

# Open access: changing the way science is published in the digital age



MAX-PLANCK-GESELLSCHAFT

Open Access and Author Rights session  
Fritz-Haber-Institut der MPG, 1<sup>st</sup> July 2009

Jan Kuras, Chemistry Central  
[www.chemistrycentral.com](http://www.chemistrycentral.com)



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# Outline

- An introduction to Open Access publishing
  - Comparing traditional and OA publishing
  - Achieving OA; and economics & funding
- BioMed Central
  - History and overview
- Open Access in chemistry
  - Open Access in other subject areas
  - Established initiatives in chemistry
  - Chemistry Central
- OA Publishing at the Max Planck Institute



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# An introduction to Open Access publishing: comparing traditional and OA publishing



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# Reality and paradox of traditional, subscription-based academic publishing

- **Economic sustainability:** *pressure on library budgets to keep up with increasing volume of research being published, and rising subscription charges*
- **Interests of scientific community, funders and society:** *concerns about authors' copyright, and access barriers to research reducing its visibility, and restricting sharing of ideas which drives scientific advancement*
- **Potential to exploit new technologies:** *the online, digital environment should be exploited for better dissemination of scientific research and data*



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# Genesis of the Open Access movement

1991: arXiv



1992: GenBank



1997: PubMed



1998: Scholarly Publishing and Academic Resources Coalition (SPARC)



1999: Open Archive Initiative; BioMed Central



2000: PubMed Central



2001: Public Library of Science (PLOS)



Budapest Open Access Initiative (2002)

Bethesda Statement on Open Access Publishing (2003)

Berlin Declaration on Open Access to Knowledge in Sciences & Humanities (2003)

# What is Open Access publishing?

- Free access → *no subscriptions; increases citation and download counts*
- Free of copyright & licensing restrictions → *increases dissemination; data can be redistributed, reused, translated & deposited freely; IP remains with authors*
- Digital, online → *exploits web technology to increase data visibility & usability*
- Full-text available immediately upon publication → *ensures rapid publication and access to research. Indexed by Google and others*

Open Access is: not self-publishing; not a means to bypass peer review; not a 2nd class, cut-price publishing route



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# Achieving Open Access



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# How Open Access to research is delivered

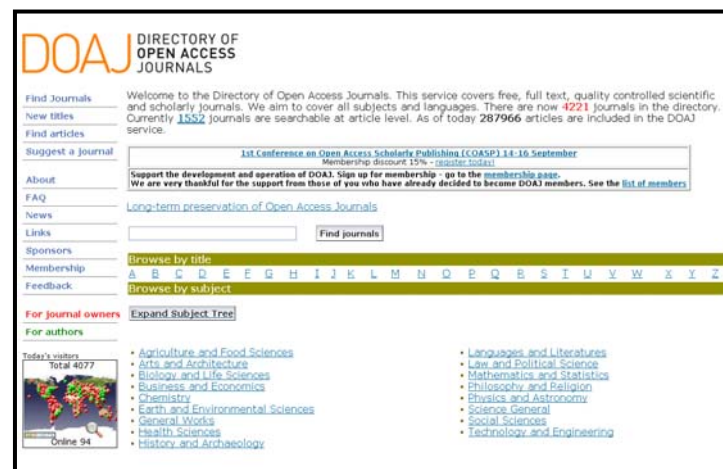
## The Green route: Open Access repositories/archives

- May contain un-refereed pre-prints and/or refereed post-prints
- May belong to individuals, institutions or be central/subject-specific



## The Gold route: Open Access journals

- Fully OA journals
- Subscription-based journals that offer an OA option to authors



- ~10% of journals are OA

# Open Access Journals: business models

*Involve charging for the service of publishing*

## Fee-based Open Access journals

- Most common model involves payment of an article processing charge (APC)



## Self-supported Open Access journals

- Sources of income include subsidies from host universities, professional societies



# What do article processing charges pay for?

- World-wide barrier-free Open Access to the full text
- Electronic tools for peer review and publication
- Pre-and post-publication tracking tools for authors
- Preparation of manuscripts in various formats for online publication
- Inclusion in PubMed as soon as possible after publication
- Full text inclusion in a number of permanent archives such as PubMed Central
- Inclusion in CrossRef (enabling electronic citation in other journals that are available electronically)
- Promoting journals through marketing activities



# Economics and Funding



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# Macro-economics are simple

- Open access publishing involves no new costs
- From the perspective of the research community as a whole, switching to an Open Access publishing model is affordable and desirable
  - It costs no more than the current model
  - It delivers more: universal access and reuse



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# Micro-economics are more challenging

- Library budgets already stretched paying the costs of the current publishing model through subscriptions
- Costs of traditional system are mostly invisible to authors, whereas article processing charges are an obstacle for authors
- During a transitional period, moves towards open access may involve additional costs
- Librarians are on a treadmill which is moving too fast to get off



# Funding: recent mandates change the landscape

- “Author pays” is misleading - authors are seldom exposed to cost of publication
- Some funding agencies mandate open access, often within 6-12 months
- Some universities mandate retention of copyright and frequently offer funds to cover OA fees

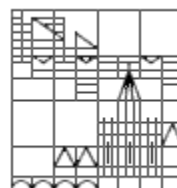
“Universities need to do more to develop institutional policies and strategies that increase access to their peer-reviewed research results to the widest range of users, to maximise the impact and visibility of university research”: **EUA, April 2008**



# Some universities & institutions fund OA publishing costs



Universität  
Konstanz



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# Funding agency mandates for Open Access

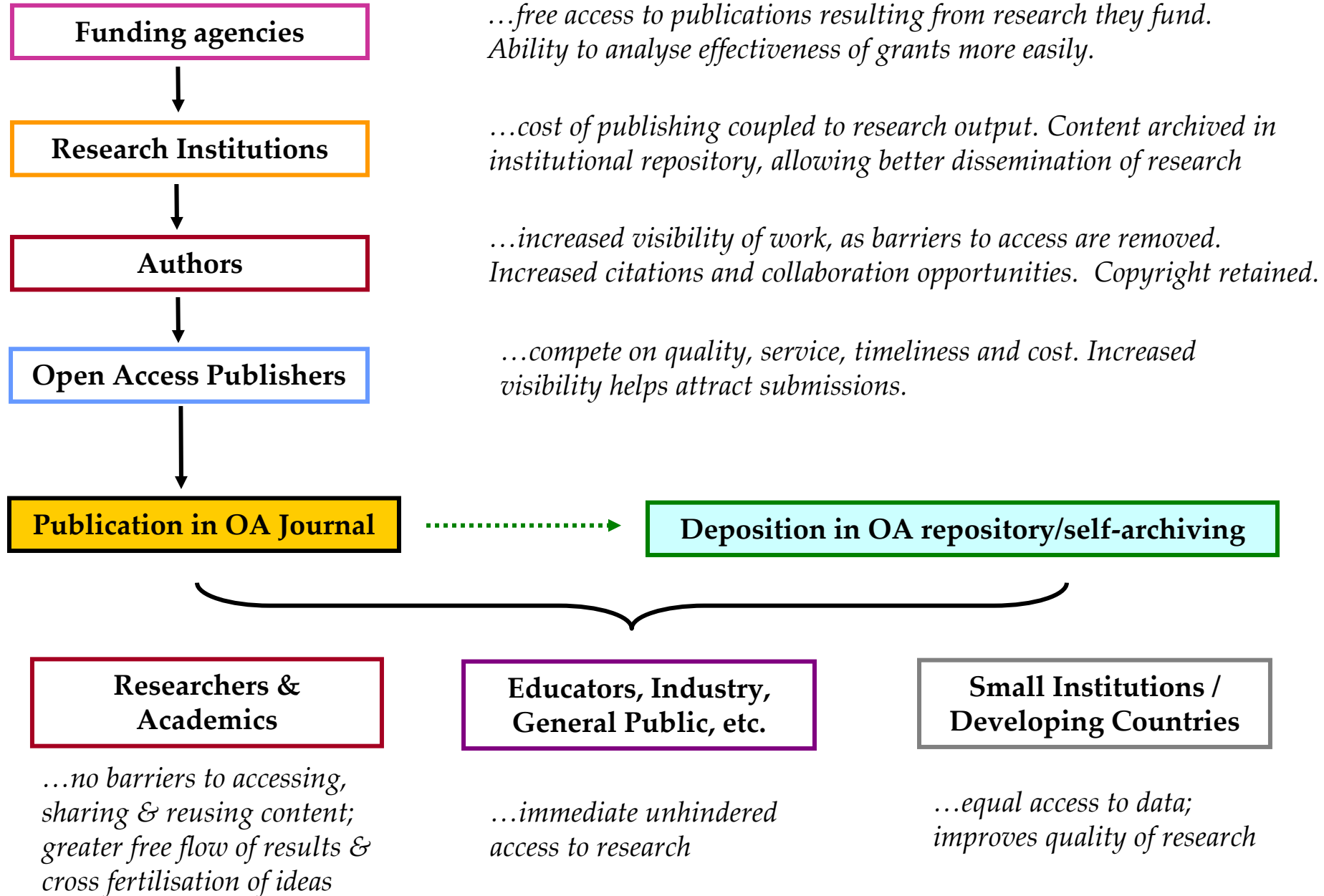


*"...NIH shall require that all investigators funded by the NIH submit ... to PubMed Central an electronic version of their final, peer-reviewed manuscripts upon acceptance... no later than 12 months after publication."*



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# Removing access barriers benefits the research community



BioMed Central



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**BioMed Central**  
The Open Access Publisher

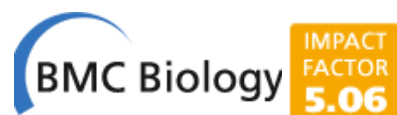
## An Overview

- Commercial open access publisher now part of Springer SBM
- Launched first open access journals in 2000
- Now publishing ~200 OA titles
- Over 30,000 peer-reviewed OA articles published
- Chemistry Central (2006) and PhysMath Central (2007) – new publishing services
- All research articles published under Creative Commons license, allowing freedom to reuse and redistribute



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## BMC series journals: *edited in-house, e.g.*



## Independent journals: *administered by independent groups*



## Hybrid journals: *e.g. charge for non-research content*



# BioMed Central Institutional Membership

Currently over 280 members in 35 countries worldwide

**Supporter Membership**

**Post-pay Membership**

**Pre-pay Membership**

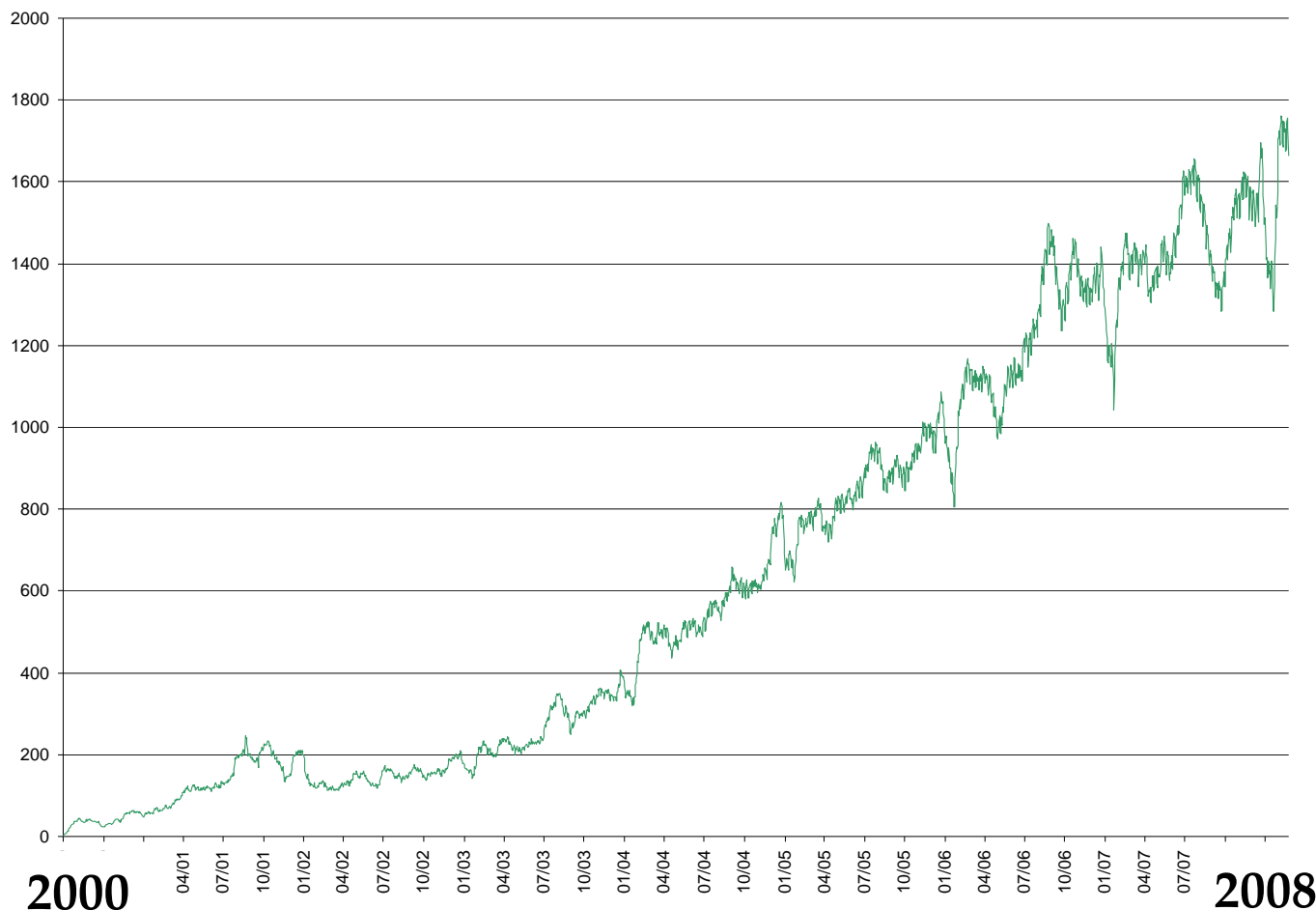
- Authors budget for APCs in their grant/funding applications
- Authors from low-income nations have APCs waived
- Discounts & waivers on a case-by-case basis e.g. new journal launches
- APC discounts to those who have acted as peer reviewers

**Myth debunked:** Charging APCs does **not** affect the independence of the editorial process



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# Growing number of submissions to OA journals



Total monthly submissions to BioMed Central, PhysMath Central & Chemistry Central



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# Open Access publishing in Chemistry and other subject areas



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# Open Access in other disciplines

## Life Sciences



**GenBank**

## Physics



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# Established open access initiatives in chemistry



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**PubChem** - part of NIH's Molecular Libraries Roadmap Initiative. Provides biological activity information on small molecules through 3 databases: Pc-Substances (>40M records), Pc-Compounds (>19M unique structures), and Pc-Bioassay (>1,000 bioassays).

**NCBI PubChem Compound**

PubChem » Compound Summary

**Ibuprofen - Compound Summary** (CID 3672)

A nonsteroidal anti-inflammatory agent with analgesic properties used in the therapy of rheumatism and arthritis.

**Table of Contents**

- Drug and Chemical Information
  - Medication Information
  - Pharmacological Action
  - Pharmacological Classification
  - Chemical Classification
  - Safety and Toxicology
  - Literature Links
  - Literature Mining
- BioActivity Results
- Synonyms
- Properties
- Descriptors
- Compound Information
- Substance Information
  - Category
- Exports

**Drug and Chemical Information:** (Total: 1)

**Ibuprofen**

**Medication Information**

**IBUPROFEN ORAL SUSPENSION USP [Actavis Mid Atlantic, LLC]**

The active ingredient in Ibuprofen Oral Suspension USP is ibuprofen, which is a member of the propionic acid group of nonsteroidal anti-inflammatory drugs (NSAIDs). Ibuprofen is a racemic mixture of [+-]S- and [+-]R-enantiomers. It is a [more...](#)

Description	Clinical Pharmacology Indication & Usage
Contraindications	Warnings
Adverse Reactions	Overdosage
How Supplied	Dosage & Administration
	Precautions

**Structure & Quick Link Bar**

2D 3D

**Compound ID** 3672

**Molecular Weight** 206.28082 [g/mol]

**Molecular Formula** C<sub>13</sub>H<sub>18</sub>O<sub>2</sub>

**XLogP3** 3.5

**H-Bond Donor** 1

**H-Bond Acceptor** 2

**Links**

- NLM Toxicology Link
- Chemical Structure Search
- BioActivity Summary: This Compound with Similar Compounds



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**ChemSpider** - chemistry search engine; aggregating & indexing chemical structures and associated information into a searchable repository and making it available to everybody, at no charge.



The screenshot displays the ChemSpider website interface. At the top, the ChemSpider logo is accompanied by the tagline "Building Community for Chemists". Navigation links for Home, Search, Services, Resources, About, and Login are present. A left sidebar lists various search options: Simple Search, Structure Search, LASSO Search, Advanced LASSO, Chemical Elements, Properties Search, Predicted Properties, Data Source Search, Literature Search, NCBI Entrez Search, PubChem Search, Advanced Search, and Searches History. Below this, there are advertisements for ChemSpider Consultancy and Prestwick Chemical.

The main content area shows the results of a search for "ibuprofen". It indicates that 1 hit was found in 0.65 seconds. The search term is "ibuprofen" and it was found by synonym. A message prompts the user to login to add spectra, identifiers, links, and publications. Below this, a table with columns "Add:", "Description", "Identifier", "CIF", "Spectrum", "Image", and "Comments" is visible. The search results are categorized under "INHERENT PROPERTIES, IDENTIFIERS AND REFERENCES".

Key information for the search result includes:

- ChemSpider ID: 3544
- Empirical Formula:  $C_{13}H_{18}O_2$
- Molecular Weight: 206.2808
- Nominal Mass: 206 Da
- Average Mass: 206.2808 Da
- Monoisotopic Mass: 206.13068 Da

The chemical structure of ibuprofen is shown as a 3D ball-and-stick model. Below the structure, the systematic name is given as "2-(4-isobutylphenyl)propanoic acid". Other identifiers provided include the SMILES string O=C(O)C(c1ccc(cc1)CC(C)C)C, the InChI string InChI=1/C13H18O2/c1-9(2)8-11-4-6-12(7-5-11)10(3)13(14)15/h4-7,9-10H,8H2,1-3H3,(H,14,15), the InChIKey HEFNWWSXXWATRW-UHFFFAOYAB, the Std. InChI string InChI=1S/C13H18O2/c1-9(2)8-11-4-6-12(7-5-11)10(3)13(14)15/h4-7,9-10H,8H2,1-3H3,(H,14,15), and the Std. InChIKey HEFNWWSXXWATRW-UHFFFAOYSA-N.

Quick Links: [Permalink](#) [Similar](#) [Isomers](#) [Wikibox](#)

Below the identifiers, there is a section for "WIKIPEDIA ARTICLE(S)" with a "LICENSE" link. The article text states: "Advil is a brand of **ibuprofen**, a **non-steroidal anti-inflammatory drug** (NSAID). Advil is manufactured by Madison NJ based **Wyeth** and has been on the market since 1984. [Read more...](#) or [Edit at Wikipedia...](#)"

The Wikipedia article further describes ibuprofen (INN) as a **non-steroidal anti-inflammatory drug** (NSAID) originally marketed as **Brufen**, and since then under various other **trademarks** (see **tradenames** section), most notably **Nurofen**, **Advil** and **Motrin**. It is used for relief of symptoms of **arthritis**, primary **dysmenorrhea**, **fever**, and as an **analgesic**, especially where there is an **inflammatory** component. Ibuprofen is known to have an **antiplatelet** effect, though it is relatively mild and short-lived when compared with that of **aspirin** or other better-known antiplatelet drugs. Ibuprofen is a core medicine in the **World Health Organization's "Essential Drugs List"**, which is a list of minimum medical needs for a basic health care system. [Read more...](#) or [Edit at](#)



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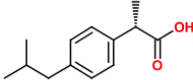
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**Structure Search**

File Edit View Help



**Choose a Category:**

- ☒ Building Blocks
- ☒ Screening Compounds
- ☐ All Compounds

(what are categories?)

[Substructure Search](#) [Exact Structure Search](#) [Choose Specific Supplier](#)

**Search Named Chemicals**

Name:  [Search](#)

Name: [Advil](#), [Ibuprofen](#) CAS Num: [15687-27-1](#) SMILES: [S=C=NC](#)

**Search from a List**

[Upload a File...](#) [Enter a List...](#)

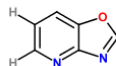
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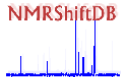
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**NMRShiftDB** - database of structures & NMR spectra. Allows prediction ( $^{13}\text{C}$ ,  $^1\text{H}$  etc.) and searching of spectra, structures & other properties. Features peer-reviewed submission of datasets by its users. Software is open source, data is published under an open content license.



**Current usage of NMRShiftDB is:**  
Registered Users: 1965  
Structures which can be searched: 31386  
Spectra: Measured 35076, calculated 550

Username:

Password:

☐ Use cookies for persistent login

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[Create New Account](#)  
(Only necessary for contributing data)

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Problems using NMRShiftDB? See our [tips on browsers to use](#) !

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### NMRShiftDB Links

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5	N. Prakash	350
6	B. Patel	305
7	M. Gericke	181
8	N. Kuznik	120
9	K. Bohn	111
10	R. Ellinger	76
11	A. Dransfeld	56
12	K. Bartussek	26
13	M. Mitchell	20
14	J. Bitzer	19
15	L. Ernst	17
16	R. Mueller	16
17	C. Steinbeck	15
18	J. Beutler	10
19	T. Nidas	8
20	R. Stenutz	6

More people have contributed.

[NMRShiftDB Servers](#)

### About NMRShiftDB

NMRShiftDB is a NMR database (web database) for organic structures and their nuclear magnetic resonance (nmr) spectra. It allows for spectrum prediction ( $^{13}\text{C}$ ,  $^1\text{H}$  and other nuclei) as well as for searching spectra, structures and other properties. Last not least, it features peer-reviewed submission of datasets by its users. The NMRShiftDB software is open source, the data is published under an open content license. Please consult the [documentation](#) for more detailed information.

### News about NMRShiftDB

**Bugfix release** 2009-04-07 10:42 - [NMRShiftDB](#)  
Bug fix release 1.3.4 is now available. It fixes some bugs and cleans up ID handling. See [here](#) for details.  
[Read More »](#)

**NMR prediction paper published** 2009-01-28 11:32 - [NMRShiftDB](#)  
A paper on prediction of  $^1\text{H}$ -NMR spectra using the data from NMRShiftDB has been published in BMC Bioinformatics. It can be read electronically on [here](#).  
[Read More »](#)


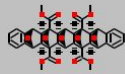
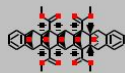
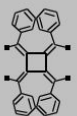
**Bioclipse-based client available** 2008-06-18 15:45 - [NMRShiftDB](#)  
Specipse, the new standalone client for NMRShiftDB, based on Bioclipse and therefore Eclipse, is available for Windows and Linux systems at [here](#) - it provides convenient access to NMRShiftDB functions including offline editing of entries.  
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**CUBIC NMRShiftDB server moved** 2008-04-15 15:39 - [NMRShiftDB](#)  
The server running at CUBIC was moved to the NMR labs of the University of Mainz, thanks to the help of the NMR department of Organic Chemistry running these facilities.  
It can now be reached at [here](#).  
Once we've completed the OS upgrade of our main servers at the Max-Planck-Institute for Chemical Ecology in Jena, the Mainz server will be integrated into the load scheduling system and you may get automatically redirected to it again.  
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**Server Upgrade** 2008-04-15 12:22 - [NMRShiftDB](#)  
The NMRShiftDB servers will get an OS upgrade over the coming weeks. This might lead to delays in replication, but should not affect availability.  
[Read More »](#)

**New NMRShiftDB paper** 2008-04-05 21:28 - [NMRShiftDB](#)  
A paper has been published evaluating the quality of the NMRShiftDB data and using it for comparing NMR prediction tools. Find details at [here](#).  
[Read More »](#)

### Latest Additions





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# OA facilitates interactive online resources

The screenshot displays the Scivee website interface. At the top, there is a navigation bar with a search box, login/register links, and icons for browse, upload, and community. Below this is a secondary navigation bar with links for pubcasts, videos, postcasts, channels, and tags. The main content area features a video player titled "Bioinformatic analyses of mammalian 5'-UTR sequence properties of mRNAs predicts alternative translation initiation sites". The video player shows a woman speaking, with the text "Jill Wegryn Bioinformatician and Project Scientist at UCSD" overlaid. The video player has a "full screen" button and a progress bar. To the left of the video player, the authors and citation information are listed: "Authors: Jill L Wegryn, Thomas M Drudge, Faramarz Valafar, Vivian Hook" and "Citation: BMC Bioinformatics. 2008 May 8; 9:232". To the right of the video player, there are links to "Listen to the podcast" and "View Original Article". Below the video player, there are tabs for "Figures", "Supplementary Materials", "References", "Tags", and "Related Content". The "Figures" tab is active, showing a series of small thumbnail images. To the right of the thumbnails, there is a section for "Linked profiles" and "Submitted by" information, including a DOI and a rating. The BMC Bioinformatics logo is visible in the bottom right corner.

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Bioinformatic analyses of mammalian 5'-UTR sequence properties of mRNAs predicts alternative translation initiation sites

Authors: Jill L Wegryn, Thomas M Drudge, Faramarz Valafar, Vivian Hook  
Citation: BMC Bioinformatics. 2008 May 8; 9:232  
Peer-Reviewed Paper

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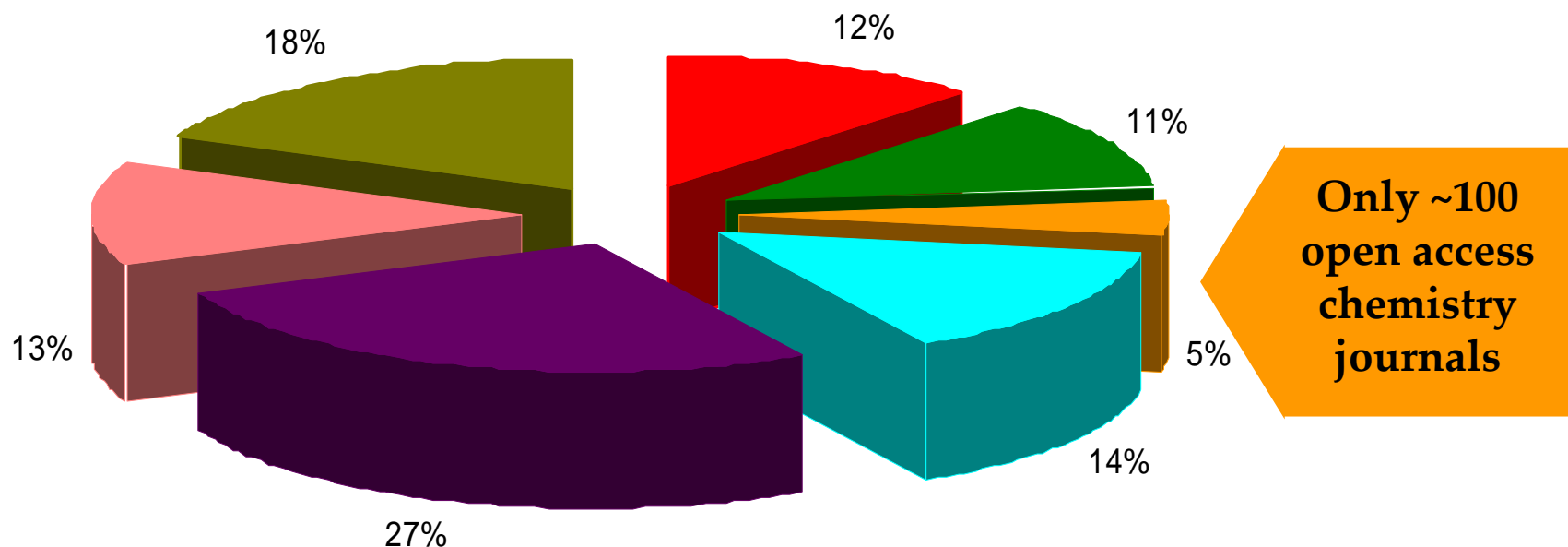
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Linked profiles: jwegryn  
Submitted by: apyl  
DOI: 10.4016/9592.01  
Rating: ★★★★★  
You must be logged in to rate a video.

BMC Bioinformatics

“Pubcasts”: Scivee allows OA full texts and videos to be tagged to, and synchronised with each other

# Open Access Journals by Subject Area



■ Agriculture and food sciences

■ Chemistry

■ Health sciences and medicine

■ Technology and engineering

■ Biology and life sciences

■ Earth and environmental science

■ Physics and mathematics

Source: Directory of Open Access Journals  
([www.doaj.org](http://www.doaj.org))



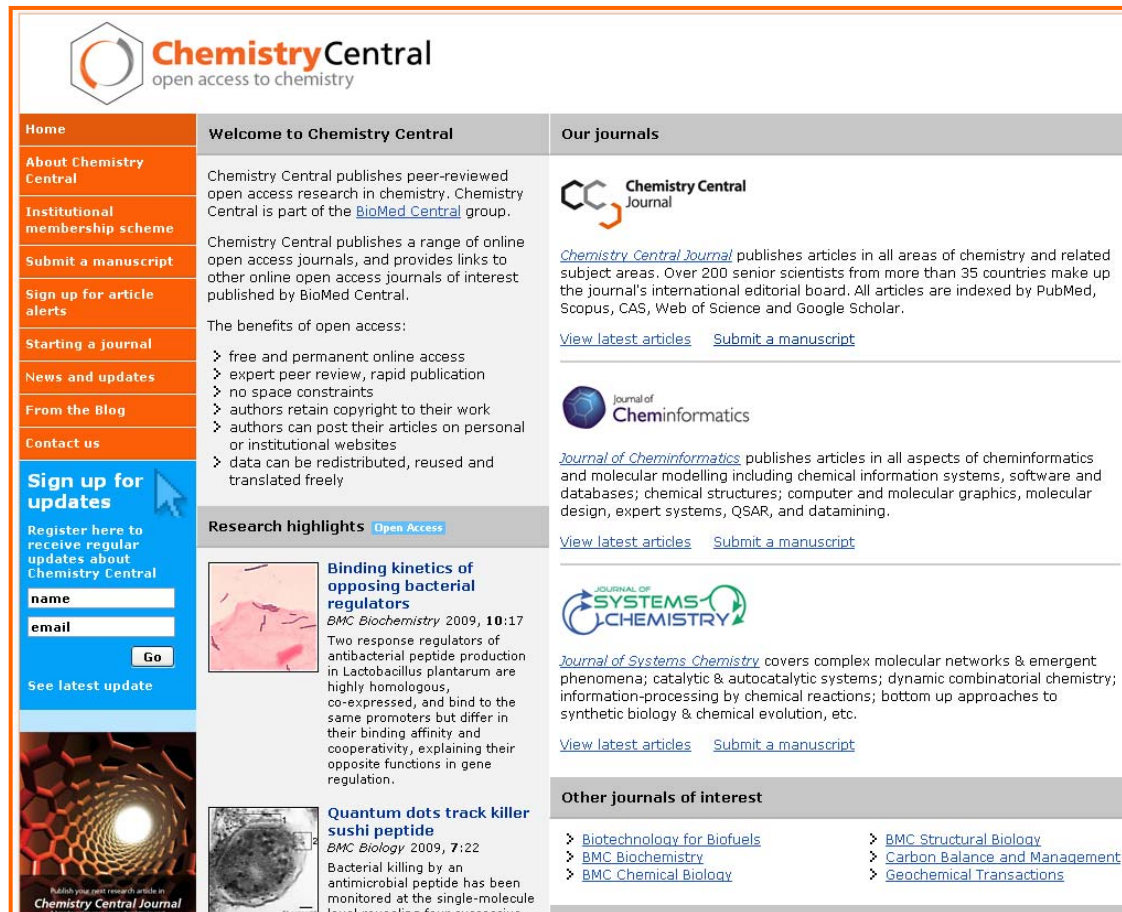
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- Covers *all areas of chemistry* through 55 subject-specific sections
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The screenshot shows the Chemistry Central Journal homepage. At the top, the logo and name 'Chemistry Central Journal' are displayed, along with the website URL 'www.journal.chemistrycentral.com'. Below this is a navigation bar with links: Home, Browse articles, Supplements, Search, Weblinks, Submit article, My Chemistry Central Journal, and About Chemistry Central Journal. The main content area is divided into several sections. On the left, under 'About the journal', there are links for 'Open access to all articles', 'View the Editorial Board', 'Tracked/indexed by PubMed, PubMed Central, Thomson Reuters (ISI), CAS, Scopus and Google Scholar', 'Instructions for authors submitting a manuscript', 'Contact us', 'View the most accessed articles', 'RSS feed of the latest articles', 'Promote the journal Posters, leaflets, T-Shirts and more.', and 'View answers to some Frequently Asked Questions'. The main content area features a 'CALL FOR PAPERS' section, a 'POSTER' section, a 'Latest supplement' section (Volume 3 Suppl 1, 4th German Conference on Chemoinformatics: 22 CIC-Workshop Meeting abstracts), a 'Latest articles' section (Correction: Heavy metal ions in wines: meta-analysis of target hazard quotients reveal health risks), a 'Research article' section (Electron ionization mass spectral fragmentation study of sulfation derivatives of polychlorinated biphenyls), and a 'Methodology' section (Automated extraction of chemical structure information from digital raster images). On the right side, there are buttons for 'REGISTER NOW', 'CLICK HERE TO REGISTER', 'Search', 'SUBMIT A MANUSCRIPT', 'CLICK HERE TO SUBMIT', and 'Sign up for article alerts!'. At the bottom right, there are links for 'Unique Heterocycles', 'Chemistry Lab Notebook', and 'Make \$5K+ Week Online'.





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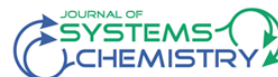
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Software

**The JSpecView Project: an Open Source Java viewer and converter for JCAMP-DX, and XML spectral data files**

**Robert J Lancashire** ✉  
Department of Chemistry, The University of the West Indies, Mona Campus, Kingston 7, Jamaica

✉ author email ✉ corresponding author email

Chemistry Central Journal 2007, 1:31 doi:10.1186/1752-153X-1-31

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**Abstract**

The JSpecView Open Source project began with the intention of providing both a teaching and research tool for the display of JCAMP-DX spectra. The development of the Java source code commenced under license in 2001 and was released as Open Source in March 2006. The scope was then broadened to take advantage of the XML initiative in Chemistry and routines to read and write AnIML and CMLspect documents were added.

JSpecView has the ability to display the full range of JCAMP-DX formats and protocols and to display multiple spectra simultaneously. As an aid for the interpretation of spectra it was found useful to offer routines such that if any part of the spectral display is clicked, that region can be highlighted and the (x, y) coordinates returned. This is conveniently handled using calls from JavaScript and the feedback results can be used to initiate links to other applets like Jmol, to generate a peak table, or even to load audio clips providing helpful hints.

Whilst the current user base is still small, there are a number of sites that already feature the applet. A tutorial video showing how to examine NMR spectra using JSpecView has appeared on YouTube and was formatted for replay on iPods and it has been incorporated into the JSpecView project.

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**Interpretation of the IR of acetophenone**



Acetophenone (thin film) 1-phenylethan-1-one

The vibrational mode corresponding to that peak is: scissors of aromatic C-H groups (~1265 cm<sup>-1</sup>)

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**acetophenone**



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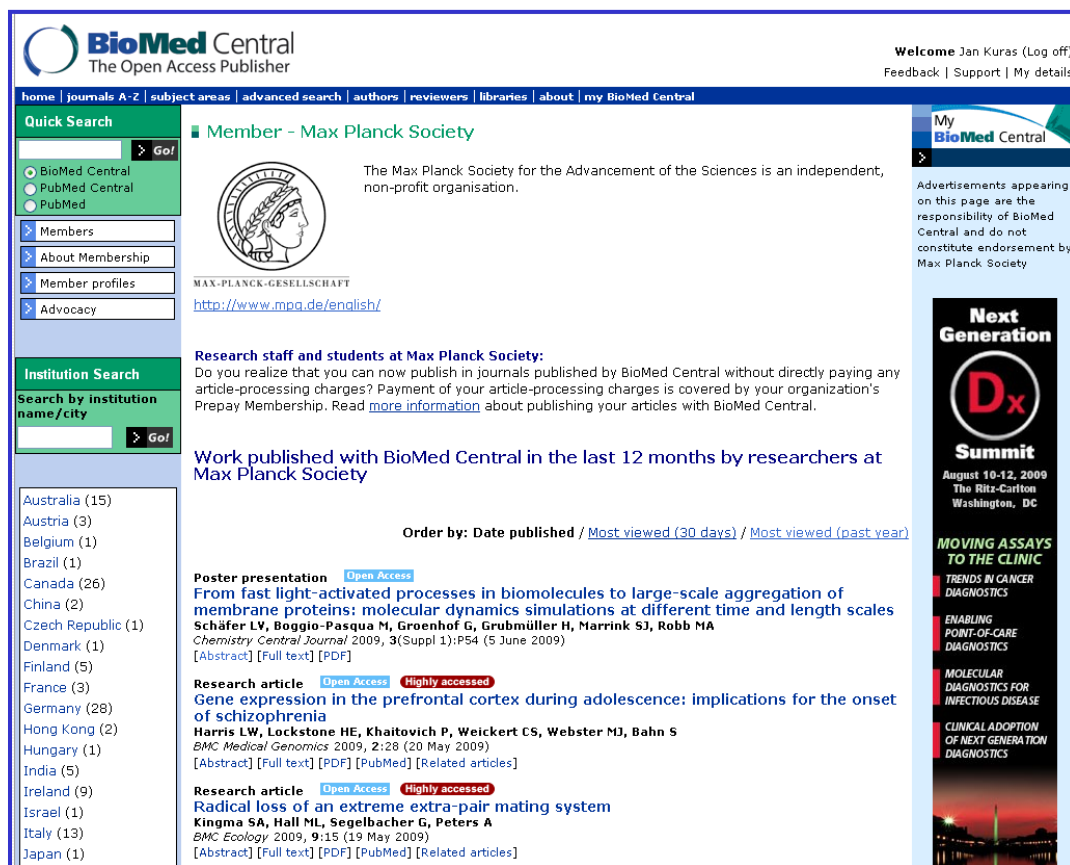
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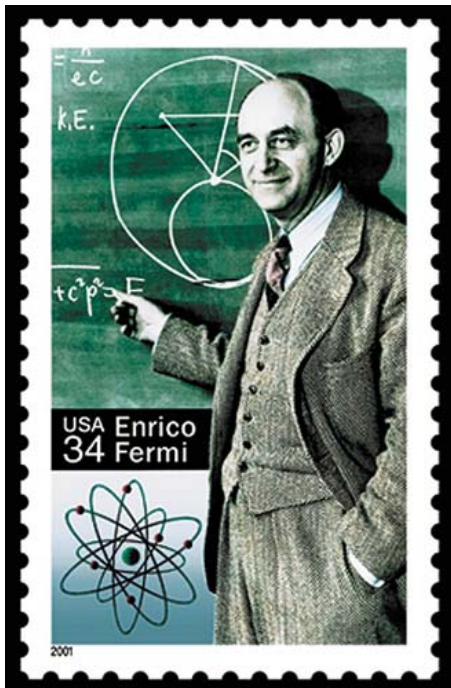
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