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## Compound Name Resolutions

## Compound Pathway Coverage

## Optimum Value of the Minimized Objective Function: 98

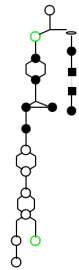

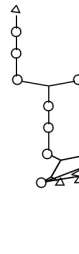
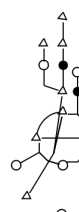
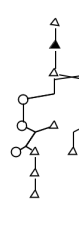



43 compound match results form the input to the covering algorithm.  
43 of the recognized compounds are substrates in 496 PGDB reactions.  
42 of the recognized compounds are substrates in 287 PGDB pathways;  
a pathway covering set of 18 pathways covers those 42 compounds:

Colored nodes are compounds in the covered set;  
Colored edges are reactions with side compounds in the covered set;  
BLUE - no indicated change in quantity; GREEN - an increase in quantity;  
RED - a decrease in quantity.

You utilized the cost function **Pathway Harmony**:

This function favors pathways where either the 'input' substrates  
are metabolites that show an increase in abundance, and the 'output'  
substrates are metabolites that show a decrease, or vice versa.

Pathway	Objective Function Value	Pathway Glyph	Covered Compounds
chlorogenic acid biosynthesis II	10		shikimate
glycerol degradation I	10		glycerol
glyoxylate cycle	6		(S)-malate citrate cis-aconitate succinate
L-alanine degradation II (to D-lactate)	4		L-glutamate 2-oxoglutarate (R)-lactate pyruvate L-alanine
L-ascorbate biosynthesis VII (plants, D-galacturonate pathway)	10		L-galactonate
L-glutamate degradation IV	1		pyruvate 4-aminobutanoate L-alanine succinate 2-oxoglutarate L-glutamate
L-methionine salvage cycle I (bacteria and plants)	7		2-oxoglutarate L-glutamine formate putrescine
L-serine biosynthesis II	2		L-serine glycine pyruvate L-alanine D-glycerate
phosphatidylethanolamine biosynthesis III	5		L-serine ethanolamine
sorbitol biosynthesis II	6		D-gluconate keto-D-fructose

superpathway of anaerobic sucrose degradation	4		$\beta$ -D-fructofuranose sucrose (S)-lactate pyruvate
superpathway of aspartate and asparagine biosynthesis	4		L-asparagine L-aspartate L-glutamine L-glutamate 2-oxoglutarate
superpathway of branched chain amino acid biosynthesis	2		L-threonine pyruvate 2-oxoglutarate L-isoleucine L-glutamate L-valine L-leucine
superpathway of L-citrulline metabolism	4		fumarate L-aspartate L-proline L-glutamate 2-oxoglutarate L-glutamine
superpathway of L-lysine, L-threonine and L-methionine biosynthesis II	2		L-lysine 2-oxoglutarate L-glutamate pyruvate L-aspartate L-cysteine L-threonine
superpathway of phenylalanine, tyrosine and tryptophan biosynthesis	6		L-phenylalanine L-tyrosine 2-oxoglutarate L-glutamate L-serine L-tryptophan L-glutamine pyruvate
trehalose degradation II (cytosolic)	5		$\alpha,\alpha$ -trehalose $\beta$ -D-glucopyranose $\alpha$ -D-glucopyranose
urate conversion to allantoin I	10		urate

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Arabidopsis thaliana col version 17.1.

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