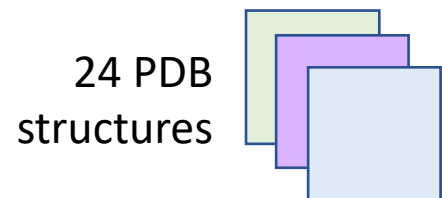


×

All-atom MD simulation

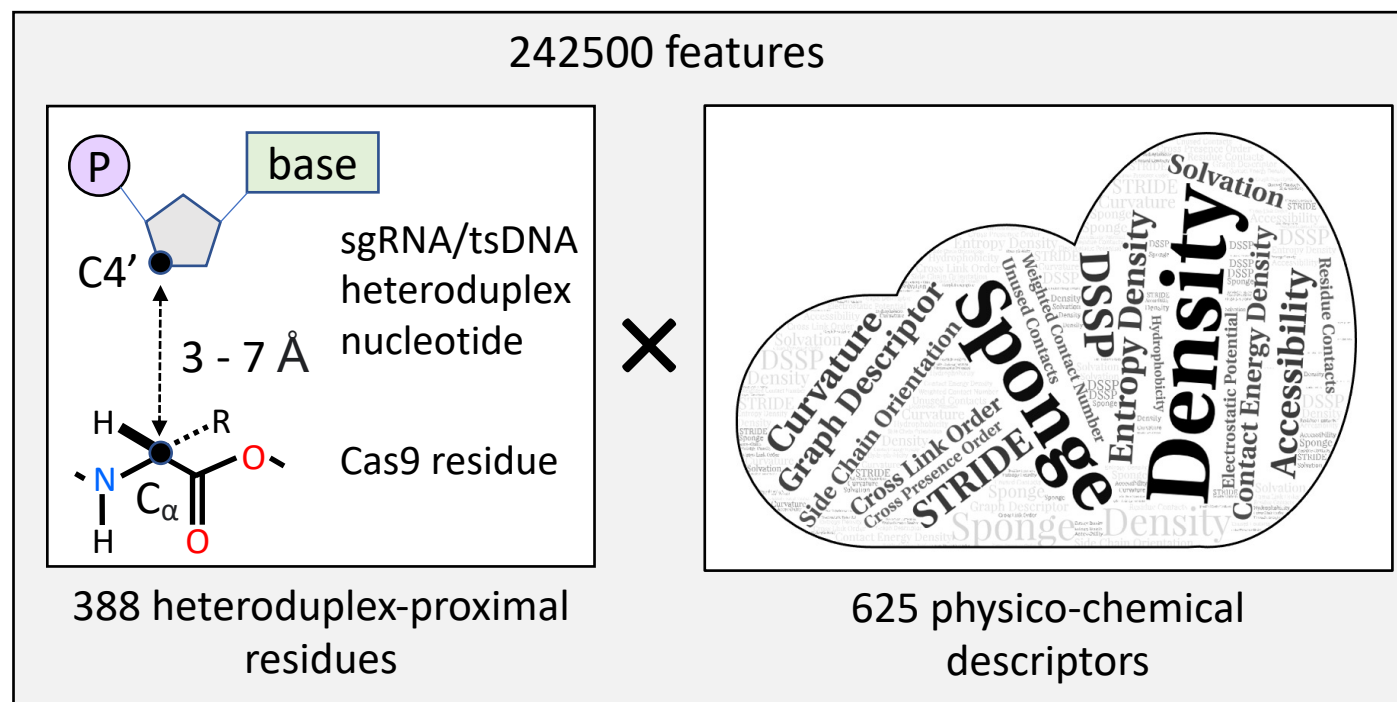


×

28 MD trajectories

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Extract BlueStar STING features



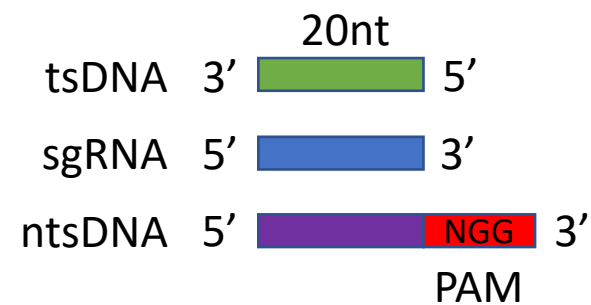
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SHAP-based feature reduction via XGBoost training

21 features XGBoost model

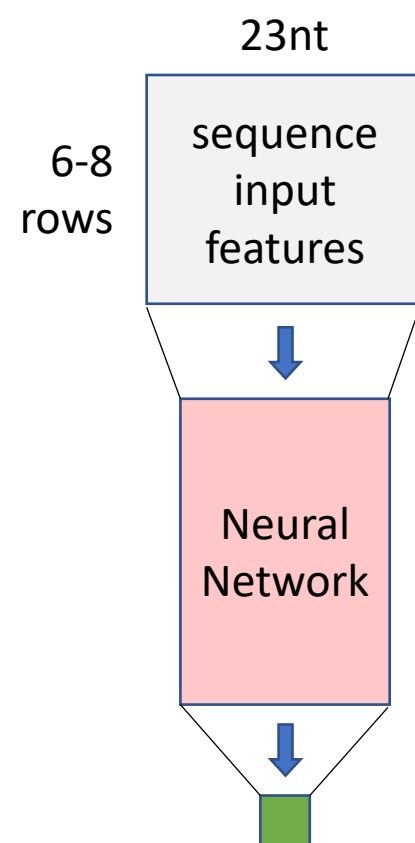


Sequence approach



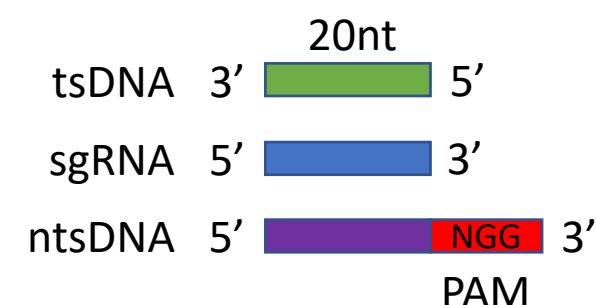
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One-hot encode



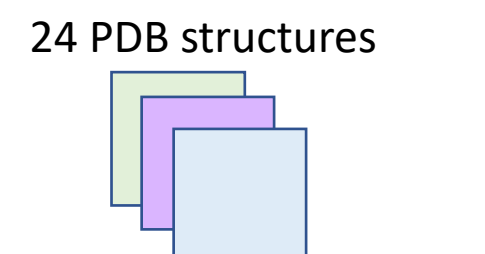
Predicted CRISPR-Cas9 cleavage activity

Nanoenvironment approach



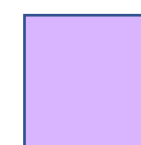
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All-atom MD simulation



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Randomly sample PDB structure



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Extract BlueStar STING features

21 input features

Nanoenv-Cas9-WNA

Predicted CRISPR-Cas9 cleavage activity

