

Within the DBPOM, we have developed a tool for distinguishing the reversed and adverse genes of a specified compound, or drug on cancer samples, by comparing the data stemming from the two groups of differential gene expression results.

Differential gene expression analyses have been performed on both cancer versus control tissues samples (E1) from TCGA and molecular-compound-treated cell lines versus DMSO-treated cell lines (E2) from the CMap database. When a cell line is treated with a compound, if the effect on a gene is oppositional, meaning it is up-regulated in E1 and down-regulated in E2 or vice versa, we consider it to have a reversed effect on said gene. Otherwise, if a gene is marked as $1(E1) \sim 1(E2)$, $-1(E1) \sim -1(E2)$, $0(E1) \sim 1(E2)$ or $0(E1) \sim -1(E2)$, with 0 standing for no change, we consider the compound to have an adverse effect on this specific gene. For each compound, if it reverses the expression of a cancer-associated gene, it is thought to be effective on the gene. On the contrary, if the gene expression substantially deviates after treatment with the compound, we believe that the drug has had an adverse effect on the gene. Moreover, we defined one score as the Reversed and Adverse of Drug Effect (RADE) which indicates the safety and effectiveness of each compound by integrating both the reversed and adverse genes.

Regarding precision medicine, we consider two commonly studied cases. One is for specific mutations, as users may want to know the differences of drug response by individual patients with vs. without a specific mutation; and the other is about the overall mutation pattern as different cell lines of the same cancer type may respond very differently to the same drug due to their distinct mutation patterns. We have developed a tool for measuring the similarity between the mutation profiles in a cell line and in the cancer of a patient. For each cancer sample, the cell line with the highest similarity score was considered as the best reference.

There are four main modules in DBPOM.

1. Compounds

User could get the drug response by inputting the cancer type, cell line ID, and compound name.

The datasets provides three options: (1) TCGA vs. CMap (2) subTCGA vs. CMap (all mutation) (3) subTCGA vs. CMap (specific mutation) :

(1) TCGA versus CMap: in E1, all of the cancer samples of the selected cancer type in TCGA are utilized. While this is the general strategy in current research, it does not consider individual differences. We provide this option in case some users need it.

(2) subTCGA-mutation versus CMap: in E1, the subset of cancer samples in TCGA which have high matching scores with selected cell line are utilized. We provide this strategy as overall mutation pattern is an important criterion for distinguishing different cell lines. So, we provide users with this option to suit diverse requirements. In practice, for each cancer patient, he or she is firstly classified into the most suitable sample group according to mutation similarity, and then to analyze effect of drugs on him or her.

(3) subTCGA-specific versus CMap: E1 utilizes a subset of cancer samples with the specific mutation that user concerns from TCGA, which match the specific mutation that user concerns of the selected cell line in E2. We proposed this strategy and expected to get a reasonable evaluation of drug effectiveness that could then assist precision medicine.

Example: BRCA, BT20, erlotinib and subTCGA (specific mutation) vs. CMap

By clicking Filter, the search result will be shown as followings:

Datasets	Cancer Type	Cell Line	Compound	Dosage	Time	Number of Reversed Gene	Number of Adverse Gene	RADE	Detail	Download
TCGA vs. CMap	PRAD	PC3	BRD-A03772856	500 nM	6 h	407	738	5.903	Detail	Download
TCGA vs. CMap	PRAD	PC3	BRD-A03772856	1 µM	6 h	514	913	4.578	Detail	Download
TCGA vs. CMap	PRAD	PC3	BRD-A03772856	10 µM	6 h	427	674	4.898	Detail	Download
TCGA vs. CMap	PRAD	PC3	BRD-A03772856	3 µM	6 h	415	552	4.346	Detail	Download
TCGA vs. CMap	PRAD	PC3	trichostatin-a	500 nM	6 h	559	1286	5.452	Detail	Download
TCGA vs. CMap	PRAD	PC3	trichostatin-a	1 µM	6 h	565	1352	5.611	Detail	Download
TCGA vs. CMap	PRAD	PC3	trichostatin-a	10 µM	6 h	567	1437	6.004	Detail	Download
TCGA vs. CMap	PRAD	PC3	trichostatin-a	3 µM	6 h	608	1541	5.523	Detail	Download
TCGA vs. CMap	PRAD	PC3	geldanamycin	500 nM	6 h	306	375	5.306	Detail	Download
TCGA vs. CMap	PRAD	PC3	geldanamycin	1 µM	6 h	360	522	5.336	Detail	Download

“Number of Reversed gene” is the gene number of reversed genes. “Number of Adverse gene” is the gene number of the adverse genes. “RADE” is a score defined by considering both the number of reversed genes and adverse genes. The lower the score, the higher the effectiveness and safety.

Users could download all the reversed genes and adverse genes, and their differentially expressed level in E1(cancer vs. normal) and E2(compound treated cell line vs. DMSO treated cell line) by clicking download.

By clicking detail, it will jump to compound detail page.

(1) Overview

User could search the detail information of this compound or drug from CMap by clicking “Jump”. For some drugs that reported in GDSC, the information is also provided in our page.

DATASET	Cell Line	Cancer Type	Drug Name	Putative Target	Pathway Name	Ln-IC50	Z-Score
GDSC2	BT20	BRCA	erlotinib	EGFR	EGFR signaling	2.64162	0.044483

(2) Reversed gene

By clicking Reversed Gene, it will list all the reversed genes with differential expression level in E1(cancer vs. normal) and E2(compound treated cell line vs. DMSO treated cell line). User could

sort the value by clicking arrows. We provide Download in three formats CSV, Excel and PDF.

erlotinib
ID: BRD-K70401845 | Dosage: 10 µM | Time: 6 h

Overview **Reversed Gene** Adverse Gene Key Pathway

Show 10 entries

Genes	Fold change of cancer samples vs. normal samples	Fold change of compound treated vs. DMSO treated cell lines
A2M	down -2.165	up 4.189
AASS	down -3.503	up 3.171
ABCA5	down -2.877	up 5.107
ABCC6	down -2.736	up 3.633
ABCG2	down -2.749	up 2.254
ABHD6	down -2.294	up 8.101
ABI3BP	down -4.456	up 4.192
ACAA2	down -2.308	up 9.532
ACACB	down -12.626	up 3.78
ACADL	down -10.111	up 2.412

Showing 1 to 10 of 963 entries

Four gene function annotation methods (GO, KEGG, PID, REACTOME) are provided by clicking the relative buttons. The pathways with pvalue < 0.05 are the significant ones.

Enrichment Result

GO
PID
KEGG
REACTOME

Show 10 entries

Pathway Name	P-value	Reverse Num	Hit Num
ACTIN_CYTOSKELETON_ORGANIZATION_AND_BIOGENESIS	2.92e-01	8	92
ACTIN_FILAMENT_BASED_MOVEMENT	5.57e-01	0	10
ACTIN_FILAMENT_BASED_PROCESS	4.04e-01	8	102
ACTIN_FILAMENT_BUNDLE_FORMATION	2.11e-01	1	11
ACTIN_FILAMENT_ORGANIZATION	2.24e-01	2	21
ACTIN_FILAMENT_POLYMERIZATION	2.41e-01	1	12
ACTIN_POLYMERIZATION_AND_OR_DEPOLYMERIZATION	4.71e-01	1	20
ACTIVATION_OF_IMMUNE_RESPONSE	2.71e-01	1	13
ACTIVATION_OF_JNK_ACTIVITY	2.41e-01	1	12
ACTIVATION_OF_MAPK_ACTIVITY	4.62e-01	2	32

Showing 1 to 10 of 626 entries

(3) In a similar way, analyses of the adverse gene are following the same way.

(4) We additionally provide 11 key pathways and their sub pathways that clinicians and drug researchers may pay much more attention.

When user selects “Cell cycle” and then “KEGG_CELL_CYCLE”, and clicks Submit, all the reversed and adverse genes are shown as

erlotinib
 ID: BRD-K70401845 | Dosage: 10 µM | Time: 6 h

Overview Reversed Gene Adverse Gene **Key Pathway**

Cell cycle Submit

Show 10 entries

Genes	Fold change of cancer samples vs. normal samples	Fold change of compound treated vs. DMSO treated cell lines
BUB3	up_2.043	down_-4.742
CCNA2	up_7.112	down_-5.55
CCND1	up_2.44	down_-4.745
CDC25A	up_4.424	down_-6.215
CDC6	up_7.841	down_-2.124
CDKN2C	down_-2.545	up_5.566
CDKN2D	up_2.25	down_-7.581
E2F5	up_2.23	down_-2.37
ESPL1	up_6.509	down_-2.208
MAD2L1	up_4.412	down_-2.207

Showing 1 to 10 of 13 entries Previous 1 2 Next

Show 10 entries

Genes	Fold change of cancer samples vs. normal samples	Fold change of compound treated vs. DMSO treated cell lines
ATR	0.0	down_-16.876
BUB1	up_9.569	up_15.559
BUB1B	up_7.564	up_5.929
CCNE1	up_6.855	up_3.095
CDC45	up_7.323	up_2.532
CDC7	up_3.313	up_11.614
CDKN2A	up_6.708	up_2.568
CHEK1	up_2.86	up_4.104
D8F4	up_2.285	up_2.874
E2F2	up_3.882	up_3.12

Showing 1 to 10 of 15 entries Previous 1 2 Next

2. Personalized Medicine

Three options are provided.

(1) Enter Patient Matched Cell Line

When user enters cell line name, it will match the relative cancer samples of the same cancer type according to mutation similarity score by choosing “subTCGA vs. CMap (specific mutation)” or “subTCGA vs. CMap (all mutation)”. We also provide an option of “TCGA vs. CMap” in case of user needs.

By clicking Detail for detail analyses information.

Personalized Medicine

This is a patient-centric module with three options for medicine recommendation.

In Datasets, "subTCGA vs. CMap (all mutation)" is short for mutation pattern matched TCGA vs. CMap, and "subTCGA vs. CMap (specific mutation)" is short for mutation pattern matched TCGA vs. CMap (cell line specific mutation).

Enter Patient Matched Cell Line Selection of Mutation Gene Upload Specific Patient Data

Search by matched cell line according to the similarity between their mutation profiles.

Show 10 entries Choose Datasets all Export CSV

Filter by Cell Line: e.g. VCAP, BT20, SK480

Filter Compound: erlotinib e.g. gefitinib, erlotinib, BMS-536924 Filter

Datasets	Cancer Type	Cell Line	Compound	Dosage	Time	Number of Reversed Gene	Number of Adverse Gene	RADE		
TCGA vs. CMap	LUAD	A549	erlotinib	10 µM	24 h	988	1299	3.698	Detail	Download
TCGA vs. CMap	LUAD	A549	erlotinib	10 µM	6 h	1071	1206	2.921	Detail	Download
TCGA vs. CMap	BRCA	BT20	erlotinib	100 nM	24 h	498	528	5.529	Detail	Download
TCGA vs. CMap	BRCA	BT20	erlotinib	500 nM	24 h	783	1041	4.409	Detail	Download
TCGA vs. CMap	BRCA	BT20	erlotinib	10 µM	24 h	759	744	3.353	Detail	Download
TCGA vs. CMap	BRCA	BT20	erlotinib	1 µM	24 h	615	902	6.193	Detail	Download
TCGA vs. CMap	BRCA	BT20	erlotinib	100 nM	6 h	813	1011	3.972	Detail	Download
TCGA vs. CMap	BRCA	BT20	erlotinib	500 nM	6 h	749	764	3.536	Detail	Download
TCGA vs. CMap	BRCA	BT20	erlotinib	10 µM	6 h	963	1111	3.111	Detail	Download
TCGA vs. CMap	BRCA	BT20	erlotinib	1 µM	6 h	727	960	4.717	Detail	Download

Showing 1 to 10 of 144 entries First Previous Next Last

(2) Selection of Mutation Gene

For each cancer type, we provide a gene list in which each gene has at least 5% mutation rate in cancer samples of TCGA. Users could know the differences of drug response by patients with vs. without a specific mutation. After selecting cancer type, specific mutation gene, cell line, compound, dosage, time and datasets data orderly, it will list both the reversed effect and adverse effect of this drug on cancer patients with vs. without the mutation. Also User could download through 3 ways.

Personalized Medicine

This is a patient-centric module with three options for medicine recommendation.

In Datasets, "subTCGA vs. CMap (all mutation)" is short for mutation pattern matched TCGA vs. CMap, and "subTCGA vs. CMap (specific mutation)" is short for mutation pattern matched TCGA vs. CMap (cell line specific mutation).

Enter Patient Matched Cell Line Selection of Mutation Gene Upload Specific Patient Data

Select key mutation gene.

Choose a Cancer: BRCA Choose a Gene: CRCCCP2 Choose a Cell Line: HS578T

Choose a Compound: ALW-3-38-3 Choose a Dosage: 10 µM Choose a Time: 24 h

Choose Datasets: TCGA vs. CMap Submit

Sample Group	Effect Type	Effect Result																																	
With mutation	Reversed	<p>Show <input type="text" value="10"/> entries Search: <input type="text"/></p> <p style="text-align: right;">CSV Excel PDF</p> <table border="1"> <thead> <tr> <th>Gene</th> <th>Fold change of cancer samples vs. normal samples</th> <th>Fold change of compound treated vs. DMSO treated cell lines</th> </tr> </thead> <tbody> <tr><td>ABAT</td><td>up_2.644</td><td>down_-6.687</td></tr> <tr><td>ABCA1</td><td>down_-2.536</td><td>up_3.517</td></tr> <tr><td>ABCA12</td><td>up_3.363</td><td>down_-6.087</td></tr> <tr><td>ABCC6</td><td>down_-3.365</td><td>up_3.044</td></tr> <tr><td>ABUM3</td><td>down_-2.984</td><td>up_3.096</td></tr> <tr><td>ACAN</td><td>up_5.308</td><td>down_-6.787</td></tr> <tr><td>ACD1</td><td>down_-4.095</td><td>up_11.046</td></tr> <tr><td>ACSL4</td><td>down_-2.511</td><td>up_5.076</td></tr> <tr><td>ACSL6</td><td>up_2.1</td><td>down_-4.111</td></tr> <tr><td>ACTL8</td><td>up_80.75</td><td>down_-7.217</td></tr> </tbody> </table> <p>Showing 1 to 10 of 766 entries Previous <input type="text" value="1"/> 2 3 4 5 ... 77 Next</p>	Gene	Fold change of cancer samples vs. normal samples	Fold change of compound treated vs. DMSO treated cell lines	ABAT	up_2.644	down_-6.687	ABCA1	down_-2.536	up_3.517	ABCA12	up_3.363	down_-6.087	ABCC6	down_-3.365	up_3.044	ABUM3	down_-2.984	up_3.096	ACAN	up_5.308	down_-6.787	ACD1	down_-4.095	up_11.046	ACSL4	down_-2.511	up_5.076	ACSL6	up_2.1	down_-4.111	ACTL8	up_80.75	down_-7.217
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(3) Upload Specific Patient Data

Furthermore, user could also upload their own files about gene mutation profile of cancer sample for analysis. We provide an example file. After selecting this file, choosing the cancer type and then clicking uploading, the best matched cell line will be shown, following with the response that all the compounds on this cell line.

Personalized Medicine

This is a patient-centric module with three options for medicine recommendation.

In Datasets, "subTCGA vs. CMap (all mutation)" is short for mutation pattern matched TCGA vs. CMap, and "subTCGA vs. CMap (specific mutation)" is short for mutation pattern matched TCGA vs. CMap (cell line specific mutation).

Enter Patient Matched Cell Line Selection of Mutation Gene **Upload Specific Patient Data**

Upload users' file (official symbols of genes having mutations).

Select File to Upload: 未选择任何文件 [Example file\(click to view\)](#)

Choose cancer type: BRCA Filter by: Special mutation gene

SKBR3

Filter by compounds: Filter Show 10 entries

Compound	Dosage	Time	Number of Reversed Gene	Number of Adverse Gene	RADE		
GSK-429286A	100 nM	24 h	476	796	9.843	Detail	Download
GSK-429286A	500 nM	24 h	651	681	4.502	Detail	Download
GSK-429286A	10 μM	24 h	596	865	6.823	Detail	Download
GSK-429286A	1 μM	24 h	644	751	5.073	Detail	Download
KIN001-127	100 nM	24 h	743	1022	5.187	Detail	Download
KIN001-127	500 nM	24 h	827	1103	4.518	Detail	Download
KIN001-127	10 μM	24 h	623	698	5.039	Detail	Download
KIN001-127	1 μM	24 h	700	870	4.974	Detail	Download
WYE-125132	100 nM	24 h	916	999	3.336	Detail	Download
WYE-125132	500 nM	24 h	1066	1409	3.474	Detail	Download

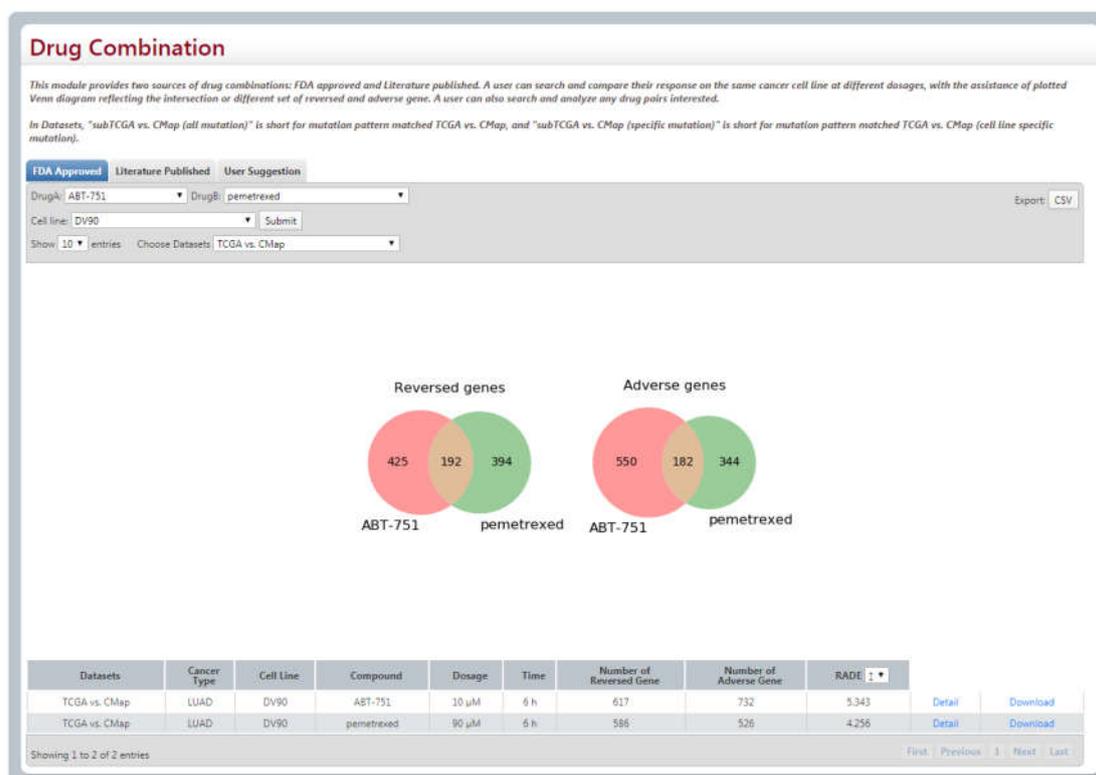
Showing 1 to 10 of 1393 entries [First](#) [Previous](#) [Next](#) [Last](#)

3 Drug combination

In this module, three options are available.

(1) 397 FDA approved drug pairs

When you select Drug A, Drug B and cell line, Two Venn Plots are provided to give the information about the intersection and different set of reserved genes and adverse genes that these two drugs affect, respectively. Besides, the detailed information are also shown as following.



(2) Literature Published. Similar with (1).

(3) User Suggestion. User could search their interested drug pairs (in the download page, user could download all the compound we used in the database) for analysis.

4 Download

User could download all the files and documents we used in DBPOM.

Download

This module allows access to all the reversed and adverse effects of 19,406 small molecular compounds and drugs and 509 drug combinations on the 12310 genes of cancer patients across 5 cancer types based on 28 kinds of cell lines and 3076 cancer samples.
Moreover, all the documents used in the database, like all the compounds, key pathways, drug combination and so on, are available for download.

We also provide detailed field descriptions for each download file.

TCGA vs. CMap : Cell Line	BRCA-BT20 COAD-SW480 COAD-MDST8 COAD-LOVO LHC-HEPG2 LUAD-NCH2073	BRCA-MDAMB231 COAD-NCH508 COAD-SNU1040 COAD-SW948 LUAD-SKLU1 PRAD-VCAP	BRCA-HS578T COAD-HTL15 COAD-RKO COAD-HT29 LUAD-NCH596 PRAD-PC3	BRCA-SKBR3 COAD-SNUC5 COAD-SW620 COAD-CL34 LUAD-DV90	BRCA-MCF7 COAD-SNUC4 COAD-HCT116 LHC-HUH7 LUAD-A549
Specific-mutation-gene subTCGA vs. CMap : Cell Line	BRCA-BT20 COAD-SW480 COAD-MDSTE COAD-LOVO LHC-HEPG2 LUAD-NCH2073	BRCA-MDAMB231 COAD-NCH508 COAD-SNU1040 COAD-SW948 LUAD-SKLU1 PRAD-VCAP	BRCA-HS578T COAD-HTL15 COAD-RKO COAD-HT29 LUAD-NCH596 PRAD-PC3	BRCA-SKBR3 COAD-SNUC5 COAD-SW620 COAD-CL34 LUAD-DV90	BRCA-MCF7 COAD-SNUC4 COAD-HCT116 LHC-HUH7 LUAD-A549
All-mutation-gene subTCGA vs. CMap : Cell Line	BRCA-BT20 COAD-SW480 COAD-HT29 LUAD-NCH596 PRAD-PC3	BRCA-MDAMB231 COAD-NCH508 COAD-CL34 LUAD-DV90	BRCA-HS578T COAD-MDST8 LHC-HUH7 LUAD-A549	BRCA-SKBR3 COAD-SW948 LHC-HEPG2 LUAD-NCH2073	BRCA-MCF7 COAD-SW620 LUAD-SKLU1 PRAD-VCAP
Description of RADB Supplement files	Database_Description 12310 gene symbols collected from CMap Detail information of cell lines in DBPOM 19406 compounds in DBPOM FDA approved and Text mining validated drug combinations for cancer in DBPOM 1882 biological processes and pathways used in DBPOM 11 key pathways (cell proliferation, cell death, etc.) used in DBPOM Mutation profile of TCGA cancer samples used in DBPOM Mutation genes of each cell line Specific mutation genes of each cell line				