COVID-disruptors

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0.1 Repurposing Therapeutics for COVID-19

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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.

[4]:
```
# 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
```

[17]:
```
df = pd.read_csv("Data/COVID-19.csv", sep = ' ', header=0)
```

[18]:
```
df
```

[18]:

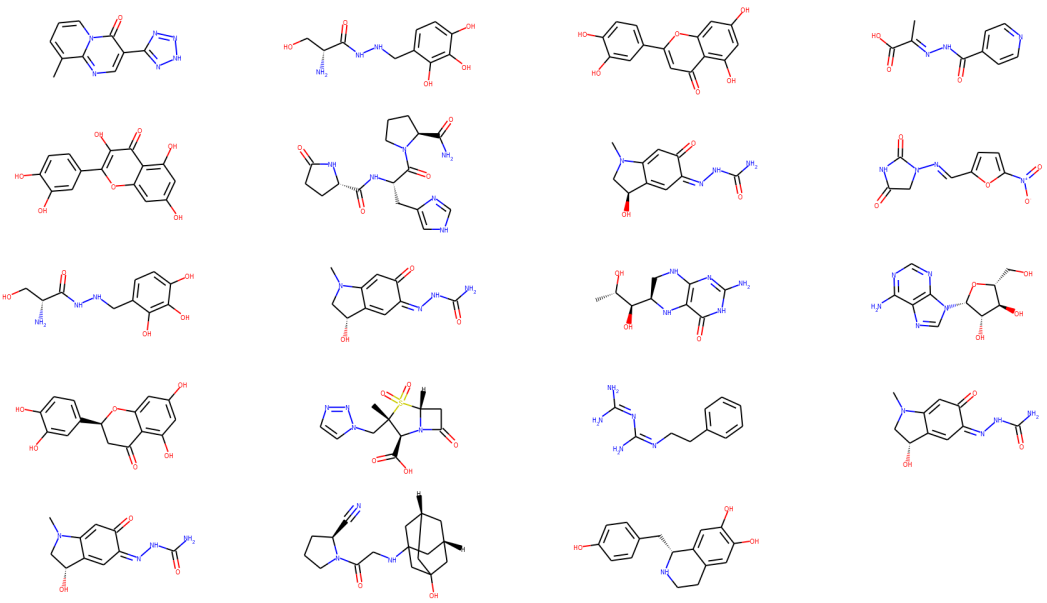
	smiles	zinc_id	\
0	Cc1cccn2c(=O)c(-c3nn[nH]n3)cnc12	ZINC000005783214	

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

[19]:
```
x = df['smiles'].values
mols = [Chem.MolFromSmiles(smi) for smi in x]
Draw.MolsToGridImage(mols, molsPerRow = 4, subImgSize=(450, 200))
```

[19]:



[20]:
```
from mordred import Calculator, descriptors
```

[21]:
```
# create descriptor calculator with all descriptors
calc = Calculator(descriptors, ignore_3D=True)

# calculate multiple molecule
mols1 = [Chem.MolFromSmiles(smi) for smi in x]

# as pandas
df1 = calc.pandas(mols1)
```

```
100%|      | 19/19 [00:03<00:00,  6.12it/s]
```

[22]:
```
df1
```

[22]:

	ABC	ABCGG	nAcid	nBase	SpAbs_A	SpMax_A	SpDiam_A	\
0	13.451608	11.497362	2	0	22.492647	2.457867	4.902998	
1	13.113111	11.885521	0	1	22.203716	2.342088	4.684176	
2	16.608204	13.330263	0	0	26.321008	2.467430	4.934859	
3	10.963281	10.033994	1	0	18.556154	2.239094	4.478187	
4	17.343821	14.207716	0	0	27.687065	2.499067	4.998133	
5	20.143738	18.489856	0	0	32.998178	2.410037	4.742169	
6	13.113111	11.698753	0	0	20.720454	2.471080	4.827489	
7	13.084601	11.840974	0	0	20.946550	2.341573	4.481647	
8	13.113111	11.885521	0	1	22.203716	2.342088	4.684176	
9	13.113111	11.698753	0	0	20.720454	2.471080	4.827489	
10	13.113111	11.268952	0	0	20.857278	2.424769	4.849537	

11	14.894331	13.336359	0	0	24.631339	2.511395	4.844357
12	16.608204	13.330263	0	0	26.321008	2.467430	4.934859
13	15.981561	15.139991	1	0	24.471027	2.692414	5.134610
14	10.934771	9.585837	0	5	18.037415	2.171121	4.342241
15	13.113111	11.698753	0	0	20.720454	2.471080	4.827489
16	13.113111	11.698753	0	0	20.720454	2.471080	4.827489
17	17.865098	14.583318	0	1	28.157662	2.577832	5.155242
18	15.763198	12.369030	0	1	26.041871	2.427752	4.855505

	SpAD_A	SpMAD_A	LogEE_A	…	SRW10	TSRW10	MW	\
0	22.492647	1.323097	3.789440	…	9.879144	63.377796	228.075959	
1	22.203716	1.233540	3.770033	…	9.543020	50.345912	257.101171	
2	26.321008	1.253381	3.987292	…	10.124509	55.372829	286.047738	
3	18.556154	1.237077	3.585883	…	9.123802	45.923073	207.064391	
4	27.687065	1.258503	4.032867	…	10.230234	56.728753	302.042653	
5	32.998178	1.269161	4.182886	…	9.992734	77.282364	362.170253	
6	20.720454	1.218850	3.759364	…	9.740204	64.085225	236.090940	
7	20.946550	1.232150	3.755768	…	9.464750	65.041652	238.033819	
8	22.203716	1.233540	3.770033	…	9.543020	50.345912	257.101171	
9	20.720454	1.218850	3.759364	…	9.740204	64.085225	236.090940	
10	20.857278	1.226899	3.757231	…	9.792947	49.951285	241.117489	
11	24.631339	1.296386	3.898836	…	10.012476	69.036959	267.096754	
12	26.321008	1.253381	3.987292	…	10.124509	55.372829	288.063388	
13	24.471027	1.223551	3.970478	…	10.543893	71.840726	300.052840	
14	18.037415	1.202494	3.579412	…	8.906664	45.409755	205.132745	
15	20.720454	1.218850	3.759364	…	9.740204	64.085225	236.090940	
16	20.720454	1.218850	3.759364	…	9.740204	64.085225	236.090940	
17	28.157662	1.279894	4.065227	…	10.451638	70.897434	303.194677	
18	26.041871	1.302094	3.935368	…	9.940542	53.806646	271.120843	

	AMW	WPath	WPol	Zagreb1	Zagreb2	mZagreb1	mZagreb2
0	9.123038	483	27	92.0	111.0	4.916667	3.722222
1	7.790945	693	26	84.0	95.0	8.166667	4.194444
2	9.227346	896	36	114.0	136.0	7.750000	4.472222
3	8.627683	414	18	68.0	74.0	6.194444	3.472222
4	9.438833	986	40	120.0	145.0	8.611111	4.694444
5	7.545214	1657	35	134.0	156.0	9.000000	5.722222
6	8.141067	518	25	88.0	103.0	7.027778	3.694444
7	10.349296	580	20	86.0	98.0	6.416667	3.722222
8	7.790945	693	26	84.0	95.0	8.166667	4.194444
9	8.141067	518	25	88.0	103.0	7.027778	3.694444
10	7.534922	504	27	88.0	103.0	7.027778	3.694444
11	8.346774	657	32	104.0	128.0	6.638889	4.194444
12	8.729194	896	36	114.0	136.0	7.750000	4.472222
13	9.376651	698	36	116.0	147.0	8.291667	4.131944
14	6.837758	450	15	66.0	69.0	5.583333	3.500000
15	8.141067	518	25	88.0	103.0	7.027778	3.694444

```
16   8.141067    518    25     88.0    103.0  7.027778  3.694444
17   6.450951   1047    35    128.0    155.0  6.680556  4.597222
18   7.327590    820    31    106.0    124.0  6.277778  4.333333

[19 rows x 1613 columns]
```