Protecting High Energy Barriers: A New Equation to Regulate Boost Energy in Accelerated Molecular Dynamics Simulations

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TITLE RUNNING HEAD: New Boost Equation for Accelerated MD

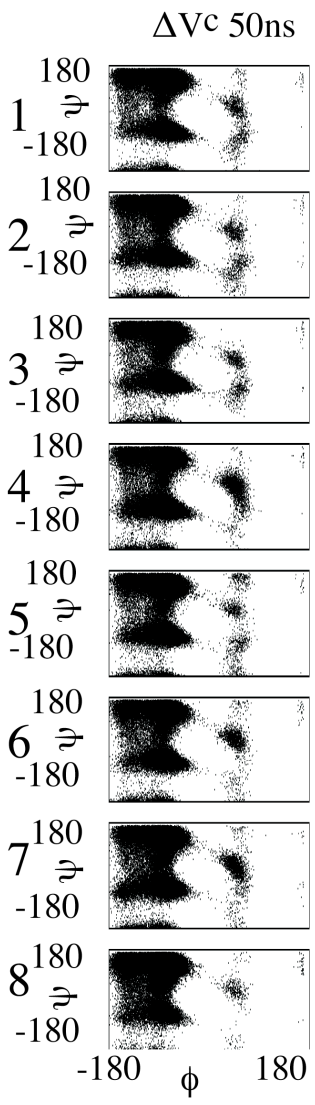

Figure S1: Decalanine Phi(Φ)-Psi(Ψ) angles distribution obtained from aMD simulations with ΔV^c. Parameters were set to E_1=74, E_2= E_1+35, α_2=5 and α_1=15. All values are in kcal/mol.

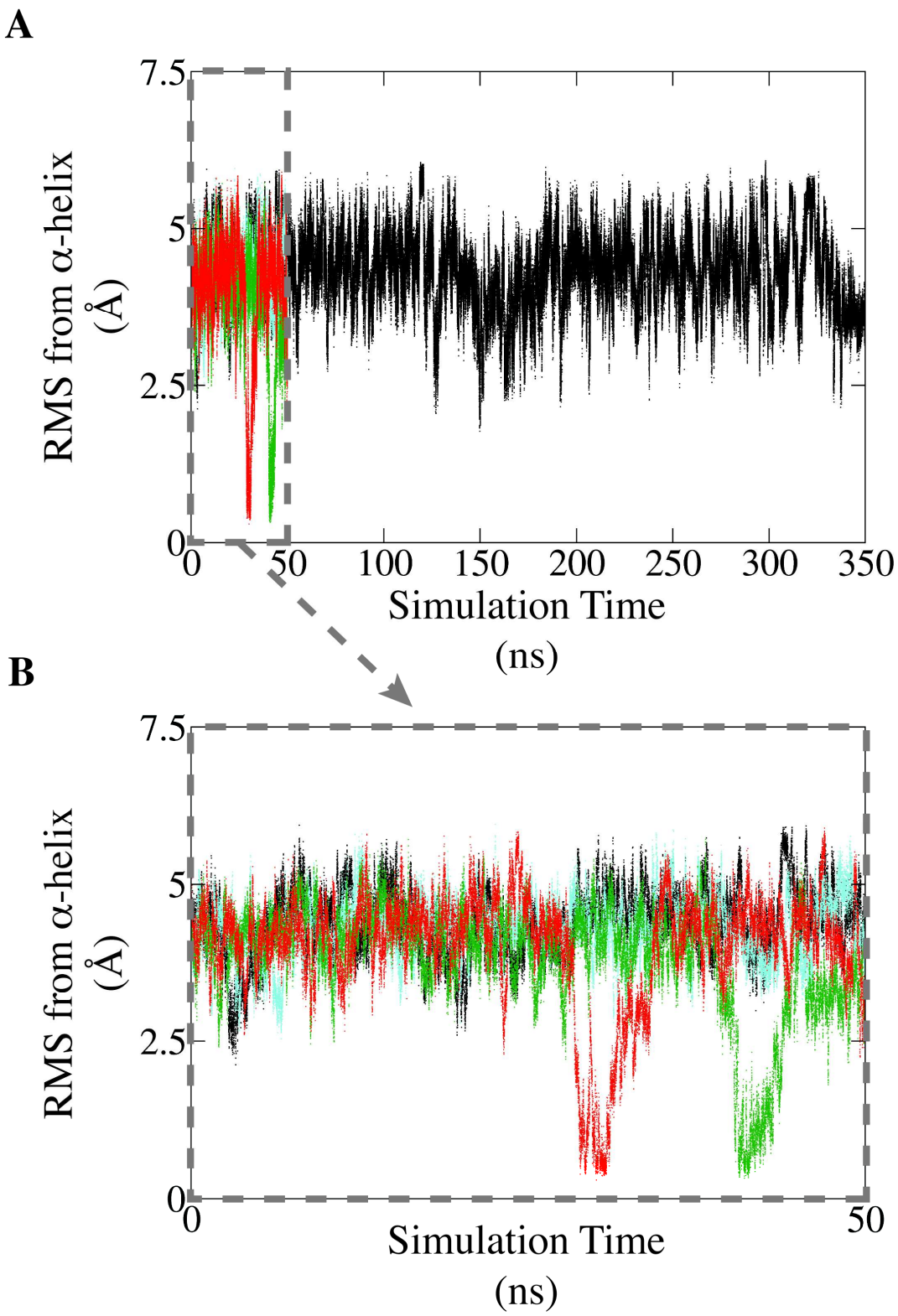
A
7.5
5
2.5
0
RMS from α-helix (Å)
0
50
100
150
200
250
300
350
Simulation Time (ns)
B
7.5
5
2.5
0
RMS from α-helix (Å)
0
50
Simulation Time (ns)

Figure S2: Decalinine root mean square (RMS) deviation from α-helix conformation calculated along: A) 350ns of cMD and 50 ns of aMD simulations, and B) the first 50ns of simulations displayed in (A). Solid lines correspond to MD (black) and aMD with parameters set to E_1=74, α_2=5 (all aMD simulations) E_2= E_1+25 and α_1=30 (cyan); E_2= E_1+25 and α_1=15 (red); E_2= E_1+35 and α_1=15 (green). All values are in kcal/mol.