

January 1st/2010

How DNA Goes A'Courtin'

Simplified model catches essential details of how DNA complements find their matches

By Jane Palmer, PhD

[pdf](#) [print](#) [leave a comment](#)

Until now, scientists have known little about how complementary single strands of DNA court one another before binding to form the classical double helix. But now, molecular dynamics simulations have identified that the binding—or hybridization—mechanism depends largely on the sequence of the DNA: Ordered sequences will meet and then slither lengthwise to find the correct match; but sequences that are random will connect at key sites then rapidly assemble along the molecule's length.

"One would have thought that random sequences would have more difficulty hybridizing, and that is not necessarily the case," says **Juan J. de Pablo, PhD**, professor of chemical and biological engineering at University of Wisconsin, Madison. The work was published in the October 5 issue of the *Proceedings of the National Academy of Sciences*.

Scientists have previously tried to simulate the pathways by which DNA strands combine, but the models they used included too much detail to enable sufficiently long computations, de Pablo says. So De Pablo's group developed a highly

simplified model, tested on experimental data, to capture essential details of the interactions between the base pairs of complementary strands of DNA. The researchers then simulated the process by which the single strands interact using molecular dynamics and Monte Carlo simulations, taking multiple "snapshots" of the double helix as it assembled. To the team's surprise, the path to a successful union depended crucially on the sequences of the molecules.

When the sequences of both single strands are ordered or repetitive, any two sites of base pairs can come together and the two strands slowly "slither" lengthwise until complementary base pairs match along the entire chain, says de Pablo. When the sequences are random, however, single sites located toward the center of the strands unite early. "The moment they come together, then the molecule just assembles perfectly and it does so very quickly," de Pablo says.

The results could influence the design of technologies that depend on the hybridization process, such as gene chips, de Pablo says. To engineer more efficient and reliable hybridization, researchers could use random sequences, which bind more efficiently and with fewer errors.

"This is an interesting step forward," says **Nadrian Seeman, PhD**, professor of chemistry at New York University. "No one had taken the time to track the pathway previously." Seeman has used the principle of random sequencing in his own hybridization studies, and he finds it reassuring to see it vindicated by the simulation data. "It does tell people who are designing sequences to avoid repetition in the sequences," he says.

Tags: [News Byte](#) [Molecular Dynamics](#)

All submitted comments are reviewed, so it may be a few days before your comment appears on the site.

POST NEW COMMENT

SHARE THIS

[Tweet](#) 83

[Email](#)

POPULAR ARTICLES

[Big Data Analytics In Biomedical Research](#)

Can the complexities of biology be boiled down to Amazon.com-style recommendations? The examples here suggest possible pathways to an intelligent healthcare system with big data at its core.

01/02/12 by Katharine Miller

[The Eyes Have It: Biomechanical Models Explore Disorders of the Eye](#)

Biomechanical models contribute to a better understanding of both the normal and the diseased eye.

02/19/13 by Katharine Miller

[The Physiome: A Mission Imperative](#)

To understand biology—and provide appropriate medical care—scientists need to understand interactions across multiple scales. Hence the Physiome.

06/01/10 by Katharine Miller

POPULAR TAGS

[DATA MINING](#) [visualization](#) [genomics](#)

[SIMULATION](#) [neuroscience](#) [biomechanics](#) [Systems Biology](#) [DRUG DISCOVERY](#) [Cancer](#) [DNA](#) [Molecular Dynamics](#) [bioinformatics](#)

SUBSCRIBE TO

[RSS Feed](#)

[Subscribe to Print Edition](#)

[Subscribe to Table of Contents: *](#)

Your name:

E-mail:

The content of this field is kept private and will not be shown publicly.

Homepage:

Subject:

Comment: *

CAPTCHA

All submitted comments are reviewed, so it may be a few days before your comment appears on the site. This question is for testing whether you are a human visitor and to prevent automated spam submissions.



What code is in the image?: *

Enter the characters shown in the image.

Save

Preview



Supported by the *Mobilize Center*,
a National Institutes of Health
Big Data to Knowledge (BD2K)
Center of Excellence
(Grant U54EB020405).

Stanford University
James H. Clark Center S271
318 Campus Drive,
MC: 5448
Stanford, CA 94305-5448

[About](#)
[Archive](#)
[Contact](#)
[Subscribe](#)

Search