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Supplementary Material: 3 figures

Molecular Dynamics Simulations of the Conformational Changes of the Glutamate Receptor Ligand-Binding Core in the Presence of Glutamate and Kainate

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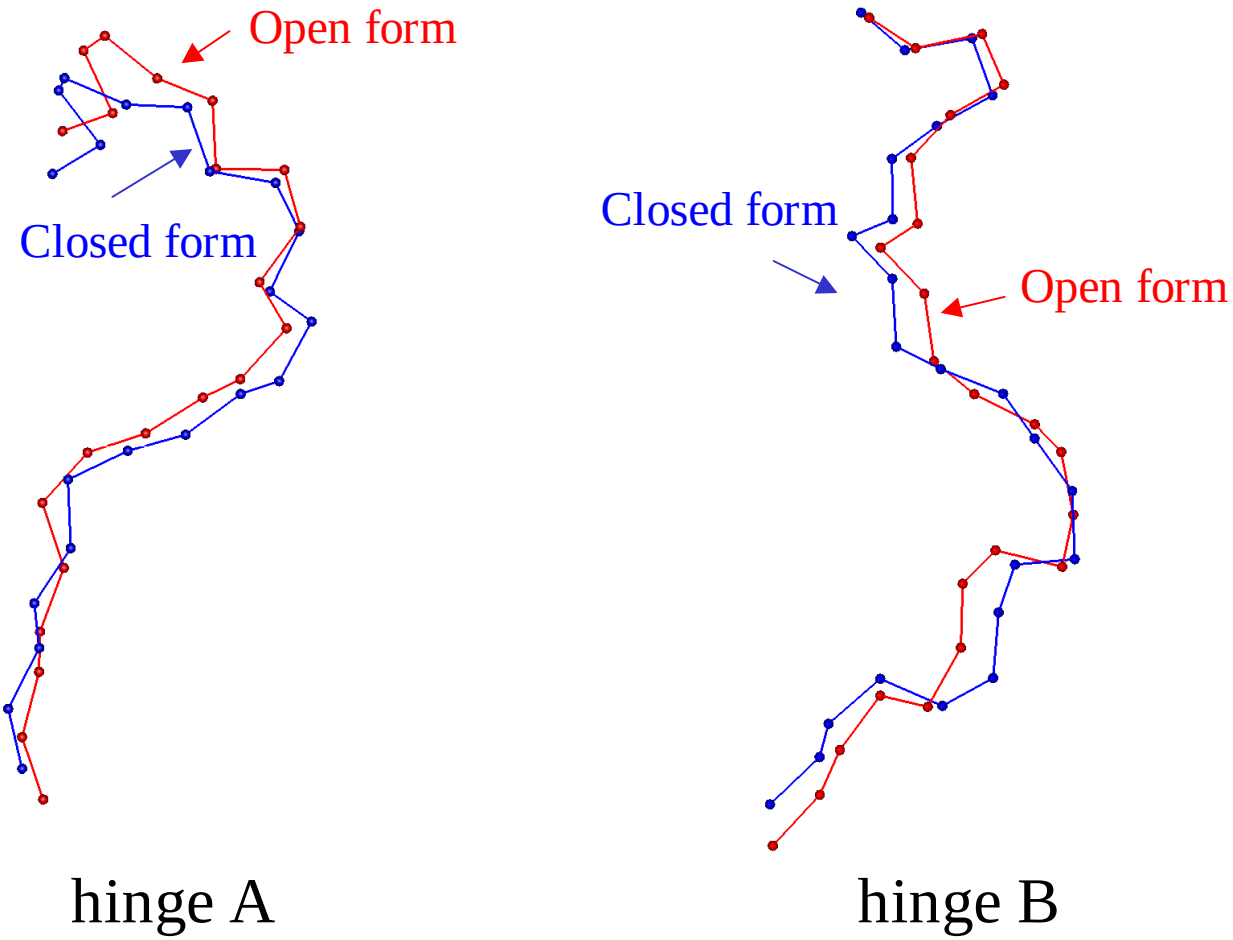

Figure 1. Superimposition of the hinge regions (A: residues 75-110; B: residues 172-193) of the closed (in blue) and open (in red) forms of QBP.

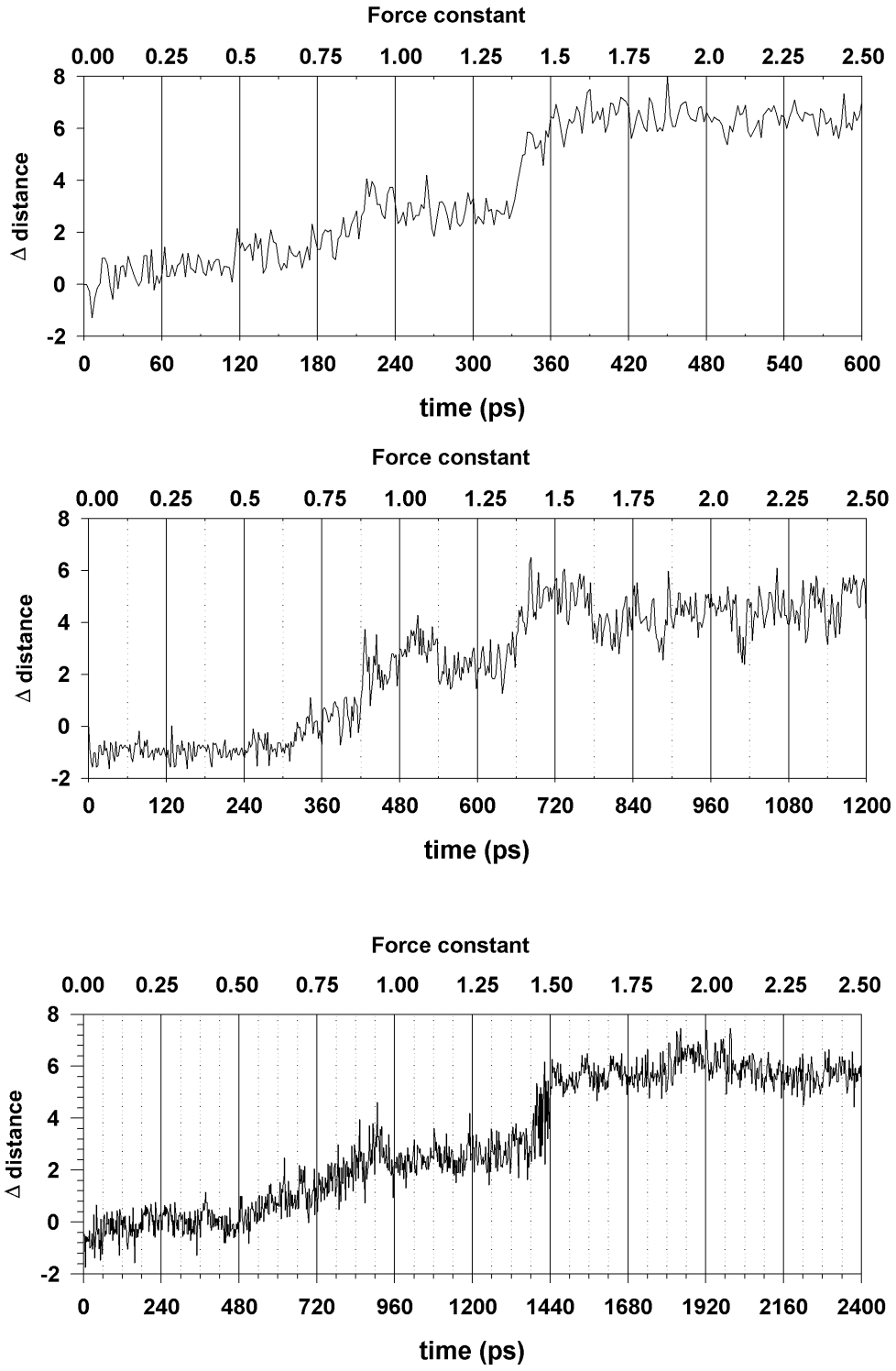

Figure 2. Degree of closure of the GluR2 ligand-binding core domain expressed as the increase in the distance between Cα atoms of residues Ser 158 and Arg 108 over different simulation times (lower axis) and incremental template force constants (upper axis).

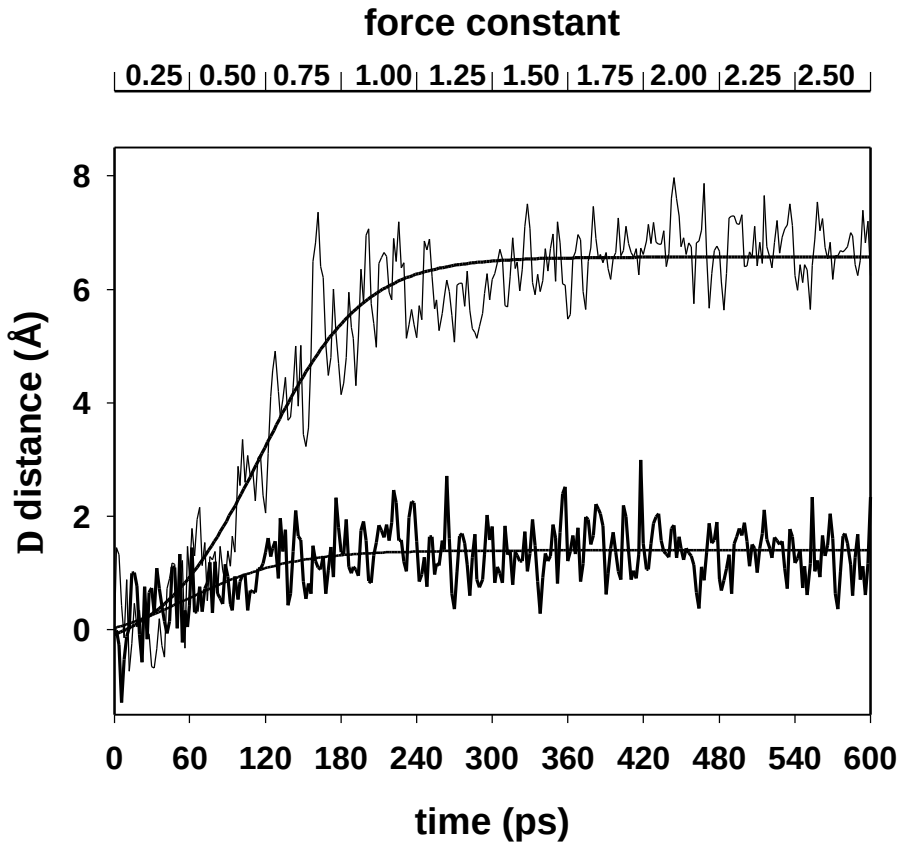

Figure 3. Degree of closure of the GluR2 ligand-binding core domains, in the absence of ligand, expressed as the increment in the distance between Cα atoms of residues Ser 158 and Arg 108 over the simulation time. Thin and thick lines correspond to the MD simulations in the absence and in the presence of torsional restraints applied to the Cα trace of the linker loop, respectively. The upper axis shows the value of the template force constant applied at different times during the simulations.