WORKING WITH NANOPARTICLE TOXICITY DATASET IN PYTHON

PROGRAMMING FOR CHEMISTS

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OUTLINE

GitHub

Process of work

Attempts

Program

Conclusions

GITHUB

WE WON IT.

BUT NOT FOR THE FIRST ATTEMPT

Belvglin Создано в Colab — a3b4da9 · 1 minute ago — **18 Commits**

Nanoparticle-Toxicity-Dataset	alo	2 weeks ago
Kirill_Nanopart_tox_dataset.ipynb	alo	51 minutes ago
Nanoparticles_Galya.ipynb	Создано в Colab	1 minute ago
README.md	first commit	2 weeks ago
aboba.txt	alo	2 weeks ago
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StuffWeDid Kirill
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Languages

PROCESS OF WORK

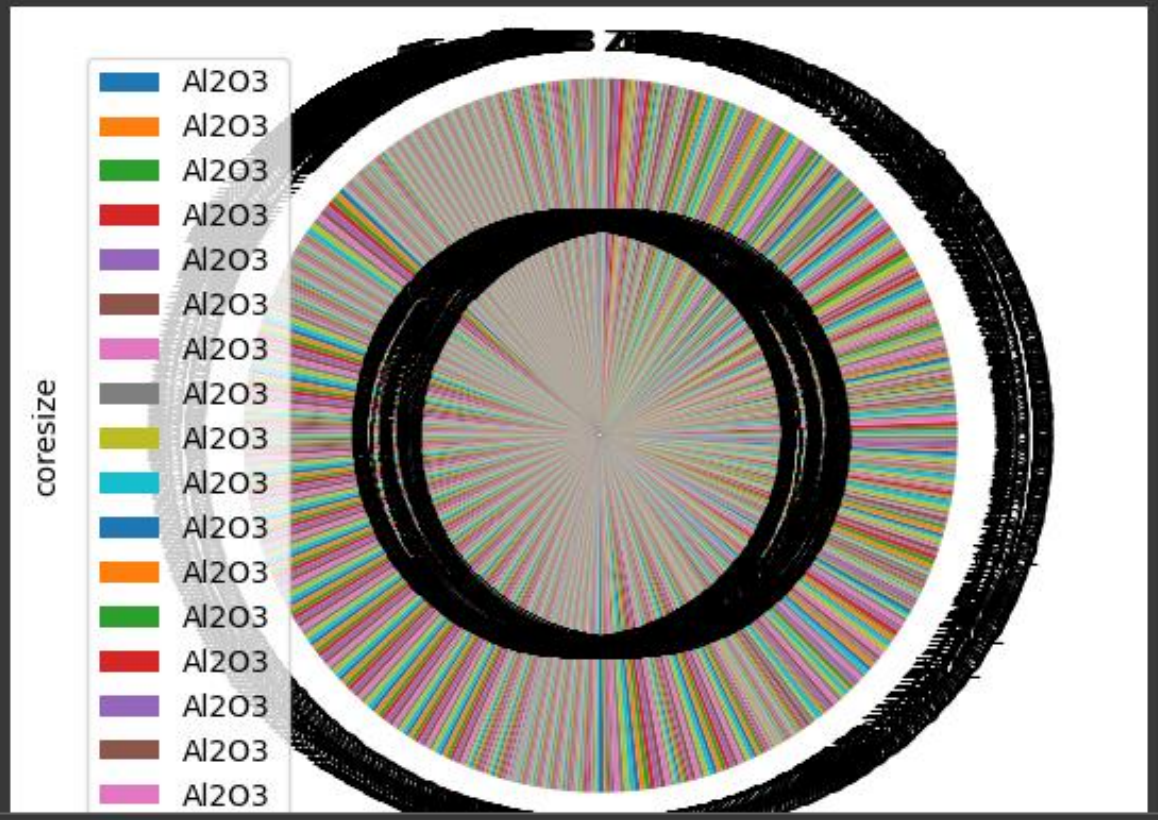
- Choosing a database
- Fighting with GitHub and GitBush: discovered tokens
- Structuring the Dataset
- Spending a lot of hours on finding the best relations of parameters and matching them to the conscious result
- Looking through a lot of courses and papers
- Finally got it.

BUT NOT WITHOUT FAILS

YES, WE ARE CHEMIST, BE TOLERANT

WE GOT THIS...

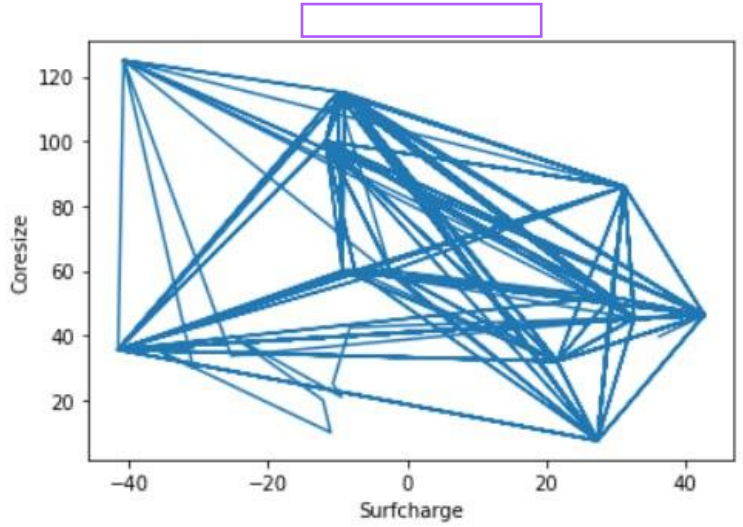
```
import pandas as pd
cvsData = pd.read_csv("nanotox_dataset.csv")
cvsData.plot.pie(y='coresize', labels=cvsData['NPs'], autopct='%1.1f%%', startangle=90)
plt.axis('equal')
plt.show()
```

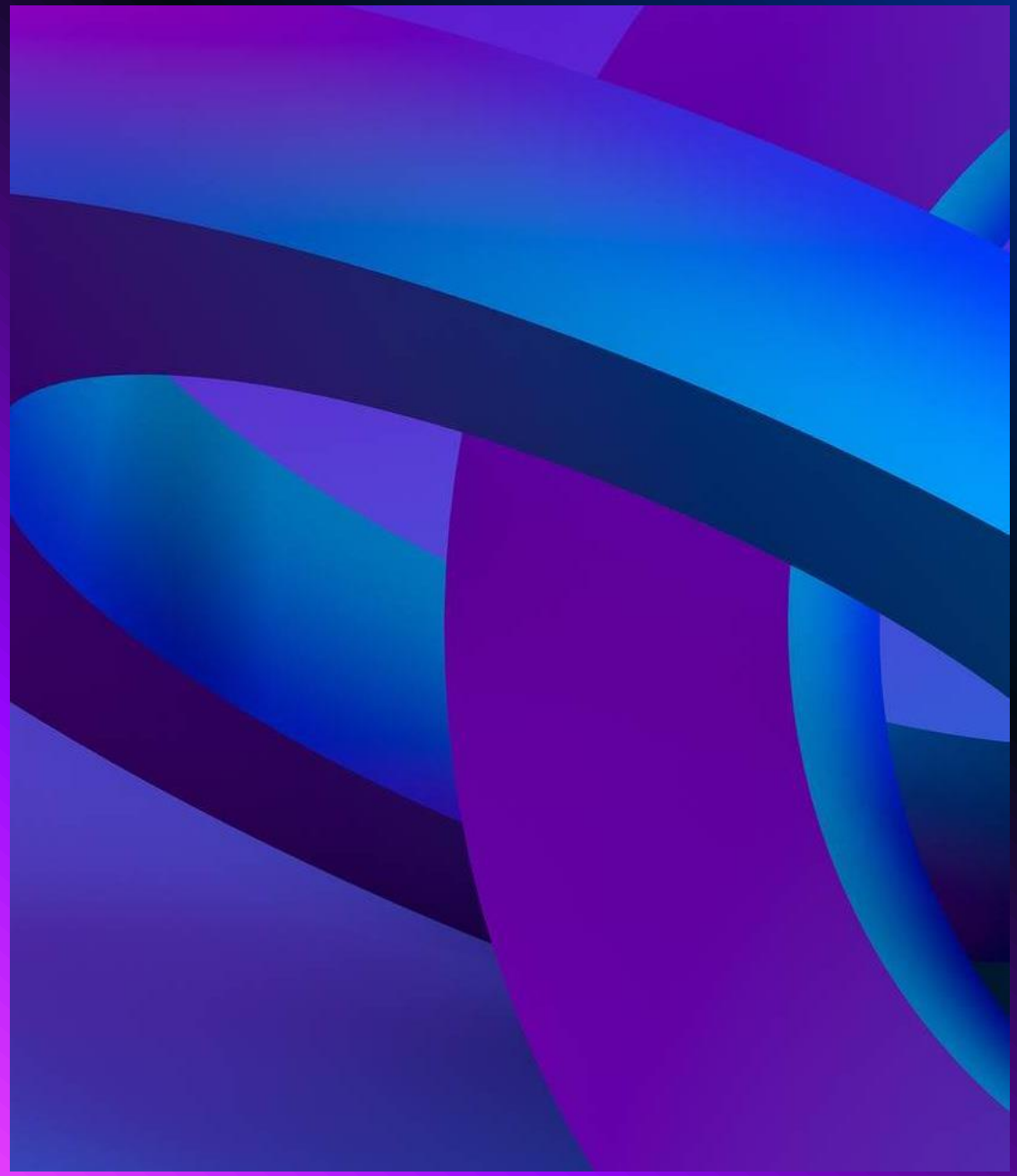


AND THIS...

Ввод [3]:

```
import matplotlib.pyplot as plt
import numpy as np
import csv

X = []
Y = []

with open('nanotox_dataset.csv', 'r', encoding='utf-8') as datafile:
    plotting = csv.reader(datafile, delimiter=',')
    for ROWS in plotting:
        X.append(float(ROWS[3]))
        Y.append(float(ROWS[1]))
plt.plot(X, Y)
plt.title(
plt.xlabel('Surfcharge')
plt.ylabel('Coresize')
plt.show()
```



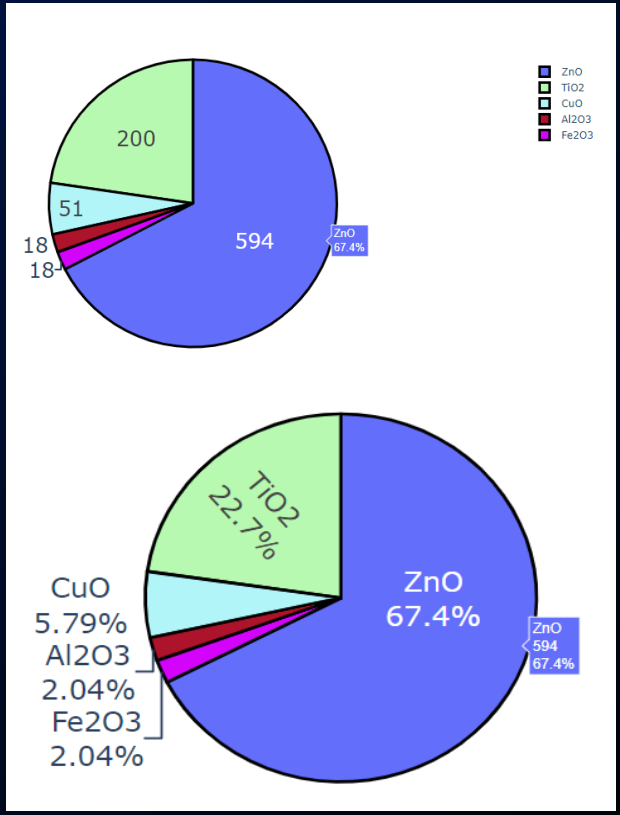


FIRST OF ALL WE FIND OUT ALL RELATIONS WE COULD

It was challenging due to:

- Experimental type of data
- Abundance of source data and only one column with results
- In addition this one parameter was uncountable and has data like ‘yes/no’

WE STRUCTURED OUR DATASET TO GET RID OF PARAMETERS WE DON'T NEED




```
# Sorting by column 'Name of column'
cvsData.sort_values(by=['hydrosize','class'],ascending=[False, False])
cvsData.drop("Ec", axis = 1) # Удалить переменную из фрейма данных
#Параметр «axis» в Pandas определяет направление выполнения операции:
#Движение вниз по строкам (по умолчанию) соответствует axis=0, что эквивалентно операциям агрега
#Движение вбок по столбцам соответствует axis=1, что эквивалентно операциям агрегации данных по
```

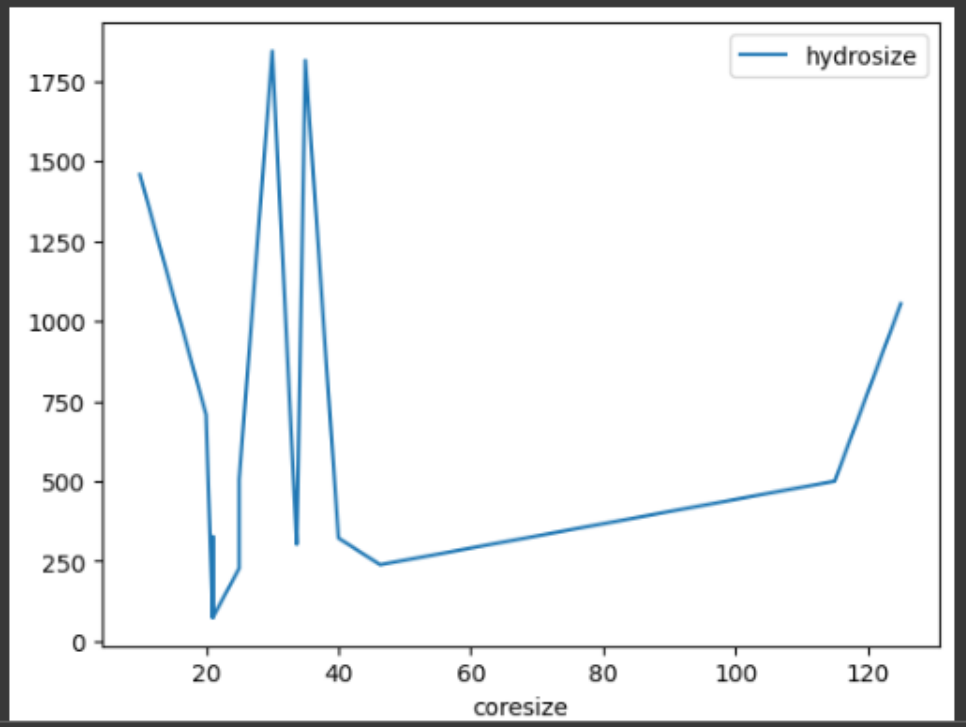
	NPs	coresize	hydrosize	surfcharge	surfarea	Expotime	dosage	e	NOxygen	class
0	Al2O3	39.7	267.0	36.3	64.7	24	0.001	1.61	3	nonToxic
1	Al2O3	39.7	267.0	36.3	64.7	24	0.010	1.61	3	nonToxic
2	Al2O3	39.7	267.0	36.3	64.7	24	0.100	1.61	3	nonToxic
3	Al2O3	39.7	267.0	36.3	64.7	24	1.000	1.61	3	nonToxic
4	Al2O3	39.7	267.0	36.3	64.7	24	5.000	1.61	3	nonToxic
...	...	...	...	...	...	...	...	...	...	...
876	ZnO	45.3	310.0	32.7	21.3	24	20.000	1.65	1	Toxic
877	ZnO	32.0	1093.0	21.6	37.0	24	25.000	1.65	1	Toxic
878	ZnO	46.3	239.0	42.8	24.1	12	100.000	1.90	1	Toxic

```
import plotly as py
import plotly.graph_objs as go
import numpy as np
groups = ['Al2O3', 'Fe2O3', 'TiO2','CuO','ZnO']
amount = [18,18,200,51,594]
colors = ['#ad132a', '#d303fc', '#b7f9b1', '#b1f5f9']

trace = go.Pie(labels=groups, values=amount,
               hoverinfo='label+percent', textinfo='value',
               textfont=dict(size=25),
               marker=dict(colors=colors,
                           line=dict(color='#000000', width=3)))
from plotly.offline import iplot
iplot([trace])
```

SO AT FIRST WE JUST DRAW SOME GRAPHS

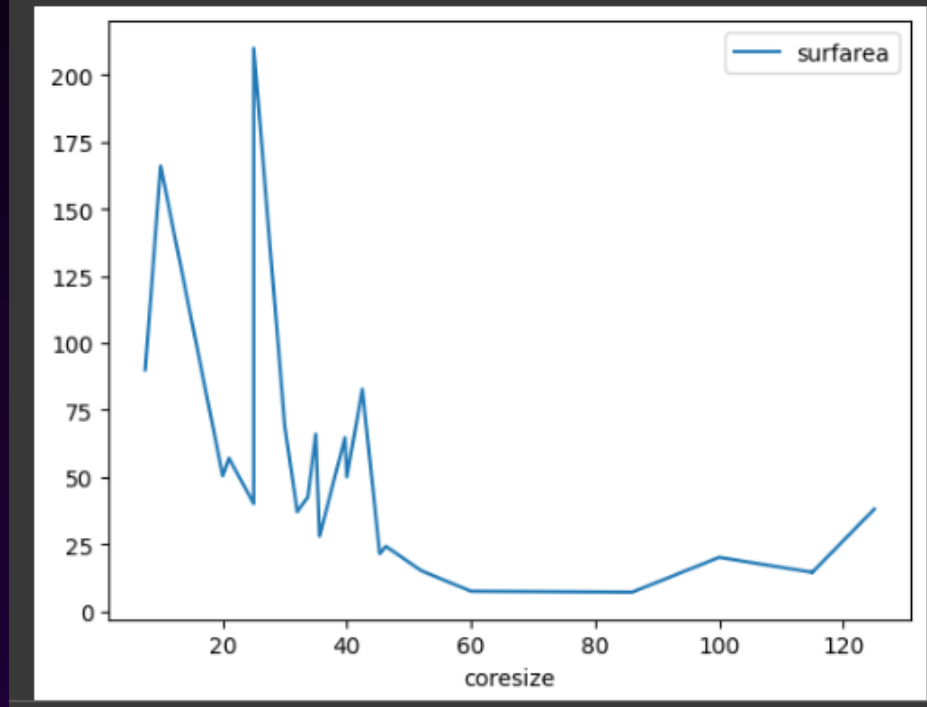
```
data.sort_values(data.columns[1],inplace=True)
filtr_data = data[data['NPs'] == 'TiO2']
filtr_data.plot(x='coresize', y='hydrosize')
```

```
<Axes: xlabel='coresize'>
```



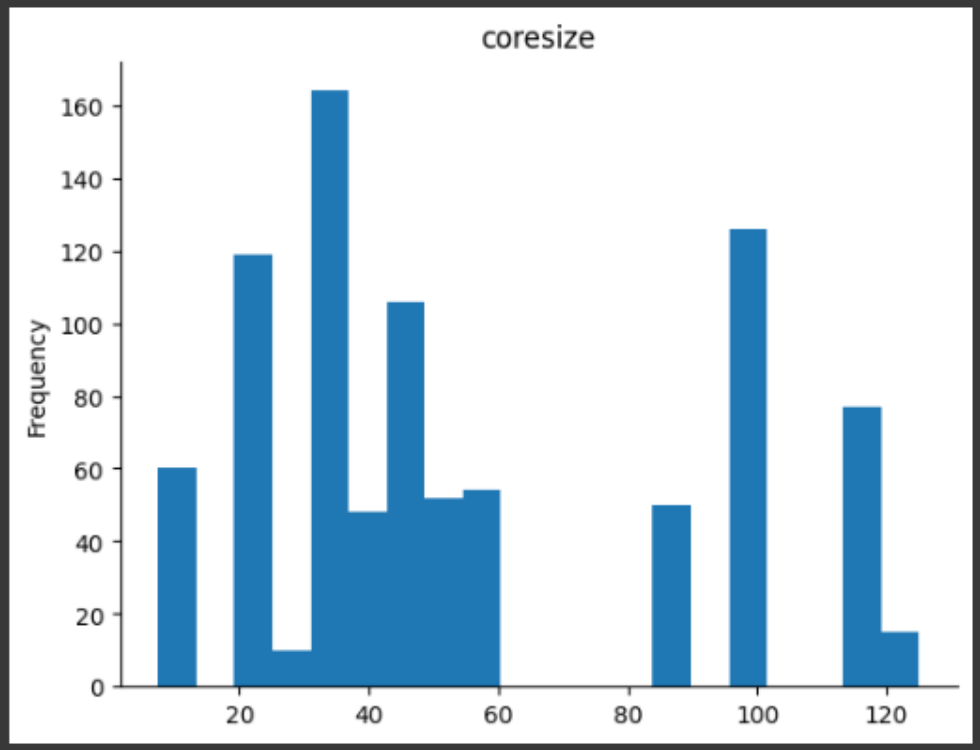

```
import pandas as pd
cvsData = pd.read_csv("nanotox_dataset.csv")
cvsData.sort_values(cvsData.columns[1],inplace=True)
cvsData.plot(x='coresize',y='surfarea')
```

```
<Axes: xlabel='coresize'>
```



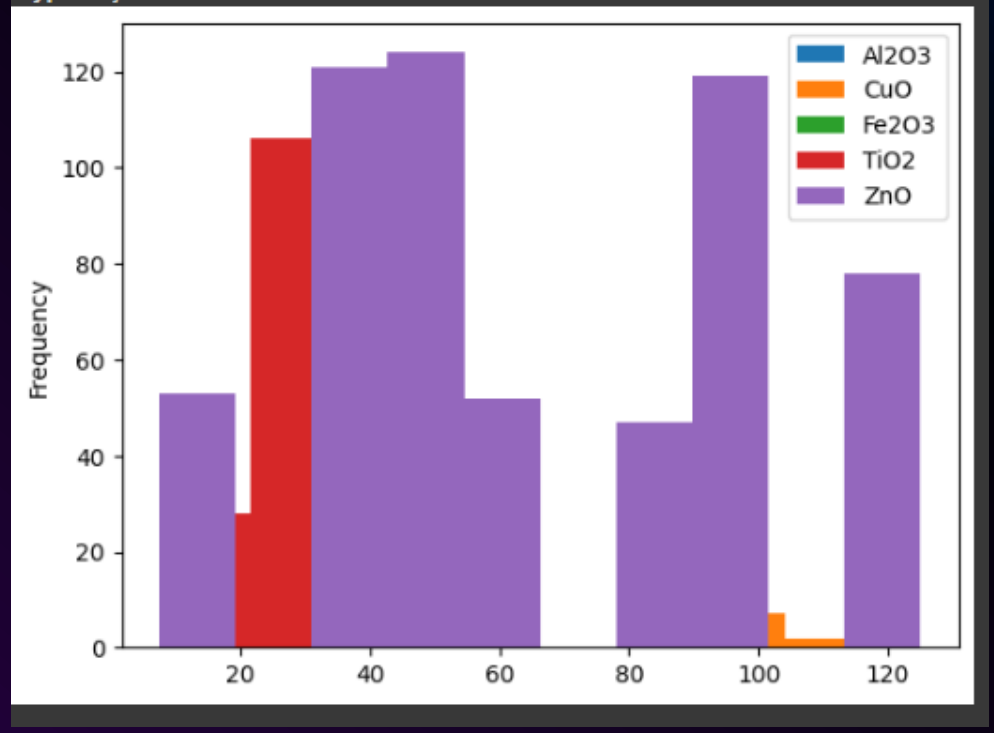
AND MORE

```
from matplotlib import pyplot as plt
df_12['coresize'].plot(kind='hist', bins=20, title='coresize')
plt.gca().spines[['top', 'right',]].set_visible(False)
```

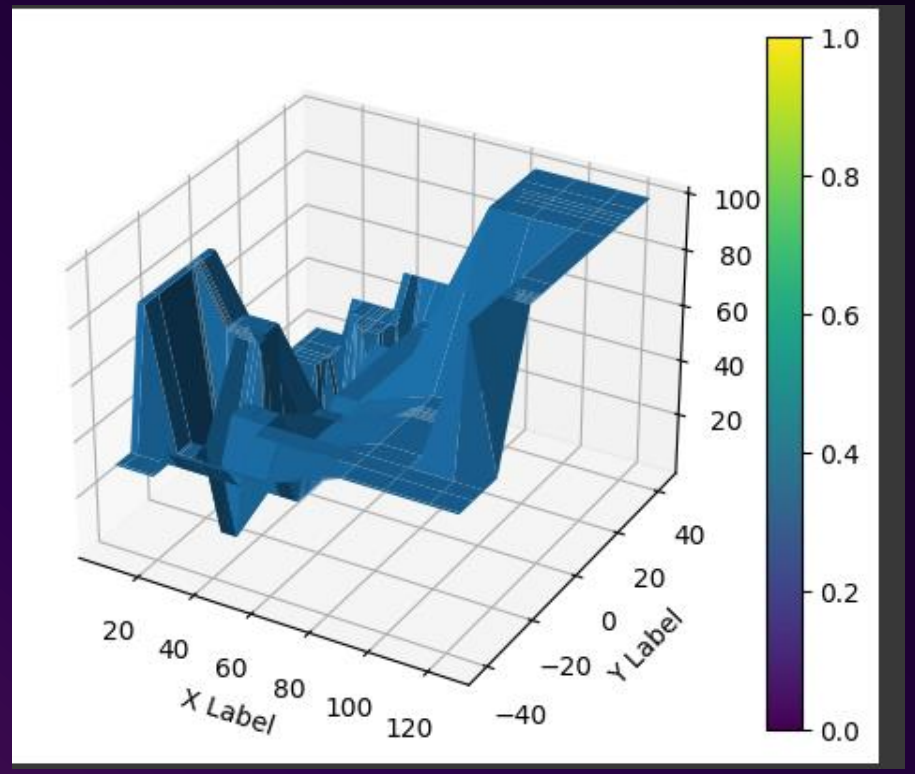



```
df.groupby('NPs')['coresize'].plot(kind='hist', legend = True)
```

```
dtype: object
```

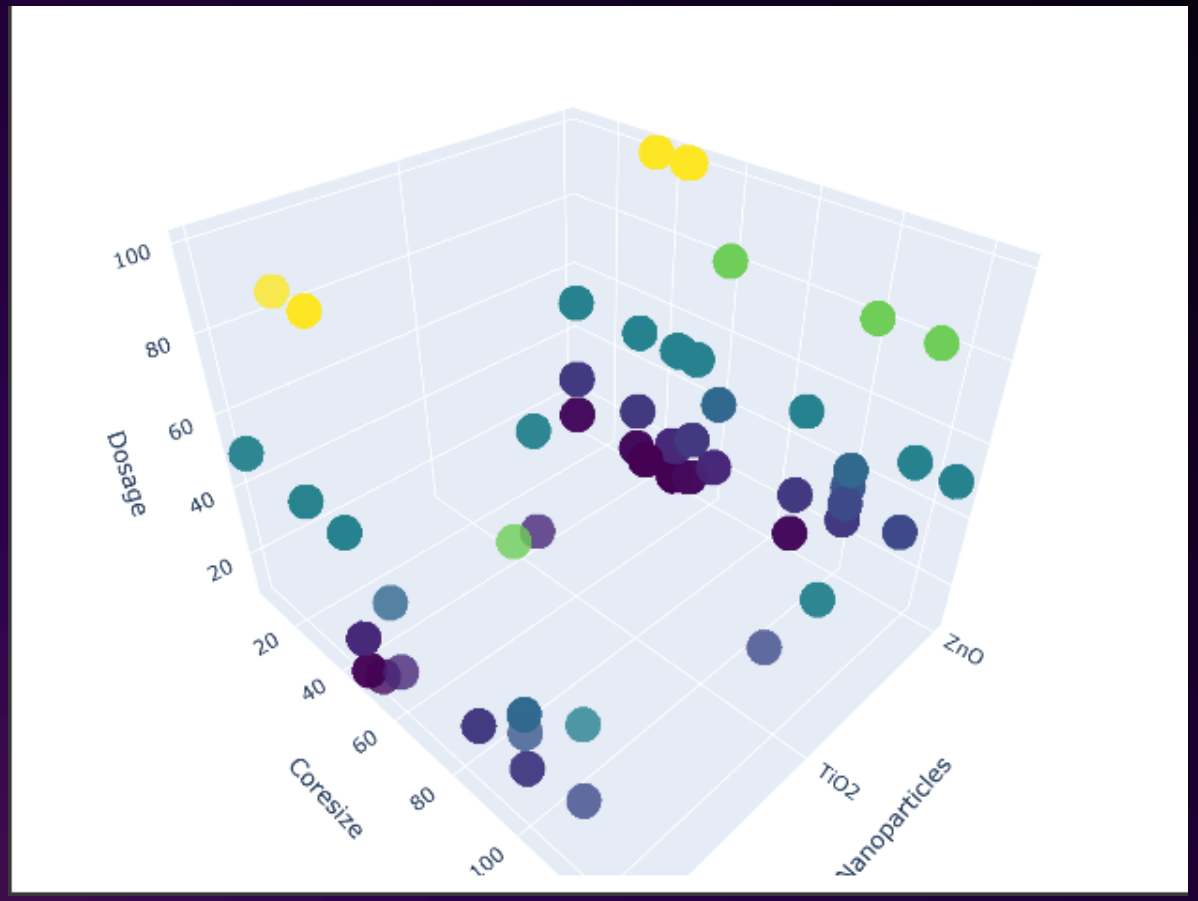


BUT WE UPGRADE OUR SKILL AND GOT THIS



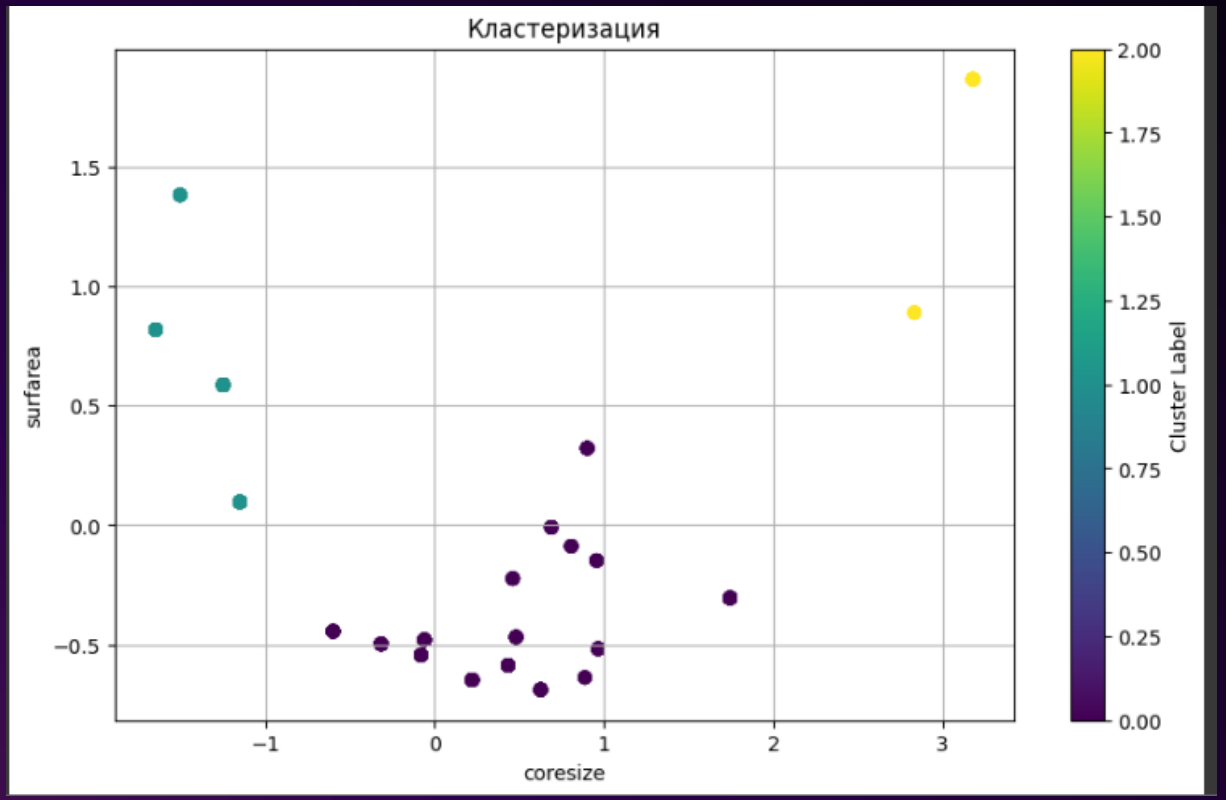

```python
x = data['coresize'].values
y = data['surfcharge'].values
z = data['dosage'].values

# Создание сетки
X = np.unique(xsurf)
Y = np.unique(ysurf)
X, Y = np.meshgrid(X, Y)

# Интерполяция Z значений
Z = griddata((xsurf, ysurf), z, (X, Y), method='nearest')

# Создание 3D графика
fig = plt.figure()
ax = fig.add_subplot(111, projection='3d')

# Построение поверхности
surf = ax.plot_surface(X, Y, Z)

# Добавление цветовой шкалы
fig.colorbar(surf)

# Добавление подписей
ax.set_xlabel('X Label')
ax.set_ylabel('Y Label')
ax.set_zlabel('Z Label')

# Отображение графика
plt.show()
```

AND ALSO THIS



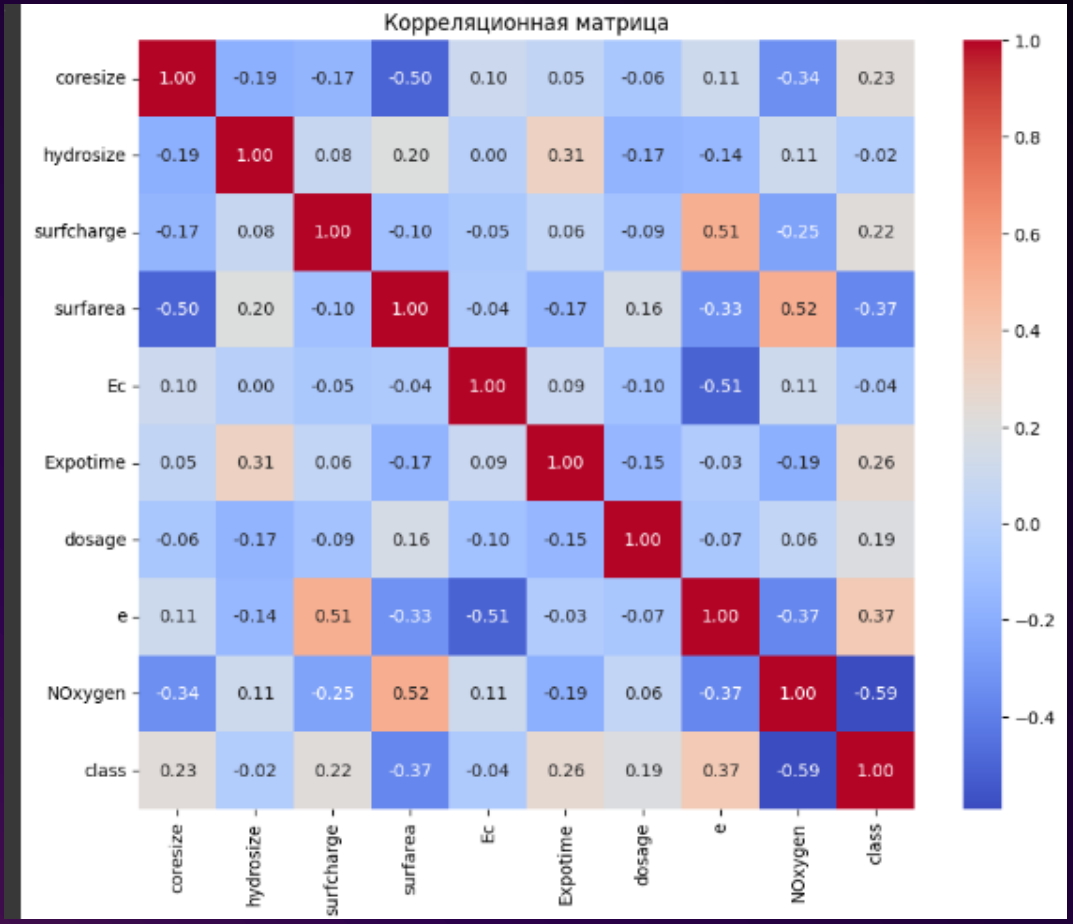

```
#Это 3д модель распределения токсичных частиц по размеру и до
x = df3['NPs']
y = df3['coresize']
z = df3['dosage']

trace2 = go.Scatter3d(
    x=x,
    y=y,
    z=z,
    mode='markers',
    marker=dict(
        size=12,
        color=z,
        colorscale='Viridis',
        opacity = 0.8))

data2 = [trace2]
fig2 = go.Figure(data=data2, layout=layout)
fig2.update_layout(scene = dict(
                    xaxis_title='Nanoparticles',
                    yaxis_title='Coresize',
                    zaxis_title='Dosage'),
                    width=700,
                    margin=dict(r=20, b=10, l=10, t=10))
iplot(fig2, filename='3d-plot')
```

WE ALSO MADE A FEW MORE THINGS



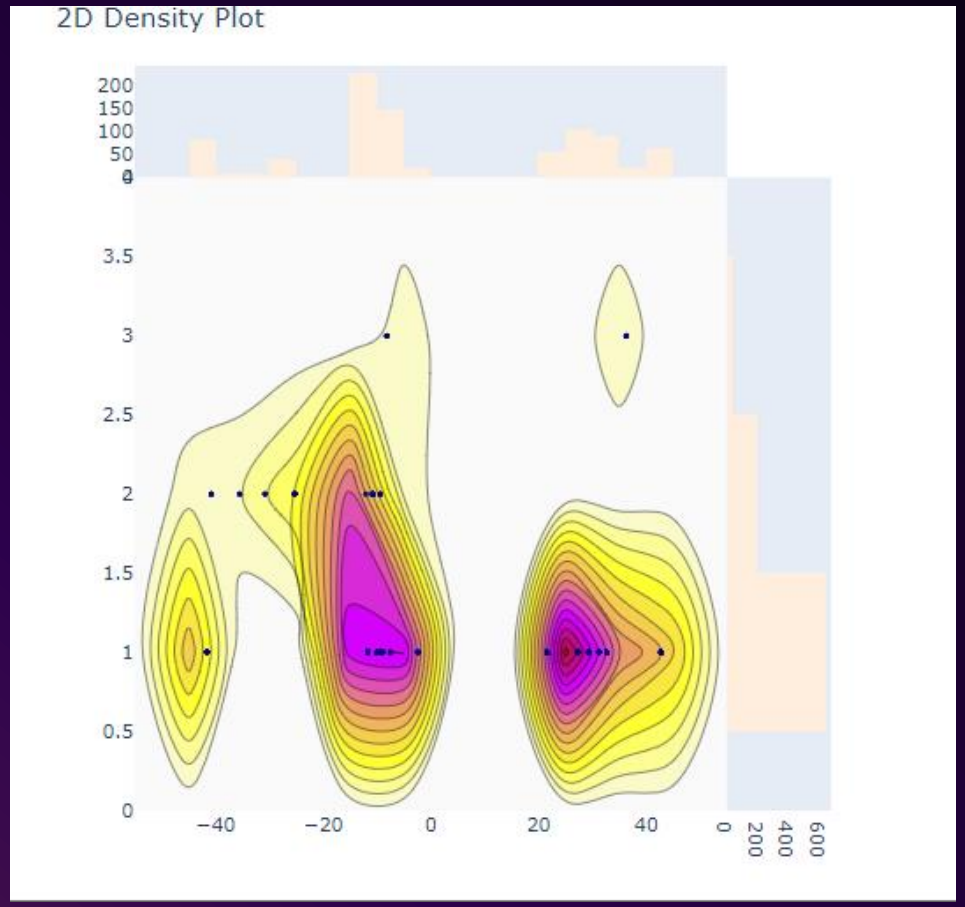

```python
# Шаг 1: Загрузка данных
df = pd.DataFrame(data, columns=['coresize', 'surfarea'])
# Шаг 2: Предобработка данных
# Удаляем строки с пропущенными значениями и выбираем только числовые колонки
data_cleaned = df.dropna()
X = data_cleaned.select_dtypes(include=[np.number])

# Нормализация данных
scaler = StandardScaler()
X_scaled = scaler.fit_transform(X)

# Шаг 3: Кластеризация K-means
kmeans = KMeans(n_clusters=3, random_state=10)  # Выберите количество кластеров
kmeans.fit(X_scaled)
labels = kmeans.labels_

# Шаг 4: Визуализация результатов
# Снижение размерности до 2D для визуализации
pca = PCA(n_components=2)
X_pca = pca.fit_transform(X_scaled)

plt.figure(figsize=(10, 6))
plt.scatter(X_pca[:, 0], X_pca[:, 1], c=labels, cmap='viridis', marker='o')
plt.title('Кластеризация')
plt.xlabel('coresize')
plt.ylabel('surfarea')
plt.colorbar(label='Cluster Label')
plt.grid()
plt.show()
```

WE ALSO MADE A FEW MORE THINGS



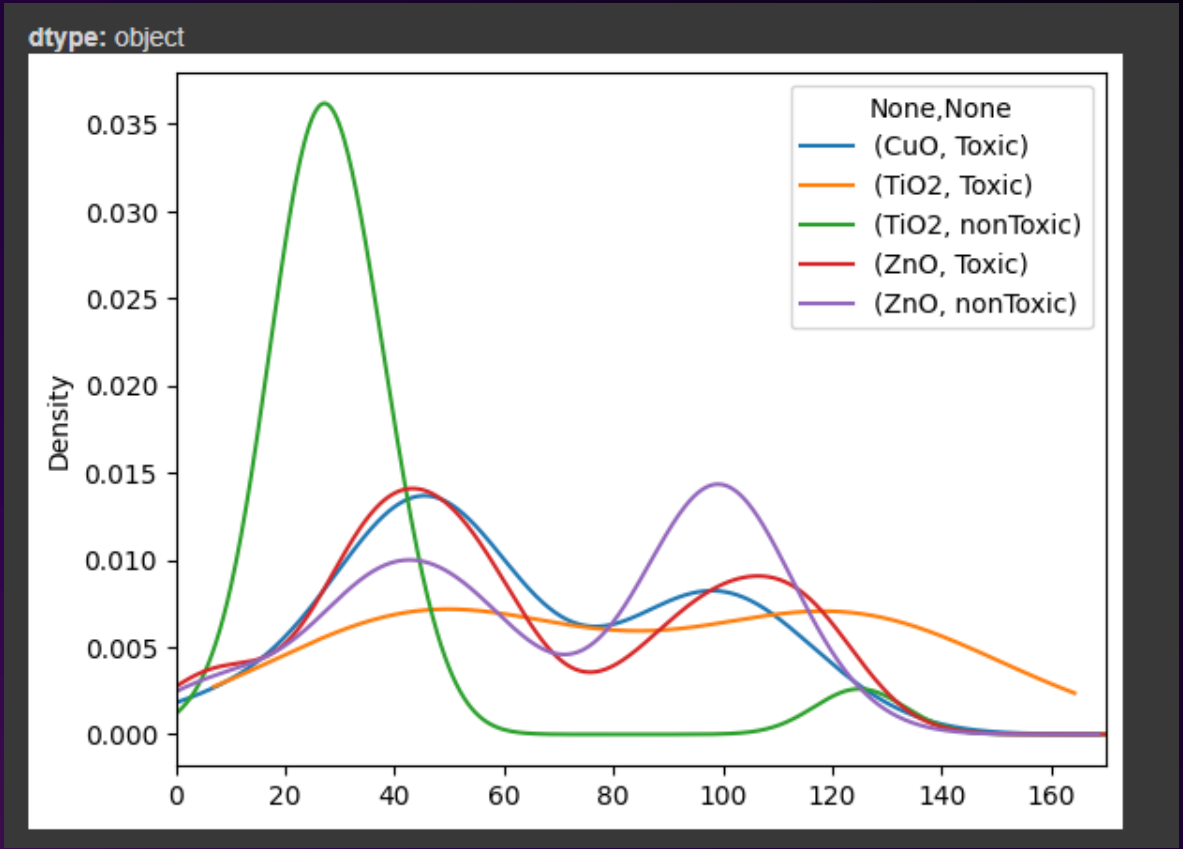

```python
# Шаг 2: Извлечение только числовых данных
numeric_data = data.select_dtypes(include=['number'])

# Шаг 3: Построение корреляционной матрицы
correlation_matrix = numeric_data.corr()

# Шаг 4: Визуализация корреляционной матрицы
plt.figure(figsize=(10, 8))  # Задаем размер графика
sns.heatmap(correlation_matrix, annot=True, cmap='coolwarm', fmt='.2f',
            xticklabels=correlation_matrix.columns,
            yticklabels=correlation_matrix.index)
plt.title('Корреляционная матрица')
plt.show()
```

WHAT ABOUT MORE SPECIFIC INFORMATION?




```
#здесь представлена плотность распределения по заряду поверхности и количеству атомов кислорода
import plotly.figure_factory as ff
x = df['surfcharge']
y = df['NOxygen']
colorscale = ['#ad132a', '#d303fc', 'rgb(236,158,105)', (1,1,0.2), (0.98,0.98,0.98)]
fig1 = ff.create_2d_density(
    x,y,colorscale=colorscale,
    hist_color='rgb(255,237,222)', point_size=3)

iplot(fig1, filename='histogram_subplots')
```

TOXICITY



- `df2.groupby(['NPs','class'])['coresize'].plot(kind='kde', xlim=[0,170], legend = True)`

THANKS FOR YOUR ATTENTION

(We really did our best)