

Comprehensive reaction and structure database

Reference source for exploring how to synthesize target molecules

Powered by the Accord Chemistry Cartridge

SPRESI for Accord Database Explorer

SPRESI* is a chemical and reaction database that acts as a comprehensive reference source to aid in the planning and synthesis of target molecules. It provides the information you need when exploring synthetic options, saving you the time and trouble of looking through the primary literature to meet your own research goals. The Accord Database Explorer (ADE) version of SPRESI lets you access the comprehensive SPRESI dataset via ADE's forms-based interface, which empowers you to customize queries and search the SPRESI dataset in conjunction with a range of other ADE-compatible databases.

SPRESI is a chemical structure and reaction database that provides you with direct access to over:

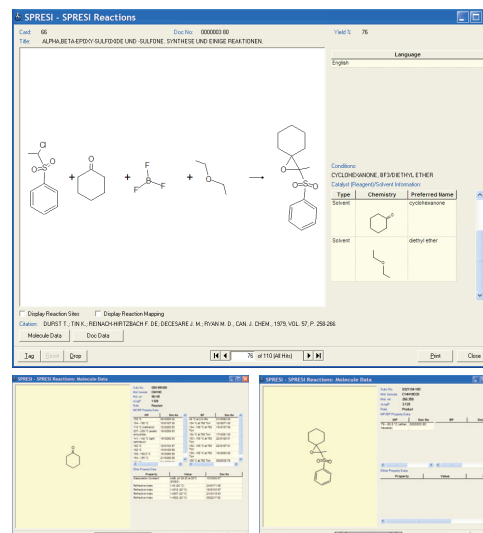
- 5 million structures
- 3.8 million reactions
- 28 million factual data entries extracted from 627,000 references and 164,000 patents

SPRESI consists of data gathered since 1974 and includes data extracted from over 565,000 patents, journals, books, and other sources.

Associated property data for structures includes boiling point, decomposition, density, dissociation, melting point, polymorphic transformation, refractive index, optical rotation, and sublimation.

Data for each reaction includes complete biographical data, short comments on experimental conditions, yield, boiling or melting points (where available) and references to spectroscopic data such as NMR, UV or IR (where available).

The All-Union Institute of Scientific and Technical Information of the Academy of Science of the USSR (VINITI) in Moscow, along with the Central Information Processing for Chemistry (ZIC) in Berlin, have abstracted this data from the world's chemical literature since 1974 to maintain this database.



Browsing a reaction record from SPRESI in ADE 3.0 (top). Drilling-down from within the selected reaction to individual product or reactant molecules enables you to find out additional property information such as melting point and boiling point (bottom).

Convenient, Forms-Based Searching

The Accord Database Explorer version of SPRESI provides you with access to the SPRESI dataset through Accord Database Explorer 3.0, a powerful, forms-based database client. ADE 3.0 provides you with a customizable, forms-based interface for browsing and querying data. Pre-built forms enable you to begin querying and browsing data immediately, or you can create forms that best suit your own way of working.

Using ADE, you can easily use target structures to search for molecules or reactions from SPRESI's comprehensive dataset, enabling you to explore synthetic methods and approaches of interest and helping you solve synthetic problems. Hitsets can be filtered by combining structural information with property criteria, such as yield or reaction conditions, to further narrow down your search and to obtain only the data that you need.

ADE 3.0's data federation capabilities enable you to extend the scope of the data that you can search. For instance, by combining searches in SPRESI and Accelrys' Chemicals Available for Purchase (CAP) database, you can locate specific reactants for experimental use and easily determine commercial sources from which the material can be ordered. Other databases, such as Accelrys Protecting Groups and Solid Phase Synthesis from the Accelrys Chemical Database range, can also be incorporated, giving you a one-stop reference resource to aid in synthetic planning and investigation.

Key Features:

- Comprehensive structure/ reaction database compiled by experts in the field
- Searchable by exact structure, substructure, free text and keywords
- Full reaction site mapping and display
- Powerful forms-based searching and browsing capabilities
- High speed installation process utilizing Oracle 10g Transportable Tablespace technology
- Powered by the Accord Chemistry Cartridge to ensure efficient and effective search capabilities and the highest quality chemistry representation
- Ideal companion to other Accord-format databases for federated querying via Accord Database Explorer 3.0

Case Number	Reaction	Reaction Conditions	Source	Citation	Citation	Index
16		NON METANOIL	DBREF 1, THE A. BRENCHAMPTON & CO. DECEMBER 1954 VOL. 10, P. 2000	DBREF 1, THE A. BRENCHAMPTON & CO. DECEMBER 1954 VOL. 10, P. 2000	DBREF 1, THE A. BRENCHAMPTON & CO. DECEMBER 1954 VOL. 10, P. 2000	<input type="checkbox"/> Page <input type="checkbox"/> Reaction <input type="checkbox"/> Structure
17		NON METANOIL	DBREF 1, THE A. BRENCHAMPTON & CO. DECEMBER 1954 VOL. 10, P. 2000	DBREF 1, THE A. BRENCHAMPTON & CO. DECEMBER 1954 VOL. 10, P. 2000	DBREF 1, THE A. BRENCHAMPTON & CO. DECEMBER 1954 VOL. 10, P. 2000	<input type="checkbox"/> Page <input type="checkbox"/> Reaction <input type="checkbox"/> Structure
18		NON METANOIL	DBREF 1, THE A. BRENCHAMPTON & CO. DECEMBER 1954 VOL. 10, P. 2000	DBREF 1, THE A. BRENCHAMPTON & CO. DECEMBER 1954 VOL. 10, P. 2000	DBREF 1, THE A. BRENCHAMPTON & CO. DECEMBER 1954 VOL. 10, P. 2000	<input type="checkbox"/> Page <input type="checkbox"/> Reaction <input type="checkbox"/> Structure
19		NON METANOIL	DBREF 1, THE A. BRENCHAMPTON & CO. DECEMBER 1954 VOL. 10, P. 2000	DBREF 1, THE A. BRENCHAMPTON & CO. DECEMBER 1954 VOL. 10, P. 2000	DBREF 1, THE A. BRENCHAMPTON & CO. DECEMBER 1954 VOL. 10, P. 2000	<input type="checkbox"/> Page <input type="checkbox"/> Reaction <input type="checkbox"/> Structure
20		NON METANOIL	DBREF 1, THE A. BRENCHAMPTON & CO. DECEMBER 1954 VOL. 10, P. 2000	DBREF 1, THE A. BRENCHAMPTON & CO. DECEMBER 1954 VOL. 10, P. 2000	DBREF 1, THE A. BRENCHAMPTON & CO. DECEMBER 1954 VOL. 10, P. 2000	<input type="checkbox"/> Page <input type="checkbox"/> Reaction <input type="checkbox"/> Structure

Customizable grid view enables you to manually assess and filter your hitset to pick out specific molecules or reactions of interest

Platform Requirements

SPRESI ADE version requires an Oracle 10g instance running on Microsoft Windows (2000, XP or 2003 Server), Red Hat Enterprise Linux (versions 3 and 4) and Solaris (9 and 10). The Accord Database Explorer 3.0 client is designed to run on Microsoft Windows 2000 and Windows XP.