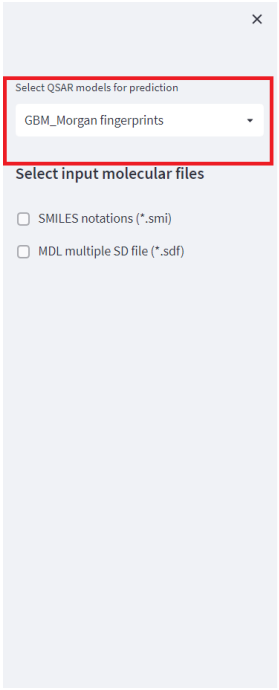
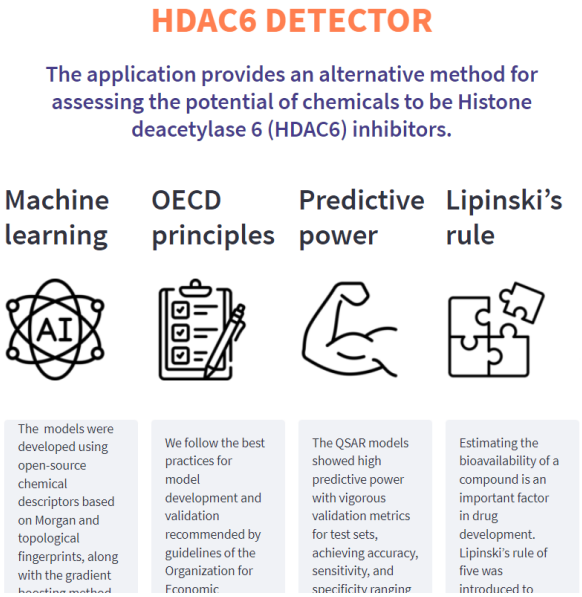
Manual of HDAC6 DETECTOR

open-source software

Step 1. *Select QSAR models for prediction*.

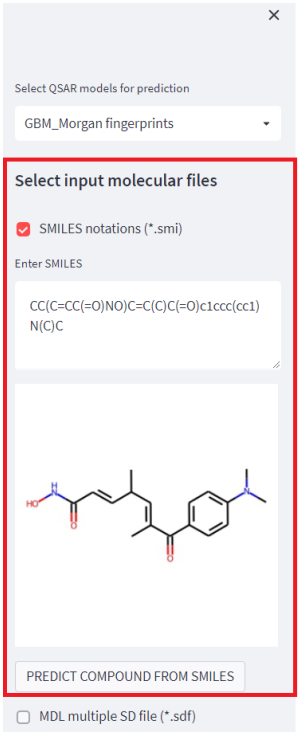
You can choose a model developed using the Morgan fingerprints and gradient boosting method (GBM) or a model developed using topological fingerprints, and multilayer perceptron (MLP) classifier.

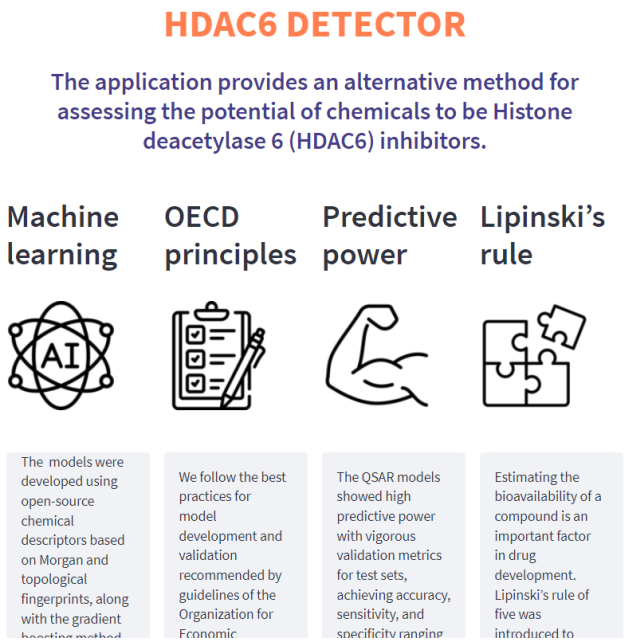




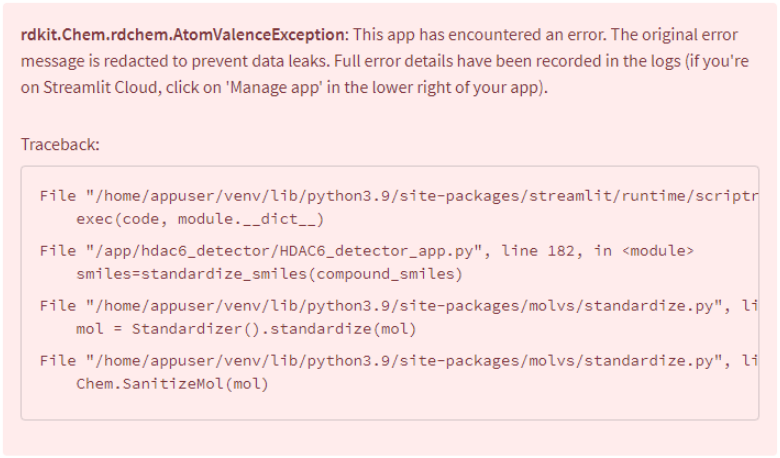
Step 2. *Select input molecular files.*

If you choose smiles, please, directly paste the SMILES representation of the desired chemical structure and press Ctrl+Enter. If the entered chemical structure is correct, the application will generate a 2D image of the studied compound. Click on the "PREDICT COMPOUND FROM SMILES" button.

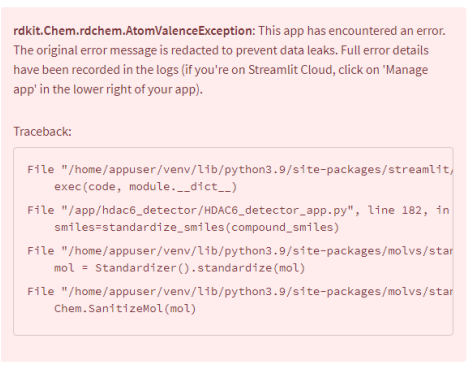


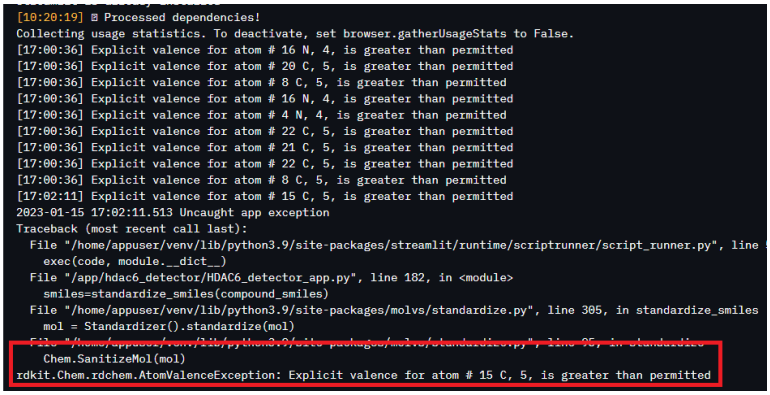


If the entered structure is incorrect, the application reports an error that has occurred, the details of which can be found through the application manager.

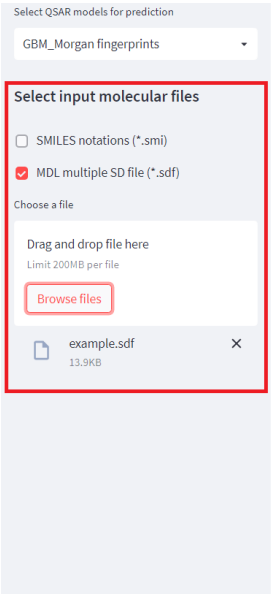


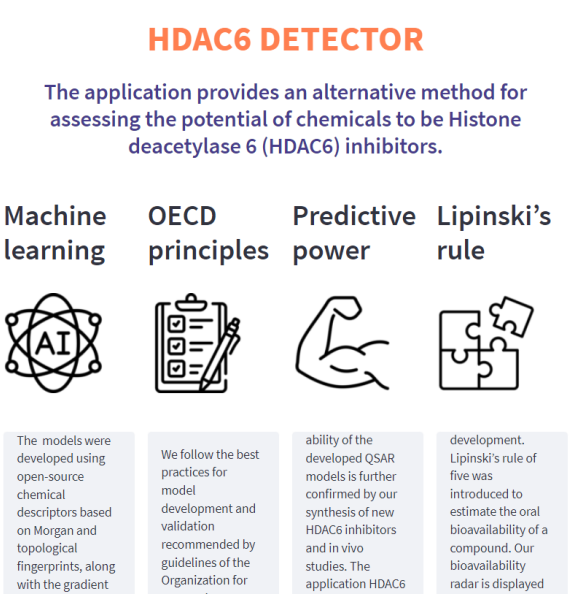
To clarify the details of the error, please click here



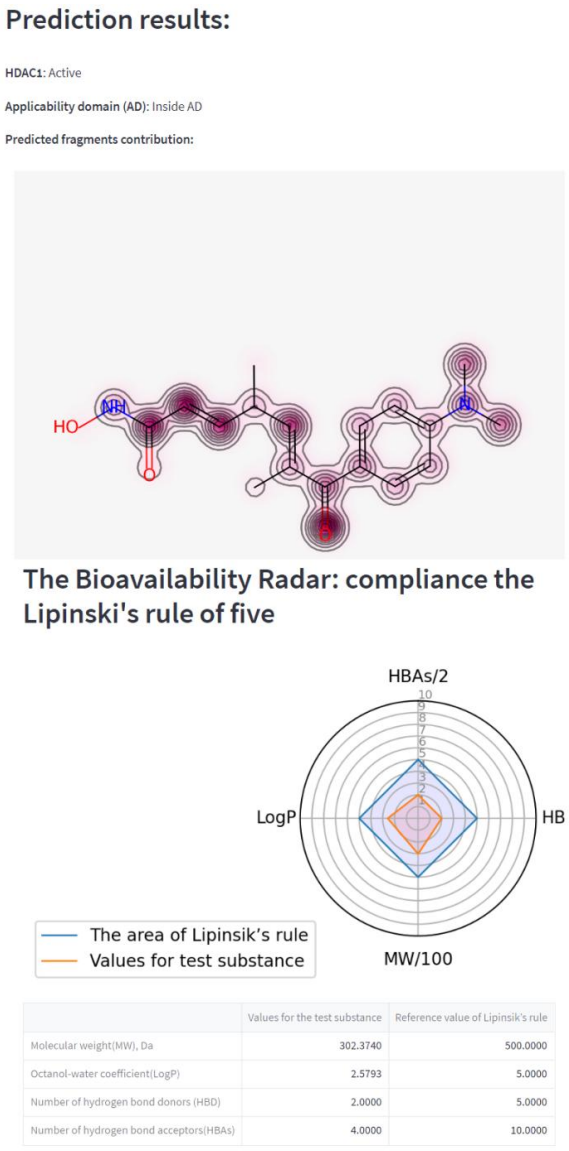


If you choose a file *sdf, that may contain a different number of chemical structures, please specify the path to this file on your computer's hard drive. In this case, you need to click the " Browse files" button.

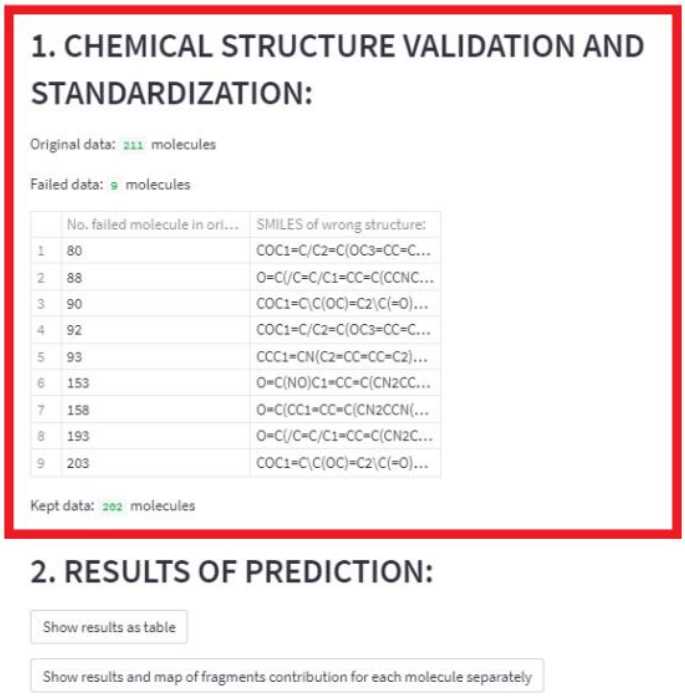




Step 3. *Prediction results*. The form of presentation of the results depends on the type of descriptors selected, as well as the format of the input chemical data. For example, when selecting SMILES, the results will be displayed for a single molecule. The chemical fragments are colored in green (predicted to reduce inhibitory activity) or magenta (predicted to increase activity HDAC6 inhibitors). The gray isolines separate positive and negative contributions.



If you select a file *sdf, the results will be presented in tabular form. If incorrect structures are detected in the file *sdf, the corresponding information will appear in the section "CHEMICAL STRUCTURE VALIDATION AND STANDARDIZATION"



1. CHEMICAL STRUCTURE VALIDATION AND STANDARDIZATION:

Original data: 211 molecules

Failed data: 9 molecules

	No. failed molecule in ori...	SMILES of wrong structure:
1	80	COC1=C/C2=C(OC3=CC=C...
2	88	O=C(/C=C/C1=CC=C(CCNC...
3	90	COC1=C\C(OC)=C2\C(=O)...
4	92	COC1=C/C2=C(OC3=CC=C...
5	93	CCC1=CN(C2=CC=CC=C2)...
6	153	O=C(NO)C1=CC=C(CN2CC...
7	158	O=C(CC1=CC=C(CN2CCN(...
8	193	O=C(/C=C/C1=CC=C(CN2C...
9	203	COC1=C\C(OC)=C2\C(=O)...

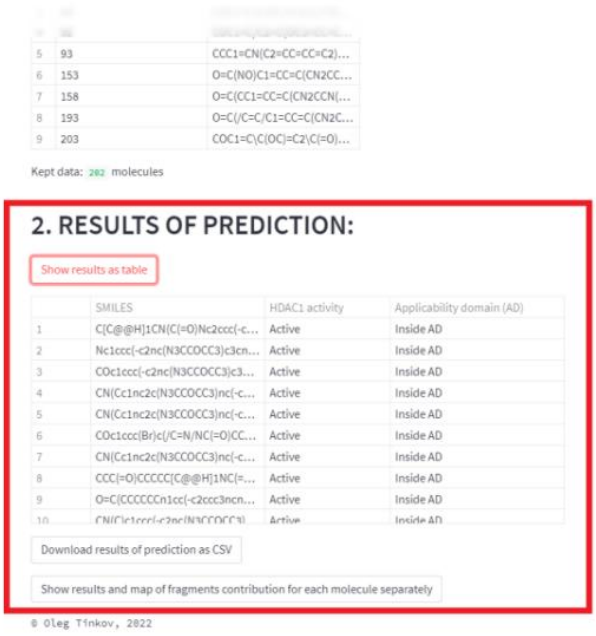
Kept data: 202 molecules

2. RESULTS OF PREDICTION:

Show results as table

Show results and map of fragments contribution for each molecule separately

The prediction results for correct chemical structures are displayed in a table that can be downloaded, or separately for each molecule if you click the " Show results and map of fragments contribution for each molecule separately" button.



5	93	CCC1=CN(C2=CC=CC=C2)...
6	153	O=C(NO)C1=CC=C(CN2CC...
7	158	O=C(CC1=CC=C(CN2CCN(...
8	193	O=C(/C=C/C1=CC=C(CN2C...
9	203	COC1=C\C(OC)=C2\C(=O)...

Kept data: 202 molecules

2. RESULTS OF PREDICTION:

Show results as table

	SMILES	HDAC1 activity	Applicability domain (AD)
1	C[C@@H]1CN(C(=O)Nc2ccc(-c...	Active	Inside AD
2	Nc1ccc(-c2nc(N3CCOCC3)c3cn...	Active	Inside AD
3	COc1ccc(-c2nc(N3CCOCC3)c3...	Active	Inside AD
4	CN(Cc1nc2c(N3CCOCC3)nc(-c...	Active	Inside AD
5	CN(Cc1nc2c(N3CCOCC3)nc(-c...	Active	Inside AD
6	COc1ccc(Br)c(/C=N/NC(=O)CC...	Active	Inside AD
7	CN(Cc1nc2c(N3CCOCC3)nc(-c...	Active	Inside AD
8	CCC(=O)CCCCC[C@@H]1NC(=...	Active	Inside AD
9	O=C(CCCCCCn1cc(-c2ccc3ncn...	Active	Inside AD
10	CN(Cc1ccc(-c2nc(N3CCOCC3)...	Active	Inside AD

Download results of prediction as CSV

Show results and map of fragments contribution for each molecule separately

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