Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Electronic Supplementary Information

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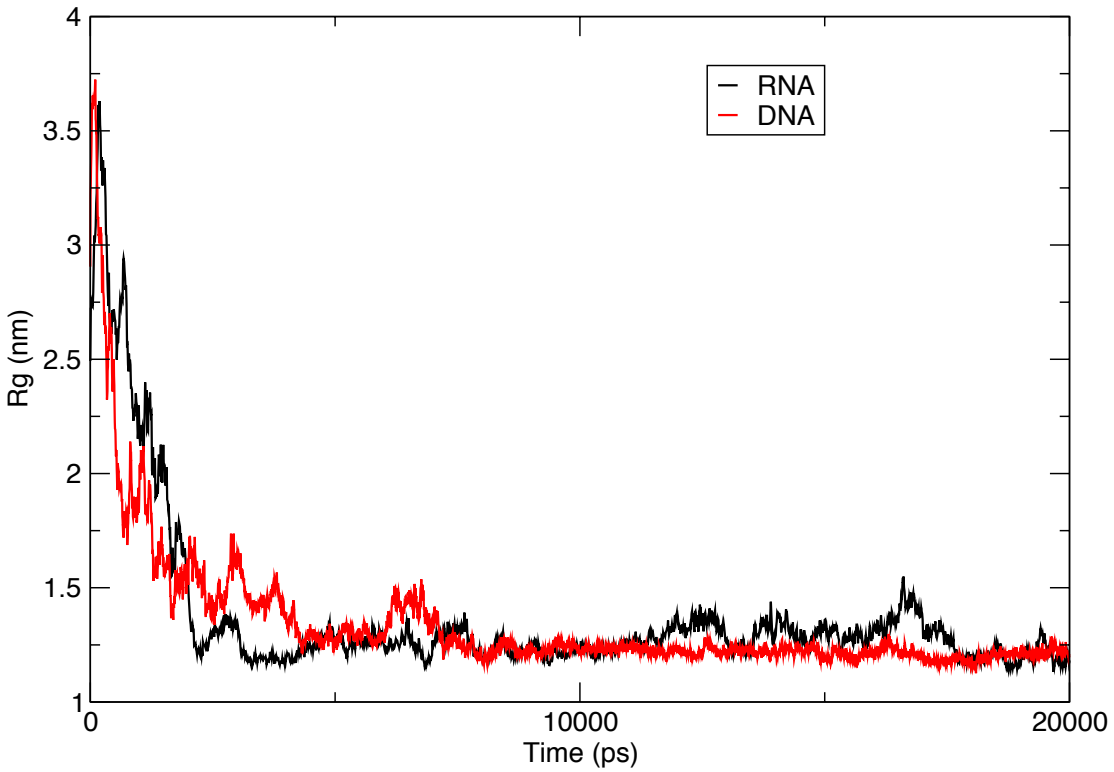


Figure 1: Radius of gyration of RNA and DNA taken from independent single trajectory molecular dynamics simulations. Both single-stranded nucleic acid chains undergo hydrophobic collapse to the globular form over the first 5 ns.

Table 1. Replica Temperatures:

273.00, 274.67, 276.35, 278.03, 279.73, 281.43, 283.14, 284.85, 286.57, 288.30, 290.04, 291.79, 293.54, 295.31, 297.08, 298.85, 300.64, 302.44, 304.24, 306.05, 307.87, 309.69, 311.53, 313.37, 315.22, 317.08, 318.95, 320.82, 322.71, 324.60, 326.50, 328.41, 330.33, 332.26, 334.20, 336.15, 338.10, 340.07, 342.04, 344.02, 346.01, 348.01, 350.02, 352.04, 354.06, 356.10, 358.15, 360.20, 362.26, 364.33, 366.42, 368.51, 370.61, 372.72, 374.84, 376.97, 379.11, 381.26, 383.42, 385.59, 387.76, 389.95, 392.15, 394.36, 396.58, 398.81, 401.05, 403.43, 405.69, 407.96, 410.24, 412.53, 414.84, 417.15, 419.47, 421.81, 424.15, 426.51, 428.87, 431.25, 433.64, 436.04, 438.45, 440.86, 443.29, 445.74, 448.19, 450.66, 453.14, 455.63, 458.13, 460.64, 463.16, 465.70, 468.26, 470.82, 473.39, 475.97, 478.56, 481.17, 483.79, 486.42, 489.06, 491.72, 494.38, 497.07, 499.76, 502.46

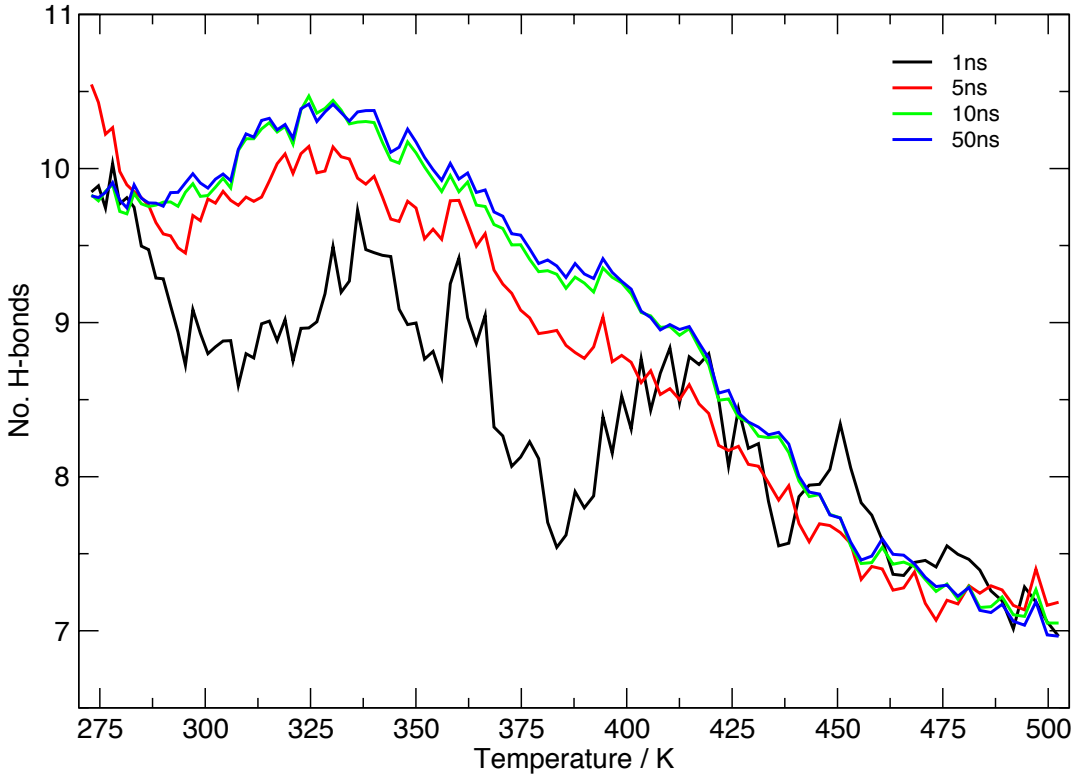
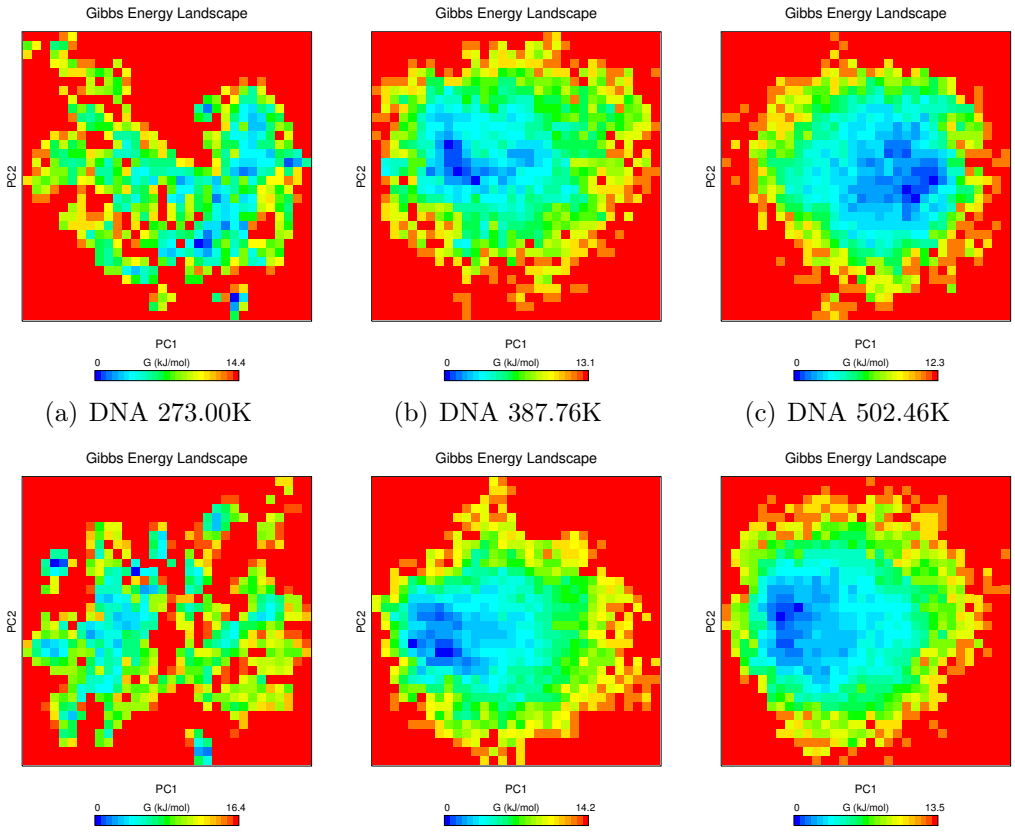


Figure 2: Average number of hydrogen bonds between RNA bases at each temperature. Values have been bootstrapped over four different ranges of data to display convergence of simulations.



(a) DNA 273.00K (b) DNA 387.76K (c) DNA 502.46K

(d) RNA 273.00K (e) RNA 387.76K (f) RNA 502.46K

Figure 3: Gibbs free energy surface of RNA and DNA at three temperatures in two dimensional principal component space. The principal components were calculated form the nucleic acid phosphate backbone atoms, producing common axes in all plots. At 273K in plots (a) and (d) the surface appears to be very rugged, with a number of low energy minima. At higher temperatures the surface, as we expect, becomes broader and less well defined. In this case, PCA was conducted independently for DNA and RNA.