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SMILES, for AI

Genome, from the land of Biology, once gets represented as a sequence of ATCG letters, comes to land of string-computation.

Similarly, molecule, from the land of Chemistry, once get represented in SMILES (Simplified Molecular Input Line Entry System) string format, comes to land of string-computation.

Example: Benzene gets represented as "c1ccccc1".

Once in the land of strings, these representations become amenable to new age techniques of Artificial Intelligence (AI), like Machine Learning (ML) and Deep Learning (DL) on sequences, via various embedding techniques.

Came across this wonderful article on the same topic at [Towards Data Science](https://lnkd.in/gFq6Z6bq)
<https://lnkd.in/gFq6Z6bq>

Immediate application is in the field of drug discovery, where screening the universe of all possible molecule combinations becomes humanly impossible, for a given target/disease. Use of AI/ML/DL looks promising in this search of a needle in the haystack.

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Basic Molecular Representation for Machine Learning

towardsdatascience.com • 2 min read

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