

MMP visualization with Cytoscape

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Who am I ?

- **kzfm (@fmkz__)**
 - **blog.kzfmix.com**
 - **github.com/kzfm**
- **Computational Chemist**
 - **chemoinformatics**
 - **S&L Based Drug Designer**



LT@RDKitUGM

RDKit has 2 MMP generators

- **mmpa**
 - Contrib/mmpa
 - python scripts
 - (I use these scripts to generate MMPs for my in house system)
- **mmpdb**
 - mmpdb repo
 - CLI tool maintained by adalke & KramerChristia
 - <http://www.dalkescientific.com/writings/diary/archive/2018/06/04/mmpdb.html>

mmpdb is easy to use !

```
mmpdb fragment smiles.txt -o CHEMBL930273.fragments    # fragmentation  
mmpdb index CHEMBL930273.fragments -o CHEMBL930273.db  # make db  
mmpdb loadprops -p act.txt CHEMBL930273.db             # load properties
```

but it doesn't have a option for visualization

What if mmpdb has a option like gengml or such?

MMP Visualization

1. create gmlfile from mmpdb with python-igraph

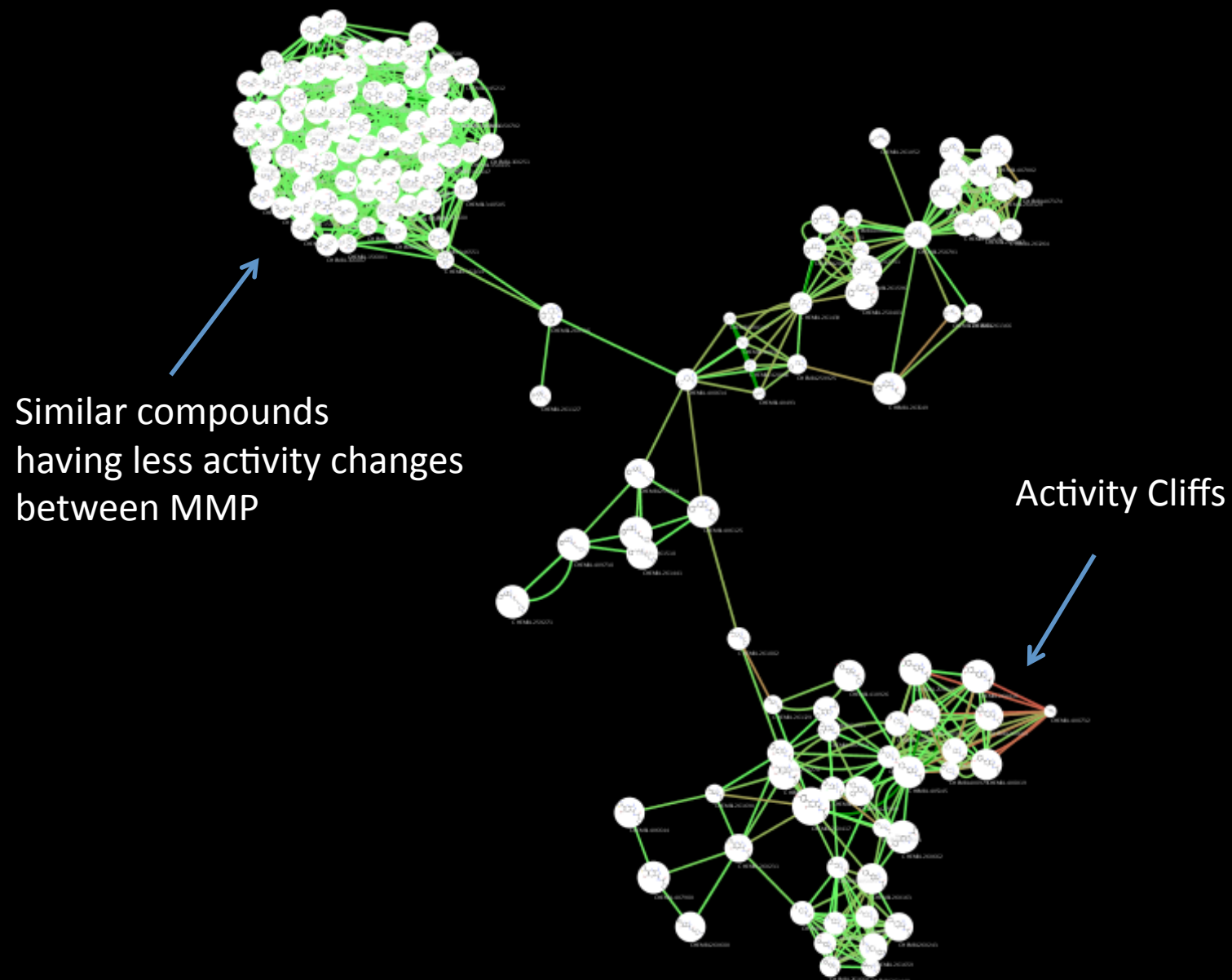
2. import gmlfile with Cytoscape 

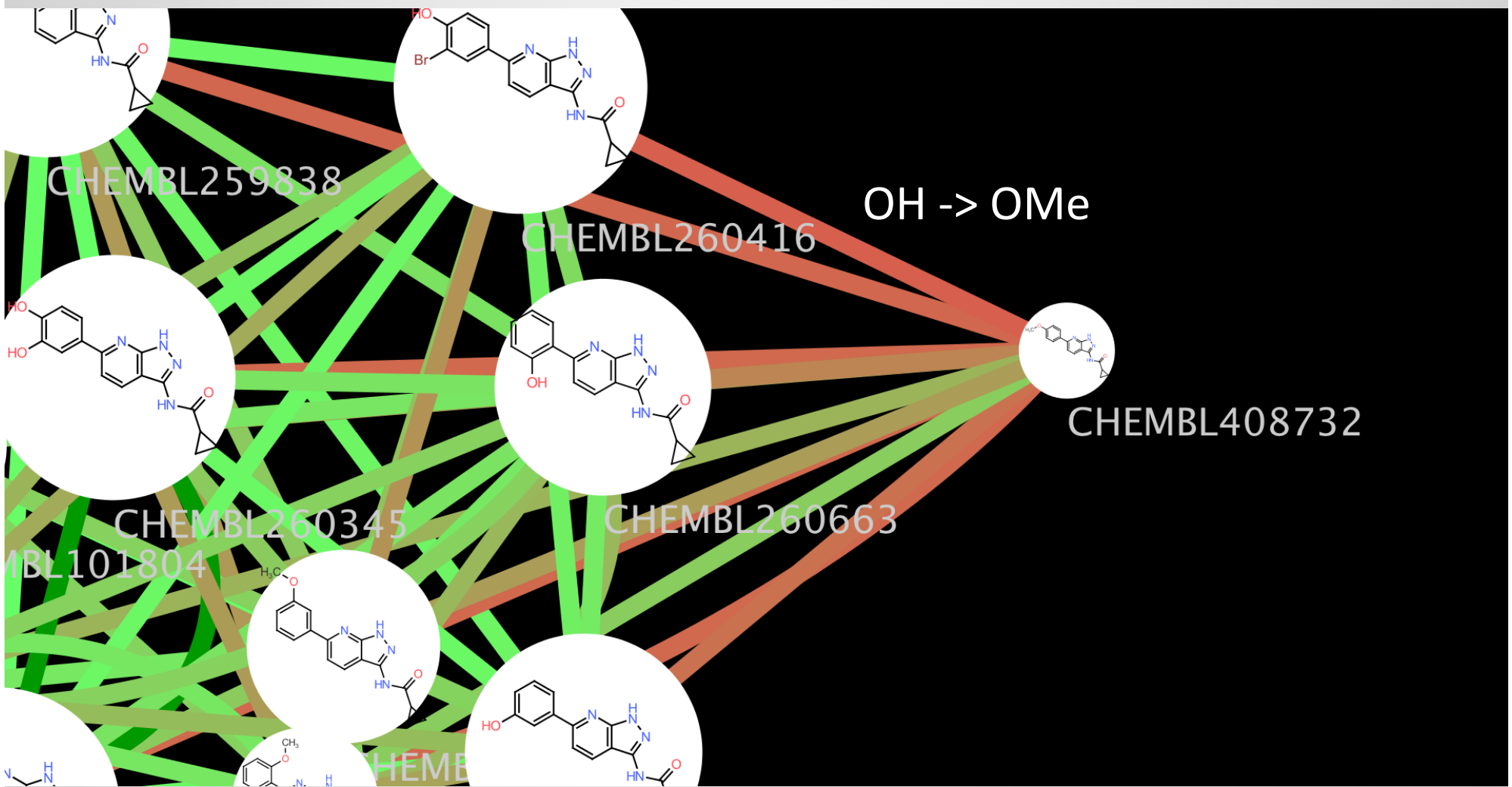
3. configure attribute of Cytoscape

- node size
- edge color
- structure rendering with chemviz2 plugin

Sample Data

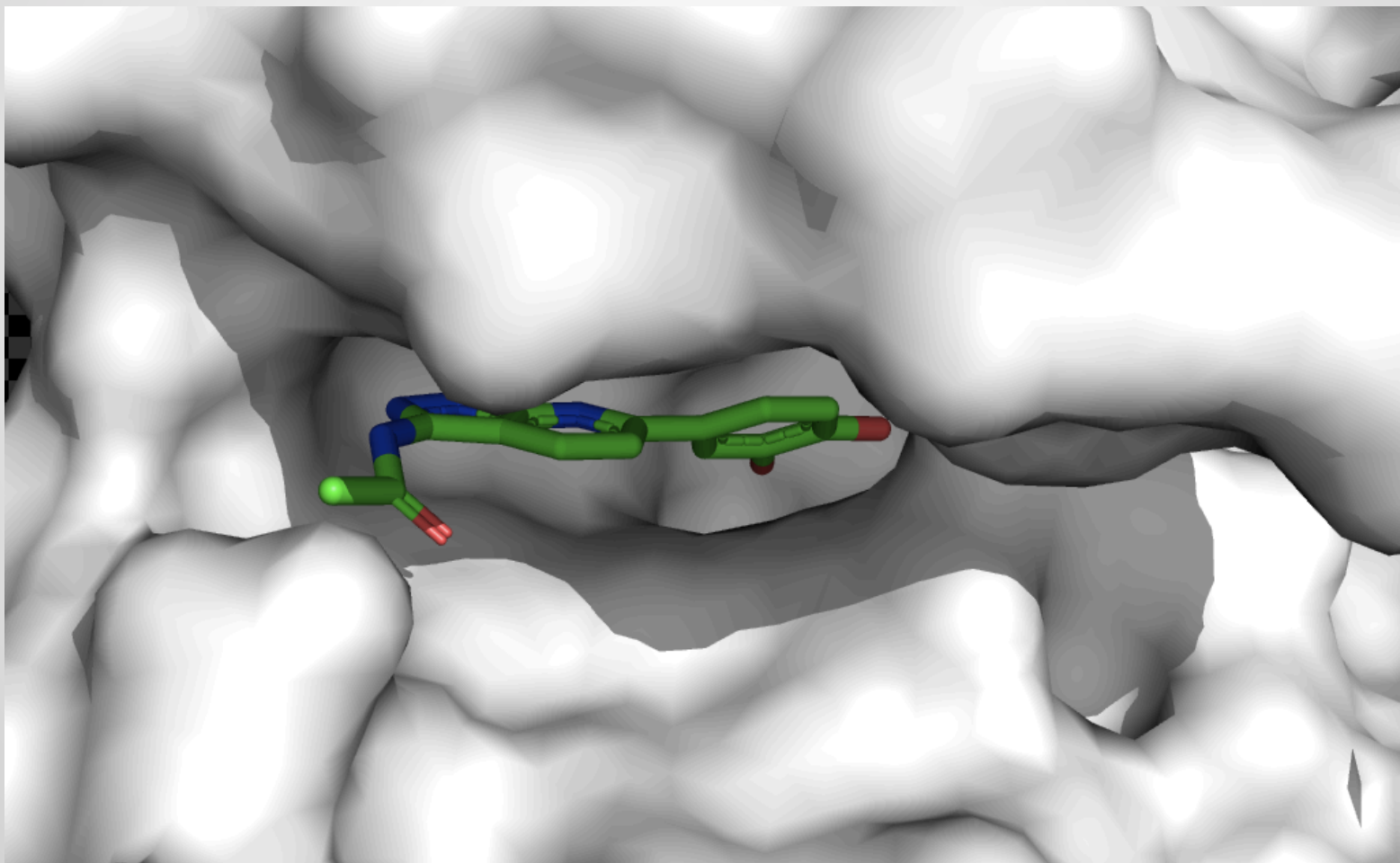
- **CHEMBL930273**
 - **Inhibition of recombinant GSK3-beta**
 - **J. Med. Chem. (2008) 51:2062-2077**
 - **151 assay data (IC50)**



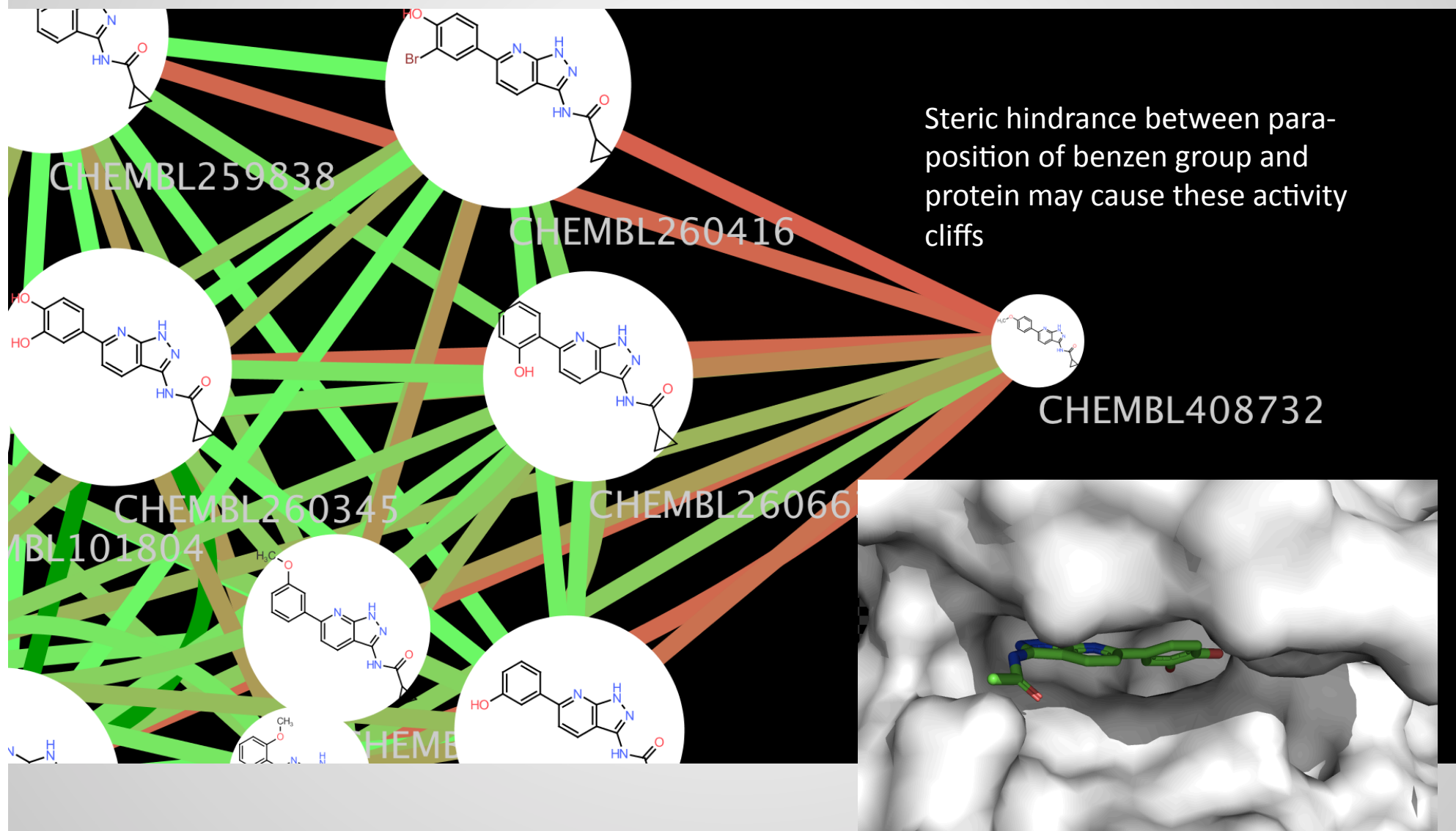


PDB-ID:5OY4

- **GSK3beta complex with N-(6-(3,4-dihydroxyphenyl)-1H-pyrazolo[3,4-b]pyridin-3-yl)acetamide**



Interpretation of AC



summary

- **Visualizing MMP is a convinient way to interprete SAR of project componds**
 - **Seeing SAR from a wide point of view**
 - **Search Activity Cliffs and get to the root of that**