

# CHEM WATCH

A T K Y N A S T O N

2003

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**CHEMWATCH NEWSLETTER**  
**QUARTERLY CD RELEASE 2003/2**

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Dear ChemWatch User,

Please find enclosed the newest release of the ChemWatch Package, CD 2003/2.

## ChemWatch Customer Satisfaction Survey

As part of an ongoing commitment to refining products and services to meet the needs of our clients, ChemWatch is currently conducting a general customer satisfaction review.

We would appreciate your assistance in completing the short survey attached and faxing it through to Chemwatch on the following number: +61 3 9572 4666. Alternatively it can be posted to:

The Quality Manager  
Chemwatch  
70 Bambra Road  
Caulfield North 3161  
Australia

## ChemWatch Program Developments

### Chemweb Gold – Preview to the New Interface

The extensive number of users of the web-based version of Chemwatch continues to grow and in order to meet this demand a new interface is currently under development. The new look Chemweb Gold integrates aesthetically pleasing graphics with increased functionality. Due for release later this year, users will be able to produce the much anticipated Hazardous Substances Register and will also have the ability to create labels to their individual needs with the Custom Label program. The new screen layout (pictured) will contain separate frames of buttons on either side, which remain constant as the material names and corresponding reports change. What does it all really mean? Less clicks and more efficient access to an increased number of reports.



### Custom Labels

The Custom Labels program, previously only available on the LAN version of Chemwatch, will soon be accessible from the web-based version of Chemwatch. Custom Label allows users to generate labels for their specific needs and to comply with their company standards. Its design ranges from a default label for each material to save you time through to complete control over the layout, where you can include company logos and other bitmaps. This will be made available as a post release patch: for the most up to date notification of its release users should subscribe to [chemtech-request@chemwatch.net](mailto:chemtech-request@chemwatch.net).

Developments to the program have also seen an increase in the barcode component and Custom Labels now supports a much larger range of barcode types, including: EAN128A, EAN128B, EAN128C, UPC A, E0 and E1.

### Mini-MSDS in Portuguese

Bom dia. Portuguese has become the seventeenth language the Chemwatch user interface has been translated for. Outside of Portugal, this will help Chemicals management in Brazil, parts of Africa and East Timor.

### Substructure Searching

Substructure search functionality – a breakthrough technology bringing theoretical chemistry to immediate chemicals applications– is now operational in both Chemwatch and ChemWeb Gold.

The tool allows the database to be trawled by chemical subunit, producing a full list of matching substances. When applied to the comprehensive pure substances collection offered by Chemwatch, the technology starts to offer the kind of power to offer real efficiency savings.

The search engine was developed for ChemWatch by Dr. Wolfgang D. Ihlenfelt, founder of German software company Xemistry GmbH. The chemoinformatics software that forms the basis of Chemwatch's search function was developed by Xemistry out of research undertaken in postdoctorate studies in Japan.

Implications for research purposes are endless, but at Chemwatch we have found the function particularly useful for identifying a group of materials related by a common functional group, finding appropriate alternatives for certain substances, and for alarming of inappropriate chemical incompatibilities.

From the main Chemwatch Search Screen, Structure search can be accessed via the main drop down menu. Select the option to either search by SMILES or to draw the molecule or fragment in question. Simple Molecular Input Line Entry Specification (SMILES) is a protocol to represent basic molecular structural connectivity through symbols based on a carbon chain.

Tutorials, and some information on the background of SMILES is available online, at <http://www.daylight.com/dayhtml/smiles/smiles-intro.html>

## ChemWeb Gold Mailing List

We are currently creating a mailing list of IT/IS people whose licensing agreement allows them to install the Intranet version of ChemWeb Gold on their own server. The list is aimed at communicating the current technical issues concerning Chemweb Gold and will include notice of downloadable patches, service packs and updates as soon as they become available. If you would like to subscribe to this list, please post an email to the following address:

[chemtech-request@chemwatch.net](mailto:chemtech-request@chemwatch.net)

## Additions to the ChemWatch Team

ChemWatch sales have boomed in the last few months, and to meet escalated demand, the Chemwatch team has been growing in concert.

To keep up with the accelerating demand of MSDS production, Chemwatch has appointed certified chemist Duncan Hind, who completed a BA in applied science at RMIT in 1993. Chemwatch has also made good use of Duncan's medley of IT talents, and has appointed him to manage the MSDS generator's operation. Most recently he has been working to automate a system to automate calculation on MSDS data, to facilitate a faster response to urgent client queries.

We have also welcomed in a new communications expert, Janet Hider Smith, to edit the weekly Bulletin Board news update, and manage the rest of our range of publications. Janet has a ranging history in media production, including a period of working through western Europe that is bringing first hand nous to our global focus. And like most of us at Chemwatch, there is some H&S in the backlogs of her resume, as she worked on safety manuals for a crane company in Germany.

## Bulletin Board

We provide a free weekly bulletin to all our clients presenting a summary of the latest developments in the scientific field. These are resourced from a large selection of material including scientific journals, magazines and websites. If you would like to subscribe please email: [chembulletin-request@chemwatch.net](mailto:chembulletin-request@chemwatch.net)

## Galleria Chemica

### QSAR– stops gaps in chemical safety data

In the past, gaps in our knowledge of safety properties for various chemicals have resulted in shortcomings in chemical H&S management. A new tool, currently being implemented at ChemWatch fills these gaps by applying modeling techniques to existing chemical structural knowledge.

QSAR (Quantitative Structure Activity Relationships) methods extrapolate physical, (thermo)chemical, (eco)toxicological and pharmacological properties of chemicals. Extensive use over the last decade, with validation via classical means, has established a powerful method of accuracy for practical applications.

Most recently, Chemwatch has been drawing on these modeling resources to consolidate our info on thermodynamic and energy release properties, in order to determine essential knowledge for proper handling protocols, transportation, and family/class incompatibility.

Also, QSAR has allowed calculation of more than 500 potentially active pharmacophores – the structure of a drug that enables its intended action - for over 250,000 pure chemicals to appear in the first release of mega database Galleria Chemica.

Chemwatch users take advantage of QSAR via the Environment screen. Where chemical data is available, users are able to view distributions for listed chemicals. However, where a property isn't known, modeling allows accurate advice to be constructed from effective Guestimates.

Fugacity models have also been added to this ChemWatch module, which use non-structural techniques to predict the fate of chemicals in the environment, employing half-lives and other physico-chemical data.



## Asian Diary

### Galleria Chemica Debut

Principal Dr. Bernie Bialkower recently made the journey to QingDao to preview the new interface for the popular Chemweb Gold program and the much anticipated Galleria Chemica.

As expected, they were extremely well received and although still in the final development stages, both projects have fostered a strong interest in the Chinese market. Fueling this interest, the NRCC have initiated an email campaign that provides potential clients access to the database and an opportunity to see first hand how powerful Chemwatch is in effective chemicals management.

Coinciding with the campaign and ten years in the making, the hazardous chemicals registration work in China officially started in early March. According to the legislative requirements set out in "Measures of Hazardous Chemicals Registration" (Decree 35 of SAWS), businesses storing and using chemicals are now required to conduct risk assessments in the workplace, submit appropriate MSDS and Label all containers appropriately. With the legislation now firmly in place and businesses looking to comply with National Standards the need for the Chemwatch Chemical Database and Management System is as strong as ever. To assist in the introduction of the new legislation the chemical advisory hotline (86-532-388,9090), originally set-up and maintained by NRCC, has now been designated as China's National Chemical Emergency Response Hotline. To better enhance the quality of service on the hotline, the NRCC is taking an active role in training and maintaining communication with AICM and foreign agency ER.

To further aid in the implementation of the new legislation for China, Ye Congsheng has been responsible for drafting a series of accredited management documents and relevant management provisions, as well as setting up test labs.

**Ye Congsheng NRCC, China**

随着NRCC的广泛宣传，越来越多的中国企业对CHEMWATCH化学品安全管理系统产生了浓厚的兴趣。NRCC已经启动了大规模的EMAIL和邮件宣传攻势，让更多的化学品用户了解具有强大功能的CHEMWATCH系统。此外，经过近10年的准备工作，中国的危险化学品登记工作已经正式启动。按照《危险化学品登记管理办法》的要求，登记单位要求对化学品的作业场所进行评估，必须提交符合要求的化学品安全技术说明书和安全标签。因此，广大的化学品用户需要一个化学品安全管理系统来帮助他们遵循法规的要求。

目前，NRCC的化学事故应急咨询专线已经被SAWS指定为国家化学事故应急咨询专线。为进一步提高NRCC的应急响应能力，NRCC与AICM、及国外化学事故应急响应机构进行了广泛的交流，同时邀请了DUPONT的应急响应专家给NRCC进行了培训。为配合危险化学品登记注册工作的顺利实施，《管理办法》要求对未分类化学品进行危险性鉴别和分类，并对鉴别与分类机构实施认可制度。NRCC负责起草了一系列的鉴别与分类机构认可文件，并即将建设自己的化学品危险性鉴别与分类实验室。

## Training Focus

Chemwatch sales have continued their strong and steady growth through an uncertain time for the ASEAN/Asian region, and training new users has become the major focus of activity for the local division in recent months.

Shannon Sim has recently completed an instruction programme in Hong Kong, for the Dangerous Goods Management staff of Cathay Pacific. The course focused on using the Chemwatch database to monitor transport regulations on hazardous goods – which are regularly shipped without adequate labelling or in passenger luggage. The Airline has recently implemented Chemwatch software and subscribed to the 24-7 Emergency Response hotline as an indispensable backup to its customs control.

Mattel Toys has also signed as another important new client in the region, and combined training courses have recently been held for local staff in Jakarta and Guangzhou, conducted by Chemwatch's

appointed local distributor Chemcare Asia Consultants. This focussed on all aspects of Chemwatch database navigation as well as introducing Hazardous Materials. Training, with classes taken in both English as well as Mandarin.



The Chemwatch Database is also building on its profile as an important education tool. Ngee Ann Polytechnic has recently purchased the database for enhanced chemical safety for students use, and for managing laboratory environments.

Within the Pharma industry, Chemwatch has recently established cooperation with Pfizer on Chemwatch as the safety database for their Singapore manufacturing facilities. In conjunction with Chemwatch contacts within the Biolab industries, a major Biolab Safety Training Program has been developed to give tailored instruction to this sector. The course is to be run by the CSIRO at the National University of Singapore.

Chemwatch's profile continues to grow in the region, the Indonesian market the latest to see a surge in the company's profile. In particular, we have been working with several of the major chemical manufacturers in the Merak Petrochemical area (Western Java), and we are preparing an introduction on enhanced safety by implementation of Hazcom programs based on the Chemwatch Safety Database.

**Barry Lynam Chemcare Asia**



## American Diary

ChemWatch continues to have an escalating presence in North America. New government clients include the Federal Bureau of Investigation (FBI) and the National Institute for Occupational Health and Safety (NIOSH). The US military continues to recognize ChemWatch as the preferred chemical emergency response tool with the addition of Robins Air Force Base in the State of Georgia. We welcome Kevin Bartoe and the hazmat team at Robins AFB to the ChemWatch family.

One of the largest and most prestigious universities in North America is adopting ChemWatch across all of its campuses. The Ohio State University in Columbus Ohio is now installing ChemWatch on its own intranet.



Our laboratory management partner, Vertere, brought several new ChemWatch clients linked to their new Chemical Management system this past quarter. Among them are Vassar college and the Cytec Corporation.

Just as important as new clients are the renewals of our current clients. Here is a photo of Richard Dell, Assistant Director of Safety Services of the renowned research institution, Case Western Reserve University in Cleveland, Ohio reviewing the new ChemWatch Collection of supplier MSDSs. Dick became one of the early subscribers to the Collection when he added it to his current ChemWatch license.

Paul reports that with well over 100 inches of snow in Northern Ohio this past winter (a record) he is looking forward to a sunny and warm spring.

**Jim Wood and Paul Ruez ChemWatchNA**



*Jim and Paul just returned from the massive Pittcon Show in Orlando Florida where they displayed their new booth as well as the ChemWatch System. Jim and Paul and the new booth will be at the Fire Department Instructors conference in early April and the American Industrial Hygiene conference in Dallas in May*

## Vertere Introduces the Inventory Manager at Pittcon 2003

Vertere debuted its exciting new inventory management software at Pittcon 2003 in Orlando, FL. The Inventory Manager includes modules for chemical, equipment and supply management, each using bar coding to reduce the time required for routine inventory tasks and increase record accuracy.

Interest at Pittcon focused on the ChIM module and its link to ChemWatch. With a single click, ChIM users move from a chemical record to the full details available in ChemWatch. ChIM's many easy-to-use functions include group and item security setup options and 21 CFR Part 11 compliance, to help customers meet stringent security requirements.

'I think it's GREAT!! It looks terrific and the test drive was fun,' reports Barbara Ray, Coordinator, Hazardous Materials, Department of Safety and Risk Management and an early version tester from the University of Rhode Island. One of hundreds of sites using Vertere's ChIM software for chemical management, URI is on the list of customers upgrading to the new ChIM module.

Users particularly like the ease of entering and updating records in the Inventory Manager. The system is delivered with more than 150,000 chemicals already defined by vendor and vendor catalog number to eliminate tedious keying of chemical names. The system includes a Chemical Information Gateway to safety, regulatory, and physical property information, as well as the ChemWatch database. As shown below, users can select a group of records and update many fields at one time. The program also allows group transfers and deletions (disposals), as well as allowing rapid reporting via e-mail.

Designed to meet the requirements of the scientific community, the Inventory Manager is equally efficient for tracking and managing corporate assets in laboratory, classroom, office, or maintenance environments. To minimize maintenance, each module uses a core set of location, user, and vendor data. Users can switch between the modules, each with its own security and customized setup. In early April, Vertere demonstrated the equipment module at the Central Region Conference of the National Property Management Association in Hot Springs, Arkansas. Long-term customers from the University of Arkansas (at Fayetteville, Little Rock, and Pine Bluff) are looking forward to the improvements offered by the Inventory Manager to simplify their capital equipment management programs.

Vertere's Customer Support Manager Harry Hickey joined Sharon Stasko, Jim Wood, and Paul Ruez at Pittcon in demonstrating the Inventory Manager and ChemWatch. He took time out to capture ChemWatch's own Jim Wood meeting Jim Wood, a chemical researcher from New Jersey.



## ChemWatch Australia Training Dates

### Adelaide

June 3 – Level 1  
June 4 – Risk Assessment/Custom Labels  
October 14 – Level 1  
October 15 – Chemweb Gold

### Brisbane

June 17 – Level 1  
June 18 – Risk Assessment/Custom Labels  
September 9 – Level 1  
September 10 – Chemweb Gold  
November 18 – Level 1  
November 19 – Risk Assessment/Custom Labels

### Cairns

May 27 – Level 1  
May 28 – Risk Assessment/Custom Labels  
October 28 – Level 1  
October 29 – Chemweb Gold

### Canberra

September 23 – Level 1  
September 24 – Chemweb Gold

### Hobart

May 20 – Level 1  
May 21 – Chemweb Gold

### Launceston

October 7 – Level 1  
October 8 – Risk Assessment/Custom Labels

### Melbourne

June 10 – Level 1  
June 11 – Chemweb Gold  
August 26 – Level 1  
August 27 – Risk Assessment/Custom Labels  
November 11 – Level 1  
November 12 – Chemweb Gold

### Newcastle

October 21 – Level 1  
October 22 – Risk Assessment/Custom Labels

### Perth

September 2 – Level 1  
September 3 – Risk Assessment/Custom Labels

### Sydney

June 24 – Level 1  
June 25 – Chemweb Gold  
September 16 – Level 1  
September 17 – Chemweb Gold  
November 25 – Level 1  
November 26 – Risk Assessment/Custom Labels

## ChemWatch Affiliate Companies

### Global Chemical Data Inc.

1913 21st Avenue South  
Nashville, Tennessee 37212  
Tel: +1-615-467-0383/+1-440-269-6872  
Fax: +1-615-269-6872  
Email: info@globalchemicaldata.com  
Web: www.globalchemicaldata.com

### Vertere

225 Chapman Street  
2nd Floor  
Providence, Rhode Island  
02905-4507  
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Fax: +1-401-528-1197  
Email: info@vertere.com  
Web: www.vertere.com

### Kemika@XXI

33 Des Agarics, Blainville QC  
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Tel: +1-450-435-7475  
Fax: +1-450-435-0677  
Email: info@kemikaxxi.com  
Web: www.kemikaxxi.com

### Applied Science Associates

70 Dean Krauss Drive  
Narrangansett, Rhode Island  
02882-1143  
Web: www.appsci.com

### National Registration Center for Chemicals (NRCC)

218 Yan An San Road  
QingDao, China  
Email: cchem@public.qd.sd.cn  
Web: www.nrcc.com.cn

### Elogix/Chemwatch

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