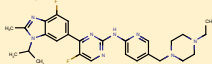


Inputs

Drug



SMILES

```
CCN1CCN(CC2=CC=C(NC3=NC=C(F)C(=N3)C3=CC(F)=C4N=C(C)N(C(C)C)C4=C3)N=C2)CC1
```

Model

Bag-of-n-grams
Model

Bag Of
Words

Select TopK and move
others to UNK (unknown)

Create
Sequence

MLP

Outputs

Output Probabilities

