Load the BINANA module

In [1]:
```
import sys
sys.path.append("../")
import binana
```

Load optional visualization module for this demo

In [2]:
```
import py3Dmol
```

Load in a receptor and ligand

In [3]:
```
ligand, receptor = binana.load_ligand_receptor.from_files("ligand.pdbqt"
, "receptor.pdbqt")
```

In [4]:
```
ligand, receptor
```

Out[4]:
```
(<binana._structure.mol.Mol at 0x7fe87141c320>,
 <binana._structure.mol.Mol at 0x7fe8713c06a0>)
```

Get information about the hydrogen bonds (example)

In [5]:
```
hbond_inf = binana.interactions.get_hydrogen_bonds(ligand, receptor)
```

In [6]:
```
# Counting/characterizing the acceptors and donors (counts)
hbond_inf["counts"]
```

Out[6]:
```
{'HDONOR_LIGAND_SIDECHAIN_OTHER': 2, 'HDONOR_RECEPTOR_SIDECHAIN_OTHER':
1}
```

In [7]:
```
# List the atoms involved in each hydrogen bond
for hbond_label in hbond_inf["labels"]:
    print(hbond_label)
```

```
('A:CHT(1):N1(14)', 'A:CHT(1):H1(16)', 'A:ASP(157):OD2(285)', 'LIGAND')
('A:CHT(1):O6(22)', 'A:ASN(156):2HD2(276)', 'A:ASN(156):ND2(274)', 'REC
EPTOR')
('A:CHT(1):O6(22)', 'A:CHT(1):HO6(23)', 'A:ASP(157):OD1(284)', 'LIGAN
D')
```

Get information about the cation-pi interactions (example)

In [8]:
```
cation_pi_inf = binana.interactions.get_cation_pi(ligand, receptor)
```

In [9]:
```
# Counting/characterizing the acceptors and donors (counts)
cation_pi_inf["counts"]
```

Out[9]:
```
{'PI-CATION_LIGAND-CHARGED_OTHER': 2,
 'PI-CATION_LIGAND-CHARGED_BETA': 2,
 'PI-CATION_RECEPTOR-CHARGED_OTHER': 1}
```

In [10]:
```
# List the atoms involved in each cation-pi interaction
for cation_pi_label in cation_pi_inf["labels"]:
    print(cation_pi_label)
```

```
('[A:CHT(1):N1(2) / A:CHT(1):C5(1) / A:CHT(1):C6(3) / A:CHT(1):C6(4) /
A:CHT(1):C7(9)]', '[A:TRP(43):CG(28) / A:TRP(43):CD1(29) / A:TRP(43):NE
1(31) / A:TRP(43):CE2(32) / A:TRP(43):CD2(30)]')
('[A:CHT(1):N1(2) / A:CHT(1):C5(1) / A:CHT(1):C6(3) / A:CHT(1):C6(4) /
A:CHT(1):C7(9)]', '[A:TRP(43):CE2(32) / A:TRP(43):CD2(30) / A:TRP(43):C
E3(33) / A:TRP(43):CZ3(35) / A:TRP(43):CH2(36) / A:TRP(43):CZ2(34)]')
('[A:CHT(1):N1(2) / A:CHT(1):C5(1) / A:CHT(1):C6(3) / A:CHT(1):C6(4) /
A:CHT(1):C7(9)]', '[A:TRP(205):CG(468) / A:TRP(205):CD1(469) / A:TRP(20
5):NE1(471) / A:TRP(205):CE2(472) / A:TRP(205):CD2(470)]')
('[A:CHT(1):N1(2) / A:CHT(1):C5(1) / A:CHT(1):C6(3) / A:CHT(1):C6(4) /
A:CHT(1):C7(9)]', '[A:TRP(205):CE2(472) / A:TRP(205):CD2(470) / A:TRP(2
05):CE3(473) / A:TRP(205):CZ3(475) / A:TRP(205):CH2(476) / A:TRP(205):C
Z2(474)]')
('[A:CHT(1):C2(17) / A:CHT(1):O1(18) / A:CHT(1):C5(19) / A:CHT(1):C4(2
0) / A:CHT(1):C3(21)]', '[A:LYS(94):NZ(144) / A:LYS(94):HZ1(146) / A:LY
S(94):HZ2(147) / A:LYS(94):HZ3(148)]')
```

Other interactions are also available

In [11]:
```
print("Available functions for detecting interactions:")
for f in dir(binana.interactions):
    if "get_" in f:
        print("    " + f)
```

```
Available functions for detecting interactions:
    get_active_site_flexibility
    get_all_interactions
    get_cation_pi
    get_close
    get_closest
    get_electrostatic_energies
    get_hydrogen_bonds
    get_hydrophobics
    get_ligand_atom_types
    get_pi_pi
    get_salt_bridges
```

Get and display PDB-formatted text

In [12]:
```
pdb_txt = binana.output.pdb_file.write(
    ligand, receptor,
    hydrogen_bonds=hbond_inf,
    cat_pi=cation_pi_inf,
    as_str=True
)
print(
    "\n".join(
        [
            l
            for l
            in pdb_txt.split("\n")
            if l.startswith("REMARK")
        ]
    )
)
```

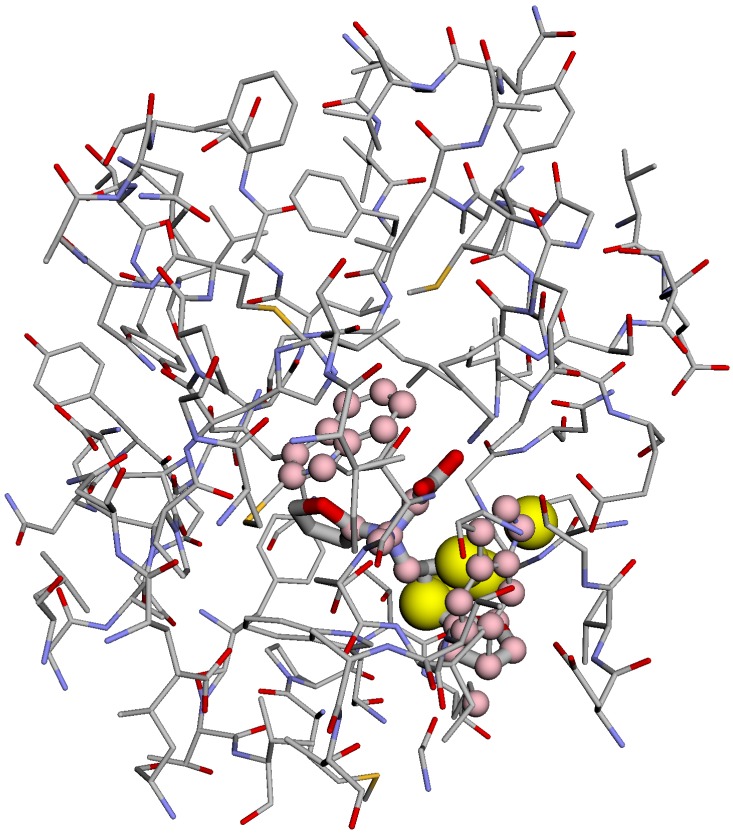
```
REMARK
REMARK The residue named "CCN" contains the closest contacts between th
e
REMARK protein and receptor. "CON" indicates close contacts. "ALP", "BE
T", and
REMARK "OTH" indicate receptor contacts whose respective protein residu
es have
REMARK the alpha-helix, beta-sheet, or "other" secondary structure. "BA
C" and
REMARK "SID" indicate receptor contacts that are part of the protein ba
ckbone
REMARK and sidechain, respectively. "HYD" indicates hydrophobic contact
s
REMARK between the protein and ligand. "HBN" indicates hydrogen bonds.
"SAL"
REMARK indicates salt bridges. "PIS" indicates pi-pi stacking interacti
ons,
REMARK "PIT" indicates T-stacking interactions, and "PIC" indicates cat
ion-pi
REMARK interactions. Protein residue names are unchanged, but the ligan
d
REMARK residue is now named "LIG".
REMARK
```

In [13]:
```
view = py3Dmol.view(data="",linked=False)

view.addModel(pdb_txt)

view.setStyle({'stick':{'radius':0.1}})
view.setStyle({"resn": "LIG"}, {'stick':{'radius':0.3}})
view.setStyle({"resn": "HBN"}, {'sphere':{'radius':1, "color": "yellow"
}})
view.setStyle({"resn": "PIC"}, {'sphere':{'radius':0.5, "color": "pink"
}})

view.zoomTo()
```



Out[13]: <py3Dmol.view at 0x7fe8502ca9e8>

Get the interactions as a dictionary for easier big-data analysis

In [14]:
```
data = binana.output.dictionary.collect(
    hydrogen_bonds=hbond_inf,
    cat_pi=cation_pi_inf
)

print("Keys:")
print(list(data.keys()))

print("")
print("Hydrogen-bond data (example):")
print(data["hydrogenBonds"])
```

```
Keys:
['hydrogenBonds', 'cationPiInteractions']

Hydrogen-bond data (example):
[{'ligandAtoms': [{'chain': 'A', 'resID': 1, 'resName': 'CHT', 'atomNam
e': 'N1', 'atomIndex': 14}, {'chain': 'A', 'resID': 1, 'resName': 'CH
T', 'atomName': 'H1', 'atomIndex': 16}], 'receptorAtoms': [{'chain':
'A', 'resID': 157, 'resName': 'ASP', 'atomName': 'OD2', 'atomIndex': 28
5}]}, {'ligandAtoms': [{'chain': 'A', 'resID': 1, 'resName': 'CHT', 'at
omName': 'O6', 'atomIndex': 22}], 'receptorAtoms': [{'chain': 'A', 'res
ID': 156, 'resName': 'ASN', 'atomName': 'ND2', 'atomIndex': 274}, {'cha
in': 'A', 'resID': 156, 'resName': 'ASN', 'atomName': '2HD2', 'atomInde
x': 276}]}, {'ligandAtoms': [{'chain': 'A', 'resID': 1, 'resName': 'CH
T', 'atomName': 'O6', 'atomIndex': 22}, {'chain': 'A', 'resID': 1, 'res
Name': 'CHT', 'atomName': 'HO6', 'atomIndex': 23}], 'receptorAtoms':
[{'chain': 'A', 'resID': 157, 'resName': 'ASP', 'atomName': 'OD1', 'ato
mIndex': 284}]}]
```

Get all the interactions at once

In [15]:
```
all_inf = binana.interactions.get_all_interactions(ligand, receptor)
```

In [16]:
```
all_inf.keys()
```

Out[16]:
```
dict_keys(['closest', 'close', 'electrostatic_energies', 'active_site_f
lexibility', 'hydrophobics', 'hydrogen_bonds', 'ligand_atom_types', 'pi
_pi', 'cat_pi', 'salt_bridges', 'ligand_rotatable_bonds'])
```

Get and dispaly PDB-formatted text containing all interactions

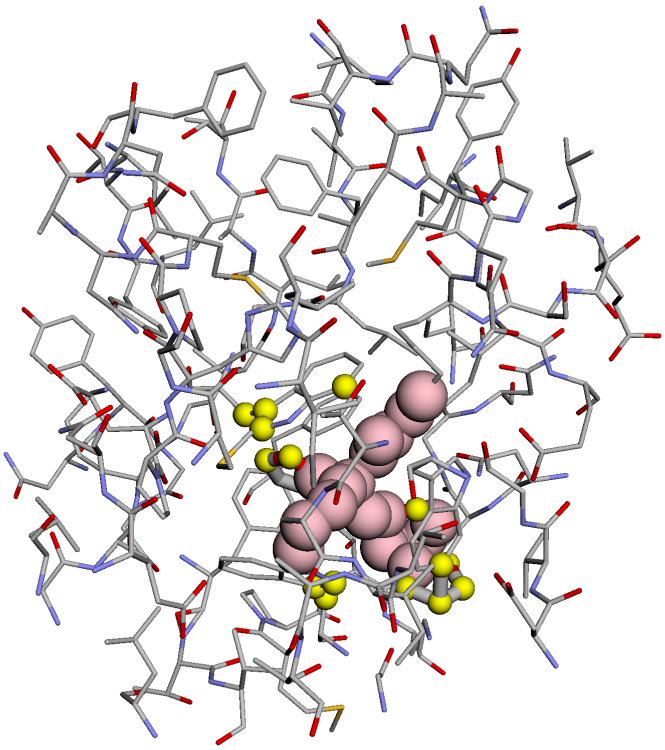
In [17]:
```
pdb_txt = binana.output.pdb_file.write_all(
    ligand, receptor,
    all_inf,
    as_str=True
)
```

In [18]:
```
view = py3Dmol.view(data="",linked=False)

view.addModel(pdb_txt)

view.setStyle({'stick':{'radius':0.1}})
view.setStyle({"resn": "LIG"}, {'stick':{'radius':0.3}})
view.setStyle({"resn": "CCN"}, {'sphere':{'radius':0.5, "color": "yello
w"}})
view.setStyle({"resn": "SAL"}, {'sphere':{'radius':1, "color": "pink"}})

view.zoomTo()
```



Out[18]: <py3Dmol.view at 0x7fe8302bdcc0>

Get all interactions as a single dictionary

In [19]:
```
all_data = binana.output.dictionary.collect_all(all_inf)

print(all_data.keys())
print()
print("Hydrogen bonds (example):")
print()
print(all_data["hydrogenBonds"])
```

```
dict_keys(['closestContacts', 'closeContacts', 'hydrophobicContacts',
'hydrogenBonds', 'piPiStackingInteractions', 'tStackingInteractions',
'cationPiInteractions', 'saltBridges', 'activeSiteFlexibility', 'electr
ostaticEnergies', 'ligandAtomTypes', 'ligandRotatableBonds'])

Hydrogen bonds (example):

[{'ligandAtoms': [{'chain': 'A', 'resID': 1, 'resName': 'LIG', 'atomNam
e': 'N1', 'atomIndex': 14}, {'chain': 'A', 'resID': 1, 'resName': 'LI
G', 'atomName': 'H1', 'atomIndex': 16}], 'receptorAtoms': [{'chain':
'A', 'resID': 157, 'resName': 'ASP', 'atomName': 'OD2', 'atomIndex': 28
5}]}, {'ligandAtoms': [{'chain': 'A', 'resID': 1, 'resName': 'LIG', 'at
omName': 'O6', 'atomIndex': 22}], 'receptorAtoms': [{'chain': 'A', 'res
ID': 156, 'resName': 'ASN', 'atomName': 'ND2', 'atomIndex': 274}, {'cha
in': 'A', 'resID': 156, 'resName': 'ASN', 'atomName': '2HD2', 'atomInde
x': 276}]}, {'ligandAtoms': [{'chain': 'A', 'resID': 1, 'resName': 'LI
G', 'atomName': 'O6', 'atomIndex': 22}, {'chain': 'A', 'resID': 1, 'res
Name': 'LIG', 'atomName': 'HO6', 'atomIndex': 23}], 'receptorAtoms':
[{'chain': 'A', 'resID': 157, 'resName': 'ASP', 'atomName': 'OD1', 'ato
mIndex': 284}]}]
```