# Task objective: To cluster the sample into "site" and "year" based on N concentrations and date

In [1]:
```
%matplotlib inline
import matplotlib.pyplot as plt
import seaborn as sns; sns.set()  # for plot styling
import numpy as np
import pandas as pd
```

In [2]:
```
data = pd.read_excel('BHL_kmeans.xlsx', sheet_name='Data_by_sub')
data.head()
```

Out[2]:

| | Site ID | Site No. | Sample date | Time stamp | Sample type | Flow (cms) | DRP (mg P/L) | TP (mg P/L) | TSS (mg/L) | VSS (mg/L) | ... | Unna |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| **0** | Sub11 | 11 | 2016-03-31 | 42460 | Base | 0.025511 | 0.001 | 0.293 | 18.666667 | 14.000000 | ... | |
| **1** | Sub11 | 11 | 2016-04-14 | 42474 | Base | 0.041794 | 0.013 | 0.040 | 2.000000 | 3.333333 | ... | |
| **2** | Sub11 | 11 | 2016-04-28 | 42488 | Base | 0.078278 | 0.001 | 0.129 | 39.333333 | 31.333333 | ... | |
| **3** | Sub11 | 11 | 2016-05-17 | 42507 | Base | 0.064980 | 0.001 | 0.177 | 63.333333 | 37.333333 | ... | |
| **4** | Sub11 | 11 | 2016-05-17 | 42507 | Base | 0.064980 | 0.001 | 0.177 | 63.333333 | 37.333333 | ... | |

5 rows × 32 columns

In [3]:
```
X = data[['Time stamp', 'Nitrate (mg/L)']]
X.head()
```

Out[3]:

| | Time stamp | Nitrate (mg/L) |
|---|---|---|
| **0** | 42460 | 35.3001 |
| **1** | 42474 | 31.7656 |
| **2** | 42488 | 30.5188 |
| **3** | 42507 | 22.9285 |
| **4** | 42507 | 22.9285 |

In [4]:
```
y_true = data['Site No.']
y_true = y_true.to_numpy()
print(type(y_true))
```

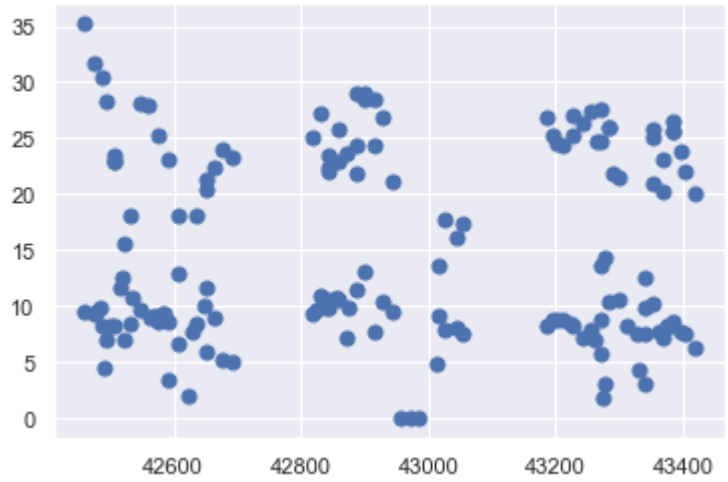
```
<class 'numpy.ndarray'>
```

In [5]:
```
X = X.to_numpy()
print(type(X))
print(X.shape)
```

```
<class 'numpy.ndarray'>
(156, 2)
```

In [6]:
```
plt.scatter(X[:, 0], X[:, 1], s=50)
```

Out[6]:
```
<matplotlib.collections.PathCollection at 0x2313b813a58>
```

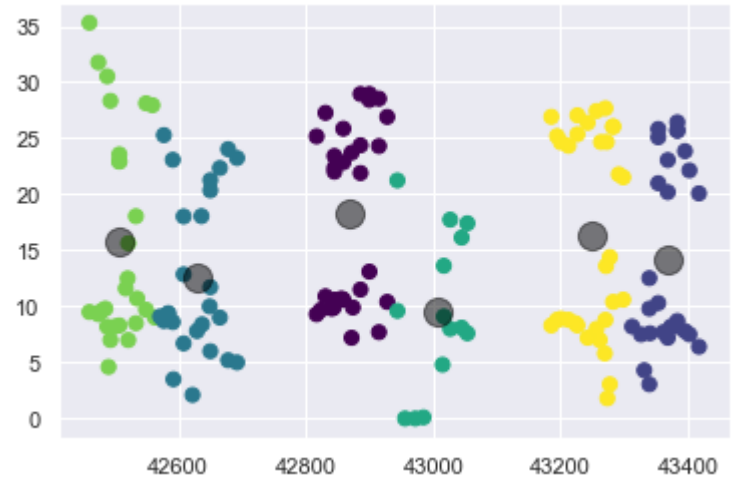



In [23]:
```
from sklearn.cluster import KMeans
kmeans = KMeans(n_clusters=6)
kmeans.fit(X)
y_kmeans = kmeans.predict(X)
```

In [30]:
```
print(y_kmeans)
```

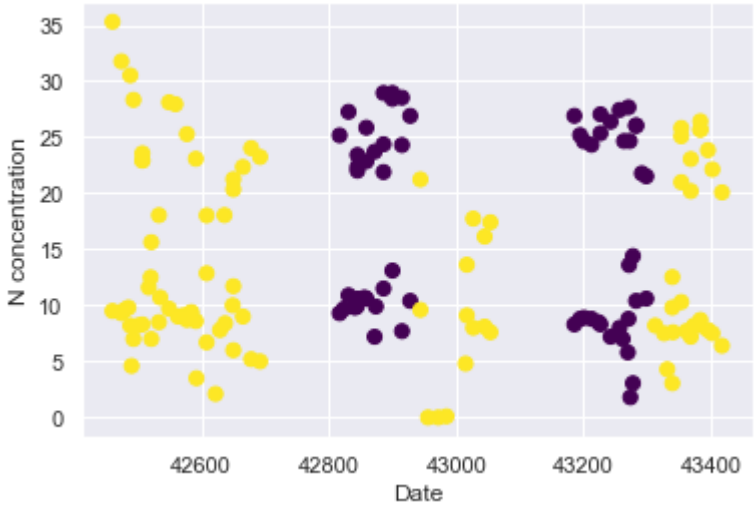
```
[4 4 4 4 4 4 4 4 4 2 2 2 2 2 2 2 0 0 0 0 0 0 0 0 0 0 0 0 3 3 3 3 5 5 5 5 5
 5 5 5 5 5 5 5 5 1 1 1 1 1 1 1 4 4 2 2 2 2 0 0 0 0 3 5 5 5 5 1 1 1 1 1 1 4 4
 4 4 4 4 4 4 2 2 2 2 2 2 2 2 0 0 0 0 0 0 0 0 0 3 3 3 3 3 3 3 3 5 5 5 5 5
 5 5 5 5 5 5 1 1 1 1 1 1 1 1 1 4 4 4 4 4 4 4 2 2 2 2 2 2 2 0 0 0 0 0 3 5 5
 5 5 5 1 1 1 1 1]
```

In [31]:
```
# plots the simulated dataset, colored by its cluster number
plt.scatter(X[:, 0], X[:, 1], c=y_kmeans, s=50, cmap='viridis')

# plot the cluster centers
centers = kmeans.cluster_centers_
plt.scatter(centers[:, 0], centers[:, 1], c='black', s=200, alpha=0.5);
```

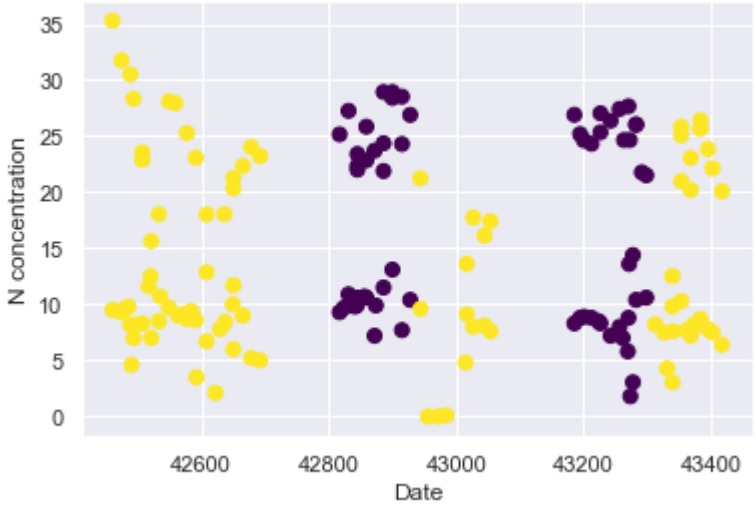


In [29]:
```
from sklearn.metrics import pairwise_distances_argmin
from scipy.stats import mode
from sklearn.metrics import accuracy_score
clusters = kmeans.fit_predict(X)

for a in range(0,7):
    print('rseed = ', a)
    def find_clusters(X, n_clusters, rseed=a):
        # 1. Randomly choose clusters
        rng = np.random.RandomState(rseed)
        i = rng.permutation(X.shape[0])[:n_clusters]
        centers = X[i]

        while True:
            # 2a. Assign labels based on closest center
            labels = pairwise_distances_argmin(X, centers)

            # 2b. Find new centers from means of points
            new_centers = np.array([X[labels == i].mean(0)
                                    for i in range(n_clusters)])

            # 2c. Check for convergence
            if np.all(centers == new_centers):
                break
            centers = new_centers

        return centers, labels

    centers, labels = find_clusters(X, 6)
    labels = np.zeros_like(clusters)
    for i in range(10):
        mask = (clusters == i)
        labels[mask] = mode(y_true[mask])[0] #Takes the mode of the true label
    plt.scatter(X[:, 0], X[:, 1], c=labels, s=50, cmap='viridis');
    plt.xlabel('Date')
    plt.ylabel('N concentration')
    plt.show()
    print('accuracy for fig above = ', accuracy_score(y_true, labels))
```

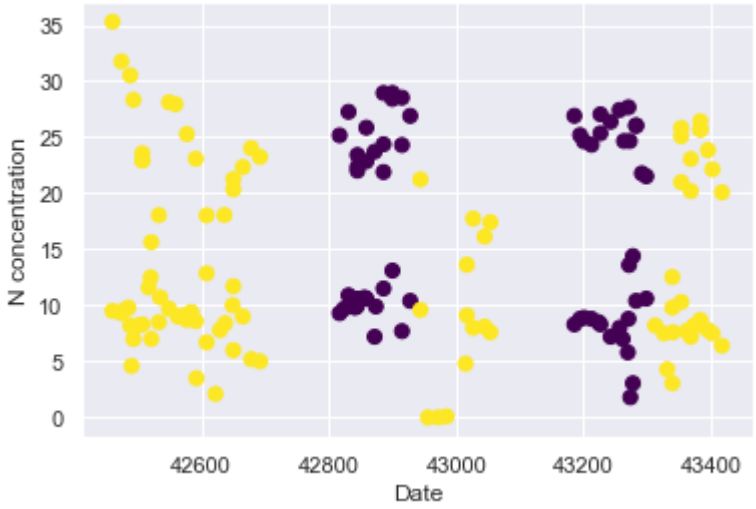
```
rseed =  0
```



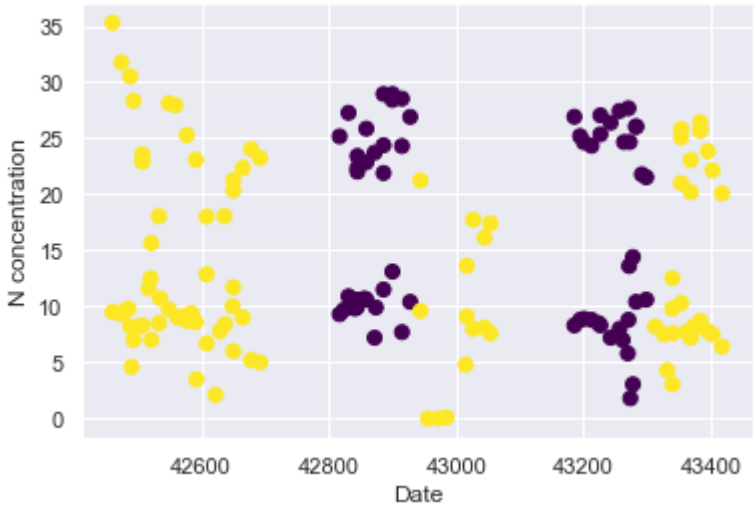

```
accuracy for fig above =  0.5512820512820513
rseed =  1
```



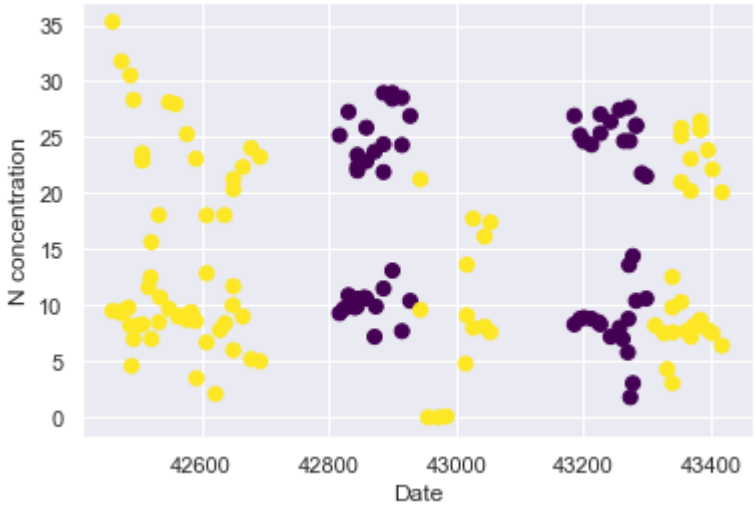

```
accuracy for fig above =  0.5512820512820513
rseed =  2
```



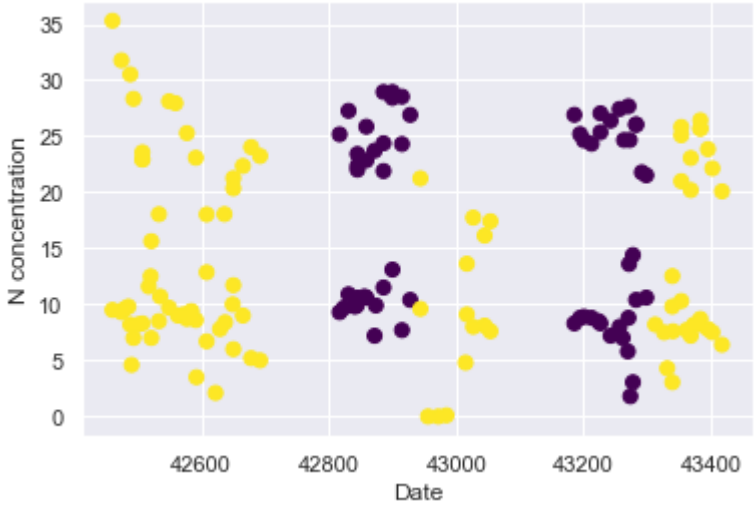
```
accuracy for fig above =  0.5512820512820513
rseed =  3
```



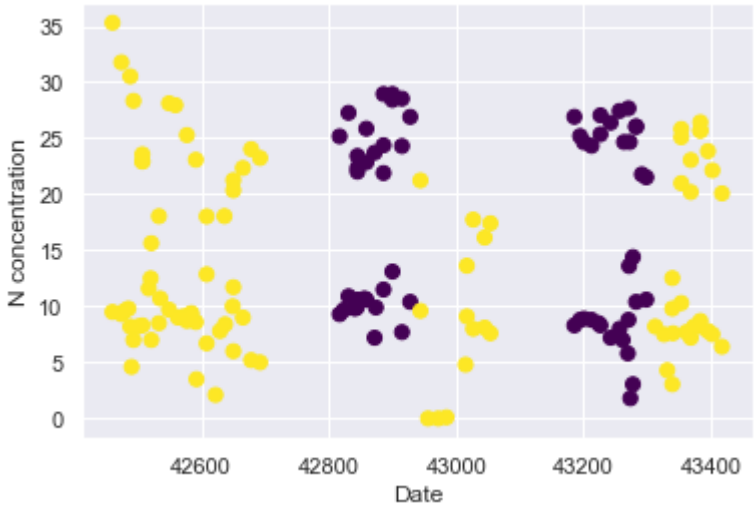

```
accuracy for fig above =  0.5512820512820513
rseed =  4
```




```
accuracy for fig above =  0.5512820512820513
rseed =  5
```




```
accuracy for fig above =  0.5512820512820513
rseed =  6
```



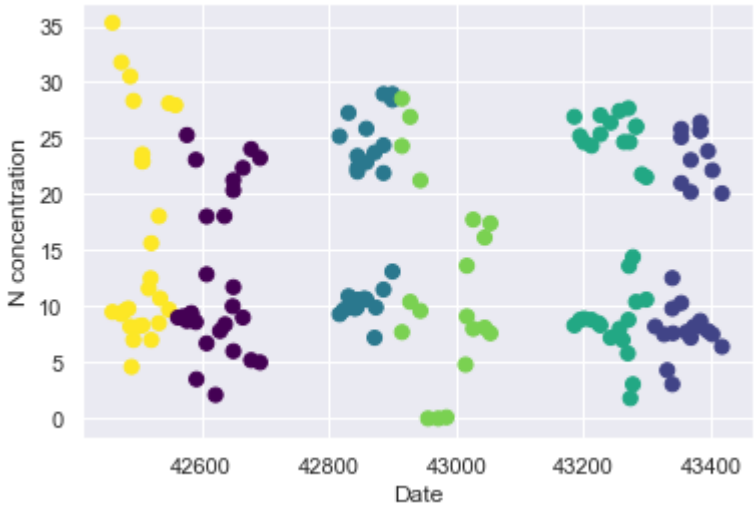

```
accuracy for fig above =  0.5512820512820513
```

# Does not cluster properly; Try SpectralClustering approach

In [27]:
```
from sklearn.cluster import SpectralClustering
model = SpectralClustering(n_clusters=6, affinity='nearest_neighbors',
                           assign_labels='kmeans')
labels = model.fit_predict(X)
plt.scatter(X[:, 0], X[:, 1], c=labels,
            s=50, cmap='viridis');
plt.xlabel('Date')
plt.ylabel('N concentration')
```

```
C:\ProgramData\Anaconda3\lib\site-packages\sklearn\manifold\spectral_embeddin
g_.py:237: UserWarning: Graph is not fully connected, spectral embedding may
not work as expected.
  warnings.warn("Graph is not fully connected, spectral embedding"
```

Out[27]:
```
Text(0, 0.5, 'N concentration')
```




## Spectral clustering did not seem to perform any better .

### The original kmeans were only able to achieve 55% accuracy (changing rseed also did not appear to improve the prediction). Clustering might not be suitable for this task or additional transformation is needed to segregate the data.

In [ ]:
```
```