Supporting material:

Study on allosteric activation mechanism of SHP2 via elastic network models and neural relational inference molecular dynamics simulation

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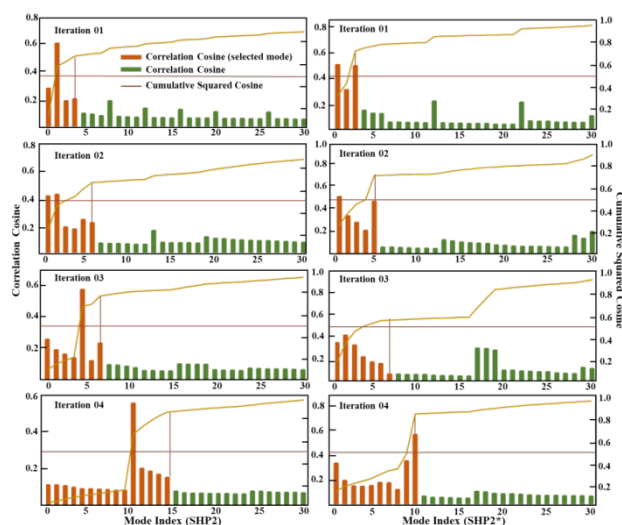[†] *These authors contributed equally to this work*

Figure S1. Correlation cosine between instantaneous distance vector and eigenmodes. The left and right columns indicate conformational iterations from inactive and active to intermediate states, respectively. Principal components whose sum of cosine squares is greater than 0.5 are shown in orange, almost exhibiting complete functional slow motion.
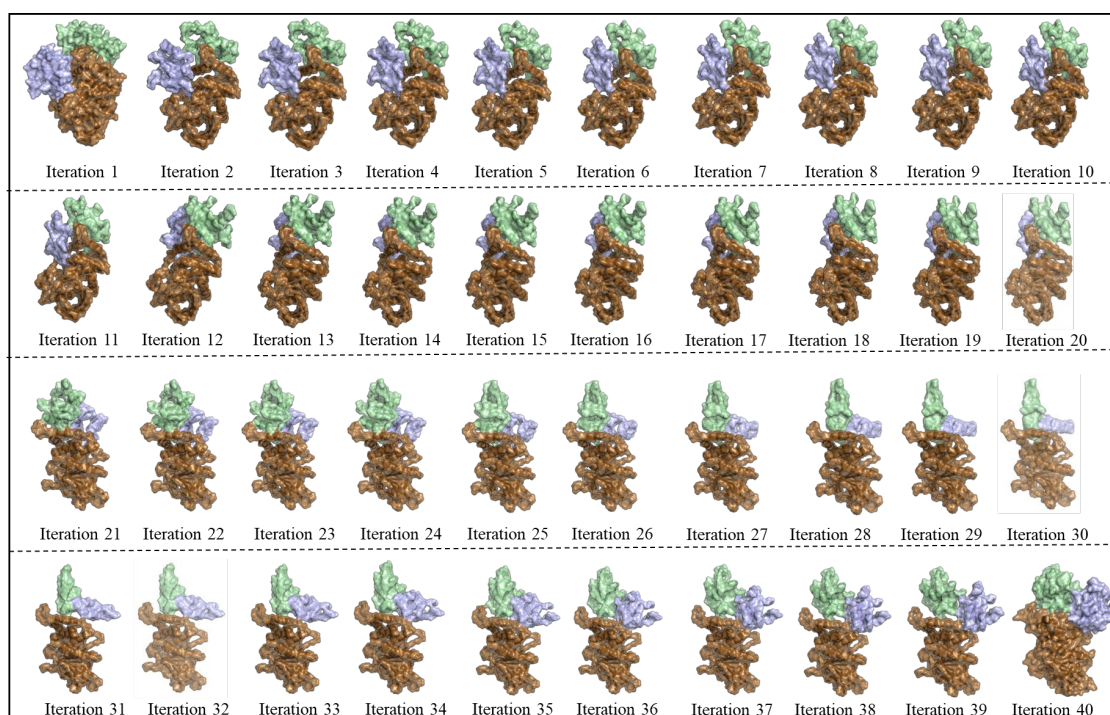

Figure S2. 40 intermediate conformations in the deformation of SHP2 from the closed to the open state.
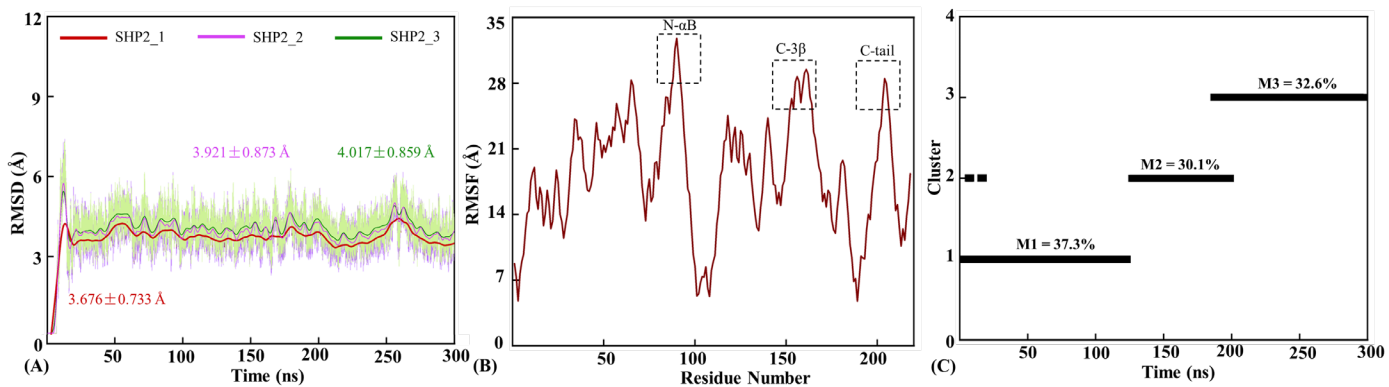
Figure S3. Three conventional molecular dynamics simulation of the SHP2 system. RMSD values of all the Cα atoms; (B) RMSF distribution at residue level. Three regions N-αB, C-3β and C-tail show high flexibility.