

MMPBSA Calculations of Small RNA Molecules Containing 3' Overhangs

Caroline Velez, Stephen Telehany, Jennifer McGinnis, and Maria C. Nagan

Adelphi University, Garden City, NY

Prior melting studies performed on RNA complexes with 3' overhangs found that two overhanging bases provide more stability than one. In addition, the first base must be a purine but the second base is more stabilizing if it is a pyrimidine rather than a purine (O'Toole *et al.*, *RNA*, 2005). To confirm these findings, MMPBSA calculations and specifically normal mode analysis (NMA) was implemented to identify the correlation in molecular dynamic (MD) trajectories of small RNA molecules with different purine and pyrimidine 3' overhangs. Once entropy and free energy of the complex were computed, a more comprehensive $\Delta\Delta G^\circ$ was determined.

