

## CHM 494: Chemical Literature Review

August 26, 2013

Prof. Jeremy Garritano

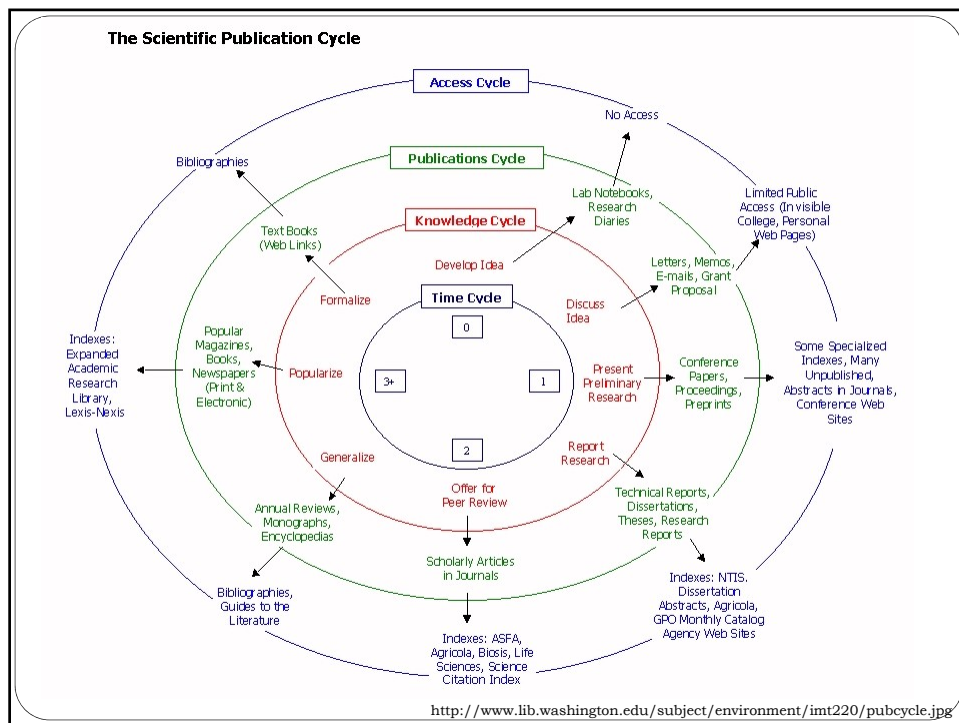
ph: 496-7279 email: [jgarrita@purdue.edu](mailto:jgarrita@purdue.edu)

<http://guides.lib.purdue.edu/chm494>

### Today...

- **Scientific Publication Cycle**
  - Scope/Purpose of Journals
  - Types of Articles
- **Review Articles**
- **Citation searching**
- **Patents**

# Scientific Publication Cycle



## Scope/Purpose of Journals

All of science



All of a discipline (chemistry)



Sub-discipline (organic, biochemistry)



Specialized area

*Nature*

*Science*

*PNAS*

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*Journal of the American Chemical Society*

*New Journal of Chemistry*

*Angewandte Chemie*

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*Journal of Organic Chemistry*

*Journal of Chemical Physics*

*Journal of Chemical Education*

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*European Journal of Mass Spectrometry*

*Photochemical and Photobiological Sciences*

*Heterocycles*

## Types of Articles

- **Original Articles/Papers** or **Research Articles/Papers**

- Original research conducted by the authors; "From the lab notebook to the page;"  
Usually first appearance of the results; Often peer-reviewed

- **Letters** or **Communications**

- Short (usually) and sweet articles that discuss important findings; Not as detailed as a research article; Published quickly; May be more theoretical

- **Reviews**

- Summarizes a particular topic over time – recent trends, advances in the field, evolving theories, etc.; Many articles are cited in support; No original research is communicated; Like a lengthy introduction or background section of an article

- **News**

- Discusses events in industry or academia; May mention specific articles; Very brief; May be written by non-scientists.

## Letters or Communications

- *Accounts of Chemical Research*
- *ChemComm (Chemical Communications)*
- *Inorganic Chemistry Communications*
- *Organic Letters*
- *Tetrahedron Letters*

## Reviews

- *Annual Review of Biochemistry*
- *Applied Spectroscopy Reviews*
- *Chemical Reviews*
- *ChemSocRev (Chemical Society Reviews)*
- *Critical Reviews in Analytical Chemistry*

## News (Trade Publications)

- *Chemical and Engineering News*
- *The Chemical Engineer*
- *Chemistry in Australia*
- *Chemistry World*
- *Chemistry and Industry*

## Review Articles

If you were not familiar with the topic, where would you start?

**Research** articles on “density functional theory”

- Time-dependent density functional theory study on electronic excited states of the hydrogen-bonded solute-solvent phenol-(H<sub>2</sub>O)(n) (n=3-5) clusters
- Density Functional Theory Modeling of the Proposed Nitrite Anhydrase Function of Hemoglobin in Hypoxia Sensing
- Density functional theory study of La<sub>2</sub>Ce<sub>2</sub>O<sub>7</sub>: Disordered fluorite versus pyrochlore structure
- Ti(N) Decoration of Single-Wall Carbon Nanotubes and Graphene by Density Functional Theory Computations

If you were not familiar with the topic, where would you start?

**Review** articles on “density functional theory”

- Density functional theory for predicting polymeric forces against surface fouling
- Calculation of Magnetic Circular Dichroism Spectra with Time-Dependent Density Functional Theory
- Recent Developments in Classical Density Functional Theory
- Dispersion interactions in density-functional theory
- Time-dependent density-functional theory for molecules and molecular solids

## Finding Background Information: Review Articles

- Provides another way to find articles (extensive bibliographies and additional keywords)
- Condenses unfamiliar (and familiar) topics into a more readable format
- Helps narrow down your topic by finding an area to focus your research
- Good place to start if you have not been given anything

## Finding Review Articles...

- Use “Refine” features in Web of Science or SciFinder after you put in your keywords or author.

The screenshot displays a Web of Science search results page. At the top, it shows 'Results: 74,585' and 'Page 1'. On the left, the 'Refine Results' sidebar is visible, containing two sections: 'Web of Science Categories' and 'Document Types'. The 'Document Types' section is highlighted with a red rectangle and includes the following options: ☐ ARTICLE (69,235), ☐ PROCEEDINGS PAPER (5,974), ☐ REVIEW (3,194), ☐ MEETING ABSTRACT (620), and ☐ LETTER (269). The main results area on the right lists three articles. Article 1 is titled 'Symmetry and surface symmetry' by Lee S. J. and Mekjian A. Z., published in PHYSICAL REVIEW C, Volume 82, with 2 citations. Article 2 is titled 'Half-metallic ferrimagnetism in the' by Bayar Eser, Kervan Nazmiye, and Kervan Nazmiye, published in JOURNAL OF MAGNETISM AND MATERIALS, December 2011, with 0 citations. Article 3 is titled 'Modulation effects of Cu doping on' by Li W. Q., Cao J. X., and Zhang J. H., published in JOURNAL OF MAGNETISM AND MATERIALS, December 2011, with 0 citations. Each article entry includes a 'FIND IT @ PURDUE LIBRARIES' button and a 'Full Text' or 'View abstract' link.

## SciFinder...before you search

REFERENCES: RESEARCH TOPIC ?

Examples:  
The effect of antibiotic residues on dairy products  
Photocyanation of aromatic compounds

**Search**

[Advanced Search](#) ☐ Always Show

---

Publication Years

Examples: 1995, 1995-1999, 1995-, -1995

Document Types

<input type="checkbox"/> Biography	<input type="checkbox"/> Historical
<input type="checkbox"/> Book	<input type="checkbox"/> Journal
<input type="checkbox"/> Clinical Trial	<input type="checkbox"/> Letter
<input type="checkbox"/> Commentary	<input type="checkbox"/> Patent
<input type="checkbox"/> Conference	<input type="checkbox"/> Preprint
<input type="checkbox"/> Dissertation	<input type="checkbox"/> Report
<input type="checkbox"/> Editorial	<input checked="" type="checkbox"/> Review

## SciFinder...after you search

Analyze **Refine** Categorize

Refine by: ?

- ☐ Research Topic
- ☐ Author
- ☐ Company Name
- ☒ Document Type
- ☐ Publication Year
- ☐ Language
- ☐ Database

Document Type(s)

- ☐ Biography
- ☐ Book
- ☐ Clinical Trial
- ☐ Commentary
- ☐ Conference
- ☐ Dissertation
- ☐ Editorial
- ☐ Historical
- ☐ Journal
- ☐ Letter
- ☐ Patent
- ☐ Preprint
- ☐ Report
- ☒ Review

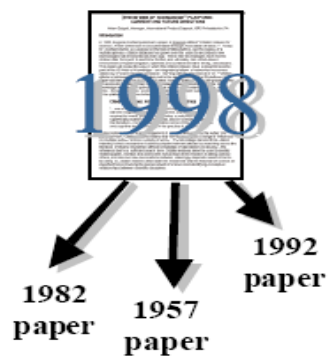
**Refine**



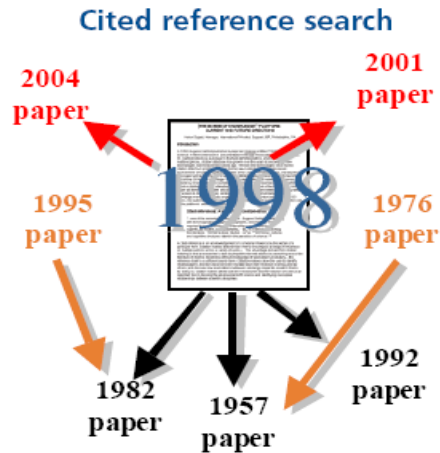
## Citation Searching

How do you *usually* use a bibliography or list of references?

**Traditional search**



## How does cited reference searching work?



## Citation indexing: A unique concept

- A way to track research concepts *forward* in time
- Identifies related topics and papers, regardless of “keyword” indexing
- Identifies other areas of research where a concept or theory is being applied or discussed

## Question

- What other problems or issues might you have if someone simply stated, “My article has been cited over 100 times”?









## Citation indexing: Problems

- Is someone citing it because it is good or bad?
- People can cite themselves (self-citation) or their boss—  
inflating the numbers
- Databases cannot cover all publications—not a “true” count.  
(Will see this in WoS and SciFinder.)
- Foreign authors may be cited more in foreign publications—  
missed citations

## Web of Science: Built for Citation Searching

<http://purl.lib.purdue.edu/db/db257>

## A full record in Web of Science...


   (0)   Save to:    more options

**Palladium-catalyzed alkynylation**

Author(s): Negishi, E (Negishi, E); Anastasia, L (Anastasia, L)

Source: CHEMICAL REVIEWS Volume: 103 Issue: 5 Pages: 1979-2017 DOI: 10.1021/cr020377i Published: MAY 2003

Times Cited: 487 (from Web of Science)

Cited References: 279 [ [view related records](#) ]  [Citation Map](#)

Document Type: Review

Language: English

**KeyWords Plus:** CROSS-COUPLING REACTION; CARBON BOND FORMATION; TRANSITION-METAL CATALYSIS; STEREODEFINED EXOCYCLIC ALKENES; ESPERAMICIN-CALICHEMICIN CLASS; STEREOSPECIFIC GROUP TRANSFER; HIGHLY SELECTIVE SYNTHESIS; ORGANO-ALUMINUM COMPOUNDS; ACETYLENIC TIN REAGENTS; ANION CAPTURE PROCESSES

Reprint Address: Negishi, E (reprint author), Purdue Univ, Herbert C Brown Labs Chem, W Lafayette, IN 47907 USA

**Addresses:**  
1. Purdue Univ, Herbert C Brown Labs Chem, W Lafayette, IN 47907 USA

**Publisher:** AMER CHEMICAL SOC, 1155 16TH ST, NW, WASHINGTON, DC 20036 USA

**Web of Science Category:** Chemistry, Multidisciplinary

**Subject Category:** Chemistry

IDS Number: 679KY

ISSN: 0009-2665

...Times Cited and References

# Can sort search results by times cited...

Web of Science<sup>SM</sup>

Results Author=(negishi e\*)  
Timespan=All Years, Databases=SCIEXPANDED, SSCL, ASHCL, CPCAS, CPCSSN  
Lemmatization=On

Results: 430

Sort by: Times Cited -- highest to lowest

Refine Results

Search within results for

Web of Science Categories

- ☐ CHEMISTRY ORGANIC (189)
- ☐ CHEMISTRY MULTIDISCIPLINARY (173)
- ☐ CHEMISTRY INORGANIC NUCLEAR (30)
- ☐ PHYSICS CONDENSED MATTER (19)
- ☐ PHARMACOLOGY PHARMACY (17)

Document Types

- ☐ ARTICLE (283)
- ☐ MEETING ABSTRACT (82)
- ☐ NOTE (38)
- ☐ LETTER (28)
- ☐ PROCEEDINGS PAPER (24)

Subject Areas

Authors

Group Authors

1. Title: PALLADIUM-CATALYZED OR NICKEL-CATALYZED CROSS COUPLING - A NEW SELECTIVE METHOD FOR CARBON-CARBON BOND FORMATION  
Author(s): NEGISHI E  
Source: ACCOUNTS OF CHEMICAL RESEARCH Volume: 15 Issue: 11 Pages: 340-348 DOI: 10.1021/ar00083a001 Published: 1982  
Times Cited: 734 (from Web of Science)  
[FIND IT @ PURDUE LIBRARY](#)
2. Title: METAL-PROMOTED CYCLIZATION. 11. REACTION OF ZIRCONOCENE DICHLORIDE WITH ALKYL LITHIUMS OR ALKYL GRIGNARD REAGENTS AS A CONVENIENT METHOD FOR GENERATING A ZIRCONOCENE EQUIVALENT AND ITS USE IN ZIRCONIUM-PROMOTED CYCLIZATION OF ALKENES, ALKYNES, DIENES, ENYNES, AND DIYNES  
Author(s): NEGISHI E; CEDERBAUM FE; TAKAHASHI T  
Source: TETRAHEDRON LETTERS Volume: 27 Issue: 25 Pages: 2829-2832 DOI: 10.1016/S0040-4039(00)84653-5 Published: 1986  
Times Cited: 530 (from Web of Science)  
[FIND IT @ PURDUE LIBRARY](#)
3. Title: SELECTIVE CARBON-CARBON BOND FORMATION VIA TRANSITION-METAL CATALYSIS. 3. HIGHLY SELECTIVE SYNTHESIS OF UNSYMMETRICAL BIARYLS AND DIARYLMETHANES BY NICKEL-CATALYZED OR PALLADIUM-CATALYZED REACTION OF ARYL DERIVATIVES AND BENZYLZINC DERIVATIVES WITH ARYL HALIDES  
Author(s): NEGISHI E; KING AD; OKUKADO N  
Source: JOURNAL OF ORGANIC CHEMISTRY Volume: 42 Issue: 10 Pages: 1821-1823 DOI: 10.1021/jo00430a041 Published: 1977  
Times Cited: 522 (from Web of Science)  
[FIND IT @ PURDUE LIBRARY](#)

# Narrowing or analyzing results...

Web of Science<sup>SM</sup>

Results Author=(negishi e\*)  
Timespan=All Years, Databases=SCIEXPANDED, SSCL, ASHCL, CPCAS, CPCSSN  
Lemmatization=On

Results: 430

Sort by: Times Cited -- highest to lowest

Refine Results

Search within results for

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[FIND IT @ PURDUE LIBRARY](#)
3. Title: SELECTIVE CARBON-CARBON BOND FORMATION VIA TRANSITION-METAL CATALYSIS. 3. HIGHLY SELECTIVE SYNTHESIS OF UNSYMMETRICAL BIARYLS AND DIARYLMETHANES BY NICKEL-CATALYZED OR PALLADIUM-CATALYZED REACTION OF ARYL DERIVATIVES AND BENZYLZINC DERIVATIVES WITH ARYL HALIDES  
Author(s): NEGISHI E; KING AD; OKUKADO N  
Source: JOURNAL OF ORGANIC CHEMISTRY Volume: 42 Issue: 10 Pages: 1821-1823 DOI: 10.1021/jo00430a041 Published: 1977  
Times Cited: 522 (from Web of Science)  
[FIND IT @ PURDUE LIBRARY](#)

...Analyze and Refine

## Analyze feature

- Make sure the records you have are within the limits chosen to be analyzed.

24 records. Topic=(antioxidant\* and chocolate)  
Analysis: Document Type=(REVIEW)

Rank the records by this field:	Analyze:	Set display options:	Sort by:
Author Conference Title Country/Territory Document Type	Up to 500 records	Show the top 10 results. Minimum record count (threshold): 2	<input checked="" type="radio"/> Record count <input type="radio"/> Selected field

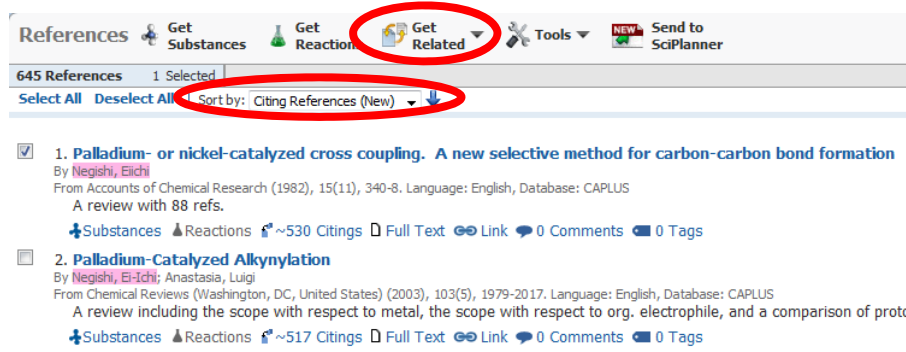
Analyze

## Citation searching on SciFinder Scholar

- Similar to WoS, but limited to citing articles published since January 1, 1997
- Note: Citation search results can vary widely for papers in “crossover” disciplines, so search in both databases for post-1996 articles!

## Citation Searching in SciFinder:

- To find who has cited an article since its publication, choose the article or articles you want, then choose “Get Related” → “Get Citing.”



## Cited vs. Citing

- **Get Cited** references = items in the article bibliography (older articles)
- **Get Citing** references = items that cite the article you are interested in (newer articles)

Note: The “Citing references” choice corresponds to the *WoS* “Cited Reference” search

## Analyzing Review Articles

- Can leave search results sorted by date (newest first) to find the latest review articles on your topic

**Or**

- Can sort by times cited to find the most influential review articles, regardless of date

Patents



## Why are patents important?

- Nearly 17% of the records in SciFinder are patents
- Most information in patents is not published elsewhere
- Patents must meet requirements for Novelty, Usefulness, and Non-obviousness
- Help avoid duplication in R&D
- Maintain current awareness
- Monitor competition
- etc.

## Why do we need to search patents?

- Often patents are the only documents for the R&D activities of a company
- If you are going to work in the chemical industry, your job may depend on your knowing about patents!

SciFinder Pubs.	Pfizer			3M		
	Patents	All	%	Patents	All	%
2010	74	1000	7	661	726	91
2011	61	960	6	597	647	92
2012	62	901	7	682	735	93

## What are some limits to patents?

- No experimental proof of prototypes or proof of chemicals actually tested or synthesized— “paper patents”
  - Many patents might be invalidated if challenged
- Classification system is difficult to navigate
- Titles can be very short and simple; not easily describing the invention
- In terms of chemical structures, patents may be too general (use of Markush groups)

## Patentability of an invention

- In order to be patentable, an invention must be:
  - **Novel:** The invention in its entirety must not have been known or used before
  - **Useful:** The invention must be fit for some desirable practical purpose.
  - **Non-obvious** in light of the prior art; not apparent to someone with “ordinary skill in the art”

## Is every invention/innovation published via patents?


- No, the other route is *trade secrets*.
- If not disclosed, they do not have the time limitations.
- So, if not disclosed, the information is not available!
- Can keep it secret indefinitely, but...
  - Depends on confidentiality
  - Can be reverse engineered

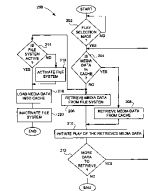
## Three Types of Patents

- **Utility** patents. For new and useful processes, machines, articles of manufacture, compositions of matter, or any useful improvements thereof. (xxxxxxx) (20 yrs) (*chemical patents usually are utility patents*)
- **Design** patents. For new, original, and ornamental design for an article of manufacture. Protects only the appearance, not structure or utilitarian features. (Dxxxxxx) (14 yrs) (*Examples: iPod case; Koosh ball design*)
- **Plant** patents. For invention, discovery or asexual reproduction of distinct and new varieties of plants. (PPxxxxx) (20 yrs)

# Example of a Utility Patent

- US Patent 6,934,812
- Title: Media player with instant play capability

	
(12) <b>United States Patent</b> Robbin et al.	
(10) <b>Patent No.:</b> <b>US 6,934,812 B1</b> (45) <b>Date of Patent:</b> <b>Aug. 23, 2005</b>	
(54) <b>MEDIA PLAYER WITH INSTANT PLAY CAPABILITY</b>	
(75) <b>Inventors:</b> Jeffrey L. Robbin, 1 in Altos, CA (US); Neil R. Hollman, Sunnyvale, CA (US); Steven Bollinger, San Jose, CA (US)	
(73) <b>Assignee:</b> Apple Computer, Inc., Cupertino, CA (US)	
(*) <b>Notice:</b> Subject to any disclaimer, the term of this patent is extended or adjusted under 35 U.S.C. (154) by 269 days.	
(21) <b>Appl. No.:</b> 09/182,217	
(22) <b>Filed:</b> Apr. 5, 2002	
<b>Related U.S. Application Data</b> (60) Provisional application No. 60/346,236, filed on Oct. 23, 2001.	
(51) <b>Int. Cl.</b> <b>G06F 13/10</b> (52) <b>U.S. Cl.</b> <b>711/108, 711/111, 711/112, 711/113, 711/119, 711/150</b> (56) <b>Field of Search</b> <b>711/112, 711/150, 711/108, 148, 149, 111-113, 704/590, 704/593, 710/52, 56</b>	
<b>References Cited</b> <b>U.S. PATENT DOCUMENTS</b> 5,698,938 A * 3/1997 Yamane et al. 360/335 5,697,796 A * 4/1997 Cho ..... 367/10 5,712,449 A * 4/1998 Kato et al. .... 386/96 5,784,412 A * 4/1998 Saitani ..... 364/233 5,822,286 A * 12/1998 Shindia ..... 360/4733 5,879,740 A * 2/1999 Quana et al. .... 365/501 6,032,175 B1 * 12/2001 Brandt et al. .... 711/112	
<b>FOREIGN PATENT DOCUMENTS</b> DE 43 44 773 A1 4/1994 DE 44 47 022 A1 6/1996 EP 1 028 425 A2 8/2000	
<b>OTHER PUBLICATIONS</b> Kennedy, "Digital Data Storage Using Video Disc," IBM Technical Disclosure Bulletin, vol. 24, No. 2, Jan. 1981. Newell, Aps, et al., "Non-Computer Remote MP3-Specker and USB-Archives," CT Magazine Ever Computer Technik, Verlag Hanser Hoes GmbH, Hannover DE, No. 25, Dec. 4, 2000. * cited by examiner Primary Examiner—T Nguyen (71) Attorney, Agent, or Firm—Reyer Weaver & Thomas, LLP	
<b>ABSTRACT</b> A media player and a method for operating a media player are disclosed. A media program is able to substantially immediately begin playing after a media player has been made. Through intelligent operations, the media program is able to start playing even before the media program has been substantially or completely loaded from disk storage into semiconductor memory (i.e., cache memory). Additionally, the media program can be loaded into semiconductor memory through use of a background process without disrupting the playing of the media program. Furthermore, if needed, the disk storage is able to be aggressively "powered off" when not being accessed, thereby enhancing battery life when in battery-powered mode.	
49 Claims, 6 Drawing Sheets	



# Example of a Design Patent

- US Patent D506,476
- Title: Media Device

U.S. Patent Jun. 21, 2005 Sheet 3 of 3 US D506,476 S



FIG. 4




FIG. 5



FIG. 6



FIG. 7

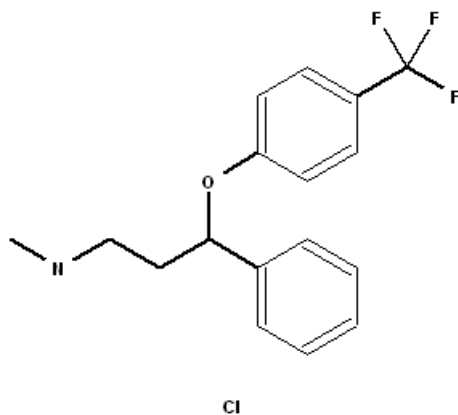
	
(12) <b>United States Design Patent</b> Andre et al.	
(10) <b>Patent No.:</b> <b>US D506,476 S</b> (45) <b>Date of Patent:</b> <b>Jun. 21, 2005</b>	
(54) <b>MEDIA DEVICE</b>	
(75) <b>Inventors:</b> Bartley K. Andre, Menlo Park, CA (US); Daniel J. Conter, San Francisco, CA (US); Dennis De La Torre, San Francisco, CA (US); Richard P. Hornum, San Francisco, CA (US); Jonathan P. Lee, San Francisco, CA (US); Steve John, Palo Alto, CA (US); Duncan Robert Kerr, San Francisco, CA (US); Mike McElroy, San Francisco, CA (US); Matthew Dean Reilich, San Francisco, CA (US); Douglas B. Sotger, Menlo Park, CA (US); Calvin Q. Seld, Palo Alto, CA (US); Christopher J. Terpago, Pacifica, CA (US); Eugene Anthony Whang, San Francisco, CA (US)	
(73) <b>Assignee:</b> Apple Computer, Inc., Cupertino, CA (US)	
(*) <b>Term:</b> 14 Years	
(21) <b>Appl. No.:</b> 28/212,343	
(22) <b>Filed:</b> Aug. 30, 2004	
<b>Related U.S. Application Data</b> (60) Continuation of application No. 29/196,632, filed on Jan. 5, 2004.	
(51) <b>Int. Cl.</b> <b>14/00</b> (52) <b>U.S. Cl.</b> <b>D04/096</b> (56) <b>Field of Search</b> <b>D14/00, 401, D14/435, 474, 498, 445, 177, D03/352, 333, 273, 149 B, 463, 43-47, 210/368, 1, 307, 308, 3, 302, 2, 24, 25, 210/342, 344</b>	
<b>References Cited</b> <b>U.S. PATENT DOCUMENTS</b> D364,069 S * 6/1992 McGarry 4,976,493 A * 4/1997 Madell et al. 5,192,082 A * 3/1993 Sano et al. .... B3/44	
<b>OTHER PUBLICATIONS</b> Andre et al., entitled "Media Device," U.S. Appl. No. 29/196,630, filed Apr. 28, 2003. * cited by examiner Primary Examiner—Prabhakar Deshmukh (71) Attorney, Agent, or Firm—Reyer Weaver & Thomas, LLP	
<b>CLAIM</b> We claim the ornamental design for a media device, substantially as shown and described.	
<b>DESCRIPTION</b> FIG. 1 is a perspective view of a media device in accordance with the present design. The media device can, for example, be a media player or a media storage device. FIG. 2 is a front view for the media device. FIG. 3 is a rear view for the media device. FIG. 4 is a top view for the media device. FIG. 5 is a bottom view for the media device. FIG. 6 is a right side view for the media device; and FIG. 7 is a left side view for the media device. The broken lines and/or dashed lines are for illustrative purposes only and form no part of the claimed design.	
1 Claim, 3 Drawing Sheets	



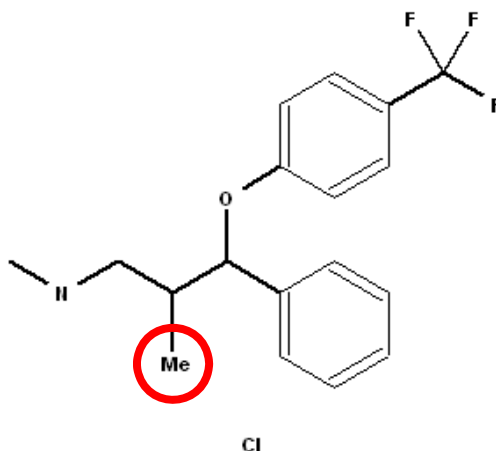
## Other features of chemical patents

- Markush groups
- Variable points of attachment

What if I patent the Prozac molecule?



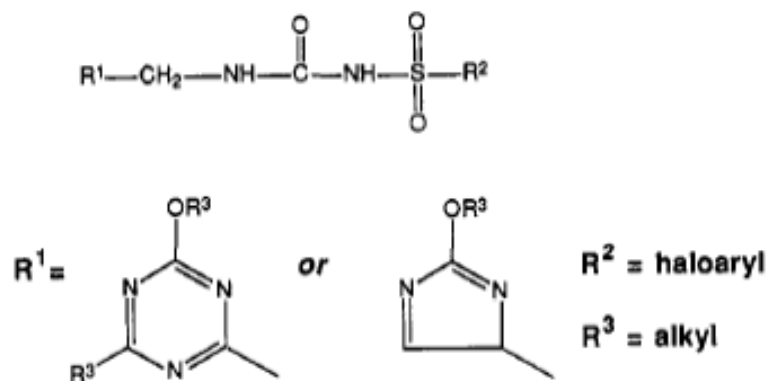
And then someone else finds the same pharmaceutical activity by simply adding another methyl group?



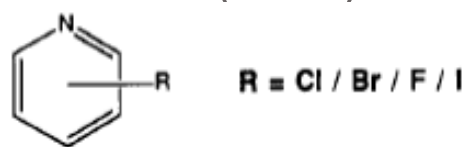
## Markush groups in chemical patents

The intent is to cover as many variations as possible in patented chemical structures by **(a)** designating one or more generic groups attached to the core molecular structure or by **(b)** designating variable points of attachment to the core (or both).

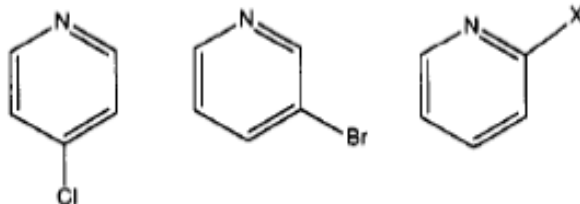
## Markush Groups in Patents



## Variable Points of Attachment (VPA)

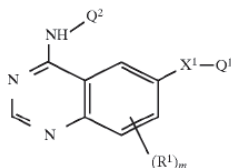


may retrieve



# Patent 5,866,572

The invention concerns quinazoline derivatives of the formula I



I

wherein  $X^1$  is a direct link or a group such as CO,  $C(R^2)_2$  and  $CH(OR^2)$ ;

wherein  $Q^1$  is phenyl, naphthyl or a 5- or 6-membered heteroaryl moiety and  $Q^1$  optionally bears up to 3 substituents;

wherein m is 1 or 2 and each  $R^1$  may be a group such as hydrogen, halogeno and trifluoromethyl; and

wherein  $Q^2$  may be phenyl or a 9- or 10-membered bicyclic heterocyclic moiety and  $Q^2$  optionally bears up to 3 substituents;

or a pharmaceutically-acceptable salt thereof;

processes for their preparation, pharmaceutical compositions containing them and the use of their receptor tyrosine kinase inhibitory properties in the treatment of proliferative disease such as cancer.

## Today...

- **Scientific Publication Cycle**

- Scope/Purpose of Journals
- Types of Articles

- **Importance of:**

- Review Articles
- Citation searching
- Patents



## Questions, help, problems?

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