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Chemical Biology

Research highlights

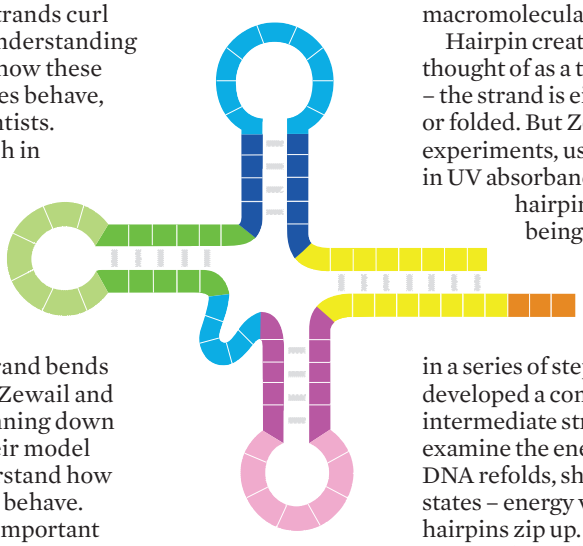
Computational model reveals how DNA and RNA fold into hairpins

Genetic code does the twist

Revealing how DNA strands curl up is the first step to understanding how structure affects how these big biological molecules behave, says a team of US scientists.

The group, at Caltech in Pasadena, has developed a computational model to discover how DNA and RNA strands fold into hairpins – loops that form when the strand bends back on itself. Ahmed Zewail and colleagues say that pinning down this process shows their model could be used to understand how larger DNA molecules behave.

'Hairpins are a very important structural feature of DNA,' says Zewail, 'and they are a manageable size to test our ideas on how long, macromolecular DNA strands fold.'



Nucleic acids can fold to form hairpin bends

Hairpin creation is typically thought of as a two-state process – the strand is either unfolded or folded. But Zewail's recent experiments, using changes in UV absorbance to follow a hairpin refolding after being subjected to a laser induced temperature jump, suggest the process occurs in a series of steps. Now Zewail has developed a computational kinetic intermediate structure model to examine the energy landscape as DNA refolds, showing intermediate states – energy valleys – as the hairpins zip up.

Zewail's model successfully predicts that the zipping process varies depending on the structure of the hairpin – including whether folding starts from the loop or the free ends of the hairpin. 'We were surprised that a simple two-coordinate model gives accurate predictions,' says Zewail. 'We're now using it to work on bigger systems, and the results are very promising.'

Philip Bevilacqua, who studies RNA folding at Pennsylvania State University, University Park, US, says the model will be a useful tool. 'It corroborates data already out there and it should make useful predictions to guide future experiments. It will be well used because it's simple to use.'

James Mitchell Crow

Reference

M M Lin *et al*, *Phys. Chem. Chem. Phys.*, 2008, DOI: 10.1039/b804675c

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