What's New from



SLA Vendor Roundtable

W. Mercier, CAS Major Account Manager June 10, 2002

CAS, as a division of the American Chemical Society, provides an integral service to the scientific and intellectual property communities.



from the the ACS charter: "to encourage the increase and diffusion of chemical knowledge for the benefit of industry and education"

CAS scientists analyze and index scientific literature























World Leading Chemistry Databases

To create the world's best digital environment to search, retrieve, analyze and link chemical information

Power of the Web Value Added Tools





The CA/CAPLUS databases keep getting better and better



- References and page images back to 1907 added
- Full Journal titles added
- ISBNs added
- new ROLES added
- Cited references added
- LEXICON added



The CAS Registry improvements continue



- Currently ~40 million substances
- 85 million calculated properties added



Calculated Physical Properties Sample Record

RN 103628-46-2 REGISTRY



Calculated Properties (CALC)

P	ROPERTY	VALUE	CONDITION	NOT	E
HD H donors		+=====+====+==== 2		ACD (1)	
HAC H acceptors		5		ACD	
olecula	r Weight	295.40		ACD	(1)
ogP		0.667+/-0.641		ACD	(1)
ogD		-2.43	pH 1	ACD	(1)
ogD		-2.43	рН 4	ACD	(1)
ogD		-1.73	рН 7	ACD	(1)
logD		-0.82	рН 8	ACD	(1)
logD		0.53	рН 10	ACD	(1)
Ka		11.31+/-0.40	Most Acidic	ACD	(1)
Ка		9.49+/-0.28	Most Basic	ACD	(1)
iolar So	lubility	>=1 mol/L	рН 1	ACD	(1)
iolar So	lubility	>=1 mol/L	рН 4	ACD	(1)
	-	>=1 mol/L	рН 7	ACD	(1)
	-	>=0.1 - <1 mol/L	рН 8		(1)
olar So	lubility	>=0.01 - <0.1 mol/L	рН 10	ACD	(1)
	donors accepto olecula: ogP ogD ogD ogD ogD Ka Ka olar So olar So olar So olar So	acceptors olecular Weight ogP ogD ogD ogD ogD Ka Ka olar Solubility olar Solubility olar Solubility olar Solubility olar Solubility	donors 2 acceptors 5 olecular Weight 295.40 ogP 0.667+/-0.641 ogD -2.43 ogD -2.43 ogD -1.73 ogD -0.82 ogD 0.53 Ka 11.31+/-0.40 Ka 9.49+/-0.28 olar Solubility >=1 mol/L olar Solubility >=0.1 - <1 mol/L	donors 2 acceptors 5 olecular Weight 295.40 ogP 0.667+/-0.641 ogD -2.43 ogD -2.43 ogD -1.73 ogD -0.82 ogD 0.53 ogD 0.53 ogD 11.31+/-0.40 Most Acidic Ka 9.49+/-0.28 olar Solubility >=1 mol/L olar Solubility >=1 mol/L olar Solubility >=1 mol/L olar Solubility >=1 mol/L olar Solubility >=0.1 - <1 mol/L	donors 2 ACD acceptors 5 ACD olecular Weight 295.40 ACD ogP 0.667+/-0.641 ACD ogD -2.43 pH 1 ACD ogD -2.43 pH 4 ACD ogD -2.43 pH 7 ACD ogD 0.53 pH 7 ACD ogD 0.53 pH 10 ACD ogD 0.53 pH 10 ACD olar Solubility >=1 mol/L pH 1 ACD olar Solubility >=1 mol/L pH 1 ACD olar Solubility >=1 mol/L pH 7 ACD olar Solubility >=1 mol/L pH 7 ACD olar Solubility >=0.1 - <1 mol/L

(1) Calculated using Advanced Chemistry Development software Solaris V4.67, 2001.

CCCS

REGISTRY will offer new tools for polymer searching

- New polymer "linking" feature

 collects related polymers into one answer set
- New polymer structure/substructure searching feature
 - allows more flexible input of polymer structures



CASREACT now contains more reactions

- 5.7 million single and multi-step reactions back to 1974 (includes reactions from InfoChem)
- Journal and patent literature
- Reactions linked to CAplus documents
- Weekly updates

TOXCENTER enhances STN's toxicology offering



- >5 million records from journal literature and patents
- CAS RNs
- robust content from 4 databases
 - BIOSIS Previews/RN[®] from 1969-present
 - CAplus from 1947-present
 - International Pharmaceutical Abstracts (IPA) from 1970present
 - MEDLINE from 1958-present



BLAST[®] searching in the CAS Registry is now available in STN on the Web (http://stnweb.cas.org)



New Patent Look-Up tool available on STN Easy

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STNEasy	Easy Advanced	CAS Number Pate	ent
Search Page			Search Page
Easy Search Advanced Search CAS Number Search Patent Lookup	1. Select Your Cates 2. Enter one or mor	Patents	gory is: low. Terms will be joined with: AND 💌
+ Help Session Cost Price List	Title:	e g. plasma wekšng	Browse Index
Preferences Search History	Subject Words:	household cleaner e.g. surface layer	Browse Index
+ Cust. Support Home Page Comments	Inventor:	Last Name	Browse Index
Log Off	r	First Name	M.I.
	Patent Assignee:	Clorox e.g. Crucial Chemical Comp	Browse Index
	IPC Classification:	e.g. B2314009-00	Browse Index
	Patent Number or Patent Country:	e.g. EP1043108, EP	Browse Index
	Publication Date:	e.g. 19991028, 1999	Browse Index
	Application Number or Application Country:	e.g. EP1999-890401, EP	Browse Index



Announcing: STN Easy for Intranets Available June 16

- Create a customized site that makes STN Easy databases accessible to end-users
- IP authentication for STN Easy (loginIDs & passwords not needed)
- Deliver current-awareness search results
- Customize content, appearance, & access to full-text

Recent SciFinder release provided new content and functionality



- Nucleotide or Protein Sequence search
- Calculated physical properties
- Retrospective reaction coverage
- "Get related" information
- Ability to link to Spotfire DecisionSite for Lead Discovery software
- Ability to create Keep Me Posted (KMP) profiles based on structures



Recent SciFinder Scholar release included many new enhancements



- Retrospective reaction coverage
- Calculated physical properties
- Citation Linking
- Get Related Substances
- eScience[®] link
- More user preferences



STN improvements

New email delivery options for search results

- multiple formats (RTF, PDF, zipped HTML, plain text)
- graphic images
- links to full-text documents

This feature also available for SDIs! Available as of June 2 See also May/June *STNews* or June *STNewsline*

CCGS

STN EXPRESS V6 offers more tools and features

- RTF transcript files now contain live (fully functional)
 hyperlinks
- Expanded formats available for transcripts (EXCEL, HTML, ASCII, and RTF)
- Expand abbreviations feature added
- Improved Registry Number wizards
- Citation hyperlinks available
- Patent number hyperlinks available
- Improved Accounting function
- Auto-upgrade capability

CCS

STN EXPRESS Version 6 offers more tools and features

• Table Tool

 create a table of data, graphics, and/or chemical structures from STN answer sets for simple analysis

Report Tool

- create customized reports from STN search results
- Predefined Reports feature
 - allows users to quickly create patent reports with a professional, customized look and feel
- Graphical statistical summaries in reports or tables
- Print preview feature added



Announcing STN EXPRESS V. 6.01

- New professional-looking report options
 - Substance Report
 - Substance Report with Properties
 - Journal Report
 - Patent & Journal (combined) Report
 - Substance Table
 - Substance Table with properties
- Enhanced editing and formatting capabilities with postprocessing tools
- Launch CAS Registry BLAST
- Include BLAST alignment data within transcripts





CAS is using the web in innovative ways to...

- Link out to full-text documents
- Link in from full-text journal articles to a CAS abstract
- Link to relevant content via web search engines



 Communicate with customers and provide technical support



ChemPort content has grown since its introduction in 1997

- 155 publishers
- 3 patent suppliers
- Aggregators (EBSCO, HighWire...)

>3300 journals!



ChemPort connections get better...

- Site Administration Tool added
- Email citation feature added

Science Spotlight has also been enhanced



Announcing: Information Professional Web Pages Debuted June 9

- www.cas.org/infopro/index.html
- Focus on products geared to information professionals
- Selected CAS presentations
- Trade show information
- What's New information



New on www.cas.org : "Ask CAS" self help





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Power of the Web Value Added Tools



What's New from



Stop by our exhibit booth

