5_TYK2_Eliminating_PAINS

April 8, 2022

[1]:
```
!git clone https://github.com/PatWalters/rd_filters ../tools
```

```
Cloning into '../tools'…
remote: Enumerating objects: 83, done.
remote: Total 83 (delta 0), reused 0 (delta 0), pack-reused 83
Unpacking objects: 100% (83/83), done.
```

[5]:
```
!pip install docopt
```

```
Collecting docopt
  Downloading docopt-0.6.2.tar.gz (25 kB)
Building wheels for collected packages: docopt
  Building wheel for docopt (setup.py) … done
  Created wheel for docopt: filename=docopt-0.6.2-py2.py3-none-any.whl
size=13705
sha256=d4a7ab80de8245e8b9d18fbfe0d8a39f0ff9c7629f5c7b4a6075515156f06dc3
  Stored in directory: /home/cv/.cache/pip/wheels/72/b0/3f/1d95f96ff986c7dfffe46
ce2be4062f38ebd04b506c77c81b9
Successfully built docopt
Installing collected packages: docopt
Successfully installed docopt-0.6.2
```

[7]:
```
!cd ../tools
```

[8]:
```
!pip install ../tools
```

```
Processing /home/cv/TECHX/tools
Requirement already satisfied: pandas in
/home/cv/anaconda3/envs/deepchem/lib/python3.7/site-packages (from rd-
filters==0.1) (1.2.4)
Requirement already satisfied: docopt in
/home/cv/anaconda3/envs/deepchem/lib/python3.7/site-packages (from rd-
filters==0.1) (0.6.2)
Requirement already satisfied: python-dateutil>=2.7.3 in
/home/cv/anaconda3/envs/deepchem/lib/python3.7/site-packages (from pandas->rd-
filters==0.1) (2.8.1)
Requirement already satisfied: pytz>=2017.3 in
/home/cv/anaconda3/envs/deepchem/lib/python3.7/site-packages (from pandas->rd-
filters==0.1) (2021.1)
Requirement already satisfied: numpy>=1.16.5 in
/home/cv/anaconda3/envs/deepchem/lib/python3.7/site-packages (from pandas->rd-
filters==0.1) (1.20.2)
Requirement already satisfied: six>=1.5 in
/home/cv/anaconda3/envs/deepchem/lib/python3.7/site-packages (from python-
dateutil>=2.7.3->pandas->rd-filters==0.1) (1.15.0)
Building wheels for collected packages: rd-filters
  Building wheel for rd-filters (setup.py) … done
  Created wheel for rd-filters: filename=rd_filters-0.1-py3-none-any.whl
size=33801
sha256=fe8bf2a4d3a9e8a02804fb53367885e106acd718b4c0b26c87f0a25d46658737
  Stored in directory: /tmp/pip-ephem-wheel-cache-
cfm_go60/wheels/de/3f/0f/9178deb02e296aabf3c32d4191e3bc9aad0e8bf9900044a50b
Successfully built rd-filters
Installing collected packages: rd-filters
Successfully installed rd-filters-0.1
```

[9]:

```
!rd_filters -h
```

```
Usage:
rd_filters filter --in INPUT_FILE --prefix PREFIX [--rules RULES_FILE_NAME]
[--alerts ALERT_FILE_NAME][--np NUM_CORES]
rd_filters template --out TEMPLATE_FILE [--rules RULES_FILE_NAME]

Options:
--in INPUT_FILE input file name
--prefix PREFIX prefix for output file names
--rules RULES_FILE_NAME name of the rules JSON file
--alerts ALERTS_FILE_NAME name of the structural alerts file
--np NUM_CORES the number of cpu cores to use (default is all)
--out TEMPLATE_FILE parameter template file name
```

[10]:

```
!pwd
```

```
/home/cv/TECHX/notebooks
```

[13]:

```
!rd_filters filter --in ../pipeline/5_PAINS_rd_filter/35_smiles.smi --prefix 22 \
--rules ../tools/rd_filters/data/rules.json --alerts ../tools/rd_filters/data/alert_collection.csv
```

```
using 8 cores
Using alerts from Inpharmatica
[21:27:49] Explicit valence for atom # 1 N, 4, is greater than permitted
[21:27:49] Explicit valence for atom # 15 N, 4, is greater than permitted
[21:27:49] Explicit valence for atom # 1 N, 4, is greater than permitted
[21:27:49] Explicit valence for atom # 19 N, 4, is greater than permitted
```

```
[21:27:49] Can't kekulize mol.  Unkekulized atoms: 1 2 4 5 6 7 8

[21:27:49] Explicit valence for atom # 5 N, 4, is greater than permitted
[21:27:49] Can't kekulize mol.  Unkekulized atoms: 16 17 18 20 22 23 24

Wrote SMILES for molecules passing filters to 22.smi
Wrote detailed data to 22.csv
22 of 35 passed filters 62.9%
Elapsed time 0.09 seconds
```

[20]:
```python
import pandas as pd

df = pd.read_csv('../pipeline/5_PAINS_rd_filter/22.smi', sep=' ', header=None)
df.columns = ['SMILES', 'Name']
```

[21]:
```python
df
```

[21]:
```
                                               SMILES          Name
0   O(c1ccc(cc1)[C@H]4n2nc(nc2NC(c3cc(OC)ccc3)C4)N)CC  ZINC13131776
1   Clc1c(ccc(Cl)c1)[C@H]3C[C@H](n2nc(nc2N3)N)c4cc…  ZINC13131298
2        O=C(c3cc2n1c(nnc1)c(nc2cc3)NC4CCCC4)c5ccccc5  ZINC06901595
3      s3c(SCc1nc(nc(n1)N)Nc2c(cccc2)C)nnc3NCc4ccccc4  ZINC09728763
4   Clc1c(Cl)ccc(c1)C3Nc2n(nc(n2)N)[C@@H](C3)c4ccc…  ZINC13131981
5   Fc1cc(ccc1)CNc3nc(c(c2onc(c2)C)cn3)c5cnc(N4CCO…  ZINC19124027
6   O=C(c3cc2n1c(nnc1C)c(nc2cc3)NC[C@@H]4N(CCC4)CC…  ZINC20939758
7     O=C(c3cc2n1c(nnc1C)c(nc2cc3)NCc4ccncc4)c5ccccc5  ZINC20939765
8       O=C(N(C)C)c3ccc(c1nc(nc(n1)N)Nc2ccc(cc2)C)cc3  ZINC32540567
9         O(C(c3ccc(c1nc(nc(n1)N)Nc2ccc(cc2)C)cc3)C)C  ZINC32541042
10        Fc1c(c(F)ccc1)CNc4n2ncnc2nc(c3ccc(OC)cc3)c4  ZINC23432014
11  O(c1ccc(cc1)[C@H]4n2nc(nc2NC(c3ccc(OC)cc3)C4)N…  ZINC02472318
12  O(c1ccc(cc1)[C@H]4n2nc(nc2NC(c3cc(OC)ccc3)C4)N…  ZINC02472304
13         S=C(Nc2nc(c1c(O)cccc1)cc(n2)c3ccc(OC)cc3)N  ZINC01084111
14  Clc1ccc(cc1)C(=O)c3sc2n(c(=O)[nH]c(=O)c2c3N)c4…  ZINC02638281
15  Fc1ccc(cc1)C3Nc2n(nc(n2)N)[C@@H](C3)c5ccc(OCc4…  ZINC02472295
16  O(c1ccc(cc1)[C@H]4n2nc(nc2N[C@@H](c3ccc(cc3)C)…  ZINC02472298
17    [nH]2c1nc(NCCN(C)C)cc(c1cc2)c4cc3c(cnc(N)c3)cc4  ZINC72143513
18        s1cnc4c1cc(c3c2c([nH]cc2)nc(NCCN(C)C)c3)cc4  ZINC72146015
19  O(c1c(cccc1)CNc3nc4c(n2c3nnc2C)cc(cc4)C(=O)c5c…  ZINC09224703
20  o1c(nnc1)c5ccc(c4c2c([nH]cc2)nc(NCc3ccncc3)c4)cc5  ZINC72454514
21     n1(ncc4c1ccc(c3c2c([nH]cc2)nc(NCCN(C)C)c3)c4)C  ZINC72168947
```

[22]:
```
!rd_filters filter --in ../pipeline/5_PAINS_rd_filter/all_smiles.smi --prefix␣
↪all \
--rules ../tools/rd_filters/data/rules.json --alerts ../tools/rd_filters/data/
↪alert_collection.csv
```

```
using 8 cores
Using alerts from Inpharmatica
```

```
[14:30:50] Explicit valence for atom # 9 N, 4, is greater than permitted
[14:30:50] Explicit valence for atom # 17 N, 4, is greater than permitted
[14:30:50] Explicit valence for atom # 17 N, 4, is greater than permitted
[14:30:50] Explicit valence for atom # 17 N, 4, is greater than permitted
[14:30:50] Explicit valence for atom # 1 N, 4, is greater than permitted
[14:30:50] Explicit valence for atom # 15 N, 4, is greater than permitted
[14:30:50] Explicit valence for atom # 19 N, 4, is greater than permitted
[14:30:50] Explicit valence for atom # 19 N, 4, is greater than permitted
[14:30:50] Explicit valence for atom # 25 N, 4, is greater than permitted
[14:30:50] Explicit valence for atom # 5 N, 4, is greater than permitted
[14:30:50] Explicit valence for atom # 5 N, 4, is greater than permitted
[14:30:50] Explicit valence for atom # 5 N, 4, is greater than permitted
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[14:30:50] Explicit valence for atom # 5 N, 4, is greater than permitted
[14:30:50] Explicit valence for atom # 5 N, 4, is greater than permitted
[14:30:50] Explicit valence for atom # 27 N, 4, is greater than permitted
[14:30:50] Explicit valence for atom # 27 N, 4, is greater than permitted
[14:30:50] Explicit valence for atom # 18 N, 4, is greater than permitted
[14:30:50] Explicit valence for atom # 18 N, 4, is greater than permitted
[14:30:50] Explicit valence for atom # 12 N, 4, is greater than permitted
[14:30:50] Explicit valence for atom # 22 N, 4, is greater than permitted
[14:30:50] Explicit valence for atom # 22 N, 4, is greater than permitted
[14:30:50] Explicit valence for atom # 22 N, 4, is greater than permitted
[14:30:50] Explicit valence for atom # 22 N, 4, is greater than permitted
[14:30:50] Explicit valence for atom # 1 N, 4, is greater than permitted
[14:30:50] Explicit valence for atom # 1 N, 4, is greater than permitted
[14:30:50] Explicit valence for atom # 4 N, 4, is greater than permitted
[14:30:50] Explicit valence for atom # 5 N, 4, is greater than permitted
[14:30:50] Explicit valence for atom # 5 N, 4, is greater than permitted
[14:30:50] Explicit valence for atom # 16 N, 4, is greater than permitted
[14:30:50] Explicit valence for atom # 5 N, 4, is greater than permitted
[14:30:50] Explicit valence for atom # 5 N, 4, is greater than permitted
[14:30:50] Explicit valence for atom # 16 N, 4, is greater than permitted
[14:30:50] Explicit valence for atom # 5 N, 4, is greater than permitted
[14:30:50] Explicit valence for atom # 5 N, 4, is greater than permitted
[14:30:50] Explicit valence for atom # 5 N, 4, is greater than permitted
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50] Explicit valence for atom # 1 N, 4, is greater than permitted
[14:30:50] Explicit valence for atom # 5 N, 4, is greater than permitted
[14:30:50] Explicit valence for atom # 5 N, 4, is greater than permitted
[14:30:50] Explicit valence for atom # 18 N, 4, is greater than permitted
[14:30:50] Explicit valence for atom # 24 N, 4, is greater than permitted
[14:30:50] Explicit valence for atom # 4 N, 4, is greater than permitted
[14:30:50] Explicit valence for atom # 1 N, 4, is greater than permitted
[14:30:50] Explicit valence for atom # 3 N, 4, is greater than permitted
[14:30:50] Explicit valence for atom # 5 N, 4, is greater than permitted
[14:30:50] Explicit valence for atom # 10 N, 4, is greater than permitted
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[14:30:50] Explicit valence for atom # 10 N, 4, is greater than permitted
[14:30:50] Explicit valence for atom # 3 N, 4, is greater than permitted
[14:30:50] Explicit valence for atom # 9 N, 4, is greater than permitted
[14:30:50] Explicit valence for atom # 10 N, 4, is greater than permitted
[14:30:50] Explicit valence for atom # 21 N, 4, is greater than permitted
[14:30:50] Explicit valence for atom # 5 N, 4, is greater than permitted
[14:30:50] Explicit valence for atom # 22 N, 4, is greater than permitted
[14:30:50] Explicit valence for atom # 10 N, 4, is greater than permitted
[14:30:50] Explicit valence for atom # 1 N, 4, is greater than permitted
[14:30:50] Explicit valence for atom # 19 N, 4, is greater than permitted
[14:30:50] Explicit valence for atom # 12 N, 4, is greater than permitted
[14:30:50] Explicit valence for atom # 5 N, 4, is greater than permitted
[14:30:50] Explicit valence for atom # 25 N, 4, is greater than permitted
[14:30:50] Explicit valence for atom # 12 N, 4, is greater than permitted
[14:30:50] Explicit valence for atom # 24 N, 4, is greater than permitted
[14:30:50] Explicit valence for atom # 25 N, 4, is greater than permitted
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[14:30:50] Explicit valence for atom # 5 N, 4, is greater than permitted
[14:30:50[] 14Explicit valence for atom # 12 N, 4, is greater than permitted:
30:50] Explicit valence for atom # 1 N, 4, is greater than permitted
[14:30:50] Explicit valence for atom # 1 N, 4, is greater than permitted
[14:30:50] Explicit valence for atom # 23 N, 4, is greater than permitted
[14:30:50] Explicit valence for atom # 25 N, 4, is greater than permitted
[14:30:50] Explicit valence for atom # 1 N, 4, is greater than permitted
[14:30:50] Explicit valence for atom # 1 N, 4, is greater than permitted
[14:30:50] Explicit valence for atom # 5 N, 4, is greater than permitted
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[14:30:50] Explicit valence for atom # 5 N, 4, is greater than permitted
[14:30:50] Explicit valence for atom # 15 N, 4, is greater than permitted
[14:30:50] Explicit valence for atom # 17 N, 4, is greater than permitted
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permitted
[14:30:50] Explicit valence for atom # 18 N, 4, is greater than permitted
[14:30:50] Explicit valence for atom # 14 N, 4, is greater than permitted
Explicit valence for atom # 21 N, 4, is greater than permitted
[14:30:50] Explicit valence for atom # 1 N, 4, is greater than permitted
[14:30:50] Explicit valence for atom # 1 N, 4, is greater than permitted
[14:30:50] Explicit valence for atom # 5 N, 4, is greater than permitted
[14:30:50] Explicit valence for atom # 13 N, 4, is greater than permitted
[14:30:50] Explicit valence for atom # 1 N, 4, is greater than permitted
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[14:30:50] Explicit valence for atom # 1 N, 4, is greater than permitted
[14:30:50] Explicit valence for atom # 4 N, 4, is greater than permitted
[14:30:50] Explicit valence for atom # 10 N, 4, is greater than permitted
[14:30:50] Explicit valence for atom # 5 N, 4, is greater than permitted
[14:30:50] Explicit valence for atom # 20 N, 4, is greater than permitted
[14:30:50] Explicit valence for atom # 20 N, 4, is greater than permitted
[14:30:50] Explicit valence for atom # 25 N, 4, is greater than permitted
[14:30:50] Explicit valence for atom # 5 N, 4, is greater than permitted
[14:30:50] Explicit valence for atom # 1 N, 4, is greater than permitted
[14:30:50] Explicit valence for atom # 24 N, 4, is greater than permitted
[14:30:50] Explicit valence for atom # 1 N, 4, is greater than permitted
[14:30:50] Explicit valence for atom # 5 N, 4, is greater than permitted
[14:30:50] Explicit valence for atom # 16 N, 4, is greater than permitted
[14:30:50] Explicit valence for atom # 16 N, 4, is greater than permitted
[14:30:50] Explicit valence for atom # 21 N, 4, is greater than permitted
[14:30:50] Explicit valence for atom # 23 N, 4, is greater than permitted
[14:30:50] Explicit valence for atom # 15 N, 4, is greater than permitted
[14:30:50] Explicit valence for atom # 5 N, 4, is greater than permitted
[14:30:50] Explicit valence for atom # 5 N, 4, is greater than permitted
[[14:3014:50:] 30Explicit valence for atom # 5 N, 4, is greater than permitted:
50] Explicit valence for atom # 5 N, 4, is greater than permitted
[[1414:30:50] Explicit valence for atom # 5 N, 4, is greater than permitted
:30:50] Explicit valence for atom # 5 N, 4, is greater than permitted
[14:30:50] Explicit valence for atom # 15 N, 4, is greater than permitted
[14:30:50] Explicit valence for atom # 5 N, 4, is greater than permitted
[14:30:50] Explicit valence for atom # 18 N, 4, is greater than permitted
[14:30:50] Explicit valence for atom # 1 N, 4, is greater than permitted
[14:30:50] Explicit valence for atom # 5 N, 4, is greater than permitted
[14:30:50] Explicit valence for atom # 1 N, 4, is greater than permitted
[14:30:50] Explicit valence for atom # 1 N, 4, is greater than permitted
[14:30:50] Explicit valence for atom # 1 N, 4, is greater than permitted
[14:30:50] Explicit valence for atom # 1 N, 4, is greater than permitted
[14:30:50] Explicit valence for atom # 11 N, 4, is greater than permitted
[14:30:50] Explicit valence for atom # 1 N, 4, is greater than permitted
[14:30:50] Explicit valence for atom # 1 N, 4, is greater than permitted
[14:30:50] Explicit valence for atom # 1 N, 4, is greater than permitted
[14:30:50] Explicit valence for atom # 5 N, 4, is greater than permitted
[14:30:50] Explicit valence for atom # 20 N, 4, is greater than permitted
[14:30:50] Explicit valence for atom # 1 N, 4, is greater than permitted
[14:30:50] Explicit valence for atom # 20 N, 4, is greater than permitted
[14:30:50] Explicit valence for atom # 27 N, 4, is greater than permitted
[14:30:50] Explicit valence for atom # 28 N, 4, is greater than permitted
[14:30:50] Explicit valence for atom # 12 N, 4, is greater than permitted
[14:30:50] Explicit valence for atom # 5 N, 4, is greater than permitted
[14:30:50] Explicit valence for atom # 10 N, 4, is greater than permitted
[14:30:50] Explicit valence for atom # 10 N, 4, is greater than permitted
[14:30:50] Explicit valence for atom # 4 N, 4, is greater than permitted
[14:30:50] Explicit valence for atom # 1 N, 4, is greater than permitted
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[14:30:50] Explicit valence for atom # 16 N, 4, is greater than permitted
[14:30:50] Explicit valence for atom # 16 N, 4, is greater than permitted
[14:30:50] Explicit valence for atom # 1 N, 4, is greater than permitted
[14:30:50] Explicit valence for atom # 22 N, 4, is greater than permitted
[14:30:50] Explicit valence for atom # 12 N, 4, is greater than permitted
[14:30:50] Explicit valence for atom # 1 N, 4, is greater than permitted
[14:30:50] Explicit valence for atom # 1 N, 4, is greater than permitted
[14:30:50] Explicit valence for atom # 13 N, 4, is greater than permitted
[14:30:50] Explicit valence for atom # 1 N, 4, is greater than permitted
[14:30:50] Explicit valence for atom # 1 N, 4, is greater than permitted
[14:30:50] Explicit valence for atom # 23 N, 4, is greater than permitted
[14:30:50] Explicit valence for atom # 1 N, 4, is greater than permitted
[14:30:50] Explicit valence for atom # 1 N, 4, is greater than permitted
[14:30:50] Explicit valence for atom # 16 N, 4, is greater than permitted
[14:30:50] Explicit valence for atom # 1 N, 4, is greater than permitted
[14:30:50] Explicit valence for atom # 5 N, 4, is greater than permitted
[14:30:50] Explicit valence for atom # 1 N, 4, is greater than permitted
[14:30:50] Explicit valence for atom # 15 N, 4, is greater than permitted
[14:30:50] Explicit valence for atom # 5 N, 4, is greater than permitted
[14:30:[5014] :30:50] Explicit valence for atom # 1 N, 4, is greater than
permitted
Explicit valence for atom # 4 N, 4, is greater than permitted
[14:30:50] Explicit valence for atom # 1 N, 4, is greater than permitted
[14:30:50] Explicit valence for atom # 1 N, 4, is greater than permitted
[14:30:50] Explicit valence for atom # 12 N, 4, is greater than permitted
[14:30:50] Explicit valence for atom # 1 N, 4, is greater than permitted
[14:30:50] Explicit valence for atom # 1 N, 4, is greater than permitted
[14:30:50] Explicit valence for atom # 5 N, 4, is greater than permitted
[14:30:50] Explicit valence for atom # 1 N, 4, is greater than permitted
[14:30:50] Explicit valence for atom # 1 N, 4, is greater than permitted
[14:30:50] Explicit valence for atom # 12 N, 4, is greater than permitted
[14:30:50] Explicit valence for atom # 5 N, 4, is greater than permitted
[14:30:50] Explicit valence for atom # 15 N, 4, is greater than permitted
[14:30:50] Explicit valence for atom # 19 N, 4, is greater than permitted
[14:30:50] Explicit valence for atom # 9 N, 4, is greater than permitted
[14:30:50] Explicit valence for atom # 9 N, 4, is greater than permitted
[14:30:50] Explicit valence for atom # 15 N, 4, is greater than permitted
[14:30:50] Explicit valence for atom # 1 N, 4, is greater than permitted
[[14:30:1450] Explicit valence for atom # 12 N, 4, is greater than permitted
[14:30:50] Explicit valence for atom # 4 N, 4, is greater than permitted
:30:50] Explicit valence for atom # 1 N, 4, is greater than permitted
[14:30:50] Explicit valence for atom # 18 N, 4, is greater than permitted
[14:30:50] Explicit valence for atom # 12 N, 4, is greater than permitted
[14:30:50] Explicit valence for atom # 16 N, 4, is greater than permitted
[14:30:50] Explicit valence for atom # 16 N, 4, is greater than permitted
[14:30:50] Explicit valence for atom # 12 N, 4, is greater than permitted
[14:30:50] Explicit valence for atom # 12 N, 4, is greater than permitted
[14:30:50] Explicit valence for atom # 15 N, 4, is greater than permitted
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[14:30:50] Explicit valence for atom # 24 N, 4, is greater than permitted
[14:30:50] Explicit valence for atom # 1 N, 4, is greater than permitted
[14:30:50] Explicit valence for atom # 15 N, 4, is greater than permitted
[14:30:50] Explicit valence for atom # 15 N, 4, is greater than permitted
[14:30:50] Explicit valence for atom # 12 N, 4, is greater than permitted
[14:30:50] Explicit valence for atom # 5 N, 4, is greater than permitted
[14:30:50] Explicit valence for atom # 1 N, 4, is greater than permitted
[14:30:50] Explicit valence for atom # 11 N, 4, is greater than permitted
[14:30:50] Explicit valence for atom # 1 N, 4, is greater than permitted
[14:30:50] Explicit valence for atom # 1 N, 4, is greater than permitted
[14:30:50] Explicit valence for atom # 1 N, 4, is greater than permitted
[14:30:50] Explicit valence for atom # 5 N, 4, is greater than permitted
[14:30:50] Explicit valence for atom # 1 N, 4, is greater than permitted
[14:30:50] Explicit valence for atom # 4 N, 4, is greater than permitted
[14:30:50] Explicit valence for atom # 1 N, 4, is greater than permitted
[14:30:50] Explicit valence for atom # 11 N, 4, is greater than permitted
[14:30:50] Explicit valence for atom # 18 N, 4, is greater than permitted
[14:30:50] Explicit valence for atom # 21 N, 4, is greater than permitted
[14:30:50] Explicit valence for atom # 1 N, 4, is greater than permitted
[14:30:50] Explicit valence for atom # 18 N, 4, is greater than permitted
[14:30:50] Explicit valence for atom # 18 N, 4, is greater than permitted
[14:30:50] Explicit valence for atom # 1 N, 4, is greater than permitted
[14:30:50] Explicit valence for atom # 20 N, 4, is greater than permitted
[14:30:50] Explicit valence for atom # 25 N, 4, is greater than permitted
[14:30:50] Explicit valence for atom # 24 N, 4, is greater than permitted
[14:30:50] Explicit valence for atom # 1 N, 4, is greater than permitted
[14:30:50] Explicit valence for atom # 1 N, 4, is greater than permitted
[14:30:50[] Explicit valence for atom # 1 N, 4, is greater than permitted
14:30:50] Explicit valence for atom # 15 N, 4, is greater than permitted
[14:30:50] Explicit valence for atom # 1 N, 4, is greater than permitted
[14:30:50] Explicit valence for atom # 1 N, 4, is greater than permitted
[14:30:50] Explicit valence for atom # 22 N, 4, is greater than permitted
[14:30:50] Explicit valence for atom # 1 N, 4, is greater than permitted
[14:30:50] Explicit valence for atom # 1 N, 4, is greater than permitted
[14:30:50] Explicit valence for atom # 1 N, 4, is greater than permitted
[14:30:50] Explicit valence for atom # 1 N, 4, is greater than permitted
[14:30:50] Explicit valence for atom # 1 N, 4, is greater than permitted
[14:30:50] Explicit valence for atom # 1 N, 4, is greater than permitted
[14:30:50] Explicit valence for atom # 1 N, 4, is greater than permitted
[14:30:50] Explicit valence for atom # 1 N, 4, is greater than permitted
[14:30:50] Explicit valence for atom # 1 N, 4, is greater than permitted
[14:30:50] Explicit valence for atom # 20 N, 4, is greater than permitted
[14:30:50] Explicit valence for atom # 9 N, 4, is greater than permitted
[14:30:50] Explicit valence for atom # 27 N, 4, is greater than permitted
[14:30:50] Explicit valence for atom # 27 N, 4, is greater than permitted
[14:30:50] Explicit valence for atom # 1 N, 4, is greater than permitted
[14:30:50] Explicit valence for atom # 8 N, 4, is greater than permitted
[14:30:50] Explicit valence for atom # 13 N, 4, is greater than permitted
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[14:30:50] Explicit valence for atom # 5 N, 4, is greater than permitted
[14:30:50] Explicit valence for atom # 1 N, 4, is greater than permitted
[14:30:50] Explicit valence for atom # 5 N, 4, is greater than permitted
[14:30:50] Explicit valence for atom # 20 N, 4, is greater than permitted
[14:30:50] Explicit valence for atom # 5 N, 4, is greater than permitted
[14:30:50] Explicit valence for atom # 18 N, 4, is greater than permitted
[14:30:50] Explicit valence for atom # 1 N, 4, is greater than permitted
[14:30:50] Explicit valence for atom # 1 N, 4, is greater than permitted
[14:30:50] Explicit valence for atom # 10 N, 4, is greater than permitted
[14:30:50] Explicit valence for atom # 10 N, 4, is greater than permitted
[14:30:50] Explicit valence for atom # 11 N, 4, is greater than permitted
[14:30:50] Explicit valence for atom # 1 N, 4, is greater than permitted
[14:30:50] Explicit valence for atom # 12 N, 4, is greater than permitted
[14:30:50] Explicit valence for atom # 18 N, 4, is greater than permitted
[14:30:50] Explicit valence for atom # 16 N, 4, is greater than permitted
[14:30:50] Explicit valence for atom # 1 N, 4, is greater than permitted
[14:30:50] Explicit valence for atom # 5 N, 4, is greater than permitted
[14:30:50] Explicit valence for atom # 1 N, 4, is greater than permitted
[14:30:50] Explicit valence for atom # 19 N, 4, is greater than permitted
[14:30:50] Explicit valence for atom # 15 N, 4, is greater than permitted
[14:30:50] Explicit valence for atom # 22 N, 4, is greater than permitted
[14:30:50] Explicit valence for atom # 15 N, 4, is greater than permitted
[14:30:50] Explicit valence for atom # 17 N, 4, is greater than permitted
[14:30:50] Explicit valence for atom # 21 N, 4, is greater than permitted
[14:30:50] Explicit valence for atom # 17 N, 4, is greater than permitted
[14:30:50] Explicit valence for atom # 2 N, 4, is greater than permitted
[14:30:50] Explicit valence for atom # 15 N, 4, is greater than permitted
[14:30:50] Explicit valence for atom # 15 N, 4, is greater than permitted
[14:30:50] Explicit valence for atom # 5 N, 4, is greater than permitted
[14:30:50] Explicit valence for atom # 1 N, 4, is greater than permitted
[14:30:50] Explicit valence for atom # 15 N, 4, is greater than permitted
[14:30:50] Explicit valence for atom # 15 N, 4, is greater than permitted
[14:30:50] Explicit valence for atom # 15 N, 4, is greater than permitted
[14:30:50] Explicit valence for atom # 14 N, 4, is greater than permitted
[14:30:50] Explicit valence for atom # 1 N, 4, is greater than permitted
[14:30:50] Explicit valence for atom # 1 N, 4, is greater than permitted
[14:30:50] Explicit valence for atom # 1 N, 4, is greater than permitted
[14:30:50] Explicit valence for atom # 25 N, 4, is greater than permitted
[14:30:50] Explicit valence for atom # 9 N, 4, is greater than permitted
[14:30:50] Explicit valence for atom # 1 N, 4, is greater than permitted
[14:30:50] Explicit valence for atom # 1 N, 4, is greater than permitted
[14:30:50] Explicit valence for atom # 21 N, 4, is greater than permitted
[14:30:50] Explicit valence for atom # 21 N, 4, is greater than permitted
[14:30:50] Explicit valence for atom # 1 N, 4, is greater than permitted
[14:30:50] Explicit valence for atom # 12 N, 4, is greater than permitted
[14:30:50] Explicit valence for atom # 1 N, 4, is greater than permitted
[14:30:50] Explicit valence for atom # 1 N, 4, is greater than permitted
[14:30:50] Explicit valence for atom # 14 N, 4, is greater than permitted
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[14:30:50] Explicit valence for atom # 18 N, 4, is greater than permitted
[14:30:50[] Explicit valence for atom # 5 N, 4, is greater than permitted
14:30:50] Explicit valence for atom # 28 N, 4, is greater than permitted
[14:30:50] Explicit valence for atom # 5 N, 4, is greater than permitted
[14:30:50] Explicit valence for atom # 1 N, 4, is greater than permitted
[14:30:50] Explicit valence for atom # 19 N, 4, is greater than permitted
[14:30:50] Explicit valence for atom # 19 N, 4, is greater than permitted
[14:30:50] Explicit valence for atom # 1 N, 4, is greater than permitted
[14:30:50] Explicit valence for atom # 1 N, 4, is greater than permitted
[14:30:50] Explicit valence for atom # 1 N, 4, is greater than permitted
[14:30:50] Explicit valence for atom # 18 N, 4, is greater than permitted
[14:30:50] Explicit valence for atom # 26 N, 4, is greater than permitted
[[14:30:1450] :30Explicit valence for atom # 1 N, 4, is greater than permitted
:50] Explicit valence for atom # 5 N, 4, is greater than permitted
[14[:30:14:50] 30:Explicit valence for atom # 1 N, 4, is greater than permitted
50] Explicit valence for atom # 5 N, 4, is greater than permitted
[14:30:50] Explicit valence for atom # 14 N, 4, is greater than permitted
[14:30:50] Explicit valence for atom # 18 N, 4, is greater than permitted
[14:30:50] Explicit valence for atom # 15 N, 4, is greater than permitted
[14:30:50] Explicit valence for atom # 23 N, 4, is greater than permitted
[14:30:50] Explicit valence for atom # 1 N, 4, is greater than permitted
[14:30:50] Explicit valence for atom # 15 N, 4, is greater than permitted
[14:30:50] Explicit valence for atom # 15 N, 4, is greater than permitted
[14:30:50] Explicit valence for atom # 1 N, 4, is greater than permitted
[14:30:50] Explicit valence for atom # 17 N, 4, is greater than permitted
[14:30:50] Explicit valence for atom # 5 N, 4, is greater than permitted
[14:30:50] Explicit valence for atom # 9 N, 4, is greater than permitted
[14:30:50] Explicit valence for atom # 1 N, 4, is greater than permitted
[14:30:50] Explicit valence for atom # 15 N, 4, is greater than permitted
[14:30:50] Explicit valence for atom # 19 N, 4, is greater than permitted
[14:30:50] Explicit valence for atom # 24 N, 4, is greater than permitted
[14:30:50] Explicit valence for atom # 1 N, 4, is greater than permitted
[14:30:50] Explicit valence for atom # 1 N, 4, is greater than permitted
[14:30:50] Explicit valence for atom # 27 N, 4, is greater than permitted
[14:30:50] Explicit valence for atom # 1 N, 4, is greater than permitted
[14:30:50] Explicit valence for atom # 1 N, 4, is greater than permitted
[14:30:50] Explicit valence for atom # 5 N, 4, is greater than permitted
[14:30:50] Explicit valence for atom # 21 N, 4, is greater than permitted
[14:30:50] Explicit valence for atom # 21 N, 4, is greater than permitted
[14:30:50] Explicit valence for atom # 1 N, 4, is greater than permitted
[14:30:50] Explicit valence for atom # 1 N, 4, is greater than permitted
[14:30:50] Explicit valence for atom # 12 N, 4, is greater than permitted
[14:30:50] Explicit valence for atom # 13 N, 4, is greater than permitted
[14:30:50] Explicit valence for atom # 13 N, 4, is greater than permitted
[14:30:50] Explicit valence for atom # 21 N, 4, is greater than permitted
[14:30:50] Explicit valence for atom # 15 N, 4, is greater than permitted
[14:30:50] Explicit valence for atom # 25 N, 4, is greater than permitted
[14:30:50] Explicit valence for atom # 1 N, 4, is greater than permitted
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[14:30:50] Explicit valence for atom # 1 N, 4, is greater than permitted
[14:30:50] Explicit valence for atom # 19 N, 4, is greater than permitted
[14:30:50] Explicit valence for atom # 1 N, 4, is greater than permitted
[14:30:50] Explicit valence for atom # 28 N, 4, is greater than permitted
[14:30:50] Explicit valence for atom # 1 N, 4, is greater than permitted
[14:30:50] Explicit valence for atom # 5 N, 4, is greater than permitted
[14:30:50] Explicit valence for atom # 22 N, 4, is greater than permitted
[14:30:50] Explicit valence for atom # 1 N, 4, is greater than permitted
[14:30:50] Explicit valence for atom # 15 N, 4, is greater than permitted
[14:30:50] Explicit valence for atom # 24 N, 4, is greater than permitted
[14:30:50] Explicit valence for atom # 15 N, 4, is greater than permitted
[14:30:50] Explicit valence for atom # 20 N, 4, is greater than permitted
[14:30:50] Explicit valence for atom # 1 N, 4, is greater than permitted
[14:30:50] Explicit valence for atom # 1 N, 4, is greater than permitted
[14:30:50] Explicit valence for atom # 5 N, 4, is greater than permitted
[14:30:50] Explicit valence for atom # 1 N, 4, is greater than permitted
[14:30:50] Explicit valence for atom # 1 N, 4, is greater than permitted
[14:30:50] Explicit valence for atom # 12 N, 4, is greater than permitted
[14:30:50] Explicit valence for atom # 21 N, 4, is greater than permitted
[14:30:50] Explicit valence for atom # 15 N, 4, is greater than permitted
[14:30:50] Explicit valence for atom # 15 N, 4, is greater than permitted
[14:30:50] Explicit valence for atom # 15 N, 4, is greater than permitted
[14:30:50] Explicit valence for atom # 15 N, 4, is greater than permitted
[14:30:50] Explicit valence for atom # 15 N, 4, is greater than permitted
[14:30:50] Explicit valence for atom # 1 N, 4, is greater than permitted
[14:30:50] Explicit valence for atom # 12 N, 4, is greater than permitted
[14:30:50] Explicit valence for atom # 1 N, 4, is greater than permitted
[14:30:50] Explicit valence for atom # 13 N, 4, is greater than permitted
[14:30:50] Explicit valence for atom # 1 N, 4, is greater than permitted
[14:30:50] Explicit valence for atom # 1 N, 4, is greater than permitted
[14:30:50] Explicit valence for atom # 18 N, 4, is greater than permitted
[14:30:50] Explicit valence for atom # 1 N, 4, is greater than permitted
[14:30:50] Explicit valence for atom # 5 N, 4, is greater than permitted
[14:30:50] Explicit valence for atom # 3 N, 4, is greater than permitted
[14:30:50] Explicit valence for atom # 29 N, 4, is greater than permitted
[14:30:50] Explicit valence for atom # 15 N, 4, is greater than permitted
[14:30:50] Explicit valence for atom # 18 N, 4, is greater than permitted
[14:30:50] Explicit valence for atom # 1 N, 4, is greater than permitted
[14:30:50] Explicit valence for atom # 1 N, 4, is greater than permitted
[14:30:50] Explicit valence for atom # 1 N, 4, is greater than permitted
[14:30:50] Explicit valence for atom # 13 N, 4, is greater than permitted
[14:30:50] Explicit valence for atom # 11 N, 4, is greater than permitted
[14:30:50] Explicit valence for atom # 11 N, 4, is greater than permitted
[14:30:50] Explicit valence for atom # 21 N, 4, is greater than permitted
[14:30:50] Explicit valence for atom # 15 N, 4, is greater than permitted[
14:30:50] Explicit valence for atom # 22 N, 4, is greater than permitted
[14:30:50] Explicit valence for atom # 1 N, 4, is greater than permitted
[14:30:50] Explicit valence for atom # 1 N, 4, is greater than permitted
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[14:30:50] Explicit valence for atom # 20 N, 4, is greater than permitted
[14:30:50] Explicit valence for atom # 1 N, 4, is greater than permitted
[14:30:50] Explicit valence for atom # 22 N, 4, is greater than permitted
[14:30:50] Explicit valence for atom # 21 N, 4, is greater than permitted
[14:30:50] Explicit valence for atom # 1 N, 4, is greater than permitted
[14:30:50] Explicit valence for atom # 1 N, 4, is greater than permitted
[14:30:50] Explicit valence for atom # 17 N, 4, is greater than permitted
[14:30:50] Explicit valence for atom # 18 N, 4, is greater than permitted
[14:30:50] Explicit valence for atom # 1 N, 4, is greater than permitted
[14:30:50] Explicit valence for atom # 1 N, 4, is greater than permitted
[14:30:50] Explicit valence for atom # 12 N, 4, is greater than permitted
[14:30:50] Explicit valence for atom # 1 N, 4, is greater than permitted
[14:30:50] Explicit valence for atom # 1 N, 4, is greater than permitted
[14:30:50] Explicit valence for atom # 9 N, 4, is greater than permitted
[14:30:50] Explicit valence for atom # 9 N, 4, is greater than permitted
[14:30:50] Explicit valence for atom # 9 N, 4, is greater than permitted
[14:30:50] Explicit valence for atom # 1 N, 4, is greater than permitted
Wrote SMILES for molecules passing filters to all.smi
Wrote detailed data to all.csv
1826 of 2608 passed filters 70.0%
Elapsed time 0.82 seconds
```

[23]:
```python
df_rd_filter = pd.read_csv('../pipeline/5_PAINS_rd_filter/all.csv')
df_rd_filter.head()
```

[23]:
```
                                              SMILES          NAME FILTER  \
0  O(c1cc(ccc1)\C=C(\c2nc(nc(n2)N)Nc3ccccc3)/C#N)…  ZINC55039390     OK
1  O(c1c(cccc1)\C=C\C(=O)Nc2nn4c(n2)N[C@@H](c3ccc…  ZINC09185435     OK
2  O(c1ccc(cc1)[C@H]4n2nc(nc2N[C@@H](c3ccccc3)C4)…  ZINC02404424     OK
3  O(c1ccc(cc1)[C@H]4n2nc(nc2N[C@@H](c3ccccc3)C4)…  ZINC05307450     OK
4  Clc1c(cccc1)\C=C\C(=O)Nc2nn4c(n2)N[C@@H](c3ccc…  ZINC09158125     OK

        MW     LogP  HBD  HBA    TPSA  Rot
0  388.431  3.28678    2    8  118.97  8.0
1  481.556  5.09350    2    7   90.30  7.0
2  439.519  4.61420    2    6   81.07  6.0
3  393.447  3.01790    2    7   90.30  6.0
4  485.975  5.73830    2    6   81.07  6.0
```

[28]:
```python
#identify which filters remove the largest number of molecules

from collections import Counter

def counter(df):
    count_list = list(Counter(df.FILTER).items())
    count_df = pd.DataFrame(count_list, columns=['Rule', 'Count'])
    count_df.sort_values('Count', inplace=True, ascending=False)
    return count_df

counter(df_rd_filter)
```

[28]:

```
                                  Rule  Count
0                                   OK   2065
1                              INVALID    399
4                    Filter9_metal > 0     52
7               Filter82_pyridinium > 0     37
6                Filter20_hydrazine > 0     10
10  Filter14_thio_oxopyrylium_salt > 0     10
2                    Filter39_imine > 0      9
9               Filter58_polyphenol2 > 0     7
3                 Filter38_aldehyde > 0      4
11     Filter4_alpha_halo_carbonyl > 0      4
8           Filter94_2_halo_pyridine > 0     3
14      Filter44_michael_acceptor2 > 0      3
5            Filter78_bicyclic_Imide > 0     2
13          Filter81_Thiocarbamate > 0      2
12           Filter69_thio_carbonate > 0     1
```

[26]:

```
len(df_rd_filter['NAME'].unique())
```

[26]: 1848

[27]:

```
df_rd_filter_unique = df_rd_filter.drop_duplicates('NAME')
df_rd_filter_unique.shape
```

[27]: (1848, 9)

[29]:

```
counter(df_rd_filter_unique)
```

[29]:

```
                                  Rule  Count
0                                   OK   1457
1                              INVALID    286
4                    Filter9_metal > 0     34
7               Filter82_pyridinium > 0     30
10  Filter14_thio_oxopyrylium_salt > 0      9
6                Filter20_hydrazine > 0      7
2                    Filter39_imine > 0      6
9               Filter58_polyphenol2 > 0     4
3                 Filter38_aldehyde > 0      3
8           Filter94_2_halo_pyridine > 0     3
11     Filter4_alpha_halo_carbonyl > 0      3
13          Filter81_Thiocarbamate > 0      2
14      Filter44_michael_acceptor2 > 0      2
5            Filter78_bicyclic_Imide > 0     1
```

```
12         Filter69_thio_carbonate > 0      1
```

[ ]:

```

```