

Additional file 2: Pathway examples

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1 geranyl pyrophosphate

1.1 pathway candidate 1: mevalonate pathway

number of active reactions: 8
starts with basic: False
reactions w/o dG: 0
sum (dG + |dG|): 0
dG: -2.154517e+02
number of heterologous enzymes: 5
number of cofactors: 8

number of side reactions: 11

R08549 : 2-Oxoglutarate dehydrogenase complex -2.723933
e+01

substrates:

1	C00026	2-Oxoglutarate
1	C00010	CoA
1	C00003	NAD+

products:

1	C00091	Succinyl-CoA
1	C00011	CO2
1	C00004	NADH
1	C00080	H+

R02084 : succinyl-CoA:3-hydroxy-3-methylglutarate CoA-
transferase -3.166626e+00

substrates:

1	C00091	Succinyl-CoA
1	C03761	3-Hydroxy-3- methylglutarate

products:

1	C00042	Succinate
1	C00356	(S)-3-Hydroxy-3- methylglutaryl-CoA

R02082 : (R)-Mevalonate:NADP+ oxidoreductase (CoA
acylating) -2.534910e+01

substrates:

1	C00356	(S)-3-Hydroxy-3-
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			methylglutaryl-CoA
	2	C00005	NADPH
	2	C00080	H+
	products:		
	1	C00418	(R)-Mevalonate
	1	C00010	CoA
	2	C00006	NADP+
R02245 : ATP:(R)-mevalonate 5-phosphotransferase			
-1.348146e+01			
	substrates:		
	1	C00002	ATP
	1	C00418	(R)-Mevalonate
	products:		
	1	C00008	ADP
	1	C01107	(R)-5-Phosphomevalonate
R03245 : ATP:(R)-5-phosphomevalonate phosphotransferase			
-2.712405e+00			
	substrates:		
	1	C00002	ATP
	1	C01107	(R)-5-Phosphomevalonate
	products:		
	1	C00008	ADP
	1	C01143	(R)-5-Diphosphomevalonate
R01121 : ATP:(R)-5-diphosphomevalonate carboxy-lyase (
adding ATP -6.741552e+01			
	substrates:		
	1	C00002	ATP
	1	C01143	(R)-5-Diphosphomevalonate
	products:		
	1	C00008	ADP
	1	C00009	Orthophosphate
	1	C00129	Isopentenyl diphosphate
	1	C00011	CO2
R01123 : Isopentenyl-diphosphate delta3-delta2-isomerase			
-4.902559e+00			

substrates:
1 C00129 Isopentenyl diphosphate

products:
1 C00235 Dimethylallyl diphosphate

R01658 : Dimethylallyl-diphosphate:isopentenyl-
diphosphate dimethylallyltranstransferase
-7.118467e+01

substrates:
1 C00235 Dimethylallyl diphosphate
1 C00129 Isopentenyl diphosphate

products:
1 C00013 Diphosphate
1 C00341 Geranyl diphosphate

1.2 overall balance

1.3 side reactions

R00089 : ATP diphosphate-lyase (cyclizing

substrates:

1 C00002 ATP

products:

1 C00575 3',5'-Cyclic AMP

1 C00013 Diphosphate

R00104 : ATP:NAD⁺ 2'-phosphotransferase

substrates:

1 C00002 ATP

1 C00003 NAD⁺

products:

1 C00008 ADP

1 C00006 NADP⁺

R00112 : NADPH:NAD⁺ oxidoreductase

substrates:

1 C00005 NADPH

1 C00003 NAD⁺

products:

1 C00006 NADP⁺

1 C00004 NADH

R00405 : Succinate:CoA ligase (ADP-forming)

substrates:

1 C00002 ATP

1 C00042 Succinate

1 C00010 CoA

products:

1 C00008 ADP

1 C00009 Orthophosphate

1 C00091 Succinyl-CoA

R02003 : Geranyl-diphosphate:isopentenyl-diphosphate
geranyltrans-transferase

substrates:
 1 C00341 Geranyl diphosphate
 1 C00129 Isopentenyl diphosphate

products:
 1 C00013 Diphosphate
 1 C00448 trans , trans-Farnesyl
 diphosphate

-R00127 : -ATP:AMP phosphotransferase

substrates:
 2 C00008 ADP

products:
 1 C00002 ATP
 1 C00020 AMP

-R00130 : -ATP:dephospho-CoA 3'-phosphotransferase

substrates:
 1 C00008 ADP
 1 C00010 CoA

products:
 1 C00002 ATP
 1 C00882 Dephospho-CoA

-R00137 : -ATP:nicotinamide-nucleotide
 adenylyltransferase

substrates:
 1 C00013 Diphosphate
 1 C00003 NAD⁺

products:
 1 C00002 ATP
 1 C00455 Nicotinamide D-
 ribonucleotide

-R00267 : -Isocitrate:NADP⁺ oxidoreductase (
 decarboxylating)

substrates:
 1 C00026 2-Oxoglutarate
 1 C00011 CO₂

	1	C00005	NADPH
	1	C00080	H+
	products:		
	1	C00311	Isocitrate
	1	C00006	NADP+
-R00519 : -formate:NAD+ oxidoreductase			
	substrates:		
	1	C00080	H+
	1	C00011	CO2
	1	C00004	NADH
	products:		
	1	C00058	Formate
	1	C00003	NAD+
-R00833 : -(R)-Methylmalonyl-CoA CoA-carbonylmutase			
	substrates:		
	1	C00091	Succinyl-CoA
	products:		
	1	C01213	(R)-Methylmalonyl-CoA

1.4 pathway candidate: non-mevalonate pathway

number of active reactions: 9
starts with basic: False
reactions w/o dG: 2
sum (dG + |dG|):0
dG: -1.998150e+02
number of heterologous enzymes: 0
number of cofactors: 3

number of side reactions: 24

R05636 : 1-Deoxy-D-xylulose 5-phosphate pyruvate-lyase (carboxylating) -2.901798e+01

substrates:

1	C00022	Pyruvate
1	C00118	D-Glyceraldehyde 3-phosphate

products:

1	C11437	1-Deoxy-D-xylulose 5-phosphate
1	C00011	CO2

R05688 : 1-Deoxy-D-xylulose 5-phosphate isomeroreductase -2.321112e+01

substrates:

1	C11437	1-Deoxy-D-xylulose 5-phosphate
1	C00005	NADPH
1	C00080	H+

products:

1	C11434	2-C-Methyl-D-erythritol 4-phosphate
1	C00006	NADP+

R05633 : CTP: 2-C-Methyl-D-erythritol 4-phosphate cytidyltransferase -4.729713e+00

substrates:

1	C11434	2-C-Methyl-D-erythritol 4-phosphate
1	C00063	CTP

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products:
  1          C11435  4-(Cytidine 5'-diphospho)
                    -2-C-methyl-D-erythritol
  1          C00013  Diphosphate

R05634 : ATP:4-(Cytidine 5'-diphospho)-2-C-methyl-D-
        erythritol 2-phosphotransferase          -5.273891e+00

substrates:
  1          C11435  4-(Cytidine 5'-diphospho)
                    -2-C-methyl-D-erythritol
  1          C00002  ATP

products:
  1          C11436  2-Phospho-4-(cytidine 5'-
                    diphospho)-2-C-methyl-D-erythritol
  1          C00008  ADP

R05637 : 2-Phospho-4-(cytidine 5'-diphospho)-2-C-methyl-D-
        -erythritol CMP-lyase (cyclizing)          0

substrates:
  1          C11436  2-Phospho-4-(cytidine 5'-
                    diphospho)-2-C-methyl-D-erythritol

products:
  1          C11453  2-C-Methyl-D-erythritol
                    2,4-cyclodiphosphate
  1          C00055  CMP

R08689 : (E)-4-hydroxy-3-methylbut-2-en-1-yl-diphosphate:
        oxidized ferredoxin oxidoreductase (hydrating) 0

substrates:
  1          C11453  2-C-Methyl-D-erythritol
                    2,4-cyclodiphosphate
  2          C00138  Reduced ferredoxin

products:
  1          C11811  1-Hydroxy-2-methyl-2-
                    butenyl 4-diphosphate
  1          C00001  H2O
  2          C00139  Oxidized ferredoxin

R08210 : dimethylallyl diphosphate:ferredoxin

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oxidoreductase -6.639758e+01

substrates:

1	C11811	1-Hydroxy-2-methyl-2-
		butenyl 4-diphosphate
2	C00138	Reduced ferredoxin
2	C00080	H+

products:

1	C00235	Dimethylallyl diphosphate
1	C00001	Oxidized ferredoxin
2	C00139	H2O

R01658 : Dimethylallyl-diphosphate:isopentenyl-
diphosphate dimethylallyltransferase
-7.118467e+01

substrates:

1	C00235	Dimethylallyl diphosphate
1	C00129	Isopentenyl diphosphate

products:

1	C00013	Diphosphate
1	C00341	Geranyl diphosphate

-R01123 : -Isopentenyl-diphosphate delta3-delta2-
isomerase 0

substrates:

1	C00235	Dimethylallyl diphosphate
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products:

1	C00129	Isopentenyl diphosphate
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1.5 overall balance

Table 2: Overall balance of the pathway candidate representing the non-mevalonate pathway

		R01658	R05633	R05634	R05636	R05637	R05688	R08210	R08689	-R01123	overall
Dimethylallyl	diphosphate	-1	0	0	0	0	0	1	0	-1	-1
Isopentenyl	diphosphate	-1	0	0	0	0	0	0	0	1	0
Diphosphate		1	1	0	0	0	0	0	0	0	2
Geranyl	diphosphate	1	0	0	0	0	0	0	0	0	1
2-C-Methyl-D-erythritol	4-phosphate	0	-1	0	0	0	1	0	0	0	0
CTP		0	-1	0	0	0	0	0	0	0	-1
4-(Cytidine	5-diphospho)-2-C-methyl-D-erythritol	0	1	-1	0	0	0	0	0	0	0
ATP		0	0	-1	0	0	0	0	0	0	-1
2-Phospho-4-(cytidine	5-diphospho)-2-C-methyl-D-erythritol	0	0	1	0	-1	0	0	0	0	0
ADP		0	0	1	0	0	0	0	0	0	1
Pyruvate		0	0	0	-1	0	0	0	0	0	-1
D-Glyceraldehyde	3-phosphate	0	0	0	-1	0	0	0	0	0	-1
1-Deoxy-D-xylulose	5-phosphate	0	0	0	1	0	-1	0	0	0	0
CO2		0	0	0	1	0	0	0	0	0	1
2-C-Methyl-D-erythritol	2,4-cyclodiphosphate	0	0	0	0	1	0	0	-1	0	0
CMP		0	0	0	0	1	0	0	0	0	1
NADPH		0	0	0	0	0	-1	0	0	0	-1
H+		0	0	0	0	0	-1	-2	0	0	-3
NADP+		0	0	0	0	0	1	0	0	0	1
1-Hydroxy-2-methyl-2-butenyl	4-diphosphate	0	0	0	0	0	0	-1	1	0	0
Reduced ferredoxin		0	0	0	0	0	0	-2	-2	0	-4
Oxidized ferredoxin		0	0	0	0	0	0	2	2	0	4
H2O		0	0	0	0	0	0	1	1	0	2

1.6 side reactions

R00004 : diphosphate phosphohydrolase

substrates:

1	C00013	Diphosphate
1	C00001	H2O

products:

2	C00009	Orthophosphate
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R00086 : ATP phosphohydrolase

substrates:

1	C00002	ATP
1	C00001	H2O

products:

1	C00008	ADP
1	C00009	Orthophosphate

R00087 : ATP diphosphohydrolase (diphosphate-forming)

substrates:

1	C00002	ATP
1	C00001	H2O

products:

1	C00020	AMP
1	C00013	Diphosphate

R00089 : ATP diphosphate-lyase (cyclizing

substrates:

1	C00002	ATP
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products:

1	C00575	3,5-Cyclic AMP
1	C00013	Diphosphate

R00199 : ATP:pyruvate,water phosphotransferase

substrates:

1	C00002	ATP
1	C00022	Pyruvate
1	C00001	H2O

products:
 1 C00020 AMP
 1 C00074 Phosphoenolpyruvate
 1 C00009 Orthophosphate

R00200 : ATP:pyruvate 2-O-phosphotransferase

substrates:
 1 C00002 ATP
 1 C00022 Pyruvate

products:
 1 C00008 ADP
 1 C00074 Phosphoenolpyruvate

R00511 : cytidine-5-monophosphate phosphohydrolase

substrates:
 1 C00055 CMP
 1 C00001 H2O

products:
 1 C00475 Cytidine
 1 C00009 Orthophosphate

R00512 : ATP:TMP phosphotransferase

substrates:
 1 C00002 ATP
 1 C00055 CMP

products:
 1 C00008 ADP
 1 C00112 CDP

R00515 : CTP diphosphohydrolase (diphosphate-forming)

substrates:
 1 C00063 CTP
 1 C00001 H2O

products:
 1 C00055 CMP
 1 C00013 Diphosphate

R00568 : CTP aminohydrolase

substrates:

1	C00063	CTP
1	C00001	H2O

products:

1	C00075	UTP
1	C00014	Ammonia

R00572 : CTP:pyruvate 2-O-phosphotransferase

substrates:

1	C00063	CTP
1	C00022	Pyruvate

products:

1	C00112	CDP
1	C00074	Phosphoenolpyruvate

R01015 : D-glyceraldehyde-3-phosphate aldose-ketose-isomerase

substrates:

1	C00118	D-Glyceraldehyde 3-phosphate
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products:

1	C00111	Glycerone phosphate
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R01123 : Isopentenyl-diphosphate delta3-delta2-isomerase

substrates:

1	C00129	Isopentenyl diphosphate
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products:

1	C00235	Dimethylallyl diphosphate
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R01195 : Ferredoxin:NADP+ oxidoreductase

substrates:

1	C00006	Reduced ferredoxin
1	C00080	NADP+
2	C00138	H+

products:

1 C00005 Oxidized ferredoxin
2 C00139 NADPH

R02003 : Geranyl-diphosphate:isopentenyl-diphosphate
geranyltrans-transferase

substrates:

1 C00341 Geranyl diphosphate
1 C00129 Isopentenyl diphosphate

products:

1 C00013 Diphosphate
1 C00448 trans , trans-Farnesyl
diphosphate

R05884 : isopentenyl-diphosphate:ferredoxin
oxidoreductase

substrates:

1 C11811 1-Hydroxy-2-methyl-2-
butenyl 4-diphosphate
2 C00138 Reduced ferredoxin
2 C00080 H+

products:

1 C00129 Isopentenyl diphosphate
1 C00001 Oxidized ferredoxin
2 C00139 H₂O

-R00104 : -ATP:NAD⁺ 2-phosphotransferase

substrates:

1 C00008 ADP
1 C00006 NAD⁺

products:

1 C00002 ATP
1 C00003 NAD⁺

-R00127 : -ATP:AMP phosphotransferase

substrates:

2 C00008 ADP

products:

1 C00002 ATP

1 C00020 AMP
 -R00132 : -carbonate hydro-lyase (carbon-dioxide-forming)
 substrates:
 1 C00011 CO2
 1 C00001 H2O
 products:
 1 C01353 Carbonic acid
 -R00216 : -(S)-Malate:NADP+ oxidoreductase(oxaloacetate-
 decarboxylating)
 substrates:
 1 C00022 Pyruvate
 1 C00011 CO2
 1 C00005 NADPH
 1 C00080 H+
 products:
 1 C00149 (S)-Malate
 1 C00006 NADP+
 -R00513 : -ATP:cytidine 5-phosphotransferase
 substrates:
 1 C00008 ADP
 1 C00055 CMP
 products:
 1 C00002 ATP
 1 C00475 Cytidine
 -R01064 : -2-dehydro-3-deoxy-6-phospho-D-galactonate D-
 glyceraldehyde-3-phospho-lyase (pyruvate-forming)
 substrates:
 1 C00022 Pyruvate
 1 C00118 D-Glyceraldehyde 3-
 phosphate
 products:
 1 C01286 2-Dehydro-3-deoxy-6-
 phospho-D-galactonate

-R05605 : -2-dehydro-3-deoxy-6-phospho-D-gluconate D-glyceraldehyde-3-phosphate-lyase (pyruvate-forming)

substrates:

1	C00118	D-Glyceraldehyde 3-phosphate
1	C00022	Pyruvate

products:

1	C04442	2-Dehydro-3-deoxy-6-phospho-D-gluconate
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-R10092 : -carbonate hydro-lyase (carbon-dioxide-forming)

substrates:

1	C00011	CO ₂
1	C00001	H ₂ O

products:

1	C00288	HCO ₃ ⁻
1	C00080	H ⁺

2 amygdalin

2.1 pathway candidate: starting from sucrose

number of active reactions: 4
starts with basic: True
reactions w/o dG: 0
sum (dG + |dG|):9.763018e-02
dG: -4.130443e+01
number of heterologous enzymes: 2
number of cofactors: 1
number of side reactions: 4

R00803 : sucrose:phosphate alpha-D-glucosyltransferase
4.881509e-02

substrates:

1	C00089	Sucrose
1	C00009	Orthophosphate

products:

1	C00095	D-Fructose
1	C00103	D-Glucose 1-phosphate

R00289 : UTP:alpha-D-glucose-1-phosphate
uridylyltransferase -8.295754e+00

substrates:

1	C00075	UTP
1	C00103	D-Glucose 1-phosphate

products:

1	C00013	Diphosphate
1	C00029	UDP-glucose

R10638 : UDP-D-glucose:(R)-mandelonitrile beta-D-
glucosyltransferase -1.412458e+01

substrates:

1	C00561	Mandelonitrile
1	C00029	UDP-glucose

products:

1	C00844	Prunasin
1	C00015	UDP

R10639 : -1.893291e+01

substrates:

1	C00844	Prunasin
1	C00029	UDP-glucose

products:

1	C08325	Amygdalin
1	C00015	UDP

2.2 thermodynamic profile

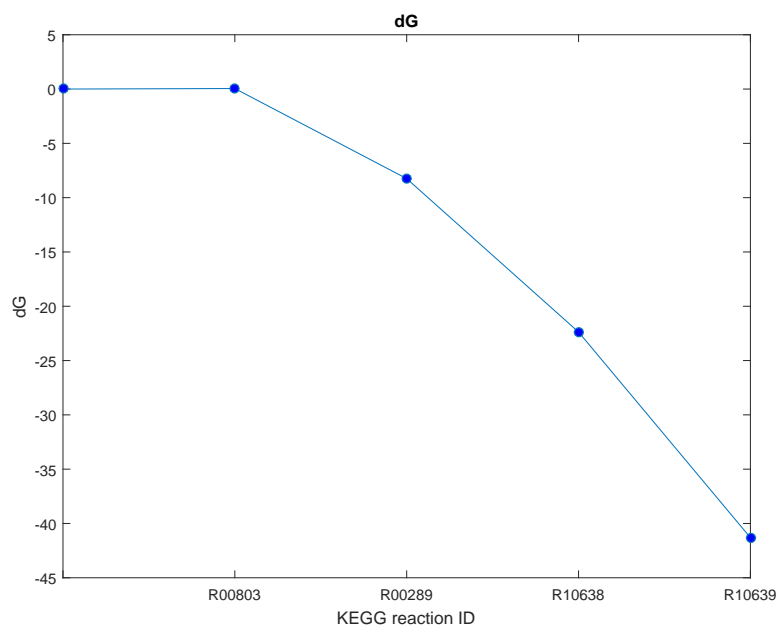


Figure 1: Thermodynamic profile for the pathway candidate for the synthesis of amygdalin from sucrose.

2.3 overall balance

reaction R00289

substrates:

1 C00013
1 C00029

products:

1 C00075
1 C00103

reaction R00803

substrates:

1 C00095
1 C00103

products:

1 C00089
1 C00009

reaction R10638

substrates:

1 C00844
1 C00015

products:

1 C00561
1 C00029

reaction R10639

substrates:

1 C08325
1 C00015

products:

1 C00844
1 C00029

overall:

C00009 1
C00013 -1
C00015 -2

C00029 1
C00075 1
C00089 1
C00095 -1
C00103 0
C00561 1
C00844 0
C08325 -1

not balanced:

C00009 1
C00013 -1
C00015 -2
C00029 1
C00075 1
C00089 1
C00095 -1
C00561 1
C08325 -1

2.4 side reactions

R00291 : UDP-glucose 4-epimerase

substrates:
1 C00029 UDP-glucose

products:
1 C00052 UDP-alpha-D-galactose

R00959 : alpha-D-Glucose 1-phosphate 1,6-phosphomutase

substrates:
1 C00103 D-Glucose 1-phosphate

products:
1 C00668 alpha-D-Glucose 6-phosphate

R08639 : alpha-D-glucose 1,6-phosphomutase

substrates:
1 C00103 D-Glucose 1-phosphate

products:
1 C00092 D-Glucose 6-phosphate

-R00878 : -alpha-D-Glucose aldose-ketose-isomerase

substrates:
1 C00095 D-Fructose

products:
1 C00267 alpha-D-Glucose

2.5 pathway candidate: starting from α -D-Glucose 6-phosphate

number of active reactions: 4
starts with basic: False
reactions w/o dG: 0
sum (dG + |dG|): 2.070859e+00
dG: -3.202206e+01
number of heterologous enzymes: 2
number of cofactors: 1
number of side reactions: 5

-R00959 : α -D-Glucose 1-phosphate 1,6-phosphomutase
4.881509e-02

substrates:

1 C00668 α -D-Glucose 6-phosphate

products:

1 C00103 D-Glucose 1-phosphate

R00289 : UTP: α -D-glucose-1-phosphate
uridylyltransferase -1.412458e+01

substrates:

1 C00075 UTP
1 C00103 D-Glucose 1-phosphate

products:

1 C00013 Diphosphate
1 C00029 UDP-glucose

R10638 : UDP-D-glucose:(R)-mandelonitrile beta-D-glucosyltransferase
-1.893291e+01

substrates:

1 C00561 Mandelonitrile
1 C00029 UDP-glucose

products:

1 C00844 Prunasin
1 C00015 UDP

R10639 : 9.866146e-01

substrates:

1	C00844	Prunasin
1	C00029	UDP-glucose

products:

1	C08325	Amygdalin
1	C00015	UDP

2.6 thermodynamic profile

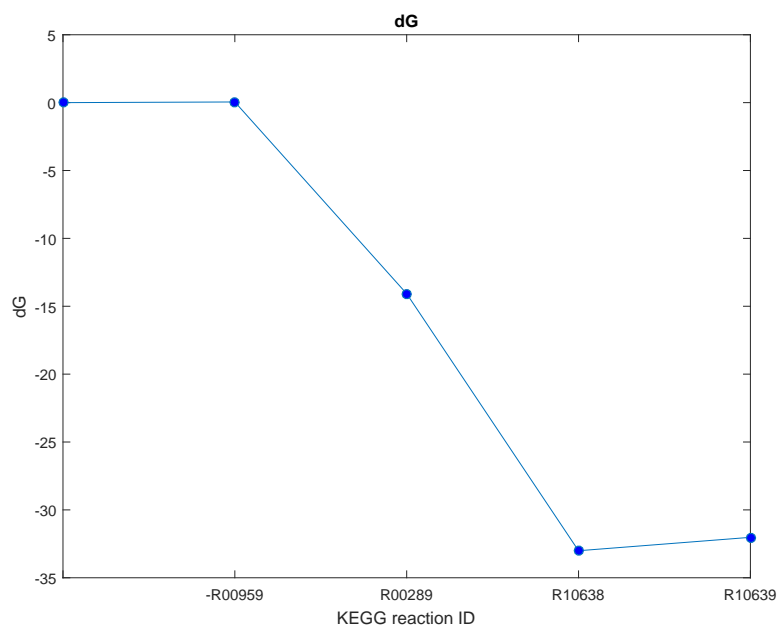


Figure 2: Thermodynamic profile for the pathway candidate for the synthesis of amygdalin from α -D-Glucose 6-phosphate.

2.7 overall balance

reaction R00289

substrates:

1 C00013
1 C00029

products:

1 C00075
1 C00103

reaction R10638

substrates:

1 C00844
1 C00015

products:

1 C00561
1 C00029

reaction R10639

substrates:

1 C08325
1 C00015

products:

1 C00844
1 C00029

reaction R00959

substrates:

1 C00668

products:

1 C00103

overall:

C00013 -1
C00015 -2
C00029 1
C00075 1
C00103 2

C00561 1
C00668 -1
C00844 0
C08325 -1

not balanced:

C00013 -1
C00015 -2
C00029 1
C00075 1
C00103 2
C00561 1
C00668 -1
C08325 -1

2.8 side reactions

R00291 : UDP-glucose 4-epimerase

substrates:
1 C00029 UDP-glucose

products:
1 C00052 UDP-alpha-D-galactose

R00959 : alpha-D-Glucose 1-phosphate 1,6-phosphomutase

substrates:
1 C00103 D-Glucose 1-phosphate

products:
1 C00668 alpha-D-Glucose 6-phosphate

R02737 : UDPglucose:D-glucose -6-phosphate 1-alpha-D-glucosyltransferase

substrates:
1 C00029 UDP-glucose
1 C00668 alpha-D-Glucose 6-phosphate

products:
1 C00015 UDP
1 C00689 alpha , alpha'-Trehalose 6-phosphate

R02740 : alpha-D-Glucose 6-phosphate ketol-isomerase

substrates:
1 C00668 alpha-D-Glucose 6-phosphate

products:
1 C05345 beta-D-Fructose 6-phosphate

R08639 : alpha-D-glucose 1,6-phosphomutase

substrates:
1 C00103 D-Glucose 1-phosphate

products:
1 C00092 D-Glucose 6-phosphate

3 pyrrolysine

3.1 pathway candidate

number of active reactions: 4
starts with basic: True
reactions w/o dG: 4
sum (dG + |dG|): 0
dG: 0
number of heterologous enzymes: 4
number of cofactors: 2
number of side reactions: 9

R10010 : L-lysine carboxy-aminomethylmutase 0

substrates:

1 C00047 L-Lysine

products:

1 C20277 (2R,3R)-3-Methylornithine

R10011 : 0

substrates:

1 C00047 L-Lysine

1 C20277 (2R,3R)-3-Methylornithine

1 C00002 ATP

products:

1 C20278 (2R,3R)-3-Methylornithinyl-N6-lysine

1 C07305 Products of ATP breakdown

R10012 : 0

substrates:

1 C20278 (2R,3R)-3-Methylornithinyl-N6-lysine

1 C00003 NAD+

1 C00001 H2O

products:

1 C20279 (2R,3R)-3-Methylglutamyl-5-semialdehyde-N6-lysine

1 C00014 Ammonia

1 C00004 NADH

R10013 : 0

substrates:

1 C20279 (2R,3R)-3-Methylglutamyl
-5-semialdehyde-N6-lysine

products:

1 C16138 L-Pyrrolysine
1 C00001 H2O

3.2 overall balance

```
reaction R10010
substrates:
    1 C20277
products:
    1 C00047
reaction R10011
substrates:
    1 C20278
    1 C07305
products:
    1 C00047
    1 C20277
    1 C00002
reaction R10012
substrates:
    1 C20279
    1 C00014
    1 C00004
products:
    1 C20278
    1 C00003
    1 C00001
reaction R10013
substrates:
    1 C16138
    1 C00001
products:
    1 C20279
overall:
C00001  0
C00002  1
```

C00003 1
C00004 -1
C00014 -1
C00047 2
C07305 -1
C16138 -1
C20277 0
C20278 0
C20279 0

not balanced:

C00002 1
C00003 1
C00004 -1
C00014 -1
C00047 2
C07305 -1
C16138 -1

3.3 side reactions

R00086 : ATP phosphohydrolase

substrates:

1	C00002	ATP
1	C00001	H2O

products:

1	C00008	ADP
1	C00009	Orthophosphate

R00087 : ATP diphosphohydrolase (diphosphate-forming)

substrates:

1	C00002	ATP
1	C00001	H2O

products:

1	C00020	AMP
1	C00013	Diphosphate

R00089 : ATP diphosphate-lyase (cyclizing)

substrates:

1	C00002	ATP
---	--------	-----

products:

1	C00575	3',5'-Cyclic AMP
1	C00013	Diphosphate

R00103 : NAD⁺ phosphohydrolase

substrates:

1	C00003	NAD ⁺
1	C00001	H2O

products:

1	C00020	AMP
1	C00455	Nicotinamide D-ribonucleotide

R00104 : ATP:NAD⁺ 2'-phosphotransferase

substrates:

1	C00002	ATP
1	C00003	NAD ⁺

products:
1 C00008 ADP
1 C00006 NADP+

R00143 : ammonia:NAD+ oxidoreductase

substrates:
1 C00014 Ammonia
1 C00003 NAD+
1 C00001 H2O

products:
1 C00192 Hydroxylamine
1 C00004 NADH
1 C00080 H+

R00462 : L-lysine carboxy-lyase (cadaverine-forming)

substrates:
1 C00047 L-Lysine

products:
1 C01672 Cadaverine
1 C00011 CO2

R00787 : ammonia:NAD+ oxidoreductase

substrates:
1 C00014 Ammonia
2 C00001 NAD+
3 C00003 H2O

products:
1 C00088 Nitrite
3 C00004 NADH
3 C00080 H+

R11104 : NADH phosphohydrolase

substrates:
1 C00004 NADH
1 C00001 H2O

products:
1 C00020 AMP

1 C21113 NMNH

4 (S)-2-phenyloxirane

4.1 pathway candidate

number of active reactions: 4
starts with basic: False
reactions w/o dG: 1
sum (dG + |dG|): 2.081496e+01
dG: -1.728943e+01
number of heterologous enzymes: 4
number of cofactors: 3
number of side reactions: 11

R02506 : cinnamaldehyde:NADP+ oxidoreductase (CoA-cinnamoylating) 6.126122e+00

substrates:

1	C00903	Cinnamaldehyde
1	C00010	CoA
1	C00006	NADP+

products:

1	C00540	Cinnamoyl-CoA
1	C00005	NADPH
1	C00080	H+

-R02255 : -trans-Cinnamate:CoA ligase (AMP-forming) 0

substrates:

1	C00020	AMP
1	C00013	Diphosphate
1	C00540	Cinnamoyl-CoA

products:

1	C00002	ATP
1	C00423	trans-Cinnamate
1	C00010	CoA

R11070 : trans-cinnamate carboxy-lyase -2.769690e+01

substrates:

1	C00423	trans-Cinnamate
---	--------	-----------------

products:

1	C07083	Styrene
1	C00011	CO2

R05488 : styrene ,FADH2:oxygen oxidoreductase 4.281356e
+00

substrates :

1	C07083	Styrene
1	C01352	FADH2
1	C00007	Oxygen

products :

1	C20782	(S)-2-Phenyloxirane
1	C00016	FAD
1	C00001	H2O

4.2 thermodynamic profile

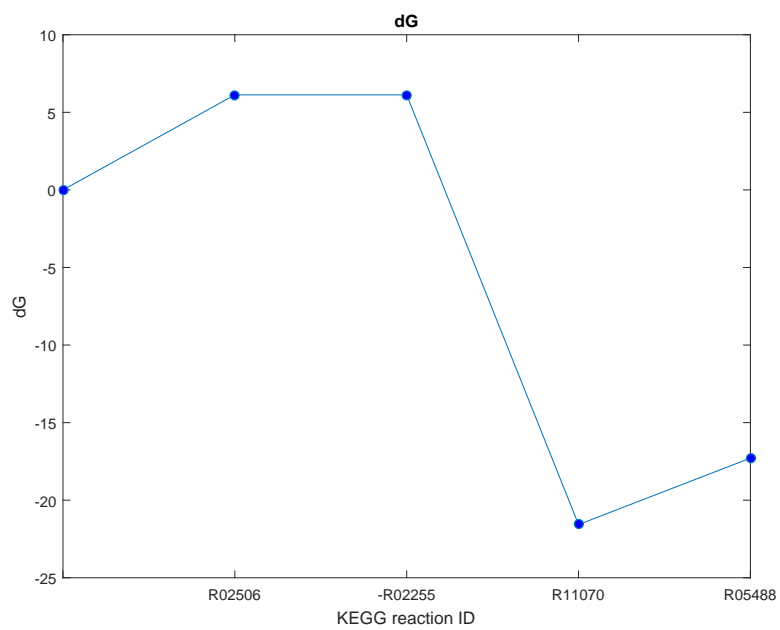


Figure 3: Thermodynamic profile for a pathway candidate for the synthesis of (S)-2-Phenyloxirane starting from cinnamaldehyde.

4.3 overall balance

reaction R02506

substrates:

1 C00540
1 C00005
1 C00080

products:

1 C00903
1 C00010
1 C00006

reaction R05488

substrates:

1 C20782
1 C00016
1 C00001

products:

1 C07083
1 C01352
1 C00007

reaction R11070

substrates:

1 C07083
1 C00011

products:

1 C00423

reaction R02255

substrates:

1 C00020
1 C00013
1 C00540

products:

1 C00002
1 C00423
1 C00010

overall:
C00001 -1
C00002 1
C00005 -1
C00006 1
C00007 1
C00010 2
C00011 -1
C00013 -1
C00016 -1
C00020 -1
C00080 -1
C00423 2
C00540 -2
C00903 1
C01352 1
C07083 0
C20782 -1

not balanced:
C00001 -1
C00002 1
C00005 -1
C00006 1
C00007 1
C00010 2
C00011 -1
C00013 -1
C00016 -1
C00020 -1
C00080 -1
C00423 2
C00540 -2
C00903 1
C01352 1
C20782 -1

4.4 side reactions

R00004 : diphosphate phosphohydrolase

substrates:

1	C00013	Diphosphate
1	C00001	H2O

products:

2	C00009	Orthophosphate
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R00086 : ATP phosphohydrolase

substrates:

1	C00002	ATP
1	C00001	H2O

products:

1	C00008	ADP
1	C00009	Orthophosphate

R00087 : ATP diphosphohydrolase (diphosphate-forming)

substrates:

1	C00002	ATP
1	C00001	H2O

products:

1	C00020	AMP
1	C00013	Diphosphate

R00089 : ATP diphosphate-lyase (cyclizing

substrates:

1	C00002	ATP
---	--------	-----

products:

1	C00575	3',5'-Cyclic AMP
1	C00013	Diphosphate

R00127 : ATP:AMP phosphotransferase

substrates:

1	C00002	ATP
1	C00020	AMP

products:
 2 C00008 ADP

R00182 : AMP phosphoribohydrolase

substrates:
 1 C00020 AMP
 1 C00001 H2O

products:
 1 C00147 Adenine
 1 C00117 D-Ribose 5-phosphate

R00183 : adenosine 5'-monophosphate phosphohydrolase

substrates:
 1 C00020 AMP
 1 C00001 H2O

products:
 1 C00212 Adenosine
 1 C00009 Orthophosphate

R00190 : AMP:diphosphate phospho-D-ribosyltransferase

substrates:
 1 C00020 AMP
 1 C00013 Diphosphate

products:
 1 C00147 Adenine
 1 C00119 5-Phospho-alpha-D-ribose 1-diphosphate

-R00132 : -carbonate hydro-lyase (carbon-dioxide-forming)

substrates:
 1 C00011 CO2
 1 C00001 H2O

products:
 1 C01353 Carbonic acid

-R00161 : -ATP:FMN adenylyltransferase

substrates:
 1 C00013 Diphosphate

1 C00016 FAD

products:

1 C00002 ATP

1 C00061 FMN

-R10092 : -carbonate hydro-lyase (carbon-dioxide-forming)

substrates:

1 C00011 CO2

1 C00001 H2O

products:

1 C00288 HCO₃⁻

1 C00080 H⁺