Addendum: molecular generation for desired transcriptome changes with adversarial...

Health & Medicine

An Addendum on

Molecular Generation for Desired Transcriptome Changes With Adversarial Autoencoders

By Shayakhmetov R, Kuznetsov M, Zhebrak A, Kadurin A, Nikolenko S, Aliper A and Polykovskiy D (2020). Front. Pharmacol. 11: 269. doi: 10. 3389/fphar. 2020. 00269

In the original article, we missed the parallel work by Méndez-Lucio et al. (2020) . This work also tackles a similar problem of generating molecular structures from transcriptomic data. The authors proposed a conditional model based on the generative adversarial networks Goodfellow et al. (2014) . Unlike their approach, our model is joint, allowing us to generate molecular structures for a given gene expression profile and vice versa.

References

Goodfellow, I., Pouget-Abadie, J., Mirza, M., Xu, B., Warde-Farley, D., Ozair, S., et al. (2014). " Generative adversarial nets," in *Advances in Neural Information Processing Systems.* (Curran Associates, Inc), vol. 27, 2672–2680.

Google Scholar

Méndez-Lucio, O., Baillif, B., Clevert, D.-A., Rouquié, D., Wichard, J. (2020). De novo generation of hit-like molecules from gene expression signatures using artificial intelligence. *Nat. Commun.* 11, 1–10. doi: 10. 1038/s41467-019-13807-w

PubMed Abstract | CrossRef Full Text | Google Scholar