In [5]:
```
import pandas as pd
import numpy as np
df1=pd.read_csv("bioactivity_data_flavormolecules_actual_datapreprocessed_output22.csv")
```

Label compounds as Active, Inactive and Intermediate

Labeling compounds as either being active, inactive or intermediate The bioactivity data is in the IC50 unit. Compounds having values of less than 1000 nM will be considered to be active while those greater than 10,000 nM will be considered to be inactive. As for those values in between 1,000 and 10,000 nM will be referred to as intermediate.

In [6]:
```
bioactivity_threshold = []
for i in df1.standard_value:
    if float(i) >= 10000:
        bioactivity_threshold.append("inactive")
    elif float(i) <= 1000:
        bioactivity_threshold.append("active")
    else:
        bioactivity_threshold.append("intermediate")
```

In [7]:
```
bioactivity_class = pd.Series(bioactivity_threshold, name='class')
df2 = pd.concat([df1, bioactivity_class], axis=1)
df2.rename(columns = {'molecule_chembl_id':'chembl_id'}, inplace = True)
df2.head()
```

Out[7]:

	chembl_id	molecule_pref_name	standard_value	target_chembl_id	target_pref_name	targ
0	CHEMBL165	RESVERATROL	0.0225	CHEMBL399	HeLa	H
1	CHEMBL19224	PAPAVERINE	0.0590	CHEMBL613633	Ileum	

	chembl_id	molecule_pref_name	standard_value	target_chembl_id	target_pref_name	targ
2	CHEMBL50	QUERCETIN	0.1100	CHEMBL2362975	No relevant target	
3	CHEMBL107	COLCHICINE	0.3600	CHEMBL3879801	NON-PROTEIN TARGET	
4	CHEMBL441687	GLYCYRRHIZIN	0.4000	CHEMBL3746	11-beta-hydroxysteroid dehydrogenase 2	H

In [8]:
```
#! conda install -c rdkit rdkit -y
import sys
sys.path.append('/usr/local/lib/python3.7/site-packages/')
import matplotlib.pyplot as plt
```

In [5]:
```
df2.head()
```

Out[5]:

	chembl_id	molecule_pref_name	standard_value	target_chembl_id	target_pref_name	targ
0	CHEMBL165	RESVERATROL	0.0225	CHEMBL399	HeLa	H
1	CHEMBL19224	PAPAVERINE	0.0590	CHEMBL613633	Ileum	
2	CHEMBL50	QUERCETIN	0.1100	CHEMBL2362975	No relevant target	
3	CHEMBL107	COLCHICINE	0.3600	CHEMBL3879801	NON-PROTEIN TARGET	
4	CHEMBL441687	GLYCYRRHIZIN	0.4000	CHEMBL3746	11-beta-hydroxysteroid dehydrogenase 2	H

Convert IC50 to pIC50

To allow **IC50** data to be more uniformly distributed, we will convert **IC50** to the negative logarithmic scale which is essentially **-log10(IC50)**.

This custom function pIC50() will accept a DataFrame as input and will:

- Take the IC50 values from the `standard_value` column and converts it from nM to M by multiplying the value by 10^{-9}
- Take the molar value and apply -log10
- Delete the `standard_value` column and create a new `pIC50` column

Point to note: Values greater than 100,000,000 will be fixed at 100,000,000 otherwise the negative logarithmic value will become negative.

In [9]:
```
df2.standard_value.describe()
```

Out[9]:
```
count    3.650000e+02
mean     5.559458e+06
std      5.365129e+07
min      2.250000e-02
25%      1.220000e+03
50%      1.700000e+04
75%      1.200000e+05
max      9.069430e+08
Name: standard_value, dtype: float64
```

In [10]:
```
#norm = []
df2['standard_value_norm']=df2['standard_value']
for i in range(len(df2['standard_value'])):
    k=df2['standard_value_norm'][i]
    if k > 100000000:
        #df['column name'] = df['column name'].replace(['old value'],'n
ew value')
        df2["standard_value_norm"]=df2["standard_value_norm"].replace([
k],100000000)
```

In [11]:
```
df2.standard_value_norm.describe()
```

Out[11]:
```
count    3.650000e+02
mean     2.328929e+06
std      1.250262e+07
```

```
min      2.250000e-02
25%      1.220000e+03
50%      1.700000e+04
75%      1.200000e+05
max      1.000000e+08
Name: standard_value_norm, dtype: float64
```

In [12]:
```
pIC50 = []
for i in df2['standard_value_norm']:
    molar = i*(10**-9) # Converts nM to M
    pIC50.append(-np.log10(molar))
```

In [13]:
```
len(df2)
```

Out[13]: 365

In [73]:
```
len(pIC50)
```

Out[73]: 365

In [14]:
```
df2['pIC50']=pIC50
df2.head()
```

Out[14]:

	chembl_id	molecule_pref_name	standard_value	target_chembl_id	target_pref_name	targ
0	CHEMBL165	RESVERATROL	0.0225	CHEMBL399	HeLa	H
1	CHEMBL19224	PAPAVERINE	0.0590	CHEMBL613633	Ileum	
2	CHEMBL50	QUERCETIN	0.1100	CHEMBL2362975	No relevant target	
3	CHEMBL107	COLCHICINE	0.3600	CHEMBL3879801	NON-PROTEIN TARGET	
4	CHEMBL441687	GLYCYRRHIZIN	0.4000	CHEMBL3746	11-beta-hydroxysteroid dehydrogenase 2	H

In [15]:
```
df2.head()
df_norm=df2.drop(columns=['standard_value','standard_value_norm'])
df_norm.head()
```

Out[15]:

	chembl_id	molecule_pref_name	target_chembl_id	target_pref_name	target_organism	cla
0	CHEMBL165	RESVERATROL	CHEMBL399	HeLa	Homo sapiens	act
1	CHEMBL19224	PAPAVERINE	CHEMBL613633	Ileum	Rattus norvegicus	act
2	CHEMBL50	QUERCETIN	CHEMBL2362975	No relevant target	NaN	act
3	CHEMBL107	COLCHICINE	CHEMBL3879801	NON-PROTEIN TARGET	NaN	act
4	CHEMBL441687	GLYCYRRHIZIN	CHEMBL3746	11-beta-hydroxysteroid dehydrogenase 2	Homo sapiens	act

In [16]:
```
df_nat=pd.read_csv('df2.csv')      #1145 ids chembl_pubchem_decriptors
df_nat.head()
```

Out[16]:

	pubchem_id	molecular_weight	hbd_count	hba_count	xlogp	natural	chembl_id
0	4	75.111	2	2	-1.0	1	CHEMBL326602
1	49	116.116	1	3	0.7	1	CHEMBL146554
2	58	102.089	1	3	0.1	1	CHEMBL171246
3	70	130.143	1	3	0.9	1	CHEMBL445647
4	72	154.121	3	4	1.1	1	CHEMBL37537

In [17]:
```
df_nat.info()
```

```
<class 'pandas.core.frame.DataFrame'>
RangeIndex: 1145 entries, 0 to 1144
Data columns (total 7 columns):
 #   Column            Non-Null Count  Dtype
```

```
---  ------            --------------  -----
 0   pubchem_id        1145 non-null   int64
 1   molecular_weight  1145 non-null   float64
 2   hbd_count         1145 non-null   int64
 3   hba_count         1145 non-null   int64
 4   xlogp             1126 non-null   float64
 5   natural           1145 non-null   int64
 6   chembl_id         1145 non-null   object
dtypes: float64(2), int64(4), object(1)
memory usage: 62.7+ KB
```

In [18]:
```
fdb_bio=df_norm.merge(df_nat,on=['chembl_id'], how="inner")
fdb_bio.info()
fdb_bio.head()
```

```
<class 'pandas.core.frame.DataFrame'>
Int64Index: 365 entries, 0 to 364
Data columns (total 13 columns):
 #   Column              Non-Null Count  Dtype
---  ------              --------------  -----
 0   chembl_id           365 non-null    object
 1   molecule_pref_name  306 non-null    object
 2   target_chembl_id    365 non-null    object
 3   target_pref_name    365 non-null    object
 4   target_organism     293 non-null    object
 5   class               365 non-null    object
 6   pIC50               365 non-null    float64
 7   pubchem_id          365 non-null    int64
 8   molecular_weight    365 non-null    float64
 9   hbd_count           365 non-null    int64
 10  hba_count           365 non-null    int64
 11  xlogp               364 non-null    float64
 12  natural             365 non-null    int64
dtypes: float64(3), int64(4), object(6)
memory usage: 39.9+ KB
```

Out[18]:

	chembl_id	molecule_pref_name	target_chembl_id	target_pref_name	target_organism	cla
0	CHEMBL165	RESVERATROL	CHEMBL399	HeLa	Homo sapiens	act

	chembl_id	molecule_pref_name	target_chembl_id	target_pref_name	target_organism	cla
1	CHEMBL19224	PAPAVERINE	CHEMBL613633	Ileum	Rattus norvegicus	act
2	CHEMBL50	QUERCETIN	CHEMBL2362975	No relevant target	NaN	act
3	CHEMBL107	COLCHICINE	CHEMBL3879801	NON-PROTEIN TARGET	NaN	act
4	CHEMBL441687	GLYCYRRHIZIN	CHEMBL3746	11-beta-hydroxysteroid dehydrogenase 2	Homo sapiens	act

In [19]:
```
df6=fdb_bio.drop(['target_organism'], axis=1)
df6.head()
```

Out[19]:

	chembl_id	molecule_pref_name	target_chembl_id	target_pref_name	class	pIC50	pu
0	CHEMBL165	RESVERATROL	CHEMBL399	HeLa	active	10.647817	
1	CHEMBL19224	PAPAVERINE	CHEMBL613633	Ileum	active	10.229148	
2	CHEMBL50	QUERCETIN	CHEMBL2362975	No relevant target	active	9.958607	
3	CHEMBL107	COLCHICINE	CHEMBL3879801	NON-PROTEIN TARGET	active	9.443697	
4	CHEMBL441687	GLYCYRRHIZIN	CHEMBL3746	11-beta-hydroxysteroid dehydrogenase 2	active	9.397940	

In [12]:
```
fdb_bio.to_csv('fdb_classification_bioactivity_pIC50.csv', index=False)
```

Intermediate Class was not considered for **Exploratory Data Analysis**

In [20]:
```
# removing the intermediate class
df_2class = fdb_bio[fdb_bio['class'] != 'intermediate']
df_2class.info()
```

```
<class 'pandas.core.frame.DataFrame'>
Int64Index: 297 entries, 0 to 364
Data columns (total 13 columns):
 #   Column              Non-Null Count  Dtype  
---  ------              --------------  -----  
 0   chembl_id           297 non-null    object 
 1   molecule_pref_name  244 non-null    object 
 2   target_chembl_id    297 non-null    object 
 3   target_pref_name    297 non-null    object 
 4   target_organism     243 non-null    object 
 5   class               297 non-null    object 
 6   pIC50               297 non-null    float64
 7   pubchem_id          297 non-null    int64  
 8   molecular_weight    297 non-null    float64
 9   hbd_count           297 non-null    int64  
 10  hba_count           297 non-null    int64  
 11  xlogp               296 non-null    float64
 12  natural             297 non-null    int64  
dtypes: float64(3), int64(4), object(6)
memory usage: 32.5+ KB
```

In [21]:
```
df_2class.to_csv('fdb_classification_bioactivity_pIC50_onlyactive_inactive.csv', index=False)
```

Exploratory Data Analysis (Chemical Space Analysis) via Lipinski descriptors

Calculate Lipinski descriptors

Christopher Lipinski, a scientist at Pfizer, came up with a set of rule-of-thumb for evaluating the **druglikeness** of compounds. Such druglikeness is based on the Absorption, Distribution, Metabolism and Excretion (ADME) that is also known as the pharmacokinetic profile. Lipinski analyzed all orally active FDA-approved drugs in the formulation of what is to be known as the **Rule-of-Five** or **Lipinski's Rule**.

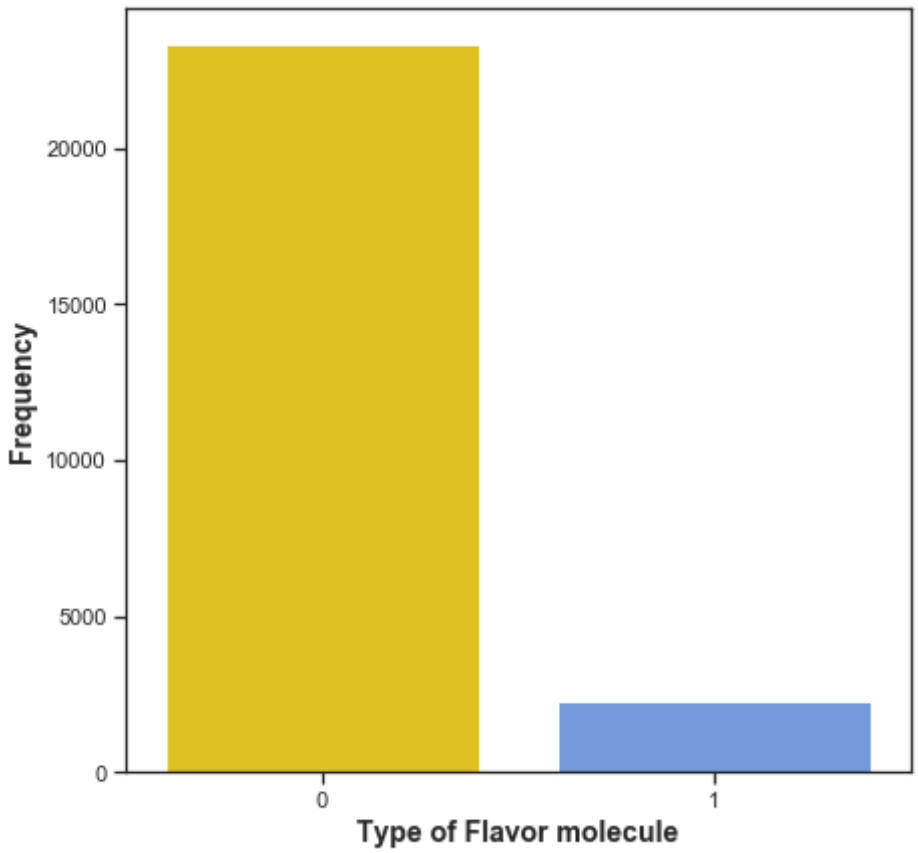
The Lipinski's Rule stated the following:

- Molecular weight < 500 Dalton
- Octanol-water partition coefficient (LogP) < 5
- Hydrogen bond donors < 5
- Hydrogen bond acceptors < 10

In [3]:
```
import pandas as pd
import seaborn as sns
#sns.set_theme(style="darkgrid")
sns.set(style='ticks')
import matplotlib.pyplot as plt
df_fla=pd.read_csv("fdb_molecules_22Nov.csv")
```

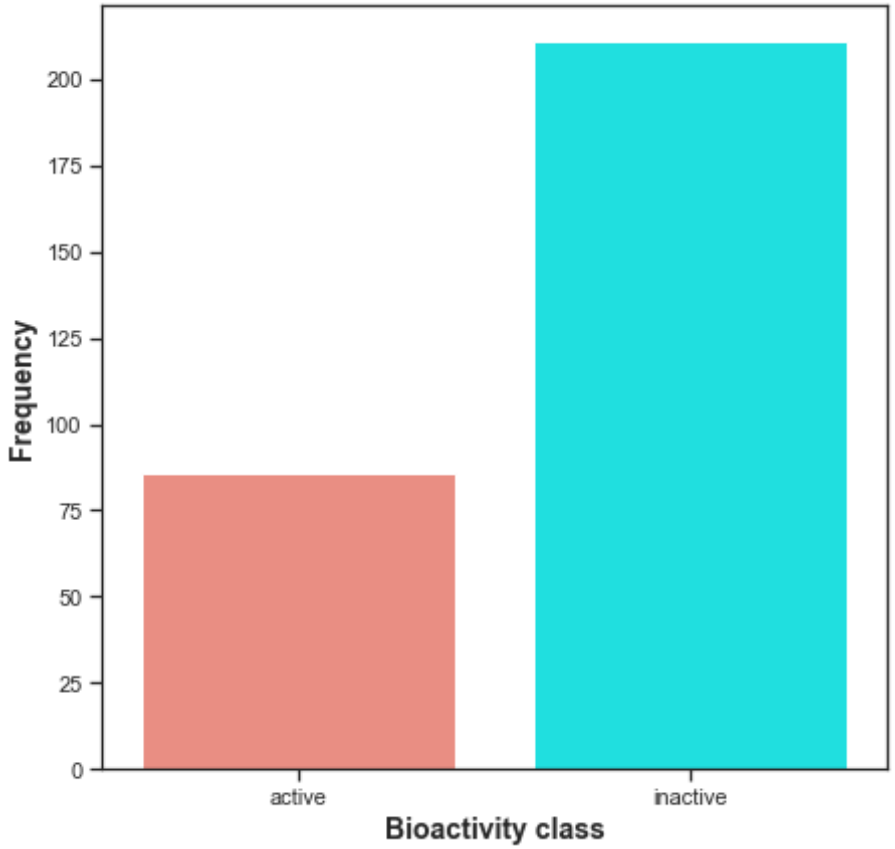
Frequency plot of the Synthetic and Natural Molecules in Flavor Db

In [4]:
```
plt.figure(figsize=(7,7))

sns.countplot(x='natural', data=df_fla,palette=['gold','cornflowerblue'
])

plt.xlabel('Type of Flavor molecule', fontsize=14, fontweight='bold')
plt.ylabel('Frequency', fontsize=14, fontweight='bold')

plt.savefig('plot_synthtic_nativecount_class.png')
```



Frequency plot of the 2 bioactivity classes

In [141]:
```
plt.figure(figsize=(7,7))

sns.countplot(x='class', data=df_2class,palette=['salmon','cyan'])

plt.xlabel('Bioactivity class', fontsize=14, fontweight='bold')
plt.ylabel('Frequency', fontsize=14, fontweight='bold')

plt.savefig('plot_bioactivity_class.png')
```

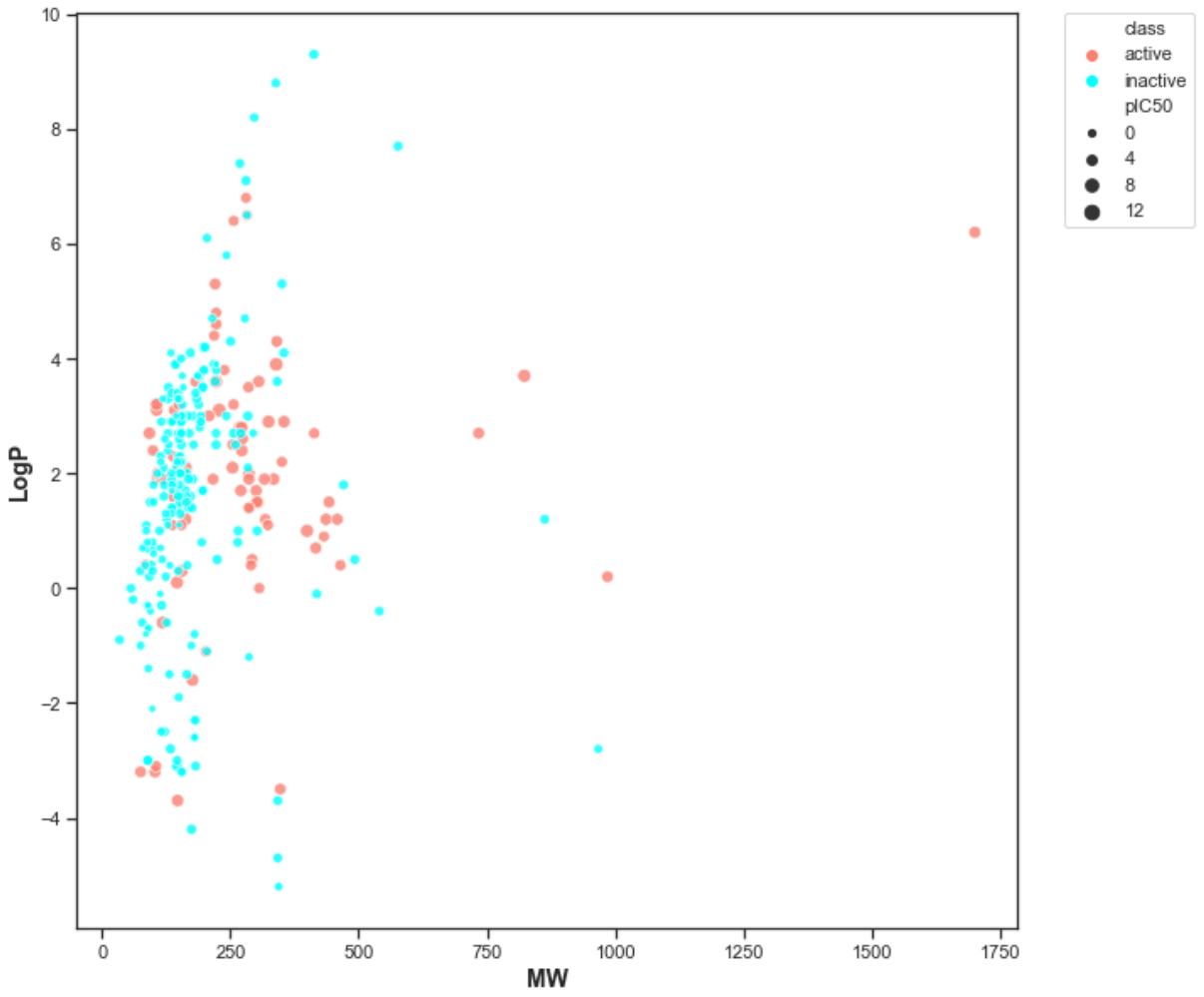


Scatter plot of MW versus LogP

It can be seen that the 2 bioactivity classes are spanning similar chemical spaces as evident by the scatter plot of MW vs LogP.

In [122]:
```
plt.figure(figsize=(10,10))

sns.scatterplot(x='molecular_weight', y='xlogp', data=df_2class, hue='class',palette=['salmon','cyan'], size='pIC50', alpha=0.8)

plt.xlabel('MW', fontsize=14, fontweight='bold')
```

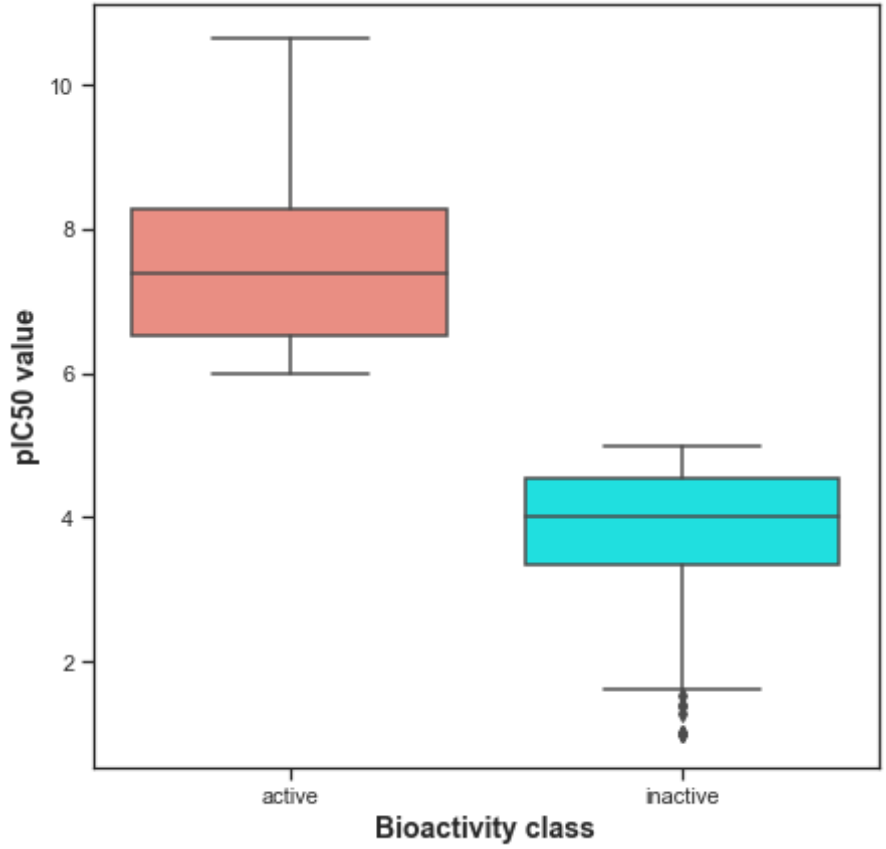
```
plt.ylabel('LogP', fontsize=14, fontweight='bold')
plt.legend(bbox_to_anchor=(1.05, 1), loc=2, borderaxespad=0)
plt.savefig('plot_MW_vs_LogP.png')
```



Box plots

pIC50 value

In [140]:
```
plt.figure(figsize=(7, 7))

sns.boxplot(x = 'class', y = 'pIC50', data = df_2class,palette=['salmo
n','cyan'])

plt.xlabel('Bioactivity class', fontsize=14, fontweight='bold')
plt.ylabel('pIC50 value', fontsize=14, fontweight='bold')

plt.savefig('plot_ic50.png') #threshold >6 active, <6 inactive
```



In [124]:
```
def mannwhitney(descriptor, verbose=False):
  # https://machinelearningmastery.com/nonparametric-statistical-signif
```

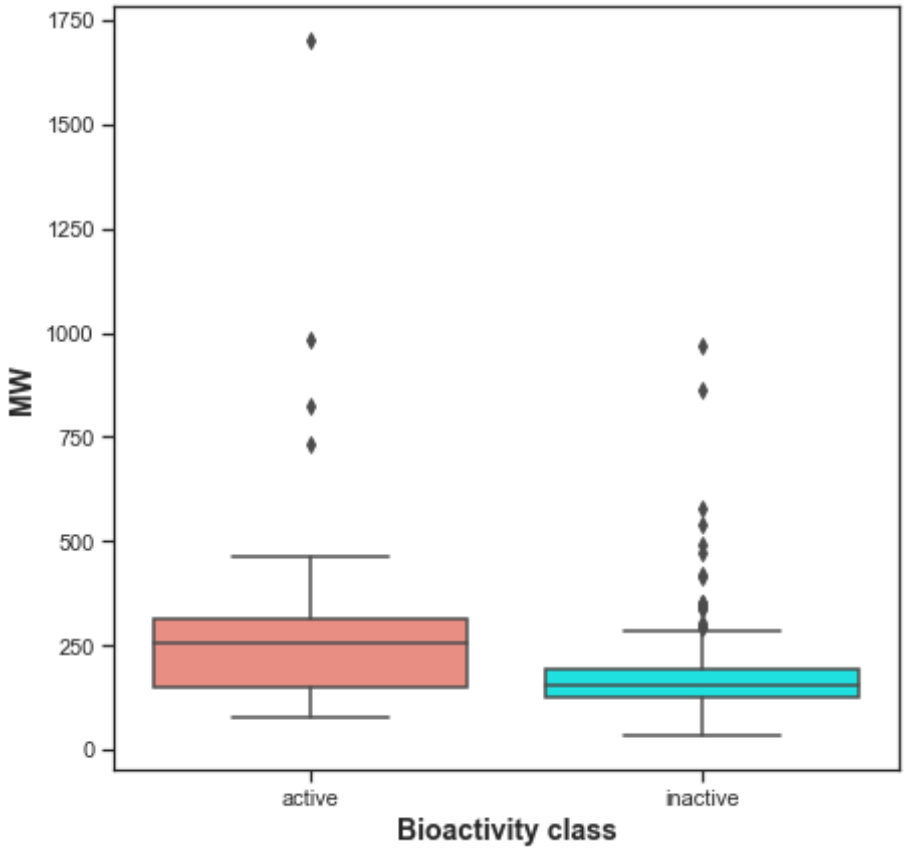
```
icance-tests-in-python/
    from numpy.random import seed
    from numpy.random import randn
    from scipy.stats import mannwhitneyu
# actives and inactives
    selection = [descriptor, 'class']
    df = df_2class[selection]
    active = df[df['class'] == 'active']
    active = active[descriptor]

    selection = [descriptor, 'class']
    df = df_2class[selection]
    inactive = df[df['class'] == 'inactive']
    inactive = inactive[descriptor]
   # compare samples
    stat, p = mannwhitneyu(active, inactive)
      #print('Statistics=%.3f, p=%.3f' % (stat, p))
      # interpret
    alpha = 0.05
    if p > alpha:
        interpretation = 'Same distribution (fail to reject H0)'
    else:
        interpretation = 'Different distribution (reject H0)'

    results = pd.DataFrame({'Descriptor':descriptor,
                            'Statistics':stat,
                            'p':p,
                            'alpha':alpha,
                            'Interpretation':interpretation}, index=[0])
    filename = 'mannwhitneyu_' + descriptor + '.csv'
    results.to_csv(filename)

    return results
```

In [125]:
```
mannwhitney('pIC50')
# compare active to inactive calss to see if there is any statistical d
ifference between active or nactive class or not
# p value < 0.05 , rejecting null hypothesis and thus we can say that a
ctive and inactive classes have different distribution
```

Out[125]:

	Descriptor	Statistics	p	alpha	Interpretation
0	pIC50	0.0	6.087553e-42	0.05	Different distribution (reject H0)

In [126]:
```
plt.figure(figsize=(7, 7))

sns.boxplot(x = 'class', y = 'molecular_weight', data = df_2class,palet
te=['salmon','cyan'])

plt.xlabel('Bioactivity class', fontsize=14, fontweight='bold')
plt.ylabel('MW', fontsize=14, fontweight='bold')

plt.savefig('plot_MW.png')
```



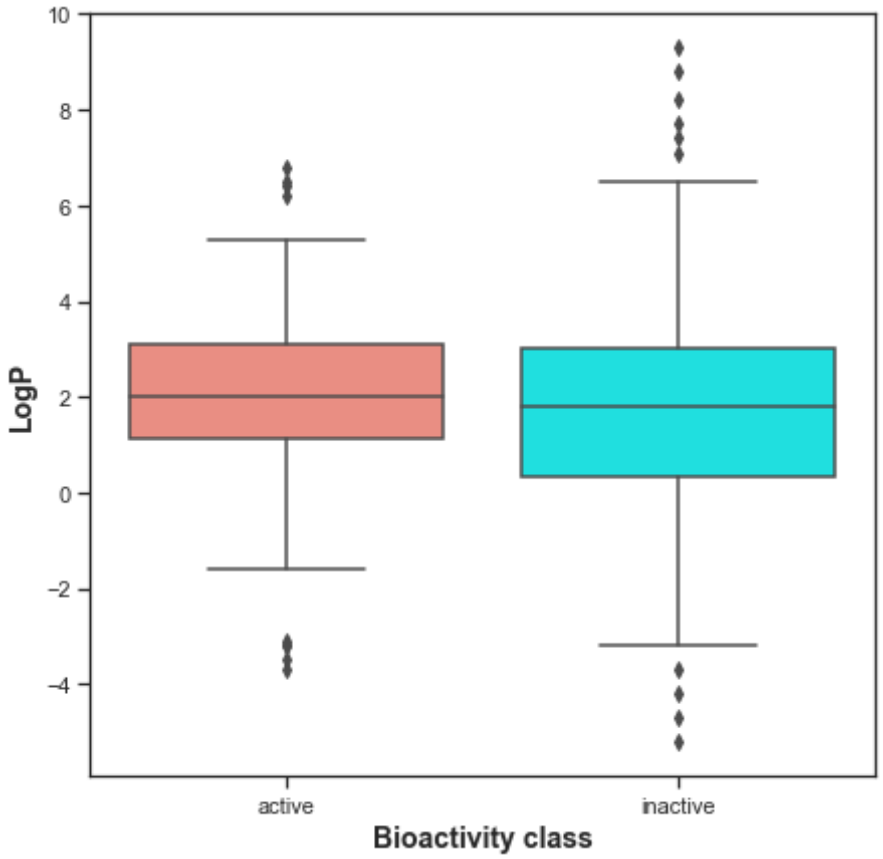
In [127]:
```
mannwhitney('molecular_weight')
```

Out[127]:

	Descriptor	Statistics	p	alpha	Interpretation
0	molecular_weight	5254.5	6.436918e-09	0.05	Different distribution (reject H0)

In [128]:
```
plt.figure(figsize=(7, 7))

sns.boxplot(x = 'class', y = 'xlogp', data = df_2class,palette=['salmo
n','cyan'])

plt.xlabel('Bioactivity class', fontsize=14, fontweight='bold')
```

```
plt.ylabel('LogP', fontsize=14, fontweight='bold')

plt.savefig('plot_LogP.png')
```



In [129]:
```
mannwhitney('xlogp')
```

Out[129]:

	Descriptor	Statistics	p	alpha	Interpretation
0	xlogp	8217.5	0.10134	0.05	Same distribution (fail to reject H0)

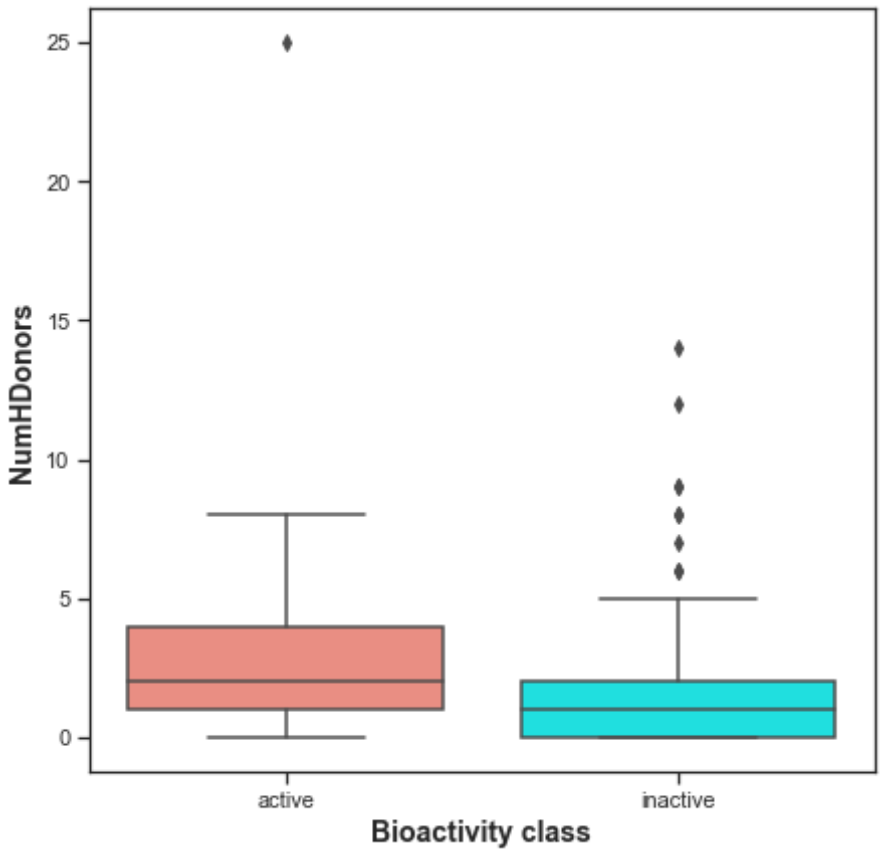
In [130]:
```
df_2class.head()
```

Out[130]:

	chembl_id	molecule_pref_name	target_chembl_id	target_pref_name	target_organism	cla
0	CHEMBL165	RESVERATROL	CHEMBL399	HeLa	Homo sapiens	act
1	CHEMBL19224	PAPAVERINE	CHEMBL613633	Ileum	Rattus norvegicus	act
2	CHEMBL50	QUERCETIN	CHEMBL2362975	No relevant target	NaN	act
3	CHEMBL107	COLCHICINE	CHEMBL3879801	NON-PROTEIN TARGET	NaN	act
4	CHEMBL441687	GLYCYRRHIZIN	CHEMBL3746	11-beta-hydroxysteroid dehydrogenase 2	Homo sapiens	act

In [131]:

```
plt.figure(figsize=(7,7))

sns.boxplot(x = 'class', y = 'hbd_count', data = df_2class,palette=['sa
lmon','cyan'])

plt.xlabel('Bioactivity class', fontsize=14, fontweight='bold')
plt.ylabel('NumHDonors', fontsize=14, fontweight='bold')

plt.savefig('plot_NumHDonors.png')
```



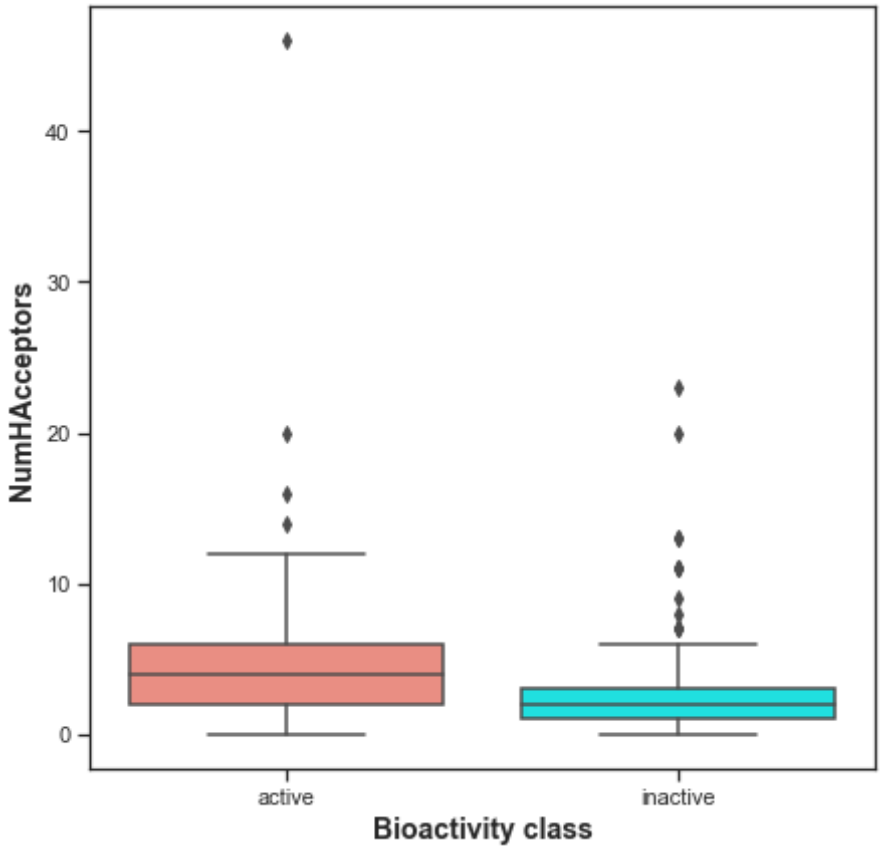
In [132]:
```
mannwhitney('hbd_count')
```

Out[132]:

	Descriptor	Statistics	p	alpha	Interpretation
0	hbd_count	5945.5	6.722676e-07	0.05	Different distribution (reject H0)

In [133]:
```
plt.figure(figsize=(7,7))

sns.boxplot(x = 'class', y = 'hba_count', data = df_2class,palette=['sa
lmon','cyan'])
```

```
plt.xlabel('Bioactivity class', fontsize=14, fontweight='bold')
plt.ylabel('NumHAcceptors', fontsize=14, fontweight='bold')
plt.savefig('plot_NumHAcceptors.png')
```



In [134]:
```
mannwhitney('hba_count')
```

Out[134]:

	Descriptor	Statistics	p	alpha	Interpretation
0	hba_count	5616.0	7.643777e-08	0.05	Different distribution (reject H0)

In [135]:
```
df_2class.head()
df3_act=df_2class[df_2class['class']=='active']
```

```
df3_inact=df_2class[df_2class['class']=='inactive']
```

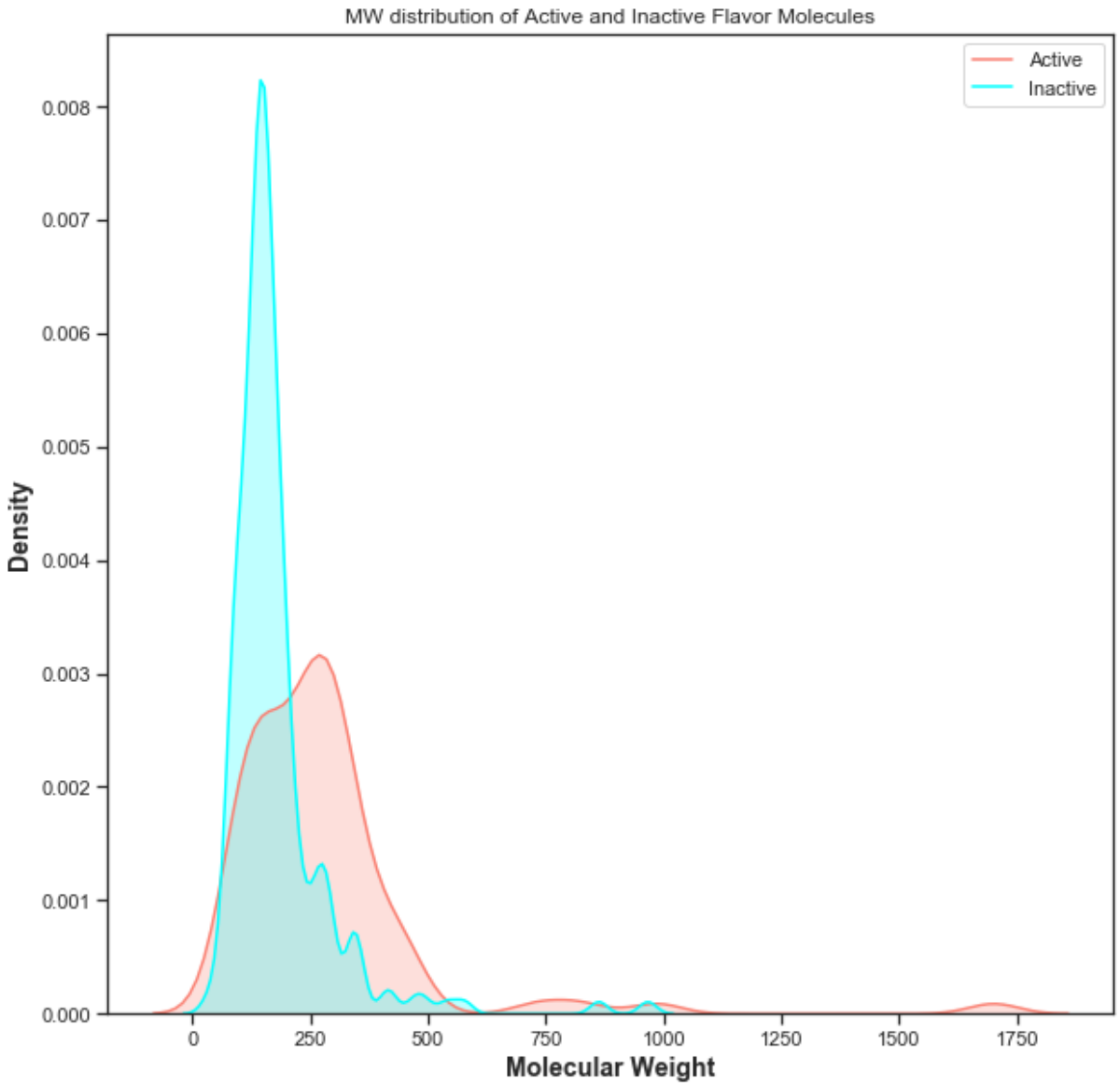
In [97]:
```
df3_act.head()
```

Out[97]:

	chembl_id	molecule_pref_name	target_chembl_id	target_pref_name	target_organism	cla
0	CHEMBL165	RESVERATROL	CHEMBL399	HeLa	Homo sapiens	act
1	CHEMBL19224	PAPAVERINE	CHEMBL613633	Ileum	Rattus norvegicus	act
2	CHEMBL50	QUERCETIN	CHEMBL2362975	No relevant target	NaN	act
3	CHEMBL107	COLCHICINE	CHEMBL3879801	NON-PROTEIN TARGET	NaN	act
4	CHEMBL441687	GLYCYRRHIZIN	CHEMBL3746	11-beta-hydroxysteroid dehydrogenase 2	Homo sapiens	act

Density Plots

In [136]:
```
fig = plt.figure(figsize =(10,10))
plt.rcParams.update({'font.size': 14})
act=sns.kdeplot(df3_act['molecular_weight'], color='salmon', shade=True
,Label='Active')
inact=sns.kdeplot(df3_inact['molecular_weight'], color='cyan', shade=Tr
ue,Label='Inactive')


# plt.vlines(x_median2, 0, y_median2,label='median_hum', color='r')
# plt.vlines(x_median, 0, y_median,label='median_ind')
plt.title("MW distribution of Active and Inactive Flavor Molecules")
plt.xlabel("Molecular Weight",fontsize=14, fontweight='bold')
plt.ylabel("Density",fontsize=14, fontweight='bold')
#plt.gca().legend(('IndiGen nsSNPs(22 residues)','HUMSAVAR nsSNPs(76 re
sidues)'),loc="upper right")
plt.legend(loc="upper right")
plt.savefig('plot_density_mw.png')
```



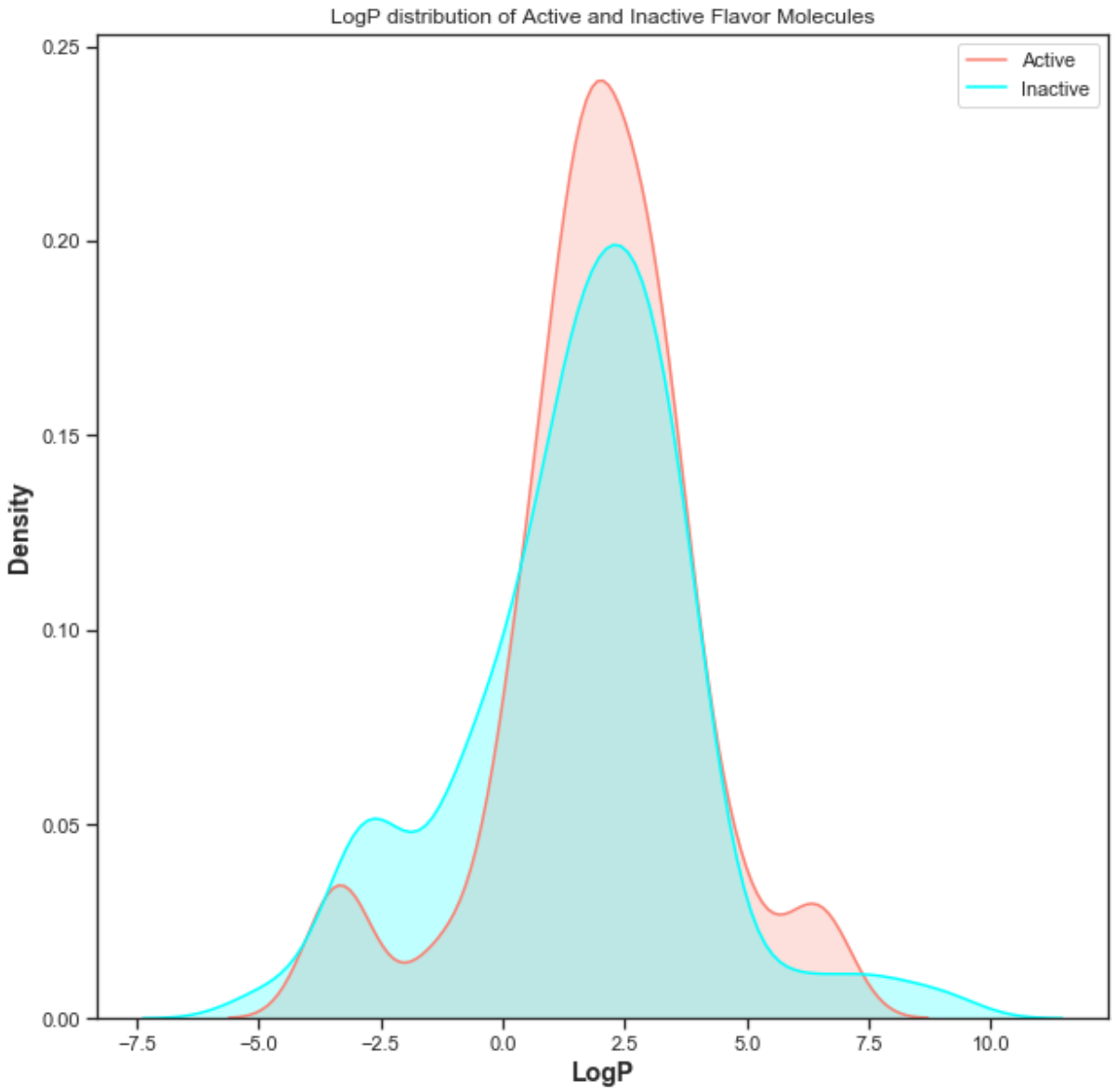
In [99]:
```
df3_act.head()
```

Out[99]:

	chembl_id	molecule_pref_name	target_chembl_id	target_pref_name	target_organism	cl
0	CHEMBL165	RESVERATROL	CHEMBL399	HeLa	Homo sapiens	act
1	CHEMBL19224	PAPAVERINE	CHEMBL613633	Ileum	Rattus norvegicus	act
2	CHEMBL50	QUERCETIN	CHEMBL2362975	No relevant target	NaN	act
3	CHEMBL107	COLCHICINE	CHEMBL3879801	NON-PROTEIN TARGET	NaN	act
4	CHEMBL441687	GLYCYRRHIZIN	CHEMBL3746	11-beta-hydroxysteroid dehydrogenase 2	Homo sapiens	act

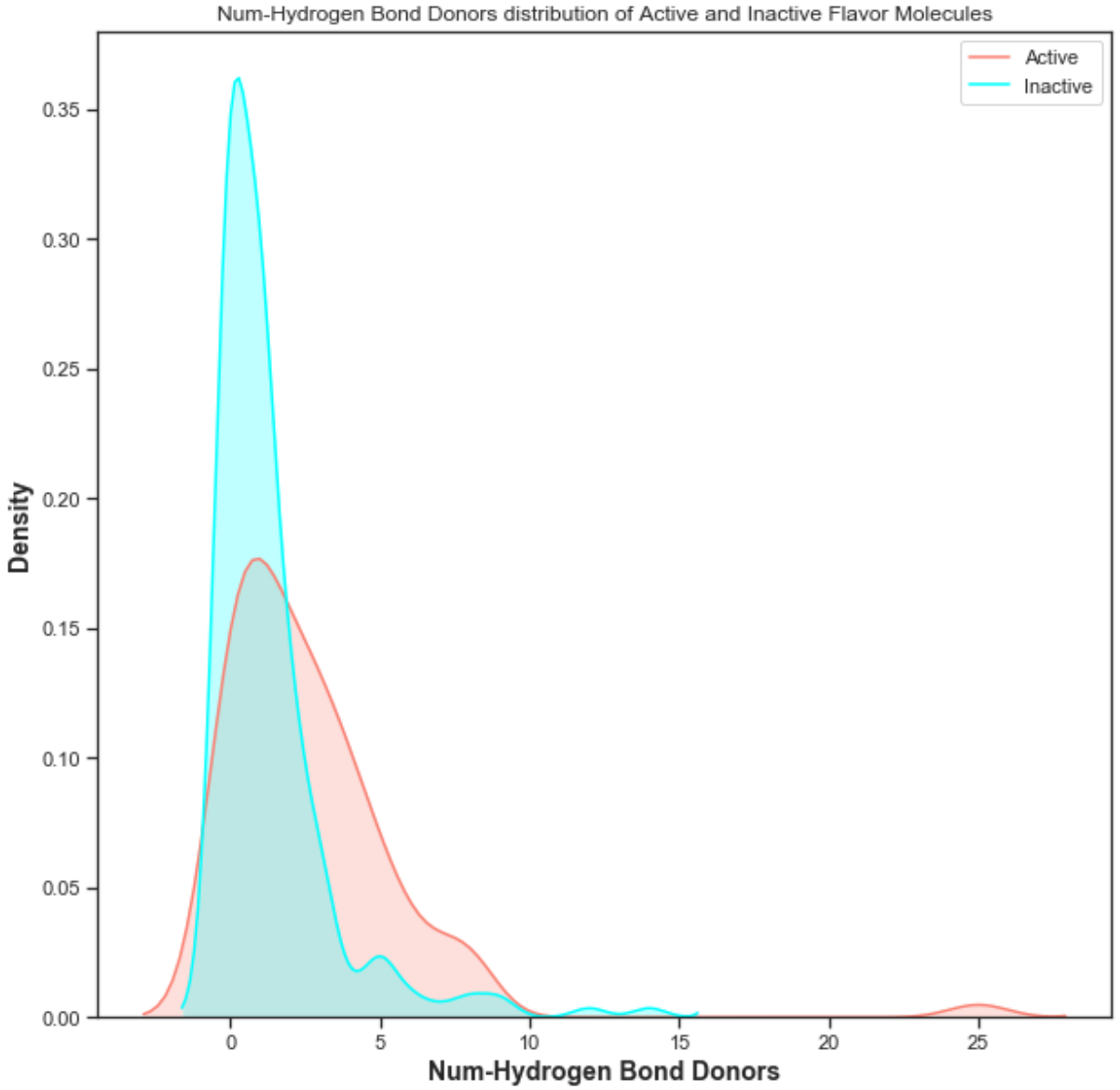
In [137]:

```
fig = plt.figure(figsize =(10,10))
plt.rcParams.update({'font.size': 14})
act=sns.kdeplot(df3_act['xlogp'], color='salmon', shade=True,Label='Act
ive')
inact=sns.kdeplot(df3_inact['xlogp'], color='cyan', shade=True,Label='I
nactive')


# plt.vlines(x_median2, 0, y_median2,label='median_hum', color='r')
# plt.vlines(x_median, 0, y_median,label='median_ind')
plt.title("LogP distribution of Active and Inactive Flavor Molecules")
plt.xlabel("LogP",fontsize=14, fontweight='bold')
plt.ylabel("Density",fontsize=14, fontweight='bold')
#plt.gca().legend(('IndiGen nsSNPs(22 residues)','HUMSAVAR nsSNPs(76 re
sidues)'),loc="upper right")
plt.legend(loc="upper right")
plt.savefig('plot_density_logp.png')
```

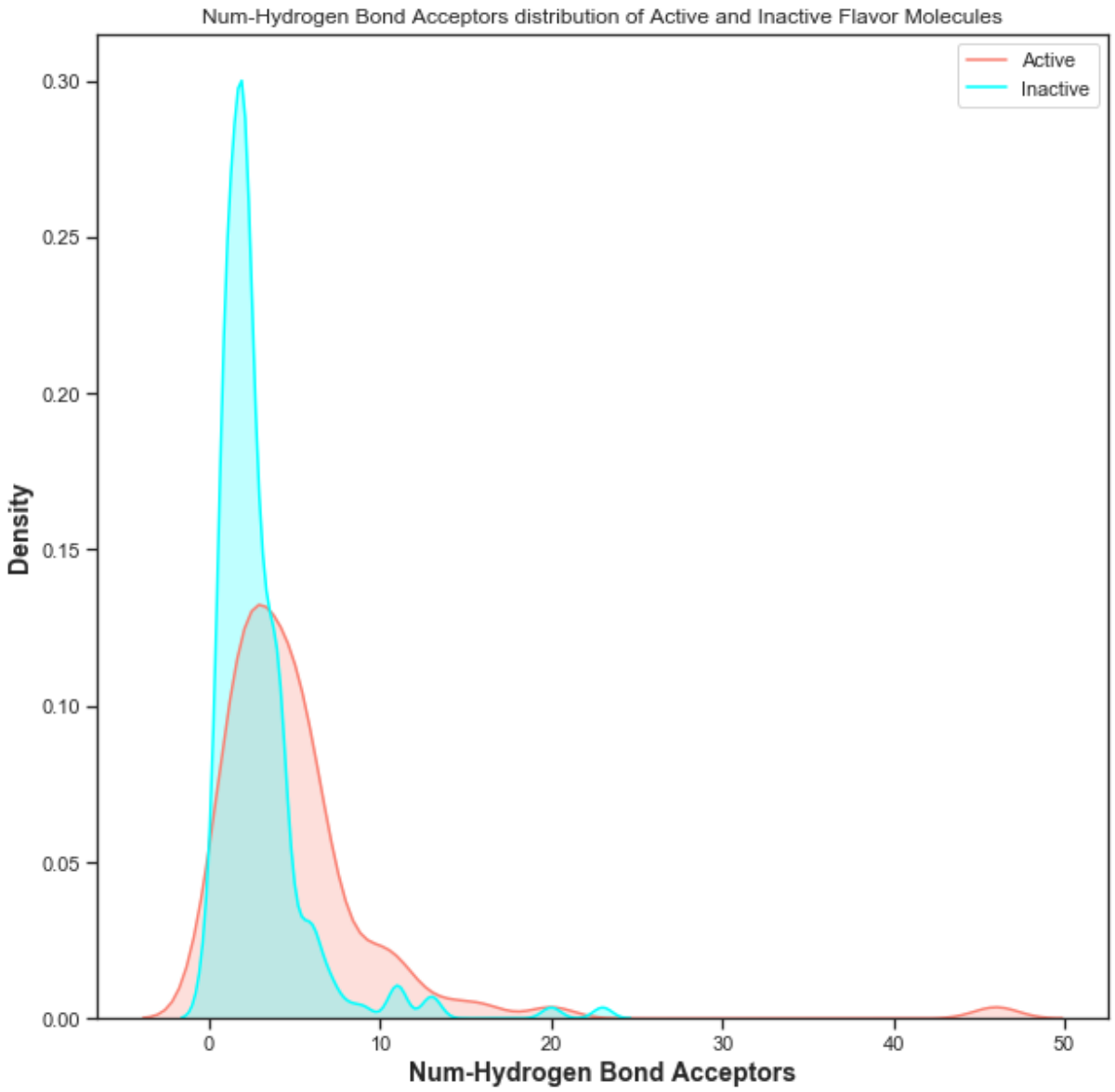


In [138]:
```
fig = plt.figure(figsize =(10,10))
```

```
plt.rcParams.update({'font.size': 14})
act=sns.kdeplot(df3_act['hbd_count'], color='salmon', shade=True,Label=
'Active')
inact=sns.kdeplot(df3_inact['hbd_count'], color='cyan', shade=True,Labe
l='Inactive')


# plt.vlines(x_median2, 0, y_median2,label='median_hum', color='r')
# plt.vlines(x_median, 0, y_median,label='median_ind')
plt.title("Num-Hydrogen Bond Donors distribution of Active and Inactive
 Flavor Molecules")
plt.xlabel("Num-Hydrogen Bond Donors",fontsize=14, fontweight='bold')
plt.ylabel("Density",fontsize=14, fontweight='bold')
#plt.gca().legend(('IndiGen nsSNPs(22 residues)','HUMSAVAR nsSNPs(76 re
sidues)'),loc="upper right")
plt.legend(loc="upper right")
plt.savefig('plot_density_hbd.png')
```



In [139]:
```
fig = plt.figure(figsize =(10,10))
plt.rcParams.update({'font.size': 14})
act=sns.kdeplot(df3_act['hba_count'], color='salmon', shade=True,Label=
'Active')
inact=sns.kdeplot(df3_inact['hba_count'], color='cyan', shade=True,Labe
l='Inactive')


# plt.vlines(x_median2, 0, y_median2,label='median_hum', color='r')
# plt.vlines(x_median, 0, y_median,label='median_ind')
plt.title("Num-Hydrogen Bond Acceptors distribution of Active and Inact
ive Flavor Molecules")
plt.xlabel("Num-Hydrogen Bond Acceptors",fontsize=14, fontweight='bold'
)
plt.ylabel("Density",fontsize=14, fontweight='bold')
#plt.gca().legend(('IndiGen nsSNPs(22 residues)','HUMSAVAR nsSNPs(76 re
sidues)'),loc="upper right")
plt.legend(loc="upper right")
plt.savefig('plot_density_hba.png')
```



Interpretation of Statistical Results

Box Plots

pIC50 values

Taking a look at pIC50 values, the actives and inactives displayed *statistically significant difference*, which is to be expected since threshold values (`IC50 < 1,000 nM = Actives while IC50 > 10,000 nM = Inactives` , corresponding to `pIC50 > 6 = Actives and pIC50 < 5 = Inactives`) were used to define actives and inactives.

Lipinski's descriptors

All of the Lipinski's descriptors except LogP exhibited *statistically significant difference* between the actives and inactives.

In [136]:
```
! zip -r results.zip . -i *.csv *.png
```

```
  adding: bioactivity_data_flavormolecules_actual_datapreprocessed_outp
ut2.csv (164 bytes security) (deflated 74%)
  adding: bioactivity_data_flavormolecules_actual_ouput1.csv (164 bytes
security) (deflated 85%)
  adding: bioactivity_data_flavormolecules_scraped_datapreprocessed_out
put2.csv (164 bytes security) (deflated 70%)
  adding: df2.csv (164 bytes security) (deflated 69%)
  adding: fdb scraped data/bioactivity_data_flavormolecules_scraped.csv
(164 bytes security) (deflated 84%)
  adding: fdb scraped data/bioactivity_data_flavormolecules_scraped_oup
ut1.csv (164 bytes security) (deflated 84%)
  adding: fdb scraped data/flavordb_molecules_scraped.csv (164 bytes se
curity) (deflated 72%)
  adding: fdb scraped data/oubch_to_chemblid.csv (164 bytes security)
(deflated 62%)
  adding: fdb scraped data/try.csv (164 bytes security) (deflated 64%)
  adding: fdb_classification_bioactivity_pIC50.csv (164 bytes security)
(deflated 69%)
  adding: fdb_molecules_22Nov.csv (164 bytes security) (deflated 73%)
```

```
  adding: fdb_natural_2254.csv (164 bytes security) (deflated 72%)
  adding: mannwhitneyu_hba_count.csv (164 bytes security) (deflated 1
0%)
  adding: mannwhitneyu_hbd_count.csv (164 bytes security) (deflated 9%)
  adding: mannwhitneyu_molecular_weight.csv (164 bytes security) (defla
ted 10%)
  adding: mannwhitneyu_pIC50.csv (164 bytes security) (deflated 9%)
  adding: mannwhitneyu_xlogp.csv (164 bytes security) (deflated 9%)
  adding: plot_bioactivity_class.png (164 bytes security) (deflated 2
3%)
  adding: plot_LogP.png (164 bytes security) (deflated 19%)
  adding: plot_MW.png (164 bytes security) (deflated 19%)
  adding: plot_MW_vs_LogP.png (164 bytes security) (deflated 3%)
  adding: plot_NumHAcceptors.png (164 bytes security) (deflated 19%)
  adding: plot_NumHDonors.png (164 bytes security) (deflated 19%)
  adding: pubchem_flavordb.csv (164 bytes security) (deflated 62%)
  adding: pubchem_tochembl.csv (164 bytes security) (deflated 62%)
  adding: till_now_bioactivity.csv (164 bytes security) (deflated 93%)
  adding: till_now_bioactivity_2.csv (164 bytes security) (deflated 8
9%)
  adding: till_now_bioactivity_3.csv (164 bytes security) (deflated 8
8%)
```

In [ ]: