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Supplemental Information

Spermine Condenses DNA, but Not RNA Duplexes

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Supporting Material

Spermine condenses DNA, but not RNA duplexes

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Contribution of spermine scattering to the WAXS signal. To determine whether the observed differences in the WAXS signals stem from scattering of the spermine itself or conformational changes in the RNA, we used CRYSOL to examine simulated scattering from two sets of models. The first set contained the same snapshots from the MD simulations for the RNA/spermine system used in the main text. The second contained the exact same set of snapshots with the spermines deleted. Therefore, the RNA geometry is the same in these two sets, which differ only in the presence (or lack thereof) of spermine. The simulated scattering profiles from these two sets of models do not change significantly, as shown in Figure S1, suggesting that the observed experimental WAXS differences are a result of changes in RNA conformation. However, as discussed in the text (Results, wide angle x-ray scattering section), we acknowledge that caution must be exercised in using CRYSOL to interpret WAXS spectra, because it is not designed to accurately model local interactions in the solute or discrete interactions between solute and solvent.

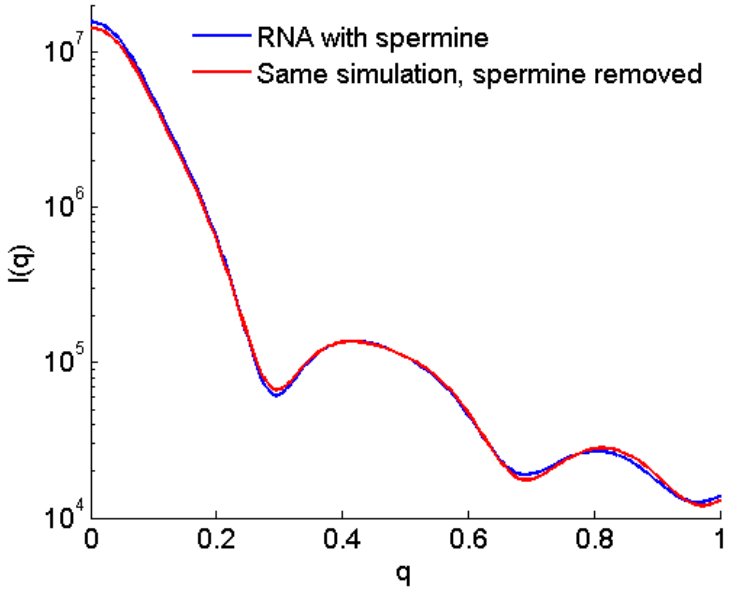

Figure S1. Scattering profiles computed with CRYSOL from (blue) snapshots from our simulations of the RNA/spermine system and (red) the exact same snapshots with the spermine removed from the PDB files before analysis with CRYSOL.

To further demonstrate the small effect of spermine on the scattering, we computed the difference profile from the curves above, shown in Figure S2, with the same scale as in Figure 6 of the main text. Figure 6 compares simulations of RNA with spermine and RNA without spermine (rather than this case, where we have deleted the spermine after the fact), and shows a larger signal. Clearly, the presence of the spermine does not cause the large changes seen in our WAXS patterns.

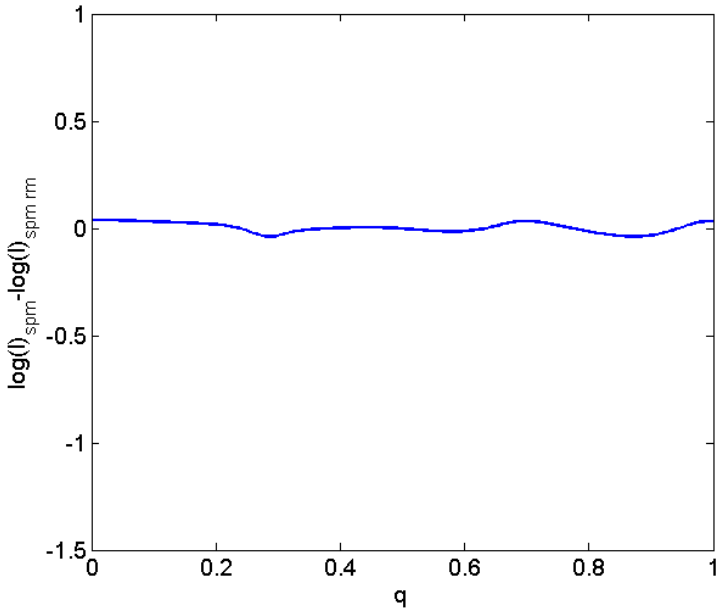

Figure S2. Difference profiles computed from the curves shown in Figure S1. The scale is the same as in Figure 6 of the main text.