IPA tips and tricks

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Senior Scientist, QIAGEN Bioinformatics
September 17, 2019

Agenda

With a dataset

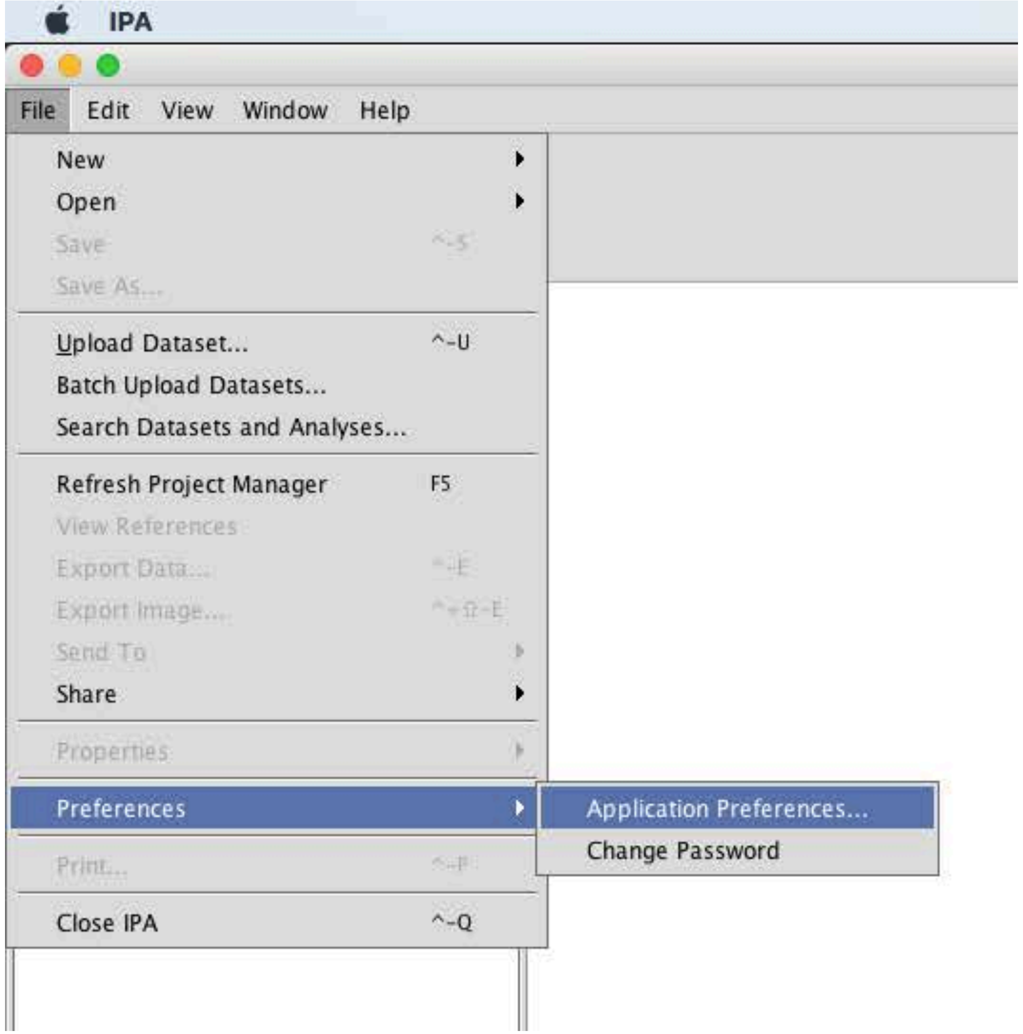
With or without a dataset

Chapters

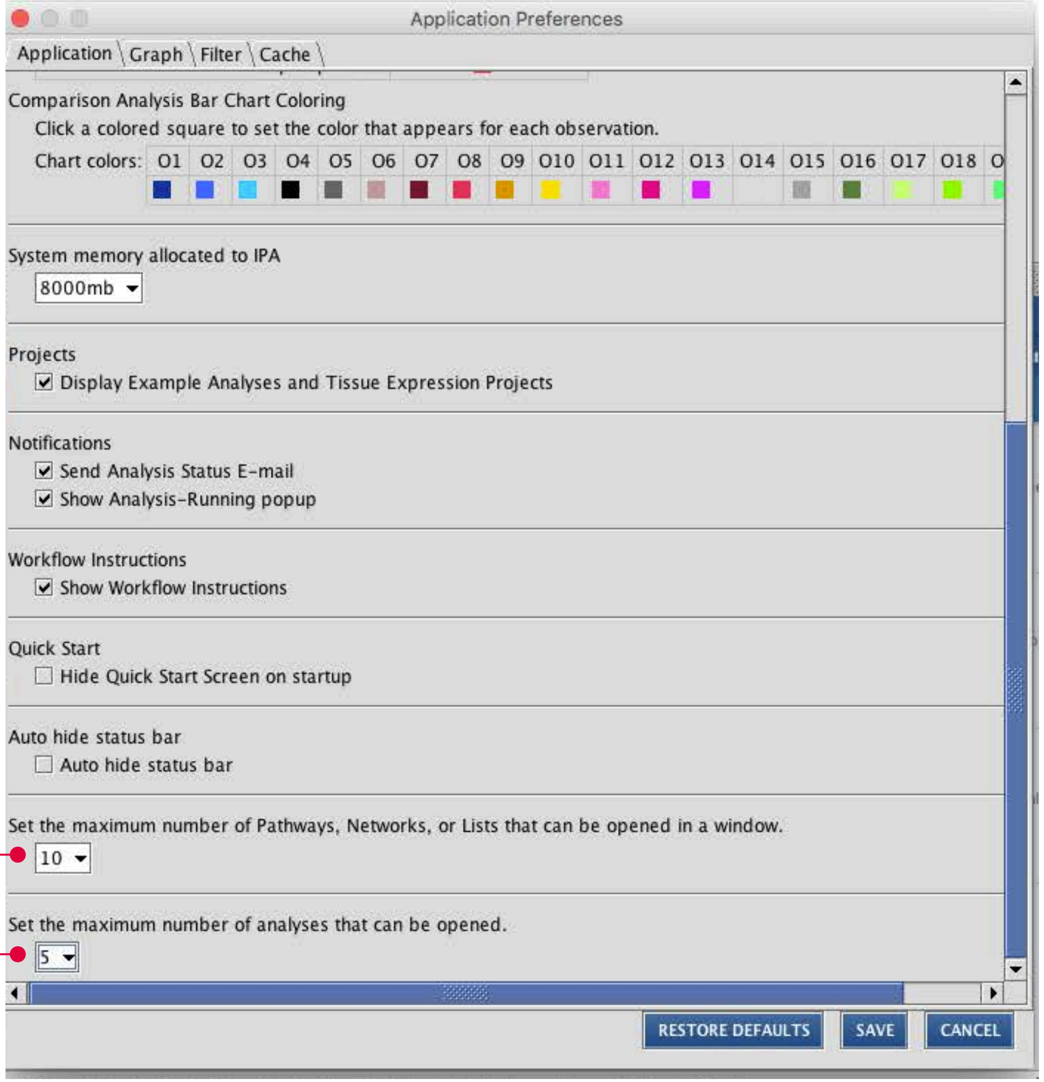
With a dataset

With or without a dataset

How to access Application Preferences



Multitask with additional windows



Comparison Analysis Bar Chart Coloring

Click a colored square to set the color that appears for each observation.

Chart colors: O1 O2 O3 O4 O5 O6 O7 O8 O9 O10 O11 O12 O13 O14 O15 O16 O17 O18 O

System memory allocated to IPA

8000mb

Projects

☑ Display Example Analyses and Tissue Expression Projects

Notifications

☑ Send Analysis Status E-mail

☑ Show Analysis-Running popup

Workflow Instructions

☑ Show Workflow Instructions

Quick Start

☐ Hide Quick Start Screen on startup

Auto hide status bar

☐ Auto hide status bar

Set the maximum number of Pathways, Networks, or Lists that can be opened in a window.

10

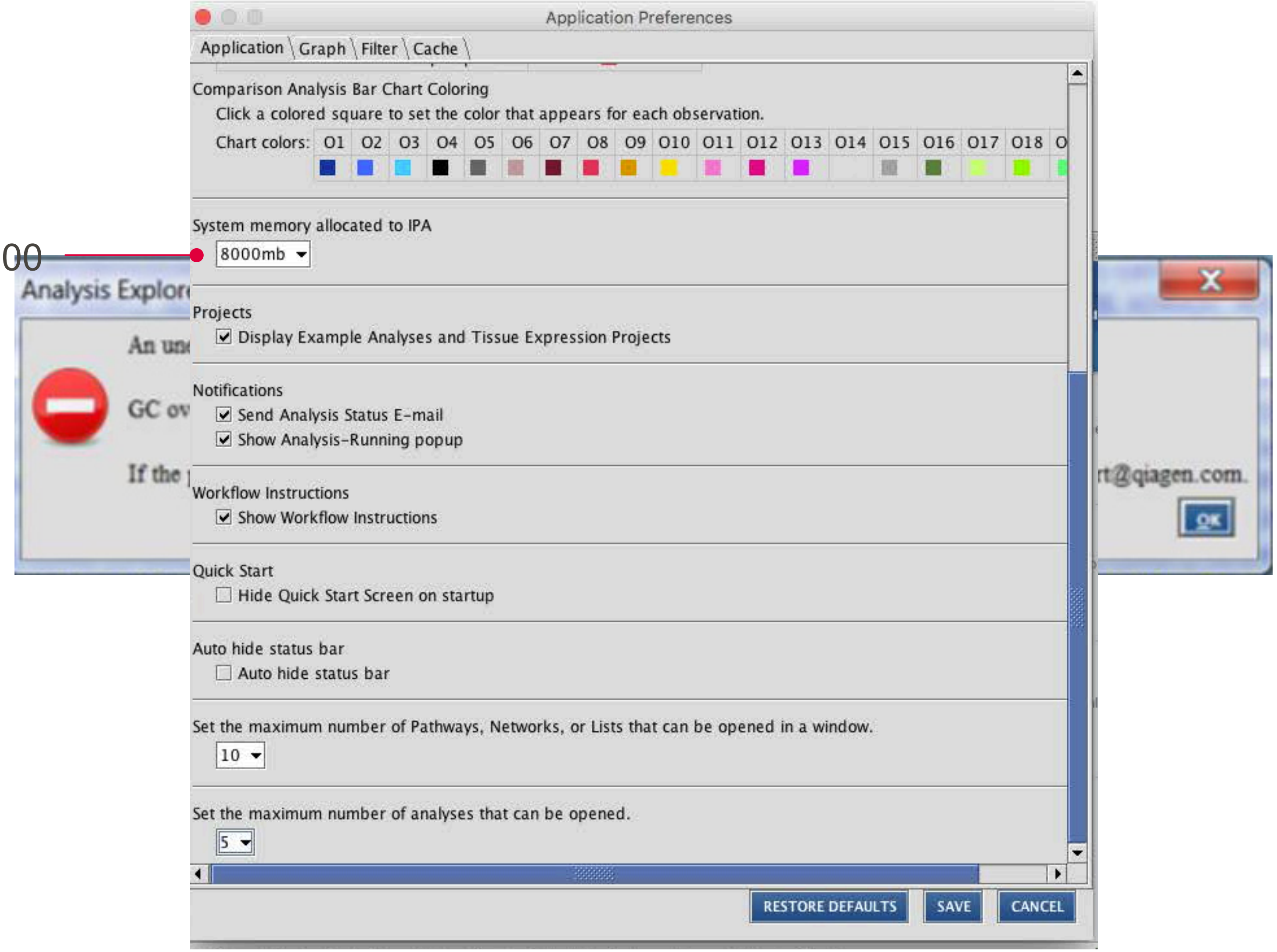
Set the maximum number of analyses that can be opened.

5

Set to up to 10

Set to up to 5

Prevent technical errors



Set to >1000

Application Preferences

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Clear the cache

The “magic wand”

IPA performance can be improved by enabling caching, or temporary storage of frequently accessed IPA publicly available data, such as Canonical Pathway information, on this local computer.
The minimum cache size is 1MB and recommended is between 200MB & 1GB.

☑ Enable Ingenuity content caching on this machine.

The current cache size is 31 MB (31023498 bytes)

Amount of disk space to use for caching: 2000 MB.

Amount of free disk space available 124462.305 MB.

Clearing the cache deletes all cached data. IPA features that use cache will temporarily be slower until the cache is restored.

Set to 200 MB to 10 GB

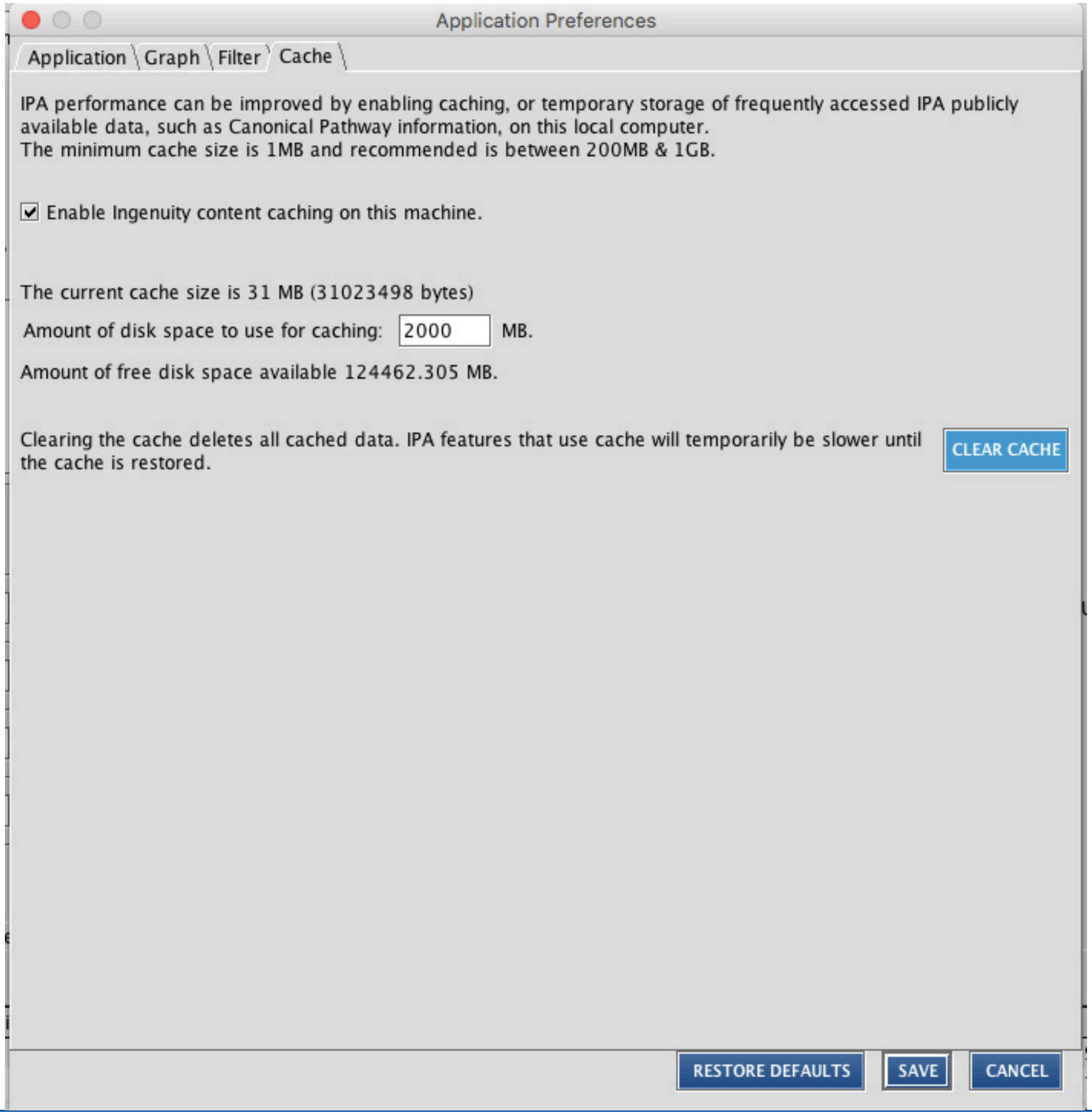
Saving your preferences

Steps:

Select Save button

Log out of IPA

Log back into the program



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Chapters

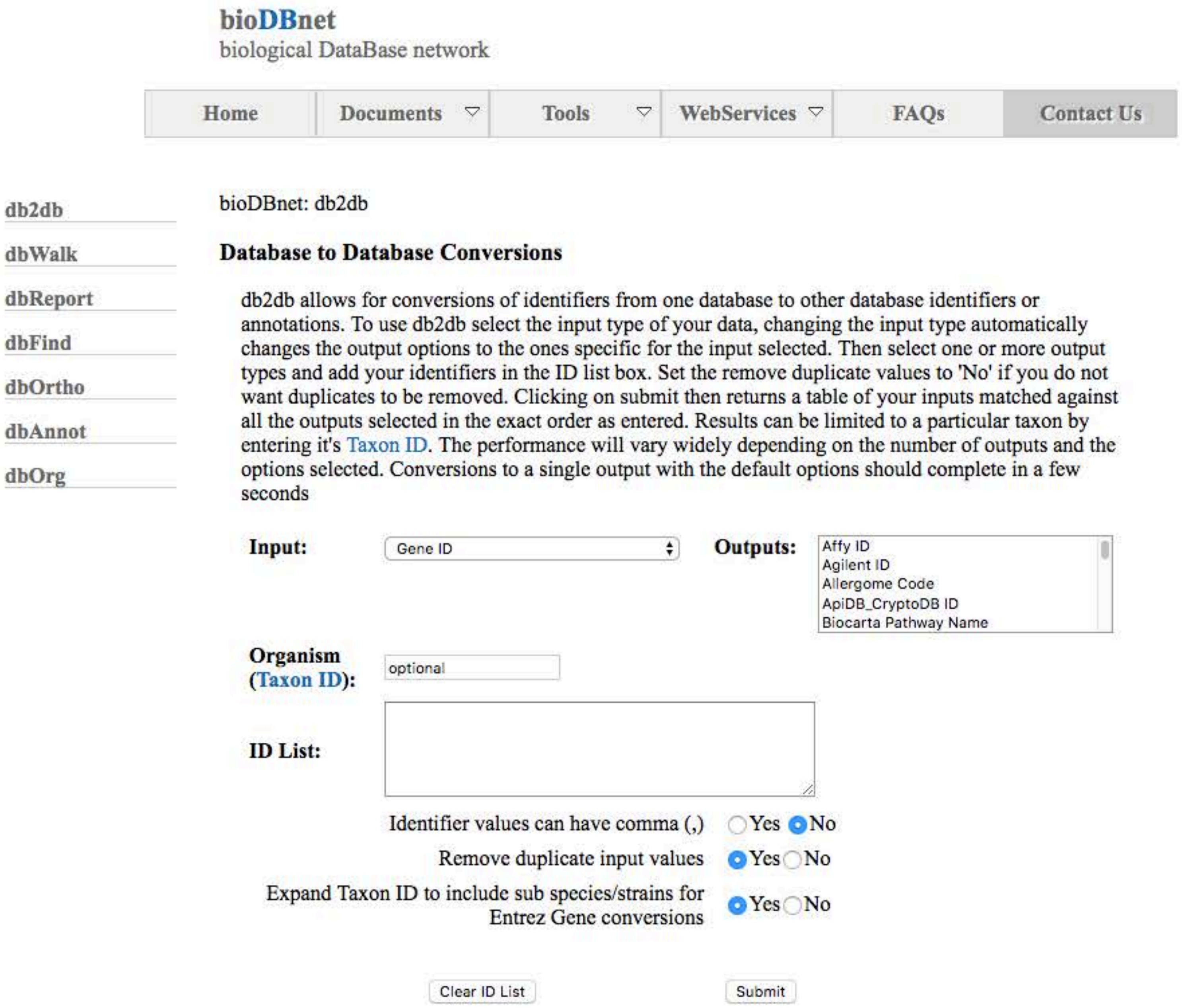
With a dataset

With or without a dataset

Convert IDs: bioDBnet

db2db

https://biodbnet-abcc.ncifcrf.gov/db/db2db.php



bioDBnet: db2db

Database to Database Conversions

db2db allows for conversions of identifiers from one database to other database identifiers or annotations. To use db2db select the input type of your data, changing the input type automatically changes the output options to the ones specific for the input selected. Then select one or more output types and add your identifiers in the ID list box. Set the remove duplicate values to 'No' if you do not want duplicates to be removed. Clicking on submit then returns a table of your inputs matched against all the outputs selected in the exact order as entered. Results can be limited to a particular taxon by entering it's Taxon ID. The performance will vary widely depending on the number of outputs and the options selected. Conversions to a single output with the default options should complete in a few seconds

Input: Gene ID

Outputs:
Affy ID
Agilent ID
Allergome Code
ApiDB_CryptoDB ID
Biocarta Pathway Name

Organism (Taxon ID): optional

ID List:

Identifier values can have comma (,) ○ Yes ● No

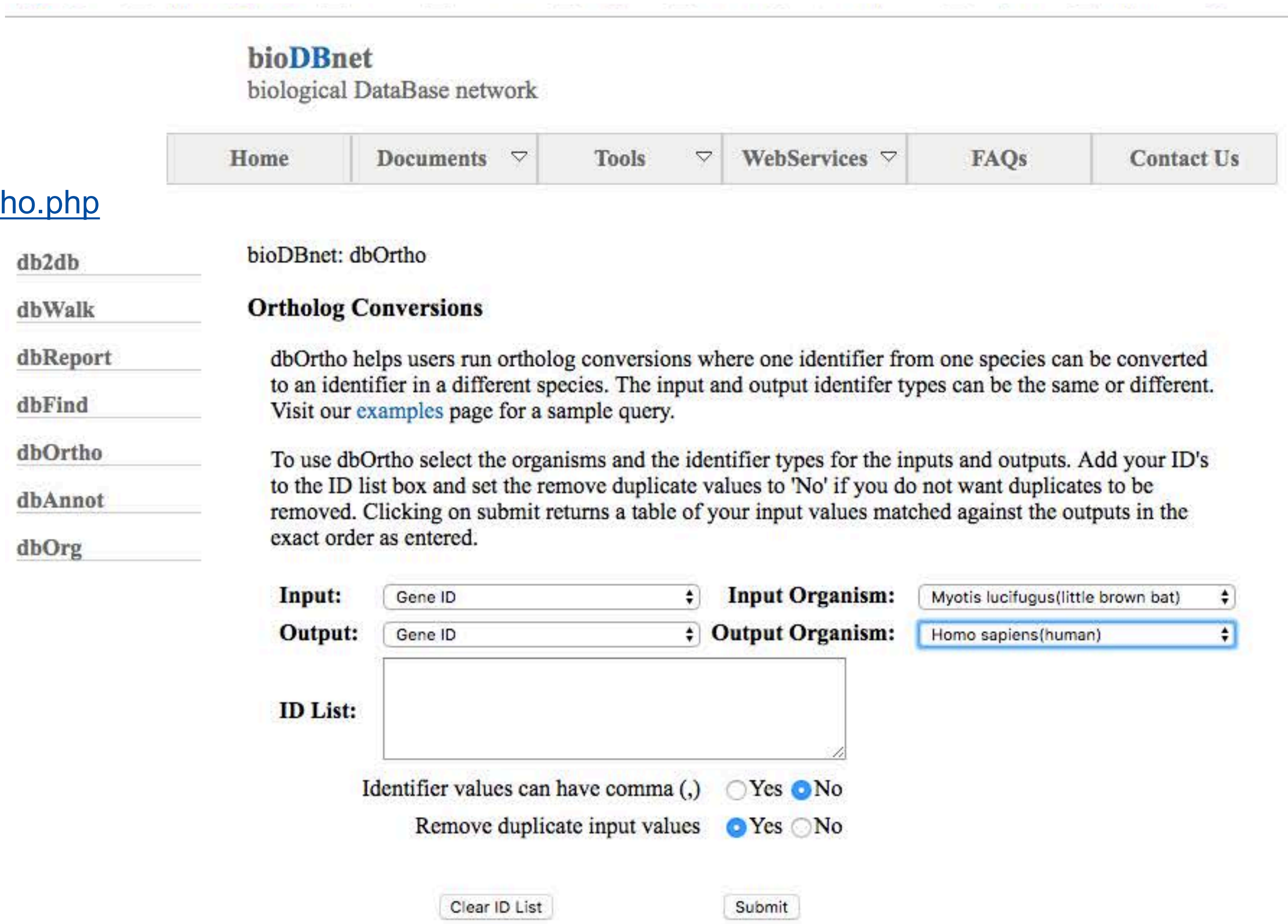
Remove duplicate input values ● Yes ○ No

Expand Taxon ID to include sub species/strains for Entrez Gene conversions ● Yes ○ No

Convert IDs: bioDBnet

dbOrtho

https://biodbnet-abcc.ncifcrf.gov/db/dbOrtho.php



bioDBnet: dbOrtho

Ortholog Conversions

dbOrtho helps users run ortholog conversions where one identifier from one species can be converted to an identifier in a different species. The input and output identifer types can be the same or different. Visit our examples page for a sample query.

To use dbOrtho select the organisms and the identifier types for the inputs and outputs. Add your ID's to the ID list box and set the remove duplicate values to 'No' if you do not want duplicates to be removed. Clicking on submit returns a table of your input values matched against the outputs in the exact order as entered.

Input: Gene ID **Input Organism:** Myotis lucifugus(little brown bat)
Output: Gene ID **Output Organism:** Homo sapiens(human)
ID List:

Identifier values can have comma (,) ○ Yes ● No
Remove duplicate input values ● Yes ○ No

Metabolomics IDs

ID types you can use:

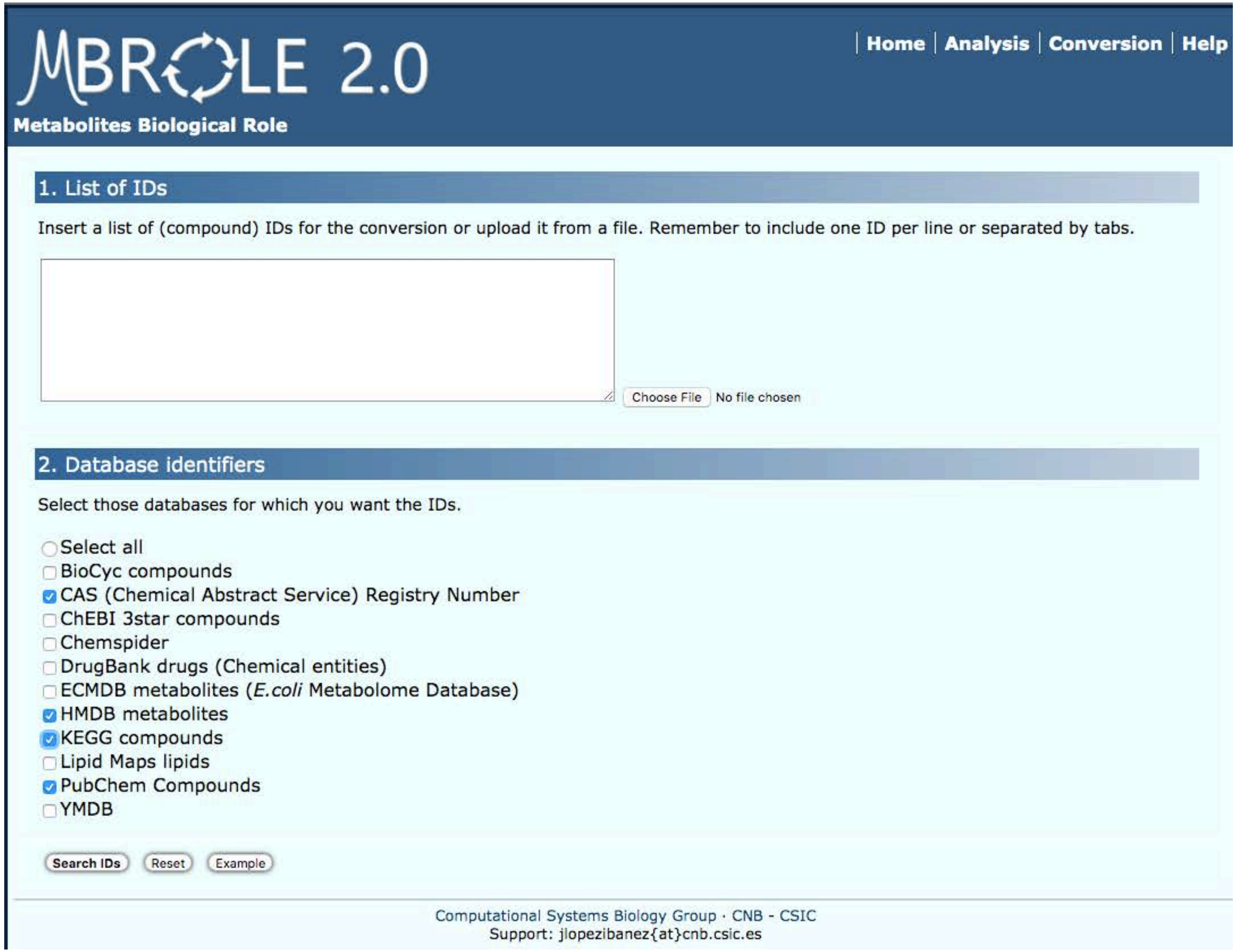
HMDB, PubChem, KEGG, and CAS Registry

Use latest HMDB ID (seven digits, not five)

Convert IDs: MBROLE*

http://csbg.cnb.csic.es/mbrole2/conversion.php

*Uses older HMDB identifiers



Metabolites Biological Role

1. List of IDs

Insert a list of (compound) IDs for the conversion or upload it from a file. Remember to include one ID per line or separated by tabs.

2. Database identifiers

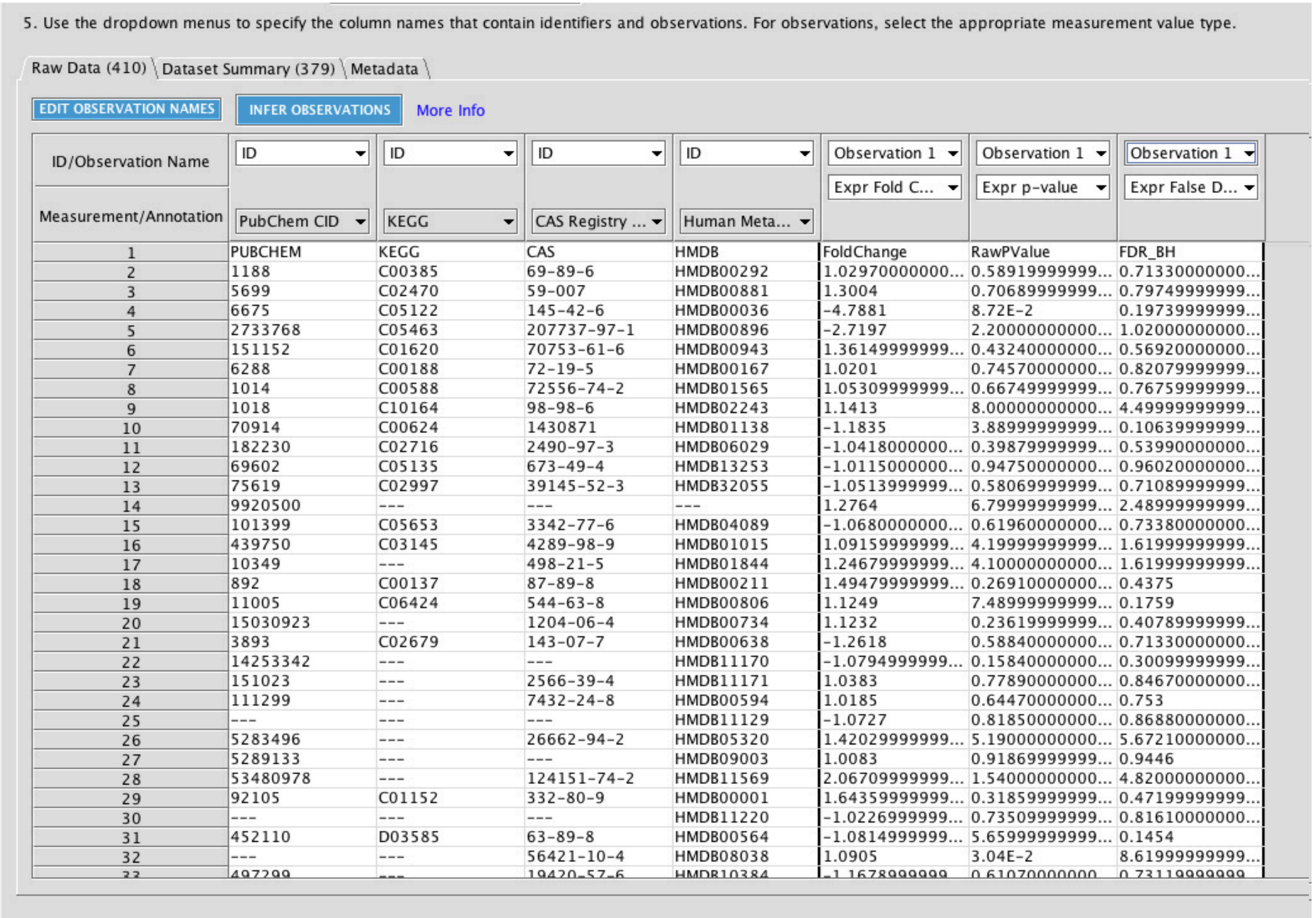
Select those databases for which you want the IDs.

○ Select all
☐ BioCyc compounds
☑ CAS (Chemical Abstract Service) Registry Number
☐ ChEBI 3star compounds
☐ Chemspider
☐ DrugBank drugs (Chemical entities)
☐ ECMDB metabolites (*E.coli* Metabolome Database)
☑ HMDB metabolites
☑ KEGG compounds
☐ Lipid Maps lipids
☑ PubChem Compounds
☐ YMDB

Computational Systems Biology Group · CNB - CSIC
Support: jlopezibanez{at}cnb.csic.es

Add multiple IDs to maximize mapping

Up to five ID columns per dataset



5. Use the dropdown menus to specify the column names that contain identifiers and observations. For observations, select the appropriate measurement value type.

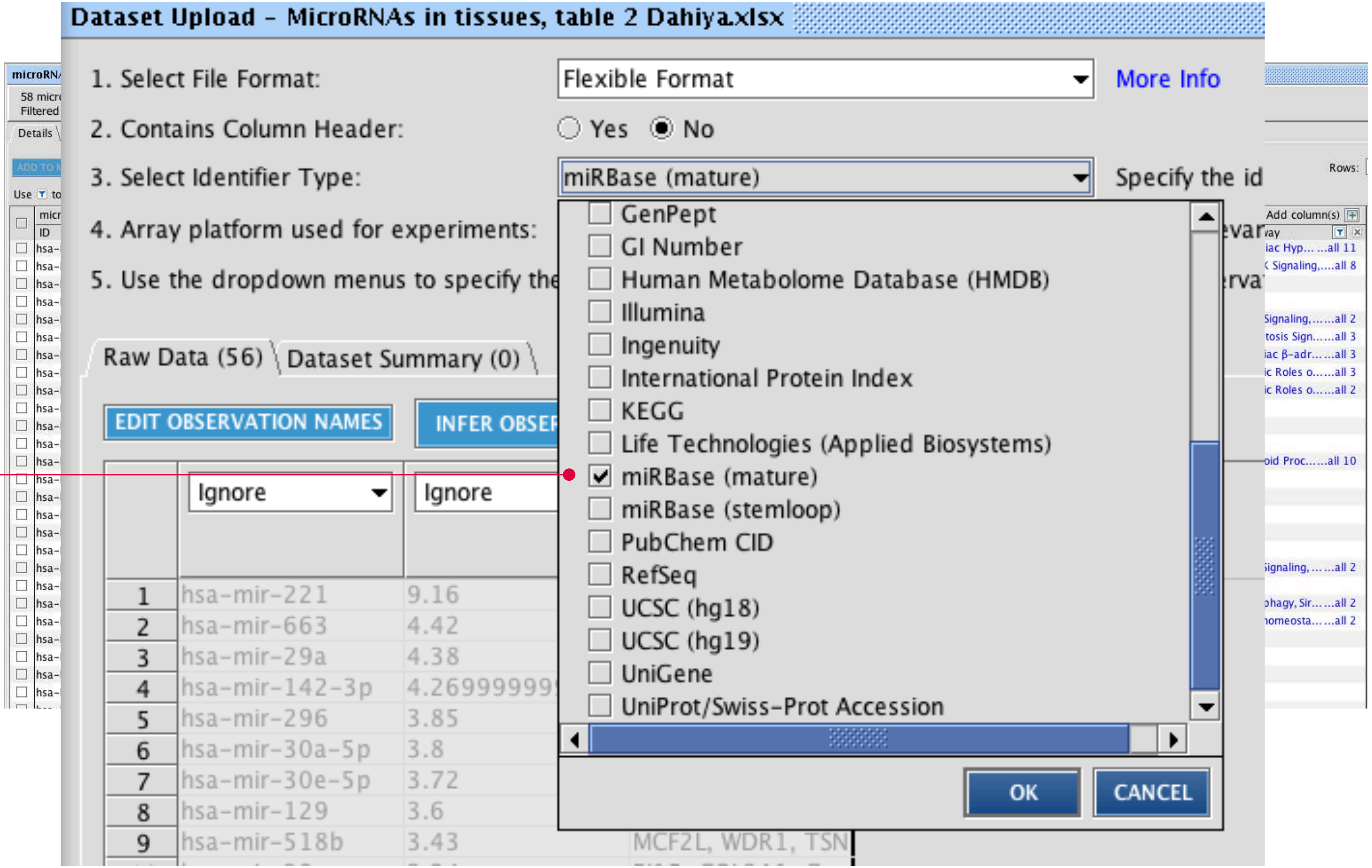
ID/Observation Name	ID	ID	ID	ID	Observation 1	Observation 1	Observation 1
Measurement/Annotation	PubChem CID	KEGG	CAS Registry ...	Human Meta...	Expr Fold C...	Expr p-value	Expr False D...
1	PUBCHEM	KEGG	CAS	HMDB	FoldChange	RawPValue	FDR_BH
2	1188	C00385	69-89-6	HMDB00292	1.02970000000...	0.58919999999...	0.71330000000...
3	5699	C02470	59-007	HMDB00881	1.3004	0.70689999999...	0.79749999999...
4	6675	C05122	145-42-6	HMDB00036	-4.7881	8.72E-2	0.19739999999...
5	2733768	C05463	207737-97-1	HMDB00896	-2.7197	2.20000000000...	1.02000000000...
6	151152	C01620	70753-61-6	HMDB00943	1.36149999999...	0.43240000000...	0.56920000000...
7	6288	C00188	72-19-5	HMDB00167	1.0201	0.74570000000...	0.82079999999...
8	1014	C00588	72556-74-2	HMDB01565	1.05309999999...	0.66749999999...	0.76759999999...
9	1018	C10164	98-98-6	HMDB02243	1.1413	8.00000000000...	4.49999999999...
10	70914	C00624	1430871	HMDB01138	-1.1835	3.88999999999...	0.10639999999...
11	182230	C02716	2490-97-3	HMDB06029	-1.04180000000...	0.39879999999...	0.53990000000...
12	69602	C05135	673-49-4	HMDB13253	-1.01150000000...	0.94750000000...	0.96020000000...
13	75619	C02997	39145-52-3	HMDB32055	-1.05139999999...	0.58069999999...	0.71089999999...
14	9920500	---	---	---	1.2764	6.79999999999...	2.48999999999...
15	101399	C05653	3342-77-6	HMDB04089	-1.06800000000...	0.61960000000...	0.73380000000...
16	439750	C03145	4289-98-9	HMDB01015	1.09159999999...	4.19999999999...	1.61999999999...
17	10349	---	498-21-5	HMDB01844	1.24679999999...	4.10000000000...	1.61999999999...
18	892	C00137	87-89-8	HMDB00211	1.49479999999...	0.26910000000...	0.4375
19	11005	C06424	544-63-8	HMDB00806	1.1249	7.48999999999...	0.1759
20	15030923	---	1204-06-4	HMDB00734	1.1232	0.23619999999...	0.40789999999...
21	3893	C02679	143-07-7	HMDB00638	-1.2618	0.58840000000...	0.71330000000...
22	14253342	---	---	HMDB11170	-1.07949999999...	0.15840000000...	0.30099999999...
23	151023	---	2566-39-4	HMDB11171	1.0383	0.77890000000...	0.84670000000...
24	111299	---	7432-24-8	HMDB00594	1.0185	0.64470000000...	0.753
25	---	---	---	HMDB11129	-1.0727	0.81850000000...	0.86880000000...
26	5283496	---	26662-94-2	HMDB05320	1.42029999999...	5.19000000000...	5.67210000000...
27	5289133	---	---	HMDB09003	1.0083	0.91869999999...	0.9446
28	53480978	---	124151-74-2	HMDB11569	2.06709999999...	1.54000000000...	4.82000000000...
29	92105	C01152	332-80-9	HMDB00001	1.64359999999...	0.31859999999...	0.47199999999...
30	---	---	---	HMDB11220	-1.02269999999...	0.73509999999...	0.81610000000...
31	452110	D03585	63-89-8	HMDB00564	-1.08149999999...	5.65999999999...	0.1454
32	---	---	56421-10-4	HMDB08038	1.0905	3.04E-2	8.61999999999...
33	497299	---	19420-57-6	HMDB10384	-1.16789999999...	0.61070000000...	0.73119999999...

MicroRNAs

Use the MicroRNA Target Filter

Use mRNA targets for Core Analyses

Map miRNAs as “mature”



Dataset Upload – MicroRNAs in tissues, table 2 Dahiya.xlsx

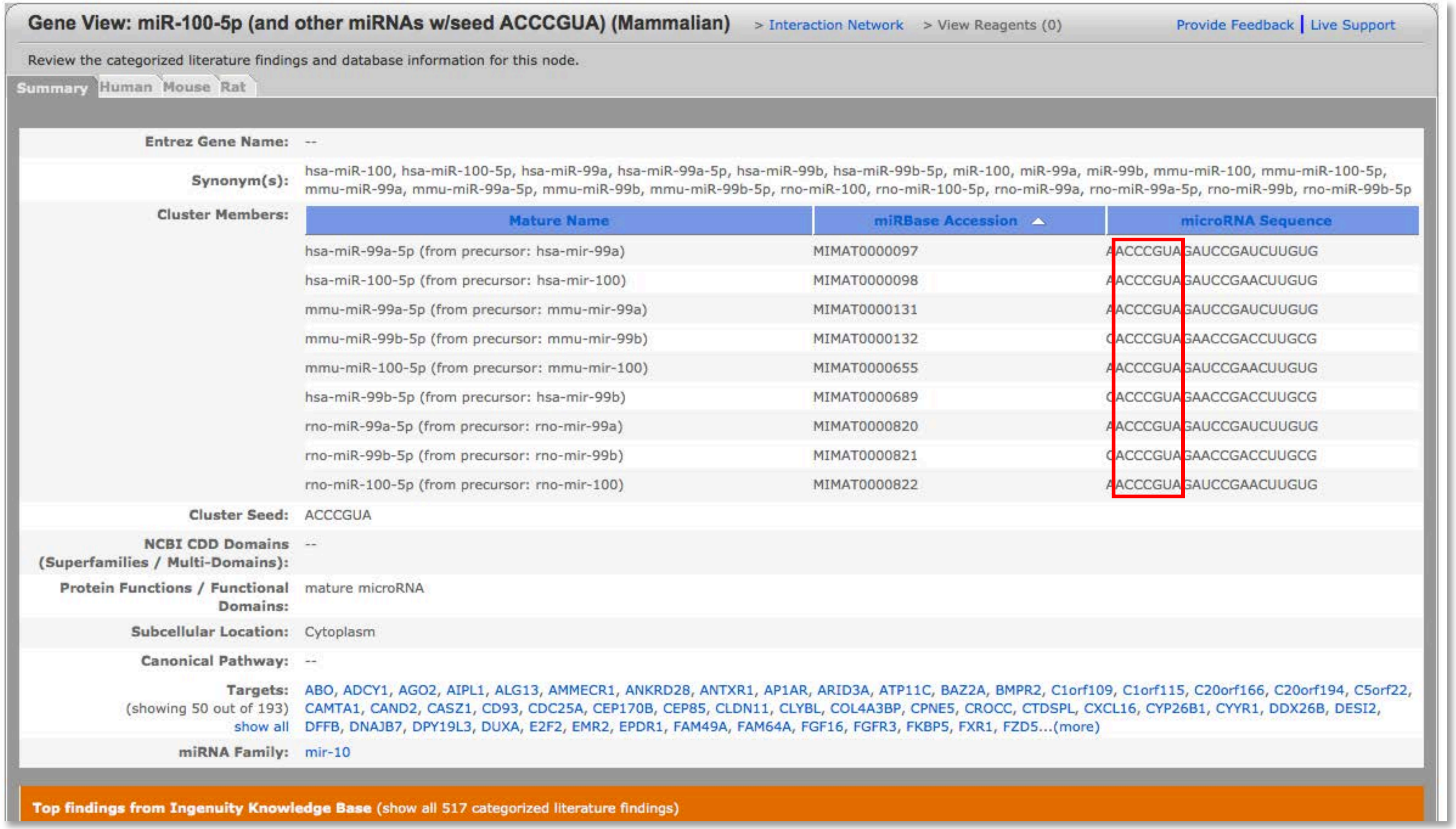
1. Select File Format: Flexible Format
2. Contains Column Header: ○ Yes ● No
3. Select Identifier Type: miRBase (mature)
4. Array platform used for experiments:
5. Use the dropdown menus to specify the

	Ignore	Ignore	
1	hsa-mir-221	9.16	
2	hsa-mir-663	4.42	
3	hsa-mir-29a	4.38	
4	hsa-mir-142-3p	4.26999999	
5	hsa-mir-296	3.85	
6	hsa-mir-30a-5p	3.8	
7	hsa-mir-30e-5p	3.72	
8	hsa-mir-129	3.6	
9	hsa-mir-518b	3.43	MCF2L, WDR1, TSN

Mature MicroRNAs

Grouped into entities based on same seven-nucleotide “seed sequence

Increases the specificity of targeting information



Gene View: miR-100-5p (and other miRNAs w/seed ACCCGUA) (Mammalian)

Review the categorized literature findings and database information for this node.

Entrez Gene Name: --

Synonym(s): hsa-miR-100, hsa-miR-100-5p, hsa-miR-99a, hsa-miR-99a-5p, hsa-miR-99b, hsa-miR-99b-5p, miR-100, miR-99a, miR-99b, mmu-miR-100, mmu-miR-100-5p, mmu-miR-99a, mmu-miR-99a-5p, mmu-miR-99b, mmu-miR-99b-5p, rno-miR-100, rno-miR-100-5p, rno-miR-99a, rno-miR-99a-5p, rno-miR-99b, rno-miR-99b-5p

Cluster Members:

Mature Name	miRBase Accession ▲	microRNA Sequence
hsa-miR-99a-5p (from precursor: hsa-mir-99a)	MIMAT0000097	AACCCGUAGAUCCGAUCUUGUG
hsa-miR-100-5p (from precursor: hsa-mir-100)	MIMAT0000098	AACCCGUAGAUCCGAACUUGUG
mmu-miR-99a-5p (from precursor: mmu-mir-99a)	MIMAT0000131	AACCCGUAGAUCCGAUCUUGUG
mmu-miR-99b-5p (from precursor: mmu-mir-99b)	MIMAT0000132	CACCCGUAGAACCGACCUUGCG
mmu-miR-100-5p (from precursor: mmu-mir-100)	MIMAT0000655	AACCCGUAGAUCCGAACUUGUG
hsa-miR-99b-5p (from precursor: hsa-mir-99b)	MIMAT0000689	CACCCGUAGAACCGACCUUGCG
rno-miR-99a-5p (from precursor: rno-mir-99a)	MIMAT0000820	AACCCGUAGAUCCGAUCUUGUG
rno-miR-99b-5p (from precursor: rno-mir-99b)	MIMAT0000821	CACCCGUAGAACCGACCUUGCG
rno-miR-100-5p (from precursor: rno-mir-100)	MIMAT0000822	AACCCGUAGAUCCGAACUUGUG

Cluster Seed: ACCCGUA

NCBI CDD Domains (Superfamilies / Multi-Domains): --

Protein Functions / Functional Domains: mature microRNA

Subcellular Location: Cytoplasm

Canonical Pathway: --

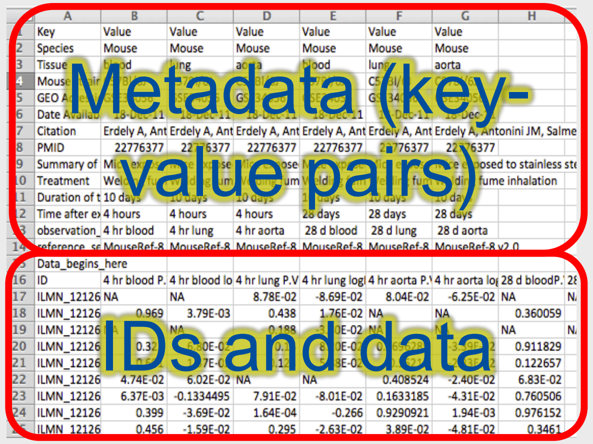
Targets: (showing 50 out of 193) show all
ABO, ADCY1, AGO2, AIPL1, ALG13, AMMECR1, ANKRD28, ANTXR1, AP1AR, ARID3A, ATP11C, BAZ2A, BMPR2, C1orf109, C1orf115, C20orf166, C20orf194, C5orf22, CAMTA1, CAND2, CASZ1, CD93, CDC25A, CEP170B, CEP85, CLDN11, CLYBL, COL4A3BP, CPNE5, CROCC, CTDSPL, CXCL16, CYP26B1, CYYR1, DDX26B, DESI2, DFFB, DNAJB7, DPY19L3, DUXA, E2F2, EMR2, EPDR1, FAM49A, FAM64A, FGF16, FGFR3, FKBP5, FXR1, FZD5...(more)

miRNA Family: mir-10

Top findings from Ingenuity Knowledge Base (show all 517 categorized literature findings)

Create results repository using Batch Upload

Format files

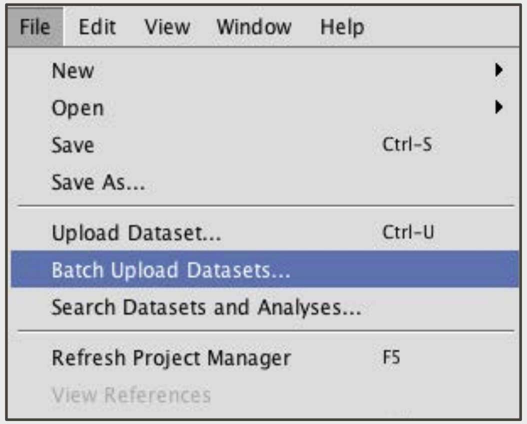


	A	B	C	D	E	F	G	H
1	Key	Value	Value	Value	Value	Value	Value	
2	Species	Mouse	Mouse	Mouse	Mouse	Mouse	Mouse	
3	Tissue	blood	lung	aorta	blood	lung	aorta	
4	Mouse [illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	
5	GEO A[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	
6	Date Availab	18-Dec-11	18-Dec-11	18-Dec-11	18-Dec-11	18-Dec-11	18-Dec-11	
7	Citation	Erdely A, Ant	Erdely A, Ant	Erdely A, Ant	Erdely A, Ant	Erdely A, Ant	Erdely A, Antonini JM, Salme	
8	PMID	22776377	22776377	22776377	22776377	22776377	22776377	
9	Summary of	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	Mice exposed to stainless ste	
10	Treatment	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	Welding fume inhalation	
11	Duration of t	10 days	10 days	10 days	10 days	10 days	10 days	
12	Time after ex	4 hours	4 hours	4 hours	28 days	28 days	28 days	
13	observation_	4 hr blood	4 hr lung	4 hr aorta	28 d blood	28 d lung	28 d aorta	
14	reference_se	MouseRef-8	MouseRef-8	MouseRef-8	MouseRef-8	MouseRef-8	MouseRef-8 v2.0	
15	Data_begins_here							
16	ID	4 hr blood P.	4 hr blood lo	4 hr lung P.V	4 hr lung logl	4 hr aorta P.\	4 hr aorta lo	28 d bloodP.
17	ILMN_12126	NA	NA	8.78E-02	-8.69E-02	8.04E-02	-6.25E-02	NA
18	ILMN_12126	0.969	3.79E-03	0.438	1.76E-02	NA	NA	0.360059
19	ILMN_12126	NA	NA	0.188	[illegible]	NA	NA	NA
20	ILMN_12126	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	0.911829
21	ILMN_12126	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	0.122657
22	ILMN_12126	4.74E-02	6.02E-02	NA	NA	0.408524	-2.40E-02	6.83E-02
23	ILMN_12126	6.37E-03	-0.1334495	7.91E-02	-8.01E-02	0.1633185	-4.31E-02	0.760506
24	ILMN_12126	0.399	-3.69E-02	1.64E-04	-0.266	0.9290921	1.94E-03	0.976152
25	ILMN_12126	0.456	-1.59E-02	0.295	-2.63E-02	3.89E-02	-4.81E-02	0.3461

1

Add metadata to dataset files

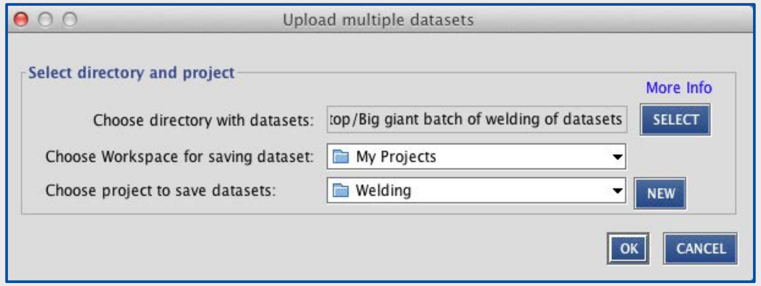
Upload data



2

Select "Batch Upload Datasets…." option

Select multiple datasets



Choose directory with datasets: top/Big giant batch of welding of datasets

Choose Workspace for saving dataset: My Projects

Choose project to save datasets: Welding

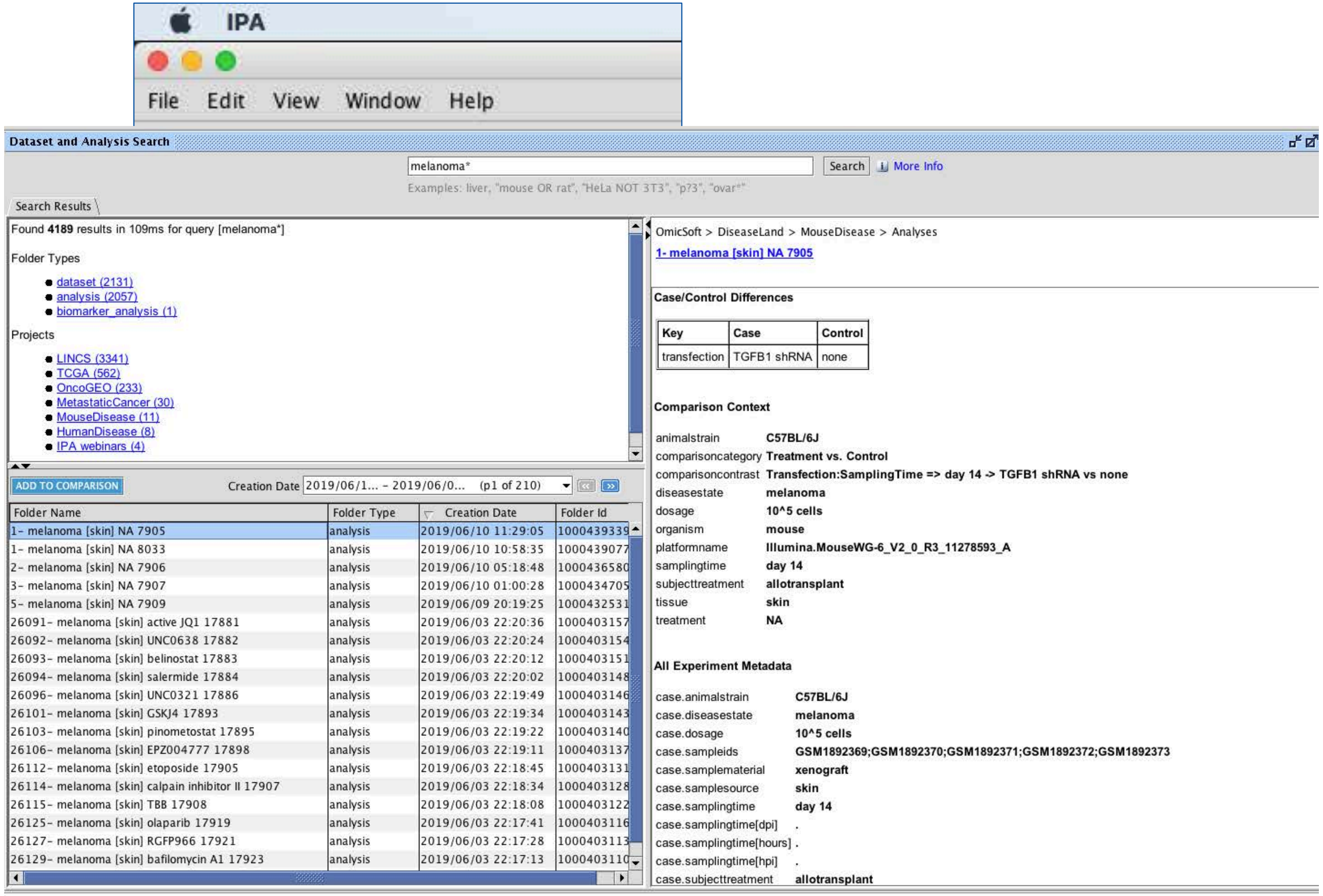
3

Select directory and destination of saved datasets

Add metadata to datasets

Easily search for related datasets/analyses

Metadata keys useful for Analysis Match



Dataset and Analysis Search

melanoma*

Examples: liver, "mouse OR rat", "HeLa NOT 3T3", "p?3", "ovar*"

Found **4189** results in 109ms for query [melanoma*]

Folder Types

- dataset (2131)
- analysis (2057)
- biomarker_analysis (1)

Projects

- LINCS (3341)
- TCGA (562)
- OncoGEO (233)
- MetastaticCancer (30)
- MouseDisease (11)
- HumanDisease (8)
- IPA webinars (4)

Creation Date 2019/06/1... – 2019/06/0... (p1 of 210)

Folder Name	Folder Type	Creation Date	Folder Id
1– melanoma [skin] NA 7905	analysis	2019/06/10 11:29:05	1000439339
1– melanoma [skin] NA 8033	analysis	2019/06/10 10:58:35	1000439077
2– melanoma [skin] NA 7906	analysis	2019/06/10 05:18:48	1000436580
3– melanoma [skin] NA 7907	analysis	2019/06/10 01:00:28	1000434705
5– melanoma [skin] NA 7909	analysis	2019/06/09 20:19:25	1000432531
26091– melanoma [skin] active JQ1 17881	analysis	2019/06/03 22:20:36	1000403157
26092– melanoma [skin] UNC0638 17882	analysis	2019/06/03 22:20:24	1000403154
26093– melanoma [skin] belinostat 17883	analysis	2019/06/03 22:20:12	1000403151
26094– melanoma [skin] salermide 17884	analysis	2019/06/03 22:20:02	1000403148
26096– melanoma [skin] UNC0321 17886	analysis	2019/06/03 22:19:49	1000403146
26101– melanoma [skin] GSKJ4 17893	analysis	2019/06/03 22:19:34	1000403143
26103– melanoma [skin] pinometostat 17895	analysis	2019/06/03 22:19:22	1000403140
26106– melanoma [skin] EPZ004777 17898	analysis	2019/06/03 22:19:11	1000403137
26112– melanoma [skin] etoposide 17905	analysis	2019/06/03 22:18:45	1000403131
26114– melanoma [skin] calpain inhibitor II 17907	analysis	2019/06/03 22:18:34	1000403128
26115– melanoma [skin] TBB 17908	analysis	2019/06/03 22:18:08	1000403122
26125– melanoma [skin] olaparib 17919	analysis	2019/06/03 22:17:41	1000403116
26127– melanoma [skin] RGFP966 17921	analysis	2019/06/03 22:17:28	1000403113
26129– melanoma [skin] bafilomycin A1 17923	analysis	2019/06/03 22:17:13	1000403110

OmicSoft > DiseaseLand > MouseDisease > Analyses

1- melanoma [skin] NA 7905

Case/Control Differences

Key	Case	Control
transfection	TGFB1 shRNA	none

Comparison Context

animalstrain	**C57BL/6J**
comparisoncategory	**Treatment vs. Control**
comparisoncontrast	**Transfection:SamplingTime => day 14 -> TGFB1 shRNA vs none**
diseasestate	**melanoma**
dosage	**10^5 cells**
organism	**mouse**
platformname	**Illumina.MouseWG-6_V2_0_R3_11278593_A**
samplingtime	**day 14**
subjecttreatment	**allotransplant**
tissue	**skin**
treatment	**NA**

All Experiment Metadata

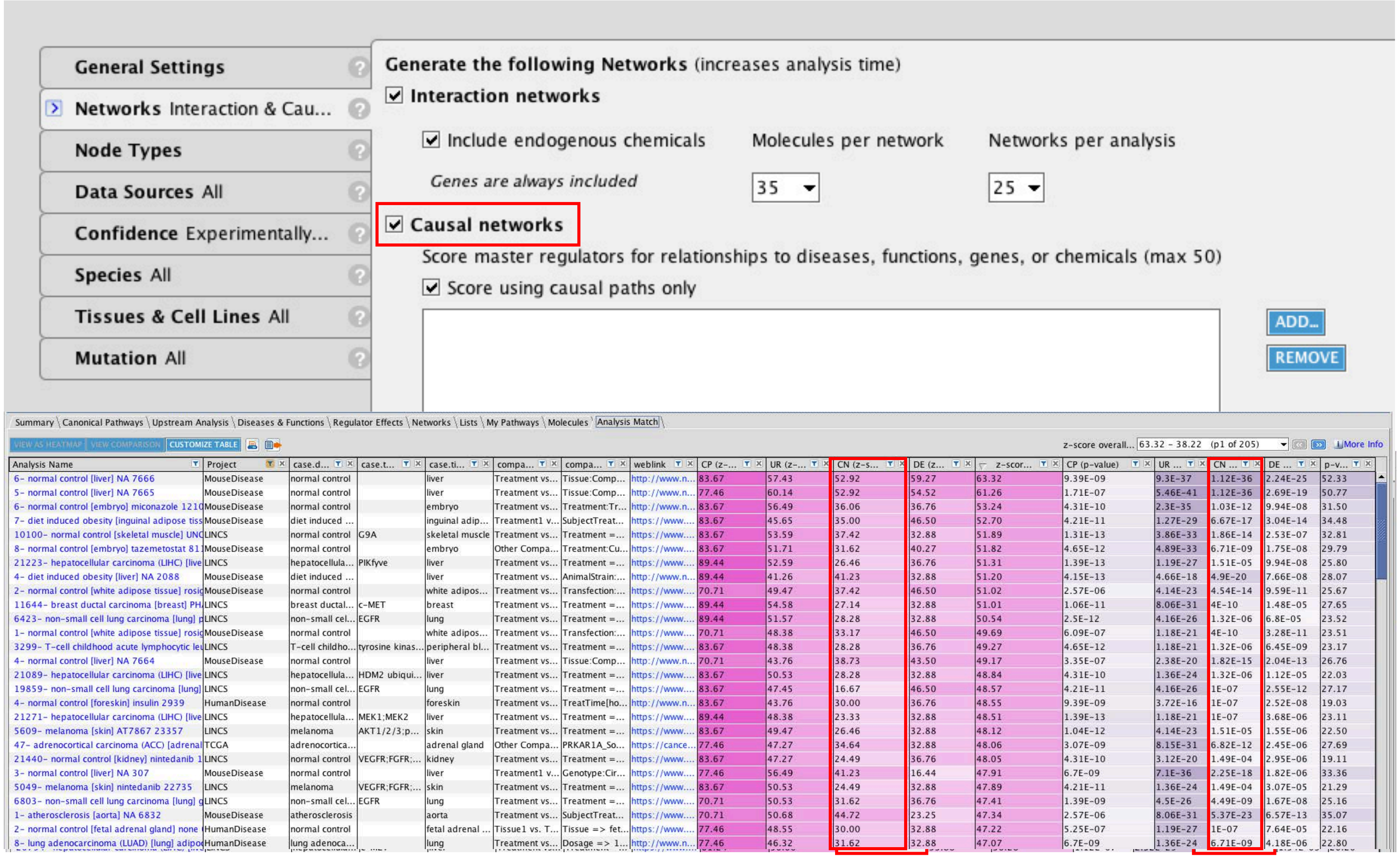
case.animalstrain	**C57BL/6J**
case.diseasestate	**melanoma**
case.dosage	**10^5 cells**
case.sampleids	**GSM1892369;GSM1892370;GSM1892371;GSM1892372;GSM1892373**
case.samplematerial	**xenograft**
case.samplesource	**skin**
case.samplingtime	**day 14**
case.samplingtime[dpi]	.
case.samplingtime[hours]	.
case.samplingtime[hpi]	.
case.subjecttreatment	**allotransplant**

Chapters

With a dataset

With or without a dataset

Enable Causal Networks



Generate the following Networks (increases analysis time)

☑ **Interaction networks**

☑ Include endogenous chemicals

Genes are always included

Molecules per network: 35

Networks per analysis: 25

☑ **Causal networks**

Score master regulators for relationships to diseases, functions, genes, or chemicals (max 50)

☑ Score using causal paths only

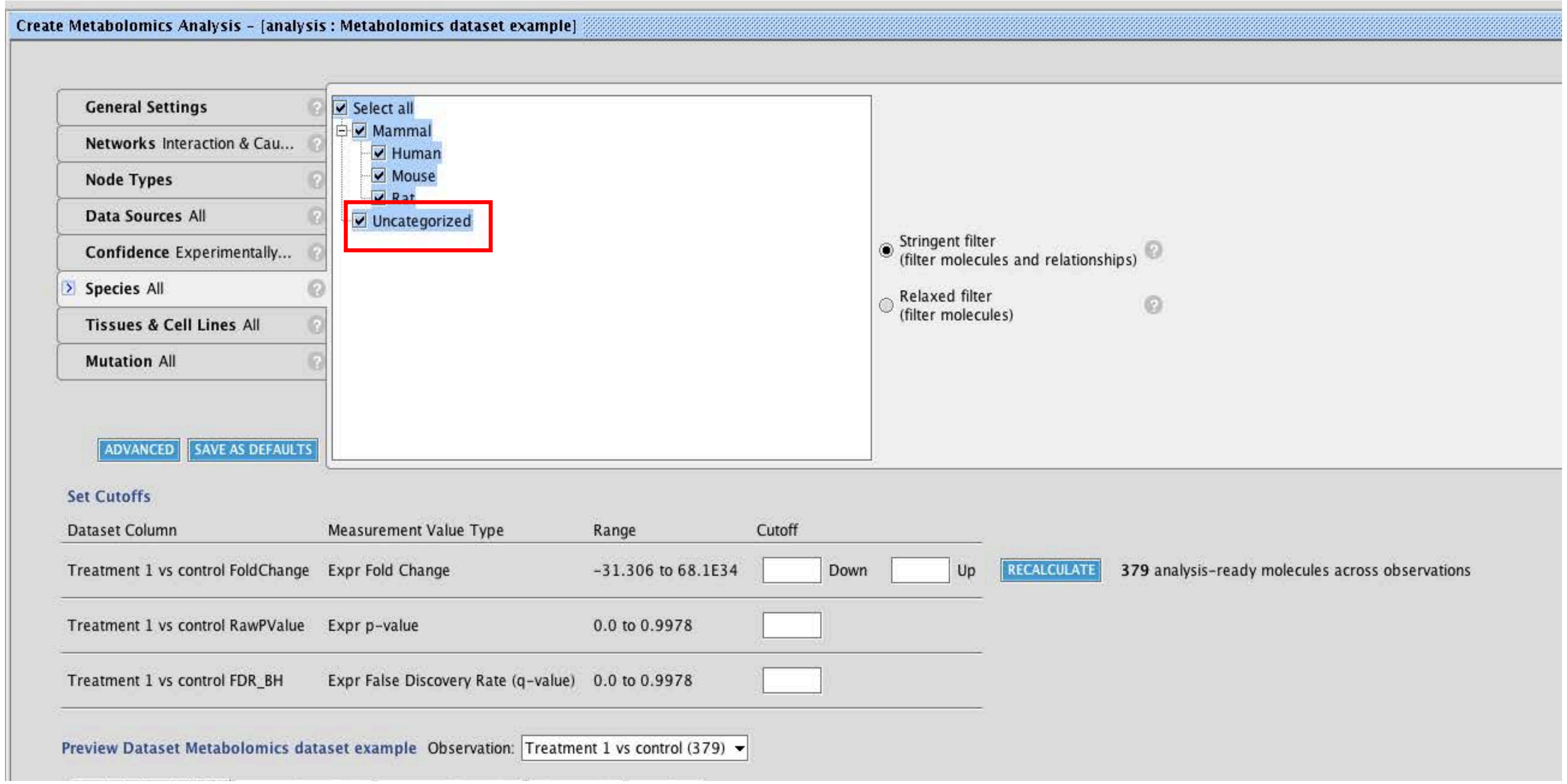
z-score overall... 63.32 - 38.22 (p1 of 205)

Analysis Name	Project	case.d...	case.t...	case.ti...	compa...	compa...	weblink	CP (z-...	UR (z-...	CN (z-s...	DE (z...	z-scor...	CP (p-value)	UR ...	CN ...	DE ...	p-v...
6- normal control [liver] NA 7666	MouseDisease	normal control		liver	Treatment vs...	Tissue:Comp...	http://www.n...	83.67	57.43	52.92	59.27	63.32	9.39E-09	9.3E-37	1.12E-36	2.24E-25	52.33
5- normal control [liver] NA 7665	MouseDisease	normal control		liver	Treatment vs...	Tissue:Comp...	http://www.n...	77.46	60.14	52.92	54.52	61.26	1.71E-07	5.46E-41	1.12E-36	2.69E-19	50.77
6- normal control [embryo] miconazole 1210	MouseDisease	normal control		embryo	Treatment vs...	Treatment:Tr...	http://www.n...	83.67	56.49	36.06	36.76	53.24	4.31E-10	2.3E-35	1.03E-12	9.94E-08	31.50
7- diet induced obesity [inguinal adipose tiss	MouseDisease	diet induced ...		inguinal adip...	Treatment1 v...	SubjectTreat...	https://www....	83.67	45.65	35.00	46.50	52.70	4.21E-11	1.27E-29	6.67E-17	3.04E-14	34.48
10100- normal control [skeletal muscle] UNC	LINCS	normal control	G9A	skeletal muscle	Treatment vs...	Treatment =...	https://www....	83.67	53.59	37.42	32.88	51.89	1.31E-13	3.86E-33	1.86E-14	2.53E-07	32.81
8- normal control [embryo] tazemetostat 811	MouseDisease	normal control		embryo	Other Compa...	Treatment:Cu...	https://www....	83.67	51.71	31.62	40.27	51.82	4.65E-12	4.89E-33	6.71E-09	1.75E-08	29.79
21223- hepatocellular carcinoma (LIHC) [live	LINCS	hepatocellula...	PIKfyve	liver	Treatment vs...	Treatment =...	https://www....	89.44	52.59	26.46	36.76	51.31	1.39E-13	1.19E-27	1.51E-05	9.94E-08	25.80
4- diet induced obesity [liver] NA 2088	MouseDisease	diet induced ...		liver	Treatment vs...	AnimalStrain:...	http://www.n...	89.44	41.26	41.23	32.88	51.20	4.15E-13	4.66E-18	4.9E-20	7.66E-08	28.07
2- normal control [white adipose tissue] rosig	MouseDisease	normal control		white adipos...	Treatment vs...	Transfection:...	https://www....	70.71	49.47	37.42	46.50	51.02	2.57E-06	4.14E-23	4.54E-14	9.59E-11	25.67
11644- breast ductal carcinoma [breast] PH	LINCS	breast ductal...	c-MET	breast	Treatment vs...	Treatment =...	https://www....	89.44	54.58	27.14	32.88	51.01	1.06E-11	8.06E-31	4E-10	1.48E-05	27.65
6423- non-small cell lung carcinoma [lung] p	LINCS	non-small cel...	EGFR	lung	Treatment vs...	Treatment =...	https://www....	89.44	51.57	28.28	32.88	50.54	2.5E-12	4.16E-26	1.32E-06	6.8E-05	23.52
1- normal control [white adipose tissue] rosig	MouseDisease	normal control		white adipos...	Treatment vs...	Transfection:...	https://www....	70.71	48.38	33.17	46.50	49.69	6.09E-07	1.18E-21	4E-10	3.28E-11	23.51
3299- T-cell childhood acute lymphocytic leu	LINCS	T-cell childho...	tyrosine kinas...	peripheral bl...	Treatment vs...	Treatment =...	https://www....	83.67	48.38	28.28	36.76	49.27	4.65E-12	1.18E-21	1.32E-06	6.45E-09	23.17
4- normal control [liver] NA 7664	MouseDisease	normal control		liver	Treatment vs...	Tissue:Comp...	http://www.n...	70.71	43.76	38.73	43.50	49.17	3.35E-07	2.38E-20	1.82E-15	2.04E-13	26.76
21089- hepatocellular carcinoma (LIHC) [live	LINCS	hepatocellula...	HDM2 ubiqui...	liver	Treatment vs...	Treatment =...	https://www....	83.67	50.53	28.28	32.88	48.84	4.31E-10	1.36E-24	1.32E-06	1.12E-05	22.03
19859- non-small cell lung carcinoma [lung]	LINCS	non-small cel...	EGFR	lung	Treatment vs...	Treatment =...	https://www....	83.67	47.45	16.67	46.50	48.57	4.21E-11	4.16E-26	1E-07	2.55E-12	27.17
4- normal control [foreskin] insulin 2939	HumanDisease	normal control		foreskin	Treatment vs...	TreatTime[ho...	http://www.n...	83.67	43.76	30.00	36.76	48.55	9.39E-09	3.72E-16	1E-07	2.52E-08	19.03
21271- hepatocellular carcinoma (LIHC) [live	LINCS	hepatocellula...	MEK1;MEK2	liver	Treatment vs...	Treatment =...	https://www....	89.44	48.38	23.33	32.88	48.51	1.39E-13	1.18E-21	1E-07	3.68E-06	23.11
5609- melanoma [skin] AT7867 23357	LINCS	melanoma	AKT1/2/3;p...	skin	Treatment vs...	Treatment =...	https://www....	83.67	49.47	26.46	32.88	48.12	1.04E-12	4.14E-23	1.51E-05	1.55E-06	22.50
47- adrenocortical carcinoma (ACC) [adrenal	TCGA	adrenocortica...		adrenal gland	Other Compa...	PRKAR1A_So...	https://cance...	77.46	47.27	34.64	32.88	48.06	3.07E-09	8.15E-31	6.82E-12	2.45E-06	27.69
21440- normal control [kidney] nintedanib 1	LINCS	normal control	VEGFR;FGFR;...	kidney	Treatment vs...	Treatment =...	https://www....	83.67	47.27	24.49	36.76	48.05	4.31E-10	3.12E-20	1.49E-04	2.95E-06	19.11
3- normal control [liver] NA 307	MouseDisease	normal control		liver	Treatment1 v...	Genotype:Cir...	https://www....	77.46	56.49	41.23	16.44	47.91	6.7E-09	7.1E-36	2.25E-18	1.82E-06	33.36
5049- melanoma [skin] nintedanib 22735	LINCS	melanoma	VEGFR;FGFR;...	skin	Treatment vs...	Treatment =...	https://www....	83.67	50.53	24.49	32.88	47.89	4.21E-11	1.36E-24	1.49E-04	3.07E-05	21.29
6803- non-small cell lung carcinoma [lung] g	LINCS	non-small cel...	EGFR	lung	Treatment vs...	Treatment =...	https://www....	70.71	50.53	31.62	36.76	47.41	1.39E-09	4.5E-26	4.49E-09	1.67E-08	25.16
1- atherosclerosis [aorta] NA 6832	MouseDisease	atherosclerosis		aorta	Treatment vs...	SubjectTreat...	https://www....	70.71	50.68	44.72	23.25	47.34	2.57E-06	8.06E-31	5.37E-23	6.57E-13	35.07
2- normal control [fetal adrenal gland] none (	HumanDisease	normal control		fetal adrenal ...	Tissue1 vs. T...	Tissue => fet...	https://www....	77.46	48.55	30.00	32.88	47.22	5.25E-07	1.19E-27	1E-07	7.64E-05	22.16
8- lung adenocarcinoma (LUAD) [lung] adipo	HumanDisease	lung adenoca...		lung	Treatment vs...	Dosage => 1...	http://www.n...	77.46	46.32	31.62	32.88	47.07	6.7E-09	1.36E-24	6.71E-09	4.18E-06	22.80

Species filter

Check “Uncategorized” for Metabolomics Analyses

Most endogenous chemicals are uncategorized



☑ Select all
- ☑ Mammal
  - ☑ Human
  - ☑ Mouse
  - ☑ Rat
- ☑ Uncategorized

● Stringent filter (filter molecules and relationships)

○ Relaxed filter (filter molecules)

Set Cutoffs

Dataset Column	Measurement Value Type	Range	Cutoff
Treatment 1 vs control FoldChange	Expr Fold Change	-31.306 to 68.1E34	Down Up
Treatment 1 vs control RawPValue	Expr p-value	0.0 to 0.9978	
Treatment 1 vs control FDR_BH	Expr False Discovery Rate (q-value)	0.0 to 0.9978	

379 analysis-ready molecules across observations

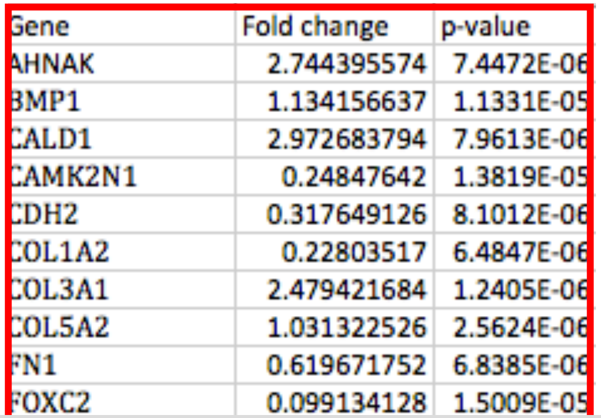
Preview Dataset Metabolomics dataset example Observation: Treatment 1 vs control (379)

Generate the right stats for “small” platforms

Use the correct Reference Set (user dataset)

All molecules identified by the ‘omics technology used

Used in p-value calculation for enrichment

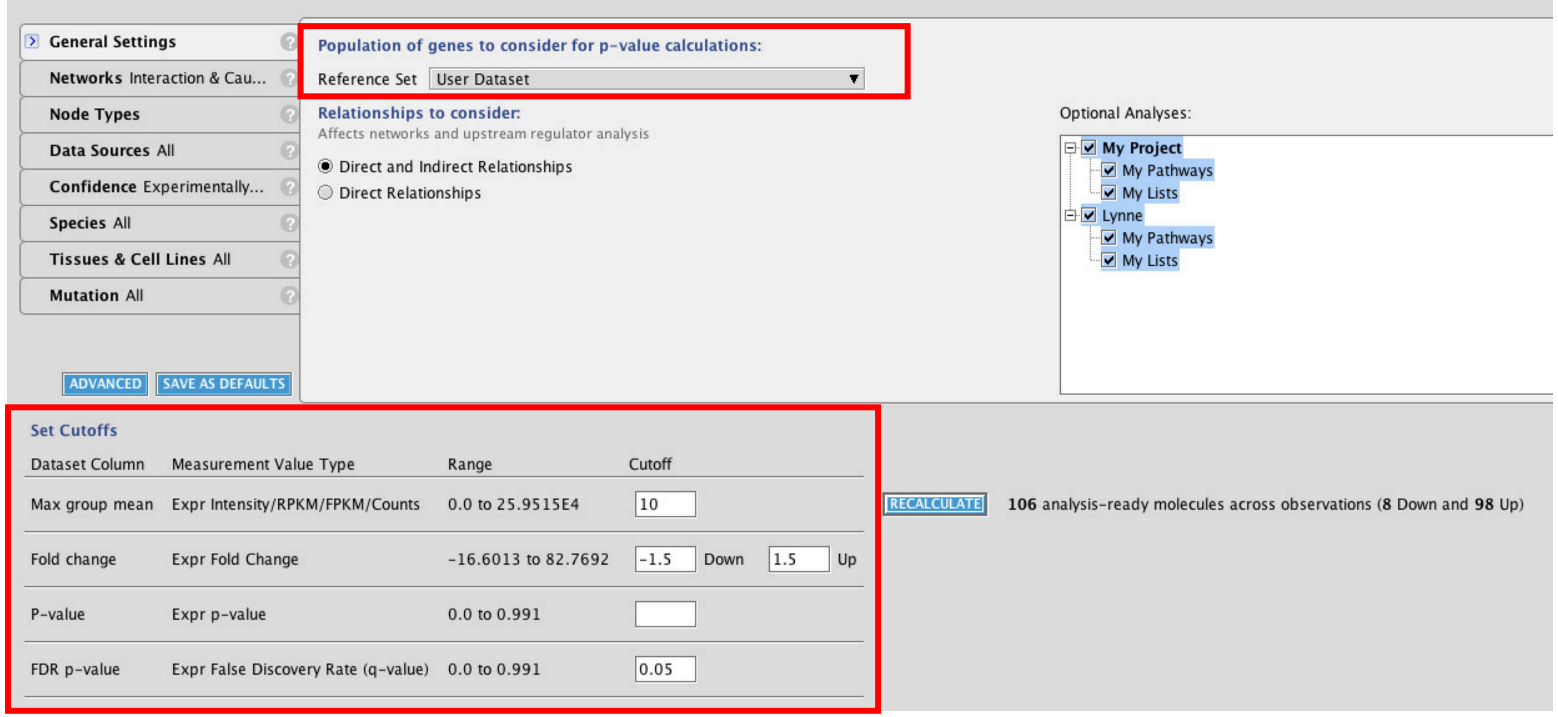


Gene	Fold change	p-value
AHNAK	2.744395574	7.4472E-06
BMP1	1.134156637	1.1331E-05
CALD1	2.972683794	7.9613E-06
CAMK2N1	0.24847642	1.3819E-05
CDH2	0.317649126	8.1012E-06
COL1A2	0.22803517	6.4847E-06
COL3A1	2.479421684	1.2405E-06
COL5A2	1.031322526	2.5624E-06
FN1	0.619671752	6.8385E-06
FOXC2	0.099134128	1.5009E-05

When setting up your Analysis:

Upload entire dataset.

Set cutoffs to find most significantly-perturbed molecules in the dataset.



Population of genes to consider for p-value calculations:

Reference Set: User Dataset

Relationships to consider:

Affects networks and upstream regulator analysis

● Direct and Indirect Relationships

○ Direct Relationships

Set Cutoffs

Dataset Column	Measurement Value Type	Range	Cutoff			
Max group mean	Expr Intensity/RPKM/FPKM/Counts	0.0 to 25.9515E4	10			
Fold change	Expr Fold Change	-16.6013 to 82.7692	-1.5	Down	1.5	Up
P-value	Expr p-value	0.0 to 0.991				
FDR p-value	Expr False Discovery Rate (q-value)	0.0 to 0.991	0.05			

106 analysis-ready molecules across observations (**8** Down and **98** Up)

Chapters

With a dataset

With or without a dataset

Select and connect multiple upstream regulators

Upstream Analysis results

Upstream Regula...	Expr Log Ratio	Molecule Type
SNAI1	↑1.041	transcription regulator
SNAI2	↑590.706	transcription regulator

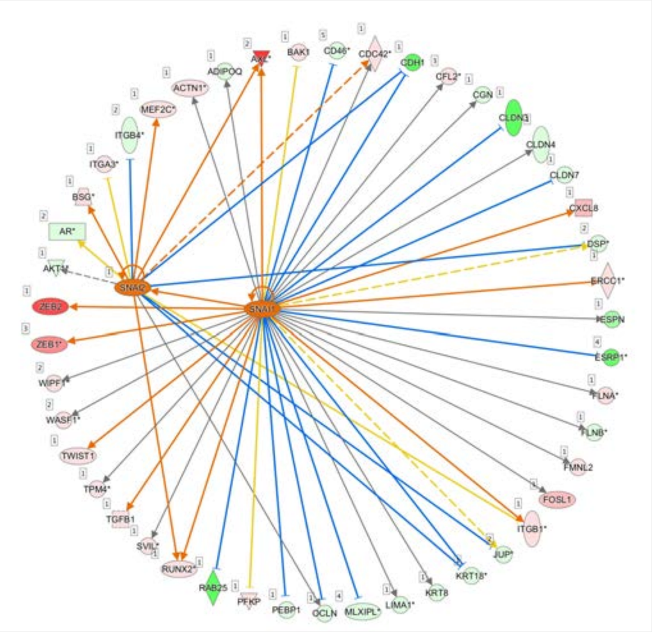
1

Select upstream regulators of interest

Generate network

2

Select “Display as Network”

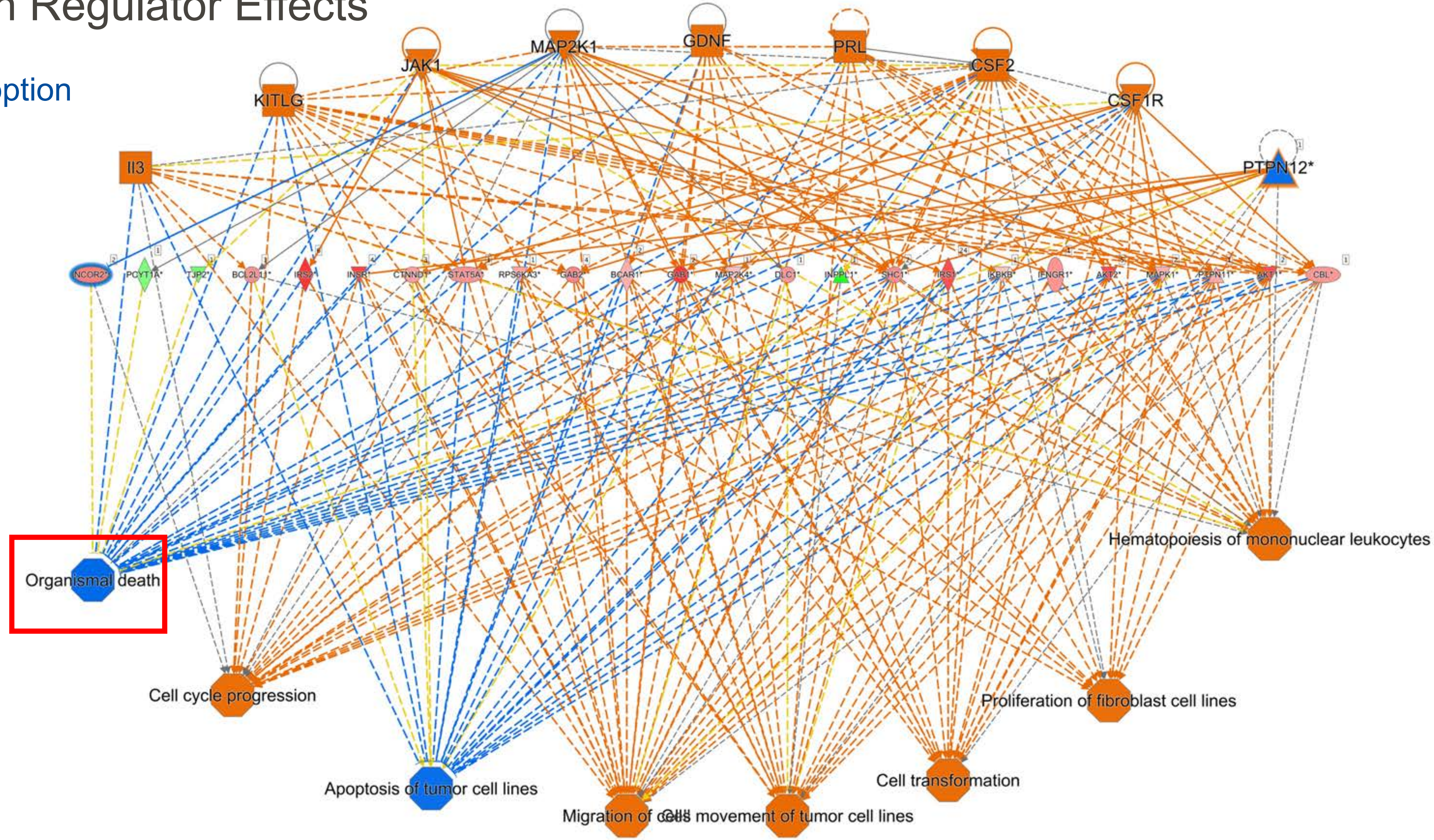


3

Network is generated

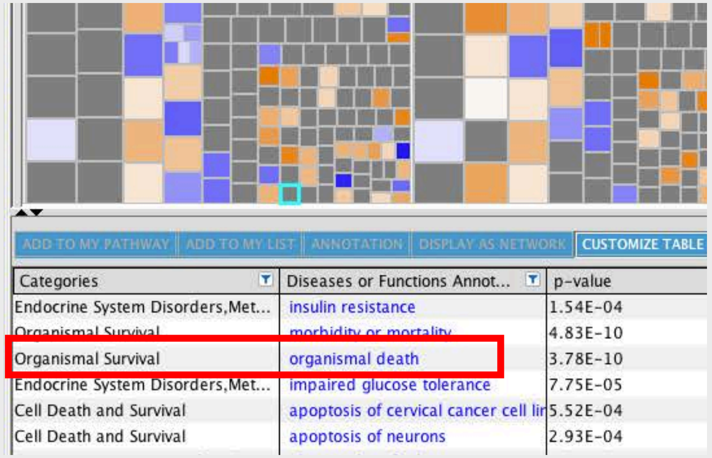
Filtering categories in Regulator Effects

Use “Generate Networks” option



Regulator Effects: Generate revised networks

Find category

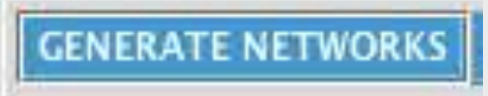


Categories	Diseases or Functions Annot...	p-value
Endocrine System Disorders,Met...	insulin resistance	1.54E-04
Organismal Survival	morbidity or mortality	4.83E-10
Organismal Survival	organismal death	3.78E-10
Endocrine System Disorders,Met...	impaired glucose tolerance	7.75E-05
Cell Death and Survival	apoptosis of cervical cancer cell lir	5.52E-04
Cell Death and Survival	apoptosis of neurons	2.93E-04

1

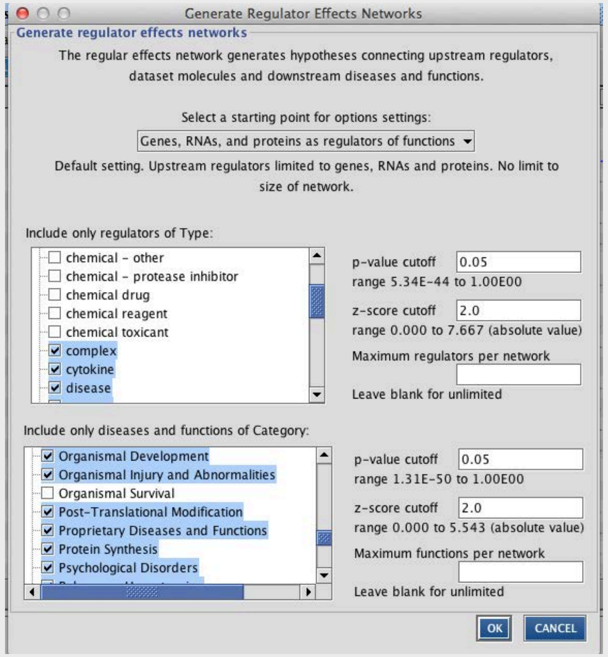
Go to Diseases and Functions results

Regenerate network



2

Select “Generate Network” button



Generate Regulator Effects Networks

Generate regulator effects networks

The regular effects network generates hypotheses connecting upstream regulators, dataset molecules and downstream diseases and functions.

Select a starting point for options settings:

Genes, RNAs, and proteins as regulators of functions

Default setting. Upstream regulators limited to genes, RNAs and proteins. No limit to size of network.

Include only regulators of Type:

- ☐ chemical - other
- ☐ chemical - protease inhibitor
- ☐ chemical drug
- ☐ chemical reagent
- ☐ chemical toxicant
- ☑ complex
- ☑ cytokine
- ☑ disease

p-value cutoff 0.05
range 5.34E-44 to 1.00E00
z-score cutoff 2.0
range 0.000 to 7.667 (absolute value)
Maximum regulators per network
Leave blank for unlimited

Include only diseases and functions of Category:

- ☑ Organismal Development
- ☑ Organismal Injury and Abnormalities
- ☐ Organismal Survival
- ☑ Post-Translational Modification
- ☑ Proprietary Diseases and Functions
- ☑ Protein Synthesis
- ☑ Psychological Disorders

p-value cutoff 0.05
range 1.31E-50 to 1.00E00
z-score cutoff 2.0
range 0.000 to 5.543 (absolute value)
Maximum functions per network
Leave blank for unlimited

3

Deselect category; click ”OK”

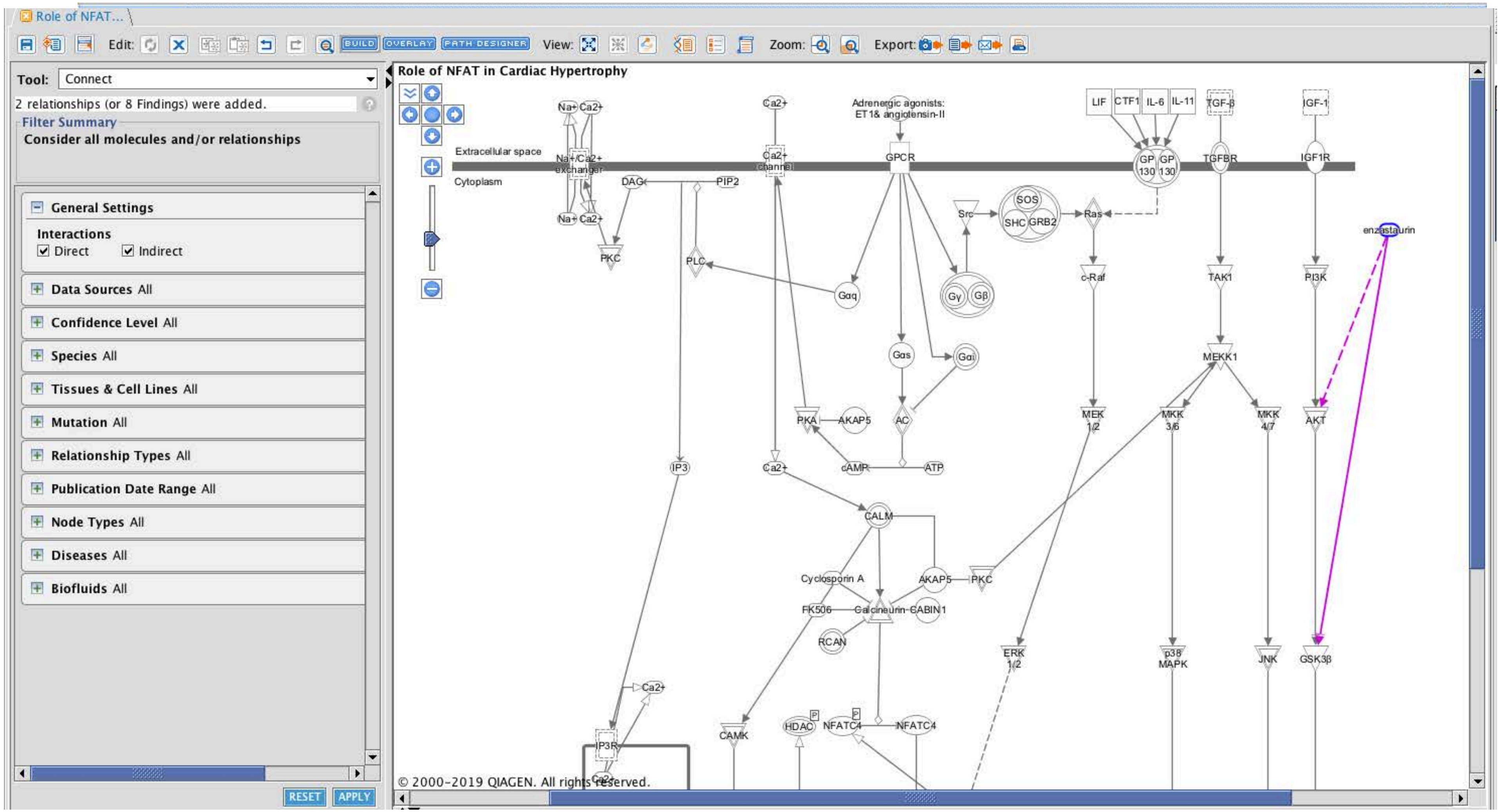
Chapters

With a dataset

With or without a dataset

Connect to/from one node

Select only ONE node



Tool: Connect

2 relationships (or 8 Findings) were added.

Filter Summary

Consider all molecules and/or relationships

General Settings

Interactions

☑ Direct ☑ Indirect

Data Sources All

Confidence Level All

Species All

Tissues & Cell Lines All

Mutation All

Relationship Types All

Publication Date Range All

Node Types All

Diseases All

Biofluids All

Role of NFAT in Cardiac Hypertrophy

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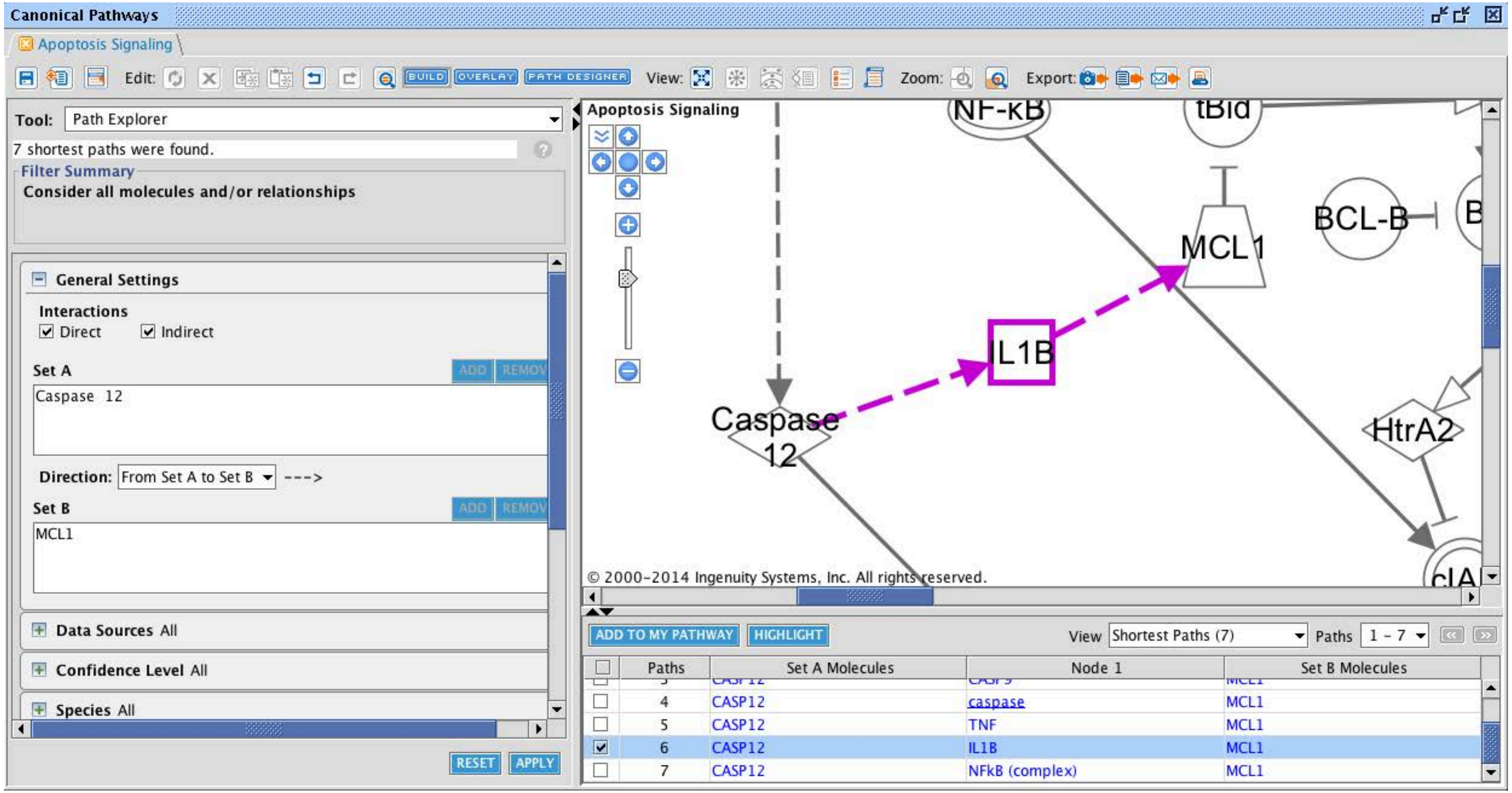
Path Explorer: Find the shortest path between nodes



Tool: Path Explorer

7 shortest paths were found.

Filter Summary

Consider all molecules and/or relationships

General Settings

Interactions

☑ Direct ☑ Indirect

Set A

Caspase 12

Direction: From Set A to Set B --->

Set B

MCL1

Data Sources All

Confidence Level All

Species All

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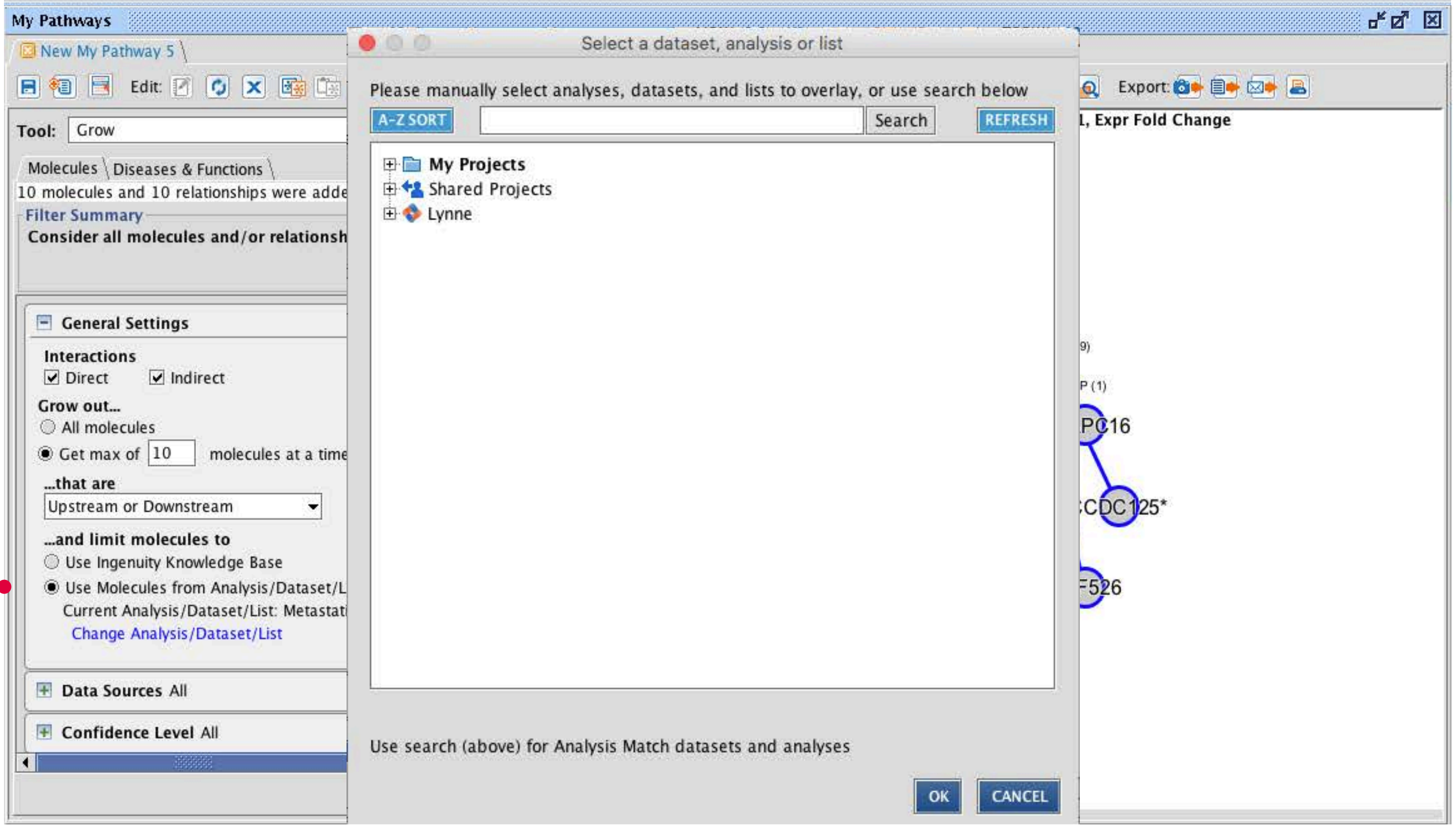
View Shortest Paths (7) Paths 1 - 7

☐	Paths	Set A Molecules	Node 1	Set B Molecules
☐	4	CASP12	caspase	MCL1
☐	5	CASP12	TNF	MCL1
☑	6	CASP12	IL1B	MCL1
☐	7	CASP12	NFkB (complex)	MCL1

Grow to a constrained set of molecules



Tool: Grow

10 molecules and 10 relationships were adde

Filter Summary

Consider all molecules and/or relationsh

General Settings

Interactions

☑ Direct ☑ Indirect

Grow out...

○ All molecules

● Get max of 10 molecules at a time

...that are

Upstream or Downstream

...and limit molecules to

○ Use Ingenuity Knowledge Base

● Use Molecules from Analysis/Dataset/L

Current Analysis/Dataset/List: Metastati

Change Analysis/Dataset/List

Data Sources All

Confidence Level All

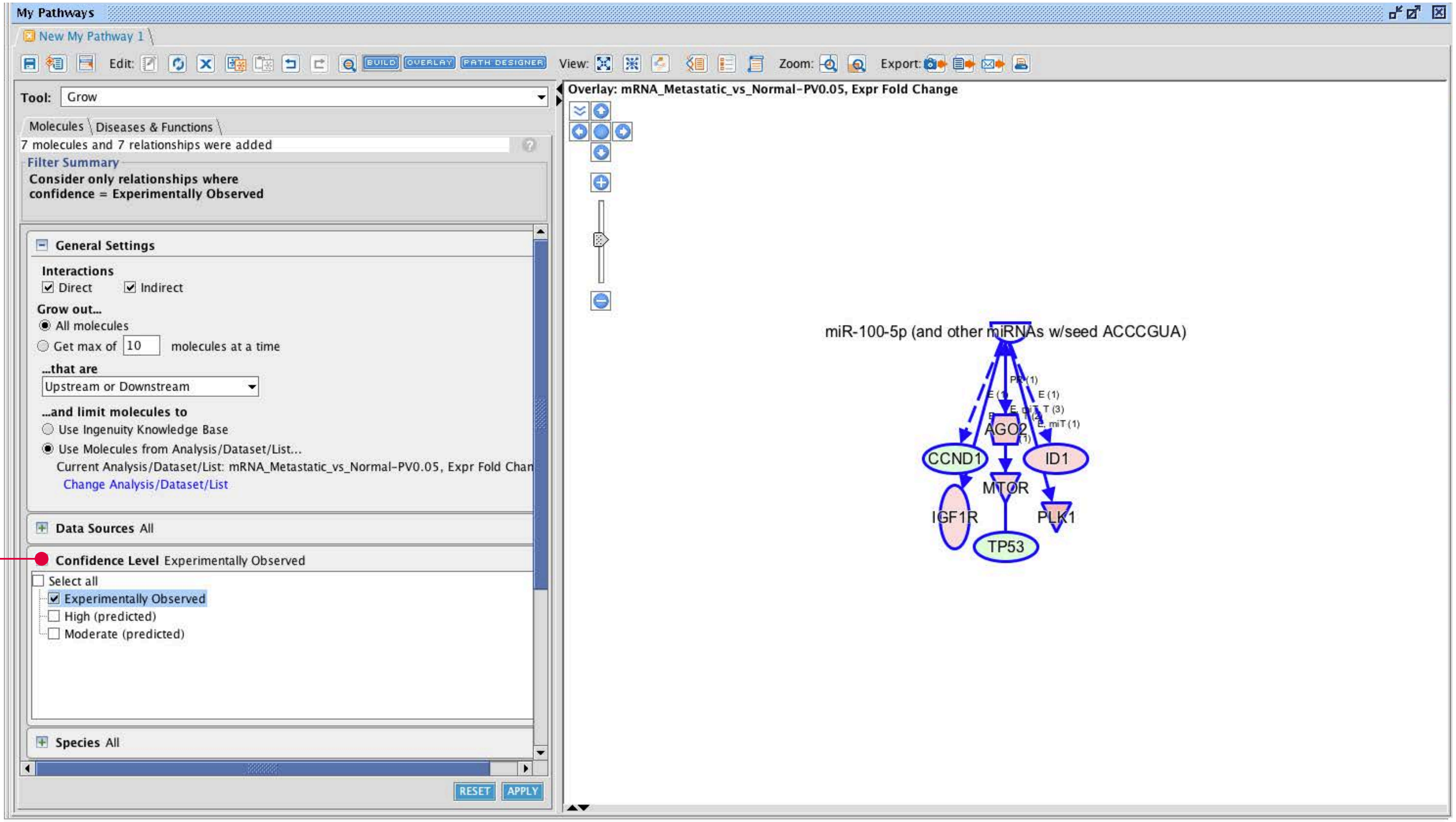
Select a dataset, analysis or list

Please manually select analyses, datasets, and lists to overlay, or use search below

Use search (above) for Analysis Match datasets and analyses

Filter to data/analysis/list of interest

Use the confidence filter to fine-tune miRNA targeting



Tool: Grow

Molecules | Diseases & Functions

7 molecules and 7 relationships were added

Filter Summary

Consider only relationships where confidence = Experimentally Observed

General Settings

Interactions

☑ Direct ☑ Indirect

Grow out...

● All molecules

○ Get max of 10 molecules at a time

...that are

Upstream or Downstream

...and limit molecules to

○ Use Ingenuity Knowledge Base

● Use Molecules from Analysis/Dataset/List...

Current Analysis/Dataset/List: mRNA_Metastatic_vs_Normal-PV0.05, Expr Fold Chan

Change Analysis/Dataset/List

Data Sources All

Confidence Level Experimentally Observed

☐ Select all

☑ Experimentally Observed

☐ High (predicted)

☐ Moderate (predicted)

Species All

Overlay: mRNA_Metastatic_vs_Normal-PV0.05, Expr Fold Change

Filter based on source of miRNA/target mRNA information

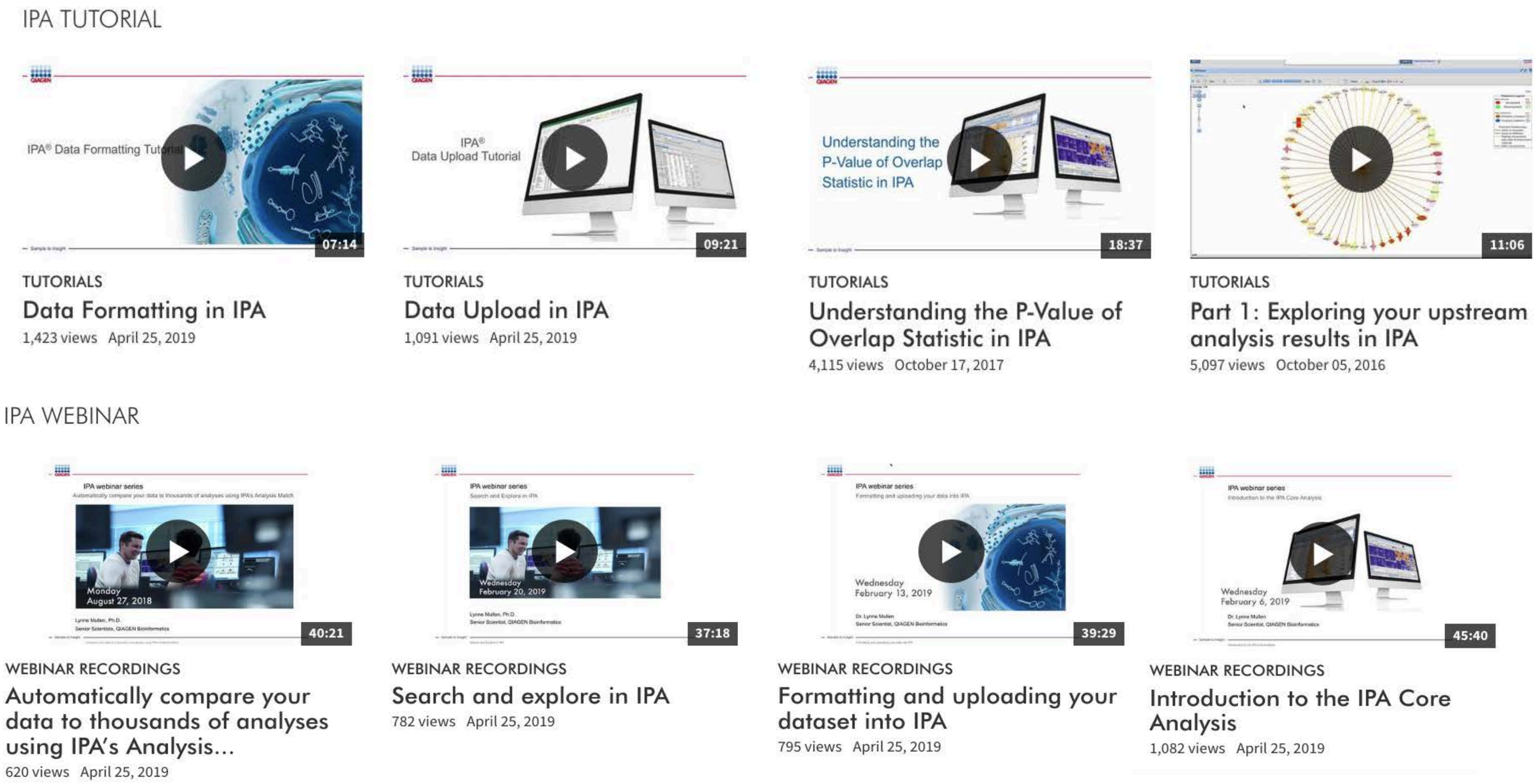
Chapters

With a dataset

With or without a dataset

Additional resources

Recorded webinars and tutorials available at tv.qiagenbioinformatics.com



IPA TUTORIAL

TUTORIALS
Data Formatting in IPA
1,423 views April 25, 2019

TUTORIALS
Data Upload in IPA
1,091 views April 25, 2019

TUTORIALS
Understanding the P-Value of Overlap Statistic in IPA
4,115 views October 17, 2017

TUTORIALS
Part 1: Exploring your upstream analysis results in IPA
5,097 views October 05, 2016

IPA WEBINAR

WEBINAR RECORDINGS
Automatically compare your data to thousands of analyses using IPA's Analysis...
620 views April 25, 2019

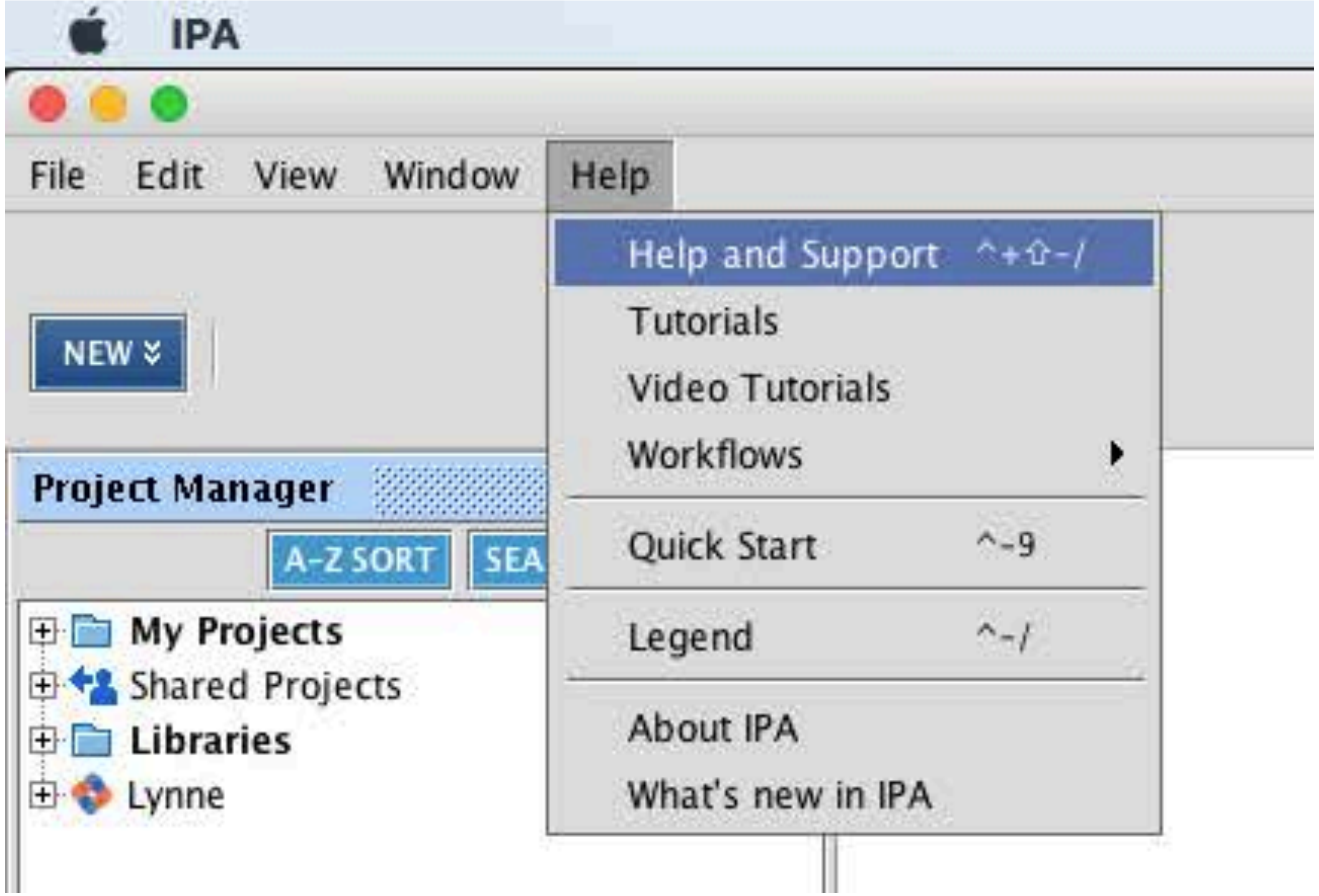
WEBINAR RECORDINGS
Search and explore in IPA
782 views April 25, 2019

WEBINAR RECORDINGS
Formatting and uploading your dataset into IPA
795 views April 25, 2019

WEBINAR RECORDINGS
Introduction to the IPA Core Analysis
1,082 views April 25, 2019

Additional resources

Online help manual available at http://qiagen.force.com/KnowledgeBase/KnowledgeIPAPage



Customer Support and additional resources

Contact

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via **email** or **telephone**

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A response
within **ONE** business day

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Thank you for attending!

Questions?