

二面角动力学分析结合 Zn^{2+} 的淀粉样蛋白 A β 40 和 A β 42 的多态性特征

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Dihedral Dynamics Analyses of the Polymorphic Properties of Zn^{2+} -Bound Amyloid β 40 (A β 40) and β 42 (A β 42)

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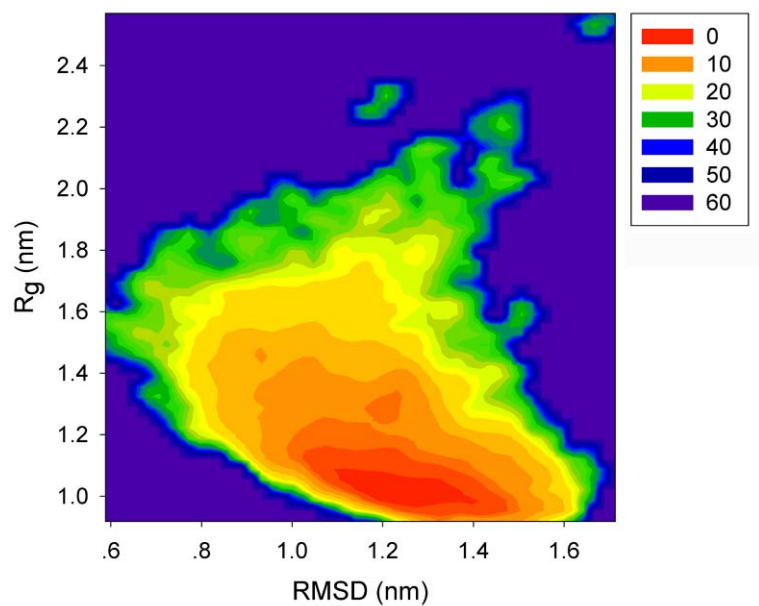


图 S1 以 RMSD 和 R_g 为变量分析得到的 A β 40 构象空间的势能分布(能量单位: $\text{kJ}\cdot\text{mol}^{-1}$)

Fig.S1 The free energy landscape (in $\text{kJ}\cdot\text{mol}^{-1}$) in terms of RMSD and R_g for A β 40
Symbol '+' indicates that $\Delta G=0$

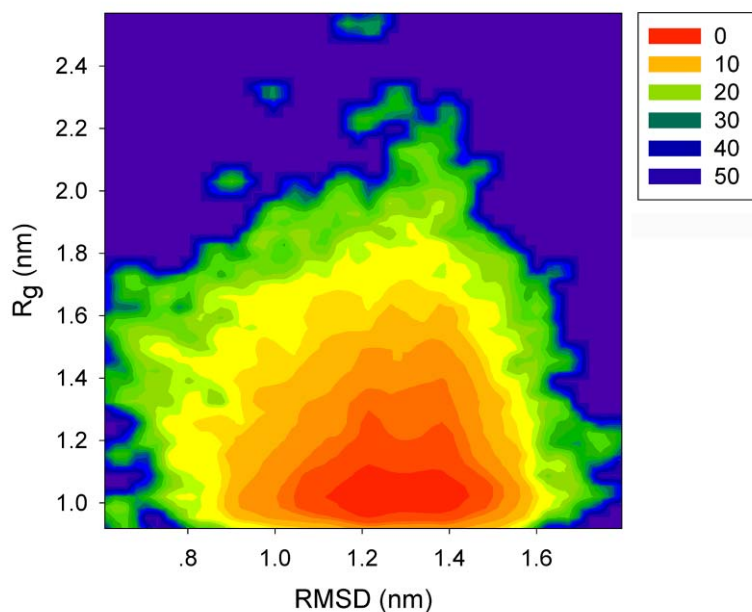


图 S2 以 RMSD 和 R_g 为变量分析得到的 A β 42 构象空间的势能分布(能量单位: $\text{kJ}\cdot\text{mol}^{-1}$)

Fig.S2 The free energy landscape (in $\text{kJ}\cdot\text{mol}^{-1}$) in terms of RMSD and R_g for A β 42
Symbol '+' indicates that $\Delta G=0$.

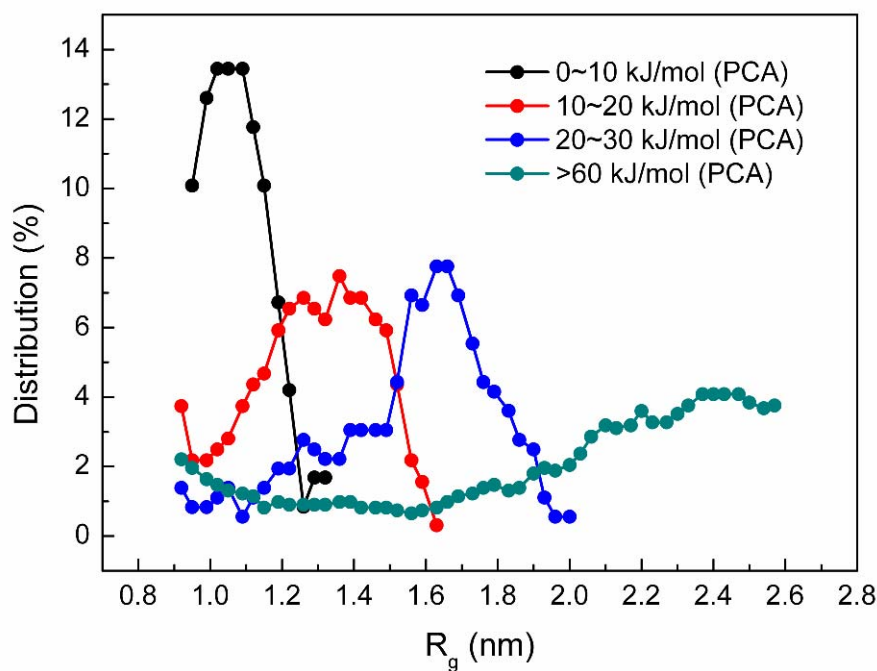


图 S3 图 S1 中不同等势面对应的构象回转半径 R_g 的分布

Fig.S3 The distribution of radius of gyration (R_g) calculated for conformations corresponding to different contour surfaces shown in Fig. S1

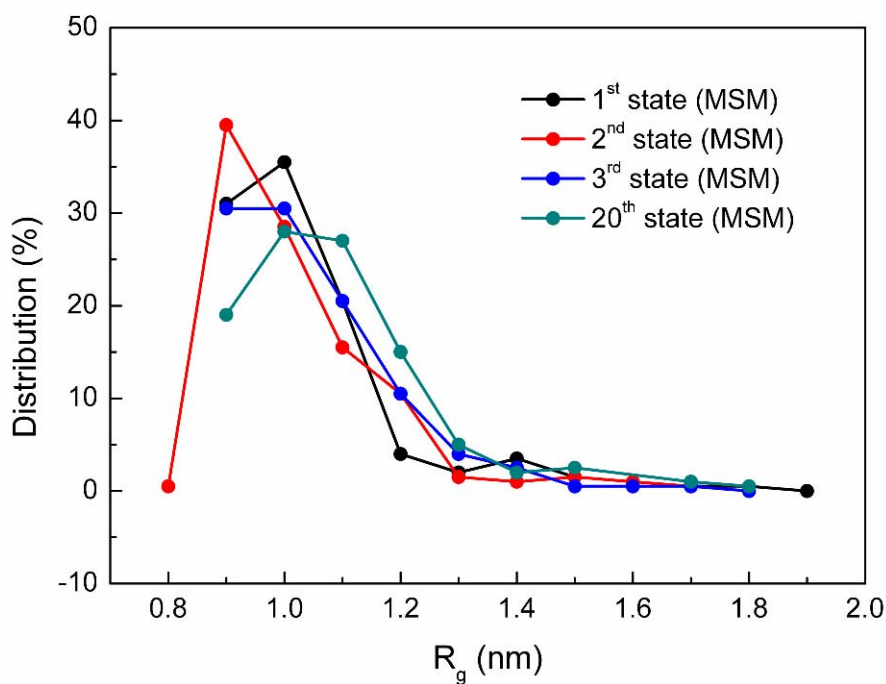


图 S4 图 8(正文) A β 40 MSM 中不同微观状态所包含的构象回转半径 R_g 的分布

Fig.S4 The distribution of radius of gyration (R_g) calculated for conformations corresponding to different microstates shown in Fig. 8 of the main text

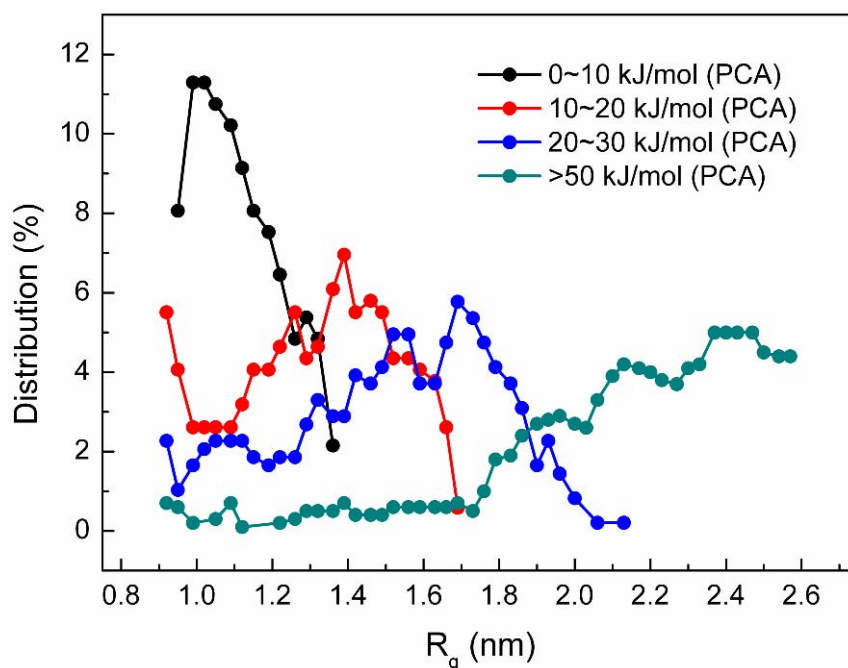


图 S5 图 S2 中不同等势面对应的构象回转半径 R_g 的分布

Fig.S5 The distribution of radius of gyration (R_g) calculated for conformations corresponding to different contour surfaces shown in Fig. S2

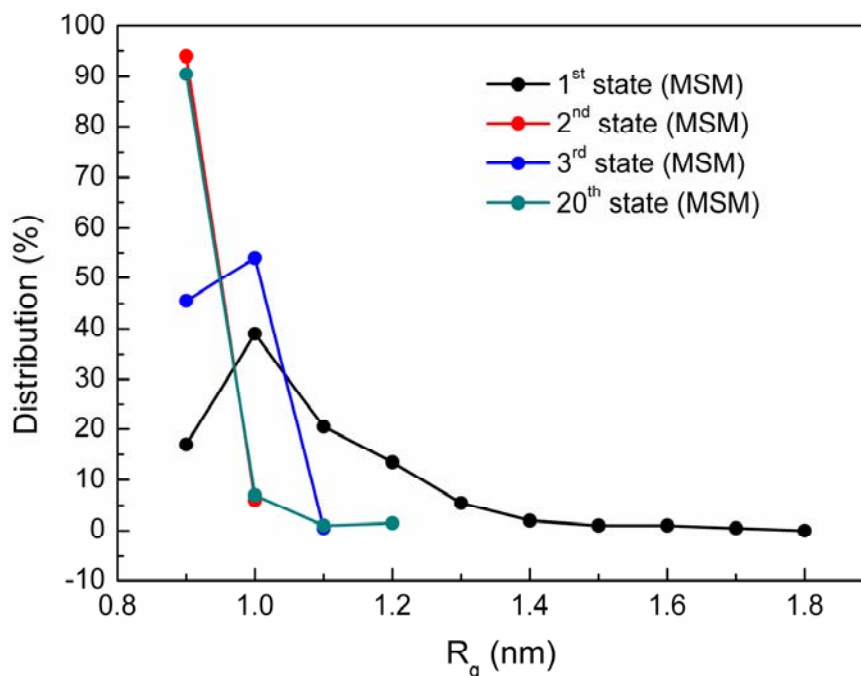


图 S6 图 9(正文)A β 42 MSM 中不同微观状态所包含的构象回转半径 R_g 的分布

Fig.S6 The distribution of radius of gyration (R_g) calculated for conformations corresponding to different microstates shown in Fig. 9 of the main text