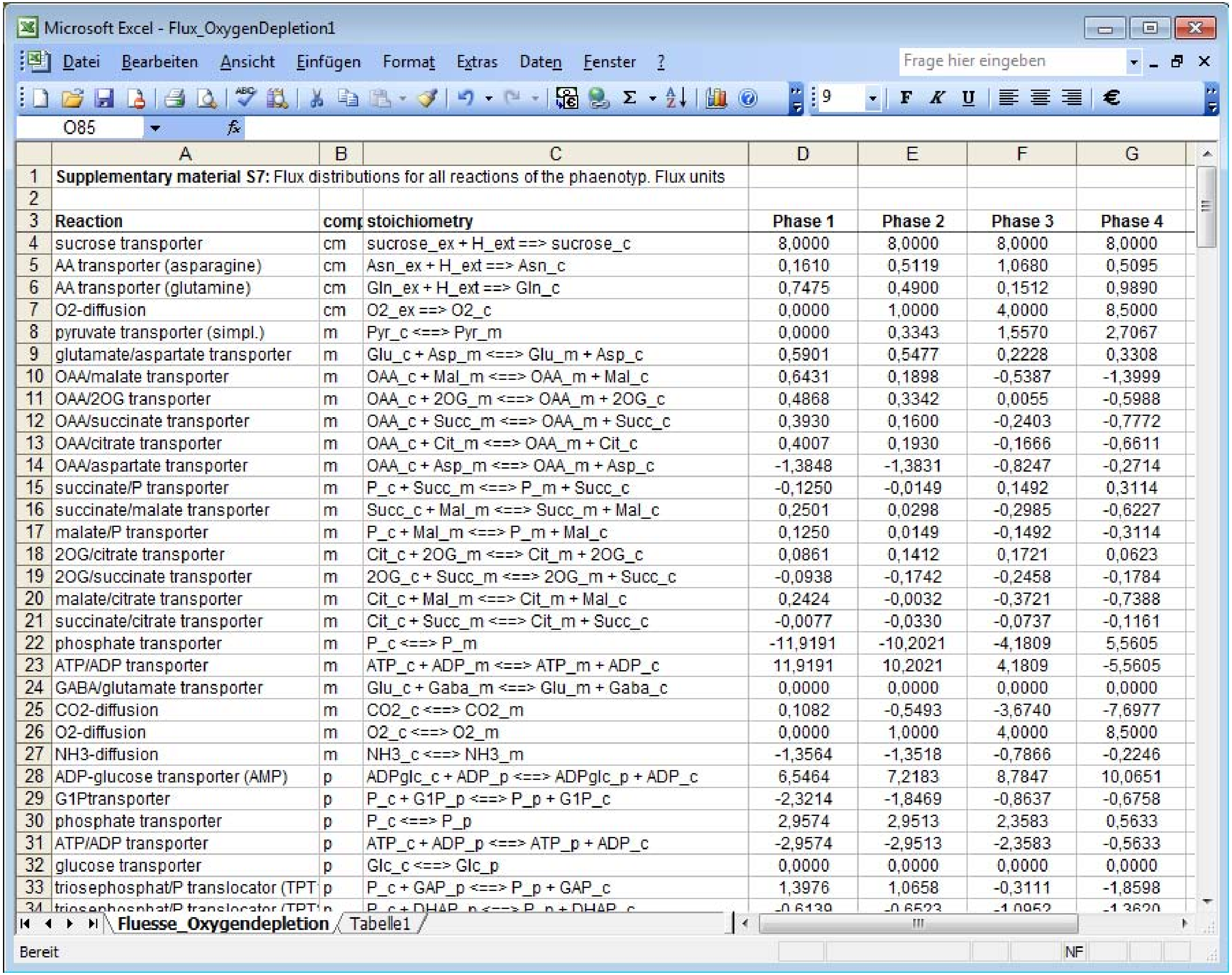
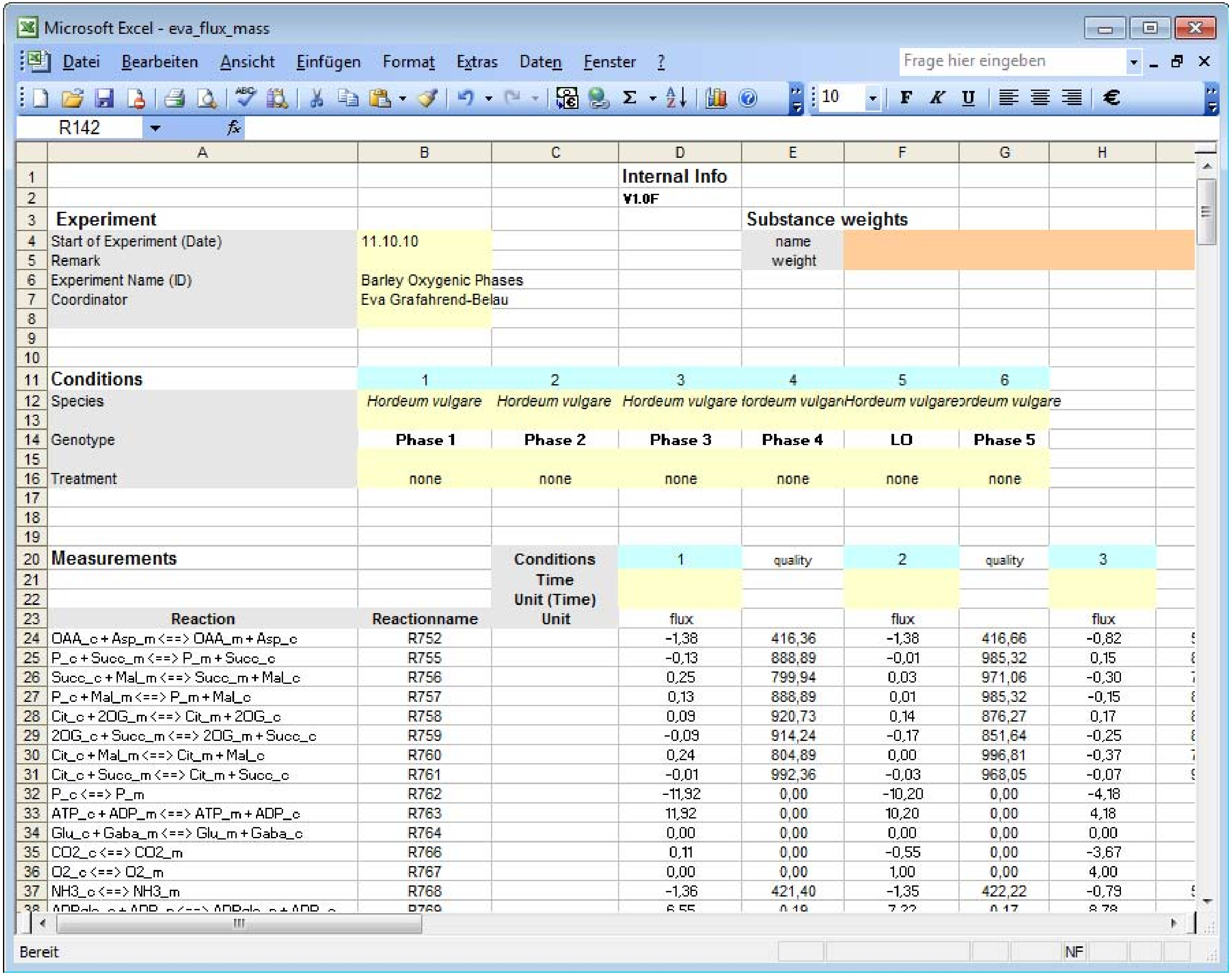


Supplementary material S7: Flux distributions for all reactions of the phaenotyp. Flux units

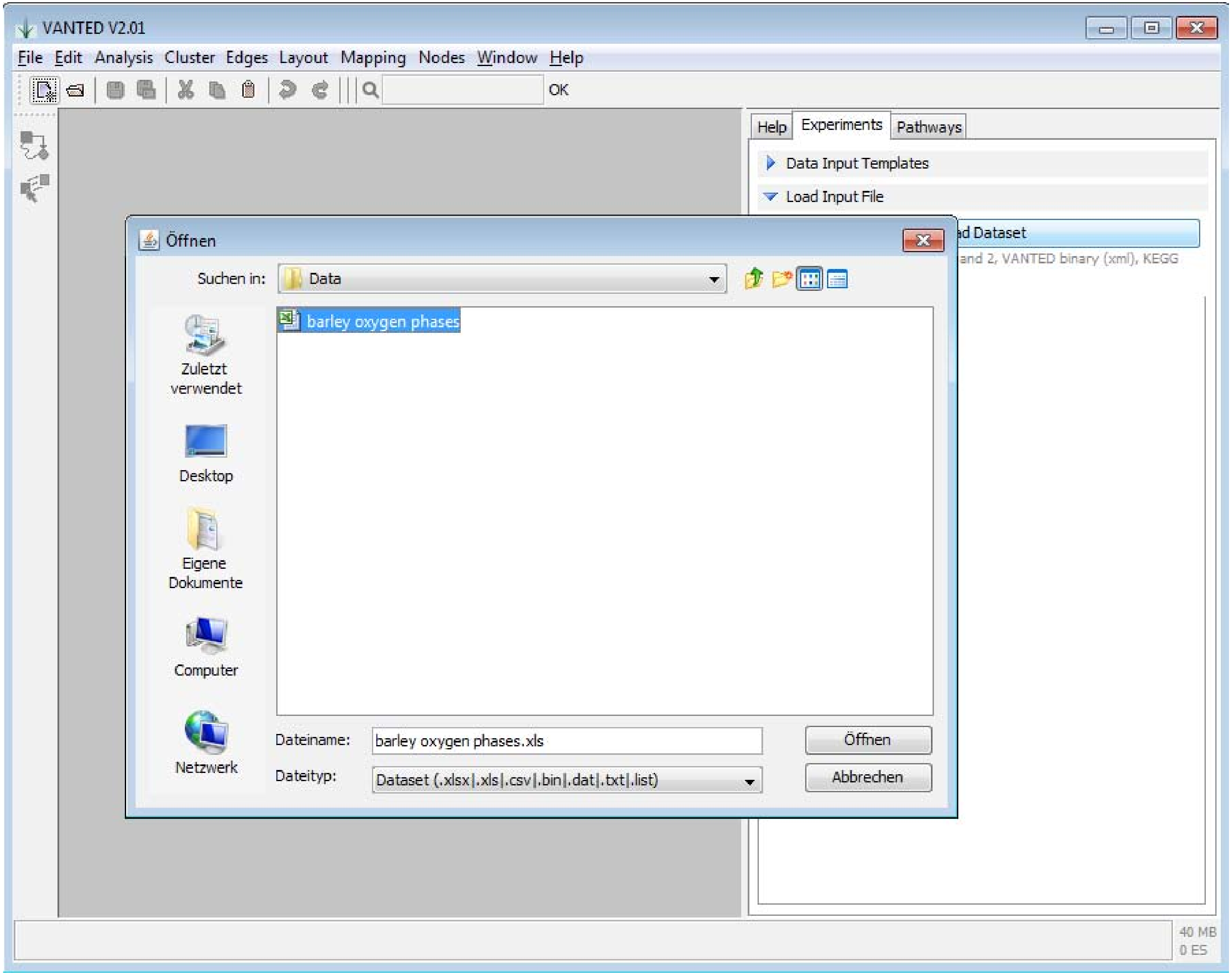
	A	B	C	D	E	F	G
1	**Supplementary material S7:** Flux distributions for all reactions of the phaenotyp. Flux units						
2							
3	**Reaction**	**comp**	**stoichiometry**	**Phase 1**	**Phase 2**	**Phase 3**	**Phase 4**
4	sucrose transporter	cm	sucrose_ex + H_ext ==> sucrose_c	8,0000	8,0000	8,0000	8,0000
5	AA transporter (asparagine)	cm	Asn_ex + H_ext ==> Asn_c	0,1610	0,5119	1,0680	0,5095
6	AA transporter (glutamine)	cm	Gln_ex + H_ext ==> Gln_c	0,7475	0,4900	0,1512	0,9890
7	O2-diffusion	cm	O2_ex ==> O2_c	0,0000	1,0000	4,0000	8,5000
8	pyruvate transporter (simpl.)	m	Pyr_c <==> Pyr_m	0,0000	0,3343	1,5570	2,7067
9	glutamate/aspartate transporter	m	Glu_c + Asp_m <==> Glu_m + Asp_c	0,5901	0,5477	0,2228	0,3308
10	OAA/malate transporter	m	OAA_c + Mal_m <==> OAA_m + Mal_c	0,6431	0,1898	-0,5387	-1,3999
11	OAA/2OG transporter	m	OAA_c + 2OG_m <==> OAA_m + 2OG_c	0,4868	0,3342	0,0055	-0,5988
12	OAA/succinate transporter	m	OAA_c + Succ_m <==> OAA_m + Succ_c	0,3930	0,1600	-0,2403	-0,7772
13	OAA/citrate transporter	m	OAA_c + Cit_m <==> OAA_m + Cit_c	0,4007	0,1930	-0,1666	-0,6611
14	OAA/aspartate transporter	m	OAA_c + Asp_m <==> OAA_m + Asp_c	-1,3848	-1,3831	-0,8247	-0,2714
15	succinate/P transporter	m	P_c + Succ_m <==> P_m + Succ_c	-0,1250	-0,0149	0,1492	0,3114
16	succinate/malate transporter	m	Succ_c + Mal_m <==> Succ_m + Mal_c	0,2501	0,0298	-0,2985	-0,6227
17	malate/P transporter	m	P_c + Mal_m <==> P_m + Mal_c	0,1250	0,0149	-0,1492	-0,3114
18	2OG/citrate transporter	m	Cit_c + 2OG_m <==> Cit_m + 2OG_c	0,0861	0,1412	0,1721	0,0623
19	2OG/succinate transporter	m	2OG_c + Succ_m <==> 2OG_m + Succ_c	-0,0938	-0,1742	-0,2458	-0,1784
20	malate/citrate transporter	m	Cit_c + Mal_m <==> Cit_m + Mal_c	0,2424	-0,0032	-0,3721	-0,7388
21	succinate/citrate transporter	m	Cit_c + Succ_m <==> Cit_m + Succ_c	-0,0077	-0,0330	-0,0737	-0,1161
22	phosphate transporter	m	P_c <==> P_m	-11,9191	-10,2021	-4,1809	5,5605
23	ATP/ADP transporter	m	ATP_c + ADP_m <==> ATP_m + ADP_c	11,9191	10,2021	4,1809	-5,5605
24	GABA/glutamate transporter	m	Glu_c + Gaba_m <==> Glu_m + Gaba_c	0,0000	0,0000	0,0000	0,0000
25	CO2-diffusion	m	CO2_c <==> CO2_m	0,1082	-0,5493	-3,6740	-7,6977
26	O2-diffusion	m	O2_c <==> O2_m	0,0000	1,0000	4,0000	8,5000
27	NH3-diffusion	m	NH3_c <==> NH3_m	-1,3564	-1,3518	-0,7866	-0,2246
28	ADP-glucose transporter (AMP)	p	ADPglc_c + ADP_p <==> ADPglc_p + ADP_c	6,5464	7,2183	8,7847	10,0651
29	G1Ptransporter	p	P_c + G1P_p <==> P_p + G1P_c	-2,3214	-1,8469	-0,8637	-0,6758
30	phosphate transporter	p	P_c <==> P_p	2,9574	2,9513	2,3583	0,5633
31	ATP/ADP transporter	p	ATP_c + ADP_p <==> ATP_p + ADP_c	-2,9574	-2,9513	-2,3583	-0,5633
32	glucose transporter	p	Glc_c <==> Glc_p	0,0000	0,0000	0,0000	0,0000
33	triosephosphat/P translocator (TPT	p	P_c + GAP_p <==> P_p + GAP_c	1,3976	1,0658	-0,3111	-1,8598
34	triosephosphat/P translocator (TPT	p	P_c + DHAP_p <==> P_p + DHAP_c	-0,6139	-0,6523	-1,0952	-1,3620

Figure 1: Take flux raw data



	A	B	C	D	E	F	G	H
1				**Internal Info**				
2				**V1.0F**				
3	**Experiment**				**Substance weights**			
4	Start of Experiment (Date)	11.10.10			name			
5	Remark				weight			
6	Experiment Name (ID)	Barley Oxygenic Phases						
7	Coordinator	Eva Grafahrend-Belau						
8								
9								
10								
11	**Conditions**	1	2	3	4	5	6	
12	Species	*Hordeum vulgare*	*Hordeum vulgare*	*Hordeum vulgare*	*lordeum vulgar*	*Hordeum vulgare*	*ordeum vulgare*	
13								
14	Genotype	**Phase 1**	**Phase 2**	**Phase 3**	**Phase 4**	**LO**	**Phase 5**	
15								
16	Treatment	none	none	none	none	none	none	
17								
18								
19								
20	**Measurements**		**Conditions**	1	quality	2	quality	3
21			**Time**					
22			**Unit (Time)**					
23	**Reaction**	**Reactionname**	**Unit**	flux		flux		flux
24	OAA_c + Asp_m <==> OAA_m + Asp_c	R752		-1,38	416,36	-1,38	416,66	-0,82
25	P_c + Succ_m <==> P_m + Succ_c	R755		-0,13	888,89	-0,01	985,32	0,15
26	Succ_c + Mal_m <==> Succ_m + Mal_c	R756		0,25	799,94	0,03	971,06	-0,30
27	P_c + Mal_m <==> P_m + Mal_c	R757		0,13	888,89	0,01	985,32	-0,15
28	Cit_c + 2OG_m <==> Cit_m + 2OG_c	R758		0,09	920,73	0,14	876,27	0,17
29	2OG_c + Succ_m <==> 2OG_m + Succ_c	R759		-0,09	914,24	-0,17	851,64	-0,25
30	Cit_c + Mal_m <==> Cit_m + Mal_c	R760		0,24	804,89	0,00	996,81	-0,37
31	Cit_c + Succ_m <==> Cit_m + Succ_c	R761		-0,01	992,36	-0,03	968,05	-0,07
32	P_c <==> P_m	R762		-11,92	0,00	-10,20	0,00	-4,18
33	ATP_c + ADP_m <==> ATP_m + ADP_c	R763		11,92	0,00	10,20	0,00	4,18
34	Glu_c + Gaba_m <==> Glu_m + Gaba_c	R764		0,00	0,00	0,00	0,00	0,00
35	CO2_c <==> CO2_m	R766		0,11	0,00	-0,55	0,00	-3,67
36	O2_c <==> O2_m	R767		0,00	0,00	1,00	0,00	4,00
37	NH3_c <==> NH3_m	R768		-1,36	421,40	-1,35	422,22	-0,79

Figure 2: Fill data input template

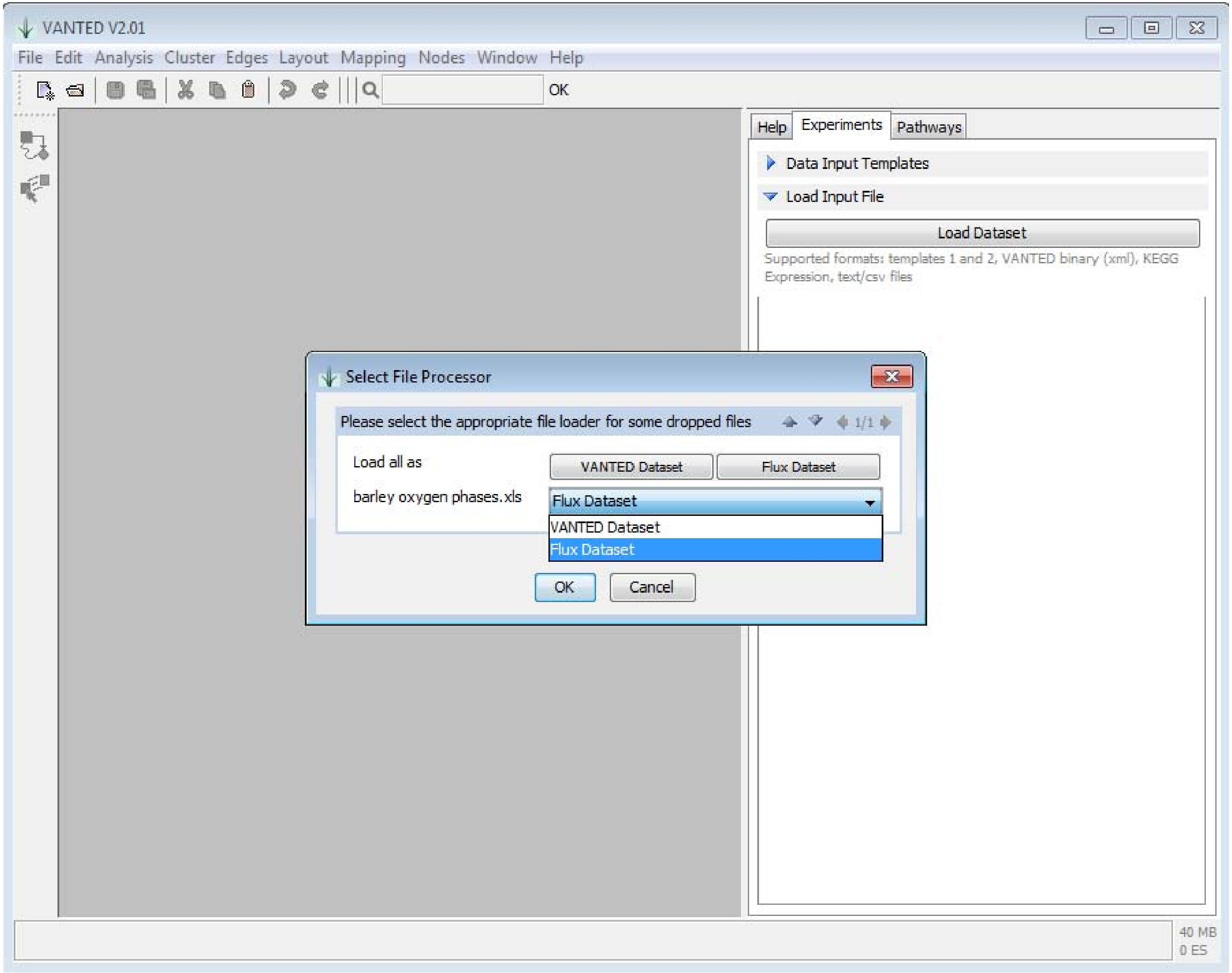


Suchen in: Data

Dateiname: barley oxygen phases.xls

Dateityp: Dataset (.xlsx|.xls|.csv|.bin|.dat|.txt|.list)

Figure 3: Load flux data



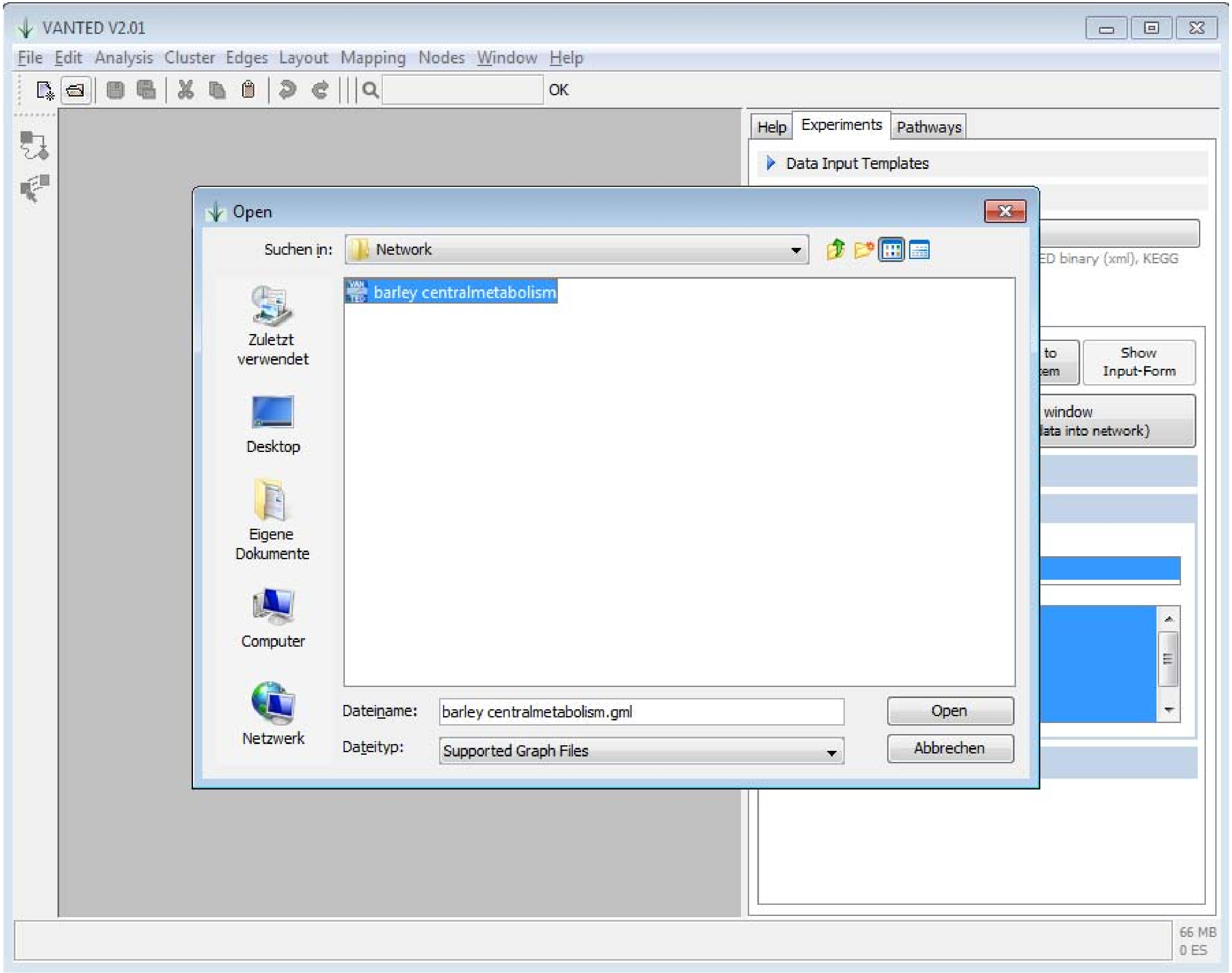
Supported formats: templates 1 and 2, VANTED binary (xml), KEGG Expression, text/csv files

Please select the appropriate file loader for some dropped files

Load all as: VANTED Dataset | Flux Dataset

barley oxygen phases.xls: Flux Dataset

Figure 4: Select correct template loader

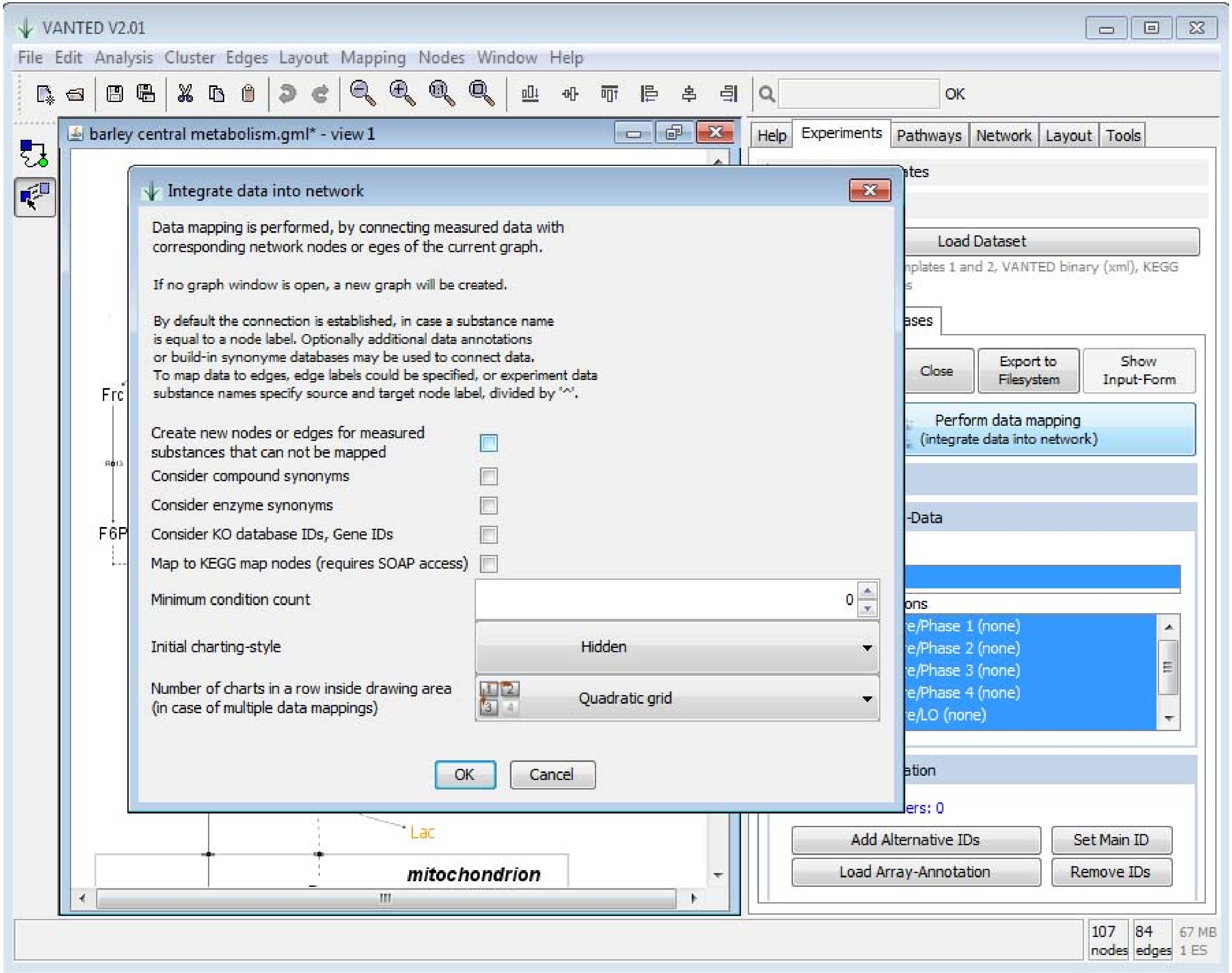


Suchen in: Network

Dateiname: barley centralmetabolism.gml

Dateityp: Supported Graph Files

Figure 5: Load network



Integrate data into network

Data mapping is performed, by connecting measured data with corresponding network nodes or eges of the current graph.

If no graph window is open, a new graph will be created.

By default the connection is established, in case a substance name is equal to a node label. Optionally additional data annotations or build-in synonyme databases may be used to connect data. To map data to edges, edge labels could be specified, or experiment data substance names specify source and target node label, divided by '^'.

- Create new nodes or edges for measured substances that can not be mapped ☐
- Consider compound synonyms ☐
- Consider enzyme synonyms ☐
- Consider KO database IDs, Gene IDs ☐
- Map to KEGG map nodes (requires SOAP access) ☐

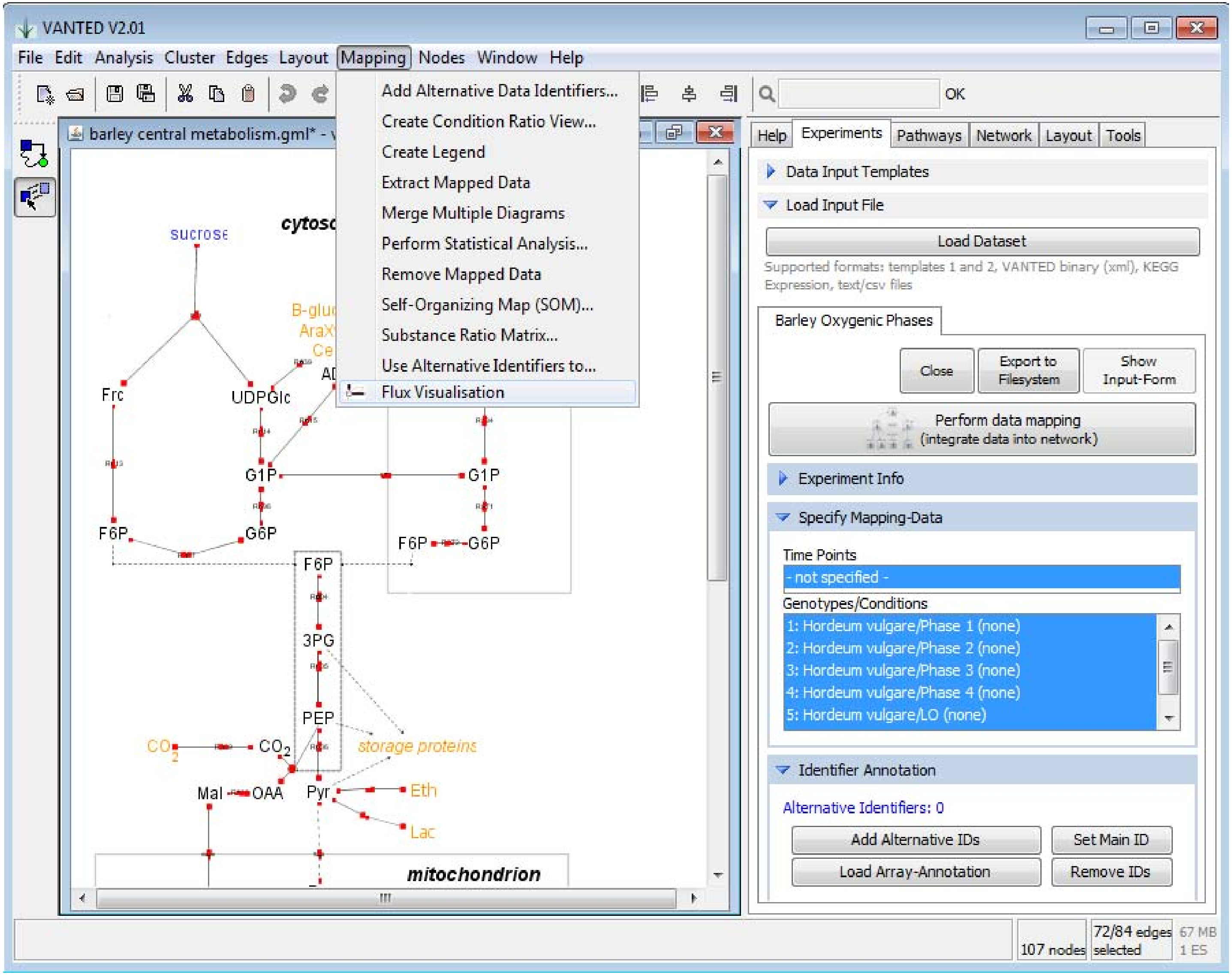
Minimum condition count: 0

Initial charting-style: Hidden

Number of charts in a row inside drawing area (in case of multiple data mappings): Quadratic grid

OK Cancel

Figure 6: Map flux data onto network



Time Points

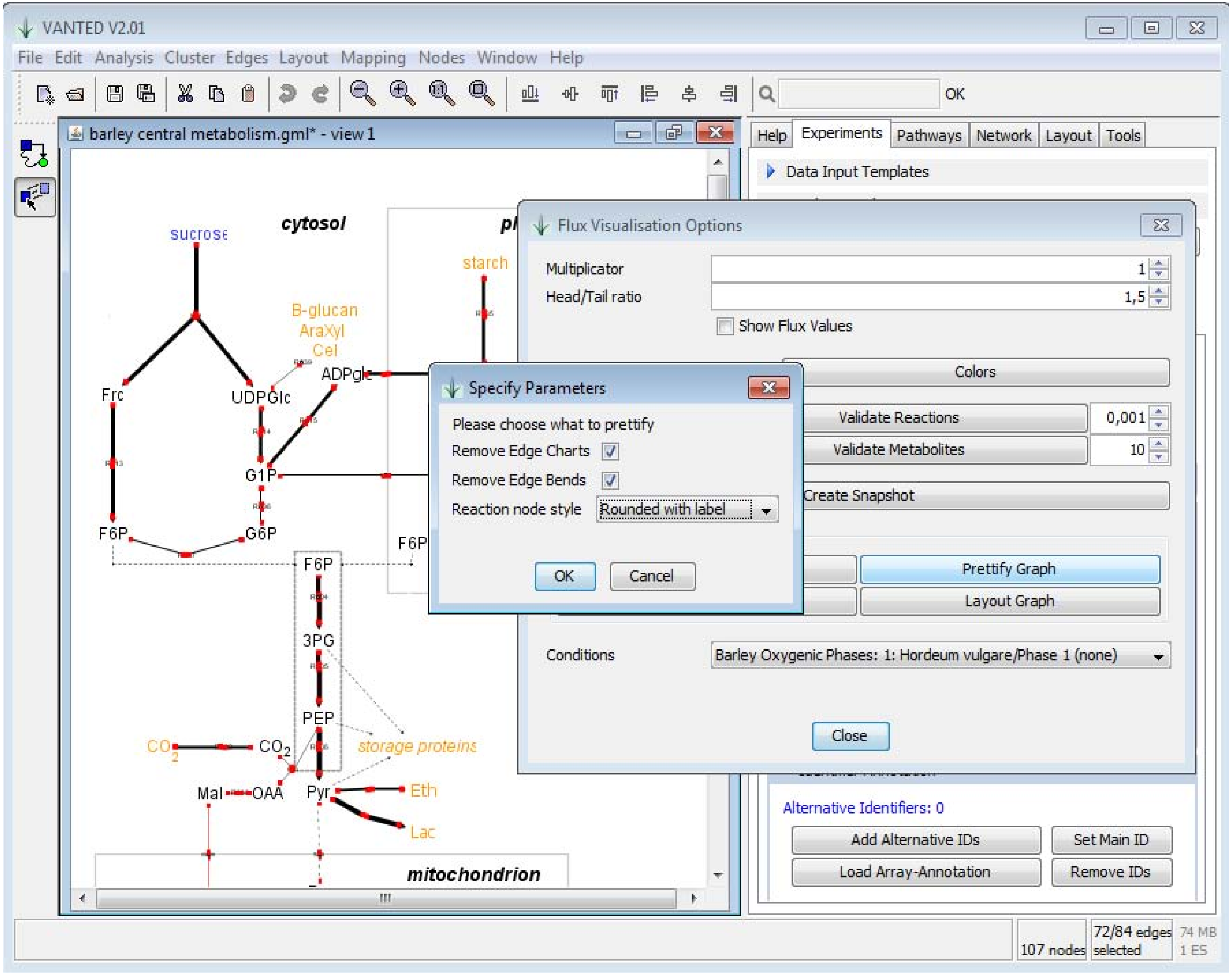
- not specified -

Genotypes/Conditions

1: Hordeum vulgare/Phase 1 (none)
2: Hordeum vulgare/Phase 2 (none)
3: Hordeum vulgare/Phase 3 (none)
4: Hordeum vulgare/Phase 4 (none)
5: Hordeum vulgare/LO (none)

Alternative Identifiers: 0

Figure 7: Summon FluxMap dialog



VANTED V2.01

barley central metabolism.gml* - view 1

Flux Visualisation Options

Multiplicator: 1

Head/Tail ratio: 1,5

☐ Show Flux Values

Validate Reactions: 0,001

Validate Metabolites: 10

Conditions: Barley Oxygenic Phases: 1: Hordeum vulgare/Phase 1 (none)

Specify Parameters

Please choose what to prettify

Remove Edge Charts ☑

Remove Edge Bends ☑

Reaction node style: Rounded with label

Alternative Identifiers: 0

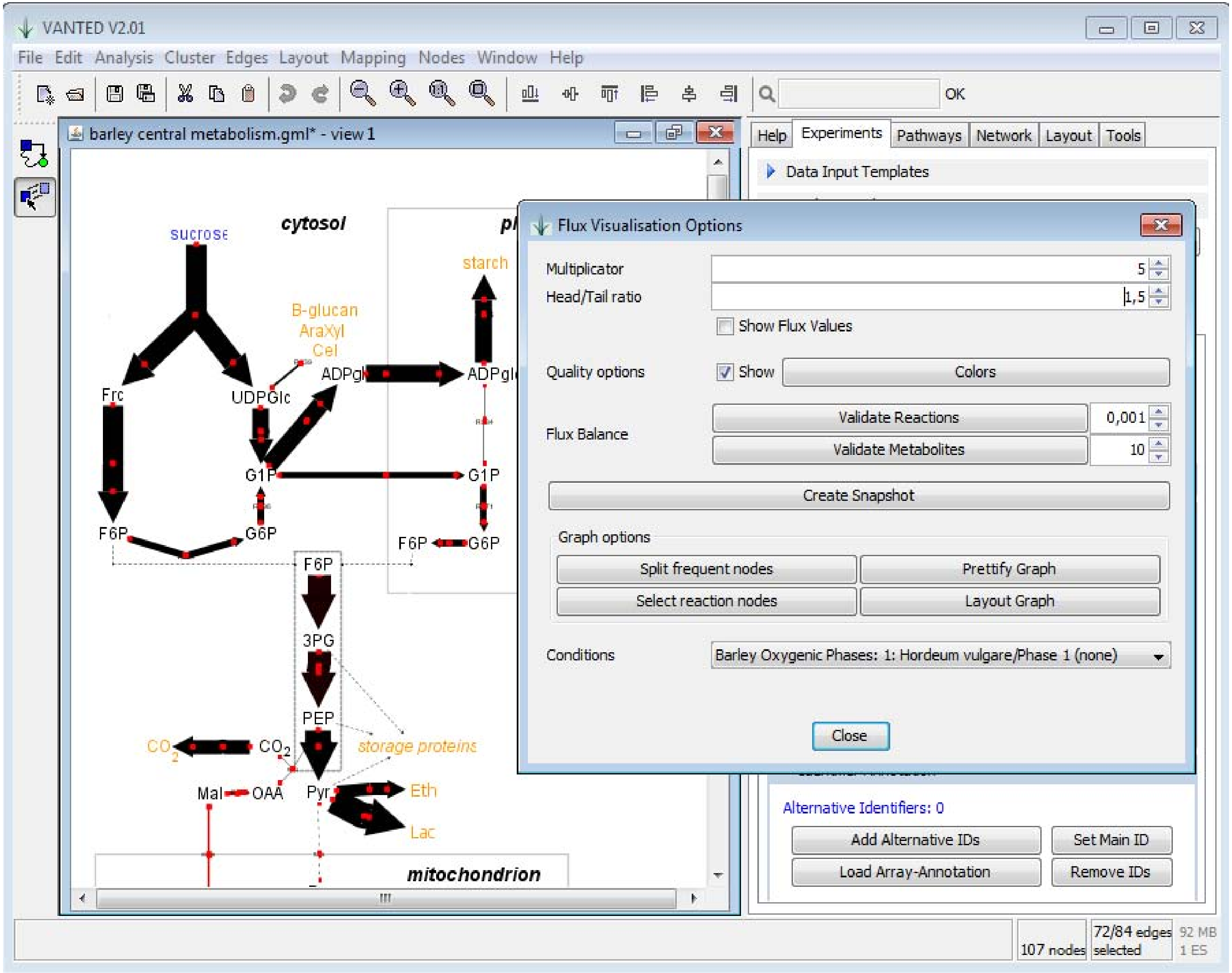
107 nodes

72/84 edges selected

74 MB

1 ES

Figure 8: Improve visualization



barley central metabolism.gml* - view 1

Flux Visualisation Options

Multiplicator: 5

Head/Tail ratio: 1,5

☐ Show Flux Values

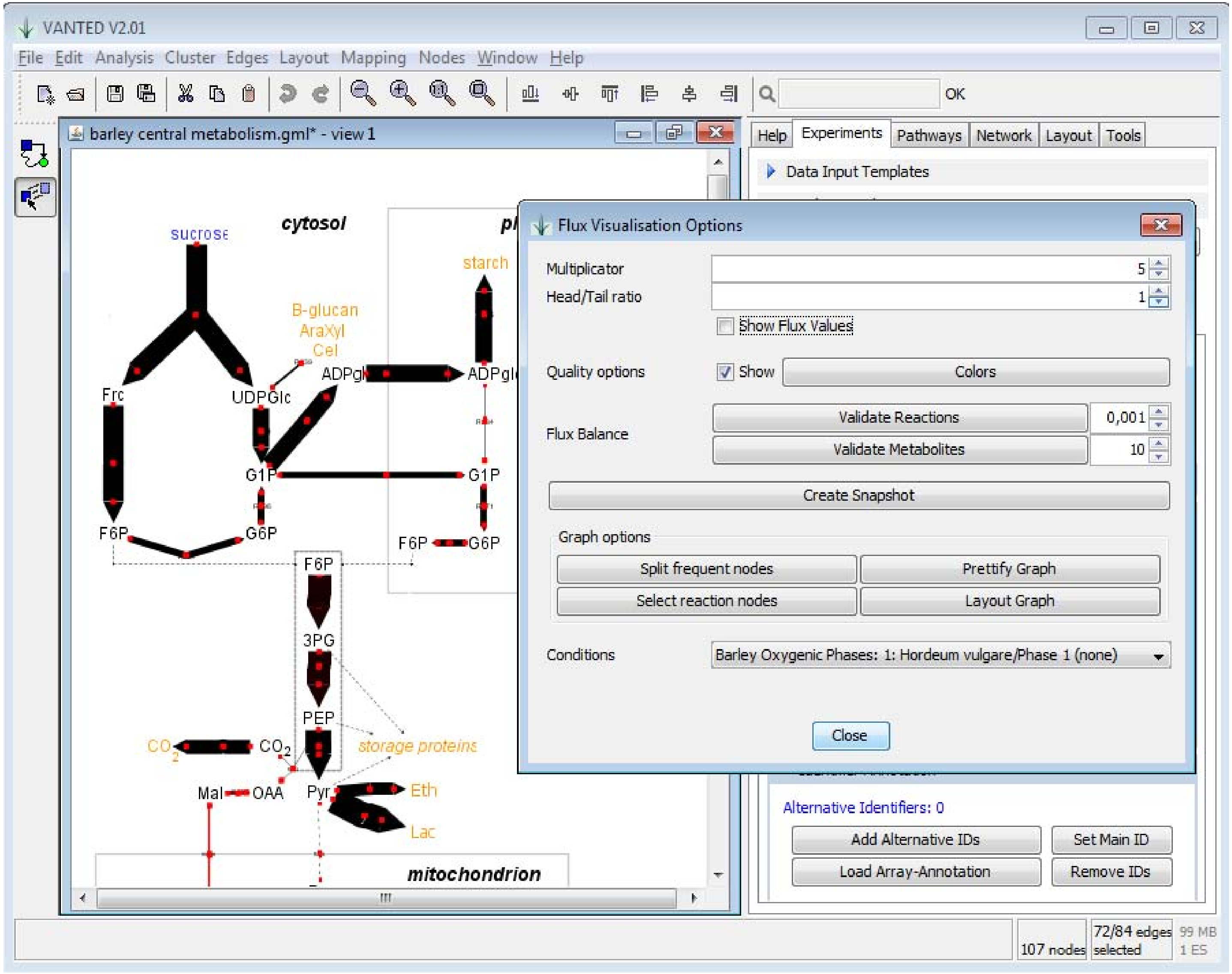
Quality options: ☑ Show

Flux Balance: Validate Reactions 0,001; Validate Metabolites 10

Conditions: Barley Oxygenic Phases: 1: Hordeum vulgare/Phase 1 (none)

107 nodes | 72/84 edges selected | 92 MB 1 ES

Figure 9: Increase global edge thickness



Multiplicator 5

Head/Tail ratio 1

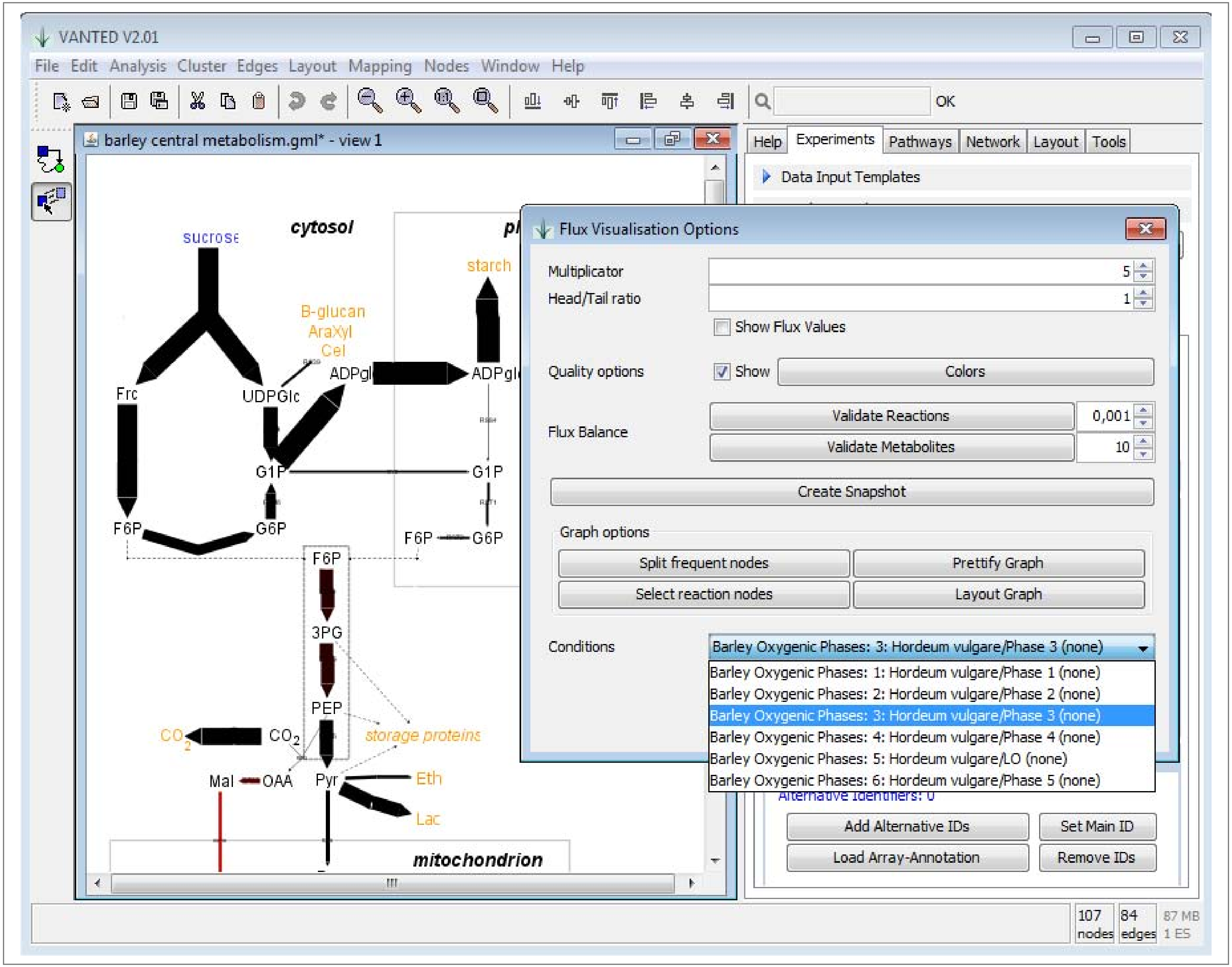
☐ Show Flux Values

Quality options ☑ Show

Flux Balance: Validate Reactions 0,001; Validate Metabolites 10

Conditions: Barley Oxygenic Phases: 1: Hordeum vulgare/Phase 1 (none)

Figure 10: Reduce arrowhead/-tail ratio



Flux Visualisation Options

Multiplicator: 5

Head/Tail ratio: 1

☐ Show Flux Values

Quality options: ☑ Show

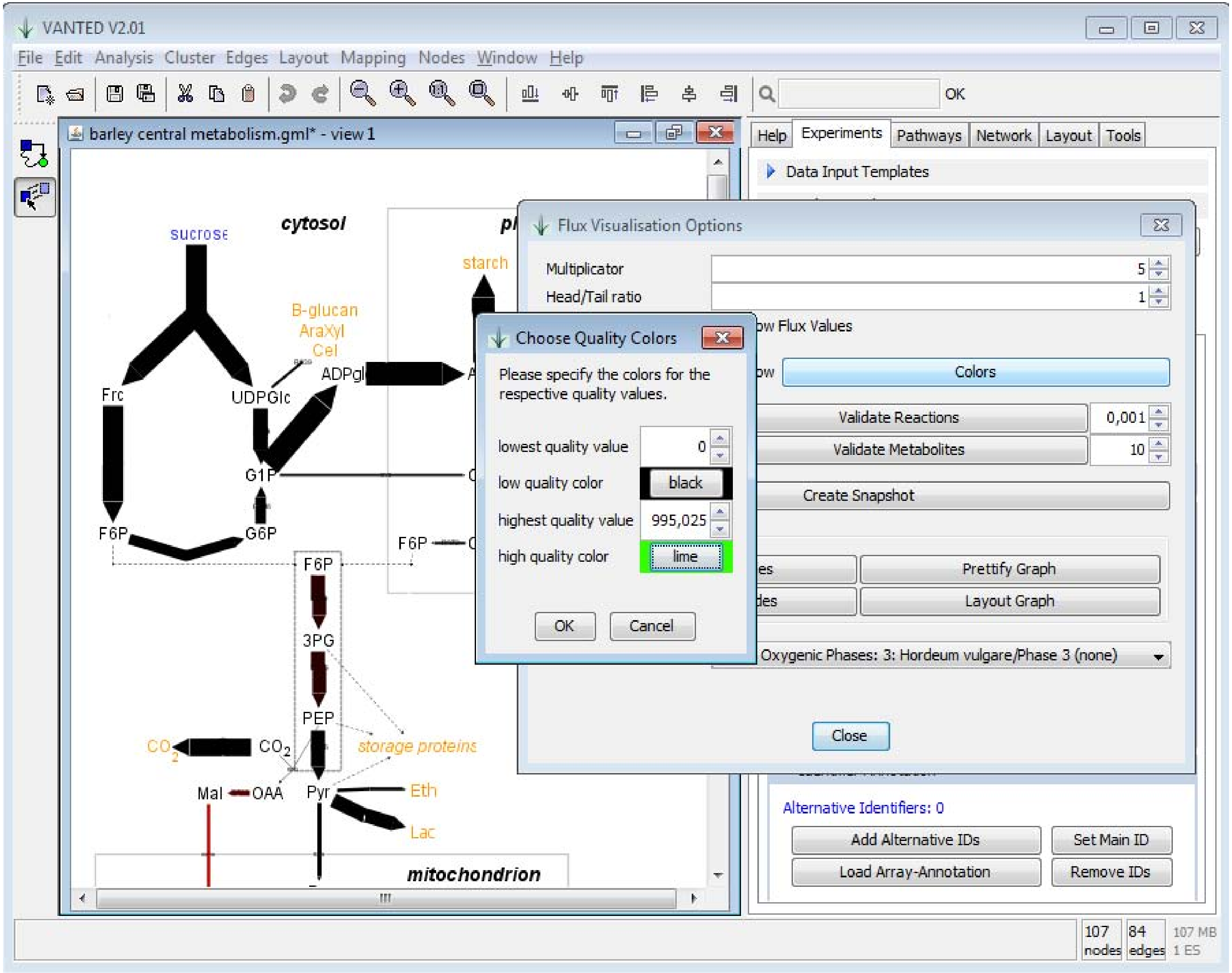
Flux Balance: Validate Reactions 0,001; Validate Metabolites 10

Conditions: Barley Oxygenic Phases: 3: Hordeum vulgare/Phase 3 (none)

- Barley Oxygenic Phases: 1: Hordeum vulgare/Phase 1 (none)
- Barley Oxygenic Phases: 2: Hordeum vulgare/Phase 2 (none)
- Barley Oxygenic Phases: 3: Hordeum vulgare/Phase 3 (none)
- Barley Oxygenic Phases: 4: Hordeum vulgare/Phase 4 (none)
- Barley Oxygenic Phases: 5: Hordeum vulgare/LO (none)
- Barley Oxygenic Phases: 6: Hordeum vulgare/Phase 5 (none)

107 nodes 84 edges 87 MB 1 ES

Figure 11: Switch between different conditions



Multiplicator 5

Head/Tail ratio 1

Please specify the colors for the respective quality values.

lowest quality value 0

low quality color black

highest quality value 995,025

high quality color lime

Validate Reactions 0,001

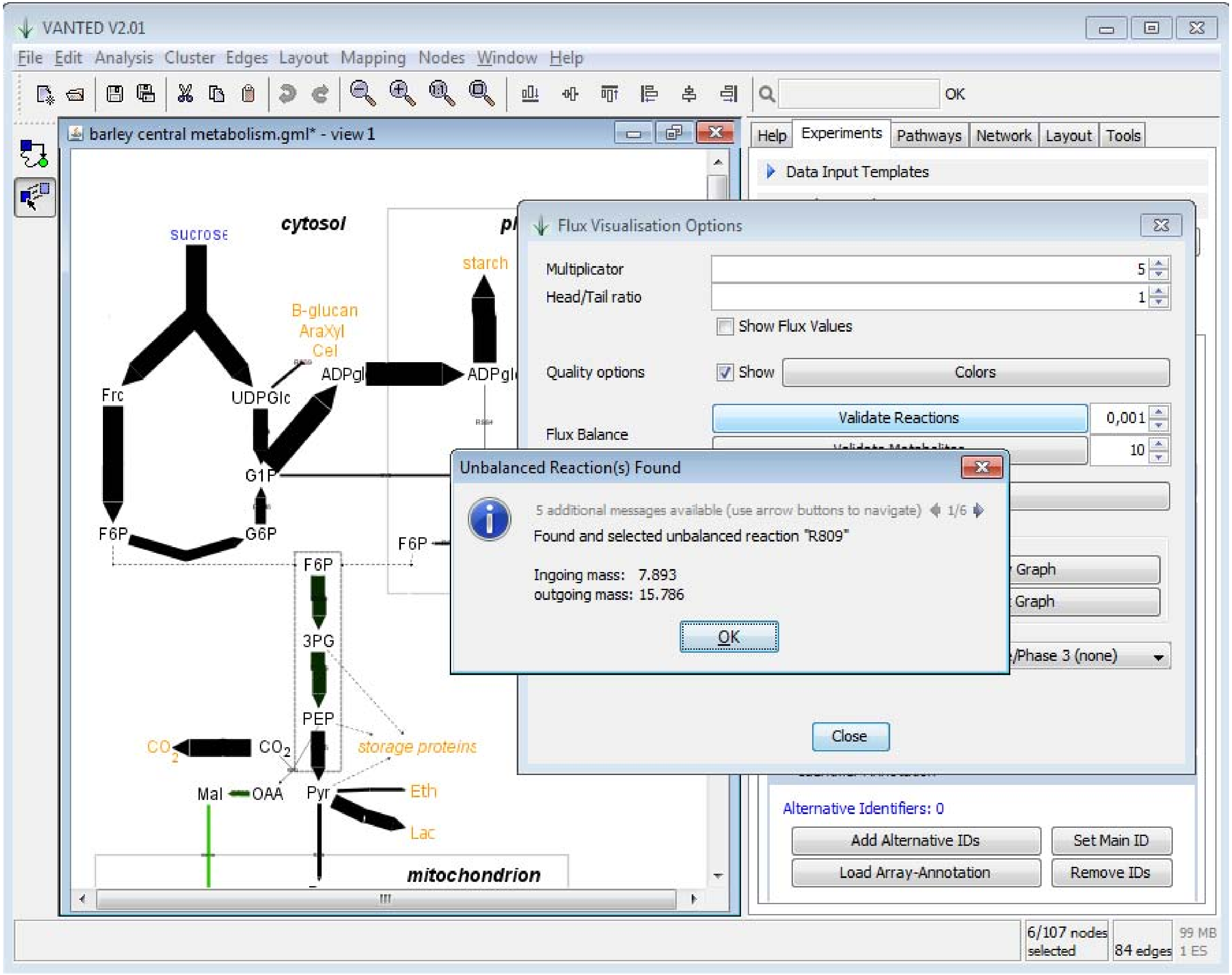
Validate Metabolites 10

Oxygenic Phases: 3: Hordeum vulgare/Phase 3 (none)

Alternative Identifiers: 0

107 nodes 84 edges 107 MB 1 ES

Figure 12: Adapt visualization of quality information



Multiplicator 5

Head/Tail ratio 1

☐ Show Flux Values

Quality options ☑ Show

Flux Balance: Validate Reactions 0,001; 10

Unbalanced Reaction(s) Found

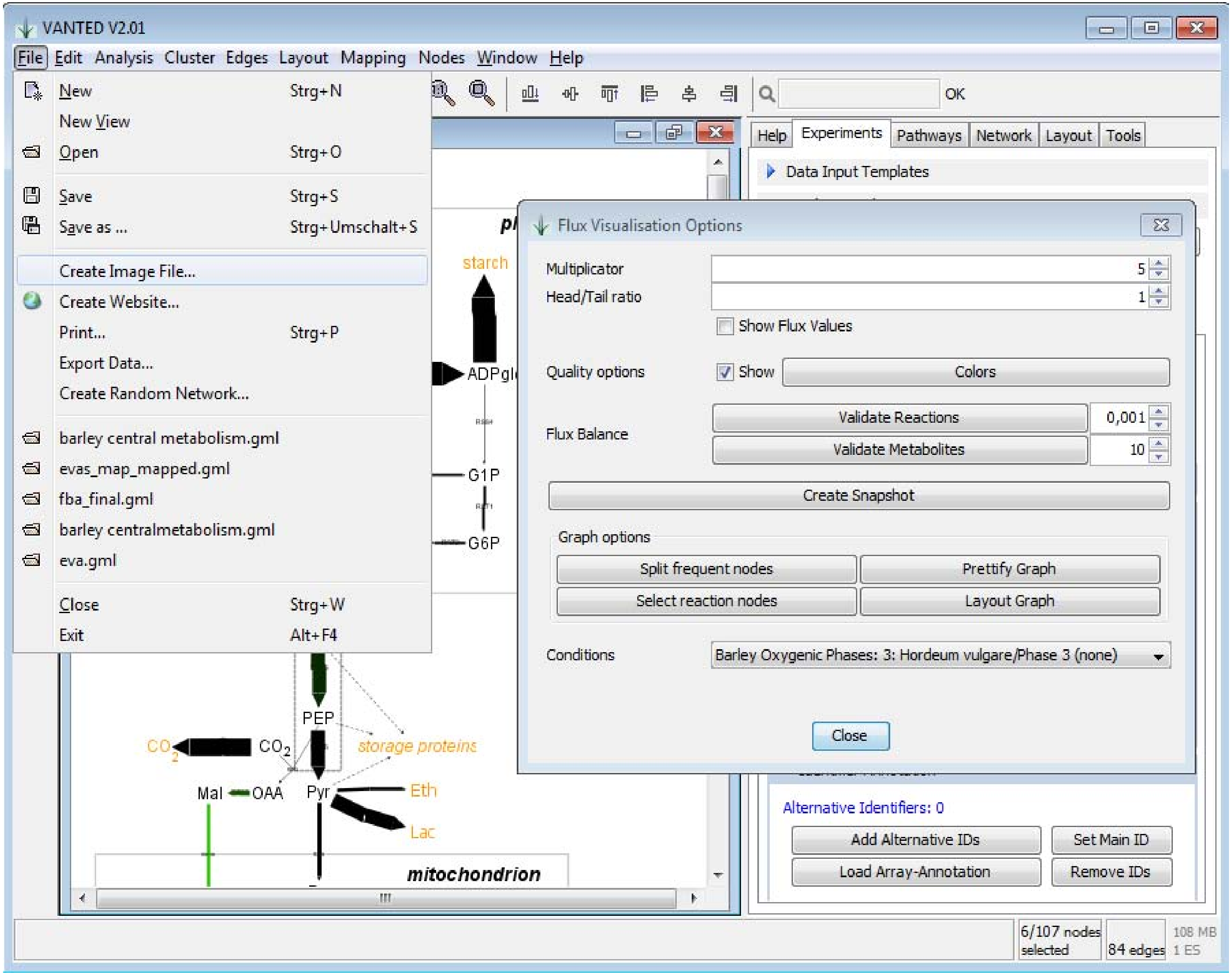
5 additional messages available (use arrow buttons to navigate) 1/6

Found and selected unbalanced reaction "R809"

Ingoing mass: 7.893
outgoing mass: 15.786

6/107 nodes selected
84 edges
99 MB
1 ES

Figure 13: Validate flux balance



Multiplicator 5

Head/Tail ratio 1

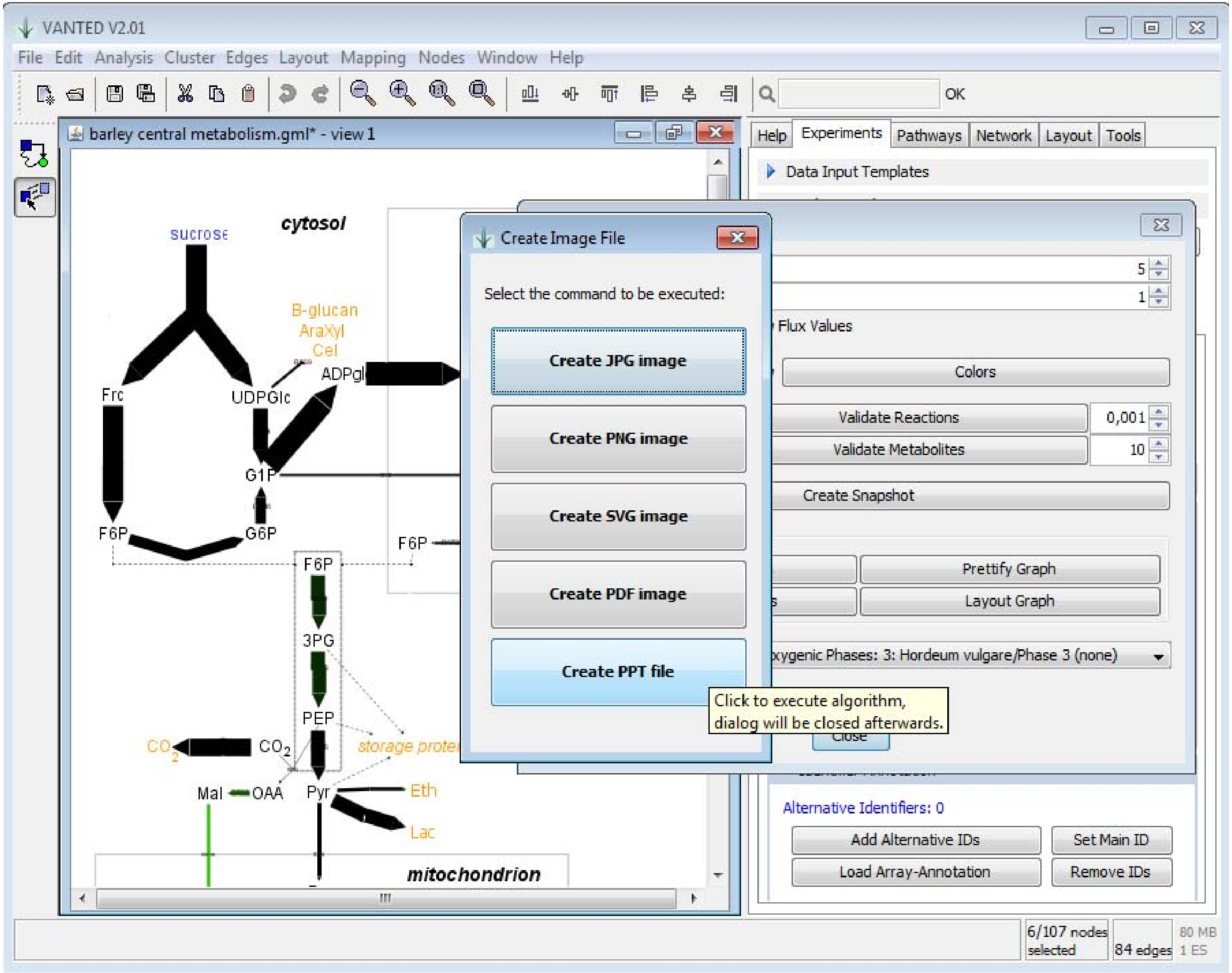
☐ Show Flux Values

Quality options ☑ Show

Flux Balance 0,001 10

Conditions Barley Oxygenic Phases: 3: Hordeum vulgare/Phase 3 (none)

Figure 14: Export data, graphics or webpage



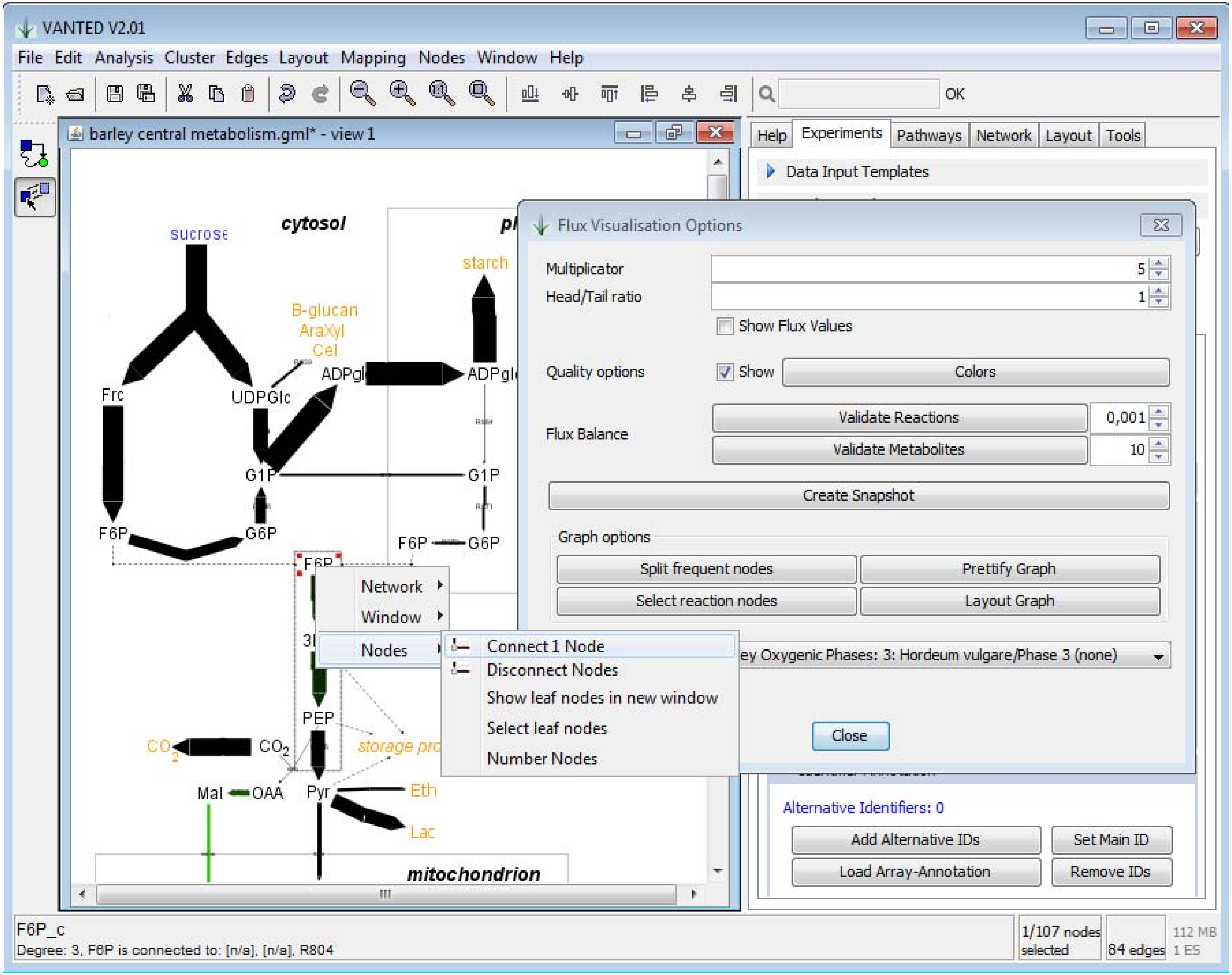
Select the command to be executed:

Click to execute algorithm, dialog will be closed afterwards.

xygenic Phases: 3: Hordeum vulgare/Phase 3 (none)

Alternative Identifiers: 0

Figure 15: Export in different graphical formats



Multiplicator 5

Head/Tail ratio 1

☐ Show Flux Values

Quality options ☑ Show

Flux Balance: Validate Reactions 0,001; Validate Metabolites 10

ey Oxygenic Phases: 3: Hordeum vulgare/Phase 3 (none)

F6P_c

Degree: 3, F6P is connected to: [n/a], [n/a], R804

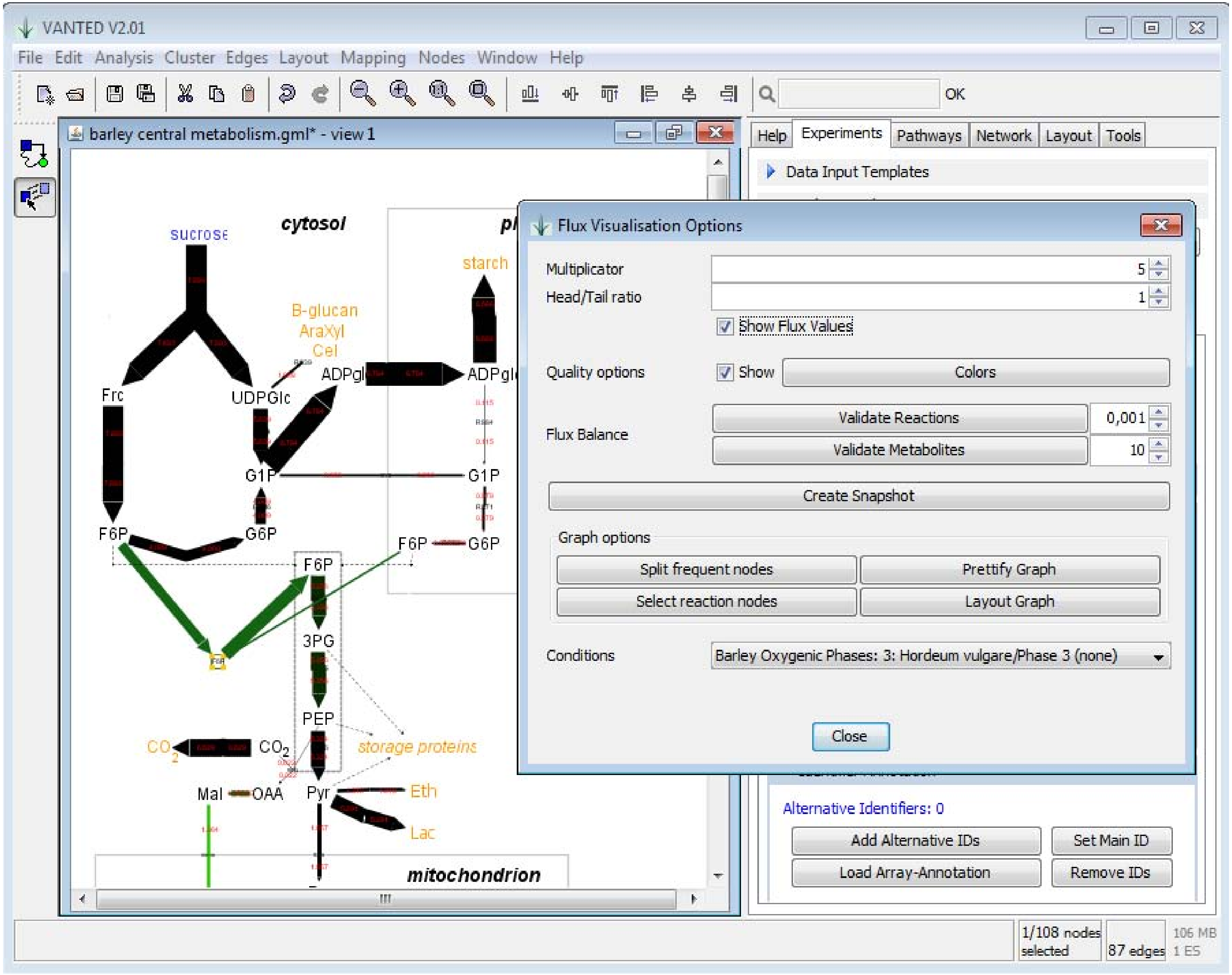
1/107 nodes selected

84 edges

112 MB

1 ES

Figure 16: Connect metabolites with the same label



Multiplicator 5

Head/Tail ratio 1

☑ Show Flux Values

Quality options ☑ Show

Flux Balance
Validate Reactions 0,001
Validate Metabolites 10

Conditions: Barley Oxygenic Phases: 3: Hordeum vulgare/Phase 3 (none)

Figure 17: Show flux values on edges