De Novo Molecular Generation with Stacked Adversarial Model

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• Introduction

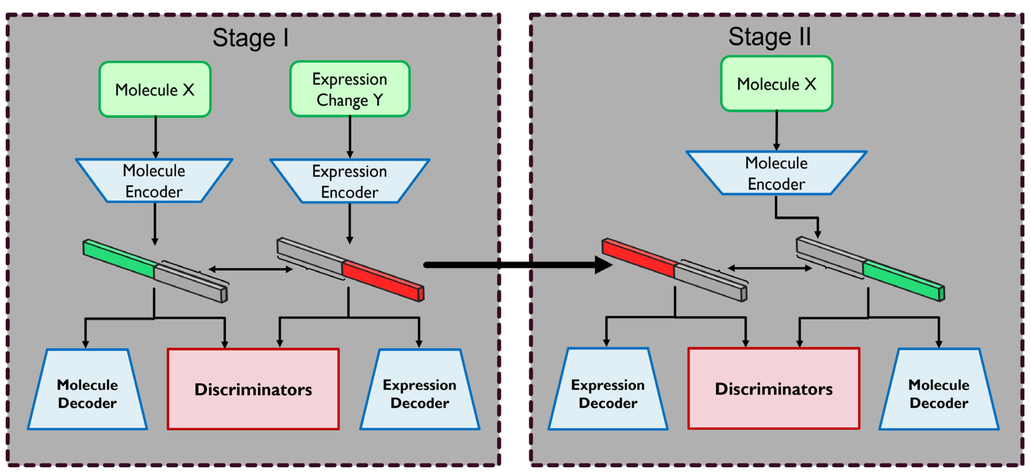
Generating novel drug molecules with **desired biological properties** is a time consuming and complex task.

Conditional **generative adversarial** models have recently been proposed as promising approaches for de novo drug design.

Can these models be further improved to generate more **valid** and **biological meaningful** molecules?

• Method

Stacking technique has been proved successful in image generation tasks. Therefore, it was adapted for molecular generation.



The **SBiAAE** model consists two similar previous proposed model, **BiAAE**.

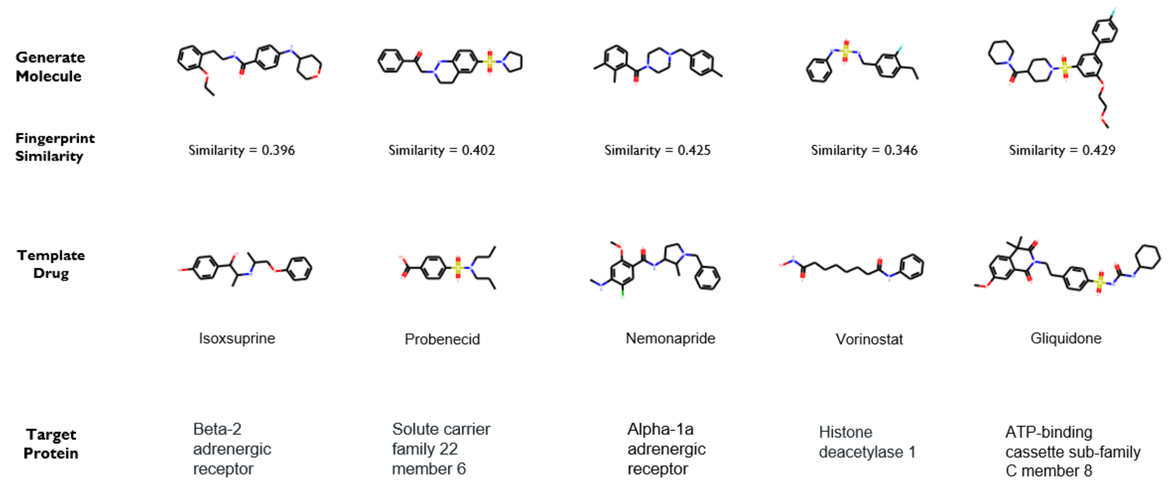
By stacking together, they are expected to learn a better **latent representation** of both **molecule** and **expression change**, so that:

1. Generating more valid molecules
2. Generating molecules that can meet the prior requirements better.

• Result

Similarity principle : compounds that are similar to biologically active ones should also be active and vice versa
The **validity** evaluates how often the model generates valid molecule.
The **similarity** measures how close the generated molecules are to their templates.

Model	Validity	Similarity
BiAAE	64.7%	0.247
SBiAAE	69.1%	0.265



• Conclusion

The stacking technique has been successfully adopted for the existing BiAAE model, formed **SBiAAE** and helped with the **De novo molecular generation** task. This may potentially increase the **productivity** of the **drug design** and benefit the human beings.

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