Computer Searchable Chemical Database

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Introduction:
Can't find that reagent? More and more software packages and solutions are available to help.

A **chemical database** is a database specifically designed to store chemical information.

The aim of this project was to simplify access to the stock of chemicals used laboratory. Although located at the same site and belonging to the same administrative unit, these laboratories were spread across several buildings. If someone needed a certain chemical that was stored in another laboratory, finding it sometimes turned resembled the search for the (in)famous needle in a haystack: It required that the person in the other laboratory was available, and this person knew their stock of chemicals and the location of the individual products by heart.

Not too many years ago, the problem of managing a chemical storehouse might have been considered a challenge, but one that could be solved with a reasonable amount of software acumen, most likely involving a mainframe database and customized programming.

Maintaining a computer-searchable chemical database.
The first step in proper recycling or disposal of chemicals is to know what you have. The best way to do this is by maintaining an inventory of all the chemicals in use or stored in your laboratory. Supply room personnel should record the receipt of all purchased chemicals. Among the data that should be recorded are the supplier, the amount of chemical purchased, its purity, its amount, the person ordering the chemical and the laboratory room number to which it was delivered.

New chemicals should be added to the database as they are purchased and old ones deleted as they are consumed. This last requirement means that laboratory personnel and not just stockroom personnel should be able to access the database to update information. Laboratory personnel should record when samples are completely consumed or transferred from one laboratory to another. This inventory can be used to tell laboratory managers and staff members when samples becomes old and disposal is necessary.

Principle
Upon arrival of the facility, each product is given a code that specifies its storage location and is immediately entered by the individual users into (and tracked by) a MySQL database. This database is, in turn, accessible from any workplace on Intranet. This contributes to improve efficiency of laboratory work and saves cost, e.g. by avoiding multiple orders of identical products.

The Problem:
The Chemicals Database is a simple yet effective approach to track a stock of products. It provides a "catalogue" that is accessible from any workplace over Intranet (and, if configures accordingly, Internet).

Although the concept described here deals in particular with chemicals in a laboratory, it can easily be adapted to other "items".

A first approach to solve this problem was developed in Microsoft Access, which uses a proprietary data format and requires the installation and maintenance of runtime modules on the individual computers - incompatible with a modern laboratory!

We wanted retrieval of information in a convenient manner - that is, from any workplace and at any time - while ensuring safe, restricted access to the data. In addition, it was important to find a solution which would not rely on a proprietary solution but that was open for future extensions and modifications.

The Solution:
To resolve these problems, we set up a central database, holding all information about the chemicals and similar products in our laboratories. The application was developed based on the Analyses Database [1] and implemented at remarkably low cost (e.g. no license fees) in short time, using standard off-the-shelf computer equipment. The system went from test phase to production in less than one week and is essentially **maintenance-free**; the installation at the author's (former) workplace is operational since 2002.

The database is set up using freely accessible tools such as the MySQL database engine, the apache web server in connection with the PHP scripting language, and the Linux operating system.

MySQL is officially, but also called "My Sequel" is (as of July 2013) the world's second most widely used open-source relational database management system (RDBMS). It is named after co-founder Michael Widenius's daughter. The SQL phrase stands for Structured Query Language.

The default port of Mysql is 3306. The MySQL development project has made its source code available under the terms of the GNU General Public License, as well as under a variety of proprietary agreements. MySQL was owned and sponsored by a single for-profit firm, the Swedish company MySQL AB, now owned by Oracle Corporation.

MySQL is a popular choice of database for use in web applications, and is a central component of the widely used LAMP open source web application software stack (and other 'AMP' stacks). LAMP is an acronym for "Linux, Apache, MySQL, Perl/PHP/Python." Free-software-open source projects that require a full-featured database management system often use MySQL.

PHP is a server-side scripting language designed for web development but also used as a general-purpose programming language. PHP is now installed on more than 244 million websites and 2.1 million web servers.[2] Originally created by Rasmus Lerdorf in 1995, the reference implementation of

PHP is now produced by The PHP Group. While PHP originally stood for *Personal Home Page*, it now stands for *PHP: Hypertext Preprocessor*, a recursive acronym.

PHP code is interpreted by a web server with a PHP processor module, which generates the resulting web page: PHP commands can be embedded directly into an HTML source document rather than calling an external file to process data. It has also evolved to include a command-line interface capability and can be used in standalone graphical applications. [6]

PHP is free software released under the PHP License, which is incompatible with the GNU General Public License (GPL) due to restrictions on the usage of the term *PHP*. PHP can be deployed on most web servers and also as a standalone shell on almost every operating system and platform, free of charge.

To ensure appropriate user-friendliness, the application is accessible from any workplace via Intranet while still ensuring safe, restricted access (login and password). The code generated is conform to publicly available standards and does *not* use any browser-specific code, so the application is accessible with any browser and on any platform.

In addition, this solution does not rely on a proprietary code but employs publicly recognised standard formats and protocols. It is freely available under the terms and conditions of the GNU Public License (GPL), thus being open for extensions and custom modifications.

The **GNU General Public License** (**GNU GPL** or **GPL**) is the most widely used free software license, which guarantees end users (individuals, organizations, companies) the freedoms to use, study, share (copy), and modify the software. Software that ensures that these rights are retained is called free software. The license was originally written by Richard Stallman of the Free Software Foundation (FSF) for the GNU project.

The GPL grants the recipients of a computer program the rights of the Free Software Definition and uses copyleft to ensure the freedoms are preserved whenever the work is distributed, even when the work is changed or added to. The GPL is a copyleft license, which means that derived works can only be distributed under the same license terms. This is in distinction to permissive free software licenses, of which the BSD licenses are the standard examples. GPL was the first copyleft license for general use.

Technical Details.
System Requirements
The system uses a database and Intranet server that centrally holds the database. This server can be a standard, off-the-shelf computer (even a rather slow machine) and uses standard Linux tools: A web server (preferably Apache), the MySQL database engine, and PHP scripting. The installation is described in detail in the documentation.

Fortunately, there are a number of chemical inventory software packages on the market, ranging from very flexible general purpose programs to those written as custom software programs for a particular industry or company. This review contains a sampling of such programs, but there are numerous customized solutions and other types of tracking software that can be used for chemical inventory tracking.

How actually the Software Works?
These computer programs vary in sophistication and features. Software search features can include one or more of the following search options: searching by chemical name, chemical supplier, the storage location, and the laboratory department and/or individual who purchased the chemical. The chemical name can be the proper IUPAC (International Union of Pure and Applied Chemistry) systematic name designation or one or more common names of the chemical. Other search options include the CAS (Chemical Abstracts Service) Number of the chemical and the date of purchase. Some programs provide storage of MSDS information.

A Material Safety Data Sheet (MSDS) is designed to provide both workers and emergency personnel with the proper procedures for handling or working with a particular substance. MSDS's include information such as physical data (melting point, boiling point, flash point, etc.), toxicity, health effects, first aid, reactivity, storage, disposal, protective equipment, and spill/leak procedures.

More sophisticated software can print barcode labels for chemicals that can be affixed to the chemical sample container and used to track movement of chemicals within the laboratory and their consumption. Should supply of a chemical be recorded as falling below a specified level, some software can automatically issue an alert informing the user of that particular chemical and that it needs to be re-ordered. Some chemicals may arrive with an expiration data beyond which the chemical should not be used. Some software offer features that include issuing an alert when a particular chemical sample usage date is due to expire.

Some software suppliers such as Chemoventory offer limited capability versions of their software for free (www.chemoventory.com) to educational and other nonprofit institutions. Other software provides more features but must be paid for. One example is Nexxis Chemical Inventory Manager (www.labtronics.com/chemical_inventory_management.htm).

Summary
Chemical inventory programs on the market each have particular strengths and areas of specialization, mainly differentiated by those designed for pharmaceutical and biochemical companies and those for other Organisations. Options are available in a range that suits everything from big corporations to small Institution, allowing small companies to use off-the-shelf products and large companies to use highly customized solutions for their computer inventory tracking needs.

Conclusion:
This database can also be a money saver by enabling lab personnel to learn from whom they can obtain a needed chemical without purchasing a new sample. Should it be necessary to purchase a fresh sample of a particular chemical, the purchaser can review the chemical inventory to identify a supplier and the chemical purity of previously purchased samples of the same chemical. Several firms offer commercially available chemical inventory database software. Using an Internet search engine and keyword phrases such as "chemical inventory management software" can identify software suppliers and retrieve a description of their products.

REFERENCE   [1] J. Hau and L. Fay. Practical Approach to Archival and Retrieval of Analytical Data in the Laboratory. Analyst 126 (2001), 1194-1199.