

Consolidated data on commercially available compounds

Regular, frequent updates with obsolete compounds flagged

Contains reagents and screening compounds

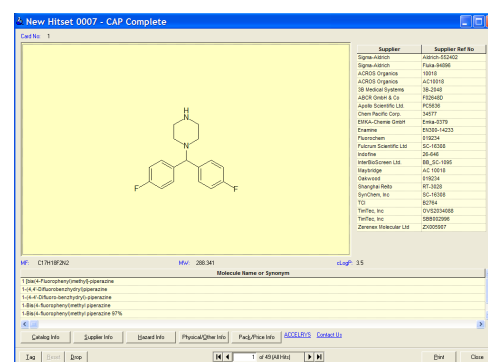
Available for various search systems

# Chemicals Available for Purchase (CAP)

Chemists engaged in activities such as chemical synthesis or screening need current information on available chemical compounds that might aid their research. Gleaning this information by searching through suppliers' catalogs is inconvenient and can be error-prone. This is especially true where some catalogs are paper-based, others are on CD, and the rest need importing to a database. The Chemicals Available for Purchase (CAP) database from Accelrys solves this problem by allowing you to electronically search the contents of multiple catalogs.

## Overview

Accelrys has consolidated the contents of many chemicals suppliers' catalogs into one easy to search relational database. Taking a compound-based approach, each chemical structure is linked to its suppliers and to the product information that they provide, such as physical properties, prices, and purity. It is now easy to find chemicals, identify their vendors, compare prices and availability, and create a report with a list of compounds of interest for easy ordering.



Example of hitset browsing using ADE.

The screenshot shows a window titled "New Hitset 0007 - CAP Complete: Supplier Information". It displays a table with columns for Supplier, Address, Phone, Fax, Internet, and eMail.

| Supplier       | Address   | Phone              | Fax                | Internet               | eMail                          |
|----------------|---|--------------------|--------------------|------------------------|--------------------------------|
| Sigma-Aldrich  | Sigma-Aldrich Company Ltd, Dorset, UK                               | +44 1202 733114    | +44 1202 715493    | www.sigmaaldrich.com   | YarFac.yarfac@sigmaaldrich.com |
| Sigma-Aldrich  | Sigma-Aldrich Corporation, Bangalore, India                         | +91 80 5112 7232   | +91 80 5112 7473   | www.sigmaaldrich.com   | YarFac.yarfac@sigmaaldrich.com |
| Sigma-Aldrich  | 12005, Sanku Lane, Houston, Texas, USA                              | 7 005 975 3201     | 7 005 975 4792     | www.sigmaaldrich.com   | YarFac.yarfac@sigmaaldrich.com |
| Sigma-Aldrich  | Sigma-Aldrich, China Inc, Shanghai, China                           | 86 21 6386 2768    | 86 21 6386 3966    | www.sigmaaldrich.com   | YarFac.yarfac@sigmaaldrich.com |
| Sigma-Aldrich  | Sigma-Aldrich Japan K.K., Tokyo, Japan                              | 81-3-6796-7300     | 81-3-6796-7300     | www.sigmaaldrich.co.jp | YarFac.yarfac@sigmaaldrich.com |
| Sigma-Aldrich  | Sigma-Aldrich Pty. Ltd, Sydney, Australia                           | 61 2 8941 8555     | 61 2 8941 8555     | www.sigmaaldrich.com   | YarFac.yarfac@sigmaaldrich.com |
| Sigma-Aldrich  | Sigma-Aldrich Corp, St. Louis, MO, USA                              | 314-771-9765       | 314-771-9757       | www.sigmaaldrich.com   | YarFac.yarfac@sigmaaldrich.com |
| Sigma-Aldrich  | Fluka Chemie GmbH, 22, D. 69126 Heidelberg, Germany                 | +49 6221 654 70 00 | +49 6221 654 70 02 | www.sigmaaldrich.com   | YarFac.yarfac@sigmaaldrich.com |
| Sigma-Aldrich  | Sigma-Aldrich Canada Ltd, Canada                                    | 905 629 9000       | 905 629 9232       | www.sigmaaldrich.com   | YarFac.yarfac@sigmaaldrich.com |
| Sigma-Aldrich  | Sigma-Aldrich Chemie GmbH, Munich, Germany                          | +49 89 8913 1100   | +49 89 8913 1100   | www.sigmaaldrich.com   | YarFac.yarfac@sigmaaldrich.com |
| ACROS Organics | Fluorochem Ltd, Buntingford Road, Loughborough, Leicestershire, UK  | +44 15 99 23 11 66 | +44 15 99 23 18 90 | www.fluorochem.co.uk   | YarFac.yarfac@sigmaaldrich.com |
| ACROS Organics | Fluorochem Ltd, 2000 Park Lane Drive, Binghampton, NY 14203, USA    | 1 800 768 7000     | 1 800 626 1166     | www.fluorochem.com     | YarFac.yarfac@sigmaaldrich.com |
| ACROS Organics | Acros Organics, Japanese Pharmaceutical SA, 2445, Belgium           | 00352 14 37 52 11  | 00352 96 655       | www.acros.be           | YarFac.yarfac@sigmaaldrich.com |
| ACROS Organics | Acros Organics USA, 100 American Road, Morris Plains, NJ 07950, USA | +1 800-768-7000    | +1 800-205-1100    | www.acros.com          | YarFac.yarfac@sigmaaldrich.com |

Comprehensive and up-to-date supplier records are provided for all chemical structures in the database

## Up-to-date information

As with any catalog, timely information is of essence. Accelrys provides regular quarterly updates. These updates aren't simply addendums that reintroduce the problem of multiple sources, they consolidate existing and updated data. Where a product has been discontinued from a catalog, it will be flagged as obsolete in the database, making it easy to formulate searches on the basis of availability.

## Versatile deployment

Accelrys CAP is available in a variety of formats, these include:

- Accord™ Database Explorer, using all the power of the Accord Chemistry Cartridge and Oracle® to give you fast, accurate, and easy access to vendor catalogs via a simple-to-use Windows® interface.
- RD files are versatile and allow the deployment of the CAP database in any chemical information management environment.

The Accord Database Explorer version of CAP utilizes Oracle Transportable Tablespace technology for installation, enabling you to rapidly plug-in and install quarterly CAP releases within a few hours for access by your end users.

Accelrys also offers a Catalyst® version of CAP that contains the associated 3D conformers of the sourced compounds. CAP is also used to generate a LUDI fragment database for *de novo* drug design.

System Requirements  
for CAP ADE:

Server - Oracle 10g,  
running on Windows,  
Linux and Solaris

Client- Windows 2000  
& XP

CAP ADE Utilizes  
Oracle Transportable  
Tablespace technology  
for rapid installation

## Finding the right compounds

CAP contains a large number of both reagents and compounds for screening. Apart from their use in commercial screening libraries, such compounds provide a pool of data on what is synthetically possible. To ensure that it is suitable for varied uses, CAP (ADE or Catalyst) has been designed to let you search only for reagents, only for screening compounds, or for all types of compound at once.

CAP (ADE or Catalyst) also allows you to perform a search based on any of a wide range of different parameters, or on a combination of these parameters. Most searches will be structure-based. Depending on your search system, such searches offer a range of exact, substructure, and similarity options. Additional parameters may include molecular formula, name, purity, quantity, price, supplier, and nature of the compound. Results are displayed in a grid that allows easy side-by-side comparison, giving you the option to quickly choose the best value for money option.

## A selected list of suppliers include:

- ABCR GmbH & Co
- ACB Blocks Ltd
- ACROS Organics
- Activate Scientific GmbH
- ACC Corporation
- Accurate
- Advanced Synthesis Group
- Adesis Inc
- Albany Molecular
- Alfa Aesar
- American Peptide
- AnaSpec Inc
- Apin Chemicals Ltd
- Apollo Scientific Ltd
- Argus Chemicals srl
- ASDI
- Asinex
- ASW MedChem
- Asta Tech
- Aurora Fine Chemicals Ltd.
- Bachem
- BetaPharma
- BioBlocks Inc
- Biosynth
- Biotage
- Boron Molecular
- Buttpark Ltd
- CB R&D Inc

- CDN Isotopes
- Cambrex
- Cambridge Isotope Labs
- Cayman Chemical
- Cerep
- Changzhou Huaren Chemical Co.
- Chem Pacific Corp.
- Chem-Impex
- ChemSampCo
- Chembridge
- Chemical Block Ltd
- Chemical Diversity
- Chemivate Ltd
- Combi-Blocks Inc
- CombiPhos
- Degussa
- Digital Specialty Chemicals
- EMC
- EMD Biosciences
- EMD Chemicals
- EMKA-Chemie GmbH
- Enamine
- Eurolabs
- Fisher
- Fluorochem
- Focus Synthesis LLC
- Frinton Labs
- Frontier Scientific
- Fulcrum Scientific
- Goss Scientific
- Gelest

- Hansa Fine Chemicals
- Honeywell
- Indofine
- InterBioScreen Ltd.
- Interchim
- J&W PharmLab, LLC
- JRD Fluorochemicals Ltd
- Kemprotec Ltd
- Key Organics
- LANXESS Deutschland GmbH
- Lancaster Inc
- Life Chemicals
- MDD Inc
- Matrix
- Maybridge
- Melford Laboratories Ltd
- Menai Organics Ltd
- Merck Biosciences
- 3B Medical Systems
- NeoMPS
- Oakwood
- Omegachem
- Organica
- Otava
- Peakdale
- Penn Specialty Chemicals
- PepTech Corp
- Pfaltz and Bauer
- Pharmcore
- Pharmeks
- Precursor Chemicals

- Promega
- ROMIL Ltd
- Rare Chemicals GmbH
- Rieke Metals, Inc
- Rintech Inc
- Ryscor Science
- SanXin ChemPharma
- Scott Medical Products
- Senn Chemicals AG
- Shanghai Reito
- Sigma-Aldrich
- Sinova
- Specs
- Strem Chemicals
- SynChem, Inc.
- SynQuest Labs
- Synchem OHG
- Synthonix Corp
- TCI
- TOSLab
- TimTec Inc
- Tocris
- Toronto Research Chemicals
- TransWorld Chemicals
- Tyger
- UkrOrgSynth
- VWR
- Vitas-M Laboratory
- Vivit Pharmatech
- Zerenex Molecular Ltd

4. New Hitset 0007 - CAP Complete: Hazard Information

| Card No. | Supplier       | Supplier Ref No | Hazard Type       | Hazard Value                  |
|----------|----------------|-----------------|-------------------|-------------------------------|
|          | Sigma-Aldrich  | Aldrich-A85131  | Hazard Codes      | Xi                            |
|          | Sigma-Aldrich  | Aldrich-255688  | Hazard Codes      | Xi                            |
|          | Lancaster Inc. | X19108          | Risk Statements   | R 36/37/38                    |
|          | Sigma-Aldrich  | Aldrich-A85131  | Risk Statements   | 20/21/22-36/37/38             |
|          | Sigma-Aldrich  | Aldrich-255688  | Risk Statements   | 20/21/22-36/37/38             |
|          | Lancaster Inc. | X19108          | Safety Statements | S 26-36                       |
|          | Sigma-Aldrich  | Aldrich-A85131  | Safety Statements | 26-37/39                      |
|          | Sigma-Aldrich  | Aldrich-255688  | Safety Statements | 26-36                         |
|          | Alfa Aesar     | L19108          | Caution           | 30                            |
|          | Lancaster Inc. | X19108          | Warnings          | H09/H41+H 411-SENSITIVE-LIGHT |
|          | Sigma-Aldrich  | Aldrich-A85131  | RETCES            | TN0002000                     |
|          | Sigma-Aldrich  | Aldrich-A85131  | WGK No            | 3                             |
|          | Sigma-Aldrich  | Aldrich-255688  | WGK No            | 3                             |

4. New Hitset 0007 - CAP Complete: Physical/Other Info

| Supplier       | Supplier Ref No | Density | Melting Pt       | Boiling Pt    | Refr Index | LogP | Flash Pt  |
|----------------|-----------------|---------|------------------|---------------|------------|------|-----------|
| Sigma-Aldrich  | Aldrich-255688  | 0.957   |                  | 172-175 (lit) | 1.426      |      | 145 F     |
| Sigma-Aldrich  | Aldrich-A85131  |         | 230 C (dec. lit) |               |            |      |           |
| ABCR GmbH & Co | L19108          |         | 172-175          |               |            |      | 103(217F) |
| Alfa Aesar     | L19108          | 0.96    |                  | 172-175       | 1.424      |      | 103(217F) |
| Lancaster Inc. | X19108          | 0.96    |                  | 172-175       | 1.424      |      | 103       |
| TCI            | A1192           | 0.96    |                  |               |            |      |           |

| Supplier         | Supplier Ref No | Type        | Value        |
|------------------|-----------------|-------------|--------------|
| Lancaster Inc.   | X19108          | Supplier No | 103354       |
| Maybridge        | AC 10483        | MDL No      | MF0200187307 |
| Alfa Aesar       | L19108          | MDL No      | MF0200099154 |
| Sigma-Aldrich    | Aldrich-A85131  | MDL No      | MF0200187307 |
| Sigma-Aldrich    | Aldrich-255688  | MDL No      | MF0200099154 |
| TCI              | A1192           | CAS Number  | 6903-85-4    |
| Pfaltz and Bauer | AS2478          | CAS Number  | 6903-85-4    |
| Maybridge        | AC 10483        | CAS Number  | 48675-60-3   |
| Lancaster Inc.   | X19108          | CAS Number  | 6903-85-4    |

Physical data, package, and price information, as well as hazard data for each compound, are easy to gather for each compound.