**Molecular generative model based on conditional variational autoencoder for novel molecular design**

Abstract

Background

A screenshot of a computer

Description automatically generated

A screenshot of a computer

Description automatically generated

Data Visualization

Clustering

* KMeans
* Agglomerative

Clustering Evaluation

* Elbow

Dimensionality Reduction

* PCA
* TSNE

Dataset Images

A molecule structure with colored lines

Description automatically generatedA structure of a molecule

Description automatically generatedA black and white drawing of a molecule

Description automatically generatedA structure of a molecule

Description automatically generatedA structure of a molecule

Description automatically generated

Generated Images

A structure of a chemical formula

Description automatically generatedA black and white drawing of a molecule

Description automatically generatedA black and white image of a molecule

Description automatically generatedA black and white image of a molecule

Description automatically generated

Method/Components

Dataset

* Preprocessing SMILES
* RDKit Images from SMILES
* Conditions
* Input File

Model Generation

* Variational Auto Encoder
* Multiple Models

Input Synthesis

* Dataset of Possible Starting Molecules
* Dataset of Conditions
* NLP for user input
* Decide Input

Generating Molecules

* Generate Multiple molecules
* Verify Molecule is Valid
* Create Molecule Profile

Docking/Simulating

Ranking

A diagram of a model

Description automatically generated

Results

A colorful dots in a circle

Description automatically generated

A colorful dots on a blue background

Description automatically generated

Conclusion

References

<https://github.com/DanielFlockhart/Molecular-Generation>

<https://www.nature.com/articles/s41597-022-01142-7>

<https://arxiv.org/pdf/2209.01712.pdf>

<https://jcheminf.biomedcentral.com/articles/10.1186/s13321-018-0286-7>