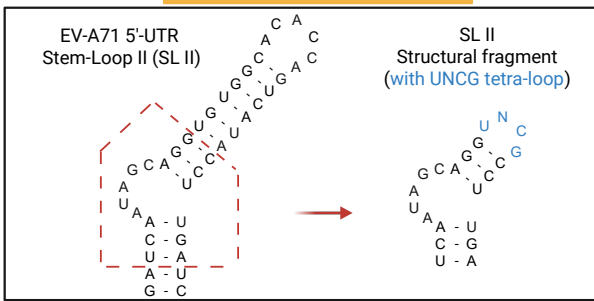
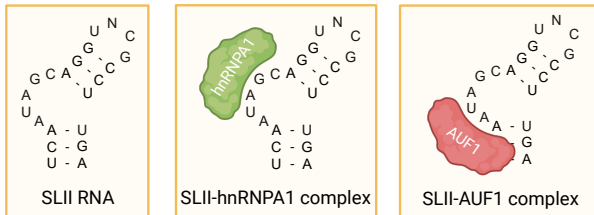


SIMULATION PIPELINE



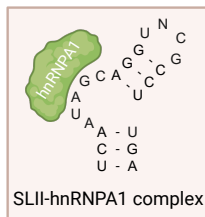
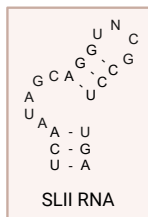
3D-structure prediction using a tool of your choice (eg: FARFAR2, AlphaFold3, DeepFoldRNA, RhoFold)



Do 3D-structure predictions of Protein-RNA complexes agree with NMR-validated Protein-RNA interface?

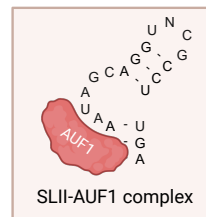
Yes

Use the predicted 3D- structures of Protein-RNA complexes



No

Build the HADDOCK models of Protein-RNA complexes



Molecular Dynamic (MD)- simulations of RNA/Proteins/Protein-RNA complexes

Docking the library of FDA-approved drugs with structures of RNA/Proteins/Protein-RNA complexes selected from MD-simulations

Drugs binding SLII

①

Drugs binding SLII-hnRNP A1 complex

②

Drugs binding hnRNP A1

③

Drugs binding SLII-AUF1 complex

④

Drugs binding AUF1

⑤

Drug candidates to modulate SLII-hnRNP A1 complex

Drug candidates to modulate SLII-AUF complex