Supporting Information

for "Gaussian Accelerated Molecular Dynamics in NAMD" by Yui Tik Pang, Yinglong Miao, Yi Wang and J. Andrew McCammon.

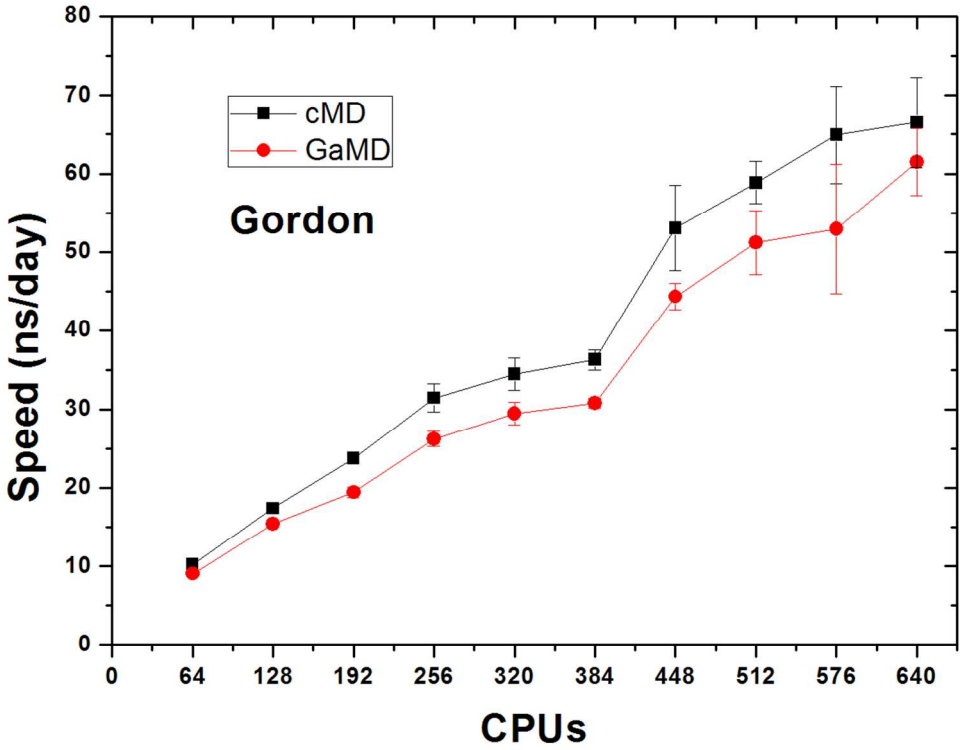

Fig. S1 Scaling performance of the conventional MD (cMD) and Gaussian accelerated molecular dynamics (GaMD) simulations using NAMD 2.11 on the M3 muscarinic G-protein-coupled receptor system (~55,500 atoms in total). The error bars were obtained as the standard deviation of six benchmarking numbers output in the NAMD 2.11 log file.

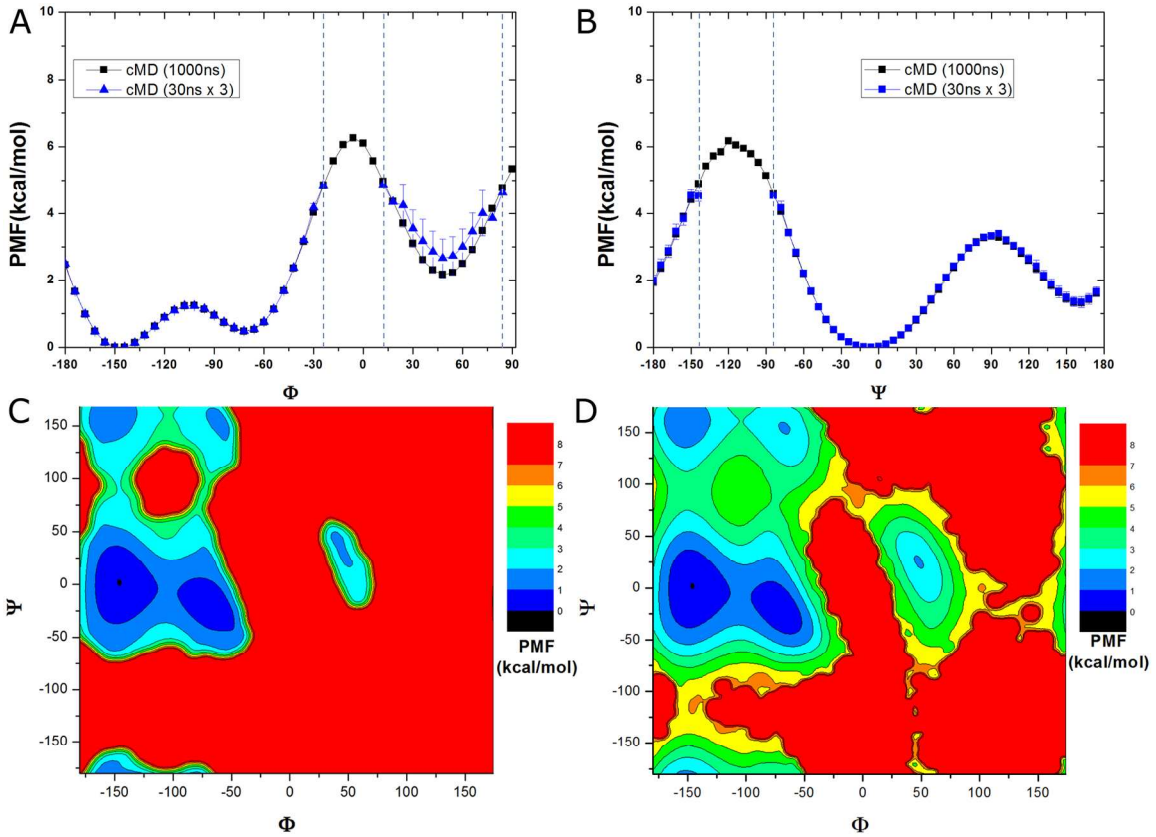

Fig. S2 Conventional MD (cMD) simulations of the alanine dipeptide: (A-B) 1D PMF profiles of (A) Φ and (B) Ψ obtained from three independent 30ns cMD simulations that hardly sample the high energy barriers and (C-D) 2D PMF profiles of (Φ, Ψ) obtained from the (C) three 30ns cMD simulations combined and (D) a converged 1000ns cMD simulation.

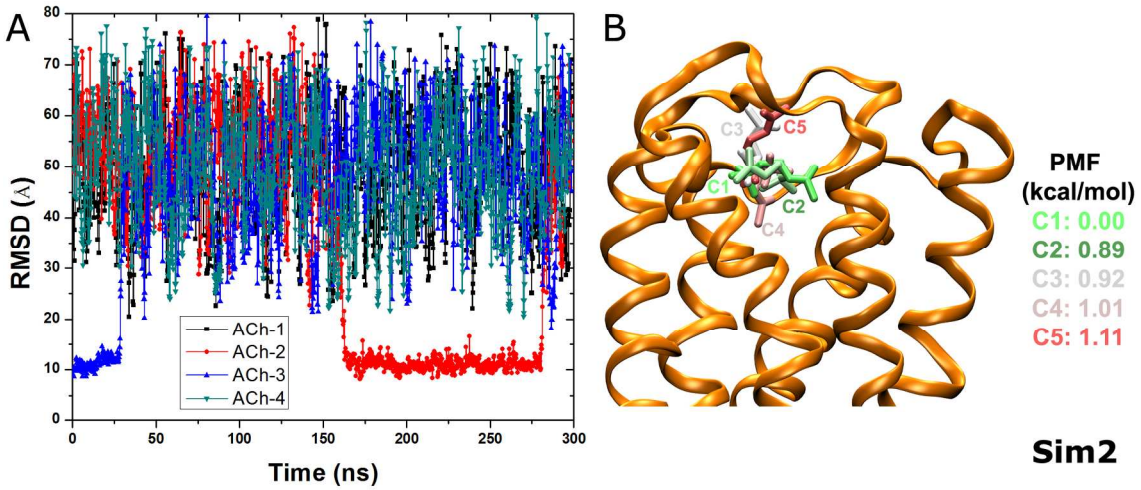

Fig. S3 The second copy of GaMD simulation of the acetylcholine (ACh) endogenous agonist binding to the M3 muscarinic GPCR: (A) the RMSD of the four diffusing ACh molecules relative to the Glide docking pose, which depicts ACh-2 and ACh-3 binds briefly to the extracellular vestibule with ~10 Å RMSD and (B) the five lowest energy structural clusters of ACh that are labeled and colored in a GWR scale according to free energy values obtained from reweighting of the GaMD simulations.

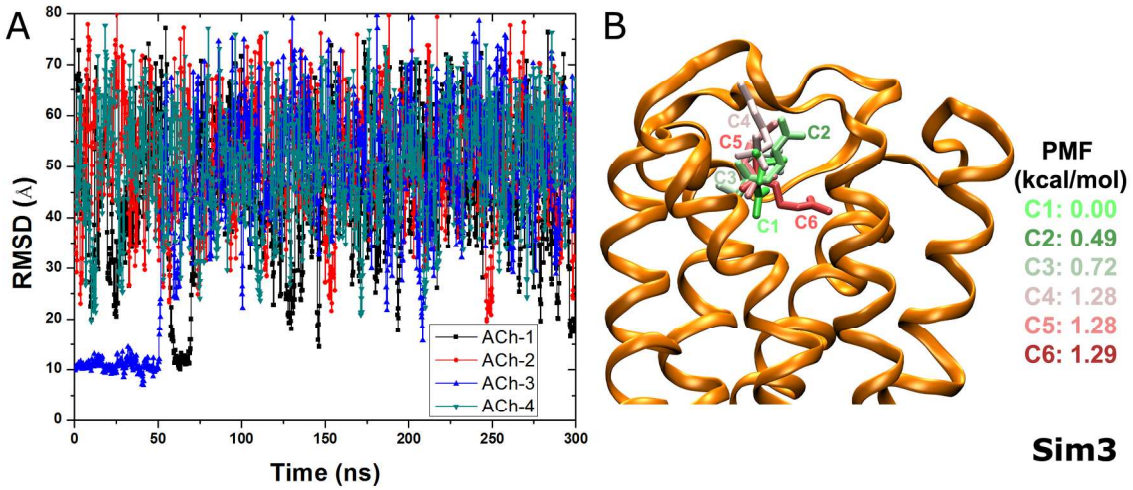

Fig. S4 The third copy of GaMD simulation of the acetylcholine (ACh) endogenous agonist binding to the M3 muscarinic GPCR: (A) the RMSD of the four diffusing ACh molecules relative to the Glide docking pose, which depicts ACh-1 and ACh-3 binds briefly to the extracellular vestibule with ~10 Å RMSD and (B) the five lowest energy structural clusters of ACh that are labeled and colored in a GWR scale according to free energy values obtained from reweighting of the GaMD simulations.