

Newsletter from STN

April 2008



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Staff News

It is with great sadness that we have to let you know that our Manager, Mike Corkill, was killed in a road accident on his way home from work at the end of March. Mike was a dedicated Team Leader, a real champion for STN, and a positive influence on all who worked with him. We all miss him very much.



STN User Update Meetings – 17th and 18th June

We are sorry to disappoint those who were intending to come to the Food Forum in April, which has had to be postponed. However, we are pleased to say that our regular User Update Meetings will go ahead as planned in June.

Take this opportunity to keep up to date with STN developments by joining us at our summer STN User Meetings, to be held this year on **Tuesday 17th June in Manchester**, and **Wednesday 18th June in London**.

Topics will include:

- STN overview and database enhancements
- STN AnaVist 2.0, STN Viewer, and STN Express 8.3
- Chemistry searching update
- Tips from the Helpdesk
- Value added by STN
- Information exchange discussion

The meetings will last from 10.00am to 3.30pm with free lunch and refreshments provided.

You can reserve your place by sending an email to STNHLPUK@RSC.ORG; we will then provide you with a finalized detailed Agenda as soon as it is available.

Remember to state your preferred venue. We look forward to meeting you in June.

Tips from the Help Desk

Search Tips: Searching for drug-like substances in CAS REGISTRY file

Property information is available for many substances in REGISTRY in one or more of three formats:

Experimental Property (EPROP) values are listed directly in REGISTRY in tabular form, with links to the references containing the information.

Experimental Property Tags (ETAG) are listed for properties that are available in the full text of the document, with links to the references containing the information.

Predicted Property (PPROP) values, calculated using software from Advanced Chemistry Development, Inc. (ACD/Labs), are listed directly in REGISTRY in tabular form.

Predicted property values may be searched to refine the results of a Registry structure or text search to a hit set of substances with molecular properties associated with oral activity in humans.

Lipinski's Rule of Five was formulated by Christopher A. Lipinski (Advanced Drug Delivery Reviews 1997 23 3-25) based on the observation that most medicines are relatively small, lipophilic molecules.

Lipinski's Rule of Five states that, in general, an orally active drug has:

- 5 or fewer hydrogen bond donors (nitrogen or oxygen atoms with one or more hydrogen atoms)
- 10 or fewer hydrogen bond acceptors (nitrogen or oxygen atoms)
- A molecular weight less than or equal to 500
- A calculated partition coefficient (log P) less than or equal to 5

The rule does not predict whether a molecule is pharmacologically active, but rather, gives an indication of its pharmacokinetics in the human body.

In REGISTRY, it is straightforward to search for substances which comply with Lipinski's Rule, as follows:

=> **S LIPINSKI/CALC**

Or

=> **S LIP/CALC**

The LIP/CALC term is expanded into the following search query:
0-5/HD AND 0-10/HAC AND LOGP<=5 AND 0-500/MW

Spotlight on KOSMET

Why use KOSMET?

Large publicly available databases can provide much useful information but articles relating to specialist subjects such as cosmetic product development may be difficult to find. If this sounds somewhat familiar, the International Federation of the Societies of Cosmetic Chemists (IFSCC) may have a solution for you: KOSMET.

What exactly is KOSMET?

Cosmetic & Perfume Science and Technology (KOSMET) is a bibliographic database containing citations to the worldwide cosmetic and perfumes literature, which has been abstracted since 1985. On April 1, 2008, the KOSMET database had over 43000 entries and it is updated by an average of 200 items a month.

What type of cosmetic literature is included in KOSMET?

Almost anything that you can think of, ranging from manuscripts of all presentations and posters presented at IFSCC Congresses and Conferences, trade exhibitions, to trade journals and industry publications, as well as journals published by member societies such as the Journal of Cosmetic Science, the International Journal of Cosmetic Science and the Journal of the Society of Cosmetic Chemists of Japan. Of course, the IFSCC Magazine is also included, not only the scientific articles but also reports of congresses and conferences and the interviews with the "Distinguished Cosmetic Scientist". But also other scientific articles such as those published in the Journal of Investigative Dermatology, Pharmaceutical Research and the Journal of the Society of Controlled Release can be found in the database. However, bear in mind that only those articles of immediate interest to the cosmetic industry are included.

What about foreign languages and full text articles ?

Even when you are dealing with articles in languages that not all of us speak, such as Japanese and Hungarian, you can still find them in the database with abstracts in English. It is possible to obtain some full papers via the click of a button from STNEasy or by using the hyperlinks in STN on the Web and Express. Another feature is that for a long time, the abstracters (the people that write the abstracts of the papers that are entered into KOSMET) only used abstracts supplied by the authors, the so-called "author-provided abstracts". If there was no abstract, or only a very short one, as for instance, in Cosmetics & Toiletries, then this one-liner would be all you got in the abstract field. In September 2002 this changed, and in such instances more useful abstracts provided by the abstracter rather than the author of the article are now also available. But you can use them with confidence as all KOSMET abstracters are professional cosmetic scientists.

Any questions or comments?

Do take the opportunity to explore this valuable resource; we will be pleased to pass on any comments you may have to the database producer on your behalf. If you need any assistance with searching KOSMET – just ask us.

STN Express version 8.3 now available

STN Express, Version 8.3, is now available for the Windows® operating system. The new version includes several important updates.

New Create L-number from STN AnaVist wizard

A new wizard in Version 8.3 creates a fully-functional [L-number from a saved STN® AnaVist™ answer set](#) (.xta file format). In addition to searching, the L-number can be used to:

- Display answers from STN AnaVist in any format
- Move full-text patent documents from STN AnaVist to STN® Viewer™ via the Evaluate with STN Viewer wizard

Enhanced Select Discover! Wizard window

The Select Discover! Wizard window has been redesigned to provide greater utility and better visibility of the search session:

- The search history window now displays the search strategy and the L-number of the items retrieved.

- The overall size of the Select Discover! Wizard window has been reduced.
- The Search and Results wizards are now accessible within tabbed menus with an option to Hide or Show the tabbed menus.

Additional software enhancements

- Support files for databases, fields, lexicons, thesauri, and other items now update automatically at login.
- The number of allowed G-group attachment points for structure drawing has increased from 20 to 200.
- The CAS RegistrySM BLAST[®] feature has been updated.
- A new toolbar button enables launching of STN AnaVist.

New software installer

A new STN Express software installer now allows for easier installation and is more consistent with Windows standards for software installation. Transcript, query, script, and other files created in previous versions of STN Express (and stored within the STN Express file structure) will be copied to a new STN Express 8.3 folder conveniently located in:

- My Documents (Windows 2000 and XP)
- Documents (Windows Vista[®])

STN Database News You May Have Missed.....

FSTA - COVERAGE DEVELOPMENT UPDATE

By the end of December 2007 a further 39373 records had been added to FSTA (Food Science & Technology Abstracts) giving a total of 776544 records in FSTA. This represents an increase of 9% on the number of records added during 2006.

More than 72% of the material added was taken from journal articles and a further 22% were patent records. The remaining content covers legislation, standards, books, conference proceedings, reports, reviews, and theses.

Each record is added to a section which reflects the appropriate subject area and, as in previous years, the largest numbers of records covered

- Fruits, Vegetables, and Nuts
- Alcoholic and Non-alcoholic Beverages and
- Food Sciences.

To produce the FSTA database, IFIS scientists scan approximately 1800 journals from a broad range of disciplines. These include food science & technology, agriculture, marine fisheries science, environmental & water sciences, public health & medicine, nutrition, biology, biotechnology, chemistry, and toxicology. The proportion of Open Access journals has steadily increased.

MARPAT – SEARCHING ENHANCED

The following enhancements were recently implemented in MARPAT:

- The number of searches that return at least one incomplete result has been reduced by more than 60%.
- The iteration and answer limits have been increased from 100,000 to 200,000 for both online and batch searches. For more information on MARPAT search limits, enter HELP SLIMITS at an arrow prompt (=>).

PCI – NOW AVAILABLE AS A REPLACEMENT TO DPCI

Patents Citation Index™ (PCI) is now available on STN and replaces Derwent Patents Citation Index® (DPCI). You may need to update existing procedures, including scripts, to work with PCI.

New features available in PCI:

- Extended coverage
- Stop words no longer used
- Additional priority application numbers
- Additional Thomson Scientific standard application numbers (/APTS and /PRTS)
- More focused content

PCI is a unique database of examiner citations from patents and literature, including 98 million patent and 11 million literature citations from more than 8 million patent families. Bibliographic patent family data from Derwent World Patents Index® (DWPISM), all patents and literature cited by examiners, and references to citing patents are included in PCI.

Coverage includes patent citations from 1973 to the present from the European Patent Office (EP), World Intellectual Property Organization (WO), and patent-issuing authorities in the following countries: Belgium (BE) France (FR) Germany (DE) Japan (JP) Netherlands (NL) Spain (ES) United Kingdom (GB) United States (US)

PCI also includes examiner and author citations from 16 patent-issuing authorities from mid-1994 to May 1997.

CAS REGISTRY ENHANCED WITH ADDITIONAL EXPERIMENTAL SPECTRA

Since the beginning of 2008, approximately 204,000 experimental spectra have been added to REGISTRY, including:

- 95,000 proton NMR spectra
- 31,000 carbon-13 NMR spectra
- 78,000 mass spectra

This enhancement is part of an ongoing effort to strengthen the collection of experimental spectra first made available in 2005. REGISTRY now includes more than 480,000 experimental spectra.

USGENE – TIMELINESS ENHANCED

The United States Patent and Trademark Office (USPTO) Genetic Sequence Database (USGENE) is now the most timely source of USPTO patent and published application sequence data, available within 3 days of publication by the USPTO.

Issued patent sequence data is therefore available within 3 days, and published application sequence data is available within 1 day of publication by the USPTO.

USGENE provides sequence data updates 10 days faster than any other comparable resource and is typically 1-3 months ahead of the USPTO sequence collection provided by the National Center for Biotechnology Information (NCBI) in GenBank®.

USPATFULL, USPAT2, AND USPATOLD – NEW CUSTOM IPC DISPLAY FORMATS

Two new custom display formats for International Patent Classification (IPC) codes have been added to U.S. Patents Original Publications (USPATFULL), U.S. Patents Latest Publications (USPAT2), and U.S. Patents Pre-1976 (USPATOLD):

- IPC.UNIQ – displays a set of unique IPC codes for a patent
- IPC.HIT – displays IPC codes matching those specified in the search query

IPC.UNIQ may be used for a more compact display of IPC information. The IPC.TAB format is available for more extensive IPC information, including IPC metadata. IPC.HIT may be used to quickly determine why a specific record has been retrieved with a complex search strategy.

WPINDEX/WPIDS/WPIX - ECLA CODES AND CURRENT US NATIONAL CLASSIFICATIONS

European Patent Classifications (ECLA) including 'In Computer Only' (ICO) codes and Current US National Patent Classifications will be added to the DWPI database (files WPINDEX/WPIDS/WPIX) from update 13 onwards. The corresponding backlog data have been added to the file on February 21, 2008. In the course of the backlog load about 8 million DWPI documents have been equipped with ECLA or US National Classification data. US National Classifications for 3.7 million patents and European Classifications for about 25 million patent publications have been added.

Training Opportunities and Updates

Hands on Workshops

The STN Agency offers all public training courses **free of charge**, but we do reserve the right to cancel courses if there is insufficient interest. We will give you notice of any cancellation at least a week in advance, and ask that you let us know if you have to cancel after registering.

May

7 th Structure Searching on STN	Manchester
15 th MARPAT	Cambridge

June

3 rd STN Refresher	Cambridge
4 th Sequence Searching on STN	Cambridge

July

10 th Introduction to STN Commands	Cambridge
15 th Patent Searching on STN	Cambridge

September

9 th Legal Status Searching on STN	Cambridge
10 th Analyzing Search Results + STN AnaVist V2.0	Cambridge

October

15 th Using STN Interfaces	Cambridge
23 rd Introduction to Chemistry Searching on STN	Cambridge

November

4 th Structure Searching on STN	Cambridge
12 th Marpat	Cambridge
25 th Sequence Searching on STN	Cambridge

December

11 th STN Refresher	Cambridge
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Registration Form:

All full-day sessions will run 10.00am to 3.30pm

e-Seminars

Live, interactive, web-based seminars bringing professional training to your desktop, each one hour long.

See <http://casevents.webex.com/casevents/mywebex/> for registration details for the following seminars from CAS:

8 May	at 2.00pm	STN: Multifile Searching for Scientific Information
12 June	at 2.00pm	STN: Searching Formulations on STN®
10 July	at 2.00pm	STN: Highlights from the 2008 STN Patent Forum
14 August	at 2.00pm	STN: Revealing the Mysteries of MARPAT®
11 Sept	at 2.00pm	STN: Finding Licensing Information on STN®

See http://www.stn-international.de/training_center/seminars.html for registration details for the following seminars from FIZ:

28 May	at 2.00pm	Setting up alerts on STN part 1
17 June	at 2.00pm	Taking command - effective use of sequence search options in USGENE, DGENE and PCTGEN
1 July	at 2.00pm	Setting up alerts on STN part 2
28 August	at 2.00pm	Patent information from East Asia on STN
9 Sept	at 2.00pm	Navigating INPADOCDB - easy recipes to get relevant results

And Finally.....

Please contact us if you have any comments or questions arising from this newsletter:

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