DiSCoVER:
Evaluating An Algorithm for Cancer-Related Medicine Recommendations

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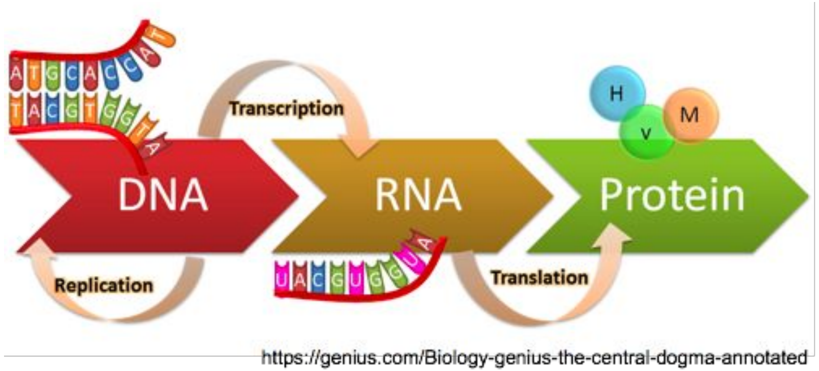
UC San Diego

Overview

- Background Information
- Proposed Solution
- Methods
- Results
- Future Steps

Background Info

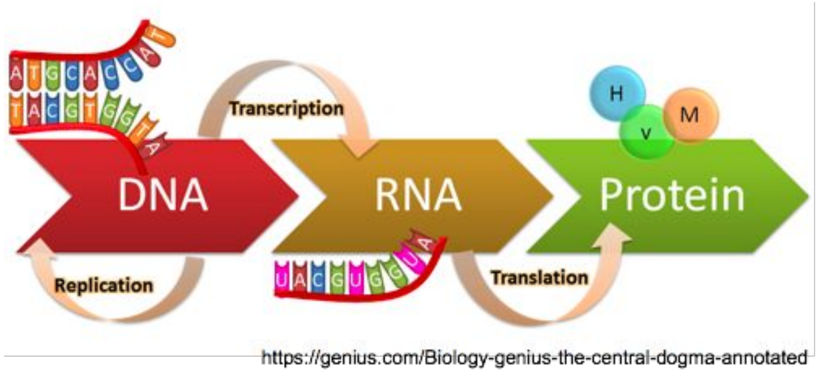
- Precision Medicine
- Protein Synthesis
- Gene Expression and Cancer



https://genius.com/Biology-genius-the-central-dogma-annotated

Background Info

- Precision Medicine
- Protein Synthesis
- Gene Expression and Cancer
- GE Lists/Datasets



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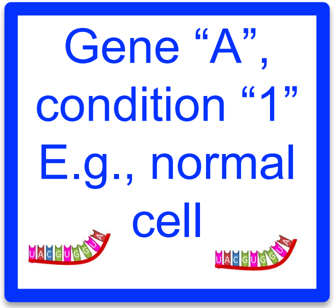
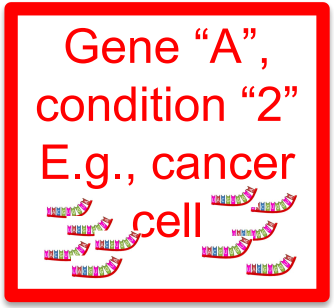
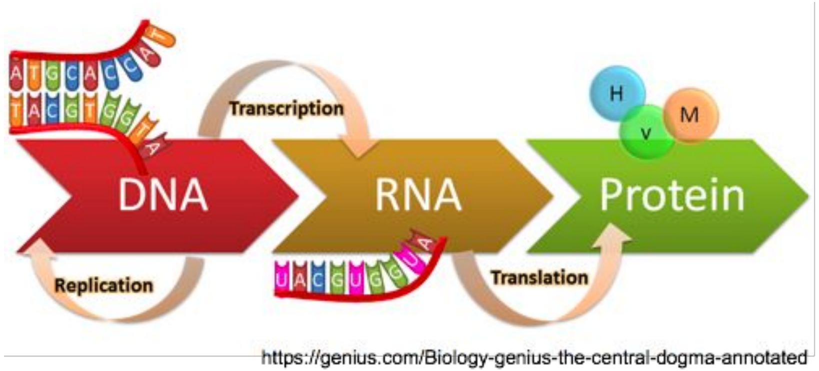

Gene “A”, condition “1” E.g., normal cell


Gene “A”, condition “2” E.g., cancer cell

Background Info

- Precision Medicine
- Protein Synthesis
- Gene Expression and Cancer
  GE lists/datasets



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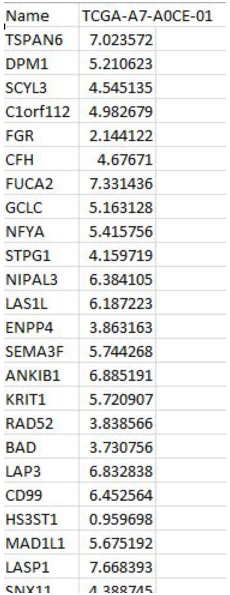
Gene "A", condition "1"
E.g., normal cell

Gene "A", condition "2"
E.g., cancer cell

Rows:
Genes

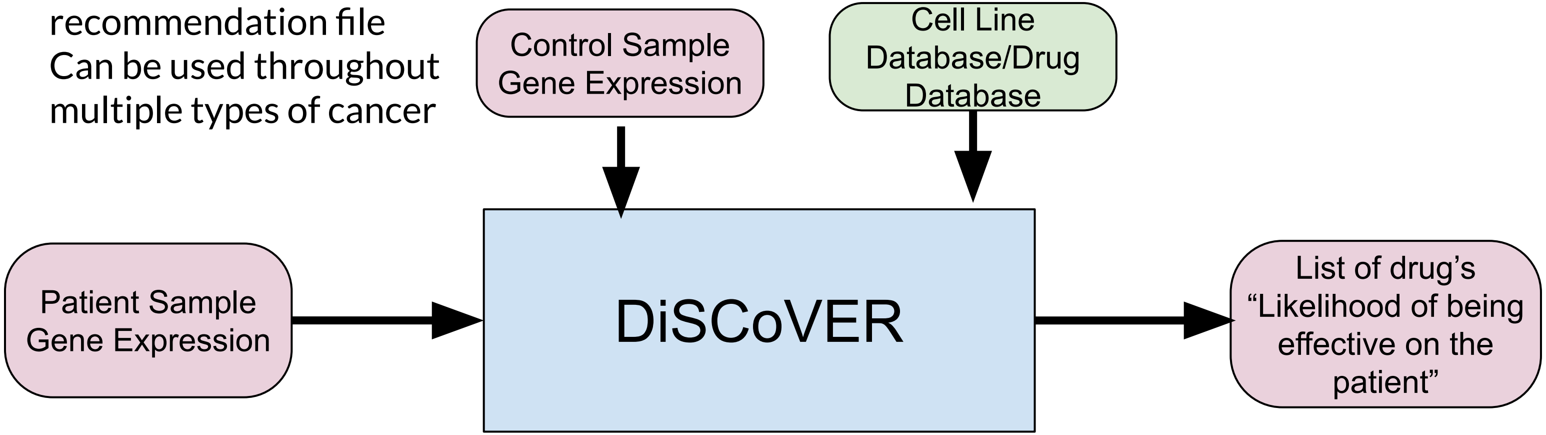


Name	TCGA-A7-A0CE-01
TSPAN6	7.023572
DPM1	5.210623
SCYL3	4.545135
C1orf112	4.982679
FGR	2.144122
CFH	4.67671
FUCA2	7.331436
GCLC	5.163128
NFYA	5.415756
STPG1	4.159719
NIPAL3	6.384105
LAS1L	6.187223
ENPP4	3.863163
SEMA3F	5.744268
ANKIB1	6.885191
KRIT1	5.720907
RAD52	3.838566
BAD	3.730756
LAP3	6.832838
CD99	6.452564
HS3ST1	0.959698
MAD1L1	5.675192
LASP1	7.668393
SNX11	4.388745

Columns:
Cell Sample
From Patients

Background Info: DiSCoVER

- "Disease-model Signature vs. Compound-Variety Enriched Response"
- Input: 2 gene expression files
- Output: 1 drug recommendation file
- Can be used throughout multiple types of cancer



Control Sample Gene Expression

Cell Line Database/Drug Database

Patient Sample Gene Expression

DiSCoVER

List of drug's "Likelihood of being effective on the patient"

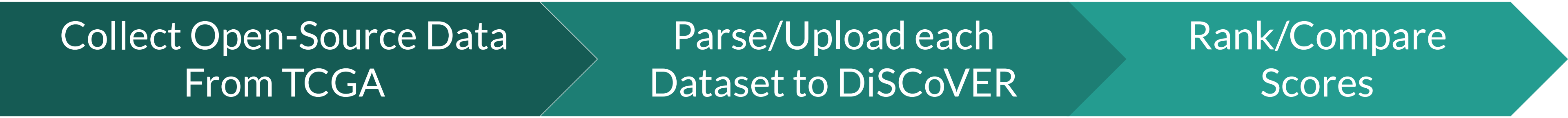
Issue At Hand

Scientists sometimes need to preprocess data before running a computer analysis. For DiSCoVER, this may result in inaccurate recommendations.

Solution

Find relationships between the outputs of DiSCoVER, where one output comes from a raw dataset and the other comes from a preprocessed dataset. If both outputs are not closely related, the accuracy of DiSCoVER's recommendations can may be questionable.

Methods

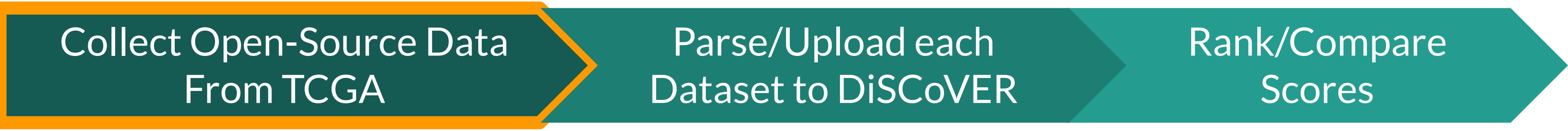


Collect Open-Source Data From TCGA

Parse/Upload each Dataset to DiSCoVER

Rank/Compare Scores

Methods



Collect Open-Source Data From TCGA

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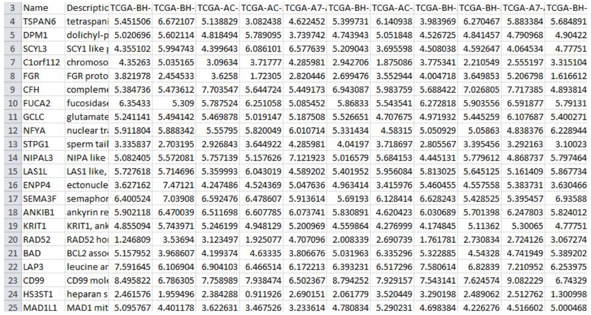
Rank/Compare Scores

Columns: Cancer Patients

Rows: Genes



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4	TSPAN6	tetraspani	5.451506	6.672107	5.138829	3.082438	4.622452	5.399731	6.140938	3.983969	6.270467	5.883384	5.684891
5	DPM1	dolichyl-p	5.020696	5.602114	4.818494	5.789095	3.739742	4.743943	5.051848	4.526725	4.841457	4.790968	4.90422
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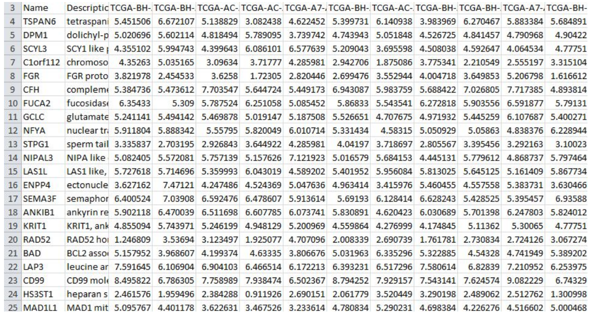
7	C1orf112	chromoso	4.35263	5.035165	3.09634	3.71777	4.285981	2.942706	1.875086	3.775341	2.210549	2.555197	3.315104
8	FGR	FGR proto	3.821978	2.454533	3.6258	1.72305	2.820446	2.699476	3.552944	4.004718	3.649853	5.206798	1.616612
9	CFH	compleme	5.384736	5.473612	7.703547	5.644724	5.449173	6.943087	5.983759	5.688422	7.026805	7.717385	4.893814
10	FUCA2	fucosidase	6.35433	5.309	5.787524	6.251058	5.085452	5.86833	5.543541	6.272818	5.903556	6.591877	5.79131
11	GCLC	glutamate	5.241141	5.494142	5.469878	5.019147	5.187508	5.526651	4.707675	4.971932	5.445259	6.107687	5.400271
12	NFYA	nuclear tr	5.911804	5.888342	5.55795	5.820049	6.010714	5.331434	4.58315	5.050929	5.05863	4.838376	6.228944
13	STPG1	sperm tail	3.335837	2.703195	2.926843	3.644922	4.285981	4.04197	3.718697	2.805567	3.395456	3.292163	3.10023
14	NIPAL3	NIPA like	5.082405	5.572081	5.757139	5.157626	7.121923	5.016579	5.684153	4.445131	5.779612	4.868737	5.797464
15	LAS1L	LAS1 like,	5.727618	5.714696	5.359993	6.043019	4.589202	5.401952	5.956084	5.813025	5.645125	5.161409	5.867734
16	ENPP4	ectonucle	3.627162	7.47121	4.247486	4.524369	5.047636	4.963414	3.415976	5.460455	4.557558	5.383731	3.630466
17	SEMA3F	semaphor	6.400524	7.03908	6.592476	6.478607	5.913614	5.69193	6.128414	6.628243	5.428525	5.395457	6.93588
18	ANKIB1	ankyrin re	5.902118	6.470039	6.511698	6.607785	6.073741	5.830891	4.620423	6.030689	5.701398	6.247803	5.824012
19	KRIT1	KRIT1, ank	4.855094	5.743971	5.246199	4.948129	5.200969	4.559864	4.276999	4.174845	5.11362	5.30065	4.77751
20	RAD52	RAD52 ho	1.246809	3.53694	3.123497	1.925077	4.707096	2.008339	2.690739	1.761781	2.730834	2.724126	3.067274
21	BAD	BCL2 asso	5.157952	3.968607	4.199374	4.63335	3.806676	5.031963	6.335296	5.322885	4.54328	4.741949	5.389202
22	LAP3	leucine ar	7.591645	6.106904	6.904103	6.466514	6.172213	6.393231	6.517296	7.580614	6.82839	7.210952	6.253975
23	CD99	CD99 mol	8.495822	6.786305	7.758989	7.938474	6.502367	8.794252	7.929157	7.543141	7.624574	9.082229	6.74329
24	HS3ST1	heparan s	2.461576	1.959496	2.384288	0.911926	2.690151	2.061779	3.520449	3.290198	2.489062	2.512762	1.300998
25	MAD1L1	MAD1 mit	5.095767	4.401178	3.622631	3.467526	3.233614	4.780834	5.290231	4.698384	4.226276	4.516602	5.000468

Raw Dataset



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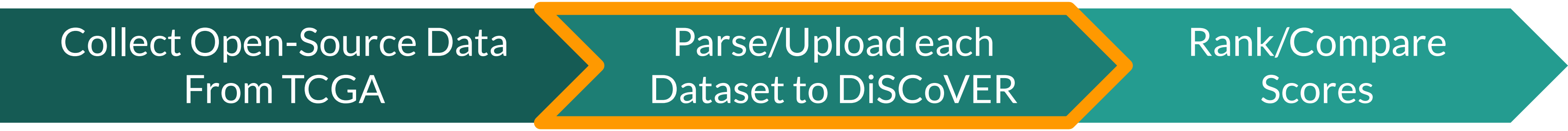
25	MAD1L1	MAD1 mit	5.095767	4.401178	3.622631	3.467526	3.233614	4.780834	5.290231	4.698384	4.226276	4.516602	5.000468

Preprocessed Dataset

- We are using RNA-Seq samples from 20 breast cancer (BRCA) patients.
- Rows represent genes, Columns represent cancerous or normal cells from each patient
- 755 columns by 40 rows

Methods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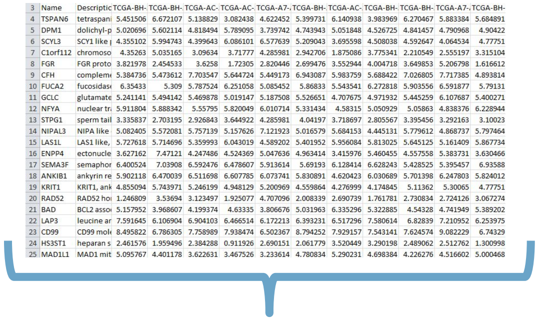
Rank/Compare Scores

TCGA Gene Expression Dataset (1 of 2)



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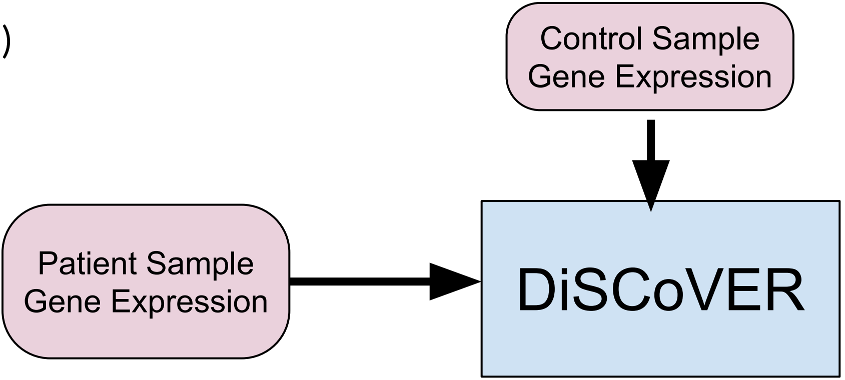
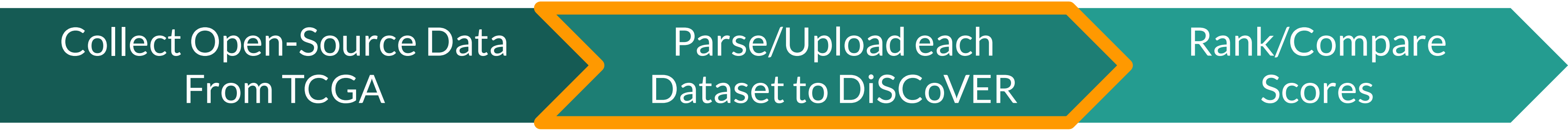
40 Columns


Control Sample Gene Expression
Patient Sample Gene Expression
DiSCoVER

Methods



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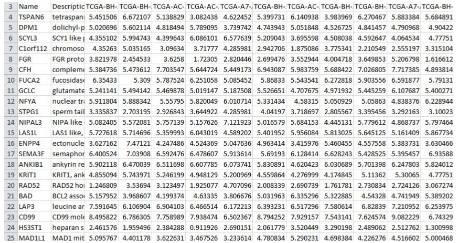

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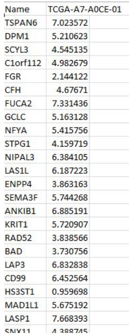
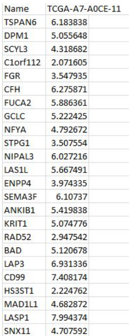
7	C1orf112	chromoso	4.35263	5.035165	3.09634	3.71777	4.285981	2.942706	1.875086	3.775341	2.210549	2.555197	3.315104
8	FGR	FGR proto	3.821978	2.454533	3.6258	1.72305	2.820446	2.699476	3.552944	4.004718	3.649853	5.206798	1.616612
9	CFH	compleme	5.384736	5.473612	7.703547	5.644724	5.449173	6.943087	5.983759	5.688422	7.026805	7.717385	4.893814
10	FUCA2	fucosidase	6.35433	5.309	5.787524	6.251058	5.085452	5.86833	5.543541	6.272818	5.903556	6.591877	5.79131
11	GCLC	glutamate	5.241141	5.494142	5.469878	5.019147	5.187508	5.526651	4.707675	4.971932	5.445259	6.107687	5.400271
12	NFYA	nuclear tr	5.911804	5.888342	5.55795	5.820049	6.010714	5.331434	4.58315	5.050929	5.05863	4.838376	6.228944
13	STPG1	sperm tail	3.335837	2.703195	2.926843	3.644922	4.285981	4.04197	3.718697	2.805567	3.395456	3.292163	3.10023
14	NIPAL3	NIPA like	5.082405	5.572081	5.757139	5.157626	7.121923	5.016579	5.684153	4.445131	5.779612	4.868737	5.797464
15	LAS1L	LAS1 like,	5.727618	5.714696	5.359993	6.043019	4.589202	5.401952	5.956084	5.813025	5.645125	5.161409	5.867734
16	ENPP4	ectonucle	3.627162	7.47121	4.247486	4.524369	5.047636	4.963414	3.415976	5.460455	4.557558	5.383731	3.630466
17	SEMA3F	semaphor	6.400524	7.03908	6.592476	6.478607	5.913614	5.69193	6.128414	6.628243	5.428525	5.395457	6.93588
18	ANKIB1	ankyrin re	5.902118	6.470039	6.511698	6.607785	6.073741	5.830891	4.620423	6.030689	5.701398	6.247803	5.824012
19	KRIT1	KRIT1, ank	4.855094	5.743971	5.246199	4.948129	5.200969	4.559864	4.276999	4.174845	5.11362	5.30065	4.77751
20	RAD52	RAD52 ho	1.246809	3.53694	3.123497	1.925077	4.707096	2.008339	2.690739	1.761781	2.730834	2.724126	3.067274
21	BAD	BCL2 asso	5.157952	3.968607	4.199374	4.63335	3.806676	5.031963	6.335296	5.322885	4.54328	4.741949	5.389202
22	LAP3	leucine ar	7.591645	6.106904	6.904103	6.466514	6.172213	6.393231	6.517296	7.580614	6.82839	7.210952	6.253975
23	CD99	CD99 mole	8.495822	6.786305	7.758989	7.938474	6.502367	8.794252	7.929157	7.543141	7.624574	9.082229	6.74329
24	HS3ST1	heparan s	2.461576	1.959496	2.384288	0.911926	2.690151	2.061779	3.520449	3.290198	2.489062	2.512762	1.300998
25	MAD1L1	MAD1 mit	5.095767	4.401178	3.622631	3.467526	3.233614	4.780834	5.290231	4.698384	4.226276	4.516602	5.000468

Cancerous Tissue Sample ("01")



Name	TCGA-A7-A0CE-01
TSPAN6	7.023572
DPM1	5.210623
SCYL3	4.545135
C1orf112	4.982679
FGR	2.144122
CFH	4.67671
FUCA2	7.331436
GCLC	5.163128
NFYA	5.415756
STPG1	4.159719
NIPAL3	6.384105
LAS1L	6.187223
ENPP4	3.863163
SEMA3F	5.744268
ANKIB1	6.885191
KRIT1	5.720907
RAD52	3.838566
BAD	3.730756
LAP3	6.832838
CD99	6.452564
HS3ST1	0.959698
MAD1L1	5.675192
LASP1	7.668393
SNX11	4.388745



Name	TCGA-A7-A0CE-11
TSPAN6	6.183838
DPM1	5.055648
SCYL3	4.318682
C1orf112	2.071605
FGR	3.547935
CFH	6.275871
FUCA2	5.886361
GCLC	5.222425
NFYA	4.792672
STPG1	3.507554
NIPAL3	6.027216
LAS1L	5.667491
ENPP4	3.974335
SEMA3F	6.10737
ANKIB1	5.419838
KRIT1	5.074776
RAD52	2.947542
BAD	5.120678
LAP3	6.931336
CD99	7.408174
HS3ST1	2.224762
MAD1L1	4.682872
LASP1	7.994374
SNX11	4.707592

Normal/Control Tissue Sample ("11")

40 Columns

X 20

Methods

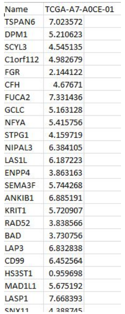
Collect Open-Source Data From TCGA

Parse/Upload each Dataset to DiSCoVER

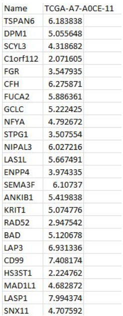
Rank/Compare Scores

Columns: Cancer Patient

Rows: Genes



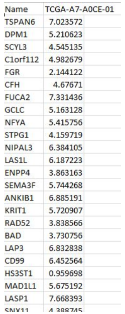
Name	TCGA-A7-A0CE-01
TSPAN6	7.023572
DPM1	5.210623
SCYL3	4.545135
C1orf112	4.982679
FGR	2.144122
CFH	4.67671
FUCA2	7.331436
GCLC	5.163128
NFYA	5.415756
STPG1	4.159719
NIPAL3	6.384105
LAS1L	6.187223
ENPP4	3.863163
SEMA3F	5.744268
ANKIB1	6.885191
KRIT1	5.720907
RAD52	3.838566
BAD	3.730756
LAP3	6.832838
CD99	6.452564
HS3ST1	0.959698
MAD1L1	5.675192
LASP1	7.668393
SNX11	4.388745



Name	TCGA-A7-A0CE-11
TSPAN6	6.183838
DPM1	5.055648
SCYL3	4.318682
C1orf112	2.071605
FGR	3.547935
CFH	6.275871
FUCA2	5.886361
GCLC	5.222425
NFYA	4.792672
STPG1	3.507554
NIPAL3	6.027216
LAS1L	5.667491
ENPP4	3.974335
SEMA3F	6.10737
ANKIB1	5.419838
KRIT1	5.074776
RAD52	2.947542
BAD	5.120678
LAP3	6.931336
CD99	7.408174
HS3ST1	2.224762
MAD1L1	4.682872
LASP1	7.994374
SNX11	4.707592

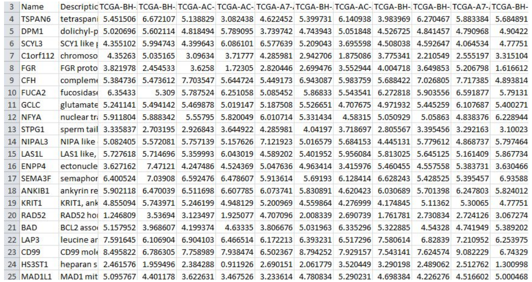
DiSCoVER

Rows: Drugs



Name	TCGA-A7-A0CE-01
TSPAN6	7.023572
DPM1	5.210623
SCYL3	4.545135
C1orf112	4.982679
FGR	2.144122
CFH	4.67671
FUCA2	7.331436
GCLC	5.163128
NFYA	5.415756
STPG1	4.159719
NIPAL3	6.384105
LAS1L	6.187223
ENPP4	3.863163
SEMA3F	5.744268
ANKIB1	6.885191
KRIT1	5.720907
RAD52	3.838566
BAD	3.730756
LAP3	6.832838
CD99	6.452564
HS3ST1	0.959698
MAD1L1	5.675192
LASP1	7.668393
SNX11	4.388745

Drug Recommendation Dataset (1 of 2)



3	Name	Descriptic	TCGA-BH-	TCGA-BH-	TCGA-AC-	TCGA-AC-	TCGA-A7-	TCGA-BH-	TCGA-AC-	TCGA-BH-	TCGA-BH-	TCGA-A7-	TCGA-BH-
4	TSPAN6	tetraspani	5.451506	6.672107	5.138829	3.082438	4.622452	5.399731	6.140938	3.983969	6.270467	5.883384	5.684891
5	DPM1	dolichyl-p	5.020696	5.602114	4.818494	5.789095	3.739742	4.743943	5.051848	4.526725	4.841457	4.790968	4.90422
6	SCYL3	SCY1 like	4.355102	5.994743	4.399643	6.086101	6.577639	5.209043	3.695598	4.508038	4.592647	4.064534	4.77751
7	C1orf112	chromoso	4.35263	5.035165	3.09634	3.71777	4.285981	2.942706	1.875086	3.775341	2.210549	2.555197	3.315104
8	FGR	FGR proto	3.821978	2.454533	3.6258	1.72305	2.820446	2.699476	3.552944	4.004718	3.649853	5.206798	1.616612
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13	STPG1	sperm tail	3.335837	2.703195	2.926843	3.644922	4.285981	4.04197	3.718697	2.805567	3.395456	3.292163	3.10023
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24	HS3ST1	heparan s	2.461576	1.959496	2.384288	0.911926	2.690151	2.061779	3.520449	3.290198	2.489062	2.512762	1.300998
25	MAD1L1	MAD1 mit	5.095767	4.401178	3.622631	3.467526	3.233614	4.780834	5.290231	4.698384	4.226276	4.516602	5.000468

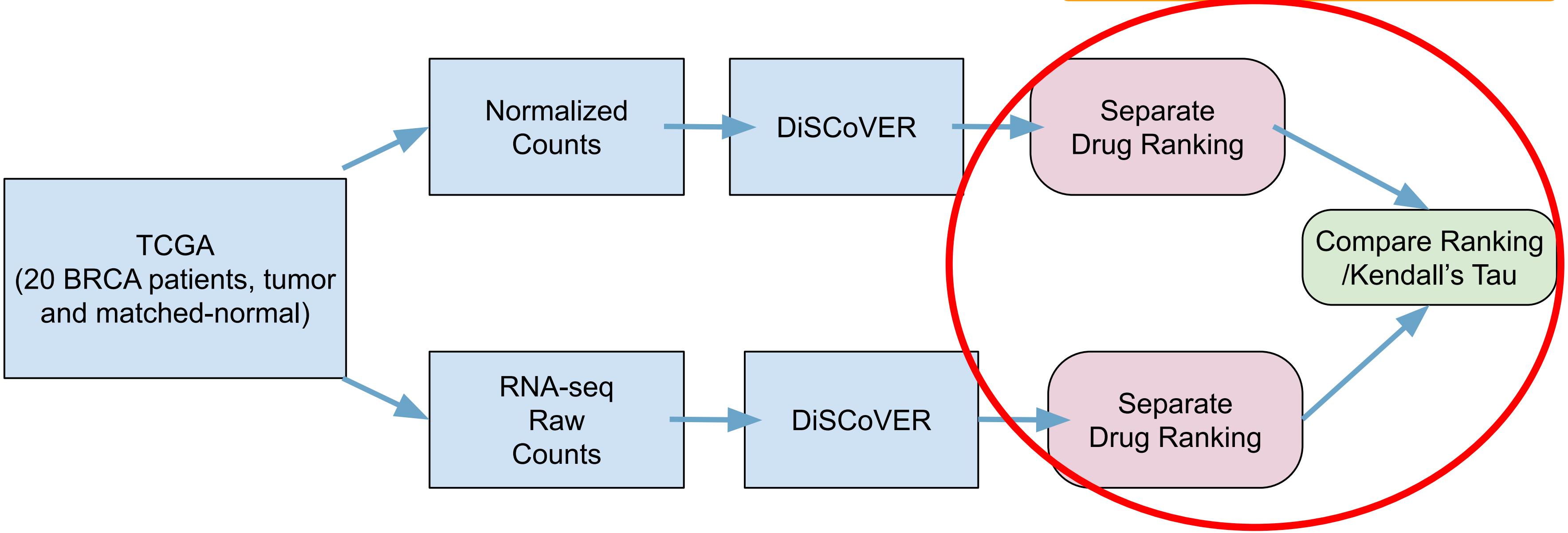
X 20

Methods

Collect Open-Source Data From TCGA

Parse/Upload each Dataset to DiSCoVER

Rank/Compare Scores



TCGA (20 BRCA patients, tumor and matched-normal)

Normalized Counts

DiSCoVER

Separate Drug Ranking

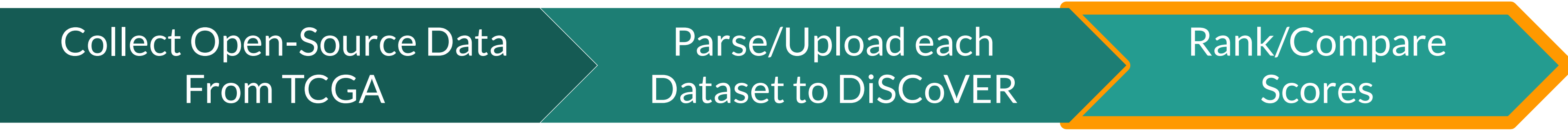
RNA-seq Raw Counts

DiSCoVER

Separate Drug Ranking

Compare Ranking /Kendall's Tau

Methods

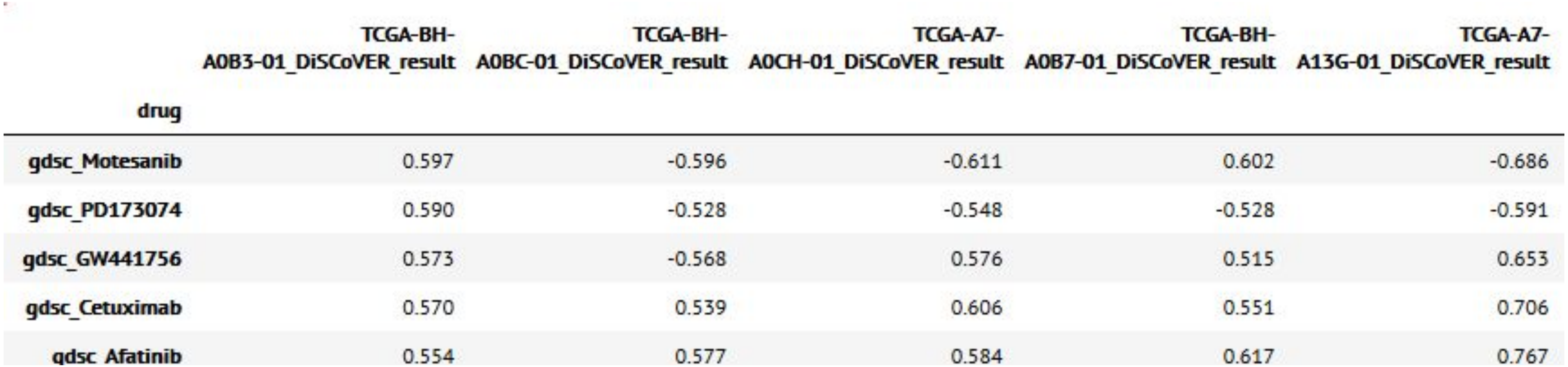


Collect Open-Source Data From TCGA

Parse/Upload each Dataset to DiSCoVER

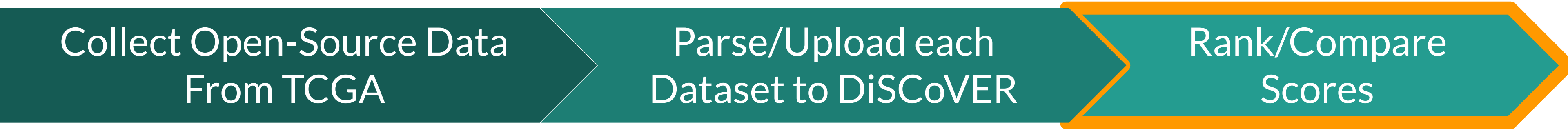
Rank/Compare Scores

Example Dataset



	TCGA-BH-A0B3-01_DiSCoVER_result	TCGA-BH-A0BC-01_DiSCoVER_result	TCGA-A7-A0CH-01_DiSCoVER_result	TCGA-BH-A0B7-01_DiSCoVER_result	TCGA-A7-A13G-01_DiSCoVER_result
drug					
gdsc_Motesanib	0.597	-0.596	-0.611	0.602	-0.686
gdsc_PD173074	0.590	-0.528	-0.548	-0.528	-0.591
gdsc_GW441756	0.573	-0.568	0.576	0.515	0.653
gdsc_Cetuximab	0.570	0.539	0.606	0.551	0.706
gdsc_Afatinib	0.554	0.577	0.584	0.617	0.767

Methods

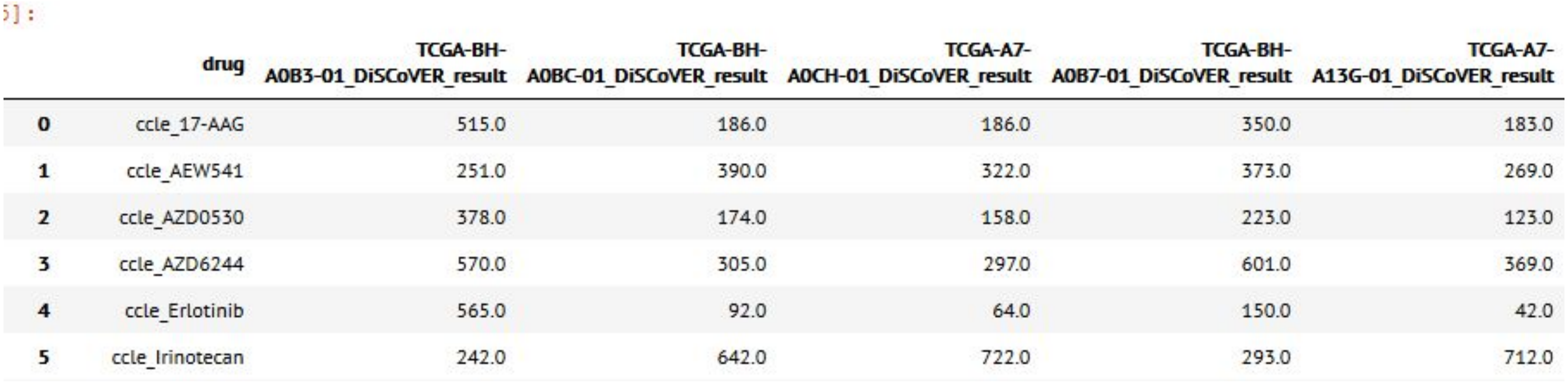


Collect Open-Source Data From TCGA

Parse/Upload each Dataset to DiSCoVER

Rank/Compare Scores

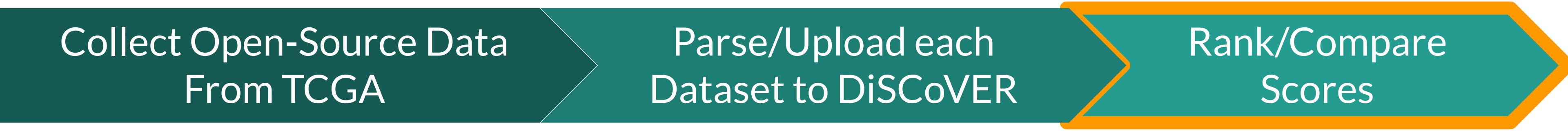
Example Dataset



5]:

	drug	TCGA-BH-A0B3-01_DiSCoVER_result	TCGA-BH-A0BC-01_DiSCoVER_result	TCGA-A7-A0CH-01_DiSCoVER_result	TCGA-BH-A0B7-01_DiSCoVER_result	TCGA-A7-A13G-01_DiSCoVER_result
0	ccle_17-AAG	515.0	186.0	186.0	350.0	183.0
1	ccle_AEW541	251.0	390.0	322.0	373.0	269.0
2	ccle_AZD0530	378.0	174.0	158.0	223.0	123.0
3	ccle_AZD6244	570.0	305.0	297.0	601.0	369.0
4	ccle_Erlotinib	565.0	92.0	64.0	150.0	42.0
5	ccle_Irinotecan	242.0	642.0	722.0	293.0	712.0

Methods

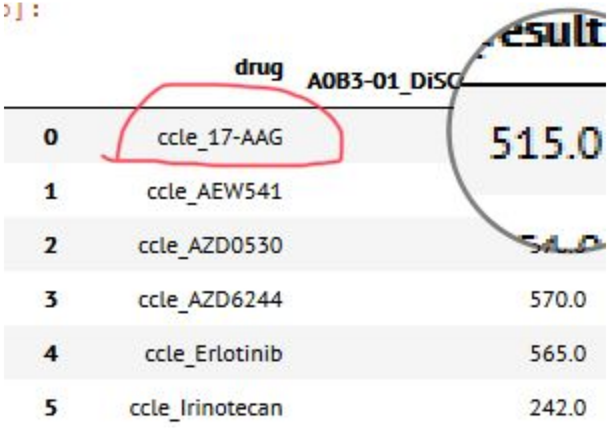


Collect Open-Source Data From TCGA

Parse/Upload each Dataset to DiSCoVER

Rank/Compare Scores

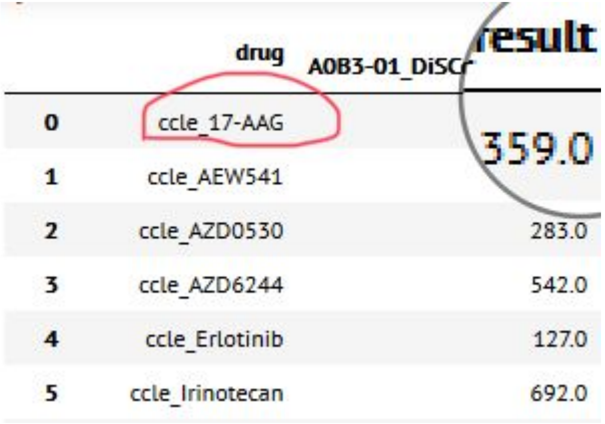
Ranking of Raw Output



]:

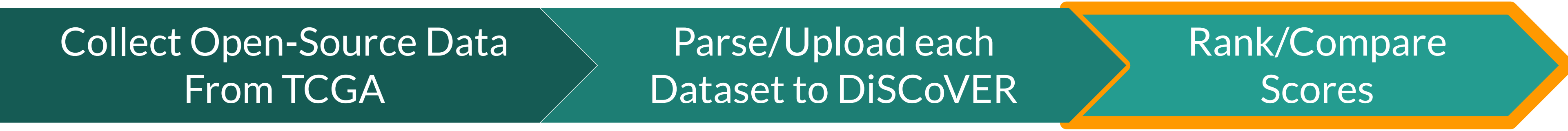
	drug	A0B3-01_DiSC result
0	ccle_17-AAG	515.0
1	ccle_AEW541	
2	ccle_AZD0530	[illegible]
3	ccle_AZD6244	570.0
4	ccle_Erlotinib	565.0
5	ccle_Irinotecan	242.0

Ranking of Preprocessed Output



	drug	A0B3-01_DiSC result
0	ccle_17-AAG	359.0
1	ccle_AEW541	
2	ccle_AZD0530	283.0
3	ccle_AZD6244	542.0
4	ccle_Erlotinib	127.0
5	ccle_Irinotecan	692.0

Methods



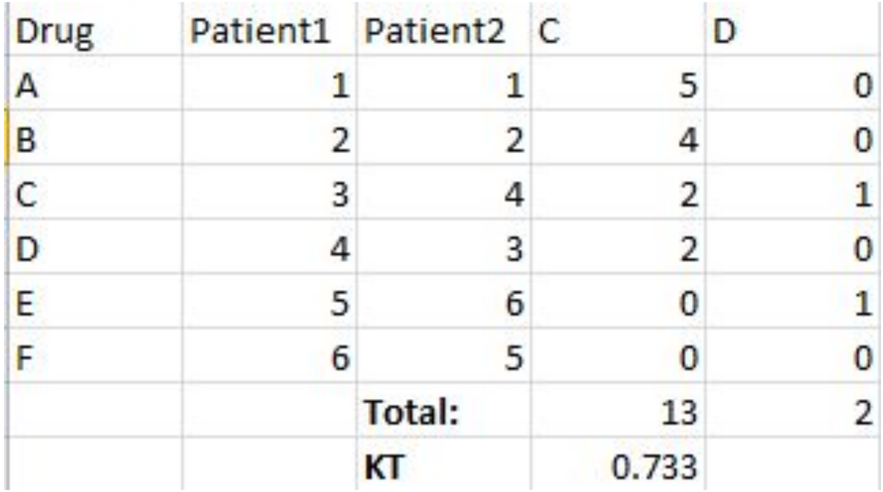
Collect Open-Source Data From TCGA

Parse/Upload each Dataset to DiSCoVER

Rank/Compare Scores

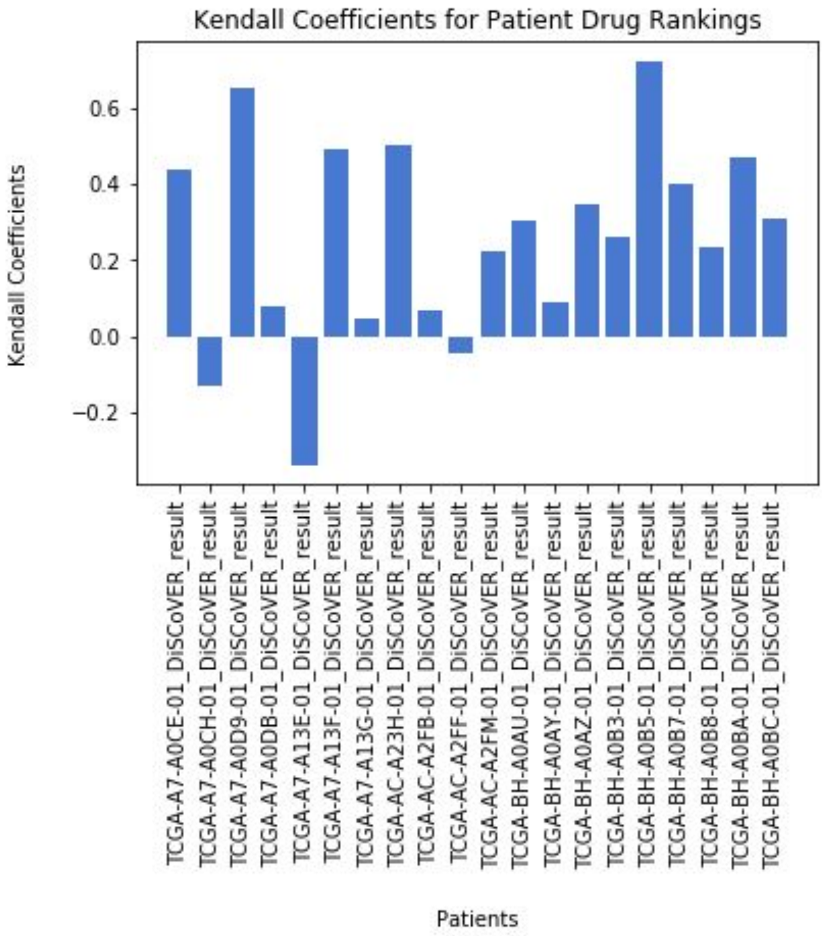
Kendall’s Tau

- Represents degree of correlation between two columns of ranked data
- Can range from -1.0 to 1.0
- Based on concordant and discordant pairs



Drug	Patient1	Patient2	C	D
A	1	1	5	0
B	2	2	4	0
C	3	4	2	1
D	4	3	2	0
E	5	6	0	1
F	6	5	0	0
		Total:	13	2
		KT	0.733	

Preliminary Results:



Possible Areas of Further Research

- Analyze possible data preprocessing methods
- Determine potential sources of “noisy data” for recommendation scores

Acknowledgments - Mesirov Lab

Dr. Jill Mesirov
PI/Lab Director

Dr. Edwin Juarez
Bioinformatics Programmer
/Research Guide

Alex Wenzel
PhD Candidate

Owen Chapman
PhD Candidate

Thank You!