Object Groups



Object Groups

- Collect and save lists of genes, metabolites, pathways...
- Transform, filter, and analyze them
- Share groups with colleagues
- Use groups in conjunction with publications
- Claim: Groups enable biologists to perform computations that required a programmer



Accessing Groups

- Desktop menu: Groups
- Web menu: Tools -> Groups
 - To use Web Object Groups, you must create a (free) BioCyc account



Creating Groups: User-Defined Groups

- Create a group by uploading a tab-delimited text file
 - Software will assist in recognizing database objects from text
- Create a group by typing in names
 - You will be presented with options for the correct object; e.g. typing "tryptophan", you will get the option to choose the compound L-tryptophan, the enzyme tryptophan synthase, and others







Add current object to group

Add quick-search result set to group

Add object-specific search result to a group

	CVC			Logged in as pkarp@ai.sri.com Logout Help My prefe	Logged in as pkarp@ai.sri.com Logout Help My preferences					
ECOCYC				Quick Search Gene Sea	rch					
A member	of the BIoCyc database col	lection		Searching Escherichia coli K-12 substr. MG1655 change organism database						
Home	Search	Tools	Help							
Escherichia coli K-12 substr. MG1655 Query Results										
			-	*						
You searched for all compounds that have a molecular weight of at least 2000.										
Your query	returned 47	results								
Your query returned 47 results.										
🧭 Turn i	nto a group									
Compound Name 🔺 🗸				Chemical Mol.						
				Formula $\triangle \nabla$ Wt. \triangle	\bigtriangledown					
(enterobacterial common antigen)x2 undecaprenyl-diphosphate				phosphate H162P2N6037C103 2138.37	78					
(enterobac	erial common a	ntigen)x3 un	decaprenyl-di	phosphate H198P2N9052C127 2744.93	38					
(enterobact	erial common a	ntigen)x4 co	e oligosaccha	ride lipid A H447N14P40160C272 6597.41	16					
(enterobacterial common antigen)x4 undecaprenyl-diphosphate				phosphate H234P2N12O67C151 3351.49	97					
(heptosyl)2	(KDO)2-lipid A			H223P2N2O51C124 2620.05	56					
(KDO)2-(lau	royl)-lipid IV _A			H170P2N2O38C96 2022.33	37					



Using Groups: Group Transformations

Use Case: Find all genes that are regulated by a transcriptional regulator.

Step 1: Create a group that contains the transcription factor.

Step 2: In the "Transforms" menu, select "Genes regulated by protein, RNA or compound".

A new column containing all genes regulated by the transcription factor is generated
Click "+" to turn that new column into a group
This group can be further transformed, e.g. into metabolic pathways



Object Group Transformations

Transform metabolite group into group of metabolic pathways, then into gene group

Transform gene group into group of regulators of those genes

Transform gene group into list of TF binding sites controlling those genes; into list of sequences

Create group of nucleotide positions; transform to closest genes; paint to cellular overview or enrich for GO terms



Using Groups: Properties

Use Case: Find the chromosome positions of all genes encoding enzymes of a pathway, sort by chromosome position. Find regulators of those genes.

Step 1: Create a group that contains the pathway.Step 2: In the "Transforms" menu, select "Genes of pathway".Step 3: Select gene column and select

- Groups > New > Group from column OR
- Click "+" at top of gene column

Step 4: Select "left-end-position" from "Add Property Column" menu and add. Sort by position by clicking on arrow in column header.

Step 5: Select "Direct regulators of gene" from "Add Transform Column" menu.



Genes of Aspartate Superpathway

Colum	nn operators	TRANSFORMS Filter to objects not in other Add	ENRICHMENTS Genes Enriched for GO (biol 🗧 Er	PROPERTIES Right-End-Position Add
	aged Show all			
	All-Genes	\ominus 📝 🌲 Left-End-Position 😂	≑ Right-End-Position 🤤	
1	thrA	337	2799	
2	thrB	2801	3733	
3	thrC	3734	5020	
4	dapB	28374	29195	
5	nadC	117752	118645	
6	dapD	185123	185947	
7	nadD	669154	669795	
8	nadA	781308	782351	
9	aspC	983742	984932	
📃 10	malY	1698981	1700153	
11	nadE	1820482	1821309	
12	dapE	2589629	2590756	
13	dapA	2596904	2597782	
🔲 14	nadB	2708442	2710064	
15	lysA	2975659	2976921	
16	metK	3084728	3085882	
17	metC	3150258	3151445	
18		3486982	3488202	
19	-	3571798	3572901	
20		3992785	3993609	
21		4011076	4013337	
22		4126695	4127855	
22		4127858	4130290	
24		4212303	4213232	
		4221851	4225534	
25				
26	lysC	4229907	4231256	

Enrichment Analysis

- Example: Does a group of genes contain more genes involved in cell division than would be expected by chance?
- More generally: Does a group contain more entities from defined classes than expected by chance?
- Check gene groups for enrichment of
 - GO terms, pathways, regulons
- Check metabolite groups for enrichment of
 - Pathways



Enrichment Analysis

- Enrichment test based on the Hypergeometric Distribution
- Can perform enrichment, depletion, or both
- Multiple testing correction optional



Enrichment Dialog

	ENRICHMENTS										
Genes Enriched for Pathway: 🖨 🕜											
		Enrichment pa	arameters			×					
<mark>∕2</mark> ∓ T4		Annalise to man		-	Enrichment Depletion						
	2.1656876	Analysis type:			 Depletion Enrichment and Depletion 						
	0.9973915	Include results less than:	whose p-va	lue 0.1			1				
	0.5333049	Algorithm deta	ils:								
	0.4431508	-		0.1111	• Fisher Exact						
	0.3669181	Statistic:			 Fisher Exact Parent-Child Union Fisher Exact Parent-Child Intersection None Bonferroni Correction Benjamini-Hochberg Correction Renjamini Yokutioli Correction 						
	1.0450248										
	0.6124025	Correction		-							
	0.4506686	Correction		-							
	1.3523909										
	1.2810624										
	2.5529437	0.88949484	1.1338782	1.0615696	0.5815946	0.88905144					



Sharing Groups

By default your groups are private

Share them with specific colleagues or make them public

Groups -> Sharing

Group URLs are permanent and can be used in publications



Lab Exercises

- 1. Search for compounds having 'glucose' in their name
- 2. Turn into group
- 3. Enrichment Analysis → Compounds Enriched for Pathways
- 4. Use defaults in Enrichment pop-up, click 'OK'
- 5. Select ten most enriched pathways
- **6.** Groups \rightarrow New \rightarrow From checked rows
- 7. Reactions of pathway
- 8. New group of reactions (green button on column)
- **9.** Groups \rightarrow Paint Data \rightarrow On cellular overview

