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左苯丙胺在多巴胺第三受体分子通道中传输分子动力学模拟

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Molecular Dynamics Simulation for Levo-Benzedrine to Transmit through Molecular Channels within D_3R

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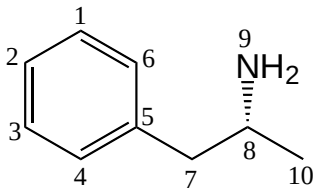
左苯丙胺分子力学参数



[RAT]

[atoms]

C1	CR61	0.025924	1
C2	CR61	-0.032764	1
C3	CR61	0.018167	1
C4	CR61	-0.046547	2
C5	CB	0.067574	2
C6	CR61	-0.054837	2
C7	CH2	-0.077805	3
C8	CH1	0.367608	3
N9	NT	-0.249178	3
C10	CH3	-0.018141	3
H11	H	0.005	3
H12	H	0.005	3

[bonds]

C1 C2
C2 C3
C3 C4
C4 C5
C5 C6
C6 C1
C5 C7
C7 C8
C8 N9
C8 C10
H11 N9
H12 N9

[angles]

; ai aj ak gromos type

C1 C2 C3
C2 C3 C4
C3 C4 C5
C4 C5 C6
C5 C6 C1
C4 C5 C7
C5 C7 C8
C7 C8 N9
C7 C8 C10
N9 C8 C10

H11 N9 H12

[impropers]

; ai aj ak al gromos type

C7 C8 N9 C10 0.000 167.360

[dihedrals]

; ai aj ak al gromos type

C1 C2 C3 C4

C2 C3 C4 C5

C3 C4 C5 C6

C4 C5 C6 C1

C3 C4 C5 C7

C4 C5 C7 C8

C5 C7 C8 C10

C5 C7 C8 N9

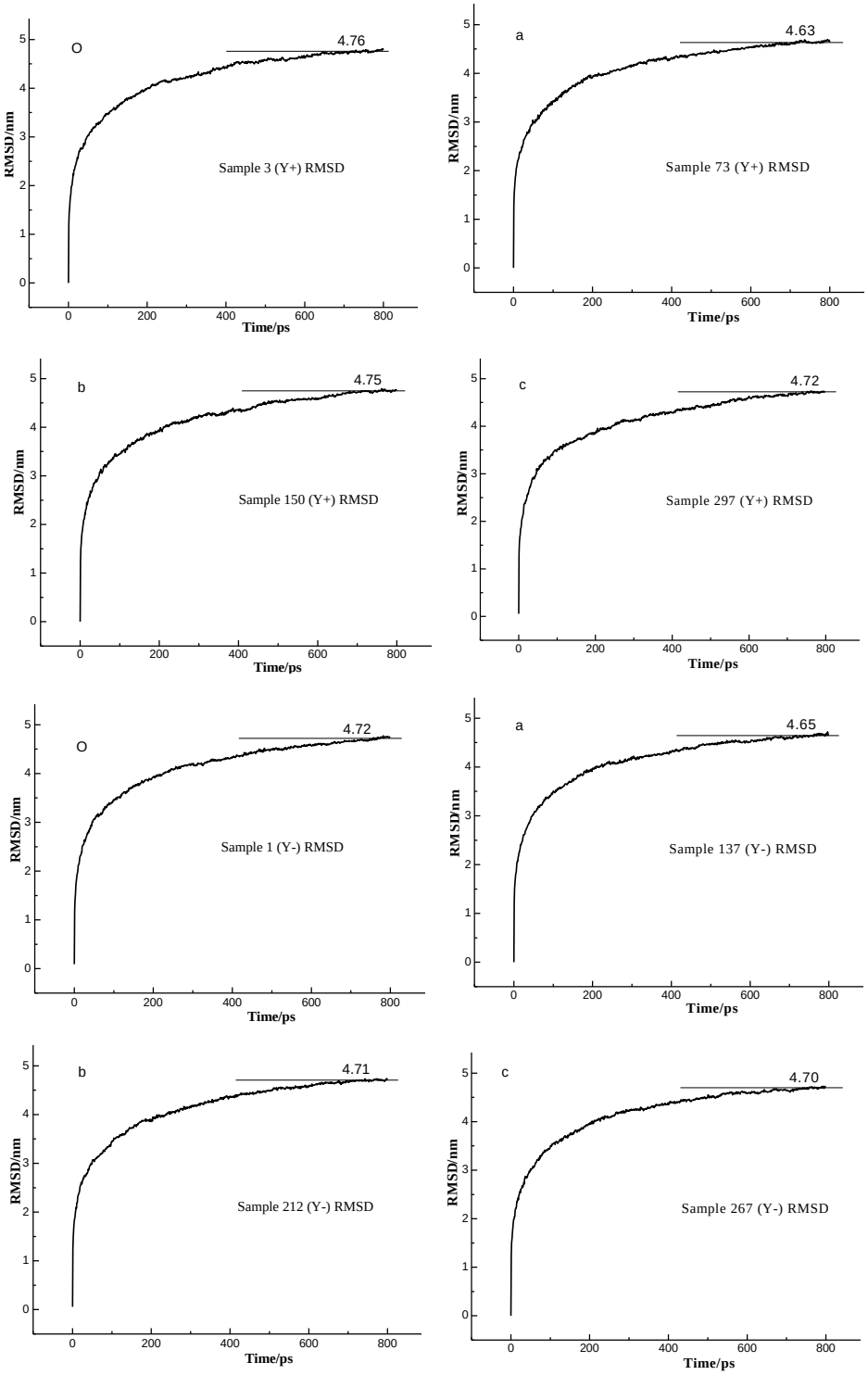


图 S1　在+*y* 和-*y* 轴方向，各自四个伞形样本分子动力学模拟体系 RMSD 模拟时间变化曲线

Fig.S1　RMSD *vs* MD simulation time within 800ps for eight samplings along the +*y* and -*y* axes

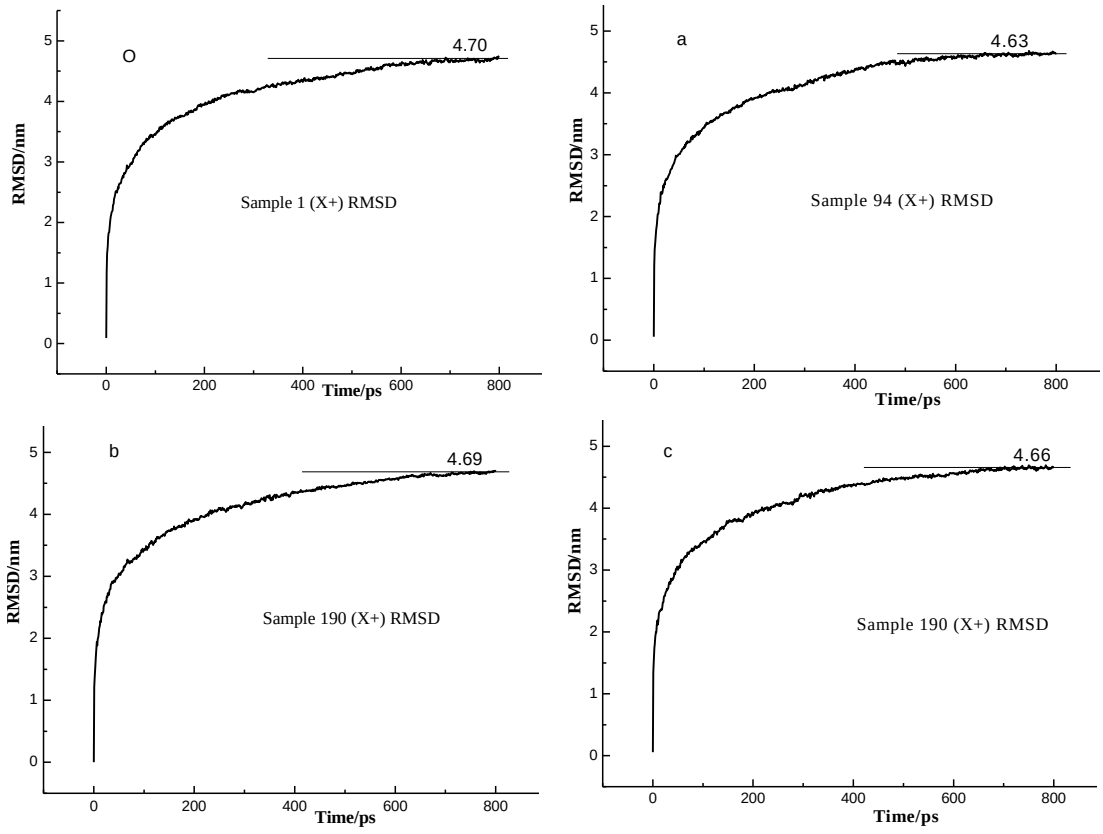
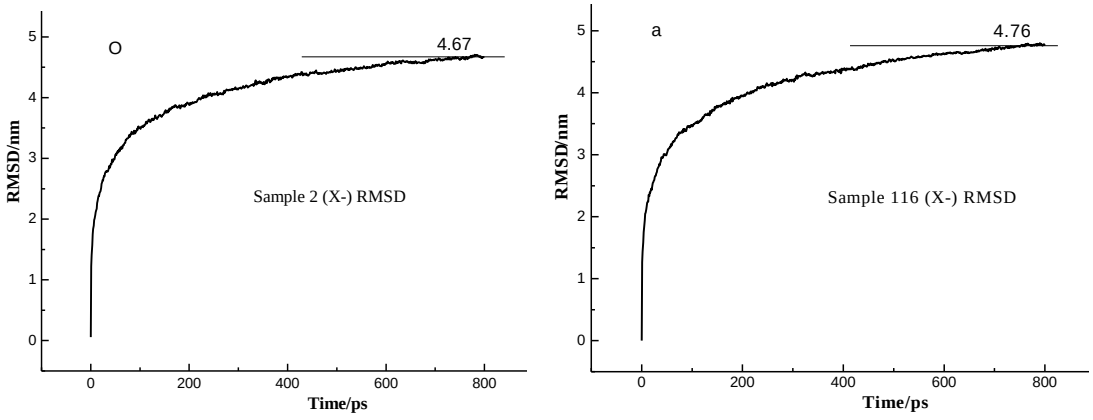


图 S2　在+*x* 轴方向，四个伞形样本分子动力学模拟体系 RMSD 随模拟时间变化曲线
Fig.S2　RMSD *vs* MD simulation time within 800ps for four samplings along the +*x* axis



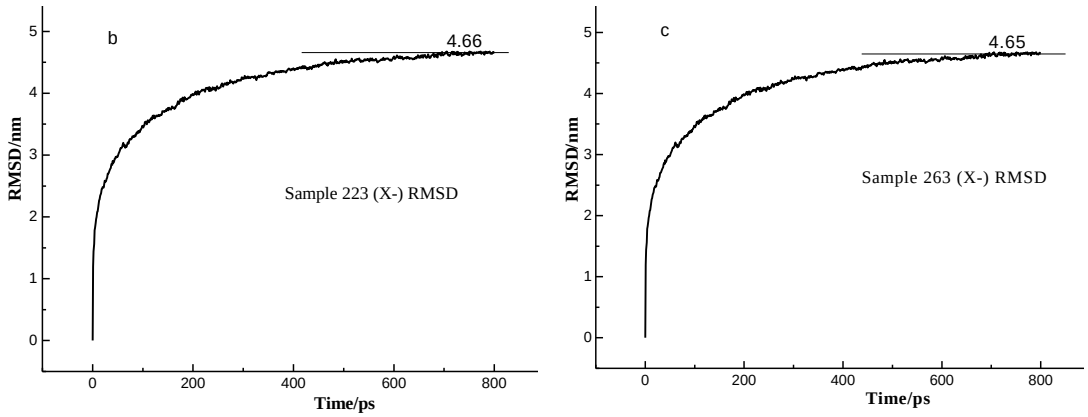


图 S3 在-*x* 轴方向，四个伞形样本分子动力学模拟体系 RMSD 随模拟时间变化曲线
Fig.S3 RMSD *vs* MD simulation time within 800ps for four samplings along the -*x* axis

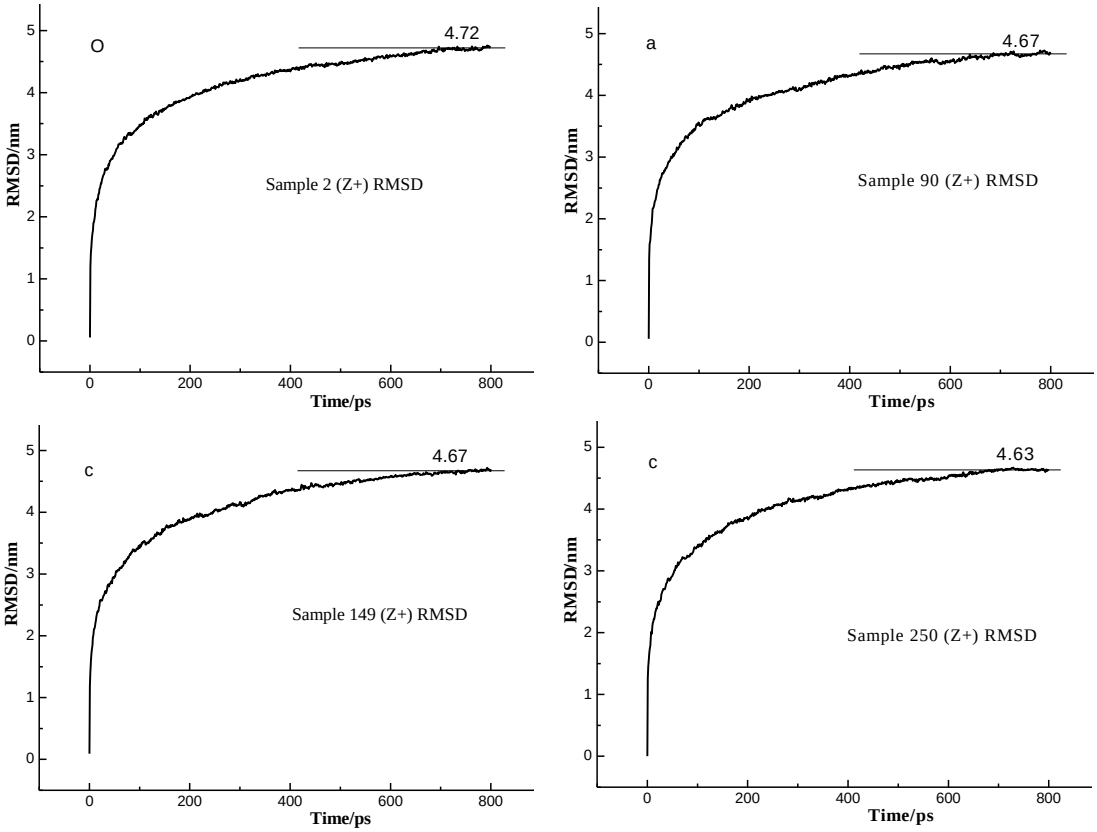


图 S4 在+*z* 轴方向，四个伞形样本分子动力学模拟体系 RMSD 随模拟时间变化曲线
Fig.S4 RMSD *vs* MD simulation time within 800ps for four samplings along the +*z* axis

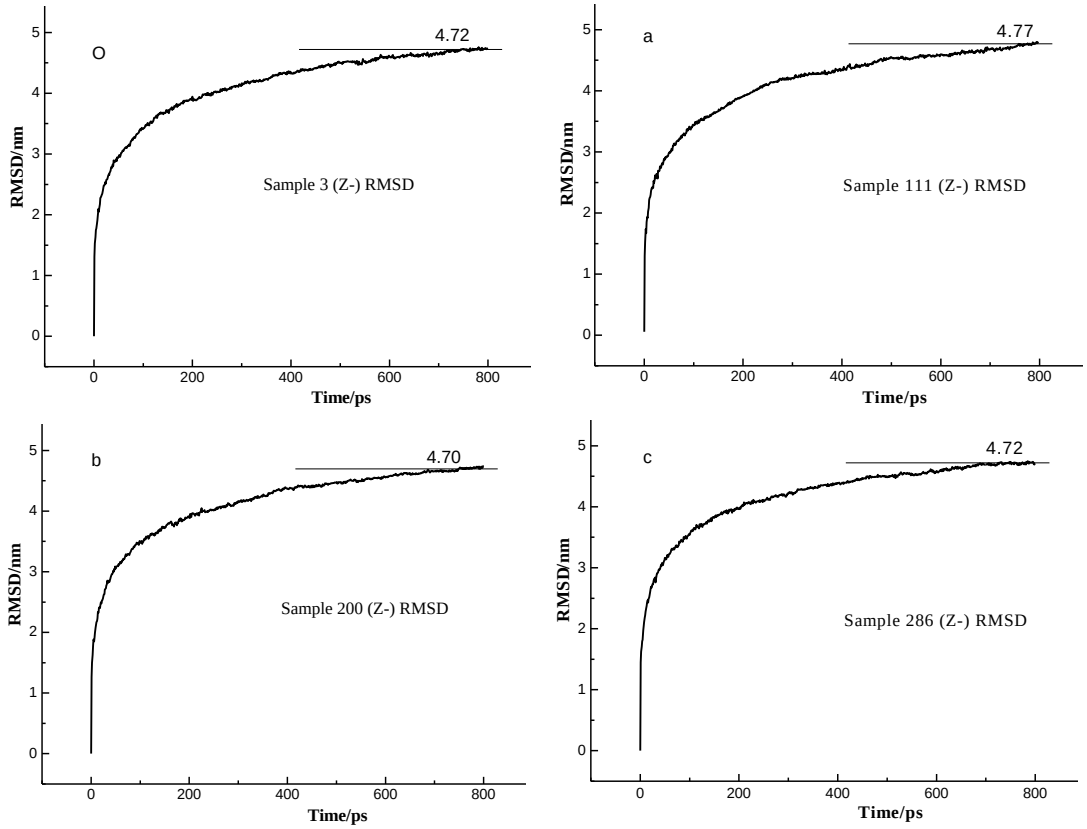


图 S5 在-*z* 轴方向，四个伞形样本分子动力学模拟体系 RMSD 随模拟时间变化曲线

Fig.S5 RMSD vs MD simulation time within 800ps for four samplings along the -*z* axis