

# ACCELRYS AVAILABLE CHEMICALS DIRECTORY (ACD)

The **Accelrys Available Chemicals Directory** (Accelrys ACD) database is one of the largest structure-searchable collections of commercially available chemicals in the world, with pricing and supplier information for over 3.2 million unique chemicals, including 3D models, from nearly 830 suppliers worldwide.

## INDUSTRY-STANDARD REFERENCE

Accelrys ACD has been the standard chemicals directory in the biopharmaceutical and chemicals industries for over 20 years.

### With Accelrys ACD, scientists can:

- Identify and locate commercial sources
- Make side-by-side comparisons of purity, quantity and price
- Save valuable time by accessing information from a single source
- Readily compile lists of chemicals of interest
- Save, refine and export results lists for use with other Accelrys applications
- See commercial availability in context of reactions

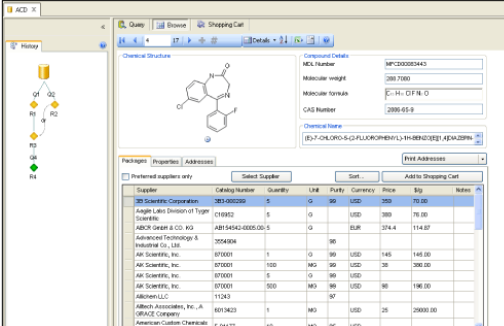
## COMPREHENSIVE AND UP-TO-DATE

Updated monthly, Accelrys ACD contains over 7.9 million structures representing over 15 million products and 42 million packages available for purchase, in bulk and research quantities from over 940 catalogs. New suppliers are continually added and we work closely with supplier partners to maintain the most current database possible, ensuring streamlined ordering and accurate catalog information.

### New: ACD includes eMolecules Catalog

Accelrys ACD now includes more than 580,000 in-stock building blocks from more than 200 trusted eMolecules suppliers. By adding eMolecules compounds and identifiers to Accelrys ACD, and with the Accelrys ACD identifiers included in the eMolecules catalog, scientists can now:

- Identify the optimal set of compounds for their synthesis or library, with confidence that those compounds will be available at the indicated prices from the selected suppliers
- Quickly, easily and confidently order their compounds from multiple suppliers using the eMolecules fulfillment service



The screenshot shows the Accelrys ACD interface. On the left is a 3D ball-and-stick model of a chemical structure. On the right, there are fields for 'Chemical Structure' (with a SMILES string: C1=CC=C(C=C1)N2C(=O)C(=O)N2), 'MEL Number' (MPC00002442), 'Molecular Weight' (289.3000), 'Molecular Formula' (C10H8F2N2O2), and 'CAS Number' (2895-65-8). Below this is a table with columns: Supplier, Catalog Number, Quantity, Unit, Purity, Currency, Price, Bq, and Notes. The table lists several suppliers and their respective product details.

Supplier	Catalog Number	Quantity	Unit	Purity	Currency	Price	Bq	Notes
Sciencelabs Corporation	289-000000	5	G	99	USD	250		
Angie Labs Division of Topp Scientific	1145852	5	G	100	USD	19.00		
ABC-Chem & CO. KG	AB154542-0000-000-5	5	G	100	EUR	324.4		114.07
Advanced Technology & Industrial Co., Ltd.	0004004			99				
AK Scientific, Inc.	070001	1	G	99	USD	145		145.00
AK Scientific, Inc.	070001	100	MG	99	USD	25		250.00
AK Scientific, Inc.	070001	5	G	99	USD			
AK Scientific, Inc.	070001	500	MG	99	USD	90		190.00
AdvancedLLC	11243			99				
AlfaTech Associates, Inc. A	6001423	1	MG	100	USD	25		20000.00
AlfaTech Company	11243			99				
Amesbury Chemical	F.24177	10	MG	99	USD			

**Figure 1:** Access Accelrys ACD from Accelrys Isentris to cherry-pick packages from chemical suppliers.

The screenshot displays the 'Search and Request Reagents' interface. At the top, there are tabs for 'Query', 'Results', and 'Shopping Cart'. Below the tabs, a search bar shows 'Search#1 (25+)' with a 'Total: 52500' and a 'Stop' button. A 'Domain(All)' dropdown and a 'Table View' button are also visible. The main area shows a grid of chemical structures with checkboxes, numbered 1 through 5. A detailed view of a reagent, '5-BROMO-N-VINYLBENZENE', is shown with its chemical structure and a table of supplier information.

Supplier Catalog	Catalog Number	Size	Price	Purity	\$/Gram	Action
3B Scientific Product List	263-234256	1000 G	USD 856	98%	0.856	Add to Cart
Abdohi One and Reagent List	020-405					Add to Cart
AAT Pharmaceutical Product List	A1-3108	1000 G	USD 785	97%	0.785	Add to Cart
AAT Pharmaceutical Product List	A1-3108	500 G	USD 510	97%	1.020	Add to Cart
AB Chem Inc. Product List	AB0241	1 KG	USD 765	97%	0.765	Add to Cart
ABCR Green Product List	AB131802-0100-00-GRM	100 G	EUR 113.00	98%	1.437	Add to Cart
ABCR Green Product List	AB131802-0025-00-GRM	25 G	EUR 38.40	98%	1.639	Add to Cart
ABCR Green Product List	AB131802-0005-00-GRM	5 G	EUR 14.90	98%	3.763	Add to Cart
Alma Organica	29400-0203	25 G	USD 258.68	98%	2.389	Add to Cart
Alfa Aesar Catalog	AC-15048	100 GRAMS	USD 100.00	97%	1.000	Add to Cart
AK Scientific Catalog	8087-MSA			98%		Add to Cart
Alkermes Chemical Co.	276216-1880	100 G	USD 153.58	97%	1.535	Add to Cart
Alkermes Chemical Co.	276216-230	25 G	USD 95.78	97%	2.229	Add to Cart
Alfa Aesar Catalog	821610-08	5 G	USD 11.18	98%	2.236	Add to Cart
Alfa Aesar Catalog	821610-14	25 G	USD 51.38	98%	2.052	Add to Cart
Alfa Aesar Catalog	821610-22	100 G	USD 144.00	98%	1.440	Add to Cart
American Custom Chemicals	HC0204587			98%		Add to Cart

Figure 2: Scientists can access reagents in ACD using both Accelrys Logistics and DiscoveryGate.

## FLEXIBLE WORKFLOW ACCESS

To help organizations integrate sourcing into multiple scientific workflows, Accelrys ACD is available via the Accelrys Isentris® informatics system (Fig. 1), the Accelrys Logistics reagent procurement and inventory tracking system (Fig. 2), the DiscoveryGate content platform at [www.discoverygate.com/dg3](http://www.discoverygate.com/dg3) (Fig. 2), and the DiscoveryGate Web Service.

## SAFETY DATA SHEETS

Accelrys ACD links to ChemADVISOR EH&S databases (available either in-house or hosted online), which contains over 20,000 Safety Data Sheets, providing comprehensive safety, hazard and regulatory information.

## ADDITIONAL FORMATS

The database can be delivered in various formats to suit specific needs:

- SDF file, containing only the 3D models (no catalog data)
- RDF file, for use with customer and third-party applications
- Relational Chemical Gateway (RCG) format for Accelrys ISIS applications
- Accelrys ACD Direct, relational Oracle® data cartridge

To learn more about Accelrys ACD, go to [accelrys.com/databases](http://accelrys.com/databases)