The Folding Mechanism and Key Metastable State
Identification of the PrP127-147 Monomer Studied by
Molecular Dynamics Simulation and Markov State Model
Analysis

Shuangyan Zhou, a Qianqian Wang, b Yuwei Wang, b Xiaojun Yao, bc Wei, Han d*,
Huanxiang Liu a

a School of Pharmacy, Lanzhou University, Lanzhou 730000, China

b State Key Laboratory of Quality Research in Chinese Medicine, Macau Institute for Applied
Research in Medicine and Health, Macau University of Science and Technology, Taipa, Macau,
China

c State Key Laboratory of Applied Organic Chemistry and Department of Chemistry, Lanzhou
University, Lanzhou 730000, China

d Laboratory of Chemical Genomics, School of Chemical biology and Biotechnology, Beijing
University Shenzhen Graduate School, Shenzhen, China

* Corresponding author

Tel.: +86-931-891-2578

Fax: +86-931-891-2582

E-mail address: hxliu@lzu.edu.cn and hanw@pkusz.edu.cn.
**Figure caption**

**Fig. S1.** The representative structures of macrostates S(16), S(8) and S(2) with β-sheet formed at the N-terminus and the hydrophobic residues are shown as sphere.

**Fig. S2.** The ensemble-averaged intrapeptide backbone H-bond map of the synthetic MSM trajectory. The contacts (i, i), (i, i+1) and (i, i+2) are not included.

**Fig. S3.** The superposition of structures in S(28). (a) the guanidyl of Arg136 was paralleled with the imidazole plane of His140, and (b) H-bond was formed between guanidyl of Arg136 and the Nδ of imidazole of His140.
Figure S2