Electronic Supplementary Material (ESI) for RSC Advances. This journal is © The Royal Society of Chemistry 2017

Electronic supplementary information: Complexes between cationic pyridylphenylene dendrimers and ovine prion protein: Do hydrophobic interactions matter?

S. A. Sorokina, P. I. Semenyuk, Yu. Y. Stroylova, V. I. Muronetz, Z. B. Shifrina

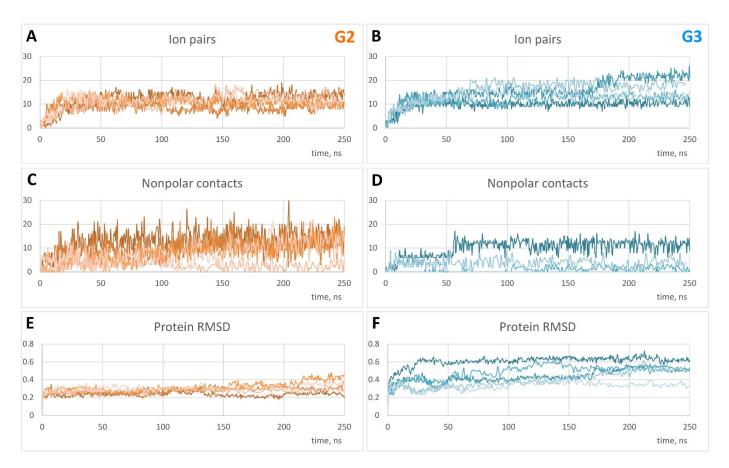


Figure S1. Time dependences of a number of ion pairs (A, B) and nonpolar contacts (C, D) between protein and dendrimer molecules and protein root-mean-square deviations (RMSD) (E, F) for all independent simulations with G2 (A, C, E) and G3 (B, D, F) dendrimers.

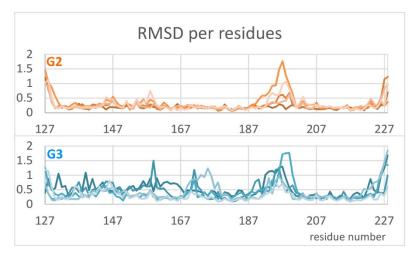


Figure S2. The protein RMSD per residues averaged on the last 10 ns of simulation with G2 (top) and G3 (bottom).