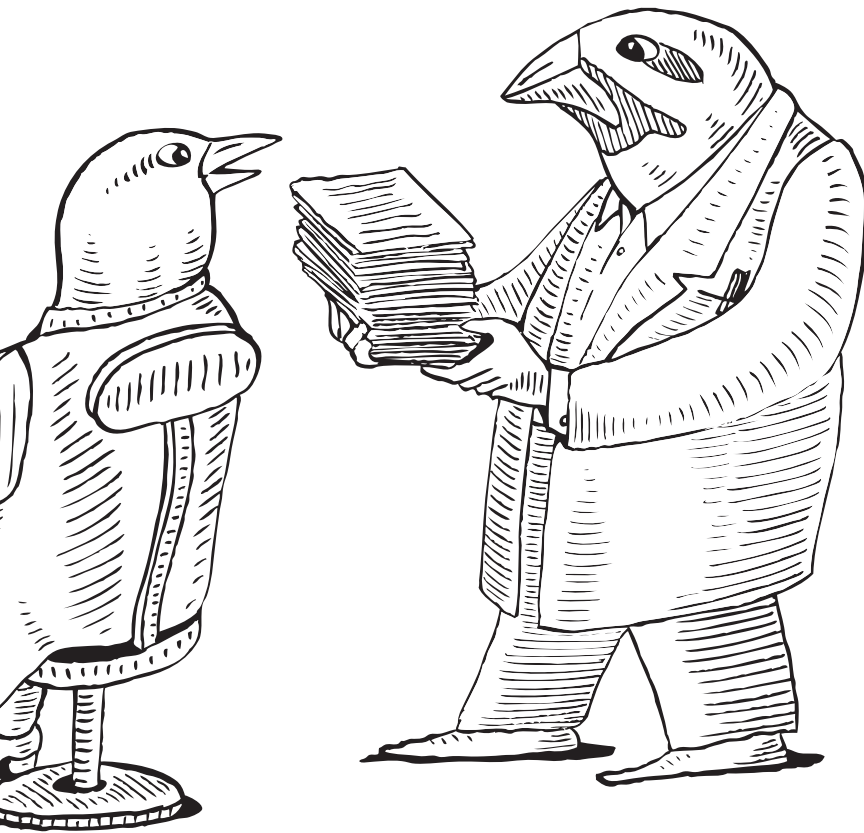


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Learning about this phenomenon may result in more than one "Aha!" moment.

Virginia Papaioannou and Ripla Arora commenting on Oral ivermectin as an unexpected initiator of CreT2-mediated deletion in T cells, published in *Nature Immunology*.

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**F11** **Protein 3D structure computed from evolutionary sequence variation.**

Marks DS, Colwell LJ, Sheridan R, Hopf TA, Pagnani A, Zecchina R, Sander C. PLoS ONE. 2011; 6(12):e28786

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**Roy Kishony and Morten Ernebjer**, Harvard University, USA. F1000 Microbiology **10** EXCEPTIONAL

22 Feb 2012 | New Finding, Technical Advance  
DOI: 10.34104/13816956.15374056

This article provides a groundbreaking approach to addressing a long-standing grand challenge of molecular and computational biology – the prediction of 3D protein structures from primary amino acid sequences – by linking evolutionary constraints on sequence divergence to the physical protein structure.

With the advent of ‘cheap and deep’ sequencing, thousands of new protein sequences are emerging, many of them from families with unknown structure and no structural homologs (1). This has brought new urgency to the thorny problem of predicting protein structure computationally without recourse to crystal structures. In this article, the authors make substantial progress towards this goal by using the fact that although a single protein sequence may not offer enough guidance for simple folding methods to work, the extant evolutionary record embodied by families of proteins often does.

The core observation is that residues in close physical proximity in a folded protein tend to co-vary across protein families, reflecting the fact that evolutionary pressures on the protein structure forces such residues to change in a coordinated fashion (2) (a fact that also underlies the exciting discovery that proteins can be decomposed into spatially contiguous evolutionary ‘sectors’ with distinct functions (4)). To overcome noise and spurious correlations, the authors apply a newly developed method (3) to efficiently translate an aligned protein family into a so-called maximum entropy distribution for all sequences in the family. Encoded in this distribution are linkage strengths between all residue pairs – linkage strengths that are based on a global model of the entire sequence rather than just the two residues in question. Such global linkages have been shown to provide an excellent guide to physical proximity of residues (2,3). The keys to that knowing which residues are close in space is tantamount to knowing the rough shape of the folded structure. The authors demonstrate that once the predicted residue proximity is encoded as geometric constraints on the protein sequence, standard folding algorithms can provide excellent structure prediction for long sequences (>200 residues) that have previously been out of reach for computational methods.

One of the great achievements of this article is that it successfully combines multiple techniques, observations, and ideas to resolve the major goal of protein folding prediction. It brings together theoretical advances in the calculation of maximum entropy distribution, existing protein folding tools, and new biological ideas to forge a practical structure-prediction pipeline that translates a protein family into a predicted structure, using only the protein sequences as input and requiring only a standard laptop computer. As such, the paper provides a tool that could prove crucial in translating the flood of new sequences into new structures and possibly also predict function.

- References**
- The Sarcocor II Global Ocean Sampling expedition: expanding the universe of protein families.**  
Yoseph B, Sutton O, Rusch DE, Halpern AL, Williamson SJ, Remington K, Eisen JA, Heidelberg KB, Manning G, Li W, Jaroszewski L, Cieplak P, Miller CS, Li H, Mashima ST, Joachimiak MP, van Belle C, Chandonna JM, Sengul DA, Zhai Y, Natarajan V, Lee S, Rajhans BJ, Balha V, Friedman R, Brenner SE, Godzik A, Eisenberg D, Dixon JE, Taylor SS, Strausberg RL, Frazier M, Venter JC. PLoS Biol. 2007 Mar; 3(5):e16  
PMID: 17355171
  - Identification of direct residue contacts in protein-protein interaction by message passing.**  
Weigt M, White RA, Szurmant H, Hoch JA, Hwa T. Proc Natl Acad Sci USA. 2009 Jan 6; 106(6):67-72  
PMID: 19119270
  - Direct-coupling analysis of residue coevolution captures native contacts across many protein families.**  
Morcos F, Pagnani A, Lunt B, Bertolino A, Marks DS, Sander C, Zecchina R, Onuchic JN, Hwa T, Weigt M. Proc Natl Acad Sci USA. 2011 Dec 6; 108(49):E1293-301  
PMID: 22110282
  - Protein sectors: evolutionary units of three-dimensional structure.**  
Halabi N, Rivore O, Leibler S, Ranganathan R. Cell. 2009 Aug 21; 138(5):774-86  
PMID: 19703402

**Disclosures**  
None declared

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**Ram Samudrala and George White**, University of Washington, WA, USA. F1000 Structural Biology **6** RECOMMENDED

09 Aug 2012 | Technical Advance, Interesting Hypothesis, Good for Teaching  
DOI: 10.34104/13816956.793153316

These authors provide a thoughtful analysis of the relation between protein structure prediction and sequence variation that supersedes the premise that sequence co-variation between residues implies physical proximity. Their structure prediction method directly tackles the problems of statistical noise in the evolutionary record, and the presence of true sequence co-variation that is unrelated to physical proximity, by using a global statistical model that incorporates comprehensive sequence information in predicting the proximity of any two residues. Their model reproduces known residue contact maps surprisingly well, and performs competitively in predicting the structures of a small set of proteins.

**Disclosures**  
None declared

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**F18** **The risk of catheter-related bloodstream infection with femoral venous catheters as compared to subclavian and internal jugular venous catheters: A systematic review of the literature and meta-analysis.**

Mark PE, Flemmer M, Harrison VV. Crit Care Med. 2012 Aug; 40(8):2478-85

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**Michael Canter**, Kantonsspital Winterthur, Switzerland. F1000 Anesthesiology & Pain Management **8** MUST READ

02 Aug 2012 | New Finding, Good for Teaching  
DOI: 10.34104/1717950485.793455721

**CHANGES CLINICAL PRACTICE** - Current guidelines recommending that femoral venous access should be avoided to decrease the risk of catheter-related bloodstream infections are not supported by current data, and the choice of site for catheter access should instead depend on the skill of the physician and the risks associated with central-line placement in the specific patient.

Until now, most guidelines from national societies, including American Society of Anesthesiologists (ASA), Center for Disease Control (CDC) and Infectious Disease Society of America (IDSA), claim that the risk of catheter-related bloodstream infections is highest with femoral venous catheters as compared to subclavian and internal jugular venous catheters. This systematic review and meta-analysis now shows that this stigma is no longer true. Indeed, the authors demonstrate with current data that there is no difference in catheter-related bloodstream infections between the femoral and subclavian, as well as subclavian and internal jugular sites. Outside specific subpopulations, there are no data to support choosing one central-line site over another.

**Disclosures**  
None declared

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Stan Falkow, Stanford University, Stanford, CA  
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