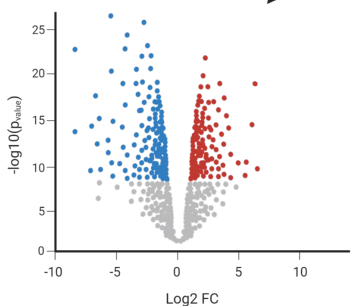
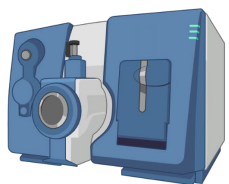
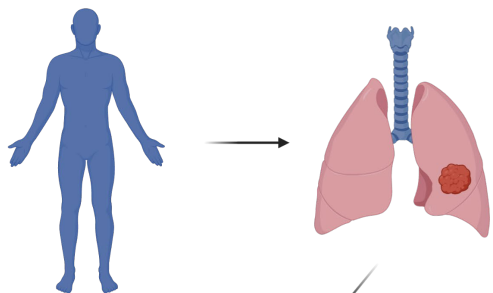




# A novel metabolic signature in malignant human lung adenocarcinomas is revealed by contextual, reaction-resolution analysis of metabolomic data

Jordan A. Berg, Youjia Zhou, Yeyun Ouyang, T. Cameron Waller, Sara M. Nowinski, Tyler Van Ry, Ian George, James E. Cox, Bei Wang, Jared Rutter

Lung adenocarcinomas and paired healthy lung tissue were obtained in Wikoff, et al. (2015), and assayed for biomarkers.



We reprocessed these metabolomics data with our tool, **Metaboverse**, to identify context-dependent patterns within the data.

1) Choose organism and output location

Select the organism you would like to analyze:  
Saccharomyces cerevisiae

Click on the folder to select output location:  
Select Output File Name

Continue

Load transcriptomics data:  
Select File No file selected

Load proteomics data:  
Select File No file selected

Load metabolomics data:  
Select File No file selected

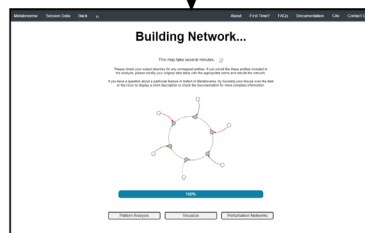
	000min_mct1_jfc	000min_mct1_bh	015min_mct1
Urea	-3.23868904	9.85E-05	-2.2272
L-Valine	1.236272279	0.001305057	0.4466
Putrescine	-1.981283414	7.02E-06	-1.5845
Methylmalonic	0.886017801	0.00095924	0.1653
Glycine	2.002589931	0.00013548	2.5797
Malonic acid	0.149937263	0.729091415	-0.0341
Fumaric acid	2.588709849	3.83E-06	1.0036
L-Alanine	2.322251455	5.26E-09	0.7780
Threonic acid	-0.382339405	0.00096726	-0.0852
D-Malic acid	2.728950429	1.97E-07	2.4007
L-Isoleucine	1.063415577	0.001035193	0.3891
Citric acid	0.183446037	0.438568557	-1.7537
L-Lysine	-2.473820035	0.003217549	-5.3311
Xanthurenic acid	0.905991059	0.169872052	0.3146
L-Glutamic acid	-0.628094548	0.203936688	-2.5799
Orotic acid	-3.96860657	0.000206079	-2.9325
L-Tyrosine	-2.309293197	0.000371556	-2.9632
Ornithine	-6.562107439	0.004785547	-8.0784
Phosphoenolpy	-0.763107235	0.01593318	-1.0192
Thymine	-0.719164516	0.000366792	-0.3706
Adenine	-1.898401034	3.13E-05	-1.3664
L-Aspartic acid	0.850815348	0.014706926	-1.8264
L-Methionine	3.386641415	0.000046418	3.3464

2) Load data

Download Metaboverse



3) Build network model and layer data



4.1) Reaction Pattern Analysis



4.2) Pathway Visualization



4.3) Perturbation Networks

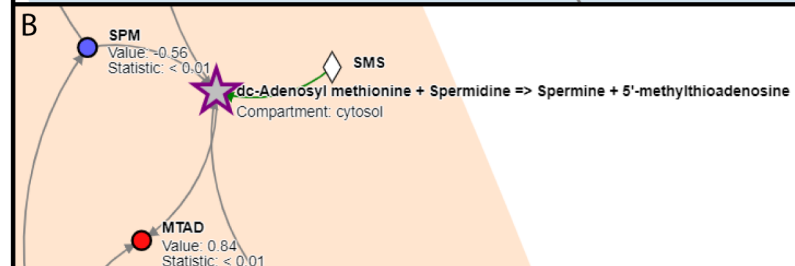
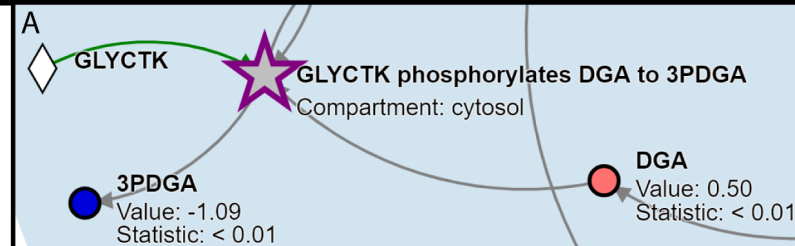


4) Analysis



Nearest Neighborhood Searches

We identified novel reaction patterns within the data, one around glycerate kinase (A), and the other around Spermine Synthase (B).



We cross-referenced the SMS pattern with the Human Protein Atlas and discovered SMS expression could be used as a prognostic marker in lung adenocarcinomas (C).

