RASPD+ web server Manual

RASPD+

RApid Screening with Physicochemical Descriptors + Machine Learning

RASPD originally developed at Supercomputing Facility for Bioinformatics and Computational Biology (SCFBio)[1] IIT Delhi and further development was continued at Heidelberg Institute for Theoretical Studies (HITS)[2] as RASPD+.

RASPD+ web server developed at Supercomputing Facility for Bioinformatics and Computational Biology (SCFBio) IIT Delhi and the Standalone version of RASPD+ was developed at Heidelberg Institute for Theoretical Studies (HITS).

1. Mukherjee, G.; Jayaram, B. **A Rapid Identification of Hit Molecules for Target Proteins via Physico-Chemical Descriptors.** *Phys. Chem. Chem. Phys.* **2013**, *15* (23), 9107–9116.
2. Holderbach, S.; Adam, L.; Jayaram, B.; Wade, R. C.; Mukherjee, G. **RASPD+: Fast Protein-Ligand Binding Free Energy Prediction Using Simplified Physicochemical Features**. *Mol Biosci.* 2020, 17;7:601065.

RASPD^{+} (RApid Screening with Physicochemical Descriptors + Machine Learning) is a computationally fast protocol for identifying lead-like molecules based on predicted binding free energy against a target protein with a 3D structure and a defined ligand binding pocket. The RASPD^{+} web server provides 4 databases against which user can screen their target protein.

The 4 databases are as follows:

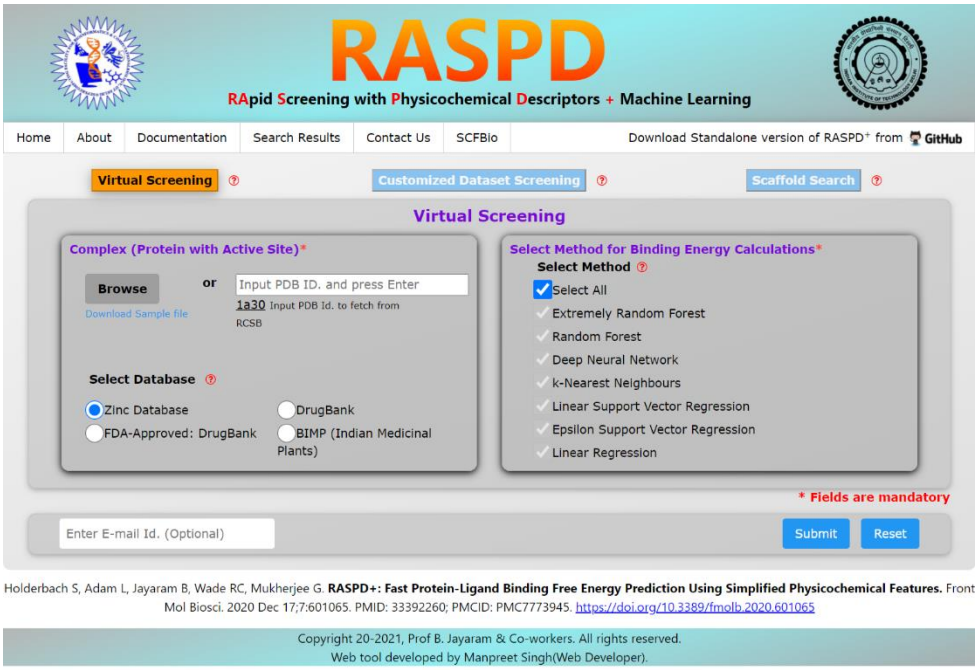
Zinc Database: This database contains 10 million small molecules from ZINC15 database.

DrugBank: This database contains small molecules from DrugBank database of Version 5.1.8. The total number of molecules are 8811.

FDA-Approved (DrugBank): This database contain only FDA (Food and Drug Administration) approved drugs from DrugBank database of Version 5.1.8. The total number of molecules are 3722.

BIMP: Bio-activity Informatics of Indian Medicinal Plants. It is a database of Indian medicinal plants containing 316 small molecules.

Availability - http://scfbio-iitd.res.in/raspd+/index.php



A help box is provided for each kind of job submission and required inputs. User can click on ⑦ icon to get detailed information instantly.

PDB Format:

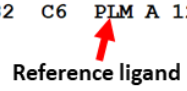
The term PDB stands for Protein Data Bank. One can download a .pdb file from RCSB website (https://www.rcsb.org/) or can generate from homology/ab-inito based tertiary structure protein modeling tool. To submit a job in RASPD^{+}, the .pdb file of protein must have one reference ligand or 1 active site identifier. A PDB file may contain multiple ligands, therefore user can select one reference ligand around which the binding energy will be calculated.

Here are shown the initial 3 residues of pdb file of PDBID 3QLM -

```
ATOM      1  N   ALA A   1      -35.373   6.813  -9.732  1.00 22.43           N
ATOM      2  CA  ALA A   1      -34.766   7.787 -10.700  1.00 24.10           C
ATOM      3  C   ALA A   1      -35.532   9.070 -10.512  1.00 24.15           C
ATOM      4  O   ALA A   1      -36.636   9.018 -10.001  1.00 25.04           O
ATOM      5  CB  ALA A   1      -34.934   7.285 -12.141  1.00 22.61           C
ATOM      6  N   LEU A   2      -35.009  10.194 -10.973  1.00 24.98           N
ATOM      7  CA  LEU A   2      -35.705  11.495 -10.850  1.00 26.29           C
ATOM      8  C   LEU A   2      -37.208  11.455 -11.123  1.00 26.82           C
ATOM      9  O   LEU A   2      -38.014  11.838 -10.259  1.00 28.78           O
ATOM     10  CB  LEU A   2      -35.066  12.562 -11.748  1.00 27.18           C
ATOM     11  CG  LEU A   2      -35.650  13.995 -11.731  1.00 28.79           C
ATOM     12  CD1 LEU A   2      -35.677  14.586 -10.354  1.00 28.02           C
ATOM     13  CD2 LEU A   2      -34.797  14.839 -12.620  1.00 28.82           C
ATOM     14  N   TRP A   3      -37.627  11.004 -12.290  1.00 26.26           N
ATOM     15  CA  TRP A   3      -39.056  11.002 -12.517  1.00 26.94           C
ATOM     16  C   TRP A   3      -39.833  10.216 -11.458  1.00 27.20           C
ATOM     17  O   TRP A   3      -40.987  10.529 -11.215  1.00 28.14           O
ATOM     18  CB  TRP A   3      -39.411  10.470 -13.902  1.00 27.00           C
ATOM     19  CG  TRP A   3      -39.275   8.941 -14.066  1.00 27.68           C
ATOM     20  CD1 TRP A   3      -38.147   8.239 -14.452  1.00 25.84           C
ATOM     21  CD2 TRP A   3      -40.324   7.957 -13.900  1.00 26.59           C
ATOM     22  NE1 TRP A   3      -38.445   6.892 -14.520  1.00 26.62           N
ATOM     23  CE2 TRP A   3      -39.760   6.692 -14.195  1.00 24.26           C
ATOM     24  CE3 TRP A   3      -41.687   8.035 -13.543  1.00 28.65           C
ATOM     25  CZ2 TRP A   3      -40.494   5.502 -14.130  1.00 28.40           C
ATOM     26  CZ3 TRP A   3      -42.441   6.827 -13.450  1.00 30.89           C
ATOM     27  CH2 TRP A   3      -41.829   5.575 -13.750  1.00 30.81           C
```

The format of reference ligand in protein file is shown below-

```
ATOM    969  CB  CYS A 124     -27.628  29.868   0.465  1.00 34.87           C
ATOM    970  SG  CYS A 124     -29.437  29.878   0.230  1.00 34.44           S
ATOM    971  OXT CYS A 124     -24.973  30.231   1.130  1.00 35.01           O
TER     972      CYS A 124
HETATM  975  C1  PLM A 127     -30.827  17.169 -12.858  0.80 58.38           C
HETATM  976  O1  PLM A 127     -30.818  15.972 -13.261  0.80 58.32           O
HETATM  977  O2  PLM A 127     -29.833  17.937 -12.733  0.80 57.59           O
HETATM  978  C2  PLM A 127     -32.185  17.751 -12.493  0.80 57.69           C
HETATM  979  C3  PLM A 127     -32.568  17.307 -11.104  0.80 57.42           C
HETATM  980  C4  PLM A 127     -33.089  18.513 -10.350  0.80 59.69           C
HETATM  981  C5  PLM A 127     -32.267  18.750  -9.062  0.80 61.33           C
HETATM  982  C6  PLM A 127     -32.685  17.756  -7.953  0.80 61.68           C
```



A PDB file having active site info will look like-

```
ATOM    931   CG LYS   778       10.475   7.812  66.858  1.00 62.24           C 0
ATOM    932   CD LYS   778        9.765   6.468  67.039  1.00 62.24           C 0
ATOM    933   CE LYS   778        9.114   6.299  68.414  1.00 62.24           C 0
ATOM    934   NZ LYS   778       10.142   6.345  69.477  1.00 62.24           N 0
ATOM    935    C LYS   778        9.742  11.355  68.249  1.00 62.24           C 0
ATOM    936    O LYS   778        9.462  11.208  69.470  1.00 62.24           O 0
ATOM    937  OXT LYS   778        9.394  12.351  67.562  1.00 62.24           O 0
TER
HETATM 1114  POL STP C   1       44.037  49.900  73.020  0.00  0.00          Ve
```

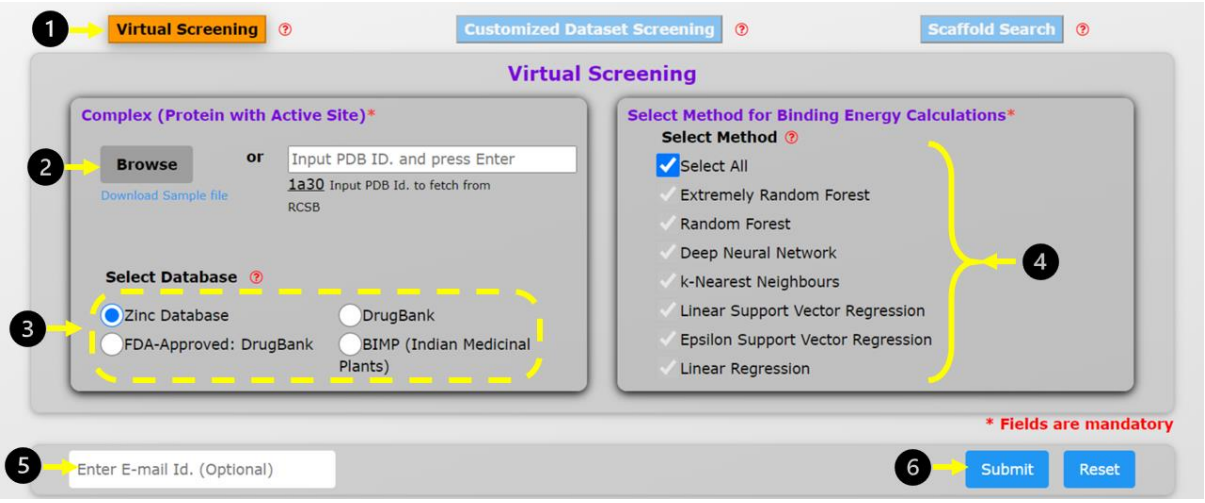
Job Submission

There are 3 methods in RASPD^{+} methodology-

Method 1: Virtual Screening:

This method estimates the binding affinity of a single protein ligand complex against one of the 4 available databases on the web tool. To submit the job-

1. Click on **Virtual Screening** button (default method).
2. Click on Browse button to upload protein and specify reference ligand (or active site identifier).
3. Out of 4 databases, select one database against which you want to screen your protein. Default selected database is Zinc database.
4. Select machine learning method for binding energy calculation. User can select one method or All methods for Binding Affinity at a time. (Default: All)
5. Specify your email id in text box to get a notification after the completion of the job. (optional)
6. Now click on submit button to run your job.



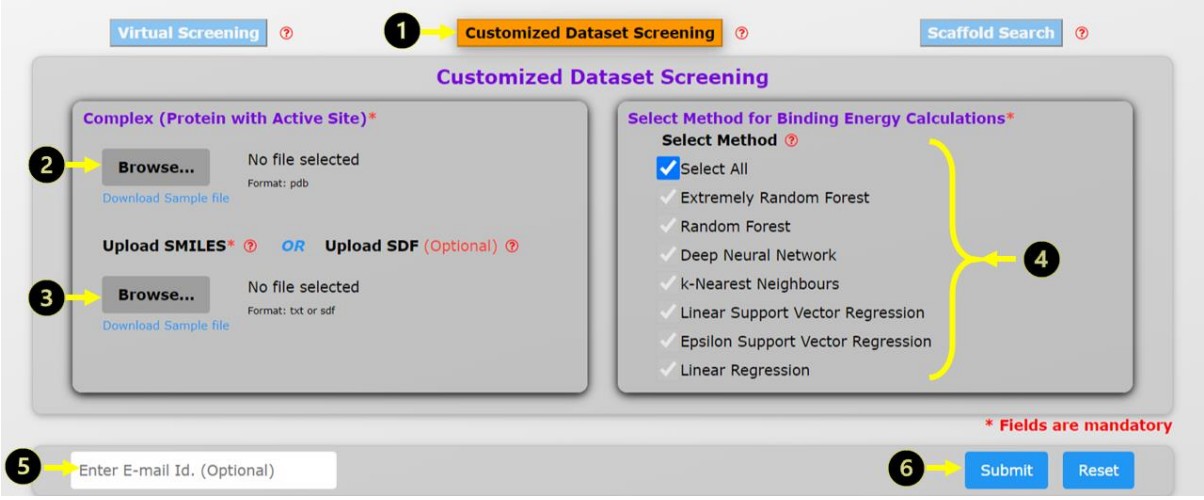
Method 2: Customised dataset Screening:

User can screen protein against their own dataset (custom dataset). User can either upload a .txt file or a .sdf file to create customised dataset. A .txt file should contain ligand information in SMILES format one in each line. Text file should not contain more than 1000 SMILES in .txt file and in .sdf file. A sample text file for SMILES is shown below-

```
CCC[C@@H](C)[N+]1=c2c(c(cc([nH]2)C)C)C(=O)[NH+]1
CC[n+]1c(c(c([nH]1)C)CNC(=O)[C@@H]1CCC(=O)N(C1)CCC[NH+]1CCOCC1)C
Cc1ccsc1C(=O)N1CCOc2c(cc(cc2OC)c2c(ncc(n2)C)C)C1
Cc1c2ccccc2oc1C(=O)N1CCN(CC1)Cc1cccc(c1)F
CC(=O)c1ccc(s1)C(=O)NC[C@@H]1Cc2cc(cc(c2O1)F)c1ccccn1
CC1=CC[C@H]2C[C@@H]([C@H]([NH+]C2=C1)N1CCN(CC1)C(=O)C)CN(C1CC1)C(=O)[C@H]1CCCO1
c1ccc2c(c1)c1ccc(cc1o2)/N=C/c1cc(ccc1O)Br
c1ccc(cc1)[C@@H]1[C@@H](C21C(=O)c1ccccc1C2=O)C(=O)c1ccc(cc1)N(=O)=O
C=CCn1nc(nn1)NC(=O)c1cccc(c1)F
CC1=C([C@H]([n+]2c([nH]cn2)N1)c1ccc(cc1)C(=O)OC)C(=O)Nc1ccc(cc1)Cl
CCCS(=O)(=O)c1ncc(c(n1)C(=O)Nc1ccc(cc1)OC(F)F)Cl
Cc1ccc(c(c1)O[C@@H](C)C(=O)Nc1ccccc1C(=O)N1CCCC1)C
CC(C)COc1ccc(cc1)CN(Cc1ccncc1)C(=O)/C=C/c1cccc(c1)F
c1ccc(cc1)SC1=CS(=O)(=O)CC1
```

To submit a customised database job,

1. Click on **Customised Dataset Screening** button.
2. Click on first Browse button to upload protein in .pdb format and specify reference ligand (or active site identifier).
3. Click on second Browse button to upload customised dataset in .txt format.
4. Select the machine learning method for binding affinity calculation (default Select All).
5. Specify your email id in text box to get a notification after the completion of the job. (optional)
6. Now click on submit button to run your job.



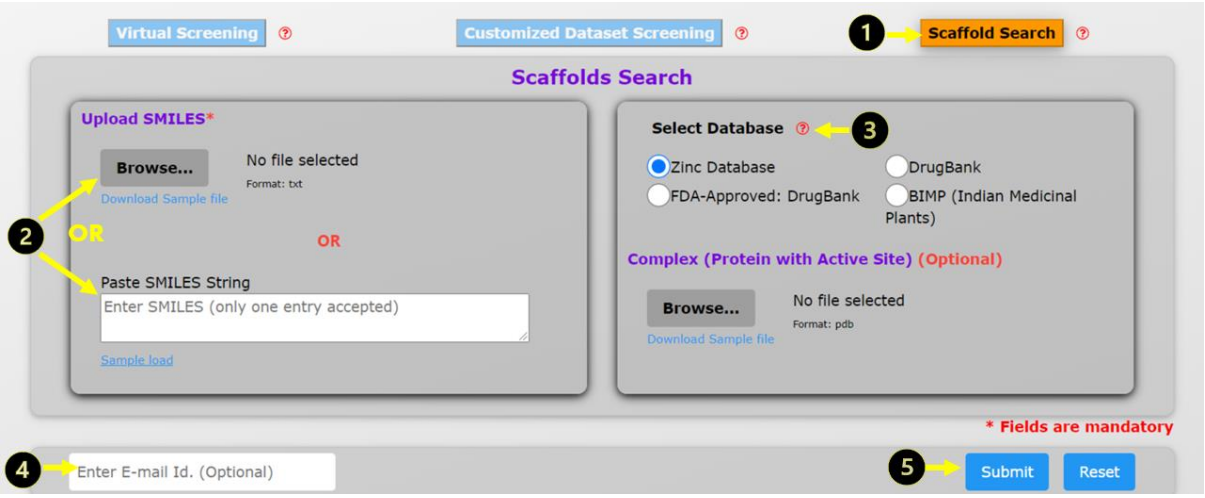
Method 3: Scaffold Search:

This option enable user to filter molecules from million/customised dataset having several scaffolds/functional groups. If one needs to select an active scaffold from it, the SMILES codes of this query active scaffold need to be supplied. User can either paste one scaffold in SMILE format in given text box or can upload a .txt file having only one scaffold. Sample file is given below-

C1=CC=CC=C1

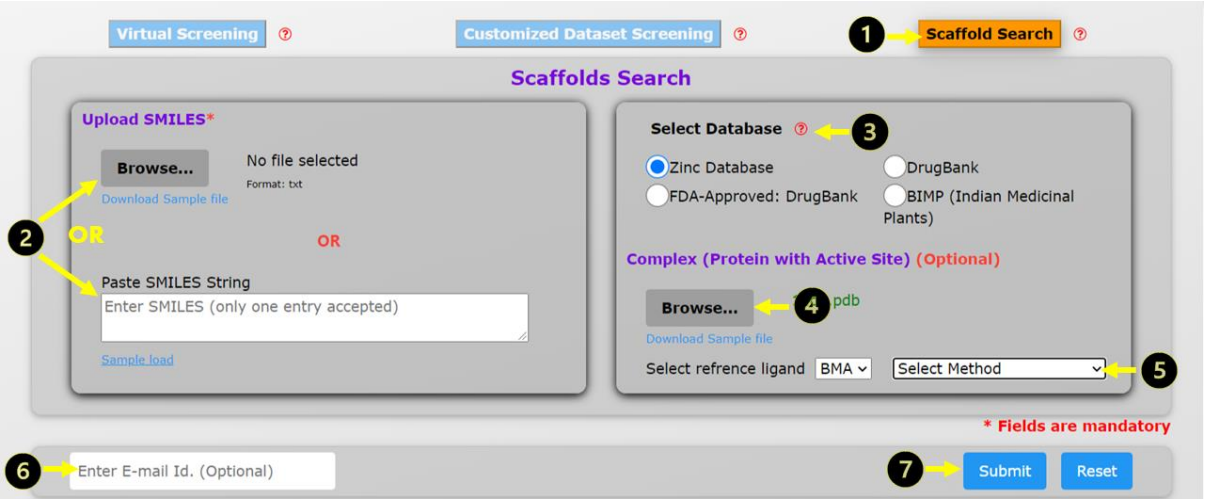
If user only wants to search small molecule having the scaffold, then

1. Click on **Scaffold Search** button.
2. Either click on Browse button to upload .txt file having one scaffold in SMILE format or paste (or type) scaffold in given text box
3. select one database against which you want to search. (Default Zinc Database)
4. Specify your email id in text box to get a notification after the completion of the job. (optional)
5. Now click on Submit button to run your job.



If user wants to search small molecule having the scaffold and want to screen target protein against search hit, then

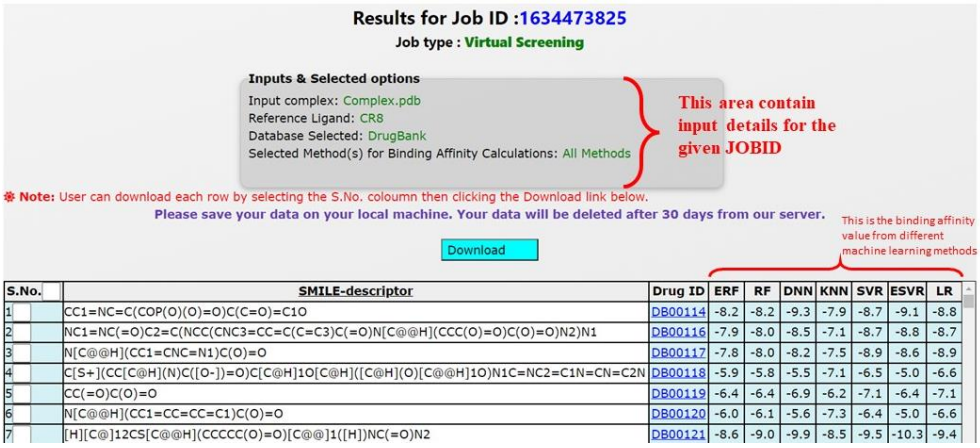
1. Click on **Scaffold Search** button.
2. Either click on browse button to upload .txt file having one scaffold in SMILE format or paste (or type) scaffold in given text box
3. select one database against which you want to search. (Default Zinc Database)
4. Click on browse button to upload protein in .pdb format and specify reference ligand (or active site identifier).
5. Select machine learning method for binding energy calculation.
6. Specify your email id in text box to get a notification after the completion of the job. (optional)
7. Now click on Submit button to run your job.



Results

Virtual Screening:

Virtual screening result of “all machine learning method” is shown below-



Results for Job ID :1634473825

Job type : Virtual Screening

Inputs & Selected options

Input complex: Complex.pdb
Reference Ligand: CR8
Database Selected: DrugBank
Selected Method(s) for Binding Affinity Calculations: All Methods

This area contain input details for the given JOBID

Note: User can download each row by selecting the S.No. coloumn then clicking the Download link below.

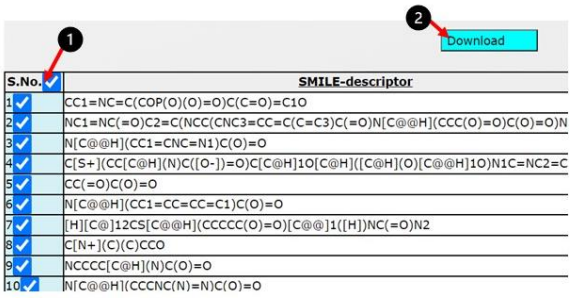
Please save your data on your local machine. Your data will be deleted after 30 days from our server.

Download

This is the binding affinity value from different machine learning methods

S.No.	SMILE-descriptor	Drug ID	ERF	RF	DNN	KNN	SVR	ESVR	LR
1	CC1=NC=C(COP(O)(O)=O)C(C=O)=C1O	DB00114	-8.2	-8.2	-9.3	-7.9	-8.7	-9.1	-8.8
2	NC1=NC(=O)C2=C(NCC(CNC3=CC=C(C=C3)C(=O)N[C@@H](CCC(O)=O)C(O)=O)N2)N1	DB00116	-7.9	-8.0	-8.5	-7.1	-8.7	-8.8	-8.7
3	N[C@@H](CC1=CNC=N1)C(O)=O	DB00117	-7.8	-8.0	-8.2	-7.5	-8.9	-8.6	-8.9
4	C[S+](CC[C@H](N)C([O-])=O)C[C@H]1O[C@H]([C@H](O)[C@@H]1O)N1C=NC2=C1N=CN=C2N	DB00118	-5.9	-5.8	-5.5	-7.1	-6.5	-5.0	-6.6
5	CC(=O)C(O)=O	DB00119	-6.4	-6.4	-6.9	-6.2	-7.1	-6.4	-7.1
6	N[C@@H](CC1=CC=CC=C1)C(O)=O	DB00120	-6.0	-6.1	-5.6	-7.3	-6.4	-5.0	-6.6
7	[H][C@]12CS[C@@H](CCCCC(O)=O)[C@@]1([H])NC(=O)N2	DB00121	-8.6	-9.0	-9.9	-8.5	-9.5	-10.3	-9.4

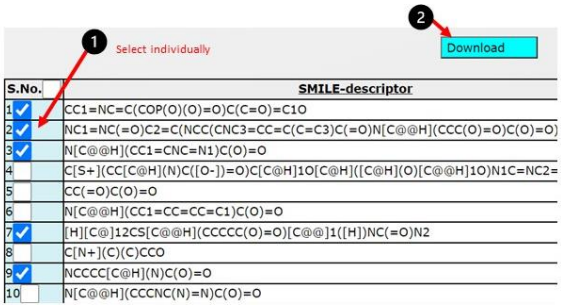
To download the whole result, check the serial number box and hit the **“Download”** button. The result will be downloaded in .csv format. User can also download only selected result by selecting individual serial number and then “**Download**” button. On clicking at Drug ID’s, users are navigated to respective database for the detailed information of ligand.



1

2 Download

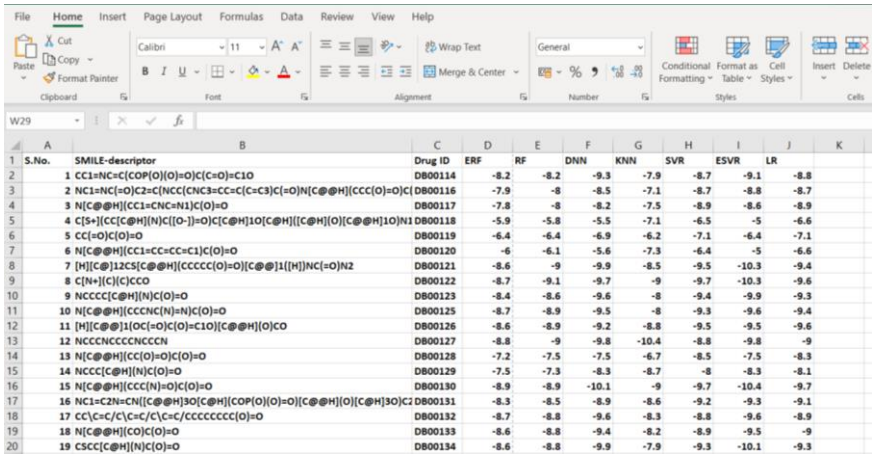
S.No.	SMILE-descriptor
1	CC1=NC=C(COP(O)(O)=O)C(C=O)=C1O
2	NC1=NC(=O)C2=C(NCC(CNC3=CC=C(C=C3)C(=O)N[C@@H](CCC(O)=O)C(O)=O)N
3	N[C@@H](CC1=CNC=N1)C(O)=O
4	C[S+](CC[C@H](N)C([O-])=O)C[C@H]1O[C@H]([C@H](O)[C@@H]1O)N1C=NC2=C
5	CC(=O)C(O)=O
6	N[C@@H](CC1=CC=CC=C1)C(O)=O
7	[H][C@]12CS[C@@H](CCCCC(O)=O)[C@@]1([H])NC(=O)N2
8	C[N+](C)(C)CCO
9	NCCCC[C@H](N)C(O)=O
10	N[C@@H](CCCNC(N)=N)C(O)=O



1 Select individually

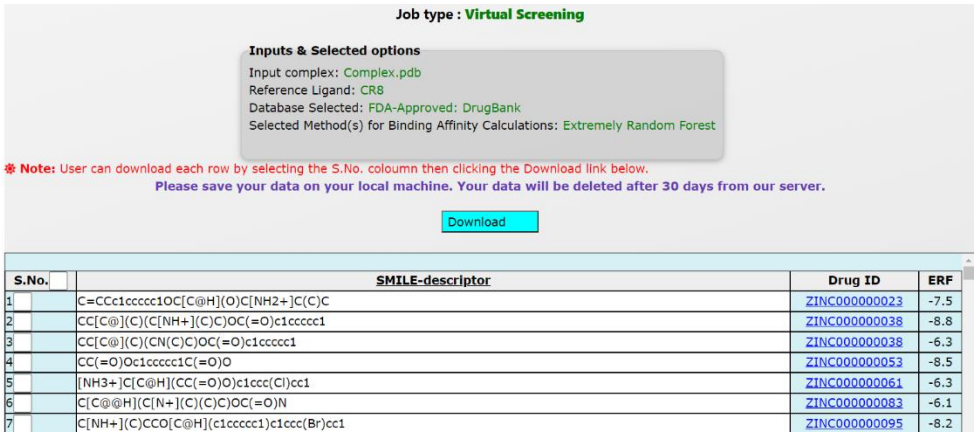
2 Download

S.No.	SMILE-descriptor
1	CC1=NC=C(COP(O)(O)=O)C(C=O)=C1O
2	NC1=NC(=O)C2=C(NCC(CNC3=CC=C(C=C3)C(=O)N[C@@H](CCC(O)=O)C(O)=O)
3	N[C@@H](CC1=CNC=N1)C(O)=O
4	C[S+](CC[C@H](N)C([O-])=O)C[C@H]1O[C@H]([C@H](O)[C@@H]1O)N1C=NC2=
5	CC(=O)C(O)=O
6	N[C@@H](CC1=CC=CC=C1)C(O)=O
7	[H][C@]12CS[C@@H](CCCCC(O)=O)[C@@]1([H])NC(=O)N2
8	C[N+](C)(C)CCO
9	NCCCC[C@H](N)C(O)=O
10	N[C@@H](CCCNC(N)=N)C(O)=O



S.No.	SMILE-descriptor	Drug ID	ERF	RF	DNN	KNN	SVR	ESVR	LR
1	CC1=NC=C(COP(O)(O)=O)C(C=O)=C1O	DB00114	-8.2	-8.2	-9.3	-7.9	-8.7	-9.1	-8.8
2	NC1=NC(=O)C2=C(NCC(CNC3=CC=C(C=C3)C(=O)N[C@@H](CCC(O)=O)C(	DB00116	-7.9	-8	-8.5	-7.1	-8.7	-8.8	-8.7
3	N[C@@H](CC1=CNC=N1)C(O)=O	DB00117	-7.8	-8	-8.2	-7.5	-8.9	-8.6	-8.9
4	C[S+](CC[C@H](N)C([O-])=O)C[C@H]1O[C@H]([C@H](O)[C@@H]1O)N1	DB00118	-5.9	-5.8	-5.5	-7.1	-6.5	-5	-6.6
5	CC(=O)C(O)=O	DB00119	-6.4	-6.4	-6.9	-6.2	-7.1	-6.4	-7.1
6	N[C@@H](CC1=CC=CC=C1)C(O)=O	DB00120	-6	-6.1	-5.6	-7.3	-6.4	-5	-6.6
7	[H][C@]12CS[C@@H](CCCCC(O)=O)[C@@]1([H])NC(=O)N2	DB00121	-8.6	-9	-9.9	-8.5	-9.5	-10.3	-9.4
8	C[N+](C)(C)CCO	DB00122	-8.7	-9.1	-9.7	-9	-9.7	-10.3	-9.6
9	NCCCC[C@H](N)C(O)=O	DB00123	-8.4	-8.6	-9.6	-8	-9.4	-9.9	-9.3
10	N[C@@H](CCCNC(N)=N)C(O)=O	DB00125	-8.7	-8.9	-9.5	-8	-9.3	-9.6	-9.4
11	[H][C@@]1(OC(=O)C(O)=C1O)[C@@H](O)CO	DB00126	-8.6	-8.9	-9.2	-8.8	-9.5	-9.5	-9.6
12	NCCCNCCCCNCCCN	DB00127	-8.8	-9	-9.8	-10.4	-8.8	-9.8	-9
13	N[C@@H](CC(O)=O)C(O)=O	DB00128	-7.2	-7.5	-7.5	-6.7	-8.5	-7.5	-8.3
14	NCCC[C@H](N)C(O)=O	DB00129	-7.5	-7.3	-8.3	-8.7	-8	-8.3	-8.1
15	N[C@@H](CCC(N)=O)C(O)=O	DB00130	-8.9	-8.9	-10.1	-9	-9.7	-10.4	-9.7
16	NC1=C2N=CN([C@@H]3O[C@H](COP(O)(O)=O)[C@@H](O)[C@H]3O)C2	DB00131	-8.3	-8.5	-8.9	-8.6	-9.2	-9.3	-9.1
17	CC\C=C/C\C=C/C\C=C/CCCCCCCC(O)=O	DB00132	-8.7	-8.8	-9.6	-8.3	-8.8	-9.6	-8.9
18	N[C@@H](CO)C(O)=O	DB00133	-8.6	-8.8	-9.4	-8.2	-8.9	-9.5	-9
19	CSCC[C@H](N)C(O)=O	DB00134	-8.6	-8.8	-9.9	-7.9	-9.3	-10.1	-9.3

Virtual screening result of one machine learning method-



Job type : Virtual Screening

Inputs & Selected options

Input complex: Complex.pdb
Reference Ligand: CR8
Database Selected: FDA-Approved: DrugBank
Selected Method(s) for Binding Affinity Calculations: Extremely Random Forest

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S.No.	SMILE-descriptor	Drug ID	ERF
1	C=CCc1ccccc1OC[C@H](O)C[NH2+]C(C)C	ZINC000000023	-7.5
2	CC[C@](C)(C)(C[NH+](C)C)OC(=O)c1ccccc1	ZINC000000038	-8.8
3	CC[C@](C)(CN(C)C)OC(=O)c1ccccc1	ZINC000000038	-6.3
4	CC(=O)Oc1ccccc1C(=O)O	ZINC000000053	-8.5
5	[NH3+]C[C@H](CC(=O)O)c1ccc(Cl)cc1	ZINC000000061	-6.3
6	C[C@@H](C[N+](C)(C)C)OC(=O)N	ZINC000000083	-6.1
7	C[NH+](C)CCO[C@H](c1ccccc1)c1ccc(Br)cc1	ZINC000000095	-8.2

Customised dataset screening:

Customised dataset screening result containing the predicted binding free energies of the query molecules is shown below for “All methods” and for “one method”-

Results for Job ID :1635831462

Job type : Customized Dataset Screening

Inputs & Selected options

Input complex: Complex.pdb
Input smiles: Molecules.txt
Reference Ligand: 486
Selected Method(s) for Binding Affinity Calculations: All Methods

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S.No.	SMILE-descriptor	ERF	RF	DNN	KNN	SVR	ESVR	LR
1	CCC[C@@H](C)[N+]1=c2c(cc([nH]2)C)C)C(=O)[NH+]1	-6.5	-6.7	-6.6	-6.8	-5.7	-7.7	-5.7
2	CC[n+]1c(c(c([nH]1)C)CNC(=O)[C@@H]1CCC(=O)N(C1)CCC[NH+]1CCOCC1)C	-7.5	-7.7	-6.7	-6.9	-6.3	-8.1	-6.2
3	Cc1ccsc1C(=O)N1CCOc2c(cc(cc2OC)c2c(ncc(n2)C)C)C1	-8.0	-8.0	-8.2	-6.8	-7.3	-9.5	-7.1
4	Cc1c2ccccc2oc1C(=O)N1CCN(CC1)Cc1cccc(c1)F	-7.7	-7.9	-7.8	-6.7	-6.8	-9.1	-6.6
5	CC(=O)c1ccc(s1)C(=O)NC[C@@H]1Cc2cc(cc(c2O1)F)c1ccccn1	-7.9	-8.0	-7.8	-6.8	-6.9	-9.1	-6.7
6	CC1=CC[C@H]2C[C@@H]([C@H]([NH+]C2=C1)N1CCN(CC1)C(=O)C)CN(C1CC1)C(=O)[C@@H]1CCCO1	-7.8	-7.7	-7.8	-7.3	-7.1	-9.1	-6.9
7	c1ccc2c(c1)c1ccc(cc1o2)/N=C/c1cc(occ1O)Br	-8.1	-8.1	-7.9	-6.8	-7.2	-9.1	-6.9
8	c1ccc(cc1)[C@@H]1[C@@H]([C21C(=O)c1ccccc1C2=O)C(=O)c1ccc(cc1)N(=O)=O	-7.9	-8.0	-8.0	-6.9	-7.1	-9.4	-6.9
9	C=CCn1nc(nn1)NC(=O)c1cccc(c1)F	-6.6	-6.8	-6.7	-6.9	-5.5	-8.0	-5.5
10	CC1=C([C@H]([n+]2c([nH]cn2)N1)c1ccc(cc1)C(=O)OC)C(=O)Nc1ccc(cc1)Cl	-7.7	-8.0	-7.4	-8.0	-7.0	-8.6	-6.8

Results for Job ID :1635833476

Job type : Customized Dataset Screening

Inputs & Selected options

Input complex: Complex.pdb
Input smiles: Molecules.txt
Reference Ligand: 486
Selected Method(s) for Binding Affinity Calculations: Extremely Random Forest

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S.No.	SMILE-descriptor	ERF
1	CCC[C@@H](C)[N+]1=c2c(cc([nH]2)C)C)C(=O)[NH+]1	-6.5
2	CC[n+]1c(c(c([nH]1)C)CNC(=O)[C@@H]1CCC(=O)N(C1)CCC[NH+]1CCOCC1)C	-7.5
3	Cc1ccsc1C(=O)N1CCOc2c(cc(cc2OC)c2c(ncc(n2)C)C)C1	-8.0
4	Cc1c2ccccc2oc1C(=O)N1CCN(CC1)Cc1cccc(c1)F	-7.7
5	CC(=O)c1ccc(s1)C(=O)NC[C@@H]1Cc2cc(cc(c2O1)F)c1ccccn1	-7.9
6	CC1=CC[C@H]2C[C@@H]([C@H]([NH+]C2=C1)N1CCN(CC1)C(=O)C)CN(C1CC1)C(=O)[C@@H]1CCCO1	-7.8
7	c1ccc2c(c1)c1ccc(cc1o2)/N=C/c1cc(occ1O)Br	-8.1
8	c1ccc(cc1)[C@@H]1[C@@H]([C21C(=O)c1ccccc1C2=O)C(=O)c1ccc(cc1)N(=O)=O	-7.9
9	C=CCn1nc(nn1)NC(=O)c1cccc(c1)F	-6.6
10	CC1=C([C@H]([n+]2c([nH]cn2)N1)c1ccc(cc1)C(=O)OC)C(=O)Nc1ccc(cc1)Cl	-7.7

Scaffold search result:

Scaffold search result without target protein contain SMILE descriptor which have query scaffold and Drug Id of small molecules while Scaffold search result with target protein have SMILE descriptor, Drug Id, and predicted binding energy values against target protein from different machine learning methods.

Results for Job ID :1635744021

Job type : Scaffold Search

Inputs & Selected options

Input smiles: Scaffold.txt
Database Selected: DrugBank

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S.No.	SMILE-descriptor	Drug ID
1	N[C@@H](CC1=CNC=N1)C(O)=O	DB00117
2	[H][C@]12CS[C@@H](CCCCC(O)=O)[C@@]1([H])NC(=O)N2	DB00121
3	C[C@H](CCCC(C)(C)O)[C@@]1([H])CC[C@@]2([H])\C(CCC[C@]12C)=C\C=C1\C[C@@H](O)C[C@H](O)C1=C	DB00136
4	[H]C(=O)[C@H](NC(C)=O)[C@@H](O)[C@H](O)[C@H](O)CO	DB00141
5	N[C@@H](CS)C(O)=O	DB00151
6	CC\C=C/C\C=C/C\C=C/C\C=C/C\C=C/CCCC(O)=O	DB00159
7	CC1=C(O)C(CO)=C(CO)C=N1	DB00165
8	CC(C)CCC[C@@H](C)[C@@]1([H])CC[C@@]2([H])\C(CCC[C@]12C)=C\C=C1\C[C@@H](O)CCC1=C	DB00169
9	NC1=NC=NC2=C1N=CN2[C@@H]1O[C@H](COP(O)(=O)OP(O)(=O)OP(O)(O)=O)[C@@H](O)[C@H]1O	DB00171
10	CCCCC(=O)N(CC1=CC=C(C=C1)C1=CC=CC=C1)C1=NNN=N1)[C@@H](C)C(C)C(O)=O	DB00177

Results for Job ID :1635832082

Job type : Scaffold Search

Inputs & Selected options

Input complex: Complex.pdb
Input smiles: Scaffold.txt
Reference Ligand: 486
Database Selected: DrugBank
Selected Method(s) for Binding Affinity Calculations: ALL

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S.No.	SMILE-descriptor	Drug ID	ERF	RF	DNN	KNN	SVR	ESVR	LR
1	CC[C@](C)(C)[C@H](C)C(=O)c1ccccc1 ZINC000000000038	DB00116	-7.2	-7.2	-7.2	-6.2	-6.4	-6.8	-6.4
2	CC[C@](C)(C)CN(C)C)OC(=O)c1ccccc1 ZINC000000000038	DB00117	-7.3	-7.4	-7.2	-5.9	-6.6	-7.1	-6.6
3	CC(=O)Oc1ccccc1C(=O)O ZINC000000000053	DB00118	-5.9	-5.8	-6.1	-5.4	-5.0	-6.3	-4.9
4	[NH3+]C[C@H](CC(=O)O)c1ccc(Cl)cc1 ZINC000000000061	DB00119	-6.3	-6.4	-6.7	-6.1	-5.6	-6.5	-5.6
5	C[C@@H](C[N+](C)(C)C)OC(=O)N ZINC000000000083	DB00120	-6.0	-6.0	-6.0	-5.8	-4.8	-6.0	-4.8
6	CN(C)CCO[C@H](c1ccccc1)c1ccc(Br)cc1 ZINC000000000095	DB00122	-8.9	-8.9	-8.6	-9.2	-7.9	-8.5	-7.8
7	C[NH+](C)CC[C@@H](c1ccc(Br)cc1)c1ccccn1 ZINC000000000096	DB00123	-8.8	-9.2	-8.7	-9.1	-7.8	-8.2	-7.9
8	C[NH+](C)CCO[C@@H](c1ccc(Cl)cc1)c1ccccn1 ZINC000000000122	DB00125	-8.4	-8.5	-8.1	-8.5	-7.2	-7.9	-7.2
9	CN(C)CCO[C@@H](c1ccc(Cl)cc1)c1ccccn1 ZINC000000000122	DB00126	-8.7	-8.7	-8.2	-8.8	-7.4	-8.3	-7.4
10	CC(C)(C)[NH2+]C[C@@H](O)COc1cccc2c1CCC(=O)N2 ZINC000000000128	DB00127	-9.1	-9.0	-9.1	-9.3	-7.8	-8.6	-8.0