X	(8,-8)	X	X
	5	X	X	X	X	(8,-10)	X
	6	X	X	X	X	X	(8,-12)

The pairs seen down the diagonal are all repeats of each other, doubling and then tripling, etc the number of source and target molecules (and excess ATP). The dominant pair is (Q_S,Q_T)=(1,1). Hence in this case the BP model recovers the (Q_S,Q_T)=(1,1) pair observed in the experimentally determined pathway.

(Q_S,Q_T) discussion for the IBP model

This pathway was not recovered with either objective (6.26) or objective (6.27). For this reason (Q_S,Q_T) pairs discussion is omitted for this pathway.

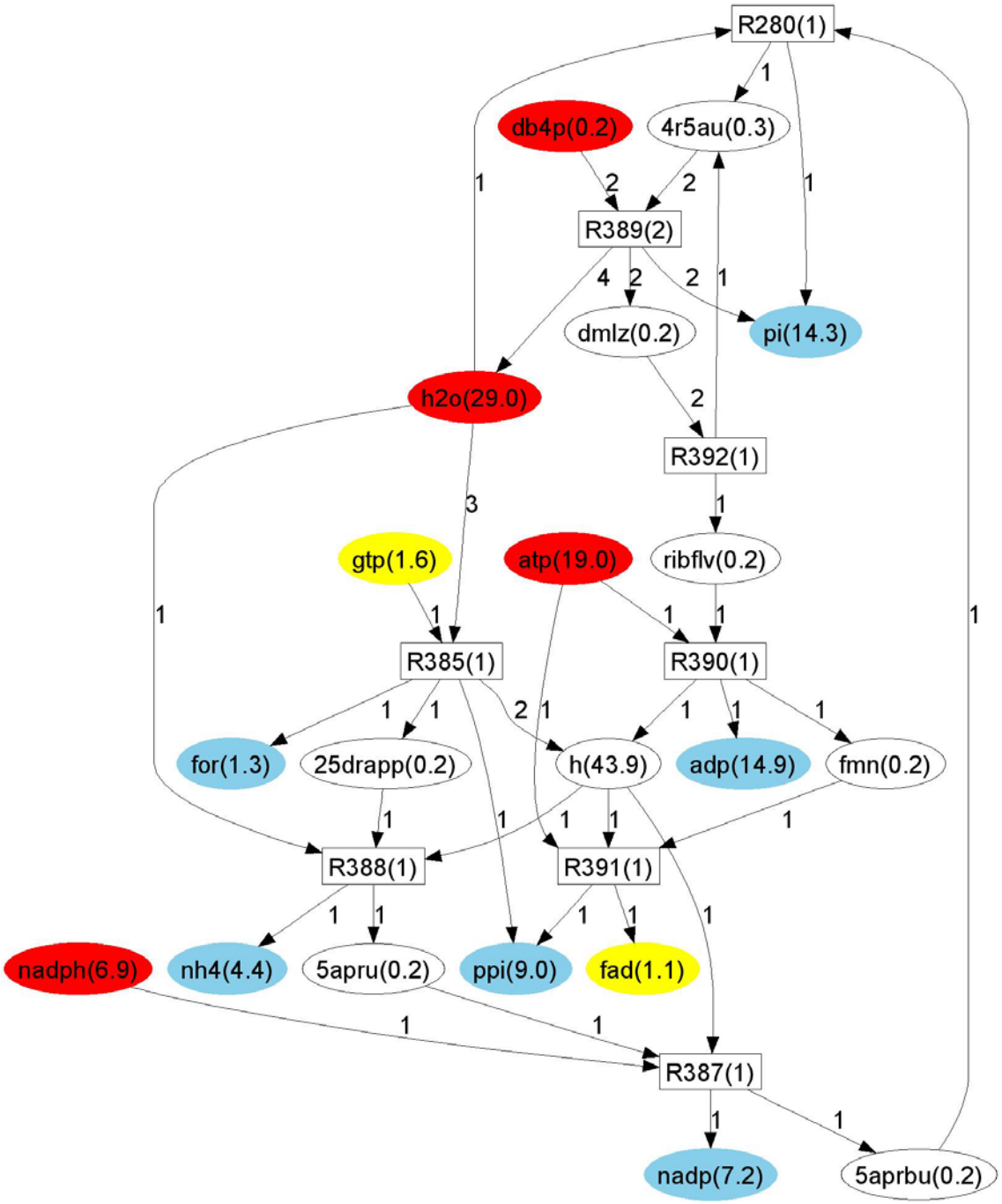
Pathway 19: Riboflavin and FMN and FAD biosynthesis

Source compound	GTP (gtp)
Target compound	FAD (fad)
(Q_S,Q_T)	(1,1)
Low presence compounds that are not forced to be balanced	3,4-dihydroxy-2-butanone 4-phosphate (db4p) Formate (for)
(Number of reactions, excess ATP)	(8,-2)
Number of unbalanced main compounds (W)	2
Specificity (Ψ)	8.23

Pathway description

This pathway has been taken from EcoCyc (http://biocyc.org/ECOLI/NEW-IMAGE?type=PATHWAY&object=RIBOSYN2-PWY).

In EcoCyc the pathway is described as being from one molecule of GTP to one molecule of FAD. The same set of reactions is present in our reaction database.


R280(1)
db4p(0.2)
4r5au(0.3)
R389(2)
dmlz(0.2)
pi(14.3)
h2o(29.0)
R392(1)
gtp(1.6)
atp(19.0)
ribflv(0.2)
R385(1)
R390(1)
for(1.3)
25drapp(0.2)
h(43.9)
adp(14.9)
fmn(0.2)
R388(1)
R391(1)
nadph(6.9)
nh4(4.4)
5apru(0.2)
ppi(9.0)
fad(1.1)
R387(1)
nadp(7.2)
5aprbu(0.2)

(Q_S,Q_T) discussion for the BP model

This pathway was not recovered with either of the objectives. Since this pathway is not recovered, (Q_S,Q_T) pairs discussion is omitted.

(Q_S,Q_T) discussion for the IBP model

This pathway was recovered with both objective (6.26) and objective (6.27). Thus, the (Q_S,Q_T) discussion is carried out for objective (6.26) and objective (6.27). The table of pairs for objective (6.26) is shown below.

(Ψ,W)		Number of molecules Q_T of target compound					
		1	2	3	4	5	6
Number of molecules Q_S of source compound	1	(8.23,2)*	(13.83,5)	(13.83,5)	(13.83,5)	(13.93,4)	(13.83,5)
	2	(10.23,3)	(8.23,2)	(12.03,6)	(12.03,6)	(12.03,6)	(12.03,6)
	3	(9.23,2)	(11.03,4)	(8.23,2)	(12.03,6)	(12.03,6)	(12.03,6)
	4	(11.03,4)	(10.23,3)	(11.03,4)	(8.23,2)	(12.03,6)	(12.03,6)
	5	(11.03,4)	(11.13,3)	(11.03,4)	(11.03,4)	(8.23,2)	(12.03,6)
	6	(11.03,4)	(9.23,2)	(10.23,3)	(11.03,4)	(11.03,4)	(8.23,2)

For this pathway the IBP model indicates that the pair (Q_S,Q_T)=(1,1) dominates all other cases. Hence in this case the IBP model recovers the (Q_S,Q_T)=(1,1) pair observed in the experimentally determined pathway.

The results for objective (6.27) are shown below.

(L,W)		Number of molecules Q_T of target compound					
		1	2	3	4	5	6
Number of molecules Q_S of source compound	1	(8,2)*	(11,5)	(11,5)	(11,5)	(11,5)	(11,5)
	2	(8,5)	(8,2)	(11,5)	(11,5)	(11,5)	(11,5)
	3	(11,5)	(11,5)	(8,2)	(11,5)	(11,5)	(11,5)
	4	(11,5)	(8,5)	(11,5)	(8,2)	(11,5)	(11,5)
	5	(11,5)	(11,5)	(11,5)	(11,5)	(8,2)	(11,5)
	6	(11,5)	(11,5)	(8,5)	(11,5)	(11,5)	(8,2)

We obtain the same dominant pair as objective (6.26). Hence for this objective the IBP model recovers the $(Q_S,Q_T)=(1,1)$ pair observed in the experimentally determined pathway.

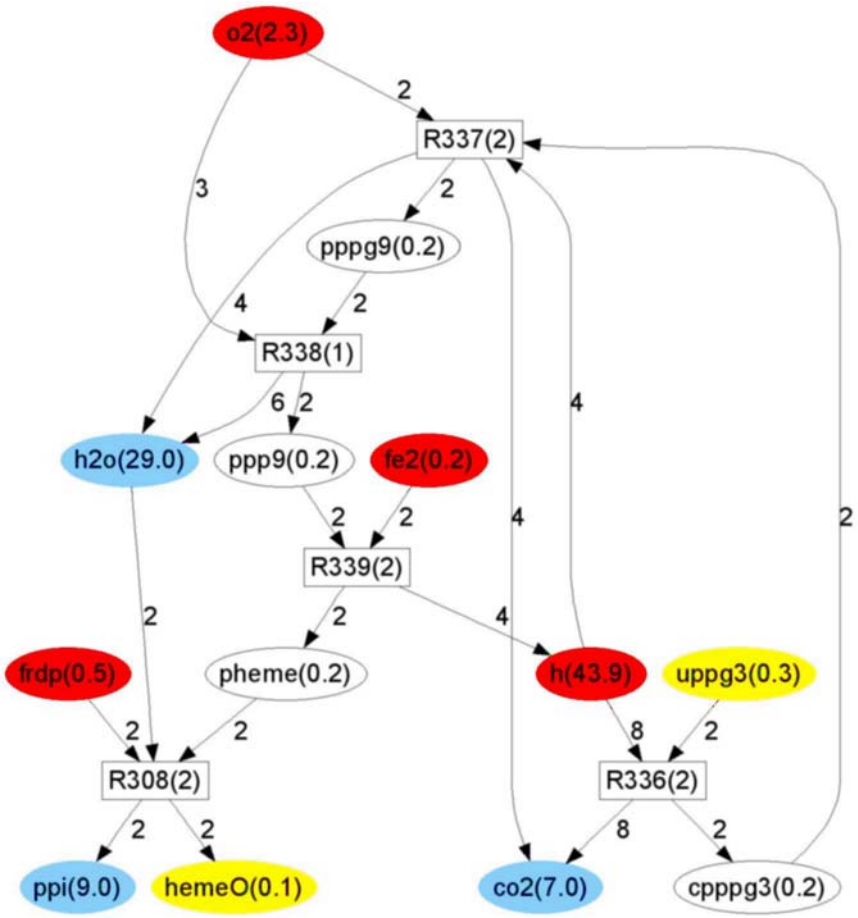
Pathway 20: Heme biosynthesis

Source compound	Uroporphyrinogen III (uppg3)
Target compound	HemeO (hemeO)
(Q_S,Q_T)	(2,2)
Low presence compounds that are not forced to be balanced	O2 (o2) Fe2+ (fe2) Farnesyl diphosphate (frdp)
(Number of reactions, excess ATP)	(5,0)
Number of unbalanced main compounds (W)	1
Specificity (Ψ)	5

Pathway description

This pathway has been taken from EcoCyc (http://biocyc.org/META/NEW-IMAGE?type=PATHWAY&object=HEME+BIOSYNTHESIS+II).

In EcoCyc the pathway is described as being from one molecule of Uroporphyrinogen III to one molecule of HemeO. However, were this to be correct, then R338 would need a non-integer number of molecules of o2 (namely 1.5). In order to avoid this difficulty, we regard the pathway as transforming two molecules of Uroporphyrinogen III to two molecules of HemeO.



(Q_S,Q_T) discussion for the BP model

This pathway was recovered with both objective (3.13) and objective (3.14). Thus, the (Q_S,Q_T) discussion is carried out for objective (3.13) and objective (3.14). The table of pairs for objective (3.13) is shown below.

(number of reactions, excess ATP)		Number of molecules Q_T of target compound					
		1	2	3	4	5	6
Number of molecules Q_S of source compound	1	X	X	X	X	X	X
	2	X	(5,0)*	X	X	X	X
	3	X	X	X	X	X	X
	4	X	X	X	(5,0)	X	X
	5	X	X	X	X	X	X
	6	X	X	X	X	X	(5,0)

The dominant pair is (Q_S,Q_T)=(2,2). Hence in this case the BP model recovers the (Q_S,Q_T)=(2,2) pair observed in the experimentally determined pathway.

On the other hand, results for objective (3.14) are shown below.

(number of reactions, excess ATP)		Number of molecules Q_T of target compound					
		1	2	3	4	5	6
Number of molecules Q_S of source compound	1	X	X	X	X	X	X
	2	X	(5,0)*	X	X	X	X
	3	X	X	X	X	X	X
	4	X	X	X	(5,0)	X	X
	5	X	X	X	X	X	X
	6	X	X	X	X	X	(5,0)

The dominant pair is $(Q_S,Q_T)=(2,2)$. Hence in this case the BP model recovers the $(Q_S,Q_T)=(2,2)$ pair observed in the experimentally determined pathway.

(Q_S,Q_T) discussion for the IBP model

This pathway was recovered with both objective (6.26) and objective (6.27). Thus, the (Q_S,Q_T) discussion is carried out for objective (6.26) and objective (6.27). The table of pairs for objective (6.26) is shown below.

(Ψ,W)		Number of molecules Q_T of target compound					
		1	2	3	4	5	6
Number of molecules Q_S of source compound	1	(19.84,9)	(19.57,9)	(20.82,10)	(20.89,9)	(20.67,9)	(20.67,9)
	2	(19.65,10)	(5,1)*	(19.63,11)	(19.47,10)	(20.7,10)	(20.72,11)
	3	(20.07,9)	(12.23,9)	(19.74,10)	(19.63,11)	(19.63,11)	(19.47,10)
	4	(21.51,9)	(12.5,9)	(19.9,11)	(5,1)	(19.63,11)	(19.63,11)
	5	(21.41,10)	(12.75,8)	(19.65,10)	(13.39,9)	(19.74,10)	(19.63,11)
	6	(21.51,9)	(13.42,8)	(19.65,10)	(12.23,9)	(19.9,11)	(5,1)

For this pathway the IBP model indicates that the pair (Q_S,Q_T)=(2,2) dominates all other cases. Hence in this case the IBP model recovers the (Q_S,Q_T)=(2,2) pair observed in the experimentally determined pathway.

The results for objective (6.27) are shown below.

(L,W)		Number of molecules Q_T of target compound					
		1	2	3	4	5	6
Number of molecules Q_S of source compound	1	(15,8)	(15,0)	(14,9)	(16,8)	(15,8)	(16,0)
	2	(16,8)	(5,1)*	(16,8)	(15,0)	(16,8)	(15,8)
	3	(17,1)	(16,3)	(15,8)	(16,8)	(15,8)	(15,0)
	4	(15,7)	(15,8)	(13,8)	(5,1)	X	(15,8)
	5	X	(16,3)	(15,8)	(16,8)	(15,8)	X
	6	(18,2)	(24,2)	(16,8)	(15,8)	X	(5,1)

We obtain the same dominant pair as objective (6.26). Hence for this objective the IBP model recovers the $(Q_S,Q_T)=(2,2)$ pair observed in the experimentally determined pathway.

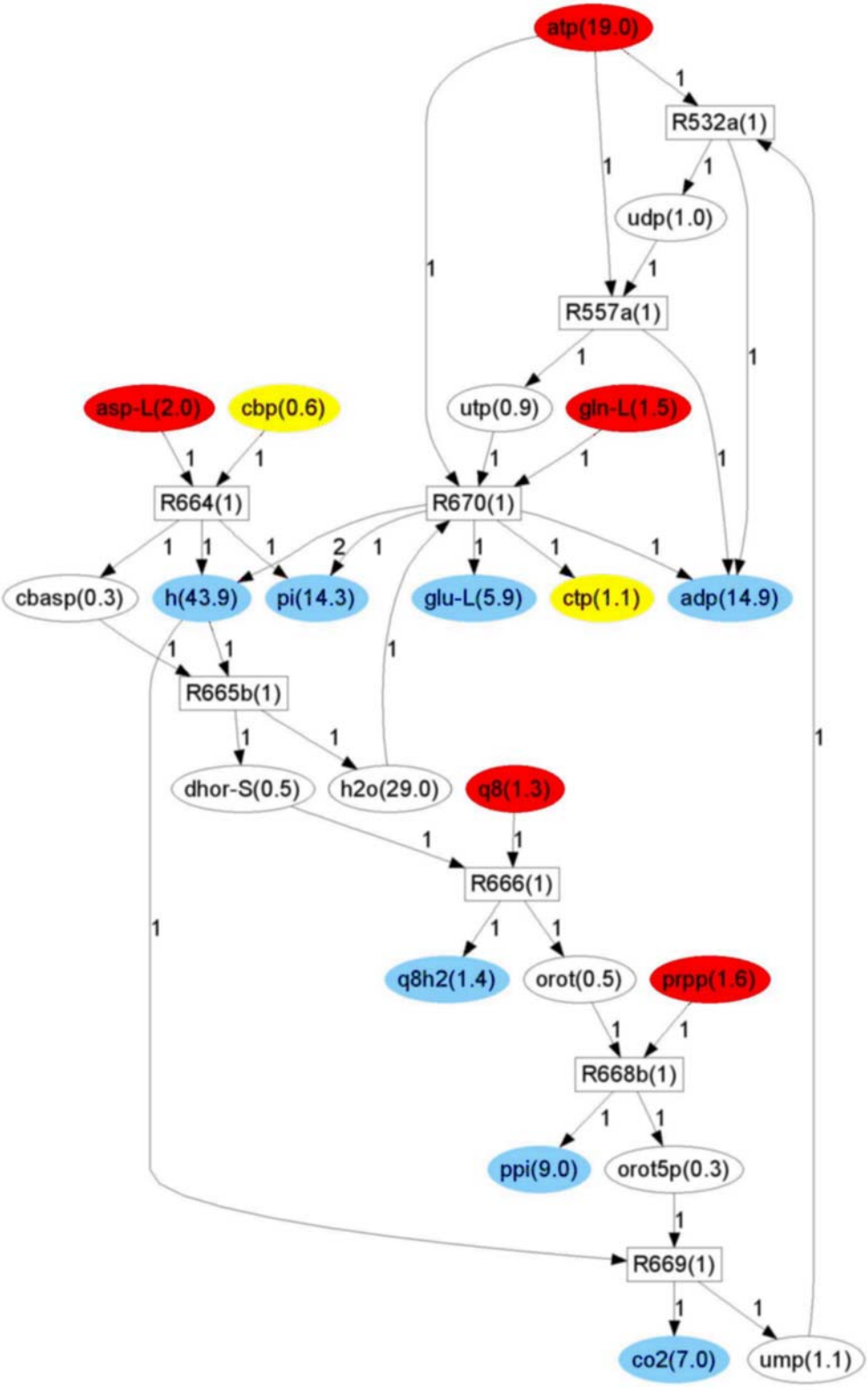
Pathway 21: De novo synthesis of pyrimidine ribonucletides

Source compound	Carbamoyl phosphate (cbp)
Target compound	CTP (ctp)
(Q_S,Q_T)	(1,1)
Low presence compounds that are not forced to be balanced	L-Aspartate (asp-L) L-Glutamine (gln-L) Ubiquinone-8 (q8) Ubiquinol-8 (q8h2) 5-Phospho-alpha-D-ribose 1-diphosphate (prpp)
(Number of reactions, excess ATP)	(8,-3)
Number of unbalanced main compounds (W)	3
Specificity (Ψ)	8

Pathway description

This pathway has been taken from EcoCyc (http://biocyc.org/ECOLI/NEW-IMAGE?type=PATHWAY&object=PWY0-162) and Lehninger (fourth edition) pages 867 and 868.

In Lehninger the pathway is described as being from one molecule of Carbamoyl phosphate to one molecule of CTP. However, this pathway is described in EcoCyc as being from one molecule of CO2 to one molecule of CDP. Since the Lehninger description appears to be the more common one it is that which has informed the pathway picture seen below.


atp(19.0)
R532a(1)
udp(1.0)
R557a(1)
asp-L(2.0)
cbp(0.6)
utp(0.9)
gln-L(1.5)
R664(1)
R670(1)
cbasp(0.3)
h(43.9)
pi(14.3)
glu-L(5.9)
ctp(1.1)
adp(14.9)
R665b(1)
dhor-S(0.5)
h2o(29.0)
q8(1.3)
R666(1)
q8h2(1.4)
orot(0.5)
prpp(1.6)
R668b(1)
ppi(9.0)
orot5p(0.3)
R669(1)
co2(7.0)
ump(1.1)

(Q_S,Q_T) discussion for the BP model

This pathway was recovered with objective (3.13). Thus, the (Q_S,Q_T) discussion is carried out for objective (3.13). The table of pairs for objective (3.13) is shown below.

(number of reactions, excess ATP)		Number of molecules Q_T of target compound					
		1	2	3	4	5	6
Number of molecules Q_S of source compound	1	(8,-3)*	X	X	X	X	X
	2	X	(8,-6)	X	X	X	X
	3	X	X	(8,-9)	X	X	X
	4	X	X	X	(8,-12)	X	X
	5	X	X	X	X	(8,-15)	X
	6	X	X	X	X	X	(8,-18)

The pairs seen down the diagonal are all repeats of each other, doubling and then tripling, etc the number of source and target molecules (and excess ATP). The dominant pair is (Q_S,Q_T)=(1,1). Hence in this case the BP model recovers the (Q_S,Q_T)=(1,1) pair observed in the experimentally determined pathway.

(Q_S,Q_T) discussion for the IBP model

This pathway was recovered with both objective (6.26) and objective (6.27). Thus, the (Q_S,Q_T) discussion is carried out for objective (6.26) and objective (6.27). The table of pairs for objective (6.26) is shown below.

(Ψ,W)		Number of molecules Q_T of target compound					
		1	2	3	4	5	6
Number of molecules Q_S of source compound	1	(8,3)*	(10.56,4)	(10.56,4)	(10.56,4)	(10.56,4)	(10.56,4)
	2	(9.85,5)	(8,3)	(10.56,4)	(10.56,4)	(10.56,4)	(10.56,4)
	3	(9.94,4)	(9.85,5)	(8,3)	(10.56,4)	(10.56,4)	(10.56,4)
	4	(9.85,5)	(9.85,5)	(9.85,5)	(8,3)	(10.56,4)	(10.56,4)
	5	(9.85,5)	(9.94,4)	(9.94,4)	(9.85,5)	(8,3)	(10.56,4)
	6	(9.85,5)	(9.85,5)	(9.85,5)	(9.85,5)	(9.85,5)	(8,3)

For this pathway the IBP model indicates that the pair (Q_S,Q_T)=(1,1) dominates all other cases. Hence in this case the IBP model recovers the (Q_S,Q_T)=(1,1) pair observed in the experimentally determined pathway.

The results for objective (6.27) are shown below.

(L,W)		Number of molecules Q_T of target compound					
		1	2	3	4	5	6
Number of molecules Q_S of source compound	1	(8,3)*	(9,5)	(9,5)	(9,5)	(9,5)	(9,5)
	2	(9,5)	(8,3)	(9,5)	(9,5)	(9,5)	(9,5)
	3	(8,4)	(9,5)	(8,3)	(9,5)	(9,5)	(9,5)
	4	(9,5)	(9,5)	(9,5)	(8,3)	(9,5)	(9,5)
	5	(9,5)	(9,5)	(9,5)	(9,5)	(8,3)	(9,5)
	6	(9,5)	(8,4)	(9,5)	(9,5)	(9,5)	(8,3)

We obtain the same dominant pair as objective (6.26). Hence for this objective the IBP model recovers the $(Q_S,Q_T)=(1,1)$ pair observed in the experimentally determined pathway.

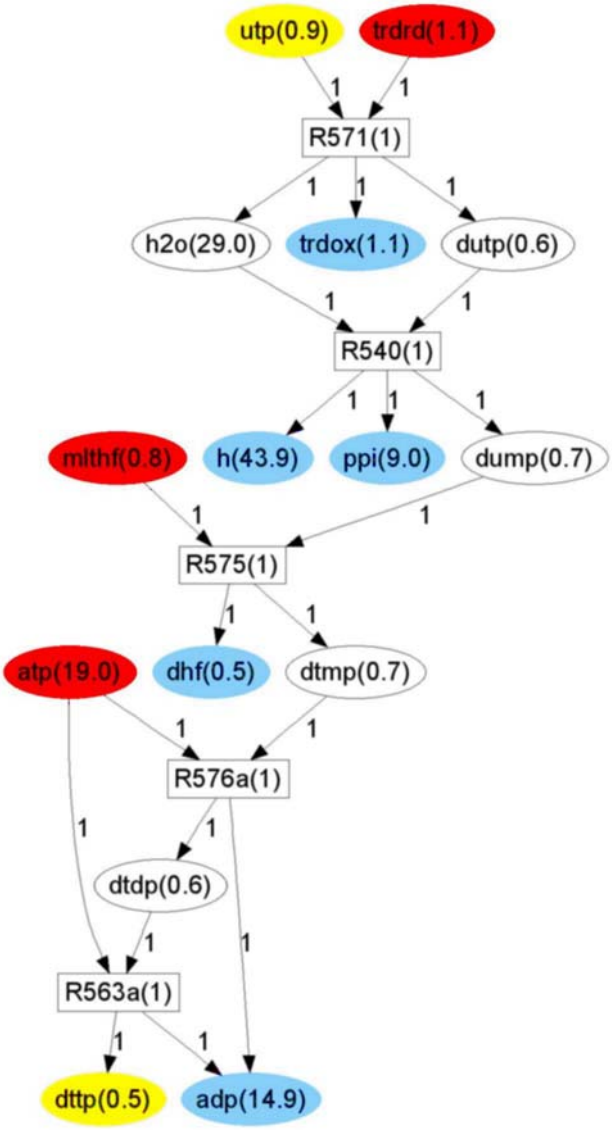
Pathway 22: De novo synthesis of pyrimidine deoxyribonucletides

Source compound	UTP (utp)
Target compound	dTTP (dttp)
(Q_S,Q_T)	(1,1)
Low presence compounds that are not forced to be balanced	7,8-Dihydrofolate (dhf) 5,10-Methylenetetrahydrofolate (mlthf) Oxidized thioredoxin (trdox) Reduced thioredoxin (trdrd)
(Number of reactions, excess ATP)	(5,-2)
Number of unbalanced main compounds (W)	4
Specificity (Ψ)	5.25

Pathway description

This pathway has been taken from EcoCyc (http://biocyc.org/ECOLI/NEW-IMAGE?type=PATHWAY&object=PWY0-166).

In EcoCyC the pathway is described as being from one molecule of UTP to one molecule of dTTP. Our database contains the same set of reactions.



(Q_S,Q_T) discussion for the BP model

This pathway was recovered with objective (3.13). Thus, the (Q_S,Q_T) discussion is carried out for objective (3.13). The table of pairs for objective (3.13) is shown below.

(number of reactions, excess ATP)		Number of molecules Q_T of target compound					
		1	2	3	4	5	6
Number of molecules Q_S of source compound	1	(5,-2)*	X	X	X	X	X
	2	X	(5,-4)	X	X	X	X
	3	X	X	(5,-6)	X	X	X
	4	X	X	X	(5,-8)	X	X
	5	X	X	X	X	(5,-10)	X
	6	X	X	X	X	X	(5,-12)

The pairs seen down the diagonal are all repeats of each other, doubling and then tripling, etc the number of source and target molecules (and excess ATP). The dominant pair is (Q_S,Q_T)=(1,1). Hence in this case the BP model recovers the (Q_S,Q_T)=(1,1) pair observed in the experimentally determined pathway.

(Q_S,Q_T) discussion for the IBP model

This pathway was recovered with both objective (6.26) and objective (6.27). Thus, the (Q_S,Q_T) discussion is carried out for objective (6.26) and objective (6.27). The table of pairs for objective (6.26) is shown below.

(Ψ,W)		Number of molecules Q_T of target compound					
		1	2	3	4	5	6
Number of molecules Q_S of source compound	1	(5.25,4)*	(6.53,3)	(6.53,3)	(6.53,3)	(6.53,3)	(6.53,3)
	2	(7.03,3)	(5.25,4)	(6.53,3)	(6.63,2)	(6.63,2)	(6.53,3)
	3	(7.03,3)	(7.13,2)	(5.25,4)	(6.63,2)	(6.63,2)	(6.53,3)
	4	(7.03,3)	(7.03,3)	(7.03,3)	(5.25,4)	(6.53,3)	(6.53,3)
	5	(7.03,3)	(7.03,3)	(7.03,3)	(7.03,3)	(5.25,4)	(6.53,3)
	6	(7.03,3)	(7.03,3)	(7.03,3)	(7.03,3)	(7.03,3)	(5.25,4)

For this pathway the IBP model indicates that the pair (Q_S,Q_T)=(1,1) dominates all other cases. Hence in this case the IBP model recovers the (Q_S,Q_T)=(1,1) pair observed in the experimentally determined pathway.

The results for objective (6.27) are shown below.

(L,W)		Number of molecules Q_T of target compound					
		1	2	3	4	5	6
Number of molecules Q_S of source compound	1	(5,4)*	(7,4)	(7,4)	(7,4)	(7,4)	(7,4)
	2	(7,4)	(5,4)	(7,4)	(7,4)	(7,4)	(7,4)
	3	(7,4)	(7,4)	(5,4)	(7,4)	(7,4)	(7,4)
	4	(7,4)	(7,4)	(7,4)	(5,4)	(7,4)	(7,4)
	5	(7,4)	(7,4)	(7,4)	(7,4)	(5,4)	(7,4)
	6	(7,4)	(7,4)	(7,4)	(7,4)	(7,4)	(5,4)

We obtain the same dominant pair as objective (6.26). Hence for this objective the IBP model recovers the $(Q_S,Q_T)=(1,1)$ pair observed in the experimentally determined pathway.

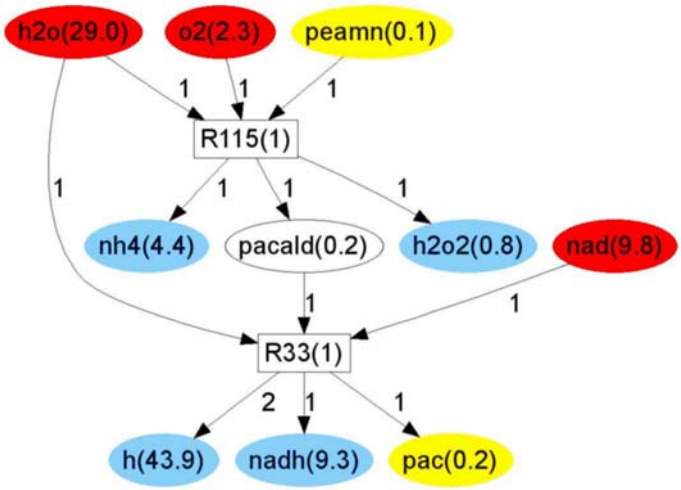
Pathway 23: Phenylethylamine degradation

Source compound	Phenethylamine (peamn)
Target compound	Phenylacetic acid (pac)
(Q_S,Q_T)	(1,1)
Low presence compounds that are not forced to be balanced	O2 (o2) Hydrogen peroxide (h2o2)
(Number of reactions, excess ATP)	(2,0)
Number of unbalanced main compounds (W)	0
Specificity (Ψ)	2

Pathway description

This pathway has been taken from EcoCyc (http://biocyc.org/ECOLI/NEW-IMAGE?type=PATHWAY&object=2PHENDEG-PWY).

In EcoCyC the pathway is described as being from one molecule of Phenethylamine to one molecule of Phenylacetic acid. Our database contains the same set of reactions.



(Q_S,Q_T) discussion for the BP model

This pathway was recovered with both objective (3.13) and objective (3.14). Thus, the (Q_S,Q_T) discussion is carried out for objective (3.13) and objective (3.14). The table of pairs for objective (3.13) is shown below.

(number of reactions, excess ATP)		Number of molecules Q_T of target compound					
		1	2	3	4	5	6
Number of molecules Q_S of source compound	1	(2,0)*	X	X	X	X	X
	2	X	(2,0)	X	X	X	X
	3	X	X	(2,0)	X	X	X
	4	X	X	X	(2,0)	X	X
	5	X	X	X	X	(2,0)	X
	6	X	X	X	X	X	(2,0)

The pairs seen down the diagonal are all repeats of each other, doubling and then tripling, etc the number of source and target molecules. The dominant pair is (Q_S,Q_T)=(1,1). Hence in this case the BP model recovers the (Q_S,Q_T)=(1,1) pair observed in the experimentally determined pathway.

On the other hand, results for objective (3.14) are shown below.

(number of reactions, excess ATP)		Number of molecules Q_T of target compound					
		1	2	3	4	5	6
Number of molecules Q_S of source compound	1	(2,0)*	X	X	X	X	X
	2	X	(2,0)	X	X	X	X
	3	X	X	(2,0)	X	X	X
	4	X	X	X	(2,0)	X	X
	5	X	X	X	X	(2,0)	X
	6	X	X	X	X	X	(2,0)

The pairs seen down the diagonal are all repeats of each other, doubling and then tripling, etc the number of source and target molecules. The dominant pair is $(Q_S,Q_T)=(1,1)$. Hence in this case the BP model recovers the $(Q_S,Q_T)=(1,1)$ pair observed in the experimentally determined pathway.

(Q_S,Q_T) discussion for the IBP model

This pathway was recovered with both objective (6.26) and objective (6.27). Thus, the (Q_S,Q_T) discussion is carried out for objective (6.26) and objective (6.27). The table of pairs for objective (6.26) is shown below.

(Ψ,W)		Number of molecules Q_T of target compound					
		1	2	3	4	5	6
Number of molecules Q_S of source compound	1	(2,0)*	X	X	X	X	X
	2	X	(2,0)	X	X	X	X
	3	X	X	(2,0)	X	X	X
	4	X	X	X	(2,0)	X	X
	5	X	X	X	X	(2,0)	X
	6	X	X	X	X	X	(2,0)

For this pathway the IBP model indicates that the pair (Q_S,Q_T)=(1,1) dominates all other cases. Hence in this case the IBP model recovers the (Q_S,Q_T)=(1,1) pair observed in the experimentally determined pathway.

The results for objective (6.27) are shown below.

(L,W)		Number of molecules Q_T of target compound					
		1	2	3	4	5	6
Number of molecules Q_S of source compound	1	(2,0)*	X	X	X	X	X
	2	X	(2,0)	X	X	X	X
	3	X	X	(2,0)	X	X	X
	4	X	X	X	(2,0)	X	X
	5	X	X	X	X	(2,0)	X
	6	X	X	X	X	X	(2,0)

We obtain the same dominant pair as objective (6.26). Hence for this objective the IBP model recovers the $(Q_S,Q_T)=(1,1)$ pair observed in the experimentally determined pathway.

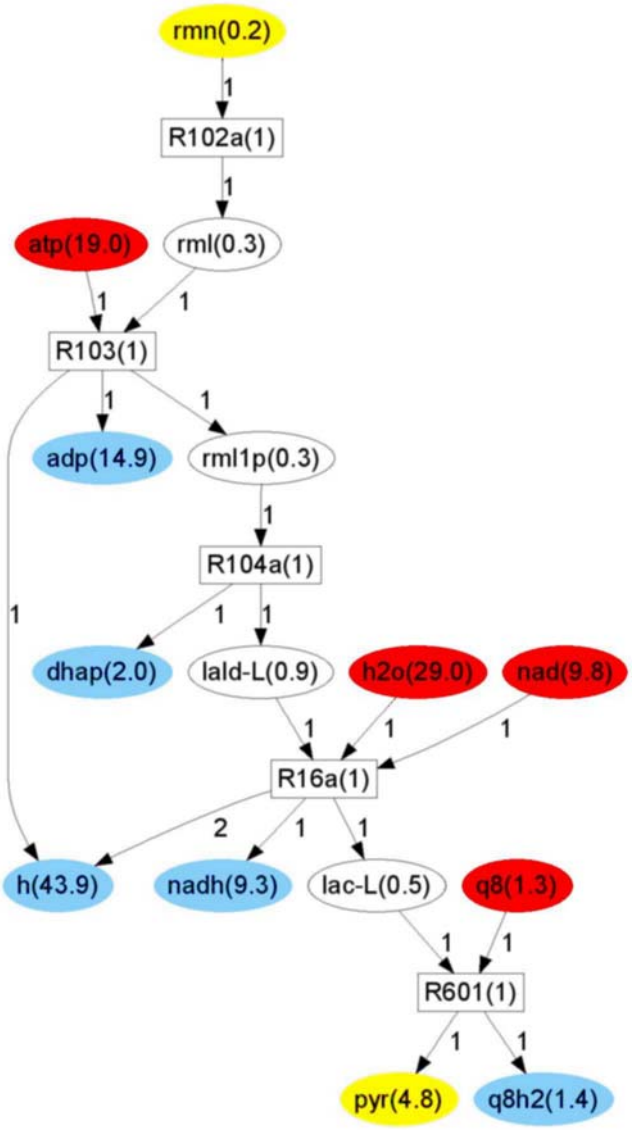
Pathway 24: Rhamnose degradation

Source compound	L-Rhamnose (rmn)
Target compound	Pyruvate (pyr)
(Q_S,Q_T)	(1,1)
Low presence compounds that are not forced to be balanced	Dihydroxyacetone phosphate (dhap) Ubiquinone-8 (q8) Ubiquinol-8 (q8h2)
(Number of reactions, excess ATP)	(5,-1)
Number of unbalanced main compounds (W)	1
Specificity (Ψ)	6.25

Pathway description

This pathway has been taken from EcoCyc (http://biocyc.org/ECOLI/NEW-IMAGE?type=PATHWAY&object=RHAMCAT-PWY).

In EcoCyC the pathway is described as being from one molecule of L-Rhamnose to one molecule of Pyruvate. Our database contains the same set of reactions.



(Q_S,Q_T) discussion for the BP model

This pathway was recovered with objective (3.13). Thus, the (Q_S,Q_T) discussion is carried out for objective (3.13). The table of pairs for objective (3.13) is shown below.

(number of reactions, excess ATP)		Number of molecules Q_T of target compound					
		1	2	3	4	5	6
Number of molecules Q_S of source compound	1	(5,-1)*	(11,1)	(11,3)	(11,5)	(11,7)	(11,9)
	2	X	(5,-2)	(12,-1)	(11,2)	(11,4)	(11,6)
	3	X	X	(5,-3)	(11,-1)	(11,1)	(11,3)
	4	X	X	X	(5,-4)	(11,-2)	(12,-2)
	5	X	X	X	X	(5,-5)	(11,-3)
	6	X	X	X	X	X	(5,-6)

The pairs seen down the diagonal are all repeats of each other, doubling and then tripling, etc the number of source and target molecules (and excess ATP). The dominant pair is (Q_S,Q_T)=(1,1). Hence in this case the BP model recovers the (Q_S,Q_T)=(1,1) pair observed in the experimentally determined pathway.

(Q_S,Q_T) discussion for the IBP model

This pathway was recovered with both objective (6.26) and objective (6.27). Thus, the (Q_S,Q_T) discussion is carried out for objective (6.26) and objective (6.27). The table of pairs for objective (6.26) is shown below.

(Ψ,W)		Number of molecules Q_T of target compound					
		1	2	3	4	5	6
Number of molecules Q_S of source compound	1	(6.25,1)*	(6.93,0)	(7.95,2)	(7.95,2)	(7.95,2)	(7.95,2)
	2	(9.81,4)	(6.25,1)	(7.95,2)	(6.93,0)	(8.05,1)	(7.95,2)
	3	(9.81,4)	(9.81,4)	(6.25,1)	(7.95,2)	(7.95,2)	(6.93,0)
	4	(9.81,4)	(9.81,4)	(9.81,4)	(6.25,1)	(7.95,2)	(7.95,2)
	5	(9.81,4)	(9.81,4)	(9.81,4)	(9.81,4)	(6.25,1)	(7.95,2)
	6	(9.81,4)	(9.81,4)	(9.81,4)	(9.81,4)	(9.81,4)	(6.25,1)

For this pathway the IBP model indicates that the pair (Q_S,Q_T)=(1,1) dominates all other cases. Hence in this case the IBP model recovers the (Q_S,Q_T)=(1,1) pair observed in the experimentally determined pathway.

The results for objective (6.27) are shown below.

(L,W)		Number of molecules Q_T of target compound					
		1	2	3	4	5	6
Number of molecules Q_S of source compound	1	(5,1)*	(9,0)	(10,2)	(10,2)	(10,2)	(10,2)
	2	(12,4)	(5,1)	(10,2)	(9,0)	(10,2)	(10,2)
	3	(12,3)	(11,6)	(5,1)	(10,2)	(10,2)	(9,0)
	4	(12,3)	(12,3)	(12,3)	(5,1)	(10,2)	(10,2)
	5	(12,3)	(12,3)	(12,3)	(12,3)	(5,1)	(10,2)
	6	(12,3)	(13,4)	(12,5)	(11,6)	(13,4)	(5,1)

We obtain the same dominant pair as objective (6.26). Hence for this objective the IBP model recovers the $(Q_S,Q_T)=(1,1)$ pair observed in the experimentally determined pathway.

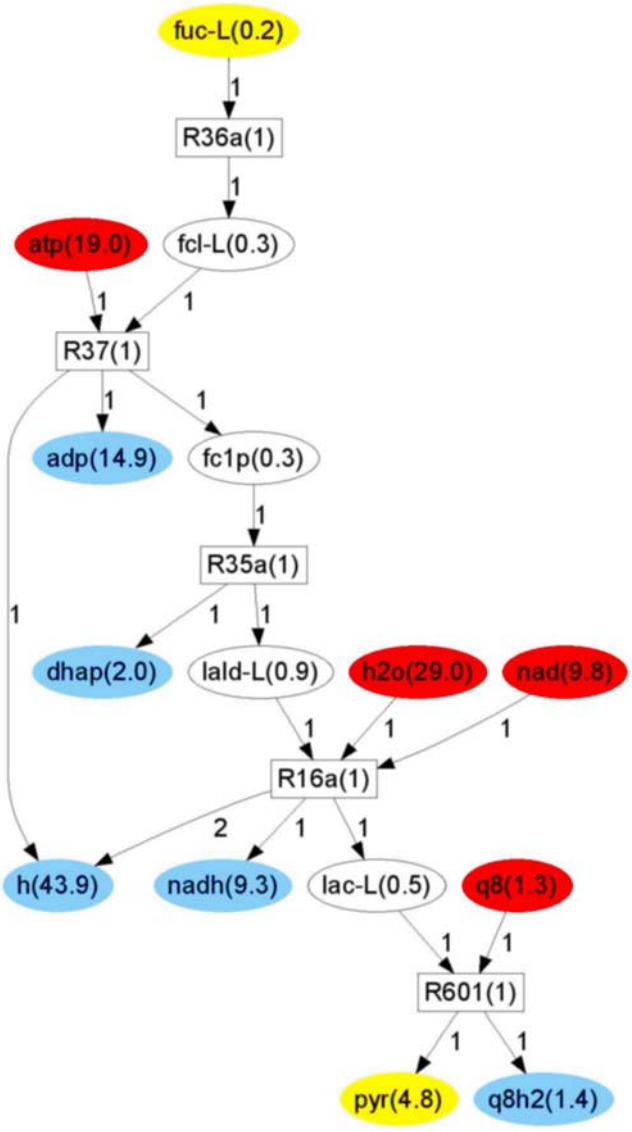
Pathway 25: Fucose degradation

Source compound	L-Fucose (fuc-L)
Target compound	Pyruvate (pyr)
(Q_S,Q_T)	(1,1)
Low presence compounds that are not forced to be balanced	Dihydroxyacetone phosphate (dhap) Ubiquinone-8 (q8) Ubiquinol-8 (q8h2)
(Number of reactions, excess ATP)	(5,-1)
Number of unbalanced main compounds (W)	1
Specificity (Ψ)	6.25

Pathway description

This pathway has been taken from EcoCyc (http://biocyc.org/ECOLI/NEW-IMAGE?type=PATHWAY&object=FUCCAT-PWY).

In EcoCyC the pathway is described as being from one molecule of L-Fucose to one molecule of Pyruvate. Our database contains the same set of reactions.



(Q_S,Q_T) discussion for the BP model

This pathway was recovered with objective (3.13). Thus, the (Q_S,Q_T) discussion is carried out for objective (3.13). The table of pairs for objective (3.13) is shown below.

(number of reactions, excess ATP)		Number of molecules Q_T of target compound					
		1	2	3	4	5	6
Number of molecules Q_S of source compound	1	(5,-1)*	(11,1)	(11,3)	(11,5)	(11,7)	(11,9)
	2	X	(5,-2)	(12,-1)	(11,2)	(11,4)	(11,6)
	3	X	X	(5,-3)	(11,-1)	(11,1)	(11,3)
	4	X	X	X	(5,-4)	(11,-2)	(12,-2)
	5	X	X	X	X	(5,-5)	(11,-3)
	6	X	X	X	X	X	(5,-6)

The pairs seen down the diagonal are all repeats of each other, doubling and then tripling, etc the number of source and target molecules (and excess ATP). The dominant pair is (Q_S,Q_T)=(1,1). Hence in this case the BP model recovers the (Q_S,Q_T)=(1,1) pair observed in the experimentally determined pathway.

(Q_S,Q_T) discussion for the IBP model

This pathway was recovered with both objective (6.26) and objective (6.27). Thus, the (Q_S,Q_T) discussion is carried out for objective (6.26) and objective (6.27). The table of pairs for objective (6.26) is shown below.

(Ψ,W)		Number of molecules Q_T of target compound					
		1	2	3	4	5	6
Number of molecules Q_S of source compound	1	(6.25,1)*	(6.93,0)	(7.95,2)	(7.95,2)	(7.95,2)	(7.95,2)
	2	(9.81,4)	(6.25,1)	(7.95,2)	(6.93,0)	(7.95,2)	(7.95,2)
	3	(9.81,4)	(9.9,3)	(6.25,1)	(7.95,2)	(7.95,2)	(6.93,0)
	4	(9.81,4)	(9.81,4)	(9.81,4)	(6.25,1)	(7.95,2)	(7.95,2)
	5	(9.81,4)	(9.81,4)	(9.81,4)	(9.81,4)	(6.25,1)	(7.95,2)
	6	(9.81,4)	(9.81,4)	(9.81,4)	(9.81,4)	(9.81,4)	(6.25,1)

For this pathway the IBP model indicates that the pair (Q_S,Q_T)=(1,1) dominates all other cases. Hence in this case the IBP model recovers the (Q_S,Q_T)=(1,1) pair observed in the experimentally determined pathway.

The results for objective (6.27) are shown below.

(L,W)		Number of molecules Q_T of target compound					
		1	2	3	4	5	6
Number of molecules Q_S of source compound	1	(5,1)*	(9,0)	(10,2)	(10,2)	(10,2)	(10,2)
	2	(12,3)	(5,1)	(10,2)	(9,0)	(10,2)	(10,2)
	3	(12,3)	(11,6)	(5,1)	(10,2)	(10,2)	(9,0)
	4	(12,3)	(12,3)	(12,3)	(5,1)	(10,2)	(10,2)
	5	(12,3)	(11,4)	(11,4)	(11,4)	(5,1)	(10,2)
	6	(11,4)	(11,4)	(11,4)	(11,4)	(11,4)	(5,1)

We obtain the same dominant pair as objective (6.26). Hence for this objective the IBP model recovers the $(Q_S,Q_T)=(1,1)$ pair observed in the experimentally determined pathway.

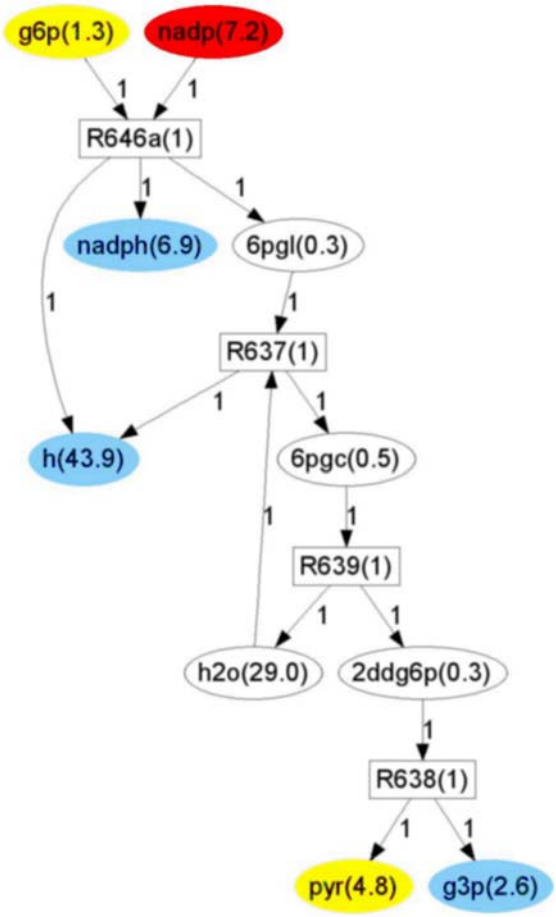
Pathway 26: Entner-Doudoroff

Source compound	D-Glucose 6-phosphate (g6p)
Target compound	Pyruvate (pyr)
(Q_S,Q_T)	(1,1)
Low presence compounds that are not forced to be balanced	None
(Number of reactions, excess ATP)	(4,0)
Number of unbalanced main compounds (W)	0
Specificity (Ψ)	4.41

Pathway description

This pathway has been taken from EcoCyc (http://biocyc.org/ECOLI/NEW-IMAGE?type=PATHWAY&object=ENTNER-DOUDOROFF-PWY).

In EcoCyC the pathway is described as being from one molecule of D-Glucose 6-phosphate to one molecule of Pyruvate. Our database contains the same set of reactions.



Note here that we have one allowable c-cycle in this pathway. More precisely the 2-cycle 6pgc-R639-h2o-R637-6pgc which contains one high presence balanced compound (h2o).

(Q_S,Q_T) discussion for the BP model

This pathway was recovered with both objective (3.13) and objective (3.14). Thus, the (Q_S,Q_T) discussion is carried out for objective (3.13) and objective (3.14). The table of pairs for objective (3.13) is shown below.

(number of reactions, excess ATP)		Number of molecules Q_T of target compound					
		1	2	3	4	5	6
Number of molecules Q_S of source compound	1	(4,0)*	(9,3)	(9,4)	(9,6)	(9,8)	(9,10)
	2	X	(4,0)	(9,2)	(9,6)	(9,6)	(9,8)
	3	X	X	(4,0)	(9,2)	(9,4)	(9,9)
	4	X	X	X	(4,0)	(9,2)	(9,4)
	5	X	X	X	X	(4,0)	(9,2)
	6	X	X	X	X	X	(4,0)

The pairs seen down the diagonal are all repeats of each other, doubling and then tripling, etc the number of source and target molecules. The dominant pair is (Q_S,Q_T)=(1,1). Hence in this case the BP model recovers the (Q_S,Q_T)=(1,1) pair observed in the experimentally determined pathway.

The results for objective (3.14) are shown below.

(number of reactions, excess ATP)		Number of molecules Q_T of target compound					
		1	2	3	4	5	6
Number of molecules Q_S of source compound	1	(4,0)	(9,3)	(9,4)	(9,6)	(9,8)	(9,10)*
	2	X	(4,0)	(9,2)	(9,6)	(9,6)	(9,8)
	3	X	X	(4,0)	(9,2)	(9,4)	(9,9)
	4	X	X	X	(4,0)	(9,2)	(9,4)
	5	X	X	X	X	(4,0)	(9,2)
	6	X	X	X	X	X	(4,0)

The dominant pair is $(Q_S,Q_T)=(1,6)$. Hence in this case the BP model does not recover the $(Q_S,Q_T)=(1,1)$ pair observed in the experimentally determined pathway.

(Q_S,Q_T) discussion for the IBP model

This pathway was not recovered with either objective (6.26) or objective (6.27). For this reason (Q_S,Q_T) pairs discussion is omitted for this pathway.

Pathway 27: Anaerobic respiration

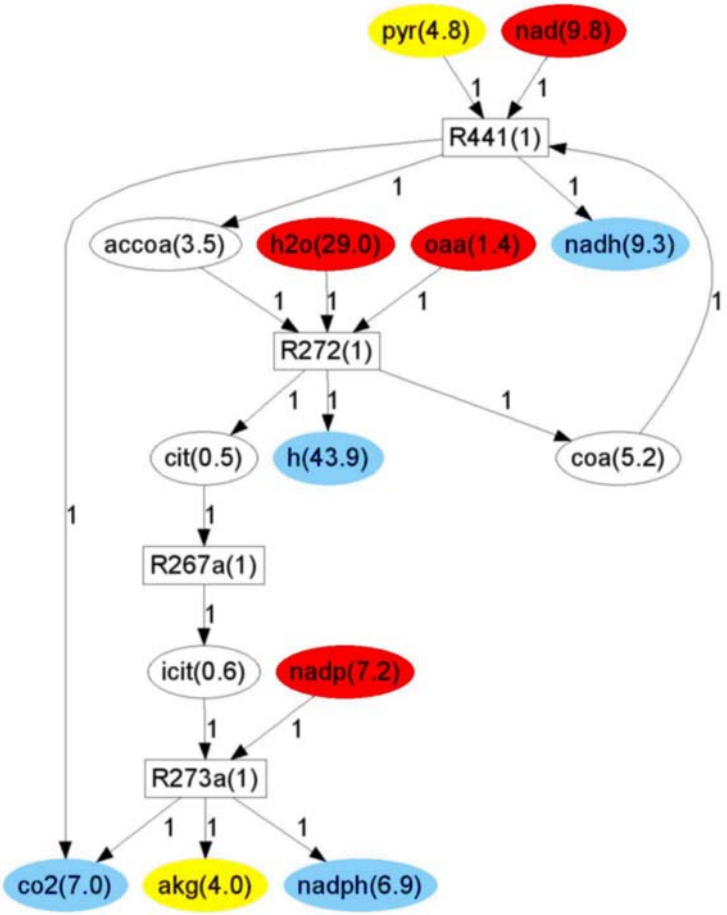
Source compound	Pyruvate (pyr)
Target compound	2-Oxoglutarate (akg)
(Q_S,Q_T)	(1,1)
Low presence compounds that are not forced to be balanced	Oxaloacetate (oaa)
(Number of reactions, excess ATP)	(4,0)
Number of unbalanced main compounds (W)	1
Specificity (Ψ)	4.79

Pathway description

This pathway has been taken from EcoCyc (http://biocyc.org/ECOLI/NEW-IMAGE?type=PATHWAY&object=ANARESP1-PWY) and Lehninger (fourth edition) page 621.

In Lehninger the pathway is described as being from one molecule of Pyruvate to one molecule of 2-Oxoglutarate. However, EcoCyc describes it as being from one molecule of Phosphoenolpyruvate to one molecule of 2-Oxoglutarate, Pyruvate being an intermediate compound.

Since the Lehninger description appears to be the clearer one it is that which has informed the pathway picture seen below.



Note here that we have one allowable c-cycle (see Chapter 3) in this pathway. More precisely the 2-cycle accoa-R272-coa-R441-accoa which contains one high presence balanced compound (coa).

(Q_S,Q_T) discussion for the BP model

This pathway was recovered with both objective (3.13) and objective (3.14). Thus, the (Q_S,Q_T) discussion is carried out for objective (3.13) and objective (3.14). The table of pairs for objective (3.13) is shown below.

(number of reactions, excess ATP)		Number of molecules Q_T of target compound					
		1	2	3	4	5	6
Number of molecules Q_S of source compound	1	(4,0)*	(5,0)	(5,0)	(5,0)	(5,0)	(5,0)
	2	(6,-1)	(4,0)	(5,0)	(5,0)	(5,0)	(5,0)
	3	X	X	(4,0)	(5,0)	(5,0)	(5,0)
	4	X	(6,-2)	(7,-2)	(4,0)	(5,0)	(5,0)
	5	X	X	X	X	(4,0)	(5,0)
	6	X	X	(6,-3)	(7,-3)	(7,-3)	(4,0)

The pairs seen down the diagonal are all repeats of each other, doubling and then tripling, etc the number of source and target molecules. The dominant pair is (Q_S,Q_T)=(1,1). Hence in this case the BP model recovers the (Q_S,Q_T)=(1,1) pair observed in the experimentally determined pathway.

The results for objective (3.14) are shown below.

(number of reactions, excess ATP)		Number of molecules Q_T of target compound					
		1	2	3	4	5	6
Number of molecules Q_S of source compound	1	(4,0)*	(5,0)	(5,0)	(5,0)	(5,0)	(5,0)
	2	(7,0)	(4,0)	(5,0)	(5,0)	(5,0)	(5,0)
	3	X	X	(4,0)	(5,0)	(5,0)	(5,0)
	4	X	(7,0)	(8,0)	(4,0)	(5,0)	(5,0)
	5	X	X	X	X	(4,0)	(5,0)
	6	X	X	(7,0)	(8,0)	(8,0)	(4,0)

The pairs seen down the diagonal are all repeats of each other, doubling and then tripling, etc the number of source and target molecules. The dominant pair is $(Q_S,Q_T)=(1,1)$. Hence in this case the BP model recover the $(Q_S,Q_T)=(1,1)$ pair observed in the experimentally determined pathway.

(Q_S,Q_T) discussion for the IBP model

This pathway was not recovered with either objective (6.26) or objective (6.27). For this reason (Q_S,Q_T) pairs discussion is omitted for this pathway.

Pathway 28: Arginine degradation

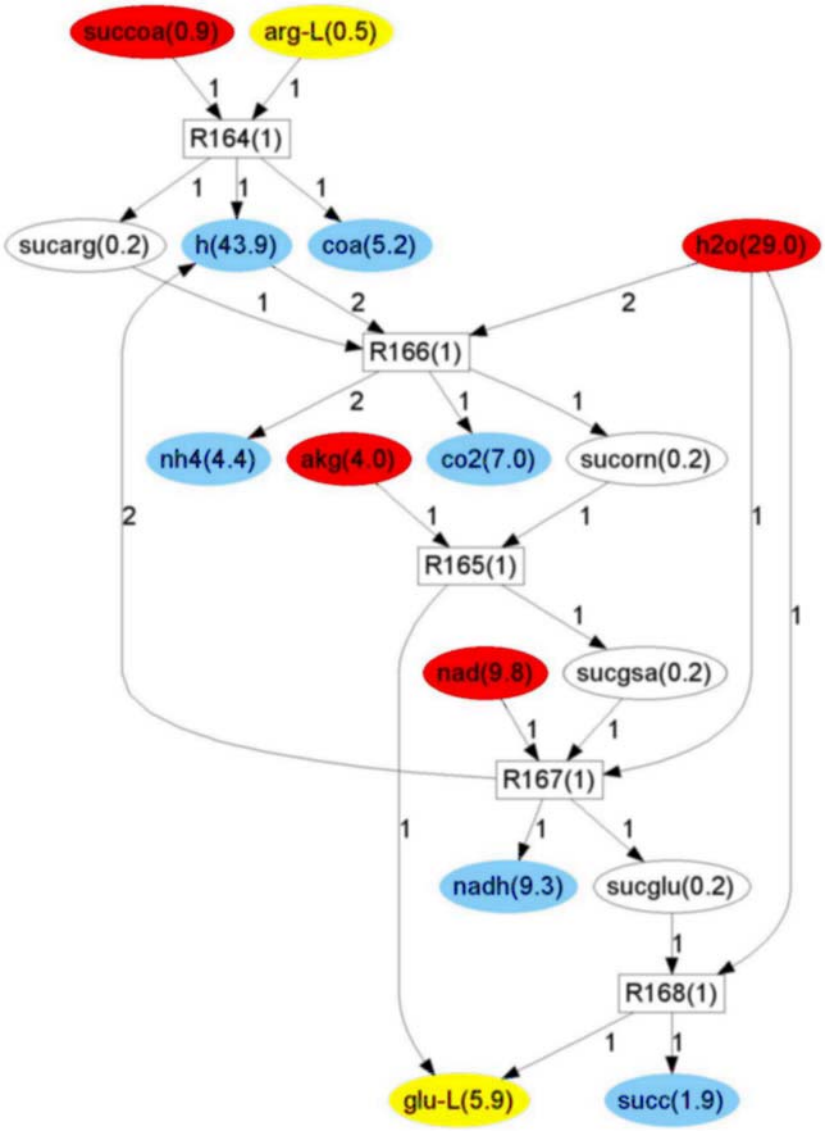
Source compound	L-Arginine (arg-L)
Target compound	L-Glutamate (glu-L)
(Q_S,Q_T)	(1,2)
Low presence compounds that are not forced to be balanced	2-Oxoglutarate (akg) Succinyl-CoA (succoa) Succinate (succ)
(Number of reactions, excess ATP)	(5,0)
Number of unbalanced main compounds (W)	2
Specificity (Ψ)	6.03

Pathway description

This pathway has been taken from EcoCyc (http://biocyc.org/ECOLI/NEW-IMAGE?type=PATHWAY&object=AST-PWY) and Lehninger (fourth edition) page 681.

Whilst the pathway is described as being from one molecule of L-Arginine to one molecule of α-Ketoglutarate in Lehninger, EcoCyc describes it as being from one molecule of L-Arginine to two molecules of L-Glutamate.

Since our reaction database does not contain the set of reactions seen in Lehninger, but does contain those seen in EcoCyc, it is that which has informed the pathway picture seen below.


succoa(0.9)
arg-L(0.5)
R164(1)
sucarg(0.2)
h(43.9)
coa(5.2)
h2o(29.0)
R166(1)
nh4(4.4)
akg(4.0)
co2(7.0)
sucorn(0.2)
R165(1)
nad(9.8)
sucgsa(0.2)
R167(1)
nadh(9.3)
sucglu(0.2)
R168(1)
glu-L(5.9)
succ(1.9)

(Q_S,Q_T) discussion for the BP model

This pathway was recovered with objective (3.13). Thus, the (Q_S,Q_T) discussion is carried out for objective (3.13). The table of pairs for objective (3.13) is shown below.

(number of reactions, excess ATP)		Number of molecules Q_T of target compound					
		1	2	3	4	5	6
Number of molecules Q_S of source compound	1	X	(5,0)*	(6,0)	(6,0)	(6,0)	(6,0)
	2	X	X	X	(5,0)	(6,0)	(6,0)
	3	X	X	X	X	X	(5,0)
	4	X	X	X	X	X	X
	5	X	X	X	X	X	X
	6	X	X	X	X	X	X

The dominant pair is (Q_S,Q_T)=(1,2). Hence in this case the BP model recovers the (Q_S,Q_T)=(1,2) pair observed in the experimentally determined pathway.

(Q_S,Q_T) discussion for the IBP model

This pathway was recovered with both objective (6.26) and objective (6.27). Thus, the (Q_S,Q_T) discussion is carried out for objective (6.26) and objective (6.27). The table of pairs for objective (6.26) is shown below.

(Ψ,W)		Number of molecules Q_T of target compound					
		1	2	3	4	5	6
Number of molecules Q_S of source compound	1	(12.74,7)	(6.03,2)*	(9.99,4)	(10.39,2)	(10.39,2)	(10.39,2)
	2	(17.27,11)	(12.74,7)	(9.48,8)	(6.03,2)	(10.39,2)	(9.99,4)
	3	(17.27,11)	(14.46,9)	(11.18,10)	(9.38,9)	(9.48,8)	(6.03,2)
	4	(17.27,11)	(15.87,11)	(12.51,12)	(11.18,10)	(9.38,9)	(9.38,9)
	5	(17.27,11)	(15.87,11)	(12.51,12)	(12.51,12)	(11.18,10)	(9.38,9)
	6	(17.27,11)	(15.87,11)	(12.51,12)	(12.51,12)	(12.51,12)	(11.18,10)

For this pathway the IBP model indicates that the pair (Q_S,Q_T)=(1,2) dominates all other cases. Hence in this case the IBP model recovers the (Q_S,Q_T)=(1,2) pair observed in the experimentally determined pathway.

The results for objective (6.27) are shown below.

(L,W)		Number of molecules Q_T of target compound					
		1	2	3	4	5	6
Number of molecules Q_S of source compound	1	(3,2)*	(5,2)	(9,4)	(10,3)	(10,5)	(11,5)
	2	(13,0)	(3,2)	(8,4)	(5,2)	(10,5)	(9,4)
	3	(12,8)	(12,8)	(3,2)	(8,4)	(8,4)	(5,2)
	4	(12,8)	(12,8)	(12,8)	(3,2)	(8,4)	(8,4)
	5	(13,0)	(12,8)	(12,8)	(12,8)	(3,2)	(8,4)
	6	(12,8)	(12,8)	(12,8)	(12,8)	(12,8)	(3,2)

In contrast with objective (6.26), the dominant pair for objective (6.27) is $(Q_S,Q_T)=(1,1)$. Hence for this objective the IBP model does not recover the $(Q_S,Q_T)=(1,2)$ pair observed in the experimentally determined pathway.

Pathway 29: Proline degradation

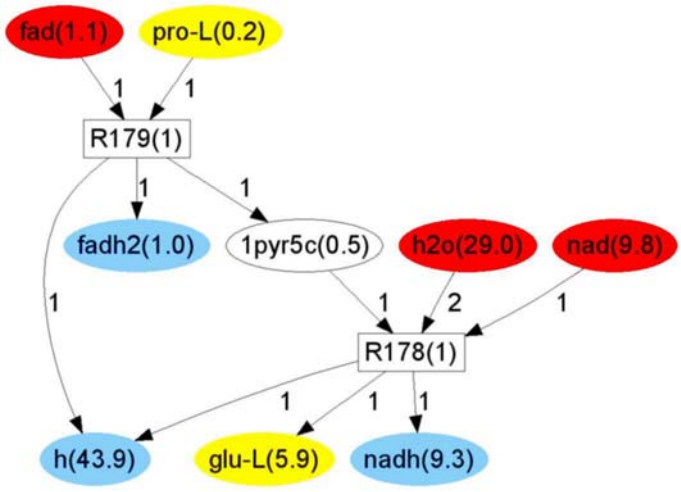
Source compound	L-Proline (pro-L)
Target compound	L-Glutamate (glu-L)
(Q_S,Q_T)	(1,1)
Low presence compounds that are not forced to be balanced	FAD (fad) FADH2 (fadh2)
(Number of reactions, excess ATP)	(2,0)
Number of unbalanced main compounds (W)	0
Specificity (Ψ)	2

Pathway description

This pathway has been taken from EcoCyc (http://biocyc.org/ECOLI/NEW-IMAGE?type=PATHWAY&object=PROUT-PWY) and Lehninger (fourth edition) page 681.

Whilst the pathway is described as being from one molecule of L-Proline to one molecule of α-Ketoglutarate (2-oxoglutarate in our database) in Lehninger, EcoCyc describes it as being from one molecule of L-Proline to one molecule of L-glutamate. Moreover, Lehninger contains two additional reactions with respect to EcoCyc.

Since our reaction database matches to those reactions seen in EcoCyc, it is that which has informed the pathway picture seen below.



(Q_S,Q_T) discussion for the BP model

This pathway was recovered with both objective (3.13) and objective (3.14). Thus, the (Q_S,Q_T) discussion is carried out for objective (3.13) and objective (3.14). The table of pairs for objective (3.13) is shown below.

(number of reactions, excess ATP)		Number of molecules Q_T of target compound					
		1	2	3	4	5	6
Number of molecules Q_S of source compound	1	(2,0)*	(10,-1)	(10,-2)	(10,-3)	(10,-4)	(10,-5)
	2	X	(2,0)	(10,-1)	(10,-2)	(10,-3)	(10,-4)
	3	X	X	(2,0)	(10,-1)	(10,-2)	(10,-3)
	4	X	X	X	(2,0)	(10,-1)	(10,-2)
	5	X	X	X	X	(2,0)	(10,-1)
	6	X	X	X	X	X	(2,0)

The pairs seen down the diagonal are all repeats of each other, doubling and then tripling, etc the number of source and target molecules. The dominant pair is (Q_S,Q_T)=(1,1). Hence in this case the BP model recovers the (Q_S,Q_T)=(1,1) pair observed in the experimentally determined pathway.

The results for objective (3.14) are shown below.

(number of reactions, excess ATP)		Number of molecules Q_T of target compound					
		1	2	3	4	5	6
Number of molecules Q_S of source compound	1	(2,0)*	(11,0)	(11,0)	(11,0)	(11,0)	(11,0)
	2	X	(2,0)	(11,0)	(11,0)	(11,0)	(11,0)
	3	X	X	(2,0)	(11,0)	(11,0)	(11,0)
	4	X	X	X	(2,0)	(11,0)	(11,0)
	5	X	X	X	X	(2,0)	(11,0)
	6	X	X	X	X	X	(2,0)

The pairs seen down the diagonal are all repeats of each other, doubling and then tripling, etc the number of source and target molecules. The dominant pair is $(Q_S,Q_T)=(1,1)$. Hence in this case the BP model recovers the $(Q_S,Q_T)=(1,1)$ pair observed in the experimentally determined pathway.

(Q_S,Q_T) discussion for the IBP model

This pathway was recovered with both objective (6.26) and objective (6.27). Thus, the (Q_S,Q_T) discussion is carried out for objective (6.26) and objective (6.27). The table of pairs for objective (6.26) is shown below.

(Ψ,W)		Number of molecules Q_T of target compound					
		1	2	3	4	5	6
Number of molecules Q_S of source compound	1	(2,0)*	(6.5,5)	(6.48,2)	X	(7.74,5)	X
	2	X	(2,0)	(7.33,3)	(6.33,5)	(6.5,5)	X
	3	X	X	(2,0)	X	(6.43,4)	X
	4	X	X	X	(2,0)	(9.49,6)	(6.33,5)
	5	X	X	X	X	(2,0)	X
	6	X	X	X	X	X	(2,0)

For this pathway the IBP model indicates that the pair (Q_S,Q_T)=(1,1) dominates all other cases. Hence in this case the IBP model recovers the (Q_S,Q_T)=(1,1) pair observed in the experimentally determined pathway.

The results for objective (6.27) are shown below.

(L,W)		Number of molecules Q_T of target compound					
		1	2	3	4	5	6
Number of molecules Q_S of source compound	1	(2,0)*	(9,3)	(9,3)	(9,3)	(10,5)	X
	2	X	(2,0)	(9,3)	(9,3)	(9,3)	(9,3)
	3	X	X	(2,0)	(9,3)	(9,3)	(9,3)
	4	X	X	X	(2,0)	(9,3)	(9,3)
	5	X	X	X	X	(2,0)	(9,3)
	6	X	X	X	X	X	(2,0)

We obtain the same dominant pair as objective (6.26). Hence for this objective the IBP model recovers the $(Q_S,Q_T)=(1,1)$ pair observed in the experimentally determined pathway.

Pathway 30: Glycolate degradation

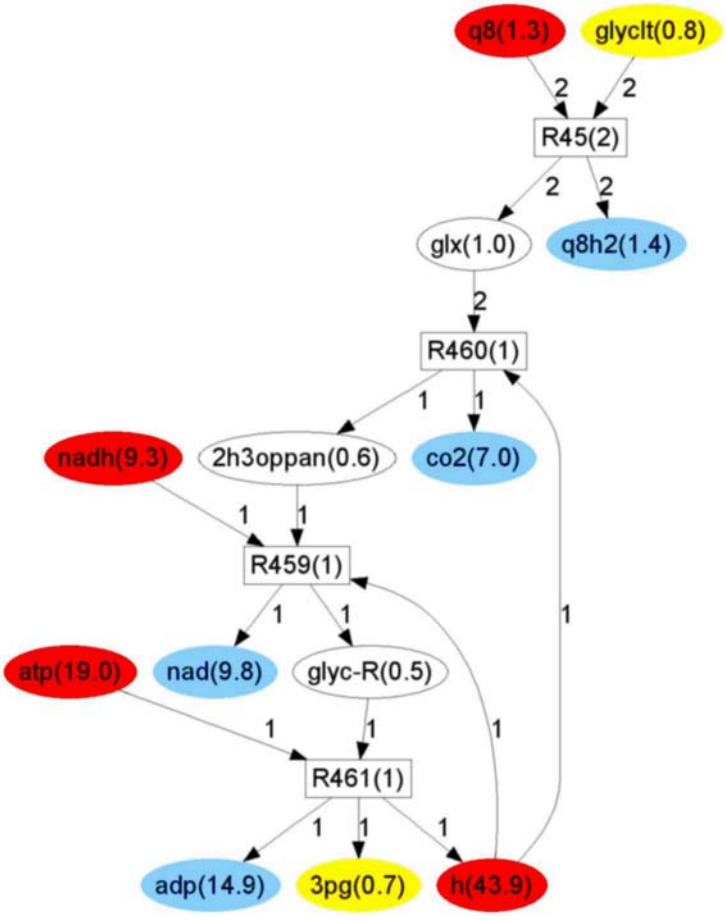
Source compound	Glycolate (glyclt)
Target compound	3-Phospho-D-glycerate (3pg)
(Q_S,Q_T)	(2,1)
Low presence compounds that are not forced to be balanced	Ubiquinone-8 (q8) Ubiquinol-8 (q8h2)
(Number of reactions, excess ATP)	(4,-1)
Number of unbalanced main compounds (W)	0
Specificity (Ψ)	4

Pathway description

This pathway has been taken from EcoCyc (http://biocyc.org/ECOLI/NEW-IMAGE?type=PATHWAY&object=GLYCOLATEMET-PWY) and Lehninger (fourth edition) page 767.

Whilst the pathway is described as being from two molecules of Glycolate to one molecule of Glycine in Lehninger, EcoCyc describes it as being from two molecules of Glycolate to one molecule of 3-Phospho-D-glycerate.

Since our reaction database matches to those reactions seen in EcoCyc, it is that which has informed the pathway picture seen below.



(Q_S,Q_T) discussion for the BP model

This pathway was recovered with objective (3.13). Thus, the (Q_S,Q_T) discussion is carried out for objective (3.13). The table of pairs for objective (3.13) is shown below.

(number of reactions, excess ATP)		Number of molecules Q_T of target compound					
		1	2	3	4	5	6
Number of molecules Q_S of source compound	1	(7,-1)	(8,-2)	(8,-3)	(8,-4)	(8,-5)	(8,-6)
	2	(4,-1)*	(7,-2)	(7,-3)	(7,-4)	(7,-5)	(7,-6)
	3	(7,-1)	(9,0)	(7,-3)	(8,-4)	(8,-5)	(8,-6)
	4	(7,-1)	(4,-2)	(7,-3)	(7,-4)	(7,-5)	(7,-6)
	5	(7,-1)	(7,-2)	(9,0)	(9,0)	(7,-5)	(8,-6)
	6	(7,-1)	(7,-2)	(4,-3)	(7,-4)	(7,-5)	(7,-6)

The dominant pair is (Q_S,Q_T)=(2,1). Hence in this case the BP model recovers the (Q_S,Q_T)=(2,1) pair observed in the experimentally determined pathway.

(Q_S,Q_T) discussion for the IBP model

This pathway was recovered with both objective (6.26) and objective (6.27). Thus, the (Q_S,Q_T) discussion is carried out for objective (6.26) and objective (6.27). The table of pairs for objective (6.26) is shown below.

(Ψ,W)		Number of molecules Q_T of target compound					
		1	2	3	4	5	6
Number of molecules Q_S of source compound	1	(6,0)	(7.38,1)	(7.38,1)	(7.38,1)	(7.38,1)	(7.38,1)
	2	(4,0)*	(6,0)	(5.92,3)	(5.92,3)	(5.92,3)	(5.92,3)
	3	(7.86,4)	(5,0)	(6,0)	(6.92,3)	(6.92,3)	(6.92,3)
	4	(7.86,4)	(4,0)	(5,0)	(6,0)	(5.92,3)	(5.92,3)
	5	(7.96,3)	(7.66,1)	(5,0)	(5,0)	(6,0)	(6.92,3)
	6	(7.86,4)	(7.66,1)	(4,0)	(5,0)	(5,0)	(6,0)

For this pathway the IBP model indicates that the pair (Q_S,Q_T)=(2,1) dominates all other cases. Hence in this case the IBP model recovers the (Q_S,Q_T)=(2,1) pair observed in the experimentally determined pathway.

The results for objective (6.27) are shown below.

(L,W)		Number of molecules Q_T of target compound					
		1	2	3	4	5	6
Number of molecules Q_S of source compound	1	(6,0)	(6,4)	(6,4)	(6,4)	(6,4)	(6,4)
	2	(4,0)*	(6,0)	(6,4)	(6,4)	(6,4)	(6,4)
	3	(6,4)	(6,4)	(6,0)	(6,4)	(6,4)	(6,4)
	4	(6,4)	(4,0)	(6,4)	(6,0)	(6,4)	(6,4)
	5	(6,4)	(6,4)	(6,4)	(6,4)	(6,0)	(6,4)
	6	(6,4)	(6,4)	(4,0)	(6,4)	(6,4)	(6,0)

We obtain the same dominant pair as objective (6.26). Hence for this objective the IBP model recovers the $(Q_S,Q_T)=(2,1)$ pair observed in the experimentally determined pathway.

Pathway 31: Phospholipid biosynthesis

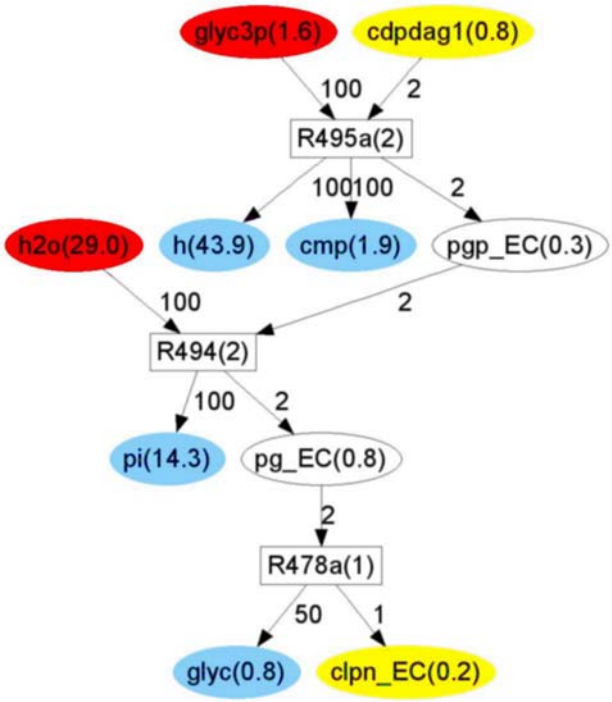
Source compound	CDPdiacilglycerol (cdpdag1)
Target compound	Cardiolipin (clpn_EC)
(Q_S,Q_T)	(2,1)
Low presence compounds that are not forced to be balanced	Glycerol 3-phosphate (glyc3p) CMP (cmp) Glycerol (glyc)
(Number of reactions, excess ATP)	(3,0)
Number of unbalanced main compounds (W)	3
Specificity (Ψ)	3

Pathway description

This pathway has been taken from EcoCyc (http://biocyc.org/ECOLI/NEW-IMAGE?type=PATHWAY&object=PHOSLIPSYN-PWY) and Lehninger (fourth edition) pages 810.

Both in Lehninger and EcoCyc, the pathway is described as being from two molecules of CDPdiacilglycerol to one molecule of cardiolipin.

Since the Lehninger description appears to be the clearer one it is that which has informed the pathway picture seen below.



(Q_S,Q_T) discussion for the BP model

This pathway was recovered with objective (3.13). Thus, the (Q_S,Q_T) discussion is carried out for objective (3.13). The table of pairs for objective (3.13) is shown below.

(number of reactions, excess ATP)		Number of molecules Q_T of target compound					
		1	2	3	4	5	6
Number of molecules Q_S of source compound	1	X	X	X	X	X	X
	2	(3,0)*	X	X	X	X	X
	3	X	X	X	X	X	X
	4	X	(3,0)	X	X	X	X
	5	X	X	X	X	X	X
	6	X	X	(3,0)	X	X	X

The dominant pair is (Q_S,Q_T)=(2,1). Hence in this case the BP model recovers the (Q_S,Q_T)=(2,1) pair observed in the experimentally determined pathway.

(Q_S,Q_T) discussion for the IBP model

This pathway was recovered with both objective (6.26) and objective (6.27). Thus, the (Q_S,Q_T) discussion is carried out for objective (6.26) and objective (6.27). The table of pairs for objective (6.26) is shown below.

(Ψ,W)		Number of molecules Q_T of target compound					
		1	2	3	4	5	6
Number of molecules Q_S of source compound	1	X	X	X	X	X	X
	2	(3,3)*	X	X	X	X	X
	3	X	X	X	X	X	X
	4	X	(3,3)	X	X	X	X
	5	X	X	X	X	X	X
	6	X	X	(3,3)	X	X	X

For this pathway the IBP model indicates that the pair (Q_S,Q_T)=(2,1) dominates all other cases. Hence in this case the IBP model recovers the (Q_S,Q_T)=(2,1) pair observed in the experimentally determined pathway.

The results for objective (6.27) are shown below.

(L,W)		Number of molecules Q_T of target compound					
		1	2	3	4	5	6
Number of molecules Q_S of source compound	1	X	X	X	X	X	X
	2	(3,3)*	X	X	X	X	X
	3	X	X	X	X	X	X
	4	X	(3,3)	X	X	X	X
	5	X	X	X	X	X	X
	6	X	X	(3,3)	X	X	X

We obtain the same dominant pair as objective (6.26). Hence for this objective the IBP model recovers the $(Q_S,Q_T)=(2,1)$ pair observed in the experimentally determined pathway.

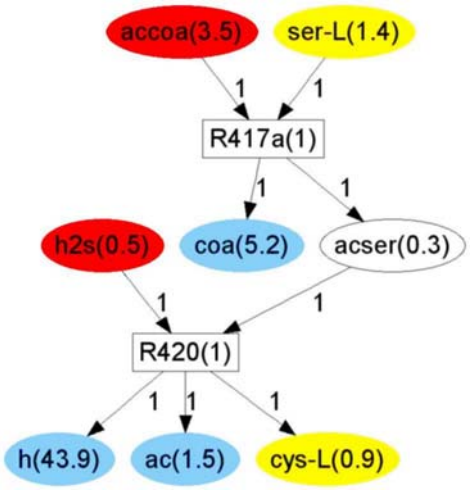
Pathway 32: Biosynthesis of cysteine

Source compound	L-Serine (ser-L)
Target compound	L-Cysteine (cys-L)
(Q_S,Q_T)	(1,1)
Low presence compounds that are not forced to be balanced	Acetyl-CoA (accoa) Hydrogen sulfide (h2s) Acetate (ac)
(Number of reactions, excess ATP)	(2,0)
Number of unbalanced main compounds (W)	1
Specificity (Ψ)	2

Pathway description

This pathway has been taken from EcoCyc (http://biocyc.org/ECOLI/NEW-IMAGE?type=PATHWAY&object=CYSTSYN-PWY) and Lehninger (fourth edition) pages 845.

In Lehninger the pathway is described as being from one molecule of L-Serine to one molecule of L-Cysteine. This pathway is described in the same way in EcoCyc with the same set of reactions.



(Q_S,Q_T) discussion for the BP model

This pathway was recovered with both objective (3.13) and objective (3.14). Thus, the (Q_S,Q_T) discussion is carried out for objective (3.13) and objective (3.14). The table of pairs for objective (3.13) is shown below.

(number of reactions, excess ATP)		Number of molecules Q_T of target compound					
		1	2	3	4	5	6
Number of molecules Q_S of source compound	1	(2,0)*	X	X	X	X	X
	2	(4,0)	(2,0)	X	X	X	X
	3	(9,0)	(5,-1)	(2,0)	X	X	X
	4	(9,0)	(4,0)	(5,-2)	(2,0)	X	X
	5	(9,0)	(9,0)	(5,-1)	(5,-3)	(2,0)	X
	6	(9,0)	(9,0)	(4,0)	(5,-2)	(5,-4)	(2,0)

The pairs seen down the diagonal are all repeats of each other, doubling and then tripling, etc the number of source and target molecules. The dominant pair is (Q_S,Q_T)=(1,1). Hence in this case the BP model recovers the (Q_S,Q_T)=(1,1) pair observed in the experimentally determined pathway.

The results for objective (3.14) are shown below.

(number of reactions, excess ATP)		Number of molecules Q_T of target compound					
		1	2	3	4	5	6
Number of molecules Q_S of source compound	1	(2,0)*	X	X	X	X	X
	2	(4,0)	(2,0)	X	X	X	X
	3	(9,0)	(6,0)	(2,0)	X	X	X
	4	(9,0)	(4,0)	(6,0)	(2,0)	X	X
	5	(9,0)	(9,0)	(6,0)	(6,0)	(2,0)	X
	6	(9,0)	(9,0)	(4,0)	(6,0)	(6,0)	(2,0)

The pairs seen down the diagonal are all repeats of each other, doubling and then tripling, etc the number of source and target molecules. The dominant pair is $(Q_S,Q_T)=(1,1)$. Hence in this case the BP model recovers the $(Q_S,Q_T)=(1,1)$ pair observed in the experimentally determined pathway.

(Q_S,Q_T) discussion for the IBP model

This pathway was recovered with both objective (6.26) and objective (6.27). Thus, the (Q_S,Q_T) discussion is carried out for objective (6.26) and objective (6.27). The table of pairs for objective (6.26) is shown below.

(Ψ,W)		Number of molecules Q_T of target compound					
		1	2	3	4	5	6
Number of molecules Q_S of source compound	1	(2,1)*	(8.17,5)	(8.46,4)	(10.88,2)	(8.61,3)	X
	2	(8.42,4)	(2,1)	(6.15,5)	(6.57,6)	X	(6.15,5)
	3	(9.67,9)	X	(2,1)	X	X	(6.15,5)
	4	(8.34,7)	(9.93,7)	(10.71,9)	(2,1)	(6.15,5)	(6.65,4)
	5	(8.43,4)	(7.13,6)	(7.71,5)	(7.13,6)	(2,1)	(6.4,5)
	6	(8.43,4)	(7.23,5)	X	(7.89,10)	(7.81,4)	(2,1)

For this pathway the IBP model indicates that the pair (Q_S,Q_T)=(1,1) dominates all other cases. Hence in this case the IBP model recovers the (Q_S,Q_T)=(1,1) pair observed in the experimentally determined pathway.

The results for objective (6.27) are shown below.

(L,W)		Number of molecules Q_T of target compound					
		1	2	3	4	5	6
Number of molecules Q_S of source compound	1	(2,1)*	(9,5)	(11,4)	(11,4)	(11,6)	(11,5)
	2	(11,4)	(2,1)	(11,6)	(9,5)	(8,4)	(8,4)
	3	(7,2)	(8,5)	(2,1)	X	(8,4)	(8,4)
	4	X	(9,4)	(13,6)	(2,1)	X	(8,4)
	5	X	(9,4)	(7,5)	(12,6)	(2,1)	(8,4)
	6	(10,7)	(7,2)	(9,4)	X	X	(2,1)

We obtain the same dominant pair as objective (6.26). Hence for this objective the IBP model recovers the $(Q_S,Q_T)=(1,1)$ pair observed in the experimentally determined pathway.

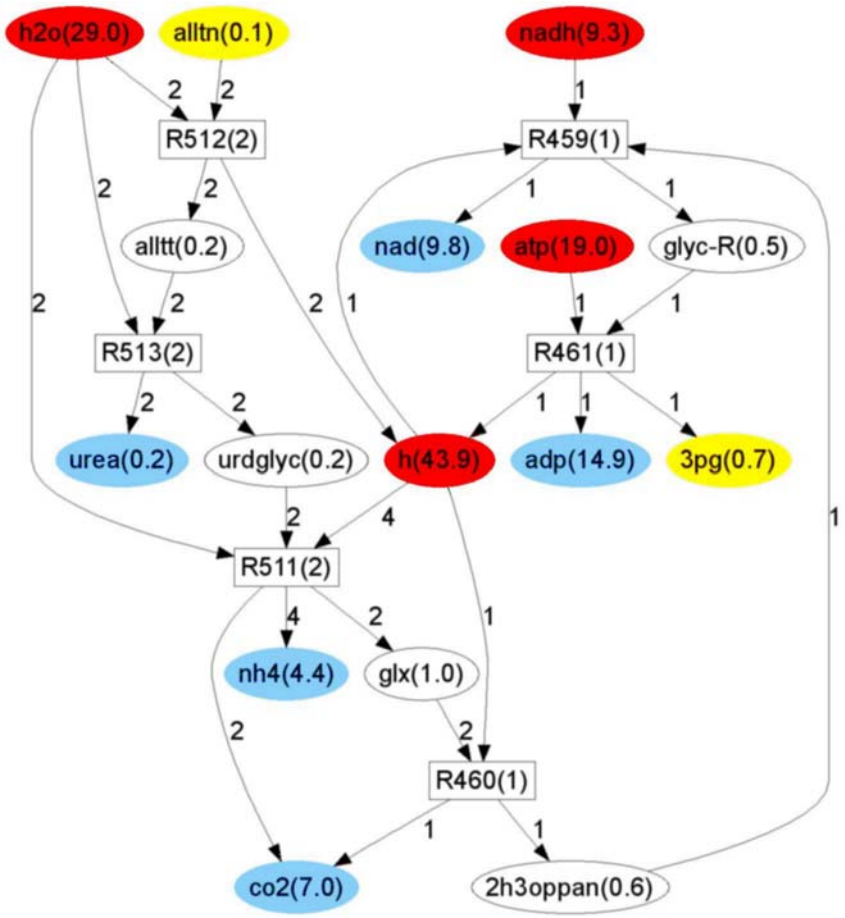
Pathway 33: Allantoin degradation

Source compound	Allantoin (alltn)
Target compound	3-Phospho-D-glycerate (3pg)
(Q_S,Q_T)	(2,1)
Low presence compounds that are not forced to be balanced	Urea (urea)
(Number of reactions, excess ATP)	(6,-1)
Number of unbalanced main compounds (W)	1
Specificity (Ψ)	6

Pathway description

This pathway has been taken from EcoCyc (http://biocyc.org/ECOLI/NEW-IMAGE?type=PATHWAY&object=PWY0-41).

In EcoCyc the pathway is described as being from two molecules of Allantoin to one molecule of 3-Phospho-D-glycerate. Our database contains the same set of reactions.



(Q_S,Q_T) discussion for the BP model

This pathway was recovered with objective (3.13). Thus, the (Q_S,Q_T) discussion is carried out for objective (3.13). The table of pairs for objective (3.13) is shown below.

(number of reactions, excess ATP)		Number of molecules Q_T of target compound					
		1	2	3	4	5	6
Number of molecules Q_S of source compound	1	(9,-1)	(10,-2)	(10,-3)	(10,-4)	(10,-5)	(10,-6)
	2	(6,-1)*	(9,-2)	(9,-3)	(9,-4)	(9,-5)	(9,-6)
	3	(9,-1)	(11,0)	(9,-3)	(10,-4)	(10,-5)	(10,-6)
	4	(9,-1)	(6,-2)	(9,-3)	(9,-4)	(9,-5)	(9,-6)
	5	(9,-1)	(9,-2)	(11,0)	(11,0)	(9,-5)	(10,-6)
	6	(9,-1)	(9,-2)	(6,-3)	(9,-4)	(9,-5)	(9,-6)

The dominant pair is (Q_S,Q_T)=(2,1). Hence in this case the BP model recovers the (Q_S,Q_T)=(2,1) pair observed in the experimentally determined pathway.

(Q_S,Q_T) discussion for the IBP model

This pathway was recovered with both objective (6.26) and objective (6.27). Thus, the (Q_S,Q_T) discussion is carried out for objective (6.26) and objective (6.27). The table of pairs for objective (6.26) is shown below.

(Ψ,W)		Number of molecules Q_T of target compound					
		1	2	3	4	5	6
Number of molecules Q_S of source compound	1	(8.1,0)	(9.38,2)	(9.38,2)	(9.38,2)	(9.38,2)	(9.48,1)
	2	(6,1)*	(8,1)	(8.93,4)	(8.93,4)	(8.93,4)	(8.93,4)
	3	(12.44,3)	(7,1)	(8,1)	(9.14,2)	(9.14,2)	(9.14,2)
	4	(12.44,3)	(6,1)	(7,1)	(8,1)	(8.93,4)	(9.02,3)
	5	(12.44,3)	(9.66,2)	(7,1)	(7,1)	(8,1)	(9.14,2)
	6	(12.44,3)	(9.66,2)	(6,1)	(7,1)	(7,1)	(8,1)

For this pathway the IBP model indicates that the pair (Q_S,Q_T)=(2,1) dominates all other cases. Hence in this case the IBP model recovers the (Q_S,Q_T)=(2,1) pair observed in the experimentally determined pathway.

The results for objective (6.27) are shown below.

(L,W)		Number of molecules Q_T of target compound					
		1	2	3	4	5	6
Number of molecules Q_S of source compound	1	(8,1)	(11,2)	(11,2)	(11,2)	(11,2)	(11,2)
	2	(6,1)*	(8,1)	(11,2)	(11,2)	(11,2)	(11,2)
	3	(12,3)	(11,1)	(8,1)	(11,2)	(11,2)	(11,2)
	4	(12,3)	(6,1)	(11,1)	(8,1)	(11,2)	(11,2)
	5	(12,3)	(12,3)	(11,1)	(11,1)	(8,1)	(11,2)
	6	(12,3)	(12,3)	(6,1)	(11,1)	(11,1)	(8,1)

We obtain the same dominant pair as objective (6.26). Hence for this objective the IBP model recovers the $(Q_S,Q_T)=(2,1)$ pair observed in the experimentally determined pathway.

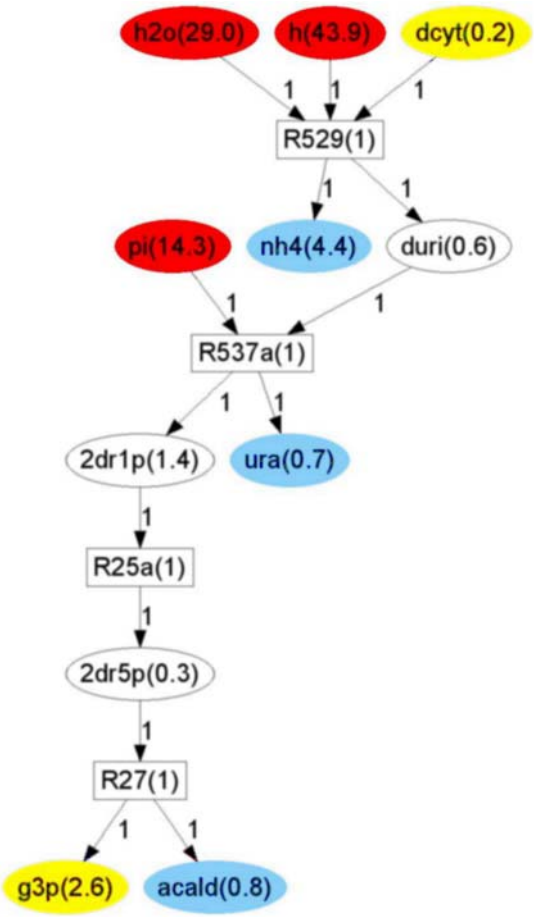
Pathway 34: Deoxycytidine degradation

Source compound	Deoxycytidine (dcyt)
Target compound	Glyceraldehyde 3-phosphate (g3p)
(Q_S,Q_T)	(1,1)
Low presence compounds that are not forced to be balanced	Acetaldehyde (acald) Uracil (ura)
(Number of reactions, excess ATP)	(4,0)
Number of unbalanced main compounds (W)	2
Specificity (Ψ)	5.63

Pathway description

This pathway has been taken from EcoCyc (http://biocyc.org/ECOLI/NEW-IMAGE?type=PATHWAY&object=PWY0-163).

In EcoCyc the pathway is described as being from one molecule of Deoxycytidine to one molecule of Glyceraldehyde 3-phosphate. Our database contains the same set of reactions.



(Q_S,Q_T) discussion for the BP model

This pathway was recovered with both objective (3.13) and objective (3.14). Thus, the (Q_S,Q_T) discussion is carried out for objective (3.13) and objective (3.14). The table of pairs for objective (3.13) is shown below.

(number of reactions, excess ATP)		Number of molecules Q_T of target compound					
		1	2	3	4	5	6
Number of molecules Q_S of source compound	1	(4,0)*	(9,-2)	(9,-4)	(9,-6)	(9,-8)	(9,-10)
	2	X	(4,0)	(9,-2)	(9,-4)	(9,-6)	(9,-8)
	3	X	X	(4,0)	(9,-2)	(9,-4)	(9,-6)
	4	X	X	X	(4,0)	(9,-2)	(9,-4)
	5	X	X	X	X	(4,0)	(9,-2)
	6	X	X	X	X	X	(4,0)

The pairs seen down the diagonal are all repeats of each other, doubling and then tripling, etc the number of source and target molecules. The dominant pair is (Q_S,Q_T)=(1,1). Hence in this case the BP model recovers the (Q_S,Q_T)=(1,1) pair observed in the experimentally determined pathway.

The results for objective (3.14) are shown below.

(number of reactions, excess ATP)		Number of molecules Q_T of target compound					
		1	2	3	4	5	6
Number of molecules Q_S of source compound	1	(4,0)*	(10,0)	(10,0)	(10,0)	(10,0)	(10,0)
	2	X	(4,0)	(10,0)	(10,0)	(10,0)	(10,0)
	3	X	X	(4,0)	(10,0)	(10,0)	(10,0)
	4	X	X	X	(4,0)	(10,0)	(10,0)
	5	X	X	X	X	(4,0)	(10,0)
	6	X	X	X	X	X	(4,0)

The pairs seen down the diagonal are all repeats of each other, doubling and then tripling, etc the number of source and target molecules. The dominant pair is $(Q_S,Q_T)=(1,1)$. Hence in this case the BP model recovers the $(Q_S,Q_T)=(1,1)$ pair observed in the experimentally determined pathway.

(Q_S,Q_T) discussion for the IBP model

This pathway was recovered with both objective (6.26) and objective (6.27). Thus, the (Q_S,Q_T) discussion is carried out for objective (6.26) and objective (6.27). The table of pairs for objective (6.26) is shown below.

(Ψ,W)		Number of molecules Q_T of target compound					
		1	2	3	4	5	6
Number of molecules Q_S of source compound	1	(5.63,2)*	X	(9.2,5)	(9.22,5)	X	(9.22,5)
	2	(12.02,7)	(5.63,2)	(9.97,4)	(8.77,7)	X	(9.2,5)
	3	(12.02,7)	(10.73,8)	(5.63,2)	(9.2,5)	(9.3,4)	(8.87,6)
	4	(12.02,7)	(10.73,8)	(10.73,8)	(5.63,2)	(9.45,6)	(10.47,3)
	5	(12.02,7)	(10.83,7)	(10.73,8)	(10.73,8)	(5.63,2)	(8.93,5)
	6	(12.02,7)	(10.73,8)	(10.83,7)	(10.73,8)	(10.83,7)	(5.63,2)

For this pathway the IBP model indicates that the pair (Q_S,Q_T)=(1,1) dominates all other cases. Hence in this case the IBP model recovers the (Q_S,Q_T)=(1,1) pair observed in the experimentally determined pathway.

The results for objective (6.27) are shown below.

(L,W)		Number of molecules Q_T of target compound					
		1	2	3	4	5	6
Number of molecules Q_S of source compound	1	(4,2)*	(8,7)	(8,7)	(8,7)	(8,7)	(8,7)
	2	(8,7)	(4,2)	(8,7)	(8,7)	(8,7)	(8,7)
	3	(8,7)	(8,7)	(4,2)	(8,7)	(8,7)	(8,7)
	4	(8,7)	(8,7)	(8,7)	(4,2)	(8,7)	(8,7)
	5	(8,7)	(8,7)	(8,7)	(8,7)	(4,2)	(8,7)
	6	(8,7)	(8,7)	(8,7)	(8,7)	(8,7)	(4,2)

We obtain the same dominant pair as objective (6.26). Hence for this objective the IBP model recovers the $(Q_S,Q_T)=(1,1)$ pair observed in the experimentally determined pathway.

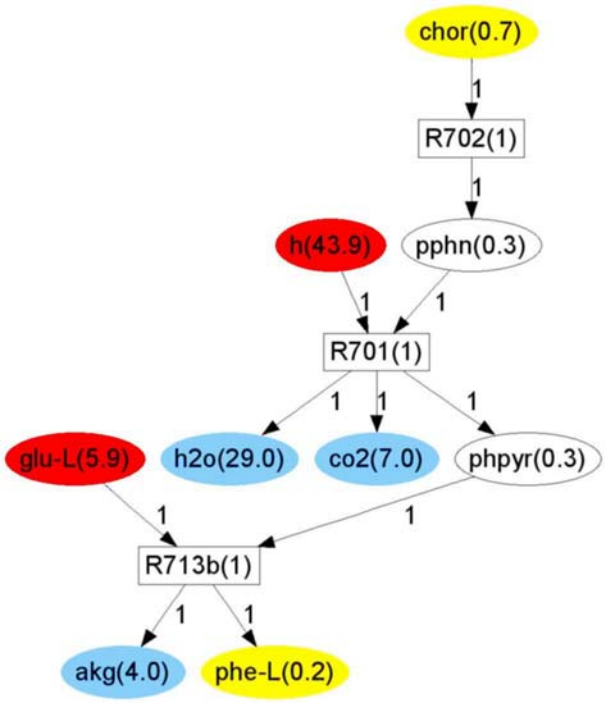
Pathway 35: Phenylalanine biosynthesis

Source compound	Chorismate (chor)
Target compound	L-Phenylalanine (phe-L)
(Q_S,Q_T)	(1,1)
Low presence compounds that are not forced to be balanced	2-Oxoglutarate (akg)
(Number of reactions, excess ATP)	(3,0)
Number of unbalanced main compounds (W)	0
Specificity (Ψ)	3

Pathway description

This pathway has been taken from EcoCyc (http://biocyc.org/ECOLI/NEW-IMAGE?type=PATHWAY&object=PHESYN) and Lehninger (fourth edition) page 851.

In Lehninger the pathway is described as being from one molecule of Chorismate to one molecule of L-Phenylalanine. This pathway is described in the same way in EcoCyc with the same set of reactions.



(Q_S,Q_T) discussion for the BP model

This pathway was recovered with both objective (3.13) and objective (3.14). Thus, the (Q_S,Q_T) discussion is carried out for objective (3.13) and objective (3.14). The table of pairs for objective (3.13) is shown below.

(number of reactions, excess ATP)		Number of molecules Q_T of target compound					
		1	2	3	4	5	6
Number of molecules Q_S of source compound	1	(3,0)*	X	X	X	X	X
	2	X	(3,0)	X	X	X	X
	3	X	X	(3,0)	X	X	X
	4	X	X	X	(3,0)	X	X
	5	X	X	X	X	(3,0)	X
	6	X	X	X	X	X	(3,0)

The pairs seen down the diagonal are all repeats of each other, doubling and then tripling, etc the number of source and target molecules. The dominant pair is (Q_S,Q_T)=(1,1). Hence in this case the BP model recovers the (Q_S,Q_T)=(1,1) pair observed in the experimentally determined pathway.

The results for objective (3.14) are shown below.

(number of reactions, excess ATP)		Number of molecules Q_T of target compound					
		1	2	3	4	5	6
Number of molecules Q_S of source compound	1	(3,0)*	X	X	X	X	X
	2	X	(3,0)	X	X	X	X
	3	X	X	(3,0)	X	X	X
	4	X	X	X	(3,0)	X	X
	5	X	X	X	X	(3,0)	X
	6	X	X	X	X	X	(3,0)

The pairs seen down the diagonal are all repeats of each other, doubling and then tripling, etc the number of source and target molecules. The dominant pair is $(Q_S,Q_T)=(1,1)$. Hence in this case the BP model recovers the $(Q_S,Q_T)=(1,1)$ pair observed in the experimentally determined pathway.

(Q_S,Q_T) discussion for the IBP model

This pathway was recovered with both objective (6.26) and objective (6.27). Thus, the (Q_S,Q_T) discussion is carried out for objective (6.26) and objective (6.27). The table of pairs for objective (6.26) is shown below.

(Ψ,W)		Number of molecules Q_T of target compound					
		1	2	3	4	5	6
Number of molecules Q_S of source compound	1	(3,0)*	X	X	X	X	X
	2	(12.44,4)	(3,0)	X	X	X	X
	3	(12.12,5)	(13.12,5)	(3,0)	X	X	X
	4	(11.97,3)	(11.97,3)	X	(3,0)	X	X
	5	(12.55,3)	X	(12.44,4)	(12.55,3)	(3,0)	X
	6	(13.12,5)	(12.44,4)	X	(12.55,3)	(12.07,3)	(3,0)

For this pathway the IBP model indicates that the pair (Q_S,Q_T)=(1,1) dominates all other cases. Hence in this case the IBP model recovers the (Q_S,Q_T)=(1,1) pair observed in the experimentally determined pathway.

The results for objective (6.27) are shown below.

(L,W)		Number of molecules Q_T of target compound					
		1	2	3	4	5	6
Number of molecules Q_S of source compound	1	(3,0)*	X	X	X	X	X
	2	X	(3,0)	X	X	X	X
	3	(15,7)	(15,7)	(3,0)	X	X	X
	4	(15,8)	(23,6)	(17,2)	(3,0)	X	X
	5	(15,8)	(15,7)	(14,8)	(15,3)	(3,0)	X
	6	(15,8)	X	X	X	X	(3,0)

We obtain the same dominant pair as objective (6.26). Hence for this objective the IBP model recovers the $(Q_S,Q_T)=(1,1)$ pair observed in the experimentally determined pathway.

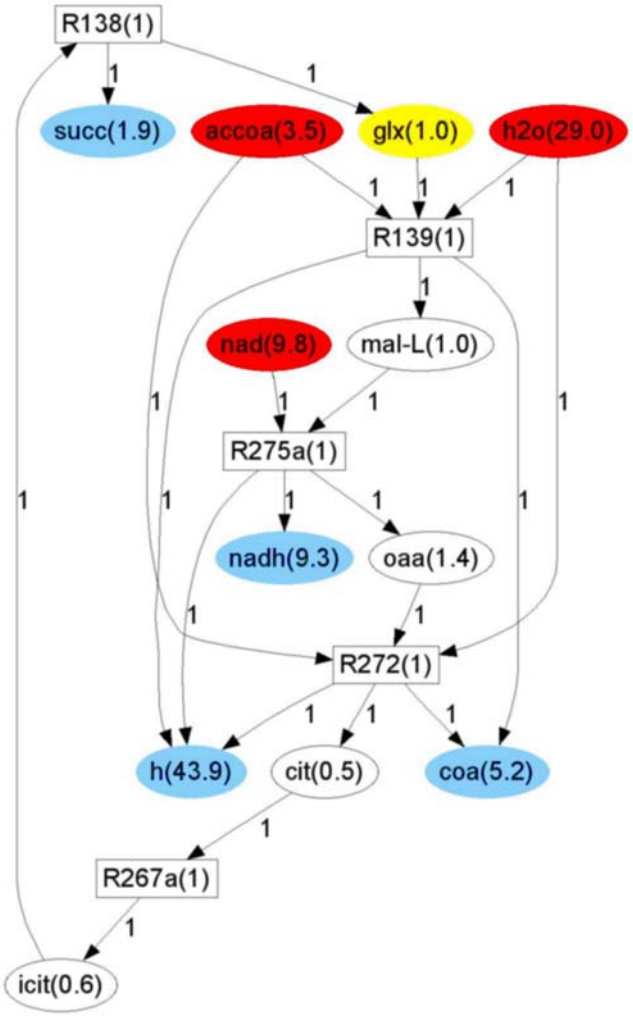
Pathway 36: Glyoxylate cycle

Source compound	Glyoxylate (glx)
Target compound	Glyoxylate (glx)
(Q_S,Q_T)	(1,1)
Low presence compounds that are not forced to be balanced	Succinate (succ) Acetyl-CoA (accoa)
(Number of reactions, excess ATP)	(5,0)
Number of unbalanced main compounds (W)	1
Specificity (Ψ)	5

Pathway description

This pathway has been taken from EcoCyc (http://biocyc.org/ECOLI/NEW-IMAGE?type=PATHWAY&object=GLYOXYLATE-BYPASS) and Lehninger (fourth edition) pages 623 and 625.

Both in Lehninger and EcoCyc, the pathway is described as being a cycle starting and finishing at glyoxylate. However, Lehninger does not include the intermediary reaction citrate -> cis-aconitate + H20, included in EcoCyc. Since our reaction database does not contain this reaction, we have selected the Lehninger pathway.



(Q_S,Q_T) discussion for the BP model

This pathway was recovered with objective (3.13). Thus, the (Q_S,Q_T) discussion is carried out for objective (3.13). The table of pairs for objective (3.13) is shown below.

(number of reactions, excess ATP)		Number of molecules Q_T of target compound					
		1	2	3	4	5	6
Number of molecules Q_S of source compound	1	(5,0)*	(6,0)	(6,0)	(6,0)	(6,0)	(6,0)
	2	(6,0)	(5,0)	(6,0)	(6,0)	(6,0)	(6,0)
	3	(6,0)	(6,0)	(5,0)	(6,0)	(6,0)	(6,0)
	4	(6,0)	(6,0)	(6,0)	(5,0)	(6,0)	(6,0)
	5	(6,0)	(6,0)	(6,0)	(6,0)	(5,0)	(6,0)
	6	(6,0)	(6,0)	(6,0)	(6,0)	(6,0)	(5,0)

The pairs seen down the diagonal are all repeats of each other, doubling and then tripling, etc the number of source and target molecules. The dominant pair is (Q_S,Q_T)=(1,1). Hence in this case the BP model recovers the (Q_S,Q_T)=(1,1) pair observed in the experimentally determined pathway.

In this pathway the source compound and the target compound are the same, moreover in the experimentally determined pathway the source/target compound is balanced (since Q_S=Q_T=1). It is therefore possible to interpret this pathway, a cycle, such that the only valid cases in the above (Q_S,Q_T) table of pairs are the diagonal entries (which are the only cases where the source/target compound is balanced). However even if we adopt this interpretation (which we did for the TCA cycle, pathway 8, above)

the dominant pair is still $(Q_S,Q_T)=(1,1)$ and the BP model still recovers the $(Q_S,Q_T)=(1,1)$ pair observed in the experimentally determined pathway.

(Q_S,Q_T) discussion for the IBP model

This pathway was not recovered with either objective (6.26) or objective (6.27). However, when applied the cyclic constraints presented in Chapter 6, we achieved recovery for objective (6.26). In particular, we found two cases where we achieved recovery, namely adding equation (6.29) or (6.30). The table of pairs for these cases are presented below. As noted above, we only examined pairs in the main diagonal. The table of pairs for (6.26) with (6.29) added is:

(Ψ,W)		Number of molecules Q_T of target compound					
		1	2	3	4	5	6
Number	1	(5,1)*	-	-	-	-	-
of	2	-	(5,1)	-	-	-	-
molecules	3	-	-	(5,1)	-	-	-
Q_S of	4	-	-	-	(5,1)	-	-
source	5	-	-	-	-	(5,1)	-
compound	6	-	-	-	-	-	(5,1)

The table of pairs for (6.26) with (6.30) added is:

(Ψ,W)		Number of molecules Q_T of target compound					
		1	2	3	4	5	6
Number of molecules Q_S of source compound	1	(5,1)*	-	-	-	-	-
	2	-	(5,1)	-	-	-	-
	3	-	-	(5,1)	-	-	-
	4	-	-	-	(5,1)	-	-
	5	-	-	-	-	(5,1)	-
	6	-	-	-	-	-	(5,1)

For both cases, the dominant pair is $(Q_S,Q_T)=(1,1)$. Hence for this objective the IBP model (adding constraints related to cyclic pathways) recovers the $(Q_S,Q_T)=(1,1)$ pair observed in the experimentally determined pathway.

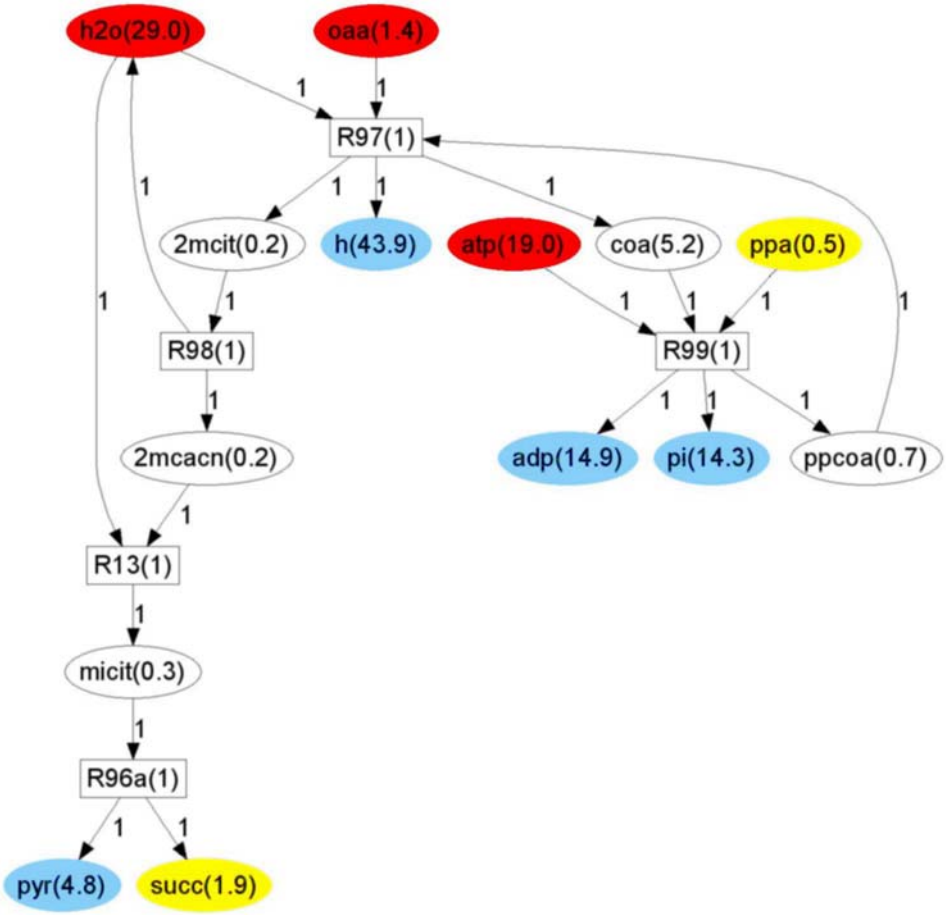
Pathway 37: Propionate degradation

Source compound	Propionate (ppa)
Target compound	Succinate (succ)
(Q_S,Q_T)	(1,1)
Low presence compounds that are not forced to be balanced	Oxaloacetate (oaa)
(Number of reactions, excess ATP)	(5,-1)
Number of unbalanced main compounds (W)	1
Specificity (Ψ)	5

Pathway description

This pathway has been taken from EcoCyc (http://biocyc.org/ECOLI/NEW-IMAGE?type=PATHWAY&object=PWY0-42).

In EcoCyc the pathway is described as being from one molecule of Propionate to one molecule of Succinate. Our database contains the same set of reactions, only changing the cofactor utilised in the first reaction of the pathway.



Note here that we have an allowable c-cycles in this pathway. More precisely the 2-cycle coa-R99-ppcoa-R97-coa which contains one high presence balanced compound (coa).

(Q_S,Q_T) discussion for the BP model

This pathway was recovered with objective (3.13). Thus, the (Q_S,Q_T) discussion is carried out for objective (3.13). The table of pairs for objective (3.13) is shown below.

(number of reactions, excess ATP)		Number of molecules Q_T of target compound					
		1	2	3	4	5	6
Number of molecules Q_S of source compound	1	(5,-1)*	(9,-1)	(8,1)	(8,2)	(8,3)	(8,4)
	2	X	(5,-2)	(8,-1)	(9,-2)	(8,1)	(8,2)
	3	X	X	(5,-3)	(8,-2)	(8,-1)	(9,-3)
	4	X	X	X	(5,-4)	(8,-3)	(8,-2)
	5	X	X	X	X	(5,-5)	(8,-4)
	6	X	X	X	X	X	(5,-6)

The pairs seen down the diagonal are all repeats of each other, doubling and then tripling, etc the number of source and target molecules (and excess ATP). The dominant pair is (Q_S,Q_T)=(1,1). Hence in this case the BP model recovers the (Q_S,Q_T)=(1,1) pair observed in the experimentally determined pathway.

(Q_S,Q_T) discussion for the IBP model

This pathway was recovered with both objective (6.26) and objective (6.27). Thus, the (Q_S,Q_T) discussion is carried out for objective (6.26) and objective (6.27). The table of pairs for objective (6.26) is shown below.

(Ψ,W)		Number of molecules Q_T of target compound					
		1	2	3	4	5	6
Number of molecules Q_S of source compound	1	(5,1)*	(7.94,2)	(7.94,2)	(7.94,2)	(7.94,2)	(7.94,2)
	2	X	(5,1)	(7.94,2)	(7.94,2)	(7.94,2)	(7.94,2)
	3	X	X	(5,1)	(7.94,2)	(7.94,2)	(7.94,2)
	4	X	X	X	(5,1)	(7.94,2)	(7.94,2)
	5	X	X	X	X	(5,1)	(7.94,2)
	6	X	X	X	X	X	(5,1)

For this pathway the IBP model indicates that the pair (Q_S,Q_T)=(1,1) dominates all other cases. Hence in this case the IBP model recovers the (Q_S,Q_T)=(1,1) pair observed in the experimentally determined pathway.

The results for objective (6.27) are shown below.

(L,W)		Number of molecules Q_T of target compound					
		1	2	3	4	5	6
Number	1	(5,1)*	(9,2)	(9,2)	(9,2)	(9,2)	(9,2)
of	2	X	(5,1)	(9,2)	(9,2)	(9,2)	(9,2)
molecules	3	X	X	(5,1)	(9,2)	(9,2)	(9,2)
Q_S of	4	X	X	X	(5,1)	(9,2)	(9,2)
source	5	X	X	X	X	(5,1)	(9,2)
compound	6	X	X	X	X	X	(5,1)

We obtain the same dominant pair as objective (6.26). Hence for this objective the IBP model recovers the $(Q_S,Q_T)=(1,1)$ pair observed in the experimentally determined pathway.

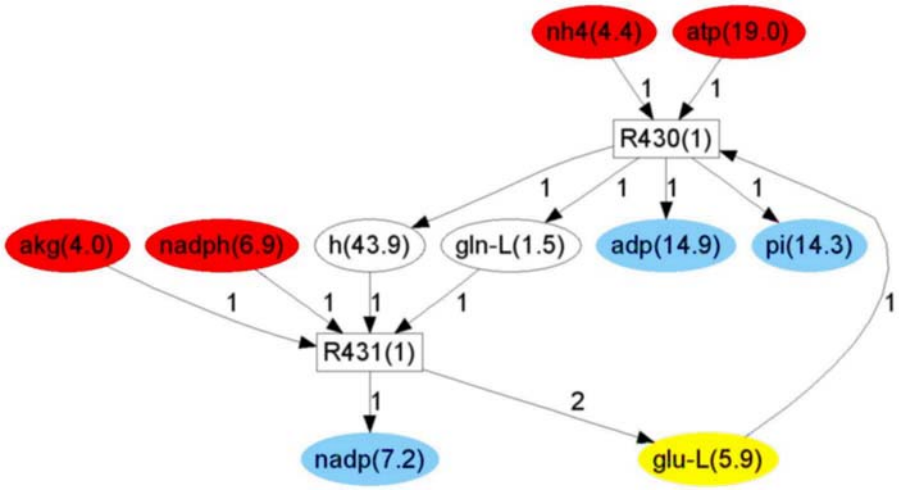
Pathway 38: Glutamate biosynthesis cycle

Source compound	L-Glutamate (glu-L)
Target compound	L-Glutamate (glu-L)
(Q_S,Q_T)	(1,2)
Low presence compounds that are not forced to be balanced	2-Oxoglutarate (akg)
(Number of reactions, excess ATP)	(2,-1)
Number of unbalanced main compounds (W)	0
Specificity (Ψ)	2.16

Pathway description

This pathway has been taken from EcoCyc (http://biocyc.org/ECOLI/NEW-IMAGE?type=PATHWAY&object=AMMASSIM-PWY) and Lehninger (fourth edition) pages 837 and 838.

In Lehninger the pathway is described as being from one molecule of L-Glutamate to two molecules of L-Glutamate. This pathway is described in the same way in EcoCyc with the same set of reactions.



(Q_S,Q_T) discussion for the BP model

This pathway was recovered with objective (3.13). Thus, the (Q_S,Q_T) discussion is carried out for objective (3.13). The table of pairs for objective (3.13) is shown below.

(number of reactions, excess ATP)		Number of molecules Q_T of target compound					
		1	2	3	4	5	6
Number of molecules Q_S of source compound	1	(2,-1)	(2,-1)*	(3,-1)	(3,-1)	(3,-1)	(3,-1)
	2	(6,-1)	(2,-2)	(3,-2)	(2,-2)	(3,-2)	(3,-2)
	3	(7,-3)	(7,-3)	(2,-3)	(3,-3)	(3,-3)	(2,-3)
	4	(7,-4)	(6,-2)	(7,-4)	(2,-4)	(3,-4)	(3,-4)
	5	(7,-5)	(7,-5)	(7,-5)	(7,-5)	(2,-5)	(3,-5)
	6	(7,-6)	(7,-6)	(6,-3)	(7,-6)	(7,-6)	(2,-6)

In this pathway a tie between the entries (Q_S,Q_T)=(1,1) and (Q_S,Q_T)=(1,2) is observed above as both entries have the same number of reactions and molecules of ATP produced, (2,-1). However, one further target molecule is produced by (Q_S,Q_T)=(1,2) with respect to (Q_S,Q_T)=(1,1). Hence, the dominant pair is (Q_S,Q_T)=(1,2) and the BP model recovers the (Q_S,Q_T)=(1,2) pair observed in the experimentally determined pathway.

(Q_S,Q_T) discussion for the IBP model

This pathway was recovered with both objective (6.26) and objective (6.27). Thus, the (Q_S,Q_T) discussion is carried out for objective (6.26) and objective (6.27). The table of pairs for objective (6.26) is shown below.

(Ψ,W)		Number of molecules Q_T of target compound					
		1	2	3	4	5	6
Number of molecules Q_S of source compound	1	(2.32,0)	(2.16,0)*	(6.94,4)	(7.59,2)	X	(9.96,6)
	2	(6.06,2)	(2.32,0)	(2.24,0)	(2.16,0)	(16.1,2)	(6.57,4)
	3	(6.09,2)	(6.9,2)	(2.32,0)	(2.24,0)	(2.24,0)	(2.16,0)
	4	X	(6.09,2)	X	(2.32,0)	(2.24,0)	(2.24,0)
	5	(5.99,1)	(6.09,1)	(6.19,2)	X	(2.32,0)	(2.24,0)
	6	(6.06,2)	(5.99,2)	(9.27,4)	(5.68,0)	X	(2.32,0)

For this pathway the IBP model indicates that the pair (Q_S,Q_T)=(1,2) dominates all other cases. Hence in this case the IBP model recovers the (Q_S,Q_T)=(1,2) pair observed in the experimentally determined pathway.

The results for objective (6.27) are shown below.

(L,W)		Number of molecules Q_T of target compound					
		1	2	3	4	5	6
Number of molecules Q_S of source compound	1	(2,0)	(2,0)*	(3,3)	(6,4)	(6,4)	(6,4)
	2	(3,1)	(2,0)	(3,0)	(2,0)	(4,3)	(3,3)
	3	(6,2)	(4,2)	(2,0)	(3,0)	(3,0)	(2,0)
	4	(6,2)	(3,1)	(4,2)	(2,0)	(3,0)	(3,0)
	5	(6,4)	(8,7)	(4,2)	(4,2)	(2,0)	(3,0)
	6	X	(6,2)	(3,1)	(4,2)	(4,2)	(2,0)

We obtain the same dominant pair as objective (6.26). Hence for this objective the IBP model recovers the $(Q_S,Q_T)=(1,2)$ pair observed in the experimentally determined pathway.

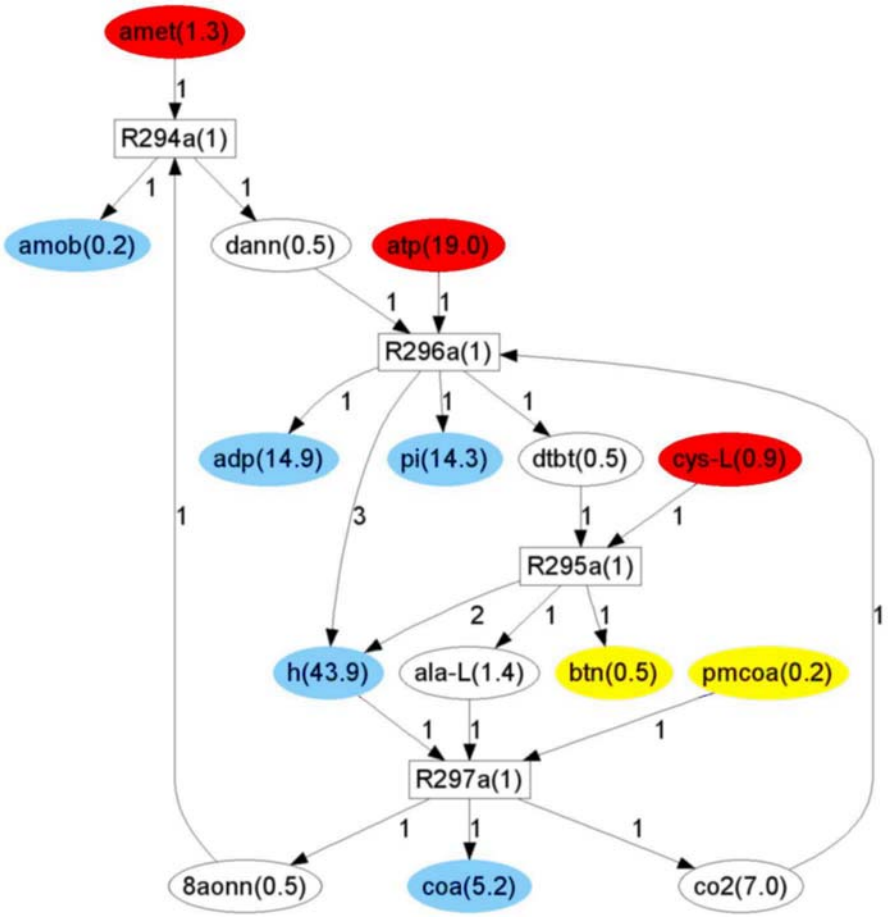
Pathway 39: Biotin biosynthesis

Source compound	Pimeloyl-CoA (pmcoa)
Target compound	Biotin (btn)
(Q_S,Q_T)	(1,1)
Low presence compounds that are not forced to be balanced	S-Adenosyl-L-methionine (amet) L-Cysteine (cys-L) S-Adenosyl-4-methylthio-2-oxobutanoate (amob)
(Number of reactions, excess ATP)	(4,-1)
Number of unbalanced main compounds (W)	3
Specificity (Ψ)	4.47

Pathway description

This pathway has been taken from EcoCyc (http://biocyc.org/ECOLI/NEW-IMAGE?type=PATHWAY&object=BIOTIN-SYNTHESIS-PWY).

In EcoCyC the pathway is described as being from one molecule of Pimeloyl-CoA to one molecule of Biotin. Our database contains the same reactions, aside from the last one in which a different cofactor is used, L-Cysteine instead of S-Adenosyl-L-methionine.



(Q_S,Q_T) discussion for the BP model

This pathway was not recovered with either of the objectives. Since this pathway is not recovered, (Q_S,Q_T) pairs discussion is omitted.

(Q_S,Q_T) discussion for the IBP model

This pathway was recovered with both objective (6.26) and objective (6.27). Thus, the (Q_S,Q_T) discussion is carried out for objective (6.26) and objective (6.27). The table of pairs for objective (6.26) is shown below.

(Ψ,W)		Number of molecules Q_T of target compound					
		1	2	3	4	5	6
Number	1	(4.47,3)*	X	X	X	X	X
of	2	X	(4.47,3)	X	X	X	X
molecules	3	X	X	(4.47,3)	X	X	X
Q_S of	4	X	X	X	(4.47,3)	X	X
source	5	X	X	X	X	(4.47,3)	X
compound	6	X	X	X	X	X	(4.47,3)

For this pathway the IBP model indicates that the pair (Q_S,Q_T)=(1,1) dominates all other cases. Hence in this case the IBP model recovers the (Q_S,Q_T)=(1,1) pair observed in the experimentally determined pathway.

The results for objective (6.27) are shown below.

(L,W)		Number of molecules Q_T of target compound					
		1	2	3	4	5	6
Number	1	(4,3)*	X	X	X	X	X
of	2	X	(4,3)	X	X	X	X
molecules	3	X	X	(4,3)	X	X	X
Q_S of	4	X	X	X	(4,3)	X	X
source	5	X	X	X	X	(4,3)	X
compound	6	X	X	X	X	X	(4,3)

We obtain the same dominant pair as objective (6.26). Hence for this objective the IBP model recover the $(Q_S,Q_T)=(1,1)$ pair observed in the experimentally determined pathway.

Pathway 40: Glycerol degradation

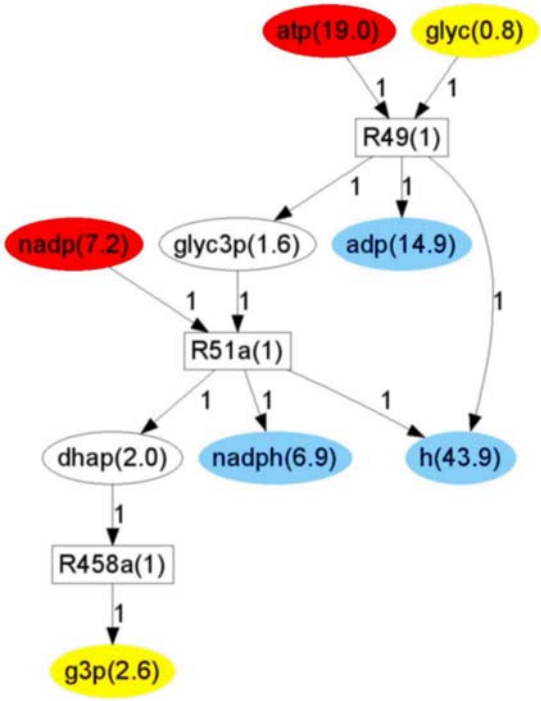
Source compound	Glycerol (glyc)
Target compound	Glyceraldehyde 3-phosphate (g3p)
(Q_S,Q_T)	(1,1)
Low presence compounds that are not forced to be balanced	
(Number of reactions, excess ATP)	(3,-1)
Number of unbalanced main compounds (W)	0
Specificity (Ψ)	3

Pathway description

This pathway has been taken from EcoCyc (http://biocyc.org/ECOLI/NEW-IMAGE?type=PATHWAY&object=PWY0-381) and Lehninger (fourth edition) page 635.

In Lehninger the pathway is described as being from one molecule of glycerol to one molecule of Glyceraldehyde 3-phosphate. This pathway is described in the same way in EcoCyc with the same set of reactions, except that EcoCyc does not include the last reaction, producing one molecule of Dihydroxyacetone phosphate instead of one molecule of Glyceraldehyde 3-phosphate.

Since the Lehninger description appears to be the clearer one it is that which has informed the pathway picture seen below.



(Q_S,Q_T) discussion for the BP model

This pathway was recovered with objective (3.13). Thus, the (Q_S,Q_T) discussion is carried out for objective (3.13). The table of pairs for objective (3.13) is shown below.

(number of reactions, excess ATP)		Number of molecules Q_T of target compound					
		1	2	3	4	5	6
Number of molecules Q_S of source compound	1	(3,-1)*	(8,-3)	(8,-5)	(8,-7)	(8,-9)	(8,-11)
	2	X	(3,-2)	(8,-4)	(8,-6)	(8,-8)	(8,-10)
	3	X	X	(3,-3)	(8,-5)	(8,-7)	(8,-9)
	4	X	X	X	(3,-4)	(8,-6)	(8,-8)
	5	X	X	X	X	(3,-5)	(8,-7)
	6	X	X	X	X	X	(3,-6)

The pairs seen down the diagonal are all repeats of each other, doubling and then tripling, etc the number of source and target molecules (and excess ATP). The dominant pair is (Q_S,Q_T)=(1,1). Hence in this case the BP model recovers the (Q_S,Q_T)=(1,1) pair observed in the experimentally determined pathway.

(Q_S,Q_T) discussion for the IBP model

This pathway was recovered with both objective (6.26) and objective (6.27). Thus, the (Q_S,Q_T) discussion is carried out for objective (6.26) and objective (6.27). The table of pairs for objective (6.26) is shown below.

(Ψ,W)		Number of molecules Q_T of target compound					
		1	2	3	4	5	6
Number of molecules Q_S of source compound	1	(3,0)*	(7.64,4)	(7.74,3)	(7.74,3)	(7.64,4)	(7.64,4)
	2	(10.29,4)	(3,0)	(6.64,3)	(6.64,3)	(6.64,3)	(6.74,2)
	3	(10.29,4)	(8.12,4)	(3,0)	(6.64,3)	(6.74,2)	(6.64,3)
	4	(10.29,4)	(9.64,5)	(8.12,4)	(3,0)	(6.64,3)	(6.64,3)
	5	(10.29,4)	(9.74,4)	(8.12,4)	(8.22,3)	(3,0)	(6.74,2)
	6	(10.29,4)	(9.64,5)	(9.64,5)	(8.22,3)	(8.22,3)	(3,0)

For this pathway the IBP model indicates that the pair (Q_S,Q_T)=(1,1) dominates all other cases. Hence in this case the IBP model recovers the (Q_S,Q_T)=(1,1) pair observed in the experimentally determined pathway.

The results for objective (6.27) are shown below.

(L,W)		Number of molecules Q_T of target compound					
		1	2	3	4	5	6
Number of molecules Q_S of source compound	1	(3,0)*	(9,4)	(9,4)	(10,3)	(9,4)	(9,4)
	2	(9,4)	(3,0)	(11,5)	(9,4)	(9,4)	(9,4)
	3	(9,4)	(9,4)	(3,0)	(9,4)	(9,4)	(9,4)
	4	(9,4)	(9,4)	(9,4)	(3,0)	(10,3)	(10,3)
	5	(9,3)	(9,4)	(9,3)	(9,3)	(3,0)	(9,4)
	6	(9,4)	(9,4)	(9,4)	X	(11,3)	(3,0)

We obtain the same dominant pair as objective (6.26). Hence for this objective the IBP model recovers the $(Q_S,Q_T)=(1,1)$ pair observed in the experimentally determined pathway.