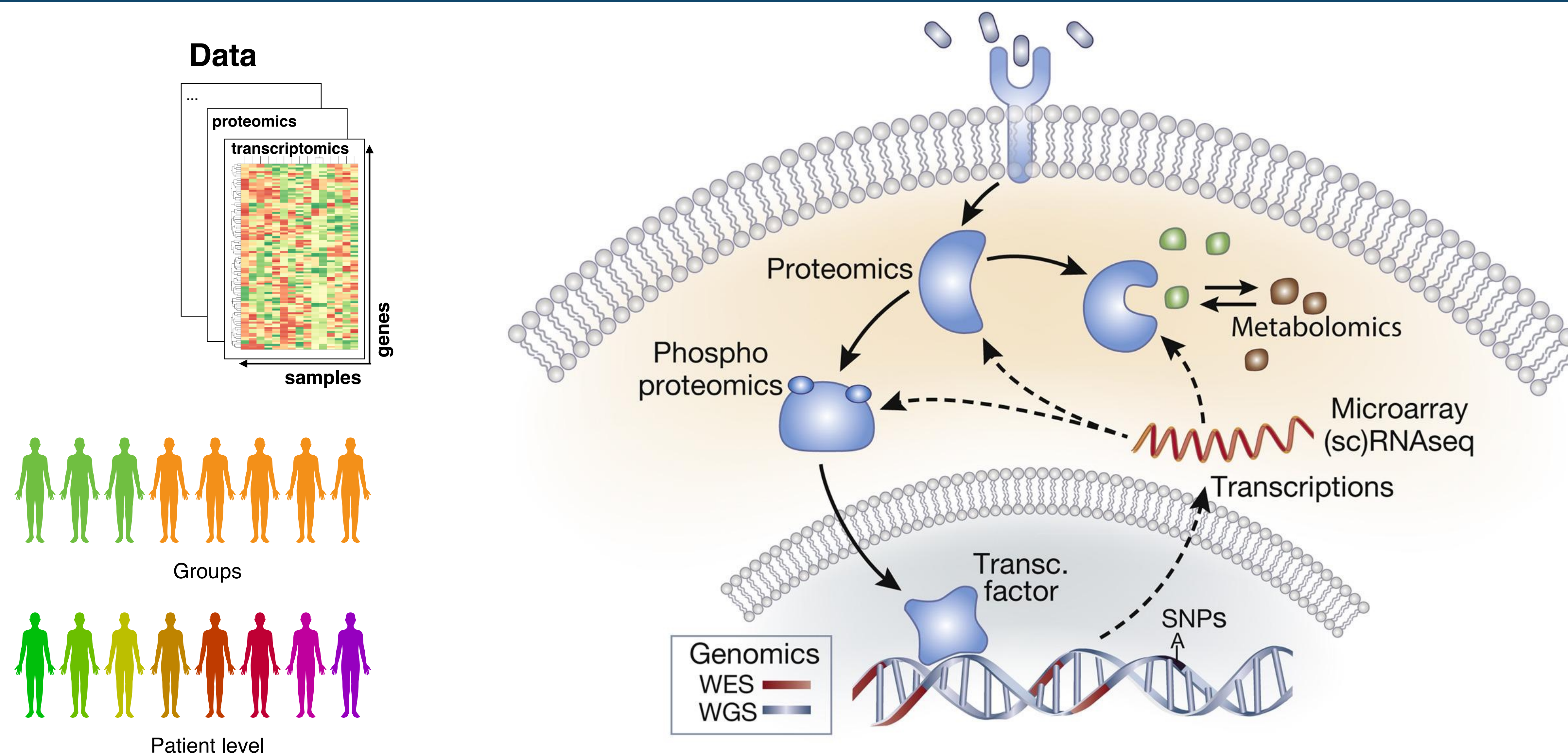
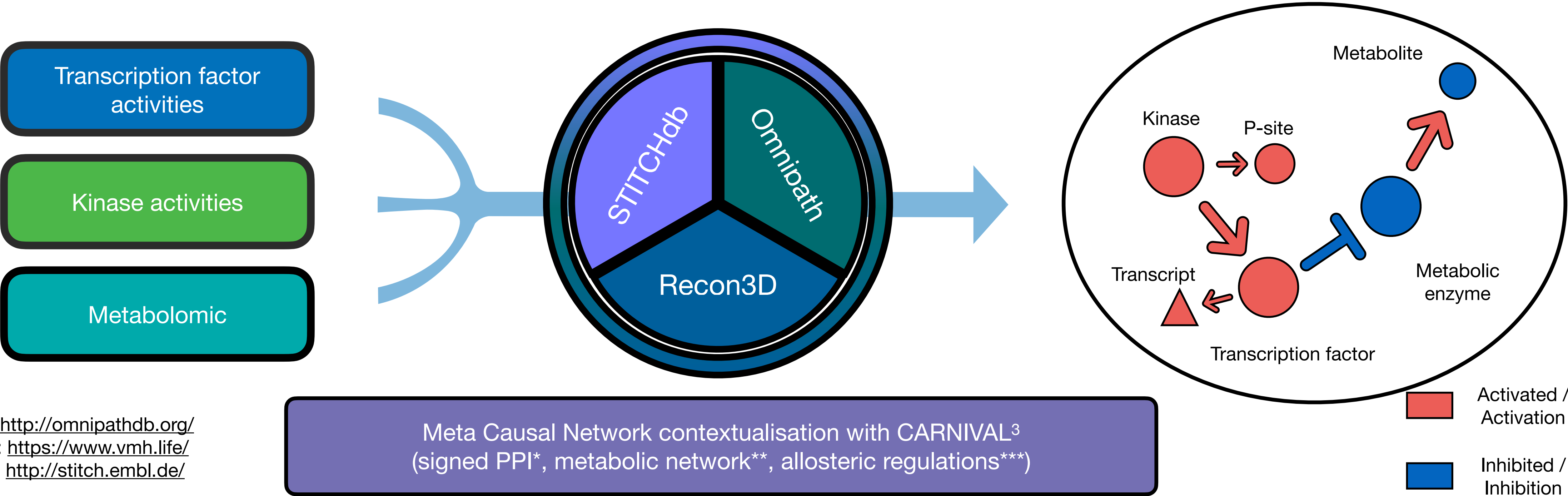


Different omics technologies to measure molecular processes





COSMOS: Multi-omic integration pipeline



*Omnipath : <http://omnipathdb.org/>

**Recon3D : <https://www.vmh.life/>

***STITCH : <http://stitch.embl.de/>

Systematic generation of testable hypothesis to connect signalling and metabolism with the NCI60 datasets

DTP Developmental Therapeutics Program

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Last Updated: 08/11/20

NCI-60 Human Tumor Cell Lines Screen

Introduction

The **NCI-60 Human Tumor Cell Lines Screen** has served the global cancer research community for >20 years. The screen was implemented in fully operational form in 1990 and utilizes 60 different human tumor cell lines to identify and characterize novel compounds with growth inhibition or killing of tumor cell lines. It is designed to screen up to 3,000 small molecules (synthetic or purified natural products) per year for potential anticancer activity. The operation of this screen utilizes 60 different human tumor cell lines, representing leukemia, melanoma and cancers of the lung, colon, brain, ovary, breast, prostate, and kidney cancers.

This screen is unique in that the complexity of a 60 cell line dose response produced by a given compound results in a biological response pattern which can be utilized in pattern recognition algorithms (**COMPARE**). Using these algorithms, it is possible to assign a putative mechanism of action to a test compound, or to determine that the response pattern is unique and not similar to that of any of the standard prototype compounds included in the NCI database. In addition, following characterization of various cellular molecular targets in the 60 cell lines, it may be possible to select compounds most likely to interact with a specific molecular target.

This screen also allows prioritization of selected agents for further evaluation by NCI in collaboration with the submitter. The screening service is offered at no cost to submitters, other than shipping costs, although requests are reviewed and only those conforming to defined guidelines are selected for screening. There is a limit of 10 structure submission requests per 30 day period.

- Compound submission for NCI-60 screening
- Data Retrieval and Testing Decisions
- List of NCI-60 human tumor cell lines
- Screening methodology (One-dose and Five-dose Assay)
- Sample handling and Preparation
- Database of Screening Results
- Molecular characterization of NCI-60
- Publications

NCI-60 Human Tumor Cell Lines Screen

Main

Compound Submission

Data Retrieval and Testing Decisions

List of NCI-60 Human Tumor Cell Lines

Screening methodology (One-dose and Five-dose Assay)

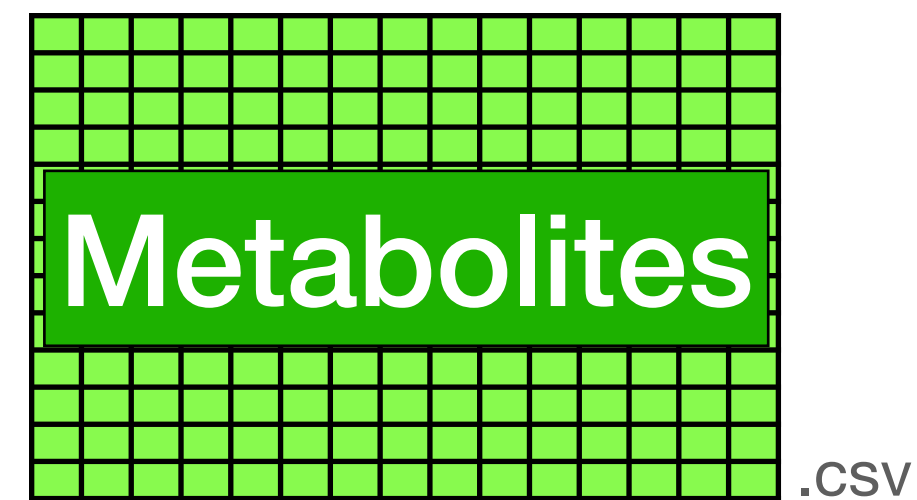
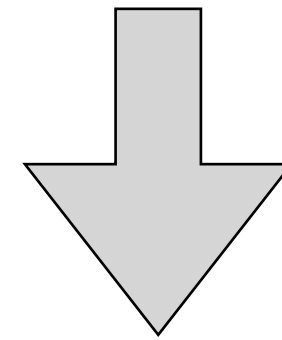
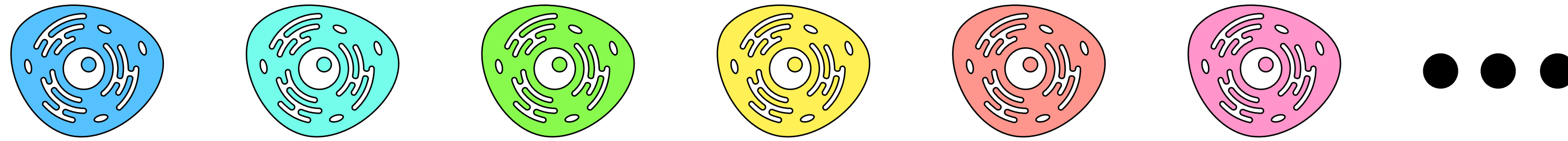
Sample Handling and Preparation

Database of Screening Results

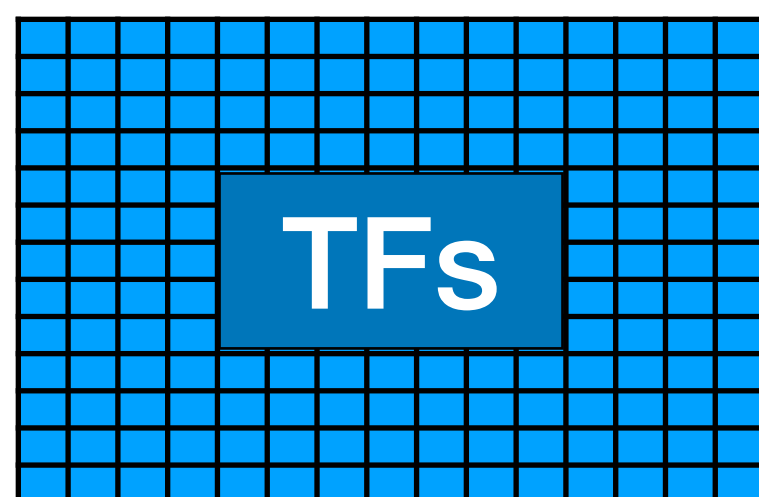
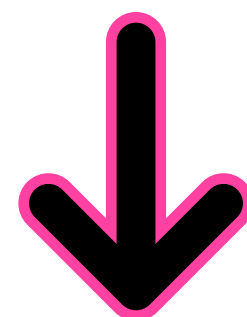
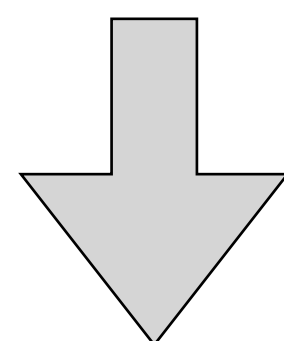
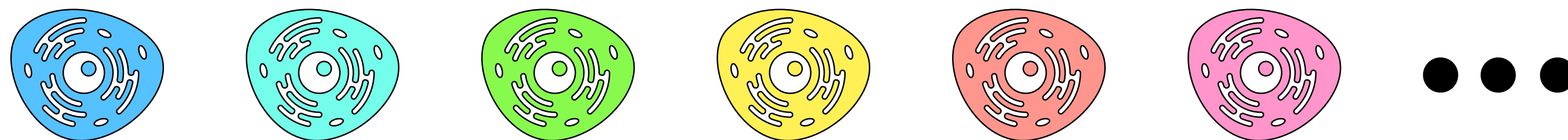
Molecular Characterization of NCI-60

Publications

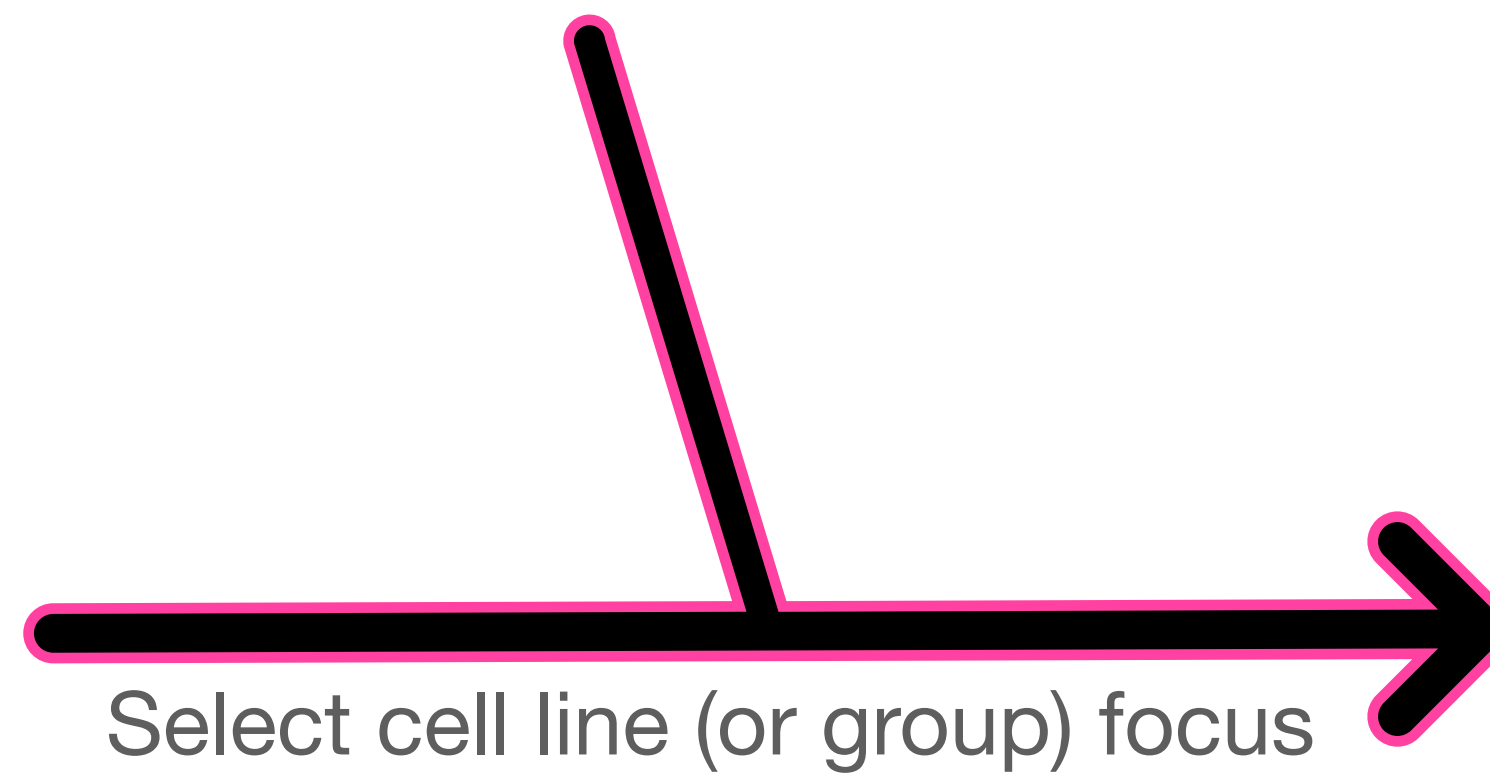
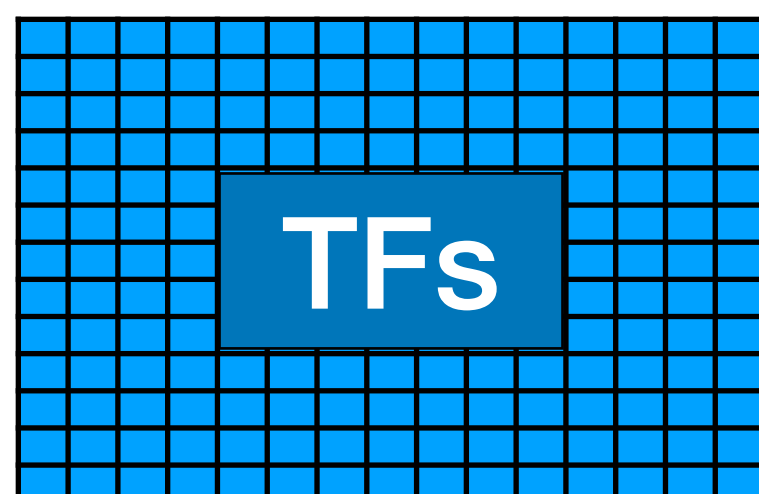
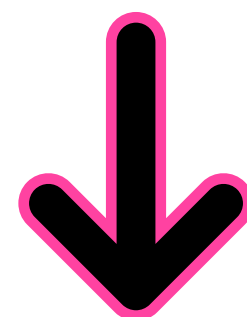
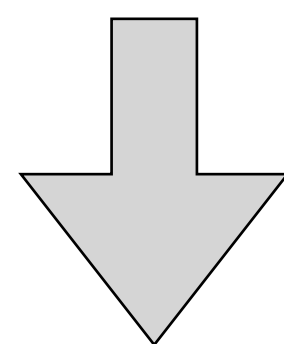
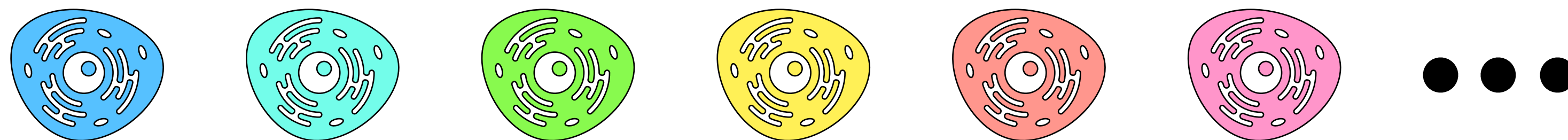
NCI60 cancer cell lines



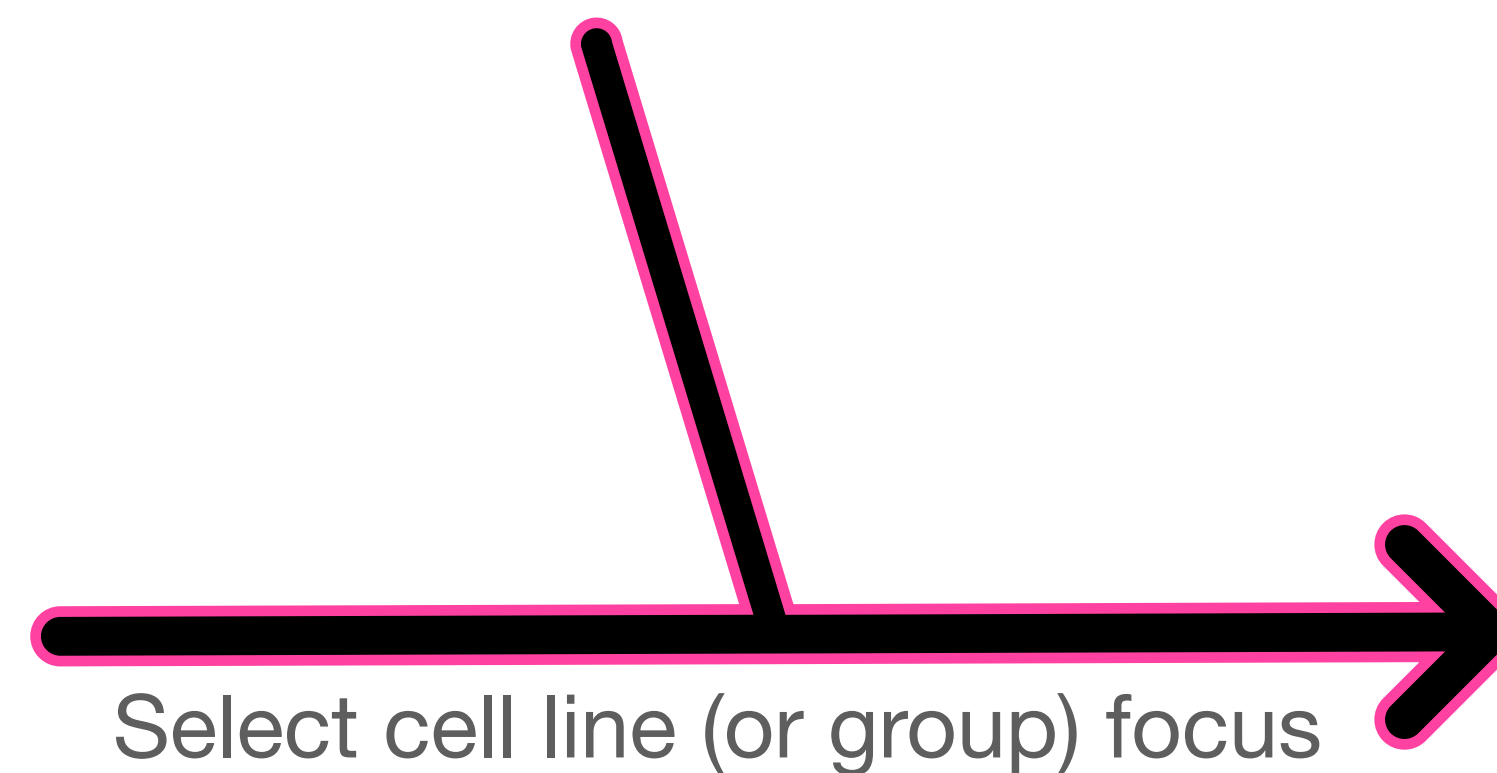
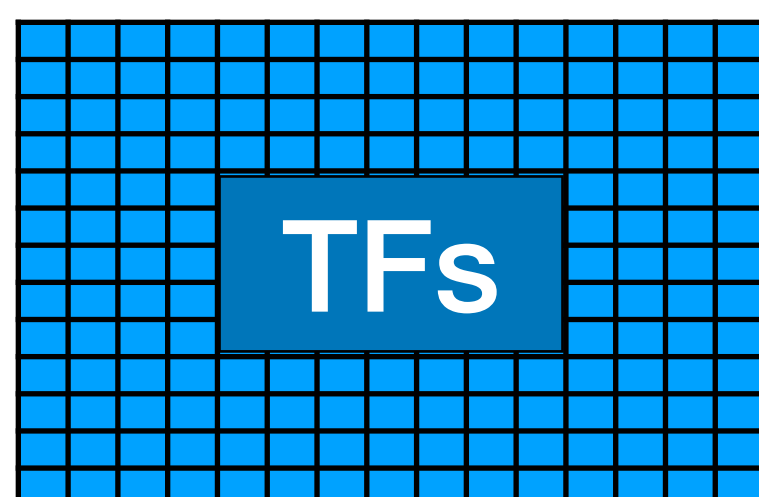
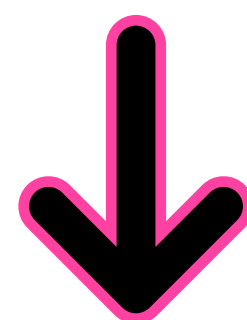
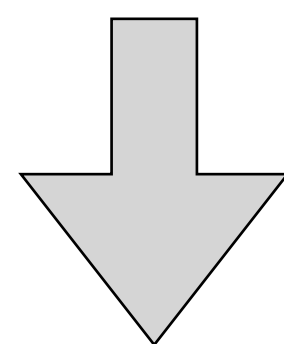
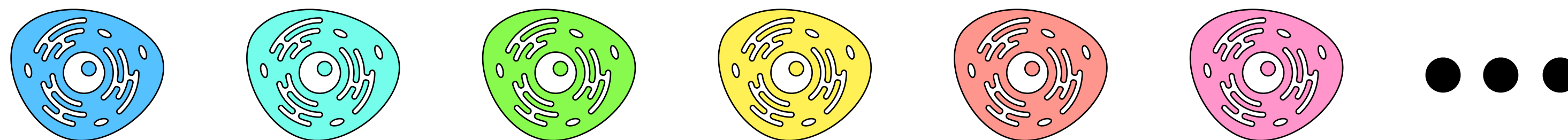
NCI60 cancer cell lines



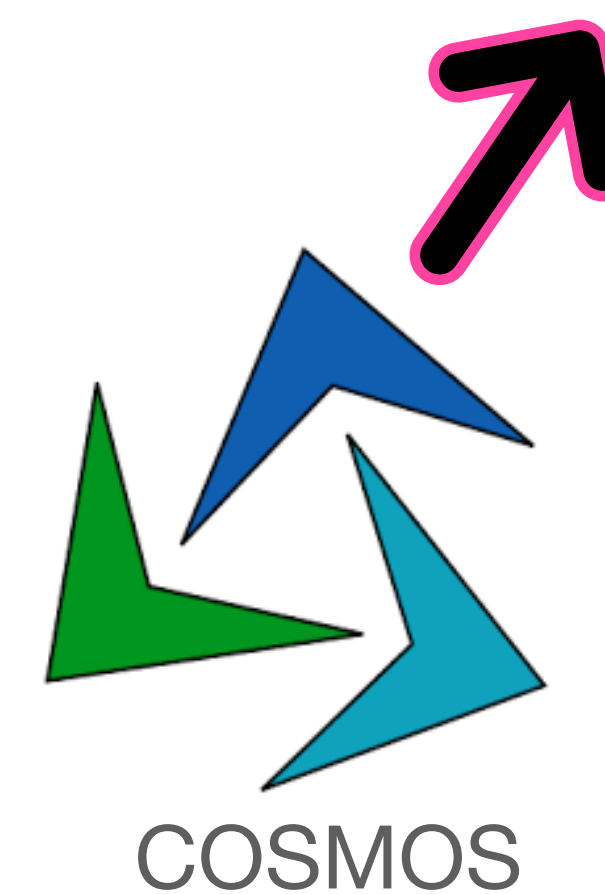
NCI60 cancer cell lines



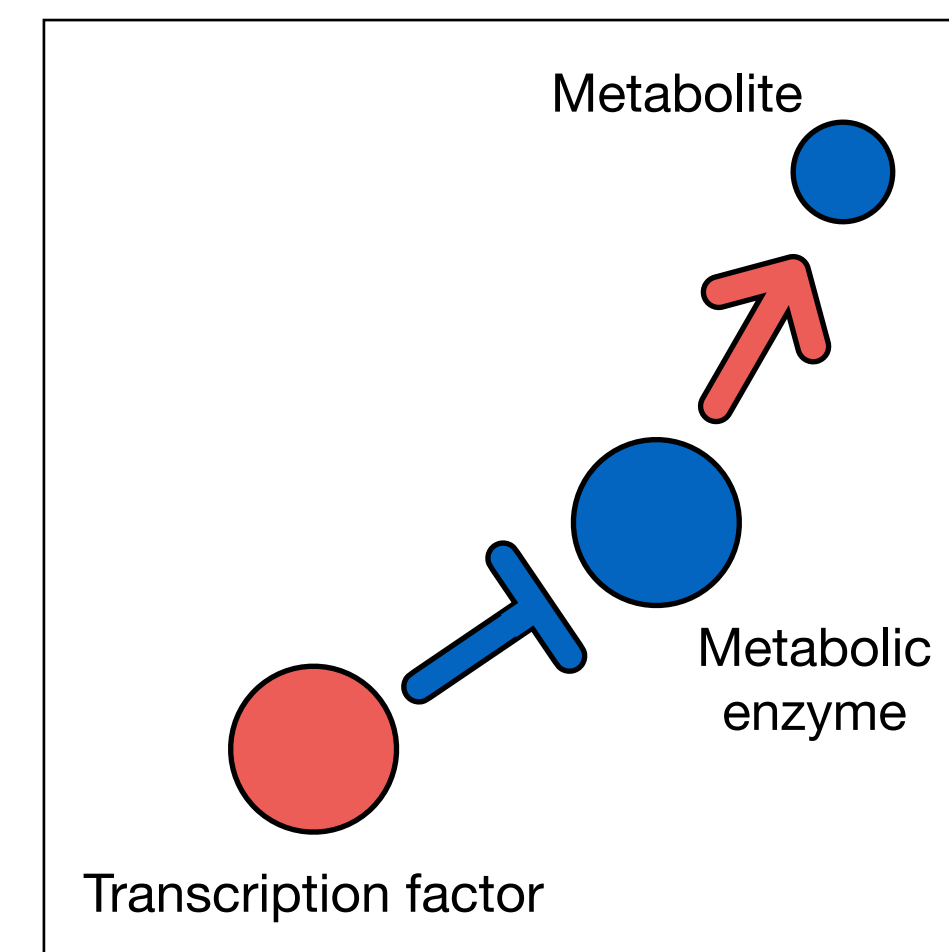
NCI60 cancer cell lines



Select cell line (or group) focus



COSMOS



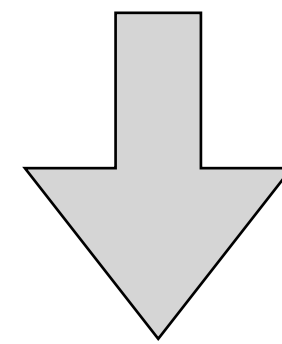
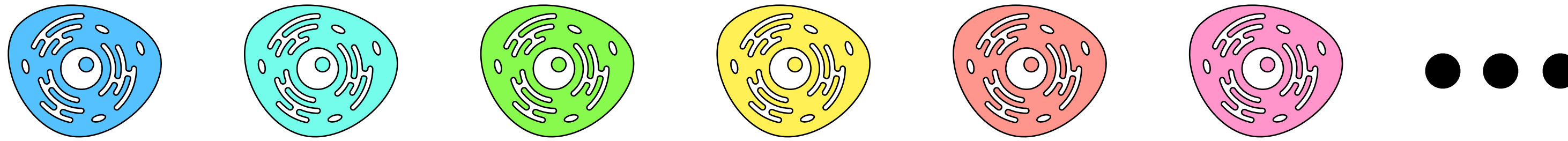
Testable hypotheses



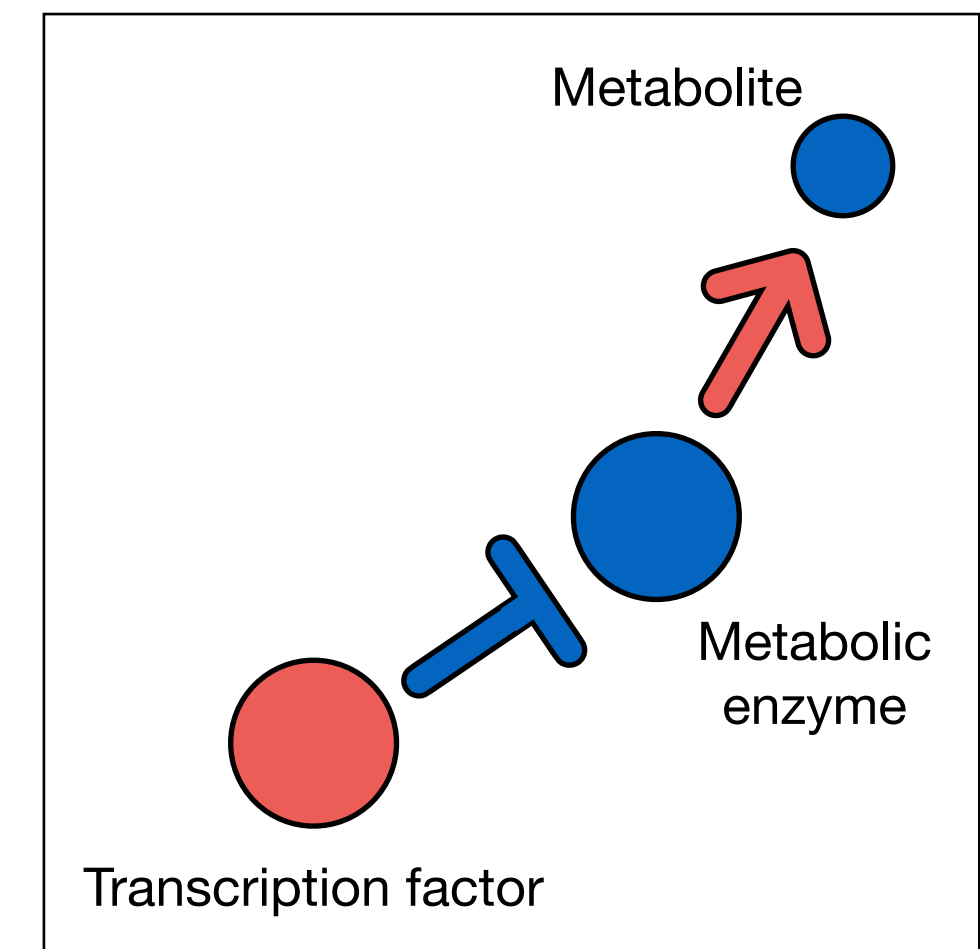
Interpretation



NCI60 cancer cell lines



```
1 library(cosmosR)
2 library(readr)
3 library(dplyr)
4
5 data("meta_network")
6 load("data/cosmos/cosmos_inputs.RData")
7
8 names(cosmos_inputs)
9
10 cell_line <- "786-0"
11
12 sig_input <- cosmos_inputs[[cell_line]]$TF_scores
13 metab_input <- cosmos_inputs[[cell_line]]$metabolomic
14 RNA_input <- cosmos_inputs[[cell_line]]$RNA
```

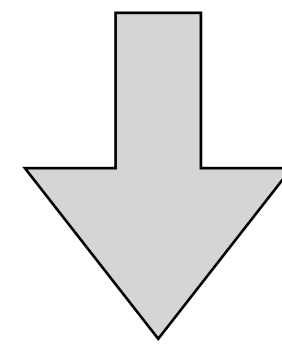
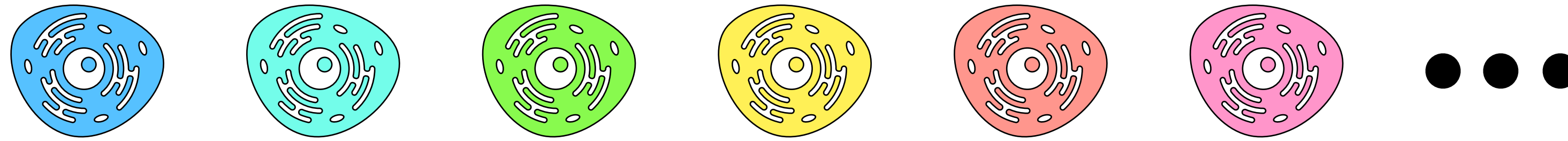


Testable hypotheses

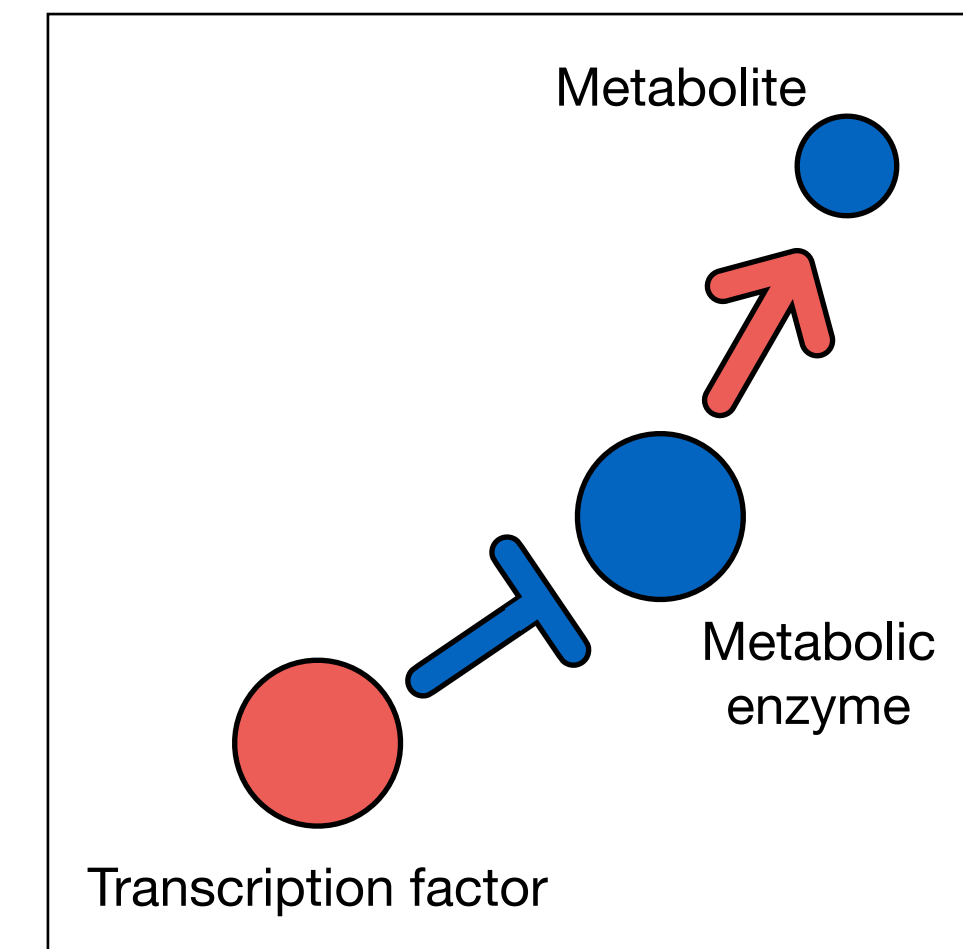
Interpretation

COSMOS

NCI60 cancer cell lines



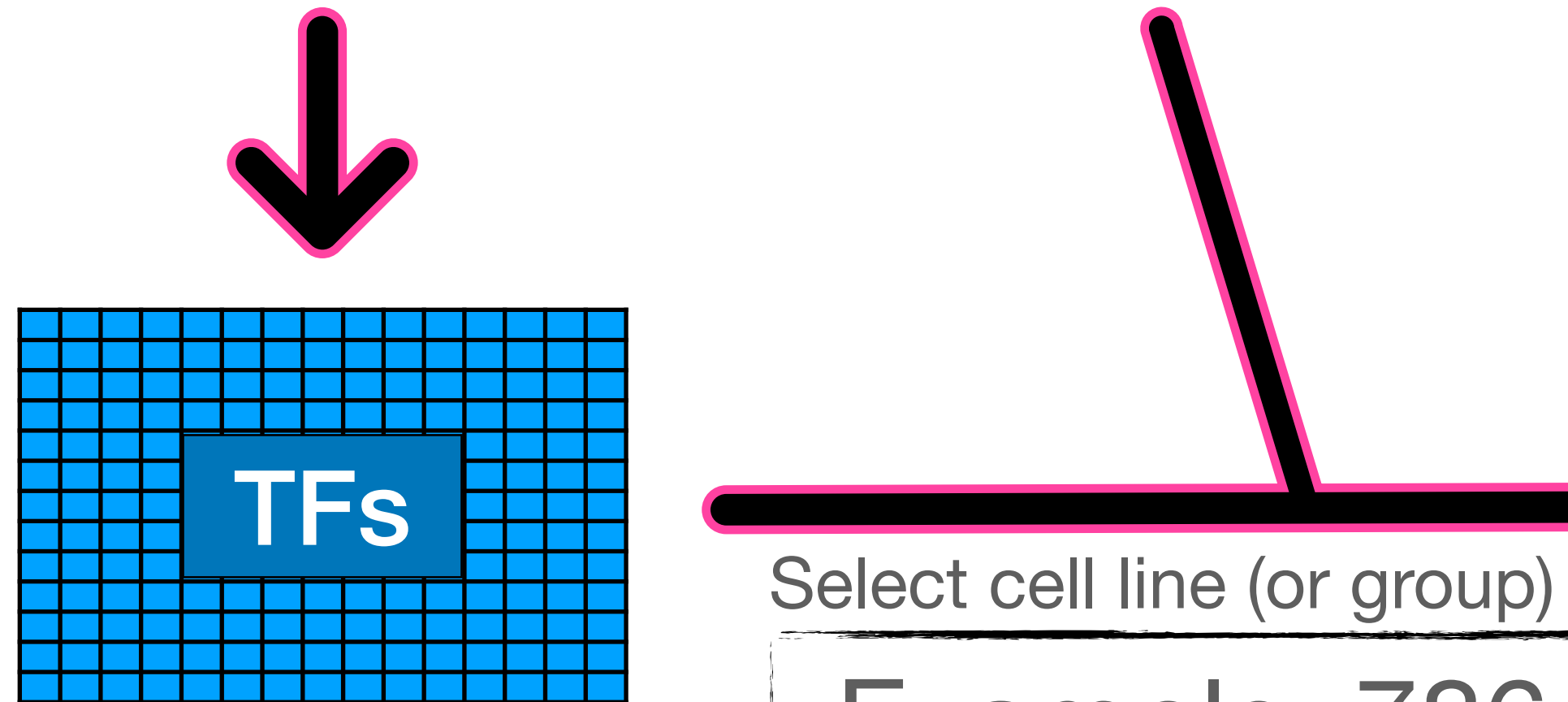
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Testable hypotheses

Interpretation 

COSMOS



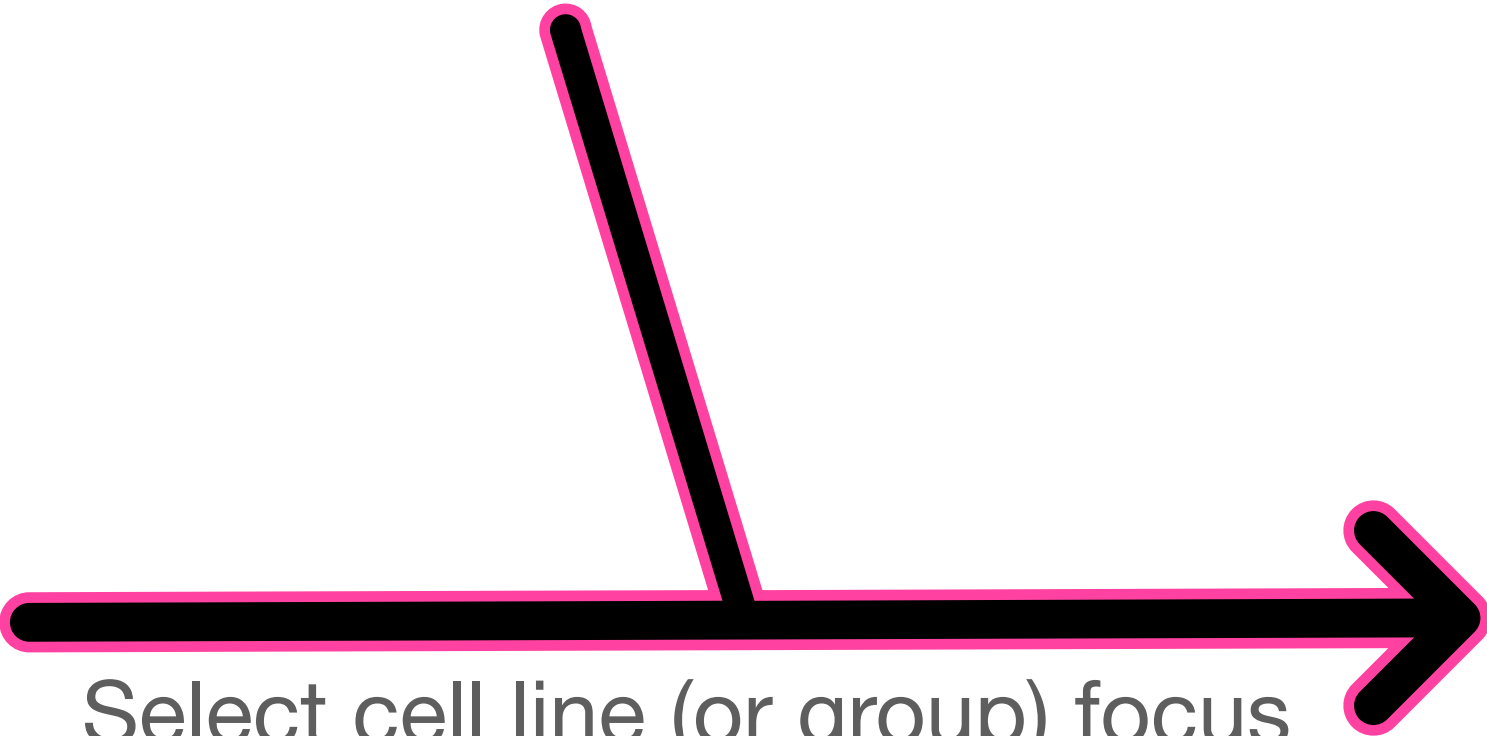
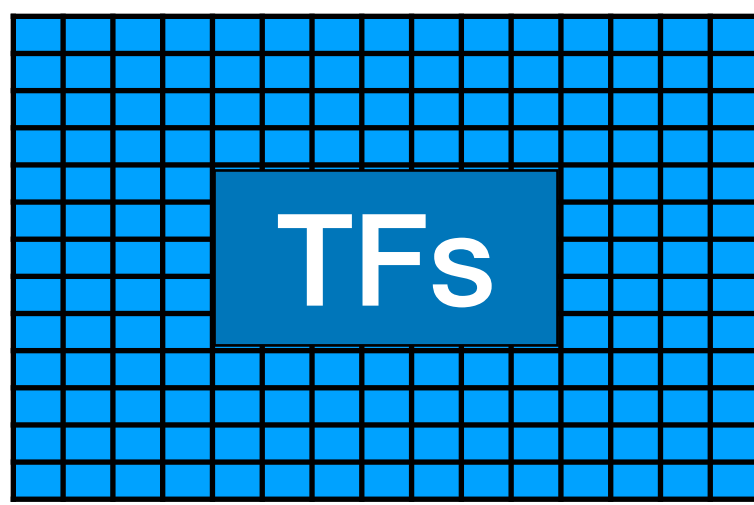
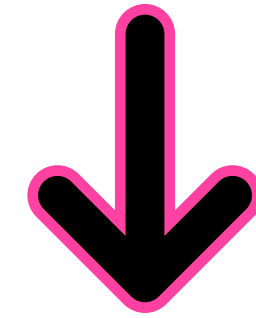
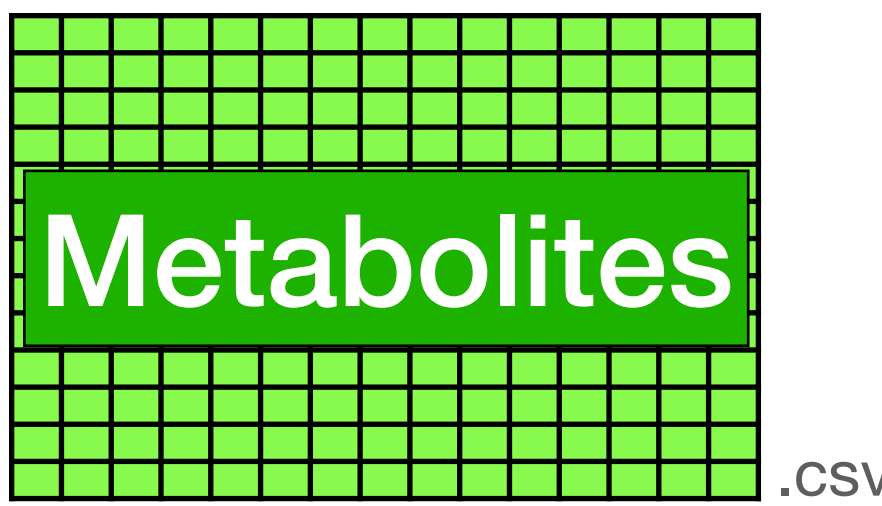
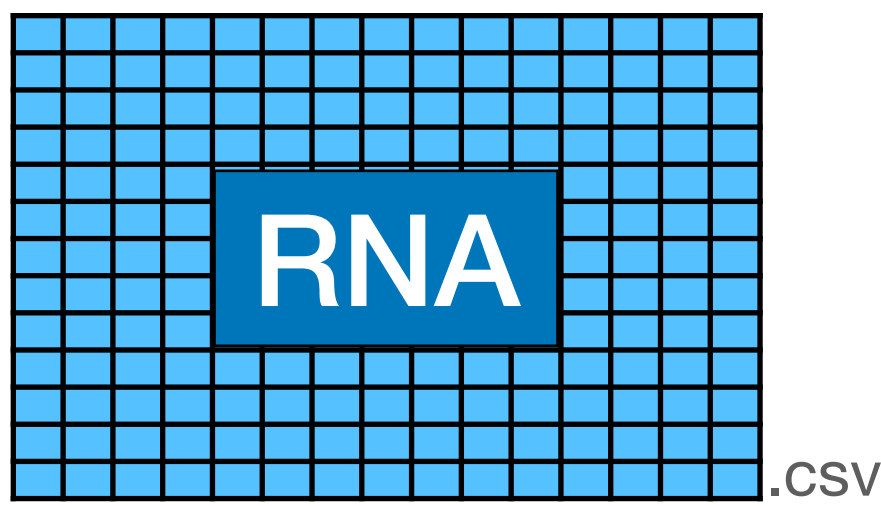
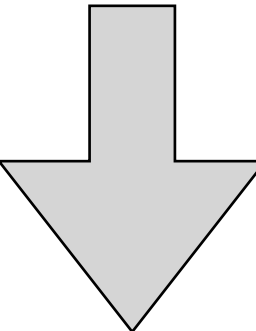
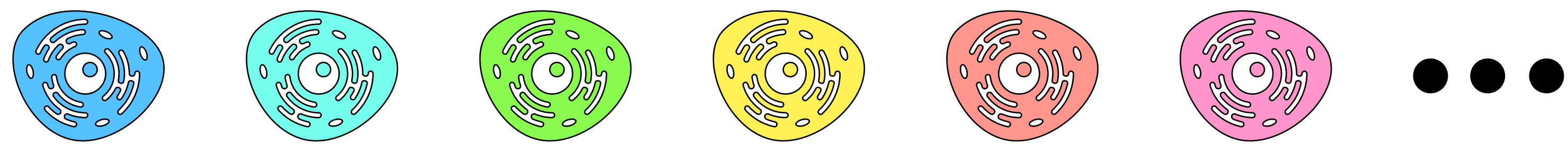
Example: 786-O



COSMOS

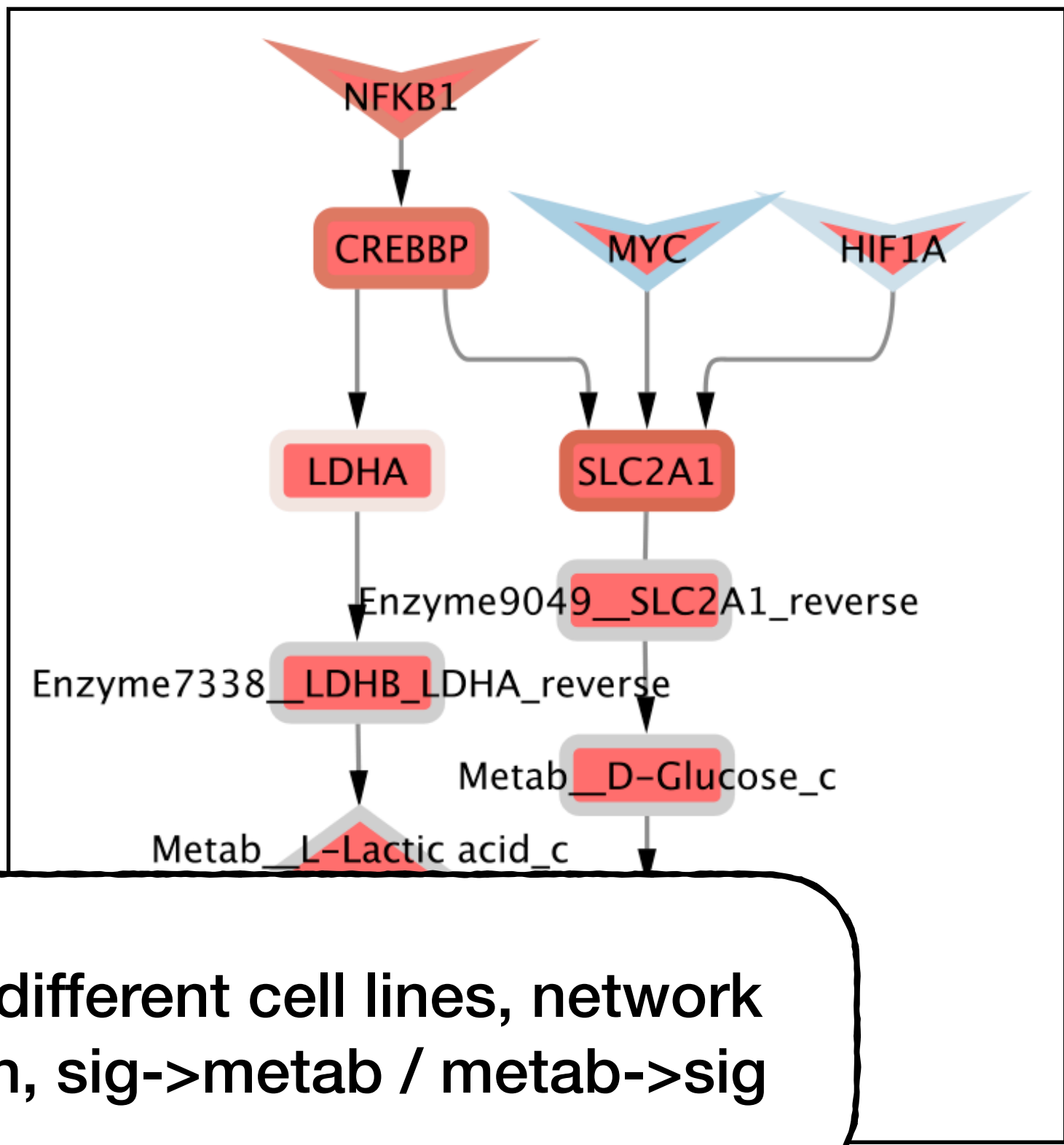
CREBBP key regulator of LDHA activity
downstream of NFKB1 in 786-O?

NCI60 cancer cell lines



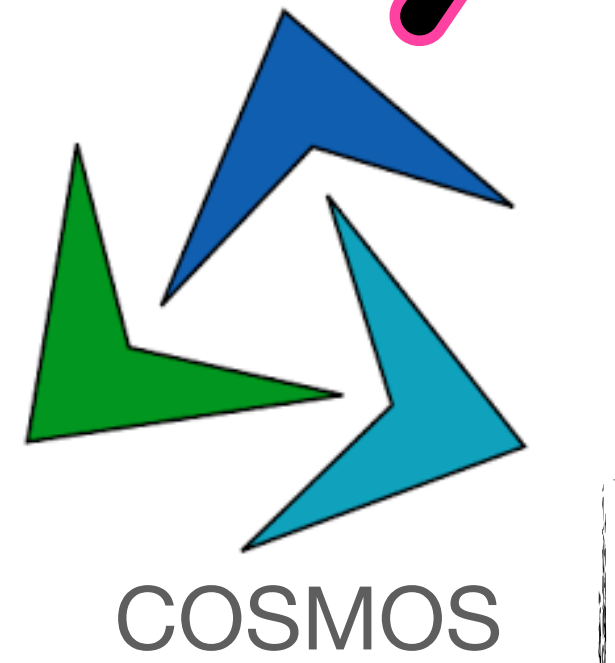
Select cell line (or group) focus

Example: 786-O



Test different cell lines, network depth, sig->metab / metab->sig

Testable hypotheses



CREBBP key regulator of LDHA activity downstream of NFKB1 in 786-O?

Formatted data and example script available in GitHub

saezlab / NCI60_cosmos

Public

<> Code

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Settings

main

1 branch

0 tags

Go to file

Add file

Code

adugourd

Update README.md

cdc8ac6 yesterday

5 commits

data	first commit	yesterday
results	first commit	yesterday
scripts	first commit	yesterday
support	first commit	yesterday
.gitignore	first commit	yesterday
EBI practical.key	first commit	yesterday
LICENSE	Create LICENSE	yesterday
NCI60.Rproj	first commit	yesterday
README.md	Update README.md	yesterday

README.md

NCI60_cosmos

Formatting NCI60 data into cosmos ready inputs and generation of testable hypothesis connecting cell-line specific TF and metabolic deregulations.

data/cosmo/cosmos_inputs.RData contains cosmos-ready inputs for each NCI60 cell lines.

scripts/run_cosmos.R to run cosmos analysis on a specific NCI60 cell line

#!/ Can only be run with the new_PKN github branch of cosmosR at the presnet time. !/

About

Formatting NCI60 data into cosmos ready inputs and generation of testable hypothesis connecting cell-line specific TF and metabolic deregulations.

Readme

GPL-3.0 License

0 stars

3 watching

0 forks

Releases

No releases published

Create a new release

Packages

No packages published

Publish your first package

Languages

R 100.0%

#!/ Can only be run with the new_PKN github branch of cosmosR at the presnet time. !/

scripts/run_cosmos.R to run cosmos analysis on a specific NCI60 cell line

data/cosmo/cosmos_inputs.RData contains cosmos-ready inputs for each NCI60 cell line

Expected outcomes:

- Explore NCI60 cell line omic datasets
- Interpreting TF activities estimated from RNA seq data
- Learning to use cosmos to integrate signalling and metabolic data with prior knowledge
- Generate and interpret testable hypotheses

Softwares:

- CBC solver executable
- R 4.1>
- cosmosR R package
- (readr and dplyr R packages)