



# SEMINARIUM INSTYTUTOWE

*przy współudziale*

Katedry Informatyki i Inżynierii Systemów  
na Wydziale Informatyki i Zarządzania  
Politechniki Wrocławskiej

10 lipca 2024 r., środa, godz. **13:15**  
Sala 200

## ***Graph neural networks in assessing the quality of 3D RNA models***

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### **Abstract**

Reliable quality assessment and ranking of 3D RNA structures are crucial to identifying limitations and practical applications of their models designed *in silico*. Currently, the accuracy of predictions generated by the increasing number of computational methods is mainly analyzed in the context of a reference structure. However, what is lacking are reliable tools for the independent evaluation of 3D RNA models when the reference structure is unknown. In our work, we face this problem and propose an application of graph neural networks (GNNs) in modeling inter-structure relationships and evaluating the quality of 3D RNA structures.

The GNN-based system developed by us operates on local descriptors of the 3D RNA structure. The system was trained on a diverse, high-quality training set, which consists of local descriptors sourced from 737 experimentally (i.e. derived by biological experiments) determined 3D RNA structures (targets) and local descriptors of 17,790 3D RNA structures predicted by RNAComposer\* for all targets considered. Next, the 870,367 descriptors derived from the predicted structures were scored in terms of their compatibility with the corresponding target descriptors. This provided us with RMSD (root mean square deviation) values that together with the respective descriptors could fuel the GNN.

Our approach was benchmarked against ARES, to our knowledge the only similar tool for reference-free evaluation of 3D RNA models. We also tested our approach on a set of predictions from the RNA-Puzzles data set. Both experiments proved the efficiency of GNNs in evaluating and ranking 3D RNA models in terms of their quality. We hope that the presented method will contribute to new standards for the assessment of 3D RNA structures and serve to filter untrustworthy conformations produced by predictive methods targeting RNA.

\* *RNAComposer is the automated RNA structure 3D modeling server developed by the scientists from the Institute of Bioorganic Chemistry of the Polish Academy of Sciences and Poznań University of Technology.*