Electronic Supplementary Material (ESI) for Chemical Communications

Supplementary Information for

Probing electronic coupling between adenine bases in RNA strands from synchrotron radiation circular dichroism experiments

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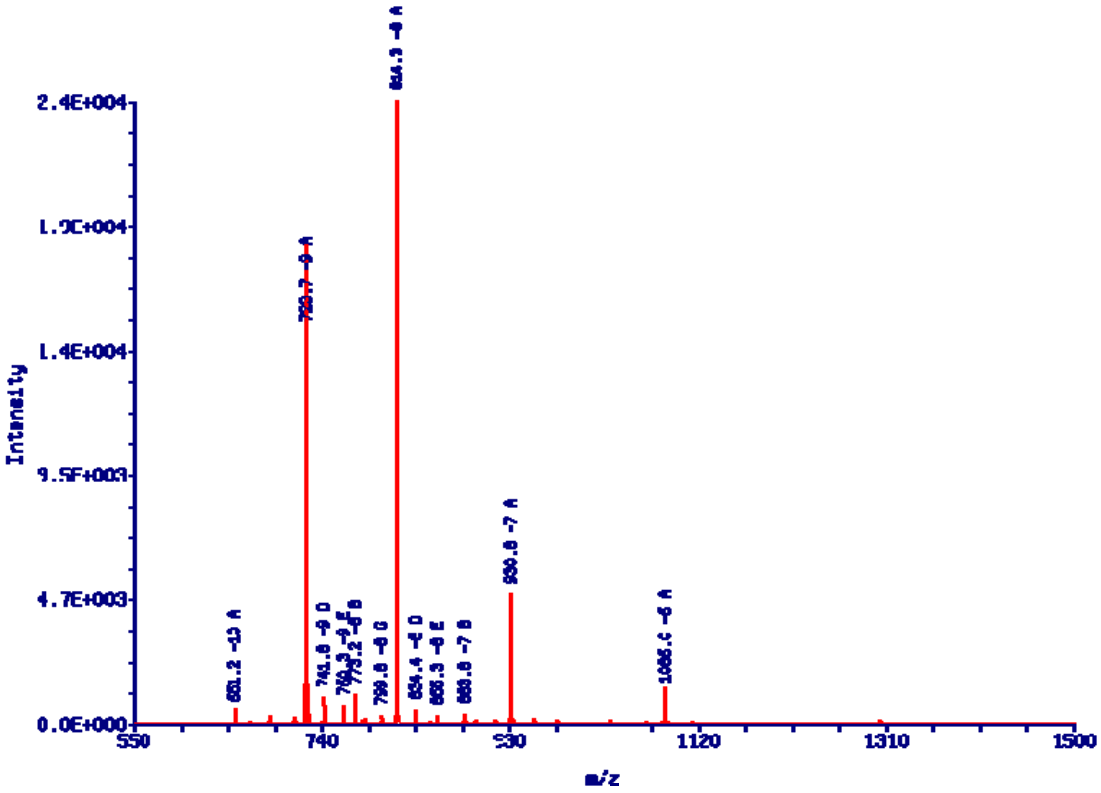

Fig. S1 Electrospray mass spectrum of $(rA)_{20}$. The ions are formed in charge states from 6- to 10-.

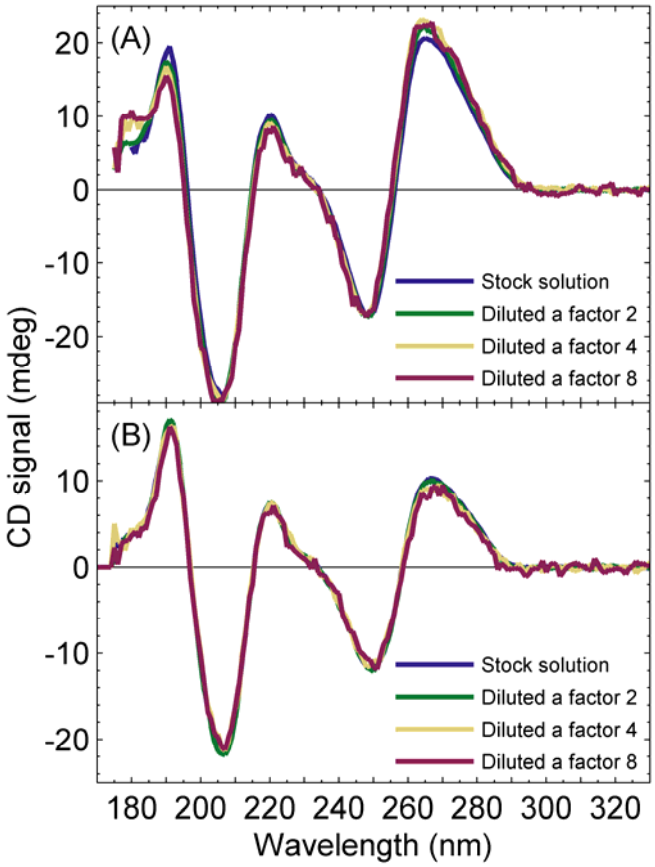

Fig. S2 Circular dichroism spectra of $(rA)_{20}$ (A) and $(rA)_4$ (B) at different concentrations. The spectra are scaled with the factor of dilution. The stock concentrations were 0.228 mM $(rA)_{20}$ and 1.15 mM $(rA)_4$.

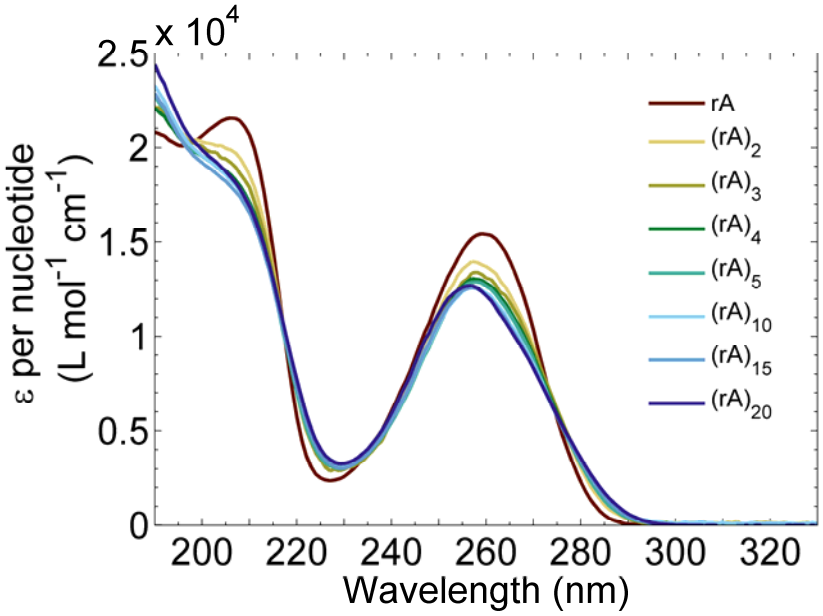

Fig. S3 A representative subset of absorption spectra of RNA strands investigated.

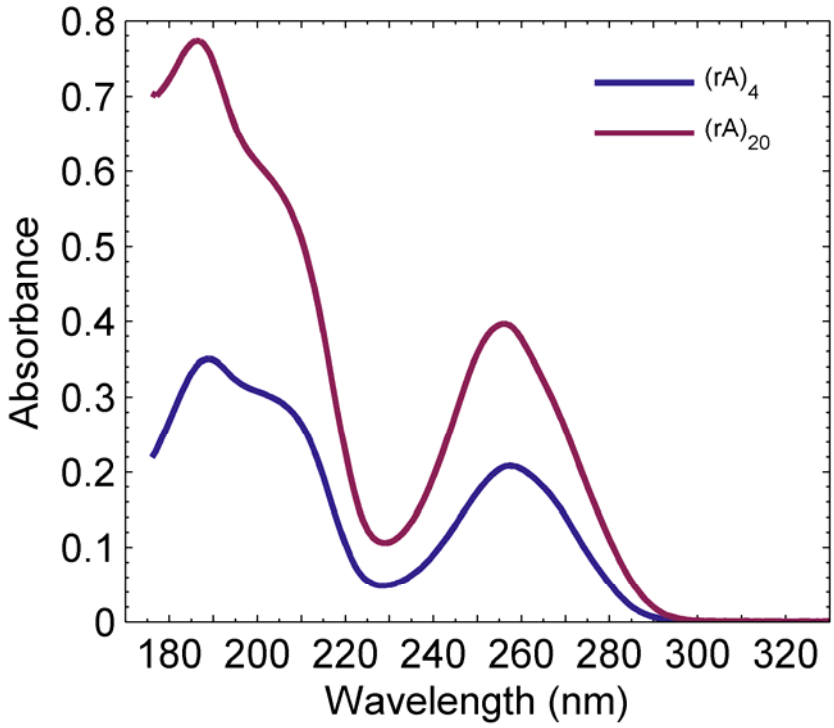

Fig. S4 SR absorption spectra of $(rA)_4$ and $(rA)_{20}$. Notice the second axis is absorbance.

Analysis of data including base-disorder as described in C. Su, C. T. Middleton and B. Kohler, *J. Phys. Chem. B*, 2012, **116**, 10266.

Assuming noncooperativity in forming stacks, the fraction of bases present in stacks of two or more bases is

$$f_b(n) = f\,(2 - f) + 2\,f\,(f - 1)/n \quad ,$$

where $f = 0.32$ according to measurements on $(rA)_4$ (based on f_g reported to be 0.43 in Table 2 in the Su et al. paper and setting f_g equal to f_b).

Correcting for base disorder implies that in the case of only two interacting neighbour bases, the CD signal should follow $c\,(n - 1)\,f_b(n)$. This function was fit to the data (curves below).