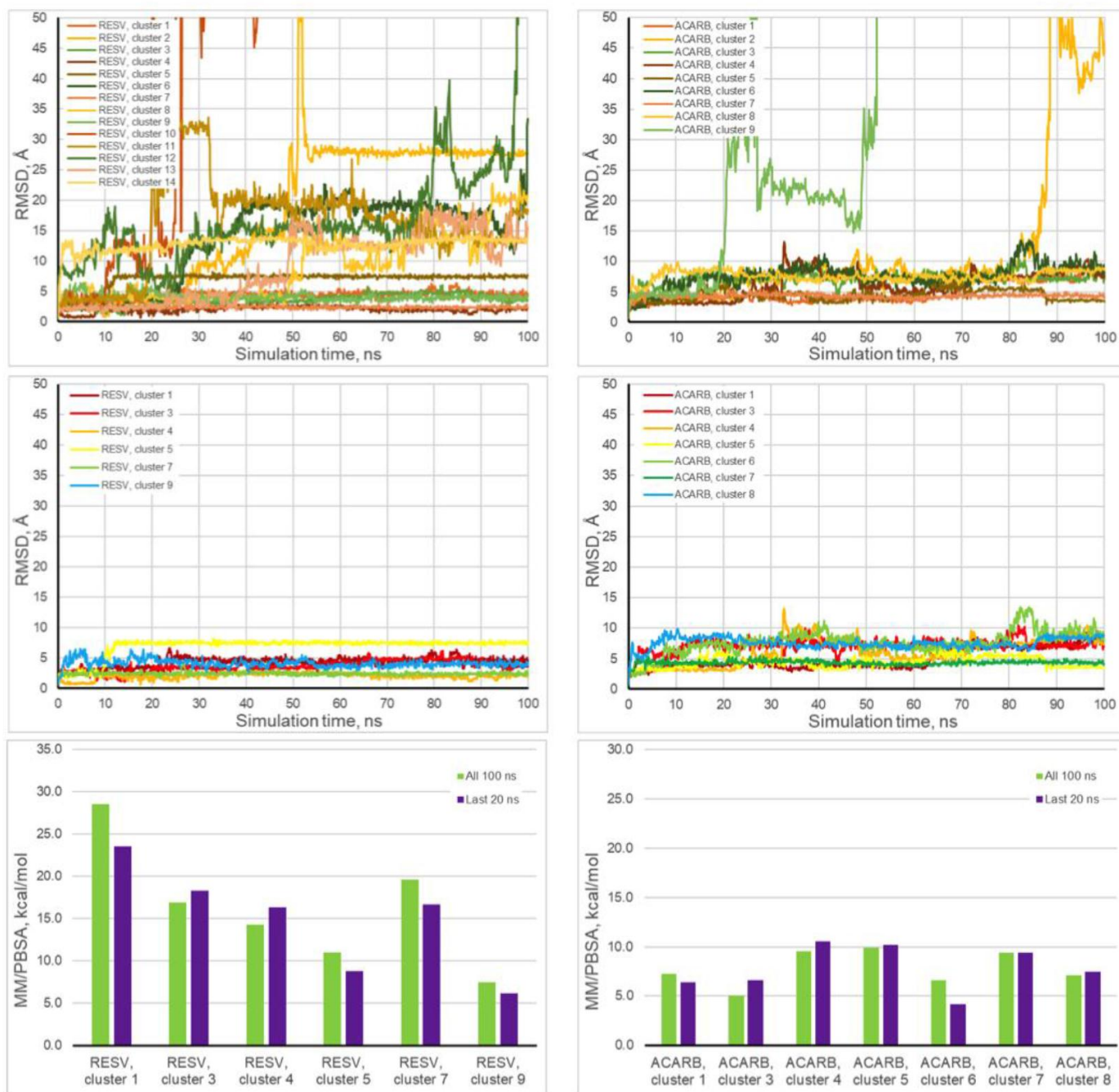


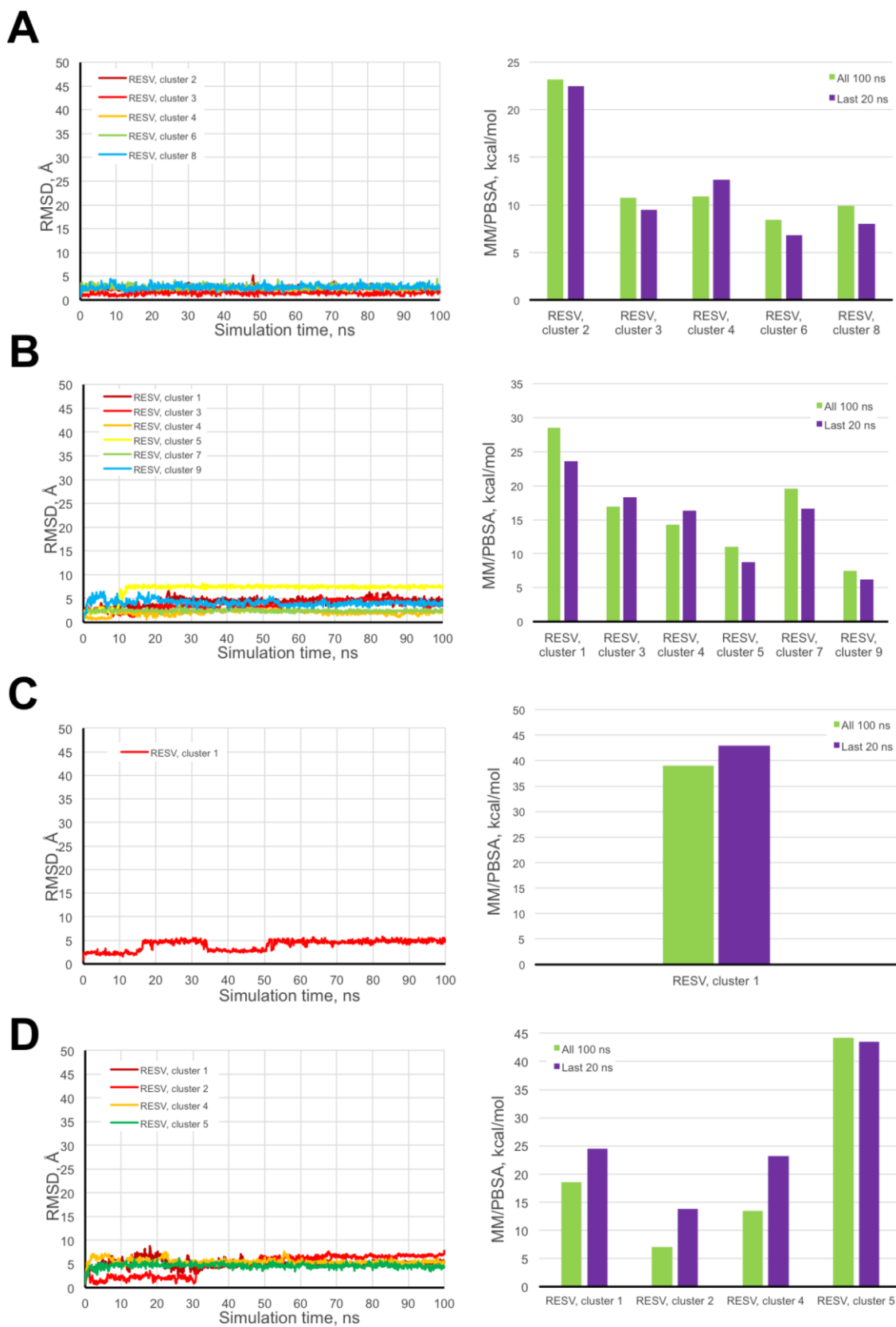
SUPPLEMENTARY FIGURES

RSV

acarbose



Supplementary Figure 1. Trajectories and MM/PBSA free energy analysis of RSV (left) and acarbose (right) forming complexes with the yeast form of GGA.



**Supplementary Figure 2.** Trajectories and MM/PBSA free energy analysis of RSV clusters forming complexes with human GAA (A), yeast GGA (B), human  $\alpha$ -Man I (C), and human  $\alpha$ -Man II homology model (D).