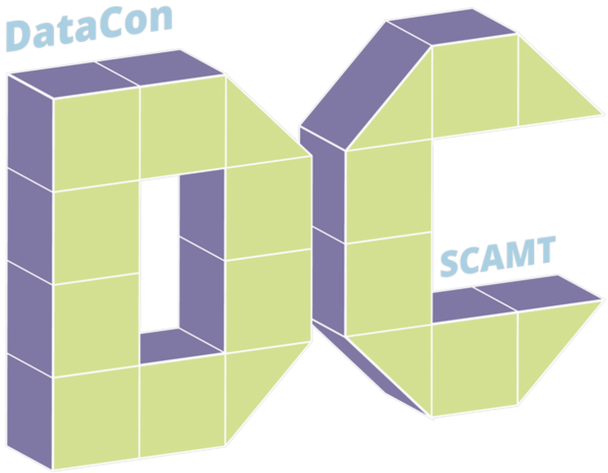
GEEK BATTLE

Предсказание токсичности наноматериалов.

Создание модели для предсказания свойств наночастиц: предсказание cell viability.



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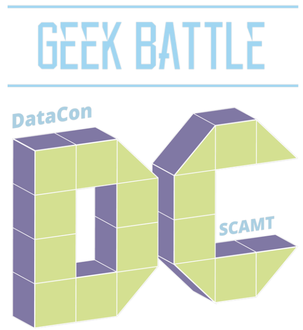
Валерий Древлянский.

План работы

1. Установка библиотек
2. Импорт данных
3. Предобработка данных
4. Создание единой базы данных
5. Анализ
6. Модели
7. Вывод



1. Установка библиотек

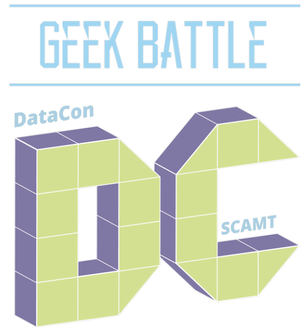
Тут все понятно и очевидно..

```
import pandas as pd
import numpy as np
import matplotlib.pyplot as plt
import seaborn as sns


from sklearn.model_selection import GridSearchCV
#from catboost import CatBoostClassifier
from sklearn.model_selection import train_test_split

import sklearn
from sklearn.ensemble import RandomForestRegressor
from sklearn import preprocessing
```

2. Импорт данных

Что мы имеем: 5 таблиц с **разным** набором признаков.

Необходимо переименовать признаки в каждом из DataFrame's и объединить их (получение уникальных значений и создание единой БД).



3.1. Предобработка данных

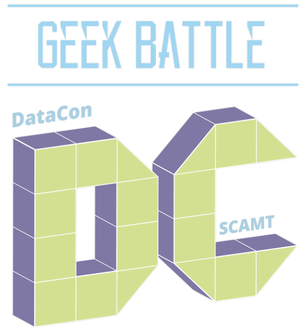
Database_1 :

```
<class 'pandas.core.frame.DataFrame'>
RangeIndex: 494 entries, 0 to 493
Data columns (total 21 columns):
 #   Column              Non-Null Count  Dtype
---  ------              --------------  -----
 0   material            494 non-null    object
 1   elements            494 non-null    object
 2   electronegativity   493 non-null    float64
 3   ionic_radius        493 non-null    float64
 4   core_size           494 non-null    float64
 5   size_in_water       493 non-null    float64
 6   surface_charge      494 non-null    float64
 7   surface_area        493 non-null    float64
 8   cell_type           494 non-null    int64
 9   concentration       494 non-null    float64
 10  number_of_atoms     494 non-null    int64
 11  mw                  493 non-null    float64
 12  tps                 494 non-null    float64
 13  a                   493 non-null    float64
 14  b                   494 non-null    float64
 15  c                   493 non-null    float64
 16  alpha               494 non-null    int64
 17  beta                494 non-null    float64
 18  gama                494 non-null    int64
 19  density             494 non-null    float64
 20  viability           494 non-null    float64
dtypes: float64(15), int64(4), object(2)
memory usage: 81.2+ KB
None
['CuO' 'ZnO' 'Mn2O3' 'CoO' 'CeO2' 'Fe2O3' 'Gd2O3' 'HfO2' 'In2O3' 'La2O3'
 'NiO' 'Sb2O3' 'SiO2' 'Al2O3']
['Cu' 'Zn' 'Mn' 'Co' 'cobalt' 'Ce' 'Fe' 'Gd' 'Hf' 'In' 'La' 'Ni' 'Sb' 'Si'
 'Al' 'Iron']
```

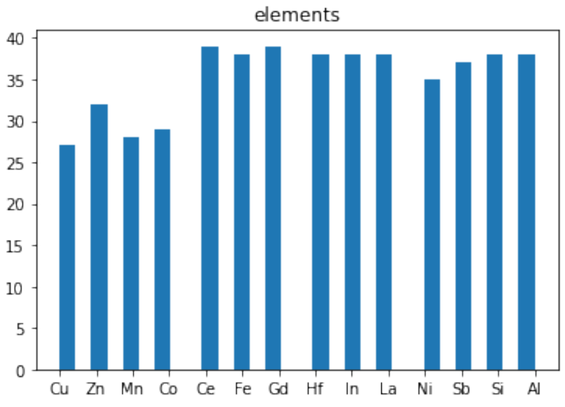
В 1 таблице (*Database_1*) все материалы-***неорганические***.

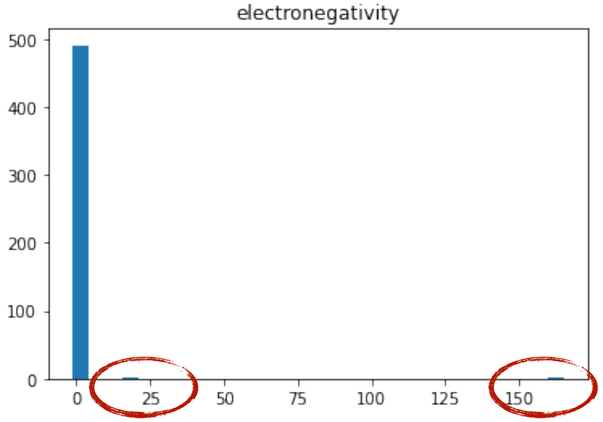
Создадим соответствующий признак.

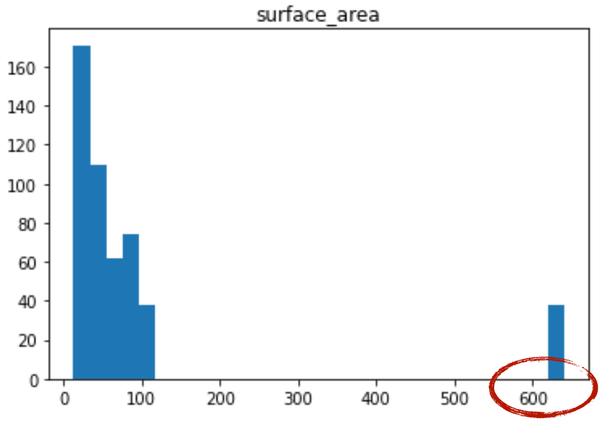
Большинство признаков - числовые. Необходимо посмотреть их распределение.

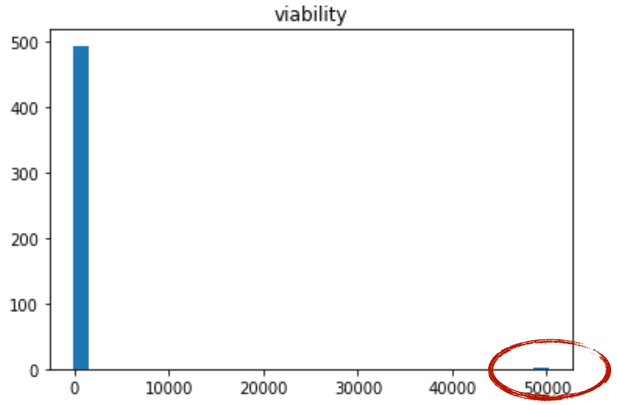


3.1. Предобработка данных



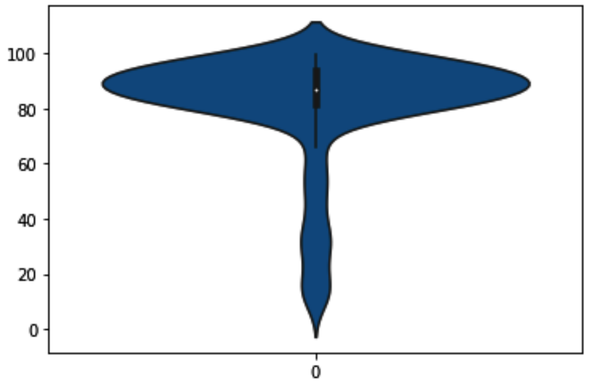




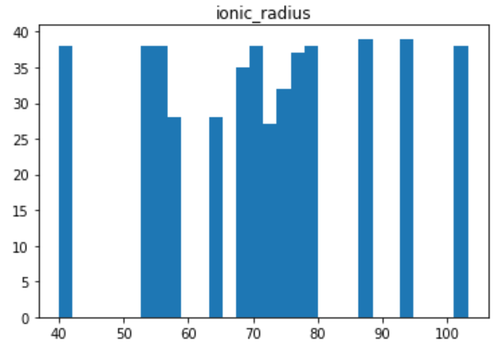


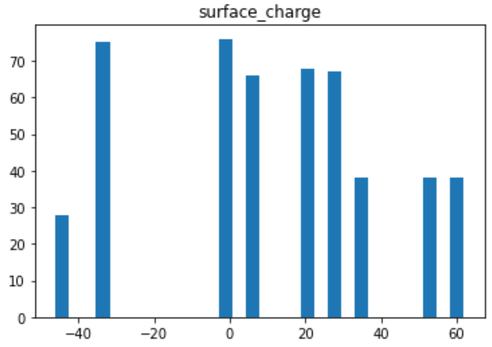

```
#Viability > 0
db_1.viability = db_1.viability[db_1['viability']<10000]
db_1.viability = db_1.viability.abs()
sns.violinplot(data=db_1.viability)
```

```
<AxesSubplot:>
```



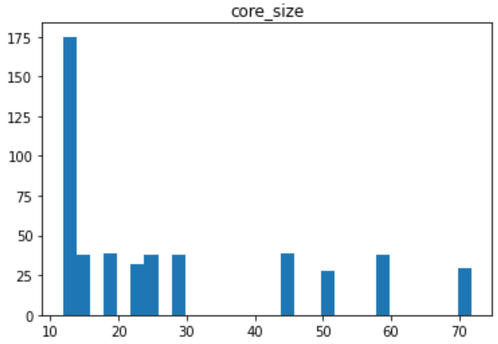
3.1. Предобработка данных

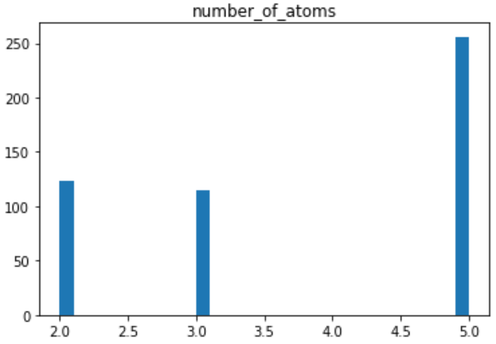


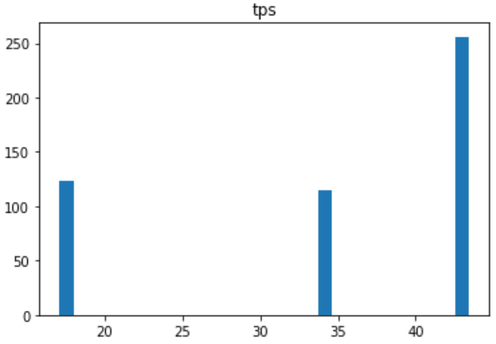


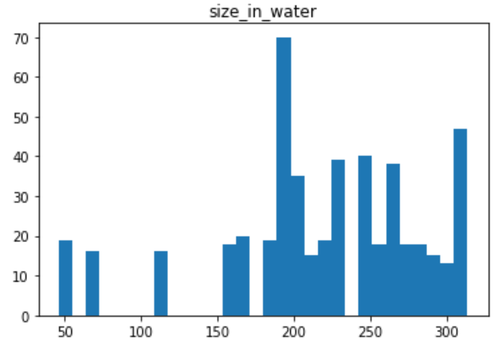
Database_1

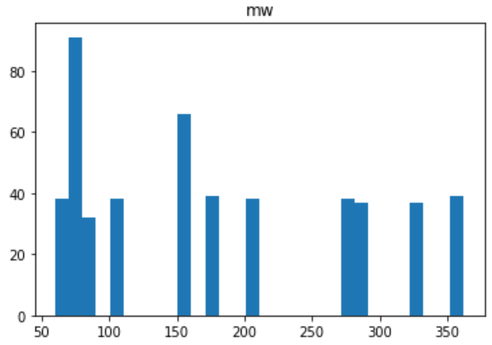
- **Ionic radius, Core_size(nm), size_in_water, Surface_charge, Exposure_dose, Number of atoms, Mw, Tps, density**, - без выбросов.

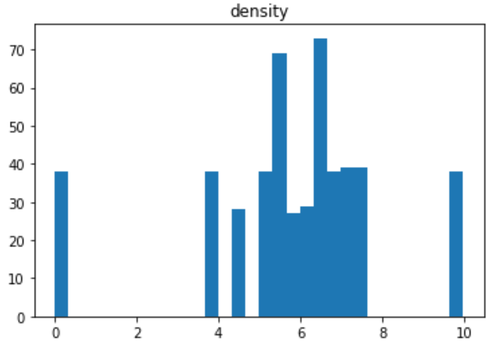












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3.2. Предобработка данных

Database_2 :

```
<class 'pandas.core.frame.DataFrame'>
RangeIndex: 2896 entries, 0 to 2895
Data columns (total 21 columns):
 #   Column                Non-Null Count  Dtype
---  ------                --------------  -----
 0   material              2896 non-null   object
 1   type_inorganic        2896 non-null   object
 2   coat                  1052 non-null   object
 3   diameter              2896 non-null   float64
 4   concentration         2896 non-null   float64
 5   surface_charge        1261 non-null   float64
 6   cell_type             2896 non-null   object
 7   cell_line             2896 non-null   object
 8   human                 2896 non-null   object
 9   animal                651 non-null    object
 10  cell_morphology       2895 non-null   object
 11  cell_age              2895 non-null   object
 12  source                2896 non-null   object
 13  exposure_time         2896 non-null   int64
 14  test                  2895 non-null   object
 15  test_indicator        2895 non-null   object
 16  biochemical_metric    2895 non-null   object
 17  viability             2896 non-null   float64
 18  interference          2896 non-null   object
 19  colloidal_stability   2896 non-null   object
 20  positive_control      2896 non-null   object
dtypes: float64(4), int64(1), object(16)
memory usage: 475.2+ KB
```

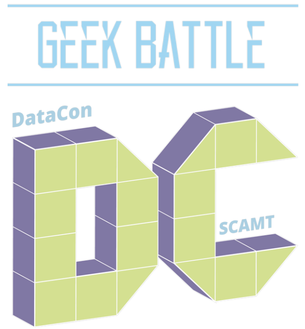
В 2 таблице (*Database_2*) были произведены следующие изменения:

1. Удаление непонятных оксидов (Copper Oxide, Zinc oxide)

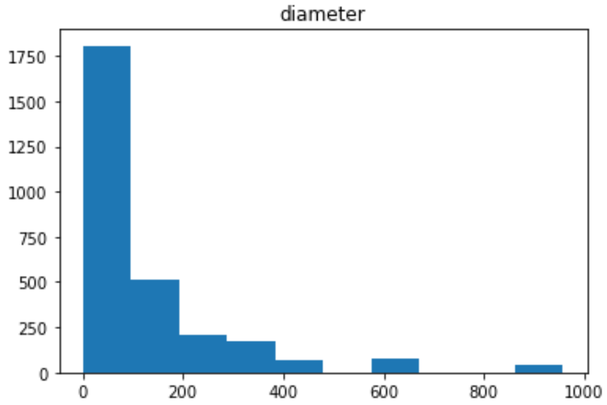
2. Замена «Iron oxide» на «Fe3O4» (Проведен поиск: статья - ссылка на реактив - сайт производителя реактива).

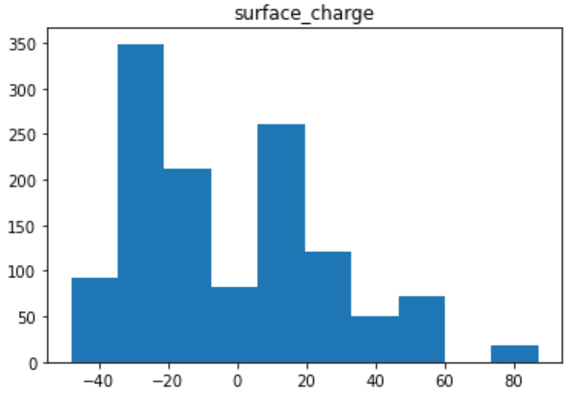
3. Проверка уникальных значений нечисловых признаков и замена на «0» и «1», где это было допустимо.

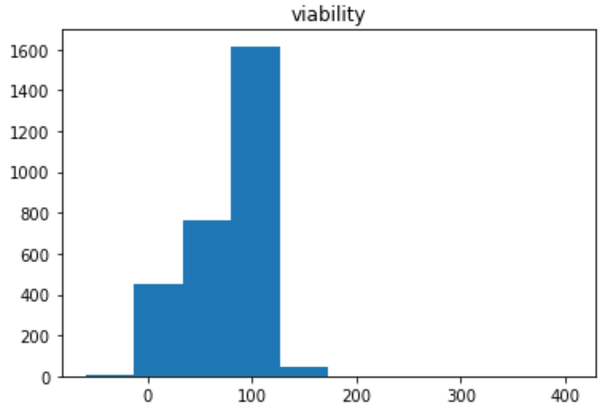
4. Анализ распределения числовых признаков.

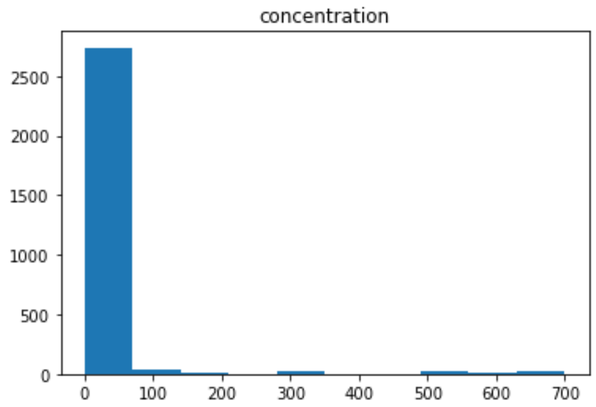


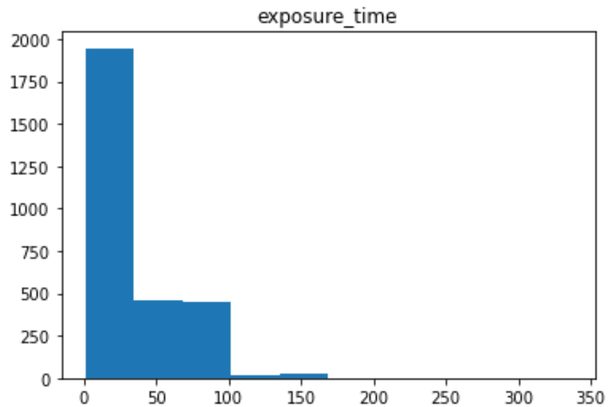
3.2. Предобработка данных







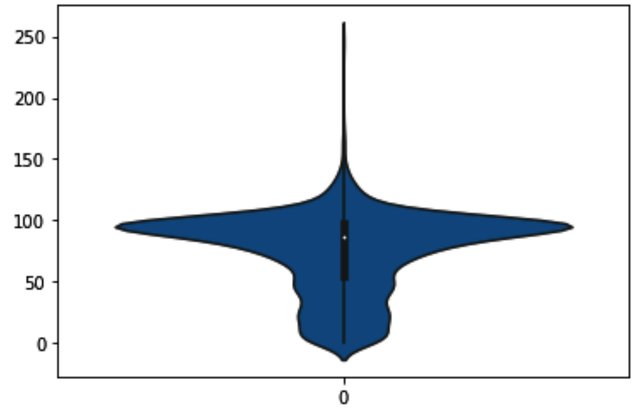





```
db_2.viability = db_2['viability'][db_2['viability']<300]
db_2.viability = db_2.viability.abs()

sns.violinplot(data=db_2.viability)
```

```
<AxesSubplot:>
```



3.3. Предобработка данных

Database_3 :

```
<class 'pandas.core.frame.DataFrame'>
RangeIndex: 4111 entries, 0 to 4110
Data columns (total 25 columns):
 #   Column            Non-Null Count  Dtype
---  ------            --------------  -----
 0   material          4111 non-null   object
 1   type_inorganic    4111 non-null   object
 2   shape             4111 non-null   object
 3   coat              4110 non-null   object
 4   synthesis_method  4111 non-null   object
 5   surfacecharge     3112 non-null   object
 6   diameter          3278 non-null   float64
 7   size_in_water     2330 non-null   float64
 8   size_in_medium    1989 non-null   float64
 9   surface_charge    2487 non-null   object
 10  zeta_in_medium    1670 non-null   float64
 11  cell_type         4111 non-null   object
 12  number_of_cells   3684 non-null   float64
 13  human             4111 non-null   object
 14  animal            4110 non-null   object
 15  source            4111 non-null   object
 16  cell_morphology   4111 non-null   object
 17  cell_age          4111 non-null   object
 18  cell_line         4111 non-null   object
 19  exposure_time     4111 non-null   int64
 20  concentration     3889 non-null   float64
 21  test              4111 non-null   object
 22  test_indicator    4111 non-null   object
 23  aspect_ratio      380 non-null    float64
 24  viability         4111 non-null   float64
dtypes: float64(8), int64(1), object(16)
memory usage: 803.1+ KB
```

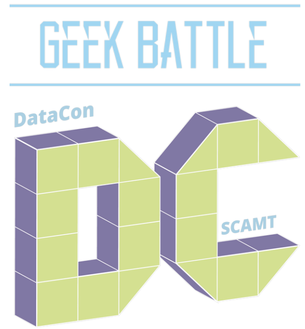
В 3 таблице (*Database_3*) были произведены следующие изменения:

1. Признак 'aspect ratio', 'zeta_in_medium' был удален, т.к. значений очень немного.

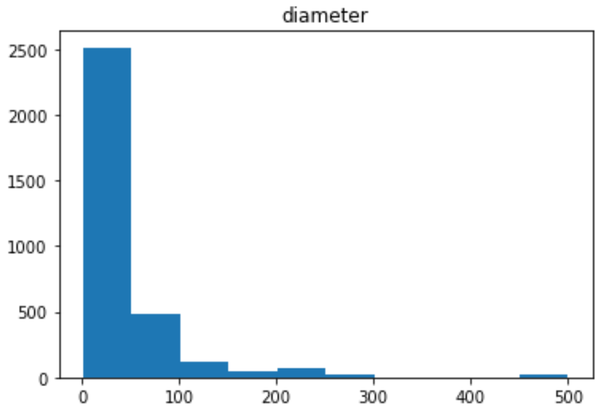
2. Замена «Iron oxide» на «Fe3O4» (Проведен поиск: статья - ссылка на реактив - сайт производителя реактива).

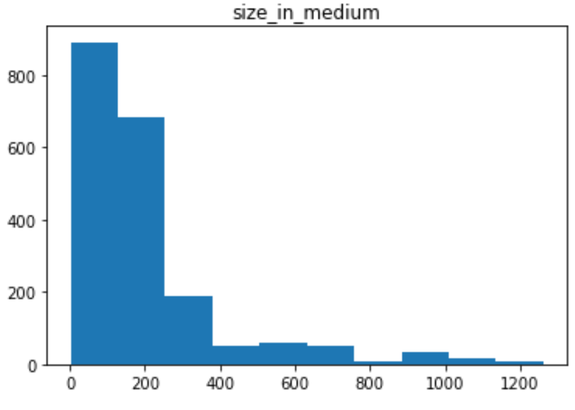
3. Проверка уникальных значений нечисловых признаков и замена на «0» и «1», где это было допустимо.

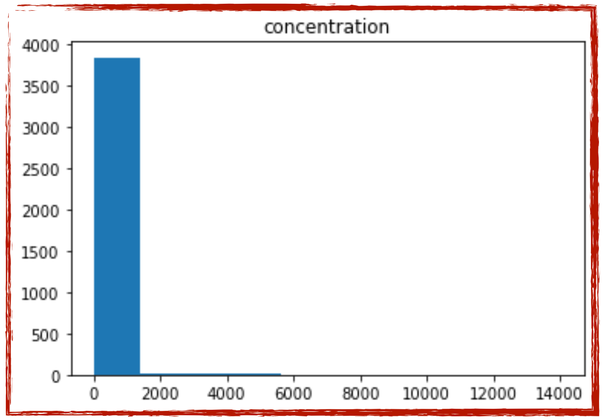
4. Анализ распределения числовых признаков.

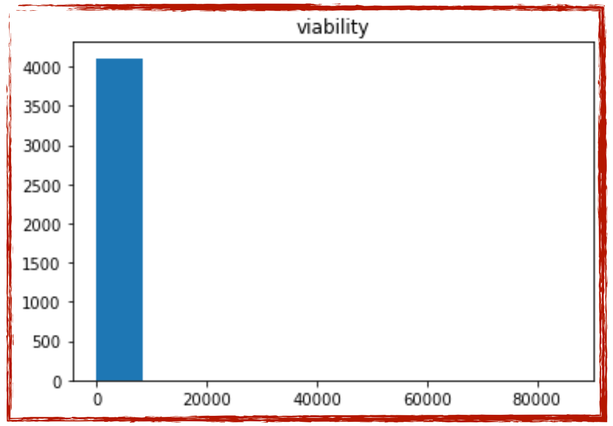


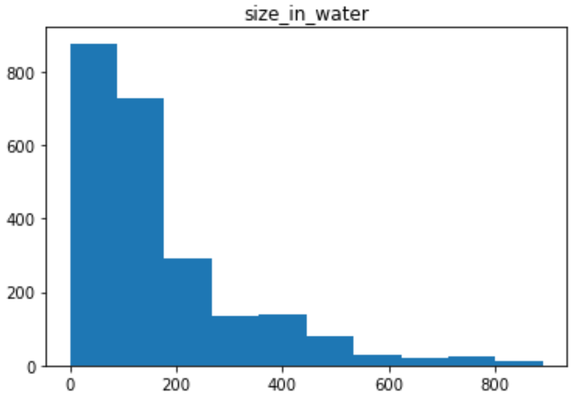
3.3. Предобработка данных

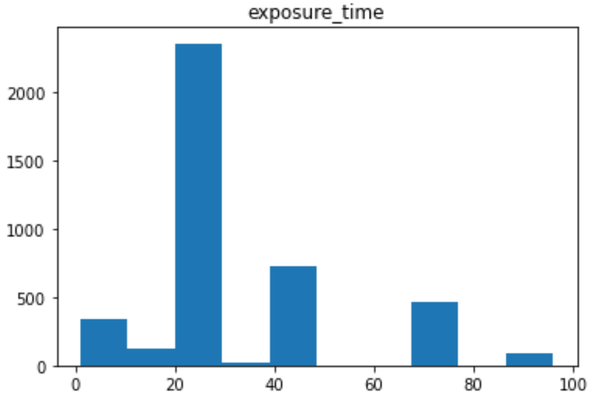


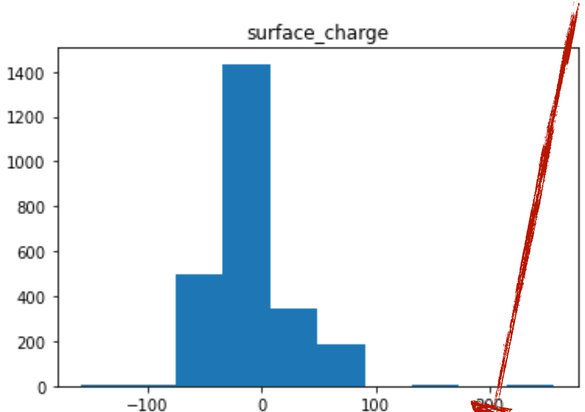












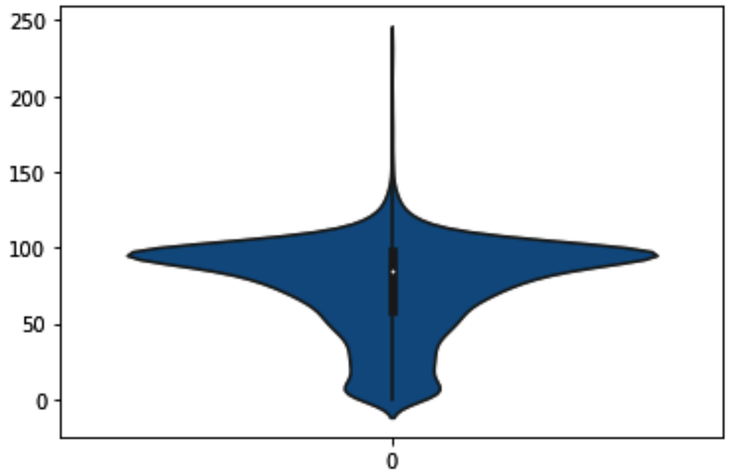
Database_3

Подозрительные значения встречаются в признаке *concentration* и *viability* .

3.3. Предобработка данных

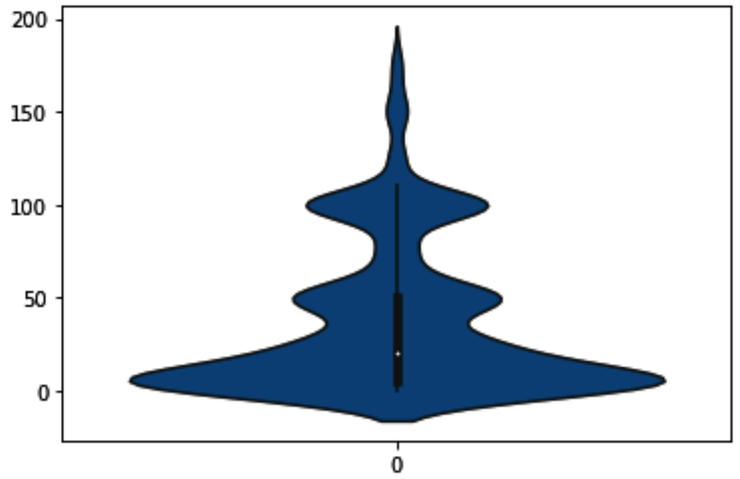
```
db_3.viability = db_3['viability'][db_3['viability']<1000]
db_3.viability = db_3.viability.abs()
sns.violinplot(data=db_3.viability)
```

```
<AxesSubplot:>
```




```
db_3.concentration = db_3['concentration'][db_3['concentration']<200]
sns.violinplot(data=db_3.concentration)
```

```
<AxesSubplot:>
```



Подозрительные значения встречаются в признаке *concentration* и *viability* .

3.4. Предобработка данных

Database_4 :

```
<class 'pandas.core.frame.DataFrame'>
RangeIndex: 1068 entries, 0 to 1067
Data columns (total 21 columns):
 #   Column              Non-Null Count  Dtype  
---  ------              --------------  -----  
 0   material            1066 non-null   object 
 1   elements            1068 non-null   object 
 2   electronegativity   1068 non-null   float64
 3   ionic_radius        1068 non-null   float64
 4   core_size           1066 non-null   float64
 5   size_in_water       1066 non-null   float64
 6   surface_charge      1066 non-null   float64
 7   surface_area        1067 non-null   float64
 8   cell_type           1068 non-null   int64  
 9   concentration       1067 non-null   float64
 10  number_of_atoms     1065 non-null   float64
 11  mw                  1065 non-null   float64
 12  tps                 491 non-null    float64
 13  a                   491 non-null    object 
 14  b                   491 non-null    object 
 15  c                   491 non-null    object 
 16  alpha               491 non-null    object 
 17  beta                491 non-null    object 
 18  gama                491 non-null    object 
 19  density             491 non-null    object 
 20  viability           1068 non-null   float64
dtypes: float64(11), int64(1), object(9)
memory usage: 175.3+ KB
```

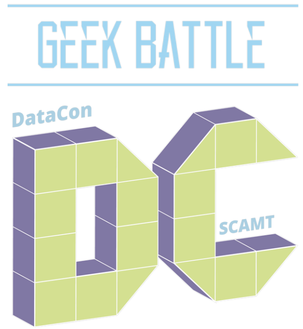
В 4 таблице (*Database_4*) были произведены следующие изменения:

1. Очистка ошибок: удаление неизвестного материала.

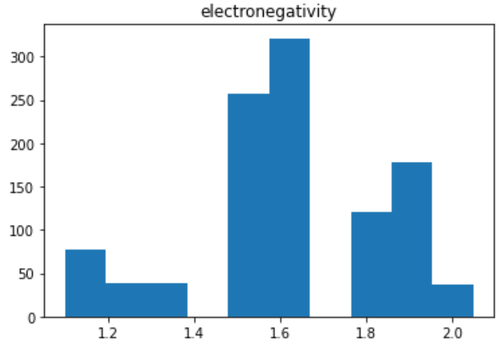
2. Создание признака.

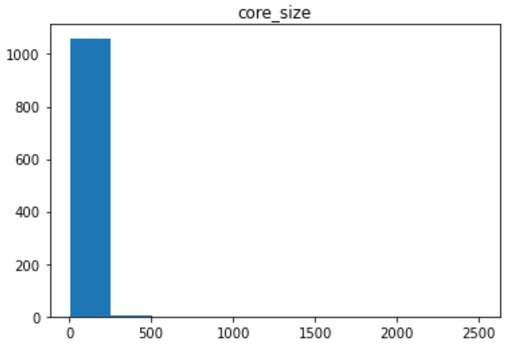
3. Замена "-" на Nan (не полностью правомерно)

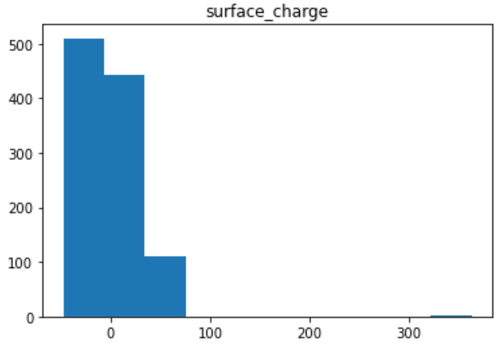
4. Анализ распределения числовых признаков.

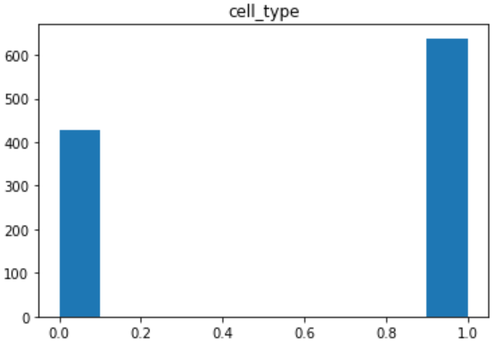


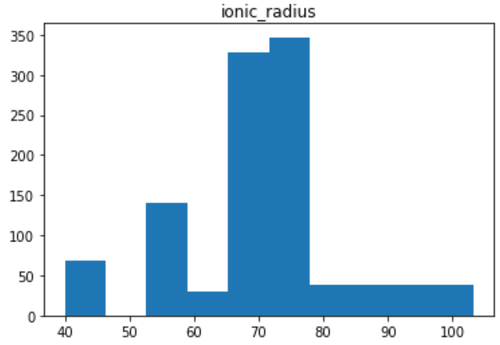
3.4. Предобработка данных

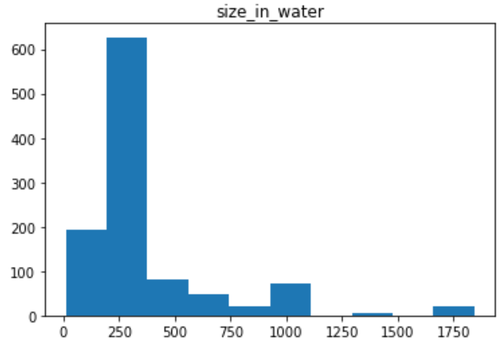


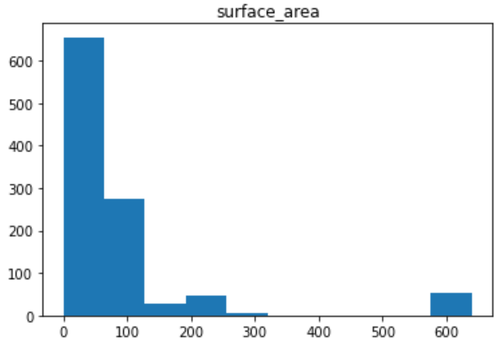


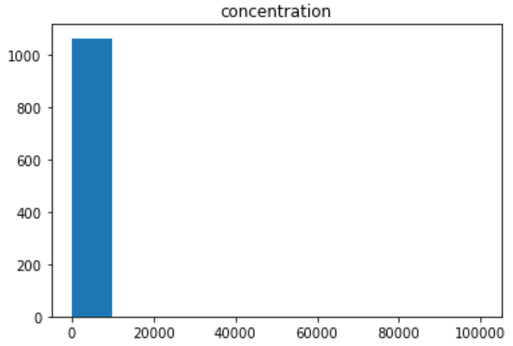


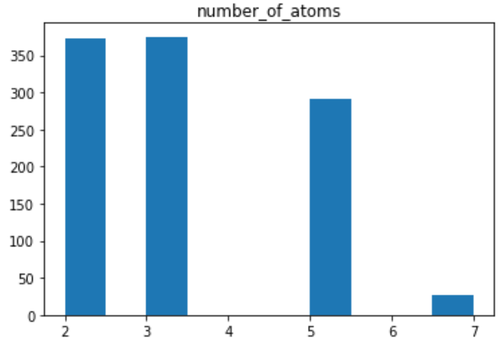


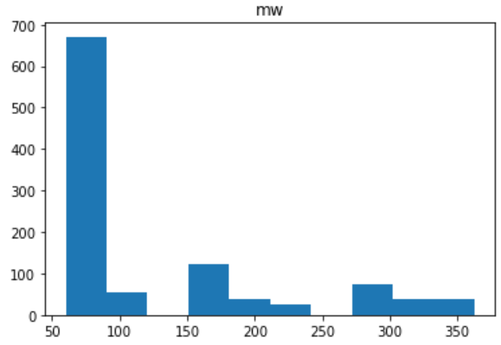


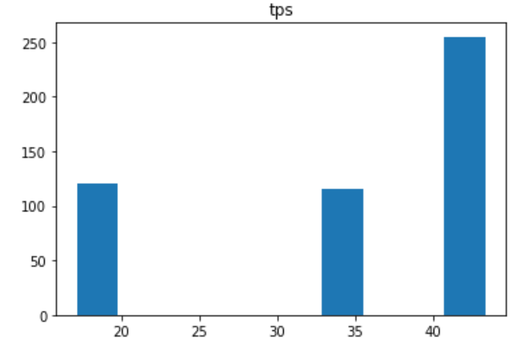


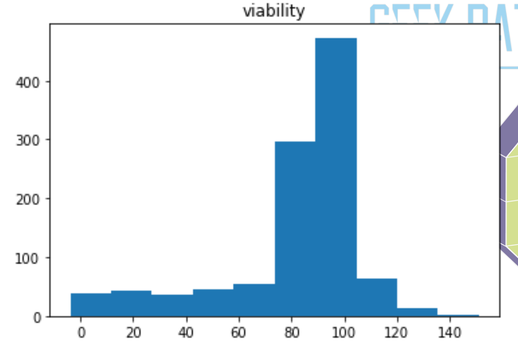












3.5. Предобработка данных

Database_5 :

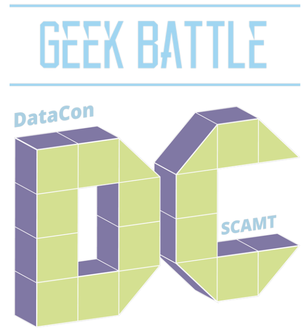
```
<class 'pandas.core.frame.DataFrame'>
RangeIndex: 574 entries, 0 to 573
Data columns (total 13 columns):
 #   Column           Non-Null Count  Dtype
---  ------           --------------  -----
 0   material         574 non-null    object
 1   core_size        572 non-null    float64
 2   size_in_water    574 non-null    float64
 3   surface_charge   573 non-null    float64
 4   surface_area     574 non-null    float64
 5   cell_line        572 non-null    object
 6   animal           574 non-null    object
 7   source           574 non-null    object
 8   cell_type        574 non-null    object
 9   exposure_time    574 non-null    int64
 10  concentration    574 non-null    float64
 11  viability        574 non-null    float64
 12  toxicity         574 non-null    object
dtypes: float64(6), int64(1), object(6)
memory usage: 58.4+ KB
```

В 5 таблице (*Database_5*) были произведены следующие изменения:

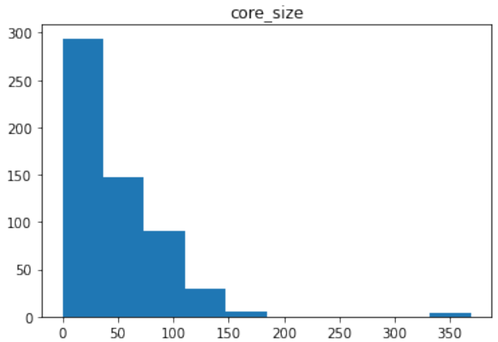
1. Очистка ошибок

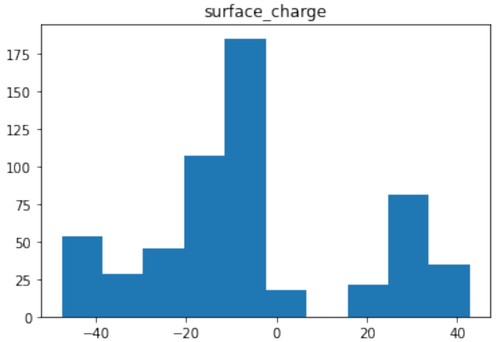
2. Создание признака.

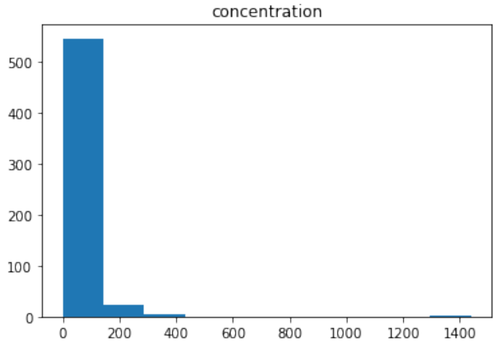
3. Анализ распределения числовых признаков.

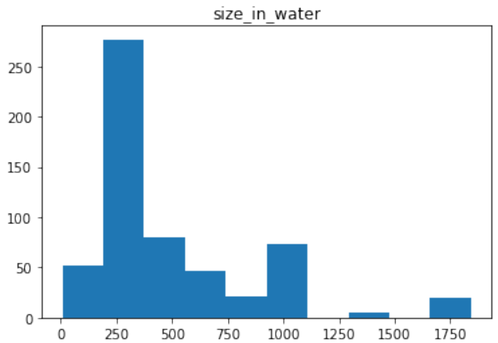


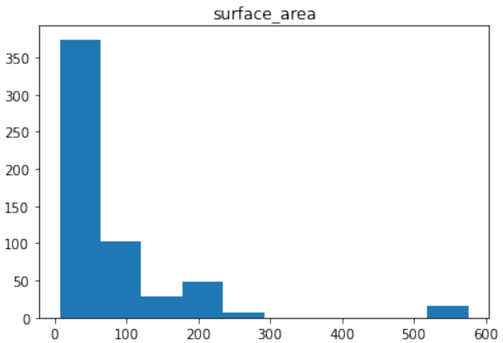
3.5. Предобработка данных

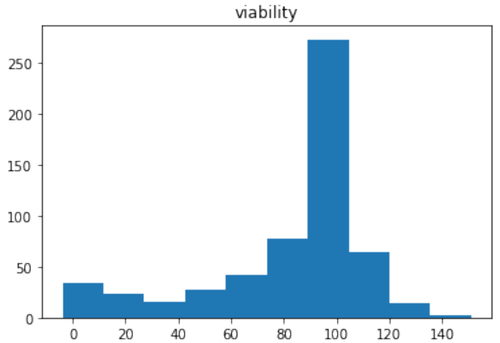


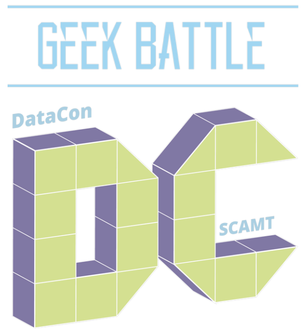




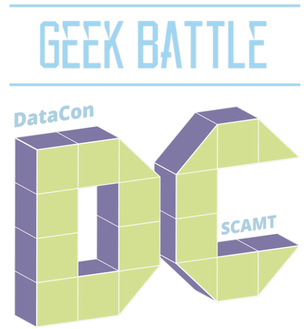






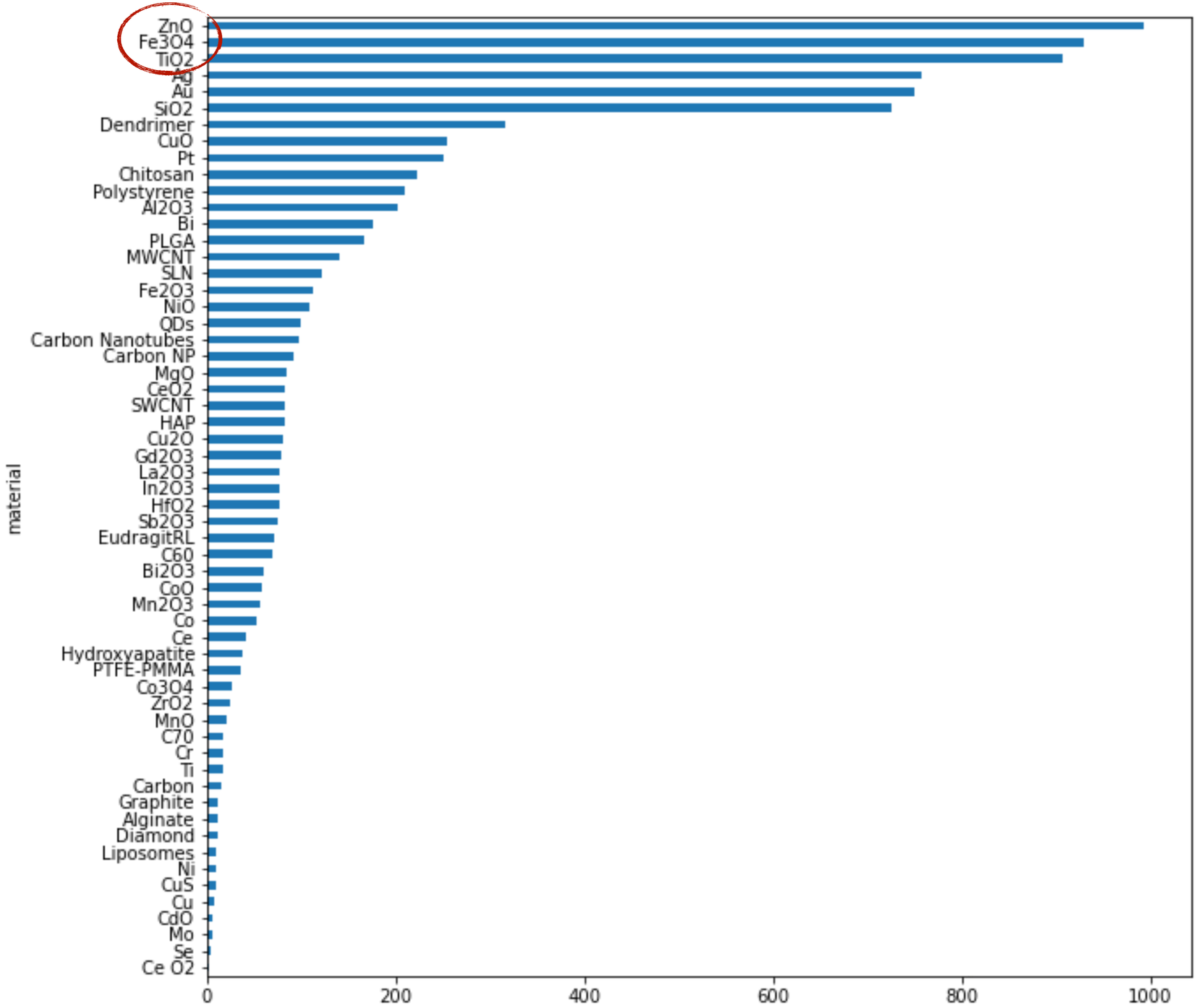


4. Создание единой базы данных - объединение таблиц.



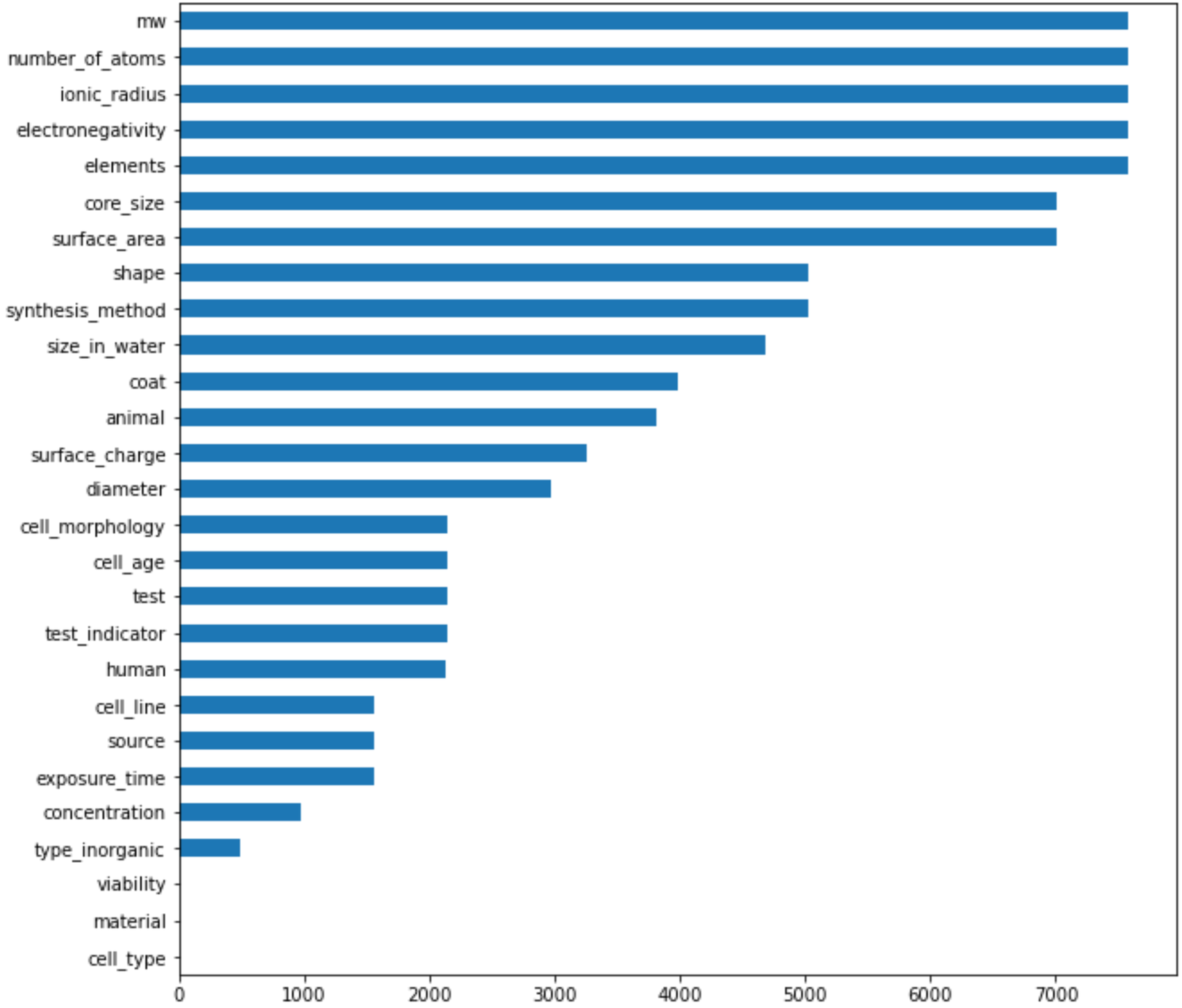
5. Анализ

- **Распределение данных по типу материала:**



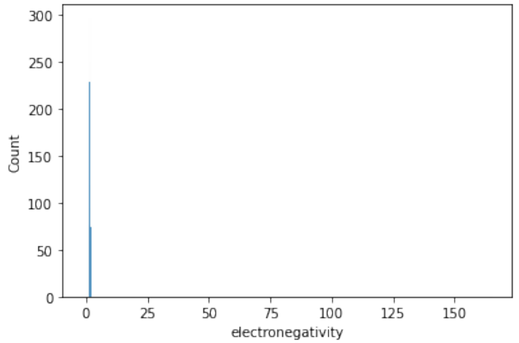
5. Анализ

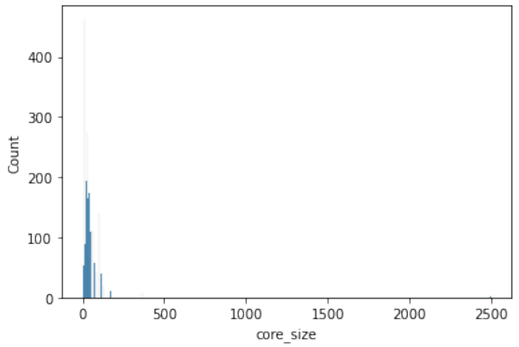
- **Распределение пропусков по признакам:**

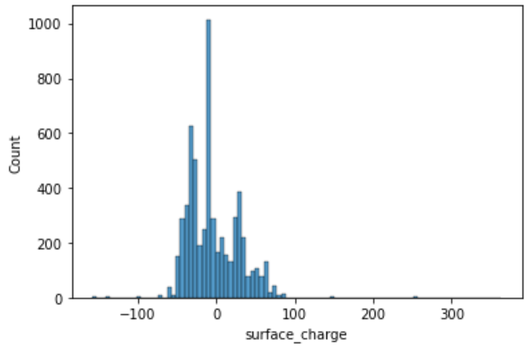


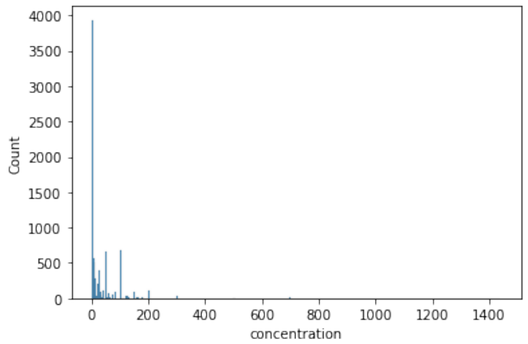
5. Анализ

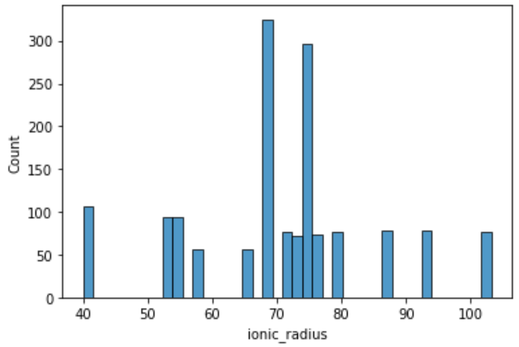
- **Распределение числовых признаков:**

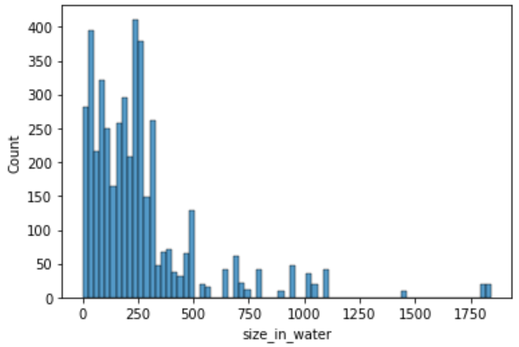


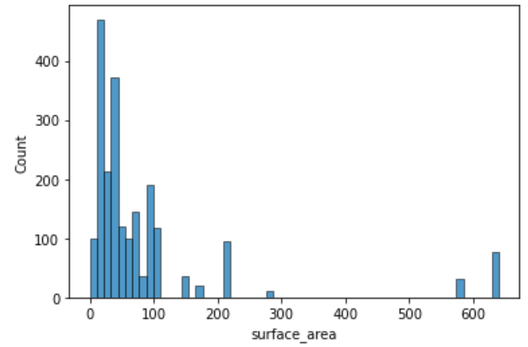


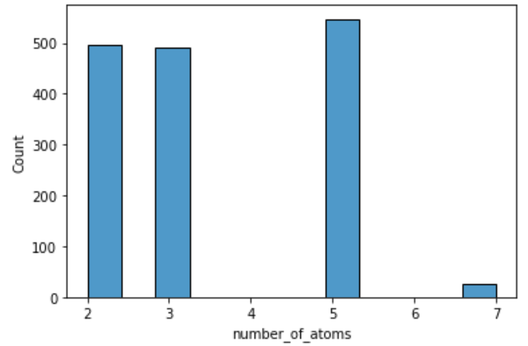


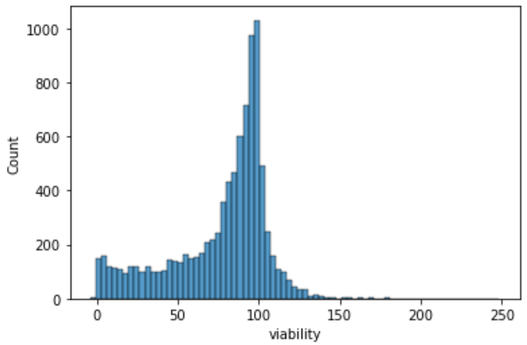


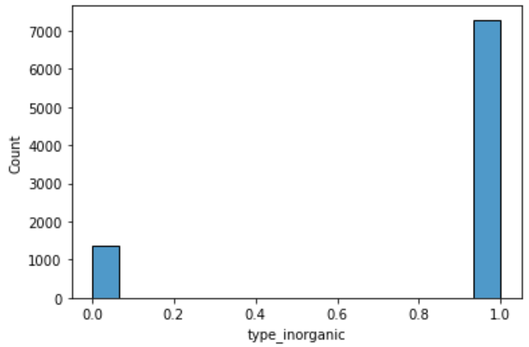


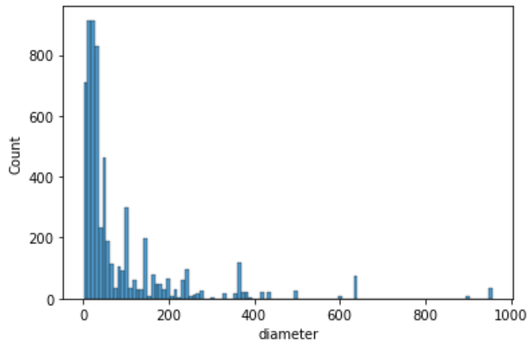


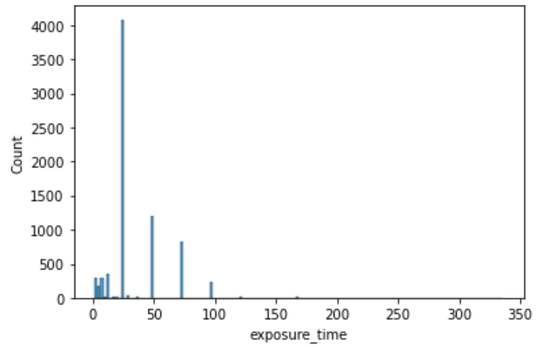






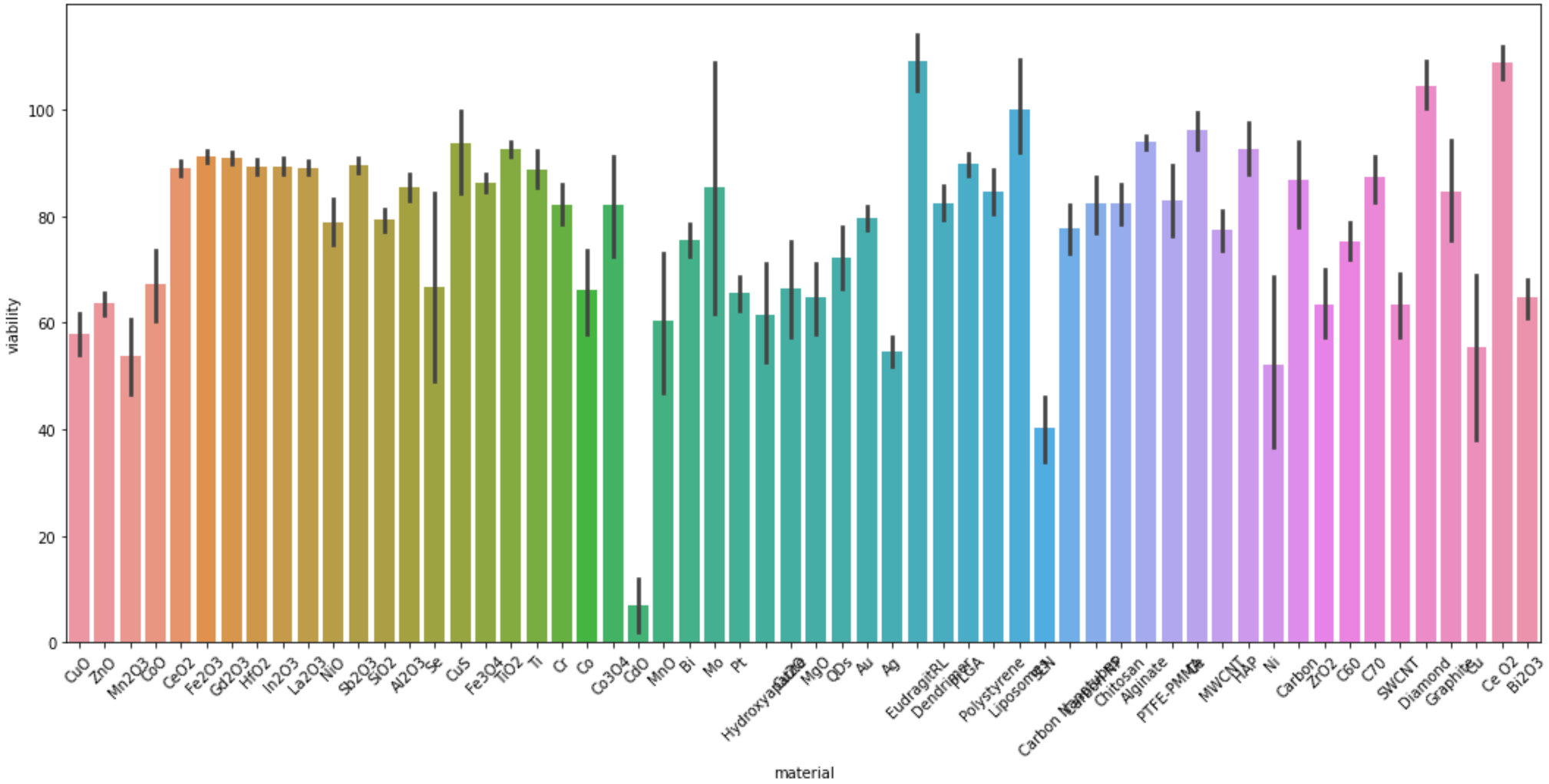






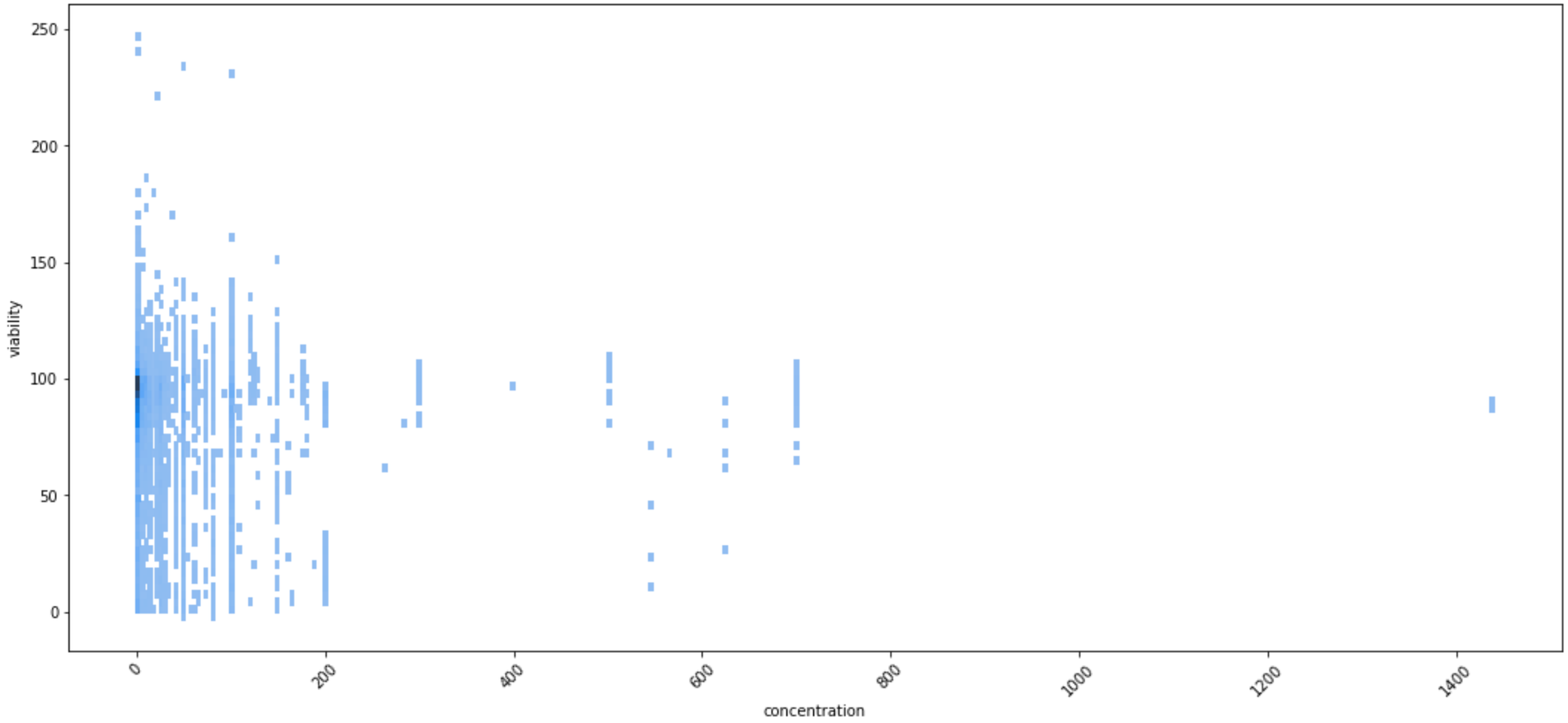
5. Анализ

- **Зависимость параметра *viability* от материала:**



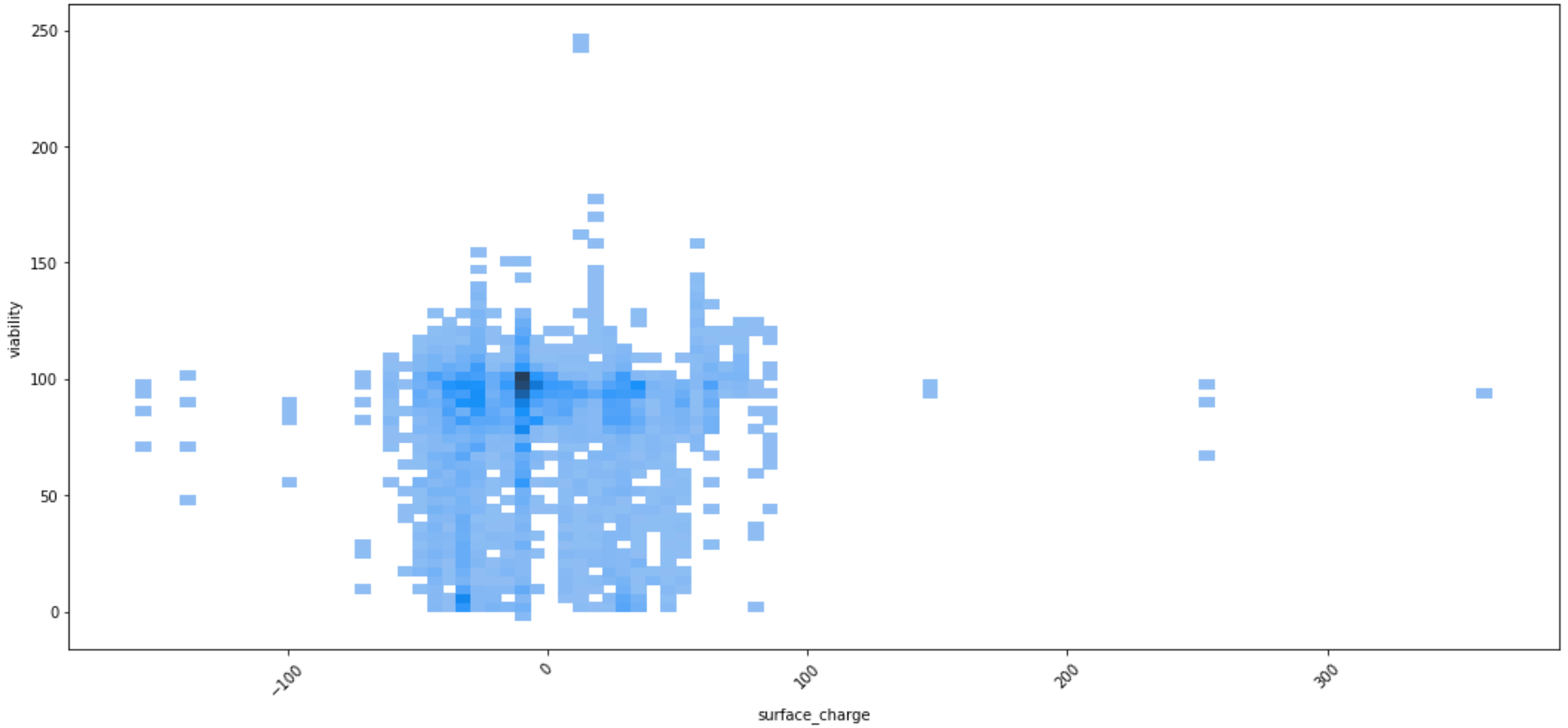
5. Анализ

- **Зависимость параметра *viability* от концентрации:**



5. Анализ

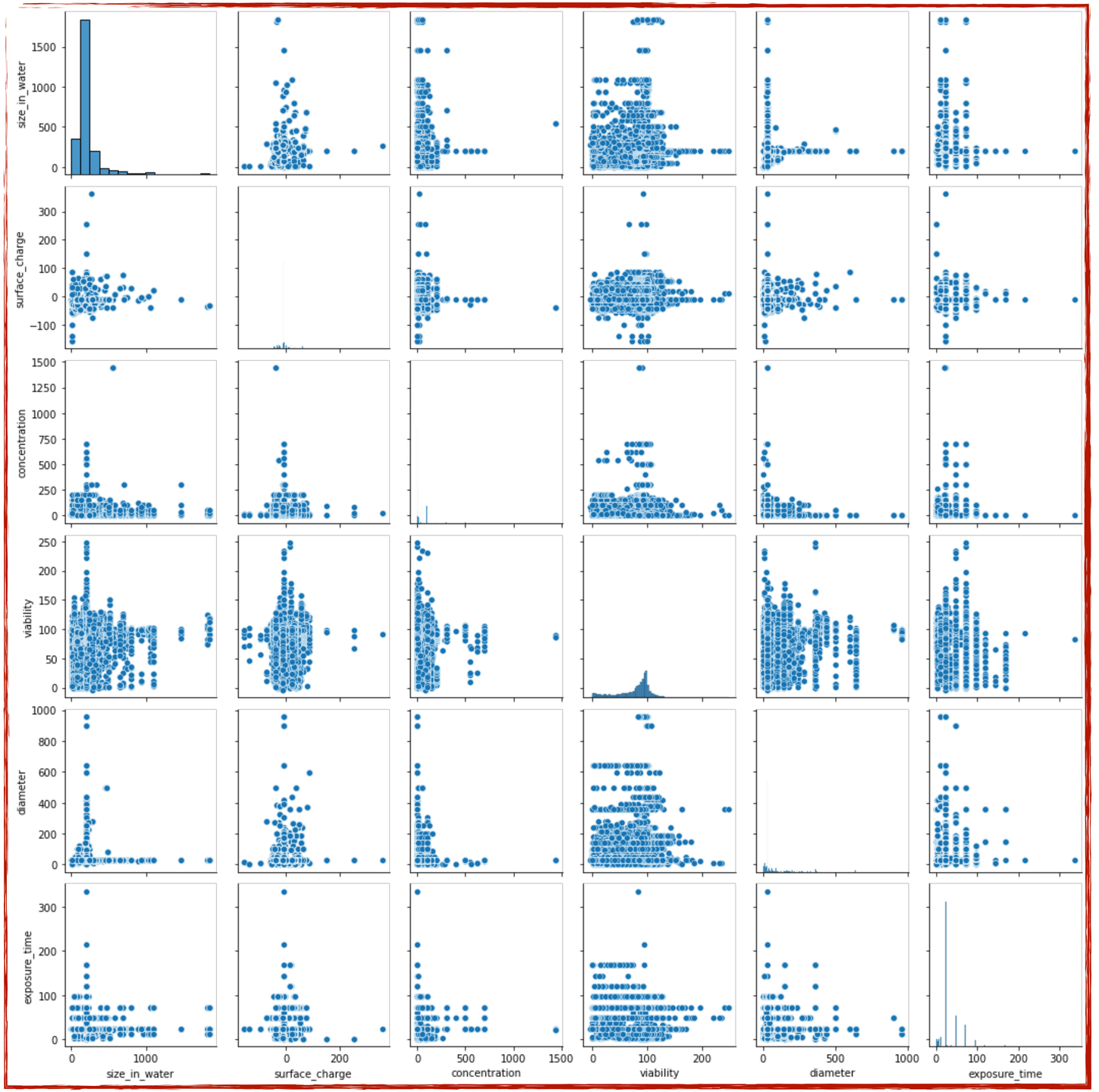
- **Зависимость параметра *viability* от заряда поверхности:**



5. Анализ

- **Корреляция признаков:** матрица графиков зависимости графиков друг от друга.

Прямолинейные зависимости и очевидные закономерности - отсутствуют



6. Модели

- **CatBoost**

```
%%time
estimator = CatBoostRegressor(random_seed = 42)
parameters = {
    'n_estimators': (200, 800, 100),
    'learning_rate': [0.1, 0.5, 0.1],
    'max_depth': [3, 6]
}


model_cb = GridSearchCV(estimator = estimator,
                        param_grid = parameters,
                        cv = 2, verbose=10)

# Обучение
model_cb.fit(features_train, target_train, cat_features=cat_features, verbose=2)
```

```
CatBoost
0.5462275143957516
{'learning_rate': 0.1, 'max_depth': 6, 'n_estimators': 800}
RMSE(CatBoost) =  19.19463126966019
```

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6. Модели

- **Random Forest Regressor**

```
estimator = RandomForestRegressor(random_state = 42)

param_grid = {
    'n_estimators': list(np.arange(50, 200, 20).astype(int)),
    'max_depth': list(np.arange(4, 20, 4).astype(int)),
}

model_rf = GridSearchCV(estimator = estimator,
                        param_grid = param_grid,
                        cv = 2, verbose=2)
# Обучение
model_rf.fit(features_train, target_train)
```

```
Random Forest Regressor
Лучшая метрика 0.525222403749226
полученная при использовании параметров: {'max_depth': 16, 'n_estimators': 190}
RMSE(RandomForest Regressor) = 20.941545331273932
```

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7. Вывод

- На основании данных о составе, свойствах, происхождении и тестах наночастиц из 5 таблиц нами построены 2 модели - **CatBoostRegressor** и **RandomForestRegressor**, предсказывающие признак viabillity.

- Была произведена предобработка данных: исправлены опечатки, удалены выбросы, обработаны пропуски. Базы данных объединены в сводную таблицу и сделана визуализация данных.

- Обе построенные модели показали близкие результаты: **RMSE(RandomForest Regressor) = 20.94, RMSE(CatBoost) = 19.19.**

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