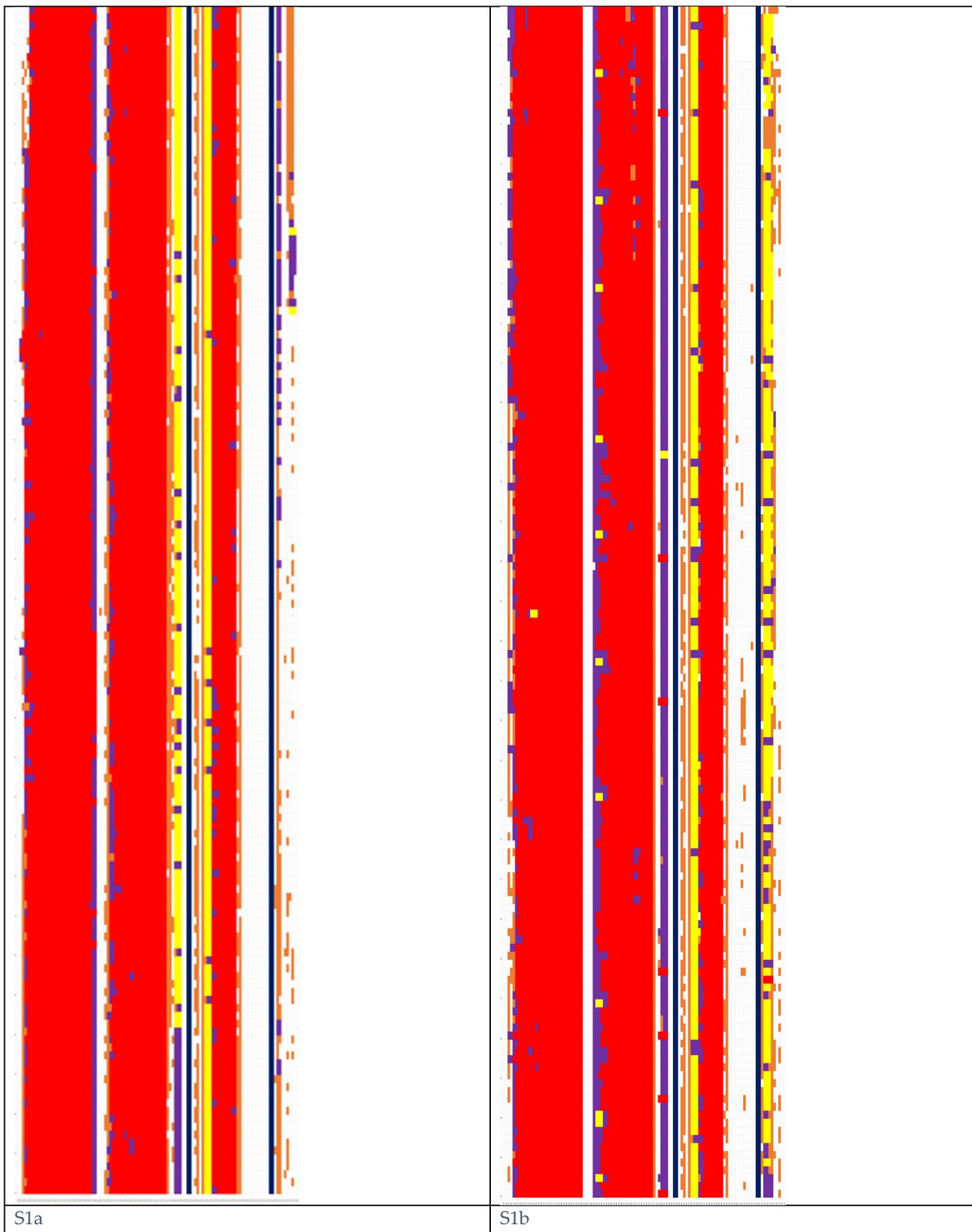
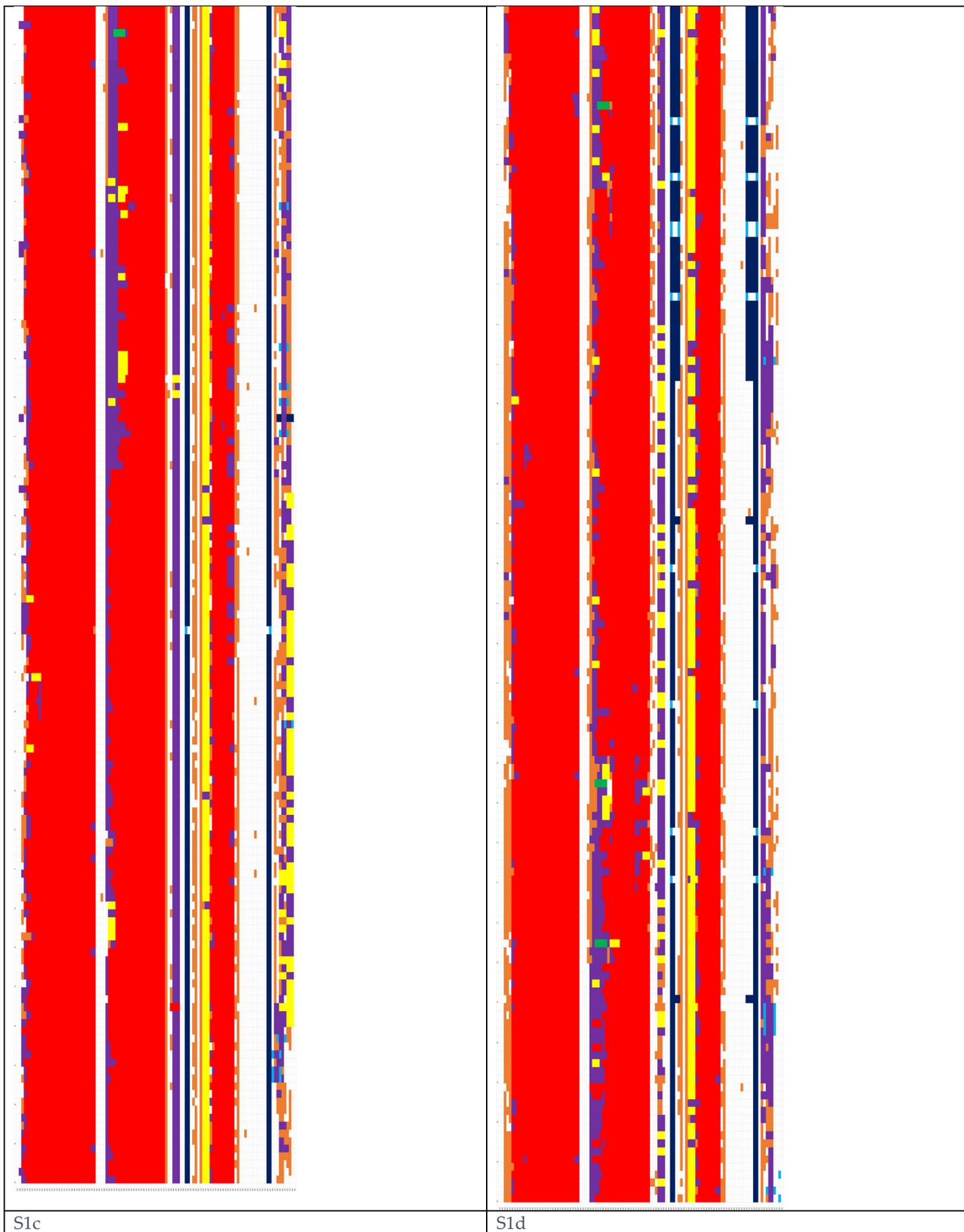

Supplementary Material: Molecular Dynamics and Optimization Studies of Horse Prion Protein Wild Type and Its S167D Mutant

Jiapu Zhang

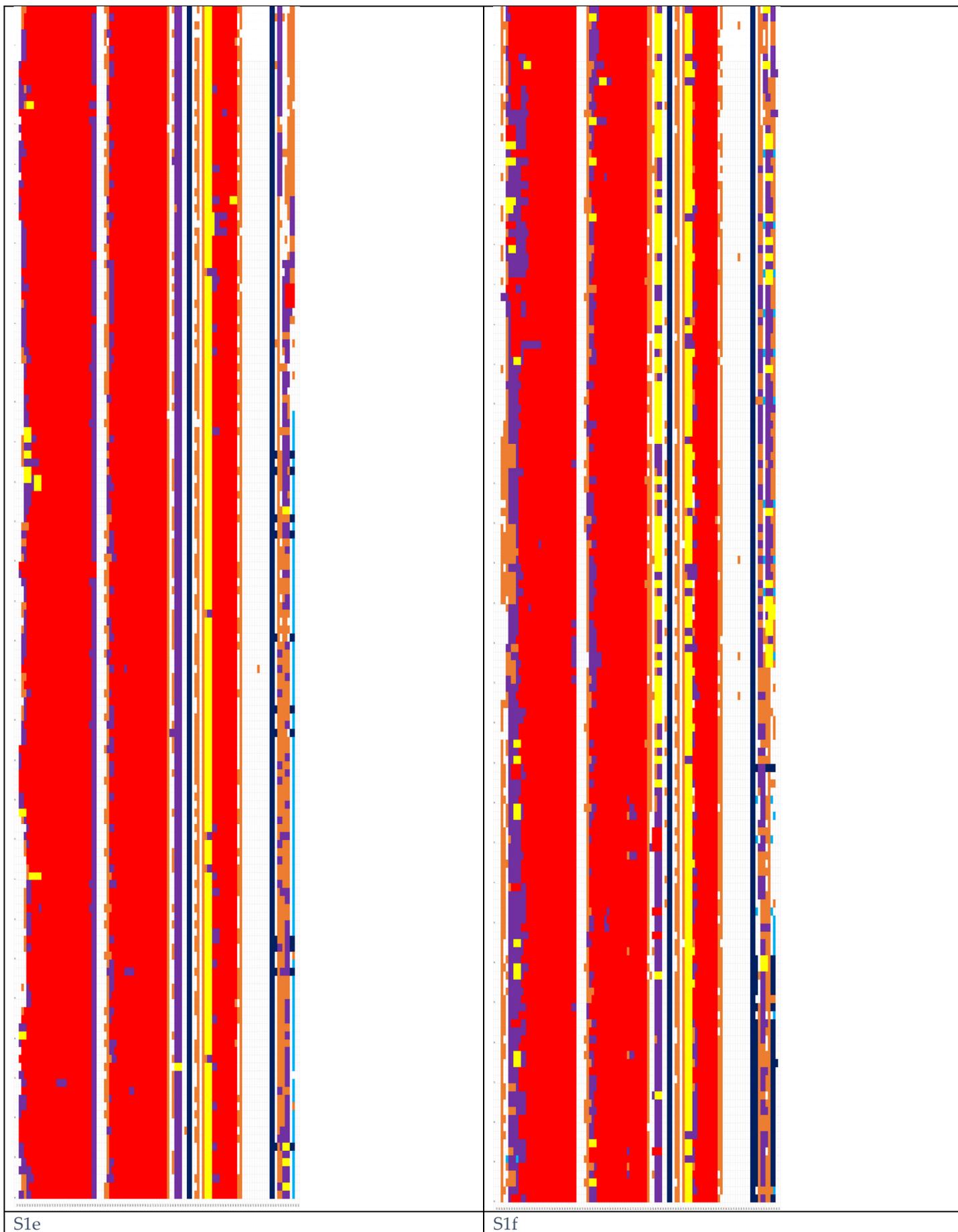
Figures S1, S2, and S3 are the MD Secondary Structures for the WT at 300 K, 350 K, 450 K respectively, where the MDs are the 30 ns' MD simulations (seed1, seed2, seed3) in neutral and low pH environments.





S1c

S1d

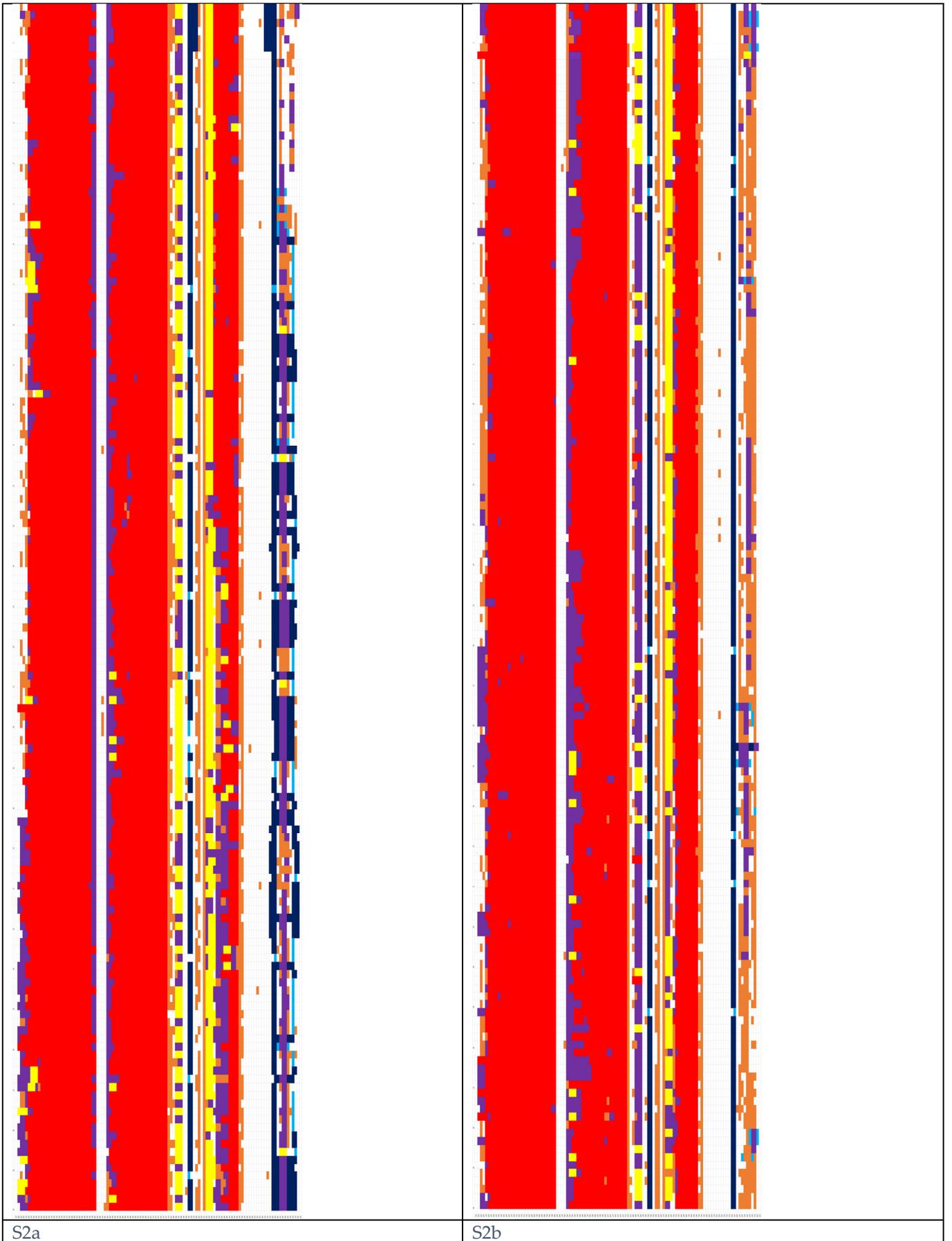


S1e

S1f

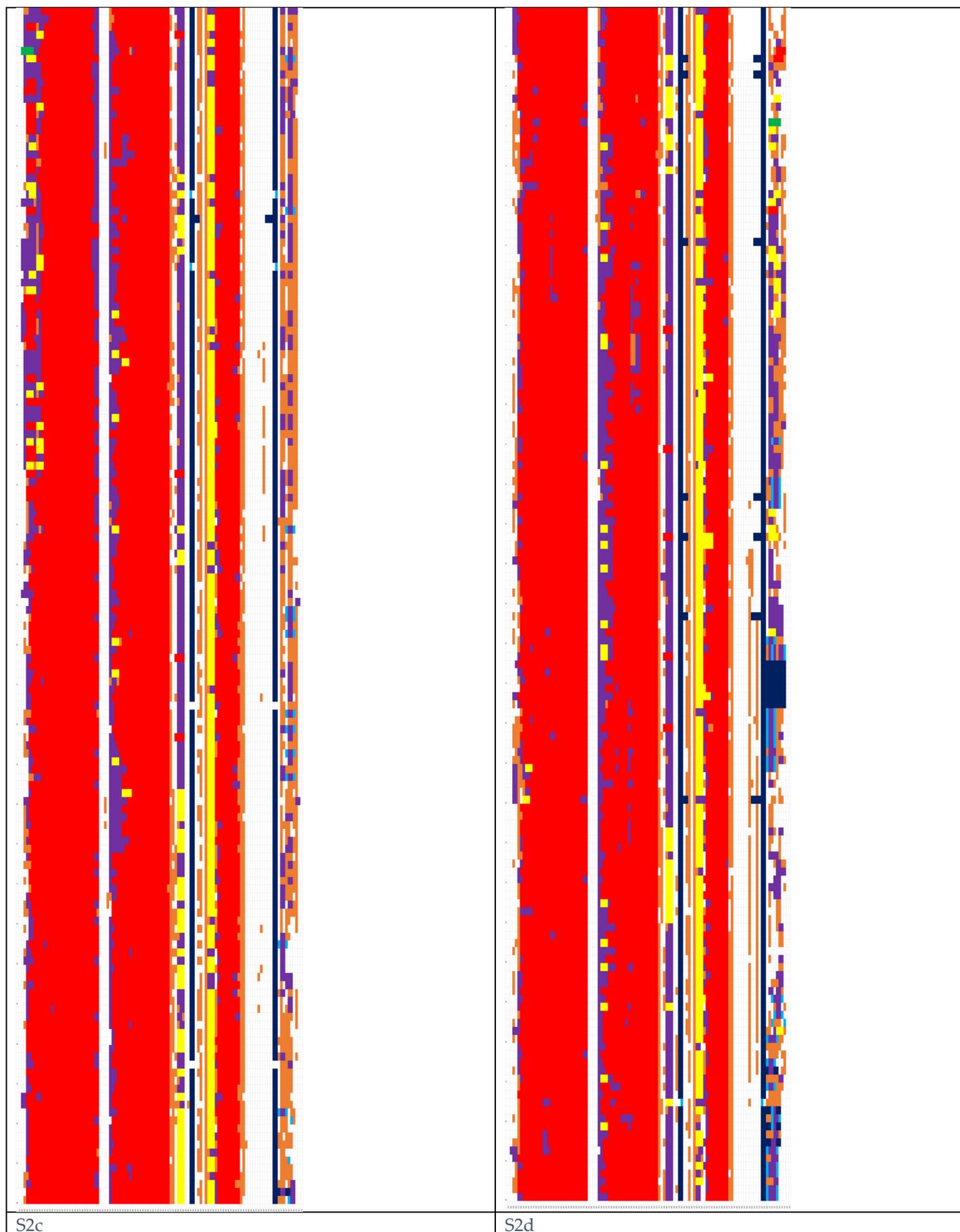


Figure S1. Secondary Structures of the WT at 300 K during 30 ns' MD simulations (up to down: seed1, seed2, seed3; left to right: neutral pH, low pH; S1a - neutral pH seed1, S1b - low pH seed1, S1c - neutral pH seed2, S1d - low pH seed2, S1e - neutral pH seed3, S1f - low pH seed3; for each of the six 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.



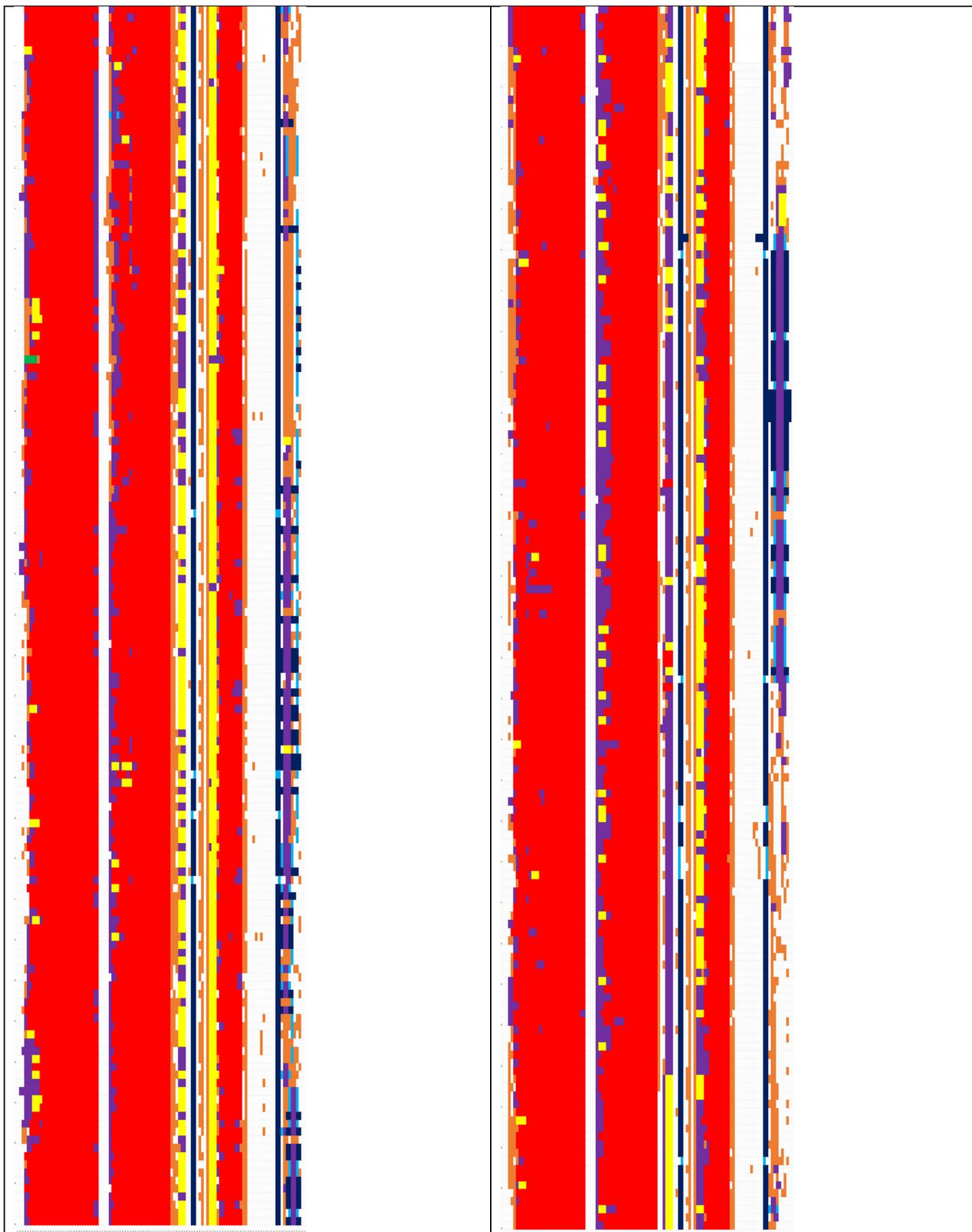
S2a

S2b



S2c

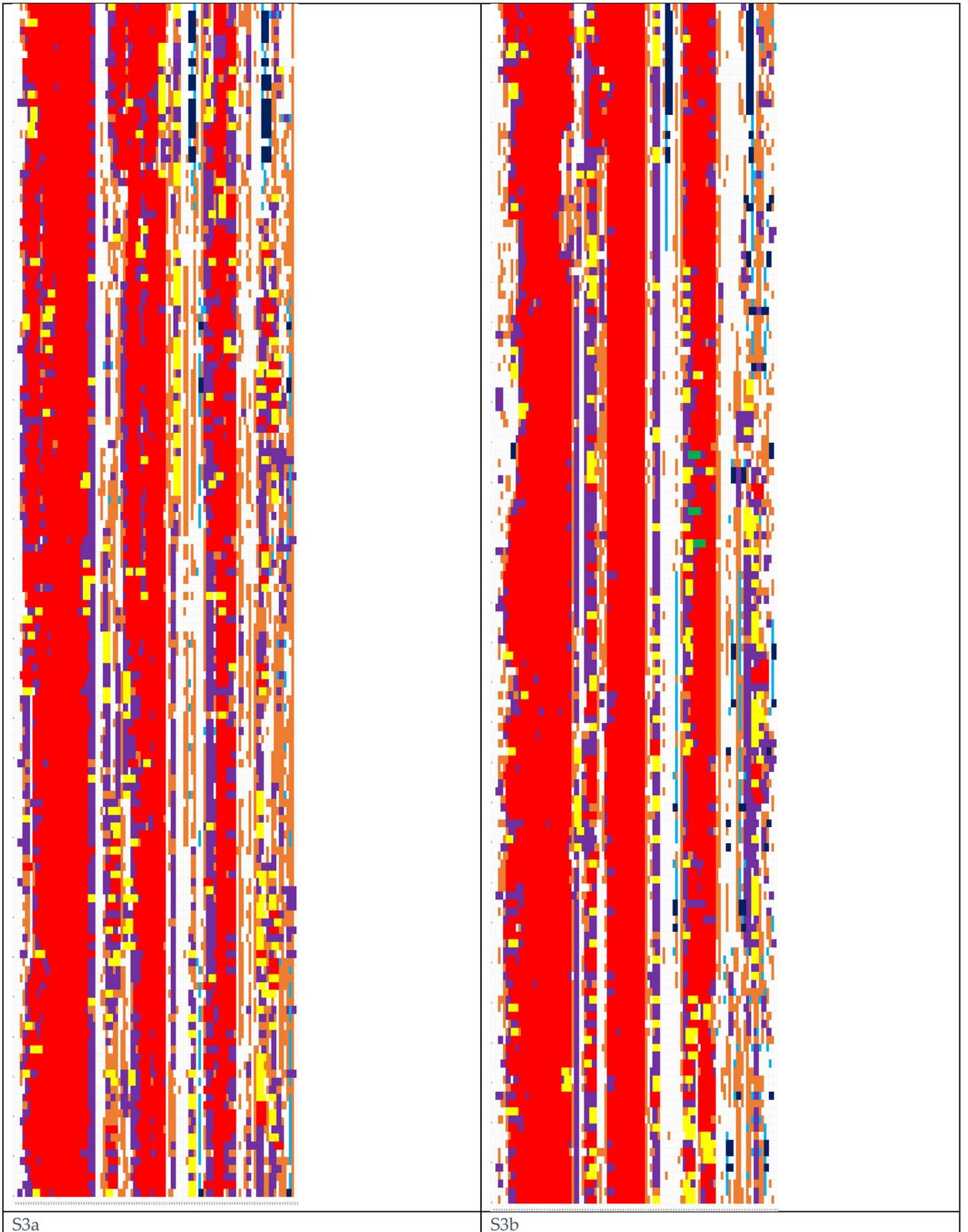
S2d



S2e

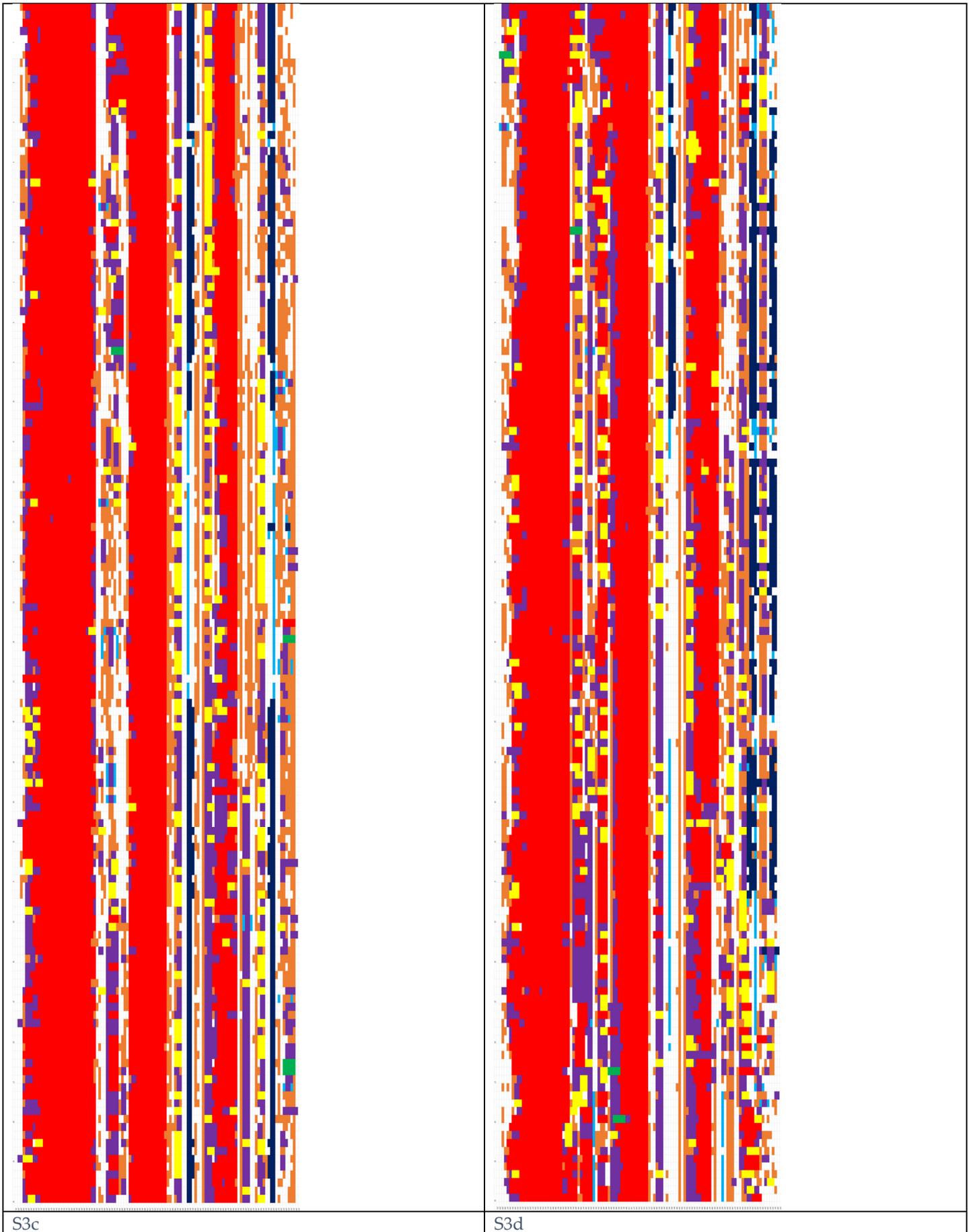
S2f

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).



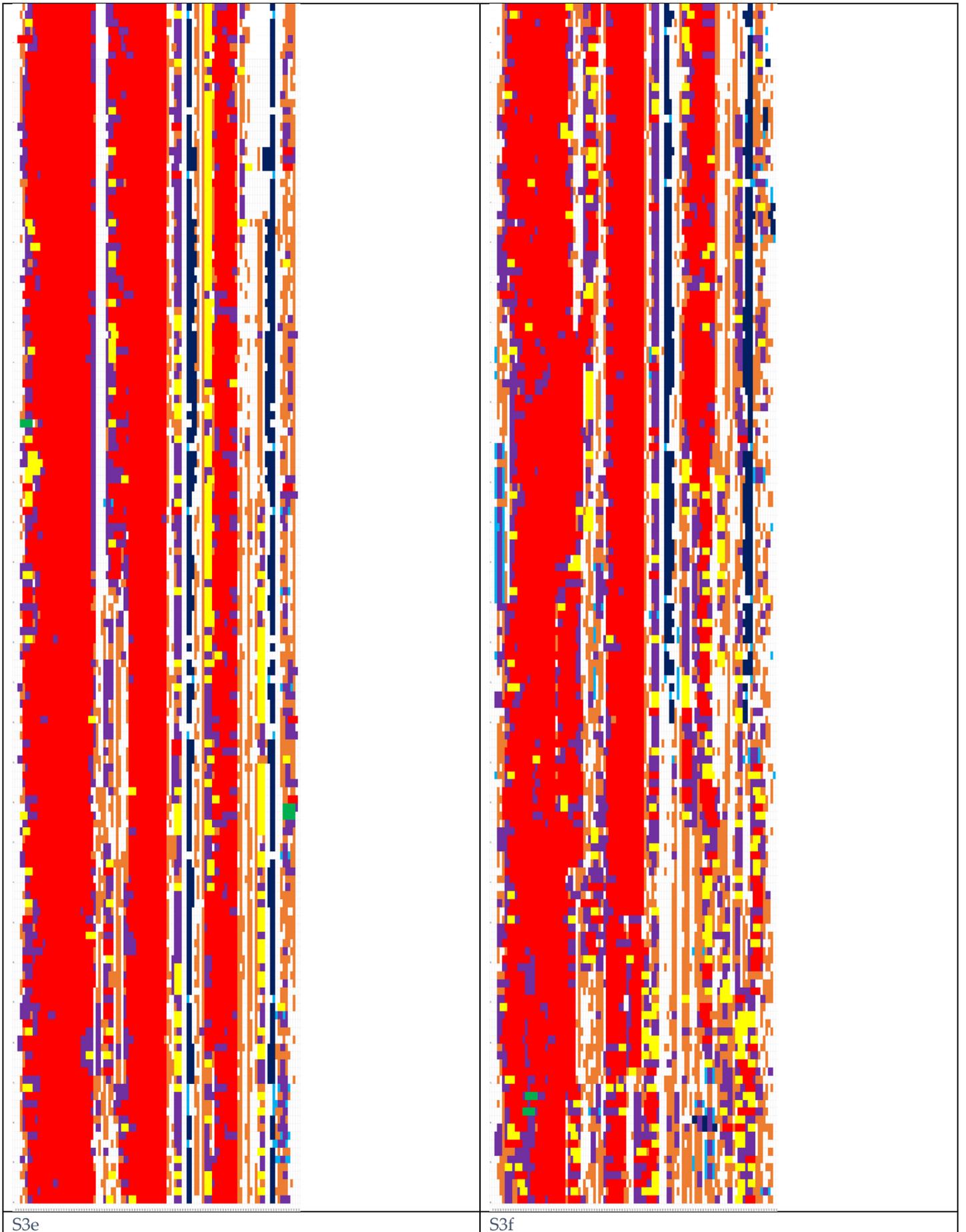
S3a

S3b



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).