

The Danish Node

Peter Løngreen, Danish ELIXIR Node

ELIXIR's Innovation and SME Forum
November 24 - 25, 2014



The Danish ELIXIR node: goals and means

“The overall purpose of the Danish ELIXIR node on bioinformatics tool interoperability and integration is to address the main problems in **tool utilization** experienced currently by the life sciences community.”

Three key concepts:

- Being user-centric
- Consultancy
- EU-wide partnerships



ELIXIR Denmark Node

- The Danish ELIXIR Node is coordinated by DTU, and includes CU, AU, and SDU as partners + Industry partners.
- The overall purpose of the Danish ELIXIR Node is :
 - The creation of a comprehensive tool registry
 - The provision of tools in the form preferred by users across academia and industry
 - Tool interoperability
 - Benchmarking, ensure tool sustainability through different interfaces

DisEMBL™

Intrinsic Protein Disorder Prediction 1.5

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SwissProt ID or AC:
(e.g. PRIO_HUMAN, P09429 or P37840)

Sequence (Amino acid single letter IUPAC code):

GLOBPLOT 2

Intrinsic Protein Disorder, Domain & Globularity Prediction

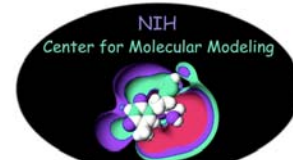
Version 2.3

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SwissProt ID or AC:
(e.g. PRIO_HUMAN or P08630)

Sequence (Amino acid single letter IUPAC code):

Center for Molecular Modeling



The CENTER FOR MOLECULAR MODELING (CMM) is part of the Division of Computational Bioscience (DCB/CIT) of the National Institutes of Health. Our research involves the development and application of theoretical and computational methodologies, from *ab initio* quantum mechanics calculations of small organic molecules to molecular mechanics simulations of macromolecular systems. Our interests include the modeling of macromolecular structure, dynamics and thermodynamics, structure-function relationships of proteins, the treatment of solvation effects, enzyme mechanism, and ligand binding. We are also interested in the application of mathematical and statistical methods (e.g., maximum entropy formalism) to data analysis and image reconstruction problems. The CMM's computational chemists and robotics maintain active collaborations with the TMpred Server.

CMM Home Page
CMM staff
Molecular Modeling Support for NIH Scientists "MMDCenter"
Software
Hardware at the NIH
Databases
Computational Molecular Biology Resources at NIH
NIH Library
U.S. National Library of Medicine

UCLA-DOE Institute for Genomics and Proteomics

Overview - Facilities Services - Seminars Lectures - People Search - Links Stats - Webmail

Welcome to the UCLA-DOE Institute for Genomics and Proteomics

News
Job Opportunity In Memory of David Slamon Training Grants 2007 Progress Report
Genes

- Protein Database - A database of proteins having functional linkages to an input protein.
- DBP Database of Interacting Proteins
- Transcriptome
- Structural Genomics of Mycobacterium tuberculosis

"DAS" - Transmembrane Prediction server

For brief description of the method read the abstract.

Please cite: M. Cerzo, E. Wallis, I. Simon, G. von Heijne and A. Elofsson: Prediction of transmembrane alpha-helices in prokaryotic membrane proteins: the Dena Alignment Surface method; Prot. Eng. vol. 10, no. 6, 673-676, 1997

The DAS server will predict transmembrane regions of a query sequence. Enter your query protein sequence into the text area below and submit it to the server. This sequence should be in one letter code.

(Use protein sequence only)

ch.EMBnet.org

TMpred - Prediction of Transmembrane Regions and Orientation

The TMpred program makes a prediction of membrane-spanning regions and their orientation. The algorithm is based on the statistical analysis of TMbase, a database of naturally occurring transmembrane proteins. The prediction is made using a combination of several weight-matrices for scoring.

[K. Hofmann & W. Stoffel \(1993\)](#)
TMbase - A database of membrane spanning proteins segments
Biol. Chem. Hoppe-Seyler **374**,166

For further information see the [TMbase](#) and [TMpred](#) documentation.

Usage: Paste your sequence in one of the supported [formats](#) into the sequence field below and press the "Run TMpred" button. Make sure that the format button (next to the sequence field) shows the correct format. Choose the minimal and maximal length of the hydrophobic part of the transmembrane helix

Output format: html | minimum: 17 | maximum: 33

Query title (optional):

Input sequence format: Plain Text

Query sequence:

BMERC

BioMolecular Engineering Research Center

BMERC 36 Cummington St. Boston, MA 02215
Phone: (617) 353-7123 Fax: (617) 353-7020
[Graduate Program in Bioinformatics](#)

The BMERC provides research support in both the development and application of SWISS-MODEL

FOLDCLASS(+)

FoldClass predicts protein fold classes and protein domains.

Following Subtopics are available:

- Example
- Output
- Algorithm
- Consideration
- Acknowledgement
- Local Data Files

TMpred Server at MIT

Identification of complete gene structures in genomic DNA



MENU

SWISS-MODEL

An Automated Comparative Protein Modelling Server

SIB - Biozentrum Basel site provided by:

Modeling requests:

- First Approach mode
- Alignment Interface
- Protein (Optimise) mode
- Disorder modeling
- GPCR mode

Model Database

PredictProtein

Structure Prediction and Sequence Analysis

Home Submission Docs Downloads Register MetaF

GeneQuiz - Home page

The GeneQuiz system provides highly automated analysis of biological sequences. Full use of GeneQuiz requires that you install certain other software at your site.

You can read a brief document [about GeneQuiz](#) explaining what it does, how it works and for what it has been used. For more details you may want to check the [list of publications](#) related to GeneQuiz.

If you use our results in your work please cite:
Andrade et al. (1999). *Bioinformatics* 15:391-412 or [Iliopoulos et al. \(2000\)](#)

Genomes that were added to GeneQuiz since its release in mid December 2000:

- 03 Nov 2003 *Shewanella oneidensis*
- 09 Feb 2002 *Listeria innocua* serovar 6a
- 16 Jan 2002 *Salmonella typhimurium* LT2 specific genes

Quick Access to genomes (most recent runs only)

Gene Finder

[http://www.bioscience.org/urllists/genefind.htm](#)

Date: 1 / 28 / 108 Time: 1:46:37 P.M.

FRONTIERS IN BIOSCIENCE; GENE FINDER

Use the database of BCM-Genefinder to find splice sites and protein coding exons, construct gene model and recognize the promoter. Place the DNA sequence < 7000 bp in the query box. For longer DNA sequences, use Email servers:

Sequence name or identifier:

Choose search method for Human, Drosophila, Nematode, Yeast and Plan

GeneQuiz

Home page

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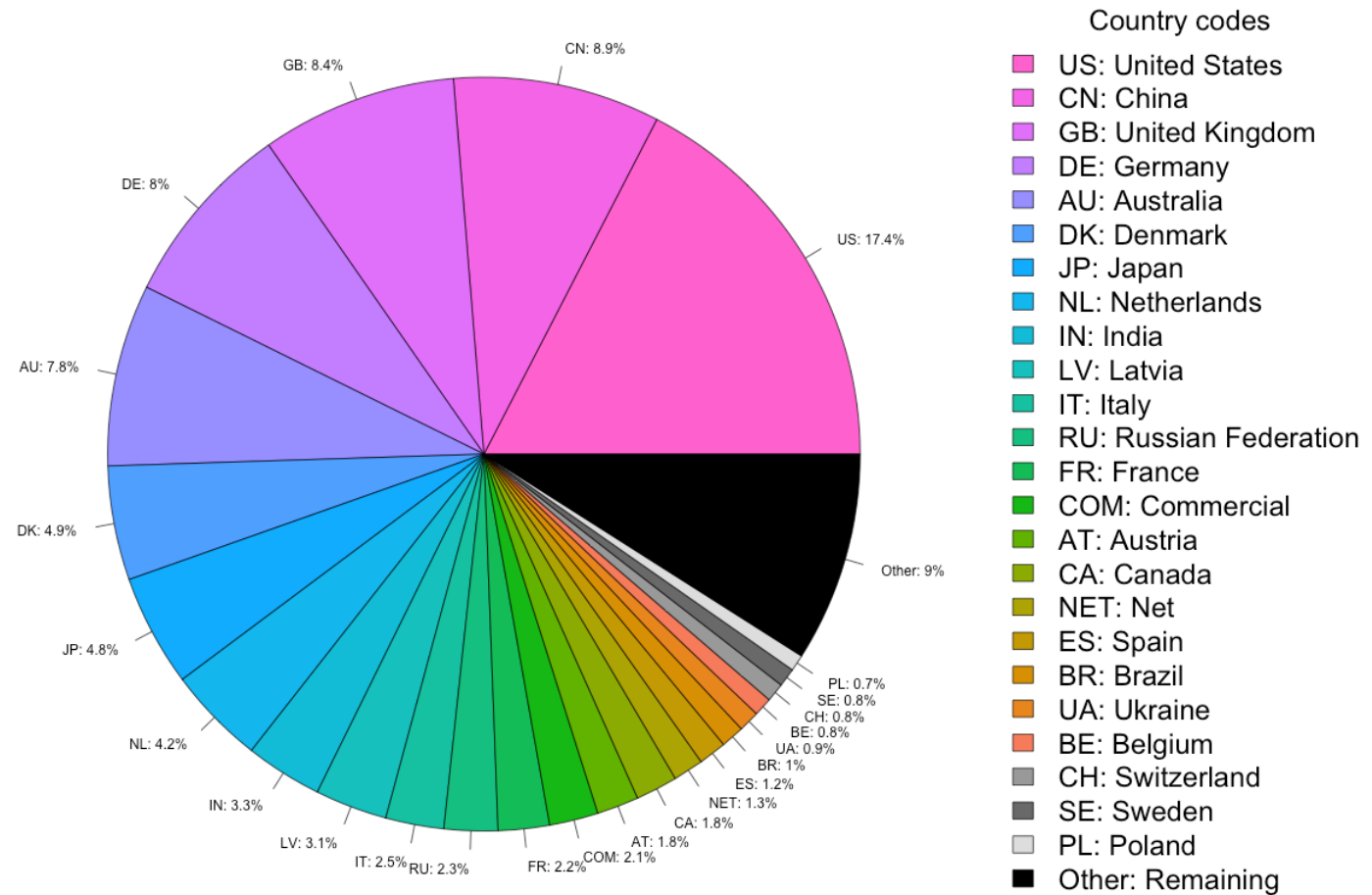
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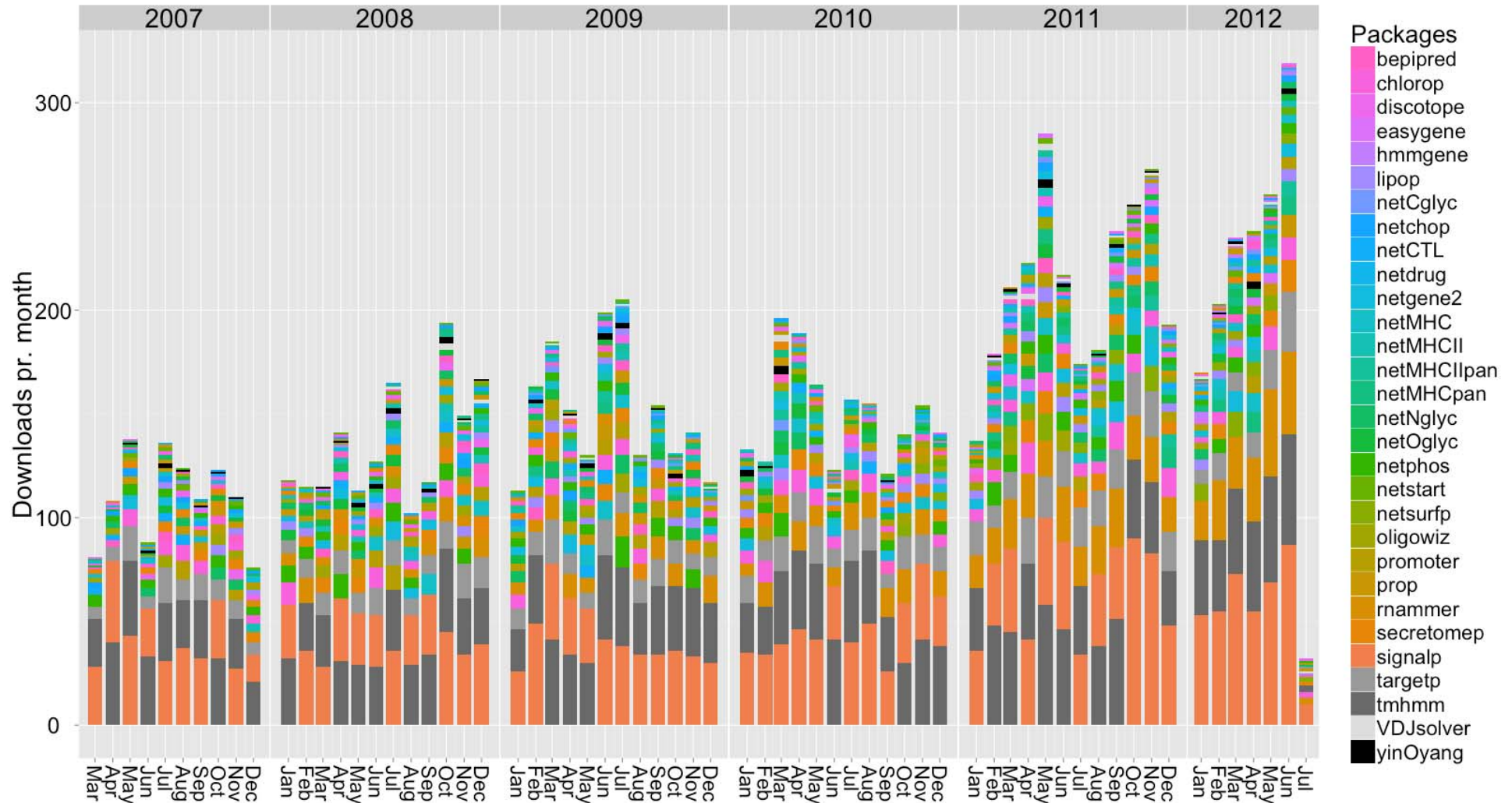
Pageviews - countries

Page views for www.cbs.dtu.dk by country

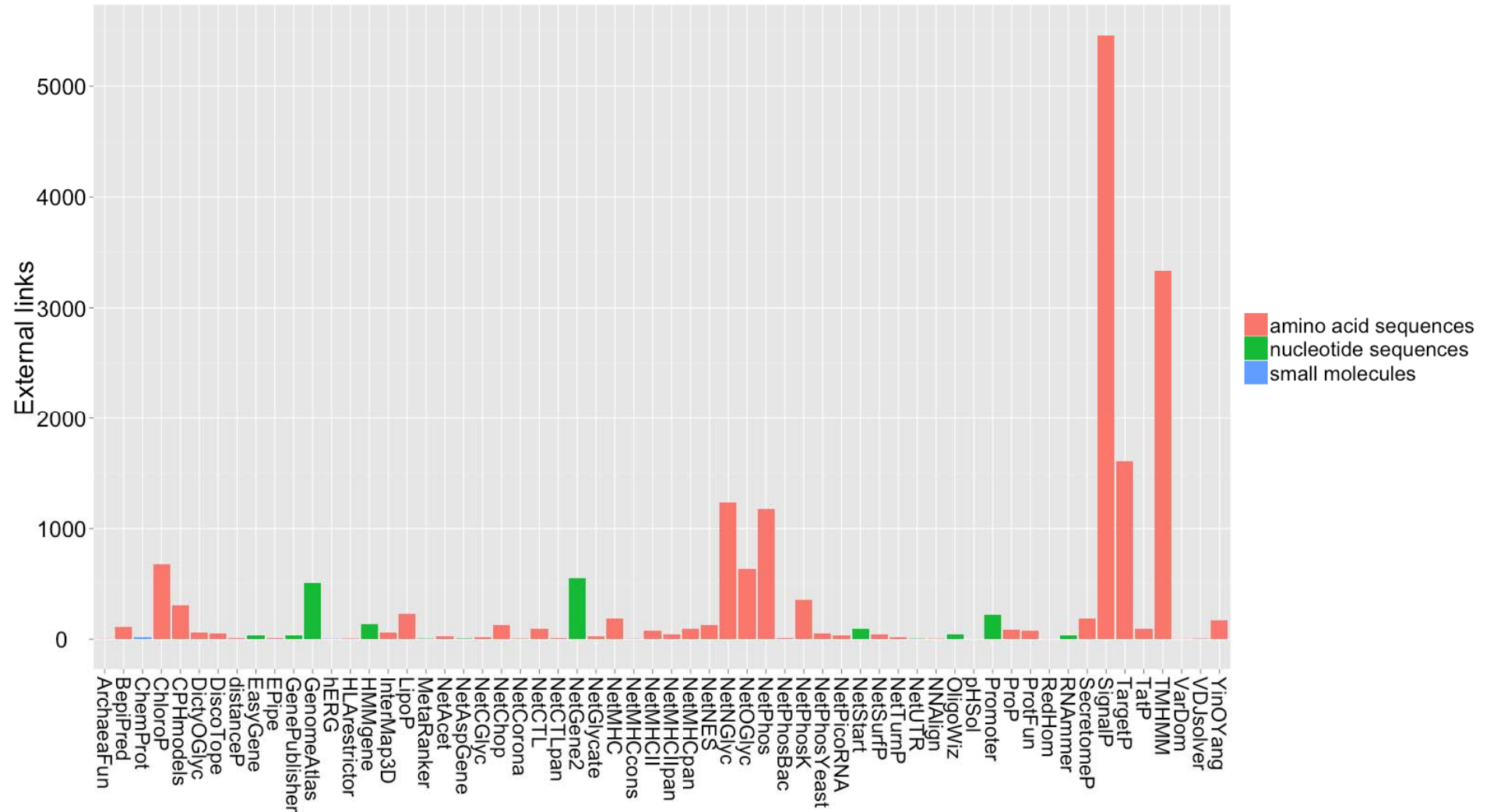


*) .gov and .edu counted as United States. Internal views not counted

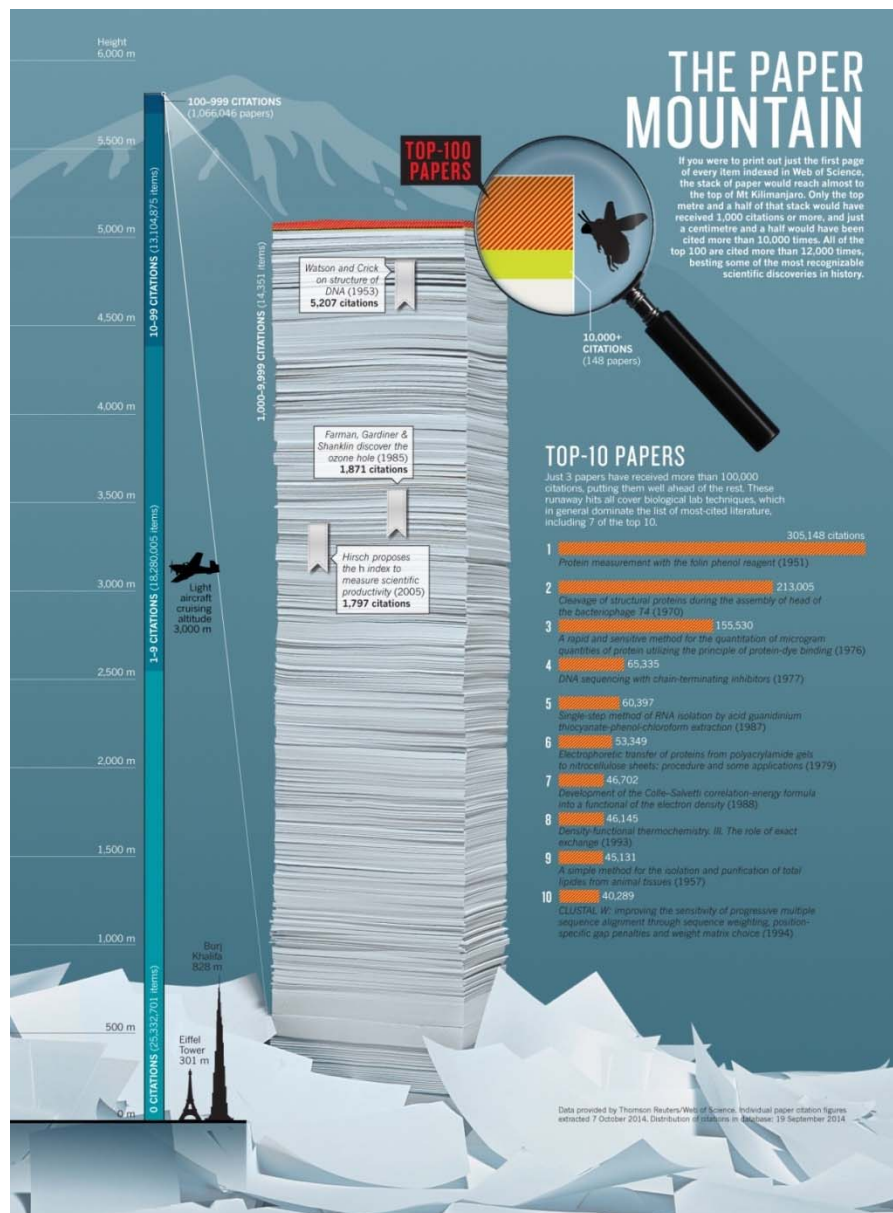
Package downloads per month



External links to www.cbs.dtu.dk



Tool benchmarking – Obsolete tools are still being cited



nature International weekly journal of science

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Archive | Volume 514 | Issue 7524 | News Feature | Article

NATURE | NEWS FEATURE

The top 100 papers

Nature explores the most-cited research of all time.

Richard Van Noorden, Brendan Maher & Regina Nuzzo

29 October 2014

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The top 100 papers

The most-cited research of all time is not what most people would expect, a Nature investigation shows.

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Tools do not always deliver on their published promises

Some old news

Biotechnology firm Amgen tried to confirm published findings related to haematology and oncology. Fifty-three papers were deemed 'landmark' studies describing something completely new, such as fresh approaches to targeting cancers or alternative clinical uses for existing therapeutics. Scientific findings were confirmed in only 6 (11%) cases.



COMMENT

RAISE STANDARDS Shift expertise to track mutations where they emerge **p.534**

DATA SYSTEMS Past climates give valuable clues to future warming **p.537**

RECOVERY BY GENES Descartes' lost letter tracked using Google **p.540**

RESEARCH Why Yale and an elusive stress hormone **p.542**

Many landmark findings in preclinical oncology research are not reproducible, in part because of inadequate cell lines and animal models.

Raise standards for preclinical cancer research

C. Glenn Begley and Lee M. Ellis propose how methods, publications and incentives must change if patients are to benefit.

Efforts over the past decade to characterize the genetic alterations in human cancers have led to a better understanding of molecular drivers of this complex set of diseases. Although we in the cancer field hoped that this would lead to more effective drugs, historically, our ability to translate cancer research to clinical success has been remarkably low. Sadly, clinical trials in oncology have the highest failure rate compared with other therapeutic areas. Given the high unmet need in oncology, it is understandable that barriers to clinical development may be lower than for other disease areas, and a larger number of drugs with suboptimal preclinical validation will enter oncology trials. However, this low success rate is not sustainable or acceptable, and investigation must reassess their approach to translating discovery research into greater clinical success and impact. Many factors are responsible for the high failure rate, notwithstanding the inherently difficult nature of this disease. Certainly, the limitations of preclinical tools such as inadequate cancer-cell-line and mouse models make it difficult for even

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REPRODUCIBILITY OF RESEARCH FINDINGS

Preclinical research generates many secondary publications, even when results cannot be reproduced.

Journal impact factor	Number of articles	Mean number of citations of non-reproduced articles*	Mean number of citations of reproduced articles
>20	21	248 (range 3–800)	231 (range 82–519)
5–19	32	169 (range 6–1,909)	13 (range 3–24)

Results from ten-year retrospective analysis of experiments performed prospectively. The term 'non-reproduced' was assigned on the basis of findings not being sufficiently robust to drive a drug-development programme.

*Source of citations: Google Scholar, May 2011.

Dimensions the Registry will address

