

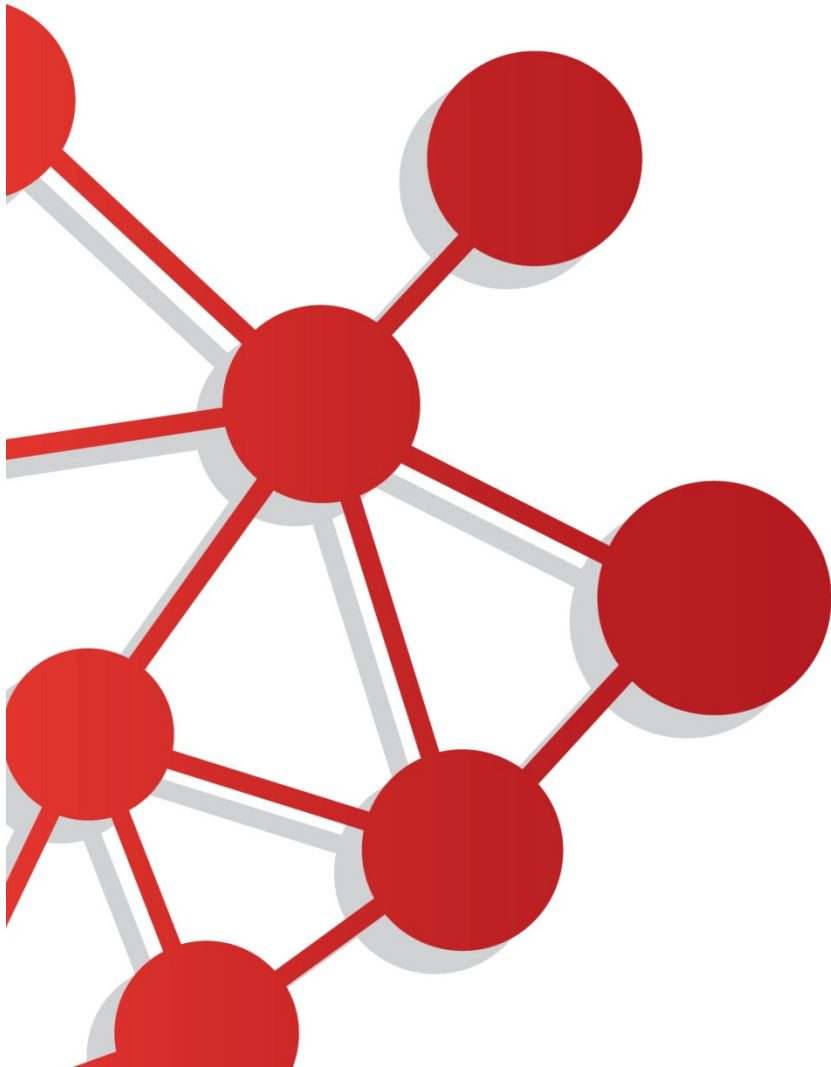
# Innovation in scientific publishing

## An editorial perspective

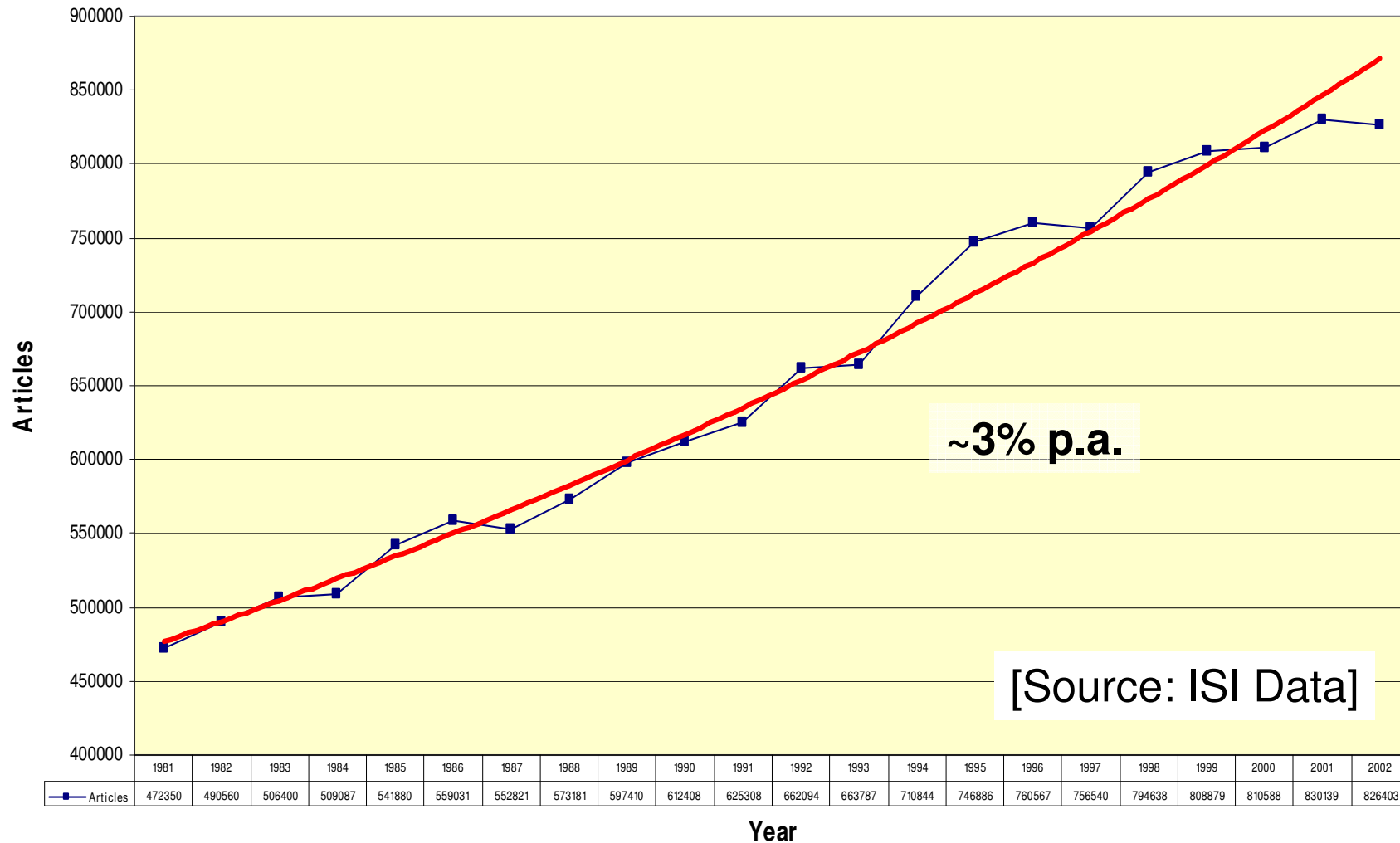
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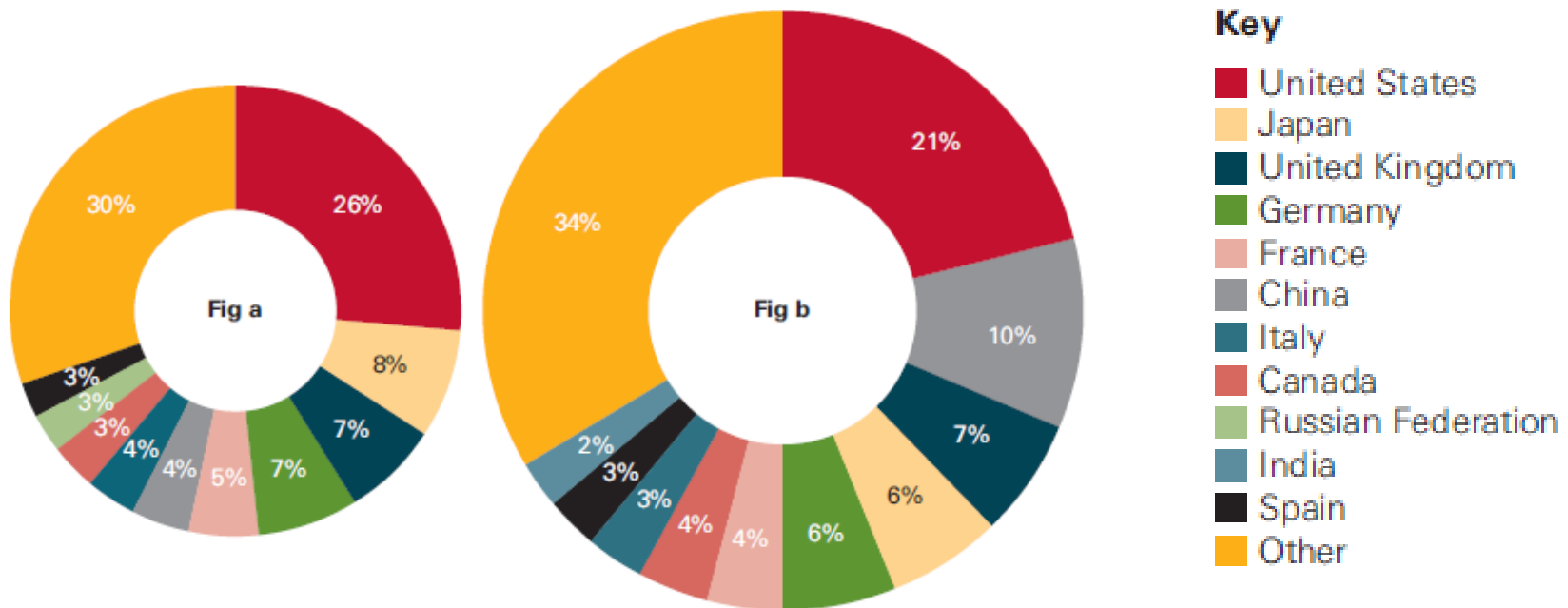
# Article Growth 1981-2002



# Global publication authorship by country

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Knowledge, networks, nations: Global scientific collaboration in the 21<sup>st</sup> century.  
RS policy document, March 2011 – data from Scopus

# DNA structure - 1953

No. 4356 April 25, 1953 NATURE 737

equipment, and to Dr. G. E. R. Doseon and the captain and officers of R.R.S. *Discovery II* for their part in making the observations.

<sup>1</sup>Young, F. B., Gerrard, H., and Jevons, W., *Phil. Mag.*, **46**, 149 (1928).

<sup>2</sup>Langset-Haggas, M. S., *Mon. Not. Roy. Astr. Soc., Geophys. Supp.*, **6**, 285 (1949).

<sup>3</sup>Von Arz, W. S., Woods Hole Papers in Phys. Oceanogr. Meteor., **11** (5) (1960).

<sup>4</sup>Ekmann, V. W., *Arkiv. Mat. Astron. Fysik. (Stockholm)*, **2** (11) (1935).

## MOLECULAR STRUCTURE OF NUCLEIC ACIDS

### A Structure for Deoxyribose Nucleic Acid

WE wish to suggest a structure for the salt of deoxyribose nucleic acid (D.N.A.). This structure has novel features which are of considerable biological interest.

A structure for nucleic acid has already been proposed by Pauling and Corey<sup>1</sup>. They kindly made their manuscript available to us in advance of publication. Their model consists of three intertwined chains, with the phosphates near the fibre axis, and the bases on the outside. In our opinion, this structure is unsatisfactory for two reasons: (1) We believe that the material which gives the X-ray diagrams is the salt, not the free acid. Without the acidic hydrogen atoms it is not clear what forces would hold the structure together, especially as the negatively charged phosphates near the axis will repel each other. (2) Some of the van der Waals distances appear to be too small.

Another three-chain structure has also been suggested by Fraser (in the press). In his model the phosphates are on the outside and the bases on the inside, linked together by hydrogen bonds. This structure as described is rather ill-defined, and for this reason we shall not comment on it.

We wish to put forward a radically different structure for the salt of deoxyribose nucleic acid. This structure has two helical chains each coiled round the same axis (see diagram). We have made the usual chemical assumptions, namely, that each chain consists of phosphate di-ester groups joining 5'-deoxy-ribofuranose residues with 3',5' linkages. The two chains (but not their bases) are related by a dyad perpendicular to the fibre axis. Both chains follow right-handed helices, but owing to the dyad the sequences of the atoms in the two chains run in opposite directions. Each chain loosely resembles Furbert's model No. 1; that is, the bases are on the inside of the helix and the phosphates on the outside. The configuration of the sugar and the atoms near it is close to Furbert's 'standard configuration', the sugar being roughly perpendicular to the attached base. There

is a residue on each chain every 3.4 Å, in the z-direction. We have assumed an angle of 36° between adjacent residues in the same chain, so that the structure repeats after 10 residues on each chain, that is, after 34 Å. The distance of a phosphorus atom from the fibre axis is 10 Å. As the phosphates are on the outside, cations have easy access to them.

The structure is an open one, and its water content is rather high. At lower water contents we would expect the bases to tilt so that the structure could become more compact.

The novel feature of the structure is the manner in which the two chains are held together by the purine and pyrimidine bases. The planes of the bases are perpendicular to the fibre axis. They are joined together in pairs, a single base from one chain being hydrogen-bonded to a single base from the other chain, so that the two lie side by side with identical z-co-ordinates. One of the pair must be a purine and the other a pyrimidine for bonding to occur. The hydrogen bonds are made as follows: purine position 1 to pyrimidine position 1; purine position 6 to pyrimidine position 6.

If it is assumed that the bases only occur in the structure in the most plausible tautomeric forms (that is, with the keto rather than the enol configurations) it is found that only specific pairs of bases can bond together. These pairs are: adenine (purine) with thymine (pyrimidine), and guanine (purine) with cytosine (pyrimidine).

In other words, if an adenine forms one member of a pair, on either chain, then on these assumptions the other member must be thymine; similarly for guanine and cytosine. The sequence of bases on a single chain does not appear to be restricted in any way. However, if only specific pairs of bases can be formed, it follows that if the sequence of bases on one chain is given, then the sequence on the other chain is automatically determined.

It has been found experimentally<sup>2,3</sup> that the ratio of the amounts of adenine to thymine, and the ratio of guanine to cytosine, are always very close to unity for deoxyribose nucleic acid.


It is probably impossible to build this structure with a ribose sugar in place of the deoxyribose, as the extra oxygen atom would make too close a van der Waals contact.

The previously published X-ray data<sup>4,5</sup> on deoxyribose nucleic acid are insufficient for a rigorous test of our structure. So far as we can tell, it is roughly compatible with the experimental data, but it must be regarded as unproved until it has been checked against more exact results. Some of these are given in the following communications. We were not aware of the details of the results presented there when we devised our structure, which rests mainly though not entirely on published experimental data and stereochemical arguments.

It has not escaped our notice that the specific pairing we have postulated immediately suggests a possible copying mechanism for the genetic material.

Full details of the structure, including the conditions assumed in building it, together with a set of co-ordinates for the atoms, will be published elsewhere.

We are much indebted to Dr. Jerry Donohue for constant advice and criticism, especially on inter-atomic distances. We have also been stimulated by a knowledge of the general nature of the unpublished experimental results and ideas of Dr. M. H. F. Wilkins, Dr. R. E. Franklin and their co-workers at



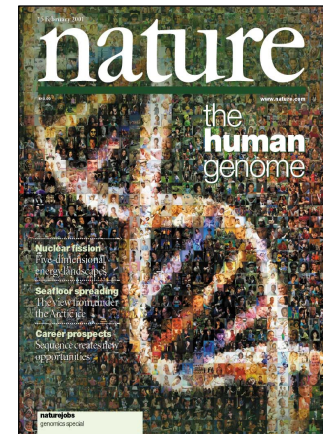
This figure is purely diagrammatic. The two ribbons symbolize the two phosphate-sugar chains, and the horizontal rods the pairs of bases holding the chains together. The vertical line marks the fibre axis.

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- 1 page
- 2 authors
- 1 figure
- no data

# The human genome - 2001

- 62 pages, 49 figures, 27 tables



**articles**

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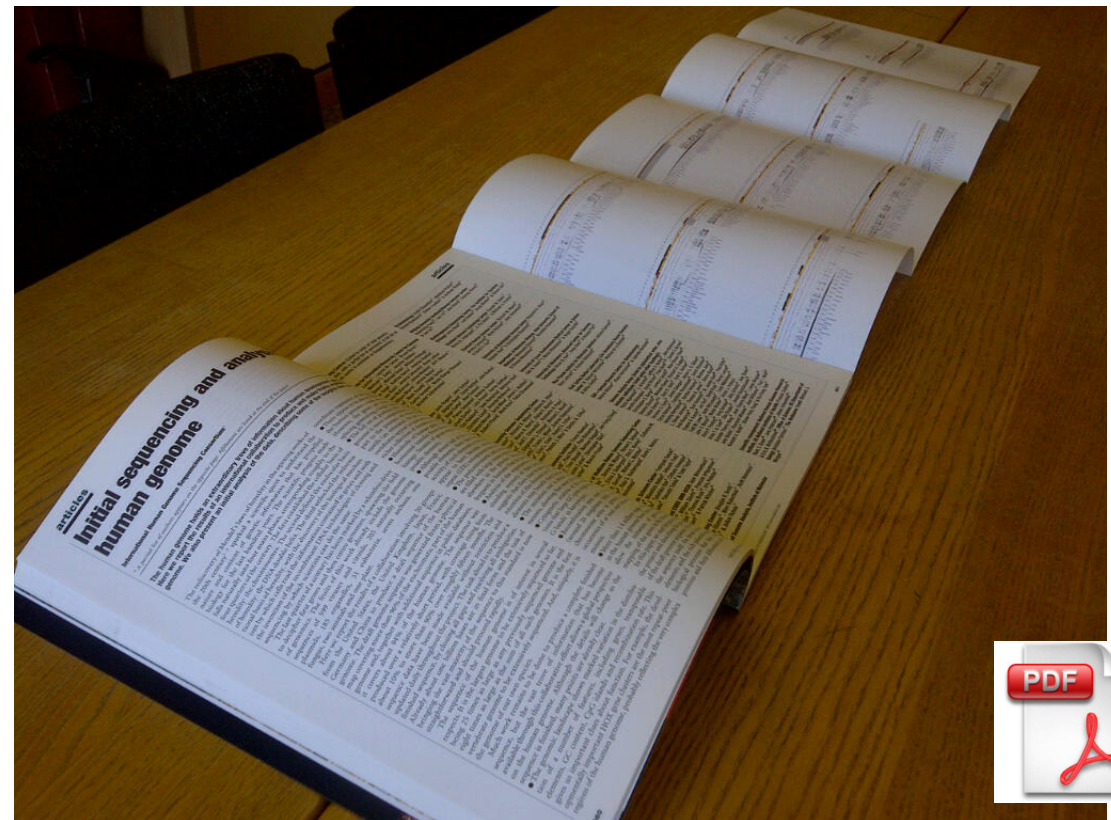
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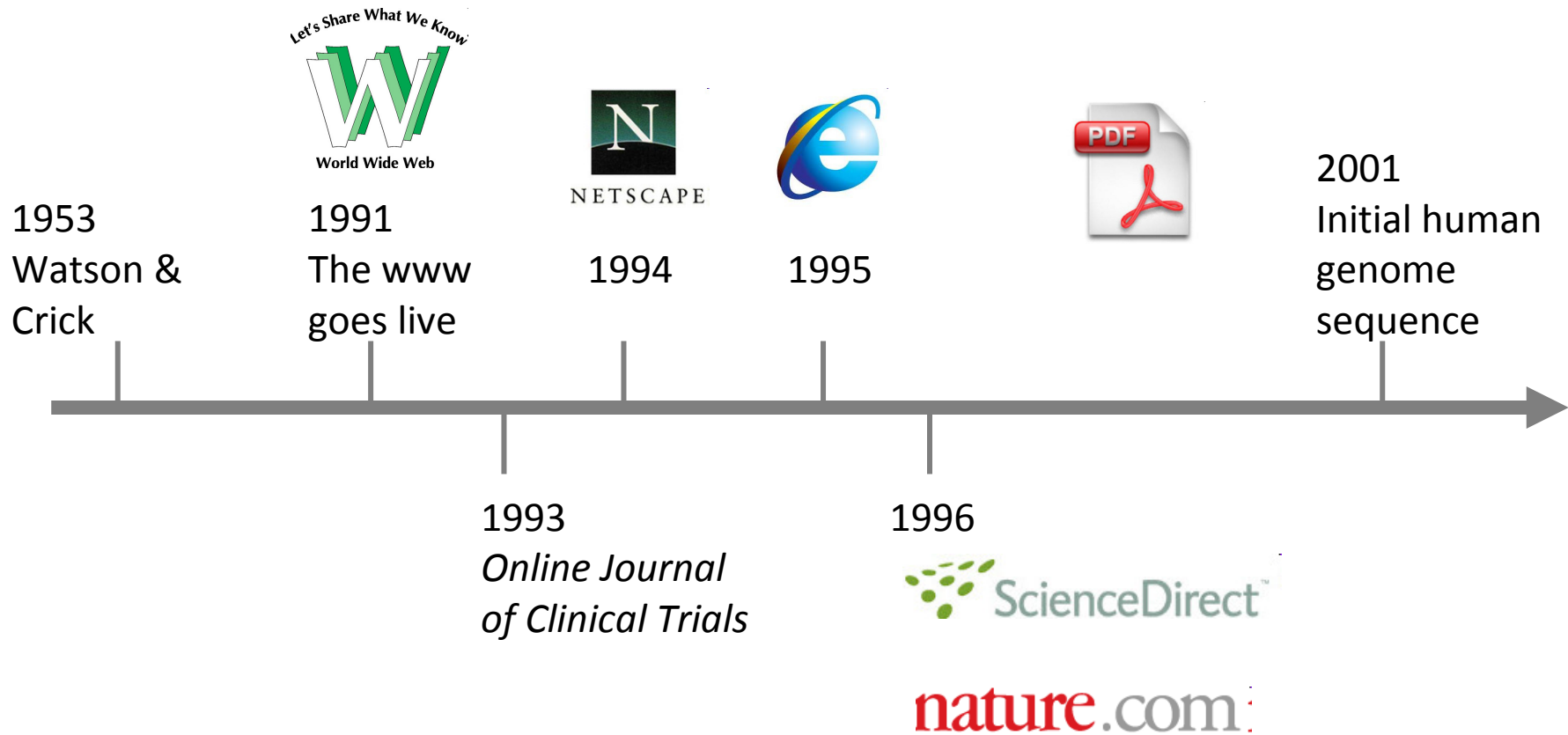
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# The human genome at 10 - 2010



# A thousand genomes – 2010

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# The rise of data: lessons learned

- Data may precede paper
  - Fort Lauderdale agreements for genomics data
  - Preprint servers in physical sciences
- Journals are key players in enforcing data deposition
  - Mandate for PDB deposition at the time of publication jointly enforced by Science and Nature
- Mandates are not enough
  - Challenges in enforcing the MIAME mandate
  - curation, data standards
  - sustainable repository infrastructure
  - community and funders support



The screenshot shows a Nature journal article page. The main title is "A map of human genome variation from population-scale sequencing". The article is from Volume 467, Issue 7319, dated 28 October 2010. The authors are from The 1000 Genomes Project Consortium. The page includes an abstract, subject terms, a "Figures at a glance" section with several small charts, and an introduction. On the right side, there are sections for "Citations to this article", "Selected feature" (with a preview of "After the Ice"), "Editor's summary", "News & Views", "Science jobs from natureJobs", and "Open Innovation challenges". A "Tool box" on the right side of the article text allows for printing, emailing, and downloading the PDF. The page also features a search bar at the top, navigation links, and a sidebar with "Spotlight On Latin America".

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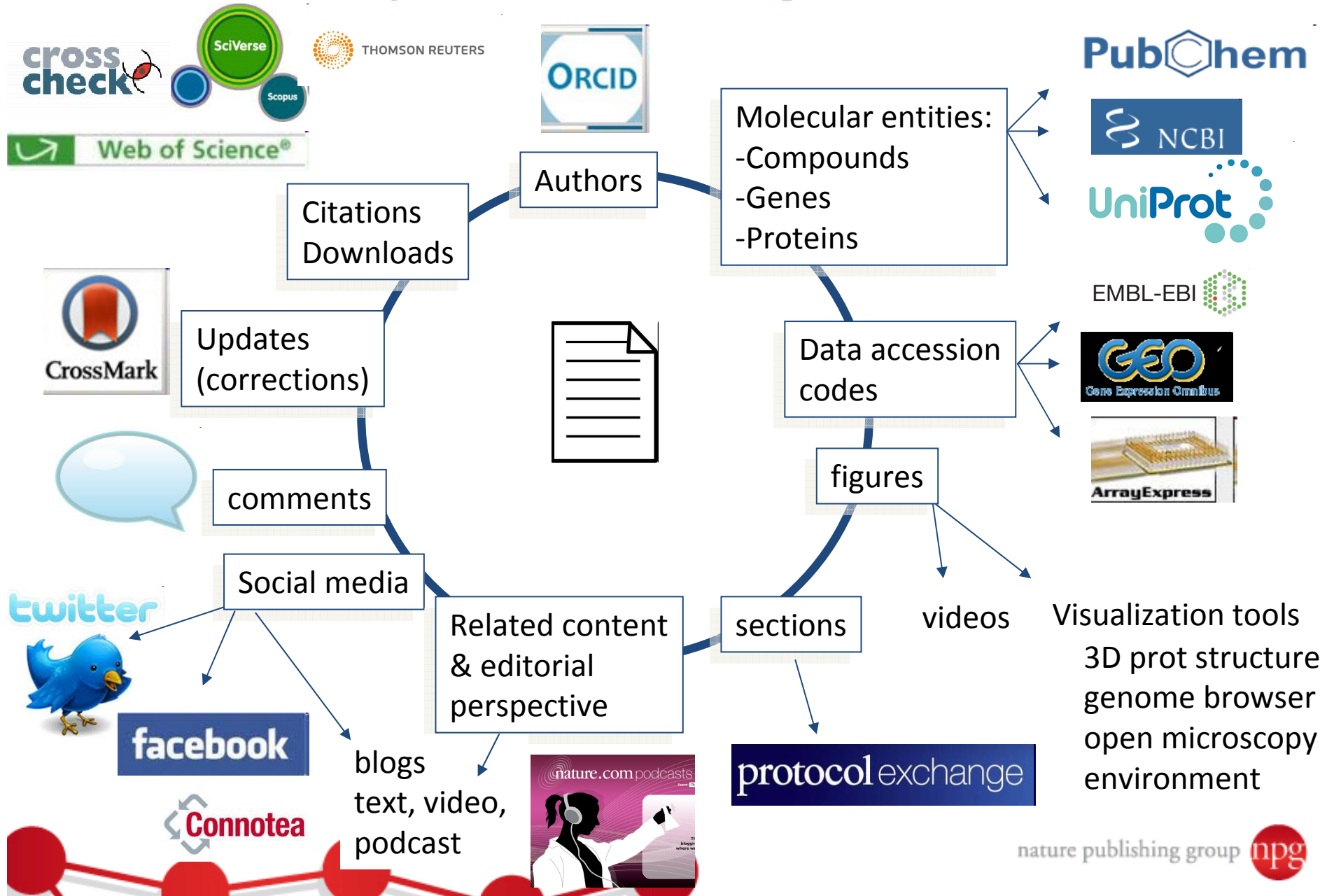
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## Acetylation regulates Cyclophilin A catalysis, immunosuppression and HIV isomerization

Michael Lammers, Heinz Neumann, Jason W Chin & Leo C James

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*Nature Chemical Biology* **6**, 331–337 (2010) | doi:10.1038/nchembio.342

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Cyclophilin A (CypA) is a ubiquitous *cis*–*trans* prolyl isomerase with key roles in immunity and viral infection. CypA suppresses T-cell activation through **cyclosporine** complexation and is required for effective HIV-1 replication in host cells. We show that CypA is acetylated in diverse human cell lines and use a synthetically evolved acetyllysyl-tRNA synthetase/tRNA<sub>CUA</sub> pair to produce recombinant acetylated CypA in *Escherichia coli*. We determined atomic-resolution structures of acetylated CypA and its complexes with **cyclosporine** and HIV-1 capsid. Acetylation markedly inhibited CypA catalysis of *cis* to *trans* isomerization and stabilized *cis* rather than *trans* forms of the HIV-1 capsid. Furthermore, CypA acetylation antagonized the immunosuppressive effects of **cyclosporine** by inhibiting the sequential steps of **cyclosporine** binding and

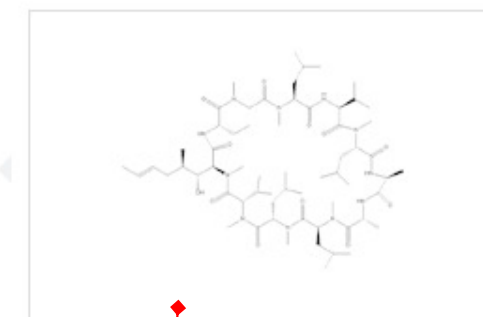
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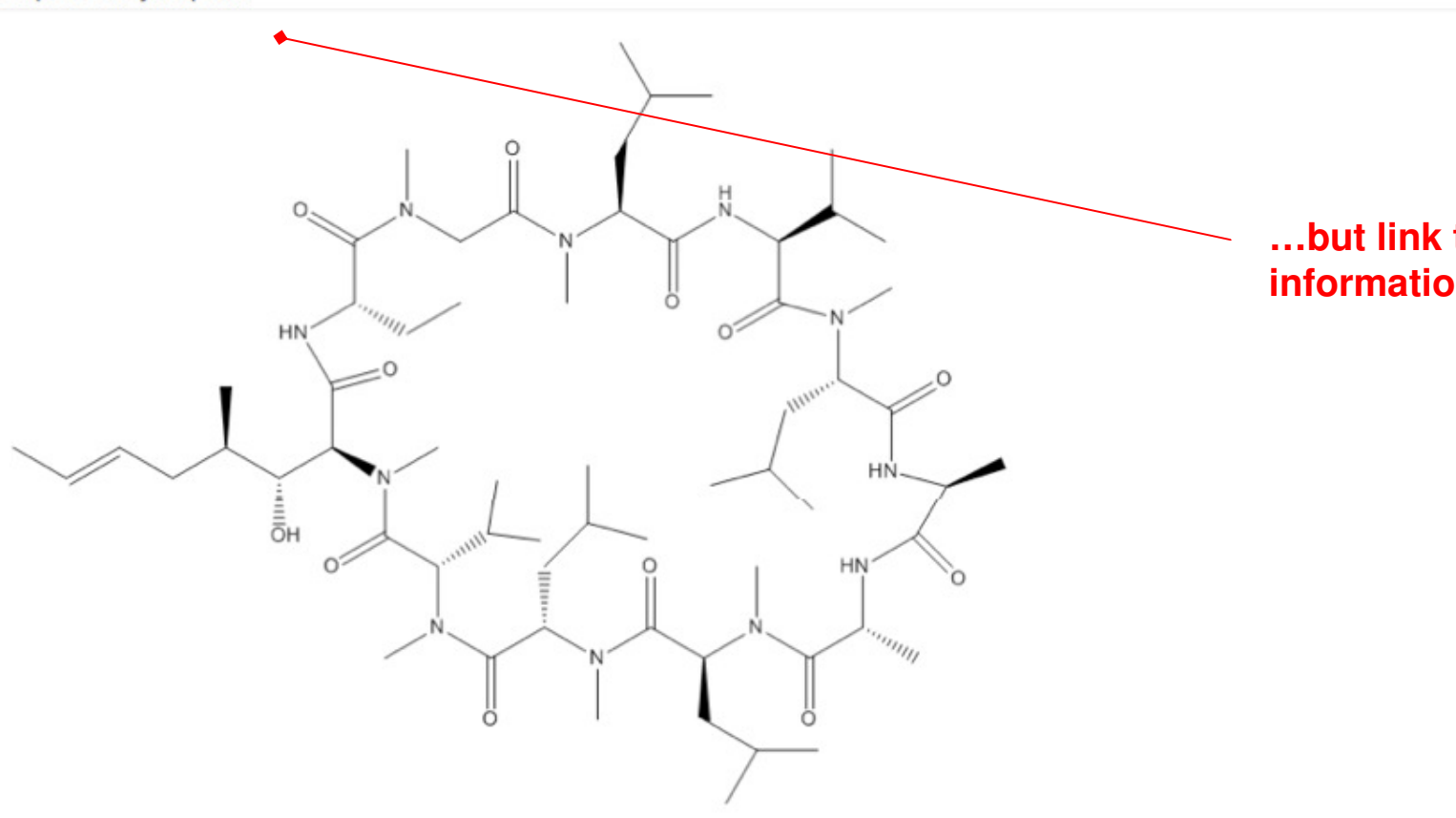
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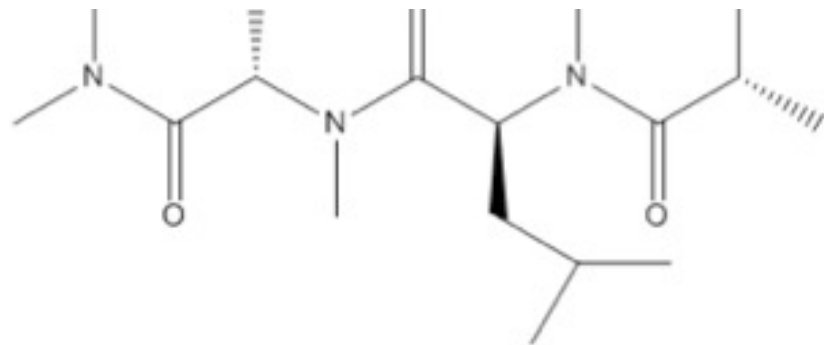
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### Synonyms

Cyclosporine

Ciclosporin

Neoral

Cyclosporine (USP)

Antibiotic S 7481F1

BMT-ABA-SAR-MLE-VAL-MLE-ALA-ALA-MLE-MLE-MVA

S-Neoral

Cipol N

HSDB 6881

S 7481F1

DRG 0275

Optimmune

(3S,6S,9S,12R,15S,18S,21S,24S,30S,33S)-30-Ethyl-33-[(1R,2R,4E)-1-hydroxy-2-methylhex-4-en-1-yl]-6,9,18,24-tetraisobutyl-3,21-diisopropyl-1,4,7,10,12,15,19,25,28-nonamethyl-1,4,7,10,13,16,19,22,25,28,31-undecaazacyclotritriacontane-2,5,8,11,14,17,20,23,26,29,32-undecone  
1,4,7,10,13,16,19,22,25,28,31-undecaazacyclotritriacontane-2,5,8,11,14,17,20,23,26,29,32-undecone, 30-ethyl-33-[(1R,2R,4E)-1-hydroxy-2-methylhex-4-en-1-yl]-6,9,18,24-tetraisobutyl-3,21-diisopropyl-1,4,7,10,12,15,19,25,28-nonamethyl-3,21-bis(1-methylethyl)-6,9,18,24-tetrakis(2-methylpropyl)-, (3S,6S,9S,12R,15S,18S,21S,24S,30S,33S)-

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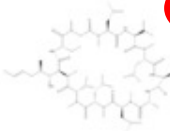
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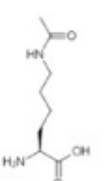
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 Michael Lammers, Heinz Neumann, Jason W Chin & Leo C James  
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cyclosporine - PubChem Public Chemical Database

http://pubchem.ncbi.nlm.nih.gov/summary/summary.cgi?sid=

index : Acetylation... cyclosporine - Pu... 1 : Acetylation reg... iGoogle Acetylation regula...

PubChem Substance

PubMed | Entrez | Structure | PubChem | Help

PubChem > Substance Summary

Chemical Structure (CID 5284373) | Deposited Record (SID 90744369)

**cyclosporine - Substance Summary (SID 90744369)**

Structure & Quick Link Bar

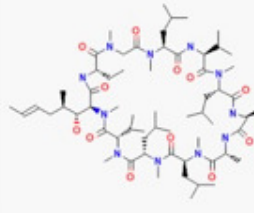


Table of Contents

- Substance Information
- Synonyms
- Comments
- Derived BioMedical Annotation
  - Medication Information
  - Pharmacological Action
  - Pharmacological Classification
  - Chemical Classification
  - Safety and Toxicology
  - Literature Links
  - Literature Mining
  - Exports

Substance Information:

SID 90744369  
 Deposit Date: 2010-03-23  
 Hold-until Date: 2010-04-04  
 Modify Date: 2010-03-23

Data Sources

Deposited in Nature Chemical Biology

Synonyms (Total: 2)

cyclosporine  
 nchembio.342-comp1

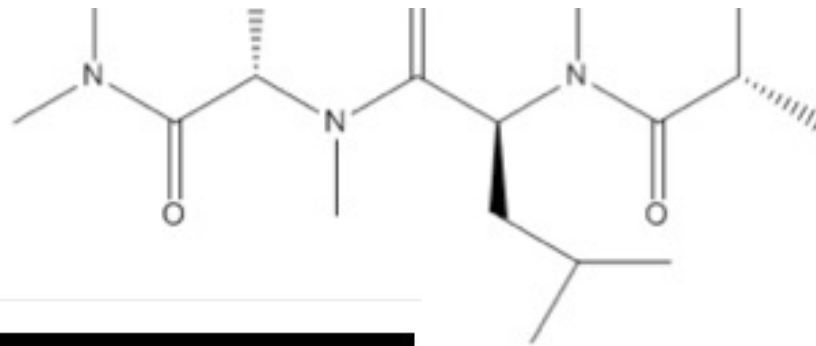
Comments

Lammers et al.  
 Acetylation regulates Cyclophilin A catalysis, immunosuppression and HIV isomerisation.  
*Nature Chemical Biology*, doi: 10.1038/nchembio.342, published online 4 April 2010  
<http://www.nature.com/naturechemicalbiology>

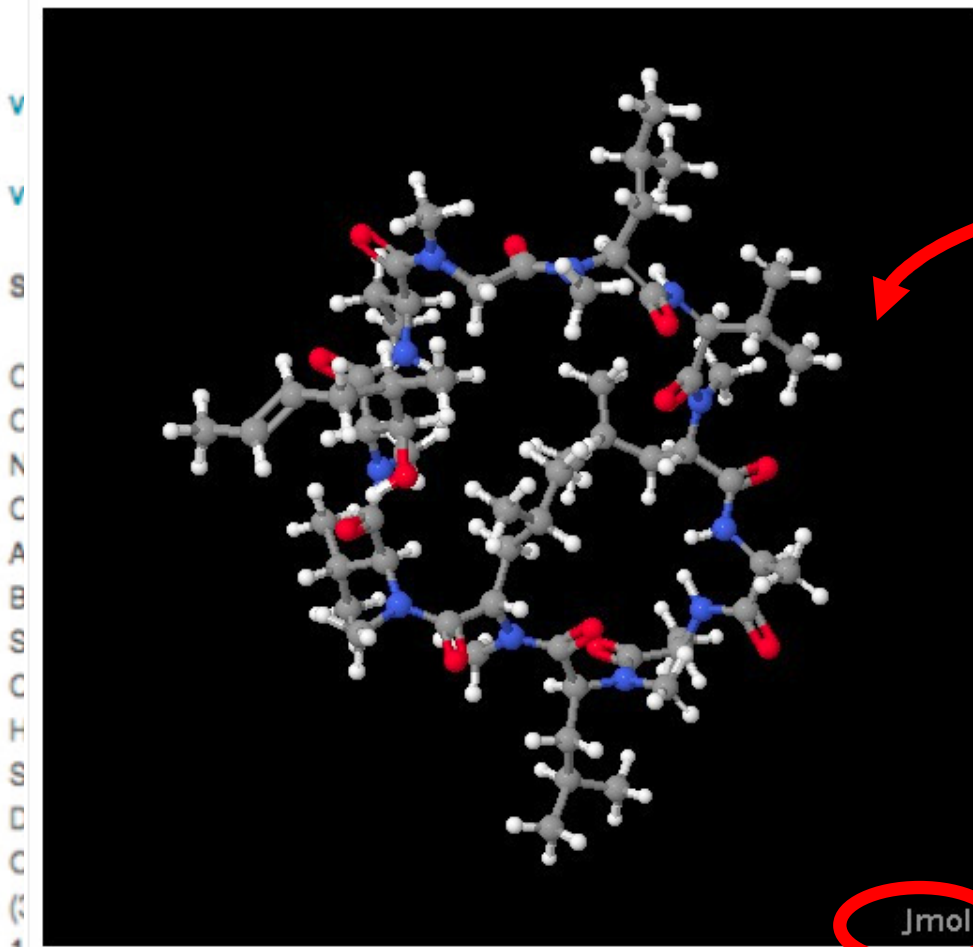
Derived Links

Related Substances:

- Same: 44 Links
- Same, Connectivity: 228 Links
- Same, Isotopes: 220 Links



Compound 1: Cyclosporine



[Molfile \(112 KB\)](#) [Download Molfile \(8 KB\)](#)

Jmol

(3S,6S,9S,12R,15S,18S,21S,24S,30S,33S)-32-undecyl-33-[(1R,2R,4E)-1-hydroxy-2-methylhex-4-en-1-yl]-6,9,18,24-tetraisobutyl-3,21-diisopropyl-1,4,7,10,13,16,19,22,25,28,31-undecaazacyclotritriacontane-2,5,8,11,14,17,20,23,26,29,32-undecone, 30-ethyl-33-[(1R,2R,4E)-1-hydroxy-2-methylhex-4-en-1-yl]-6,9,18,24-tetrakis(2-methylpropyl)-, (3S,6S,9S,12R,15S,18S,21S,24S,30S,33S)-



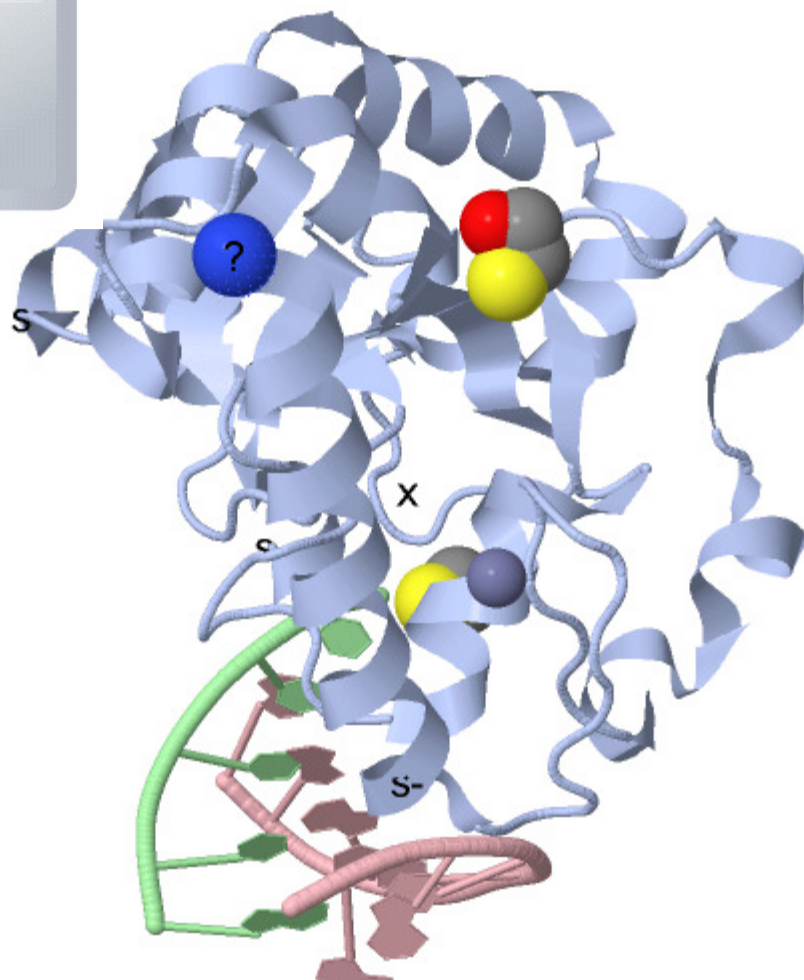
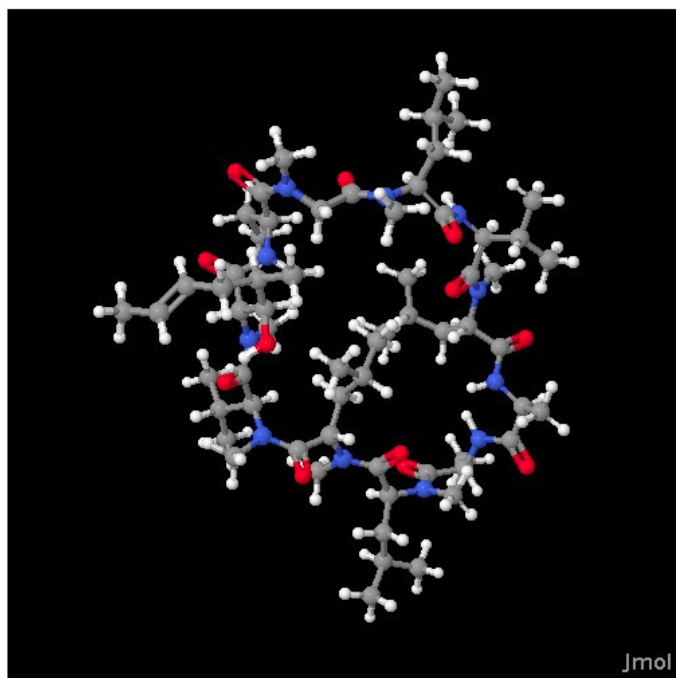
# A piece in the monkey puzzle



Trailer ▶ high ▶ low

Full film ▶ high ▶ low

Compound 1: Cyclosporine



Jmol

[Can't see the molecule?](#) [FirstGlance in Jmol](#) (ver. 1.45)

**345,517 Visitors**

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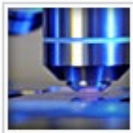


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### Most Commented

### Most Recent

### Most Popular



#### A protocol for *in vivo* detection of reactive oxygen species

Authors: Edward Owusu-Ansah, Amir Yavari, Utpal Banerjee

Lab groups: [Banerjee Lab \(University of California\)](#)

Associated Publications: [Distinct mitochondrial retrograde signals control the G1-S cell cycle checkpoint](#)

2',7'-dichlorofluorescein (H2DCF) and Dihydroethidium (DHE), have been used extensively in tissue culture experiments to evaluate reactive oxygen species (ROS) production. However, i...



#### Chromatin immunoprecipitation (ChIP) assay

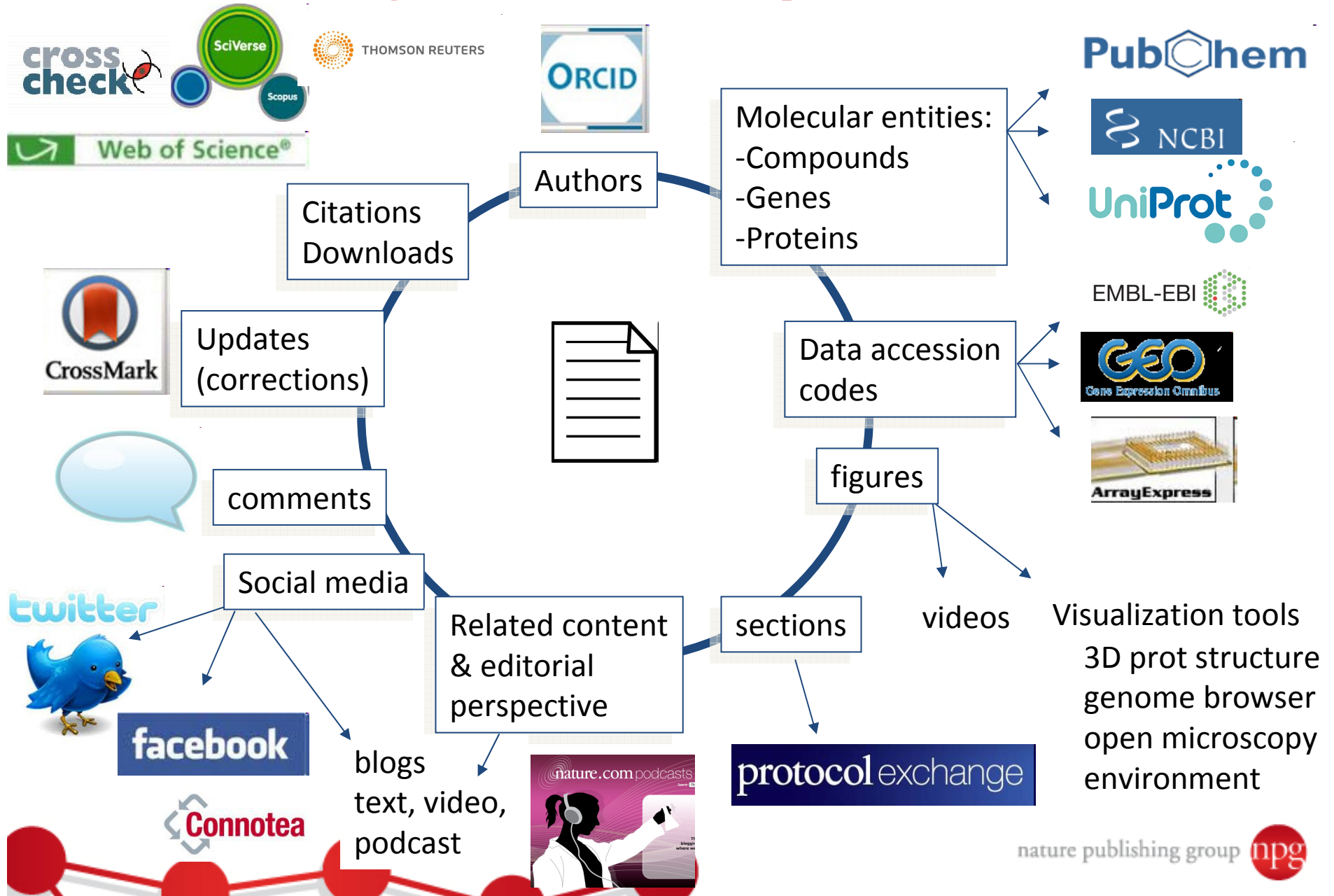
Authors: Zhongfu Ni, Danny W.-K. Ng, Jianxin Liu, Z. Jeffrey Chen

Lab groups: [Chen Lab \(The University of Texas at Austin\)](#)

Associated Publications: [Altered circadian rhythms regulate growth vigor in hybrids and allopolyploids](#)

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- Posted directly by their authors.
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- Users join online groups, align their identify their Labs.

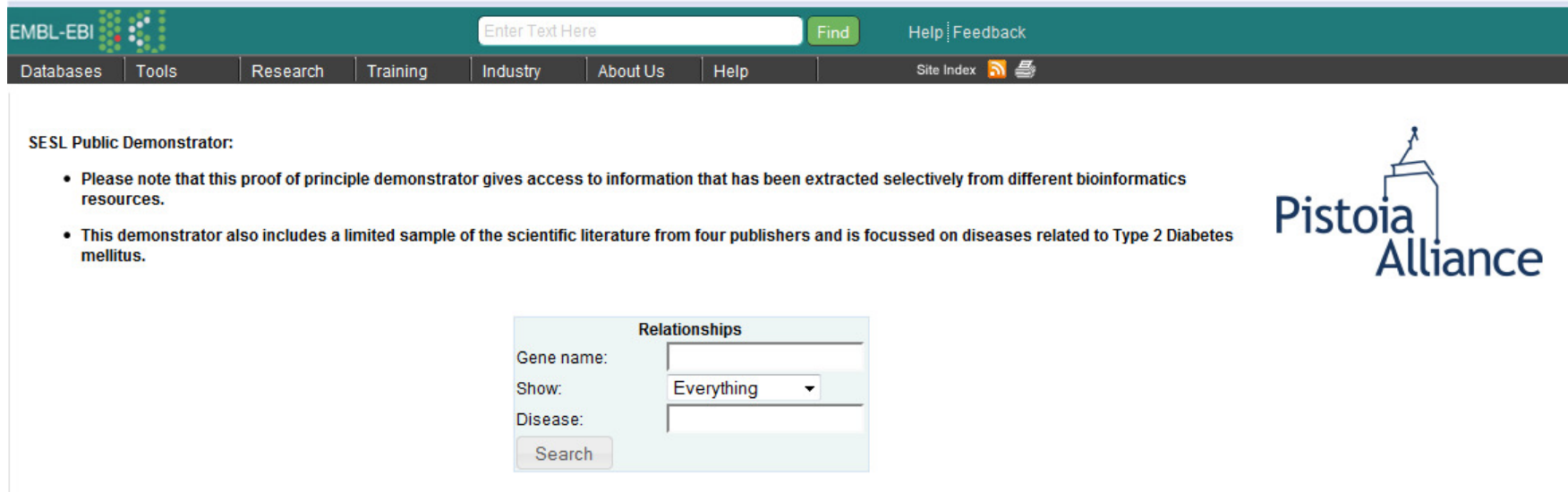
# Atomising the unit of publication



# Cross industry standards

- Credit where credit is due
  - Disambiguation
    - doi, ORCID
  - Performance measures
    - ISI impact factor, COUNTER, PIRUS, SUSHI
  - Editorial quality control
    - crosscheck, crossmark
- Openness
  - Broadcasting in machine readable format
    - Opensearch, RDF triple stores, linked data
    - APIs and external developers programmes

# Experimenting with push versus pull



The screenshot shows the top navigation bar of the Pistoia Alliance website, including the EMBL-EBI logo, a search bar with the text "Enter Text Here" and a "Find" button, and a menu with options like "Databases", "Tools", "Research", "Training", "Industry", "About Us", and "Help". Below the navigation bar, the "SESL Public Demonstrator" section is visible, containing two bullet points and a search form titled "Relationships".

**SESL Public Demonstrator:**

- Please note that this proof of principle demonstrator gives access to information that has been extracted selectively from different bioinformatics resources.
- This demonstrator also includes a limited sample of the scientific literature from four publishers and is focussed on diseases related to Type 2 Diabetes mellitus.

**Relationships**

Gene name:

Show:

Disease:



- Pistoia SESL project
- Databases: Uniprot, OMIM, and ArrayExpress
- 5 publishers: Nature Publishing Group, Oxford University Press, the Royal Society of Chemistry, UK Pubmed Central, and Elsevier.

# An expanding remit

Pre Publication	Publication	Post Publication
	traditional remit of publishers	
<div data-bbox="191 659 720 854">facilitate networking &amp; informal peer discussions and collaboration</div> <div data-bbox="191 894 653 1057">content discoverability -indexing -push and pull models</div> <div data-bbox="191 1114 747 1248">organizing: tagging, bookmarking, bibliography</div>	<div data-bbox="919 781 1163 1049">selectivity editing preservation distribution credit</div>	<div data-bbox="1291 662 1738 708">data discovery &amp; reuse</div> <div data-bbox="1291 737 1696 1084">broadcasting article information -semantic mark up -linked data -open search -APIs</div> <div data-bbox="1291 1105 1955 1200">authors disambiguation – article and subarticle level metrics</div> <div data-bbox="1291 1235 1818 1341">targeted filtering, personal delivery</div>

# More will happen...

