

# SMCVdbTutorial

**Case 1: Searching the database**

**Case 2: Filtering compounds based on molecular weight**

**Case 3: Filtering compounds based on viability value**

**Case 4 : Downloading microscopy image data of a specific compound**

**Case 5: Commercial procurement information for a specific compound**

**Case 6: Downloading compound in molecular docking-supported format**

**Case 7: Accessing PubChem Information for a specific compound**

**Case 8: Performing ADME(T) analysis of a selected compound**

**Case 9: Target prediction for a specific compound**

**Case 10: User support**

# Case 1 : Searching the database

## Example 1: Using Chemical group name

- For example **Benzofuran**, a key building block in nature, finds itself not only in biologically active natural products but also in synthetic materials. This versatile scaffold boasts a range of potential health benefits, including anti-inflammatory, antimicrobial, antifungal, antidiabetic, pain-relieving, antiparasitic, and antitumor properties.

Enter "Benzofuran"

322 entries found

SMCV ID	Source ID	PubChem CID	MW	IUPAC Name	SMILES	Viability	Reference Image
RCB_C50351	10587705	74230129	351.4	N-(2,1,3-benzoxadiazol-5-ylmethyl)-6-methoxy-N,3-dimethyl-1-benzofuran-2-carboxamide	<chem>Cc1c(C(N(C)C)C2cc3nonc3cc2)=O)oc2c1ccc(OC)c2</chem>	83.43	
RCB_C50641	11091641	72838317	295.3	2-ethyl-N-[(3-methyl-1-benzofuran-2-yl)methyl]-5-pyrimidinecarboxamide	<chem>CCc(nc1)nc1C(NC1c(C)cccc2)c2o1=O</chem>	94.27	
RCB_C50671	11139671	70705295	316.4	6-methoxy-3-methyl-N-[2-(1,3-thiazol-2-yl)ethyl]-1-benzofuran-2-carboxamide	<chem>Cc1c(C(NCCC2nccs2)=O)oc2c1ccc(OC)c2</chem>	82.06	
RCB_CS1172	11948397	77078991	340.5	1-[(2,2-dimethyl-2,3-dihydro-1-benzofuran-5-yl)methyl]-4-[(1-methyl-1H-imidazol-2-yl)methyl]piperazine	<chem>CC(C)(C1)Oc2c1cc(CN1CCN(Cc3nccn3C)CC1)cc2</chem>	103.01	
RCB_CS1228	12045054	91760515	315.4	N-[2,3-dihydro-1-benzofuran-5-yl]-(cis-3-hydroxycyclobutyl)methylcyclopentanecarboxamide	<chem>O[C@H](C1)C[C@H]1C(c1cc1)cc2c1OCC2)NC(C1CCCC1)=O</chem>	100.11	
RCB_CS1314	12119974	72839553	354.4	N-[(3S*,4R*)-1-(2,3-dihydro-1-benzofuran-5-yl)carbonyl]-4-(5-methyl-2-furyl)pyrrolidin-3-yl]acetamide	<chem>CC(N[C@@H](CN(C)C1C(c1cc1)cc3c2OCC3)=O)[C@H]1c1ccc(Co1)=O</chem>	91.32	
		NA	270.3	1-methyl-N-[(2-methyl-2,3-dihydro-1-benzofuran-5-yl)methyl]-1H-pyrrole-2-carboxamide	<chem>CC(C1)Oc2c1cc(CNC(c1cccn1C)=O)cc2</chem>	84.39	
		70707064	317.4	2-(ethoxymethyl)-1-[(6-methoxy-3-methyl-1-benzofuran-2-yl)carbonyl]pyrrolidine	<chem>CCOCC(CCC1)N1C(c1c(C)ccc(OC)c2)c2o1=O</chem>	71.31	
RCB_CS3449	14930133	91761793	357.4	N-[[cis-3-hydroxycyclobutyl]([1-methyl-1H-pyrazol-4-yl)methyl]-2-methyl-4-oxo-4,5,6,7-tetrahydro-1-benzofuran-3-carboxamide	<chem>Cc1c(C(NC([C@H](C2)C[C@H]2O)c2cn(C)nc2)=O)c(C(C)CC2)=O)c2o1</chem>	40.05	
RCB_CS3883	15288886	70709146	352.4	N-[(4-methoxy-3,5-dimethyl-2-pyridinyl)methyl]-N,3,6-trimethyl-1-benzofuran-2-carboxamide	<chem>Cc1c(C(N(C)C)C2ncc(C)c(OC)c2C)=O)oc2c1ccc(C)c2</chem>	118.89	

Showing 1 to 10 of 322 entries (filtered from 24,361 total entries)

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# Case 1 : Searching the database

## Example 1: Using Chemical group name

- For example **Pyrazole**, Pyrazole-containing molecules display a broad range of biological activities, including anti-inflammatory, anticonvulsant, anticancer, antiviral, antidepressant, analgesic, antibacterial, antifungal, and selective enzyme inhibition.

The screenshot displays the SMCVdb search results for the query "pyrazole". A yellow callout box at the top right points to the search input field with the text "Enter 'Pyrazole'". A yellow callout box at the bottom left points to the search results with the text "585 entries found". The search results are displayed in a table with columns: SMCV\_id, Source ID, MW, Name, Smiles, Viability, and Reference image. The table shows 10 entries, with the first entry being RCB\_CS0194 and the last entry being RCB\_CS0985. The search bar at the top right contains the text "pyrazole".

SMCV_id	Source ID	MW	Name	Smiles	Viability	Reference image
RCB_CS0194	10307499	353.4	N-[(1-isobutyl-1H-imidazol-5-yl)methyl]-1-(2-methoxyphenyl)-1H-pyrazole-4-carboxamide	CC(C)Cn1c(CNC(c2cn-c(ccc3)c3OC)n2)=O)cnc1	102.41	
RCB_CS0335	10565134	364.4	5-oxo-1-phenyl-N-[1-pyrimidin-2-ylpiperidin-3-yl]-2,5-dihydro-1H-pyrazole-3-carboxamide	O=C(C(=NN1c2ccccc2)=CC1=O)NC(CCC1)CN1c1ncccc1	95.91	
RCB_CS0339	10574260	316.4	3-(5-methyl-2-thienyl)-N-[2-(4-methyl-1H-1,2,3-triazol-1-yl)ethyl]-1H-pyrazole-5-carboxamide	Cc1cn(CCNC(c2cc-c3ccc(C)s3)n[nH]2)=O)nn1	84.08	
RCB_CS0548	10947938	326.3	3-(3-fluorophenyl)-N-[2-hydroxy-2-(2-pyridinyl)ethyl]-1H-pyrazole-4-carboxamide	OC(CNC(c1c[nH]ncl-c1cccc(F)c1)=O)c1ncccc1	82.53	
RCB_CS0616	11046036	297.3	3-(5-methyl-2-furyl)-N-[[5-methyl-2-pyrazinyl)methyl]-1H-pyrazole-5-carboxamide	Cc1ccc(-c2[nH]c(C)NCC3ncc(C)nc3=O)c2)o1	89.56	
RCB_CS0643	11098879	327.4	1-methyl-3-propyl-N-(2,3,4,5-tetrahydro-1-benzoxepin-4-ylmethyl)-1H-pyrazole-5-carboxamide	CCCC1nn(C)c(C)NCC2Cc(cccc3)c3OCC2=O)c1	100.27	
		353.5	5-[1-(cyclohexylmethyl)-1H-1,2,4-triazol-5-yl]-1,1,1,3,3,5,5-tetramethyl-1H,1H,3,4-bispyrazole	Cc(n(C)nc1c1-c1nn(C)c1-c2nccn2CC2CCCCC2)c1	83.76	
		323.4	1-propyl-N-[[1-(1H-pyrazol-1-ylmethyl)cyclopropyl)methyl]-1H-pyrazole-5-sulfonamide	CCCN1ncccc1N(Cc1(Cn2ncccc2)CC1)(=O)=O	75.37	
RCB_CS0885	11390180	354.5	1-ethyl-3-methyl-N-[1-(4,5,6,7-tetrahydro-1,3-benzothiazol-2-yl)ethyl]-1H-pyrazole-5-sulfonamide	CCnInc(C)cc1S(NC(C)c1nc(CCCC2)c2s1)(=O)=O	88.68	
RCB_CS0985	11543696	263.4	5-methyl-1-propyl-N-(3-thienylmethyl)-1H-pyrazole-4-carboxamide	CCCC1ncc(C)NCC2csc2=O)c1C	98.18	

Showing 1 to 10 of 585 entries (filtered from 24,361 total entries)

# Case 1 : Searching the database

## Example 2: Using other strings related to SMCVdb entries

- Users can search the database using string search, Such as using SMILES. For example “CSCCN(CC1)CCN1C(c1cc(-c2c(CO)cccc2)ccc1)=O”

When you enter this string, The database will return the matched result.

Enter "CSCCN(CC1)CCN1C(c1cc(-c2c(CO)cccc2)ccc1)=O"

SMCV ID	Source ID	PubChem CID	MW	IUPAC Name	SMILES	Viability	Reference Image
RCB_C50030	10045854	NA	370.5	[3'''-(4-[2-(methylthio)ethyl]piperazin-1-yl)carbonyl]biphenyl-2-yl)methanol	<chem>CSCCN(CC1)CCN1C(c1cc(-c2c(CO)cccc2)ccc1)=O</chem>	93.1	

Showing 1 to 1 of 1 entries (filtered from 24,361 total entries)

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# Case 1 : Searching the database

## Example 2: Using other strings related to SMCVdb entries

- Users can search the database using 'partial' string search, Such as using SMILES. For example "CSCCN(CC1)"

When you enter this string, The database will return the matched result.

The screenshot displays the SMCVdb search interface. The search bar at the top right contains the string "CSCCN(CC1)". Below the search bar, a table lists the search results. The table has columns for SMCV ID, Source ID, PubChem CID, MW, IUPAC Name, SMILES, Viability, and Reference Image. Four entries are shown, each with a small reference image. A yellow callout box with a red arrow points to the search input field, containing the text "Enter 'CSCCN(CC1)'". Another yellow callout box with a red arrow points to the search results, containing the text "4 entries found".

SMCV ID	Source ID	PubChem CID	MW	IUPAC Name	SMILES	Viability	Reference Image
RCB_C50030	10045854	NA	370.5	[3]~-[4-2-(methylthio)ethyl]piperazin-1-yl carbonyl(biphenyl-2-yl) methanol	CSCCN(CC1)CCN1C(c1cc-c2c(CO)cccc2)ccc1=O	93.1	
RCB_C52837	14588266	NA	370.5	3-[6-aminopyridin-2-yl]-N-[1-[2-(methylthio)ethyl]piperidin-4-yl]benzamide	CSCCN(CC1)CCC1NC(c1cc-c2nc(N)ccc2)ccc1=O	38.59	
RCB_C69906	43539244	74237969	305.4	2-([4-2-(methylthio)ethyl]piperazin-1-yl carbonyl pyrazolo[1,5-a]pyrimidine	CSCCN(CC1)CCN1C(c1nnc2c2c1)=O	69.44	
RCB_C83479	68537889	70759302	370.5	(4-methyl-5-[1-[2-methylimidazo[1,2-a]pyridin-6-yl carbonyl]piperidin-4-yl]-4H-1,2,4-triazol-3-yl)methanol	CSCCN(CC1)CCC1NC(c1cc-c(ncc2)c2N)ccc1=O	68.69	

Showing 1 to 4 of 4 entries (filtered from 24,361 total entries)

# Case 2: Filtering compounds based on molecular weight

## Step 1 : Open the home page

SMCVdb

Home

ADME(T) Analysis

Target prediction

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Show 10 entries

Search:

SMCV ID	Source ID	PubChem CID	MW	IUPAC Name	SMILES	Viability	Reference Image
RCB_CS0009	10015705	134067281	350.4	N,5,6-trimethyl-2-oxo-N-[1-(5-phenyl-1H-pyrazol-3-yl)ethyl]-1,2-dihydro-3-pyridinecarboxamide	<chem>CC(c1n[nH]c(-c2cccc2)c1)N(C)C(C1=CC(C)=C(C)NC1=O)=O</chem>	113.28	
RCB_CS0011	10022643	72837098	351.4	N-allyl-3-(((3-ethyl-4,5-dihydroisoxazol-5-yl)methyl)amino)sulfonyl)benzamide	<chem>CCC1=NOC(CNS(c2cc(C(NCC=C)O)ccc2)(=O)=O)C1</chem>	96.62	
RCB_CS0013	10025975	NA	435.4	1-methyl-4-[5-(morpholin-4-ylmethyl)-3-furoyl]-1,4,9-triazaspiro[5.5]undecane dihydrochloride	<chem>CN(CC1)C2(CCNC2)CN1C(c1ccc(CN2CCOCC2)c1)=O</chem>	72.72	
RCB_CS0024	10037740	70704262	362.5	2-(((3-amino-2-thienyl)carbonyl)amino)methyl)-N,N-dimethyl-7,8-dihydro-4H-pyrazolo[1,5-a][1,4]diazepine-5(6H)-carboxamide	<chem>CN(C)C(N1Cc2cc(CNC(c3cc3)c3N)=O)nn2CCCC1=O</chem>	104.81	
RCB_CS0027	10041741	70704267	362.5	N-cyclopropyl-N-(3-hydroxybenzyl)-2-(2,4,7-trimethyl-1H-indol-3-yl)acetamide	<chem>Cc1c(CC N(Cc2cc(O)ccc2)C2CC2)=O)c2c(C)ccc(C)c2[nH]1</chem>	103.84	
RCB_CS0029	10045111	NA	316.4	N-((3S*,4R*)-4-ethoxytetrahydrofuran-3-yl)-N''''-(1-phenyl-1H-pyrazol-5-yl)urea	<chem>CCO[C@@H](COC1)[C@H]1NC(Nc1ccnn1-c1cccc1)=O</chem>	99.86	
RCB_CS0030	10045854	NA	370.5	[3''''-(4-[2-(methylthio)ethyl]piperazin-1-yl)carbonyl)biphenyl-2-yl]methanol	<chem>CSCCN(CC1)CCN1C(c1cc(-c2c(CO)cccc2)ccc1)=O</chem>	93.1	
RCB_CS0033	10048011	91759616	333.4	5-([2-[2-(4-methylpiperazin-1-yl)ethyl]piperidin-1-yl]carbonyl)pyrazin-2-ol	<chem>CN1CCN(CCC(CCCC2)N2C(c(cn2)ncc2O)=O)CC1</chem>	79.25	
RCB_CS0034	10049170	NA	370.5	N-(2,1,3-benzoxadiazol-5-ylmethyl)-2-[2-(2-thienyl)ethyl]piperidine-1-carboxamide	<chem>O=C(NCc1cc2nonc2cc1)N1C(CCc2cccs2)CCCC1</chem>	131.62	
RCB_CS0038	10057755	70704288	374.9	N-((3S*,4R*)-1-((6-chloro-1,3-benzodioxol-5-yl)methyl)-4-isopropyl-3-pyrrolidinyl)methanesulfonamide	<chem>CC(C)[C@@H](CN(Cc(cc1OCCc1c1)c1C1C1)[C@H]1NS(C)(=O)=O</chem>	105.68	

Showing 1 to 10 of 24,361 entries

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## Case 2: Filtering compounds based on molecular weight

### Step 2 : Click on the MW slider

SMCVdb

Home  
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User guide **New**  
Contact Us  
Download Data  
Update

Show 10 entries

Search:

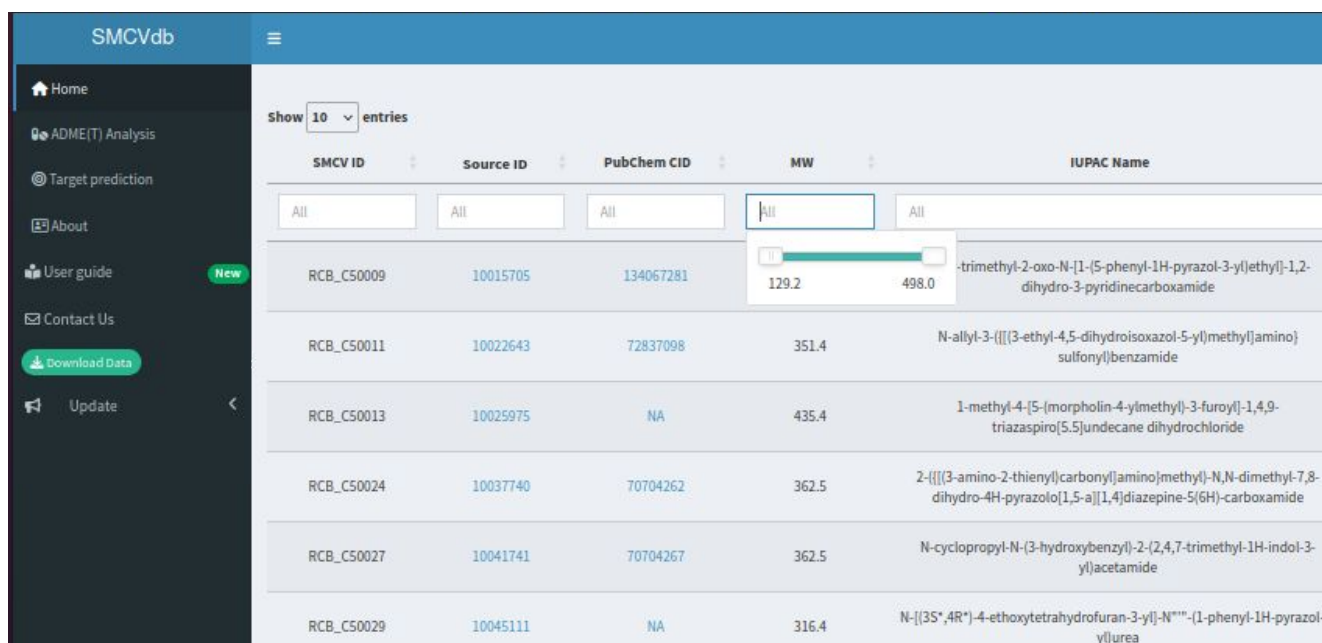
SMCV ID	Source ID	PubChem CID	MW	IUPAC Name	SMILES	Viability	Reference Image
All	All	All	All	All	All	All	All
RCB_C50009	10015705	134067281	129.2	1-trimethyl-2-oxo-N-[1-(5-phenyl-1H-pyrazol-3-yl)ethyl]-1,2-dihydro-3-pyridinecarboxamide	<chem>CC(c1n[nH]c(-c2ccccc2)c1)N(C)C(C1=CC=C(C)N(C1=O)=O</chem>	113.28	
RCB_C50011	10022643	72837098	351.4	N-allyl-3-(((3-ethyl-4,5-dihydroisoxazol-5-yl)methyl)amino)sulfonyl)benzamide	<chem>CCC1=NOC(CNS(c2cc(C(NCC=C)O)ccc2)(=O)=O)C1</chem>	96.62	
RCB_C50013	10025975	NA	435.4	1-methyl-4-[5-(morpholin-4-ylmethyl)-3-furoyl]-1,4,9-triazaspiro[5.5]undecane dihydrochloride	<chem>CN(CC1)C2(CNCC2)CN1C(c1ccc(CN2CCOCC2)c1)=O</chem>	72.72	
RCB_C50024	10037740	70704262	362.5	2-(((3-amino-2-thienyl)carbonyl)amino)methyl)-N,N-dimethyl-7,8-dihydro-4H-pyrazolo[1,5-a][1,4]diazepine-5(6H)-carboxamide	<chem>CN(C)C(N1Cc2cc(CNC(c3cc3)N)=O)nn2CCC1=O</chem>	104.81	
RCB_C50027	10041741	70704267	362.5	N-cyclopropyl-N-(3-hydroxybenzyl)-2-(2,4,7-trimethyl-1H-indol-3-yl)acetamide	<chem>Cc1c(CC(N)Cc2cc(O)ccc2)C2CC2=O)c2c(C)ccc(C)c2[nH]1</chem>	103.84	
RCB_C50029	10045111	NA	316.4	N-((3S*,4R*)-4-ethoxytetrahydrofuran-3-yl)-N''''-(1-phenyl-1H-pyrazol-5-yl)urea	<chem>CCO[C@@H](COCC1)[C@H]1NC(Nc1ccnn1-c1ccccc1)=O</chem>	99.86	
RCB_C50030	10045854	NA	370.5	[3''''-[[4-[2-(methylthio)ethyl]piperazin-1-yl]carbonyl]biphenyl-2-yl)methanol	<chem>CSCCN(CC1)CCN1C(c1cc(-c2c(CO)cccc2)ccc1)=O</chem>	93.1	
RCB_C50033	10048011	91759616	333.4	5-[[2-[2-(4-methylpiperazin-1-yl)ethyl]piperidin-1-yl]carbonyl]pyrazin-2-ol	<chem>CN1CCN(CCC(CCCC2)N2C(c(cn2)ncc2O)=O)CC1</chem>	79.25	
RCB_C50034	10049170	NA	370.5	N-(2,1,3-benzoxadiazol-5-ylmethyl)-2-[2-(2-thienyl)ethyl]piperidine-1-carboxamide	<chem>O=C(NCc1cc2nonc2cc1)N1C(CCC2cccs2)CCCC1</chem>	131.62	
RCB_C50038	10057755	70704288	374.9	N-((3S*,4R*)-1-[[6-chloro-1,3-benzodioxol-5-yl)methyl]-4-isopropyl-3-pyrrolidinyl)methanesulfonamide	<chem>CC(C)[C@@H](CN(Cc1cc1OCOC1c1c1C1)[C@H]1NS(C)(=O)=O</chem>	105.68	

Showing 1 to 10 of 24,361 entries

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## Case 2: Filtering compounds based on molecular weight

### Step 3 : Select the range



The screenshot shows the SMCVdb interface. On the left is a navigation menu with options: Home, ADME(T) Analysis, Target prediction, About, User guide (marked as New), Contact Us, Download Data, and Update. The main area displays a table of compounds with columns: SMCV ID, Source ID, PubChem CID, MW, and IUPAC Name. Above the table, there are filters for each column, with the MW filter set to a range of 129.2 to 498.0. A dropdown menu for 'Show 10 entries' is also visible.

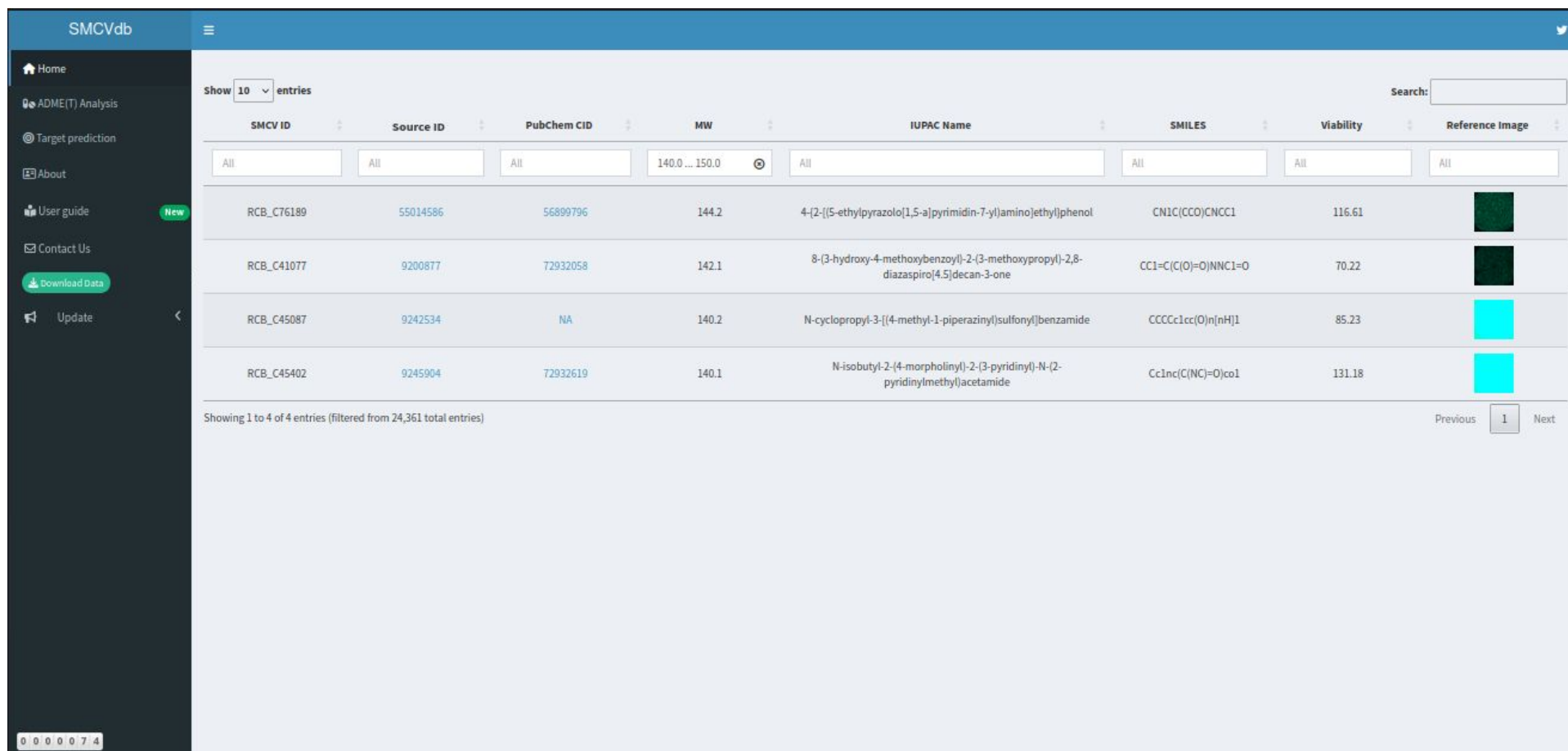
SMCV ID	Source ID	PubChem CID	MW	IUPAC Name
RCB_C50009	10015705	134067281	129.2 - 498.0	-trimethyl-2-oxo-N-[1-(5-phenyl-1H-pyrazol-3-yl)ethyl]-1,2-dihydro-3-pyridinecarboxamide
RCB_C50011	10022643	72837098	351.4	N-allyl-3-(((3-ethyl-4,5-dihydroisoxazol-5-yl)methyl)amino)sulfonyl)benzamide
RCB_C50013	10025975	NA	435.4	1-methyl-4-[5-(morpholin-4-ylmethyl)-3-furoyl]-1,4,9-triazaspiro[5.5]undecane dihydrochloride
RCB_C50024	10037740	70704262	362.5	2-(((3-amino-2-thienyl)carbonyl)amino)methyl)-N,N-dimethyl-7,8-dihydro-4H-pyrazolo[1,5-a][1,4]diazepine-5(6H)-carboxamide
RCB_C50027	10041741	70704267	362.5	N-cyclopropyl-N-(3-hydroxybenzyl)-2-(2,4,7-trimethyl-1H-indol-3-yl)acetamide
RCB_C50029	10045111	NA	316.4	N-((3S*,4R*)-4-ethoxytetrahydrofuran-3-yl)-N''''-(1-phenyl-1H-pyrazol-yl)urea

Note : For manual entry in MW use “100...150” format



## Case 2: Filtering compounds based on molecular weight





Step 4 : Result page will appear



SMCVdb

Show 10 entries

Search:

SMCV ID	Source ID	PubChem CID	MW	IUPAC Name	SMILES	Viability	Reference Image
All	All	All	140.0 ... 150.0	All	All	All	All
RCB_C76189	55014586	56899796	144.2	4-[2-[(5-ethylpyrazolo[1,5-a]pyrimidin-7-yl)amino]ethyl]phenol	CN1C(CCO)CNCC1	116.61	
RCB_C41077	9200877	72932058	142.1	8-[3-hydroxy-4-methoxybenzoyl]-2-(3-methoxypropyl)-2,8-diazaspiro[4.5]decan-3-one	CC1=C(C(O)=O)MNC1=O	70.22	
RCB_C45087	9242534	NA	140.2	N-cyclopropyl-3-[(4-methyl-1-piperazinyl)sulfonyl]benzamide	CCCCc1cc(O)n[nH]1	85.23	
RCB_C45402	9245904	72932619	140.1	N-isobutyl-2-(4-morpholinyl)-2-(3-pyridinyl)-N-(2-pyridinylmethyl)acetamide	Cc1nc(C(NC)=O)co1	131.18	

Showing 1 to 4 of 4 entries (filtered from 24,361 total entries)

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0 0 0 0 0 7 4

# Case 3: Filtering compounds within a range of viability information

## Step 1 : Open the home page

SMCVdb

Home

ADME(T) Analysis

Target prediction

About

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Update

Show 10 entries

Search:

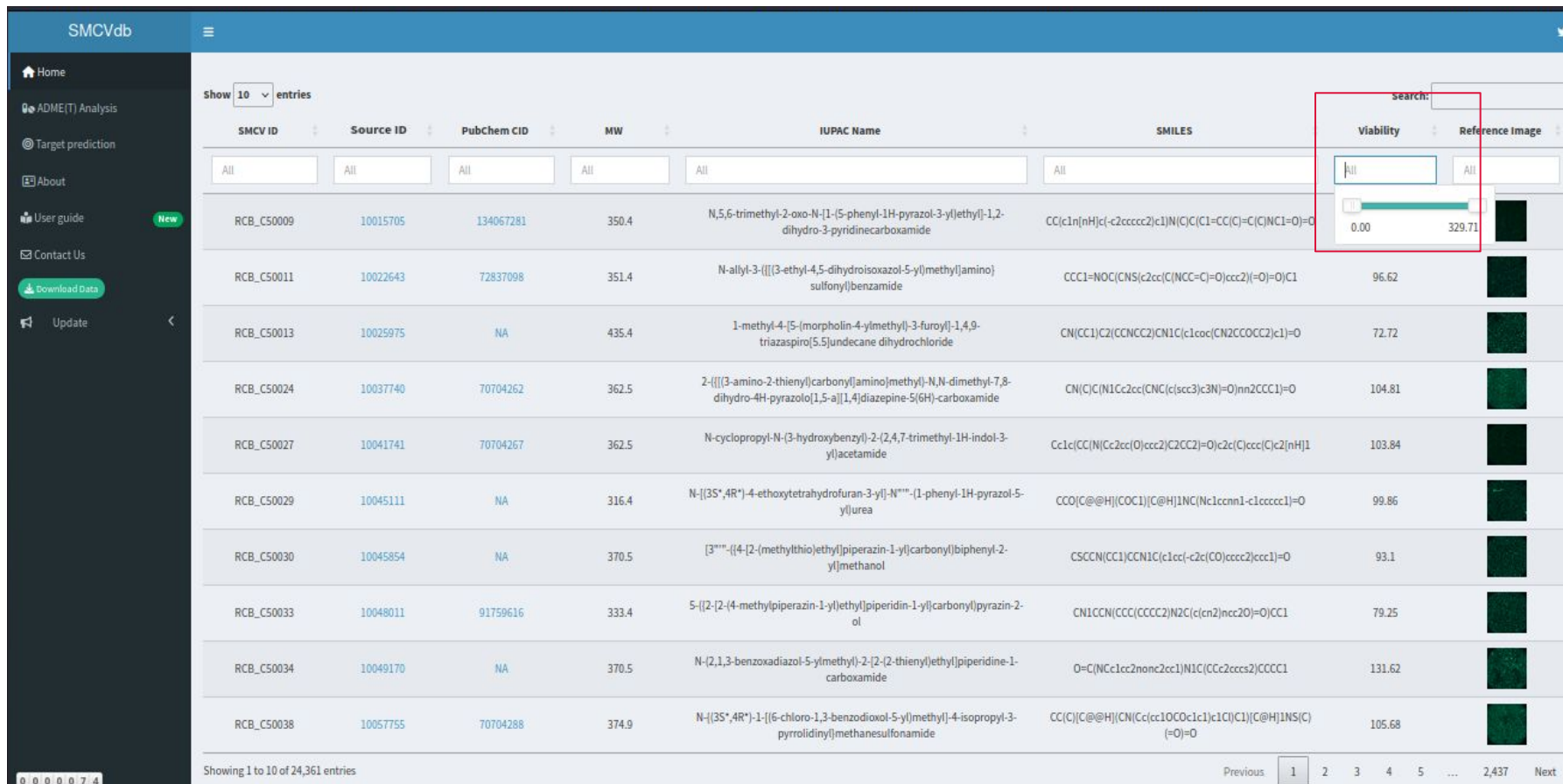
SMCV ID	Source ID	PubChem CID	MW	IUPAC Name	SMILES	Viability	Reference Image
All	All	All	All	All	All	All	All
RCB_CS0009	10015705	134067281	350.4	N,5,6-trimethyl-2-oxo-N-[1-(5-phenyl-1H-pyrazol-3-yl)ethyl]-1,2-dihydro-3-pyridinecarboxamide	<chem>CC(c1n[nH]c(-c2cccc2)c1)N(C)C(C1=CC(C)=C(C)NC1=O)=O</chem>	113.28	
RCB_CS0011	10022643	72837098	351.4	N-allyl-3-(((3-ethyl-4,5-dihydroisoxazol-5-yl)methyl)amino)sulfonylbenzamide	<chem>CCC1=NOC(CNS(c2cc(C)NCC=C)O)ccc2(=O)=O)C1</chem>	96.62	
RCB_CS0013	10025975	NA	435.4	1-methyl-4-[5-(morpholin-4-ylmethyl)-3-furoyl]-1,4,9-triazaspiro[5.5]undecane dihydrochloride	<chem>CN(CC1)C2(CCNC2)CN1C(c1ccc(CN2CCOCC2)c1)=O</chem>	72.72	
RCB_CS0024	10037740	70704262	362.5	2-(((3-amino-2-thienyl)carbonyl)amino)methyl)-N,N-dimethyl-7,8-dihydro-4H-pyrazolo[1,5-a][1,4]diazepine-5(6H)-carboxamide	<chem>CN(C)C(N1Cc2cc(CNC(c(scc3)c3N)=O)nn2CCCC1)=O</chem>	104.81	
RCB_CS0027	10041741	70704267	362.5	N-cyclopropyl-N-(3-hydroxybenzyl)-2-(2,4,7-trimethyl-1H-indol-3-yl)acetamide	<chem>Cc1c(CC)N(Cc2cc(O)ccc2)C2CC2(=O)c2c(C)ccc(C)c2[nH]1</chem>	103.84	
RCB_CS0029	10045111	NA	316.4	N-((3S*,4R*)-4-ethoxytetrahydrofuran-3-yl)-N''''-(1-phenyl-1H-pyrazol-5-yl)urea	<chem>CCO[C@@H](COC1)[C@H]1NC(Nc1ccnn1-c1cccc1)=O</chem>	99.86	
RCB_CS0030	10045854	NA	370.5	[3''''-(4-[2-(methylthio)ethyl]piperazin-1-yl)carbonyl]biphenyl-2-yl)methanol	<chem>CSCCN(CC1)CCN1C(c1cc(-c2c(CO)cccc2)ccc1)=O</chem>	93.1	
RCB_CS0033	10048011	91759616	333.4	5-((2-[2-(4-methylpiperazin-1-yl)ethyl]piperidin-1-yl)carbonyl)pyrazin-2-ol	<chem>CN1CCN(CCC(CCCC2)N2C(c(cn2)ncc2O)=O)CC1</chem>	79.25	
RCB_CS0034	10049170	NA	370.5	N-(2,1,3-benzoxadiazol-5-ylmethyl)-2-[2-(2-thienyl)ethyl]piperidine-1-carboxamide	<chem>O=C(NC1cc2nonc2cc1)N1C(CCc2cccs2)CCCC1</chem>	131.62	
RCB_CS0038	10057755	70704288	374.9	N-((3S*,4R*)-1-((6-chloro-1,3-benzodioxol-5-yl)methyl)-4-isopropyl-3-pyrrolidinyl)methanesulfonamide	<chem>CC(C)[C@@H](CN(Cc(cc1OCCc1c1)c1C1)C1)[C@H]1NS(C)(=O)=O</chem>	105.68	

Showing 1 to 10 of 24,361 entries

Previous 1 2 3 4 5 ... 2,437 Next

# Case 3: Filtering compounds within a range of viability information

## Step 2 : Click on the Viability slider



The screenshot displays the SMCVdb interface. On the left is a navigation sidebar with options like Home, ADMET Analysis, Target prediction, About, User guide, Contact Us, Download Data, and Update. The main area shows a table of compounds with columns for SMCV ID, Source ID, PubChem CID, MW, IUPAC Name, and SMILES. A search bar is at the top right. Below the search bar, there are filters for Viability and Reference Image. The Viability filter is currently set to 'All' and has a slider below it ranging from 0.00 to 329.71. The Reference Image filter is also set to 'All'. The table lists 10 entries, each with a corresponding reference image. At the bottom, it shows 'Showing 1 to 10 of 24,361 entries' and a pagination control with 'Previous', '1', '2', '3', '4', '5', '...', '2,437', and 'Next'.

SMCV ID	Source ID	PubChem CID	MW	IUPAC Name	SMILES	Viability	Reference Image
RCB_CS0009	10015705	134067281	350.4	N,5,6-trimethyl-2-oxo-N-[1-[5-phenyl-1H-pyrazol-3-yl]ethyl]-1,2-dihydro-3-pyridinecarboxamide	<chem>CC(c1n[nH](c(-c2cccc2)c1)N(C)C(C1=CC(C)=C(C)N(C1)=O)=O</chem>		
RCB_CS0011	10022643	72837098	351.4	N-allyl-3-(((3-ethyl-4,5-dihydroisoxazol-5-yl)methyl)amino)sulfonylbenzamide	<chem>CCCC1=NO(C)N(C)S(=O)(=O)C2=CC=CC=C2C1=O</chem>	96.62	
RCB_CS0013	10025975	NA	435.4	1-methyl-4-[5-(morpholin-4-ylmethyl)-3-furoyl]-1,4,9-triazaspiro[5.5]undecane dihydrochloride	<chem>CN(CC1)C2(CCNCC2)CN1C(c1ccc(CN2CCOCC2)c1)=O</chem>	72.72	
RCB_CS0024	10037740	70704262	362.5	2-(((3-amino-2-thienyl)carbonyl)amino)methyl)-N,N-dimethyl-7,8-dihydro-4H-pyrazolo[1,5-a][1,4]diazepine-5(6H)-carboxamide	<chem>CN(C)C(N1Cc2cc(CNC(c1scc3)c3N)=O)nn2CCC1=O</chem>	104.81	
RCB_CS0027	10041741	70704267	362.5	N-cyclopropyl-N-(3-hydroxybenzyl)-2-(2,4,7-trimethyl-1H-indol-3-yl)acetamide	<chem>Cc1c(C)N(Cc2cc(O)ccc2)C2CC2=O)c2c(C)ccc(C)c2[nH]1</chem>	103.84	
RCB_CS0029	10045111	NA	316.4	N-((3S*,4R*)-4-ethoxytetrahydrofuran-3-yl)-N''''-(1-phenyl-1H-pyrazol-5-yl)urea	<chem>CCO[C@@H](COC1)[C@H]1NC(Nc1ccnn1-c1cccc1)=O</chem>	99.86	
RCB_CS0030	10045854	NA	370.5	[3''''-(4-[2-(methylthio)ethyl]piperazin-1-yl)carbonyl)biphenyl-2-yl)methanol	<chem>CSCCN(CC1)CCN1C(c1cc(-c2c(CO)cccc2)ccc1)=O</chem>	93.1	
RCB_CS0033	10048011	91759616	333.4	5-[[2-[2-(4-methylpiperazin-1-yl)ethyl]piperidin-1-yl]carbonyl]pyrazin-2-ol	<chem>CN1CCN(CCC(CCCC2)N2C(c1cn2)ncc2O)=O)CC1</chem>	79.25	
RCB_CS0034	10049170	NA	370.5	N-(2,1,3-benzoxadiazol-5-ylmethyl)-2-[2-(2-thienyl)ethyl]piperidine-1-carboxamide	<chem>O=C(NC1cc2nonc2cc1)N1C(Cc2cccs2)CCCC1</chem>	131.62	
RCB_CS0038	10057755	70704288	374.9	N-((3S*,4R*)-1-[[6-chloro-1,3-benzodioxol-5-yl)methyl]-4-isopropyl-3-pyrrolidinyl)methanesulfonamide	<chem>CC(C)[C@@H](CN(Cc1cc1OCOC1c1c1C1)[C@H]1NS(C)=O)=O</chem>	105.68	

## Case 3: Filtering compounds within a range of viability information

Step 3 : Select the range

The screenshot shows a web interface with a search bar at the top. Below it, there are two filter sections: 'Viability' and 'Reference.Image'. The 'Viability' filter is currently set to a range of '100.23 |.. 100.23', which is highlighted with a red box. Below this, a slider control is visible, also showing the range '100.23' to '100.23'. The 'Reference.Image' filter is set to 'All'. On the left side, there is a chemical structure input field containing the SMILES string N(CCO1)C1=O)=O.

Note : For manual entry of range use “100...150” format

## Case 3: Filtering compounds within a range of viability information

### Step 4 : Result will appear

SMCVdb

Home  
ADME(T) Analysis  
Target prediction  
About  
User guide New  
Contact Us  
Download Data  
Update

Show 10 entries

Search:

SMCV ID	Source ID	PubChem CID	MW	IUPAC Name	SMILES	Viability	Reference Image
All	All	All	All	All	All	100.23 ... 100.23	All
RCB_C73397	49884402	70741622	334.4	3-[1-([1-ethyl-3-isopropyl-1H-pyrazol-5-yl)carbonyl]-4-piperidinyl]-1,3-oxazolidin-2-one	<chem>CCn1nc(C(C)C)cc1C(N(CC1)CCC1N(CCO1)C1=O)=O</chem>	100.23	
RCB_C83661	68834698	72905026	372.5	N,1,3-trimethyl-N-[1-methyl-2-(4-methylpyridin-2-yl)ethyl]-1H-pyrazolo[3,4-d][1,3]thiazol-5-amine	<chem>CCCC(N1CC)=NN(CC(N(CC2)CCN2c2ncccc2)=O)C1=O</chem>	100.23	
RCB_C86705	74473279	118786151	333.4	1-methyl-N-[1-(1-propyl-1H-1,2,4-triazol-5-yl)ethyl]-5-(2-thienyl)-1H-pyrazole-3-carboxamide	<chem>CCN(CC1OCCC1)Cc1c(nH)nc1-c(ccc(O)c1)c1F</chem>	100.23	
RCB_C91530	83644642	70773533	375.5	N-[[4-(dimethylamino)tetrahydro-2H-pyran-4-yl]methyl]-3-isopropyl-1-methyl-1H-pyrazole-5-carboxamide	<chem>Cc1cc(-c2cccc(N3CCN(Cc4ccco4)CC3)=O)c2)nc(C)c1</chem>	100.23	
RCB_C45386	9245764	47001547	376.4	6-(3,4-dimethylphenyl)-3-(1-piperidinylmethyl)[1,2,4]triazolo[3,4-b][1,3,4]thiadiazole	<chem>CCNc1nc(C)cc(N(CC2)CCN2C(Nc(ccc(F)c2c2F)=O)n1</chem>	100.23	

Showing 1 to 5 of 5 entries (filtered from 24,361 total entries)

Previous 1 Next

0 0 0 0 0 7 4

# Case 4 : Downloading microscopy image data of a specific compound











Step 1 : Choose your compound using case 1-3

SMCVdb

Home  
ADME(T) Analysis  
Target prediction  
About  
User guide New  
Contact Us  
Download Data  
Update

Show 10 entries

Search:

SMCV ID	Source ID	PubChem CID	MW	IUPAC Name	SMILES	Viability	Reference Image
All	All	All	All	All	All	All	All
RCB_CS0009	10015705	134067281	350.4	N,5,6-trimethyl-2-oxo-N-[1-(5-phenyl-1H-pyrazol-3-yl)ethyl]-1,2-dihydro-3-pyridinecarboxamide	<chem>CC(c1n[nH]c(-c2ccccc2)c1)N(C)C(C1=CC(C)=C(C)NC1=O)=O</chem>	113.28	
RCB_CS0011	10022643	72837098	351.4	N-allyl-3-(((3-ethyl-4,5-dihydroisoxazol-5-yl)methyl)amino)sulfonyl)benzamide	<chem>CCC1=NOC(CNS)(c2cc(C(NCC=C)O)ccc2)(=O)C1</chem>	96.62	
RCB_CS0013	10025975	NA	435.4	1-methyl-4-[5-(morpholin-4-ylmethyl)-3-furoyl]-1,4,9-triazaspiro[5.5]undecane dihydrochloride	<chem>CN(CC1)C2(CCNC2)CN1C(c1ccc(CN2CCOCC2)c1)=O</chem>	72.72	
RCB_CS0024	10037740	70704262	362.5	2-(((3-amino-2-thienyl)carbonyl)amino)methyl)-N,N-dimethyl-7,8-dihydro-4H-pyrazolo[1,5-a][1,4]diazepine-5(6H)-carboxamide	<chem>CN(C)C(N1Cc2cc(CNC(c(scc3)c3N)=O)nn2CCCC1)=O</chem>	104.81	
RCB_CS0027	10041741	70704267	362.5	N-cyclopropyl-N-(3-hydroxybenzyl)-2-(2,4,7-trimethyl-1H-indol-3-yl)acetamide	<chem>Cc1c(CC N(Cc2cc(O)ccc2)C2CC2)=O)c2c(C)ccc(C)c2[nH]1</chem>	103.84	
RCB_CS0029	10045111	NA	316.4	N-((3S*,4R*)-4-ethoxytetrahydrofuran-3-yl)-N''''-(1-phenyl-1H-pyrazol-5-yl)urea	<chem>CCO[C@@H](COC1)[C@H]1NC(Nc1ccnn1-c1ccccc1)=O</chem>	99.86	
RCB_CS0030	10045854	NA	370.5	[3''''-(4-[2-(methylthio)ethyl]piperazin-1-yl)carbonyl)biphenyl-2-yl]methanol	<chem>CSCCN(CC1)CCN1C(c1cc(-c2c(CO)cccc2)ccc1)=O</chem>	93.1	
RCB_CS0033	10048011	91759616	333.4	5-([2-[2-(4-methylpiperazin-1-yl)ethyl]piperidin-1-yl]carbonyl)pyrazin-2-ol	<chem>CN1CCN(CCC(CCCC2)N2C(c(cn2)ncc2O)=O)CC1</chem>	79.25	
RCB_CS0034	10049170	NA	370.5	N-(2,1,3-benzoxadiazol-5-ylmethyl)-2-[2-(2-thienyl)ethyl]piperidine-1-carboxamide	<chem>O=C(NC1cc2nonc2cc1)N1C(Cc2cccs2)CCCC1</chem>	131.62	
RCB_CS0038	10057755	70704288	374.9	N-((3S*,4R*)-1-((6-chloro-1,3-benzodioxol-5-yl)methyl)-4-isopropyl-3-pyrrolidinyl)methanesulfonamide	<chem>CC(C)[C@@H](CN(Cc(cc1OCCo1c1)c1Cl)C1)[C@H]1NS(C)(=O)=O</chem>	105.68	

Showing 1 to 10 of 24,361 entries

Previous 1 2 3 4 5 ... 2,437 Next

# Case 4 : Downloading microscopy image data of a specific compound

## Step 2 : Click on the reference image link

SMCVdb

Home  
ADME(T) Analysis  
Target prediction  
About  
User guide **New**  
Contact Us  
Download Data  
Update

Show 10 entries

Search:

SMCV ID	Source ID	PubChem CID	MW	IUPAC Name	SMILES	Viability	Reference Image
RCB_CS0009	10015705	134067281	350.4	N,5,6-trimethyl-2-oxo-N-[1-(5-phenyl-1H-pyrazol-3-yl)ethyl]-1,2-dihydro-3-pyridinecarboxamide	<chem>CC(c1n[nH]c(-c2cccc2)c1)N(C)C(C1=CC(C)=C(C)NC1=O)=O</chem>	113.28	
RCB_CS0011	10022643	72837098	351.4	N-allyl-3-(((3-ethyl-4,5-dihydroisoxazol-5-yl)methyl)amino)sulfonyl)benzamide	<chem>CCC1=NOC(CNS(c2cc(C(NCC=C)O)ccc2)(=O)=O)C1</chem>	96.62	
RCB_CS0013	10025975	NA	435.4	1-methyl-4-[5-(morpholin-4-ylmethyl)-3-furoyl]-1,4,9-triazaspiro[5.5]undecane dihydrochloride	<chem>CN(CC1)C2(CCNC2)CN1C(c1ccc(CN2CCOCC2)c1)=O</chem>	72.72	
RCB_CS0024	10037740	70704262	362.5	2-(((3-amino-2-thienyl)carbonyl)amino)methyl)-N,N-dimethyl-7,8-dihydro-4H-pyrazolo[1,5-a][1,4]diazepine-5(6H)-carboxamide	<chem>CN(C)C(N1Cc2cc(CNC(c(scc3)c3N)=O)nn2CCCC1)=O</chem>	104.81	
RCB_CS0027	10041741	70704267	362.5	N-cyclopropyl-N-(3-hydroxybenzyl)-2-(2,4,7-trimethyl-1H-indol-3-yl)acetamide	<chem>Cc1c(CC N(Cc2cc(O)ccc2)C2CC2)=O)c2c(C)ccc(C)c2[nH]1</chem>	103.84	
RCB_CS0029	10045111	NA	316.4	N-((3S*,4R*)-4-ethoxytetrahydrofuran-3-yl)-N''''-(1-phenyl-1H-pyrazol-5-yl)urea	<chem>CCO[C@@H](COC1)[C@H]1NC(Nc1ccnn1-c1cccc1)=O</chem>	99.86	
RCB_CS0030	10045854	NA	370.5	[3''''-(4-[2-(4-methylthio)ethyl]piperazin-1-yl)carbonyl)biphenyl-2-yl]methanol	<chem>CSCCN(CC1)CCN1C(c1cc(-c2c(CO)cccc2)ccc1)=O</chem>		
RCB_CS0033	10048011	91759616	333.4	5-([2-[2-(4-methylpiperazin-1-yl)ethyl]piperidin-1-yl]carbonyl)pyrazin-2-ol	<chem>CN1CCN(CCC(CCCC2)N2C(c(cn2)ncc2O)=O)CC1</chem>	79.25	
RCB_CS0034	10049170	NA	370.5	N-(2,1,3-benzoxadiazol-5-ylmethyl)-2-[2-(2-thienyl)ethyl]piperidine-1-carboxamide	<chem>O=C(NC1cc2nonc2cc1)N1C(Cc2cccs2)CCCC1</chem>	131.62	
RCB_CS0038	10057755	70704288	374.9	N-((3S*,4R*)-1-((6-chloro-1,3-benzodioxol-5-yl)methyl)-4-isopropyl-3-pyrrolidinyl)methanesulfonamide	<chem>CC(C)[C@@H](CN(Cc(cc1OCCc1c1)c1Cl)C1)[C@H]1NS(C)(=O)=O</chem>	105.68	

Showing 1 to 10 of 24,361 entries

Previous 1 2 3 4 5 ... 2,437 Next

# Case 4 : Downloading microscopy image data of a specific compound

Step 3 : A pop up window will appear

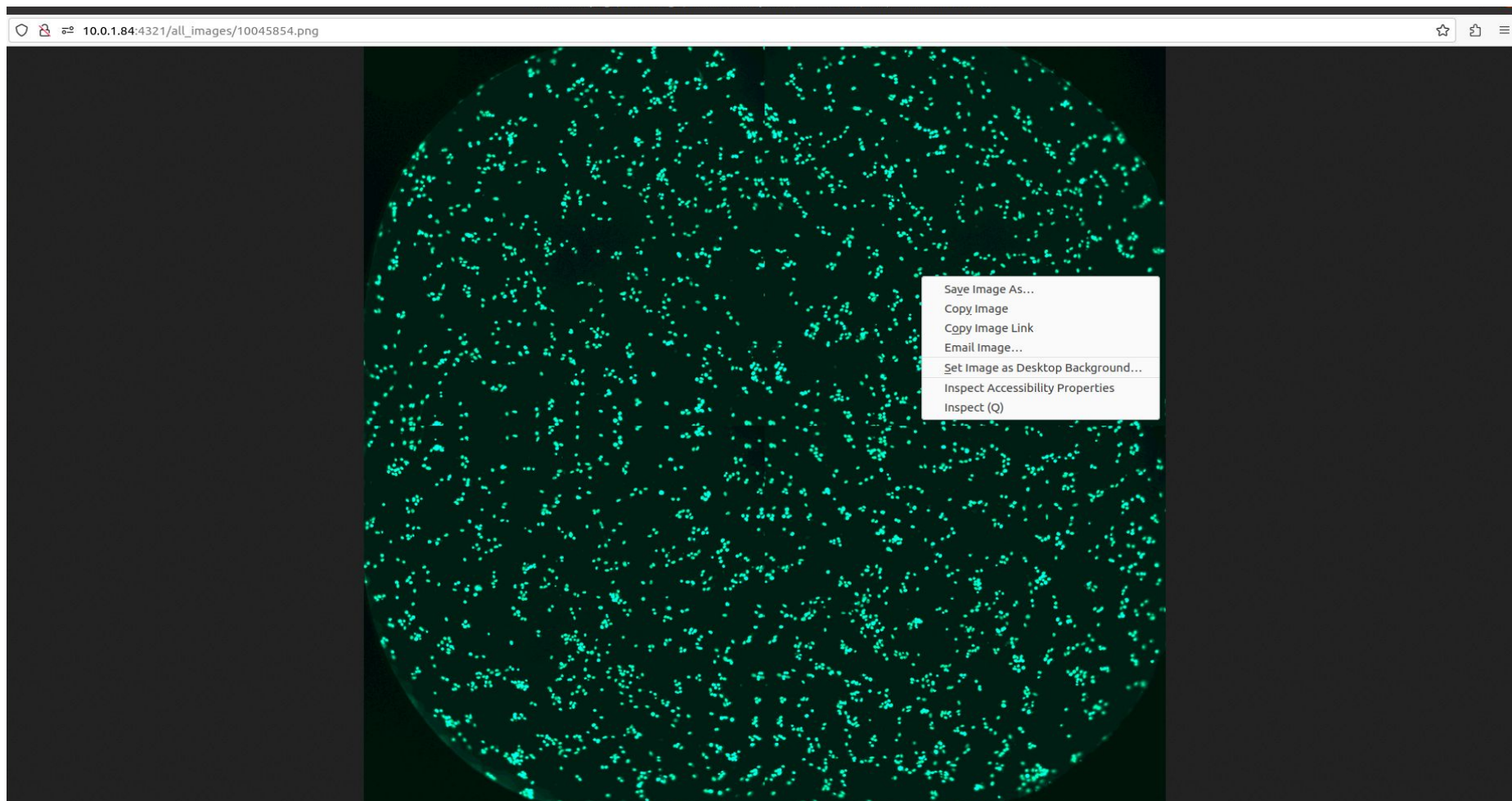
The screenshot shows the SMCVdb web application interface. On the left is a dark sidebar with navigation links: Home, ADME(T) Analysis, Target prediction, About, User guide (marked 'New'), Contact Us, Download Data, and Update. The main content area features a table with columns: SMCV ID, Source ID, PubChem CID, MW, IUPAC Name, SMILES, Viability, and Reference Image. A search bar is located in the top right. A pop-up window titled '10045854.png (PNG Image, 100...' is overlaid on the table, displaying a circular microscopy image with green fluorescent spots. The table entry for Source ID 10045854 is highlighted, showing its IUPAC Name and SMILES string. At the bottom, a pagination bar indicates 'Showing 1 to 10 of 24,361 entries' and includes page numbers 1 through 5, followed by an ellipsis and '2,437', and a 'Next' button.

SMCV ID	Source ID	PubChem CID	MW	IUPAC Name	SMILES	Viability	Reference Image
RCB_CS0009	10015705	134067281	350.4		<chem>Cc1n[nH]c(-c2cccc2)c1N(C)C(C1=CC(C)=C(C)NC1=O)=O</chem>	113.28	
RCB_CS0011	10022643	72837098	351.4		<chem>CCC1=NOC(CNS(c2cc(C(NCC=C)O)ccc2)(=O)=O)C1</chem>	96.62	
RCB_CS0013	10025975	NA	435.4		<chem>CN(CC1)C2(CCNCC2)CN1C(c1ccc(CN2CCOCC2)c1)=O</chem>	72.72	
RCB_CS0024	10037740	70704262	362.5		<chem>CN(C)C(N1Cc2cc(CNC(c1ccc3c3N)=O)nn2CCC1)=O</chem>	104.81	
RCB_CS0027	10041741	70704267	362.5		<chem>Cc1c(CC(N(Cc2cc(O)ccc2)C2CC2)=O)c2c(C)ccc(C)c2[nH]1</chem>	103.84	
RCB_CS0029	10045111	NA	316.4		<chem>CCO[C@@H](COCl)[C@H]1NC(Nc1ccn1-c1cccc1)=O</chem>	99.86	
RCB_CS0030	10045854	NA	370.5		<chem>CSCCN(CC1)CCNIC(c1cc(-c2c(CO)cccc2)ccc1)=O</chem>	93.1	
RCB_CS0033	10048011	91759616	333.4		<chem>CN1CCN(CCC(CCCC2)N2C(c1cn2)ncc2O)=O)CC1</chem>	79.25	
RCB_CS0034	10049170	NA	370.5		<chem>O=C(NCc1cc2none2cc1)N1C(Cc2cccs2)CCCC1</chem>	131.62	
RCB_CS0038	10057755	70704288	374.9	N-([3S*,4R*]-1-[(6-chloro-1,3-benzodioxol-5-yl)methyl]-4-isopropyl-3-pyrrolidiny]methanesulfonamide	<chem>CC(C)[C@@H](CN(Cc1cc1OCoc1c1c1)Cl)[C@H]1NS(C)(=O)=O</chem>	105.68	



# Case 4 : Downloading microscopy image data of a specific compound

**Step 4** : Save the image using right click



# Case 5: Commercial procurement information for a specific compound

## Step 1 : Choose your compound using case 1-3

SMCVdb

Home  
ADME(T) Analysis  
Target prediction  
About  
User guide New  
Contact Us  
Download Data  
Update

Show 10 entries

Search:

SMCV ID	Source ID	PubChem CID	MW	IUPAC Name	SMILES	Viability	Reference Image
RCB_CS0009	10015705	134067281	350.4	N,5,6-trimethyl-2-oxo-N-[1-(5-phenyl-1H-pyrazol-3-yl)ethyl]-1,2-dihydro-3-pyridinecarboxamide	<chem>CC(c1n[nH]c(-c2cccc2)c1)N(C)C(C1=CC(C)=C(C)NC1=O)=O</chem>	113.28	
RCB_CS0011	10022643	72837098	351.4	N-allyl-3-(((3-ethyl-4,5-dihydroisoxazol-5-yl)methyl)amino)sulfonylbenzamide	<chem>CCC1=NOC(CNS(c2cc(C(NCC=C)O)ccc2)(=O)=O)C1</chem>	96.62	
RCB_CS0013	10025975	NA	435.4	1-methyl-4-[5-(morpholin-4-ylmethyl)-3-furoyl]-1,4,9-triazaspiro[5.5]undecane dihydrochloride	<chem>CN(CC1)C2(CCNC2)CN1C(c1ccc(CN2CCOCC2)c1)=O</chem>	72.72	
RCB_CS0024	10037740	70704262	362.5	2-(((3-amino-2-thienyl)carbonyl)amino)methyl)-N,N-dimethyl-7,8-dihydro-4H-pyrazolo[1,5-a][1,4]diazepine-5(6H)-carboxamide	<chem>CN(C)C(N1Cc2cc(CNC(c3cc3)c3N)=O)nn2CCCC1=O</chem>	104.81	
RCB_CS0027	10041741	70704267	362.5	N-cyclopropyl-N-(3-hydroxybenzyl)-2-(2,4,7-trimethyl-1H-indol-3-yl)acetamide	<chem>Cc1c(CC N(Cc2cc(O)ccc2)C2CC2)=O)c2c(C)ccc(C)c2[nH]1</chem>	103.84	
RCB_CS0029	10045111	NA	316.4	N-((3S*,4R*)-4-ethoxytetrahydrofuran-3-yl)-N''''-(1-phenyl-1H-pyrazol-5-yl)urea	<chem>CCO[C@@H](COC1)[C@H]1NC(Nc1ccnn1-c1cccc1)=O</chem>	99.86	
RCB_CS0030	10045854	NA	370.5	[3''''-(4-[2-(4-methylthio)ethyl]piperazin-1-yl)carbonyl)biphenyl-2-yl]methanol	<chem>CSCCN(CC1)CCN1C(c1cc(-c2c(CO)cccc2)ccc1)=O</chem>	93.1	
RCB_CS0033	10048011	91759616	333.4	5-([2-[2-(4-methylpiperazin-1-yl)ethyl]piperidin-1-yl]carbonyl)pyrazin-2-ol	<chem>CN1CCN(CCC(CCCC2)N2C(c(cn2)ncc2O)=O)CC1</chem>	79.25	
RCB_CS0034	10049170	NA	370.5	N-(2,1,3-benzoxadiazol-5-ylmethyl)-2-[2-(2-thienyl)ethyl]piperidine-1-carboxamide	<chem>O=C(NC1cc2nonc2cc1)N1C(Cc2cccs2)CCCC1</chem>	131.62	
RCB_CS0038	10057755	70704288	374.9	N-((3S*,4R*)-1-((6-chloro-1,3-benzodioxol-5-yl)methyl)-4-isopropyl-3-pyrrolidinyl)methanesulfonamide	<chem>CC(C)[C@@H](CN(Cc(cc1OCCc1c1)c1C1)[C@H]1NS(C)(=O)=O</chem>	105.68	

Showing 1 to 10 of 24,361 entries

Previous 1 2 3 4 5 ... 2,437 Next

# Case 5: Commercial procurement information for a specific compound

## Step 2 : Click on ID of selected entry

SMCVdb

Show 10 entries

Search:

SMCV ID	Source ID	PubChem CID	MW	IUPAC Name	SMILES	Viability	Reference Image
RCB_CS0009	10015705	134067281	350.4	N,5,6-trimethyl-2-oxo-N-[1-(5-phenyl-1H-pyrazol-3-yl)ethyl]-1,2-dihydro-3-pyridinecarboxamide	<chem>CC(c1n[nH]c(-c2ccccc2)c1)N(C)C(C1=CC(C)=C(C)NC1=O)=O</chem>	113.28	
RCB_CS0011	10022643	72837098	351.4	N-allyl-3-(((3-ethyl-4,5-dihydroisoxazol-5-yl)methyl)amino)sulfonylbenzamide	<chem>CCC1=NOC(CNS(c2cc(C(NCC=C)O)ccc2)(=O)=O)C1</chem>	96.62	
RCB_CS0013	10025975	NA	435.4	1-methyl-4-[5-(morpholin-4-ylmethyl)-3-furoyl]-1,4,9-triazaspiro[5.5]undecane dihydrochloride	<chem>CN(CC1)C2(CCNCC2)CN1C(c1coc(CN2CCOCC2)c1)=O</chem>	72.72	
RCB_CS0029	10045854	62	362.5	2-(((3-amino-2-thienyl)carbonyl)amino)methyl)-N,N-dimethyl-7,8-dihydro-4H-pyrazolo[1,5-a][1,4]diazepine-5(6H)-carboxamide	<chem>CN(C)C(N1Cc2cc(CNC(c3cc3)c3N)=O)nn2CCC1=O</chem>	104.81	
RCB_CS0029	10045854	67	362.5	N-cyclopropyl-N-(3-hydroxybenzyl)-2-(2,4,7-trimethyl-1H-indol-3-yl)acetamide	<chem>Cc1c(CC[N](Cc2cc(O)ccc2)C2CC2=O)c2c(C)ccc(C)c2[nH]1</chem>	103.84	
RCB_CS0029	10045854	NA	316.4	N-((3S*,4R*)-4-ethoxytetrahydrofuran-3-yl)-N''''-(1-phenyl-1H-pyrazol-5-yl)urea	<chem>CCO[C@@H](COC1)[C@H]1NC(Nc1ccnn1-c1ccccc1)=O</chem>	99.86	
RCB_CS0030	10045854	NA	370.5	[3''''-(4-[2-(methylthio)ethyl]piperazin-1-yl)carbonyl]biphenyl-2-yl)methanol	<chem>CSCCN(CC1)CCN1C(c1cc(-c2c(CO)ccc2)ccc1)=O</chem>	93.1	
RCB_CS0033	10048011	91759616	333.4	5-((2-[2-(4-methylpiperazin-1-yl)ethyl]piperidin-1-yl)carbonyl)pyrazin-2-ol	<chem>CN1CCN(CCC(CCCCC)N2C(c(cn2)ncc2O)=O)CC1</chem>	79.25	
RCB_CS0034	10049170	NA	370.5	N-(2,1,3-benzoxadiazol-5-ylmethyl)-2-[2-(2-thienyl)ethyl]piperidine-1-carboxamide	<chem>O=C(NC1cc2nonc2cc1)N1C(CCC2CCCS2)CCCC1</chem>	131.62	
RCB_CS0038	10057755	70704288	374.9	N-((3S*,4R*)-1-((6-chloro-1,3-benzodioxol-5-yl)methyl)-4-isopropyl-3-pyrrolidiny])methanesulfonamide	<chem>CC(C)[C@@H](CN(Cc(cc1OCC1c1c1)C1)[C@H]1NS(C)(=O)=O</chem>	105.68	

Showing 1 to 10 of 24,361 entries

Previous 1 2 3 4 5 ... 2,437 Next



# Case 6: Downloading compound in molecular docking-supported format

Step 1 : Choose your compound using case 1-3

SMCVdb

Home  
ADME(T) Analysis  
Target prediction  
About  
User guide New  
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Download Data  
Update

Show 10 entries

Search:

SMCV ID	Source ID	PubChem CID	MW	IUPAC Name	SMILES	Viability	Reference Image
All	All	All	All	All	All	All	All
RCB_CS0009	10015705	134067281	350.4	N,5,6-trimethyl-2-oxo-N-[1-(5-phenyl-1H-pyrazol-3-yl)ethyl]-1,2-dihydro-3-pyridinecarboxamide	<chem>CC(c1n[nH]c(-c2cccc2)c1)N(C)C(C1=CC(C)=C(C)NC1=O)=O</chem>	113.28	
RCB_CS0011	10022643	72837098	351.4	N-allyl-3-(((3-ethyl-4,5-dihydroisoxazol-5-yl)methyl)amino)sulfonylbenzamide	<chem>CCC1=NOC(CNS(c2cc(C(NCC=C)O)ccc2)(=O)=O)C1</chem>	96.62	
RCB_CS0013	10025975	NA	435.4	1-methyl-4-[5-(morpholin-4-ylmethyl)-3-furoyl]-1,4,9-triazaspiro[5.5]undecane dihydrochloride	<chem>CN(CC1)C2(CCNC2)CN1C(c1coc(CN2CCOCC2)c1)=O</chem>	72.72	
RCB_CS0024	10037740	70704262	362.5	2-(((3-amino-2-thienyl)carbonyl)amino)methyl)-N,N-dimethyl-7,8-dihydro-4H-pyrazolo[1,5-a][1,4]diazepine-5(6H)-carboxamide	<chem>CN(C)C(N1Cc2cc(CNC(c(scc3)c3N)=O)nn2CCCC1)=O</chem>	104.81	
RCB_CS0027	10041741	70704267	362.5	N-cyclopropyl-N-(3-hydroxybenzyl)-2-(2,4,7-trimethyl-1H-indol-3-yl)acetamide	<chem>Cc1c(CC N(Cc2cc(O)ccc2)C2CC2)=O)c2c(C)ccc(C)c2[nH]1</chem>	103.84	
RCB_CS0029	10045111	NA	316.4	N-((3S*,4R*)-4-ethoxytetrahydrofuran-3-yl)-N''''-[1-phenyl-1H-pyrazol-5-yl]urea	<chem>CCO[C@@H](COC1)[C@H]1NC(Nc1ccnn1-c1cccc1)=O</chem>	99.86	
RCB_CS0030	10045854	NA	370.5	[3''''-[4-[2-(methylthio)ethyl]piperazin-1-yl]carbonyl]biphenyl-2-yl)methanol	<chem>CSCCN(CC1)CCN1C(c1cc(-c2c(CO)cccc2)ccc1)=O</chem>	93.1	
RCB_CS0033	10048011	91759616	333.4	5-((2-[2-(4-methylpiperazin-1-yl)ethyl]piperidin-1-yl)carbonyl)pyrazin-2-ol	<chem>CN1CCN(CCC(CCCC2)N2C(c(cn2)ncc2O)=O)CC1</chem>	79.25	
RCB_CS0034	10049170	NA	370.5	N-(2,1,3-benzoxadiazol-5-ylmethyl)-2-[2-(2-thienyl)ethyl]piperidine-1-carboxamide	<chem>O=C(NC1cc2nonc2cc1)N1C(Cc2cccs2)CCCC1</chem>	131.62	
RCB_CS0038	10057755	70704288	374.9	N-((3S*,4R*)-1-[[6-chloro-1,3-benzodioxol-5-yl)methyl]-4-isopropyl-3-pyrrolidinyl)methanesulfonamide	<chem>CC(C)[C@@H](CN(Cc(cc1OCC1c1)c1C1)C1)[C@H]1NS(C)(=O)=O</chem>	105.68	

Showing 1 to 10 of 24,361 entries

Previous 1 2 3 4 5 ... 2,437 Next

# Case 6: Downloading compound in molecular docking-supported format

## Step 2 : Click on ID of selected entry

The screenshot displays the SMCVdb interface with a table of chemical compounds. The table has columns for SMCV ID, Source ID, PubChem CID, MW, IUPAC Name, SMILES, Viability, and Reference Image. The entry with Source ID 10045854 is highlighted with a red box, and a callout bubble points to this ID.

SMCV ID	Source ID	PubChem CID	MW	IUPAC Name	SMILES	Viability	Reference Image
RCB_CS0009	10015705	134067281	350.4	N,5,6-trimethyl-2-oxo-N-[1-(5-phenyl-1H-pyrazol-3-yl)ethyl]-1,2-dihydro-3-pyridinecarboxamide	<chem>CC(c1n[nH]c(-c2cccc2)c1)N(C)C(C1=CC(C)=C(C)NC1=O)=O</chem>	113.28	
RCB_CS0011	10022643	72837098	351.4	N-allyl-3-(((3-ethyl-4,5-dihydroisoxazol-5-yl)methyl)amino)sulfonyl)benzamide	<chem>CCC1=NOC(CNS(c2cc(C(NCC=C)O)ccc2)(=O)=O)C1</chem>	96.62	
RCB_CS0013	10025975	NA	435.4	1-methyl-4-[5-(morpholin-4-ylmethyl)-3-furoyl]-1,4,9-triazaspiro[5.5]undecane dihydrochloride	<chem>CN(CC1)C2(CCNCC2)CN1C(c1coc(CN2CCOCC2)c1)=O</chem>	72.72	
RCB_CS0029	10045854	NA	362.5	2-(((3-amino-2-thienyl)carbonyl)amino)methyl)-N,N-dimethyl-7,8-dihydro-4H-pyrazolo[1,5-a][1,4]diazepine-5(6H)-carboxamide	<chem>CN(C)C(N1Cc2cc(CNC(c3cc3)c3N)=O)nn2CCC1=O</chem>	104.81	
RCB_CS0029	10045854	NA	362.5	N-cyclopropyl-N-(3-hydroxybenzyl)-2-(2,4,7-trimethyl-1H-indol-3-yl)acetamide	<chem>Cc1c(CC[N](Cc2cc(O)ccc2)C2CC2)=O)c2c(C)ccc(C)c2[nH]1</chem>	103.84	
RCB_CS0029	10045854	NA	316.4	N-((3S*,4R*)-4-ethoxytetrahydrofuran-3-yl)-N''''-(1-phenyl-1H-pyrazol-5-yl)urea	<chem>CCO[C@@H](COC1)[C@H]1NC(Nc1ccnn1-c1cccc1)=O</chem>	99.86	
RCB_CS0030	10045854	NA	370.5	[3''''-(4-[2-(methylthio)ethyl]piperazin-1-yl)carbonyl]biphenyl-2-yl)methanol	<chem>CSCCN(CC1)CCN1C(c1cc(-c2c(CO)cccc2)ccc1)=O</chem>	93.1	
RCB_CS0033	10048011	91759616	333.4	5-([2-[2-(4-methylpiperazin-1-yl)ethyl]piperidin-1-yl]carbonyl)pyrazin-2-ol	<chem>CN1CCN(CCC(CCCC2)N2C(c(cn2)ncc2O)=O)CC1</chem>	79.25	
RCB_CS0034	10049170	NA	370.5	N-(2,1,3-benzoxadiazol-5-ylmethyl)-2-[2-(2-thienyl)ethyl]piperidine-1-carboxamide	<chem>O=C(NC1cc2nonc2cc1)N1C(CCC2CCCS2)CCCC1</chem>	131.62	
RCB_CS0038	10057755	70704288	374.9	N-((3S*,4R*)-1-((6-chloro-1,3-benzodioxol-5-yl)methyl)-4-isopropyl-3-pyrrolidiny])methanesulfonamide	<chem>CC(C)[C@@H](CN(Cc(cc1OCOc1c1c1)C1)[C@H]1NS(C)(=O)=O</chem>	105.68	

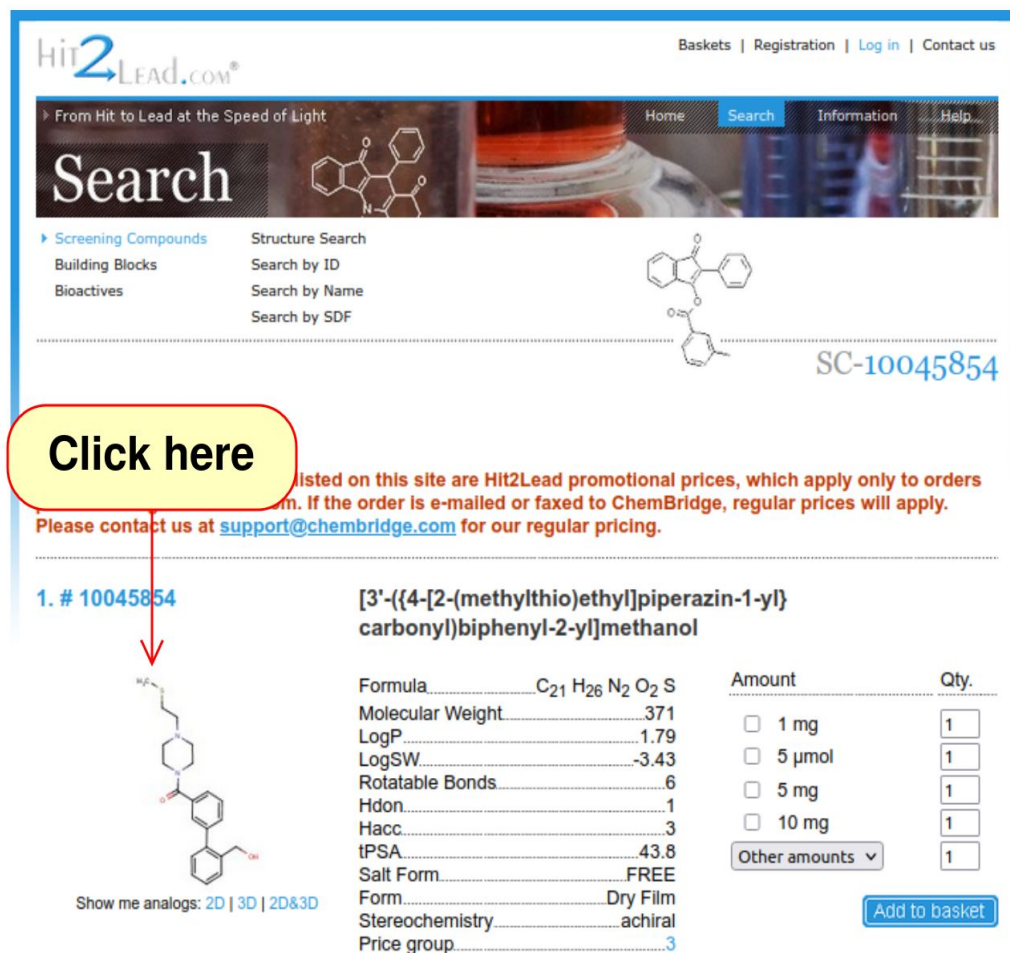
Showing 1 to 10 of 24,361 entries

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# Case 6: Downloading compound in molecular docking-supported format

Step 4 : click on image



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 Building Blocks Search by ID  
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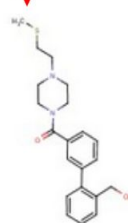
SC-10045854

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1. # 10045854

[3'-({4-[2-(methylthio)ethyl]piperazin-1-yl} carbonyl)biphenyl-2-yl]methanol



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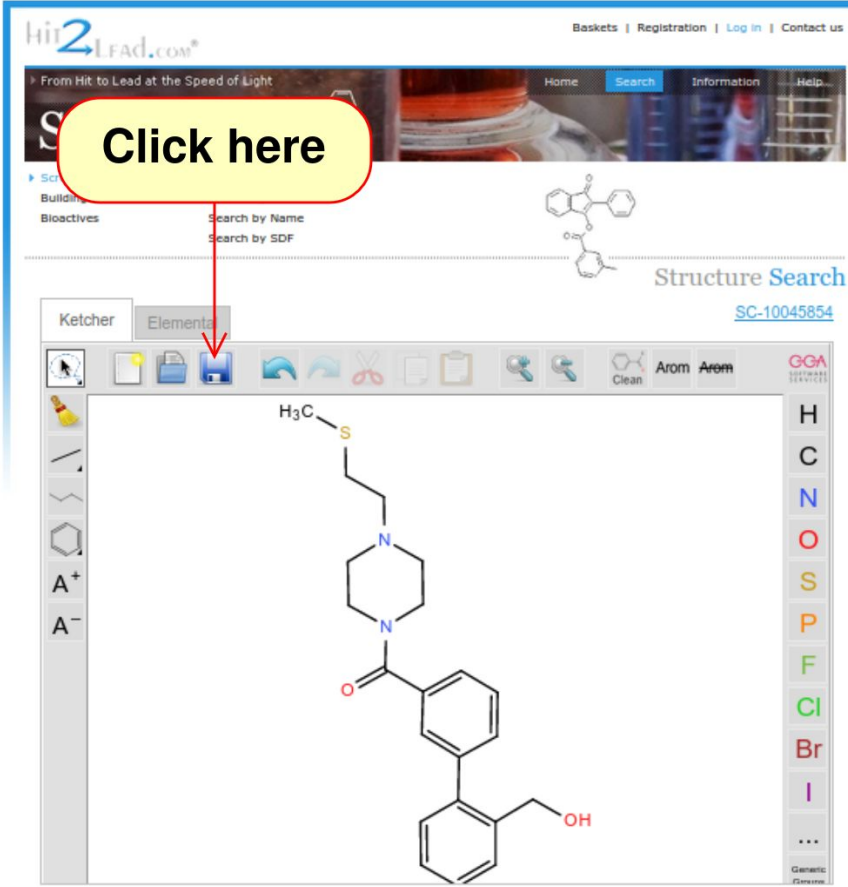
Formula.....	C <sub>21</sub> H <sub>26</sub> N <sub>2</sub> O <sub>2</sub> S	Amount	Qty.
Molecular Weight.....	371	<input type="checkbox"/> 1 mg	<input type="text" value="1"/>
LogP.....	1.79	<input type="checkbox"/> 5 µmol	<input type="text" value="1"/>
LogSW.....	-3.43	<input type="checkbox"/> 5 mg	<input type="text" value="1"/>
Rotatable Bonds.....	.6	<input type="checkbox"/> 10 mg	<input type="text" value="1"/>
Hdon.....	.1	Other amounts ▾	<input type="text" value="1"/>
Hacc.....	.3		
tPSA.....	43.8		
Salt Form.....	FREE		
Form.....	Dry Film		
Stereochemistry.....	achiral		
Price group.....	.3		

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# Case 6: Downloading compound in molecular docking-supported format

Step 5 : Click save icon (  )



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Structure Search  
SC-10045854

Recent structures

Ketcher Elements

H<sub>3</sub>C-S

H  
C  
N  
O  
S  
P  
F  
Cl  
Br  
I  
...

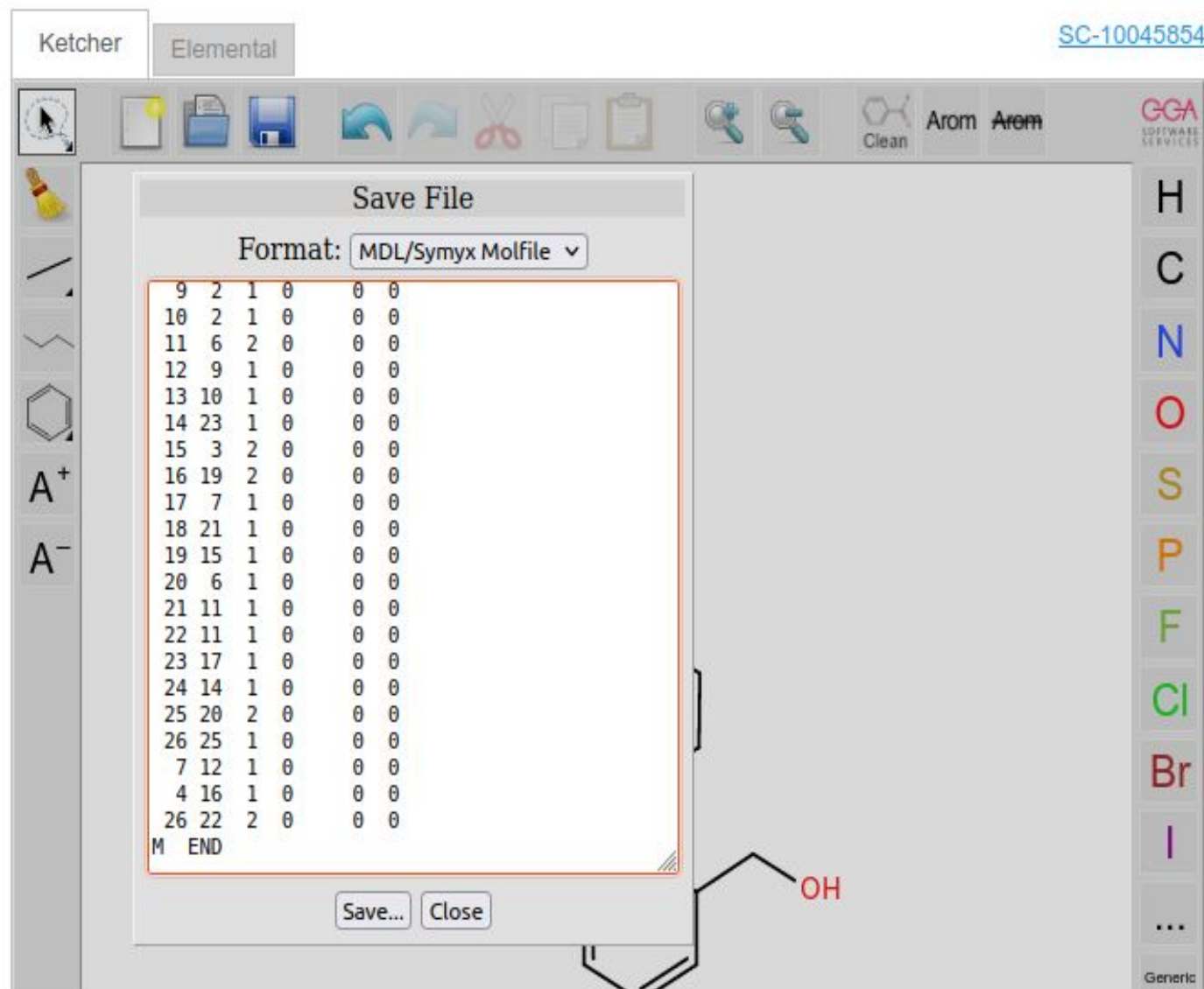
Search parameters

Substructure Search  
 Exact Match

Search

# Case 6: Downloading compound in molecular docking-supported format

Step 6 : save it in MOL format.



NOTE : MOL format is acceptable for molecular docking tools

Source : [www.hit2lead.com/](http://www.hit2lead.com/)

# Case 7: Accessing PubChem Information for a specific compound

**Step 1 :** Choose your compound using case 1-3, then go to “PubChem CID”

SMCVdb

Home  
ADME(T) Analysis  
Target prediction  
About  
User guide **New**  
Contact Us  
Download Data  
Update

Show 10 entries

Search:

SMCV_id	Source ID	PubChem CID	MW	IUPAC Name	SMILES	Viability	Reference Image
RCB_CS0009	10015705	134067281	350.4	N,5,6-trimethyl-2-oxo-N-[1-(5-phenyl-1H-pyrazol-3-yl)ethyl]-1,2-dihydro-3-pyridinecarboxamide	<chem>CC(c1n[nH]c(-c2cccc2)c1)N(C)C(C1=CC(C)=C(C)NC1=O)=O</chem>	113.28	
RCB_CS0011	10022643	72837098	351.4	N-allyl-3-(((3-ethyl-4,5-dihydroisoxazol-5-yl)methyl)amino)sulfonyl)benzamide	<chem>CCC1=NOC(CNS(c2cc(C(NCC=C)O)ccc2)(=O)=O)C1</chem>	96.62	
RCB_CS0013	10025975	NA	435.4	1-methyl-4-[5-(morpholin-4-ylmethyl)-3-furoyl]-1,4,9-triazaspiro[5.5]undecane dihydrochloride	<chem>CN(CC1)C2(CNCC2)CN1C(c1ccc(CN2CCOCC2)c1)=O</chem>	72.72	
RCB_CS0024	10037740	70704262	362.5	2-(((3-amino-2-thienyl)carbonyl)amino)methyl)-N,N-dimethyl-7,8-dihydro-4H-pyrazolo[1,5-a][1,4]diazepine-5(6H)-carboxamide	<chem>CN(C)C(N1Cc2cc(CNC(c(scc3)c3N)=O)nn2CCC1)=O</chem>	104.81	
RCB_CS0027	10041741	70704267	362.5	N-cyclopropyl-N-(3-hydroxybenzyl)-2-(2,4,7-trimethyl-1H-indol-3-yl)acetamide	<chem>Cc1c(CC(N(Cc2cc(O)ccc2)C2CC2)=O)c2c(C)ccc(C)c2[nH]1</chem>	103.84	
RCB_CS0029	10045111	NA	316.4	N-[(3S*,4R*)-4-ethoxytetrahydrofuran-3-yl]-N''''-(1-phenyl-1H-pyrazol-5-yl)urea	<chem>CCO[C@@H](COC1)[C@H]1NC(Nc1ccn1-c1cccc1)=O</chem>	99.86	
RCB_CS0030	10045854	NA	370.5	[3''''-[[4-[2-(methylthio)ethyl]piperazin-1-yl]carbonyl]biphenyl-2-yl]methanol	<chem>CSCCN(CC1)CCN1C(c1cc(-c2c(CO)cccc2)ccc1)=O</chem>	93.1	
RCB_CS0033	10048011	91759616	333.4	5-([2-[2-(4-methylpiperazin-1-yl)ethyl]piperidin-1-yl]carbonyl)pyrazin-2-ol	<chem>CN1CCN(CCC(CCCC2)N2C(c(cn2)ncc2O)=O)CC1</chem>	79.25	
RCB_CS0034	10049170	NA	370.5	N-(2,1,3-benzoxadiazol-5-ylmethyl)-2-[2-(2-thienyl)ethyl]piperidine-1-carboxamide	<chem>O=C(NC1cc2nonc2cc1)N1C(CCC2cccc2)CCCC1</chem>	131.62	
RCB_CS0038	10057755	70704288	374.9	N-[(3S*,4R*)-1-[[6-chloro-1,3-benzodioxol-5-yl)methyl]-4-isopropyl-3-pyrrolidinyl]methanesulfonamide	<chem>CC(C)[C@@H](CN(Cc(cc1OCOc1c1)c1C)C1)[C@H]1NS(C)(=O)=O</chem>	105.68	

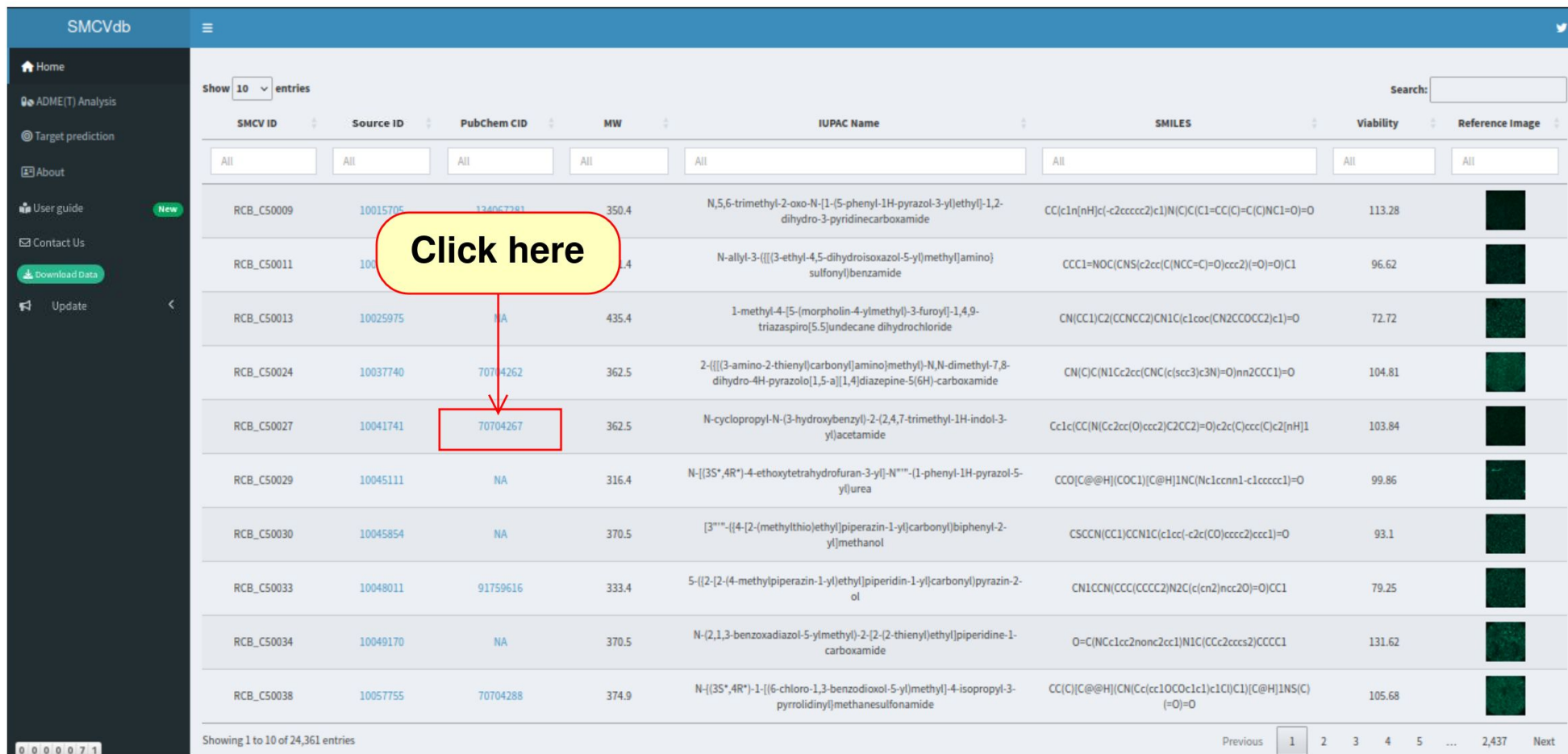
Showing 1 to 10 of 24,361 entries

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**Note :** Compounds with available cytotoxicity data in PubChem are Highlighted in navy

# Case 7: Accessing PubChem Information for a specific compound











## Step 2 : Click the link



SMCVdb

Show 10 entries

Search:

SMCV ID	Source ID	PubChem CID	MW	IUPAC Name	SMILES	Viability	Reference Image
RCB_C50009	10015705	134067381	350.4	N,5,6-trimethyl-2-oxo-N-[1-(5-phenyl-1H-pyrazol-3-yl)ethyl]-1,2-dihydro-3-pyridinecarboxamide	<chem>CC(c1n[nH]c(-c2ccccc2)c1)N(C)C(C1=CC(C)=C(C)NC1=O)=O</chem>	113.28	
RCB_C50011	10015705	134067381	350.4	N-allyl-3-(((3-ethyl-4,5-dihydroisoxazol-5-yl)methyl)amino)sulfonylbenzamide	<chem>CCCC=NO(C)NS(Cc2cc(C)ccc2)(=O)=O)C1</chem>	96.62	
RCB_C50013	10025975	NA	435.4	1-methyl-4-[5-(morpholin-4-ylmethyl)-3-furoyl]-1,4,9-triazaspiro[5.5]undecane dihydrochloride	<chem>CN(CC1)C2(CCNCC2)CN1C(c1ccc(CN2CCOCC2)c1)=O</chem>	72.72	
RCB_C50024	10037740	70704262	362.5	2-(((3-amino-2-thienyl)carbonyl)amino)methyl)-N,N-dimethyl-7,8-dihydro-4H-pyrazolo[1,5-a][1,4]diazepine-5(6H)-carboxamide	<chem>CN(C)C(N1Cc2cc(CNC(c3cc3)c3N)=O)nn2CCC1=O</chem>	104.81	
RCB_C50027	10041741	70704267	362.5	N-cyclopropyl-N-(3-hydroxybenzyl)-2-(2,4,7-trimethyl-1H-indol-3-yl)acetamide	<chem>Cc1c(CC(N(Cc2cc(O)ccc2)C2CC2)=O)c2c(C)ccc(C)c2[nH]1</chem>	103.84	
RCB_C50029	10045111	NA	316.4	N-((3S*,4R*)-4-ethoxytetrahydrofuran-3-yl)-N''''-(1-phenyl-1H-pyrazol-5-yl)urea	<chem>CCO[C@@H](COC1)[C@H]1NC(Nc1ccn1-c1ccccc1)=O</chem>	99.86	
RCB_C50030	10045854	NA	370.5	[3''''-[[4-[2-(methylthio)ethyl]piperazin-1-yl]carbonyl]biphenyl-2-yl]methanol	<chem>CSCCN(CC1)CCN1C(c1ccc(-c2c(CO)cccc2)ccc1)=O</chem>	93.1	
RCB_C50033	10048011	91759616	333.4	5-[[2-[2-(4-methylpiperazin-1-yl)ethyl]piperidin-1-yl]carbonyl]pyrazin-2-ol	<chem>CN1CCN(CCC(CCCC2)N2C(c3cn2)ccc3=O)CC1</chem>	79.25	
RCB_C50034	10049170	NA	370.5	N-(2,1,3-benzoxadiazol-5-ylmethyl)-2-[2-(2-thienyl)ethyl]piperidine-1-carboxamide	<chem>O=C(NC1cc2nonc2cc1)N1C(CCC2cccs2)CCCC1</chem>	131.62	
RCB_C50038	10057755	70704288	374.9	N-((3S*,4R*)-1-((6-chloro-1,3-benzodioxol-5-yl)methyl)-4-isopropyl-3-pyrrolidinyl)methanesulfonamide	<chem>CC(C)[C@@H](N)(CC(cc1OCOc1c1c1Cl)Cl1)[C@H]1NS(C)(=O)=O</chem>	105.68	

Showing 1 to 10 of 24,361 entries

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# Case 7: Accessing PubChem Information for a specific compound

Step 3 : The Pubchem page associated with selected name will appear

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National Center for Biotechnology Information

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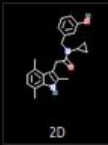
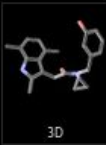
COMPOUND SUMMARY

## N-cyclopropyl-N-(3-hydroxybenzyl)-2-(2,4,7-trimethyl-1H-indol-3-yl)acetamide

Cite Download

CONTENTS

- Title and Summary
- 1 Structures
- 2 Names and Identifiers
- 3 Chemical and Physical Properties
- 4 Related Records
- 5 Chemical Vendors
- 6 Information Sources

PubChem CID	70704267
Structure	 
Molecular Formula	C <sub>23</sub> H <sub>26</sub> N <sub>2</sub> O <sub>2</sub>
Synonyms	MCULE-7573708121 N-cyclopropyl-N-(3-hydroxybenzyl)-2-(2,4,7-trimethyl-1H-indol-3-yl)acetamide
Molecular Weight	362.5 g/mol <small>Computed by PubChem 2.1 (PubChem release 2021.05.07)</small>
Dates	Create: 2013-03-04 Modify: 2024-04-20

# Case 8: Performing ADME(T) analysis of a selected compound

Step 1 : Choose your compound using case 1-3 and copy the smile notation

SMCVdb

Show 10 entries

Search:

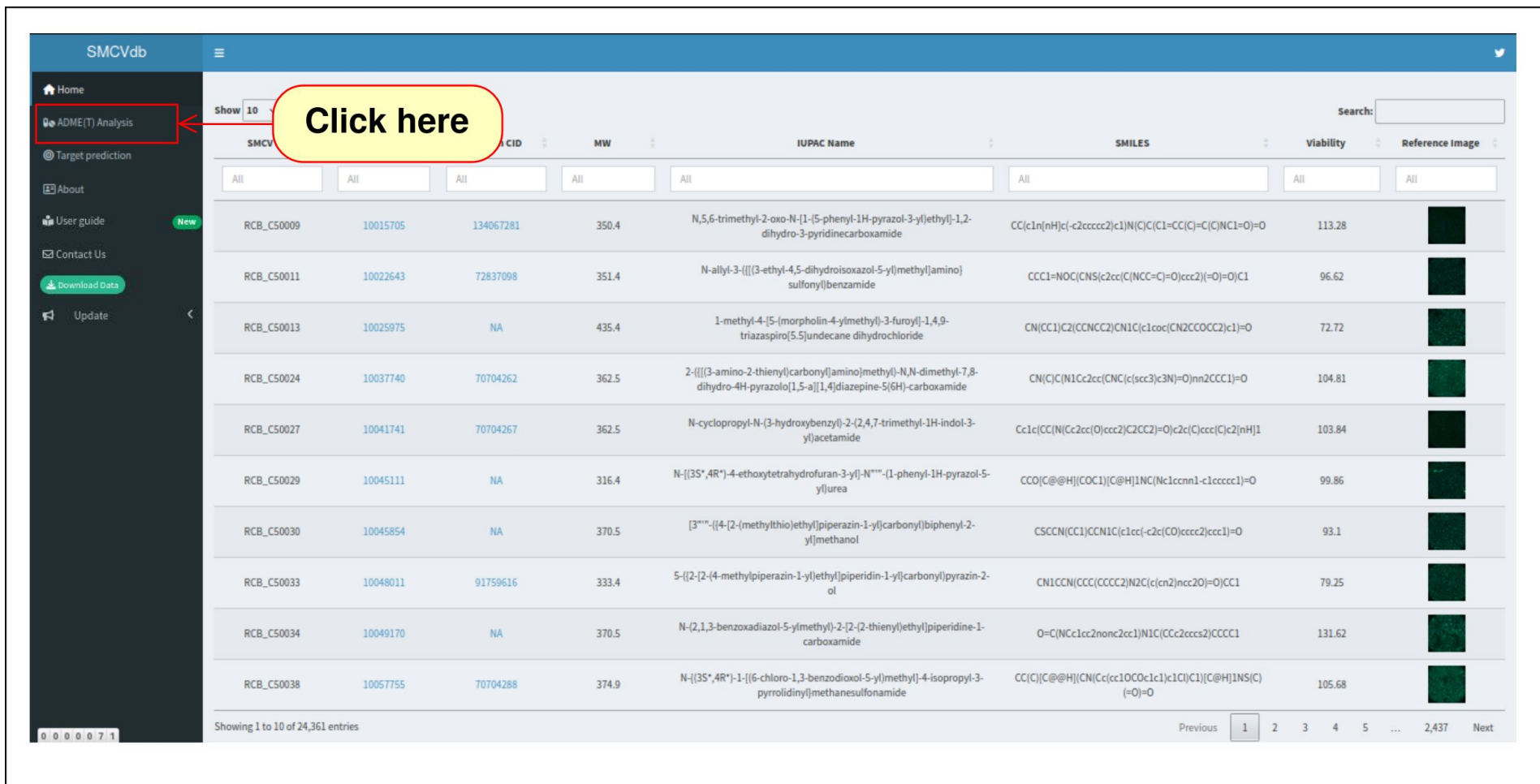
SMCV ID	Source ID	PubChem CID	MW	IUPAC Name	SMILES	Viability	Reference Image
All	All	All	All	All	All	All	All
RCB_C50009	10015705	134067281	350.4	N,5,6-trimethyl-2-oxo-N-[1-(5-phenyl-1H-pyrazol-3-yl)ethyl]-1,2-dihydro-3-pyridinecarboxamide	<chem>CC(c1n[nH]c(-c2cccc2)c1)N(C)C(C1=CC(C)=C(C)NC1=O)=O</chem>	113.28	
RCB_C50011	10022643	72837098	351.4	N-allyl-3-(((3-ethyl-4,5-dihydroisoxazol-5-yl)methyl)amino)sulfonylbenzamide	<chem>CCCC=NOC(CNS)(c2cc(C(NCC=C)O)ccc2)(=O)C1</chem>	96.62	
RCB_C50013	10025975	NA	435.4	1-methyl-4-[5-(morpholin-4-ylmethyl)-3-furoyl]-1,4,9-triazaspiro[5.5]undecane dihydrochloride	<chem>CN(CC1)C2(CCNC2)CN1C(c1ccc(CN2CCOCC2)c1)=O</chem>	72.72	
RCB_C50024	10037740	70704262	362.5	2-(((3-amino-2-thienyl)carbonyl)amino)methyl-N,N-dimethyl-7,8-dihydro-4H-pyrazolo[1,5-a][1,4]diazepine-5(6H)-carboxamide	<chem>CN(C)C(N1Cc2cc(CNC(c(ccc3c3N)=O)nn2CCC1)=O</chem>	104.81	
RCB_C50027	10041741	70704267	362.5	N-cyclopropyl-N-(3-hydroxybenzyl)-2-(2,4,7-trimethyl-1H-indol-3-yl)acetamide	<chem>Cc1c(CC(N(Cc2cc(O)ccc2)C2CC2)=O)c2c(C)ccc(C)c2[nH]1</chem>	103.84	
RCB_C50029	10045111	NA	316.4	N-([3S*,4R*]-4-ethoxytetrahydrofuran-3-yl)-N''''-[1-phenyl-1H-pyrazol-5-yl]urea	<chem>CCO[C@@H](COC1)[C@H]1NC(Nc1ccnn1-c1cccc1)=O</chem>	99.86	
RCB_C50030	10045854	NA	370.5	[3''''-[[4-[2-(methylthio)ethyl]piperazin-1-yl]carbonyl]biphenyl-2-yl]methanol	<chem>CSCCN(CC1)CCN1C(c1cc(-c2c(CO)ccc2)ccc1)=O</chem>	93.1	
RCB_C50033	10048011	91759616	333.4	5-([2-[2-(4-methylpiperazin-1-yl)ethyl]piperidin-1-yl]carbonyl)pyrazin-2-ol	<chem>CN1CCN(CCC(CCCC)N2C(c(cn2)nc2O)=O)CC1</chem>	79.25	
RCB_C50034	10049170	NA	370.5	N-(2,1,3-benzoxadiazol-5-ylmethyl)-2-[2-(2-thienyl)ethyl]piperidine-1-carboxamide	<chem>O=C(NC1cc2nonc2cc1)N1C(CCc2ccsc2)CCCC1</chem>	131.62	
RCB_C50038	10057755	70704288	374.9	N-([3S*,4R*]-1-[[6-chloro-1,3-benzodioxol-5-yl)methyl]-4-isopropyl-3-pyrroloindinyl]methanesulfonamide	<chem>CC(C)[C@@H](CN(Cc(cc1OCOC1c1c1Cl)Cl)[C@H]1NS(C)(=O)=O</chem>	105.68	

Showing 1 to 10 of 24,361 entries











Previous 1 2 3 4 5 ... 2,437 Next

# Case 8: Performing ADME(T) analysis of a selected compound

Step 2 : Click on 'ADME(T) Analysis' from side panel



The screenshot displays the SMCVdb web application interface. The side panel on the left contains a navigation menu with the following items: Home, ADME(T) Analysis (highlighted with a red box and a yellow callout bubble saying "Click here"), Target prediction, About, User guide (marked as "New"), Contact Us, Download Data, and Update. The main content area shows a table of compounds with columns for SMCV, CID, MW, IUPAC Name, SMILES, Viability, and Reference image. The table lists 10 entries, with the first entry being RCB\_CS0009 (CID 10015705, MW 350.4). The bottom of the page shows "Showing 1 to 10 of 24,361 entries" and a pagination control with "Previous", "1", "2", "3", "4", "5", "...", "2,437", and "Next".

SMCV	CID	MW	IUPAC Name	SMILES	Viability	Reference image	
RCB_CS0009	10015705	134067281	350.4	N,5,6-trimethyl-2-oxo-N-[[1-(5-phenyl-1H-pyrazol-3-yl)ethyl]-1,2-dihydro-3-pyridinecarboxamide	CC(c1n[nH]c(-c2ccccc2)c1)N(C)C(C1=CC(C)=C(C)N)C1=O	113.28	
RCB_CS0011	10022643	72837098	351.4	N-allyl-3-[[[3-ethyl-4,5-dihydroisoxazol-5-yl)methyl]amino]sulfonyl]benzamide	CCC1=NO(C)CNS(c2cc(C(NCC=C)O)ccc2)(=O)=O)C1	96.62	
RCB_CS0013	10025975	NA	435.4	1-methyl-4-[5-(morpholin-4-ylmethyl)-3-furoyl]-1,4,9-triazaspiro[5.5]undecane dihydrochloride	CN(CC1)C2(CCNCC2)CN1C(c1ccc(CN2CCOCC2)c1)=O	72.72	
RCB_CS0024	10037740	70704262	362.5	2-[[[3-amino-2-thienyl]carbonyl]amino]methyl]-N,N-dimethyl-7,8-dihydro-4H-pyrazolo[1,5-a][1,4]diazepine-5(6H)-carboxamide	CN(C)C(N1Cc2cc(CNC(c(ccc3c3N)=O)nn2)CCC1)=O	104.81	
RCB_CS0027	10041741	70704267	362.5	N-cyclopropyl-N-(3-hydroxybenzyl)-2-(2,4,7-trimethyl-1H-indol-3-yl)acetamide	Cc1c(C(C(N(Cc2cc(O)ccc2)C2CC2)=O)c2c(C)ccc(C)c2[nH]1	103.84	
RCB_CS0029	10045111	NA	316.4	N-[[3S*,4R*]-4-ethoxytetrahydrofuran-3-yl]-N''''-(1-phenyl-1H-pyrazol-5-yl)urea	CCO[C@@H](COC1)[C@H]1NC(Nc1ccnn1-c1ccccc1)=O	99.86	
RCB_CS0030	10045854	NA	370.5	[3''''-[[4-[2-(methylthio)ethyl]piperazin-1-yl]carbonyl]biphenyl-2-yl]methanol	CSCCN(CC1)CCN1C(c1ccc(-c2c(CO)ccc2)ccc1)=O	93.1	
RCB_CS0033	10048011	91759616	333.4	5-[[2-[2-(4-methylpiperazin-1-yl)ethyl]piperidin-1-yl]carbonyl]pyrazin-2-ol	CN1CCN(CCC(CCCC)N2C(c(cn2)ncc2)=O)CC1	79.25	
RCB_CS0034	10049170	NA	370.5	N-(2,1,3-benzoxadiazol-5-ylmethyl)-2-[2-(2-thienyl)ethyl]piperidine-1-carboxamide	O=C(NC1cc2nonc2cc1)N1C(CCC2cccs2)CCCC1	131.62	
RCB_CS0038	10057755	70704288	374.9	N-[[3S*,4R*]-1-[[6-chloro-1,3-benzodioxol-5-yl)methyl]-4-isopropyl-3-pyrrolidinyl]methanesulfonamide	CC(C)[C@@H](CNC(Cc(cc1OCC1c1c1C1)[C@H]1NS(C)(=O)=O	105.68	

# Case 8: Performing ADME(T) analysis of a selected compound

**Step 3** : Click on the server link eg: SwissADME

The screenshot shows the SMCVdb website interface. The left sidebar contains navigation links: Home, ADME(T) Analysis, Target prediction, About, User guide (marked as 'New'), Contact Us, Download Data, and Update. The main content area is titled 'Recommended Web servers for ADME(T) analysis' and lists three servers: ADMETlab 2.0, SwissADME, and admetSAR. Below this list is a 'References' section with three entries:

1. Xiong, G., Wu, Z., Yi, J., Fu, L., Yang, Z., Hsieh, C., Yin, M., Zeng, X., Wu, C., Lu, A., Chen, X., Hou, T., & Cao, D. (2021). ADMETlab 2.0: an integrated online platform for accurate and comprehensive predictions of ADMET properties. *Nucleic acids research*, 49(W1), W5–W14. <https://doi.org/10.1093/nar/gkab255>
2. Daina, A., Michielin, O., & Zoete, V. (2017). SwissADME: a free web tool to evaluate pharmacokinetics, drug-likeness and medicinal chemistry friendliness of small molecules. *Scientific reports*, 7, 42717. <https://doi.org/10.1038/srep42717>
3. Yang, H., Lou, C., Sun, L., Li, J., Cai, Y., Wang, Z., Li, W., Liu, G., & Tang, Y. (2019). admetSAR 2.0: web-service for prediction and optimization of chemical ADMET properties. *Bioinformatics (Oxford, England)*, 35(6), 1067–1069. <https://doi.org/10.1093/bioinformatics/bty707>

At the bottom left of the page, there is a small box containing the number 0000042.



# Case 8: Performing ADME(T) analysis of a selected compound

## Step 4 : Paste the SMILES notation and click RUN

The screenshot displays the SwissADME web application interface. The browser address bar shows [www.swissadme.ch/index.php](http://www.swissadme.ch/index.php). The page header includes the SIB logo (Swiss Institute of Bioinformatics) and navigation links: Home, FAQ, Help, Contact, Terms of Use. A main text block describes the website's purpose: "This website allows you to compute physicochemical descriptors as well as to predict ADME parameters, pharmacokinetic properties, druglike nature and medicinal chemistry friendliness of one or multiple small molecules to support drug discovery." It also provides references for the underlying methodologies: iLOGP, GB/SA, and BOILED-Egg. Below this is a text input field labeled "Enter a list of SMILES here:" containing the SMILES string CSCCN(CC1)CCN1C(c1cc(-c2c(CO)cccc2)ccc1)=O. A red "Run!" button is positioned below the input field. To the left of the input field is a Marvin JS chemical editor interface with a toolbar and a list of elements (H, C, N, O, S, F, P, Cl, Br, I, \*). A "Show BOILED-Egg" button is visible at the bottom left. The footer includes "Retrieve data:" with icons for CSV and PDF, and "POWERED BY ChemAxon".

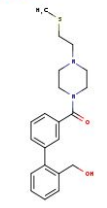
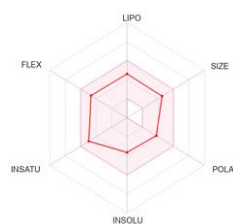
# Case 8: Performing ADME(T) analysis of a selected compound

## Step 5 : Result page will appear

← → ↻ [www.swissadme.ch/index.php](http://www.swissadme.ch/index.php)

Show BOILED-Egg Retrieve data: POWERED BY

**Molecule 1**

SMILES CSCCN1CCN(CC1)C(=O)c1cccc(c1)c1ccccc1CO

Physicochemical Properties	
Formula	C <sub>21</sub> H <sub>26</sub> N <sub>2</sub> O <sub>2</sub> S
Molecular weight	370.51 g/mol
Num. heavy atoms	26
Num. arom. heavy atoms	12
Fraction Csp <sup>3</sup>	0.38
Num. rotatable bonds	7
Num. H-bond acceptors	3
Num. H-bond donors	1
Molar Refractivity	116.14
TPSA	69.08 Å <sup>2</sup>

Lipophilicity	
Log P <sub>0/w</sub> (ILOGP)	3.47
Log P <sub>0/w</sub> (XLOGP3)	2.58
Log P <sub>0/w</sub> (WLOGP)	2.05
Log P <sub>0/w</sub> (MLOGP)	2.55
Log P <sub>0/w</sub> (SILICOS-IT)	3.71
Consensus Log P <sub>0/w</sub>	2.87

Water Solubility	
Log S (ESOL)	-3.64
Solubility	8.45e-02 mg/ml ; 2.28e-04 mol/l
Class	Soluble
Log S (All)	-3.68
Solubility	7.76e-02 mg/ml ; 2.09e-04 mol/l
Class	Soluble
Log S (SILICOS-IT)	-5.73
Solubility	6.93e-04 mg/ml ; 1.87e-06 mol/l
Class	Moderately soluble

Pharmacokinetics	
GI absorption	High
BBB permeant	Yes
P-gp substrate	Yes
CYP1A2 inhibitor	No
CYP2C19 inhibitor	Yes
CYP2C9 inhibitor	No
CYP2D6 inhibitor	Yes
CYP3A4 inhibitor	Yes
Log K <sub>p</sub> (skin permeation)	-6.73 cm/s

Druglikeness	
Lipinski	Yes; 0 violation
Ghose	Yes
Veber	Yes
Egan	Yes
Muegge	Yes
Bioavailability Score	0.55

Medicinal Chemistry	
PAINS	0 alert
Brenk	0 alert
Leadlikeness	No; 1 violation: MW>350
Synthetic accessibility	2.75

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# Case 9: Target prediction for a specific compound

Tutorial main

Step 1 : Choose your compound using case 1-3 and copy the smile notation

SMCV ID	Source ID	PubChem CID	MW	IUPAC Name	SMILES	Viability	Reference Image
RCB_C50009	10015705	134067281	350.4	N,5,6-trimethyl-2-oxo-N-[1-(5-phenyl-1H-pyrazol-3-yl)ethyl]-1,2-dihydro-3-pyridinecarboxamide	<chem>CC(c1n[nH]c(-c2cccc2)c1)N(C)C(C1=CC(C)=C(C)NC1=O)=O</chem>	113.28	
RCB_C50011	10022643	72837098	351.4	N-allyl-3-(((3-ethyl-4,5-dihydroisoxazol-5-yl)methyl)amino)sulfonylbenzamide	<chem>CCCC=NOC(CNS)(c2cc(C(NCC=C)O)ccc2)(=O)=O)C1</chem>	96.62	
RCB_C50013	10025975	NA	435.4	1-methyl-4-[5-(morpholin-4-ylmethyl)-3-furoyl]-1,4,9-triazaspiro[5.5]undecane dihydrochloride	<chem>CN(CC1)C2(CCNC2)CN1C(c1ccc(CN2CCOCC2)c1)=O</chem>	72.72	
RCB_C50024	10037740	70704262	362.5	2-(((3-amino-2-thienyl)carbonyl)amino)methyl)-N,N-dimethyl-7,8-dihydro-4H-pyrazolo[1,5-a][1,4]diazepine-5(6H)-carboxamide	<chem>CN(C)C(N1Cc2cc(CNC(c(scc3c3N)=O)nn2CCC1)=O</chem>	104.81	
RCB_C50027	10041741	70704267	362.5	N-cyclopropyl-N-(3-hydroxybenzyl)-2-(2,4,7-trimethyl-1H-indol-3-yl)acetamide	<chem>Cc1c(CC(N(Cc2cc(O)ccc2)C2CC2)=O)c2c(C)ccc(C)c2[nH]1</chem>	103.84	
RCB_C50029	10045111	NA	316.4	N-([3S*,4R*]-4-ethoxytetrahydrofuran-3-yl)-N''''-[1-phenyl-1H-pyrazol-5-yl]urea	<chem>CCO[C@@H](COC1)[C@H]1NC(Nc1ccnn1-c1cccc1)=O</chem>	99.86	
RCB_C50030	10045854	NA	370.5	[3''''-[[4-[2-(methylthio)ethyl]piperazin-1-yl]carbonyl]biphenyl-2-yl]methanol	<chem>CSCCN(CC1)CCN1C(c1cc(-c2c(CO)ccc2)ccc1)=O</chem>	93.1	
RCB_C50033	10048011	91759616	333.4	5-([2-[2-(4-methylpiperazin-1-yl)ethyl]piperidin-1-yl]carbonyl)pyrazin-2-ol	<chem>CN1CCN(CCC(CCCC)N2C(c(cn2)nc2O)=O)CC1</chem>	79.25	
RCB_C50034	10049170	NA	370.5	N-(2,1,3-benzoxadiazol-5-ylmethyl)-2-[2-(2-thienyl)ethyl]piperidine-1-carboxamide	<chem>O=C(NC1cc2nonc2cc1)N1C(CCc2ccsc2)CCCC1</chem>	131.62	
RCB_C50038	10057755	70704288	374.9	N-([3S*,4R*]-1-[[6-chloro-1,3-benzodioxol-5-yl)methyl]-4-isopropyl-3-pyrroloindinyl]methanesulfonamide	<chem>CC(C)[C@@H](CN(Cc(cc1OCOc1c1c1Cl)Cl1)[C@H]1NS(C)(=O)=O</chem>	105.68	

# Case 9: Target prediction for a specific compound

Step 2 : Click on 'Target prediction' from side panel

The screenshot shows the SMCVdb web application interface. On the left side, there is a dark sidebar with navigation options: Home, ADME(T) Analysis, Target prediction (highlighted with a red box and a yellow callout box saying "Click here"), About, User guide, Contact Us, Download Data, and Update. The main content area displays a table of chemical compounds. The table has columns for SMCV, CID, MW, IUPAC Name, SMILES, Viability, and Reference Image. The first row of data is for RCB\_C50009, with CID 10015705 and MW 350.4. The IUPAC Name is N,5,6-trimethyl-2-oxo-N-[1-(5-phenyl-1H-pyrazol-3-yl)ethyl]-1,2-dihydro-3-pyridinecarboxamide. The SMILES string is CC(c1n[nH]c(-c2cccc2)c1)N(C)C(CI=CC(C)=C(C)NC1=O)=O. The Viability is 113.28. The Reference Image is a small green square. The table shows 10 entries, and the total number of entries is 24,361. The page number is 1, and there are 2,437 pages in total.

SMCV	CID	MW	IUPAC Name	SMILES	Viability	Reference Image
RCB_C50009	10015705	350.4	N,5,6-trimethyl-2-oxo-N-[1-(5-phenyl-1H-pyrazol-3-yl)ethyl]-1,2-dihydro-3-pyridinecarboxamide	<chem>CC(c1n[nH]c(-c2cccc2)c1)N(C)C(CI=CC(C)=C(C)NC1=O)=O</chem>	113.28	
RCB_C50011	10022643	351.4	N-allyl-3-[[[(3-ethyl-4,5-dihydroisoxazol-5-yl)methyl]amino]sulfonyl]benzamide	<chem>CCC1=NOC(CNS(c2cc(C(NCC=C)=O)ccc2)(=O)=O)C1</chem>	96.62	
RCB_C50013	10025975	NA	1-methyl-4-[5-(morpholin-4-ylmethyl)-3-furoyl]-1,4,9-triazaspiro[5.5]undecane dihydrochloride	<chem>CN(CC1)C2(CCNC2)CN1C(c1ccc(CN2CCOCC2)c1)=O</chem>	72.72	
RCB_C50024	10037740	362.5	2-[[[(3-amino-2-thienyl)carbonyl]amino]methyl]-N,N-dimethyl-7,8-dihydro-4H-pyrazolo[1,5-a][1,4]diazepine-5(6H)-carboxamide	<chem>CN(C)C(N1Cc2cc(CNC(c3cc3)c3N)=O)nn2CCC1=O</chem>	104.81	
RCB_C50027	10041741	362.5	N-cyclopropyl-N-(3-hydroxybenzyl)-2-(2,4,7-trimethyl-1H-indol-3-yl)acetamide	<chem>Cc1c(CC(N(Cc2cc(O)ccc2)C2CC2)=O)c2c(C)ccc(C)c2[nH]1</chem>	103.84	
RCB_C50029	10045111	NA	N-[(3S*,4R*)-4-ethoxytetrahydrofuran-3-yl]-N''''-(1-phenyl-1H-pyrazol-5-yl)urea	<chem>CCO[C@@H](COC1)[C@H]1NC(Nc1ccn1-c1cccc1)=O</chem>	99.86	
RCB_C50030	10045854	NA	[3''''-[[4-[2-(methylthio)ethyl]piperazin-1-yl]carbonyl]biphenyl-2-yl]methanol	<chem>CSCCN(CC1)CCN1C(c1cc(-c2c(CO)cccc2)ccc1)=O</chem>	93.1	
RCB_C50033	10048011	333.4	5-[[2-[2-(4-methylpiperazin-1-yl)ethyl]piperidin-1-yl]carbonyl]pyrazin-2-ol	<chem>CN1CCN(CCC(CCCC2)N2C(c1cn2)ncc2O)=O)CC1</chem>	79.25	
RCB_C50034	10049170	NA	N-(2,1,3-benzoxadiazol-5-ylmethyl)-2-[2-(2-thienyl)ethyl]piperidine-1-carboxamide	<chem>O=C(NC1cc2nonc2cc1)N1C(CCC2cccs2)CCCC1</chem>	131.62	
RCB_C50038	10057755	374.9	N-[(3S*,4R*)-1-[(6-chloro-1,3-benzodioxol-5-yl)methyl]-4-isopropyl-3-pyrrolidinyl]methanesulfonamide	<chem>CC(C)[C@@H](CN(Cc(cc1OCOc1c1)c1C)C1)[C@H]1NS(C)(=O)=O</chem>	105.68	

# Case 9: Target prediction for a specific compound

Tutorial main

## Step 3 : Click on SwissTargetPrediction

The screenshot shows the SMCVdb website interface. The top navigation bar is blue with the SMCVdb logo and a hamburger menu icon. A dark sidebar on the left contains navigation links: Home, ADME(T) Analysis, Target prediction (highlighted with a green 'New' badge), About, User guide, Contact Us, Download Data (green button), and Update. The main content area has a light blue background and is titled 'Recommended Web servers for Target prediction'. Below the title is a link for 'SwissTargetPrediction'. A 'References' section contains a single entry: '1. Gfeller, D., Grosdidier, A., Wirth, M., Daina, A., Michielin, O., & Zoete, V. (2014). SwissTargetPrediction: a web server for target prediction of bioactive small molecules. Nucleic acids research, 42(Web Server issue), W32-W38. https://doi.org/10.1093/nar/gku293'. A version number '0 0 0 0 0 4 2' is visible in the bottom left corner of the sidebar.

# Case 9: Target prediction for a specific compound

## Step 4 : Paste the SMILES notation and click RUN

The screenshot displays the SwissTargetPrediction web application interface. At the top, there is a navigation bar with links for SwissDrugDesign, SwissDock, SwissParam, SwissSidechain, SwissBioSostere, SwissTargetPrediction (highlighted), SwissADME, SwissSimilarity, and About us. The main header includes the SIB logo (Swiss Institute of Bioinformatics) and the site title "SwissTargetPrediction", along with links for Home, FAQ, Help, Download, Contact, and Disclaimer.

A text box explains the tool's purpose: "This website allows you to estimate the most probable macromolecular targets of a small molecule, assumed as bioactive. The prediction is founded on a combination of 2D and 3D similarity with a library of 370'000 known actives on more than 3000 proteins from three different species." It also provides references: "The webtool is described in detail here: [SwissTargetPrediction: updated data and new features for efficient prediction of protein targets of small molecules, Nucl. Acids Res. \(2019\)](#). For technical information about the prediction algorithm, you can refer to: [Shaping the interaction landscape of bioactive molecules, Bioinformatics \(2013\) 29:3073-3079](#)."

The interface features a "Select a species" section with radio buttons for Homo sapiens (selected), Mus musculus, and Rattus norvegicus. Below this is a "Paste a SMILES in this box, or draw a molecule" section containing a text input field with the SMILES string CSCCN(CC1)CCN1C(c1cc(-c2c(CO)cccc2)ccc1)=O, an "Examples:" dropdown menu, and a "Clear" button. A "Predict targets" button is located below the input field, with a note "(Provide a SMILES before submitting)".

On the right side, the Marvin JS editor is visible, showing a blank canvas with the Marvin JS logo and "by ChemAxon" text. The editor includes a toolbar with various drawing tools and a legend on the right side listing elements like H, C, N, O, S, F, P, Cl, Br, I, and \*.

At the bottom of the page, it says "POWERED BY ChemAxon" and "Swiss Institute of Bioinformatics - © 2023 | SIB privacy policy".

# Case 9: Target prediction for a specific compound

Tutorial main

## Step 5 : Result page will appear

The screenshot displays the SwissTargetPrediction website interface. At the top, there is a navigation bar with links for SwissDrugDesign, SwissDock, SwissParam, SwissSidechain, SwissBioisostere, SwissTargetPrediction (selected), SwissADME, SwissSimilarity, and About us. The main header features the SIB logo (Swiss Institute of Bioinformatics) and the site title 'SwissTargetPrediction'. Below the header, there are two main panels: 'Query Molecule' and 'Target Classes'. The 'Query Molecule' panel shows the chemical structure of the query compound. The 'Target Classes' panel displays a pie chart showing the distribution of predicted targets across various classes. Below these panels, there are export options (CSV, PDF, etc.) and a search bar. The main content area is a table of predicted targets.

Target	Common name	Uniprot ID	ChEMBL ID	Target Class	Probability*	Known actives (3D/2D)
Cathepsin D	CTSD	P07339	CHEMBL2581	Protease	<div style="width: 100%;"></div>	345 / 0 <a href="#">↓</a>
Phosphodiesterase 10A (by homology)	PDE10A	Q9Y233	CHEMBL4409	Phosphodiesterase	<div style="width: 100%;"></div>	1058 / 0 <a href="#">↓</a>
Protein kinase C delta	PRKCD	Q05655	CHEMBL2996	Kinase	<div style="width: 100%;"></div>	128 / 0 <a href="#">↓</a>
Protein kinase C alpha	PRKCA	P17252	CHEMBL299	Kinase	<div style="width: 100%;"></div>	219 / 0 <a href="#">↓</a>
Liver glycogen phosphorylase	PYGL	P06737	CHEMBL2568	Enzyme	<div style="width: 100%;"></div>	100 / 0 <a href="#">↓</a>
Matrix metalloproteinase 3	MMP3	P08254	CHEMBL283	Protease	<div style="width: 100%;"></div>	278 / 0 <a href="#">↓</a>
Serine/threonine-protein kinase Aurora-B	AURKB	Q96GD4	CHEMBL2185	Kinase	<div style="width: 100%;"></div>	212 / 0 <a href="#">↓</a>
Cyclin-dependent kinase 1	CDK1	P06493	CHEMBL308	Kinase	<div style="width: 100%;"></div>	209 / 0 <a href="#">↓</a>
Serine/threonine-protein kinase Aurora-A	AURKA	O14965	CHEMBL4722	Kinase	<div style="width: 100%;"></div>	376 / 0 <a href="#">↓</a>
Serine/threonine-protein kinase PIM1	PIM1	P11309	CHEMBL2147	Kinase	<div style="width: 100%;"></div>	164 / 0 <a href="#">↓</a>

Source : <http://www.swisstargetprediction.ch/>

# Case 10: User support

Option 1 : Use contact us option

Step 1 : Click Contact Us link

The screenshot shows the SMCVdb website interface. On the left sidebar, the 'Contact Us' link is highlighted with a red box. A yellow callout bubble with the text 'Click here' points to this link. The main content area displays a table of chemical entries with columns for SMCV ID, Source ID, PubChem CID, MW, IUPAC Name, SMILES, Viability, and Reference Image. The table shows 10 entries, with the first entry being RCB\_CS0007 (MW 350.4) and the last being RCB\_CS0038 (MW 374.9). The bottom of the page indicates 'Showing 1 to 10 of 24,361 entries' and includes pagination controls.

SMCV ID	Source ID	PubChem CID	MW	IUPAC Name	SMILES	Viability	Reference Image
RCB_CS0007	All	77281	350.4	N,5,6-trimethyl-2-oxo-N-[1-(5-phenyl-1H-pyrazol-3-yl)ethyl]-1,2-dihydro-3-pyridinecarboxamide	<chem>CC(c1n[nH]c(-c2ccccc2)c1)N(C)C(C1=CC(C)=C(C)N(C1)=O)=O</chem>	113.28	
RCB_CS0008	All	77298	351.4	N-allyl-3-(((3-ethyl-4,5-dihydroisoxazol-5-yl)methyl)amino)sulfonylbenzamide	<chem>CCCC1=NOC(CNS(c2cc(C(NCC=C)=O)ccc2)(=O)=O)C1</chem>	96.62	
RCB_CS0013	10025075	NA	435.4	1-methyl-4-[5-(morpholin-4-ylmethyl)-3-furoyl]-1,4,9-triazaspiro[5.5]undecane dihydrochloride	<chem>CN(CC1)C2(CCNC2)CN1C(c1coc(CN2CCOCC2)c1)=O</chem>	72.72	
RCB_CS0024	10037740	70704262	362.5	2-(((3-amino-2-thienyl)carbonyl)amino)methyl)-N,N-dimethyl-7,8-dihydro-4H-pyrazolo[1,5-a][1,4]diazepine-5(6H)-carboxamide	<chem>CN(C)C(N1Cc2cc(CNC(c3cc3)N)=O)nn2CCC1)=O</chem>	104.81	
RCB_CS0027	10041741	70704267	362.5	N-cyclopropyl-N-(3-hydroxybenzyl)-2-(2,4,7-trimethyl-1H-indol-3-yl)acetamide	<chem>Cc1c(CC(N(Cc2cc(O)ccc2)C2CC2)=O)c2c(C)ccc(C)c2[nH]1</chem>	103.84	
RCB_CS0029	10045111	NA	316.4	N-((3S*,4R*)-4-ethoxytetrahydrofuran-3-yl)-N''''-(1-phenyl-1H-pyrazol-5-yl)urea	<chem>CCO[C@@H](COC1)(C@H)1NC(Nc1ccn1-c1ccccc1)=O</chem>	99.86	
RCB_CS0030	10045854	NA	370.5	[3''''-(4-[2-(methylthio)ethyl]piperazin-1-yl)carbonyl)biphenyl-2-yl]methanol	<chem>CSCCN(CC1)CCN1C(c1cc(-c2c(CO)cccc2)ccc1)=O</chem>	93.1	
RCB_CS0033	10048011	91759616	333.4	5-((2-[2-(4-methylpiperazin-1-yl)ethyl]piperidin-1-yl)carbonyl)pyrazin-2-ol	<chem>CN1CCN(CCC(CCCC2)N2C(c3cn2)ncc2O)=O)CC1</chem>	79.25	
RCB_CS0034	10049170	NA	370.5	N-(2,1,3-benzoxadiazol-5-ylmethyl)-2-[2-(2-thienyl)ethyl]piperidine-1-carboxamide	<chem>O=C(NC1cc2nonc2cc1)N1C(Cc2cccs2)CCCC1</chem>	131.62	
RCB_CS0038	10057755	70704288	374.9	N-((3S*,4R*)-1-[[6-chloro-1,3-benzodioxol-5-yl)methyl]-4-isopropyl-3-pyrrolidinyl)methanesulfonamide	<chem>CC(C)[C@@H](CN(Cc1cc1OCoc1c1c1C1)1)[C@H]1NS(C)(=O)=O</chem>	105.68	



# Case 10: User support

Option 1 : Use contact us option

Step 2 : Submit the form with details

The screenshot shows a web application interface for SMCVdb. On the left is a dark sidebar with navigation links: Home, ADME(T) Analysis, Target prediction, About, User guide (marked 'New'), Contact Us, Download Data, and Update. The main content area is titled 'Contact Us' and contains a message: 'We value your feedback and would love to hear from you! Please feel free to use the form below to provide your comments, suggestions, or any questions you may have. We will get back to you as soon as possible.' Below the message is a legend: '\* Indicates required question'. The form consists of three input fields: 'Name \*', 'Email \*', and 'Comments', each with a 'Your answer' placeholder. At the bottom, there are 'Submit' and 'Clear form' buttons. A footer note states: 'Never submit passwords through Google Forms.' and 'Google Forms This content is neither created nor endorsed by Google.'

# Case 10: User support

## Option 2 : Follow us on social media page

The screenshot displays the SMCVdb web application interface. At the top right, a yellow callout box with a red arrow points to a 'Follow us' button with a Twitter icon. The main content area features a table with 10 columns: SMCV ID, Source ID, PubChem CID, MW, IUPAC Name, SMILES, Viability, and Reference Image. The table lists 10 chemical entries, each with its corresponding SMILES string and viability value. A search bar is located at the top right of the table area. The left sidebar contains navigation links for Home, ADME(T) Analysis, Target prediction, About, User guide (marked as 'New'), Contact Us, Download Data, and Update. At the bottom of the table, it indicates 'Showing 1 to 10 of 24,361 entries' and includes a pagination control showing 'Previous', '1', '2', '3', '4', '5', '...', '2,437', and 'Next'.

SMCV ID	Source ID	PubChem CID	MW	IUPAC Name	SMILES	Viability	Reference Image
RCB_C50009	10015705	134067281	350.4	N,5,6-trimethyl-2-oxo-N-[1-(5-phenyl-1H-pyrazol-3-yl)ethyl]-1,2-dihydro-3-pyridinecarboxamide	<chem>CC(c1n[nH]c(-c2cccc2)c1)N(C)C(C1=CC(C)=C(C)NC1=O)=O</chem>	113.28	
RCB_C50011	10022643	72837098	351.4	N-allyl-3-(((3-ethyl-4,5-dihydroisoxazol-5-yl)methyl)amino)sulfonylbenzamide	<chem>CCC1=NOC(CNS(c2cc(C(NCC=C)O)ccc2)(=O)=O)C1</chem>	96.62	
RCB_C50013	10025975	NA	435.4	1-methyl-4-[5-(morpholin-4-ylmethyl)-3-furoyl]-1,4,9-triazaspiro[5.5]undecane dihydrochloride	<chem>CN(CC1)C2(CCNCC2)CN1C(c1coc(CN2CCOCC2)c1)=O</chem>	72.72	
RCB_C50024	10037740	70704262	362.5	2-(((3-amino-2-thienyl)carbonyl)amino)methyl)-N,N-dimethyl-7,8-dihydro-4H-pyrazolo[1,5-a][1,4]diazepine-5(6H)-carboxamide	<chem>CN(C)C(N1Cc2cc(CNC(c3cc3)c3N)=O)nn2CCC1=O</chem>	104.81	
RCB_C50027	10041741	70704267	362.5	N-cyclopropyl-N-(3-hydroxybenzyl)-2-(2,4,7-trimethyl-1H-indol-3-yl)acetamide	<chem>Cc1c(CC(N(Cc2cc(O)ccc2)C2CC2)=O)c2c(C)ccc(C)c2(nH)1</chem>	103.84	
RCB_C50029	10045111	NA	316.4	N-((3S*,4R*)-4-ethoxytetrahydrofuran-3-yl)-N''''-(1-phenyl-1H-pyrazol-5-yl)urea	<chem>CCO[C@@H](COC1)[C@H]1NC(Nc1ccn1-c1cccc1)=O</chem>	99.86	
RCB_C50030	10045854	NA	370.5	[3''''-(((4-[2-(methylthio)ethyl]piperazin-1-yl)carbonyl)biphenyl-2-yl)methanol	<chem>CSCCN(CC1)CCN1C(c1ccc(-c2c(CO)cccc2)ccc1)=O</chem>	93.1	
RCB_C50033	10048011	91759616	333.4	5-([2-[2-(4-methylpiperazin-1-yl)ethyl]piperidin-1-yl]carbonyl)pyrazin-2-ol	<chem>CN1CCN(CCC(CCCC)N2C(c(cn2)nc2O)=O)CC1</chem>	79.25	
RCB_C50034	10049170	NA	370.5	N-(2,1,3-benzoxadiazol-5-ylmethyl)-2-[2-(2-thienyl)ethyl]piperidine-1-carboxamide	<chem>O=C(NCc1cc2nonc2cc1)N1C(Cc2ccsc2)CCCC1</chem>	131.62	
RCB_C50038	10057755	70704288	374.9	N-((3S*,4R*)-1-((6-chloro-1,3-benzodioxol-5-yl)methyl)-4-isopropyl-3-pyrrolidiny)methanesulfonamide	<chem>CC(C)[C@@H](CN(Cc(cc1OCoc1c1c1Cl)C1)[C@H]1NS(C)(=O)=O</chem>	105.68	