

Connection to ChEMBL database and active molecules for Zika virus collection

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```
# 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

# DIRECTORIES
data_path = "../data/raw/"
```

1 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)
```

2 SAVE MOLECULES TO CSV

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