

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

ORGAN

Junction Tree VAE

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 Contributions

METRICS

FCD

Diversity

Uniqueness

Validity

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 Contributions

LEADERBOARD

