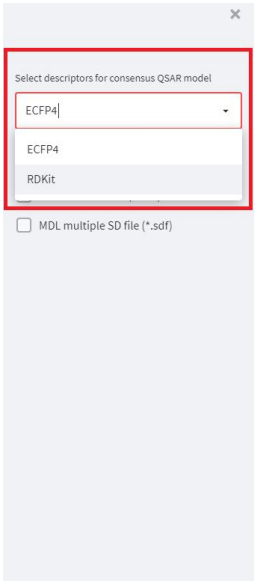
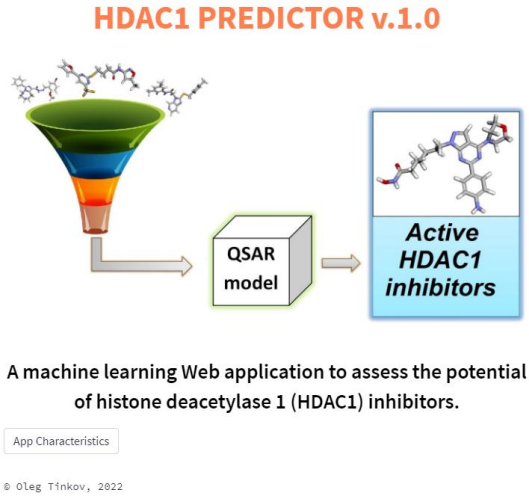
Manual of HDAC1 Predictor

open-source software

version 1.0.

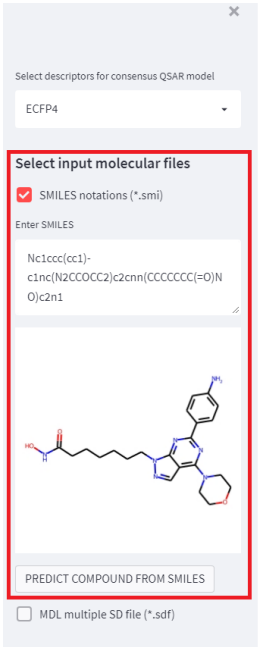
Step 1. Select descriptors for consensus QSAR model. You can choose one of two types of molecular descriptors that were used in the development of the QSAR model. If you choose ECFP4 descriptors, an additional analysis of the contributions of molecular fragments of the studied compound to the inhibition of HDAC1 will be carried out.

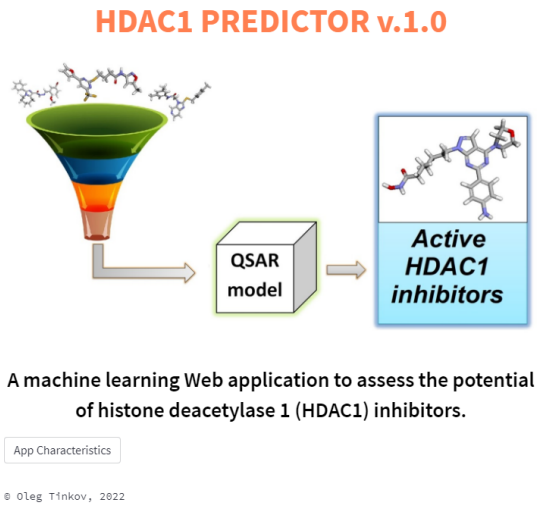




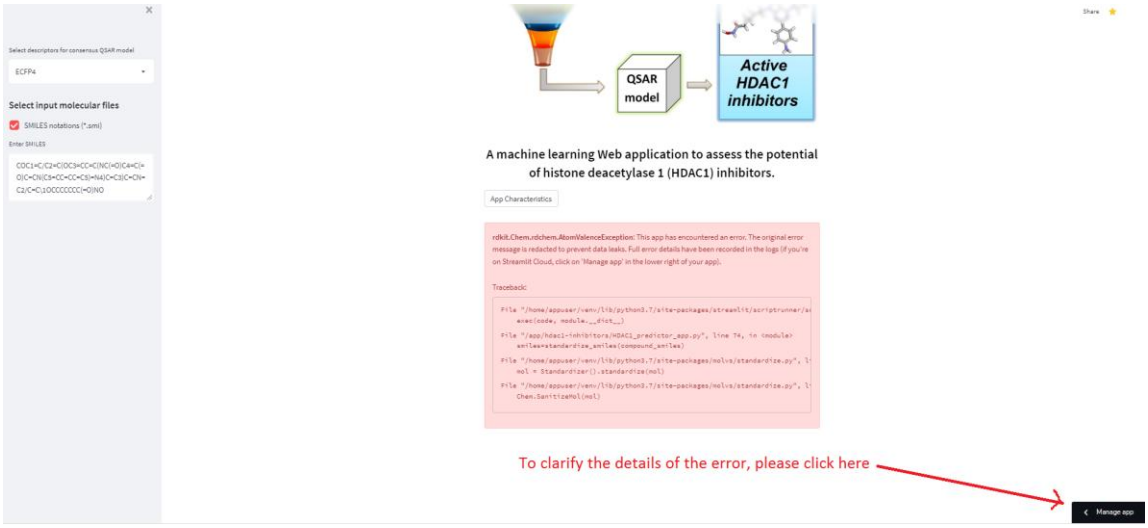
Step 2. Select input molecular files.

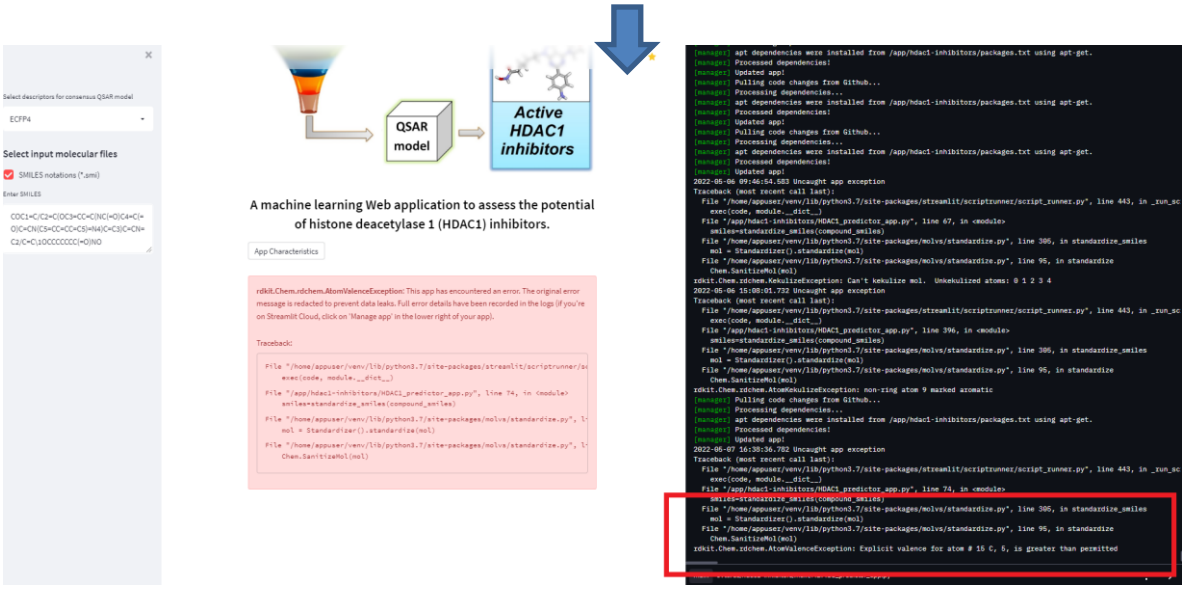
If you choose smiles, please, directly paste the SMILES representation of the desired chemical structure and press Ctrl+Enter. If the entered chemical structure is correct, the application will generate a 2D image of the studied compound. Click on the “PREDICT COMPOUND FROM SMILES” button.



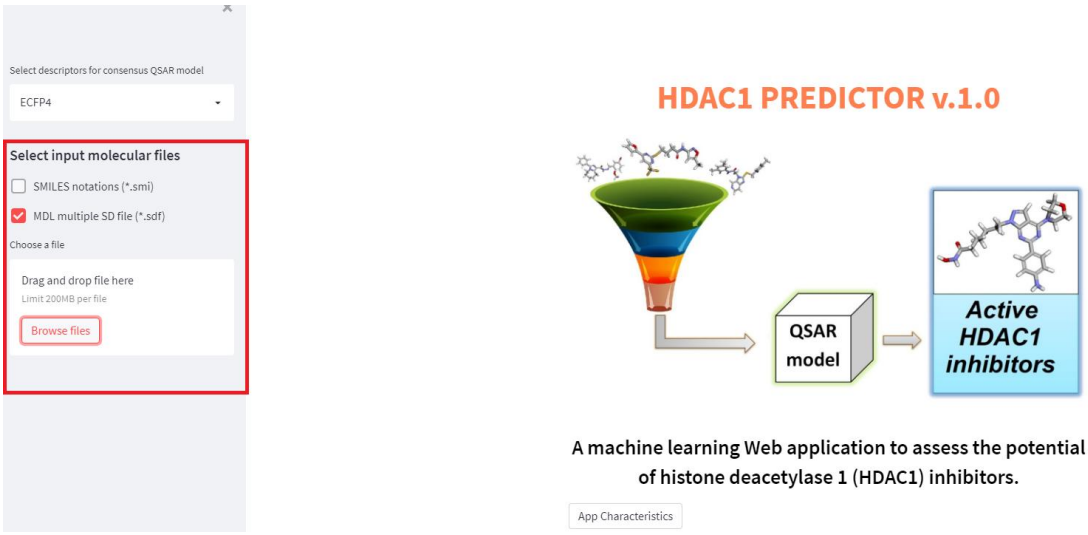


If the entered structure is incorrect, the application reports an error that has occurred, the details of which can be found through the application manager.

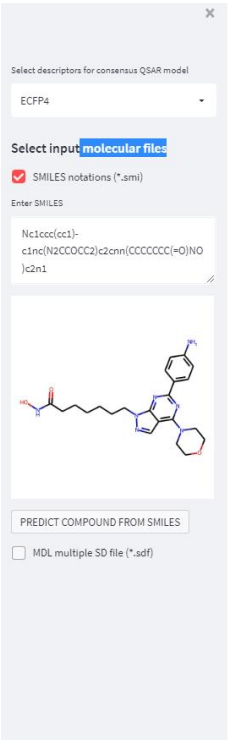


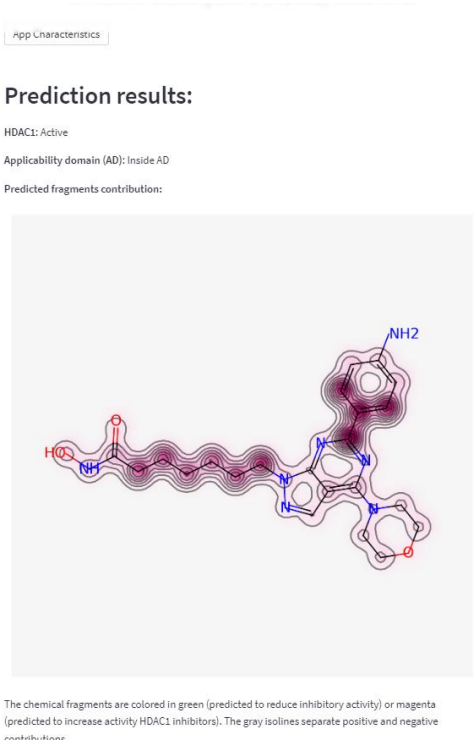


If you choose a file *sdf, that may contain a different number of chemical structures, please specify the path to this file on your computer's hard drive. In this case, you need to click the " Browse files" button.

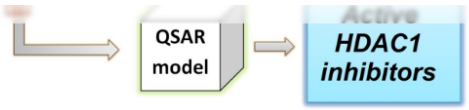


Step 3. Prediction results. The form of presentation of the results depends on the type of descriptors selected, as well as the format of the input chemical data. For example, when selecting SMILES, the results will be displayed for a single molecule.





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"



A machine learning Web application to assess the potential of histone deacetylase 1 (HDAC1) inhibitors.

App Characteristics

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)...

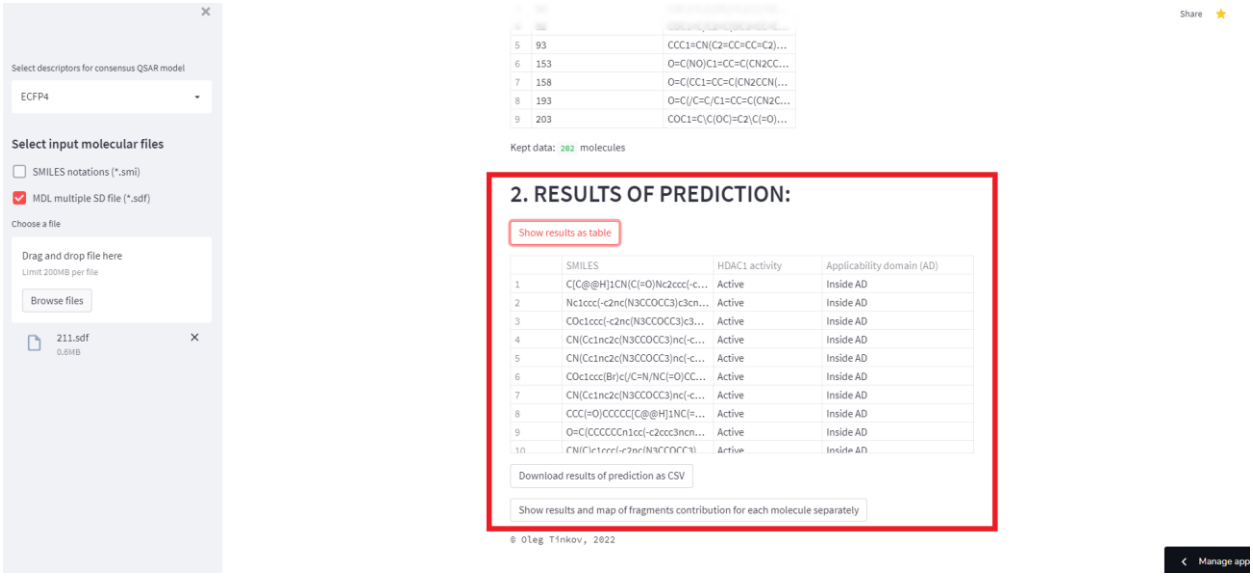
Kept data: 202 molecules

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.



A more detailed description of the application is available if you click the " Application description" button on the main page of the application