Indian Journal of Biochemistry & Biophysics
Vol. 63, August 2026, pp. 958-968
DOI: 10.56042/ijbb.v63i8.20784

Simulated docking and binding of Conantokin-P and Conantokin-Pr3 to NMDA receptor GluN2B subunit: Roles of calcium ions and gamma-carboxyglutamate residues

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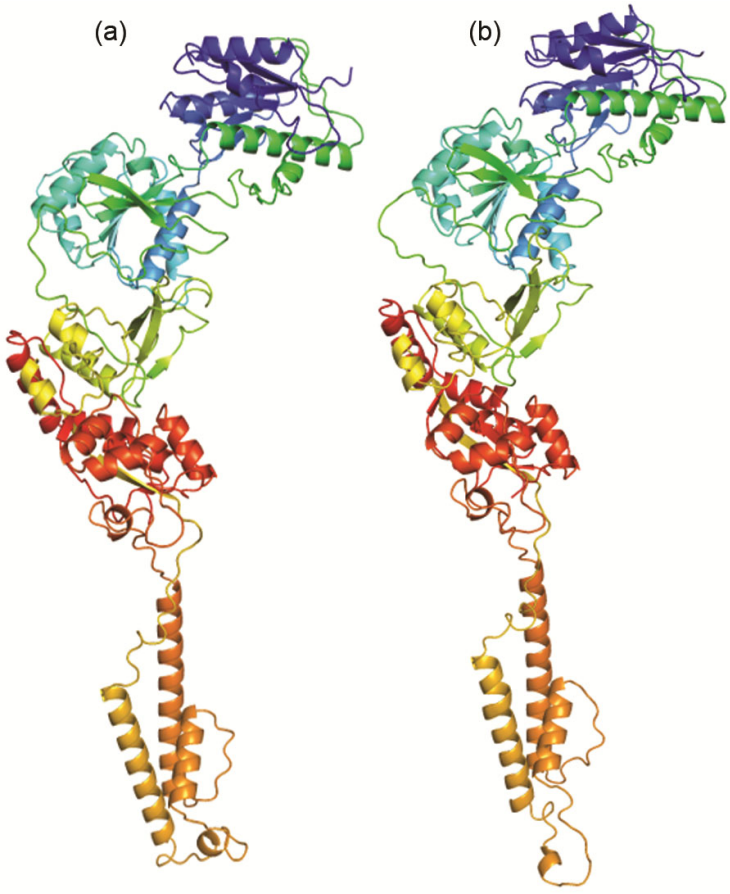
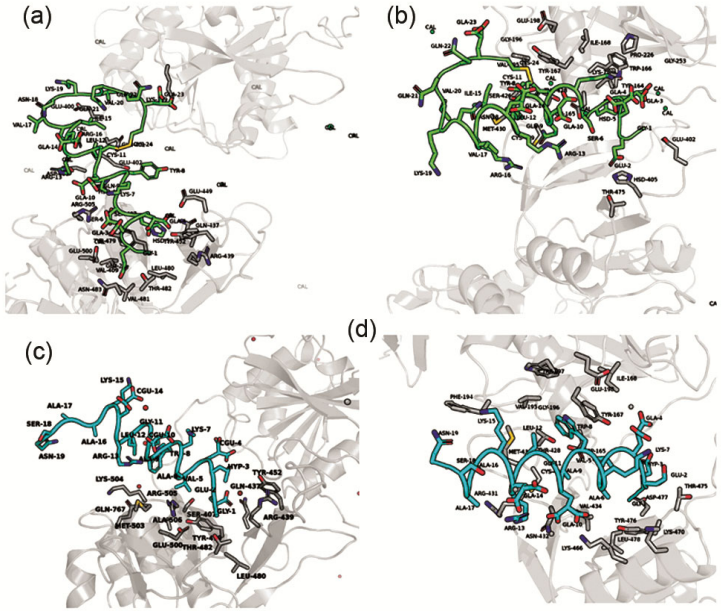
Received 18 June 2025; *revised 16 March 2026*

Supplementary data



Suppl. Fig. S1 — Aligned NMDA receptor GluN2B structures generated using (a) I-TASSER and (b) Alphafold



Suppl. Fig. S2 — 3Å Interaction networks of conantokin-GluN2B complexes. Detailed residue-level contacts for (a) con-P external, (b) con-P internal, (c) con-Pr3 external, and (d) con-Pr3 internal orientations. Interacting GluN2B residues are shown in gray sticks, highlighting the electrostatic complementarity with the peptide Gla and basic residues