

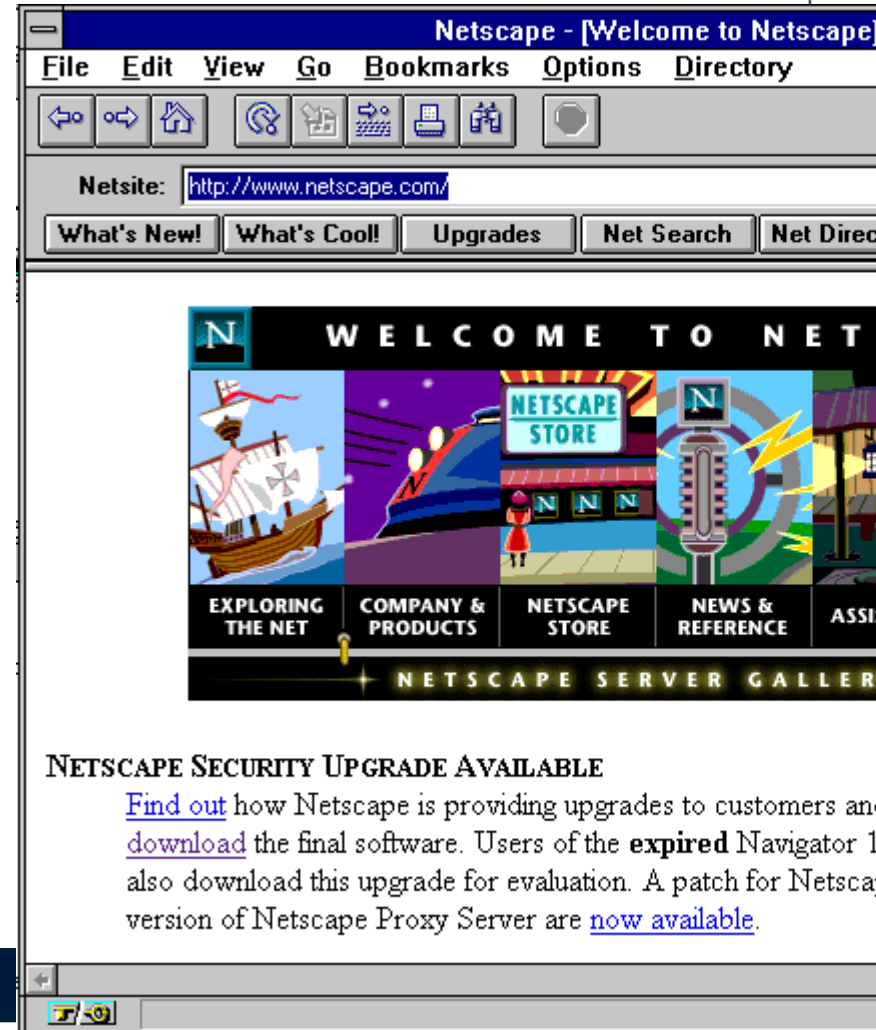
The Web - What is the Issue?

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21 Oct 2014, What's in a Name, Burlington House, London, UK

Web → `<html></html>`

- World Wide Web
 - *hyperlinked* web pages
- Web Browser
- Nowadays:
 - dynamically created
 - Interactive
- Is there an issue?



Data in HTML

doi:[10.1021/ja01193a005](https://doi.org/10.1021/ja01193a005).

Table I: Normal Paraffins

Cpd.	t_0	w_0	p_0	SMILES
n-Butane	-0.5	10	1	CCCC
n-Pentane	36.1	20	2	CCCCC
n-Hexane	68.7	35	3	CCCCCC
n-Heptane	98.4	56	4	CCCCCCC
n-Octane	125.7	84	5	CCCCCCCC
n-Nonane	150.8	120	6	CCCCCCCCC
n-Decane	174.0	165	7	CCCCCCCCCC
n-Undecane	195.8	220	8	CCCCCCCCCCC
n-Dodecane	216.2	286	9	CCCCCCCCCCCC

What is HTML?

- Aimed at human
 - “Hypertext”
 - later applets, flash, javascript, HTML5's canvas
- Terminology
 - title, paragraph, link, list, ...
- Visualization
 - bold, italic, ...
- CSS: separate content from looks

HTML draft version timeline [\[edit\]](#)

October 1991

HTML Tags, [\[5\]](#) an informal CERN document listing 18 HTML tags, was first mentioned in p

June 1992

First informal draft of the HTML DTD, [\[22\]](#) with seven [\[23\]](#)[\[24\]](#)[\[25\]](#) subsequent revisions (July 1!
August 18, November 17, November 19, November 20, November 22)

November 1992

HTML DTD 1.1 (the first with a version number, based on RCS revisions, which start with 1
than 1.0), an informal draft [\[25\]](#)

June 1993

Hypertext Markup Language [\[26\]](#) was published by the [IETF](#) IIR Working Group as an Interi
rough proposal for a standard). It was replaced by a second version [\[27\]](#) one month later, fol
further drafts published by IETF itself [\[28\]](#) that finally led to HTML 2.0 in RFC1866

November 1993

HTML+ was published by the IETF as an Internet-Draft and was a competing proposal to th
May 1994.

April 1995 (authored March 1995)

[\[20\]](#)

Where are the semantics?



Where are the semantics?



<p lang="nl">Mama, die, die, die...</p>

Solution #1: <head> + mime types

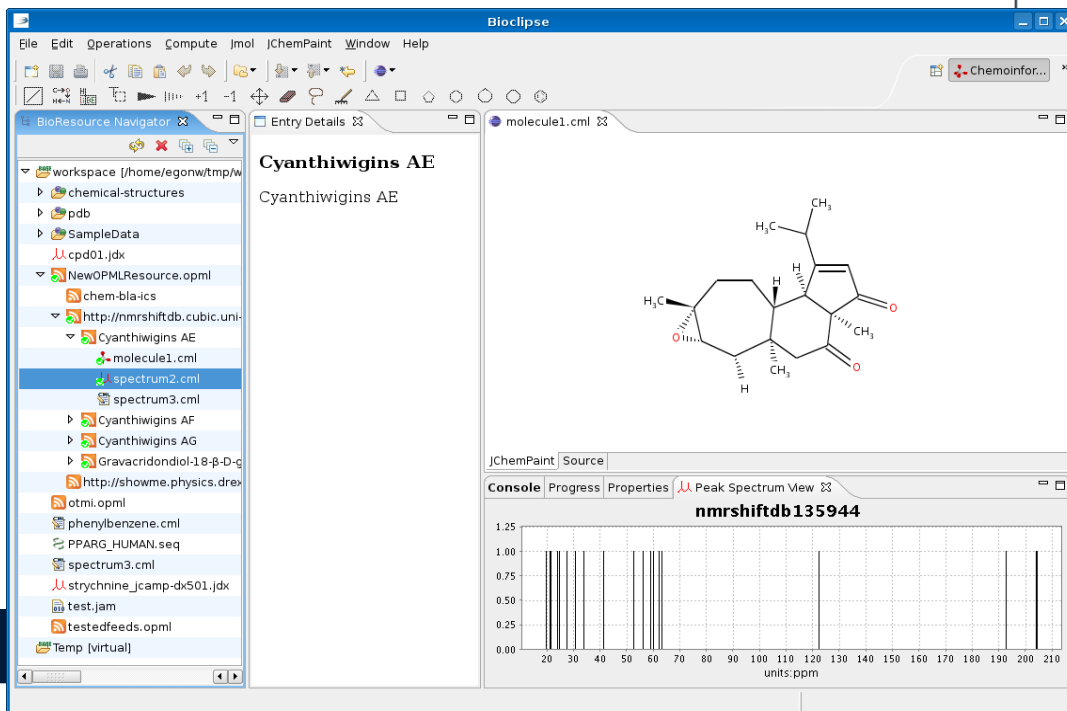
<head>

<link rel="alternate"

type="application/rss+xml" title="RSS"

href="http://some.website.org/rss/" />

</head>



Bioclipse

File Edit Operations Compute Jmol JChemPaint Window Help

Chemoinfor...

BioResource Navigator

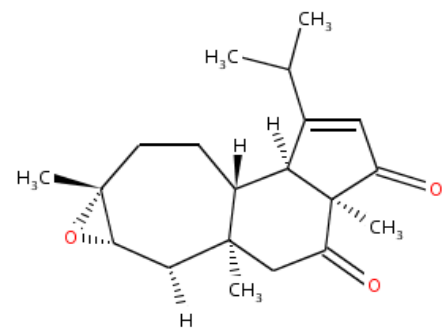
- workspace [/home/egonw/tmp/w
 - chemical-structures
 - pdb
 - SampleData
 - cpd01.jdx
 - NewOPMLResource.opml
 - chem-bla-ics
 - http://nmrshiftdb.cubic.uni-
 - Cyanthiwigins AE
 - molecule1.cml
 - spectrum2.cml
 - spectrum3.cml
 - Cyanthiwigins AF
 - Cyanthiwigins AG
 - Gravacridondiol-18-β-D-g
 - http://showme.physics.drex
 - otmi.opml
 - phenylbenzene.cml
 - PPARG_HUMAN.seq
 - spectrum3.cml
 - strychnine_jcamp-dx501.jdx
 - test.jam
 - testedfeeds.opml
 - Temp [virtual]

Entry Details

Cyanthiwigins AE

Cyanthiwigins AE

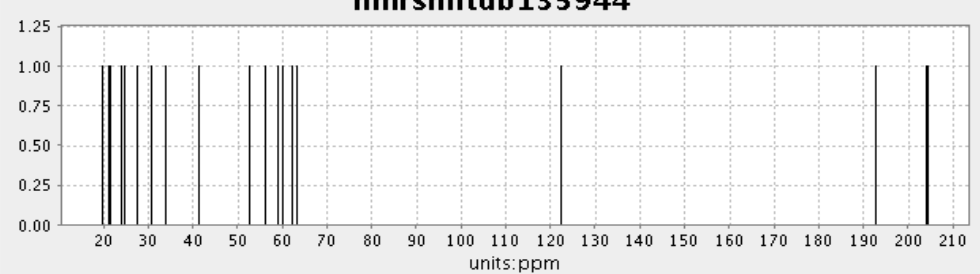
molecule1.cml



JChemPaint Source

Console Progress Properties Peak Spectrum View

nmrshiftdb135944



Murray-Rust, P., Rzepa, H.S., Williamson, M.J. & Willighagen, E.L. Chemical markup, XML, and the world wide web. 5. applications of chemical metadata in RSS aggregators. *J Chem Inf Comput Sci* 44, 462-469 (2004)

Solution #1: <head> + mime types

- <head>
 <link rel="meta" type="application/rdf+xml"
 href="meta.rdf"/>
 </head>
- Any format. Yes, also JSON.
- Any Chemical MIME type!
H. S. Rzepa, P. Murray-Rust and B. J. Whitaker, J. Chem. Inf. Comp. Sci., 1998, 38, 976-982.

Also JavaScript Object Notation (JSON)



Search ▾ Nanomaterials ▾ OpenTox ▾ Dem {

Substance > [NWKI-71060af4-1613-35cf-95ee-2a039be0388a](#) > Study

Show structures

Show composition

Substance search ?

External identifier ▾

Search

Study ? : [P-Chem](#)
[ENV](#) [ECO](#) [TOX](#)

Reliability ? : [1](#) [2](#) [3](#)
[4](#) [5](#) [6](#)

Study purpose ? :
[K](#) [S](#) [WoE](#) [D](#) [N/A](#)

JSON

IUC Substance Composition **P-Chem (1)**

Filter...

CuO

4.5 Particle size distribution (Granulometry) (1)

Test Material Form	Distribution type	Passage num.	Endpoint	Value
-	-	-	PARTICLE SIZE	= 76 nm

Showing 1 study(s) (1 to 1)

```

- study: [
  - {
    uuid: "NWKI-580091eb-bale-4500-...",
    owner: {
      - substance: {
        uuid: "NWKI-71060af4-1613-35cf-95ee-2a039be0388a",
      },
      - company: {
        uuid: "NWKI-9f4e86d0-c851-4100-8000-000000000000",
        name: "NanoWiki"
      }
    },
  },
  - citation: {
    title: null,
    year: "0",
    owner: null
  },
  - protocol: {
    topcategory: "P-CHEM",
    - category: {
      code: "PC_GRANULOMETRY_S",
      title: "4.5 Particle size distribution (Granulometry)"
    },
    endpoint: "PARTICLE SIZE",
    - guideline: [
      ""
    ]
  },
  - parameters: {
    DISTRIBUTION_TYPE: null,
    TESTMAT_FORM: null
  },
  - reliability: {

```

Solution #2: microformats

- for SMILES: `CCO`
- for CAS registry numbers: `50-00-0`
- for InChI: `InChI=1/CH4/h1H4`

1,4-naphthoquinone

InChI=1S/C10H6O2/c11-9-5-6-10(12)8-4-2-1-3-7(8)9/h1-6H-N

PubChem: [8530](#)
[\[RDF\]](#)

Posts

[Intentionally dirty fragments](#)



posted to [Practical Fragments](#) on Wed 13th Aug 14

Practical Fragments has tried to publicize the dangers of pan-assay interference assays. So what are we to make of a new paper in Curr. Opin. Microb

Solution #2: microformats

```
<html xmlns="http://www.w3.org/1999/xhtml"  
  xmlns:chem="http://www.blueobelisk.org/chemistryblogs/">
```

```
<head>  
  <title>m1</title>  
  <script type="text/javascript" src="sechemtic.js" />  
</head>
```

```
<body onload="addGoogleAndPubChemLinks(1,1)">  
  <h1>The Output</h1>  
  <p>This article is about <span class="chem:compound">m1</span>  
  (SMILES:<span class="chem:smiles">CCCO</span>).</p>
```

```
</body>
```

```
</html>
```

The Output

This article is about m1 [PubChem](#) (SMILES:CCCO [Google](#), [PubChem](#)).

Willighagen, E. et al. Userscripts for the life sciences. BMC Bioinformatics 8, 487+ (2007)

Solution #3: schema.org

schema.org

Documentation for health/medical types

Without Markup

Microdata

RDFa

JSON-LD

```
<div itemscope itemtype="http://schema.org/Drug">
  <h1>Drug Info: <span itemprop="name">PainAwayMax</span></h1>
  PainAwayMax is a brand of
  <span itemprop="alternateName">ibuprofen</span> manufactured by
  <span itemprop="manufacturer" itemscope itemtype="http://schema.org/Organization">
    <span itemprop="name">FooCorp</span>
  </span>.
  It is an
  <span itemprop="drugClass" itemscope itemtype="http://schema.org/DrugClass">
    <span itemprop="name">analgesic</span>
  </span> in the class of
```

Solution #4: HTML+RDFa

doi:[10.1021/ja01193a005](https://doi.org/10.1021/ja01193a005).

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n-Heptane	98.4	56	4	CCCCCCC
n-Octane	125.7	84	5	CCCCCCCC
n-Nonane	150.8	120	6	CCCCCCCCC
n-Decane	174.0	165	7	CCCCCCCCCC
n-Undecane	195.8	220	8	CCCCCCCCCCC
n-Dodecane	216.2	286	9	CCCCCCCCCCCC

Solution #4: HTML+RDFa

<h2>Table I: Normal Paraffins</h2>

```

<table>
  <tr>
    <td>Cpd.</td>
    <td>t<sub>0</sub></td>
    <td>w<sub>0</sub></td>
    <td>p<sub>0</sub></td>
    <td>SMILES</td>
  </tr>
  <tr typeof="cc:molecule" about="http://rdf.openmolecules.net/?InChI=1/C4H10/c1-3-4-2/h3-4H2,1-2H3">
    <td><span property="dc:title">n-Butane</span></td>
    <td><span property="cc:t0" datatype="xs:float">-0.5</span></td>
    <td><span property="cc:w0" datatype="xs:integer">10</span></td>
    <td><span property="cc:p0" datatype="xs:integer">1</span></td>
    <td><span property="chem:smiles">CCCC</span></td>
  </tr>
  <tr typeof="cc:molecule" about="http://rdf.openmolecules.net/?InChI=1/C5H12/c1-3-5-4-2/h3-5H2,1-2H3">
    <td><span property="dc:title">n-Pentane</span></td>
    <td><span property="cc:t0" datatype="xs:float">36.1</span></td>
    <td><span property="cc:w0" datatype="xs:integer">20</span></td>
  </tr>

```

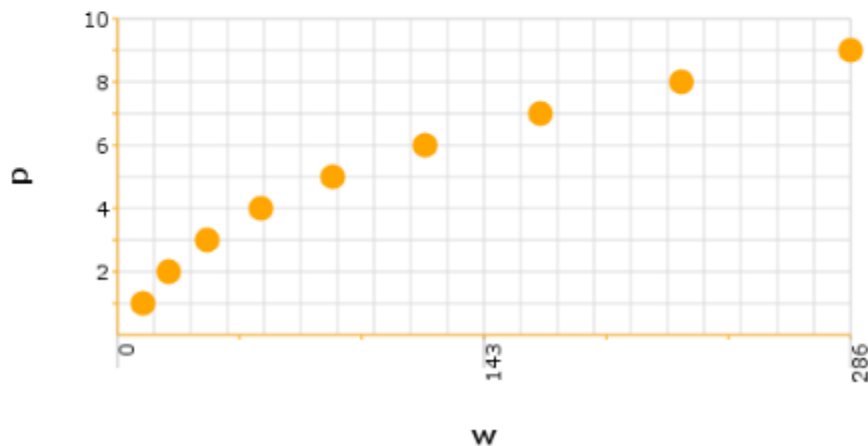


```

PREFIX cc: <http://github.com/egonw/cheminformatics.classics/1/#>
SELECT *
FROM
<http://www.w3.org/2007/08/pyRdfa/extract?
uri=http%3A%2F%2Fegonw.github.com%2Fcheminformatics.classics%2Fclassicl.html&format=pretty-xml&warnings=false&parser=lax&space-preserve=true>
(
  ?mol cc:w0 ?w ;
  cc:p0 ?p .
)

```

Plot Results



Orion Jankowski, *SPARQL to Chart*, 2010

<http://www.pharmash.com/posts/2010-09-27-sparql-to-chart.html>

Solution #5: Semantic MediaWiki


page
discussion
edit
history
delete
move
protect
watch
refresh






JRC2011 NM-401

Measurements

Material	
JRC2011 NM-401	
Label	NM-401
Source	JRC2011
Identifier	359
Chemical Composition	C

Properties	
Type	CarbonNanotube

Facts about JRC2011 NM-401 ⓘ
RDF feed 

- Has Chemical Composition C + 
- Has Identifier 359 + 
- Has Label NM-401 + 
- Has NM Type CarbonNanotube + 
- Has Source JRC2011 + 

Solution #6: RDF/XML + XSLT

OpenMolecules RDF

About <http://rdf.openmolecules.net/?InChI=1/CH4/h1H4>

Identifier <info:inchi/InChI=1/CH4/h1H4>

InChI <InChI=1/CH4/h1H4>

Source Chemical blogspace

Source ChEBI

Source DBPedia

owl:sameAs <http://dbpedia.org/resource/Methane>

Source ChemSpider

owl:sameAs <http://www.chemspider.com/Chemical-Structure.291.rdf#Compound>

foaf:homepage <http://www.chemspider.com/Chemical-Structure.291.html>

Source OpenTox

foaf:homepage <http://apps.ideaconsult.net:8080/ambit2/compound/738>

More about the Semantic Web

RDF technologies in chemistry

Edited by: Dr Martin Paul Braendle, Dr Egon Willighagen

Collection published: 13 May 2011

Last updated: 19 May 2011



The American Chemical Society (ACS) Division of Chemical Information (CINF) invited scientists from around the world to present their use of RDF technologies in chemistry on 22nd-23rd August 2010 at the 240th ACS National Meeting in Boston, USA. During three half-day sessions, the speakers demonstrated a mix of smaller and larger initiatives where Resource Description Framework (RDF) technologies are used in cheminformatics and bioinformatics as Open Standards for data exchange, common languages (ontologies), and problem solving. This Thematic Series introduces work presented at that meeting, showing the current advances in cheminformatics using these RDF technologies.

Article processing charges for this Thematic Series have been partially funded by Pfizer, Inc. Pfizer, Inc. has had no input into the content of the publication or the articles themselves. All articles in the series have been independently prepared by the authors and have been subject to the journal's standard peer review process.

Methodology **Open Access** **Highly accessed**

Chemical Entity Semantic Specification: Knowledge representation for efficient semantic cheminformatics and facile data integration

Leonid L Chepelev, Michel Dumontier

Journal of Cheminformatics 2011, **3**:20 (19 May 2011)

[Abstract](#) | [Full text](#) | [PDF](#) | [PubMed](#) | [Cited on BioMed Central](#) | [Graphical abstract](#)

Chemical Entity

The Web - What is the issue?

We're not using these innovative solutions enough.

Acknowledgments

- People whom I worked with on solutions
 - H. Rzepa, P. Murray-Rust, P. Maas, N. Jeliaskova, N. O'Boyle, R. Guha, C. Steinbeck, D. Wild, ...
- Projects that allow(ed) me to continue adoption of these methods
 - Open PHACTS (IMI-funded)
 - eNanoMapper (EC-funded)
- Wikipedia contributors (for images)