

Markush Searching in the Patent Literature

April 2008



At the end of this workshop, you will be able to

- Find unique patents from MARPAT[®] and CAplusSM by directly searching the databases, as well as by using the CASLINK tool
- Refine the results of a CASLINK search using keywords
- Use MARPAT precision tools
- Set up current awareness alerts for substances in the patent literature

Before you begin

This workshop is designed for individuals who want to extend their structure search skills of the patent literature. This workshop highlights the use of STN Express[®] software.

Prerequisites for this seminar include *Basic Substance Search Techniques* and *Structure Searching in CAS REGISTRYSM*, or equivalent experience.

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OVERVIEW

In this section, you will

- Discover the breadth of CAS patent coverage
- Identify indexing strategies used by CAS to index substances in patents
- Learn about the content and coverage of MARPAT
- Identify a comprehensive strategy to search substance information in the patent literature


CAS Patent Coverage

CAS has included chemical patents in its coverage of scientific literature since 1907. CAS covers patents from 51 patent-issuing offices worldwide (2008 data).

Patent Selection

Selection of patent documents for coverage is determined by

- Patent country
- Patent kind code
- International Patent Classification (IPC) code or U.S. National Patent Classification Codes
 - ◆ Guaranteed coverage for codes (listed at web site below)
 - ◆ Selective coverage for additional codes based on chemical content
- Patent families covered by the family member encountered; further family information is added to the CA record

 **Web Resource** Detailed information on CAS patent coverage is available at www.cas.org/expertise/cascontent/caplus/patcoverage/

Patent Currency

Patent records from the following 9 major patent-issuing offices appear in the CAplus database within 2 days of publication of the patent: United States (USPTO), Germany (GPO), Japan (JPO), Great Britain (UKPO), France, (INPI), Russia (ROSPATENT), Canada (CIPO), the European Patent Office (EPO), and the World Intellectual Property Organization (WIPO). CAplus records are fully indexed within 27 days.

Indexing of Substances in Patents

A patent may contain two kinds of substance representations:

- Specific substances, represented by specific chemical structures
- Generic (prophetic) substances, represented by generic Markush structures. Each Markush structure may represent hundreds, or even thousands, of chemical substances.

Specific Substances

Specific chemical substances described in the patent claims are indexed in the CAPlus database. If a specific substance occurs elsewhere in the patent, it is indexed only when accompanied by evidence of its real existence, e.g., properties or experimental detail. If the specific substance is new, it will receive a CAS Registry Number[®] (CAS RN).

Illustration: New substance reported in a patent

Example 1

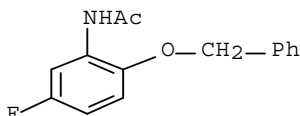
2-Benzyloxy-5-fluoroacetanilide (Formula I; R=CH₃ and X=F)

In a 500-ml flask, place 44.8 g (0.4 m) of 4-fluorophenol (1a; X=F) and 132 ml of acetic acid and stir to a solution. Add 0.6 g of sodium nitrite and cool the solution to 15° C. Add 36.0 g (0.4 m) of 70% nitric acid in drop wise keeping the temperature at 22–27° C. over 10–15 min. Stir the resulting yellow slurry at room temperature for 3 hrs. Warm the mixture to 65° C. to make a clear solution and add 132 ml of warm (65° C.) water slowly. Stir the resulting slurry

This specific substance received a CAS RN (475287-70-8) and was indexed in the CAplus record for the patent.

REGISTRY record:

RN 475287-70-8 REGISTRY
ED Entered STN: 06 Dec 2002
CN Acetamide, N-[5-fluoro-2-(phenylmethoxy)phenyl]- (CA INDEX NAME)
MF C15 H14 F N O2
SR CA
LC STN Files: CA, CAPLUS, USPATFULL



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

CAplus record highlighting the specific substance:

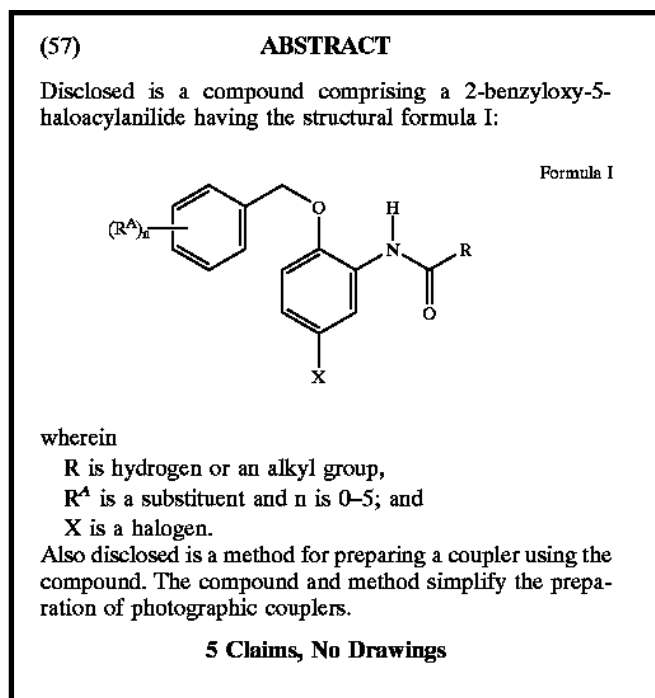
ACCESSION NUMBER: 2002:889225 CAPLUS
DOCUMENT NUMBER: 137:371374
TITLE: 2-(Benzyloxy)-5-halo-N-acylanilines
INVENTOR(S): Kim, Chang-Kyu
PATENT ASSIGNEE(S): Eastman Kodak Company, USA
SOURCE: U.S., 14 pp.
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:
PATENT NO. KIND DATE APPLICATION NO. DATE

US 6482985 B1 20021119 US 2001-11550 20011203
PRIORITY APPLN. INFO.: US 2001-11550 20011203
OTHER SOURCE(S): MARPAT 137:371374
REFERENCE COUNT: 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR
THIS RECORD. ALL CITATIONS AVAILABLE IN
THE RE FORMAT
IT **475287-70-8P**
RL: IMF (Industrial manufacture); RCT (Reactant); PREP
(Preparation); RACT (Reactant or reagent)
(prodn. of benzyloxyhaloacetanilides as intermediates for cyan
dye couplers)

Generic Substances

Generic substances, represented by Markush structures, are indexed in MARPAT. They do not receive CAS RNs.

Illustration: Generic substances reported in patent

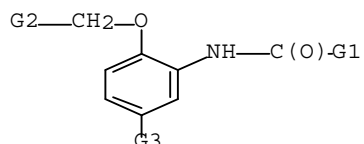


These generic substances, represented by Markush structures, are indexed in the MARPAT record for the patent.

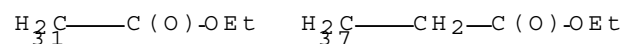
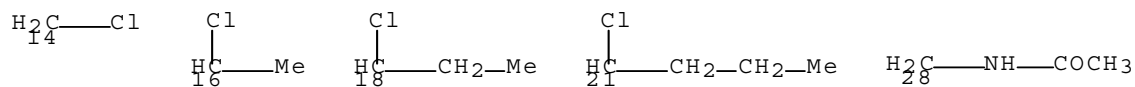
AN 137:371374 MARPAT
 TI 2-(Benzyloxy)-5-halo-N-acylanilines
 IN Kim, Chang-Kyu



MSTR 1



G1 = H / alkyl (opt. substd.) / (Specifically claimed: Me / Et / Pr-n / Pr-i / Bu-n / pentyl / nonyl / undecyl / tridecyl / pentadecyl / 14 / 16 / 18 / 21 / 28 / 31 / 37)



G2 = Ph (opt. substd. by (1-5) G4)
 G3 = F / Cl / Br / I
 G4 = R / (Examples: alkyl / F / Cl / I)
 Patent location: claim 1

MARPAT Content and Coverage

The MARPAT database contains the Markush structures for patents in CPlus from 1988–present. In addition, the database contains information licensed from Institut National de la Propriété Industrielle (INPI) for 1961-1987. MARPAT contains more than 300,000 records containing more than 750,000 Markush structures (December 2007 data). MARPAT is updated weekly with ca. 375 new records.

Structure Coverage

MARPAT contains all the Markush structures described in the claims section of chemical patents. Markush structures mentioned in the disclosures may also be indexed if broader than the claims:

- The base structure from the patent is retained, if possible.
- The variable group definitions are listed as G-number alternatives.
- Definitions given in the disclosure are used in the MARPAT diagram.
- Specific alternatives from the dependent claims are added, preceded by the “specifically claimed” (SC) qualifier.

note

→ All compound classes are covered except

- Alloys
- Metal oxides
- Inorganic salts
- Polymers

MARPAT Record

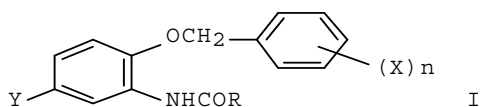
AN 137:371374 MARPAT
 TI 2-(Benzyloxy)-5-halo-N-acylanilines
 IN Kim, Chang-Kyu
 PA Eastman Kodak Company, USA
 SO U.S., 14 pp.
 CODEN: USXXAM
 DT Patent
 LA English
 IC ICM C07C233-05
 NCL 564219000
 CC 41-11 (Dyes, Organic Pigments, Fluorescent Brighteners, and
 Photographic Sensitizers)
 Section cross-reference(s): 25, 74

*The bibliographic data, the abstract, and the indexing in the CC, ST, and IT fields are the same as in the CAPLUS record. This data is only **displayable** in MARPAT.*

FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	US 6482985	B1	20021119	US 2001-11550	20011203
PRAI	US 2001-11550		20011203		

GI



AB Disclosed are 2-(optionally substituted benzyloxy)-5-halo-N-acylanilines (I; R = H, alkyl; X = substituent; n = 0-5; Y = halogen). I can be used to prepare phenolic cyan dye-forming couplers with improved efficiency. In an example, I (R = Me; Y = F; n = 0) was prepared starting with 4-fluorophenol followed by steps of nitration, reduction, acetylation, and benzylation.

ST benzyloxyhaloacetanilide prodn cyan dye coupler intermediate

IT Cyan couplers

(production of benzyloxyhaloacetanilides for)

IT 102604-67-1P 475287-72-0P

RL: IMF (Industrial manufacture); TEM (Technical or engineered material use); PREP (Preparation); USES (Uses)

(cyan dye coupler; production of benzyloxyhaloacetanilides as intermediates for)

IT 394-33-2P, 4-Fluoro-2-nitrophenol 399-97-3P, 2-Amino-4-fluorophenol 26488-93-7P 112900-44-4P 460048-17-3P
 475280-95-6P 475280-99-0P 475287-74-2P 475287-75-3P
 475287-76-4P

RL: IMF (Industrial manufacture); RCT (Reactant) (Preparation); RACT (Reactant or reagent) (intermediate; production of benzyloxyhaloacetanilides as intermediates for cyan dye couplers)

CAS RNs indicate specific substances indexed from the patent.

IT 475287-70-8P 475287-71-9P

RL: IMF (Industrial manufacture); RCT (Reactant); PREP (Preparation); RACT (Reactant or reagent)

(production of benzyloxyhaloacetanilides as intermediates for cyan dye couplers)

(continued on next page)

IT 102-36-3, 3,4-Dichlorophenyl isocyanate 150-76-5, 4-Methoxyphenol
63059-55-2 71130-54-6, Phenyl 4-cyanophenylcarbamate 475287-73-1
RL: RCT (Reactant); RACT (Reactant or reagent)

(starting material; in production of cyan dye couplers)

IT 95-85-2, 2-Amino-4-chlorophenol 100-39-0, Benzyl bromide
108-24-7, Acetic anhydride 371-41-5, 4-Fluorophenol
7697-37-2, Nitric acid, reactions

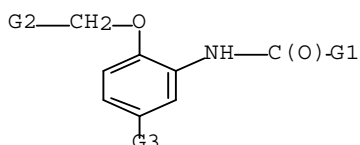
RL: RCT (Reactant); RACT (Reactant or reagent)

(starting material; production of benzyloxyhaloacetanilides as
intermediates for cyan dye couplers)

RE.CNT 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD
RE

- (1) Anon; JP 03-48603 1991 CAPLUS
- (2) Aoki; US 4579813 A 1986 CAPLUS
- (3) Itoh; US 4743595 A 1988 CAPLUS
- (4) Lau; US 5962198 A 1999 CAPLUS
- (5) Yale; J Med Chem 1970, V13(4), P713 CAPLUS
- (6) Zaltsgendler; Tetrahedron Lett 1993, V34(15) CAPLUS

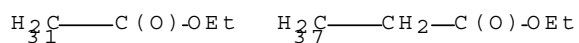
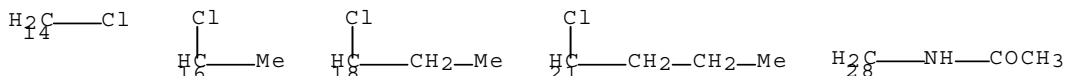
MSTR 1



MSTR 1 means Markush structure number 1.

G-numbers represent variability in the Markush structure.

G1 = H / alkyl (opt. substd.) / (Specifically claimed: Me / Et /
Pr-n / Pr-i / Bu-n / pentyl / nonyl / undecyl / tridecyl /
pentadecyl / 14 / 16 / 18 / 21 / 28 / 31 / 37)



G2 = Ph (opt. substd. by (1-5) G4)

G3 = F / Cl / Br / I

G4 = R / (Examples: alkyl / F / Cl / Br / I)

Patent location: claim 1

note

Further details concerning MARPAT displays may be found in the
MARPAT User Guide:

www.cas.org/support/stngen/stdoc/marpat.html

Markush Structures

Generally, one Markush structure from the patent is represented by one MARPAT structure, but there are exceptions.

Multiple diagrams

Markush structures may be split into two or more diagrams to

- Add the maximum amount of information for very large Markush structures
- Use the correct structure convention for all implied structures
- Code for author provisos that cannot be included in a single Markush structure

Same base structure

Markush structures sharing a base structure may be combined. One example is the case of starting materials from several claims. A note (NTE field) is added to the MARPAT structure:

Patent location:	claim 4
Note:	also incorporates claim 6

Structure in disclosure

Alternatives from a broad Markush structure in the disclosure may be added to the claimed structure. This occurs when the Markush structure

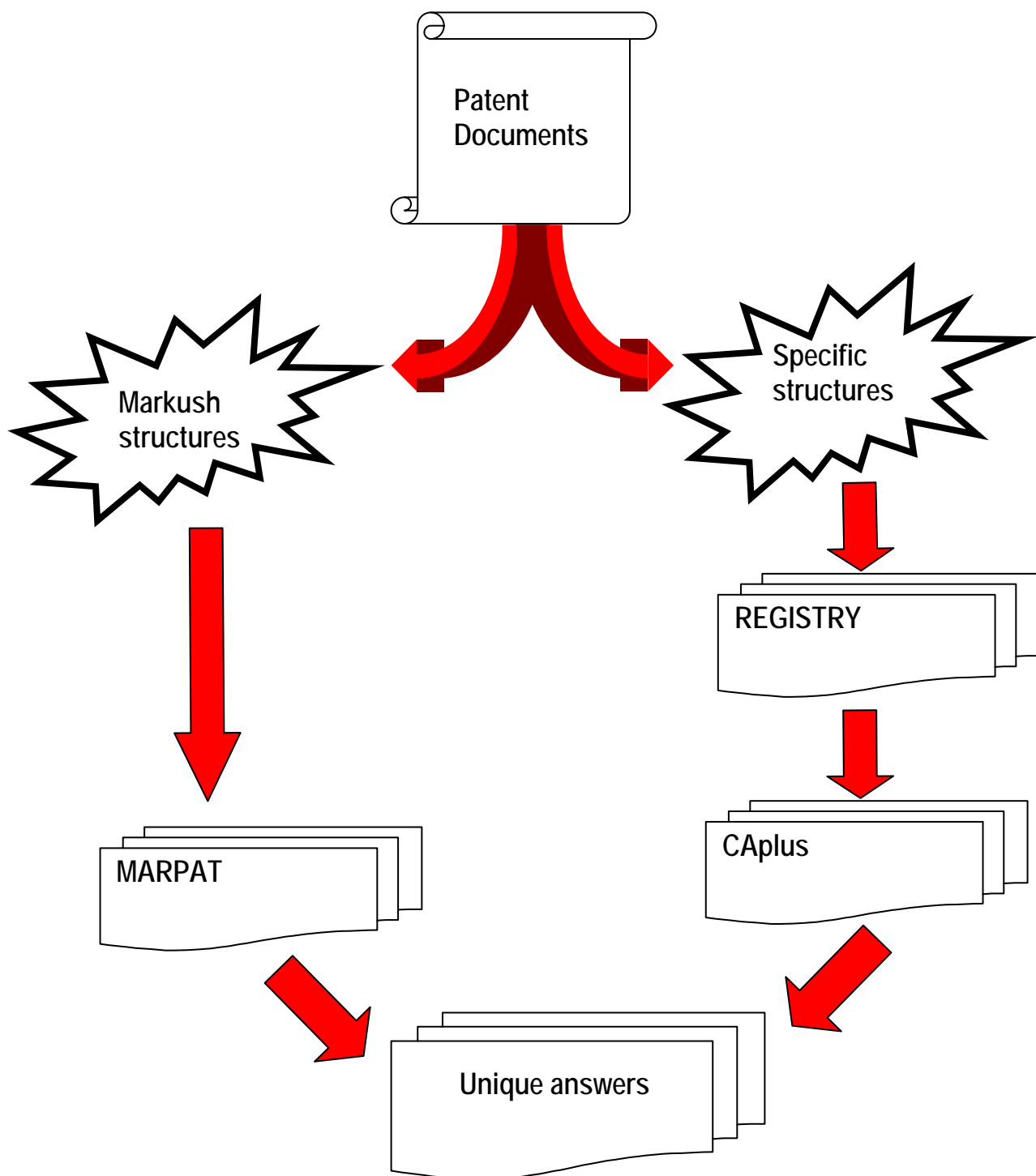
- In the disclosure is broader than the claimed structure
- Covers the products of a process patent

Patent location:	claim 9
Note:	also incorporates broader disclosure

Comprehensive Structure Searching

Comprehensive substance searching for patent information includes steps to search both

- Specific substances reported in patents, in the REGISTRY/CAplus databases
- Generic substances reported in patents, in MARPAT database



MARKUSH STRUCTURE SEARCHING

In this section, you will review MARPAT-specific structure search requirements.

Structure Search Queries

Unique requirements exist for structure search queries used in MARPAT.

Ring/Chain Bonds

Ring/chain bond characteristics are not allowed.

Illustration: Error message

```
=> S L17 FUL
```

```
RC BOND NOT ALLOWED IN A GENERIC STRUCTURE FILE
```

Searching a Markush structure file requires that all bonds in a query structure have definite specifications as ring bonds or chain bonds. The bond type 'RC', representing Ring or Chain, is not allowed for searching a Markush structure file. You may respecify the 'RC' bond in the structure as 'R' or 'C' by using the STRUCTURE command to RECALL this structure and then using the BOND command at the colon prompt (:). For more information on using these commands, enter "STRUCTURE" at an arrow prompt (=>) and then at the colon prompt (:) enter "HELP RECALL" or "HELP BOND".

Single L-Number

MARPAT search queries may include only a single L-number

- Uploaded from STN Express or STN[®] on the WebSM
- Created using the STRUCTURE command
- Resulting from a REGISTRY search

Structure Filters

Structure filters (screens) may not be used in Markush searching. REGISTRY search queries containing structure filters may be used, but the filters will be ignored.

note

Structure queries consisting of both structure terms and filters can only be uploaded directly into MARPAT with Use Filters turned off.

Structure Searching

Two search types are available in MARPAT:

- Substructure
- Closed substructure

Four choices are available for scope of the database searched:

- SAMPLE — Runs on a fixed 5% of the database
- FULL
- RANGE — Restricts searches to CA Collective Periods, CA Volumes, file entry years, or Accession Numbers
- SUBSET — Limits the size of the search database to facilitate searches running to completion

System Limits

Information about processing limits is available in a HELP message.

```
=> ? SLIMITS
```

```
The system limits for structure searches in the MARPAT File are as follows:
```

Search Scope	Iterations	Answers	Minutes
Online SAMPLE	2,000	50	5
Subset SAMPLE	2,000	50	5
Online FULL	200,000	200,000	30
Subset FULL	200,000	200,000	30
BATCH FULL	200,000	200,000	360
Online RANGE	200,000	200,000	30
Subset RANGE	200,000	200,000	30
BATCH RANGE	200,000	200,000	360

Iteration Incompletes

Answers in MARPAT answer sets may be marked Iteration Incomplete, which occurs when it could not be determined whether a candidate answer was a valid answer within the allotted processing time. The answer is included in the answer set, but marked Iteration Incomplete. These may be valid answers, but often are not.

Iteration incompletes may be isolated from answer sets.

To do this with Iteration Incomplete answers	Use this search strategy:
Remove them from the answer set	=> S L4/COM
Create a set containing only these answers	=> S L4/INC

EXTEND Structure Searches

If you wish to view the candidate answers from the first step in the two-step structure search, then add the keyword EXTEND to the SEARCH command. The keyword must be entered in the command line. An L-number answer set including all candidate answers (prior to iteration) will be created along with the usual L-number answer set. For further details enter HELP EXTEND at an arrow prompt (=>).

```
L1          STRUCTURE UPLOADED

=> S L1 EXTEND FULL

FULL SEARCH INITIATED 12:47:07

L2          24025 SEA SSS FUL L1 EXTEND

CANDIDATE STRUCTURE SEARCH COMPLETED - 24025 TO ITERATE

100.0% PROCESSED 24025 ITERATIONS ( 3 INCOMPLETE) 1960 ANSWERS
SEARCH TIME: 00.00.11

L3          1960 SEA SSS FUL L1
```

For novice mode

```
=> SEARCH EXTEND
```

CASLINK

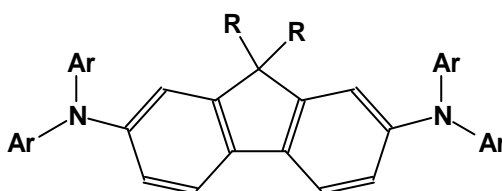
In this section, you will learn to

- Use CASLINK, the automatic Markush structure search tool
- Refine CASLINK results using keywords
- Display MARPAT answers

CASLINK

CASLINK automatically searches for both specific substances in REGISTRY and generic substances in MARPAT. REGISTRY database results are crossed into CAplus to locate the associated document records. Duplicates are removed between the MARPAT and CAplus records. The resulting answer set includes unique answers from each of the two databases.

Search Question: *Diarylaminofluorenes are good electrical conductors. Find patents concerning the electroluminescent or electrophotographic properties of such substances.*



Requirements:

- *Ar = aryl*
 - *R = anything but H*
-
-

Search Strategy

To use CASLINK to locate patent references

- Step 1 Build the structure.
 - Step 2 Enter CASLINK.
 - Step 3 Upload the structure.
 - Step 4 Run a sample structure search.
 - Step 5 Run the full-file structure search.
 - Step 6 (Option) Refine results with keywords.
 - Step 7 Display results.
-

Step 1: Build the Structure

The query may be built with STN Express, STN on the Web, or the online STRUCTURE command.

Step 2: Enter CASLINK

The FILE command is used to enter CASLINK's multifile environment.

```
=> FILE CASLINK
```

```
FILE 'CAPLUS' ENTERED AT ...
```

```
FILE 'MARPAT' ENTERED AT ...
```

```
FILE 'REGISTRY' ENTERED AT ...
```

```
CLUSTER 'CASLINK' ENTERED
```

```
Predefined command sequences will be executed in  
REGISTRY, MARPAT, and CAPLUS.
```

The CASLINK multifile environment includes the REGISTRY, CAPLUS, and MARPAT databases.

Step 3: Upload the Structure

```
=>
```

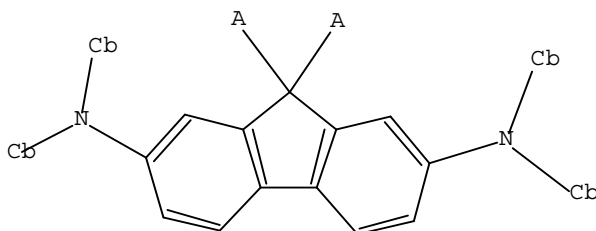
```
Uploading C:\Program Files\stnexp\Queries\caslink06.str
```

```
L1 STRUCTURE UPLOADED
```

```
=> DIS L1
```

```
L1 HAS NO ANSWERS
```

```
L1 STR
```



Tip: Display an uploaded structure query as a final check.

Note: the A nodes were set to Ring/Chain for comprehensive retrieval.

Step 4: Run a Sample Structure Search

A sample structure search searches a fixed 5% of the REGISTRY and MARPAT databases only. It is a no-cost option that is used to evaluate the effectiveness of a structure search by

- Testing the structure search to ensure it will run within system limits
- Verifying that the types of answers retrieved are the types of answers desired

```
=> S L1 SSS SAM
```

```
S L1 SSS SAM FILE=REGISTRY  
FILE 'REGISTRY'  
SAMPLE SEARCH INITIATED 12:26:34  
SAMPLE SCREEN SEARCH COMPLETED - 18317 TO ITERATE
```

```
13.1% PROCESSED      2000 ITERATIONS  
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)  
SEARCH TIME: 00.00.01  
  
FULL FILE PROJECTIONS:  ONLINE  **COMPLETE**  
                        BATCH   **COMPLETE**  
PROJECTED ITERATIONS:   358236 TO 374444  
PROJECTED ANSWERS:     235 TO 863
```

3 ANSWERS

Sample searches may fail to complete within system limits, however, the full file search will run to completion. Examine the full-file projections, as well as any answers obtained.

```
L2          3 SEA SSS SAM L1
```

```
S L2 SSS SAM FILE=MARPAT  
SAMPLE SEARCH INITIATED 12:26:35  
SAMPLE SCREEN SEARCH COMPLETED - 2027 TO ITERATE
```

```
98.7% PROCESSED      2000 ITERATIONS  
SEARCH TIME: 00.00.01  
  
FULL FILE PROJECTIONS:  ONLINE  **COMPLETE**  
                        BATCH   **COMPLETE**  
PROJECTED ITERATIONS:   38017 TO 43063  
PROJECTED ANSWERS:     1 TO 80
```

1 ANSWERS

In CASLINK, there are two answer sets to look at: one from REGISTRY and one from MARPAT.

```
L3          1 SEA SSS SAM L1
```

Summary

The REGISTRY search retrieved three answers; the MARPAT search found one. The full-file projections indicate that system limits will not be a problem.

Verify the answers:

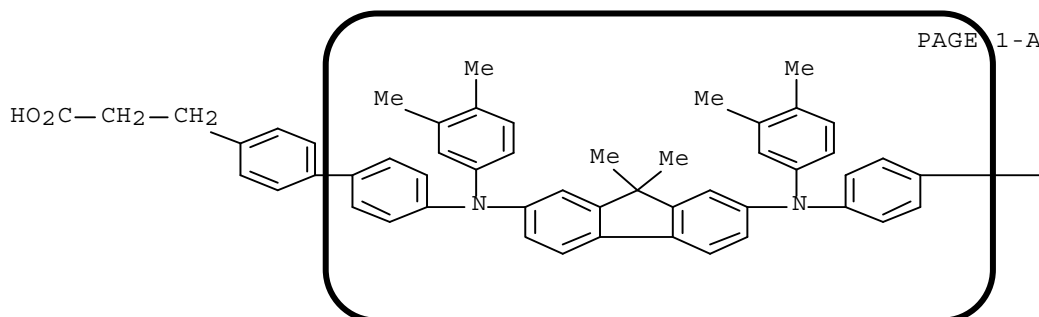
The D SCAN command is used to review results.

=> D SCAN L2

L2 3 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN
IN [1,1'-Biphenyl]-4-propanoic acid, 4',4'''-[(9,9-dimethyl-9H-fluorene-2,7-diyl)bis[(3,4-dimethylphenyl)imino]]bis-, polymer with 1,2-cyclohexanediol (9CI)
MF (C61 H56 N2 O4 . C6 H12 O2)x
CI PMS

RELATED POLYMERS AVAILABLE WITH POLYLINK

The box encloses the portion of the answer that caused the hit. This answer matches the query.



HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):0

=> D SCAN L3

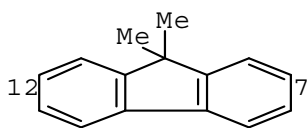
L3 1 ANSWERS MARPAT COPYRIGHT 2008 ACS on STN
IC ICM C07C209-10
ICS C07C209-04; C07C211-58; C07C211-60; C07C211-61; C07B061-00
CC 25-4 (Benzene, Its Derivatives, and Condensed Benzenoid Compounds)
TI Preparation of aromatic amines by amination using transition metal compounds and phosphine ligands

•
•
•

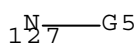
G5—₇G4—G1—₂G4—G5

(continued on next page)

G1 = 12-75 7-2



G4 = 127



G5 = Ph

Patent location: claim 8

ALL ANSWERS HAVE BEEN SCANNED

Step 5: Run the Full-File Structure Search

```
=> S L1 SSS FULL

S L1 SSS FUL FILE=REGISTRY
FULL SEARCH INITIATED 12:31:55
FULL SCREEN SEARCH COMPLETED - 365172 TO ITERATE

100.0% PROCESSED 365172 ITERATIONS 752 ANSWERS
SEARCH TIME: 00.00.05

L4 752 SEA SSS FUL L1

S L4 SSS FUL FILE=MARPAT
FILE 'MARPAT'
FULL SEARCH INITIATED 12:32:04
FULL SCREEN SEARCH COMPLETED - 43221 TO ITERATE

100.0% PROCESSED 43221 ITERATIONS 74 ANSWERS
SEARCH TIME: 00.00.19

L5 74 SEA SSS FUL L1

S L4 FILE=CAPLUS
L6 233 FILE CAPLUS

DUP REM L5 L6
PROCESSING COMPLETED FOR L5
PROCESSING COMPLETED FOR L6
L7 265 DUP REM L5 L6 (42 DUPLICATES REMOVED)
ANSWERS '1-74' FROM FILE MARPAT
ANSWERS '75-265' FROM FILE CAPLUS
```

Summary

CASLINK found 32 unique answers in MARPAT (74 answers minus 42 duplicates) and 191 unique answers in CAPLUS. The MARPAT answers are unique and would have been "missed" in a search of REGISTRY alone. Remember, the MARPAT answers are all patents, and the CAPLUS records are a combination of patent and non-patent references.

Step 6: Refine CASLINK Results with Keywords

The answer set retrieved by the CASLINK search may be refined using text terms while still in the CASLINK environment.

```
=> S L7 AND (ELECTROLUMIN? OR ELECTROPHOTO? OR ELECTRICAL CONDUCT?)

S L6 AND (ELECTROLUMIN? OR ELECTROPHOTOG? OR ELECTRICAL CONDUCT?)
FILE=CAPLUS
L8          166 FILE CAPLUS

S L5 AND (ELECTROLUMIN? OR ELECTROPHOTOG? OR ELECTRICAL CONDUCT?)
FILE=CAPLUS
L9          66 FILE CAPLUS

S L9 AND L5 FILE=MARPAT
L10         66 FILE MARPAT

DUP REM L10 L8
PROCESSING COMPLETED FOR L10
PROCESSING COMPLETED FOR L8
L11         193 DUP REM L10 L8 (39 DUPLICATES REMOVED)
              ANSWERS '1-66' FROM FILE MARPAT
              ANSWERS '67-193' FROM FILE CAPLUS
```

Summary

The number of unique MARPAT hits is now 27. The unique answers have been sorted by file (1–66 from MARPAT and 67–193 from CAplus).

Step 7: Display Results

In addition to the CAPlus display formats, MARPAT has its own special display formats.

This display format	Contains this information:
MSTR	All Markush structure(s) and related text information in the answer
MSTR(n)	Markush structure “n” and its related text
IDE	Accession Number and MSTR
FHIT	First hit MSTR with hit text terms highlighted
FQHIT	Query-focused first hit MSTR showing the hit structure and hit text terms
HIT	All hit MSTR’s with hit text terms highlighted
QHIT	Query-focused hit MSTR’s and hit text term

The query-focused formats (FQHIT, QHIT) will display that portion of the Markush structure relating to the search query. It can happen that the central core structure of the Markush structure is not the part of the structure that caused the hit. Therefore, it is not always displayed using these formats.

Usually different display formats will be used for each database's answers.

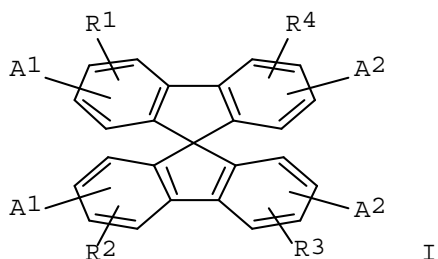
```
=> D L11 IBIB ABS FQHIT 12; D L11 123 IBIB ABS HITSTR
```

```
L11 ANSWER 12 OF 193 MARPAT COPYRIGHT 2008 ACS on STN      DUPLICATE 12
ACCESSION NUMBER:      140:254983  MARPAT
TITLE:                  Spirobifluorene dyes and organic
                        electroluminescent devices using them
INVENTOR(S) :          Suzuki, Koichi; Hiraoka, Mizuho; Senoo, Akihiro;
                        Yamada, Naoki; Negishi, Chika; Saito, Akihito
PATENT ASSIGNEE(S) :   Canon Kabushiki Kaisha, Japan
SOURCE:                 PCT Int. Appl., 91 pp.
                        CODEN: PIXXD2
DOCUMENT TYPE:         Patent
LANGUAGE:              English
FAMILY ACC. NUM. COUNT: 1
```

(continued on next page)

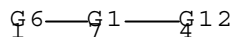
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004020373	A1	20040311	WO 2003-JP10258	20030812
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
JP 2004083483	A2	20040318	JP 2002-246601	20020827
PRIORITY APPLN. INFO.:			JP 2002-246601	20020827
GI				

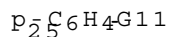


AB Provided are novel spirobifluorenes (I; A1, A2 = optionally substituted polycyclic arom. of heterocyclic group; R1-R4 = H, org. group, substituted amino, CN, halogen). Org. electroluminescence devices using the spiro compd. have an optical output with an extremely high efficiency and a high luminance, and an extremely high durability. In an example, 2,2',7,7'-tetrabromo-9,9'-spirobifluorene was treated with 9,9-dimethylfluorene-2-boronic acid in the presence of Pd(PPh₃)₄ to give a spirobifluorene compd. contg. 4 dimethylfluorene groups.

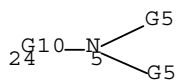
MSTR 2A



G5 = 25

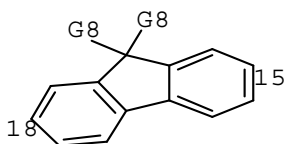


G6 = 24



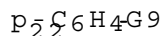
(continued on next page)

G7 = (1-5) 18-1 15-4



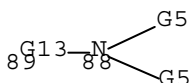
In this answer, the FQHIT format shows the core structure. Improvements to the FQHIT format (see G10 and G13) make it a much more useful display.

G8 = 22



G10 = bond

G12 = 89



G13 = bond

Patent location: claim 9
Note: substitution is restricted
Note: also incorporates claim 11

REFERENCE COUNT: 11 THERE ARE 11 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L11 ANSWER 123 OF 193 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2005:1049152 CAPLUS [Full-text](#)
DOCUMENT NUMBER: 143:356540
TITLE: Method for manufacturing **electrophotographic** photoreceptor containing triaryl amine in process cartridge for **electrophotographic** image-forming apparatus
INVENTOR(S): Ogaki, Harunobu; Tanaka, Takakazu; Kako, Kenichi
PATENT ASSIGNEE(S): Canon Inc., Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 34 pp.
CODEN: JKXXAF

DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

Hit term highlighting is available in CAplus (not in MARPAT).

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 2005266495	A2	20050929	JP 2004-80646	20040319
PRIORITY APPLN. INFO.:			JP 2004-80646	20040319

AB The title method is for preparation of a triarylamine charge-transporting compound in an **electrophotog.** photoreceptor and includes the steps of: reacting a halogenated aromatic compound with an amine in the base presence, wherein catalysts, which are alkylphosphine with a P-H bond and a metal compound, are used for the preparation The method provides high yield triaryl amine preparation

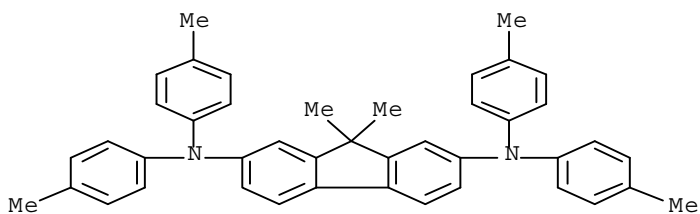
(continued on next page)

IT 143886-09-3P

RL: SPN (Synthetic preparation); TEM (Technical or engineered material use); PREP (Preparation); USES (Uses)
(preparation of charge-transporting compound)

RN 143886-09-3 CAPLUS

CN 9H-Fluorene-2,7-diamine, 9,9-dimethyl-N,N,N',N'-tetrakis(4-methylphenyl)-
(CA INDEX NAME)



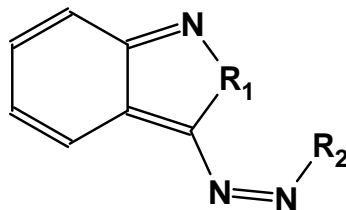
note

CASLINK features a special price benefit: The REGISTRY structure search is the regular price but the MARPAT search price is reduced.

There is also the HCASLINK cluster with REGISTRY, HCAplus, and MARPAT for those customers who prefer to use HCAplus.

Skills Practice

1. Use CASLINK to locate references discussing substances with the following structure.



$R_1 = \text{O or S}$

$R_2 = \text{Any heterocycle}$

Any type of substitution allowed at open sites

The nitrogen-containing ring system may be isolated or embedded in a larger ring system

- a. Will the query run to completion in REGISTRY and MARPAT?
- b. Do the sample search results meet the query requirements?
- c. Record the number of hits retrieved in the full-file search:

REGISTRY	_____
MARPAT	_____
CAplus	_____
Total unique hits	_____

- d. Display the final answer set using the following formats:

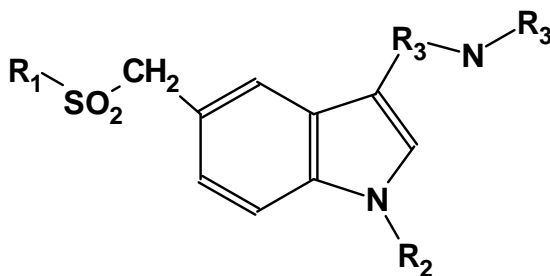
For MARPAT use BIB ABS FQHIT

For CAplus use BIB ABS HITSTR

- e. Display the full Markush structure (FHIT) for answer 3.

Skills Practice

2. Use CASLINK to locate references covering substances with the following structure in relation to headaches.



R₁ = nitrogen in a ring or a chain

R₂ = anything, including hydrogen

R₃ = carbon chain with any substitution

Nitrogen-containing ring may be isolated or embedded in a larger ring system

Any substitution is allowed at open sites

- Do the sample search results meet query requirements?
- Record the number of hits retrieved in the full-file search:

REGISTRY	_____
MARPAT	_____
CAplus	_____

- Display results using the following formats:

For MARPAT use IBIB ABS FHIT

For CAplus use IBIB ABS HITSTR

PRECISION TOOLS FOR MARPAT STRUCTURE QUERIES

In this section, you will learn to

- Use match level to control the precision of search results
- Use structure drawing tools — generic definitions and element counts — to enhance retrieval

Overview

Techniques for modifying structure queries for Markush searching are available. These structure drawing tools will either expand or reduce the number of answers retrieved from a structure search in MARPAT:

- Match level
- Generic definitions
- Element count

Match Level

Markush structures include both real atoms and generic nodes, both of which may be matched against the real atoms and generic nodes (Ak, Cb, Hy, Cy) of the search query.

Match Level determines the degree to which query nodes match with nodes in the candidate answers. Changing the degree of matching will increase or decrease the number of answers retrieved.

There are three match levels:

- Atom
- Class
- Any

Match Level Atom

Match Level Atom is the most restrictive match level. It retrieves the most precise set of answers: Specific atoms in the query match only specific atoms in candidate answers. Generic nodes in the query match only specific atoms in candidate answers.

Illustration:

Query node	Candidate answer node	Match?
Cl	Cl	Yes
Cl	Br	No
Cl	X	No
X	Cl or Br or F or I or At	Yes
X	X	No

Match Level Class

Match Level Class causes more answers to be retrieved than match level atom. Specific atoms in the query match specific atoms and generic nodes in candidate answers. Generic nodes in the query match specific atoms and generic nodes in candidate answers.

Illustration:

Query node	Candidate answer node	Match?
Cl	Cl	Yes
Cl	Br	No
Cl	X	Yes
X	Cl or Br or F or I or At	Yes
X	X	Yes

Match Level Any

Match Level Any is the least restrictive match level option. In addition to specific atoms and generic nodes, candidate answers also include R-nodes. R-nodes are indefinite substituents in the database structure described with text terms such as

- “Organic group”
- “Group to form ring”
- “Anion”
- “Protecting group”

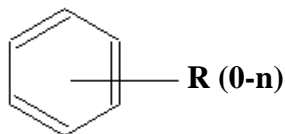
Illustration:

Query node	Candidate answer node	Match?
Cl	Cl	Yes
Cl	Br	No
Cl	X	Yes
Cl	R-node	Yes
X	Cl or Br or F or I or At	Yes
X	X	Yes
X	R-node	Yes

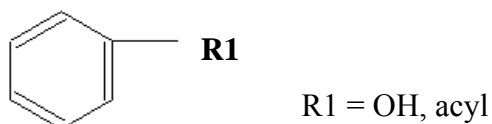
note

If the textual information for a group is SO (optional substitution) or SR (required substitution), that information is translated into an R-node (0-n).

G1=X/NO2/**phenyl (SR)** in a MARPAT structure is expanded into



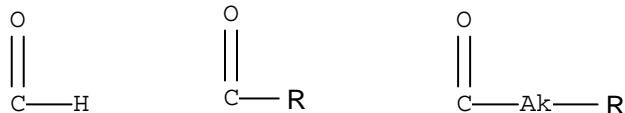
If, in the text of a patent claim, a substituent is defined as acyl:



This structure is entered into MARPAT as:



With acyl expanded into 3 fragments:



**Helpful
HINT**

Using Match Level Any for an entire query is not recommended. It retrieves far too many irrelevant answers and greatly extends the search time. Assign match level any to selected nodes in the query to

- Broaden the query
- Increase the recall
- Match R-nodes like “*protecting group*”

Default Match Levels

Structure queries automatically include default match level assignment. This assignment is only taken into account when searching MARPAT, it has no effect in any other structure searchable database.

The default settings for match levels for structures drawn with STN Express or STN on the Web are

- Atom, for ring atoms and the ring generic groups Cy, Cb, and Hy
- Class, for chain atoms and the chain generic group Ak

note

Searchers who use the STRUCTURE command to build queries may have different default settings.

Default match level settings may be changed in the structure drawing programs. From the **Setup** pulldown menu, select **Preferences**. A side-menu appears. Select **Structure Drawing**. Select the **Chemistry** tab and make changes in the area labeled **Markush Match Level Defaults**.

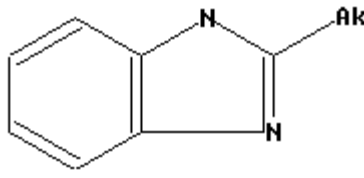
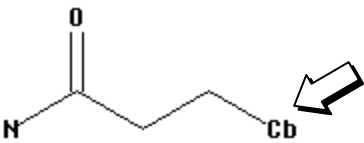
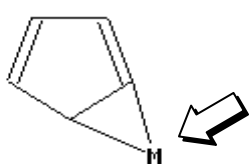
Match level any may not be assigned as the default match level.

When to Change Match Level

From atom to class

Changing from atom to class match level

- Broadens the query
- Generally increases the number of iterations in the search

If the query contains	Consider Match Level Class
A specific real atom ring system	<p data-bbox="667 615 1370 674">When you want to retrieve the real atom ring system, plus generic groups that encompass the ring definition</p> <div data-bbox="743 701 1390 877"><p data-bbox="1122 747 1390 877"><i>Change match level for all ring atoms to class.</i></p></div>
Hy, Cb, Cy	<p data-bbox="667 942 1370 1001">When you want to retrieve real atom rings represented by the ring generic group, plus the generic group</p> <div data-bbox="743 1026 1338 1167"><p data-bbox="1122 1037 1338 1125"><i>Change match level to class.</i></p></div>
M, Q, X, or A as part of a ring system	<p data-bbox="667 1257 1284 1316">When you want to match specific elements, as well as the corresponding generic groups</p> <div data-bbox="743 1331 1338 1493"><p data-bbox="1013 1341 1338 1461"><i>Change match level to class. The rest of the ring atoms are set to atom.</i></p></div>

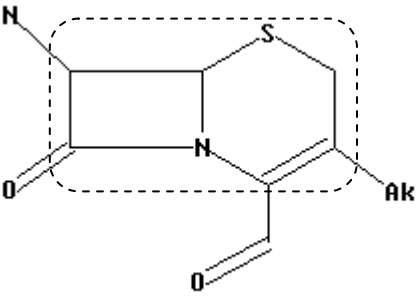
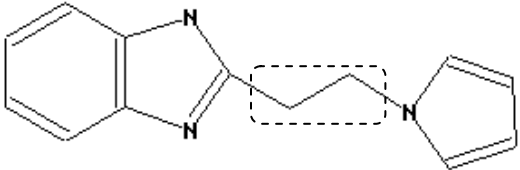
Helpful HINT

To make a specific ring system Match Level Class, change *all* of the atoms in the ring system.

From class to atom

Changing from class to atom match level

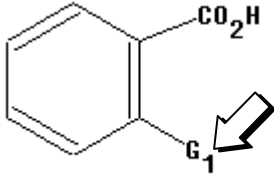
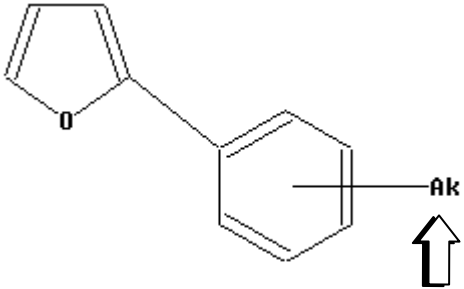
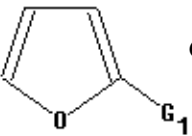
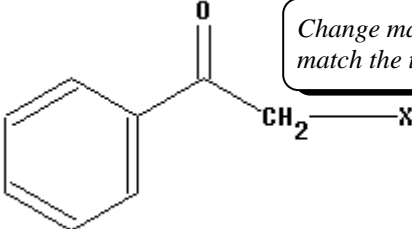
- Narrows the query
- Generally decreases the number of iterations in the search

Consider Match Level Atom, if the query contains	For example:
An important ring system that must be explicitly present in each retrieval	 <p><i>Leave the default match level setting for the ring system.</i></p>
A chain spacer of a certain length that must be present	 <p><i>Change match level for the circled chain atoms to atom.</i></p>

From atom or class to any

Changing to match level any

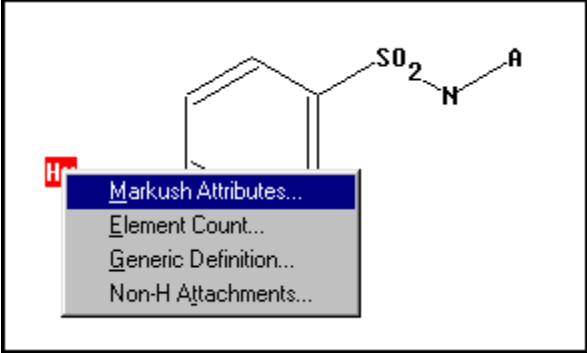
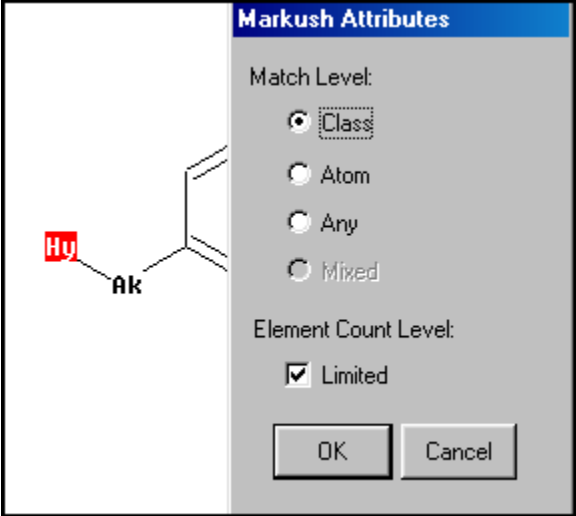
- Broadens the query
- Generally increases the number of iterations in the search

Consider Match Level Any, if the query contains	For example:
A substituent often described generically by text in patent claims, e.g., "an electron withdrawing group"	 <p><i>Change match level for the G1 substituent to any to also match an R-node which might be defined as an "electron withdrawing group".</i></p> <p>G1=NO₂, CN, X</p>
A substituent that you want to also match on that substituent with "substitution optional" (SO) or "substitution required" (SR) in the textual information	 <p><i>Change match level to any to retrieve hits such as</i></p>  <p>G1=X/NO₂/phenyl (SR)</p>
A portion that could match on "acyl" as a textual description of the attachment	 <p><i>Change match level for X to any to match the textual phrase "acyl".</i></p>


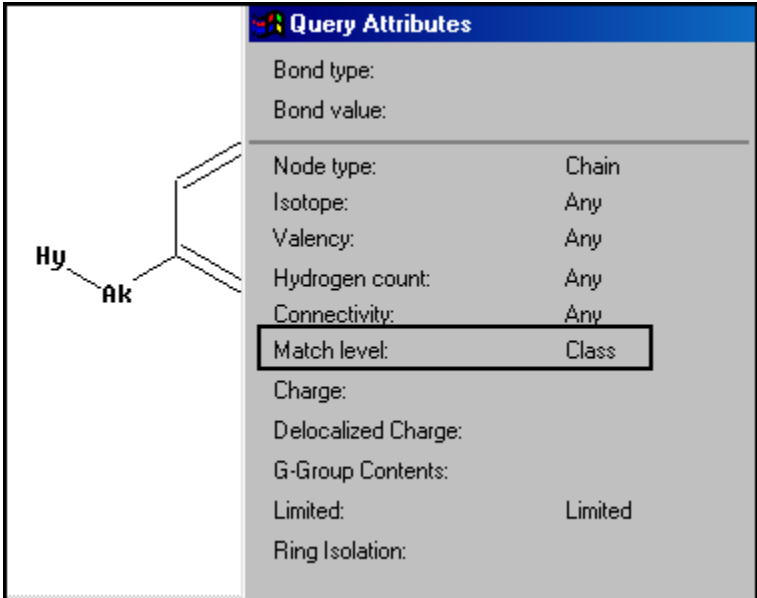
Changing Match Level Assignments

Match level assignments may be altered as needed to make the query more specific or more general.

How to

Step	Action
1	<p>Right-click on the node of interest. A side-menu appears. Select <i>Markush Attributes</i>.</p>  <p>The screenshot shows a chemical structure of a benzene ring with a substituent group $\text{SO}_2\text{N}^{\text{A}}$. A red 'H' icon is positioned to the left of the ring. A context menu is open over the ring, listing the following options: 'Markush Attributes...' (highlighted in blue), 'Element Count...', 'Generic Definition...', and 'Non-H Attachments...'.</p>
2	<p>Click to select the radio button associated with the match level of interest. Click <i>OK</i>.</p>  <p>The screenshot shows the 'Markush Attributes' dialog box. On the left is a chemical structure with a red 'H' icon and a node labeled 'Ak'. The dialog box has a blue title bar and contains the following settings: 'Match Level:' with radio buttons for 'Class' (selected), 'Atom', 'Any', and 'Mixed'; 'Element Count Level:' with a checked checkbox for 'Limited'. At the bottom are 'OK' and 'Cancel' buttons.</p>

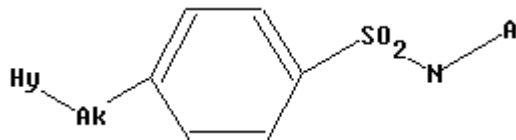
(continued on next page)

Step	Action																												
3	<p data-bbox="475 289 1377 352">(Option) Verify the setting change. Click the Query Attribute icon , and then position it on the node of interest. A <i>Query Attributes</i> summary will appear.</p> <div data-bbox="475 369 1227 963">  <table border="1" data-bbox="716 369 1227 963"> <thead> <tr> <th colspan="2" data-bbox="716 369 1227 411">Query Attributes</th> </tr> </thead> <tbody> <tr> <td data-bbox="716 411 1227 453">Bond type:</td> <td data-bbox="716 453 1227 495"></td> </tr> <tr> <td data-bbox="716 495 1227 537">Bond value:</td> <td data-bbox="716 537 1227 579"></td> </tr> <tr> <td data-bbox="716 579 1227 621">Node type:</td> <td data-bbox="716 621 1227 663">Chain</td> </tr> <tr> <td data-bbox="716 663 1227 705">Isotope:</td> <td data-bbox="716 705 1227 747">Any</td> </tr> <tr> <td data-bbox="716 747 1227 789">Valency:</td> <td data-bbox="716 789 1227 831">Any</td> </tr> <tr> <td data-bbox="716 831 1227 873">Hydrogen count:</td> <td data-bbox="716 873 1227 915">Any</td> </tr> <tr> <td data-bbox="716 915 1227 957">Connectivity:</td> <td data-bbox="716 957 1227 999">Any</td> </tr> <tr> <td data-bbox="716 999 1227 1041">Match level:</td> <td data-bbox="716 1041 1227 1083">Class</td> </tr> <tr> <td data-bbox="716 1083 1227 1125">Charge:</td> <td data-bbox="716 1125 1227 1167"></td> </tr> <tr> <td data-bbox="716 1167 1227 1209">Delocalized Charge:</td> <td data-bbox="716 1209 1227 1251"></td> </tr> <tr> <td data-bbox="716 1251 1227 1293">G-Group Contents:</td> <td data-bbox="716 1293 1227 1335"></td> </tr> <tr> <td data-bbox="716 1335 1227 1377">Limited:</td> <td data-bbox="716 1377 1227 1419">Limited</td> </tr> <tr> <td data-bbox="716 1419 1227 1461">Ring Isolation:</td> <td data-bbox="716 1461 1227 1503"></td> </tr> </tbody> </table> </div>	Query Attributes		Bond type:		Bond value:		Node type:	Chain	Isotope:	Any	Valency:	Any	Hydrogen count:	Any	Connectivity:	Any	Match level:	Class	Charge:		Delocalized Charge:		G-Group Contents:		Limited:	Limited	Ring Isolation:	
Query Attributes																													
Bond type:																													
Bond value:																													
Node type:	Chain																												
Isotope:	Any																												
Valency:	Any																												
Hydrogen count:	Any																												
Connectivity:	Any																												
Match level:	Class																												
Charge:																													
Delocalized Charge:																													
G-Group Contents:																													
Limited:	Limited																												
Ring Isolation:																													

Summary

In general, for a given set of atoms, match level class retrieves more answers than match level atom, but fewer answers than match level any.

Illustration: Note how the changes in match level affect the number of answers retrieved in MARPAT for the following query. The phenyl ring is isolated.



The changed match level(s) is/are shown in boldface type.

Hy	Ak	Ring	N	A	Answers
Atom	Class	Atom	Class	Class	1267 (default)
<i>Class</i>	Class	Atom	Class	Class	1853
Atom	<i>Atom</i>	Atom	Class	Class	1207
Atom	Class	Atom	Class	<i>Atom</i>	652
Atom	Class	<i>Class</i>	Class	Class	2306
<i>Class</i>	Class	<i>Class</i>	Class	Class	3876
<i>Class</i>	Class	Atom	<i>ANY</i>	Class	1860
<i>Class</i>	Class	Atom	<i>Class</i>	<i>ANY</i>	2135

Helpful HINT

Changing match level to ANY will match *any* R-node in the database which is described textually at that position. It may NOT encompass your query. For instance, changing the N node to ANY match level retrieves a hit with the text description “vinyl polymer” at that node.

Generic Definitions

Markush structures may include the following generic groups:

- Hy Heterocyclic ring systems
- Cb Carbocyclic ring systems
- Cy Any ring system
- Ak Any carbon chain

Generic groups may be defined more precisely with **generic definitions**. Not all definitions apply to all generic groups. The generic definitions are:

Generic Definition	Options	Applicable groups
Saturation	<ul style="list-style-type: none"> ■ Saturated: all bonds single exact ■ Unsaturated: at least one bond is double, triple, or normalized 	Hy, Cb, Cy, Ak
Type of chain	<ul style="list-style-type: none"> ■ Linear: all of the Ak carbon atoms have only one or two attachments to other carbon atoms ■ Branched: at least one of the Ak carbon atoms has more than two attachments to a carbon atom 	Ak
No. of hetero atoms	<ul style="list-style-type: none"> ■ 1 hetero atom ■ >1 hetero atom 	Hy, Cb, Cy
Type of ring system	<ul style="list-style-type: none"> ■ Monocyclic ■ Polycyclic 	Hy, Cb, Cy
No. of C atoms	<ul style="list-style-type: none"> ■ <7 C atoms ■ ≥7 C atoms 	Hy, Cb, Cy, Ak

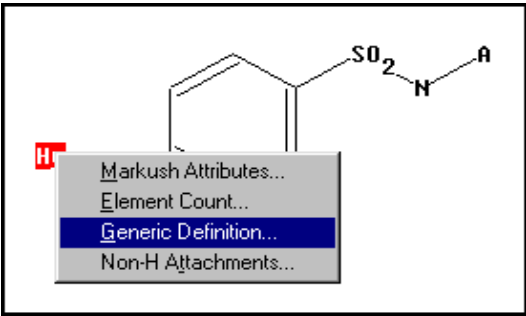
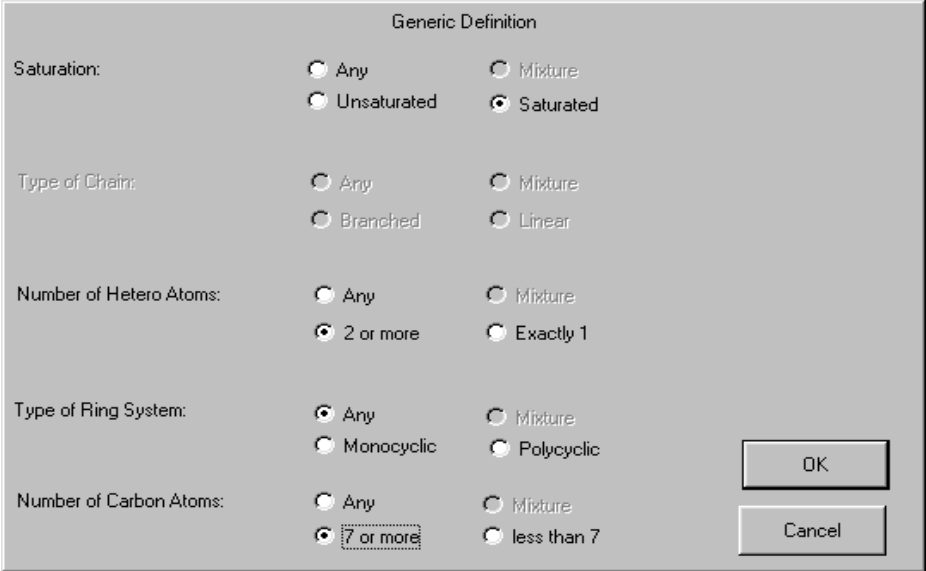
Default Generic Definitions

The default setting for a structure query in each case is "any"; that is, no further definition, with broadest retrieval.


Changing Generic Definitions

Generic definitions may be altered as needed to make the query as specific as required.

How to

Step	Action
1	<p>Right-click on the node of interest. A side-menu appears. Select <i>Generic Definition</i>.</p> 
2	<p>Click to select the radio button associated with the generic definition of interest. Click <i>OK</i>.</p> 

(continued on next page)

Step	Action
3	(Option) Verify the setting change. Click the Query Attribute icon  , and then position it on the node of interest. A <i>Query Attributes</i> summary will appear.

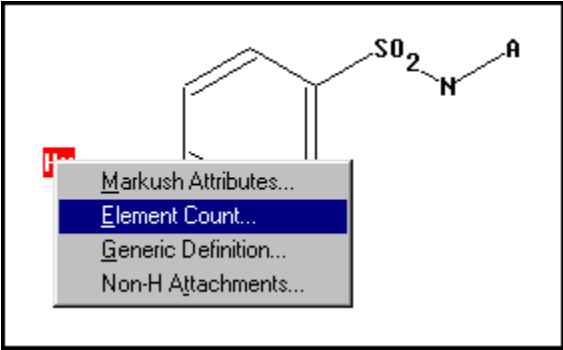
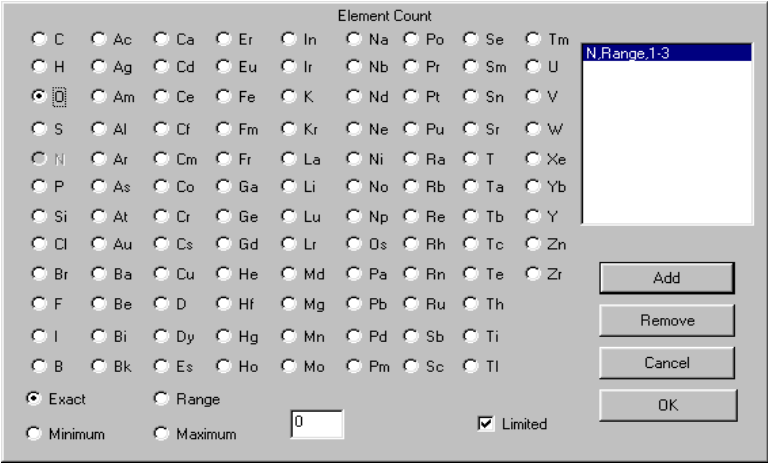
Element Count

The number and kind of elements in a generic group may be specified using **element count**.

Default Element Counts

By default, no element count is specified for a generic group.

Changing Element Counts

Step	Action
1	<p>Right-click on the node of interest. A side-menu appears. Select Element Count.</p> 
2	<p>For each element, do the following: (1) Click the radio button associated with the element of interest. (2) Click the radio button associated with the count of interest. (3) Click Add. When all element counts have been specified, click OK.</p> 

Helpful HINT

To specify that an element may not be present, an element count of Exactly 0 should be used.

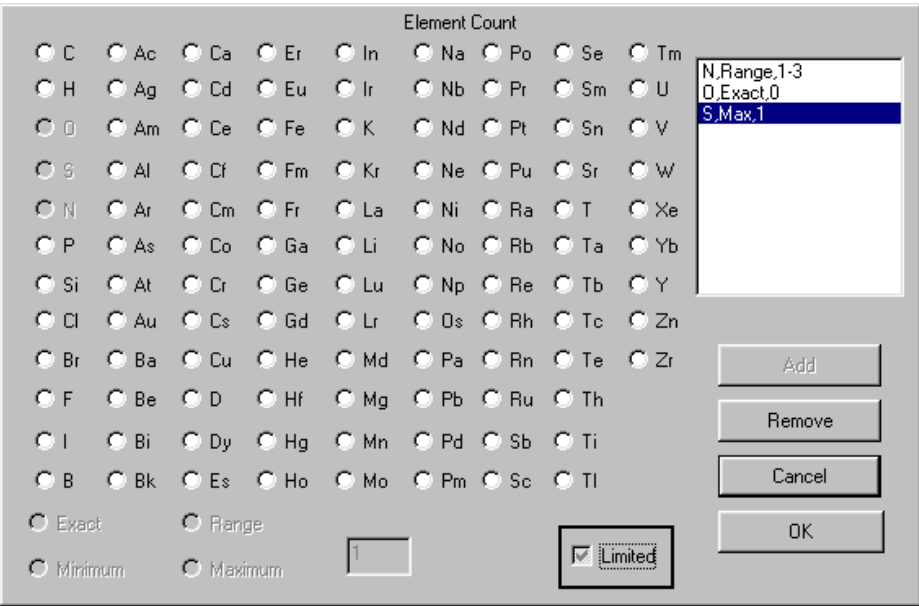
note

For the Ak and Cb generic groups, carbon is the only element count that may be assigned.

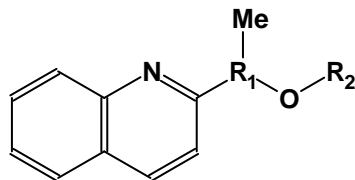
Element Count Unlimited

By default, element counts are Limited — That is, an element count in the query must match corresponding element counts in an answer. Using the “unlimited” feature, the default is over-ridden and generic groups in an answer that have no element counts may also be matched to increase the number of answers retrieved.

How to

Step	Action
1	<p>Once all element counts are specified, click to remove the checkmark from the box labeled <i>Limited</i>. Click <i>OK</i>.</p> 

Search Question: Find patents for substances with the following structure:



Requirements:

- The quinoline ring may not be part of larger ring systems.
- R₁ = heterocycle (match level class), which is unsaturated with at least 2 C atoms, a maximum of 1 O atom, and 1–5 N atoms, but at least 2 hetero atoms.
- R₂ = saturated carbon chain with 1–8 C atoms.
- The query should match against answers with no element counts specified.

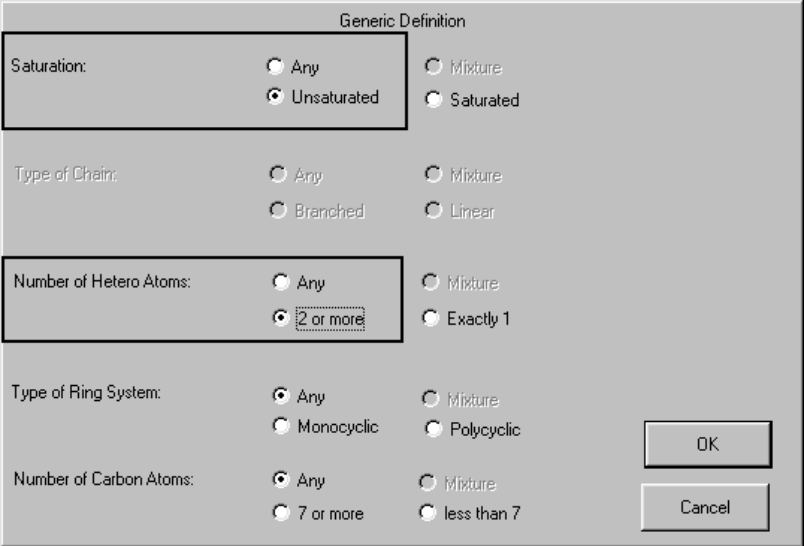
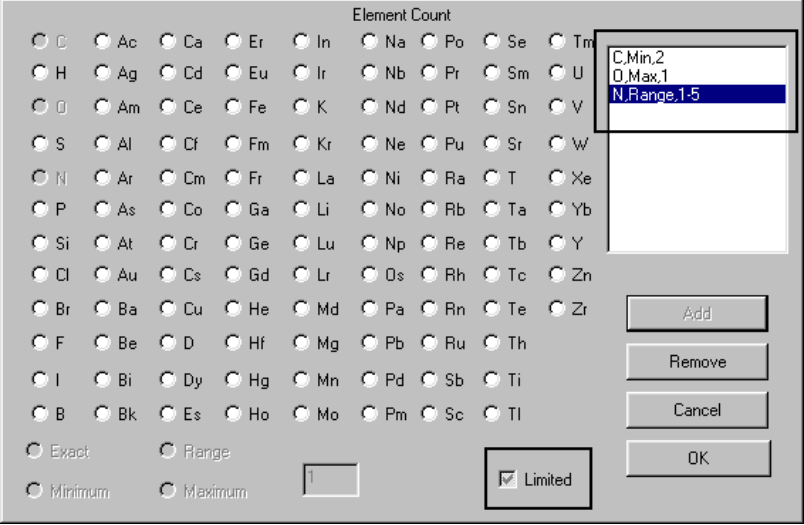
Search Strategy

To locate patent references to a structure of interest

- Step 1 Build the structure.
- Step 2 Locate specific substance matches in REGISTRY.
- Step 3 Locate generic substance matches in MARPAT.
- Step 4 Retrieve CPlus references to REGISTRY substances.
- Step 5 Remove duplicates.
- Step 6 Display results.

Step 1: Build the Structure

The query may be built with STN Express, STN on the Web, or the online STRUCTURE command.

This structure requirement	Was achieved using the following technique:
Quinoline ring not part of a larger ring system Unsaturated heterocycle	<p>The quinoline ring was "isolated".</p> <p>Unsaturated heterocycle and 2 hetero atoms specified via generic definition:</p>  <p>Element requirements specified via element count:</p> 

(continued on next page)

This structure requirement

Was achieved using the following technique:

Saturated carbon chain

Saturated chain specified via generic definition:

Generic Definition

Saturation: Any Mixture
 Unsaturated Saturated

Type of Chain: Any Mixture
 Branched Linear

Number of Hetero Atoms: Any Mixture
 2 or more Exactly 1

Type of Ring System: Any Mixture
 Monocyclic Polycyclic

Number of Carbon Atoms: Any Mixture
 7 or more less than 7

OK
Cancel

Element count range specified via element count:

Element Count

C Ac Ca Er In Na Po Se Tm
 H Ag Cd Eu Ir Nb Pr Sm U
 O Am Ce Fe K Nd Pt Sn V
 S Al Cf Fm Kr Ne Pu Sr W
 N Ar Cm Fr La Ni Ra T Xe
 P As Co Ga Li No Rb Ta Yb
 Si At Cr Ge Lu Np Re Tb Y
 Cl Au Cs Gd Lr Os Rh Tc Zn
 Br Ba Cu He Md Pa Rn Te Zr
 F Be D Hf Mg Pb Ru Th
 I Bi Dy Hg Mn Pd Sb Tl
 B Bk Es Ho Mo Pm Sc Tl

Exact Range
 Minimum Maximum

1

Limited

Add
Remove
Cancel
OK

C,Range,1-8

Step 2: Locate Specific Substances in REGISTRY

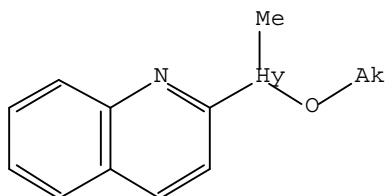
=> FILE REGISTRY

L1 STRUCTURE UPLOADED

=> D L1

L1 HAS NO ANSWERS

L1 STR



=> S L1 SSS SAM

SAMPLE SEARCH INITIATED 13:12:16

SAMPLE SCREEN SEARCH COMPLETED - 38708 TO ITERATE

5.2% PROCESSED 2000 ITERATIONS 0 ANSWERS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**

L2 0 SEA SSS SAM L1

=> S L1 SSS FUL

FULL SEARCH INITIATED 13:12:59

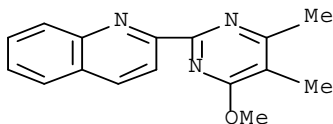
FULL SCREEN SEARCH COMPLETED - 774842 TO ITERATE

100.0% PROCESSED 774842 ITERATIONS 19 ANSWERS
SEARCH TIME: 00.00.07

L3 19 SEA SSS FUL L1

=> D SCAN

L3 19 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN
IN Quinoline, 2-(4-methoxy-5,6-dimethyl-2-pyrimidinyl) - (9CI)
MF C16 H15 N3 O



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):0

Step 3: Locate Generic Substances in MARPAT

There is a special price available for MARPAT searches when done sequentially in this order:

1. In MARPAT, use the *REGISTRY database answer set L-number* as the search term.

```
=> FILE MARPAT

=> S L3 SSS SAM

SAMPLE SEARCH INITIATED 13:20:21
SAMPLE SCREEN SEARCH COMPLETED -          398 TO ITERATE

100.0% PROCESSED          398 ITERATIONS          29 ANSWERS
SEARCH TIME: 00.00.02

FULL FILE PROJECTIONS:  ONLINE  **COMPLETE**
                        BATCH   **COMPLETE**
PROJECTED ITERATIONS:   6776 TO   9144
PROJECTED ANSWERS:     257 TO   903

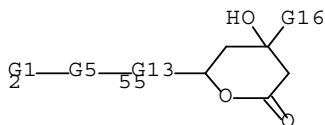
L4          29 SEA SSS SAM L1

=> D SCAN

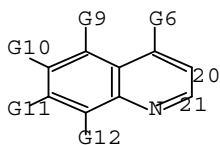
L4  29 ANSWERS  MARPAT  COPYRIGHT 2008 ACS on STH
IC  C07D215-14; C07D405-06; A61K031-55; A61K031-365; A61K031-47
CC  30-20 (Terpenes and Terpenoids)
    Section cross-reference(s): 1, 27
TI  Preparation of 5-[3-(quinolinyl)vinyl- or ethyl]mevalonates as
    HMG-CoA reductase inhibitors
ST  quinolinylvinylmevalonate prepn HMGCoA reductase inhibitor;
    mevalonate quinolinylvinyl prepn HMGCoA reductase inhibitor
IT  Atherosclerosis
    (treatment of, (quinolinylvinyl- or ethyl)mevalonates for)
IT  Lipoproteins
    RL: ADV (Adverse effect, including toxicity)
        (metabolic disorders, hyperlipoproteinemia, treatment of,
        (quinolinylvinyl- or ethyl)mevalonates for)
    ●
    ●
    ●
IT  105-45-3, Methylacetoacetate  460-00-4, 4-Bromofluorobenzene
    547-63-7, Methylisobutyrate  20061-84-1, Diethyl-2-
    (cyclohexylamino)vinylphosphonate  32249-35-7  60288-17-7
    RL: RCT (Reactant); RACT (Reactant or reagent)
        (reaction of, in preparation of HMG-CoA reductase inhibitors)
```

(continued on next page)

MSTR 1A



G1 = heterocycle <containing 1-4 heteroatoms,
zero or more N, zero or more O,
zero or more S (no other heteroatoms),
up to 7-membered monocyclic ring>
(opt. substd. by (up to 3) G2)
G2 = OCF3 / alkyl <containing up to 8 C>
G5 = 21-2 20-55



Derivative: and salts
Patent location: claim 1

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):0

=> S L3 SSS FULL

FULL SEARCH INITIATED 13:20:24

FULL SCREEN SEARCH COMPLETED - 8400 TO ITERATE

95.1% PROCESSED	7991 ITERATIONS	451 ANSWERS
98.4% PROCESSED	8263 ITERATIONS	470 ANSWERS
100.0% PROCESSED	8400 ITERATIONS (1 INCOMPLETE)	480 ANSWERS

SEARCH TIME: 00.00.44

L5 480 SEA SSS FUL L1

=> S L5/COM

L6 479 L5/COM

=> D SCAN

L6 479 ANSWERS MARPAT COPYRIGHT 2008 ACS on STN

IC ICM C07D471-22

ICS C07D513-22; A61K031-437; A61K031-4375; A61K031-4365;
A61P015-10; A61P009-00; A61P019-10; A61P037-00

CC 28-17 (Heterocyclic Compounds (More Than One Hetero Atom))
Section cross-reference(s): 1, 63

TI preparation of ring fused pyrazinopyridoindole derivatives as cyclic
GMP-specific phosphodiesterase inhibitors

ST pyrazinopyridoindole deriv prepn cyclic GMP phosphodiesterase
inhibitor prepn; tetraazaindenoanthracenedione prepn cyclic GMP
phosphodiesterase inhibitor prepn

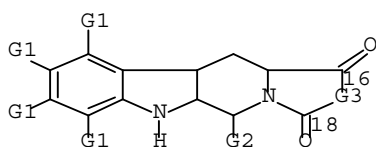
(continued on next page)

IT 9068-52-4
RL: BCP (Biochemical process); BIOL (Biological study); PROC
(Process)
(preparation of ring fused pyrazinopyridoindole derivs. as cyclic
GMP-specific phosphodiesterase inhibitors)



IT 191739-36-3P 385765-07-1P 385765-08-2P 385765-09-3P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation);
RACT (Reactant or reagent)
(preparation of ring fused pyrazinopyridoindole derivs. as cyclic
GMP-specific phosphodiesterase inhibitors)

MSTR 1



G2 = quinolinyl
G3 = heterocycle <containing 1-3 heteroatoms,
1 or more N, zero or more O, zero or more S (no other
heteroatoms), attached through 1 or more N, 1 or more C,
0 or more double bonds, 5- to 7-membered monocyclic ring>
(opt. substd. by (1-2) G4)
G4 = OCF3
G7 = alkylene <containing 1-4 C>
Patent location: claim 1
Note: and pharmaceutically acceptable salts and
solvates
HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):0

Step 4: Retrieve CAPLUS References to REGISTRY Substances

=> FILE CAPLUS

=> S L3

L7 13 L3

Step 5: Remove Duplicates

```
=> DUPLICATE REM
```

```
ENTER L# LIST OR (END):L6 L7
DUPLICATE PREFERENCE IS 'MARPAT, CAPLUS'
KEEP DUPLICATES FROM MORE THAN ONE FILE? Y/(N):N

L8          486 DUP REM L72 L75 (6 DUPLICATES REMOVED)
           ANSWERS '1-479' FROM FILE MARPAT
           ANSWERS '480-486' FROM FILE CAPLUS
```

Step 6: Display Answers

```
=> D L8 IBIB ABS FHIT 4; D L8 IBIB ABS HITSTR 484
```

```
L8 ANSWER 4 OF 486 MARPAT COPYRIGHT 2008 ACS on STN DUPLICATE 4
ACCESSION NUMBER:      133:5839 MARPAT Full-text
TITLE:                  Conjugated heterocyclic type leuco dyes with
                        high sensitivity and their use on laser imaging
                        sheets
INVENTOR(S):           Obayashi, Tatsuhiko; Okawa, Atsuhiko
PATENT ASSIGNEE(S):   Fuji Photo Film Co., Ltd., Japan
SOURCE:                Jpn. Kokai Tokkyo Koho, 44 pp.
                        CODEN: JKXXAF
DOCUMENT TYPE:        Patent
LANGUAGE:             Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:
```

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 2000144004	A2	20000526	JP 1999-221521	19990804
US 6143480	A	20001107	US 1999-388390	19990901
PRIORITY APPLN. INFO.:			JP 1998-250081	19980903

```
AB The dyes are obtained from I-type compds. or their mutual isomers bearing
a transferable H atom which is formed via the heat- or acid-induced
displacement of a substituent P where I has a structure of
HXC(R1):C(R2)C(R3):NR4 provided that R1 and R2 together form an N-containing
heterocyclic ring, R3 and R4 together form a 6-membered heterocyclic ring
with groups where they attach to, X is (optionally substituted) O, S, N.
Heat-mode laser imaging using the dyes can be done at a low output below
the ablation. Thus, dissolving an IR pigment with a I-type dye and
polystyrene beads in CHCl3 and coating the resulting solution on a PET
polyester film gave a recording sheet.
```

(continued on next page)

MSTR 1

G1—G4

G1 = SH (opt. substd.) / OH (opt. substd.) /
NH2 (opt. substd.) / (Example: 9)

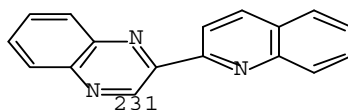
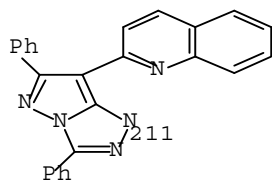
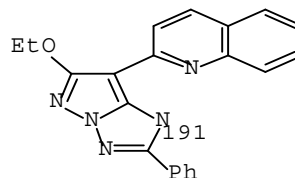
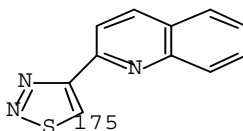
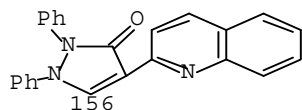
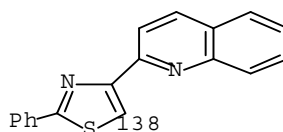
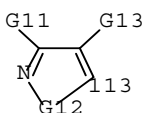
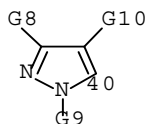
G6—G5

G2 = heterocycle <containing 1 or more N,
1 or more double bonds, attached through 2 or more C>

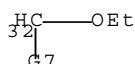
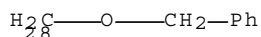
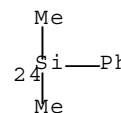
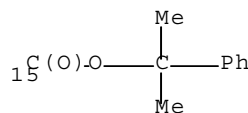
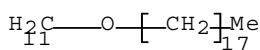
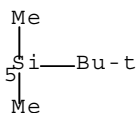
G3 = heterocycle <containing 1 or more N,
1 or more double bonds, 1 or more 6-membered rings only>

G4 = 2 / (**Examples: 40** / 113 / 138 / 156 / 175 / 191 /
211 / 231)

G2—G3

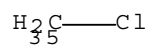


G5 = CO2Bu-t / 5 / 11 / C(=O)Ph / 15 / 24 / 28 / 32

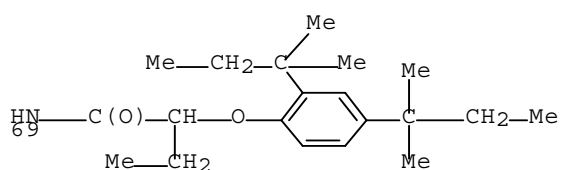


(continued on next page)

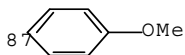
G6 = O / NMe
G7 = Ph / Me / 35



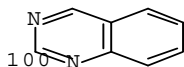
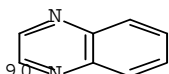
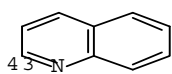
G8 = CO₂Et / **Me** / OEt / 54 / 57 / 69 / tridecyl / Ph / OMe



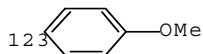
G9 = Ph / 87



G10 = **43** / 2-pyridyl / 90 / 100

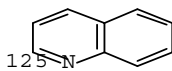


G11 = Me / Ph / 123 / OMe / CF₃ / CN / Bu-t



G12 = O / S

G13 = 125 / 2-pyridyl



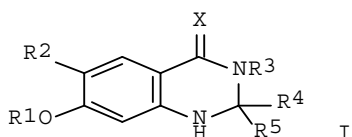
Patent location:

claim 1

L8 ANSWER 480 OF 486 CAPLUS COPYRIGHT 2008 ACS on STN
 ACCESSION NUMBER: 2004:182874 CAPLUS [Full-text](#)
 DOCUMENT NUMBER: 140:235742
 TITLE: Preparation of quinazolinones as inosine
 5'-monophosphate dehydrogenase (IMPDH)
 inhibitors.
 INVENTOR(S): Haughan, Alan Findlay; Buckley, George Martin; Dyke,
 Hazel Joan; Hannah, Duncan Robert; Richard, Marianna
 Dilani; Sharpe, Andrew; Williams, Sophie Caroline
 PATENT ASSIGNEE(S): Celltech R & D Limited, UK
 SOURCE: PCT Int. Appl., 81 pp.
 CODEN: PIXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
-----	---	-----	-----	-----
WO 2004018462	A1	20040304	WO 2003-GB3600	20030818
W:	AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW			
RW:	GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG			
PRIORITY APPLN. INFO.:			GB 2002-19638	A 20020823
			GB 2003-3866	A 20030220
			GB 2003-12773	A 20030604

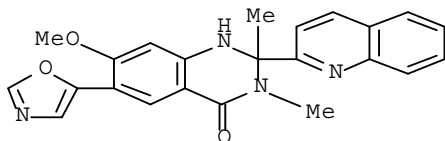
OTHER SOURCE(S): MARPAT 140:235742
 GI



AB Title compds. [I; X = O, S; R1 = aliphatic, cycloaliph., cycloalkylalkyl; R2 = (substituted) heteroaryl, cyano; R3 = (Alk1)mL1(Alk2)nR6; m, n, p, q = 0, 1; Alk1-Alk4 = (substituted) aliphatic, heteroaliph. chain; L1, L2 = bond, linker atom or group; R6 = H, (substituted) cycloaliph., heterocycloaliph., aryl, heteroaryl; R4 = (Alk3)pL2(Alk4)qR7; R7 = H, halo, cyano, (substituted) cycloaliph., heterocycloaliph., aryl, heteroaryl; R5 = H, (substituted) aliphatic; and the salts, solvates, hydrates, tautomers, isomers or N-oxides thereof], were prepared. Thus, 2-amino-4-methoxy-N-(2-morpholin-4-ylethyl)-5-oxazol-5-ylbenzamide (preparation given) was refluxed 6 h with MgSO4 and p-TsOH in acetone to give 16% 7-methoxy-2,2-dimethyl-3-(2-morpholin-4-ylethyl)-6-oxazol-5-yl-2,3-dihydro-1H-quinazolin-4-one. I inhibited IMPDH with IC50.ltoreq. 5 .mu.M.

(continued on next page)

IT 667939-56-2P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU
(Therapeutic use); BIOL (Biological study); PREP (Preparation); USES
(Uses)
(preparation of quinazolinones as IMP dehydrogenase (IMPDH) inhibitors)
RN 667939-56-2 CAPLUS
CN 4(1H)-Quinazolinone, 2,3-dihydro-7-methoxy-2,3-dimethyl-6-(5-oxazolyl)-2-
(2-quinolinyl)- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

note

Effect of Element Count Unlimited

Had the preceding search been run with "limited" turned on, 81 fewer answers would have been retrieved in the MARPAT database. The effect on other searches including Element Counts will vary with the specific search query.

The Element Count unlimited feature found results where the answers had no element counts specified such as:

```
G3 = aryl (opt. substd. by 1 or more G4) /  
heteroaryl (opt. substd. by 1 or more G4)  
G4 = CN / alkyl (opt. substd.) / alkenyl (opt. substd.) /  
aralkyl (opt. substd.) / alkoxy (opt. substd.) /  
aryloxy (opt. substd.) / acyl /
```

Summary

Element Count and Match Level

The effect of element count assignment on retrieval is also related to the match level assigned to the generic group.

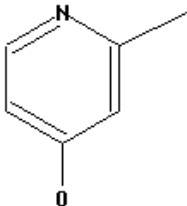
Illustration: Hy with specific element counts

Hy Match Level	Element Count level	Result
Atom	Limited	Matches only specific heterocyclic rings with matching element counts
Class	Limited	Also matches generic Hy in answer if it has element counts that encompass those required by the query
Class	Unlimited	Also matches generic Hy in answers with no element counts assigned

Generic Group Implicit Element Counts

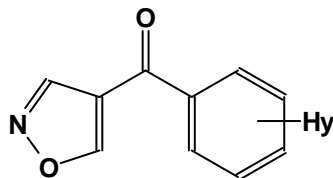
For *specific structural fragments* (see the ring illustrated below) with match level set to class, MARPAT generates element counts and generic group definitions for use in matching against generic groups in the answer file. A match will be found if the corresponding generic group

- **Has** assigned generic group definitions and element counts that encompass those generated by the specific structural fragment
- **Has no** further generic definitions or element counts attributes, but the query has element count level set to *unlimited*. This is a broader definition and will pick up answers where the file answer has no element count specified from the original document.

If the query contains	Matches include
<p>A specific heterocyclic ring that is isolated and set to match level class, e.g.,</p>  <p>The image shows a skeletal structure of a pyridine ring. The nitrogen atom is at the top vertex of the six-membered ring. A methyl group is attached to the carbon atom at the 2-position (top-right). An oxygen atom is attached to the carbon atom at the 4-position (bottom).</p>	<p>With element count level limited:</p> <ul style="list-style-type: none">■ Pyridine ring■ Hy with any specification that allows: UNSATURATED MONOCYCLIC Exactly 5 Carbons Exactly 1 Nitrogen <p><i>Examples:</i> heterocycle <containing 3 or more atoms, 1 or more N, zero or more O, zero or more S</p> <p>heterocycle <containing 1-3 heteroatoms, zero or more N, zero or more O, zero or more S (no other heteroatoms), 3- to 6-membered monocyclic ring></p> <p>With element count level unlimited:</p> <ul style="list-style-type: none">■ Pyridine ring■ Hy with any specification that allows: Containing 1-5 carbons, unsaturated, monocyclic, 1 heteroatom■ Hy with no further qualification <p><i>Example:</i> heterocycle (opt. substd.)</p>

Skills Practice

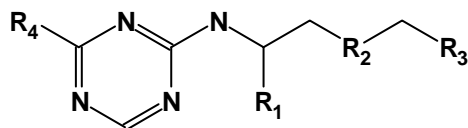
1. Locate patents concerning anti-inflammatory agents of the following type:



Requirements:

- Hy should match specific heterocycles with up to 4 N and exactly 1 S. It should also match on any Hy. The Hy may be attached to any position on the phenyl ring.
- The phenyl ring is isolated and should only match phenyl rings.
- The oxazole ring may match real atom rings or generic groups with or without element counts

2. Locate references discussing compounds with the following structure:



Requirements:

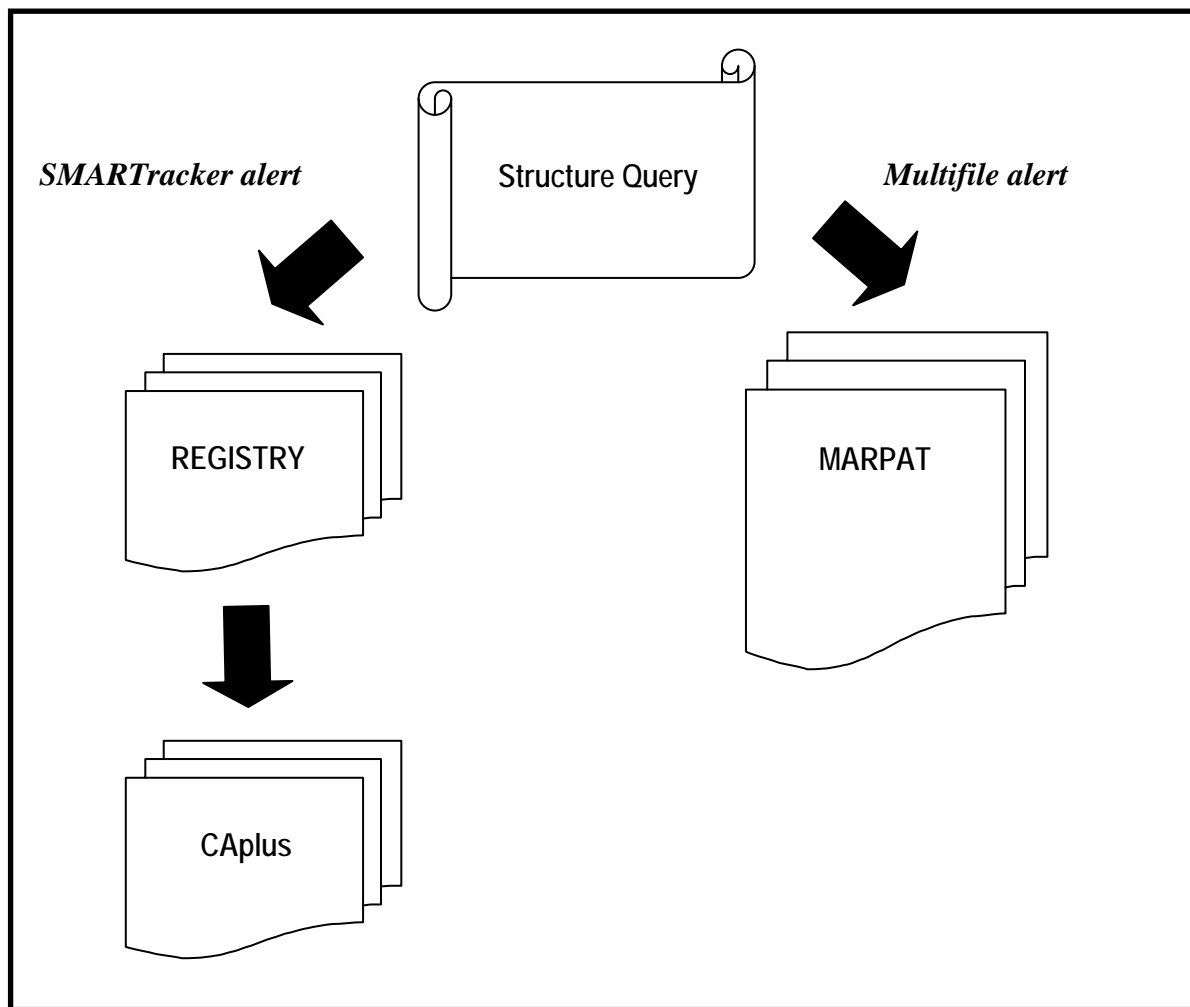
- R₁ = carbon chain (substituted or unsubstituted) or a carbocyclic ring
- R₂ = O, S, N
- R₃ = Any type of ring system
- R₄ = N in a chain
- The nitrogen containing ring may be isolated or embedded
- All of the atoms in the structure must match real atoms in Markush structures, except for R₁ and R₃ which may also match generic groups.

CURRENT AWARENESS ALERTS

In this section, you will learn to set up a current awareness alert for substances reported in the patent literature.

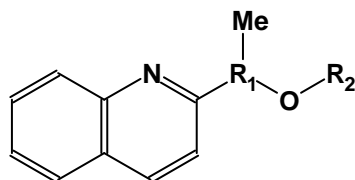
Overview

Alerts to monitor new specific substances and Markush structures require the setup of two separate current awareness searches.



The results of these two alerts must be manually merged.

Search Question: Set up a current awareness alert for substances with the following structure:



Requirements:

- The quinoline ring may not be part of a larger ring system.
- R₁ is a heterocycle (match level class). It is unsaturated with at least 2 C atoms, a maximum of one O atom, and 1–5 N atoms. There are at least 2 heteroatoms.
- R₂ is a saturated carbon chain with 1–8 C atoms.
- The query should match against answers with no element counts specified.

Search Strategy

To set up a current awareness alert for substances in the patent literature

- Step 1 Build the structure.
- Step 2 Upload the structure.
- Step 3 Set up a SMARTTracker alert for specific substances.
- Step 4 Set up a MARPAT alert for generic substances.

Step 1: Build the Structure

The query may be built with STN Express, STN on the Web, or the online STRUCTURE command.

Step 2: Upload the Structure

```
=> FILE REGISTRY CAPLUS
```

```
=>
```

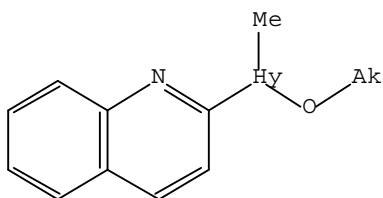
```
Uploading C:\Program Files\stnexp\Queries\ALKOXYQUIN.str
```

```
L1 STRUCTURE UPLOADED
```

```
=> D L1
```

```
L1 HAS NO ANSWERS
```

```
L1 STR
```



Step 3: Set Up a SMARTracker Alert

SMARTracker is an alert option that monitors the latest CPlus references to a REGISTRY substance. SMARTracker alerts may be run either weekly or biweekly.

=> **SMARTRACKER**

SMARTracker INITIATED

```
ENTER QUERY L# FOR SDI REQUEST OR (END):L1
ENTER UPDATE FIELD CODE (UP) OR ?:UP
ENTER SDI REQUEST NAME, (AA045/S), OR END:QUINOLINES/S
ENTER COST CENTER (NONE) OR NONE:HERBICIDE PROJECT
ENTER TYPE OF SEARCH (SSS), CSS, FAMILY, OR EXACT:SSS
ENTER TITLE (NONE):ALKOXYHETEROCYCLIC QUINOLINES
ENTER METHOD OF DELIVERY (OFFLINE), ONLINE, OR EMAIL:EMAIL
ENTER EMAIL ID (5584C): WILEYCOYOTE@REDROCK.ORG
WILEYCOYOTE@REDROCK.ORG
RECEIVE DELIVERY NOTIFICATION? (Y)/N:N
ELIMINATE PREVIOUSLY SEEN ANSWERS WITH EACH SDI RUN? Y/(N):Y
ENTER PRINT FORMAT (BIB) OR ?:IBIB ABS HITSTR
HIGHLIGHT HIT TERMS? (Y)/N:Y
ARCHIVE ANSWERS? Y/(N):N
REDISTRIBUTE ANSWERS? Y/(N):N
ENTER MAXIMUM NUMBER OF HITS TO BE PRINTED PER RUN (100):.
SORT SDI ANSWER SET (N)/Y?:N
SEND SDI WITH NO ANSWERS? (Y)/N:Y
DISPLAY CURRENCY INFORMATION? (Y)/N:Y
ENTER SDI RUN FREQUENCY - (WEEKLY), BIWEEKLY, OR ?:BIWEEKLY
ENTER SDI EXPIRATION DATE 'YYYYMMDD' OR (NONE):20091231
QUERY L1 HAS BEEN SAVED AS SDI REQUEST 'QUINOLINES/S'
```

 **Web
Resource**

A Quick Reference Card on SMARTracker is available:
www.cas.org/support/stngen/qrc/

Step 4: Set Up a MARPAT Alert

MARPAT alerts are run every 2 weeks.

```
=> FILE MARPAT

=> SDI

ENTER QUERY L# FOR SDI REQUEST OR (END):L1
ENTER SDI REQUEST NAME, (AA045/S), OR END:QUINOLMARPAT/S
ENTER COST CENTER (NONE) OR NONE:HERBICIDE PROJECT
ENTER TYPE OF SEARCH (SSS) OR CSS:SSS
ENTER TITLE (NONE):ALKOXYHETEROCYCLIC QUINOLINE MARKUSH
ENTER METHOD OF DELIVERY (OFFLINE), ONLINE, OR EMAIL:EMAIL
ENTER EMAIL ID (5584C):WILEYCOYOTE@REDROCK.ORG
WILEYCOYOTE@REDROCK.ORG
RECEIVE DELIVERY NOTIFICATION? (Y)/N:N
ELIMINATE PREVIOUSLY SEEN ANSWERS WITH EACH SDI RUN? Y/(N):Y
ENTER PRINT FORMAT (BIB) OR ?:BIB ABS FHIT
HIGHLIGHT HIT TERMS? (Y)/N:Y
ARCHIVE ANSWERS? Y/(N):N
REDISTRIBUTE ANSWERS? Y/(N):N
ENTER MAXIMUM NUMBER OF HITS TO BE PRINTED PER RUN (100):.
SORT SDI ANSWER SET (N)/Y?:N
SEND SDI WITH NO ANSWERS? (Y)/N:Y
ENTER SDI EXPIRATION DATE 'YYYYMMDD' OR (NONE):20091231
QUERY L1 HAS BEEN SAVED AS SDI REQUEST 'QUINOLMARPAT/S'
```

Helpful HINT

It is good practice to display the saved queries to verify that SDIs are set up correctly.

```
=> D SAVE/S
```

NAME	CREATED	NOTES/TITLE
QUINOLINES/S	30 JAN 2008	SDI REQUEST FOR CAPLUS FROM REGISTRY ALKOXYHETEROCYCLIC QUINOLINES
QUINOLMARPAT/S	30 JAN 2008	SDI REQUEST FOR FILE MARPAT ALKOXYHETEROCYCLIC QUINOLINE MARKUSH

MARKUSH SEARCHING IN THE PATENT LITERATURE

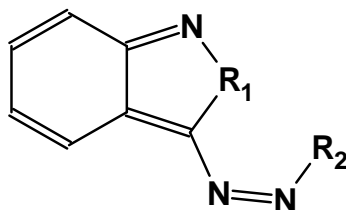
SUGGESTED SOLUTIONS TO SKILLS PRACTICE PROBLEMS

APRIL 2008

The solutions presented here are solutions that can be attained using techniques and search tools presented in the accompanying workbook.

Skills Practice (page 32):

Question 1: Use CASLINK to locate references discussing substances with the following structure.



- $R_1 = O$ or S
 - $R_2 =$ Any heterocycle
 - Any type of substitution allowed at open sites
 - The nitrogen-containing ring system may be isolated or embedded in a larger ring system
-
-

Suggested Approach:

1. Build the structure:
 $R_1 =$ a G-group defined as O or S
 $R_2 =$ an Hy
2. Enter the CASLINK multifile environment and upload and display the query
3. Run a SAMPLE SSS search and examine full-file projections; use D SCAN to see results
4. Run a FULL SSS search
5. Display results using BIB ABS FQHIT for MARPAT and BIB ABS HITSTR for CAplus

```
=> FILE CASLINK
```

```
FILE 'CAPLUS' ENTERED AT 11:17:58 ON ...
```

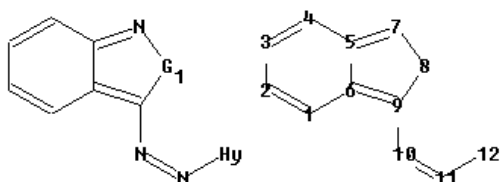
(continued on next page)

FILE 'MARPAT' ENTERED AT 11:17:58 ON...

FILE 'REGISTRY' ENTERED AT 11:17:58 ON ...

Predefined command sequences will be executed in
REGISTRY, MARPAT, and CAPLUS.

=> UPLOADING C:\CASNC\STN EXPRESS\QUERIES\34.STR



G1:O,S

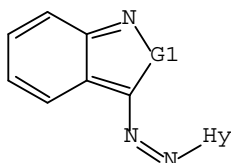
L1 STRUCTURE UPLOADED

=> D L1

The Hy group has not been further qualified.

L1 HAS NO ANSWERS

L1 STR



G1 O,S

Structure attributes must be viewed using STN Express query preparation.

=> S L1 SSS SAM

S L1 SSS SAM FILE=REGISTRY

FILE 'REGISTRY'

SAMPLE SEARCH INITIATED 11:18:36

SAMPLE SCREEN SEARCH COMPLETED - 134 TO ITERATE

100.0% PROCESSED 134 ITERATIONS

8 ANSWERS

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**

BATCH **COMPLETE**

PROJECTED ITERATIONS: 1986 TO 3374

PROJECTED ANSWERS: 8 TO 329

L2 8 SEA SSS SAM L1

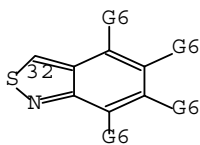
S L2 SSS SAM FILE=MARPAT

FILE 'MARPAT'

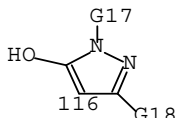
SAMPLE SEARCH INITIATED 11:18:36

SAMPLE SCREEN SEARCH COMPLETED - 144 TO ITERATE

(continued on next page)



G2 = 116



Patent location: claim 1

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):0

=> S L1 FULL

S L1 SSS FUL FILE=REGISTRY
 FILE 'REGISTRY'
 FULL SEARCH INITIATED 11:19:53
 FULL SCREEN SEARCH COMPLETED - 2797 TO ITERATE

100.0% PROCESSED 2797 ITERATIONS 147 ANSWERS
 SEARCH TIME: 00.00.01

L4 147 SEA SSS FUL L1

S L4 SSS FUL FILE=MARPAT
 FILE 'MARPAT'
 FULL SEARCH INITIATED 11:19:54
 FULL SCREEN SEARCH COMPLETED - 2932 TO ITERATE

100.0% PROCESSED 2932 ITERATIONS 67 ANSWERS
 SEARCH TIME: 00.00.03

L5 67 SEA SSS FUL L1

S L4 FILE=CAPLUS
 L6 49 FILE CAPLUS

Markush searching found an additional 67 answers not found in a REGISTRY search.

DUP REM L5 L6
 PROCESSING COMPLETED FOR L5
 PROCESSING COMPLETED FOR L6
 L7 102 DUP REM L5 L6 (14 DUPLICATES REMOVED)
 ANSWERS '1-67' FROM FILE MARPAT
 ANSWERS '68-102' FROM FILE CAPLUS

(continued on next page)

=> D 2 BIB ABS FQHIT; D 69 BIB ABS HITSTR

L7 ANSWER 2 OF 102 MARPAT COPYRIGHT 2008 ACS on STN DUPLICATE 2

AN 142:299354 MARPAT [Full-text](#)

TI Process for printing or dyeing cellulose fibers or cellulose/polyester mixed fibers with disperse dyes

IN Hall-Gouille, Veronique; Tzikas, Athanassios

PA Ciba Specialty Chemicals Holding Inc., Switz.

SO PCT Int. Appl., 25 pp.

CODEN: PIXXD2

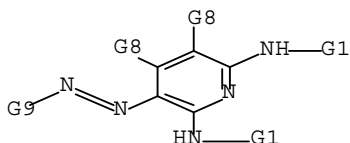
DT Patent

LA English

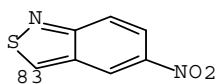
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2005024123	A2	20050317	WO 2004-EP51952	20040830
	WO 2005024123	A3	20050602		
	W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
	RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
	EP 1664420	A2	20060607	EP 2004-766635	20040830
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, FI, RO, CY, TR, BG, CZ, EE, HU, PL, SK				
	CN 1846028	A	20061011	CN 2004-80025594	20040830
	US 20070000076	A1	20070104	US 2006-570473	20060301
	IN 2006CN00804	A	20070629	IN 2006-CN804	20060306
PRAI	EP 2003-405656		20030908		
	WO 2004-EP51952		20040830		
AB	The process comprises treating cellulose fibers or cellulose/polyester blend fibers in any sequence with water, a water-soluble organic solvent having b.p.>150°, and a specific disperse dye.				

MSTR 1



G9 = 83

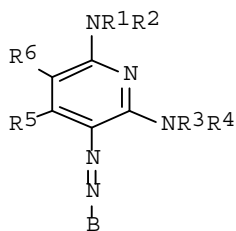


Patent location: claim 1

(continued on next page)

L7 ANSWER 69 OF 102 CAPLUS COPYRIGHT 2008 ACS on STN
 AN 2004:533766 CAPLUS [Full-text](#)
 DN 141:96759
 TI Optical information recording medium
 IN Mikoshiba, Hisashi
 PA Fuji Photo Film Co., Ltd., Japan
 SO U.S. Pat. Appl. Publ., 22 pp.
 CODEN: USXXCO
 DT Patent
 LA English
 FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	US 2004126702	A1	20040701	US 2003-737815	20031218
	JP 2004209771	A2	20040729	JP 2002-381013	20021227
PRAI	JP 2002-381013	A	20021227		
OS	MARPAT 141:96759				
GI					

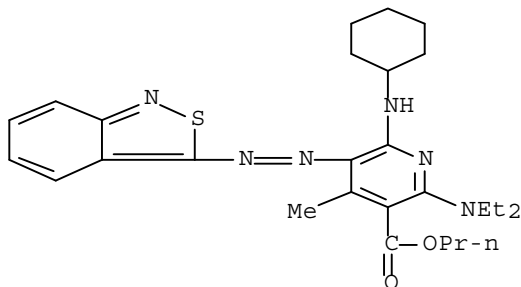


AB The present invention relates to an optical information recording medium containing a substrate having provided thereon a recording layer capable of recording information by laser beam irradiation, wherein the recording layer contains a dye represented by I (R1-4 = H, substituent group; R5,6 = H, substituent group; and B = aryl, heterocyclic group, which are derivable from a diazonium salt).

IT 714236-90-5
 RL: TEM (Technical or engineered material use); USES (Uses)
 (dye; optical information recording medium containing)

RN 714236-90-5 CAPLUS

CN 3-Pyridinecarboxylic acid, 5-(2,1-benzisothiazol-3-ylazo)-6-(cyclohexylamino)-2-(diethylamino)-4-methyl-, propyl ester (9CI)
 (CA INDEX NAME)



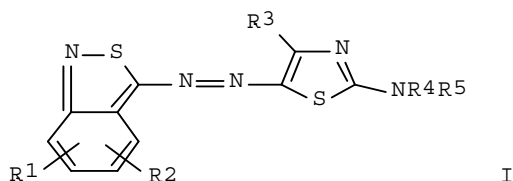
(continued on next page)

=> D 5 BIB ABS FHIT

L7 ANSWER 5 OF 102 MARPAT COPYRIGHT 2006 ACS on STN DUPLICATE 5
 AN 122:42797 MARPAT [Full-text](#)
 TI Sublimable cyan dye, its ink compositions, and sublimation-type thermal-transfer recording sheets
 IN Takuma, Hirosuke; Shimokawa, Yasushi; Matsuzaki, Yoriaki; Aida, Isamu; Koshida, Hitoshi; Kafuku, Masaaki; Eguchi, Hiroshi; Takiguchi, Ryohei
 PA Mitsui Toatsu Chemicals, Japan; Dai Nippon Printing Co., Ltd.
 SO Jpn. Kokai Tokkyo Koho, 8 pp.
 CODEN: JKXXAF
 DT Patent
 LA Japanese
 FAN.CNT 1

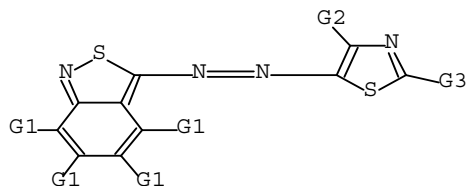
	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	JP 06206383	A2	19940726	JP 1993-3305	19930112
	JP 3370713	B2	20030127		
PRAI	JP 1993-3305		19930112		

GI



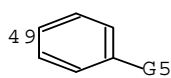
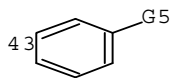
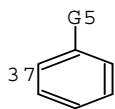
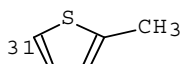
AB Claimed are the cyan dye I [R1-2 = H, C1-4 alkyl, C1-4 alkoxy, NO₂, halo; R₃ = C1-4 alkyl, C5-8 (un)substituted cycloalkyl, C6-10 (un)substituted Ph, (un)substituted heterocyclyl; R₄-5 = H, C1-6 = alkyl, C3-8 = alkoxyalkyl, C6-10 alkoxyalkoxyalkyl, C3-7 alkylcarbonyloxyalkyl, C5-10 alkylcarbonyloxyalkoxyalkyl] for sublimation-type thermal-transfer recording, its ink compns. containing I, a binder resin, and an organic solvent and/or H₂O, and the recording sheets comprising a base sheet and a dye-supporting layer containing I. The recording sheets provide lightfast and rubbing-resistant images.

MSTR 1

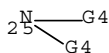
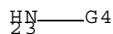


G1 = 2 or more H / alkyl <containing 1-4 C> / alkoxy <containing 1-4 C> / NO₂ / halo
 G2 = alkyl <containing 1-4 C> / cycloalkyl <containing 5-8 C> (opt. substd.) / Ph (opt. substd.) / heterocycle (opt. substd.) / (Examples: 37 / 43 / 49 / pyridyl / furyl / thienyl / 31)

(continued on next page)



G3 = NH₂ / 23 / 25



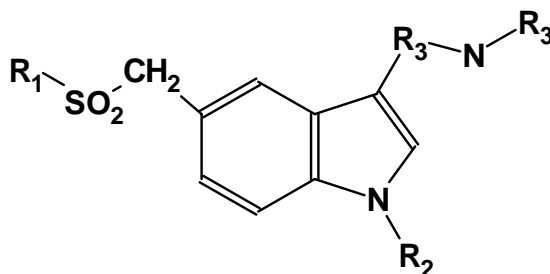
G4 = alkyl <containing 1-6 C>
 (opt. substd. by alkoxy <containing 2-7 C>
 (opt. substd. by alkoxy <containing 4-8 C>)) /
 alkyl <containing 1-6 C> (substd. by alkylcarbonyloxy
 <containing 1-5 C>) / alkyl <containing 1-7 C>
 (substd. by alkoxy <containing 1-7 C>
 (substd. by alkylcarbonyloxy <containing 2-7 C>))

G5 = Me / OMe / Cl / NHCHO / NHCOMe

Patent location: claim 1

Skills Practice (page 33)

Question 2: Use CASLINK to locate references covering substances with the following structure in relation to headaches.



- R_1 = nitrogen in a ring or a chain
 - R_2 = anything, including hydrogen
 - R_3 = carbon chain with any substitution
 - Nitrogen-containing ring may be isolated or embedded in a larger ring system
 - Any substitution is allowed at open sites
-
-

Suggested Approach:

1. Build the structure:
 R_1 = N with node characteristics ring/chain
 R_2 = represented by an open position
 R_3 = represented by an Ak
2. Enter the CASLINK multifile environment and upload and display the query
3. Run a SAMPLE SSS search and examine full-file projections; use D SCAN to see results
4. Run a FULL SSS search
5. Display results using BIB ABS FHIT for MARPAT and BIB ABS HITSTR for CPlus

=> **FILE CASLINK**

FILE 'CAPLUS' ENTERED AT 11:25:58 ON ...

FILE 'MARPAT' ENTERED AT 11:25:58 ON...

FILE 'REGISTRY' ENTERED AT 11:25:58 ON ...

Predefined command sequences will be executed in
REGISTRY, MARPAT, and CAPLUS.

=>

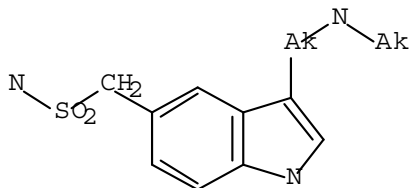
Uploading C:\CASNC\STN Express\Queries\35.str

L1 STRUCTURE UPLOADED

=> **D L1**

L1 HAS NO ANSWERS

L1 STR



Structure attributes must be viewed using STN Express query preparation.

=> **S L1 SSS SAM**

S L1 SSS SAM FILE=REGISTRY

FILE 'REGISTRY'

SAMPLE SEARCH INITIATED 11:27:07

SAMPLE SCREEN SEARCH COMPLETED - 262 TO ITERATE

100.0% PROCESSED 262 ITERATIONS 12 ANSWERS

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**

BATCH **COMPLETE**

PROJECTED ITERATIONS: 4269 TO 6211

PROJECTED ANSWERS: 33 TO 447

L2 12 SEA SSS SAM L1

S L2 SSS SAM FILE=MARPAT

FILE 'MARPAT'

SAMPLE SEARCH INITIATED 11:27:08

SAMPLE SCREEN SEARCH COMPLETED - 1138 TO ITERATE

100.0% PROCESSED 1138 ITERATIONS 3 ANSWERS

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**

BATCH **COMPLETE**

PROJECTED ITERATIONS: 20807 TO 24713

PROJECTED ANSWERS: 3 TO 163

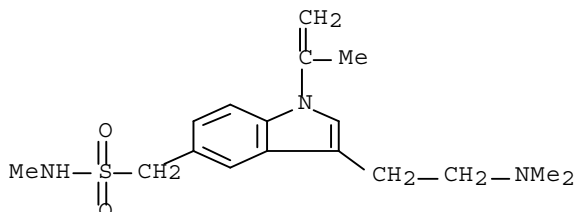
L3 3 SEA SSS SAM L1

(continued on next page)

=> D SCAN L2

L2 12 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN
 IN Butanedioic acid, compd. with 3-[2-(dimethylamino)ethyl]-N-methyl-1-(methylene)-1H-indole-5-methanesulfonamide (1:1) (9CI)
 MF C17 H25 N3 O2 S . C4 H6 O4

CM 1



CM 2

HO₂C-CH₂-CH₂-CO₂H

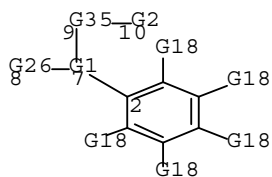
HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):0

=> D SCAN L3

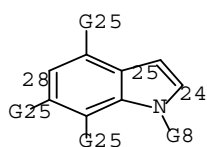
L3 3 ANSWERS MARPAT COPYRIGHT 2008 ACS on STN
 IC ICM A61K031-47
 ICS A61K031-445; A61K031-405; A61K031-38; A61K031-35; C07D209-04;
 C07D209-14; C07D333-52; C07D409-14; C07D401-10; C07D401-14;
 C07D405-10; C07D405-14; C07D409-10; C07D217-02; C07D217-12
 CC 27-11 (Heterocyclic Compounds (One Hetero Atom))
 Section cross-reference(s): 1
 TI Preparation of aminoalkylindoles as gonadotropin releasing hormone antagonists
 ST aminoalkylindole prepn gonadotropin releasing hormone antagonist
 IT Gonadotropin-releasing hormone receptor
 RL: BSU (Biological study, unclassified); MSC (Miscellaneous); BIOL (Biological study)
 (mediated disorders; treatment; preparation of aminoalkylindoles as gonadotropin releasing hormone antagonists)
 IT 223611-02-7P
 RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
 (preparation of aminoalkylindoles as gonadotropin releasing hormone antagonists)
 IT 123-72-8, Butyraldehyde 19910-33-9, 2-(4-Nitrophenyl)propionic acid 25081-39-4, Methyl 3,5-dimethylbenzoate 98244-48-5, (S)-3-Bromo-2-methyl-1-propanol
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (preparation of aminoalkylindoles as gonadotropin releasing hormone antagonists)
 IT 36924-81-9P 50712-64-6P 65284-00-6P 83397-45-9P 217189-83-8P 217192-25-1P 217192-27-3P 217192-28-4P 217192-29-5P 217192-34-2P 217192-35-3P 217192-36-4P 217192-38-6P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 (preparation of aminoalkylindoles as gonadotropin releasing hormone antagonists)

(continued on next page)

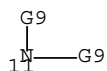
MSTR 1



G1 = 28-8 25-9 24-2



G2 = 11



G9 = alkyl <containing 1-6 C> (opt. substd.)

G28 = SO₂G29 = NH₂ (opt. substd.)

G30 = alkylene <containing 1-6 C> (opt. substd.)

G35 = alkylene <containing 1 or more C>

(opt. substd. by 1 or more G36)

Derivative: or N-oxides, pharmaceutically acceptable addition salts and/or hydrates

Patent location: claim 1

Note: substitution is restricted

Note: additional substitution and ring formation also claimed

Stereochemistry: or geometric or optical isomers or racemic mixtures

ALL ANSWERS HAVE BEEN SCANNED

(continued on next page)

=> S L1 SSS FULL

S L1 SSS FUL FILE=REGISTRY
 FILE 'REGISTRY'
 FULL SEARCH INITIATED 11:28:05
 FULL SCREEN SEARCH COMPLETED - 5723 TO ITERATE

100.0% PROCESSED 5723 ITERATIONS 214 ANSWERS
 SEARCH TIME: 00.00.01

L4 214 SEA SSS FUL L1

S L4 SSS FUL FILE=MARPAT
 FILE 'MARPAT'
 FULL SEARCH INITIATED 11:28:13
 FULL SCREEN SEARCH COMPLETED - 23241 TO ITERATE

100.0% PROCESSED 23241 ITERATIONS 67 ANSWERS
 SEARCH TIME: 00.00.16

L5 67 SEA SSS FUL L1

S L4 FILE=CAPLUS
 L6 1369 FILE CAPLUS

DUP REM L5 L6
 PROCESSING COMPLETED FOR L5
 PROCESSING COMPLETED FOR L6
 L7 1416 DUP REM L5 L6 (20 DUPLICATES REMOVED)
 ANSWERS '1-67' FROM FILE MARPAT
 ANSWERS '68-1416' FROM FILE CAPLUS

=> D 6 IBIB ABS FHIT; D 564 IBIB ABS HITSTR

L7 ANSWER 6 OF 1416 MARPAT COPYRIGHT 2008 ACS on STN DUPLICATE 6
 ACCESSION NUMBER: 130:139254 MARPAT [Full-text](#)
 TITLE: Process for the production of indole derivatives
 INVENTOR(S): Waite, David Charles
 PATENT ASSIGNEE(S): Pfizer Limited, UK; Pfizer Inc.
 SOURCE: PCT Int. Appl., 41 pp.
 CODEN: PIXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9902493	A1	19990121	WO 1998-EP3996	19980616
W: AU, BR, CA, CN, CZ, HU, ID, IL, JP, KR, MX, PL, RU, TR, US, YU				
RW: AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
CA 2286720	AA	19990121	CA 1998-2286720	19980616
AU 9883397	A1	19990208	AU 1998-83397	19980616
EP 975594	A1	20000202	EP 1998-933651	19980616
EP 975594	B1	20020918		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, PT, IE, FI				
AT 224367	E	20021015	AT 1998-933651	19980616
PT 975594	T	20021231	PT 1998-933651	19980616
ES 2182342	T3	20030301	ES 1998-933651	19980616
ZA 9805918	A	20000110	ZA 1998-5918	19980706
US 6281357	B1	20010828	US 2000-381072	20000324

(continued on next page)

PRIORITY APPLN. INFO.:

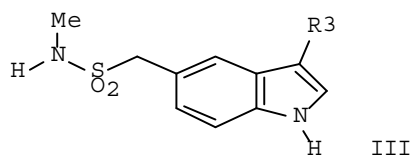
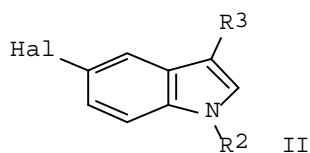
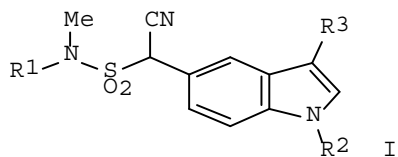
GB 1997-14383 19970708

WO 1998-EP3996 19980616

OTHER SOURCE(S):

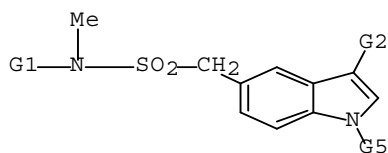
CASREACT 130:139254

GI

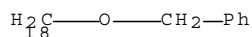


AB The title compds. I [R1, R2 = N-protecting groups; R3 = C1-6 alkyl substituted by (un)substituted 5-6 membered N-containing saturated heterocyclic group or di(C1-6 alkyl)amino] were prepared by reacting indole II [Hal = Cl, Br, I] with R1(Me)NSO₂CH₂CN in the presence of a strong base and a palladium(0) catalyst at an elevated temperature in a solvent which does not adversely affect the reaction. Compds. I may be further processed to compds. III which are useful in the treatment of inter alia migraine (no data).

MSTR 5

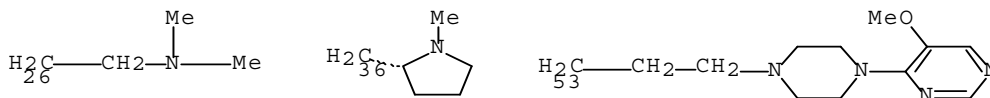


G1 = R <"protecting group"> /
(Specifically claimed: CH₂Ph / 18 / CHPh₂ / Bu-t)

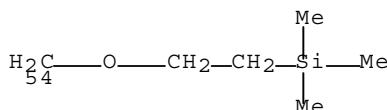
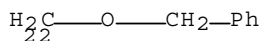


G2 = **alkyl** <containing 1-6 C> (substd. by G3) /
(Specifically claimed: 26 / 36 / 53)

(continued on next page)



- G3 = heterocycle <containing 1 or more heteroatoms, 1 or more N, non-aromatic, saturated, 5- to 6-membered monocyclic ring> (opt. substd. by G4) / **dialkylamino <each alkyl containing 1-6 C>**
- G4 = alkyl <containing 1-6 C> / pyrimidinyl (substd. by alkoxy <containing 1-6 C>)
- G5 = R <"protecting group"> / (Specifically claimed: CH2Ph / 22) / (Examples: 54 / CH2CH=CH2)



Patent location: claim 6

REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L7 ANSWER 564 OF 1416 CAPLUS COPYRIGHT 2008 ACS on STN
 ACCESSION NUMBER: 2003:830556 CAPLUS [Full-text](#)
 DOCUMENT NUMBER: 139:345813
 TITLE: Pain-free results with sumatriptan taken at the first sign of migraine pain: 2 randomized, double-blind, placebo-controlled studies
 AUTHOR(S): Winner, Paul; Mannix, Lisa K.; Putnam, D. Gayla; McNeal, Scott; Kwong, Jackie; O'Quinn, Stephen; Richardson, Mary S.
 CORPORATE SOURCE: Palm Beach Headache Center, West Palm Beach, FL, USA
 SOURCE: Mayo Clinic Proceedings (2003), 78(10), 1214-1222
 CODEN: MACPAJ; ISSN: 0025-6196
 PUBLISHER: Dowden Health Media, Inc.
 DOCUMENT TYPE: Journal
 LANGUAGE: English

AB Objective: To evaluate the efficacy and tolerability of sumatriptan, 50-mg and 100-mg tablets, compared with placebo for treatment of migraine at the first sign of pain. Patients and Methods: Two identical multicenter randomized, double-blind, placebo-controlled, single-attack studies were conducted from May through Nov. 2000 in adults (aged 18-65 yr). Patients treated migraine at the first sign of pain, while pain was mild, but not more than 2 h after onset with oral sumatriptan, 50 mg or 100 mg, or matching placebo. The primary end point was pain-free relief at 2 h after treatment with 50 mg of sumatriptan compared with placebo. Results: There were 354 patients in study 1 and 337 patients in study 2. Significantly more patients treated with sumatriptan, 50 mg and 100 mg, were completely free from pain 2 and 4 h after treatment vs. patients treated with placebo (at 2 h, 50% and 57% vs. 29%; at 4 h, 61% and 68% vs. 30%; for both, $P < .001$). Also, significantly more patients treated with sumatriptan, 50 mg

(continued on next page)

and 100 mg, were migraine-free (no pain or associated symptoms) vs. those treated with placebo at 2 and 4 h after treatment (at 2 h, 43% and 49% vs. 24%; at 4 h, 54% and 63% vs. 28%; for both, $P < .001$). The incidence of overall adverse events was low with the 50- and 100-mg dose of sumatriptan (placebo, 7%; sumatriptan at 50 mg, 14%; sumatriptan at 100 mg, 16%).
 Conclusions: Treatment of migraine at the first sign of pain with sumatriptan, 50-mg and 100-mg tablets, provides superior pain-free relief at 2 and 4 h after treatment compared with placebo. Results of these studies suggest that sumatriptan at 100 mg may be more efficacious than at 50 mg when used in the early treatment paradigm. Because these studies were not powered to detect statistical differences between active doses, studies to investigate this finding are warranted.

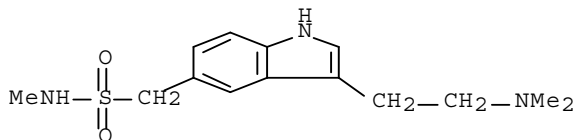
IT 103628-46-2, Sumatriptan

RL: ADV (Adverse effect, including toxicity); PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)

(pain-free results with sumatriptan taken at the first sign of migraine pain)

RN 103628-46-2 CAPLUS

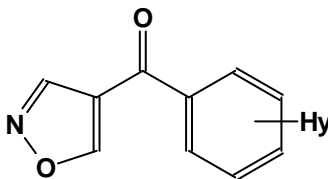
CN 1H-Indole-5-methanesulfonamide, 3-[2-(dimethylamino)ethyl]-N-methyl- (9CI)
 (CA INDEX NAME)



REFERENCE COUNT: 20 THERE ARE 20 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

Skills Practice (page 67):

Question 1: Locate patents concerning anti-inflammatory agents of the following type:



Requirements:

- Hy should match specific heterocycles with up to 4 N and exactly 1 S. It should also match on any Hy. The Hy may be attached to any position on the phenyl ring
 - The phenyl ring is isolated and should only match phenyl rings
 - The 1,2-oxazole ring may match real atom rings or generic groups with or without element counts
-
-

Suggested Approach:

1. Build the structure:
Hy = has 0-4 N, 1 S Element Count unlimited and Match Level CLASS
Phenyl ring = isolated
1,2-Oxazole ring = isolated/embedded; Match Level CLASS, Element Count unlimited
2. Enter the CASLINK multifile environment and upload and display the query
3. Run CASLINK searches and display results

```
=> FILE CASLINK  
  
FILE 'CAPLUS' ENTERED AT 11:37:30 ON ...  
  
FILE 'REGISTRY' ENTERED AT 11:37:30 ON ...  
  
FILE 'MARPAT' ENTERED AT 11:37:30 ON ...
```

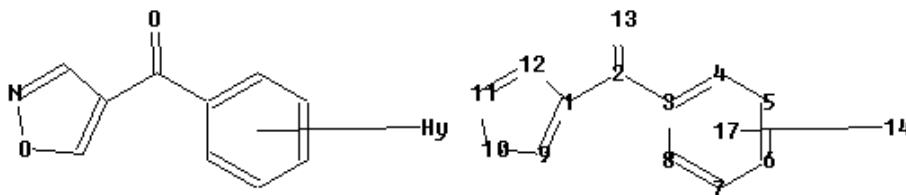
(continued on next page)

CLUSTER 'CASLINK' ENTERED

Predefined command sequences will be executed in
REGISTRY, MARPAT, and CAPLUS.

=>

Uploading C:\CASNC\STN Express\Queries\75 1.str



isolated ring systems :
containing 3 :

Match level :

1:CLASS 2:CLASS 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:CLASS
10:CLASS 11:CLASS 12:CLASS 13:CLASS 14:CLASS 17:CLASS

Element Count :

Node 14: Unlimited

N,N0-4

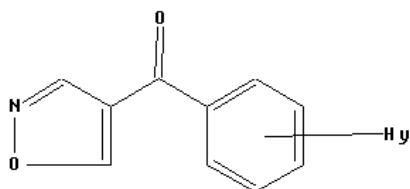
S,S1

L1 STRUCTURE UPLOADED

=> D L1

L1 HAS NO ANSWERS

L1 STR



Structure attributes must be viewed using STN Express query preparation.

=> S L1 SSS SAM

S L1 SSS SAM FILE=REGISTRY

FILE 'REGISTRY'

SAMPLE SEARCH INITIATED 11:39:48

SAMPLE SCREEN SEARCH COMPLETED - 213 TO ITERATE

100.0% PROCESSED 213 ITERATIONS

0 ANSWERS

SEARCH TIME: 00.00.01

(continued on next page)

```

FULL FILE PROJECTIONS:  ONLINE  **COMPLETE**
                        BATCH   **COMPLETE**
PROJECTED ITERATIONS:   3385 TO   5135
PROJECTED ANSWERS:      0 TO     0

L2          0 SEA SSS SAM L1

S L2 SSS SAM FILE=MARPAT
FILE 'MARPAT'
SAMPLE SEARCH INITIATED 11:39:49
SAMPLE SCREEN SEARCH COMPLETED -      2518 TO ITERATE

100.0% PROCESSED      2000 ITERATIONS      50 ANSWERS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.02

FULL FILE PROJECTIONS:  ONLINE  **COMPLETE**
                        BATCH   **COMPLETE**
PROJECTED ITERATIONS:   47601 TO  53119
PROJECTED ANSWERS:      1933 TO   3303

L3          50 SEA SSS SAM L1

=> D SCAN

L3  50 ANSWERS  MARPAT  COPYRIGHT 2008 ACS on STN
IC  ICM  C07D277-04
    ICS  C07D277-08; C07D257-12; C07C006-12
NCL 544179000
CC  28-17 (Heterocyclic Compounds (More Than One Hetero Atom))
    Section cross-reference(s): 25, 27, 33
TI  Iron catalyzed cross coupling reactions of aromatic compounds with
    organometallic reagents.
ST  arom organometallic cross coupling iron catalyst; aryl halide
    tosylate
    triflate grignard reagent coupling iron catalyst
IT  Cross-coupling reaction
    Cross-coupling reaction catalysts
    (iron catalyzed cross coupling reactions of aromatic compds. with
    organometallic reagents)
IT  Aromatic compounds
    RL: IMF (Industrial manufacture); RCT (Reactant); SPN (Synthetic
    preparation); PREP (Preparation); RACT (Reactant or reagent)
    (iron catalyzed cross coupling reactions of aromatic compds. with
    organometallic reagents)
IT  Ligroine
    RL: NUU (Other use, unclassified); USES (Uses)
    (iron catalyzed cross coupling reactions of aromatic compds. with
    organometallic reagents)
IT  Grignard reagents
    RL: RCT (Reactant); RACT (Reactant or reagent)
    (iron catalyzed cross coupling reactions of aromatic compds. with
    organometallic reagents)

```

(continued on next page)

IT Organometallic compounds
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (iron catalyzed cross coupling reactions of aromatic compds. with organometallic reagents)

IT 7439-89-6D, Iron, intermetallic compds. with magnesium
 RL: CAT (Catalyst use); USES (Uses)
 (intermetallic compound; iron catalyzed cross coupling reactions of aromatic compds. with organometallic reagents)

IT 93-58-3P, Methyl benzoate
 RL: BYP (Byproduct); PREP (Preparation)
 (iron catalyzed cross coupling reactions of aromatic compds. with organometallic reagents)

●
 ●
 ●

MSTR 1

G1—G2

G1 = Ph (opt. substd. by 1 or more G3)
 G2 = heteroaryl (opt. substd.)
 G3 = 21

$2_1^C(O)-G4$

G4 = heterocycle <containing up to 20 C, aromatic>
 Patent location: claim 1

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):0

=> S L1 FULL

S L1 SSS FUL FILE=REGISTRY
 FILE 'REGISTRY'
 FULL SEARCH INITIATED 11:40:29
 FULL SCREEN SEARCH COMPLETED - 3929 TO ITERATE

100.0% PROCESSED 3929 ITERATIONS 1 ANSWERS
 SEARCH TIME: 00.00.01

L4 1 SEA SSS FUL L1

S L4 SSS FUL FILE=MARPAT
 FILE 'MARPAT'
 FULL SEARCH INITIATED 11:40:30
 FULL SCREEN SEARCH COMPLETED - 51833 TO ITERATE

(continued on next page)

96.4% PROCESSED 49976 ITERATIONS 2129 ANSWERS
 100.0% PROCESSED 51833 ITERATIONS 2271 ANSWERS
 SEARCH TIME: 00.00.29

L5 2271 SEA SSS FUL L1

S L4 FILE=CAPLUS

L6 1 FILE CAPLUS

DUP REM L5 L6

PROCESSING COMPLETED FOR L5

PROCESSING COMPLETED FOR L6

L7 2271 DUP REM L5 L6 (1 DUPLICATE REMOVED)

ANSWERS '1-2271' FROM FILE MARPAT

=> D 305 IBIB ABS FQHIT

L7 ANSWER 305 OF 2271 MARPAT COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 147:52902 MARPAT [Full-text](#)

TITLE: Preparation of heterobicyclic compounds as P38 kinase inhibiting agents

INVENTOR(S): Chen, Meng-Hsin; Doherty, James B.; Tynebor, Robert

PATENT ASSIGNEE(S): USA

SOURCE: U.S. Pat. Appl. Publ., 41pp.

CODEN: USXXCO

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 20070129372	A1	20070607	US 2006-602782	20061121
WO 2007067478	A2	20070614	WO 2006-US46217	20061201
WO 2007067478	A3	20070726		

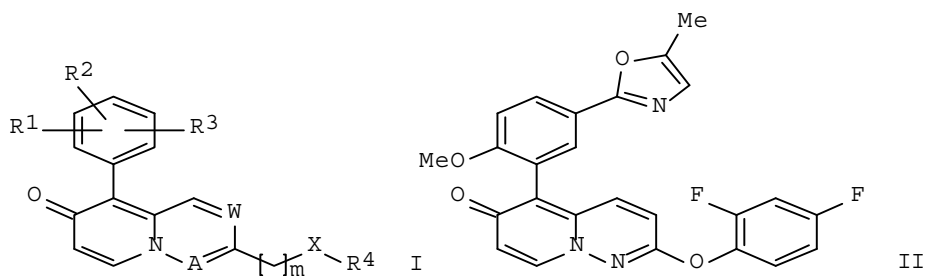
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, GT, HN, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KN, KP, KR, KZ, LA, LC, LK, LR, LS, LT, LU, LV, LY, MA, MD, MG, MK, MN, MW, MX, MY, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RS, RU, SC, SD, SE, SG, SK, SL, SM, SV, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, ZA, ZM, ZW

RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AP, EA, EP, OA

PRIORITY APPLN. INFO.: US 2005-742225P 20051205

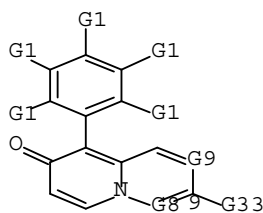
GI

(continued on next page)



AB The title compds. I [A = CH or N; W = (un)substituted CH or N; X = absent, O, alkylene, etc.; R1-R3 = H, alkoxy, cycloalkyl, etc.; R4 = aryl, H, halo, etc.; m = 0-3] that are inhibitors of p38 and are useful in the treatment of inflammation such as in the treatment of rheumatoid arthritis, rheumatoid spondylitis, osteoarthritis, gouty arthritis and other arthritic conditions; inflamed joints, eczema, psoriasis or other inflammatory skin conditions such as sunburn; inflammatory eye conditions including conjunctivitis; pyresis, pain and other conditions associated with inflammation, were prepared E.g., a multi-step synthesis of II, starting from Me 4-methoxy-3-methylbenzoate, was given. Compds. I showed IC₅₀ of < 10 μM when tested in p38 kinase assay or TNF-α release assay (specific data given for representative compds. I). Pharmaceutical composition comprising compound I is claimed.

MSTR 1



G1 = heteroaryl <containing up to 10 atoms,
1-4 heteroatoms, zero or more N, zero or more O,
zero or more S (no other heteroatoms), mono- or bicyclic>
(opt. substd.) / 135

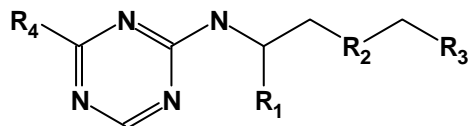
$1\text{G}^{(0)}\text{G}26$

G26 = heterocycle <containing 5-7 atoms, 1 or more N,
zero or more O, zero or more S,
attached through 1 or more N, 0 or more double bonds>
(opt. substd.)

Patent location: claim 1
Note: additional oxo substitution also claimed
Note: additional ring formation also claimed
Note: or pharmaceutically acceptable salts

Skills Practice (page 67):

Question 2: Locate references discussing compounds with the following structure:



Requirements:

- R₁ = carbon chain (substituted or unsubstituted) or a carbocyclic ring
 - R₂ = O, S, N
 - R₃ = Any type of ring system
 - R₄ = N in a chain
 - The nitrogen containing ring may be isolated or embedded
 - **All** of the atoms in the structure must match real atoms in Markush structures, except for R₁ and R₃ which may also match generic groups.
-
-

Suggested Approach:

1. Build the structure:

R₁ = G1 = Ak or Cb, Match Level CLASS (This is the default since the g-group is part of a chain)

R₂ = G2 = O, S, N, Match Level Atom (Each element must be drawn as a fragment, to be able to change Match Level to ATOM)

R₃ = Cy, Match Level CLASS

R₄ = Chain N, Match Level ATOM

Nitrogen-containing ring = isolated/embedded, Match Level ATOM

Nitrogen and carbon chain, Match Level ATOM

2. Enter the CASLINK multifile environment and upload and display the query

3. Run CASLINK searches and display results

=> FILE CASLINK

FILE 'CAPLUS' ENTERED AT 11:17:58 ON ...

FILE 'MARPAT' ENTERED AT 11:17:58 ON ...

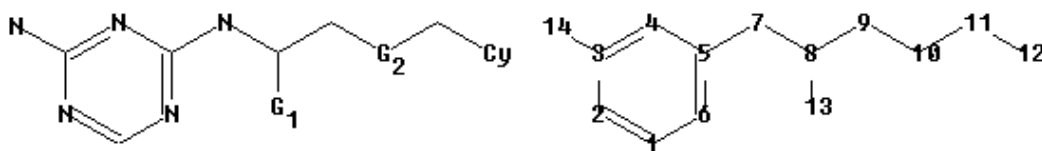
FILE 'REGISTRY' ENTERED AT 11:17:58 ON ...

CLUSTER 'CASLINK' ENTERED

Predefined command sequences will be executed in
REGISTRY, MARPAT, and CAPLUS.

=>

Uploading C:\CASNC\STN Express\Queries\Page 75 Ques 2.str



0 * 1 S * 2 N * 3

14 * 1 17 * 2 18 * 3

chain nodes :

7 8 9 10 11 12 13 14 16 17 18

ring nodes :

1 2 3 4 5 6

chain bonds :

3-14 5-7 7-8 8-9 8-13 9-10 10-11 11-12

ring bonds :

1-2 1-6 2-3 3-4 4-5 5-6

exact/norm bonds :

3-14 5-7 7-8 8-13 9-10 10-11 11-12

exact bonds :

8-9

normalized bonds :

1-2 1-6 2-3 3-4 4-5 5-6

G1:Cb,Ak

G2:[*1],[*2],[*3]

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom

10:CLASS 11:Atom 12:CLASS 13:CLASS 14:Atom 16:Atom 17:Atom

18:Atom

Node 10 (G2) shows up as CLASS in the Match Level summary, even though the fragments in G2 are set to Atom match. The more specific definition of Atom match will be searched.

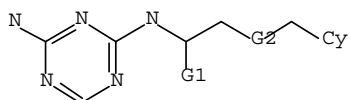
(continued on next page)

L1 STRUCTURE UPLOADED

=> D L1

L1 HAS NO ANSWERS

L1 STR



O 1 S 2 N 3

G1 Cb,Ak

G2 [@1], [@2], [@3]

=> S L1

S L1 SSS SAM FILE=REGISTRY

FILE 'REGISTRY'

SAMPLE SEARCH INITIATED 11:56:20

SAMPLE SCREEN SEARCH COMPLETED - 558 TO ITERATE

100.0% PROCESSED 558 ITERATIONS 13 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**

BATCH **COMPLETE**

PROJECTED ITERATIONS: 9743 TO 12577

PROJECTED ANSWERS: 44 TO 476

L2 13 SEA SSS SAM L1

S L2 SSS SAM FILE=MARPAT

FILE 'MARPAT'

SAMPLE SEARCH INITIATED 11:56:21

SAMPLE SCREEN SEARCH COMPLETED - 569 TO ITERATE

100.0% PROCESSED 569 ITERATIONS 2 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**

BATCH **COMPLETE**

PROJECTED ITERATIONS: 9972 TO 12788

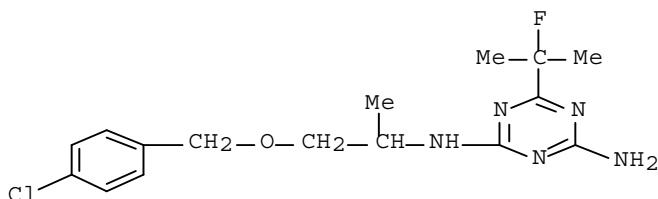
PROJECTED ANSWERS: 2 TO 125

L3 2 SEA SSS SAM L1

(continued on next page)

=> D SCAN L2

L2 13 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN
 IN 1,3,5-Triazine-2,4-diamine, N-[2-[(4-chlorophenyl)methoxy]-1-methylethyl]-6-(1-fluoro-1-methylethyl)- (9CI)
 MF C16 H21 Cl F N5 O



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):0

=> D SCAN L3

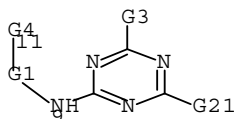
L3 2 ANSWERS MARPAT COPYRIGHT 2008 ACS on STN
 IC ICM C07D251-18
 ICS C07D405-12; C07D409-12; A01N043-68
 CC 28-19 (Heterocyclic Compounds (More Than One Hetero Atom))
 TI Preparation of formylaminotriazines as herbicides.
 ST formylaminotriazine prepn herbicide; triazine formylamino prepn herbicide
 IT Herbicides
 (preparation of formylaminotriazines as herbicides)

-
-
-

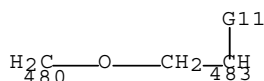
IT 234761-28-5 263907-82-0
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (preparation of formylaminotriazines as herbicides)
 IT 234761-08-1P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation);
 RACT (Reactant or reagent)
 (preparation of formylaminotriazines as herbicides)

(continued on next page)

MSTR 1A



G1 = 480-11 483-9



G4 = cyclopentyl
 G11 = Me
 G21 = 7



Patent location: claim 1
 Note: also incorporates structures 2 and 3 from claim 7

ALL ANSWERS HAVE BEEN SCANNED

=> S L1 FUL

S L1 SSS FUL FILE=REGISTRY
 FILE 'REGISTRY'
 FULL SEARCH INITIATED 11:57:08
 FULL SCREEN SEARCH COMPLETED - 11214 TO ITERATE

100.0% PROCESSED 11214 ITERATIONS 216 ANSWERS
 SEARCH TIME: 00.00.01

L4 216 SEA SSS FUL L1

S L4 SSS FUL FILE=MARPAT
 FILE 'MARPAT'
 FULL SEARCH INITIATED 11:57:10
 FULL SCREEN SEARCH COMPLETED - 11251 TO ITERATE

100.0% PROCESSED 11251 ITERATIONS 19 ANSWERS
 SEARCH TIME: 00.00.09

L5 19 SEA SSS FUL L1

(continued on next page)

S L4 FILE=CAPLUS
L6 8 FILE CAPLUS

DUP REM L5 L6
PROCESSING COMPLETED FOR L5
PROCESSING COMPLETED FOR L6
L7 22 DUP REM L5 L6 (5 DUPLICATES REMOVED)
ANSWERS '1-19' FROM FILE MARPAT
ANSWERS '20-22' FROM FILE CAPLUS

=> D L7 1 IBIB ABS FHIT; D L7 22 IBIB ABS HITSTR

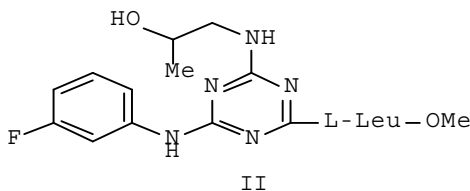
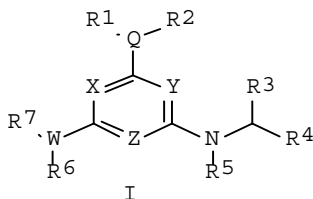
L7 ANSWER 1 OF 22 MARPAT COPYRIGHT 2008 ACS on STN DUPLICATE 1
ACCESSION NUMBER: 142:134918 MARPAT [Full-text](#)
TITLE: Preparation of novel 2,4,6-trisubstituted heterocycle
amino acid derivatives for treatment of neurological
disorders
INVENTOR(S): Brown, Dean; Cacciola, Joseph; Jacobs, Robert T.;
McLaren, Frances M.; Shenvi, Ashokkumar Bhikkappa;
Smith, Reed W., Jr.
PATENT ASSIGNEE(S): Astrazeneca AB, Swed.; Astrazeneca UK Limited
SOURCE: PCT Int. Appl., 116 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2005003103	A2	20050113	WO 2004-GB2723	20040624
WO 2005003103	A3	20051103		

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CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD,
GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC,
LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI,
NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY,
TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM,
AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK,
EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE,
SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE,
SN, TD, TG

PRIORITY APPLN. INFO.: US 2003-484250P 20030630

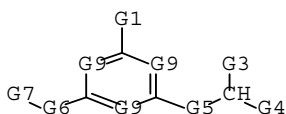
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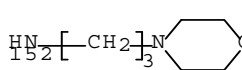
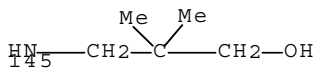
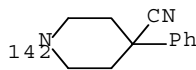
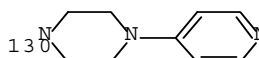
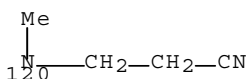
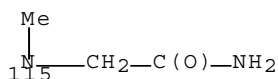
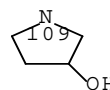
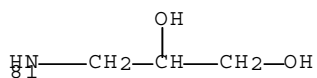
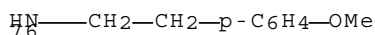
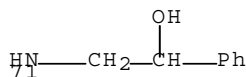
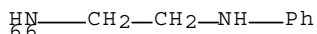
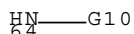
(continued on next page)

AB Triazine, pyrimidine and pyridine amino acid derivs. I [Q is C, CH or N; W is N or S (R6 not present); X, Y, Z are independently C or N (at least one is N); R1, R2 are independently H, Me, (un)substituted alkyl, carbocyclyl or heterocyclyl or R1 and R2 in combination can form an (un)substituted heterocycle or carbocycle; R3 is H or (un)substituted alkyl; R4 is H, (un)substituted alkyl or carbocyclyl, CO2Me, CONHCH2Me or CONHCH2-heterocyclyl; R5 is H or Me; R6 is H; R7 is (un)substituted carbocyclyl] were prepared for the treatment of neurol. disorders related to amyloid β protein production, e.g., Alzheimer's disease. Thus, treatment of cyanuric chloride with 3-fluoroaniline in THF in the presence of DIEA for 1 h and then leucine Me ester hydrochloride at reflux for 4 h afforded Me N-[4-[(3-fluorophenyl)amino]-6-chloro-1,3,5-triazin-2-yl]-L-leucinate. The latter formed a resin with polystyrene-hydroxybenzotriazole and was reacted with 2-hydroxy-1-propylamine to afford compound II. Compds. of the invention inhibit amyloid β production (IC50 = 0.010-5.50 μ M in the γ -secretase detergent extract assay).

MSTR 1

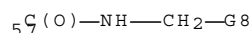


G1 = 51 / 56 / 54 / heterocycle <containing 3-20 atoms, 1 or more heteroatoms, 1 or more N, zero or more O, zero or more S (no other heteroatoms), attached through 1 or more N> (opt. substd.) / carbocycle <containing 3-7 C, mono- or bicyclic> (opt. substd.) / carbocycle <containing 7-13 C, 2-3 rings> (opt. substd.) / (Specifically claimed: 35 / morpholino / 61 / 64 / 66 / 71 / 76 / 81 / 109 / 115 / 120 / 130 / 142 / 145 / 152 / 155 / 165 / 170 / 178 / 189 / 190 / 193 / 205 / 212 / 222 / 231 / 240)

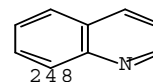
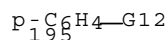
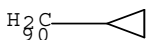
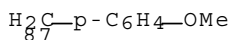
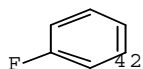


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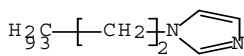
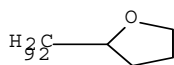
- G2 = H / Me / alkyl <containing 1-6 C> (opt. substd.) / carbocycle <containing 3-7 C, mono- or bicyclic> (opt. substd.) / carbocycle <containing 7-13 C, 2-3 rings> (opt. substd.) / heterocycle <containing 3-20 atoms, zero or more N, zero or more O, zero or more S (no other heteroatoms)> (opt. substd.)
- G3 = H / **alkyl <containing 1-6 C> (opt. substd.)** / (Specifically claimed: Bu-i)
- G4 = H / alkyl <containing 1-6 C> (opt. substd.) / CO₂Me / carbocycle <containing 3-7 C, mono- or bicyclic> (opt. substd.) / carbocycle <containing 7-13 C, 2-3 rings> (opt. substd.) / **57** / (Specifically claimed: CH₂OH / Ph)



- G5 = **NH** / NMe
- G6 = **NH** / S
- G7 = carbocycle <containing 3-7 C, mono- or bicyclic> (opt. substd.) / carbocycle <containing 7-13 C, 2-3 rings> (opt. substd.) / (Specifically claimed: 42 / 87 / 90 / 195 / 248)



- G8 = **heterocycle <containing 3-20 atoms, zero or more N, zero or more O, zero or more S (no other heteroatoms)> (opt. substd.)** / Et / (Specifically claimed: 2-tetrahydrofuryl)
- G9 = **N** / CH
- G10 = 92 / 93



- G11 = Me / alkyl <containing 1-6 C> (opt. substd.) / carbocycle <containing 3-7 C, mono- or bicyclic> (opt. substd.) / carbocycle <containing 7-13 C, 2-3 rings> (opt. substd.) / heterocycle <containing 3-20 atoms, zero or more N, zero or more O, zero or more S (no other heteroatoms)> (opt. substd.)
- G12 = OMe / NH₂
- Patent location: claim 1
- Note: substitution is restricted
- Note: or pharmaceutically acceptable salts

(continued on next page)

L7 ANSWER 22 OF 22 CAPLUS COPYRIGHT 2008 ACS on STN
 ACCESSION NUMBER: 1966:85080 CAPLUS [Full-text](#)
 DOCUMENT NUMBER: 64:85080
 ORIGINAL REFERENCE NO.: 64:16032f-h
 TITLE: Naphthotriazolylstilbene brightening agents
 PATENT ASSIGNEE(S): J. R. Geigy A.-G.
 SOURCE: 16 pp.
 DOCUMENT TYPE: Patent
 LANGUAGE: Unavailable
 FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
NL 6508811		19660110	NL 1965-8811	19650708
BE 666692			BE	
FR 1440403			FR	

PRIORITY APPLN. INFO.: CH 19640709

AB 4,2-H₂N(HO₃S)C₆H₃CH:CHC₆H₃Cl₂-3,4 (I) (34.4 g.) diazotized and coupled with 14.5 g. 2-C₁₀H₇NH₂ in 900 g. C₅H₅N, basified with NaOH to phenolphthalein, treated with 180 g. NaCl, and the upper organic layer treated with a Cu catalyst solution of 2.5 g. CuSO₄.5H₂O in 100 g. H₂O and 10 g. H₂NCH₂CH₂OH, heated to 95-7°, treated with stirring with a strong air stream and then with excess Na₂S, filtered, C₅H₅N steam distilled in the presence of 5 g. Na₂S₂O₄, the residue cooled, and the precipitate purified from C₅H₅N gave the Na salt of II (X = Cl, X' = H) (III), m. >300°. Na salt of 34.4 g. I diazotized similarly and treated with 22.7 g. 2,1-H₂NClO₆SO₃H (IV) also gave III. 2',4'-Dichloro isomer of I (34.4 g.) gave similarly with 22.7 g. IV the pale yellowish I (X = H, X' = Cl), m. >300°. Examples are given for the optical brightening of cellulose and polyamide fibers with III and for the incorporation of the I into soap powders and detergents, etc. N₂-Substituted 2-amino-s-triazines. J. R. Geigy A.-G. Neth. Appl. 6,506,935 (Cl. C 07d), Dec. 3, 1965; Swiss Appl. June 2, 1964, and May 3, 1965; 26 pp. Various title compds. were prepared for improving the gas-fastness of

●
●
●

IT 6923-57-5, s-Triazine, 2,4-diamino-6-[[2-(benzylamino)-1-methylpropyl]amino]-
 (preparation of)

RN 6923-57-5 CAPLUS

CN s-Triazine, 2,4-diamino-6-[[2-(benzylamino)-1-methylpropyl]amino]- (7CI, 8CI) (CA INDEX NAME)

