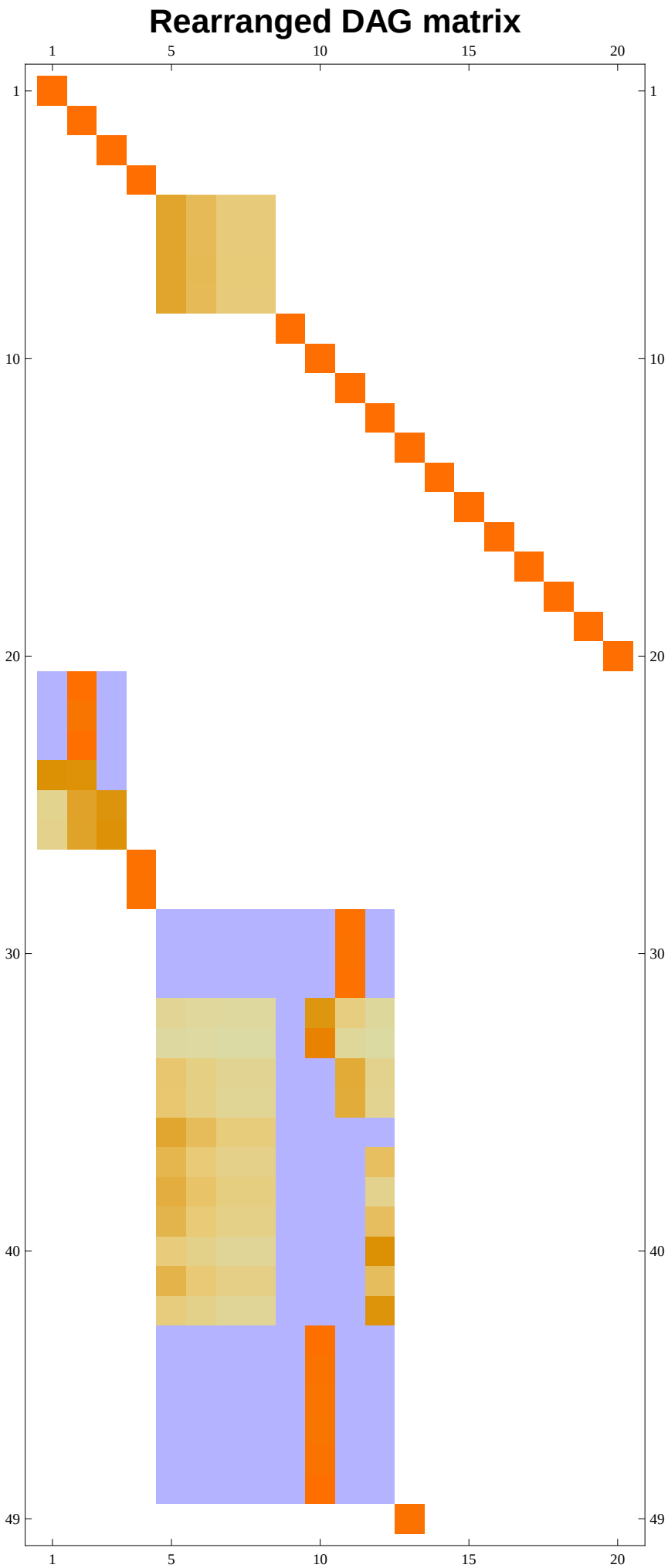
Netsplitter results: Netsplitter_V1.2

Stoichiometry input file: H:\My Documents\Research\Projects\SubNetExtraction\Netsplitter_V1.2\Demo.tsv
A total of 117 reactions were imported and 3 of these specified as reversible.
A total of 137 metabolites were listed, of which 27 were specified as external in the stoichiometry file.
No external metabolites input file was read.
No flux values input file was read.
No target metabolites input file was read.
Calculated at Thu 25 Nov 2010 10:17:10
A total of 2 selection rounds were performed resolving 4 non-trivial subnet blocks and 7 orphans.
Split Efficacy = 64% (input externals only); 76% (after selection and reincorporation); and no merging was done.
Running time for this calculation = 0.47 seconds.

Optional parameters used

Reactions omitted with ID containing: No omissions
Max connectivity kept as internal: 8
Binary vector similarity measure: SokalSneathDissimilarity
Intercluster distance: Single
Interblock overlap cutoff value = 0.215
Grouplevel search interval = {0.3, 0.7}
Optimised Grouplevel value = 0.5833
Reversibility ignored - only explicit reaction directions included.


Rearranged DAG matrix
1
5
10
15
20
1
10
20
30
40
49

49 Internal Metabolites

- **Metabolites in each block**

Numbering as in the plot; target metabolites are highlighted.

Block 1	1 LEUCOPELARGONIDIN−CMPD SYSTEM 21 CPD−590 SYSTEM 24 DIHYDROKAEMPFEROL−CMPD SYSTEM	2 CPD−591 SYSTEM 22 CPD−6994 SYSTEM 25 APIGENIN SYSTEM	3 CPD−431 SYSTEM 23 CPD−474 SYSTEM 26 NARINGENIN−CMPD SYSTEM
Block 2	4 3−DEHYDRO−SHIKIMATE SYSTEM	27 3−DEOXY−D−ARABINO−HEPTULOSONATE−7−P SYSTEM	28 DEHYDROQUINATE SYSTEM
Block 3	5 O−SINAPOYLCHOLINE SYSTEM 8 SINAPATE SYSTEM 11 CPD−8096 SYSTEM 30 CPD−8095 SYSTEM 33 CINNAMALDEHYDE SYSTEM 36 5−HYDROXY−FERULIC−ACID SYSTEM 39 FERULOYL−COA SYSTEM 42 5−HYDROXY−CONIFERALDEHYDE SYSTEM 45 HYDROXYCINNAMOYL−COA SYSTEM 48 BENZOATE SYSTEM	6 1−O−SINAPOYL−BETA−D−GLUCOSE SYSTEM 9 TYRAMINE SYSTEM 12 SINAPYL−ALCOHOL SYSTEM 31 CPD−8094 SYSTEM 34 COUMARATE SYSTEM 37 CAFFEOYL−COA SYSTEM 40 SINAPALDEHYDE SYSTEM 43 BENZOYLCOA SYSTEM 46 CINNAMOYL−COA SYSTEM	7 CHOLINE SYSTEM 10 CPD−110 SYSTEM 29 CPD−8098 SYSTEM 32 CPD−674 SYSTEM 35 CAFFEATE SYSTEM 38 FERULIC−ACID SYSTEM 41 CONIFERYL−ALDEHYDE SYSTEM 44 OXOCINNAMOYL−COA SYSTEM 47 BENZALDEHYDE SYSTEM
Block 4	13 CPD−7417 SYSTEM	49 CPD−459 SYSTEM	

- **7 Orphans (subnets with a single internal metabolite)**

14 4−COUMAROYLQUINATE SYSTEM 15 SHIKIMATE−5P SYSTEM 16 CPD−8013 SYSTEM
17 CPD−663 SYSTEM 18 CPD−412 SYSTEM 19 CPD−3041 SYSTEM
20 COUMARALDEHYDE SYSTEM

- **Externals/internals overlap between blocks**

No block overlaps found

88 External Metabolites

- **0 Metabolites refused status as externals**

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- **66 Structural externals**

These are metabolites that only ever appear as either an inflow or an outflow

- **4 High connectivity metabolites (with connectivity counts)**

42: WATER SYSTEM 31: NADP SYSTEM 31: NADPH SYSTEM
18: CO−A SYSTEM

- **17 Metabolites specified in the stoichiometry specification**

2−COUMARATE SYSTEM 3−ENOLPYRUVYL−SHIKIMATE−5P SYSTEM CAFFEOYLQUINATE SYSTEM
CAFFEOYLSHIKIMATE SYSTEM CONIFERYL−ALCOHOL SYSTEM CPD−1777 SYSTEM
CPD1F−420 SYSTEM CPD1F−437 SYSTEM CPD1F−453 SYSTEM
CPD1F−461 SYSTEM CPD1F−90 SYSTEM CPD−520 SYSTEM
CPD−7418 SYSTEM PELARGONIDIN−CMPD SYSTEM QUINATE SYSTEM
SHIKIMATE SYSTEM UDP−L−RHAMNOSE SYSTEM

- **0 Metabolites proposed in the externals file**

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- **1 Metabolites chosen interactively**

COUMARYL−COA SYSTEM

- **0 Ex-orphans becoming external due to reincorporation**

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Blockwise details for external metabolites

Block 1	Inflows	Crossflows	Outflows
	UDP−GLUCOSE SYSTEM	COUMARYL−COA SYSTEM	CPD−1961 SYSTEM
	MALONYL−COA SYSTEM	WATER SYSTEM	CPD−1962 SYSTEM
	OXYGEN−MOLECULE SYSTEM	CO−A SYSTEM	UDP SYSTEM
	2−KETOGLUTARATE SYSTEM	NADPH SYSTEM	5734−TETRAHYDROXYFLAVONE SYSTEM
		NADP SYSTEM	SUC SYSTEM
		CPD1F−90 SYSTEM	CARBON−DIOXIDE SYSTEM
		CPD−520 SYSTEM	CPD1F−766 SYSTEM
		PELARGONIDIN−CMPD SYSTEM	NARINGENIN−7−O−BETA−D−GLUCOSIDE SYSTEM

Block 2	Inflows	Crossflows	Outflows
	ERYTHROSE−4P SYSTEM	WATER SYSTEM	Pi SYSTEM
	PHOSPHO−ENOL−PYRUVATE SYSTEM	NADPH SYSTEM	
		NADP SYSTEM	
		SHIKIMATE SYSTEM	

Block 3	Inflows	Crossflows	Outflows
	NAD SYSTEM	COUMARYL−COA SYSTEM	PROTON SYSTEM
	SALICYLOYL−COA SYSTEM	WATER SYSTEM	NADH SYSTEM
	ATP SYSTEM	CO−A SYSTEM	CPD−6443 SYSTEM
	UDP−GLUCOSE SYSTEM	NADPH SYSTEM	CPD−6442 SYSTEM
	MANDELONITRILE SYSTEM	NADP SYSTEM	CPD−6441 SYSTEM
	TYR SYSTEM	CONIFERYL−ALCOHOL SYSTEM	PYRUVATE SYSTEM
	BENZYL−ALCOHOL SYSTEM	CAFFEOYLQUINATE SYSTEM	PPI SYSTEM
	MAL SYSTEM	QUINATE SYSTEM	AMP SYSTEM
	S−ADENOSYLMETHIONINE SYSTEM	CAFFEOYLSHIKIMATE SYSTEM	HCN SYSTEM
	CPD−676 SYSTEM	SHIKIMATE SYSTEM	UDP SYSTEM
	OXYGEN−MOLECULE SYSTEM	2−COUMARATE SYSTEM	CPD−79 SYSTEM
	CINNAMYL−ALC SYSTEM		CPD−8097 SYSTEM
	ISOCHORISMATE SYSTEM		CPD−81 SYSTEM
	PHE SYSTEM		CPD−63 SYSTEM
			SINAPOYL−S−MALATE SYSTEM
			ADENOSYL−HOMO−CYS SYSTEM
			12−BIS−O−SINAPOYL−BETA−D−GLUCOSIDE SYSTEM
			HYDROGEN−PEROXIDE SYSTEM
			AMMONIA SYSTEM
			CARBON−DIOXIDE SYSTEM
			GLC SYSTEM
			CPD−440 SYSTEM
			ACETYL−COA SYSTEM

Block 4	Inflows	Crossflows	Outflows
	UDP−GLUCOSE SYSTEM	WATER SYSTEM	UDP SYSTEM
		CPD−7418 SYSTEM	GLC SYSTEM
		2−COUMARATE SYSTEM	

Orphan Block	Inflows	Crossflows	Outflows
	ATP SYSTEM	COUMARYL−COA SYSTEM	Pi SYSTEM
	UDP−GLUCOSE SYSTEM	WATER SYSTEM	ADP SYSTEM
	PHOSPHO−ENOL−PYRUVATE SYSTEM	CO−A SYSTEM	UDP SYSTEM
	MALONYL−COA SYSTEM	NADPH SYSTEM	CPD−8011 SYSTEM
	OXYGEN−MOLECULE SYSTEM	NADP SYSTEM	COUMARYL−ALCOHOL SYSTEM
		3−ENOLPYRUVYL−SHIKIMATE−5P SYSTEM	CPDQT−26 SYSTEM
		CAFFEOYLQUINATE SYSTEM	CPD−3061 SYSTEM
		QUINATE SYSTEM	CARBON−DIOXIDE SYSTEM
		CAFFEOYLSHIKIMATE SYSTEM	
		UDP−L−RHAMNOSE SYSTEM	
		SHIKIMATE SYSTEM	
		CPD−520 SYSTEM	

- **Items deleted from Stoichiometry**

```
No reactions removed

No metabolitess removed
```

- **Record of interactive choices**

Selection Round	Restrict to blocks	Refused externals
1	All	None

Merge step	Merged Blocks	Included Orphans	New Block