

# The effect of carbon nanotube on the structure of H-NS protein and its interactions with DNA: molecular dynamics approach

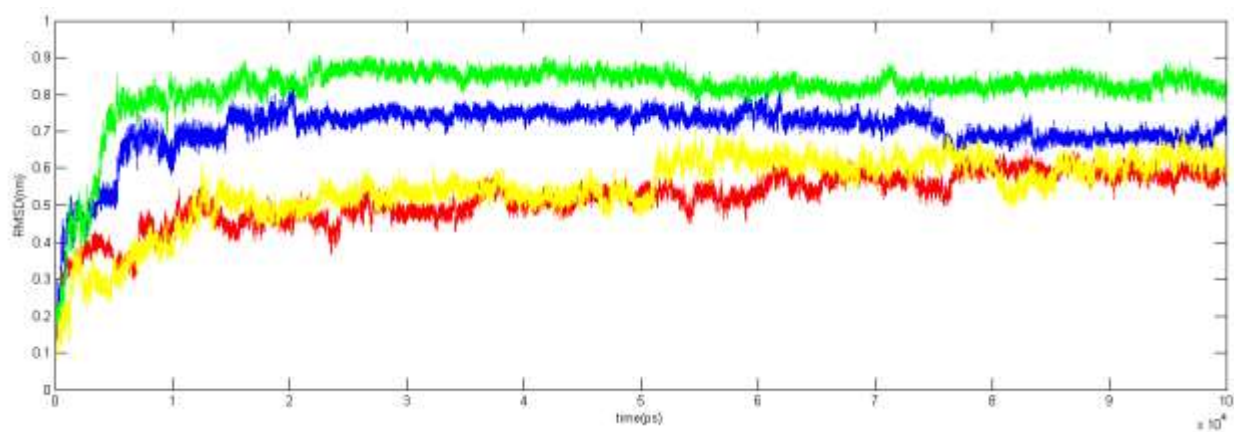
Najmeh Mahdavi-pour, Mohammad Reza Bozorgmehr, Mohammad Momen-Heravi

## Supplementary Data

### No. contents

- 1 Fig. S1 The  $C\alpha$ -RMSD (nm) of H-NS vs. time (ps). Red: *protein* blue: *protein-SWCNT* green: *protein-DNA* yellow: *protein-SWCNT-DNA*
- 2 Fig. S2 The  $R_g$  (nm) of H-NS vs. time (ps). Red: *protein* blue: *protein-SWCNT* green: *protein-DNA* yellow: *protein-SWCNT-DNA*
- 3 Fig. S3 2D Free Energy Landscape of the *protein* simulated system
- 4 Fig. S4 2D Free Energy Landscape of the *protein-SWCNT* simulated system
- 5 Fig. S5 2D Free Energy Landscape of the *protein-DNA* simulated system
- 6 Fig. S6 2D Free Energy Landscape of the *protein-SWCNT-DNA* simulated system
- 7 Fig. S7 3D Free Energy Landscape of the *protein* simulated system
- 8 Fig. S8 3D Free Energy Landscape of the *protein-SWCNT* simulated system
- 9 Fig. S9 3D Free Energy Landscape of the *protein-DNA* simulated system
- 10 Fig. S10 3D Free Energy Landscape of the *protein-SWCNT-DNA* simulated system

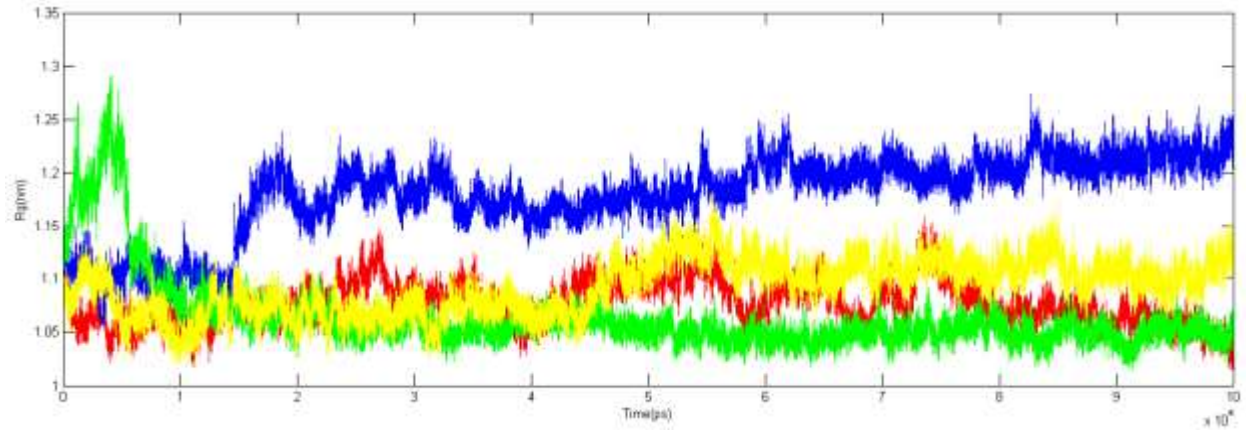
S. 1



S. 1 The  $C\alpha$ -RMSD (nm) of H-NS vs. time (ps).

Red: *protein*    blue: *protein-SWCNT*    green: *protein-DNA*    yellow: *protein-SWCNT-DNA*

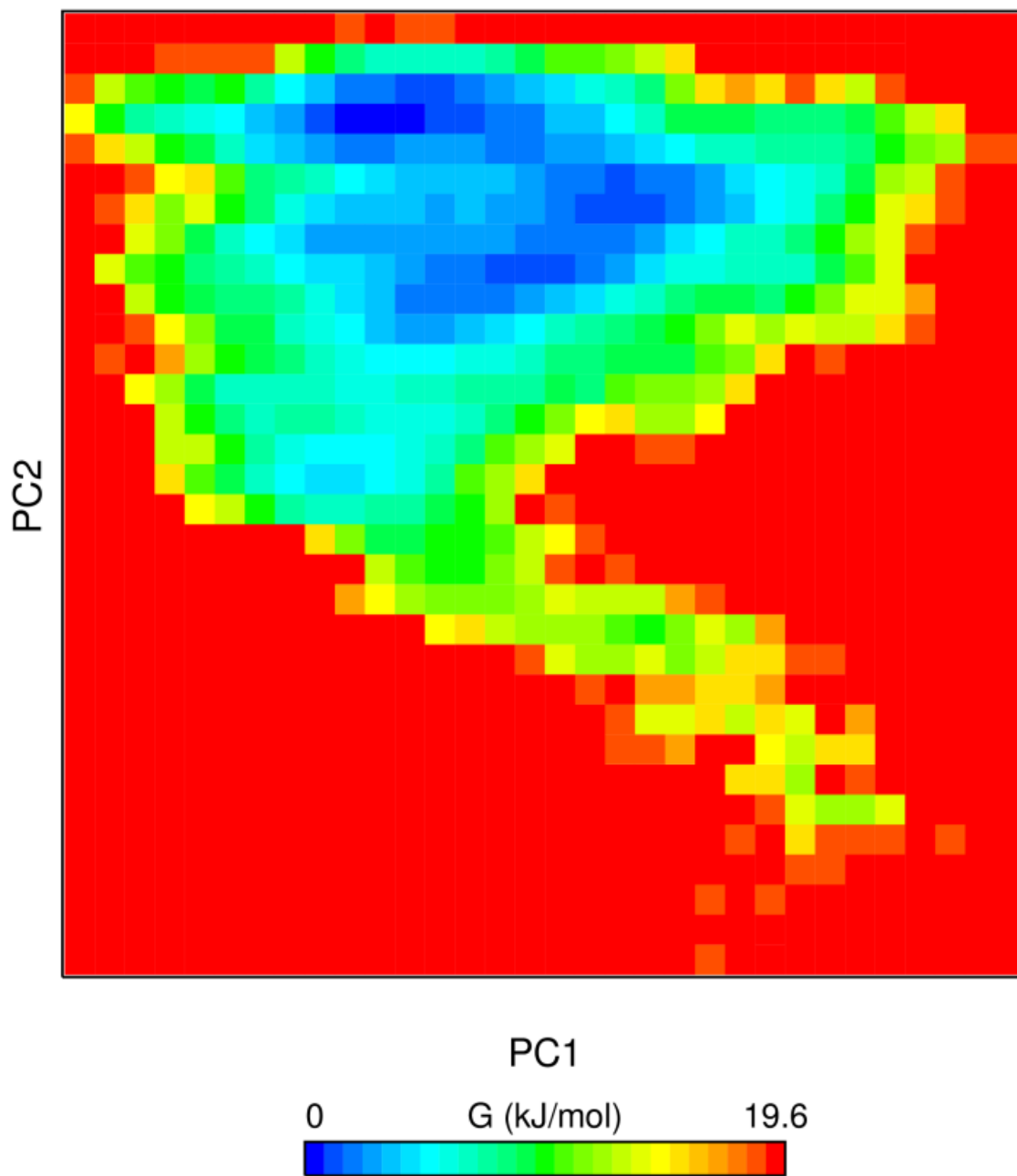
S. 2



S. 2 The Rg (nm) of H-NS vs. time (ps).

Red: *protein*      blue: *protein-SWCNT*      green: *protein-DNA*      yellow: *protein-SWCNT-DNA*

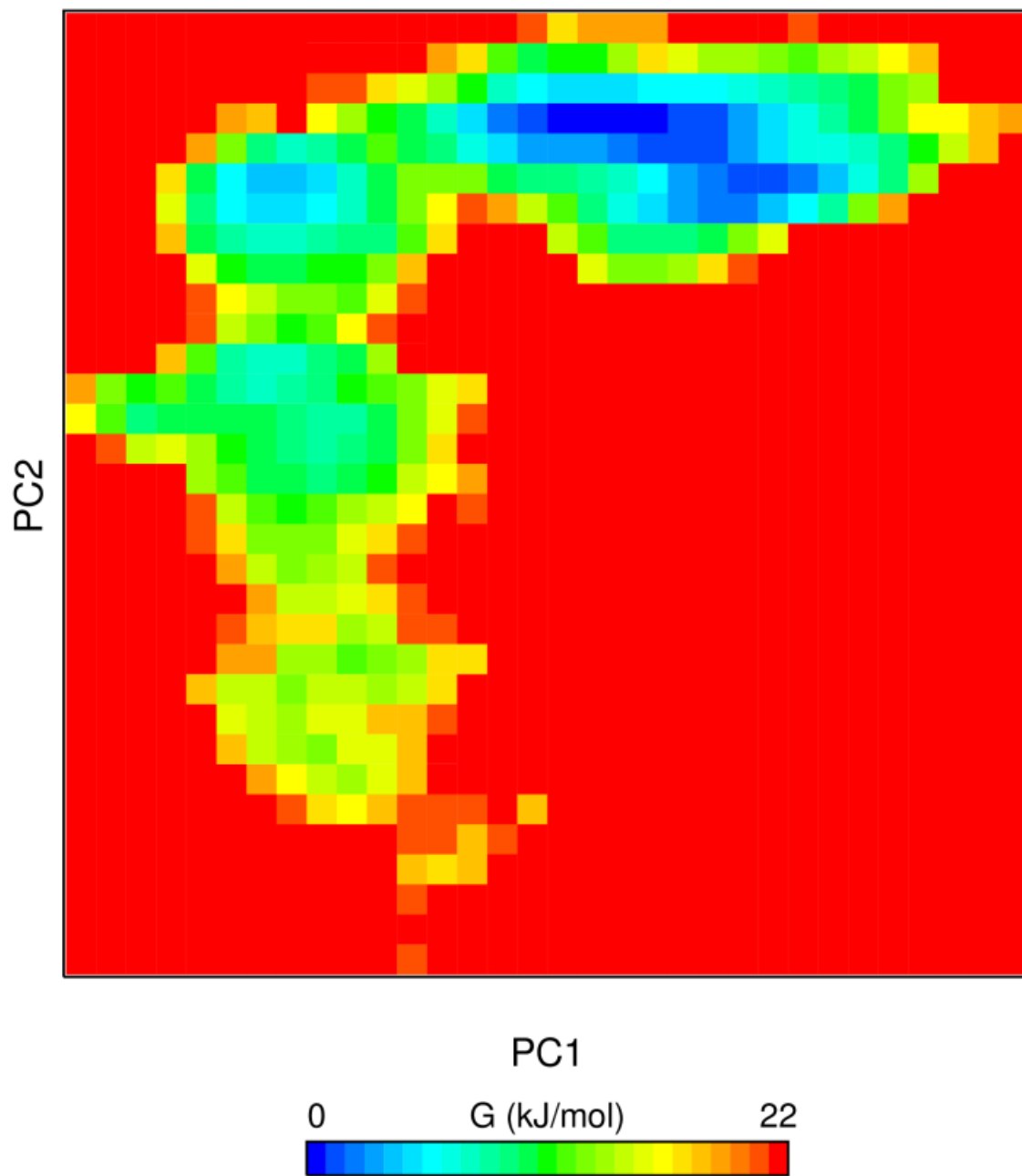
## Gibbs Energy Landscape



S. 3 2D Free Energy Landscape of the *protein* simulated system

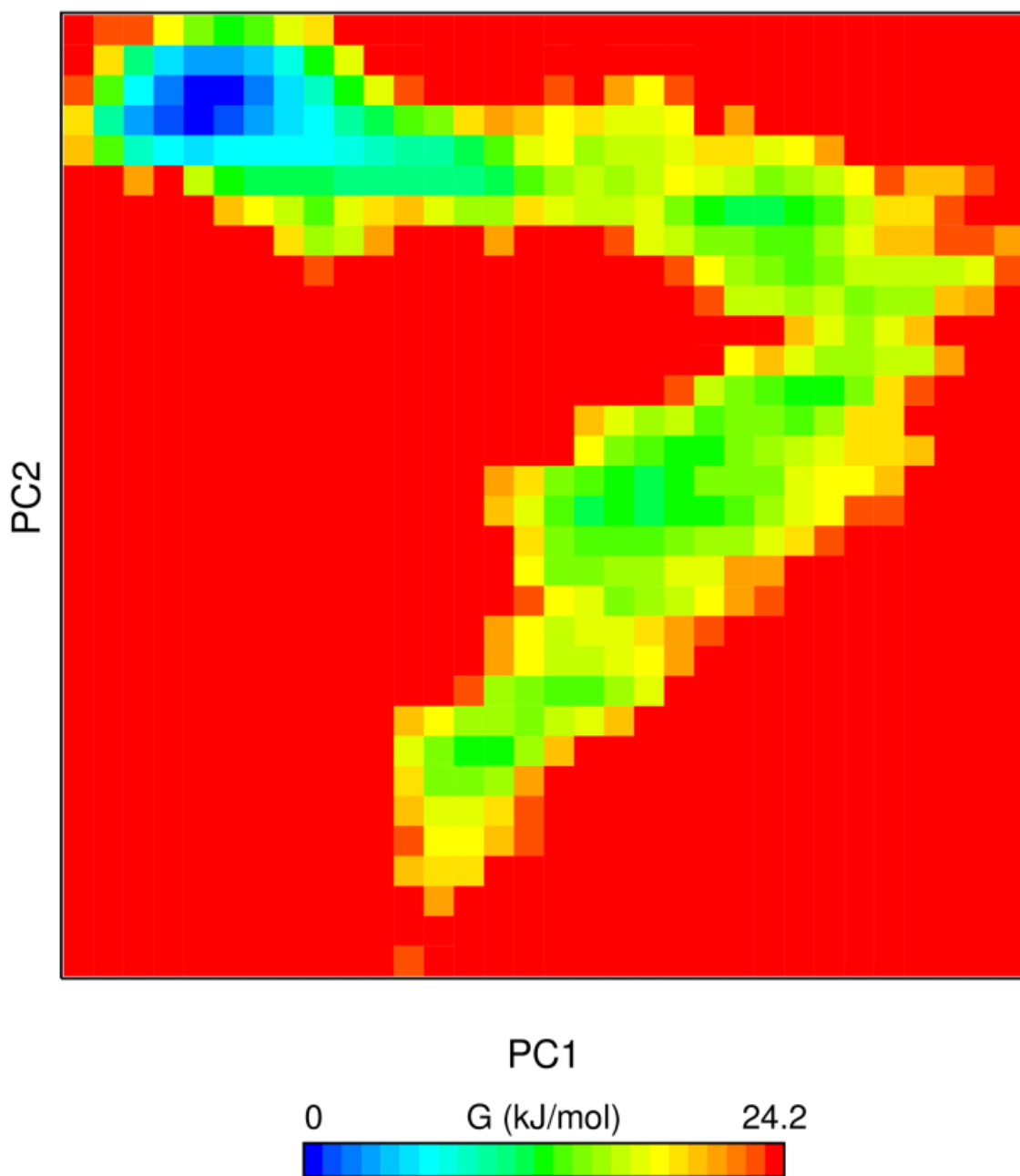
S. 4

## Gibbs Energy Landscape



S. 4 2D Free Energy Landscape of the *protein-SWCNT* simulated system

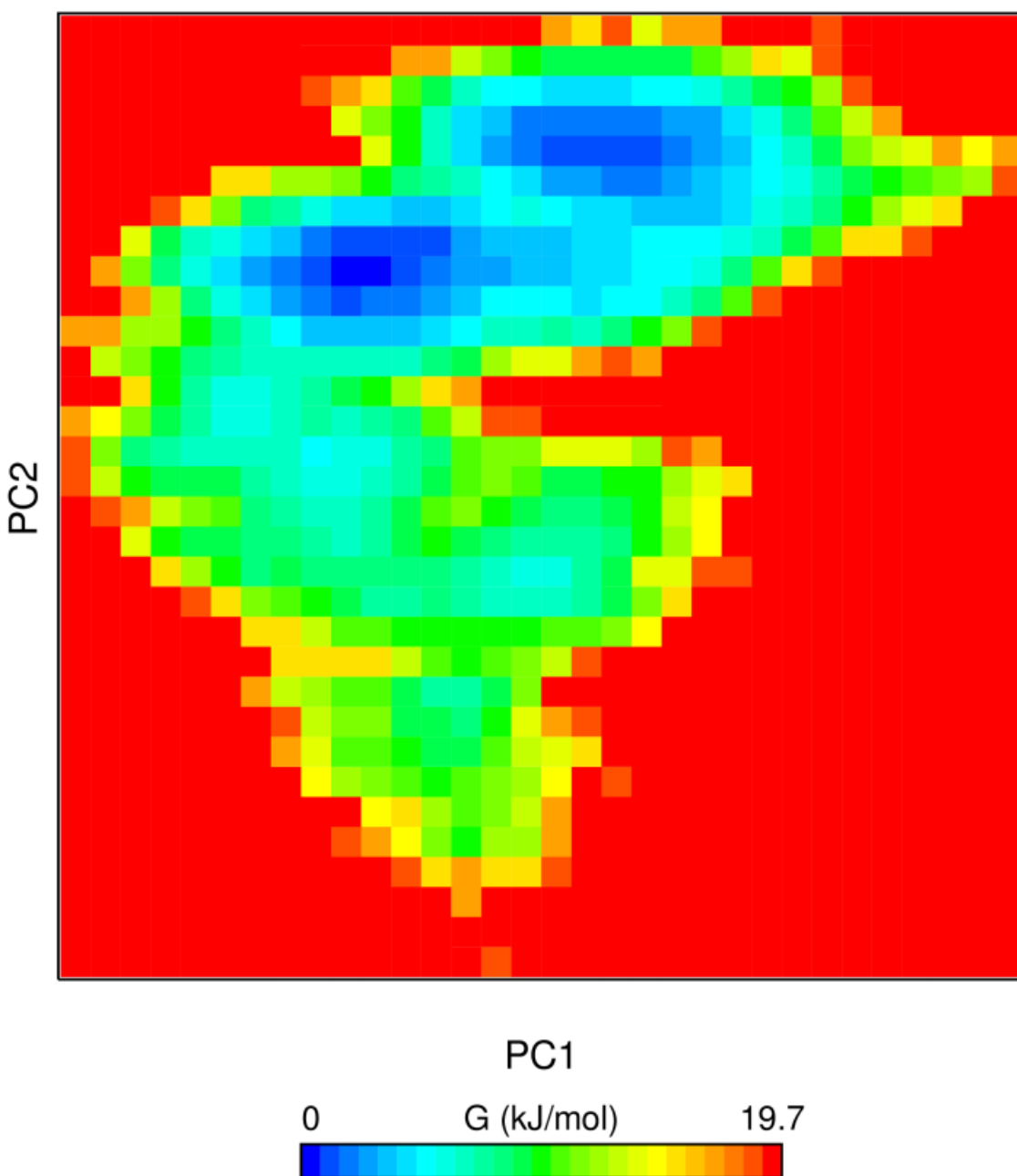
## Gibbs Energy Landscape



S. 5 2D Free Energy Landscape of the *protein-DNA* simulated system

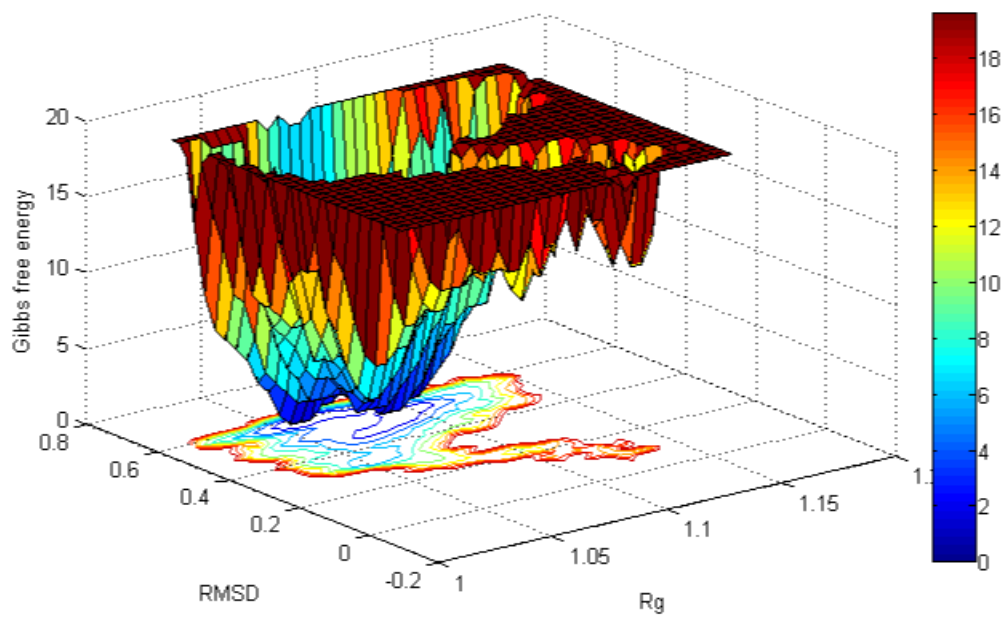
S. 6

## Gibbs Energy Landscape



S. 6 2D Free Energy Landscape of the *protein-SWCNT-DNA* simulated system

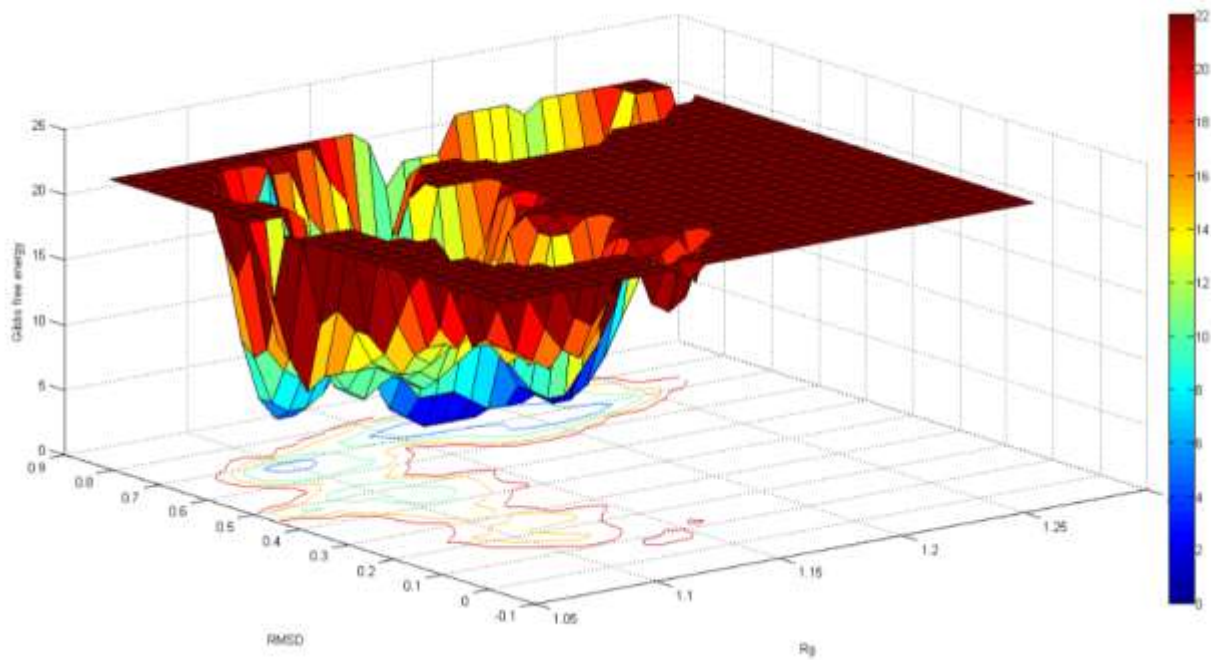
S. 7



S. 7 3D Free Energy Landscape of the *protein* simulated system

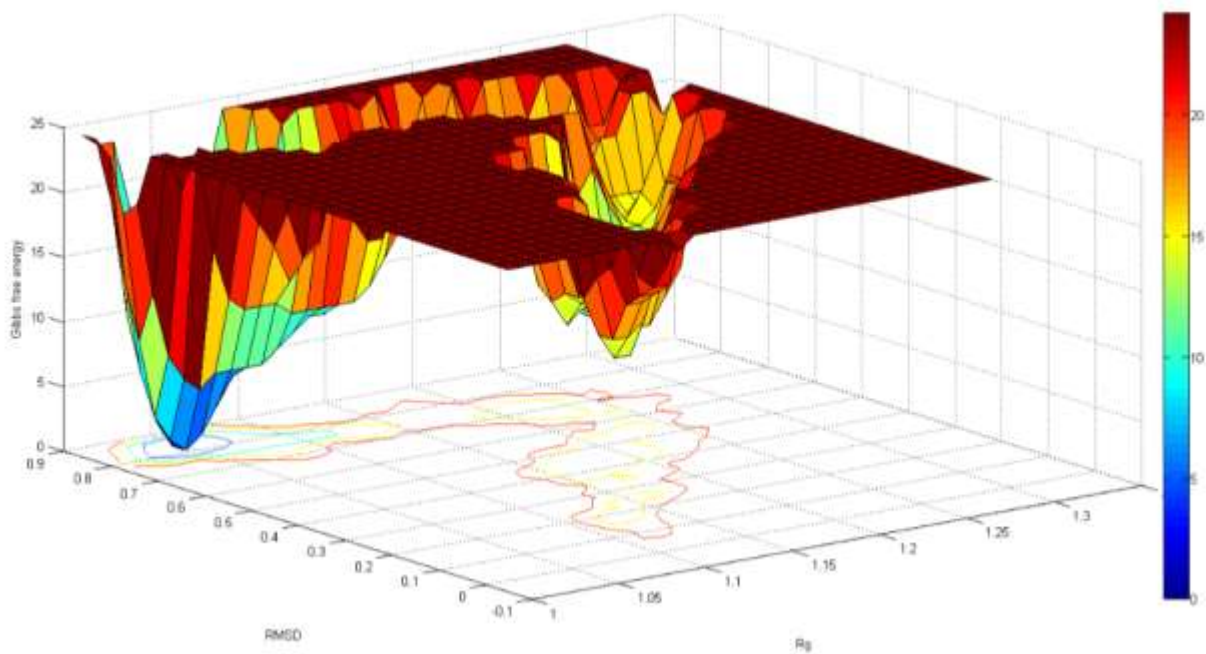


S. 8



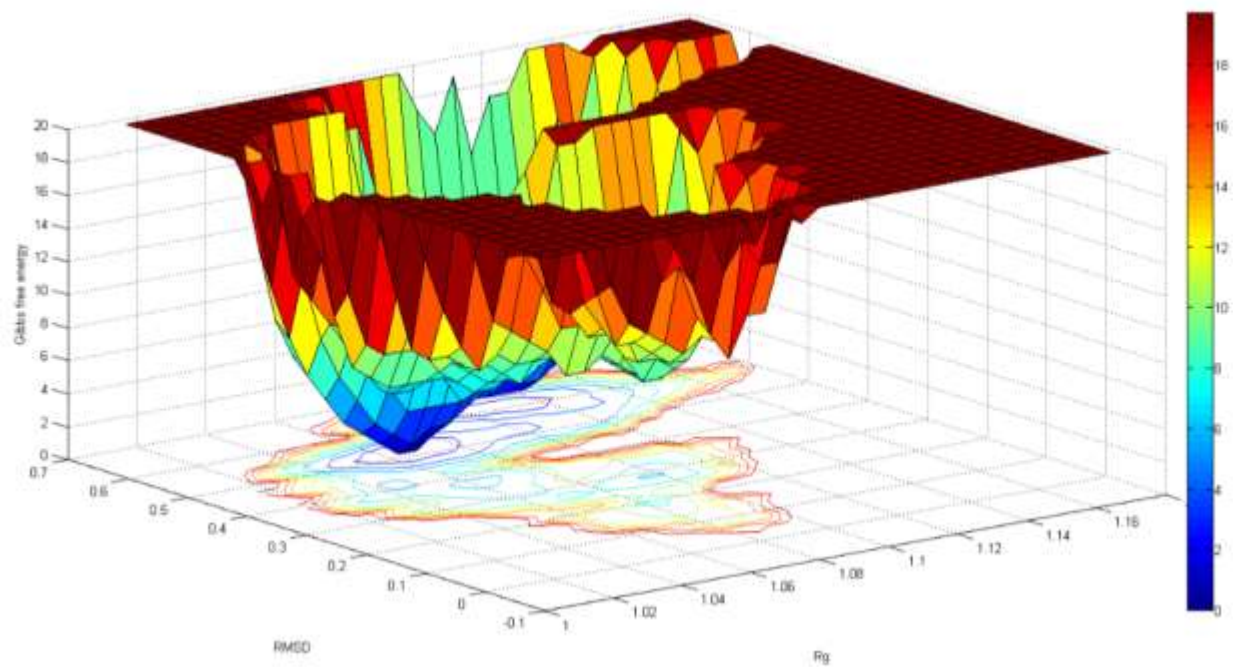
S. 8 3D Free Energy Landscape of the *protein-SWCNT* simulated system

S. 9



S. 9 3D Free Energy Landscape of the *protein-DNA* simulated system

S. 10



S. 10 3D Free Energy Landscape of the *protein-SWCNT-DNA* simulated system