

ZINC Clean Leads



4 591 276
molecules



- Macrocycles
- Atom types
- MCF
- PAINS

MOSES dataset



1 936 962
molecules


Training


Test


Test with new
scaffolds

MODELS

Language model

VAE

AAE

LatentGAN

Junction Tree VAE

...

METRICS

FCD

Diversity

Uniqueness


Validity

...

LEADERBOARD



 Contributions

 Contributions