

The SOR Database on WebLibrarian

1 July 2009

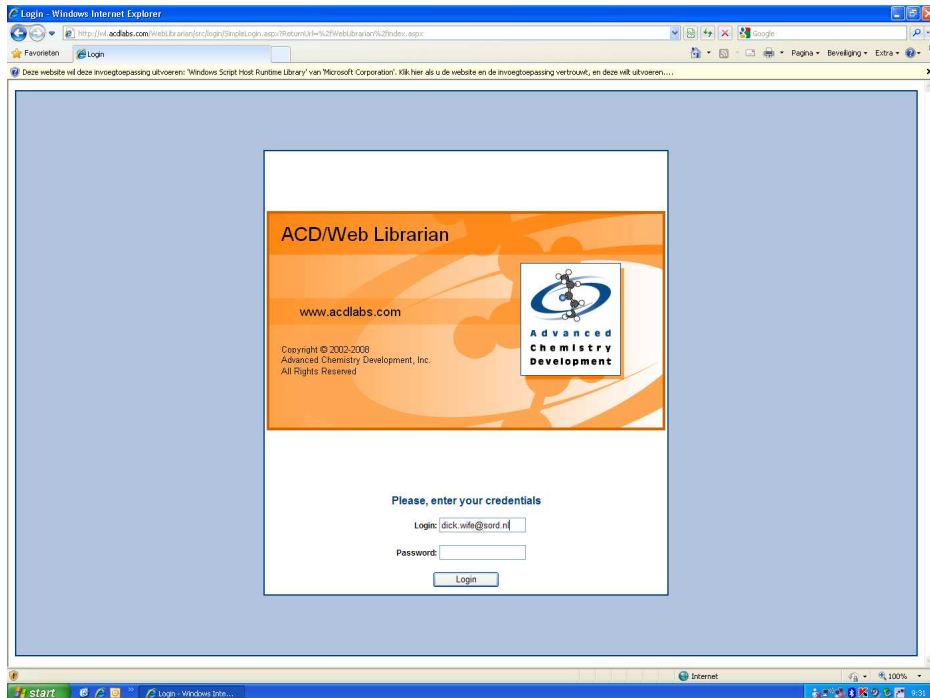
SORD is collaborating with Advanced Chemistry Development Inc. (ACD/Labs) to provide chemists with access to useful chemical reaction data. Much of the chemistry contained in the SOR Database is unpublished ("Lost Chemistry") and all of the entries are in machine-readable format.

The first SOR Databases are now accessible using WebLibrarian. You will need Internet Explorer 6.0 or higher (http://www.acdlabs.com/products/glob_sol_lab/web_librarian/).

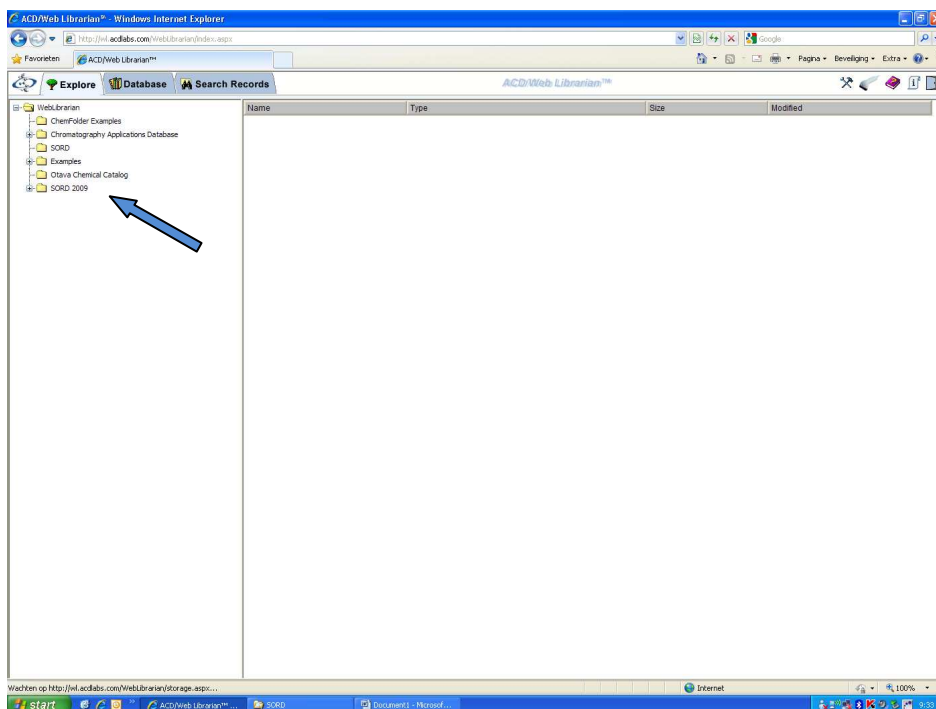
To see the databases available on WebLibrarian, use this link:

<http://wl.acdlabs.com/WebLibrarian/>

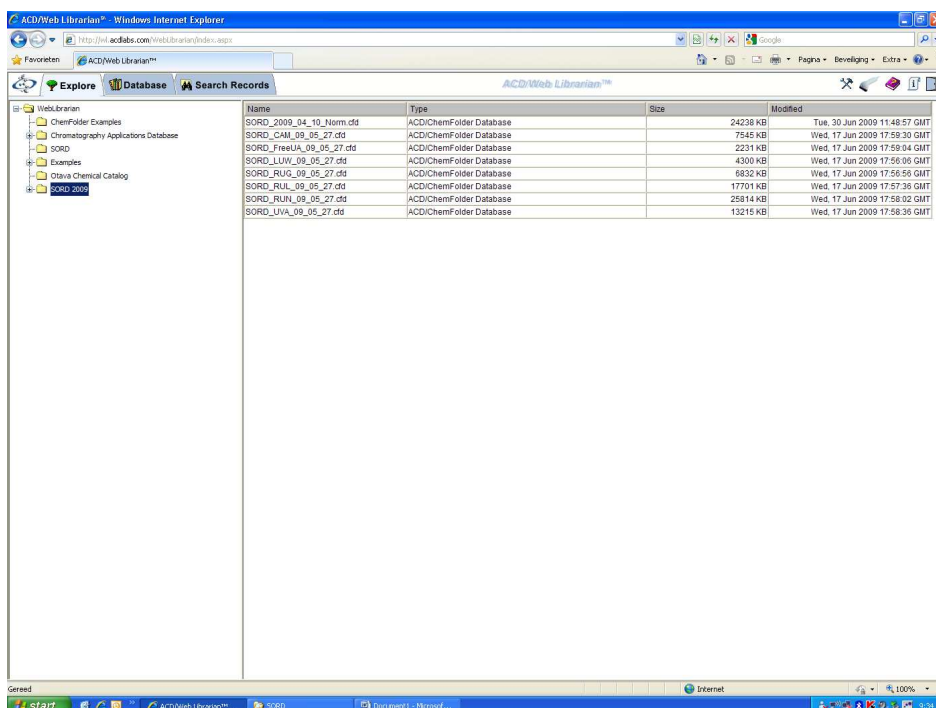
[You may need make ACD/Labs a trusted site and allow pop-ups]



Enter your e-mail address and leave the password empty. Now click on Login.



On the left side of the screen you will see a list of databases. Double click on "SORD 2009" and a menu appears with 8 databases.



Now, double-click on the top entry (SORD_2009_04_10_Norm.cfd).

The screenshot shows the ACD/WEB LIBRARIAN interface in a Windows Internet Explorer browser. The main window displays a list of databases under the 'WebLibrarian' section. A dialog box titled 'Dialogvenster van webpagina' is overlaid on the interface, prompting for a password. The dialog box contains a text field with a masked password '*****' and 'OK' and 'Cancel' buttons.

Name	Type	Size	Modified
SORD_2009_04_10_Norm.cdf	ACD/ChemFolder Database	24238 KB	Tue, 30 Jun 2009 11:48:57 GMT
SORD_CAM_09_05_27.cdf	ACD/ChemFolder Database	7545 KB	Wed, 17 Jun 2009 17:59:30 GMT
SORD_FreeUA_09_05_27.cdf	ACD/ChemFolder Database	2231 KB	Wed, 17 Jun 2009 17:59:04 GMT
SORD_LUW_09_05_27.cdf	ACD/ChemFolder Database	4300 KB	Wed, 17 Jun 2009 17:56:08 GMT
SORD_RUG_09_05_27.cdf	ACD/ChemFolder Database	8832 KB	Wed, 17 Jun 2009 17:56:56 GMT
SORD_RUL_09_05_27.cdf	ACD/ChemFolder Database	17701 KB	Wed, 17 Jun 2009 17:57:26 GMT
SORD_RUN_09_05_27.cdf	ACD/ChemFolder Database	25814 KB	Wed, 17 Jun 2009 17:58:02 GMT
SORD_LVA_09_05_27.cdf	ACD/ChemFolder Database	13215 KB	Wed, 17 Jun 2009 17:58:36 GMT

You will be asked for the password (which is provided in the e-mail for which this document is an attachment). The first record then appears:

The screenshot shows the ACD/WEB LIBRARIAN interface displaying a specific record. The record title is 'SORD 2009|SORD_2009_04_10_Norm.cdf'. The record ID is 1/4966. The record contains a chemical reaction scheme showing the conversion of a complex bicyclic structure to a mixture of two products. The record also includes a detailed experimental procedure and user data.

Note:
 Iodomethane (13 mL, 0.21 mol) was added to a stirred solution of crude taxine (28.0 g) in diethyl ether (175 mL) at room temperature. After 30 hr, the pale yellow amorphous quaternary ammonium salts of the taxines were filtered off, washed with diethyl ether (50 mL), and dried under reduced pressure. The powder was dissolved in ethanol (600 mL), and K₂CO₃ (32.5 g, 235 mmol) in water (800 mL) was added. The reaction mixture was stirred at room temperature for 3 hr. The mixture was then concentrated to 600 mL under reduced pressure, acidified with a 4 M aqueous HCl solution (130 mL), diluted with brine (100 mL), and extracted three times with chloroform (3 x 150 mL). The combined organic fractions were washed with a saturated aqueous NaHCO₃ solution and brine, dried with anhydrous Na₂SO₄, filtered, and concentrated under reduced pressure, affording a crude mixture of 32 and 33 (16.8 g, max. 33.8 mmol).

User Data:
 RXNREGNO: 61
 EXTRNREGNO: 1620002005001
 EXPERIMENTALHEADER: Preparation of a mixture of 6-O-cinnamoyltaxine I (32) and 5-O-cinnamoyltaxine II (33) from crude taxine
 RXN_SYMBOL: 3a -> 32 + 33 ?
 PAGE_SCHEME: 4142
 PAGE_EXPERIMENTAL: 50
 EXTRNREGNO_OLD: 1620002004201
 AUTHOR: Beuster, PH
 INSTITUTION: Radboud University Nijmegen, Department of Organic Chemistry, Toernooiveld, NL-6525 ED Nijmegen, the Netherlands
 COUNTRY: NL
 LANGUAGE: EN
 SOURCE_HEADER: D-Ring Modified Pacitaxel Analogues And Approaches Towards 17-Dideoxypacitaxel Analogues From Taxine
 PROFESSOR: Nolte, R.J.M./Schoenen, J.W.
 YEAR: 2002
 UNIVERSITY: Radboud University Nijmegen
 PDF_DOC: [wfPDF162002005001.pdf](#)

SORD_2009_04_10_Norm.cfd

This is a database of 4,966 records from Universities where author permission has been obtained to make these records public. Only you, and the other Universities who collaborate with SORD, can access this database.

When you enter SORD_2009_04_10_Norm.cfd, you will see the reaction scheme (RS) in the box named "Molecule". On the right is the experimental (EX) in the box named "Note". Below are the data concerning most of the chemical reaction as abstracted by SORD in the box named "User Data".

The link to the PDF ("PDF_DOC") will bring up the PDF for the record you are looking at. *Please note that SORD does no abstract spectral data but that this can be viewed in the PDF that is attached.*

Play with the database using the many useful tools and commands from ChemFolder and the Help function for complete instruction.

SORD_XYZ_09_05_27.cfd

If you return to the page with the list of available SORD databases, you will find 7 entries containing reaction data from 7 Universities. These are also password-protected and you will only be able to access the database from your University. The password for your access has also been provided in the e-mail accompanying this document. Only some of the records in each database have received author permission for public viewing (and these records also appear in SORD_2009_04_10_Norm.cfd). The remainder await the granting of author permission but are visible to members of the University.

These records are displayed with ALL of the data abstracted by SORD. The extra fields not displayed in SORD_2009_04_10_Norm.cfd are:

Yield

Melting Point (where appropriate)

Optical Rotation

Solvent(s) in steps used

Reagent(s) in steps used

This is the so-called High level access database; everything that SORD has abstracted is displayed. As for the Norm database, the link to the reaction PDF is provided.

Problems/Questions

Unless you are really familiar with WebLibrarian, you might have encountered problems or have questions about these databases. Whatever it is you have to tell us, we want to know. Please send all such queries to:

dick.wife@sord.nl

Dick will pass the queries on to the best qualified people to respond.

Database record errors

SORD is rigorous about Quality Assurance. Nevertheless, if you spot any errors in the databases, please let us know!

Feedback

Let us know what you think about the data you can now access. Also, please feel free to suggest any improvements beyond what WebLibrarian offers you now.

Together with ACD/Labs, SORD is adding to the knowledge contained in this section of the database.

What you see now is only the beginning!