Overcoming Issues in Implementing Chemical Structure Searching

Ron Kaminecki

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ICIC Barcelona, ES

Abstract

Overcoming Issues in Implementing Chemical Structure Searching Across Disparate Data Sets

▸ Ron Kaminecki (Dialog, USA)

Consider data mining a data set for chemical nomenclature. As long as the data set contains relevant names for chemicals, processing can be systematised with the inevitable exceptions and special cases handled by the programmers as these issues occur. However, consider that the data sets are from disparate sources in which correct systematic names are *not* used by design or are intentionally made ambiguous as would be the case in, say, the open press or even patents. Also, consider literature sources such as newspapers or even trade journals which may make chemical names easier to read but not easier to resolve; but these sources cannot be dismissed simply because they make the problem of extracting and searching chemical names more difficult. Also, consider other technical sources such as dissertations or trade journals in which the level of resolution can vary not only by publication, but also from issue to issue. This presentation discusses some of the issues and solutions involved with implementing a chemical information system using various information sources.

Basic Agenda

Background

- Chemical market
- Chemical information sources
- Meeting the needs of one with the other

Developments

- Findings from customers
- Issues
- Going forward

Chemical market

- Dialog entered the chemical information market in the early 1970's
- Most users were librarians
  - Academic
  - Non-technical searchers at technical companies
  - Eventually, technical searchers were segmented from the business/legal/general searchers
- Images were limited due to sources, limited bandwidth for transmission, general technology
- Text was king

Chemical market

- Business blossomed with new features added
- Brunt of the business was on text searching
- Non-technical searchers found searching using terms easier than drawing pictures
- The use of structural data was often left to more technical searchers
- Quick name lookups, general articles, any information that could be found by a name was useful

Chemical market

- Name searching had to include IUPAC, CAS Systematic, trade names, trivial names, lab codes, trademarks, etc.
- Such names were indexed by themselves (e.g., “Klaritin” or “Acetominophen”) or algorithmically segmented
- All users found segmented terms useful and a bit easier to understand than images
- Algorithm broke up names starting from the back of the name and worked its way forward, identifying segments along the way

Chemical market

- Segments could be searched using proximity and also the searcher could specify if the segments were simply next to each other or taken from a specific substance in any order
- Segments could be searched across many databases using the same terms and logic
- Users could then output the type of data that they wished based upon where the hits were found
- Classes on searching chemical databases by non-chemists were amongst the most popular

Chemical market

- Data sources have changed with new technologies allowing the identification and extraction of substance data from text
- Text is now available that incorporates both technical and non-technical data, plus somewhere in between
- Many value added chemical substance dictionaries are available
- Based on user needs and available data the system is developing

Dialog®

What would a non-chemist professional searcher want?

Chemical information sources
Chemical Dictionaries

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DIALOG(R)File 398: Chemsearch
(c) 2011 Amer.Chem.Soc. All rights reserved.
FLD003:79794-75-5|
FLD004:201105|
FLD005:RNF201105^200912^200703^200309^200307^200301^200211^200202^199902^199703^
       199612|
FLD006:RAF199104|
FLD080:(01)_(nr=01;_sr=6;_ar=C5N.01;_fr=NC5.01;_ir=46 -156 -1 )^(01)_(nr=03;_sr=
       6,6,7;_ar=C5N.01-C6.01-C7.01;_fr=NC5.01-C6.01-C7.01;_ir=3068 -10 -3 )|
FLD101:C22H23ClN2O2|
FLD120:1-Piperidinecarboxylic acid_(9CI)|
FLD122:4-(8-chloro-5,6-dihydro-11H-benzo(5,6)cyclohepta(1,2-b)pyridin-11-ylidene
       )-|
FLD124:ethyl ester|
FLD160:11H-Benzo(5,6)cyclohepta(1,2-b)pyridine|
FLD164:1-piperidinecarboxylic acid deriv.|
FLD250:Alavert^Anhissen^Bonalerg^Civeran^Claratyne^Claritin^Claritine^Clarityn^C
       larityne^Clarotadin^Cronopen^Erolin^Flonidan^Fristamin^Histaloran^Klarife
       r^Klaritin^Lertamine^Lisino^Loracert^Loradex^Loranox^Lorastine^Loratadine
       ^Loratidine^Loratyne^Lorfast^Lowadina^Optimin^Polaratyne^Pylor^Restamine^
       Sch 29851^Sensibit^Sohotin^Tadine^Velodan^Zeos|
FLD010:CHEMNAME|
FLD011:1673|
FLD999:398|
```

Chemical information sources
Chemical Dictionaries

- Traditional data from Chemical Abstracts
- Very directed to substances
- Segmentation of CAS Systematic Names and appropriate synonyms
- Value added
  - Key identifiers
  - Human indexing
  - Reliable, reviewed, edited, corrected

Chemical information sources
Press Releases

DIALOG(R)File 781: ProQuest Newsstand

Codexis Names David Anton CTO & SVP, Process Development & Manufacturing
Credits, Codexis, Inc.
PRNewswire , P n/a
Thursday , February 24, 2011

REDWOOD CITY, Calif., Feb. 24, 2011 /PRNewswire/ -- Codexis, Inc. (Nasdaq: CDXS) today announced that David Anton, Ph.D. has been promoted to Chief Technology Officer and Senior Vice President, Process Development and Manufacturing, a new position. He will continue to report to Alan Shaw, Ph.D., President and Chief Executive Officer.

Chemical information sources
Press Releases

Dr. Anton joined DuPont in 1983, and held a variety of senior research management positions across bioprocessing and biocatalysis. He led the process research, development and commercialization of several products, including 1,3 propanediol (a chemical intermediate used in a variety of industrial applications ranging from airplane deicing fluids to textiles and carpet). As Vice President, Research and Development for DuPont's joint venture with Tate and Lyle, he directed technology start-up activities for the first 100 million-pound plant for 1,3 propanediol, commissioned in Loudon, TN in 2006. As Venture Manager, Biofuels, he was global business lead for development of DuPont's advanced biofuel, biobutanol.

Chemical information sources
Press Releases

- Probably a good hit, giving the players in the field, some capacity information, partners
- Certainly not too technical; more business information
- This is a press release
- Dr. David Anton. Dr. Alan Shaw – would it make sense to link their doctoral dissertations
  - Dr. David Anton has a 1980 thesis on the characterization of Cobalamin (Vitamin B-12)
  - Dr. Alan Shaw – there are nine dissertations with variations of the name Alan Shaw

Chemical information sources
Newspapers

DIALOG(R)File 781: ProQuest Newsstand

Water-basedsealants protectgarage floors
Chicago Daily Herald , All ED , P 1
Sunday , August 21, 2011

Text:
Q. I recently purchased a condo with a one-car garage. The floor is cracked in three places coming from the drain in the lower center of the floor. I want to put some type of coating over the entire garage floor after the cracks are fixed. I live in western Pennsylvania and need something that would hold up to the salt that is used in the winter months. What would you recommend?

Chemical information sources
Newspapers

A. Some concrete or masonry sealants are not available in a number of states because of the solvent in them. So the industry is moving toward water-based sealants, which have proved to be effective and more environmentally acceptable. Euclid Chemical makes Baracade WB 244, a siloxane/silane-based blend that provides deep penetration and good surface repellency. There are others. Call a masonry-supply house in your area to get the brand they carry. The garage floor will need to be thoroughly clean and dry. You can clean it with TSP-PF (phosphate free), following directions on the container.

Chemical information sources
Newspapers

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Chemical information sources

- Very general information, though potentially useful to a non-technical user
- Could still be useful to a patent searcher
- Tradenames for chemicals
- General category of chemicals using a tradename
- TSP-PF

Chemical information sources
Combined News

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DIALOG(R)File 781: ProQuest Newsstand
(c) 2011 ProQuest Info&Learning. All rights reserved.
FLD001:THE WONDER STUFF ; It's bendy -- yet so strong a sheet of it as thin as c
       lingfilm could support an elephant. The discovery that could change the w
       orld (Eire Region)|
FLD006:   The 'miracle material' was discovered in Britain just seven years\ago,
        and the buzz around it is extraordinary. Last year, it won two\scientist
       s, from Manchester University in north England, the Nobel\Prize for physi
       cs, and this week Pounds 50million (EUR 58 million)\was pledged towards d
       eveloping technologies based on the super-\strong substance. In terms of
       its economics, one of the most\exciting parts of the graphene story is it
       s cost. Normally when\scientists develop a new wonder material, the price
        is eye-\wateringly high.^   But graphene is made by chemically processin
       g graphite -- the\cheap material in the 'lead' of pencils. Every few mont
       hs\researchers come up with new, cheaper ways of mass producing\graphene,
        so that some experts believe it could eventually cost less\than EUR 5 pe
       r pound.^   But is graphene really the wonder stuff of the 21st century?
       For\a material with so much promise, it has an incredibly simple\chemical
        structure. A sheet of graphene is just a single layer of\carbon atoms, l
       ocked together in a strongly-bonded honeycomb\pattern.^   That makes it t
       he thinnest material ever made. You would need to\stack three million gra
       phene sheets on top of each other to get a\pile one millimetre high. It i
       s also the strongest substance known\to mankind -- 200 times stronger tha
       n steel and several times\tougher than diamond.^   A sheet of graphene as
        thin as clingfilm could hold the weight of\an elephant. In fact, accordi
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Chemical information sources
Combined News

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Chemical information sources
Combined News

- Potential for mistakes is high in a combined source
- Loose usage of language and proximity to actual chemical terms confuses the issues

Chemical information sources
Ship Manifests

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DIALOG(R)File 571: Piers Exports(US Ports)
(c) 2011 Commonwealth Bus. Media. All rights reserved.
FLD001:64285425|
FLD005:NETHLDS|
FLD007:NETHERLANDS|
FLD010:EASTMAN CHEMICAL|
FLD015:2 2 DIMETHYL PROPANE 1 3 DIOL^2 DIMETHYL PROPANE 1 3 DIOL // 2^DIMETHYL P
       ROPANE 1 3 DIOL // 2 2^PROPANE 1 3 DIOL // 2 2 DIMETHYL^1 3 DIOL // 2 2 D
       IMETHYL PROPANE^3 DIOL // 2 2 DIMETHYL PROPANE 1^DIOL // 2 2 DIMETHYL PRO
       PANE 1 3|
FLD025:DIOL, SULFONATED & POLYALCOHOLS^SULFONATED & POLYALCOHOLS // DIOL,^& POLY
       ALCOHOLS // DIOL, SULFONATED^POLYALCOHOLS // DIOL, SULFONATED &|
```

Chemical information sources
Ship Manifests

- Varied data – this record has specifics, others list more generic data
- Indexing is more generic
- Chemical names are at term level
- Next level would be segmentation of the chemical names (some are illustrated)
- Decisions regarding locants

Chemical information sources
Dissertations

DIALOG(R)File 35: Dissertation Abs Online

FLD002:Piezoelectricity in Polyvinylidene Fluoride (PVDF) was observed long back and significant development has been made since its discovery. The theory on this property has predominantly revolved about the polymorphism and unique structure of PVDF. Of the four structures PVDF can be fabricated namely α, β, γ and δ, apart from the α phase
the other 3 have piezoelectricity property in them. This thesis concentrates on the β phase PVDF as they have the highest piezoelectric effect present due to non cancellation of dipoles. In the past, research in the β phase PVDF was conducted in stretched films. This thesis concentrates on the film properties in the unstretched condition. Flexoelectricity is a property which was first observed in 1969 in crystalline dielectric materials. The extension of this phenomenon in PVDF films is discussed in the thesis. Flexoelectricity is more dominant in the micro and nano sc

Chemical information sources
Dissertations

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FLD003:The direct flexoelectric effect observed in polyvinylidene fluoride films
       |
FLD004:ENGINEERING, MECHANICAL ^ENGINEERING, MATERIALS SCIENCE|
FLD007:2665|
FLD008:50|
FLD009:AADAAI1488981|
FLD012:3|
FLD014:4904|
FLD031:02559027|
FLD032:Ramachandran, Narayanan|
FLD033:0548^0794|
FLD034:0656|
FLD036:978-1-124-47705-3|
FLD037:State University of New York at Buffalo|
FLD040:Adviser: John Y. Fu|
FLD041:Fu, John Y.|
FLD043:2011|
FLD044:M.S.|
FLD099:MAI|
FLD100:Engineering, Materials Science|
FLD999:035|
```

Chemical information sources
Dissertations

- Record shows only abstract
- Would fulltext be useful?
- How about the dissertation's bibliography?
- Chemical names tend to be spelled out, then abbreviations are used for readability
- Maybe link out to the documents in the bibliography and incorporate them…

Chemical information sources
Combined News

```
DIALOG(R)File 991: Newsroom 2010
(c) 2011 Dialog. All rights reserved.
FLD001:High-mobility graphene nanoribbons prepared using polystyrene dip-pen nan
       olithography.|
FLD002:20110420|
FLD007:Dip-pen nanolithography and polystyrene etching techniques are utilized t
       o fabricate graphene nanoribbons (GNRs) on a SrTi[O.sub.3]/Nb-doped SrTi[
       O.sub.3] substrate. The atomically flat surface and the large dielectric
       constant of the insulating SrTi[O.sub.3] layer, respectively are responsi
       ble for the bipolar FET behavior with a high mobility and low operation v
       oltage at room temperature exhibited by the GNR field-effect transistor (
       FET).^Copyright (c) 2011 Gale, Cengage Learning. All rights reserved.|
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Chemical information sources

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Chemical information sources

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       oltage at room temperature exhibited by the GNR field-effect transistor (
       FET).^Copyright (c) 2011 Gale, Cengage Learning. All rights reserved.|
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Chemical information sources

- Molecular formulae can be identified easily
- Terms of art
- Semi-scientific abbreviations, acronyms

ProQuest Dialog DataStar

Advanced search

Search tips

Full text

Search industries Image view

Patents Search »

Databases

- Americas Patent Collection
- Asia Patents Collection
- Derwent Patents Citation Index®
- Derwent World Patents Index®
- European Patents Fulltext
- Europe Patent Collection
- Fulltext Patent Collection
- IMS Patent Focus
- INPADOC / Family and Legal Status
- JAPIO - Patent Abstracts of Japan
- LitAlert®

Pharmaceutical & Biomedical Search »

Databases

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Trademarks Search »

Databases

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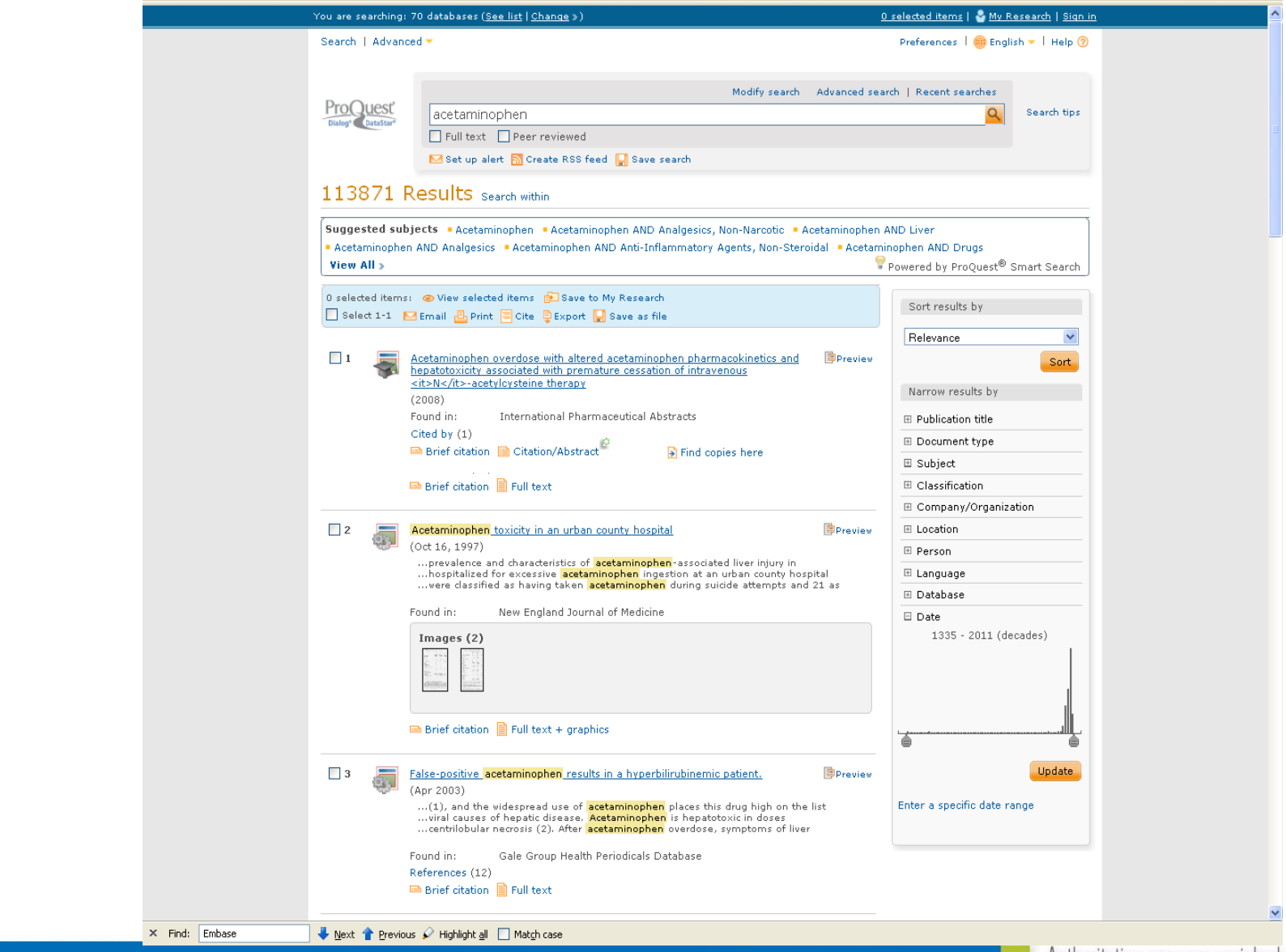
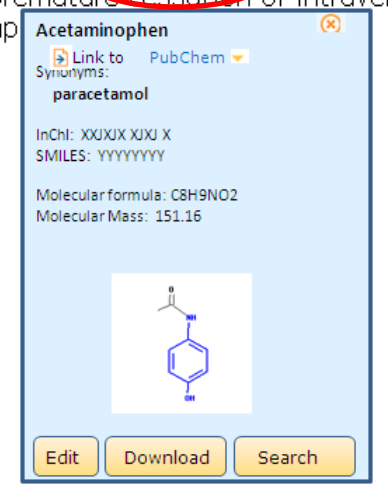
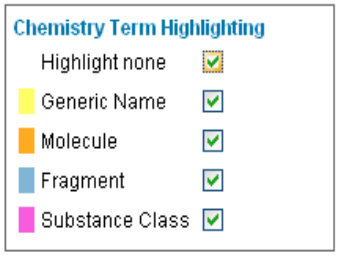
Possible solution



Possible solution

Acetaminophen overdose with altered acetaminophen pharmacokinetics and hepatotoxicity associated with premature cessation of intravenous <it>N</it>-acetylcysteine therap





OBJECTIVE: To report a case of erratic absorption, double peak serum concentrations, and hepatotoxicity following premature cessation of intravenous N-acetylcysteine (NAC) treatment in the setting of a massive acetaminophen overdose.
CASE SUMMARY: A 78-year-old man reportedly ingested approximately 96 immediate-release acetaminophen 500-mg tablets (48 g) over a one-hour period in an apparent suicide attempt. The acetaminophen concentration at 2.25 hours was 264 mug/mL. Intravenous NAC was initiated 5 hours postingestion. At 6.25 hours postingestion, the acetaminophen concentration was 281 mug/mL. Following administration of intravenous NAC for 21 hours, therapy was discontinued despite a residual acetaminophen concentration of 116 mug/mL. The patient experienced hepatotoxicity, coagulopathy, and renal injury. Pharmacokinetic analysis revealed significantly prolonged acetaminophen absorption and a second peak acetaminophen concentration of 228 mug/mL approximately 48 hours postingestion. Direct in-hospital monitoring of the patent made a second ingestion unlikely.
DISCUSSION: Acetaminophen overdose is usually effectively managed with NAC. Patients with massive ingestions may have altered absorption kinetics due to acetaminophen's solubility being exceeded, physiologically or chemically altered gastrointestinal emptying or motility, or other factors. These patients may benefit from gastrointestinal decontamination and prolonged NAC therapy.
CONCLUSIONS: In patients with massive acetaminophen ingestion, erratic absorption may occur, and toxic serum concentrations may persist beyond a standard 21-hour course of intravenous NAC therapy. Acetaminophen concentrations and aminotransferase levels should be evaluated at the completion of the intravenous NAC infusion to ensure complete elimination of acetaminophen and absence of hepatotoxicity and to exclude the need for prolonged treatment.

Findings from customers

You are searching: 1 database (See list | Change ») 2 Recent searches | 0 Selected items | My Research | Sign in

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United States Patents Fulltext

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Full text « Back to results Document 1 of 1

Add to selected items Save to My Research
Email Print Cite Export Save as file Tags

More like this
See similar documents

Objective with fluoride crystal lenses

Krähmer, Daniel; Gruner, Toralf; Ulrich, Wilhelm; Enkisch, Birgit; Gerhard, Michael; et al. United States Patents Fulltext

Other formats: Brief citation Link to PDF

Bibliographic information | Claims | Legal status | Specification | Cited references | Citing patents | Family members (1)

Abstract (summary) Translate

eng English An objective for a microlithography projection system has at least one fluoride crystal lens. The effects of birefringence, which are detrimental to the image quality, are reduced if the lens axis of the crystal lens is oriented substantially perpendicular to...
Show all

Indexing (details) Cite

Assignee	Carl Zeiss SMT AG DE
Inventor	Krähmer, Daniel Aalen, DE Gruner, Toralf Aalen-Hofen, DE Ulrich, Wilhelm Aalen, DE Enkisch, Birgit Aalen, DE Gerhard, Michael Aalen, DE Brunotte, Martin Aalen, DE Wagner, Christian KS Eersel, NL Kaiser, Winfried Aalen, DE Maul, Manfred Aalen, DE Zaczek, Christof Heubach, DE
Publication number	US 7145720 B2 (05 December 2006)
Application number	US 10367989 (08 May 2002)
Priority number	DE 10123725 (15 May 2001) DE 10123727 (15 May 2001) DE 10125487 (23 May 2001) DE 10127320 (06 June 2001)

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Possible solution

Other formats: Brief citation Link to PDF

Bibliographic information | Claims | Legal status | Specification | Cited references | Citing patents | Family members (1)

Abstract (summary) Translate

eng English An objective for a microlithography projection system has at least one fluoride crystal lens. The effects of birefringence, which are detrimental to the image quality, are reduced if the lens axis of the crystal lens is oriented substantially perpendicular to...
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Priority number	DE 10123725 (15 May 2001) DE 10123727 (15 May 2001) DE 10125487 (23 May 2001) DE 10127320 (06 June 2001) DE 10210782 (12 March 2002)
Related application	PCT: WO EP0205050 (2002-05-08) Continuation: US PCT/EP02/05050 (2002-05-08)
IPC classification	Current v8: G02B 5/30 (main); G02B 13/24 (main); G02B 1/00; G02B 1/02; G02B 17/08; G03F 7/20; H01L 21/02; H01L 21/027 More details
ECLA classification	G02B 1/02; G02B 1/08; G02B 5/30 R; G03F 7/20 T12; G03F 7/20 T26
US classification	359/499 (main)
Language	English
Application language	English
Legal representative	Fish & Richardson P.C. (Attorney)
Examiner	Sugarman, Scott J (examiner)
US field of search	359/355; 359/497; 359/499; 359/720; 359/724; 359/726
Document features	23 literature citations; 114 cited patents; 4 citing patents 98 claims; 2 legal status entries
Accession number	US7145720B2
Document URL	http://stable.aa1.proquest.com/patents/docview/15262931?accountid=91509

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Findings from customers

Findings from customers

- Does coverage of newspapers/newswires, etc., have value in chemical searches?
- Do dissertations hold their own
  - Titles/Abstracts
  - Full text
  - bibliographies
- What about annual reports, quarterly reports/investment newsletters

Findings from customers

- Any new system would have to merge a technical database with a non-technical one and leave the searcher to output what is desired
- Additional indexing, metadata, even linking to chemical structures/images would be a bonus

Findings from customers

- Markush is not a high priority, but reactions are
- Any structure searching should work with major programs, browsers, compatible with major output formatting (Bizint, Excel, etc.), and work with normal tools/formats (Java,etc.)
- Price sensitivity
- Structure searching in non-technical databases
- Highlighting in full text

Findings from customers

- Semantics
  - Users still see it as a “black box”
  - Extremely useful for a different viewpoint
- Markush
  - On newspapers?
  - Do non-technical searchers need this level?
- Substructure searching?
- Tautomers, optical activity, isotopes, etc., level of detail?

Overall

- New market, new data unlike the old, though users want old and new data combined
- Linking considerations
  - Fields like authors, companies
  - Other data sources like bibliographies
- Treatment of non-scientific and scientific text changes meaning of chemical terms and their structures
- Incorporation of dictionary data with non-technical information

Thank you for your time

Ron Kaminecki

Dialog LLC

Ron.kaminecki@dialog.com

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