SPRESIweb Online reaction database at the Chemical Database Service

What is SPRESIweb?

SPRESIweb is the online interface to the SPRESI structure and reaction database of:

- 5.62 million compounds
- 4.34 million reactions

Search for molecules and reactions

Searchable parameters include:

Chemical structure	Catalyst
Bibliographic information	Solvent
Reaction conditions / name	Yield
Reaction similarity	Physicochemical property

2 Reaction Regno: 1788479

Reaction Data
All-In-One Reaction: Similar Reaction
Yield: 56%
Conditions: methanal, Na[BH3(CN)]

Reference
HIEBERT, CHARLES K.;SILVERMAN, RICHARD B.:
»1-METHYL-4-PHENYL-1,2,3,6-TETRAHYDROPYRIDINE ANALOGUES. INACTIVATION OF MONOAMINE OXIDASE BY CONFORMATIONALLY RIGID ANALOGUES OF N,N-DIMETHYLCINNAMYLAMINE
J. MED. CHEM., 31,(1988) N 8, 1566
📄 View abstract/full paper on publisher's page

Access SPRESIweb via the
Chemical Database Service
at spresi.cds.rsc.org   email: cds@rsc.org

SPRESIweb   Online reaction database

Where is the data from?

The data accessible via SPRESIweb has been collected by the All-Union Institute of Scientific and Technical Information of the Academy of Sciences in the USSR (VINITI) and the German Zentrale Informationsverarbeitung Chemie in Berlin (ZIC) since 1974.

Synthesis Tree Search

The Synthesis Tree Search allows the retrieval of reaction trees for a given target molecule, and can be used in two directions:

- all published synthesis **reactions leading to the target**

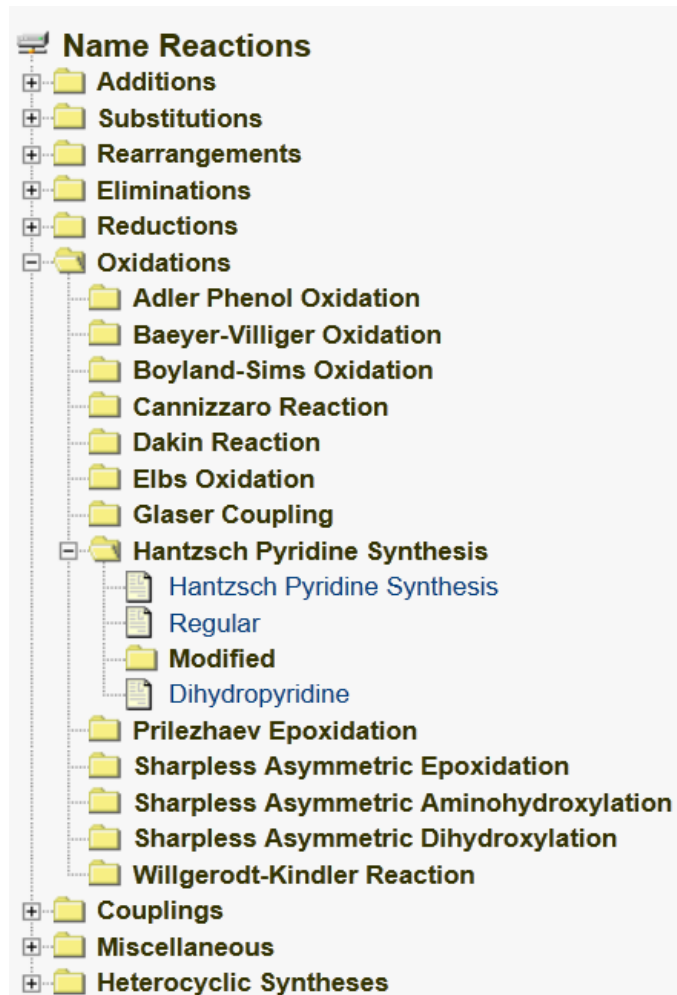- all published reactions **starting from the target**

Named Reactions

SPRESIweb has over **>600 named reaction classes** that allow the user to browse and search real-life, experimental examples of classic literature reactions.

How do I access SPRESIweb?

SPRESIweb is provided to the UK academic community via the **Royal Society of Chemistry-hosted Chemical Database Service** at **cds.rsc.org**. SPRESIweb has been developed by InfoChem GmbH. The Chemical Database Service is funded by the EPSRC.

Access is authenticated by UK academic IP address via **spresi.cds.rsc.org**. If working off-campus, a Chemical Database Service username and password will be issued.

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🖳 Name Reactions
  ⊞ 📁 Additions
  ⊞ 📁 Substitutions
  ⊞ 📁 Rearrangements
  ⊞ 📁 Eliminations
  ⊞ 📁 Reductions
  ⊟ 📂 Oxidations
        📁 Adler Phenol Oxidation
        📁 Baeyer-Villiger Oxidation
        📁 Boyland-Sims Oxidation
        📁 Cannizzaro Reaction
        📁 Dakin Reaction
        📁 Elbs Oxidation
        📁 Glaser Coupling
     ⊟ 📂 Hantzsch Pyridine Synthesis
           📄 Hantzsch Pyridine Synthesis
           📄 Regular
           📁 Modified
           📄 Dihydropyridine
        📁 Prilezhaev Epoxidation
        📁 Sharpless Asymmetric Epoxidation
        📁 Sharpless Asymmetric Aminohydroxylation
        📁 Sharpless Asymmetric Dihydroxylation
        📁 Willgerodt-Kindler Reaction
  ⊞ 📁 Couplings
  ⊞ 📁 Miscellaneous
  ⊞ 📁 Heterocyclic Syntheses
```

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