

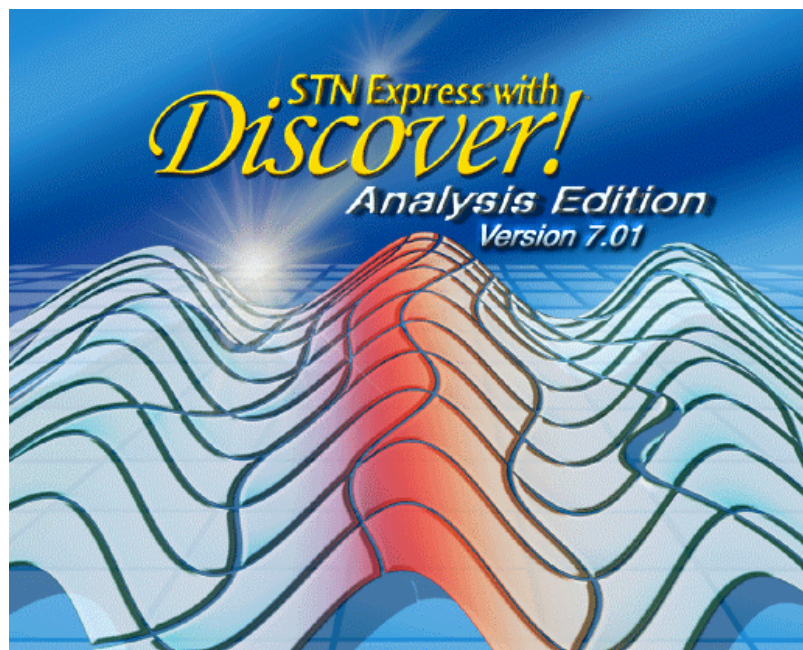
STN[®]

**New Analysis and Visualization Tools
in STN Express[®]
with *Discover!*[™], Version 7.01**

STN Patent Forum
July 2004

STN Express with *Discover!*, Analysis Edition, Version 7.01, extends your ability to analyze and visualize search results

- **Free** upgrade for Version 7.0 users
- New Analyze Plus Wizard
- New interactive Cross-tab capability
- REGISTRY Wizard enhancements
- Improved post-processing of patent information in tables and reports



The *Analyze Plus Wizard* provides improved statistics and saves time

- May now be used with multiframe answer sets
- Allows **data grouping** of Inventor/Author and Patent Assignee/Company Names
 - Automatic grouping of similar names
 - Grouping may be manually adjusted as desired
 - Specific groupings may be saved for future use
- Other selected fields may be manually grouped

The *Analyze Plus Wizard* allows field selection and grouping of terms

STN Analyze Plus

STN Express with Discover!

Analyze this L-number on 1 or 2 fields. Select "Group similar terms" to be able to group terms within a field. The results will be charted in MS Excel.

Click Analyze to process the information. Click Cancel to exit.

One field analysis

Two field analysis

Select first field

- Author/Inventor Name
- Corporate Source/Patent Assignee
- Company Name
- Publication Year
- Controlled Terms
- Patent Country
- National Classification
- WIPO International Classification

by SubClass by Main group All

Group similar terms

Options

Select second field

- Author/Inventor Name
- Corporate Source/Patent Assignee
- Company Name
- Publication Year
- Controlled Terms
- Patent Country
- National Classification
- WIPO International Classification

by SubClass by Main group All

Group similar terms

< Back Analyze Cancel

278 answers are available to analyze.

Options limit by number of terms and length, or add custom fields

Analyze Plus Wizard Options

First Field - (Author/Inventor)

Terms to view All

Truncate text to

Fields

None Alternate Custom

Field Name

Field Code

Sort

alphanumerically by frequency

Second Field - (Publication Year)

Terms to view All

Truncate text to

Fields

None Alternate Custom

Field Name

Field Code

Sort

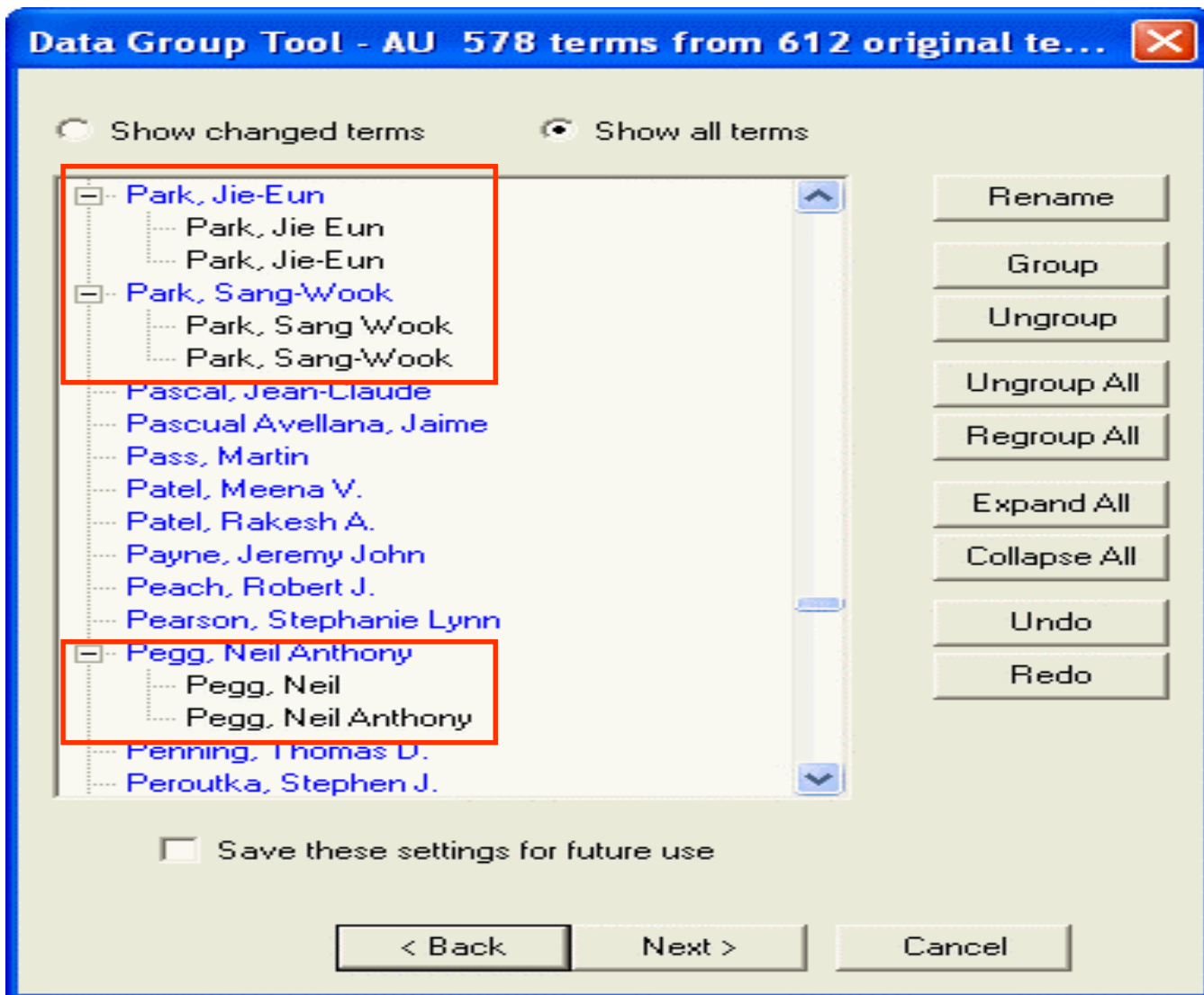
alphanumerically by frequency

OK

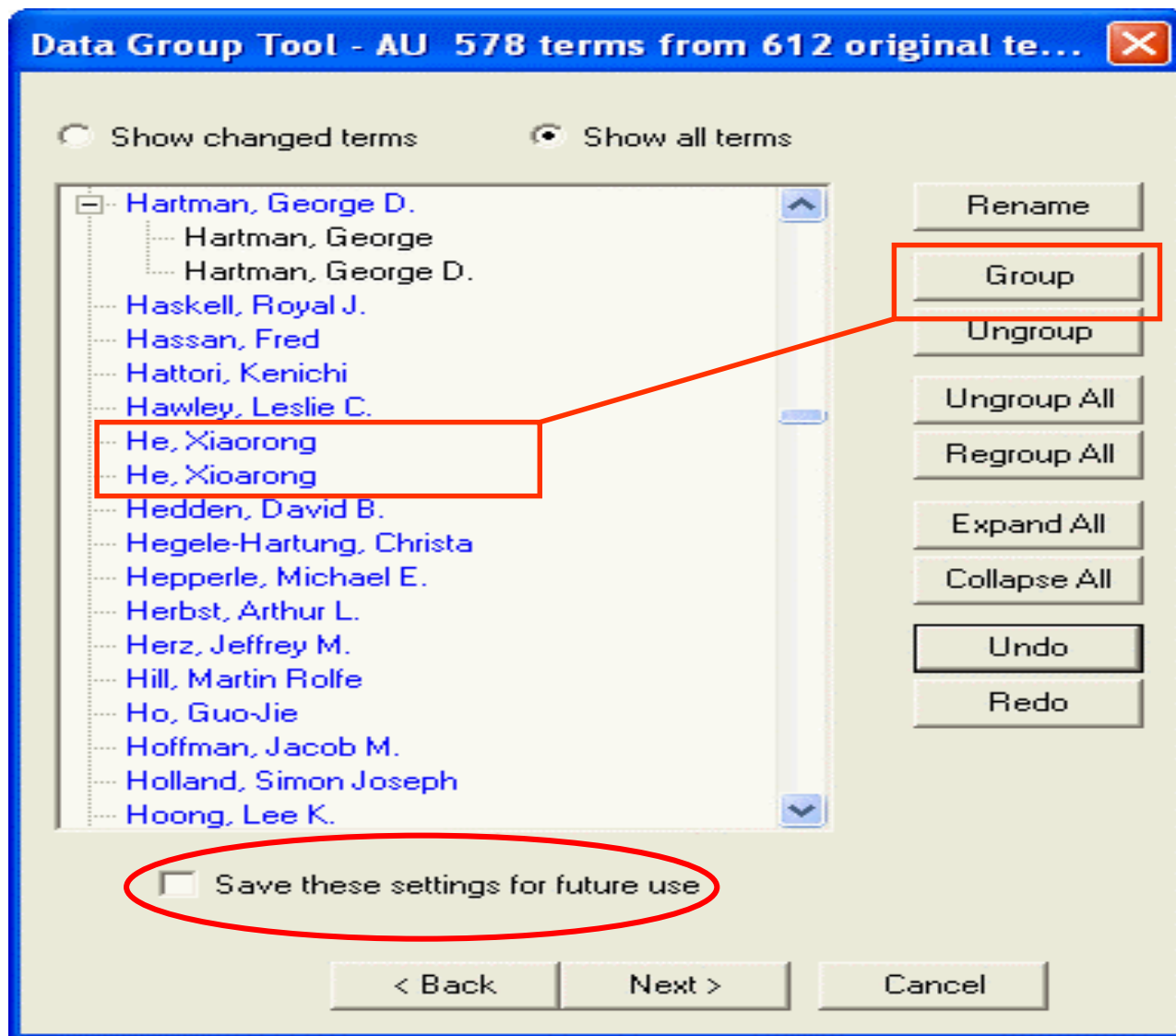
Cancel

Help

Similar inventor names are automatically grouped



Additional inventor names may be manually grouped and saved



Analyze answer sets to determine trends, new research areas, and competitive intelligence

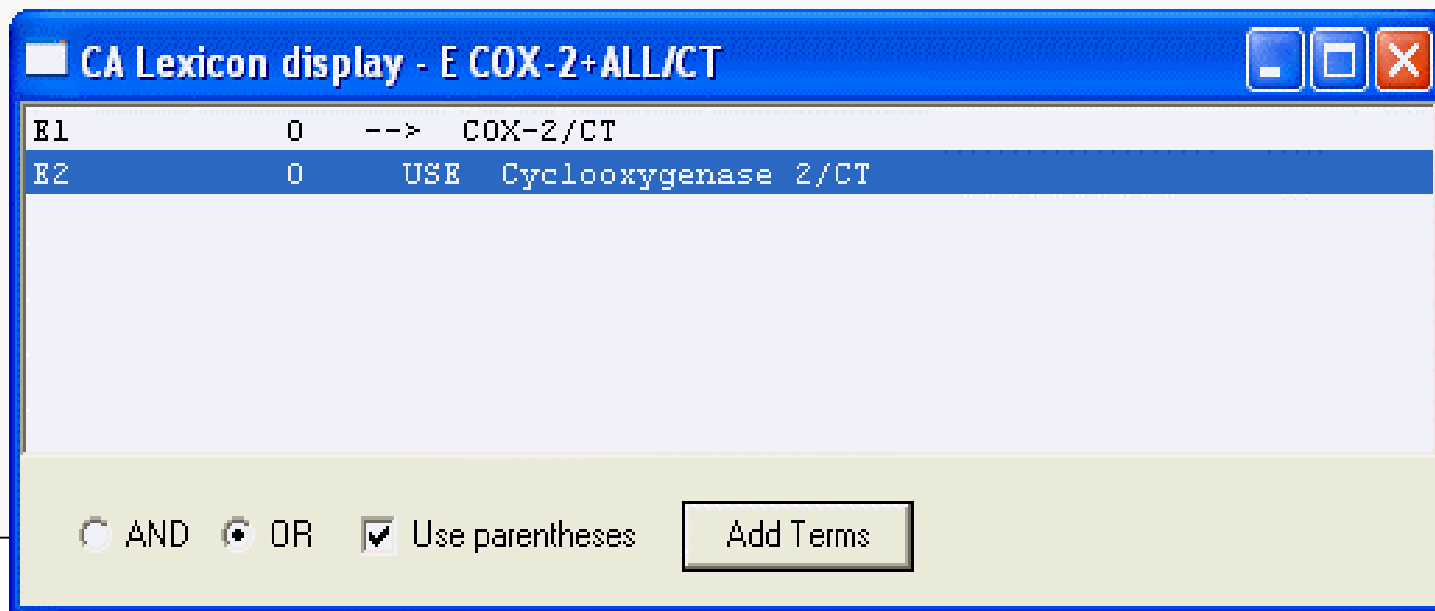
Search Question:

- Determine the top 10 companies with new patent publications on Cox-2 inhibitors from 2001-2004.
- Identify therapeutic uses defined in these patents.
- Find new analgesic substances reported in these patents containing a carboxamide functional group.

The CA Lexicon interface guides you to appropriate controlled terminology

=> FILE CAPLUS
=> SET PLURALS ON
=> S **COX-2**

Search terms in the CA Lexicon are highlighted. Right-click to view the hierarchy of terms.



Create the answer set enhanced with terms from the CA Lexicon

```
=> S (COX-2 OR "Cyclooxygenase 2")
L1      8636 COX-2 OR "CYCLOOXYGENASE 2"

=> S L1(L)INHIBITOR(L)THU/RL
L2      968 L1(L)INHIBITOR(L)THU/RL

=> S L2 AND P/DT
L3      421 L2 AND P/DT

=> S L3 AND PY.B>=2001
      3266449 PY.B>=2001
L4      278 L3 AND PY.B>=2001
```

Select the *Analyze Plus* button to start the visualization of search results

STN Online and Results

File Edit Online Query Results Preferences! Web Window Help

STN

465145 INHIBITORS
717228 INHIBITOR
(INHIBITOR)
603179 THU/RL
968 L1 (L) INHIBITORS

L2

=> S L2 AND P/DT
4379014 P/DT

L3

421 L2 AND P/DT

=> S L3 AND PY.B>=2001
3266449 PY.B>=2001

L4

278 L3 AND PY.B>=2001

Select Discover! Wizard

Choose a search wizard:

- Select Database
- Author
- CAS Registry Number
- Chemical Name
- Corporate Source
- Subject
- Edit alert

Select an L-number:

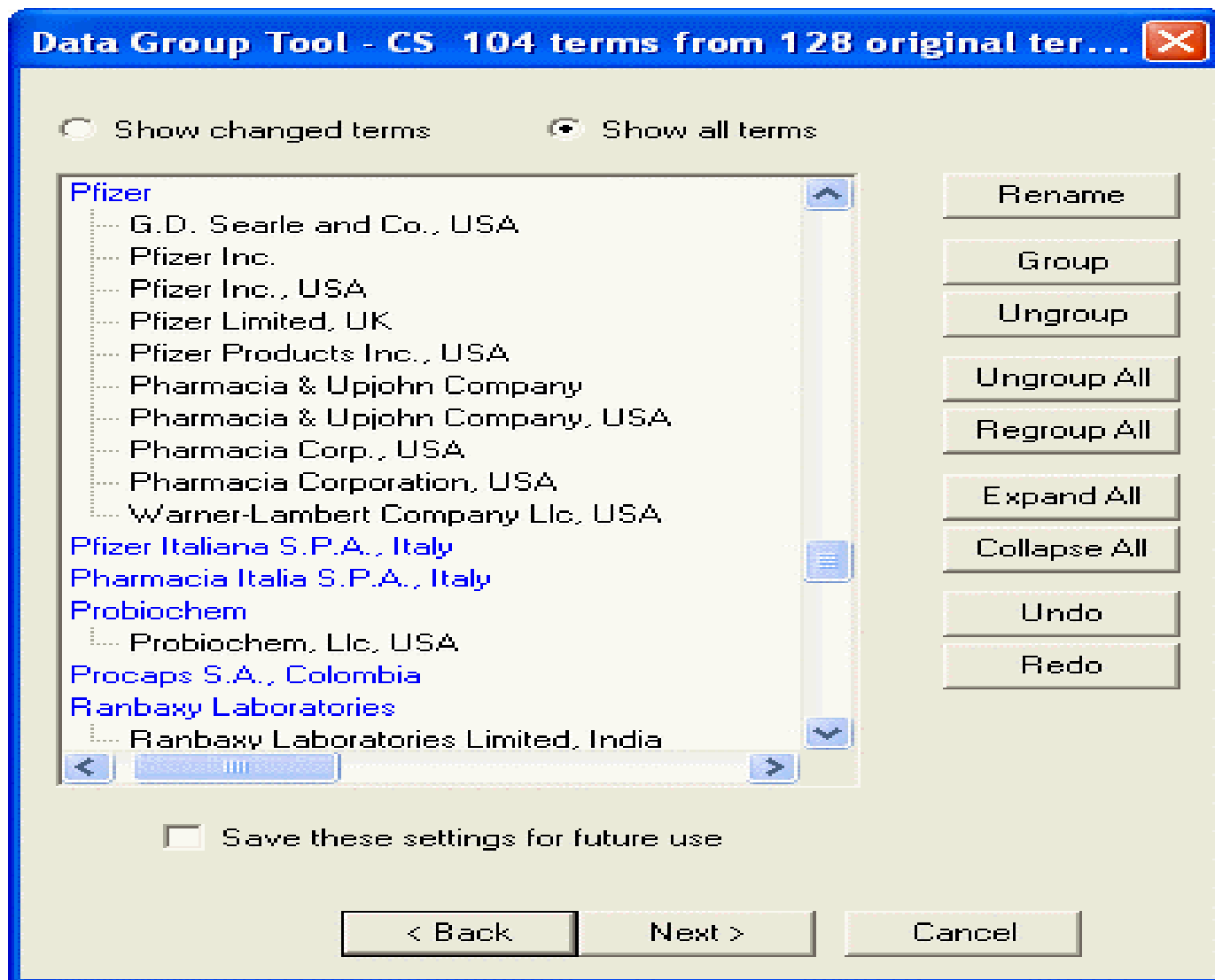
- L1 8636 ...
- L2 968 ...
- L3 421 ...
- L4 278 ...

Choose a results wizard:

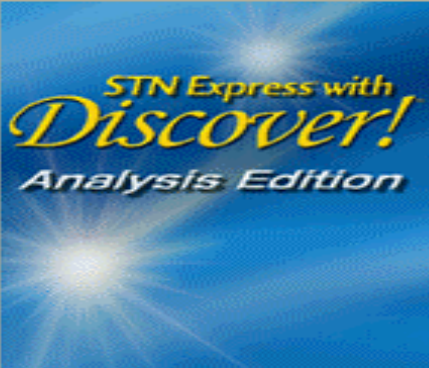
- Analyze Plus**
- Display
- Refine
- Save
- Save R-group data
- Save for SciFinder
- Get related polymers
- Get related sequences
- Create Single-file SDI
- Go to L-number

Discover! Transcript: C:\CASNC\STN Express\Trnsript\cox.tr CAPLUS INS Hold Off Print Off Online 00:07:14

Automatic grouping of assignee names provides more accurate statistics

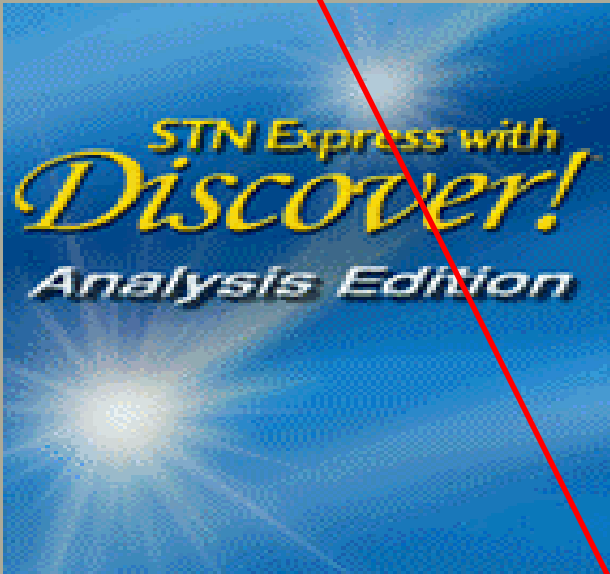


The *Cross-tab* automatically appears with live links back to STN

	A	B	C	D	E	F	G	H
1		2001	2002	2003	2004			
2	Pfizer	14	18	32	14			
3	Merck	8	4	9	4			
4	USA	2	9	8	6			
5	GlaxoSmithKline	5	5	2	3			
6	Immunomedics			6	4			
7	Novartis A.-G., Switz.			7	2			
8	Novartis Pharma			7	2			
9	Nitromed	1	1	1	5			
10	Bristol-Myers Squibb	1	2	3	1			
11	Cj			3	4			


The *Display Wizard* shows the selected answers

The screenshot shows the STN software interface. The 'Display Wizard' dialog box is open, showing a preview of the 'STN Express with Discover! Analysis Edition' logo. The dialog box is titled 'Display Records' and has a red box around it. A red arrow points from the dialog box to the data table below. The data table has columns labeled A, B, C, D, and E, and rows labeled 1, 2, and 3. The data in the table is as follows:

	A	B	C	D	E
1		2001	2002	2003	2004
2	Pfizer	14	18	32	14
3	Merck	8	4	9	4

All valid formats are included as advanced display options

STN Analyze Plus



To display retrieved answers, select an Answer range and a Display format, then click Display.

Click Finish to return to STN.

78 answers have been retrieved.

Answer range:

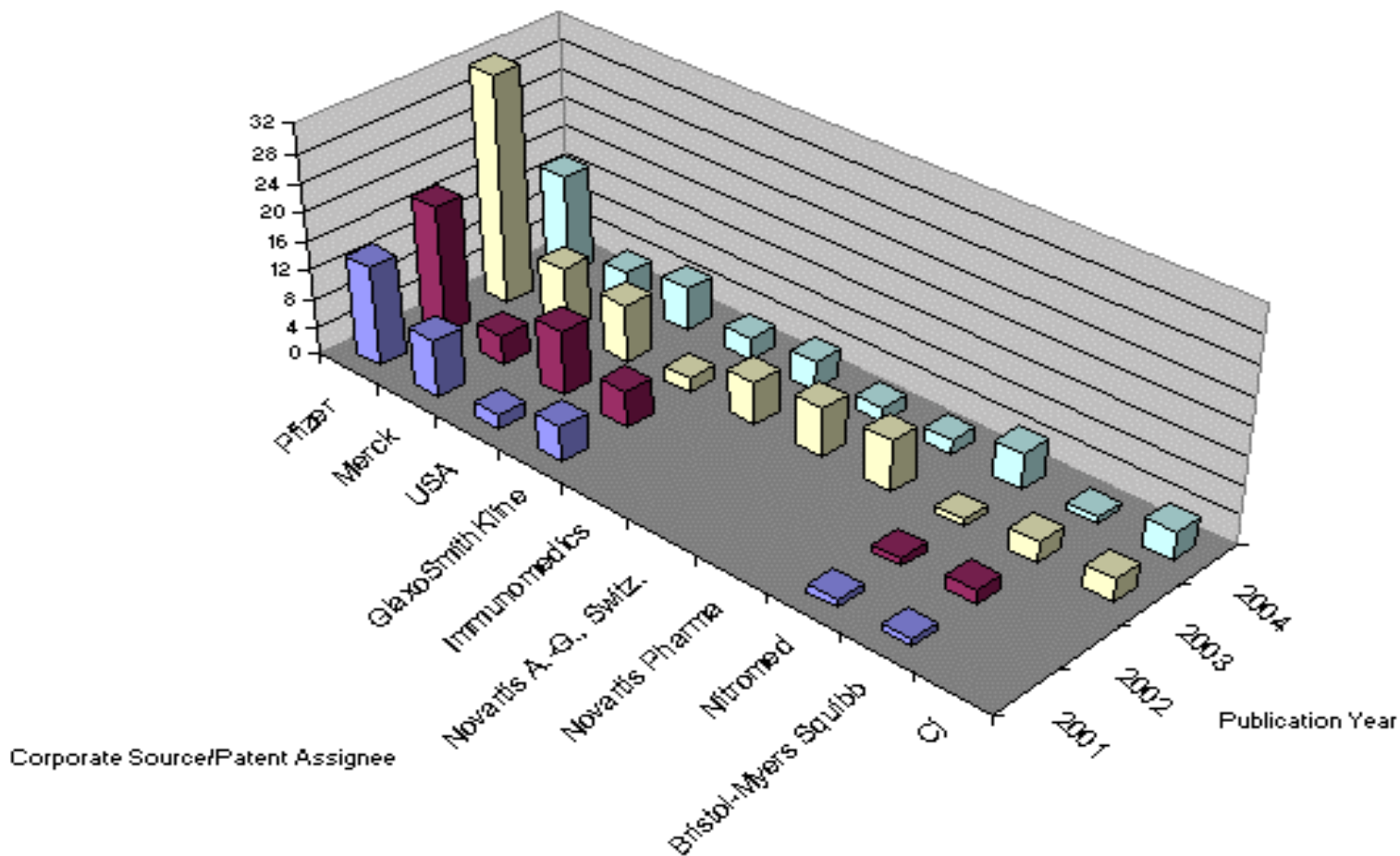
Display format: Basic Advanced

ALL
ALL
APPS
BIB
CAN
CBIB
DALL
DMAX
FAM
FBIB
IABS

< Back Display Finish

A 3-D bar chart is also provided on a separate Excel worksheet

Analysis of "Corporate Source/Patent Assignee" by Publication Year



Select the Pfizer records identified by the ANALYZE command

```
=> D L6 CS 1-
```

```
L6          ANALYZE L4 1- CS PY.B :      132 TERMS
```

```
TERM #      # OCC  # DOC  % DOC  CS PY.B
```

```
-----
```

5	48	48	17.27	PHARMACIA CORPORATION, USA
6	25	25	8.99	USA
7	17	17	6.12	PFIZER PRODUCTS INC., USA
8	16	16	5.76	MERCK & CO., INC., USA
9	13	13	4.68	GLAXO GROUP LIMITED, UK

```
  O O O
```

```
=> SELECT L6 5 7 20 25 32 64 100-103
```

```
E1 THROUGH E10 ASSIGNED
```

Combine the selected company names with the Cox-2 search

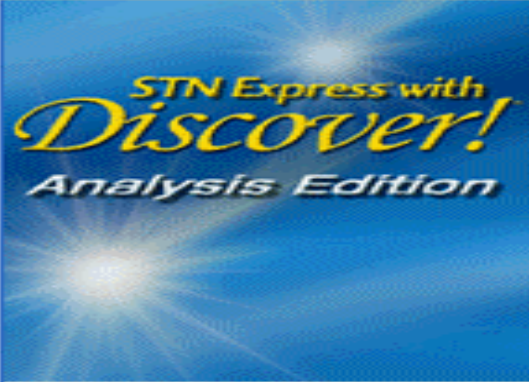
=> D SEL

E1	48	PHARMACIA CORPORATION, USA/CS
E2	17	PFIZER PRODUCTS INC., USA/CS
E3	4	PHARMACIA & UPJOHN COMPANY, USA/CS
E4	3	WARNER-LAMBERT COMPANY LLC, USA/CS
E5	2	PHARMACIA CORP., USA/CS
E6	1	G.D. SEARLE AND CO., USA/CS
E7	1	PFIZER INC./CS
E8	1	PFIZER INC., USA/CS
E9	1	PFIZER LIMITED, UK/CS
E10	1	PHARMACIA & UPJOHN COMPANY/CS

=> S L4 AND E1-E10

L7	78	L4 AND ("PHARMACIA CORPORATION,USA"/CS OR O O O
----	----	--

Uses can be identified by additional analysis of the Controlled Terms

	A	B	C	D	E
1		2001	2002	2003	2004
2	Drug Delivery Systems	10	13	21	14
3	Human	1	12	26	3
4	Anti-Inflammatory Agents	6	7	17	6
5	Analgesics	5	8	16	2
6	Pain		2	18	6
7	Heart, Disease	3	3	12	4
8	Antitumor Agents	2	3	12	4
9	Antiarthritics	3	1	13	3
10	Neoplasm	1	1	14	4



Substances can be identified by transferring CAS RNs into REGISTRY

```
=> S L7 AND ANALGESICS/CT
```

```
L9          31 L7 AND ANALGESICS/CT
```

```
=> FILE REGISTRY
```

```
=> TRANSFER L9 1- RN
```

```
L10         TRANSFER L9 1- RN      1510 1510
```

```
L11         1510 L10
```

```
=> S L11 RAN=312487-43-7,
```

```
L12         517 L11
```

```
=> D SCAN IN
```

```
L12  517 ANSWERS      REGISTRY  COPYRIGHT 2004 ACS on STN  
IN   1H-Indole-1-carboxamide, 5-chloro-2,3-dihydro-3-[(5-  
methylpyrazinyl)carbonyl]-2-oxo-N-propyl- (9CI)
```

A range of CAS RNs is used to restrict answers to new substances only. Use **HELP RNYEAR** to determine the appropriate starting point.

Run a SUBSET search on CAS RNs that appeared in the CAplusSM records

```
=> S L13 SUB=L12 FULL
```

```
FULL SUBSET SEARCH INITIATED 14:17:06 FILE 'REGISTRY'
```

```
FULL SUBSET SCREEN SEARCH COMPLETED - 255 TO ITERATE
```

```
100.0% PROCESSED 255 ITERATIONS 253 ANSWERS
```

```
SEARCH TIME: 00.00.01
```

```
L18 253 SEA SUB=L12 SSS FUL L16
```

Refine set and Save R-group data for R-group Analysis Table Tool

Limit to single component substances. Remove metal-containing compounds and incompletely defined substances.



=> S L15 AND 1/NC NOT (M/ELS OR IDS/CI)
L16 225 L18 AND 1/NC NOT (M/ELS OR IDS/CI)

The largest common structure is derived from the saved data

R-group Analysis Table Tool

Define the common structure upon which to conduct an R-group analysis of the answer set:

- Use the largest common structure
- Use a saved structure query file

Define Structure

Rename R-groups

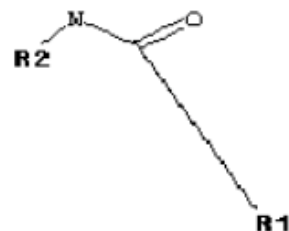
Include only answers in which

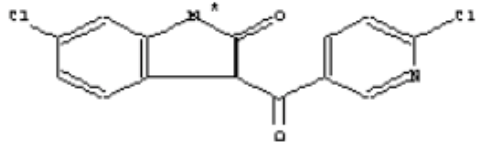

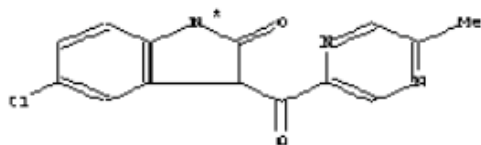
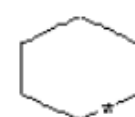
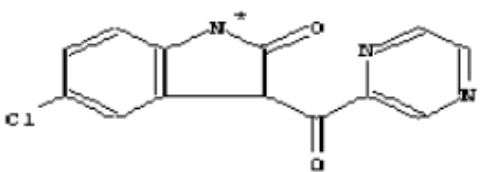
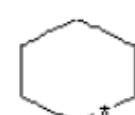
R-group:

Attaches at the following atom(s):

Save Template **Finish** **< Back** **Next >** **Cancel**

The completed table shows core structure, R-groups, and selected fields



CAS Registry Number®	IndexName	R1	R2
618903-23-4 REGISTRY	1H-Indole-1-carboxamide,6-chloro-3-[(6-chloro-3-pyridinyl)carbonyl]-N-ethyl-2,3-dihydro-2-oxo-(9CI)		
618903-22-3 REGISTRY	1H-Indole-1-carboxamide,5-chloro-N-cyclohexyl-2,3-dihydro-3-[(5-methylpyrazinyl)carbonyl]-2-oxo-(9CI)		
618903-21-2 REGISTRY	1H-Indole-1-carboxamide,5-chloro-N-cyclohexyl-2,3-dihydro-2-oxo-3-(pyrazinylcarbonyl)-(9CI)		

REGISTRY wizard enhancements provide easier and more comprehensive search results

- REGISTRY properties (experimental and calculated) are available from redesigned wizards
- POLYLINK and SEQLINK Wizards may be initiated from L-number hyperlinks

The *CAS Registry Number Wizard* finds property information

CAS Registry Number® Wizard

Select one of the following options.
Click Search to search.

REGISTRY File properties now included!

Get REGISTRY data
Full substance record

Get regulatory data
Complete CHEMLIST record

Get CAplus references
Agricultural Use

Get MSDS data
Complete MSDS-OHS record

Get U.S. patents
Complete patent (ASCII)

Get spectra
List of available spectra

Get property data
Enthalpies

Get related data
Polymers

Get catalog data
Complete CHEMCATS record

Structure search
Exact search - Free sample

- Flash Point
- Freely Rotatable Bonds
- Gibbs Energy of Formation
- Glass Transition Temperature
- Heat Capacity
- Hydrogen Acceptors
- Hydrogen Donors
- LogD
- LogP
- Ignition Properties
- Ionization Potential
- Kinematic Viscosity
- Liquid Properties
- Magnetic Moment
- Median Lethal Dose
- Melting Point
- Moisture Content
- Molar Properties
- Molecular Weight
- Nuclear Properties
- Optical Properties
- Optical Rotatory Power
- pKa
- Refractive Index
- Relative Density
- Safety
- Solubility
- Specific Gravity

Use HELP PROPERTIES in the REGISTRY File for the complete list.

Find properties using a hyperlinked CAS Registry Number

=> D 10

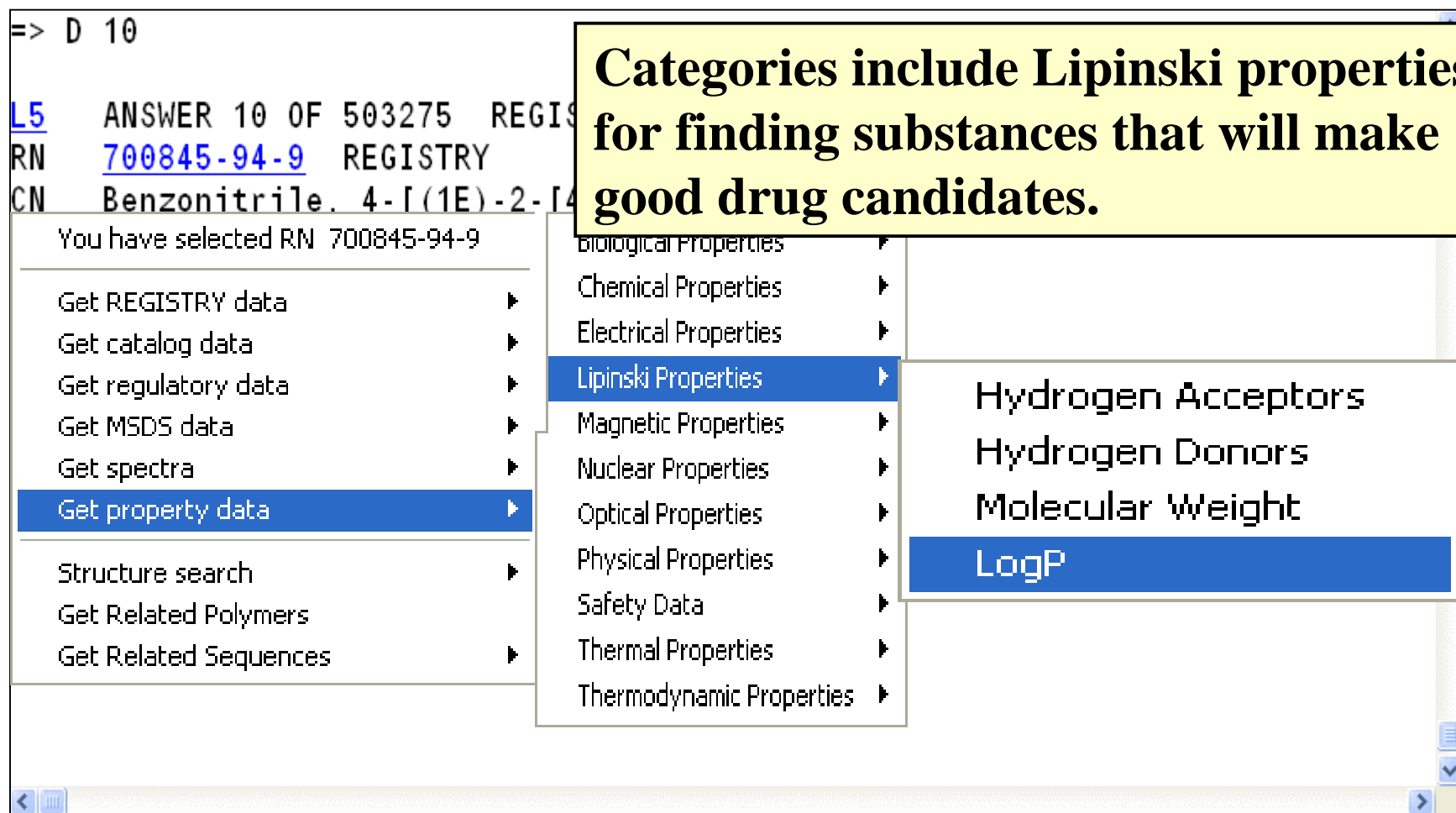
L5 ANSWER 10 OF 503275 REGIS
RN [700845-94-9](#) REGISTRY
CN Benzonitrile, 4-[(1E)-2-[4

You have selected RN 700845-94-9

- Get REGISTRY data ▶
- Get catalog data ▶
- Get regulatory data ▶
- Get MSDS data ▶
- Get spectra ▶
- Get property data ▶**
- Structure search ▶
- Get Related Polymers ▶
- Get Related Sequences ▶

- biological Properties ▶
- Chemical Properties ▶
- Electrical Properties ▶
- Lipinski Properties ▶**
- Magnetic Properties ▶
- Nuclear Properties ▶
- Optical Properties ▶
- Physical Properties ▶
- Safety Data ▶
- Thermal Properties ▶
- Thermodynamic Properties ▶

- Hydrogen Acceptors
- Hydrogen Donors
- Molecular Weight
- LogP**



Categories include Lipinski properties for finding substances that will make good drug candidates.

POLYLINK and *SEQLINK* Wizards are available from L-number hyperlinks

The screenshot shows the STN interface with a search result on the left and the 'Select Discover! Wizard' dialog box on the right. The search result includes the L5 number 49721-26-8 and a list of other CA index names. The wizard dialog box has three columns: 'Choose a search wizard', 'Select an L-number', and 'Choose a results wizard'. The 'Get Related Polymers' button in the results wizard column is highlighted with a red box, and a red arrow points from this box to a red-bordered box at the bottom of the search result containing the text '**RELATED POLYMERS AVAILABLE WITH POLYLINK**'.

STN

L5 ANSWER 1 OF 1 REGISTRY COPYRI
RN **49721-26-8** REGISTRY
CN Butanedioic acid, polymer with
OTHER CA INDEX NAMES:
CN 2,3-Butanediol, polymer with bu
MF (C4 H10 02 . C4 H6 04)x
CI PMS, COM
PCT Polyester, Polyester formed
LC STN Files: [CA](#), [CAPLUS](#), [USPATF](#)
DT.CA Caplus document type: Journa
RL.P Roles from patents: BIOL (Bi
RL.NP Roles from non-patents: BIOL

Select Discover! Wizard

Choose a search wizard:	Select an L-number:	Choose a results wizard:
Select Database	L1 1 ...	Analyze Plus
Author	L2 1 ...	Display
CAS Registry Number	L3 5424 ...	Refine
Chemical Name	L4 2411 ...	Save
Corporate Source	L5 1 ...	Save R-group data
Subject		Save for SciFinder
Edit alert		Get Related Polymers
		Get Related Sequences
		Create Single-file SDI
		Go to L-number

****RELATED POLYMERS AVAILABLE WITH POLYLINK****

Blank cells may be removed when limiting by country for individual patent fields

Individual PI | Individual PRAI | Individual AI

Patent Number Derwent Week
 Kind Code Language
 Publication Date Page Count
 Application Number Main IPC
 Application Date Designated States

All

Multiline

Number of patent rows per answer

All (maxm is 10)
 First members of family

By country

US
WO
EP
BR
JP
All

Remove blank cells

The table only shows cells with patent numbers for the desired country

Table (Untitled)			
Compositions for the treatment and prevention of pain and inflammation with a cyclooxygenase-2selective inhibitor and glucosamine	US 2003114418		
Preparation of pyrazolylbenzenesulfonamides as cyclooxygenaseinhibitors for treatment of inflammation.	US 6492411	US 5466823	US 5521207
Preparation of azolyphenylsulfonamide prodrugs of cyclooxygenase-2 (cox-2)inhibitors	US 2003105144	US 2003055012	US 6613790
Preparation of heterocyclo substituted hydroxamic acid derivatives as cyclooxygenase-2 and 5-lipoxygenase inhibitors	US 2002058810	US 6696477	
Oral fast-melt dosage form of a cyclooxygenase-2inhibitor	US 2002049233		

Blank cells from countries not selected are eliminated. Only the minimum number of columns needed are shown.

STN Express with *Discover!*, Analysis Edition, Version 7.01, provides more accurate data conveniently

- Analyze Plus Wizard provides more accurate charts and spreadsheets
- Cross-tab capability provides live links from data in charts to records on STN
- REGISTRY Wizards provide more property data and are hyperlinked to L-numbers
- Post-processing of patent information is more streamlined

STN[®]

**New Analysis and Visualization Tools
in STN Express[®]
with *Discover!*[™], Version 7.01**

STN Patent Forum
July 2004