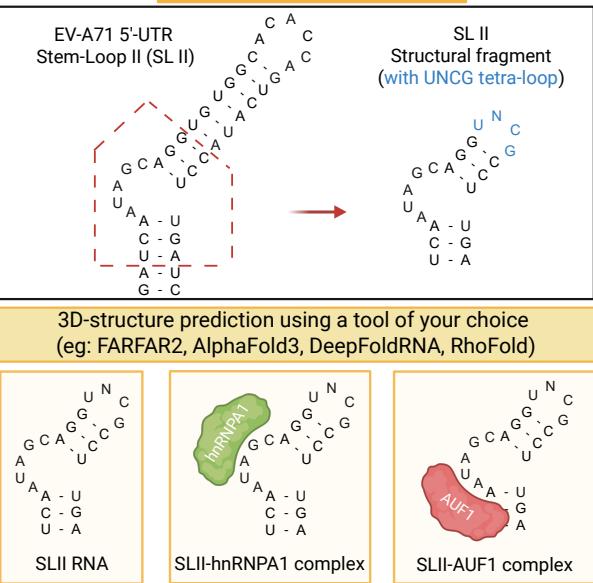
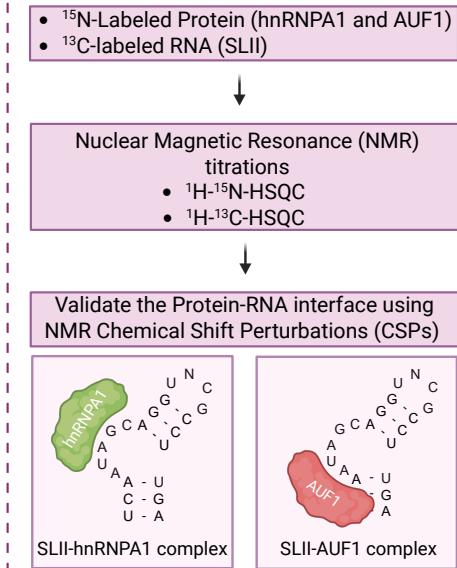


SIMULATION PIPELINE



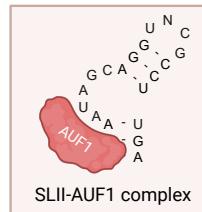
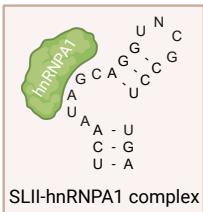
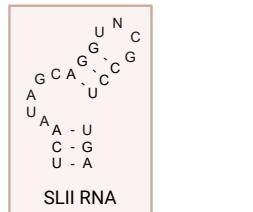
EXPERIMENTAL VALIDATION



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

Yes

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

Drugs binding SLII-hnRNPA1 complex

Drugs binding hnRNPA1

Drugs binding SLII-AUF1 complex

Drugs binding AUF1

①

②

③

④

⑤

