

Importance of Anion- π Interactions in RNA GAAA and GGAG Tetraloops: A Combined MD and QM Study

RNA tetraloops are an important component of RNA hairpin structure. Many such tetraloops are stabilized by the phosphate at position three pointing towards the purine ring of the first base (Guanine). While cation- π interactions are prevalent in the literature, anion- π interactions have garnered less attention. We use a combination of experimental and molecular dynamics structures to investigate the stabilizing effect of these interactions in tetraloop structure.