

# ACCELRYS ISENTRIS PHARMACOLOGY PACKAGE

**For Smarter Lead Generation:** Explore pharmacophores and lead compound structure-activity relationships, select scaffolds and R-groups for combinatorial libraries, compare ecotoxicology and biodegradation profiles, apply data about metabolic fate and toxic effects early in the discovery process, and monitor industry trends.

## ISENTRIS PROVIDES RICH FUNCTIONALITY TO ACCESS THE PHARMACOLOGY DATABASES:

- Drag-and-drop SAR table creation
- Rgroup decomposition for rapidly exploring the effects of substitution on the biological activity of a pharmacophore
- Citation hyper-linking to source literature information so scientists can obtain literature information without delay
- Customizable search, display, and report forms
- Metabolite explorer enabling researchers to explore known metabolite routes quickly
- Automatic links in metabolic pathways to toxicity data indicating toxic metabolic intermediates
- Support for integration of in-house and Accelrys databases so information can be searched as a single source
- Support for integration of content into existing scientific applications

**MDDR:** Bioactivity information for newly launched and developing drugs

**CMC:** Information on marketed and clinically studied drugs

Title	References
1-Poly(fluoroalkyl)benzodiazepines	Steinman, M. et al. <i>J Med Chem</i> 1973, 16(12): 1354. DOI: 10.1021/JM00270A008
Use of the selective benzodiazepine-1 (BZ-1) ligand [3H]-2-oxo-quazepam (SCH 15-725) to localize BZ-1 receptors in	Yezouff, J.P. et al. <i>Neurosci Lett</i> 1988, 88.
Several new benzodiazepines selectively interact with a benzodiazepine receptor subtype	Sieghart, W. <i>Neurosci Lett</i> 1983, 38(1): 73. DOI: 10.1016/0304-3940(83)90113-1
Time effects of food intake on the pharmacokinetics and pharmacodynamics of quazepam	Yasui-Furukori, N. et al. <i>Br J Clin Pharmacol</i> 2003, 55(4): 382. DOI: 10.1046/J.1365-2125.2003.01775.X
Benzodiazepine receptor binding of benzodiazepine hypnotics: Receptor and ligand specificity	Miller, L. G. et al. <i>Pharmacol Biochem Behav</i> 1992, 43(2): 413. DOI: 10.1016/0091-3057(92)90170-K
Effect of dietary fat content in meals on pharmacokinetics of quazepam	Yasui-Furukori, N. et al. <i>J Clin Pharmacol</i> 2002, 42(12): 1335. DOI: 10.1177/0891270002342012004

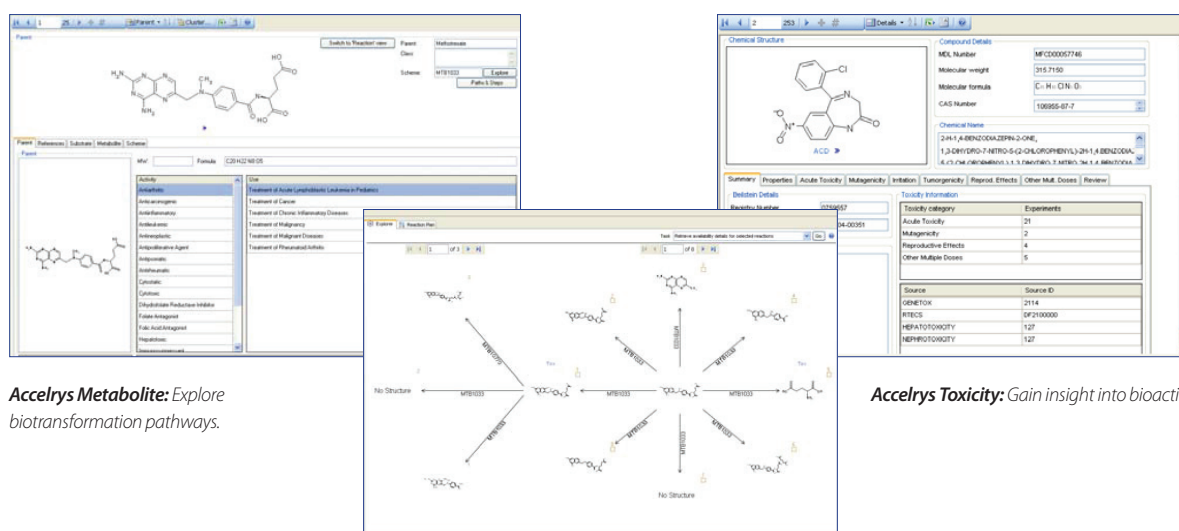
Drill down and link to citation information online

## INCLUDED DATABASES

**MDDR** provides current bioactivity findings for newly launched and developmental drugs including calculated properties based on chemical structures and 3D models. The database is produced by Accelrys and Thomson Reuters.

**National Cancer Institute Databases**, including CAS Registry (127,000 structures), Plated Compounds, AIDS, and Cancer databases, are offered as a public service to Accelrys customers.

**Accelrys Toxicity** is a structure-searchable bioactivity database of toxic chemical substances containing data from in vivo and in vitro studies of acute toxicity, mutagenicity, skin and eye irritation, tumorigenicity and carcinogenicity, reproductive effects, and multiple dose effects. Toxicity Database includes the complete contents of the Registry of Toxic Effects of Chemical Substances database, the GENE-TOX database (US Environmental Protection Agency), and the Chemical Carcinogenesis Research Information System database (National Cancer Institute).



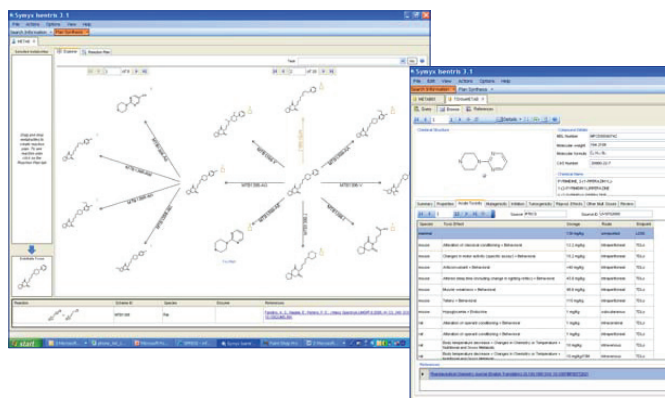
**Accelrys Metabolite:** Explore biotransformation pathways.

**Accelrys Toxicity:** Gain insight into bioactivity

**Accelrys Metabolite** is the world's most comprehensive collection of xenobiotic compounds and biotransformations (primarily medicinal drugs), which also indexes path and scheme information and experimental data from in vivo and in vitro studies compiled from primary literature, conference proceedings, and New Drug Applications. Accelrys Metabolite can be used in conjunction with Accelrys Toxicity.

**Accelrys Comprehensive Medicinal Chemistry (CMC)** offers information on marketed and clinically studied drugs including biochemical properties, drug class, measured logP and pKa, and searchable 3D models. CMC is derived from the Drug Compendium in Elsevier's Comprehensive Medicinal Chemistry.

To learn more about Isestris, go to [accelrys.com/isestris](http://accelrys.com/isestris)



Scientists can readily correlate biotransformations from Accelrys Metabolite Database with corresponding adverse effects in the Accelrys Toxicity Database.