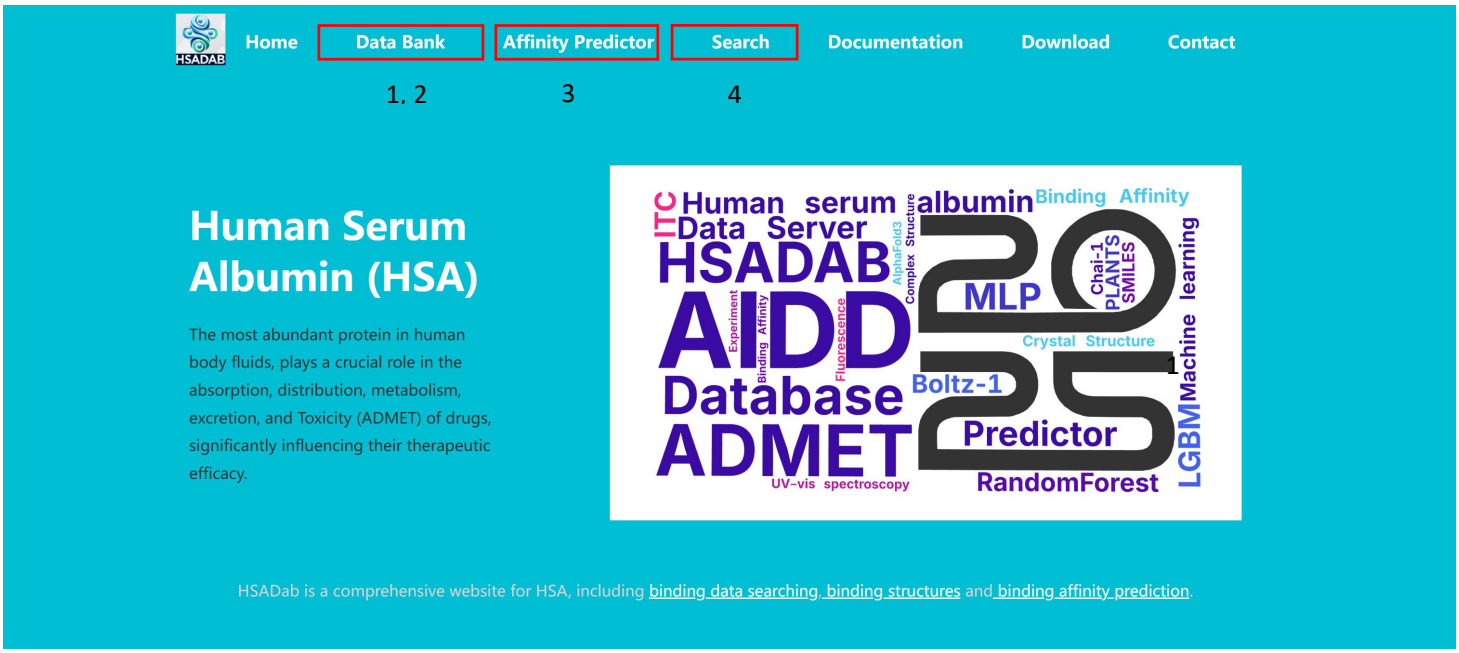
User's Manual

Home page.

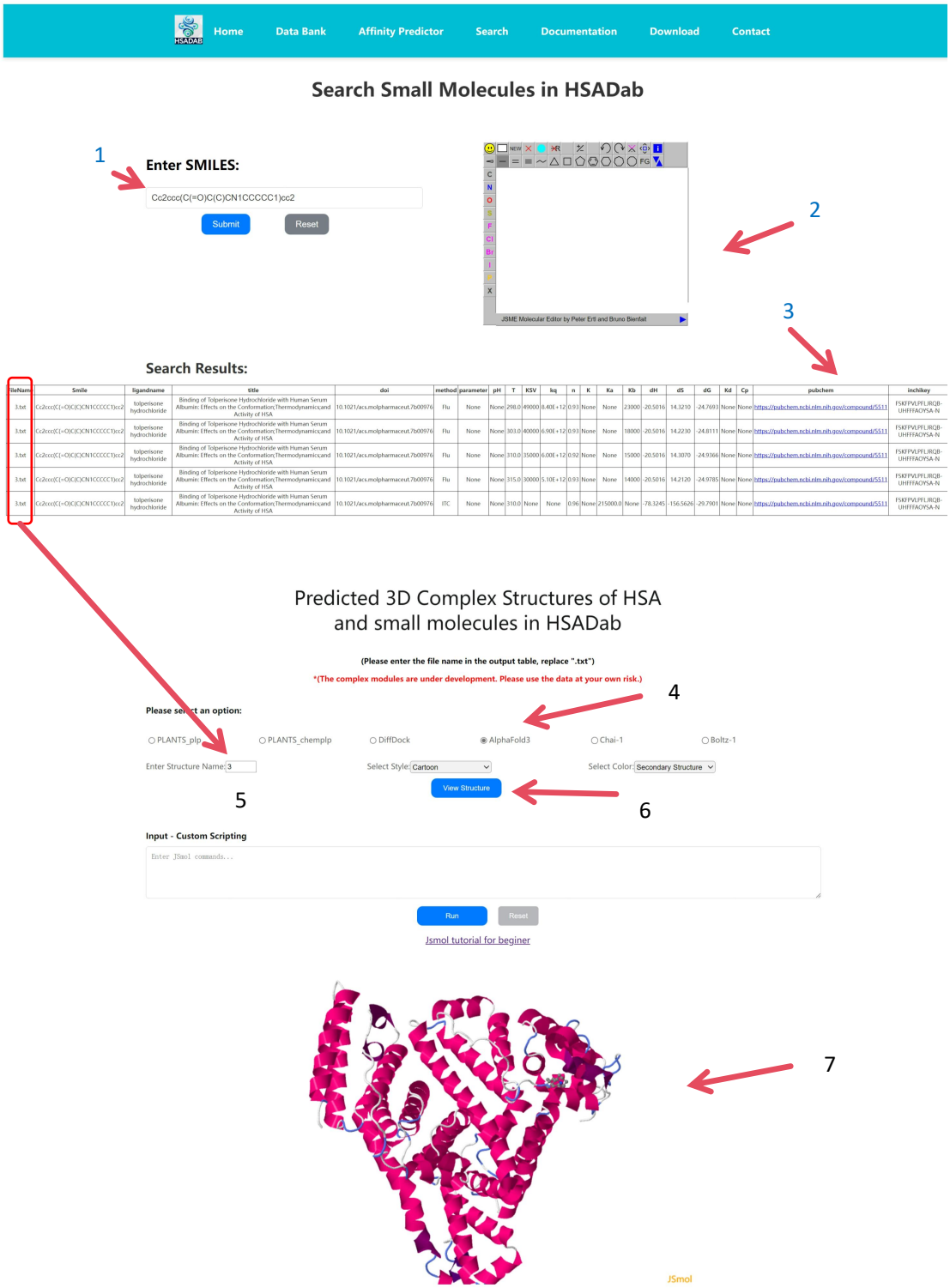


Our website can perform the following functions:

1. Binding data searching according to ligand SMILES (Data Bank)
2. 3D Binding Complex Structure Searching including prediction by Difusion Model and Docking (Data Bank)
3. Binding affinity prediction (Affinity Predictor)
4. Binding data searching according to other condition (Search)

There are also the qucik start link to these three functions.

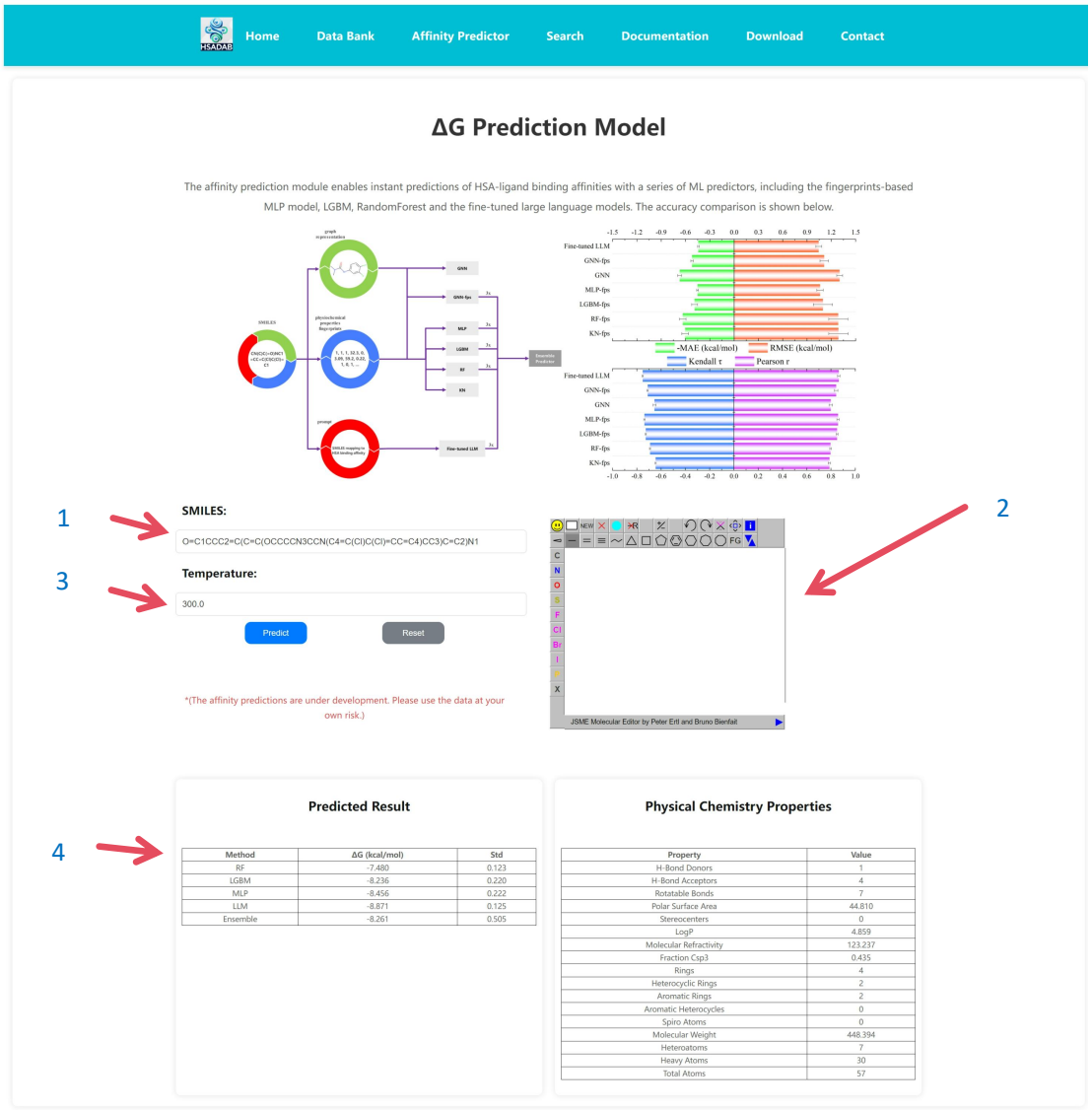
Data Bank



You can directly input SMILES in the input(1) or draw the structure in the JSME web plugin(2), where the SMILES can be updataed in the input(1). If the structure in our database, it will output a table, in which we put the link to Pubchem of the small molecules. And if you want search the

predicted 3D complex structure between the small molecules and HSA, you just need choose the method (4) and put in the filename from the table into input 5. After click view structure button (6), the docking structure will show in Jsmol web plugin (7).

Affinity Predictor



Method	ΔG (kcal/mol)	Std
RF	-7.480	0.123
LGBM	-8.236	0.220
MLP	-8.456	0.222
LLM	-8.871	0.125
Ensemble	-8.261	0.505

Property	Value
H-Bond Donors	1
H-Bond Acceptors	4
Rotatable Bonds	7
Polar Surface Area	44.810
Stereocenters	0
LogP	4.859
Molecular Refractivity	123.237
Fraction Csp3	0.435
Rings	4
Heterocyclic Rings	2
Aromatic Rings	2
Aromatic Heterocycles	0
Spiro Atoms	0
Molecular Weight	448.394
Heteroatoms	7
Heavy Atoms	30
Total Atoms	57

You can directly input SMILES in the input(1) or draw the structure in the JSME web plugin(2), where the SMILES can be updataed in the input(1). Then you should input temperature(unit is K) in the input(3). Click the “Predict” , you will see the prediction data(4). The prediction data consists of 4 kinds of machine learning model, which is a average of 3 models. Moreover, we present the physical chemistry properties.

Search

Condition Search

3 **Search Results:**

Smile	ligandname	title	doi	method	inchikey	dG	T	dG
C/C(=N\OC1OC(C)C(O)C(O)C1O)C1=CC(O)=C2C(=O)C3C=CC=CC3C(=O)C2=C1O	AORha	Modeling techniques and fluorescence imaging investigation of the interactions of an anthraquinone derivative with HSA and ctDNA	10.1016/j.saa.2015.09.011	Flu	ZCPWMSYDOMSSFR-LIMNOBDPSA-N	-30.880000	300.0	-30.880000
[H][C@@]12CCC(C(C)C)[C@@]1(C)CCC1(C)[C@]2([H])CC[C@]2([H])[C@@]3(C)CCC(O)C(C)(C)[C@]3([H])CC[C@]12C	lupeol derivative	Comparative binding mechanism of lupeol compounds with plasma proteins and its pharmacological importance	10.1039/c4mb00635f	Flu	SBTXBGJCUSLCNL-AQBVTWMUSA-N	-30.124800	298.0	-30.124800
CC1=C(C(CCC1)(C)C)/C=C/C(=C\C=C\C(=C/C=C/C=C(\C)/C=C/C=C(\C)/C=C\C2=C(CCCC2(C)C)C)\C)/C	碲?Carotene	Isorenieratene interaction with human serum albumin: Multi-spectroscopic analyses and docking.	10.1016/j.foodchem.2018.02.105	Flu	OENHQHLEOONYIE-QGWNBGMGSA-N	-30.370000	298.0	-30.370000
CC1=C(C(C[C@@H](C1O)(C)C)/C=C/C(=C/C=C/C(=C/C=C/C=C(\C)/C=C/C=C(\C)/C=C/[C@H]2C(=C[C@@H](CC2(C)C)O)C)/C)/C	Lutein	Isorenieratene interaction with human serum albumin: Multi-spectroscopic analyses and docking.	10.1016/j.foodchem.2018.02.105	Flu	KBPHJBAIARWVSC-RGZFRNHPSA-N	-30.460000	298.0	-30.460000
CC1=C(C(=C(C=C1)C)/C=C/C(=C/C=C/C(=C/C=C/C=C(/C=C/C=C(/C=C/C2=C(C=CC(=C2C)C)C)\C)\C)/C)/C)C	Isorenieratene	Isorenieratene interaction with human serum albumin: Multi-spectroscopic analyses and docking.	10.1016/j.foodchem.2018.02.105	Flu	ZCIHMQAPACOQHT-YSEOPJLNSA-N	-30.600000	298.0	-30.600000
C1=CC(=CC=C1C2=COC3=CC(=CC(=C3C2=O)O)O)O	Genistein	Delivery Mechanism of the Pharmaceutical Complex of Genistein-Adenine Based on Spectroscopic and Molecular Modelling at Atomic Scale	10.1002/cbdv.202000944	Flu	TZBJGXHYKVUXJN-UHFFFAOYSA-N	-30.500000	298.0	-30.500000
C[C@@H]1CC2=CC(=C(C(=C2C3=C(C(=C(C=C3C[C@@H]1C)OC)OC)OC)OC)OC)OC	deoxyschizandrin	Study on the interactions of Chinese medicine component deoxyschizandrin and its metal ion complexes with serum albumin	NaN	Flu	JEJFTTRHGBKKEI-OKILXGFUSA-N	-30.600000	298.0	-30.600000

You can input conditions in the input(1) , where you can also add the range. Furthermore, you can click ‘Add+’ button(2) to add other condition Click the “Search” , you will see the searched data(3). The searched data should include the search condition.