

# Untitled2

January 8, 2019

```
In [1]: from rdkit import Chem
        from rdkit.Chem import PandasTools
        import pandas as pd
```

```
In [3]: frame = PandasTools.LoadSDF('data/TR_WS_3158.sdf')
```

```
In [4]: frame.head()
```

```
Out[4]:
```

	CAS	Canonical_QSARr
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