FAST BREAKING PAPERS - 2009

December 2009

PDF

Liisa Holm talks with *ScienceWatch.com* and answers a few questions about this month's Fast Breaking Paper in the field of Computer Science.

Article Title: Searching protein structure databases with DaliLite v.3
Authors: **Holm, L**;Kaariainen, S;Rosenstrom, P;Schenkel, A
Journal: BIOINFORMATICS
Volume: 24
Issue: 23
Page: 2780-2781
Year: DEC 1 2008
* Univ Helsinki, Dept Biol & Environm Sci, POB 56,Viikinkaari 5, FIN-00014 Helsinki, Finland.
* Univ Helsinki, Dept Biol & Environm Sci, FIN-00014 Helsinki, Finland.
* Univ Helsinki, Inst Biotechnol, FIN-00014 Helsinki, Finland.

SW: Why do you think your paper is highly cited?

The paper is given as the reference on the Dali server web site. The server has been running for about 15 years at a series of locations. The Dali server is used by structural biologists to compare newly solved protein structures against the Protein Data Bank (PDB). Similarities to other proteins can help to elucidate the function of an uncharacterized protein and shed light on molecular evolution.

SW: Does it describe a new discovery, methodology, or synthesis of knowledge?

The paper describes an update of the original Dali algorithm (Holm L; Sander C, "Protein structure comparison by alignment of distance matrices" *J. Mol. Biol.* 233: 123-38, 1993).

SW: Would you summarize the significance of your paper in layman's terms?

Hundreds of new structures are added to the PDB each week. The paper reports a change to a data structure within Dali which speeds up database updates. The Dali server uses pre-computed similarities between PDB structures in order to find all the structural neighbors of the query structure.

The idea is that one usually finds a few highly similar structures using quick heuristics. Restricting the search space to neighbors of these previously found matches allows the exclusion of large parts of the database without explicit comparison.

"Our goal is to integrate protein sequence and structural comparisons for function prediction."

SW: How did you become involved in this research, and were there any problems along the way?

I was initially interested in protein structure prediction, where the problem of optimizing a sum-of-pairs function comes up in aligning—a contact map predicted from—a sequence to the contact map of a

protein with known structure.

Structure comparison by aligning two known contact maps was a similar problem, where the correctness of the result was easy to check visually. The structure comparison program yielded biologically interesting results so I ended up pursuing that line of research.

Our formulation of the protein structure alignment problem belongs to a class of problems that computer scientists call NP-complete. This means that algorithms with a practical running time cannot be guaranteed to find the exact optimum. Therefore, the server has to compromise between speed and robustness.

SW: Where do you see your research leading in the future?

Our goal is to integrate protein sequence and structural comparisons for function prediction.

Liisa Holm, Ph.D.
Professor & Group Leader
Bioinformatics Group
Institute of Biotechnology
Department of Biological and Environmental Sciences
University of Helsinki
Helsinki, Finland
Web

KEYWORDS: SEQUENCES.

PDF

back to top

2009 : December 2009 - Fast Breaking Papers : Liisa Holm Discusses DaliLite v.3

Science Home | About Thomson Reuters | Site Search