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Supplemental Information

**Probing the Structural Dynamics of the NMDA Receptor Activation by
Coarse-Grained Modeling**

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Supporting Information

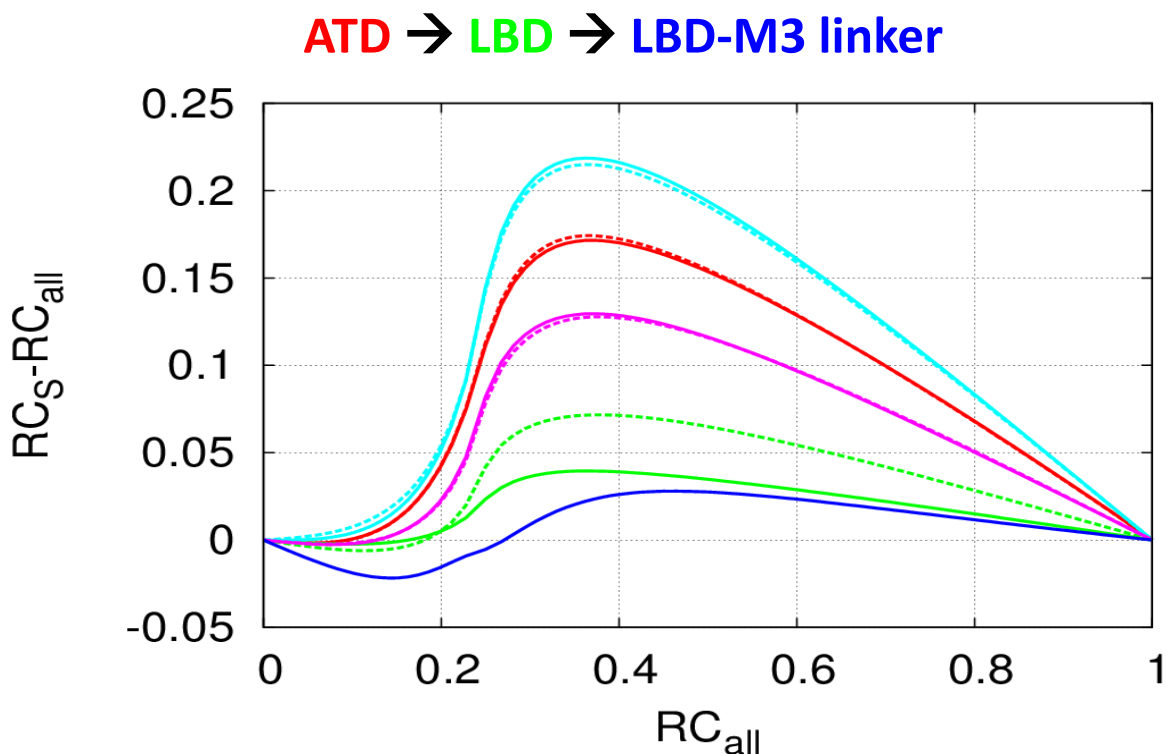


Figure S1. Reaction Coordinate (RC) analysis of transition pathway from the allosterically inhibited state to the active state as obtained from the MinActionPath server (<http://lorentz.dynstr.pasteur.fr/joel/index.php>). RC_S measures the motional progress for domain S colored as follows: ATD heterodimers (red), LBD homodimers (green), R2-D1 in GluN2A (cyan), R2-D1 between GluN2A and GluN1 (magenta), LBD-M3 linkers in GluN2A (blue). RC_{all} measures the motional progress for the whole receptor. $RC=0$ and 1 at the beginning and end of the transition, respectively. The inferred motional order for the above domains is shown, which is largely similar to the order predicted by iENM (see Fig 5).

Movie S1. A 10-frame trajectory of flexible fitting to the active-state cryo-EM map. The two GluN2A subunits are colored red (chain B) and orange (chain D), and the two GluN1 subunits are colored blue (chain A) and green (chain C). The same side view as Fig 1d is used.

Movie S2. A trajectory of the activation transition from the allosterically inhibited structure to the active-state structure of the GluN1/GluN2A receptor as predicted by iENM: (a) in the top view, (b) in the side view. The GluN2A domains are colored as follows: R1 of ATD (red transparent), R2 of ATD (red), D1 of LBD (green), D2 of LBD (green transparent), the LBD-M3 linkers (blue), M3 (cyan), whereas the rest of receptor is omitted for clarity. The gate residues

A650 of GluN2A are shown as balls in cyan. The same side view as Fig 1d is used. The corresponding trajectory file (in PDB format) is provided (file name: trajectory.pdb).