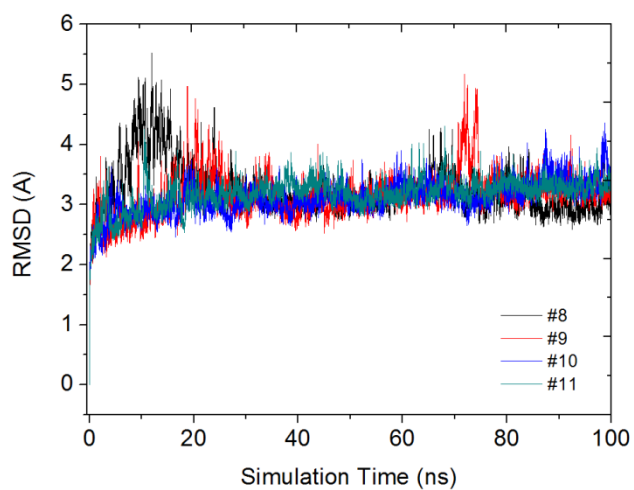
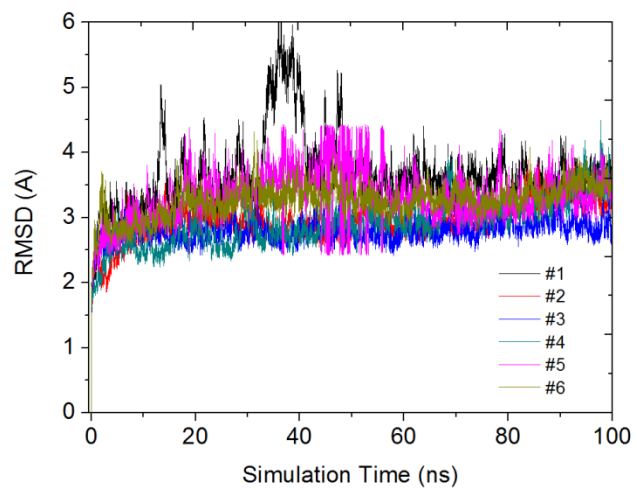


Fig. S1



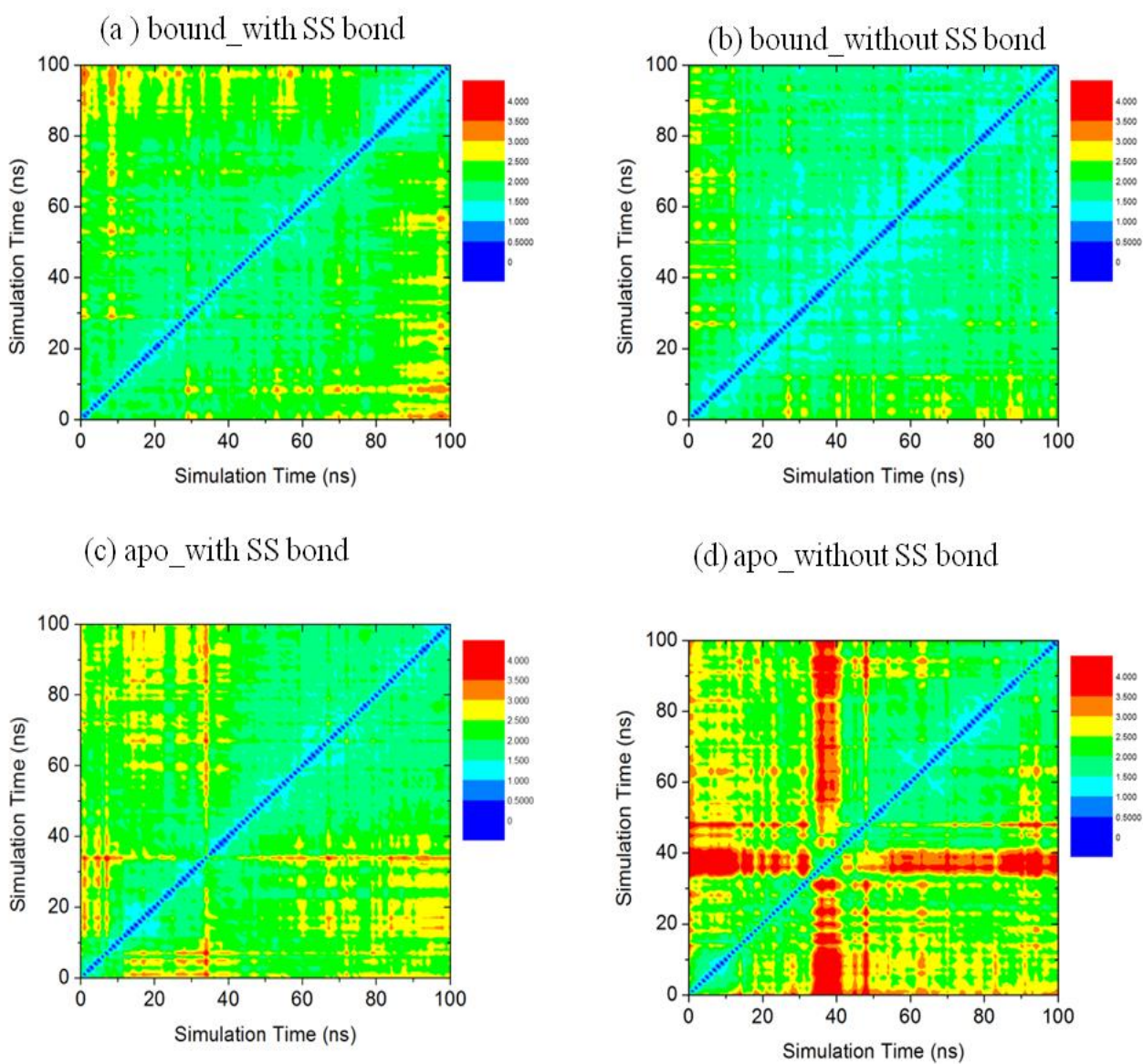
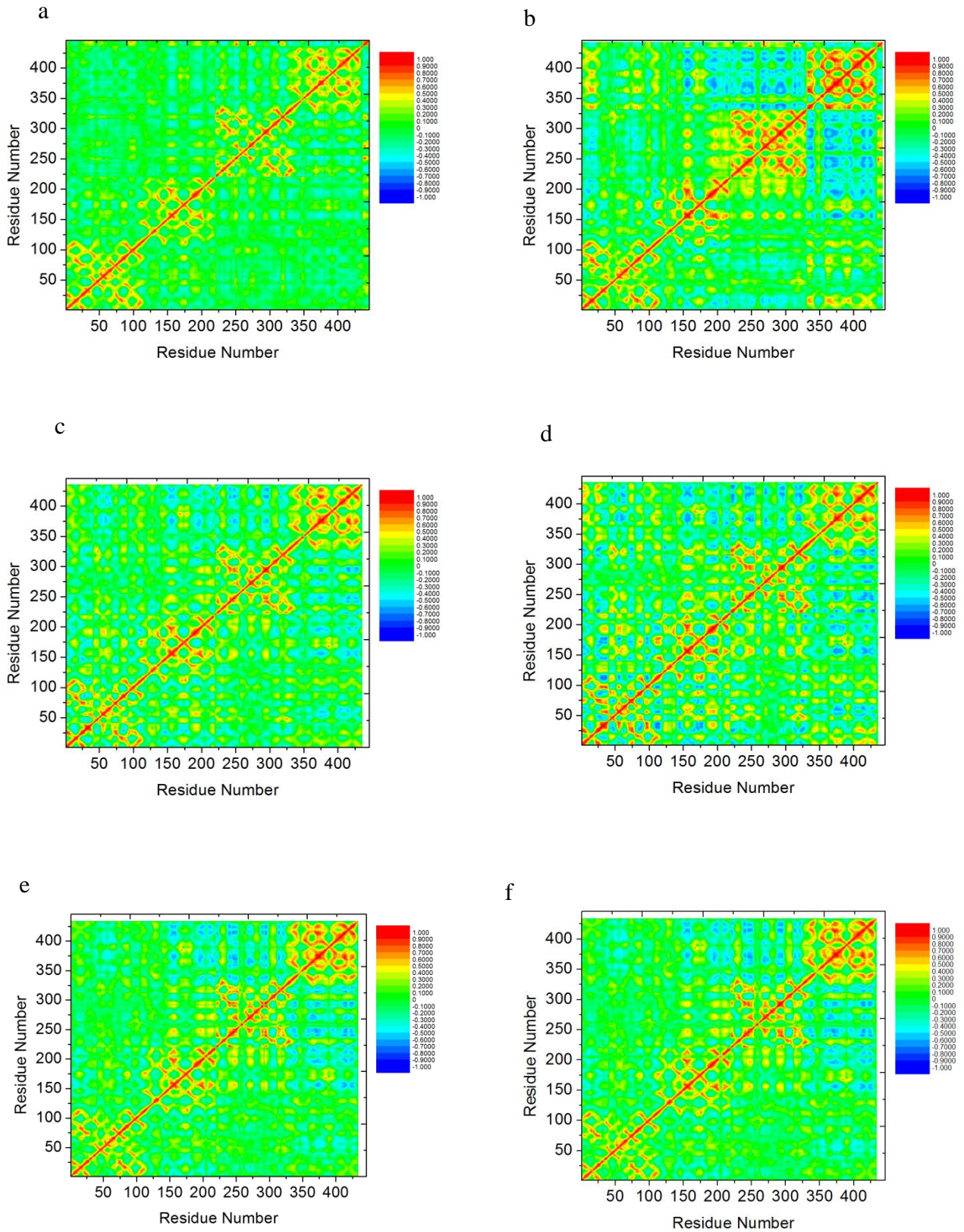


Fig. S2. 2-D RMSDs during the 100ns MD simulation

Fig. S3





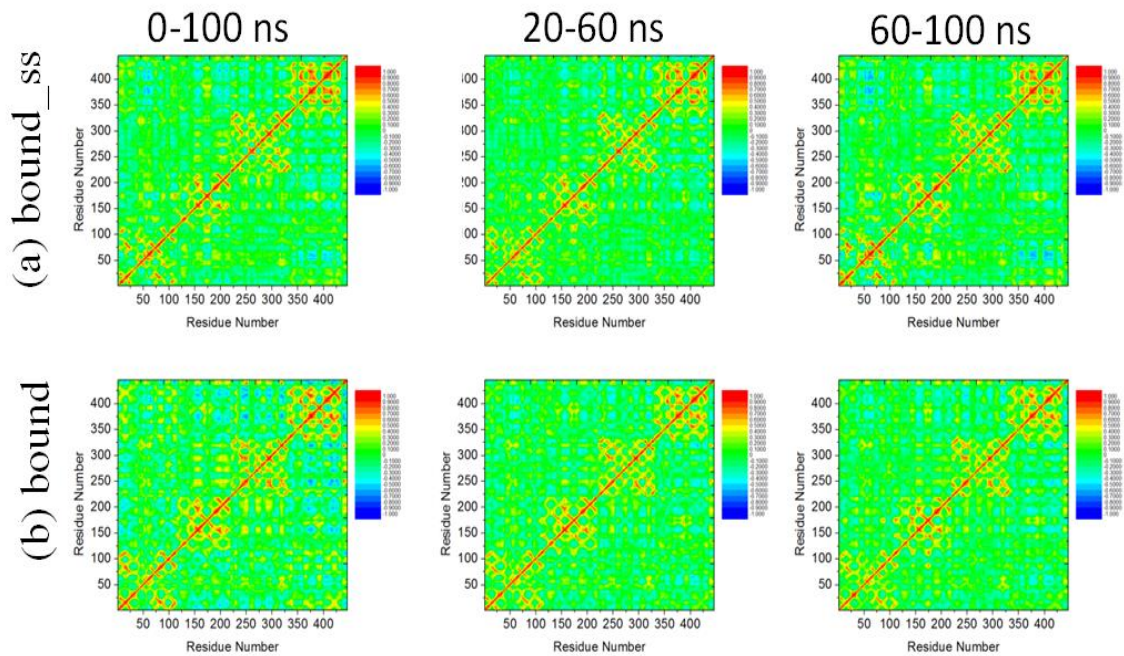
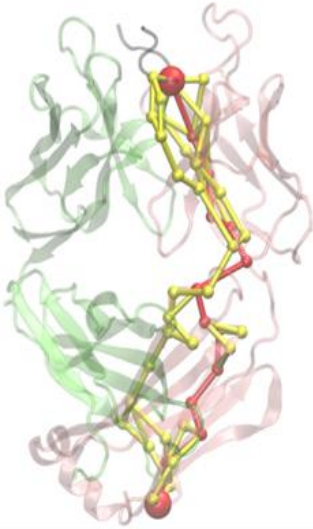


Fig. S4. Motion correlation among the Fab sub-domains in the time frame of 0-100ns, 20-60 ns and 60-100 ns

0-100

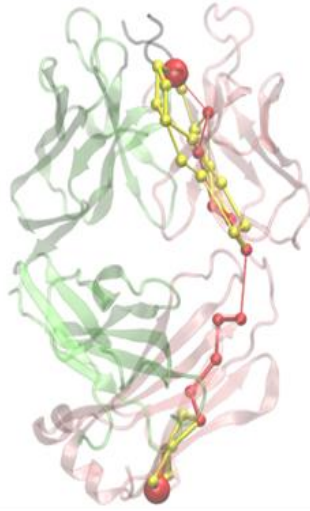
P-Met442



L-Asp156

20-60

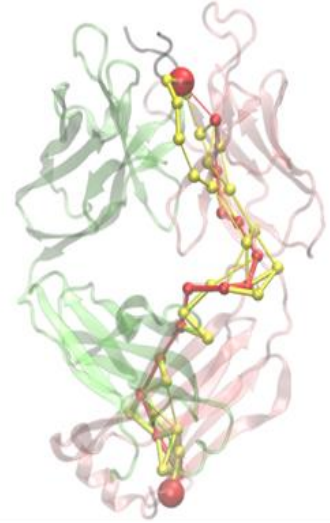
P-Met442



L-Asp156

60-100

P-Met442



L-Asp156

Fig. S5. Network analysis and flow properties from Met442 of peptide and Asp156 of light chain (the bound form without inter-SS bond) in the time frame of 0-100ns, 20-60 ns and 60-100 ns