

# Library Databases and Software

Grace Baysinger, [graceb@stanford.edu](mailto:graceb@stanford.edu)  
Swain Chemistry and Chemical Engineering Librarian

Stanford Mass Spectrometry Users Meeting 2014



# SciFinder<sup>®</sup>

- Most comprehensive database in chemistry
  - About 40% of the CAS content is biochemistry
  - SF also includes the Medline database
  - Covers 10,000 journals, plus conference proceedings, patents, books, theses, technical reports, major reference works
  - Updated daily
- Search interface includes “power tools”
  - Search by topic, substance, and reaction
  - Analyze – get statistical frequency summary of fields in search results
  - Refine –filter search results
  - Categorize – view detailed terms used in papers
  - Sort by most cited
  - Keep me posted alerts
- Individual registration and login required

# REAXYS®

## INSPIRING CHEMISTRY

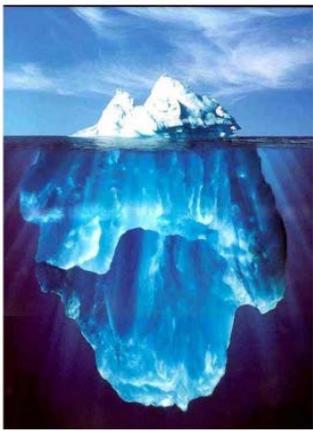


- Based on the Beilstein Handbook of Organic Chemistry, Gmelin Handbook of Inorganic and Organometallic Chemistry, and a Chemistry Patent database
  - Largest chemistry database of physical properties
  - In-depth chemical indexing for about 400 journals
  - Updated quarterly
- Search by substance, reaction, and topic
  - Tool to convert name to structure
  - Power tools to analyze and filter results
  - Compact display, PDF output
  - Alerts
- Personal login not required



- Covers the most important titles
  - Includes citation indexes for journals (1900-), conference proceedings (1990-), and books (2005-)
  - Also includes two chemistry databases
  - Indexes content “cover-to-cover”
  - Updated weekly
- Search interface includes
  - Search by subject, cited reference, or structure
  - Browse some indexes (author, organization, source title)
  - Filters for refining and analyzing search results
  - Sort by latest or most cited
  - Create graphical citation report
  - Set up alert
- Current Contents Connect contains articles before issues

- Most comprehensive citation database
  - Strongest coverage in Science, Engineering, and Medicine; also covers Social Sciences and humanities
  - Nearly 20,000 journals, conference proceedings, adding books
  - Includes “articles in press” for nearly 4,000 journals
  - Coverage began 1996- and includes some older content
  - Updated daily
- Search interface
  - Search, refine, analyze, sort, alerts
  - Results has look and feel of a spreadsheet
  - Links out to a patent database
  - Alerts



# xSearch

- Collaborative effort between Stanford University Libraries and Deep Web Technologies
  - Resources selected by bibliographers in libraries
  - Search up to 260 resources at one time
  - Includes databases, full-text ebooks and ejournals, data sets, funding, images, patents, streaming media
- Search interface
  - Select subject categories or document types
  - Can view results while search is still running
  - Retrieves up to 100 items per resource
  - Sort by relevance, date
  - Jump to a favorite resource
  - Filter by topic, author, publication, etc.
  - View topics graphically
  - Create a “custom engine” with your favorite databases
  - Set up alerts

# Sample Search Results - xSearch

Search: **Keyword: (VCP OR valosin-containing protein)**

[Create an alert from this search](#)

**AND (cancer\* OR tumor\*)**

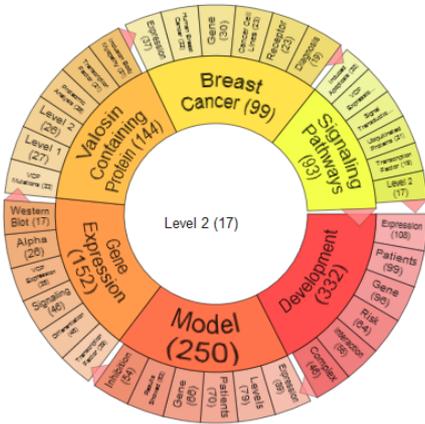
Search My Selections (0) [Icons] Search Builder Collection Status Logout

2,885 top results from at least 1,240,566 found.

137 of 137 sources complete

Topics Visual

All Results



All (2925) Archives (0) Data (181) Databases (1435) eBooks (102) eJournals (523) Funding (29)  
 Gov Docs (161) Images (62) Multimedia (0) News (102) Patents (14) Primary Sources (156) Reference (223)  
 Reports (1) Theses (159)

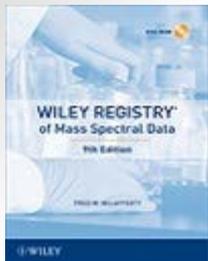
Results 1 - 10 of 2,925 Sort by: Rank Limit to: All Collections [Navigation icons] Refine Search

- 1** Novel antibody capable of recognizing modified valosine-containing protein VCP, useful for diagnosis, prognosis and determination of neurodegenerative disease and malignant tumor concerned with VCP expression

★★★★★  
 Derwent Innovations Index  
 Patent Number: WO2005058964-A1 Assignee: JAPAN SCI&TECHNOLOGY AGENCY Derwent Primary Accession Number: 2005506113  
 KAKIZUKA A; OHIZUMI H; HORI S; MAEDA R; NOGUCHI M; KOIKE M
- 2** Identification of potent VCP/p97/CDC48 inhibitors with distinct biochemical mechanisms including a reversible, allosteric inhibitor that activates the unfolded protein response, induce autophagy and cancer cell death

★★★★★  
 Environmental Sciences & Pollution Management  
 Magnaghi, Paola; D'Alessio, Roberto; Valsasina, Barbara; Avanzi, Nilla; Rizzi, Simona; Asa, Daniela; Gasparri, Fabio; Cozzi, Liviana; Cucchi, Ulisse; Orrenius, Cristian; Polucci, Paolo; Ballinari, Dario; Perrera, Claudia; Leone, Antonella; Cervi, Giovanni...  
 2012 American Association for Cancer Research Annual Meeting  
 2012-03-31
- 3** Structural basis for ovarian tumor domain-containing protein 1 (otu1) binding to p97/valosin-containing protein (vcp)

★★★★★  
 Engineering Village



# Wiley Registry of Mass Spectral Data

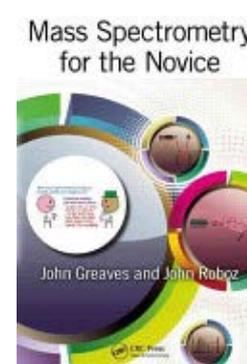
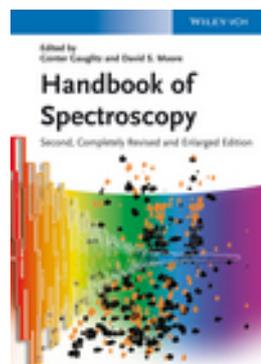
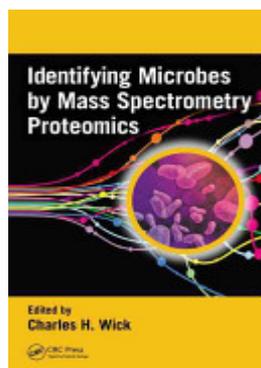
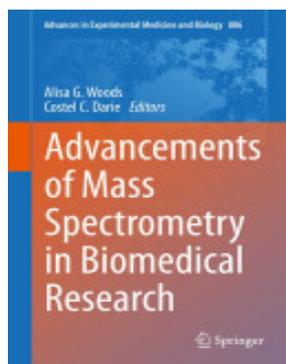
- This database contains three collections of MS data:
  - (1) Wiley Registry 9th – 670,000 classical EI spectra, 570,000 searchable structures
  - (2) NIST/EPA/NIH 2011 – 240,000 classical EI spectra, 210,000 searchable structures
  - (3) Wiley MS – 100,000 classical EI spectra, 100,000 searchable structures
- It is the largest mass spectral library that is commercially available. Coverage includes pharmaceuticals, illegal drugs, poisons, pesticides, steroids, natural products, chemical warfare agents, and environmental pollutants.
- Search by structure, name, and spectral peak. Can also upload and search by spectral diagram.

# Software and Mobile Apps

- Swain Library has site licenses for
  - ACD Labs/i-Lab (PC)
    - Spectrus Processor (1D and 2D NMR) & Physical Prop. Prediction
    - i-Lab – spectral, properties, and ADME Tox Predictions
  - ChemBioOffice Ultra
  - PyMOL
- MestreNova is under consideration (PC, Mac, Linux)
  - Includes spectral processing and prediction (1D and 2D NMR)
  - Also includes MS analysis tools
  - Your input wanted
- Mobile apps
  - Browzine for looking at journal table of contents
  - Falconer Biology and Swain Chemistry & Chemical Engineering Libraries have circulating iPads

# Books / eBooks

- Many recent books are only available online in the Stanford Libraries
- Use [SearchWorks](#) to look by author, title, and subject
- Use [xSearch](#) to do full-text searching
- Use publisher websites to use special search features
- Covers below are for some recently received ebooks



# Mass Spectrometry Guide

“One-stop shopping guide” to mass spec library resources:

**<http://library.stanford.edu/guides/mass-spectrometry>**

*Many thanks to Allis Chien  
for the invitation to speak at SUMS!*

Grace Baysinger  
graceb@stanford.edu