

Connection to ChEMBL database and get molecules for Zika virus

Apuntes de clase

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Tabla de contenidos

1	IMPORT LIBRARIES	1
2	PATHS	3
3	GET MOLECULES FOR ZIKA VIRUS	5
4	SAVE MOLECULES TO CSV	7

Capítulo 1

IMPORT LIBRARIES

(Adam, Lee, y Wang 2023)

```
# PATH TO CUSTOM MODULES
import sys

sys.path.append("../src")

# IMPORT LIBRARIES
from chembl_webresource_client.new_client import new_client
import pandas as pd

# IMPORT CUSTOM MODULES
import repository.chembl_api_connection as chembl
```


Capítulo 2

PATHS

```
# PATHS TO SAVE DATA  
data_path = "../data/raw/"
```


Capítulo 3

GET MOLECULES FOR ZIKA VIRUS

```
# GET THE TARGET ID WITH MAXIMUM NUMBER OF IC50 MOLECULES FOR A GIVEN ORGANISM
organism = "Zika virus"
activity = "IC50"
target_id = chembl.get_target_id_maximum_activity(organism, activity)

# GET MOLECULES FOR TARGET ID AND ACTIVITY TYPE
molecules = chembl.get_molecules_from_target_activity(target_id, activity)
```


Capítulo 4

SAVE MOLECULES TO CSV

```
# SAVE MOLECULES TO CSV  
molecules.to_csv(data_path + target_id + "_raw.csv", index=False)
```

Adam, Awadalkareem, Christy Lee, y Tian Wang. 2023. «Rational Development of Live-Attenuated Zika Virus Vaccines». *Pathogens* 12 (2): 194. <https://doi.org/10.3390/pathogens12020194>.

