STANFORD UNIVERSITY LIBRARIES

Library Databases and Software

Grace Baysinger, graceb@stanford.edu
Swain Chemistry and Chemical Engineering Librarian

Stanford Mass Spectrometry Users Meeting 2014

SciFinder®

- 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

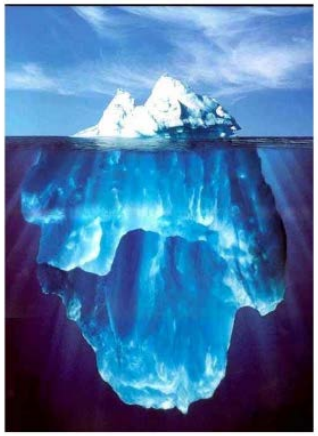
- Search interface includes
  - Search by subject, cited reference, or structure
  - Browse some indexes (author, organization, source title)
  - Filters for refining and analyzing search results
  - Sort by latest or most cited
  - Create graphical citation report
  - Set up alert

  - Current Contents Connect contains articles before issues

Scopus

- Most comprehensive citation database
  - Strongest coverage in Science, Engineering, and Medine; 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

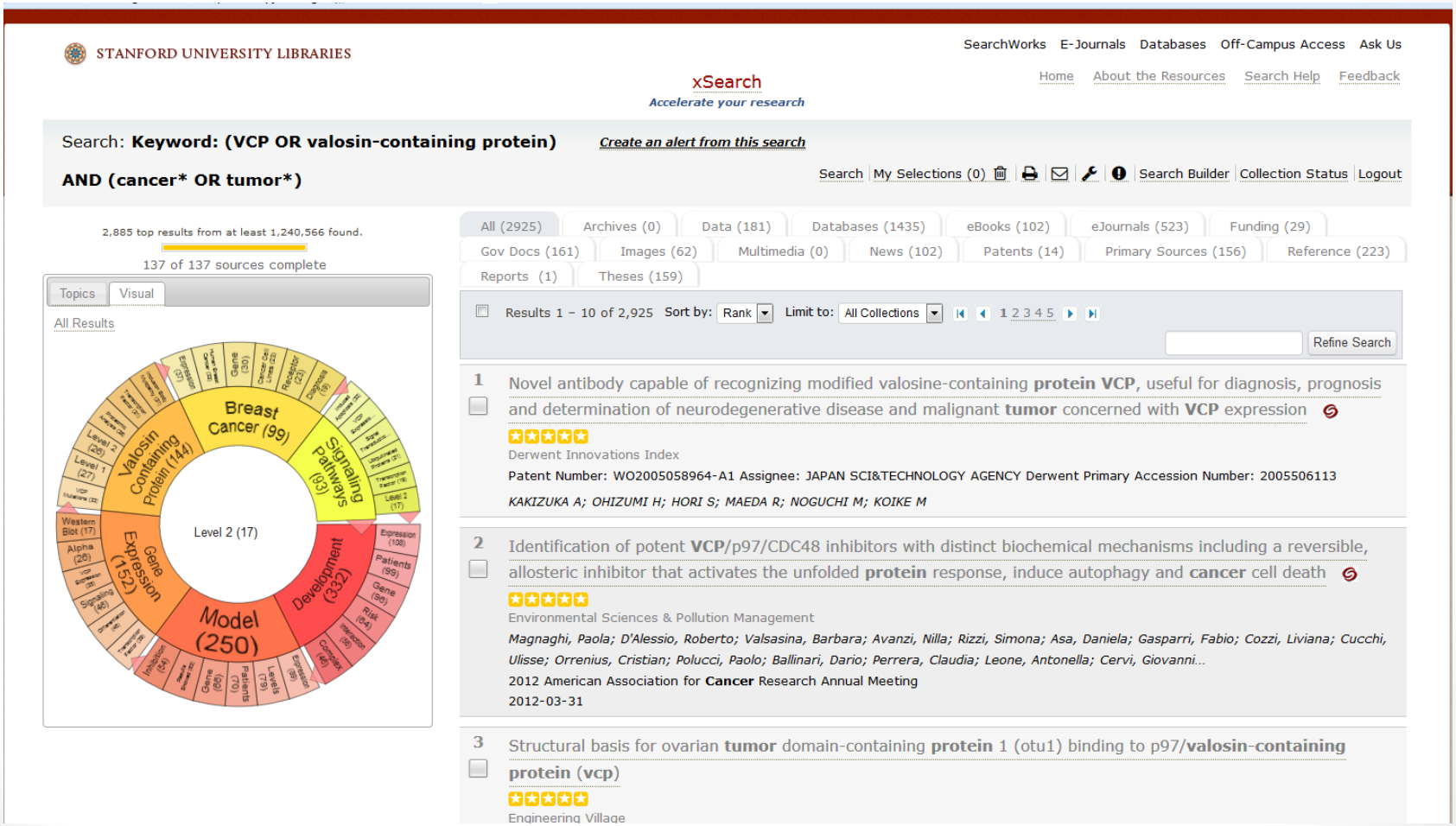


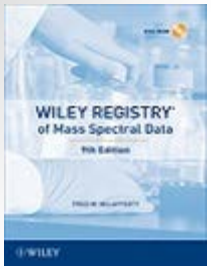
xSearch

- 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





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

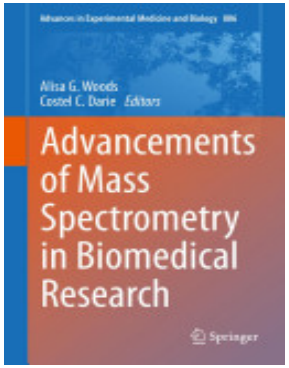
  - MestreNova is under consideration (PC, Mac, Linux)
    - Includes spectral processing and prediction (1D and 2D NMR)
    - Also includes MS analysis tools
    - Your input wanted

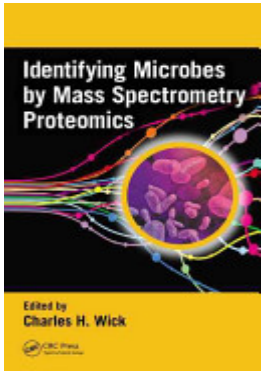
  - Mobile apps
    - Browzine for looking at journal table of contents
    - Falconer Biology and Swain Chemistry & Chemical Engineering Libraries have circulating iPads

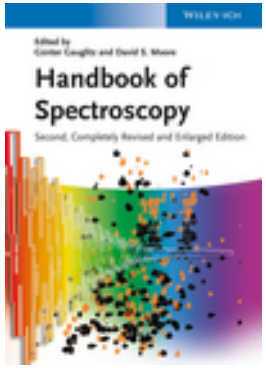
Books / eBooks

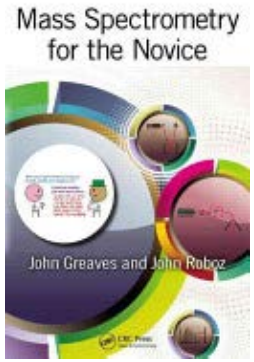
- Many recent books are only available online in the Stanford Libraries
- Use **SearchWorks** to look by author, title, and subject
- Use **xSearch** to do full-text searching
- Use publisher websites to use special search features

- 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

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Grace Baysinger

graceb@stanford.edu