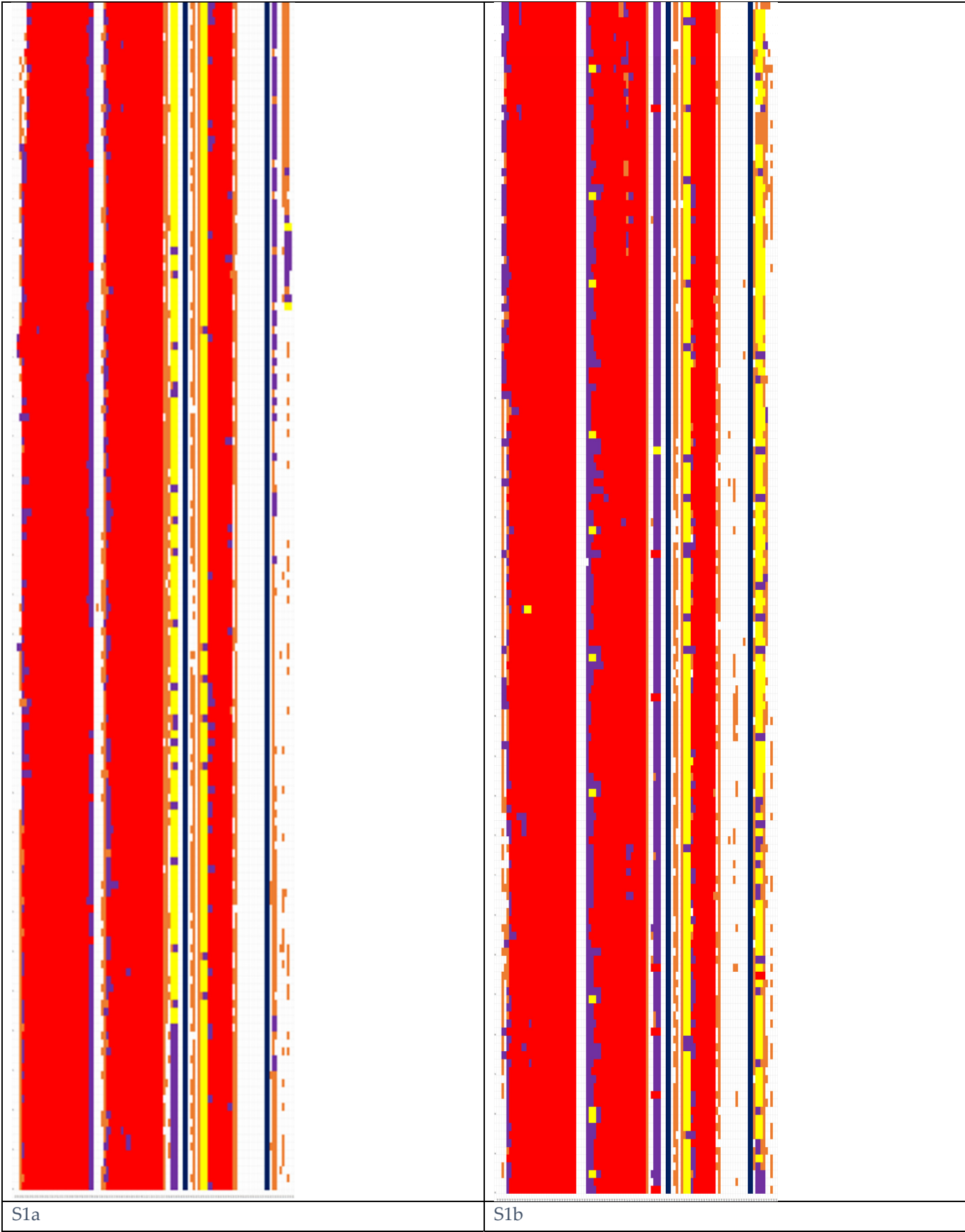
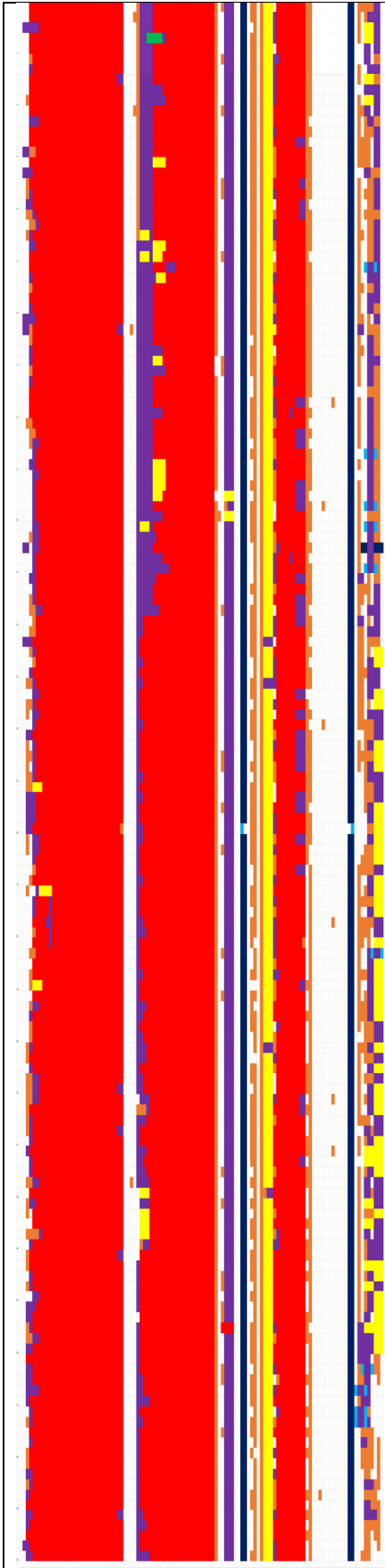


# Supplementary Material: Molecular Dynamics and Optimization Studies of Horse Prion Protein Wild Type and Its S167D Mutant

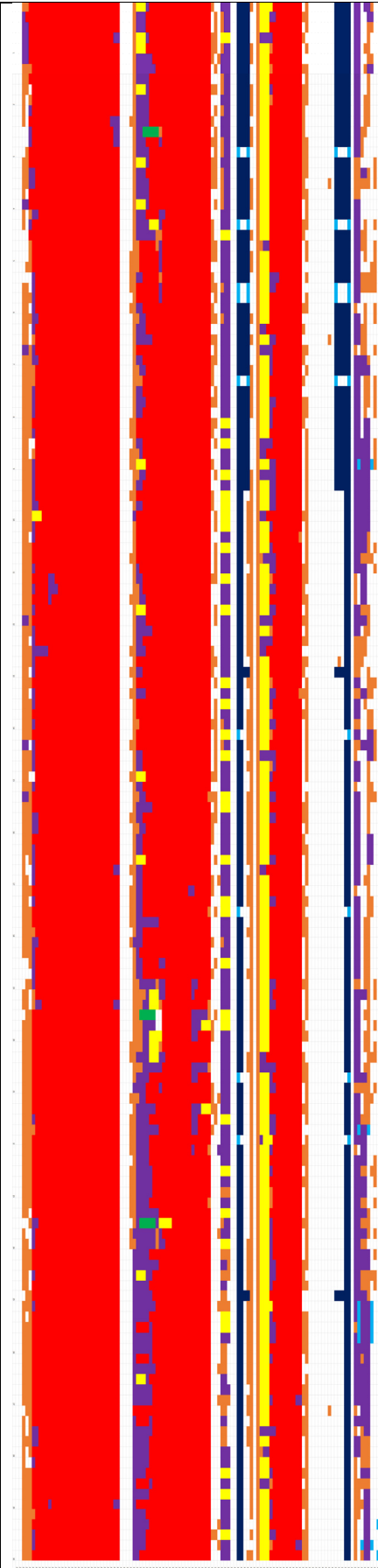
Jiapu Zhang

Figures S1, S2, and S3 are the MD Secondary Structures for the WT at 300 K, 350 K, 450 K respectively, where the MDs are the 30 ns' MD simulations (seed1, seed2, seed3) in neutral and low pH environments.

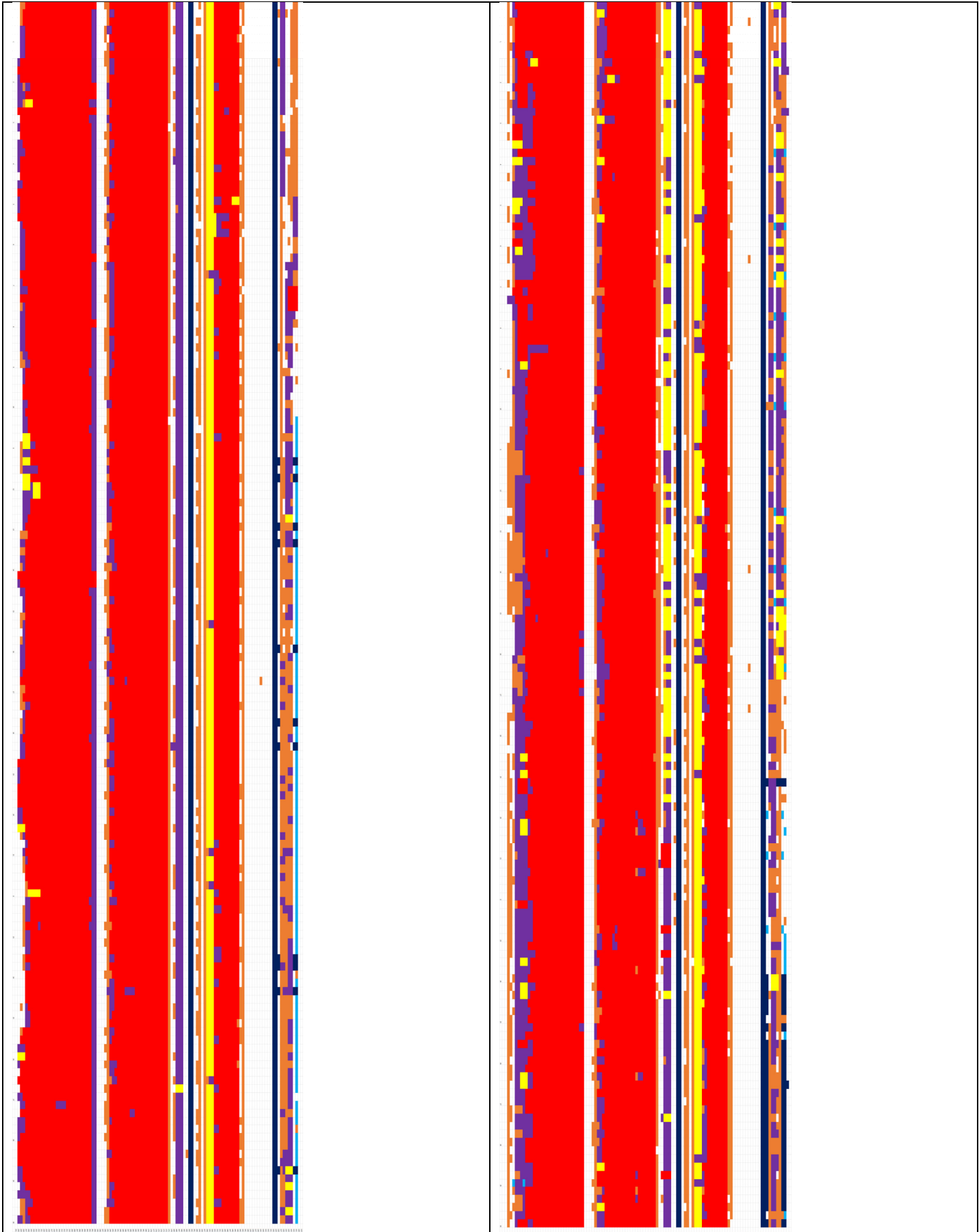




S1c



S1d



S1e

S1f



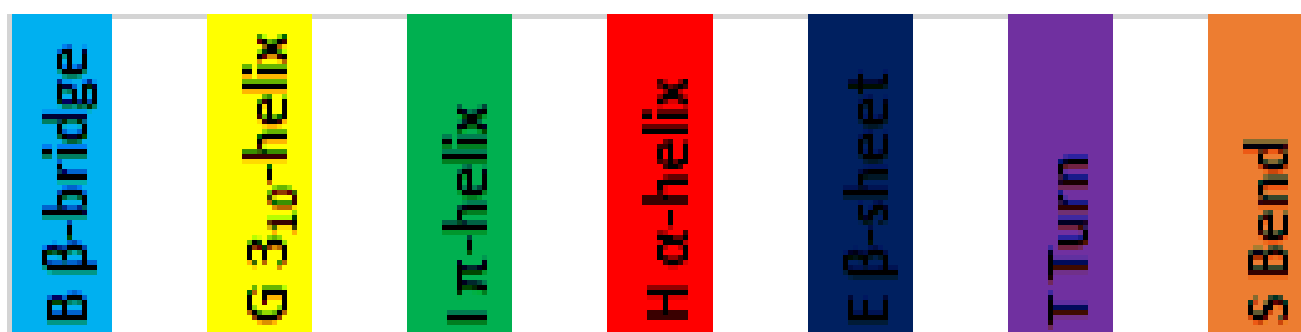
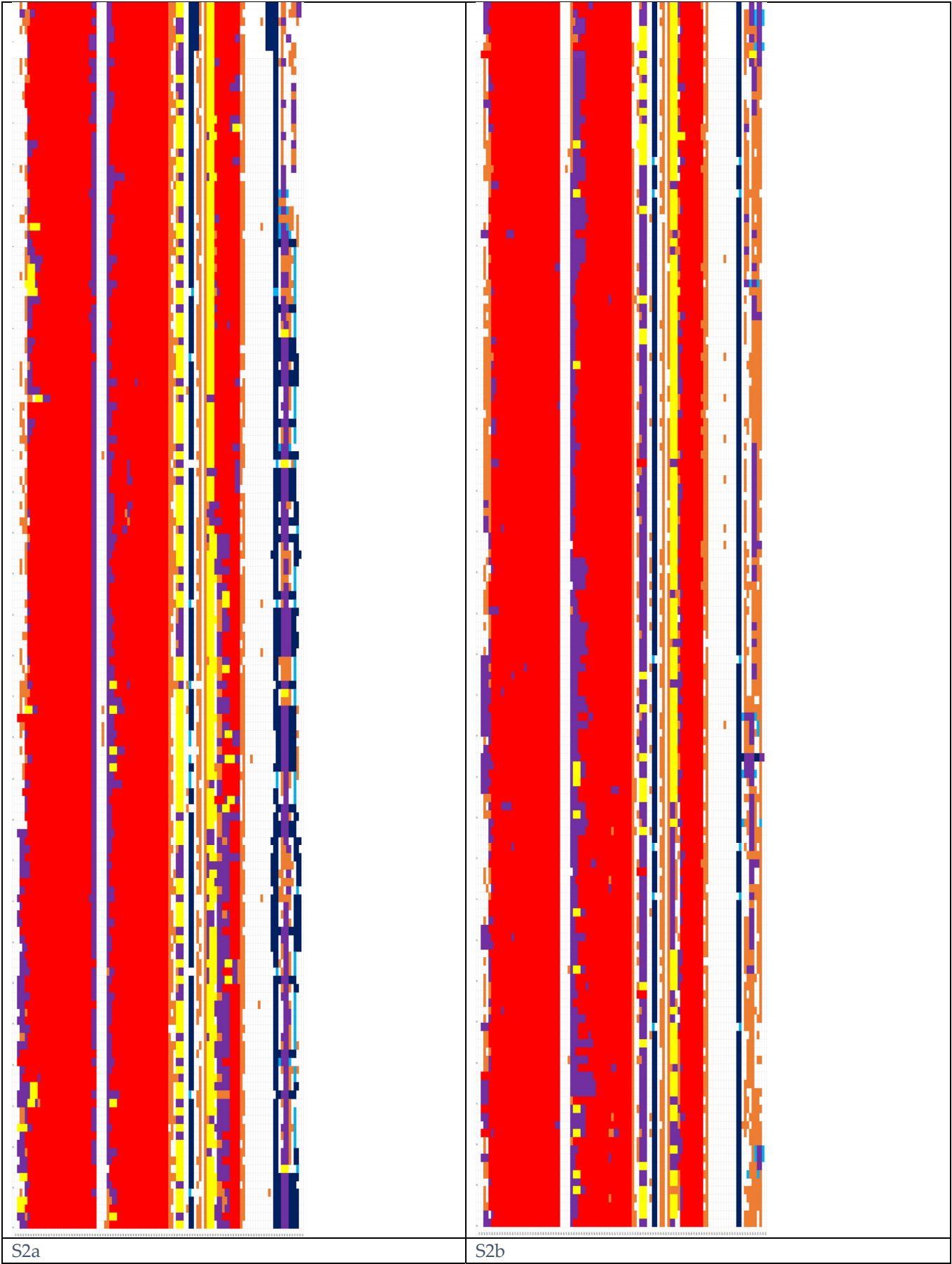
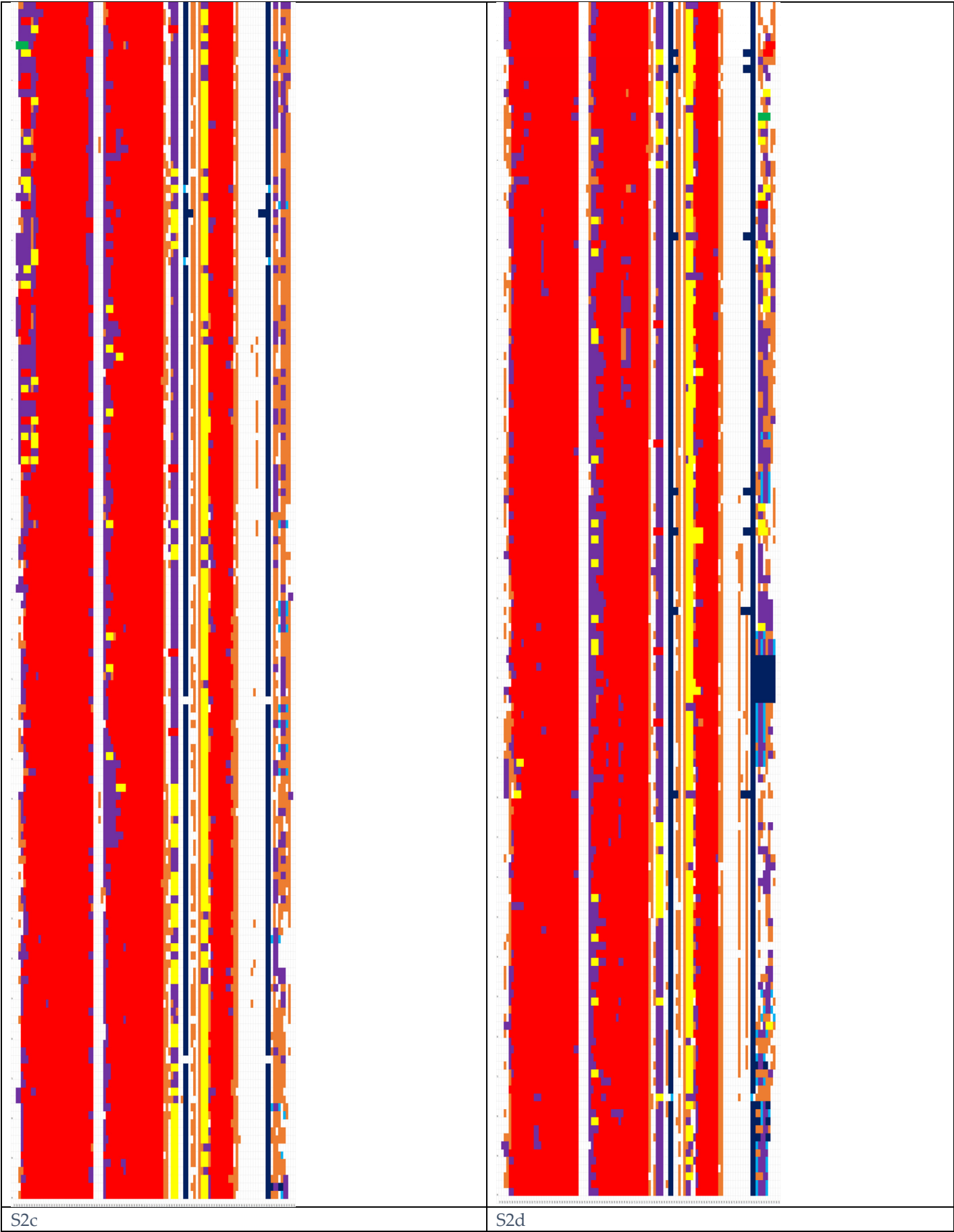
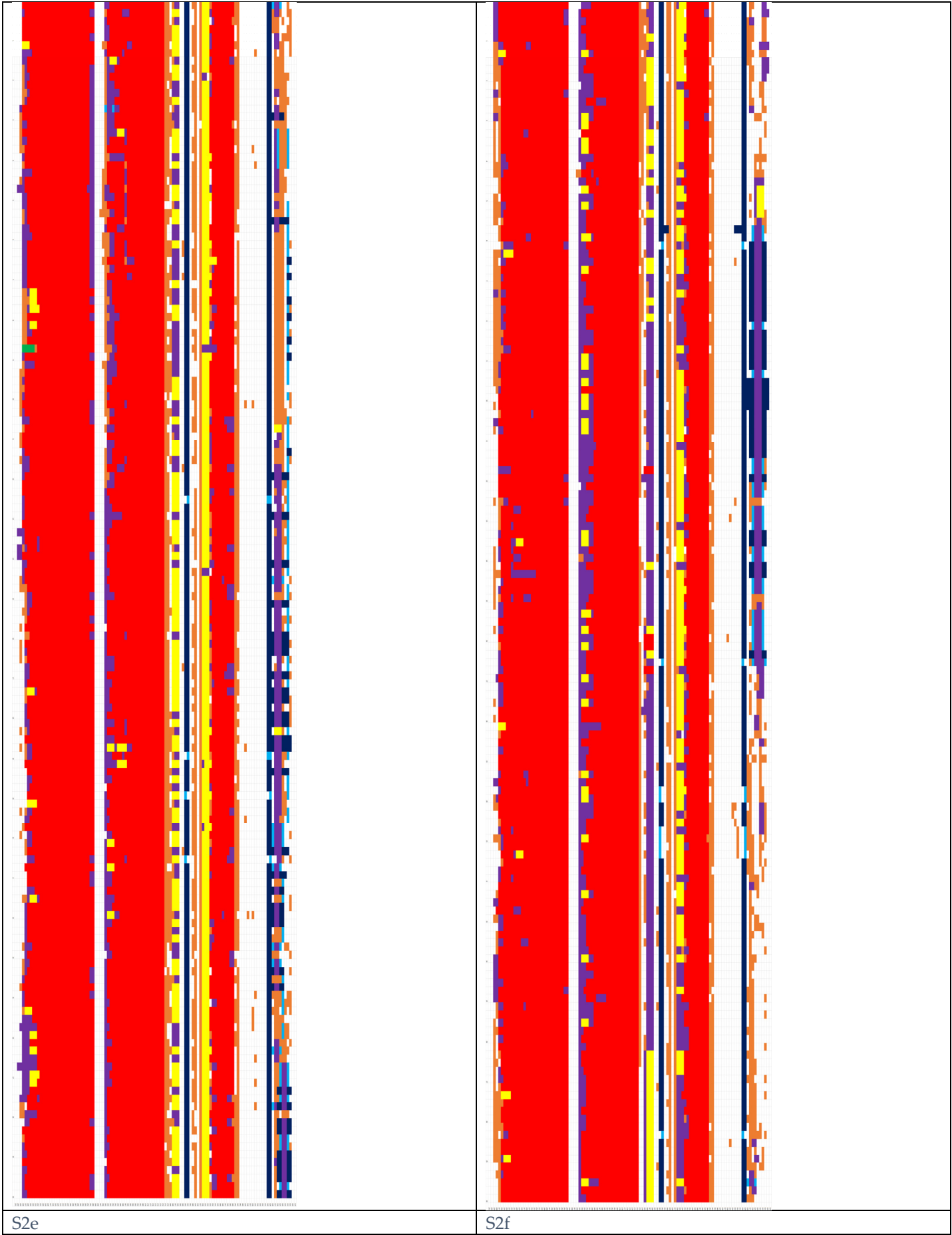


Figure S1. Secondary Structures of the WT at 300 K during 30 ns' MD simulations (up to down: seed1, seed2, seed3; left to right: neutral pH, low pH; S1a - neutral pH seed1, S1b - low pH seed1, S1c - neutral pH seed2, S1d - low pH seed2, S1e - neutral pH seed3, S1f - low pH seed3; for each of the six graphs its labels from up to down is 1 to 30 ns and its labels from right to left is PrP residue numbers 119-231). The meaning of each colours is also illuminated in the last graph.



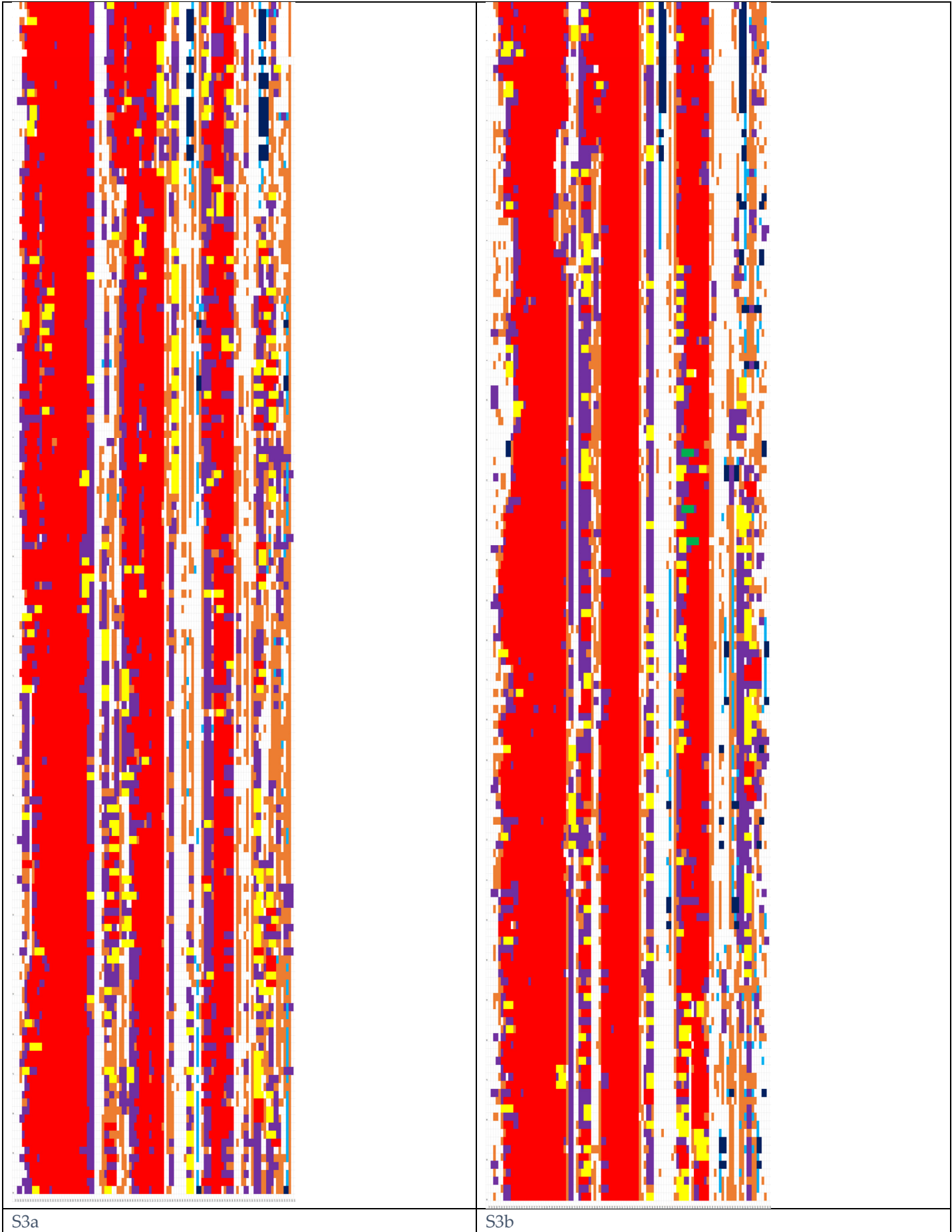


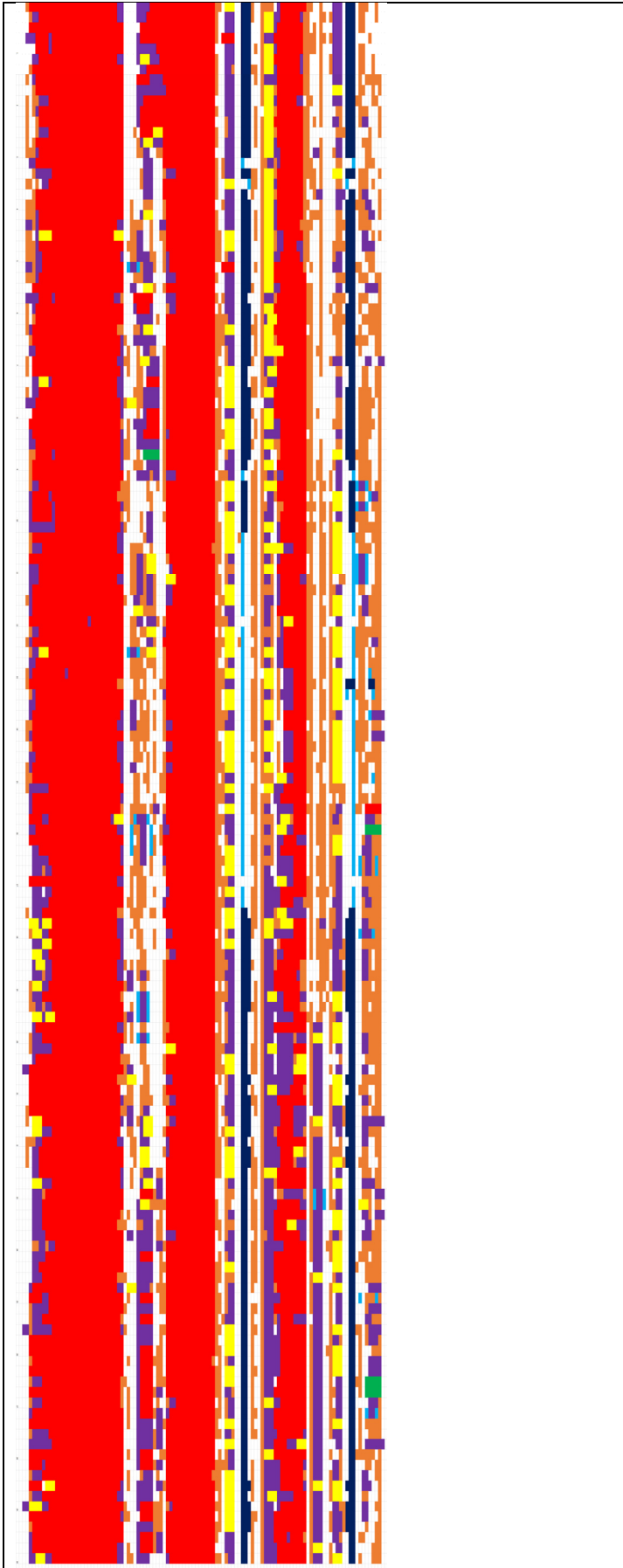
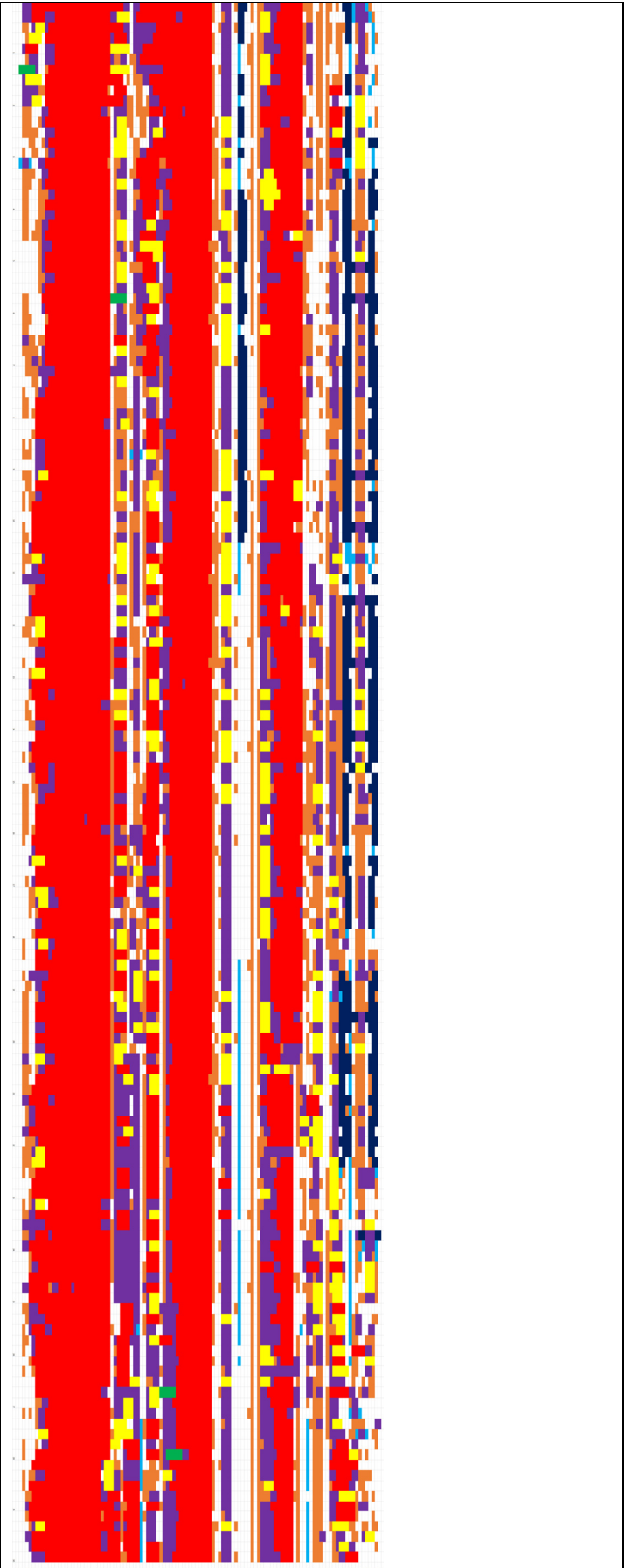


S2e

S2f

Figure S2. Secondary Structures of the WT at 350 K during 30 ns' MD simulations (up to down: seed1, seed2, seed3; left to right: neutral pH, low pH; S2a - neutral pH seed1, S2b - low pH seed1, S2c - neutral pH seed2, S2d - low pH seed2, S2e - neutral pH seed3, S2f - low pH seed3; for each of the six graphs its labels from up to down is 1 to 30 ns and its labels from right to left is PrP residue numbers 119-231).



	
S3c	S3d



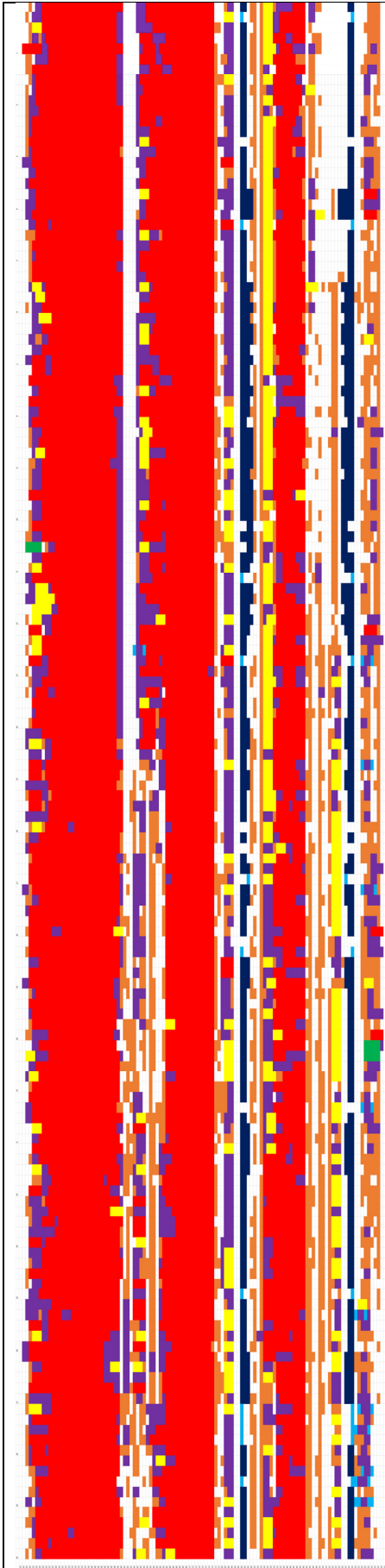
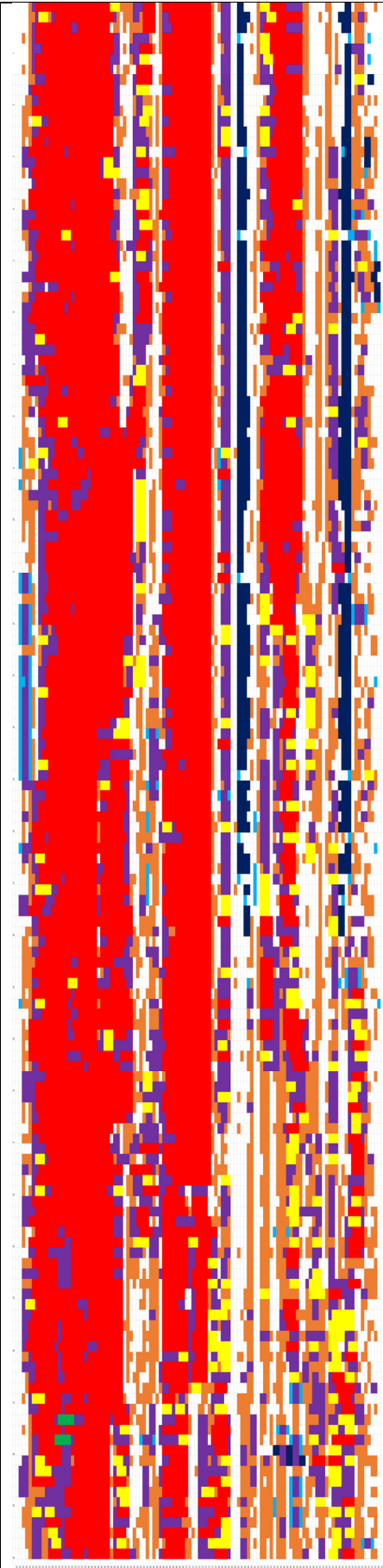
	
S3e	S3f



Figure S3. Secondary Structures of the WT at 4S20 K during 30 ns' MD simulations (up to down: seed1, seed2, seed3; left to right: neutral pH, low pH; S3a - neutral pH seed1, S3b - low pH seed1, S3c - neutral pH seed2, S3d - low pH seed2, S3e - neutral pH seed3, S3f - low pH seed3; for each of the six graphs its labels from up to down is 1 to 30 ns and its labels from right to left is PrP residue numbers 119-231).