COVID-19-Sprotein-binding-disruptors

March 19, 2020

0.1 Repurposing Therapeutics for COVID-19

Micholas Dean Smith and Jeremy C. Smith from University of Tennessee and ORNL have published a molecular modeling paper and identified 47 potential small-molecule hits (20 are available for purchase) that could limit severe acute respiratory syndrome coronavirus-2 (SARS-CoV-2), the culprit of the COVID-19 pandemic. Please note that SARS-Cov-2 is the name of the new virus and the disease name is COVID-19. You can read the naming convention for viruses from here, WHO-technical-guide.

Micholas Dean Smith and Jeremy Smith used Summit (IBM AC922 Summit to screen a small molecule library (~ 8000 compounds) and carried out Docking and Molecular Dynamics calculations to identify hits that could bind to the main "spike" protein (aka S-protein) of the caronavirus. You can read the article from The Preprint Server for Chemistry server, ChemRxiv

I have taken the top-19 best-ranked compounds from the manuscript and used the chemoinformatics python library to display the compounds. You can also visit my GitHub and download the Python code.

[48]:
```
# install anaconda
# install the following llibraries: pandas and rdkit
# libraries needed pandas and rdkit
# copy and run the code

import pandas as pd
from rdkit import Chem
from rdkit.Chem import AllChem
from rdkit.Chem import Draw
from rdkit.Chem.Draw import IPythonConsole
from rdkit.Chem.Draw.MolDrawing import MolDrawing, DrawingOptions
from rdkit.Chem import PandasTools
from rdkit.Chem.Draw import IPythonConsole
```

[49]:
```
df = pd.read_csv("Data/COVID-19.csv", sep = ' ', header=0)
```

[50]:
```
df
```

[50]:

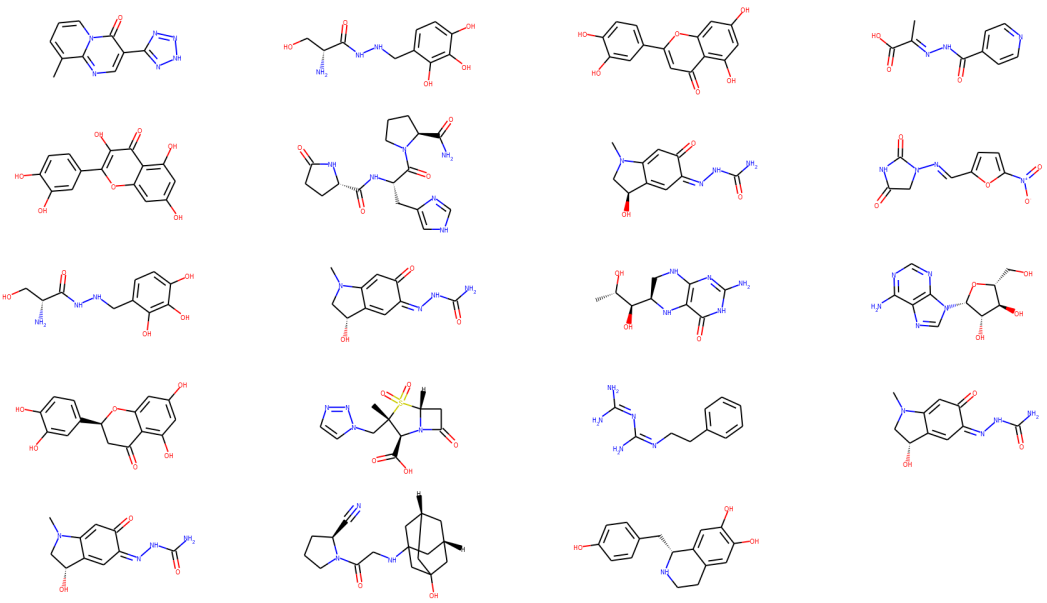
	smiles	zinc_id	\
0	Cc1cccn2c(=O)c(-c3nn[nH]n3)cnc12	ZINC000005783214	
1	N[C@H](CO)C(=O)NNCc1ccc(O)c(O)c1O	ZINC000003830273	
2	O=c1cc(-c2ccc(O)c(O)c2)oc2cc(O)cc(O)c12	ZINC000018185774	

3	C/C(=N\NC(=O)c1ccncc1)C(=O)O	ZINC000004974291
4	O=c1c(O)c(-c2ccc(O)c(O)c2)oc2cc(O)cc(O)c12	ZINC000003869685
5	NC(=O)[C@@H]1CCCN1C(=O)[C@H](Cc1c[nH]cn1)NC(=O…	ZINC000004096261
6	CN1C[C@H](O)C2=C/C(=N/NC(N)=O)C(=O)C=C21	ZINC000100029428
7	O=C1CN(/N=C/c2ccc([N+](=O)[O-])o2)C(=O)N1	ZINC000003875368
8	N[C@H](CO)C(=O)NNCc1ccc(O)c(O)c1O	ZINC000003830273
9	CN1C[C@@H](O)C2=C/C(=N/NC(N)=O)C(=O)C=C21	ZINC000100045148
10	C[C@H](O)[C@H](O)[C@H]1CNc2nc(N)[nH]c(=O)c2N1	ZINC000013585233
11	Nc1ncnc2c1ncn2[C@@H]1O[C@H](CO)[C@@H](O)[C@@H]1O	ZINC000000970363
12	O=C1C[C@@H](c2ccc(O)c(O)c2)Oc2cc(O)cc(O)c21	ZINC000000058117
13	C[C@]1(Cn2ccnn2)[C@H](C(=O)O)N2C(=O)C[C@H]2S1(…	ZINC000003787060
14	NC(N)=N/C(N)=N\CCc1ccccc1	ZINC000005851063
15	CN1C[C@@H](O)C2=C/C(=N/NC(N)=O)C(=O)C=C21	ZINC000100045148
16	CN1C[C@@H](O)C2=C/C(=N/NC(N)=O)C(=O)C=C21	ZINC000100045148
17	N#C[C@@H]1CCCN1C(=O)CNC12C[C@@H]3C[C@H](CC(O)(…	ZINC000100003507
18	Oc1ccc(C[C@H]2NCCc3cc(O)c(O)cc32)cc1	ZINC000000896041

	Name
0	Permirolast
1	Benserazide
2	NP-Luteolin-monoarbinoside
3	Pyruvic-acid-Calcium-isoniazid
4	NP-Quercetol;quercetin
5	Protirelin
6	Carbazochrome
7	Nitrofurantoin
8	Benserazide
9	Carbazochrome
10	Sapropterin
11	Vidarbine
12	NP:Eriodictyol
13	Tazobactum
14	Phenformin-hcl
15	Carbazochrome
16	Carbazochrome
17	Vildagliptin
18	NP:Demethyl-coclaurine

[51]:
```
x = df['smiles'].values
mols = [Chem.MolFromSmiles(smi) for smi in x]
Draw.MolsToGridImage(mols, molsPerRow = 4, subImgSize=(450, 200))
```

[51]:



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