chem-bla-ics

The Internet Journal of Chemistry

Published August 11, 2025

Citation
Willighagen, E. (2025, August 11). The Internet Journal of Chemistry. *Chem-bla-ics*. https://doi.org/10.59350/2ss5b-jpr33

Keywords
Publishing, Wikidata, Scholia

The Internet Journal of Chemistry (IJC, issn:1099-8292) was one of the first scientific journals to get published on the world wide web (part of *the Internet*), see doi: 10.1080/00987913.2000.10764578. Issues were published from 1998 to 2004. But because it predates systematic archiving of webpages by libraries, a lot is lost. The nature of the journal, however, makes it unique, and quite a number of articles are cited a lot, and should be part of the *scientific record*. But I soon realized it actually is quite hard to track down content of the journal. I knew some articles have been *author accepted manuscripts* online. One of that was my own first (and single) author-article, self-archived on Zenodo (doi:10.5281/zenodo.1495470), green open access style.

I wanted to see what I could recover, and here I describe what I did and what could be done next.

A list of all articles

The first step is actually to create a list of all articles published in the IJC and collect as much metadata about them as possible. With just over 100 articles, I decided to use Wikidata, as a machine-readable database, supporting the curation and reporting. I wanted at least two independent sources, and for Wikidata, use public resources. That means, while Web of Science does have a list of all articles, I only used this for validation, and **not** as information source. Instead, I used citations to IJC articles and, of course, the Internet Archive (IA). It turns out a query like this does wonders (well, for the abstracts; I did not find full-texts archived on IA):

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https://web.archive.org/web/*/http://www.ijc.com/abstracts/*
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I found that all but one article had the abstract archived in the IA. Here's an example:

Internet Journal of Chemistry, **2003**, *6*, 2 [ISSN: 1099-8292].

Article 2

Helical Net Plots and Lipid Favourable Surface Mapping of Transmembrane Helices of Integral Membrane Proteins: Aids to Structure Determination of Integral Membrane Proteins

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Keywords: bacteriorhodopsin, molecular mechanics, lipids, lipophilicity

Publication date: April 23, 2003 17:25:00 GMT

Abstract:
Molecular mechanics calculations were used to determine the lipid favourable surfaces of transmembrane helices. The symmetric hydrophobic dodecane molecule was chosen as a lipophilic probe, since it has no polar groups, and only van der Waals interaction would be encountered. To evaluate the effectiveness of this approach the transmembrane helices of *bacteriorhodopsin* (BR) were chosen as the model system since both its helix - helix and lipid - helix interfaces have been structurally defined by crystallography. The ideal alpha-helix geometry of the TM helices of the BR, mimicking the transmembrane helices, were used to study the interaction with the lipophilic probe and hence to map the surface as a test case. The calculated lipid facing surfaces of three TM helices substantially agreed with lipid observed interacting surfaces of TM helices in the crystal structure. The two lipophilic surfaces were predicted for the other four TM helices. One surface for each of those helices was in excellent agreement with lipid facing surfaces determined by crystallography data. The other surface was poor prediction of the lipid facing surface, but the rest of the surface could be assigned as a helix - helix interfaces. These will be used the study of more complex helices and lipids in the same way. The results for the interaction of dodecane with BR were encouraging and it should provide a basis for obtaining extra information in determination of lipid favourable surfaces of helices of other integral membrane proteins with unknown three-dimensional structure.

This gave my a lot of information to add to Wikidata. Title, publication date, volume, article number, keywords, an absstract, and, of course, the list of authors. Some authors I know

personally, many I did not. But it did allow me to enter all articles to Wikidata along with the authors and “author” (P50) or “author name string” (P2093).

The article authors

It also turned out that multiple authors listed their IJC article on their public ORCID profile. That greatly helped identification. I managed to link many authors to mostly existing Wikidata items:

Authors Reload

Show 10 entries Search:

Count	Author	Orcid	Example work
8	Henry S. Rzepa	0000-0002-8635-8390	Chemstock: A Web-based Chemical Inventory system built from OpenSource Software Components
6	Peter Murray-Rust	0000-0003-3386-3972	CMLSnap: Animated Reaction Mechanisms
5	Georgios V. Gkoutos	0000-0002-2061-091X	A Mechanism for Creating Chemically Oriented Internet Search Channels
4	Francis Muguet		Coupling Between Molecular Orbital Shape Evolution and Inversion Vibration within the Hydronium Radical
4	Paul Kiprof	0000-0003-0097-5783	Theoretical Studies of Hypervalent Iodine Compounds
2	Steven Bachrach	0000-0002-7628-7947	Organoselenium Compounds: Comparisons of Computational Methods, Geometries and Electron Density Distribution
2	Razif Gabdoulline	0000-0001-8719-6234	Classification of auxin related compounds based on similarity of their interaction fields: Extension to a new set of compounds
2	Razif Gabdoulline	0000-0002-4780-1134	Classification of auxin related compounds based on similarity of their interaction fields: Extension to a new set of compounds
2	Luc Patiny	0000-0002-4943-2643	MolBank: First fully web-based publication of chemical reaction data of individual molecules with structure search a submission
2	Herbert H H Homeier	0000-0001-9517-8458	On Convergence Acceleration of Multipolar and Orthogonal Expansions

WDQS legacy-full-graph venue: authors.sparql

Showing 1 to 10 of 50 entries

Previous 1 2 3 4 5 Next

I already mentioned that I used Wikidata to collect this information. Besides the interactive visualization with Scholia, it also gave me the option to track my progress with SPARQL queries. For example, this query helped me do that author FAIR-ification:

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Wikidata Query Service | Examples | Help | More tools | Query Builder | English

```
PREFIX target: <http://www.wikidata.org/entity/Q27211732>

SELECT DISTINCT (MIN(?publication_date_) AS ?publication_date) ?vol ?issue ?work ?workLabel
  (GROUP_CONCAT(DISTINCT ?authorLabel_; separator=", ") AS ?authors)
  (GROUP_CONCAT(DISTINCT ?authorName_; separator=", ") AS ?authorNames)
WHERE {
  ?work wdt:P1433 target: .
  OPTIONAL { ?work wdt:P478 ?vol }
  OPTIONAL { ?work wdt:P433 ?issue }
  OPTIONAL {
    ?work wdt:P50 ?author_ .
    SERVICE wdsubgraph:wikidata_main {
      ?author_ rdfs:label ?authorLabel_ ; FILTER (lang(?authorLabel_) = "en")
    }
  }
  OPTIONAL { ?work wdt:P2093 ?authorName_ }
  OPTIONAL {
    ?work wdt:P577 ?publication_datetime .
    BIND(xsd:date(?publication_datetime) AS ?publication_date_)
  }
  SERVICE wikibase:label { bd:serviceParam wikibase:language "[AUTO_LANGUAGE],mul,en". }
} GROUP BY ?work ?workLabel ?wos ?abstract ?fulltext ?vol ?issue
  ORDER BY # ASC(?publication_date)
  ASC(?vol) ASC(xsd:integer(?issue))

```

Table | 107 results in 2254 ms | Code | Download | Link

publication_date	vol	issue	work	workLabel	authors	authorNames
1998-01-01	1	1	wd:Q99508579	Self-consistent Quantum Monte Carlo Simulations of the Structure in the Liquid and Liquid-Vapor Interfaces of Gallium and Aluminum	Stuart A. Rice	Meishan Zhao
1998-01-01	1	2	wd:Q135313949	Correlation Between Photochemical Activity and Excited State Electronic Structure of Aromatic Azides	Mikhail Budyka	T. S. Zyubina, M. M. Kantor
1998-01-01	1	3	wd:Q135315720	Organoselenium Compounds: Comparisons of Computational Methods, Geometries and Electron Density Distribution	Steven Bachrach	Sulin Jiang
1998-01-09	1	4	wd:Q135315721	New Evidences on photoemission electron impact ionization in time-of-flight mass spectrometer		Richang Lu, Jiling Bai, Haiyang Li, Li Wang
1998-01-13	1	5	wd:Q135315814	Dual Fluorescence: A Theoretical Study of the Electronic Excitations of (N,N)-bridged 4-Aminobenzonitriles		Rudolf Schamschule, Andreas B. J. Parusel, Gottfried Köhler
				Computational chemistry study of polymethylsiloxane structure		Vladimir D. Khavrytchenko, Andrey V.

You can see here two columns with author information, one for P50 and the other for P2093. There is quite some identification left to be done, and additional information is welcome:

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Table ▾ 107 results in 640 ms Code Download ▾ Link ▾

publication_date	vol	issue	work	workLabel	wos	abstract	fulltext
1998-01-01	1	1	wd:Q99508579	Self-consistent Quantum Monte Carlo Simulations of the Structure in the Liquid and Liquid-Vapor Interfaces of Gallium and Aluminum	000173141600001	<https://web.archive.org/web/20020109191947/http://www.ijc.com:80/abstracts/abstract1n1.html>	<https://www.researchgate.net/profile/Meishan_Zhao/publication/291346646_Self--consistent_Quantum_Monte_Carlo_Simulations_of_the_Structure_in_the_Liquid_and_Liquid--Vapor_Interfaces_of_Gallium_and_Aluminum/links/56a148bf08ae984c4498dc03/Self--consistent-Quantum-Monte-Carlo-Simulations-of-the-Structure-in-the-Liquid-and-Liquid--Vapor-Interfaces-of-Gallium-and-Aluminum.pdf>
1998-01-01	1	2	wd:Q135313949	Correlation Between Photochemical Activity and Excited State Electronic Structure of Aromatic Azides	000173141800001	<https://web.archive.org/web/20000925050026/http://www.ijc.com:80/abstracts/abstract1n2.html>	
1998-01-01	1	3	wd:Q135315720	Organoselenium Compounds: Comparisons of Computational Methods, Geometries and Electron Density Distribution	000173141900001	<https://web.archive.org/web/20000925050015/http://www.ijc.com:80/abstracts/abstract1n3.html>	
1998-01-09	1	4	wd:Q135	New Evidences on photoemission electron impact ionization in time-of-flight mass	000173142000001	<https://web.archive.org/web/20010306042753/http://ww	

Sources

So, that brings us to this list of sources:

- Internet Archive: abstracts and metadata
- ORCID profiles: ORCIDs of (some) authors
- Google Scholar: metadata and citations
- Web of Science: independent list for external validation

Because there is plenty of work left to be done and I hope the collected information will further spread in library collections, I added sources as much as possible. This query lists for all articles the Web of Science identifier (recorded so that everyone can check the consistency), the link to the Internet Archive-d abstract page, and a link to a known full text (five).

If you wonder, neither OpenAlex or Europe PMC have a full list.

What's next?

I do not have a formal training in archiving, but I am happy with the minimal viable metadata collection. I know more can be done (and love to hear your pointers and suggestions): more author identies, better coverage of keyword annotation, etc. But I think an important addition is adding citations to and from the IJC articles are important. The journal predates efforts like the I4OC and Open Citations, so I may have to manually recover citations from Google Scholar. I will have to report on that later. But you can enjoy the citations that are already there. And now that we have sufficient metadata, I can use this to find more full texts.

Btw, I have made contact with Prof. Steven Bachrach, who founded the journal and was the Editor-in-Chief.