



CancerDR Manual

Developed at Dr. G.P.S. Raghava Group

CONTENTS

Introduction.....	3
1. Search Tool.....	4
1.1 Drug Targets.....	4
1.2 Cell Lines.....	4
1.3 Drugs.....	5
1.4 Structure.....	5
3. Browse Tool.....	7
2.1 Major Fields.....	7
2.2 Drug Targets.....	9
2.3 Cell Line.....	9
2.4 Drugs.....	9
3. Alignment/Mutation.....	11
3.1 Total Align.....	11
3.2 Custom Align.....	13
3.3 Mutants.....	15
3.4 Structure Alignment.....	15
4. Target Structure.....	17
4.1 Tertiary.....	17
4.2 Secondary.....	21
4.3 Compare.....	21
4.4 User Sequence.....	22

4.5 Structures in PDB.....	22
5. Map/Alignment.....	24
5.1 Short Reads.....	24
5.2 Contigs.....	27
5.3 Genes.....	28
6. Clustering Tool.....	30
6.1 Drug Targets.....	30
6.2 Cell Lines.....	32
6.3 Drugs.....	35
7. Downloads.....	37
7.1 Sequences.....	37
7.2 Alignments.....	38
7.3 Structures.....	39
7.4 PDB structures.....	39

Introduction

CancerDR is the compilation of mutation data and pharmacological drug profiles from Catalogue Of Somatic Mutations (COSMIC) and Cancer Cell Line Encyclopedia (CCLE). In COSMIC, 138 anticancer drugs targeting a wide range of therapeutic targets were screened on 275-507 cell lines and in case of CCLE, 24 anticancer drugs were screened on more than 500 cell lines. We have compiled both of these data on a single platform in user-friendly format to make out some useful conclusions on cancer drug resistance. Methods of drug screening on cancer cell lines are available on COSMIC and CCLE websites respectively. We obtained the mutational status of 116 unique drug targets in cell lines from the parallel sequencing data available at CCLE website. Then we tried to correlate the mutation status of targets with IC50 values of the drugs. Along with this, we have been predicted the structures of these therapeutic targets. To correlate the effect of mutation on target structure, we predicted the tertiary structures of all mutants reported in CCLE for 116 drug targets. In addition to this, structural alignments of wild type drug targets with their mutants are generated and covered in the CancerDR. For sequence alignment purpose, all the given mutations were mapped on the target sequence. Then alignment of wild type and their mutants were generated. These sequences can also be used for the alignment of short reads to find out the mutations in a given target gene. After sequence alignment, we generated the phylogenetic trees of mutants to show the distance between them. We also tried to cluster the cell lines on the basis of IC50 values of anticancer drugs assayed on them. This will help to identify the most sensitive or most resistant cell lines for a particular drug. Similarly, we cluster the drugs to identify which drug is most effective or less effective on a particular cell line.

This manual will help users to understand the tools integrated in the CancerDR for their efficient use.

Note: Most of the CancerDR tool requires Java. So, make sure that Java is installed on your system.

1. Search Tool

Search tool is divided into four parts:

1.1 Drug Targets: CancerDR contains the information about 116 anticancer drug targets. For the efficient retrieval of this information, we have integrated this tool. If user wants the information about some drug target e.g. AKT1, just type AKT1 in the input box and click search button at the bottom of the page. This will return only that information, which is checked by the user in their corresponding check box. User can check, CHECK ALL button to display all the information (Figure 1).

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Home General Information Mutation Acknowledgement Guide Links Team Contact

Search
Browse
Alignment/Mutation
Target Structure
Map/Alignment
Clusters/Groups
Downloads

Go to Search Menu and select Drug Target

Enter Query

Enter the Target name

Select Fields to be Searched:
☒ Target (eg.)
☒ cDNA Mutation (eg.)
☐ Codon Mutation (eg.)
☐ Protein Mutation (eg.)

Select Fields to be Displayed:
☒ Target
☐ cDNA Mutation
☐ Target Structure
☐ DIP
☐ Number of wild type cells
☒ Codon Mutation
☐ MINT
☐ Reactome
☐ Number of Mutated cells
☐ Protein Mutation
☐ String
☐ QuickGO
☐ CHECK ALL

Submit Clear Data

Displayed all the field selected by the user

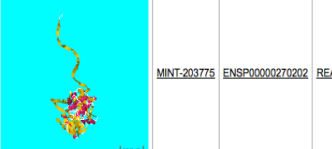
Drug Targets	Wild type CLs	Mutated CLs	cDNA Mutation	Codon Mutation	Protein Mutation	Target Structure	MINT	STRING	REACTOME	DIP	GO
AKT1	874	33	c.145G>A, c.175C>T, c.49G>A, c.745C>T, c.797C>T, c.7G>A,	c.(145-147)GAG>AAG, c.(175-177)CAG>TAG, c.(49-51)GAG>AAG, c.(745-747)CGG>TGG, c.(796-798)TCG>TTG, c.(7-9)GAC>AAC,	p.E49K, p.Q59*, p.E17K, p.R249W, p.S266L, p.D3N,		MINT:203775	ENSP00000270202	REACT_111045	DIP:24269N	P31749

Figure 1. Drug target Search tool showing the result of searching AKT1 as drug target.

1.2 Cell Lines: User can use this tool to find out the information about any of the cell line available in CancerDR. Type the cell line name in input box (e.g. A498) and click submit button. It will return the information like tissue type and number of drugs tried against

that cell line with their respective IC₅₀ (μM) values (Figure 2).

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Home General Submission Acknowledgement Guide Links Team Contact

Search
Browse
Alignment/Mutation
Target Structure
Map/Alignment
Clusters/Groups
Downloads

Go to Search Menu and select Cell Line

Cell Lines Search in CancerDR

This page is designed to help you search for a specific query in CancerDR. This page allows user to search in any/all field of Cell Lines in CancerDR, their genes and mutations with target sequences. Page also allows to DISPLAY selected/all corresponding fields. For more information, please click [HERE](#).

Search Options

Enter Query

Select Fields to be Searched:

☒ Cell line (eg.) ☐ Tissue Type (eg.)

Select Fields to be Displayed:

☒ Cell line ☒ Tissue type ☐ CHECK ALL ☒ Number of drugs tried ☐ Number of targets

Result

Cell Line	Tissue Type	No of drugs tried
A498	KIDNEY	132

Click to see the no. of drug tried

Drug	Cell Line	Tissue Type	IC ₅₀ (μM)	Source
17AAG	A498	KIDNEY	0.10	COSMIC
681640	A498	KIDNEY	58.16	COSMIC
A443654	A498	KIDNEY	67.18	COSMIC
A770041	A498	KIDNEY	237.12	COSMIC
ABT263	A498	KIDNEY	179.45	COSMIC
ABT888	A498	KIDNEY	338.45	COSMIC
AG014699	A498	KIDNEY	191.39	COSMIC
AlCAR	A498	KIDNEY	15351.95	COSMIC
AKTInhibitor/VIII	A498	KIDNEY	1.08	COSMIC

Figure 2. Cell line search tool showing the search of A498 cell line.

1.3 Drugs: 148 drugs available in the CancerDR can be explored by the drugs search tool. Type the drug name user wish to search e.g. ABT888 and click submit button after checking the box user wants to display. This tool can obtain information like drug target(s), H-bond donor, H-bond acceptor, molecular weight and structure of the drug (Figure 3).

1.4 Structure: If user wishes to search some drug on the basis of structure or wants to find some drug similar to a given molecule, this tool can help in that case. User either has to draw the structure by using JME editor or can upload a MOL/SDF/SMILE file of test molecule and click submit button. It will return all the molecules from CancerDR, which has same structure like test molecule (Figure 4).

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Home General Search Alignment Acknowledgement Guide Links Team Contact

Search
Browse
Alignment/Mutation
Target Structure
Map/Alignment
Clusters/Groups
Downloads

Go to Search Menu and select Drug

Search in CancerDR

Enter Query **ABT888**

Enter the Drug name

Displayed all the field selected by the user


Select Fields to be Searched:

☒ Drug (eg. **ABT888**) ☒ Drug targets (eg. **PARP1**) ☒ H-bond donor ☒ H-bond acceptor (eg. **1**) ☒ Molecular weight (eg. **2**)

Select Fields to be Displayed:

☒ Number of targets ☒ Structure ☒ Molecular weight ☒ H-bond donor ☒ H-bond acceptor ☒ CHECK ALL

Search Clear Data

Drug	Pubchem ID	Targets	No of Targets	Chemical Formula	Mol Weight	Polarizability	pI	Volume	HBA	HBD	Structure
ABT888	11960529	PARP1, PARP2	2	C13H16N4O	244.2923	26.57	9.72	220.62	3	3	

1/1 50

Figure 3. Drug search tool showing the search of ABT888 anticancer drug.

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Home General Search Alignment Acknowledgement Guide Links Team Contact

Search
Browse
Alignment/Mutation
Target Structure
Map/Alignment
Clusters/Groups
Downloads

Go to Search Menu and select Structure

Upload Smile/Mol or SDF Format

Drug with similar structure

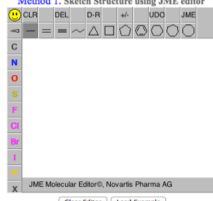
CancerDR search molecule Form

CancerDR allow to find similar molecules. You may submit a single molecules using any of the 3 methods. Please only one method at a time.

- Sketch using JME editor.
- Paste molecules in the box.
- Upload file containing molecules in standard format.

Please select type of search: ☒ Substructure Search ☐ Exact Search ☐ Exact Fragment search ☐ Superstructure Search

Method 1. Sketch Structure using JME editor



Method 2. Paste structure in Mol/SMILE/SDF format (use an example)

Method 3. Upload File :

Select the input format (If used Method 2 or 3)
☐ MOL ☒ SMILE ☐ SDF

RUN CLEAR

Compound Molecule ID	Pubchem ID	Targets	Molecular Formula
B1BW2992	44569596	EGFR, ERBB2	C25H26ClFN4O3

1/1 50

Figure 4. Structure search tool for similarity search of drugs.

2. Browse Tool

Browse tool divided into four parts

2.1 Major Fields: This tool is integrated to explore the database on the basis of fields like tissue type, target class and mutated targets. User can know how many cell lines are belonging to which particular tissue type and how many drugs are tried on each of these cell lines with their respective IC50 (μM) values (Figure 5a).

The screenshot shows the CancerDR website interface. The header includes the database name and the institute. The navigation menu has options like Home, General, Information, Submission, Acknowledgement, Guide, Links, Team, and Contact. A 'Browse' button is highlighted with a callout: 'Go to Browse Menu and select Major Fields'. Below the navigation menu, there is a section titled 'Go To Browse by Drug Target Class'. A callout points to a table titled 'Browse by Tissue Type' with the following data:

Tissue type	Cell lines
AUTONOMIC GLANDIA	10
BILIARY TRACT	1
BLADDER	18
BLOOD	113
BONE	37
BREAST	51
CENTRAL NERVOUS SYSTEM	88
ENDOMETRIUM	20

A callout points to this table: 'Table with Tissue Types'. An arrow points from this table to a 'Result' table, with a callout: 'Click to see the cell lines of each Tissue Type'. The 'Result' table has the following data:

Drug	Cell Line	Tissue	IC50 (μM)	Source
17AAG	CHP212	AUTONOMIC GLANDIA	0.029792815	CCLE
17AAG	IMR32	AUTONOMIC GLANDIA	1.724061966	CCLE
17AAG	KELLY	AUTONOMIC GLANDIA	2.224541187	CCLE
17AAG	KPNSI9S	AUTONOMIC GLANDIA	0.082642227	CCLE
17AAG	SIMA	AUTONOMIC GLANDIA	1.778700352	CCLE
17AAG	SKNAS	AUTONOMIC GLANDIA	0.385245234	CCLE
17AAG	SKNBE2	AUTONOMIC GLANDIA	1.170010686	CCLE

Figure 5a. Tissue types browse option in CancerDR to browse data according to the tissue types.

User can know how many drugs hitting which target or pathway and on how many cell lines that drug was tried with their respective IC50 (μM) values (Figure 5b). Along with this, user can know how many mutants are present for a particular target and which cell line has which mutants. Further they can also get the drug sensitivity information of a particular drug on particular cell line, which can help in relating the effect of mutations on drug sensitivity (Figure 5c).

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[Home](#) [General](#) [Information](#) [Submission](#) [Acknowledgement](#) [Guide](#) [Links](#) [Team](#) [Contact](#)

Search >
Browse >
Alignment/Mutation >
Target Structure >
Map/Alignment >
Clusters/Groups >
Downloads >

Fields browse in CancerDR

This page allow user to browse the drug targets according to the therapeutic class of the drug targets. For more information, click [HERE](#).

Go To Browse by Tissue type

Go To Browse by Target Mutants

Table with Target Class

Target Class ^	Number of drugs ^
Apoptosis	22
Cell cycle	16
Chromatin	3
Cytoskeleton	5
DNA repair	19

Click to see the drugs in each class

Drug ^	Target Class ^
ABT263	Apoptosis
AEW541	Apoptosis
AUY922	Apoptosis
AZD6482	Apoptosis
BMS536924	Apoptosis
Bryostatins	Angiogenesis, Apoptosis
Embelin	Apoptosis
GDC0941	Apoptosis
JNJ26854165	Apoptosis
L685458	Cell cycle, Apoptosis
LBW242	Apoptosis
MG132	Apoptosis
Nutlin3	Apoptosis

Figure 5b. Browse according to the drug target class.

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[Home](#) [General](#) [Information](#) [Submission](#) [Acknowledgement](#) [Guide](#) [Links](#) [Team](#) [Contact](#)

Search >
Browse >
Alignment/Mutation >
Target Structure >
Map/Alignment >
Clusters/Groups >
Downloads >

Fields browse in CancerDR

This page allow user to browse the drug targets according to the mutants of target proteins. For more information, click [HERE](#).

Go To Browse by Drug Target Class

Go To Browse by Tissue type

Table with Mutants

Gene ^	No. of Mutations ^
ABL1	24
ABL2	5
AKT1	7
AKT2	5
AKT3	8

Click to see the type of mutants for each target

Mutants of target [ABL1](#) and drug assayed

Cell Line ^	cDNA Mutation ^	Codon Mutation ^	Protein Mutation ^	Drug assayed ^	IC50 (μM) ^	Source ^
639V	c.700T>C	c.(700-702)TAT>CAT	p.Y234H	AZD0530	8	CCLE
639V	c.700T>C	c.(700-702)TAT>CAT	p.Y234H	Nilotinib	8	CCLE
639V	c.700T>C	c.(700-702)TAT>CAT	p.Y234H	AP24534	2.45	COSMIC
639V	c.700T>C	c.(700-702)TAT>CAT	p.Y234H	Bosutinib	98.34	COSMIC
639V	c.700T>C	c.(700-702)TAT>CAT	p.Y234H	Nilotinib	97.2	COSMIC
A253	c.1823G>A	c.(1822-1824)CGC>CAC	p.R608H	AZD0530	8	CCLE
A253	c.1823G>A	c.(1822-1824)CGC>CAC	p.R608H	Nilotinib	8	CCLE

Figure 5c. Browsing on the basis of types of mutations present in drug targets.

2.2 Drug Targets: Drug target browsing facilitates the user to get the comprehensive information of drug targets such as links for mutations, protein-protein interactions, pathway interactions, gene ontologies, genome browser, phylogenetic tree, chromosomal position and number of cell lines with mutated drug targets. All the databases are linked to a single window for gathering fast information about a drug target (Figure 6).

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Home | General | Information | Acknowledgement | Guide | Links | Team | Contact

Search >
Browse >
Alignment/Mutation >
Target Structure >
Map/Alignment >
Clusters/Groups >
Downloads >

Go to Browse Menu and select Drug Targets

No. of Mutated cell lines for particular target

Drug Target	Refseq ID	COSMIC	MINT	STRING	DIP	Reactome	QuickGO	NCBI Genome Browser	Ensembl Genome Browser	Gene Atlas	Tree Families	Mutated Cell Lines
ABL1	NP_006097	ABL1	MINT-57668	P08519	QIP-1042N	REACT_111045	P08519	NM_007313	ENSP0000023315	ABL1	ABL1	38
ABL2	NP_006298	ABL2	MINT-1347081	P49984	QIP-81N	REACT_111046	P49984	NM_007314	ENSP0000023929	ABL2	ABL2	187
AKT1	NP_006154	AKT1	MINT-203775	P31749	QIP-24289N	REACT_111045	P31749	NM_005183	ENSP0000027002	AKT1	AKT1	33
AKT2	NP_006167	AKT2	MINT-87790	P31751	NA	REACT_111045	P31751	NM_005182	ENSP0000027582	AKT2	AKT2	21
AKT3	NP_006456	AKT3	MINT-222821	Q9Y243	NA	REACT_111045	Q9Y243	NM_005465	ENSP0000026382	AKT3	AKT3	24
ALK	NP_004295	ALK	NA	Q9UM73	NA	NA	Q9UM73	NM_004304	ENSP0000027200	ALK	ALK	70
AR	NP_000035	AR	MINT-54801	P10275	QIP-125N	REACT_71	P10275	NM_000064	ENSP0000026382	AR	AR	82
ATM	NP_000042	ATM	MINT-184471	Q13315	QIP-182N	REACT_111183	Q13315	NM_000061	ENSP0000027816	ATM	ATM	144
AURKA	NP_000035	AURKA	NA	Q14965	QIP-33068N	REACT_111556	Q14965	NM_198433	ENSP0000021591	AURKA	AURKA	22
AURKB	MINT-141297	AURKB	Q96G04	QIP-34530N	REACT_111556	Q96G04	NM_004217	ENSP0000021380	ENSP0000021380	AURKB	AURKB	11
AURKC	NA	AURKC	Q9UGB9	NA	NA	NA	Q9UGB9	NM_001015878	ENSP0000020288	AURKC	AURKC	290
BCL2	MINT-87089	BCL2	P10415	QIP-1043N	REACT_578	P10415	NM_000833	ENSP0000022953	ENSP0000022953	BCL2	BCL2	18
BIM	MINT-143204	BIM	P31813	NA	REACT_578	P31813	NM_203081	ENSP0000024082	ENSP0000024082	BIM	BIM	48
BRAF	MINT-110643	BRAF	Q08182	QIP-34071N	REACT_5900	Q08182	NM_000061	ENSP0000028662	ENSP0000028662	BRAF	BRAF	118
CDK2	MINT-147180	CDK2	P42674	QIP-266N	REACT_111102	P42674	NM_004346	ENSP0000021102	ENSP0000021102	CDK2	CDK2	30

Select any of the field to open the respective links

Drug	Cell Line	Tissue Type	IC50(μM)	Source
17AAG	639V	URINARY TRACT	0.150094494	CCLE
17AAG	639V	BLADDER	0.15	COSMIC
681640	639V	BLADDER	5.38	COSMIC
ABT263	639V	BLADDER	51.54	COSMIC
ABT888	639V	BLADDER	325.64	COSMIC
AEW541	639V	URINARY TRACT	1.736181378	CCLE
AGO14699	639V	BLADDER	319.47	COSMIC

Drug Profiling on 639V Cell line

Cell Lines
639V
A253
BCP1
CA46

Figure 6. Screen shots showing the usage of drug targets tool in browse menu.

2.3 Cell Line: Here user can browse according to cell lines. This browsing option enables the user to look at the number of drugs and their targets along with the information regarding the histology of the cell lines (Figure 7).

2.4 Drugs: This tool enables the user to get as much as information about the drugs on a single window with their structures. With this option, the user can look at different

descriptors of drugs like pI, Volume, Hydrogen Bond Acceptor, Hydrogen Bond Donor, Structure link, molecular target, along with other chemical properties and structures of drugs (Figure 8).

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Home General Information Submission Acknowledgement Guide Links Team Contact

Search >
Browse >
Alignment/Mutation >
Target Structure >
Map/Alignment >
Clusters/Groups >
Downloads >

Line browse in CancerDR

This page summarizes the Primary site, Histology, and Number of Targets in different Cell Lines. For more information, please click [HERE](#).

Cell Line	Tissue Type	CCL/CCOSMIC Link	Number of drugs Tried	No. of Targets
1321N1	CENTRAL NERVOUS SYSTEM	1321N1	21	34
22RV1	PROSTATE	22RV1	122	195
22RV1	PROSTATE	22RV1	24	38
2313287	GI TRACT	2313287	78	125
42MGBA	CENTRAL NERVOUS SYSTEM	42MGBA	20	32
5637	BLADDER	5637		
5637	URINARY TRACT	5637		
639V	BLADDER	639V		
639V	URINARY TRACT	639V		
647V	BLADDER	647V		
697	BLOOD	697		
697	HAEEMATOPNETIC AND LYMPHOID TISSUE	697		

Result

Drug	Cell Line	Tissue Type	IC50(μM)	Source
17AAG	2313287	GI TRACT	0.07	COSMIC
ABT888	2313287	GI TRACT	339.84	COSMIC
AG014699	2313287	GI TRACT	18.27	COSMIC
AICAR	2313287	GI TRACT	2764.86	COSMIC
AKTInhibitorVIII	2313287	GI TRACT	0.76	COSMIC
AP24534	2313287	GI TRACT	40.81	COSMIC
AS601245	2313287	GI TRACT	7.06	COSMIC
ATRA	2313287	GI TRACT	40.09	COSMIC

Go to Browse Menu and select Cell lines

No. of Drugs Tried on each cell line

Information and useful link about each cell line

Figure 7. Browse cell lines option.





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CSIR - Institute of Microbial Technology, India

Home General Information Submission Acknowledgement Guide Links Team Contact

Search >
Browse >
Alignment/Mutation >
Target Structure >
Map/Alignment >
Clusters/Groups >
Downloads >

Drug browse in CancerDR

This page summarizes the Drugs with different descriptors like pI, Volume, HBA, HBD, and Molecular Targets. For more information, please click [HERE](#).

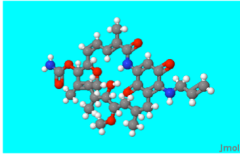
Drug Name	Pubchem ID	Molecular Targets	Number of Targets	Chemical Formula	Molecular Weight	Polarizability	pI	Volume	HBA	HBD	Structure
17AAG	6505803	HSP90	1	C31H43N3O8	585.6884	61.68	5.85	550.26	8	4	
661640	10384972	WEE1, CHK1	2	C20H11CN2O3	362.766	36.39		282.6	3	3	
64	10172843	AKT1, AKT2, AKT3	3	C24H23N5O	397.4723	44.62	11.61	356.81	4	3	
69602	11360381	AMPKagonist	1	C20H12N2O3S	360.386	36.58		294.79	5	3	

Go to Browse Menu and select Drugs

Drug Structure

Information and useful link about each Drug

3D Structure of 17AAG



be opened below the list of the mutants of ABL2. Upper part of the main window shows the multiple sequence alignment, which can be presented by number of ways using menu bar options. Base of this window contains a button, upon clicking which opens a popup window displaying more intuitive sequence alignment with Coverage, Consensus and Quality information of alignment (Figure 10).



Figure 10. Multiple sequence alignment display.

Each mutant in that uppermost list is clickable which opens into next page having link of Jalview button. Upon clicking this button, two popup windows open: one showing the sequence alignment of ABL2 with its mutants (including the selected one) and second window shows the predicted structure of selected mutant for comparison with the multiple sequence alignment in the first window. Moving the cursor over the structure shows the corresponding sequence alignment portion in the other window. Jalview gives

the users different options to highlight the desired regions in the alignment through the menu bar (Figure 11).

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Total Align page of CancerDR

This page is designed to view multiple sequence alignments of Wild type Targets with the Mutants and Natural Variants. It helps user to view variable regions in the sequences among mutants and respective targets in CancerDR. Click "Start Jalview" button to compare structure of Mutant with wild type and its mutants' sequences.

Click on button to compare V.A183T with complete sequence alignment

Jalview window showing sequence alignment of ABL2 with its mutants

Predicted structure of V.A183T mutant of ABL2

Figure 11. Multiple sequence alignment with structure of mutant.

3.2 Custom align: This module allows users to perform multiple sequence alignment of selected sequences of mutants of a drug target. This option also allows users to align their own sequence against any selected mutant's sequence of a drug target. Further, mutants are sorted based upon the increasing IC₅₀ values for a given drug at a given time and then can be selected for the alignment (Figure 12).

For instance, by clicking on AKT2, we get three drugs, which have been tested, on these targets (A443654, AKT inhibitor and MK2206). By selecting A443654 and submitting, we get three hits (*i.e.* for target AKT2 using drug A443654 three cell lines have been reported with three different kind of mutations and IC₅₀ values). Now, we can select any two mutants or one mutant and user defined/provided sequence. After selecting

any two hits and clicking on Align button, Jalview window opens, which shows the alignment of selected mutants in the interactive way (as described in the previous section). This module is useful to select mutants based upon IC50 values and compares their sequences interactively (Figure 13, 14).

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Home General Information Submission Acknowledgement Guide Links Team Contact

Search
Browse
Alignment/Mutation
Target Structure
Map/Alignment
Clusters/Groups
Downloads

Align selected target sequences

This module allows users to perform multiple sequence alignment of selected sequences of a drug target. This option also allows users to align their own sequence against selected sequence of a drug target. Further, mutants can be sorted based upon the ic50 values for a given drug at a given time and then can be selected for the alignment. For more information, please click [Help](#)

Select any one of the Targets

<input type="checkbox"/> ABL1	<input type="checkbox"/> ABL2	<input type="checkbox"/> AKT1	<input type="checkbox"/> AKT2	<input type="checkbox"/> AKT3	<input type="checkbox"/> ALK	<input type="checkbox"/> AR	<input type="checkbox"/> ATM	<input type="checkbox"/> AURKA	<input type="checkbox"/> AURKB
<input type="checkbox"/> AURKC	<input type="checkbox"/> BCL2	<input type="checkbox"/> BMX	<input type="checkbox"/> BRAF	<input type="checkbox"/> BTK	<input type="checkbox"/> CASP3	<input type="checkbox"/> CCR5	<input type="checkbox"/> CDK1	<input type="checkbox"/> CDK2	<input type="checkbox"/> CDK4
<input type="checkbox"/> CDK6	<input type="checkbox"/> CDK7	<input type="checkbox"/> CTNNB1	<input type="checkbox"/> DHFR	<input type="checkbox"/> EGFR	<input type="checkbox"/> ERBB2	<input type="checkbox"/> FGFR1	<input type="checkbox"/> FGFR3	<input type="checkbox"/> FLT1	<input type="checkbox"/> FLT3
<input type="checkbox"/> FNTA	<input type="checkbox"/> GSK3A	<input type="checkbox"/> GSK3B	<input type="checkbox"/> HDAC1	<input type="checkbox"/> HDAC2	<input type="checkbox"/> HDAC3	<input type="checkbox"/> HDAC6	<input type="checkbox"/> HDAC8	<input type="checkbox"/> HSP90AA1	<input type="checkbox"/> HSP90AB1
<input type="checkbox"/> HSP90AB4P	<input type="checkbox"/> HSP90B1	<input type="checkbox"/> HSP90B3P	<input type="checkbox"/> IGF1R	<input type="checkbox"/> IKKBE	<input type="checkbox"/> ITK	<input type="checkbox"/> JAK2	<input type="checkbox"/> KDR	<input type="checkbox"/> KIT	<input type="checkbox"/> MAP2K1
<input type="checkbox"/> MAP2K2	<input type="checkbox"/> MAPK11	<input type="checkbox"/> MAPK12	<input type="checkbox"/> MAPK13	<input type="checkbox"/> MAPK14	<input type="checkbox"/> MAPK7	<input type="checkbox"/> MAPK8	<input type="checkbox"/> MCL1	<input type="checkbox"/> MDM2	<input type="checkbox"/> MET
<input type="checkbox"/> MTOR	<input type="checkbox"/> NFKB1	<input type="checkbox"/> NTRK1	<input type="checkbox"/> P4HB	<input type="checkbox"/> PAK1	<input type="checkbox"/> PARP1	<input type="checkbox"/> PDGFRA	<input type="checkbox"/> PDGFRB	<input type="checkbox"/> PDK1	<input type="checkbox"/> PIK3CA
<input type="checkbox"/> PIK3CB	<input type="checkbox"/> PIK3CG	<input type="checkbox"/> PLK1	<input type="checkbox"/> PLK2	<input type="checkbox"/> PLK3	<input type="checkbox"/> PPM1D	<input type="checkbox"/> PRKAA1	<input type="checkbox"/> PRKCA	<input type="checkbox"/> PRKCB	<input type="checkbox"/> PRKCD
<input type="checkbox"/> PRKCE	<input type="checkbox"/> PRKCG	<input type="checkbox"/> PRKCH	<input type="checkbox"/> PRKCI	<input type="checkbox"/> PRKCO	<input type="checkbox"/> PRKCSH	<input type="checkbox"/> PRKCZ	<input type="checkbox"/> PRKDC	<input type="checkbox"/> PSENEN	<input type="checkbox"/> RPS6KA1
<input type="checkbox"/> RPS6KA2	<input type="checkbox"/> RPS6KA3	<input type="checkbox"/> RPS6KA4	<input type="checkbox"/> RPS6KA5	<input type="checkbox"/> RPS6KA6	<input type="checkbox"/> RPS6KB2	<input type="checkbox"/> RXRA	<input type="checkbox"/> RXRB	<input type="checkbox"/> SGK3	<input type="checkbox"/> SMO
<input type="checkbox"/> SRC	<input type="checkbox"/> SYK	<input type="checkbox"/> TBC1	<input type="checkbox"/> TEC	<input type="checkbox"/> TNF	<input type="checkbox"/> TOP1	<input type="checkbox"/> WEE1	<input type="checkbox"/> XIAP		

Click on button against the AKT2

Figure 12. Customized sequence alignment.

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Home General Information Submission Acknowledgement Guide Links Team Contact

Align selected target sequences

This module allows users to perform multiple sequence alignment of selected sequences of a drug target. This option also allows users to align their own sequence against selected sequence of a drug target. Further, mutants can be sorted based upon the ic50 values for a given drug at a given time and then can be selected for the alignment. For more information, please click [Help](#)

AKT2

Select Drug against which you want to select mutants for selected Target.

☐ A443654 ☐ AKTInhibiti ☐ MK2206

submit

Upload the sequence you want to align.

Table is sorted based upon decreasing ic50 values

#	Drug	Target	Mutation	Cell Line	ic50
1	A443654	AKT2	p.S130D	CLO668	0.41
2	A443654	AKT2	p.E360A	NCH1694	0.51
3	A443654	AKT2	p.A139V	CW2	143.35

Click button to view alignment for selected sequence

Select any one of the Targets

<input type="checkbox"/> ABL1	<input type="checkbox"/> ABL2	<input type="checkbox"/> AKT1	<input type="checkbox"/> AKT2	<input type="checkbox"/> AKT3	<input type="checkbox"/> ALK	<input type="checkbox"/> AR	<input type="checkbox"/> ATM	<input type="checkbox"/> AURKA	<input type="checkbox"/> AURKB
<input type="checkbox"/> AURKC	<input type="checkbox"/> BCL2	<input type="checkbox"/> BMX	<input type="checkbox"/> BRAF	<input type="checkbox"/> BTK	<input type="checkbox"/> CASP3	<input type="checkbox"/> CCR5	<input type="checkbox"/> CDK1	<input type="checkbox"/> CDK2	<input type="checkbox"/> CDK4
<input type="checkbox"/> CDK6	<input type="checkbox"/> CDK7	<input type="checkbox"/> CTNNB1	<input type="checkbox"/> DHFR	<input type="checkbox"/> EGFR	<input type="checkbox"/> ERBB2	<input type="checkbox"/> FGFR1	<input type="checkbox"/> FGFR3	<input type="checkbox"/> FLT1	<input type="checkbox"/> FLT3
<input type="checkbox"/> FNTA	<input type="checkbox"/> GSK3A	<input type="checkbox"/> GSK3B	<input type="checkbox"/> HDAC1	<input type="checkbox"/> HDAC2	<input type="checkbox"/> HDAC3	<input type="checkbox"/> HDAC6	<input type="checkbox"/> HDAC8	<input type="checkbox"/> HSP90AA1	<input type="checkbox"/> HSP90AB1
<input type="checkbox"/> HSP90AB4P	<input type="checkbox"/> HSP90B1	<input type="checkbox"/> HSP90B3P	<input type="checkbox"/> IGF1R	<input type="checkbox"/> IKKBE	<input type="checkbox"/> ITK	<input type="checkbox"/> JAK2	<input type="checkbox"/> KDR	<input type="checkbox"/> KIT	<input type="checkbox"/> MAP2K1
<input type="checkbox"/> MAP2K2	<input type="checkbox"/> MAPK11	<input type="checkbox"/> MAPK12	<input type="checkbox"/> MAPK13	<input type="checkbox"/> MAPK14	<input type="checkbox"/> MAPK7	<input type="checkbox"/> MAPK8	<input type="checkbox"/> MCL1	<input type="checkbox"/> MDM2	<input type="checkbox"/> MET
<input type="checkbox"/> MTOR	<input type="checkbox"/> NFKB1	<input type="checkbox"/> NTRK1	<input type="checkbox"/> P4HB	<input type="checkbox"/> PAK1	<input type="checkbox"/> PARP1	<input type="checkbox"/> PDGFRA	<input type="checkbox"/> PDGFRB	<input type="checkbox"/> PDK1	<input type="checkbox"/> PIK3CA
<input type="checkbox"/> PIK3CB	<input type="checkbox"/> PIK3CG	<input type="checkbox"/> PLK1	<input type="checkbox"/> PLK2	<input type="checkbox"/> PLK3	<input type="checkbox"/> PPM1D	<input type="checkbox"/> PRKAA1	<input type="checkbox"/> PRKCA	<input type="checkbox"/> PRKCB	<input type="checkbox"/> PRKCD
<input type="checkbox"/> PRKCE	<input type="checkbox"/> PRKCG	<input type="checkbox"/> PRKCH	<input type="checkbox"/> PRKCI	<input type="checkbox"/> PRKCO	<input type="checkbox"/> PRKCSH	<input type="checkbox"/> PRKCZ	<input type="checkbox"/> PRKDC	<input type="checkbox"/> PSENEN	<input type="checkbox"/> RPS6KA1
<input type="checkbox"/> RPS6KA2	<input type="checkbox"/> RPS6KA3	<input type="checkbox"/> RPS6KA4	<input type="checkbox"/> RPS6KA5	<input type="checkbox"/> RPS6KA6	<input type="checkbox"/> RPS6KB2	<input type="checkbox"/> RXRA	<input type="checkbox"/> RXRB	<input type="checkbox"/> SGK3	<input type="checkbox"/> SMO
<input type="checkbox"/> SRC	<input type="checkbox"/> SYK	<input type="checkbox"/> TBC1	<input type="checkbox"/> TEC	<input type="checkbox"/> TNF	<input type="checkbox"/> TOP1	<input type="checkbox"/> WEE1	<input type="checkbox"/> XIAP		

Click to see alignment

Click on button against the A443654 and submit

Drugs tested against AKT2 in different cell lines

Upload own sequence

Check boxes to select any two mutants based on IC50

Mutants sorted according to increasing IC50 values

Figure 13. Customized sequence alignment.

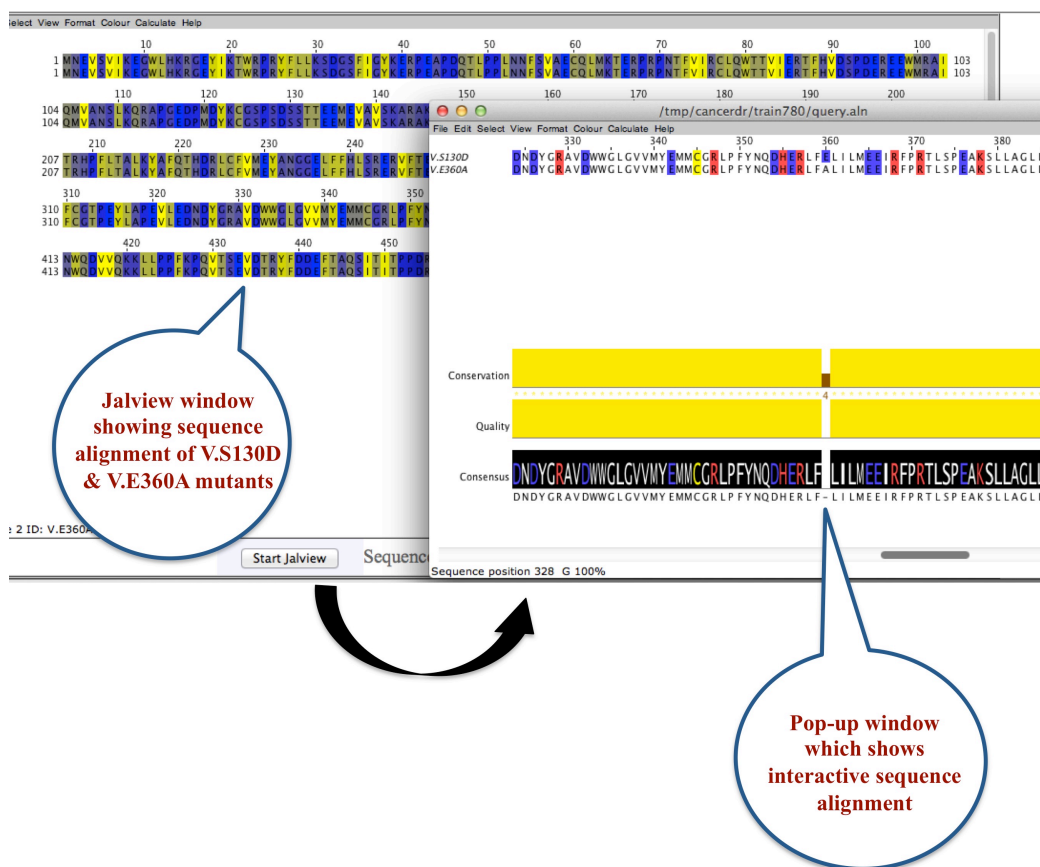


Figure 14. Customized sequence alignment.

3.3 Mutants: This page allows the user to display different types of mutations reported for a drug target at amino acid level, codon level and cDNA level (Figure 15).

3.4 Structure alignment: This module allows users to visualize structure alignment of mutants/variants of a target. User can select mutants by clicking on RED button and natural variants by clicking on BLUE button of a target. Structure sequence alignment (using MUSTANG software) is visible in jmol applet, which is accompanied by the details of the sequences aligned to achieve that alignment. Also download option is given to download the structurally aligned file above the Jmol applet. In few cases, where extremely variable length of sequences is present, a few sequences have been removed to achieve the multiple structure alignment (Figure 16).

**Mutations at
amino acid level,
cDNA level &
Codon level**

Sequence alignment of wild type MAPK12 and its mutants

Figure 16. Structure alignment.

4. Target structure

4.1 Tertiary: Predicted tertiary structure (using HHsuite) of each drug target and their mutants are available through this module. This page is designed to view structures of wild type targets and their mutants. It helps the user to see 3D view in Jmol against selected targets in CancerDR. Also, user can download the selected structure for analysis (Figure 17a,b). This page also shows the reliability score of modelled structure, which include percent coverage, identity with the template and percentage of allowed region in ramachandran plot.

CancerDR: Cancer Drug Resistance Database
CSIR - Institute of Microbial Technology, India

Home | General | Information | Submission | Acknowledgement | Guide | Links | Team | Contact

Tertiary structure of target mutants

We predicted tertiary structure of each drug target and their mutants. This page is designed to view structures of wild type targets and their Mutants. It helps user to see 3D view in Jmol against selected Targets in CancerDR. Note: Java should be enabled in your browser for proper functioning of the this module. For more information, please click [Help](#)

Example

Structure Quality Statistics of CDK6

Query Sequence Length	Mapped query sequence	Query sequence covered	Identity of aligned region	Ramachandran allowed region	Ramachandran map	Template alignment
327	1-326	99.69%	100.00%	88.2%	CDK6	CDK6.hhr

3D-Structure of CDK6

List of Mutants

- VA197S
- VD246E
- VH119Q
- VR168H
- VS57P

CancerDR: Cancer Drug Resistance Database
CSIR - Institute of Microbial Technology, India

Home | General | Information | Submission | Acknowledgement | Guide | Links | Team | Contact

Tertiary structure page of CancerDR

This page is designed to view structures of Wild-type targets with the Mutants. It helps user to see 3D view in Jmol against selected Targets in CancerDR. For more information, please click [Help](#)

Structure Quality Statistics of VA197S

Length	Area Covered	Coverage	Identity	Procheck	Download	Alignment
327	1-326	99.69%	100.00%	88.2%	VA197S.hhr	VA197S.hhr

3D-Structure of VA197S

Figure 17 (a). Tertiary structure information.

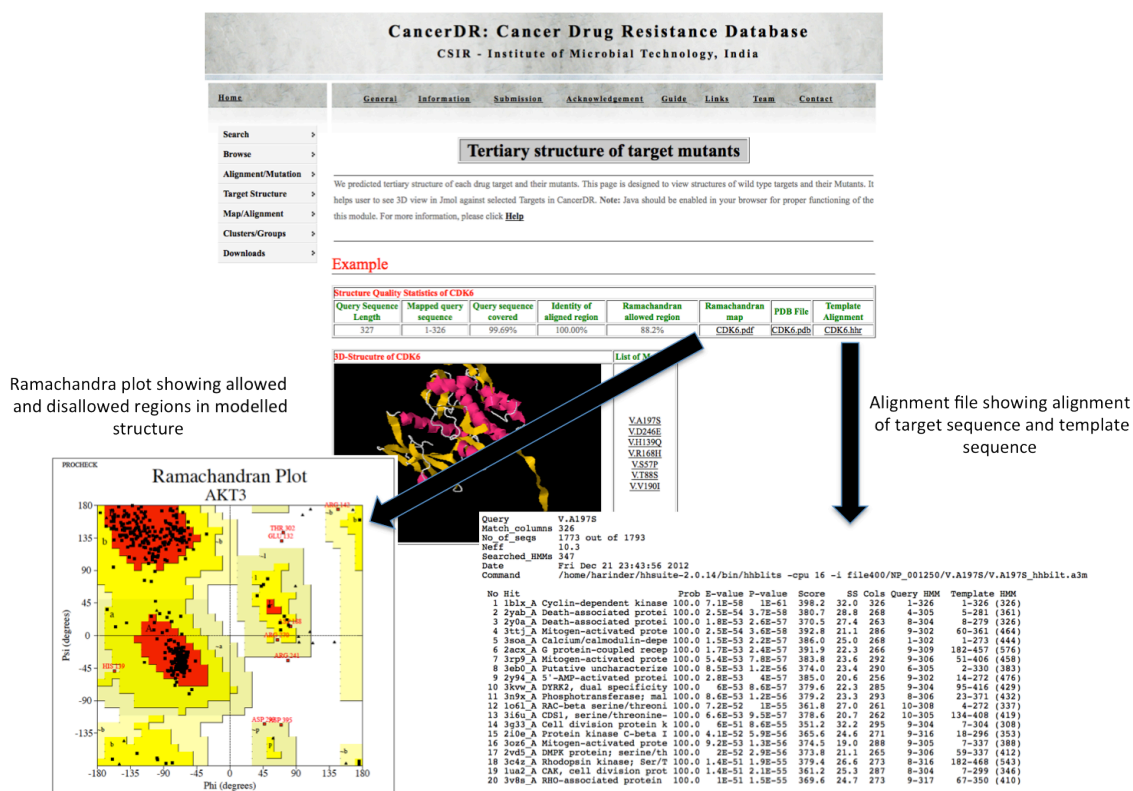


Figure 17 (b). Aignment file and ramachandran plot.

Reliability Parameters:

Mapped query sequence: This score indicates, which part of the query sequence is covered by the templates.

Query sequence covered: It is the percentage of the length of query sequence covered by the templates.

Identity of aligned region: This indicates, what is the identity of query and template in the aligned regions.

Ramachandran allowed region: This parameter tells about how much

percentage of the modeled structure falls in the allowed region of ramachandran plot.

HHR file format:

No: the index of the database match.

Hit: the first 30 characters of the name line.

Prob: the Probability of template to be a true positive. For the probability of being a true positive, the secondary structure score in column SS is taken into account, together with the raw score in column Score. True positives are de_fined to be either globally homologous or they are at least homologous in parts, and thereby locally similar in structure. More precisely, the latter criterion demands that the MAXSUB score between query and hit is at least 0.1. In almost all cases the structural similarity will be due to a global OR LOCAL homology between query and template.

E-value: The E-value gives the average number of false positives ('wrong hits') with a score better than the one for the template when scanning the database. It is a measure of reliability: Evalues near to 0 signify a very reliable hit, an E-value of 10 means about 10 wrong hits are expected to be found in the database with a score at least this good. Note that E-value and P-value are calculated without taking the secondary structure into account!

P-value: The P-value is the E-value divided by the number of sequences in the database. It is the probability that in a pairwise comparison a wrong hit will score at least this good.

Score: the raw score is what comes out of the (Viterbi) HMM-HMM alignment excluding the secondary structure score. Informally speaking, it is the sum over the similarities of aligned pro_le colmunns minus the gap penalties.

SS: the secondary structure score. This score tells you how well the PSIPRED-predicted (3-state) or actual DSSP-determined (8-state) secondary structure sequences agree with each other. PSIPRED con_dence values are used in the scoring, low con_dences getting less statistical weight.

Cols: the number of aligned Match columns in the HMM-HMM alignment.

Query HMM: the range of aligned match states from query HMM.

Template HMM: the range of aligned match states from the database/template HMM and, in parenthesis, the number of match states in the database HMM.

For further information, please visit <http://toolkit.tuebingen.mpg.de/hhblits>.

The screenshot displays the CancerDR: Cancer Drug Resistance Database interface. The main navigation bar includes links for Home, General, Information, Submission, Acknowledgement, Guide, Links, Team, and Contact. The left sidebar contains a search bar and a list of navigation options: Search, Browse, Alignment/Mutation, Target Structure, Map/Alignment, Clusters/Groups, and Downloads. The main content area is titled "Compare structure of target mutants" and includes a form for selecting two mutants for structural alignment. A callout bubble points to this form, stating "Select any two mutants of ABL2". Below the form, a table lists various protein targets, including AKT1, BRAF, ERK1, ERK2, ERK3, ERK4, ERK5, ERK6, ERK7, ERK8, ERK9, ERK10, ERK11, ERK12, ERK13, ERK14, ERK15, ERK16, ERK17, ERK18, ERK19, ERK20, ERK21, ERK22, ERK23, ERK24, ERK25, ERK26, ERK27, ERK28, ERK29, ERK30, ERK31, ERK32, ERK33, ERK34, ERK35, ERK36, ERK37, ERK38, ERK39, ERK40, ERK41, ERK42, ERK43, ERK44, ERK45, ERK46, ERK47, ERK48, ERK49, ERK50, ERK51, ERK52, ERK53, ERK54, ERK55, ERK56, ERK57, ERK58, ERK59, ERK60, ERK61, ERK62, ERK63, ERK64, ERK65, ERK66, ERK67, ERK68, ERK69, ERK70, ERK71, ERK72, ERK73, ERK74, ERK75, ERK76, ERK77, ERK78, ERK79, ERK80, ERK81, ERK82, ERK83, ERK84, ERK85, ERK86, ERK87, ERK88, ERK89, ERK90, ERK91, ERK92, ERK93, ERK94, ERK95, ERK96, ERK97, ERK98, ERK99, ERK100. A callout bubble points to the "Welcome to cancerdr result page" message, stating "Intermediate page showing message about processing of job". Below the message, a "Wait..." button is visible. A callout bubble points to the "Structure alignment in 3D" section, stating "Structure alignment of selected mutants". The bottom section shows the "Alignment of sequences" results, including the program name (MUSTANG v3.2.1), authors (A. S. Konagurthu, J. C. Whisstock, and P. J. Stuckey, A. M. Lesk), and the alignment statistics for two structures: V.A183T.pdb and V.P986fs.pdb. The alignment statistics are as follows:

Length:	1230
Identity:	556/1230 (45.2%) (Calculated as the percentage of conserved columns in the a
Similarity:	556/1230 (45.2%) (Calculated as the percentage of semi-conserved columns in
Gaps:	290/1230 (23.6%) (Calculated as the percentage of columns with atleast one g

Figure 19. Structure alignment of selected mutants selected by the user.

4.4 User sequence: This module allows users to predict the structure of their sequence using homology modeling (using MODELLER). User has to either paste the query sequence in FASTA format or upload the corresponding file containing query sequence and select any one of the targets against which structure has to be built. The selected target serves as a template for the structure prediction (Figure20).

4.5 Structures in PDB: We have also collected available PDB structures available for all the targets. There are multiple structures available for every target. These can be accessed via the PDB ID hyperlink for that target (Figure 21).

[illegible]

Figure 20. Tertiary structure prediction of user sequence.

[illegible]

Figure 21. Experimentally validated structure information (PDB structures).

5. Map/Alignment

Due to advancement in Next Generation Sequencing (NGS) technologies whole genome, transcriptome and exome sequencing have been frequently used to find out the mutations in the cancer samples. The data produced by the NGS technologies could be in form of short reads; contigs (if short reads were assembled) or genes, predicted from assembled contigs (or genomic fragments). Map/Alignment sections of our CancerDR allow the user to align Short reads, contigs and genes to cancer targets mentioned in this database. We have three separate modules for all three purposes.

5.1 Short Reads: This module allows the user to align and visualize short reads (i.e. Illumina reads) to cancer targets. Any mutation, at a particular position in the cancer sequencing sample can be easily visualized. User can provide single end reads (i.e. .fastq files) or paired end reads (i.e. .fastq file) for the alignment. Short reads file should be in .fastq format. For the paired end reads alignment two separate files of forward read and reversed reads are necessary. Single end reads file should be provided in third box (Figure 22).

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CSIR - Institute of Microbial Technology, India

Home General Information Submission Acknowledgement Guide Links Team

Short Read Mapping in CancerDR

Upload mate-1 (Forward) and mate-2 (Reversed) files (.fastq) for alignment. Both files should be provide together.

or

User can upload a single end read file.

Email is necessary for this module

Example files and Alignment Result

Forward read (Mate-1) [Download](#)

Reversed read (mate-2) [Download](#)

Single end file [Download](#)

Results of Mate-1 and Mate-2 files

Tablet viewer [Alignment Result](#)

Figure 22. Submission page for short reads alignment to cancer targets.

User can check the example file results by clicking **Alignment Results** link in the example section of the page. User must provide a valid Email address in this section so that results link can be send though email in case short reads alignment taking time (Figure 23).

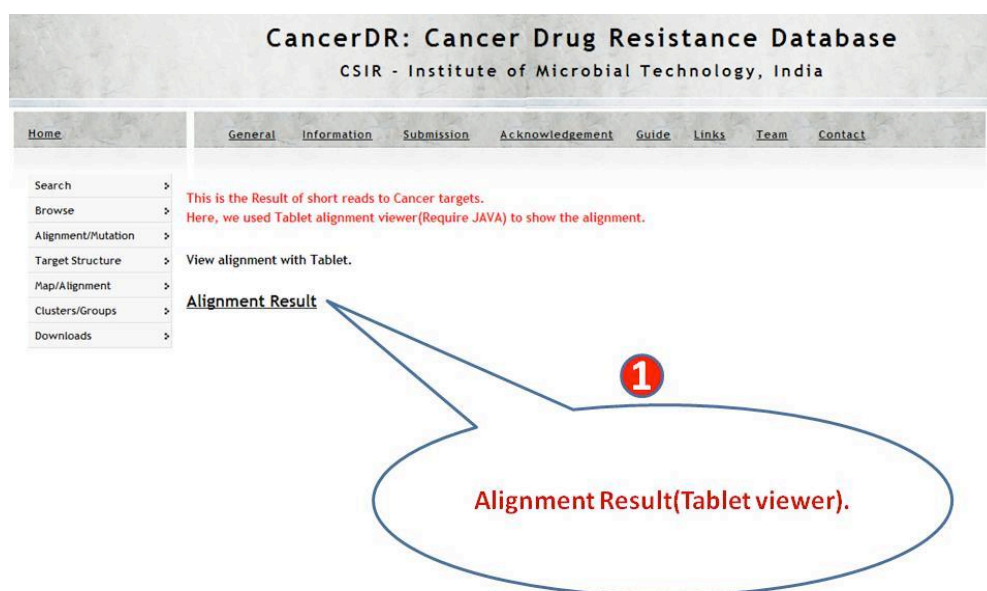


Figure 23. Alignment result link, appear after submission of short reads.

After submitting the short reads files, Alignment results will be available after some time (depends upon the amount of data and load on our server) (Figure 24). User should have JAVA to view the alignment results.

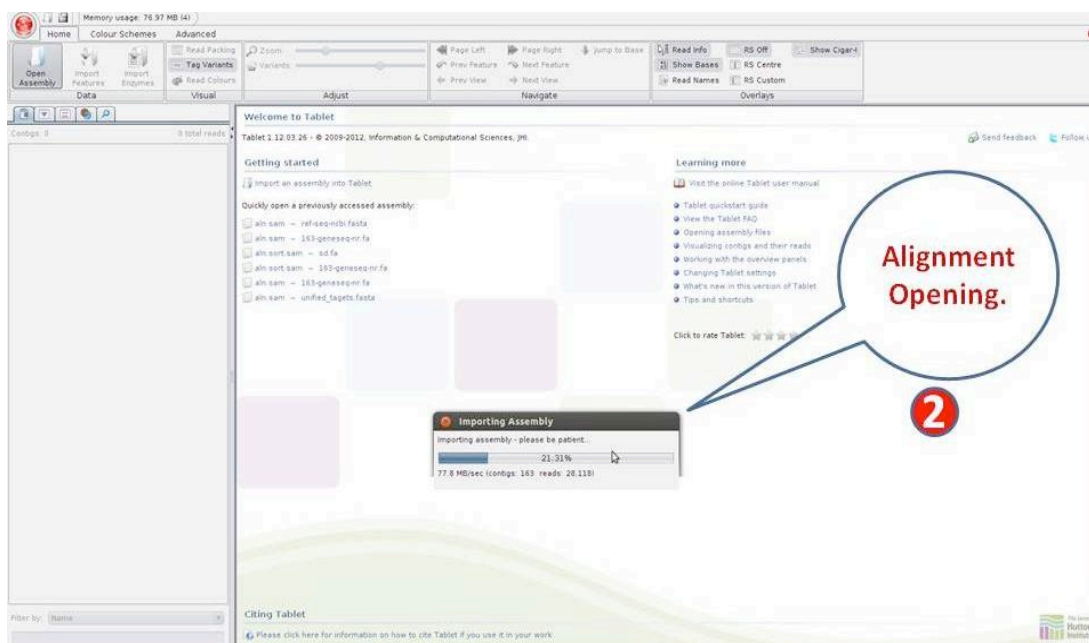


Figure 24. Processing of alignment results in Tablet viewer.

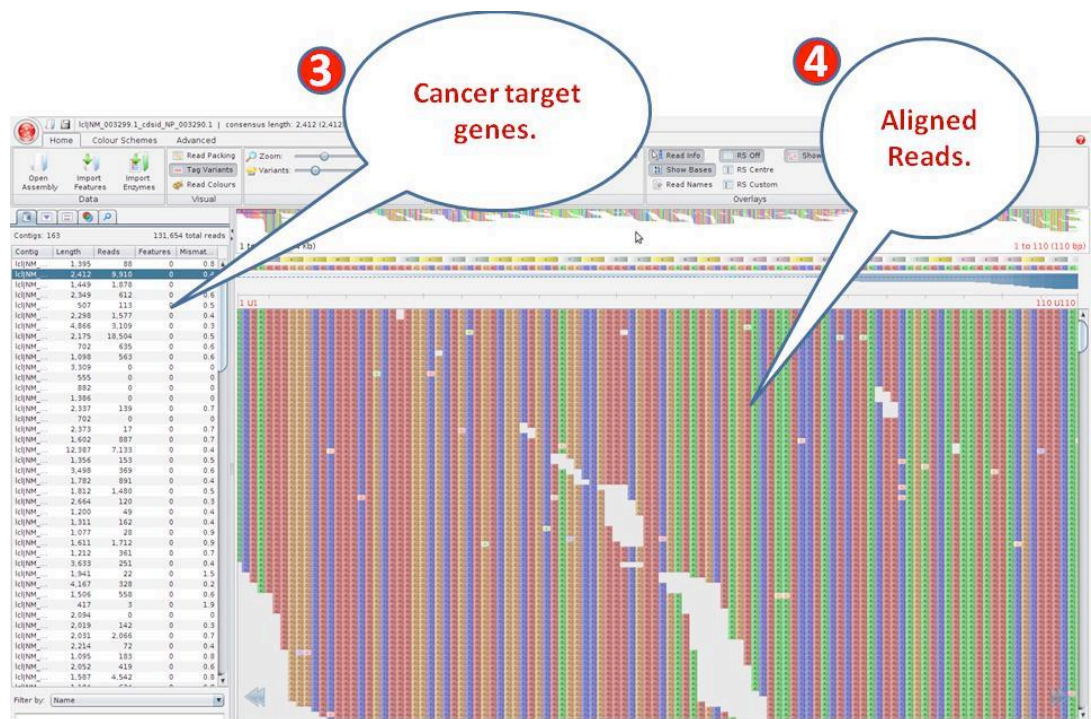


Figure 25. Alignment of short reads to cancer targets.

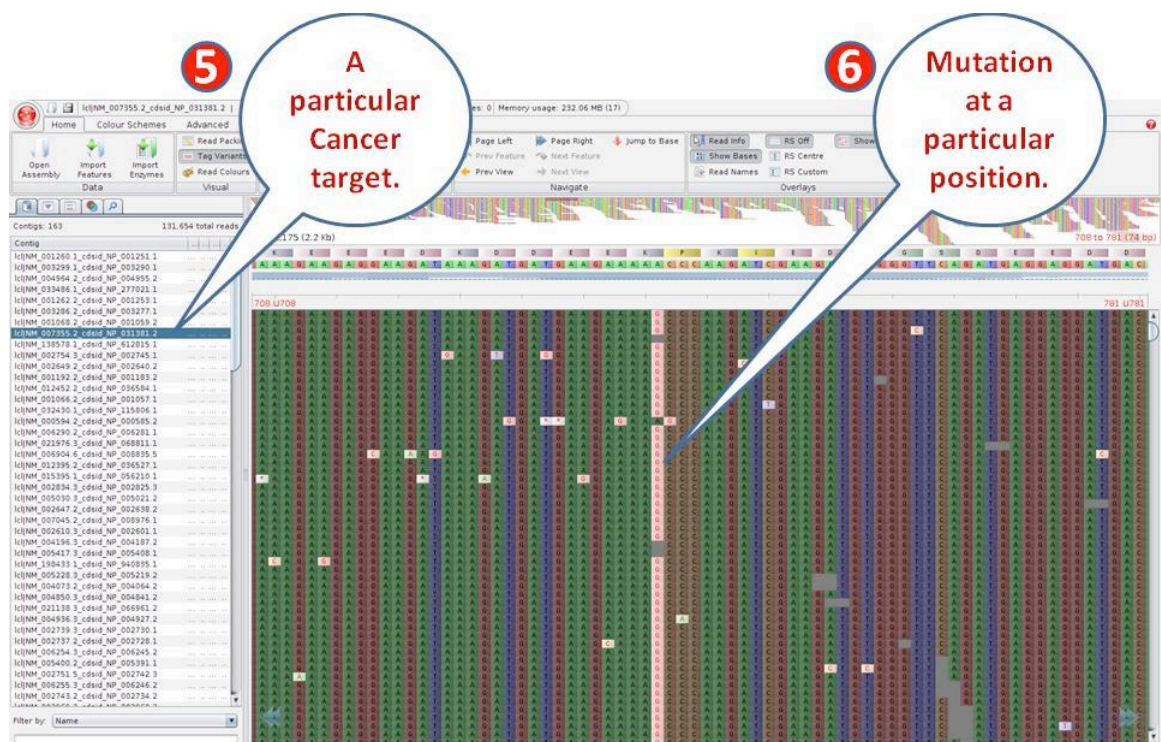


Figure 26. Visualization of a mutation in cancer sequence sample for a particular gene.

Tablet viewer window will start opening the alignment files in the next step (Figure 25). Alignment results will provide the information about number of reads align to each cancer target (i.e. gene). User can select a particular gene and check for mutation present at any position in the sequenced cancer sample (Figure 26).

Please contact Dr. G P S Raghava (raghava@imtech.res.in) in case you want to align bulk amount of data to Cancer targets, we will provide ftp service for the purpose.

5.2 Contigs: This module is prepared for the alignment of genes (both nucleotide and protein sequences), predicted from user provided contigs. At this module, user can provide contigs (or genomic fragments) of cancer sequenced samples and find out any change in the sequence by aligning to our cancer targets (i.e. wild type genes) by BLAST (Figure 27).

CancerDR: Cancer Drug Resistance Database
CSIR - Institute of Microbial Technology, India

Home | General | Information | Submission | Acknowledgement | Guide | Links | Team | Contact

Search > | Browse > | Alignment/Mutation > | Target Structure > | Map/Alignment > | Clusters/Groups > | Downloads >

Contigs Alignment in CancerDR

It is possible to sequence any or all or selected set of genes in a single shots with Next Generation Sequencing(NGS) technologies, produced short reads. There are number of assemblers which use these reads and produce contigs. These contigs have genes. This web page first predict the genes from contigs and then align genes to selected drug targets with BLAST.

[HELP](#)

Submit contigs file: <input type="button" value="Choose File"/> No file chosen Expect Value for BLAST search: <input type="text" value="1e-5"/> <input type="button" value="Search All"/> <input type="button" value="Run Analysis"/>	Example Contig file Download Predicted Genes from contigs Download Predicted Proteins from contigs Download BLAST result of Predicted Genes and Proteins Genes Protein
------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------	---------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------

Upload a contig file (FASTA format.)

Expected value (e Value) of BLAST for alignment of genes to Cancer targets.

Example files and Alignment Result

Figure 27. Contigs (or genomic fragments) submission page.

Nucleotide sequenced (contigs of genomic fragments) should be in fasta file format. User can select variable E value cutoff for the alignment. This module works in two steps. First, genes have been predicted from contigs with the help of Augustus software. Second, predicted genes have been aligned to cancer targets with BLAST.

BLAST alignment results can be downloaded and checked for any variation present in the genes predicted from cancer genome fragments at nucleotide and protein level both.

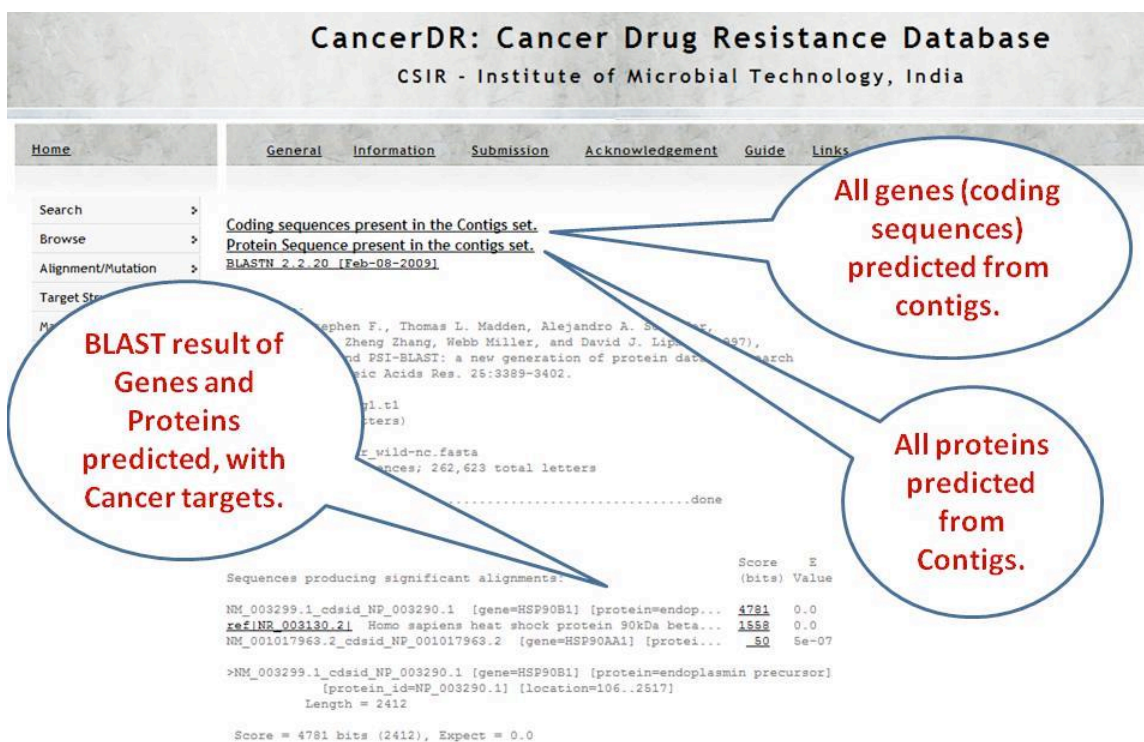


Figure 28. Alignment (i.e. BLAST) results page of genes predicted from contigs.

5.3 Genes: This module has been prepared for the alignment of gene (both nucleotide and amino acid) sequences with cancer target at this database. This strategy provides the idea about any variation in the sequenced cancer genes with respect to wild type sequences of same gene present at our database. These web pages have the option for both single and multiple fasta sequences with multiple E value options for BLAST alignment. Nucleotide and protein sequences both can be provided at this module to align with cancer targets. Example section provides the idea about input and output files used at this module.

CancerDR: Cancer Drug Resistance Database
CSIR - Institute of Microbial Technology, India

Home Submission Acknowledgement Guide Links Team

Search
Browse
Alignment/Mutation
Target Structure
Map/Alignment
Clusters/Groups
Downloads

Gene Sequence Alignment in CancerDR

For the comparison of sequences (i.e., Nucleotide or Protein) with Cancer drug targets with the help of BLAST.

Type/paste query sequences in FASTA format:

Example Sequence protein Example Sequence Nucleotide

or Upload your sequence
[Choose File](#) No file chosen

Sequence type: ☐ Nucleotide sequence ☒ Protein Sequence

Expect Value:

BLAST type:

[Run All](#) [Run Analysis](#)

Example

Gene sequence(Fasta) file	Download
Cancer target Protein(Fasta)file	Download
BLAST result of Gene Sequence	Download
BLAST result of Cancer target Proteins	Download

Annotations:

- Upload Multiple FASTA sequence of Genes or Proteins for BLAST search with Cancer targets.
- User can provide a file of genes or Proteins.
- Type of sequence(i.e. Nucleotide or Protein)
- Type of BLAST program.
- Expected value(e Value) of BLAST for alignment.
- Example files and Alignment Result

Figure 29. Genes (i.e. Nucleotide or proteins) sequence submission page.

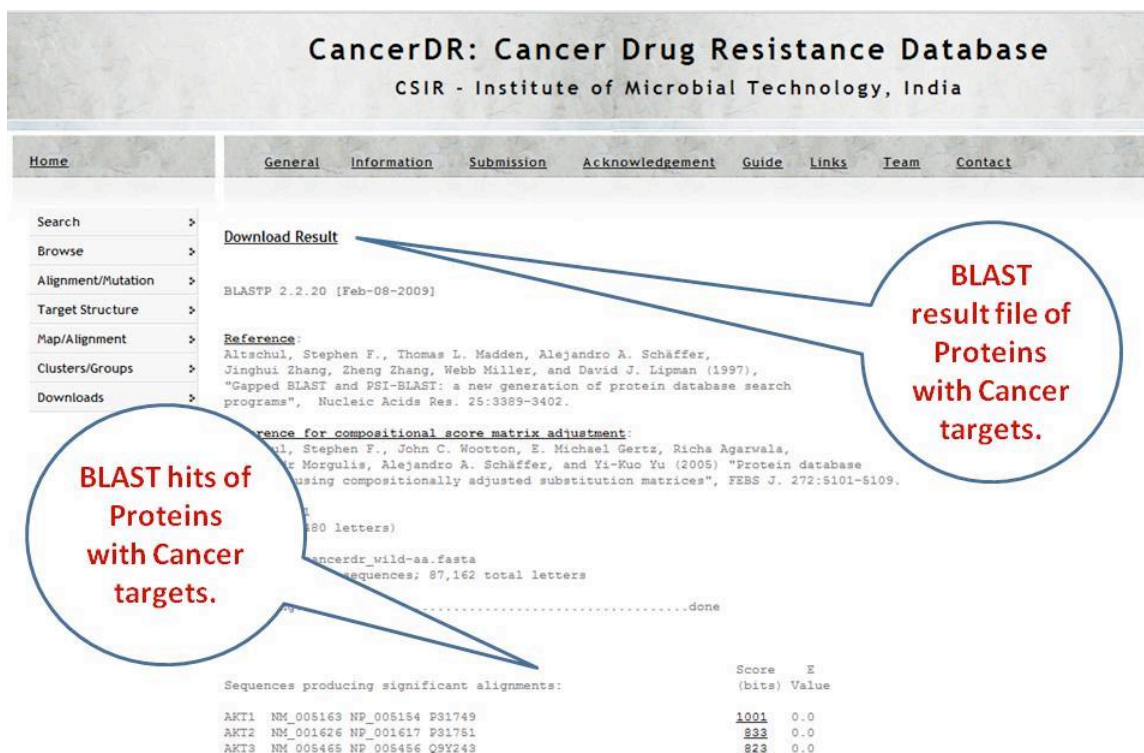


Figure 30. Alignment (i.e. BLAST) results page of genes.

6. Clustering Tool

Clustering tool is subdivided into three parts:

6.1 Clustering of sequences in a drug target: We have provided this tool to look at the distance of different mutated sequences of a selected target as an alignment tree. Here user can select a drug target from the given list. The Alignment-tree diagram will be displayed creating the tree of all possible mutated protein sequences for that selected drug target. There are two different selection options (Figure 31a) for drug targets, i) Red button- for mutants of given drug target, ii) Blue button for natural variants of the query drug target. Clicking red or blue buttons displays name of query with 'Start Jalview' button in middle table, which on submission/starting, displays windows for Clustal-W alignment and alignment tree (Figure 31b). Finally the user can look at the distance of different mutant sequences in the alignment against selected target.

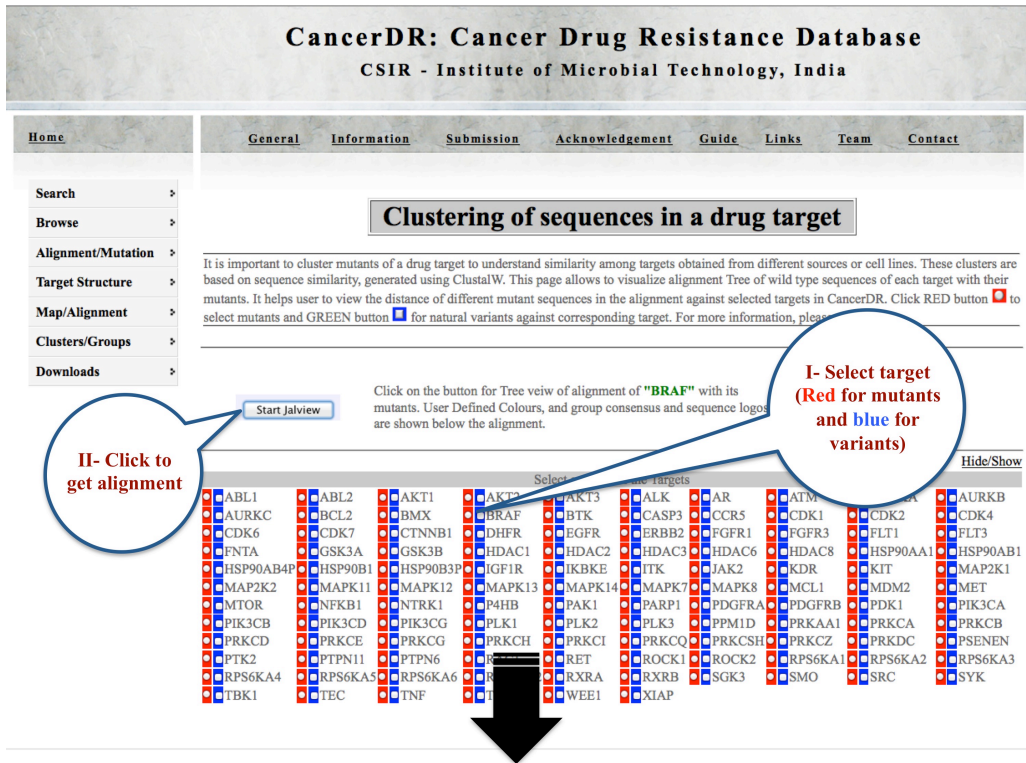


Figure 31a. Tool for the drug target clustering on the basis of their sequences.

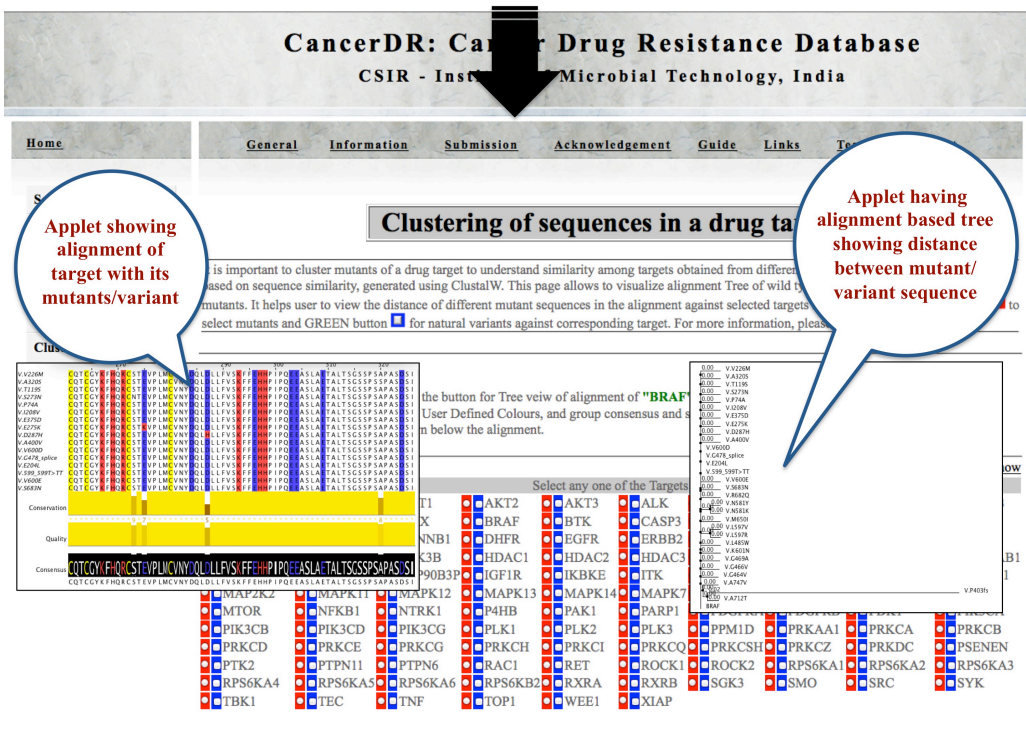


Figure 31b. Jalview showing the clustered drug target sequences.

6.2 Clustering of Cell lines: This page allows user to cluster cell lines based on their sensitivity towards a drug. We group cell lines for each drug based on their relative sensitivity to reference (highest sensitivity) or inhibition IC50 value in a given range. User can either choose tissue type or all cell lines (Figure 32a) or can select the cell lines with mutated drug targets (Figure 33a). The second column gives the number of cell lines screened against the drug as it is equal to or greater than reference IC50 (lowest of all). Subsequent columns, up to eight, give grouping based on IC50 value equal to or greater than 3, 5, 25, 100 and 250 times of reference IC50. The columns from nine to sixteen show the group of cell lines having absolute value of IC50 lying in different ranges (R1, R2, R3, R4, R5, R6, R7 and R8) (Figure 32b & c).

In addition, 'MUTANTS' button in the tissue list leads to a table on the next page (Figure 33a), which has similar ranges of IC50 along with links to bar plots at the last column. The bar plots show the distribution of IC50 values along different mutants of the drug-target coming from various cell line (Figure 33b).

CancerDR: Cancer Drug Resistance Database
CSIR - Institute of Microbial Technology, India

Home General Information Submission Acknowledgement Guide Links Team Contact

Search >
Browse >
Alignment/Mutation >
Target Structure >
Map/Alignment >
Clusters/Groups >
Downloads >

Clustering of Cell lines

This page allows user to cluster cell lines based on their sensitivity towards a drug. We group cell lines for each drug based on their relative sensitivity to reference (highest sensitivity) or inhibition IC50 value in a given range. User can either choose tissue type or all cell lines or can select the cell lines with mutated drug targets. The second column gives the number of cell lines screened against the drug as it is equal to or greater than reference IC50 (lowest of all). Subsequent columns, up to eight, give grouping based on IC50 value equal to or greater than 3, 5, 25, 100, 250 times of reference IC50. The columns from nine to sixteen shows the group of cell lines having absolute value of IC50 lying in different ranges (R1, R2, R3, R4, R5, R6, R7 and R8). The cell line in groups with lower value may be preferred and higher values may be less preferred. For more information, please click [HERE](#).

at IC-50s, xRef: times of reference value(column two to seven) , Range of IC50 value(column eight to fifteen)- R1: 0-0.001 μ M, R2: 0.001-0.005 μ M, R3: 0.005-0.025 μ M, R4: 0.025-0.125 μ M, R5: 0.125-0.625 μ M, R6: 0.625-15 μ M, R7: 15-390 μ M, R8: greater than 390 μ M.

Select Tissue type against which you want to see Cell Line clusters

☐ BILIARY TRACT ☐ BLADDER ☐ BLOOD ☐ BONE ☐ BREAST ☐ CENTRAL NERVOUS SYSTEM
☐ ENDOMETRIUM ☐ PANCREAS ☐ HAEMATOPOIETIC AND LYMPHOID TISSUE ☐ KIDNEY ☐ LARGE INTESTINE ☐ LIVER ☐ LUNG
☐ ESOPHAGUS ☐ OTHER ☐ OVARY ☐ PANCREAS ☐ PLEURA ☐ PROSTATE ☐ SALIVARY GLAND
☐ SKIN ☐ SOFT TISSUE ☐ STOMACH ☐ THYROID ☐ UPPER AERODIGESTIVE TRACT ☐ UTERINE TRACT ☐ UTERUS
☐ ALL ☐ MUTANTS

Cell Line clusters for **OVARY** tissue type

Drug	IC50 > Ref	IC50 > 3xRef	IC50 > 5xRef	IC50 > 25xRef	IC50 > 100xRef	IC50 > 250xRef	IC50 > 390xRef	R1	R2	R3	R4	R5	R6	R7	R8
17AAG	88	14	28	18	11	8	8	0	0	0	21	42	11	2	0
NUB304	34	8	8	8	8	8	8	0	0	0	0	0	0	0	0
HA5004	0	0	0	0	0	0	0	0	0	0	1	2	0	0	0
AC25041	3	0	0	0	0	0	0	0	0	0	0	0	0	0	0
NU2263	18	14	14	11	11	11	11	0	0	0	0	1	8	11	0
NU2388	18	14	11	11	11	11	11	0	0	0	0	0	0	0	0
NU2041	20	48	19	0	0	0	0	0	0	0	0	0	0	0	0
NU2388	18	14	11	11	11	11	11	0	0	0	0	0	0	0	0
NU2388	18	14	11	11	11	11	11	0	0	0	0	0	0	0	0

Select any tissue of origin to get list of grouped cell lines

Table having rows of different drugs assayed with cell lines grouped in different columns for e.g. 17AAG drug have many groups of cell lines based on ranges of IC50

Figure 32a. Screen shot showing the cell lines clustering function.

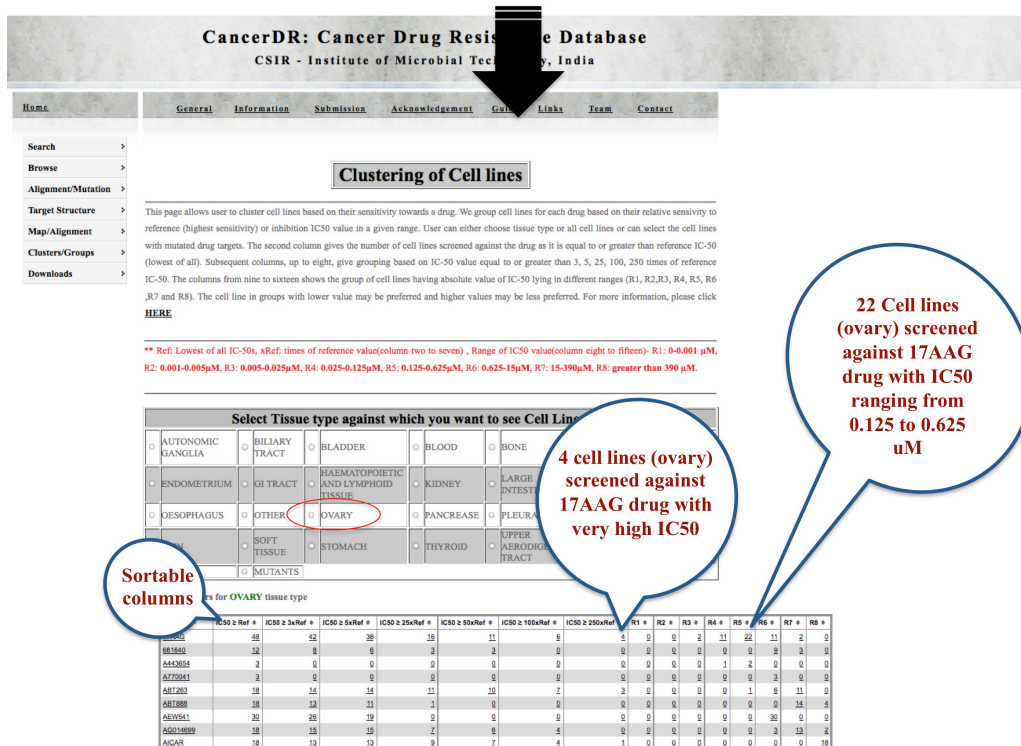


Figure 32b. Result of clustering of ovary cell lines.

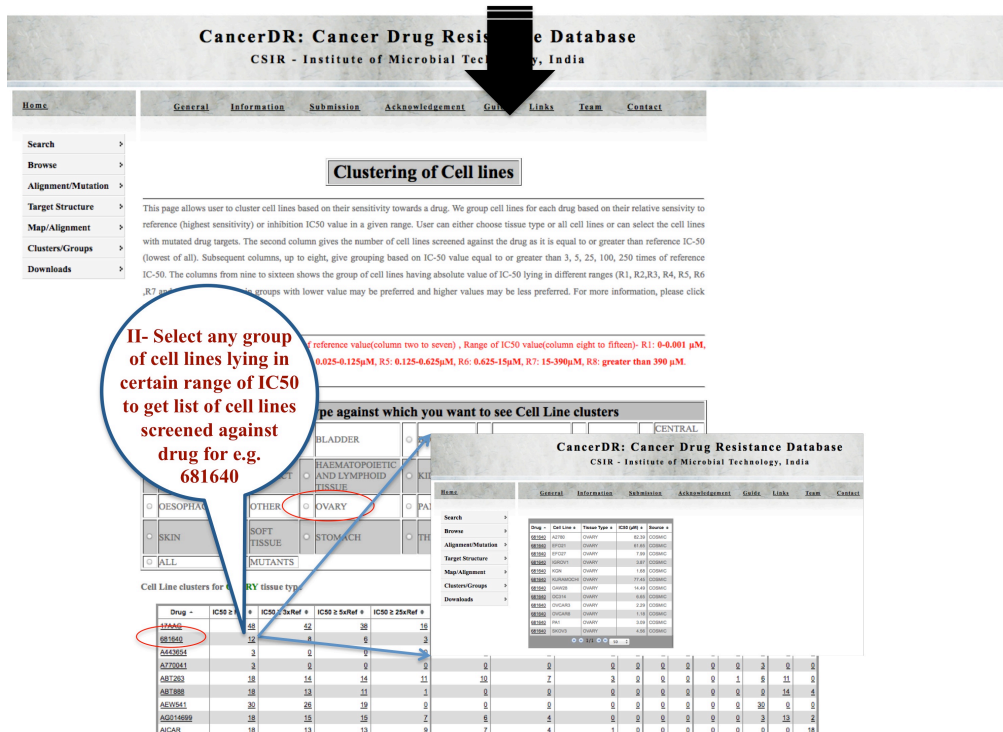


Figure 32c. Further exploration of the clustering tool to obtain IC50 values.

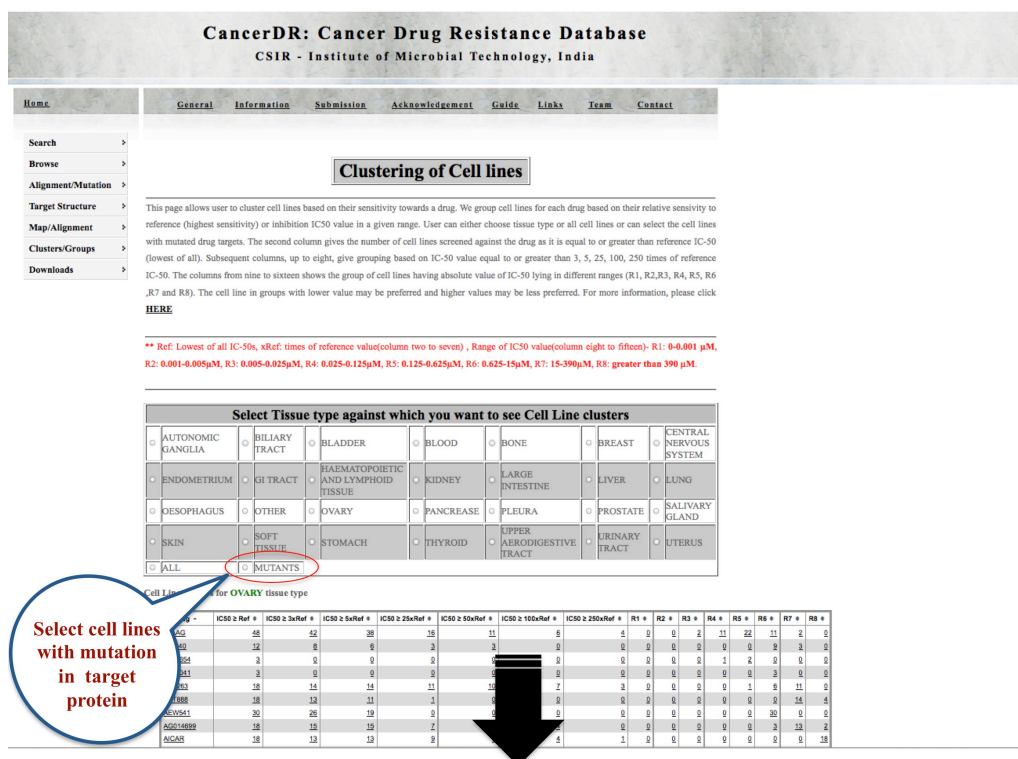


Figure 33a. Clustering of cell lines which are mutated in some drug target.

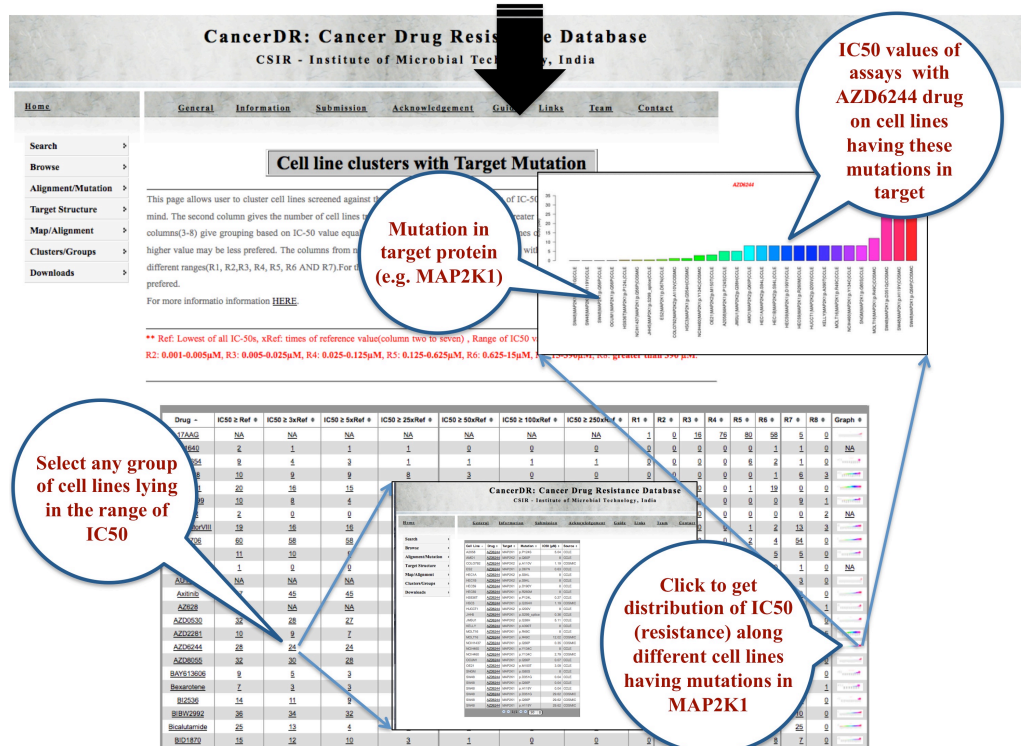


Figure 33b. Screenshot showing the Pharmacological profiling of AZD6244 drug.

6.3 Clustering of drugs: It is important to know which drugs have similar level of effectiveness for a given cell line or tissue type. This page allows the user to cluster drugs screened against selected cell line and group on the basis of IC50 or relative drug sensitivity. User can either choose the tissue type, all cell lines or can select the cell lines with mutated drug targets (Figure 34a). The second column gives the number of drugs screened against the particular cell line as it is equal to or greater than reference IC50 (lowest of all IC50s). Subsequent columns, up to eighth, give grouping based on IC50 value equal or greater than 3, 5, 25, 100, and 250 times of reference IC50. The columns from nine to sixteen show the group of drugs with absolute value of IC50 lying in different ranges (R1, R2, R3, R4, R5, R6, R7 and R8). The drugs in groups with higher value are important for resistance-mechanism related studies (Figure 34b).

The ‘MUTANTS’ button in the tissue list leads to a table on the next page, which has similar ranges of IC50 along with links to bar plots at the last column. The bar plots show the distribution of IC50 values along different cell lines having mutation in the targets of corresponding drugs.

Clicking on any number in displayed table leads to a new table having list of drugs grouped in that range of IC50 (Figure 34c).

CancerDR: Cancer Drug Resistance Database
CSIR - Institute of Microbial Technology, India

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Clustering of drugs

It is important to know which drugs have similar level of effectiveness for a given cell line or tissue type. This page allows the user to cluster drugs screened against selected cell line and grouped on the basis of IC-50 or relative drug sensitivity. User can either choose the tissue type, all cell lines or can select the cell lines with mutated drug targets. The second column gives the number of drugs screened against the particular cell line as it is equal to or greater than reference IC-50 (lowest of all IC-50s). Subsequent columns, up to eighth, give grouping based on IC-50 value equal or greater than 3, 5, 25, 100, 250 times of reference IC-50. The columns from nine to sixteen show the group of drugs with absolute value of IC-50 lying in different ranges (R1, R2, R3, R4, R5, R6, R7 and R8). The drugs in groups with lower value may be preferred and higher values may be less preferred. For more information, please click [HERE](#).

all IC-50s, xRef: times of reference value(column two to seven) , Range of IC50 value(column eight to fifteen)- R1: 0-0.001 μ M, R2: 0.001-0.005 μ M, R3: 0.005-0.025 μ M, R4: 0.025-0.125 μ M, R5: 0.125-0.625 μ M, R6: 0.625-15 μ M, R7: 15-390 μ M, R8: greater than 390 μ M.

Select any tissue of origin to get list of grouped drugs

Select Tissue type against which you want to see Drug clusters

<input type="checkbox"/> BILIARY TRACT	<input type="checkbox"/> BLADDER	<input type="checkbox"/> BLOOD	<input type="checkbox"/> BONE	<input type="checkbox"/> BREAST	<input type="checkbox"/> CENTRAL NERVOUS SYSTEM
<input type="checkbox"/> ENDOMETRIUM	<input type="checkbox"/> ESOPHAGUS	<input type="checkbox"/> HAEMATOPOIETIC AND LYMPHOID TISSUE	<input type="checkbox"/> KIDNEY	<input type="checkbox"/> LARGE INTESTINE	<input type="checkbox"/> LIVER
<input type="checkbox"/> LUNG	<input type="checkbox"/> OTHER	<input type="checkbox"/> OVARY	<input type="checkbox"/> PANCREAS	<input type="checkbox"/> PLEURA	<input type="checkbox"/> PROSTATE
<input type="checkbox"/> SALIVARY GLAND	<input type="checkbox"/> SKIN	<input type="checkbox"/> SOFT TISSUE	<input type="checkbox"/> STOMACH	<input type="checkbox"/> THYROID	<input type="checkbox"/> UPPPER AERODIGESTIVE TRACT
<input type="checkbox"/> UTERUS	<input type="checkbox"/> ALL	<input type="checkbox"/> MUTANTS			

Drug cluster for **OVARY** tissue type

Cell Line	IC50 \pm Ref	IC50 \geq 3xRef	IC50 \geq 5xRef	IC50 \geq 25xRef	IC50 \geq 100xRef	IC50 \geq 250xRef	R1	R2	R3	R4	R5	R6	R7	R8
A2780	NA	NA	NA	NA	NA	NA	NA	7	1	4	11	8	11	23
Caov3	27	36	20	30	31	30	22	0	0	1	3	2	4	18
Caov4	23	10	10	9	8	0	5	0	0	0	0	0	0	0
DOV18	24	23	23	21	18	0	0	0	0	0	0	1	0	0
DOV904	22	22	22	20	20	19	17	0	0	1	1	1	20	0
DOV13	24	23	22	21	20	19	18	0	1	0	2	2	18	0
EP021	102	117	118	110	100	92	0	0	0	0	10	68	65	11
EP027	NA	NA	NA	NA	NA	NA	0	0	0	0	0	13	64	32
ES2	24	22	18	18	17	15	13	0	1	4	1	18	0	0

Table having rows of different cell lines assayed with drugs grouped in different columns for e.g. Caov3 cell line assayed with many drugs which are grouped on the basis of ranges of IC50

Figure 34a. Clustering of drugs assayed on ovary cell lines.

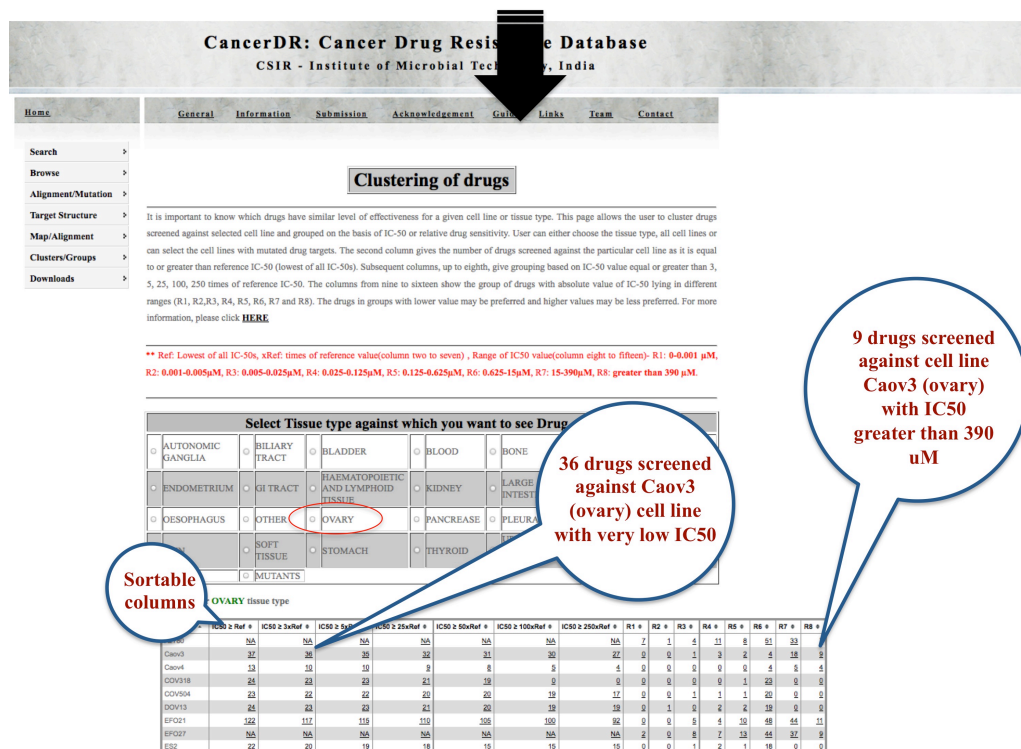


Figure 34b. Result showing clustered drugs.

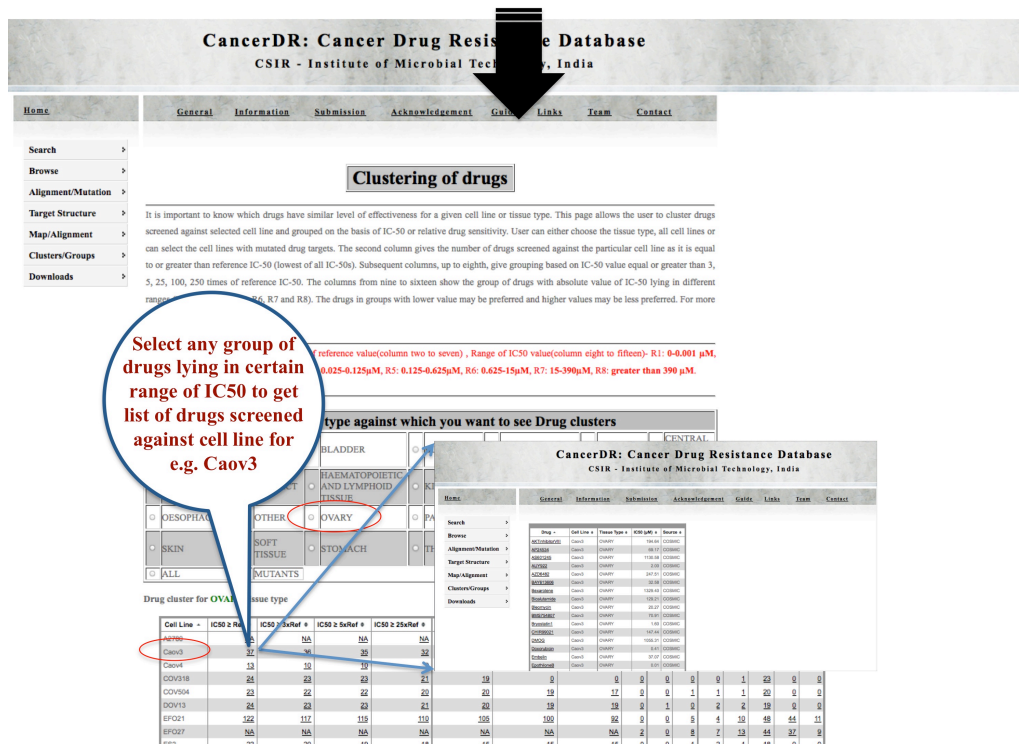


Figure 34c. IC50 values of assayed drugs on the respective cell lines.

7. Downloads

This section is divided into 4 modules: for downloading all target sequences and their mutants/variants, for downloading multiple sequence alignments of targets and their mutants/variants, for downloading predicted structures and for downloading experimental PDB structures (whichever are available).

8.1 Sequences: This page allows the users to download the sequences of drug targets (wild type) and their mutants/natural variants. User can download either a specific or all target sequences. User has to click on RED button to select mutants and BLUE button for natural variants against corresponding targets. User can either download a specific target and its mutants/natural variants or can browse whole directory containing all targets and their mutants/variants. Further, facility has been provided to synchronize whole sequence data at user's local disc using rsync command (Figure 35).

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Home | General | Information | Submission | Acknowledgement | Guide | Links | Team | Contact

Search > | Browse > | Alignment/Mutation > | Target Structure > | Map/Alignment > | Clusters/Groups > | Downloads >

Download Sequence of Drug Targets

This page allow users to download the sequences of drug targets (wild type) and their mutants/natural variants. Further, facility is provided to synchronize data at your local disk using rsync command. User can click on RED button for natural variants against corresponding target. For more information, click on BLUE button.

Download wild type sequence of drug target **ABL2** and its cancer mutants in FASTA format.

Browse Directory: This folder contains sequences of all targets and their mutants in FASTA format. User can download all the files.

Rsync Facility: This server allows the user to synchronize any sequence data folder in CancerDR using following command:
`rsync -avz --delete cdd.cdri.ac.in:/cancerdr/data/align/mut/fa /user_local_directory/`

Select any one of the Targets

ABL1	ABL2	AKT1	AKT2	AKT3	ALK	AR	ATM	AURKA	CDK1	CDK2	CDK4	CDK5	CDK6	CDK7	CDK8	CDK9	CDK10	CDK11	CDK12	CDK13	CDK14	CDK15	CDK16	CDK17	CDK18	CDK19	CDK20	CDK21	CDK22	CDK23	CDK24	CDK25	CDK26	CDK27	CDK28	CDK29	CDK30	CDK31	CDK32	CDK33	CDK34	CDK35	CDK36	CDK37	CDK38	CDK39	CDK40	CDK41	CDK42	CDK43	CDK44	CDK45	CDK46	CDK47	CDK48	CDK49	CDK50	CDK51	CDK52	CDK53	CDK54	CDK55	CDK56	CDK57	CDK58	CDK59	CDK60	CDK61	CDK62	CDK63	CDK64	CDK65	CDK66	CDK67	CDK68	CDK69	CDK70	CDK71	CDK72	CDK73	CDK74	CDK75	CDK76	CDK77	CDK78	CDK79	CDK80	CDK81	CDK82	CDK83	CDK84	CDK85	CDK86	CDK87	CDK88	CDK89	CDK90	CDK91	CDK92	CDK93	CDK94	CDK95	CDK96	CDK97	CDK98	CDK99	CDK100	CDK101	CDK102	CDK103	CDK104	CDK105	CDK106	CDK107	CDK108	CDK109	CDK110	CDK111	CDK112	CDK113	CDK114	CDK115	CDK116	CDK117	CDK118	CDK119	CDK120	CDK121	CDK122	CDK123	CDK124	CDK125	CDK126	CDK127	CDK128	CDK129	CDK130	CDK131	CDK132	CDK133	CDK134	CDK135	CDK136	CDK137	CDK138	CDK139	CDK140	CDK141	CDK142	CDK143	CDK144	CDK145	CDK146	CDK147	CDK148	CDK149	CDK150	CDK151	CDK152	CDK153	CDK154	CDK155	CDK156	CDK157	CDK158	CDK159	CDK160	CDK161	CDK162	CDK163	CDK164	CDK165	CDK166	CDK167	CDK168	CDK169	CDK170	CDK171	CDK172	CDK173	CDK174	CDK175	CDK176	CDK177	CDK178	CDK179	CDK180	CDK181	CDK182	CDK183	CDK184	CDK185	CDK186	CDK187	CDK188	CDK189	CDK190	CDK191	CDK192	CDK193	CDK194	CDK195	CDK196	CDK197	CDK198	CDK199	CDK200	CDK201	CDK202	CDK203	CDK204	CDK205	CDK206	CDK207	CDK208	CDK209	CDK210	CDK211	CDK212	CDK213	CDK214	CDK215	CDK216	CDK217	CDK218	CDK219	CDK220	CDK221	CDK222	CDK223	CDK224	CDK225	CDK226	CDK227	CDK228	CDK229	CDK230	CDK231	CDK232	CDK233	CDK234	CDK235	CDK236	CDK237	CDK238	CDK239	CDK240	CDK241	CDK242	CDK243	CDK244	CDK245	CDK246	CDK247	CDK248	CDK249	CDK250	CDK251	CDK252	CDK253	CDK254	CDK255	CDK256	CDK257	CDK258	CDK259	CDK260	CDK261	CDK262	CDK263	CDK264	CDK265	CDK266	CDK267	CDK268	CDK269	CDK270	CDK271	CDK272	CDK273	CDK274	CDK275	CDK276	CDK277	CDK278	CDK279	CDK280	CDK281	CDK282	CDK283	CDK284	CDK285	CDK286	CDK287	CDK288	CDK289	CDK290	CDK291	CDK292	CDK293	CDK294	CDK295	CDK296	CDK297	CDK298	CDK299	CDK300	CDK301	CDK302	CDK303	CDK304	CDK305	CDK306	CDK307	CDK308	CDK309	CDK310	CDK311	CDK312	CDK313	CDK314	CDK315	CDK316	CDK317	CDK318	CDK319	CDK320	CDK321	CDK322	CDK323	CDK324	CDK325	CDK326	CDK327	CDK328	CDK329	CDK330	CDK331	CDK332	CDK333	CDK334	CDK335	CDK336	CDK337	CDK338	CDK339	CDK340	CDK341	CDK342	CDK343	CDK344	CDK345	CDK346	CDK347	CDK348	CDK349	CDK350	CDK351	CDK352	CDK353	CDK354	CDK355	CDK356	CDK357	CDK358	CDK359	CDK360	CDK361	CDK362	CDK363	CDK364	CDK365	CDK366	CDK367	CDK368	CDK369	CDK370	CDK371	CDK372	CDK373	CDK374	CDK375	CDK376	CDK377	CDK378	CDK379	CDK380	CDK381	CDK382	CDK383	CDK384	CDK385	CDK386	CDK387	CDK388	CDK389	CDK390	CDK391	CDK392	CDK393	CDK394	CDK395	CDK396	CDK397	CDK398	CDK399	CDK400	CDK401	CDK402	CDK403	CDK404	CDK405	CDK406	CDK407	CDK408	CDK409	CDK410	CDK411	CDK412	CDK413	CDK414	CDK415	CDK416	CDK417	CDK418	CDK419	CDK420	CDK421	CDK422	CDK423	CDK424	CDK425	CDK426	CDK427	CDK428	CDK429	CDK430	CDK431	CDK432	CDK433	CDK434	CDK435	CDK436	CDK437	CDK438	CDK439	CDK440	CDK441	CDK442	CDK443	CDK444	CDK445	CDK446	CDK447	CDK448	CDK449	CDK450	CDK451	CDK452	CDK453	CDK454	CDK455	CDK456	CDK457	CDK458	CDK459	CDK460	CDK461	CDK462	CDK463	CDK464	CDK465	CDK466	CDK467	CDK468	CDK469	CDK470	CDK471	CDK472	CDK473	CDK474	CDK475	CDK476	CDK477	CDK478	CDK479	CDK480	CDK481	CDK482	CDK483	CDK484	CDK485	CDK486	CDK487	CDK488	CDK489	CDK490	CDK491	CDK492	CDK493	CDK494	CDK495	CDK496	CDK497	CDK498	CDK499	CDK500	CDK501	CDK502	CDK503	CDK504	CDK505	CDK506	CDK507	CDK508	CDK509	CDK510	CDK511	CDK512	CDK513	CDK514	CDK515	CDK516	CDK517	CDK518	CDK519	CDK520	CDK521	CDK522	CDK523	CDK524	CDK525	CDK526	CDK527	CDK528	CDK529	CDK530	CDK531	CDK532	CDK533	CDK534	CDK535	CDK536	CDK537	CDK538	CDK539	CDK540	CDK541	CDK542	CDK543	CDK544	CDK545	CDK546	CDK547	CDK548	CDK549	CDK550	CDK551	CDK552	CDK553	CDK554	CDK555	CDK556	CDK557	CDK558	CDK559	CDK560	CDK561	CDK562	CDK563	CDK564	CDK565	CDK566	CDK567	CDK568	CDK569	CDK570	CDK571	CDK572	CDK573	CDK574	CDK575	CDK576	CDK577	CDK578	CDK579	CDK580	CDK581	CDK582	CDK583	CDK584	CDK585	CDK586	CDK587	CDK588	CDK589	CDK590	CDK591	CDK592	CDK593	CDK594	CDK595	CDK596	CDK597	CDK598	CDK599	CDK600	CDK601	CDK602	CDK603	CDK604	CDK605	CDK606	CDK607	CDK608	CDK609	CDK610	CDK611	CDK612	CDK613	CDK614	CDK615	CDK616	CDK617	CDK618	CDK619	CDK620	CDK621	CDK622	CDK623	CDK624	CDK625	CDK626	CDK627	CDK628	CDK629	CDK630	CDK631	CDK632	CDK633	CDK634	CDK635	CDK636	CDK637	CDK638	CDK639	CDK640	CDK641	CDK642	CDK643	CDK644	CDK645	CDK646	CDK647	CDK648	CDK649	CDK650	CDK651	CDK652	CDK653	CDK654	CDK655	CDK656	CDK657	CDK658	CDK659	CDK660	CDK661	CDK662	CDK663	CDK664	CDK665	CDK666	CDK667	CDK668	CDK669	CDK670	CDK671	CDK672	CDK673	CDK674	CDK675	CDK676	CDK677	CDK678	CDK679	CDK680	CDK681	CDK682	CDK683	CDK684	CDK685	CDK686	CDK687	CDK688	CDK689	CDK690	CDK691	CDK692	CDK693	CDK694	CDK695	CDK696	CDK697	CDK698	CDK699	CDK700	CDK701	CDK702	CDK703	CDK704	CDK705	CDK706	CDK707	CDK708	CDK709	CDK710	CDK711	CDK712	CDK713	CDK714	CDK715	CDK716	CDK717	CDK718	CDK719	CDK720	CDK721	CDK722	CDK723	CDK724	CDK725	CDK726	CDK727	CDK728	CDK729	CDK730	CDK731	CDK732	CDK733	CDK734	CDK735	CDK736	CDK737	CDK738	CDK739	CDK740	CDK741	CDK742	CDK743	CDK744	CDK745	CDK746	CDK747	CDK748	CDK749	CDK750	CDK751	CDK752	CDK753	CDK754	CDK755	CDK756	CDK757	CDK758	CDK759	CDK760	CDK761	CDK762	CDK763	CDK764	CDK765	CDK766	CDK767	CDK768	CDK769	CDK770	CDK771	CDK772	CDK773	CDK774	CDK775	CDK776	CDK777	CDK778	CDK779	CDK780	CDK781	CDK782	CDK783	CDK784	CDK785	CDK786	CDK787	CDK788	CDK789	CDK790	CDK791	CDK792	CDK793	CDK794	CDK795	CDK796	CDK797	CDK798	CDK799	CDK800	CDK801	CDK802	CDK803	CDK804	CDK805	CDK806	CDK807	CDK808	CDK809	CDK810	CDK811	CDK812	CDK813	CDK814	CDK815	CDK816	CDK817	CDK818	CDK819	CDK820	CDK821	CDK822	CDK823	CDK824	CDK825	CDK826	CDK827	CDK828	CDK829	CDK830	CDK831	CDK832	CDK833	CDK834	CDK835	CDK836	CDK837	CDK838	CDK839	CDK840	CDK841	CDK842	CDK843	CDK844	CDK845	CDK846	CDK847	CDK848	CDK849	CDK850	CDK851	CDK852	CDK853	CDK854	CDK855	CDK856	CDK857	CDK858	CDK859	CDK860	CDK861	CDK862	CDK863	CDK864	CDK865	CDK866	CDK867	CDK868	CDK869	CDK870	CDK871	CDK872	CDK873	CDK874	CDK875	CDK876	CDK877	CDK878	CDK879	CDK880	CDK881	CDK882	CDK883	CDK884	CDK885	CDK886	CDK887	CDK888	CDK889	CDK890	CDK891	CDK892	CDK893	CDK894	CDK895	CDK896	CDK897	CDK898	CDK899	CDK900	CDK901	CDK902	CDK903	CDK904	CDK905	CDK906	CDK907	CDK908	CDK909	CDK910	CDK911	CDK912	CDK913	CDK914	CDK915	CDK916	CDK917	CDK918	CDK919	CDK920	CDK921	CDK922	CDK923	CDK924	CDK925	CDK926	CDK927	CDK928	CDK929	CDK930	CDK931	CDK932	CDK933	CDK934	CDK935	CDK936	CDK937	CDK938	CDK939	CDK940	CDK941	CDK942	CDK943	CDK944	CDK945	CDK946	CDK947	CDK948	CDK949	CDK950	CDK951	CDK952	CDK953	CDK954	CDK955	CDK956	CDK957	CDK958	CDK959	CDK960	CDK961	CDK962	CDK963	CDK964	CDK965	CDK966	CDK967	CDK968	CDK969	CDK970	CDK971	CDK972	CDK973	CDK974	CDK975	CDK976	CDK977	CDK978	CDK979	CDK980	CDK981	CDK982	CDK983	CDK984	CDK985	CDK986	CDK987	CDK988	CDK989	CDK990	CDK991	CDK992	CDK993	CDK994	CDK995	CDK996	CDK997	CDK998	CDK999	CDK1000
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Click on RED button for mutants or BLUE button for variants of ABL2

Click to download ABL2 sequence and its mutants' sequences

Command to synchronize all sequence data at local disc

Click to download all targets' sequences and their mutants' sequences

Figure 35. Sequence download.

7.2 Alignments: This module is to download the sequence alignment files in the CLUSTALW format of drug targets (wild type) with their mutants/natural variants. User can download either a specific or all sequence alignments. User has to click on RED button to select mutants' alignment and BLUE button for natural variants' alignment for the corresponding selected targets. User can either download alignment file containing a specific target and its mutants/natural variants or can browse whole directory containing all alignment files. Further, facility has been provided to synchronize all alignment data at user's local disc using rsync command (Figure 36).

CancerDR: Cancer Drug Resistance Database
CSIR - Institute of Microbial Technology, India

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Search > | Browse > | Alignment/Mutation > | Target Structure > | Map/Alignment > | Clusters/Groups > | Downloads >

Download Sequence Alignment of Drug Targets

This page allows users to download the sequence alignments of Target (wild type) and their mutants/variants. User can download either a specific or all sequence alignments. User has to click on RED button to select mutants' alignment and BLUE button for natural variants' alignment for the corresponding selected targets. User can either download alignment file containing a specific target and its mutants/natural variants or can browse whole directory containing all alignment files. Further, facility has been provided to synchronize all alignment data at user's local disc using rsync command (Figure 36).

Download ABL2 & mutants | **Browse Directory** | **rsync Facility**

This folder contains alignments of all targets and their mutants. User can download all the files.

This server allows the user to synchronize any alignment data folder in CancerDR using following command:
`rsync -avz --delete crdd.osdd.net::cancerdr/data/align/mut/abn/user_local_directory`

Select any one of the Targets

<input type="checkbox"/> ABL1	<input type="checkbox"/> ABL2	<input type="checkbox"/> AKT1	<input type="checkbox"/> AKT2	<input type="checkbox"/> AKT3	<input type="checkbox"/> ALK	<input type="checkbox"/> AR	<input type="checkbox"/> ATM	<input type="checkbox"/> AURKA	<input type="checkbox"/> AURKB
<input type="checkbox"/> AURKC	<input type="checkbox"/> BCL2	<input type="checkbox"/> CDK1	<input type="checkbox"/> CDK2	<input type="checkbox"/> CDK3	<input type="checkbox"/> CDK4	<input type="checkbox"/> CDK5	<input type="checkbox"/> CDK6	<input type="checkbox"/> CDK7	<input type="checkbox"/> CDK8
<input type="checkbox"/> CDK9	<input type="checkbox"/> CDK10	<input type="checkbox"/> CDK11	<input type="checkbox"/> CDK12	<input type="checkbox"/> CDK13	<input type="checkbox"/> CDK14	<input type="checkbox"/> CDK15	<input type="checkbox"/> CDK16	<input type="checkbox"/> CDK17	<input type="checkbox"/> CDK18
<input type="checkbox"/> CDK19	<input type="checkbox"/> CDK20	<input type="checkbox"/> CDK21	<input type="checkbox"/> CDK22	<input type="checkbox"/> CDK23	<input type="checkbox"/> CDK24	<input type="checkbox"/> CDK25	<input type="checkbox"/> CDK26	<input type="checkbox"/> CDK27	<input type="checkbox"/> CDK28
<input type="checkbox"/> CDK29	<input type="checkbox"/> CDK30	<input type="checkbox"/> CDK31	<input type="checkbox"/> CDK32	<input type="checkbox"/> CDK33	<input type="checkbox"/> CDK34	<input type="checkbox"/> CDK35	<input type="checkbox"/> CDK36	<input type="checkbox"/> CDK37	<input type="checkbox"/> CDK38
<input type="checkbox"/> CDK39	<input type="checkbox"/> CDK40	<input type="checkbox"/> CDK41	<input type="checkbox"/> CDK42	<input type="checkbox"/> CDK43	<input type="checkbox"/> CDK44	<input type="checkbox"/> CDK45	<input type="checkbox"/> CDK46	<input type="checkbox"/> CDK47	<input type="checkbox"/> CDK48
<input type="checkbox"/> CDK49	<input type="checkbox"/> CDK50	<input type="checkbox"/> CDK51	<input type="checkbox"/> CDK52	<input type="checkbox"/> CDK53	<input type="checkbox"/> CDK54	<input type="checkbox"/> CDK55	<input type="checkbox"/> CDK56	<input type="checkbox"/> CDK57	<input type="checkbox"/> CDK58
<input type="checkbox"/> CDK59	<input type="checkbox"/> CDK60	<input type="checkbox"/> CDK61	<input type="checkbox"/> CDK62	<input type="checkbox"/> CDK63	<input type="checkbox"/> CDK64	<input type="checkbox"/> CDK65	<input type="checkbox"/> CDK66	<input type="checkbox"/> CDK67	<input type="checkbox"/> CDK68
<input type="checkbox"/> CDK69	<input type="checkbox"/> CDK70	<input type="checkbox"/> CDK71	<input type="checkbox"/> CDK72	<input type="checkbox"/> CDK73	<input type="checkbox"/> CDK74	<input type="checkbox"/> CDK75	<input type="checkbox"/> CDK76	<input type="checkbox"/> CDK77	<input type="checkbox"/> CDK78
<input type="checkbox"/> CDK79	<input type="checkbox"/> CDK80	<input type="checkbox"/> CDK81	<input type="checkbox"/> CDK82	<input type="checkbox"/> CDK83	<input type="checkbox"/> CDK84	<input type="checkbox"/> CDK85	<input type="checkbox"/> CDK86	<input type="checkbox"/> CDK87	<input type="checkbox"/> CDK88
<input type="checkbox"/> CDK89	<input type="checkbox"/> CDK90	<input type="checkbox"/> CDK91	<input type="checkbox"/> CDK92	<input type="checkbox"/> CDK93	<input type="checkbox"/> CDK94	<input type="checkbox"/> CDK95	<input type="checkbox"/> CDK96	<input type="checkbox"/> CDK97	<input type="checkbox"/> CDK98
<input type="checkbox"/> CDK99	<input type="checkbox"/> CDK100	<input type="checkbox"/> CDK101	<input type="checkbox"/> CDK102	<input type="checkbox"/> CDK103	<input type="checkbox"/> CDK104	<input type="checkbox"/> CDK105	<input type="checkbox"/> CDK106	<input type="checkbox"/> CDK107	<input type="checkbox"/> CDK108
<input type="checkbox"/> CDK109	<input type="checkbox"/> CDK110	<input type="checkbox"/> CDK111	<input type="checkbox"/> CDK112	<input type="checkbox"/> CDK113	<input type="checkbox"/> CDK114	<input type="checkbox"/> CDK115	<input type="checkbox"/> CDK116	<input type="checkbox"/> CDK117	<input type="checkbox"/> CDK118
<input type="checkbox"/> CDK119	<input type="checkbox"/> CDK120	<input type="checkbox"/> CDK121	<input type="checkbox"/> CDK122	<input type="checkbox"/> CDK123	<input type="checkbox"/> CDK124	<input type="checkbox"/> CDK125	<input type="checkbox"/> CDK126	<input type="checkbox"/> CDK127	<input type="checkbox"/> CDK128
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7.3 Structures: This section assists the users to download the predicted structures of drug targets (wild type) along with their mutants/natural variants. User can download either a specific target structure and structure of its mutants/variants or can browse directory containing all targets' structures and their mutants/variants. User has to click on RED button to select mutants and BLUE button for natural variants against corresponding targets. Facility has been provided to synchronize data at user's local disc using rsync command (Figure 37).

7.4 PDB structures: This section allows the users to download the experimentally determined structures of drug targets (wild type) available from the Protein Data Bank. User can download either a specific target PDBs or can browse directory containing all targets'. User can also avail rsync facility to synchronize the structural data from the server to the local disc (Figure 38).

CancerDR: Cancer Drug Resistance Database
CSIR - Institute of Microbial Technology, India

Home General Information Submission Acknowledgement Guide Links Team Contact

Search
Browse
Alignment/Mutation
Target Structure
Map/Alignment
Clusters/Groups
Downloads

Download Tertiary Structure of Drug Targets

This allows users to download the predicted tertiary structures of Targets (wild type) and their mutants/natural variants predicted using highly accurate software HHSuite. User can download either a specific or all target structures. To synchronize structural data at your local disk using rsync. Click RED button to select mutants and BLUE button to select natural variants against corresponding target. For more information, please click [HERE](#).

Download ABL2 & variants Download wild type structure of drug target **ABL2** and its natural variants.

Browse Directory This folder contains structures of all targets and their variants. User can download all the files.

rsync Facility This server allows the user to synchronize any structure data folder in CancerDR using following command:
`rsync -avz --delete crdd.osdd.net::cancerdr/data/algo/var/fa/user_local_directory/`

Select any one of the Targets

<input type="checkbox"/> ABL1	<input type="checkbox"/> ABL2	<input type="checkbox"/> AKT1	<input type="checkbox"/> AKT2	<input type="checkbox"/> AKT3	<input type="checkbox"/> ALK	<input type="checkbox"/> AR	<input type="checkbox"/> ATM	<input type="checkbox"/> AURKA	<input type="checkbox"/> AURKB
<input type="checkbox"/> AURKC	<input type="checkbox"/> BCL2	<input type="checkbox"/> BRAF	<input type="checkbox"/> BTK	<input type="checkbox"/> CASP3	<input type="checkbox"/> CCR5	<input type="checkbox"/> CDK1	<input type="checkbox"/> CDK2	<input type="checkbox"/> CDK4	<input type="checkbox"/> CDK6
<input type="checkbox"/> CDK7	<input type="checkbox"/> CENP	<input type="checkbox"/> DHFR	<input type="checkbox"/> EGFR	<input type="checkbox"/> ERBB2	<input type="checkbox"/> FGFR1	<input type="checkbox"/> FGFR3	<input type="checkbox"/> FLT1	<input type="checkbox"/> FLT3	<input type="checkbox"/> HSP90A1
<input type="checkbox"/> FNTA	<input type="checkbox"/> GSK3A	<input type="checkbox"/> GSK3B	<input type="checkbox"/> HDAC1	<input type="checkbox"/> HDAC2	<input type="checkbox"/> HDAC3	<input type="checkbox"/> HDAC6	<input type="checkbox"/> HDAC8	<input type="checkbox"/> HSP90AB1	<input type="checkbox"/> HSP90AB2
<input type="checkbox"/> HSP90B1	<input type="checkbox"/> HSP90B2	<input type="checkbox"/> HSP90B3	<input type="checkbox"/> HSP90B4	<input type="checkbox"/> HSP90B5	<input type="checkbox"/> HSP90B6	<input type="checkbox"/> HSP90B7	<input type="checkbox"/> HSP90B8	<input type="checkbox"/> HSP90B9	<input type="checkbox"/> HSP90B10
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CancerDR: Cancer Drug Resistance Database
CSIR - Institute of Microbial Technology, India

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Browse >
Alignment/Mutation >
Target Structure >
Map/Alignment >
Clusters/Groups >
Downloads >

Download experimental structure of targets

We have extracted structures of drug targets/proteins from Protein DataBank (PDB). This module allows user to download experimentally determined structures of drug targets available in the PDB site. User can download either all the targets or specific target. Synchronization facility is provided to synchronize the data using rsync.

Download ABL2 PDB
This folder contains experimental structures of all targets in PDB format. User can download all the files.
rsync facility
This server allows the user to synchronize any structure data folder in CancerDR using following command:
`rsync -avz --delete crdd.osdd.net:casocdr/data/ser/exp_sst/ /user_local_directory/`

Select any one of the Targets

<input type="checkbox"/> ABL1	<input type="checkbox"/> ABL2	<input type="checkbox"/> AKT1	<input type="checkbox"/> AKT2	<input type="checkbox"/> AKT3	<input type="checkbox"/> ALK	<input type="checkbox"/> AR	<input type="checkbox"/> ATM	<input type="checkbox"/> AURKA	<input type="checkbox"/> AURKB
<input type="checkbox"/> AURKC	<input type="checkbox"/> BCL2	<input type="checkbox"/> CDK7	<input type="checkbox"/> CDK9	<input type="checkbox"/> BRAF	<input type="checkbox"/> BTK	<input type="checkbox"/> CASP3	<input type="checkbox"/> CCR5	<input type="checkbox"/> CDK1	<input type="checkbox"/> CDK2
<input type="checkbox"/> CDK6	<input type="checkbox"/> CDK7	<input type="checkbox"/> CDK9	<input type="checkbox"/> DHFR	<input type="checkbox"/> EGFR	<input type="checkbox"/> ERBB2	<input type="checkbox"/> FGFR1	<input type="checkbox"/> FGFR3	<input type="checkbox"/> FLT1	<input type="checkbox"/> FLT3
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