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Prediction of RNA structure with equivariant neural networks

A new deep-learning system called Atomic Rotationally Equivariant Scorer (ARES) significantly improves the prediction of RNA structures over previous artificial intelligence (AI) models. The advance, described by Stanford University researchers in a paper in Science may help scientists uncover the biological functions of RNA and pave the way to the discovery of novel RNA-targeted drugs ("ARES deep-learning system improves 3D RNA structure prediction").

When paired with software to sample the space of possible RNA structural models, ARES is able to achieve improved performance in the prediction of 3D RNA structure. Such a method could be useful for structure-based virtual screening, assuming the predicted structures are sufficiently accurate. This approach uses an atomistic representation of the RNA structural models.

ARES outperformed at least nine other methods to come out on top in a community-wide RNA-puzzles contest.

Applications

- Development of RNA-targeted drugs for a wide variety of diseases, particularly infectious (e.g., viral) diseases, hereditary chronic conditions, and currently "untreatable" diseases
- Identification of specific RNA molecules as drug targets
- Customers include pharmaceutical companies, biotech companies, and organization that offer services to these companies

Advantages

- This method allows for substantially more accurate prediction of RNA structure than the previous state of the art
- Tremendous commercial interest in computational prediction of RNA 3D structure

Publications

- Townshend et al. Science (2021) "Geometric deep learning of RNA structure" *Science* (2021).
- Eismann et al. Proteins (2020) "Hierarchical, rotation-equivariant neural networks to select structural models of protein complexes
- Swafford, Isabel. Stanford News (8.26.2021) Stanford machine learning algorithm predicts biological structures more accurately than ever before

Patents

- Published Application: WO2022246473
- Published Application: 20240233861

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