**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

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

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>