



SPRESI^{web} is a chemical **STRUCTURE** and **REACTION** database that provides direct access to over:

- 6.0 million structures
- 3.8 million reactions
- 28 million factual data entries

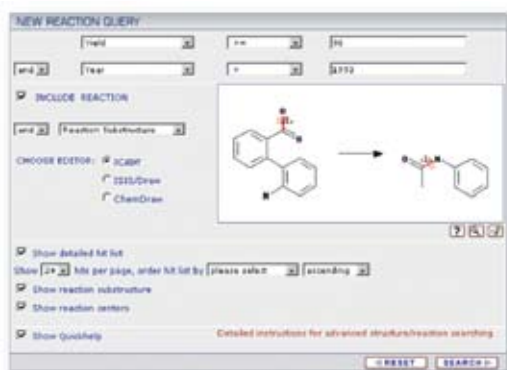
extracted from

- 627,000 references
- 164,000 patents.

SPRESI^{web} is the ideal web-based research tool:

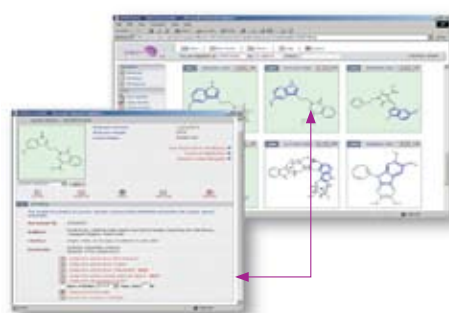
Scientists can search the database easily thanks to the user-friendly, highly intuitive web interface.

Synthesis of given target molecules can be planned interactively with the synthesis-planning tool "Synthesis Tree Search" (STS).



Structures

- Choose your favourite structure editor (ISIS/Draw, ChemDraw or our Java applet ICEDIT) to formulate your query.



- Perform exact and substructure search as well as parent, tautomer and isomer search.
- Retrieve property data (physical properties and keywords) as well as trivial/trade names and synonyms.
- See immediately if the compounds in your hit list are commercially available.
- Download your result lists as SDfiles.

Reactions

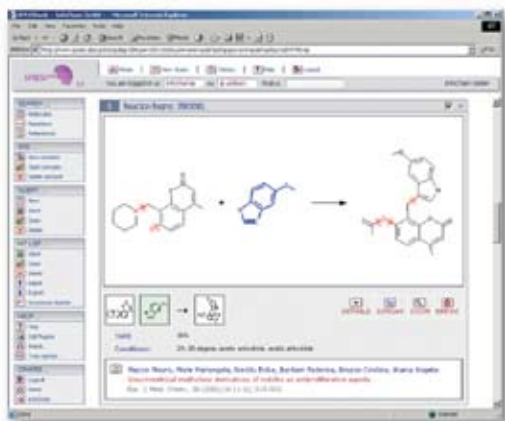
Discover new individual synthesis pathways with SPRESI^{web}.

- Define reactant and/or product to perform a reaction substructure search.
- Look for *similar reactions* having the same chemical transformation.
- Search for a particular reaction mechanism with the unique "name reactions" tool ICNameRXN.
- Retrieve reaction conditions (catalyst, temperature, solvent, etc.).
- See at a glance if the reactants or products of your hit list are commercially available.
- Download your hit list as an Rdf file.

References

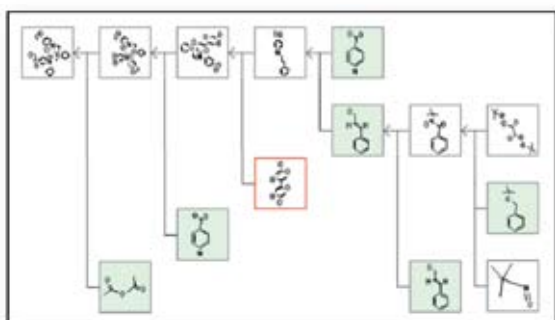
Access patent references and scientific literature published by the most relevant chemistry journals back to 1974.

File your literature references by downloading hit lists in BibTex and EndNote format.



STS

Choose the best synthesis pathway to your target molecule! With this highly interactive synthesis-planning tool you will be able to build an individual synthesis strategy based on millions of published reactions.



Access

Start your web browser; log in; and off you go!

- SSL (Secure Socket Layer) guarantees safe transactions.
- An intranet version is available for in-house installation.

Links

Thanks to the web-based architecture, SPRESI^{web} offers direct links to:

- catalogue data of several chemicals suppliers
- a full text article or abstract on the publisher's web site
- document delivery services
- direct view or purchase of patents
- cheminformatics services such as Chem-Navigator, ACD/Labs Online, Chemie.de.

Customer-specific solutions, such as linking to in-house databases or document delivery services, can also be provided.

History

In the 1970s the All-Union Institute of Scientific and Technical Information of the Academy of Sciences of the USSR (VINITI) in Moscow and the German Zentrale Informationsverarbeitung Chemie in Berlin (ZIC) began to build a chemistry database. This data collection was designed to include structures, chemical properties, physical properties, keywords, and factual data for the substances. Ever since, VINITI has provided regular updates. Since 2002 the research application SPRESI^{web} has enabled access to this database.

System Requirements

Browsers supported in this version are Internet Explorer 5.5 (SP2) or higher, Firefox 1.0 and higher, Netscape Navigator 7.1, 7.2. JavaScript must be enabled.