



DIALOG

**Chemical Information
on Dialog**

Featuring DialogClassic



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Seminar Development Team

Stella Shandelman
Susan Kelly
Beverley Crane
Raymond Niro

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Preface

Introduction to Chemical Science Searching on Dialog provides an introduction to searching the chemical databases using DialogClassic for users who need to locate information pertinent to research and development interests within the chemical industry. The information in the chemical databases also provides a unique springboard for searching in other scientific disciplines: biology, medicine, pharmaceuticals, physics, and engineering. This information may also be used for expanding the scope of a search to include patent, toxicity and environmental interests.

Audience

This half-day class is intended for Dialog searchers who have the need to locate chemical information online and are familiar with the basic Dialog commands. Several simple techniques will be discussed and are designed to help the searcher locate chemical information in several related areas.

Seminar Overview

This seminar is divided into five sections:

1. Introduction to Chemical Searching
2. Chemical Substance Searching
3. The MAP Command
4. Applications
5. Wrap Up

Class Time

The class is scheduled for 3 hours with online practice sessions.

Learning Objectives

Attendees will understand more about chemical searching by:

Becoming familiar with classes of chemicals

- Locating CAS Registry Numbers and synonyms
- Demonstrating knowledge of the MAP command
- Locating toxicity, environmental, and patent information

Workbook Conventions

Search Examples

In this workbook all search examples are presented using **Dialog Command Language**. All of the features illustrated in the search examples—search functionality, database indexing and content—are available using Dialog Command Language through the DialogWeb–Command Search, DialogClassicWeb, and DialogLink[®] interfaces. Dialog Command Language is not case sensitive; therefore, you will see examples in both upper- and lowercase.

Database Tables

Key features of individual databases appear in one or more tables in this workbook. The tables are intended to simplify comparison by grouping the key features in an easy-to-digest format.

Learning Checks

Learning Checks are provided to help reinforce material presented in the Section.

Online Practice

Practice exercises are included at the end of most sections in order to help you learn the concepts and techniques presented. Your instructor will provide you with practice passwords to enable you to complete the online practice free of charge.

Tips

Tips to help you get the most from using Dialog appear in shaded boxes. Be sure to look for these throughout the text.

Ellipses

Occasionally search results are truncated in order to save space. Omitted text is indicated with a series of dots or “ellipsis points”:

Section 1: Introduction

This seminar introduces Dialog searchers to the chemical information databases. It is designed to train users to retrieve information pertinent to research and development interests within the chemical industry.

The chart below describes two types of chemical questions you may want to research. For example, you may want to conduct a subject search to obtain information from the chemical literature files. On the other hand, you may need to do a substance search, either specific or generic. Using the Dialog MAP command you can use chemical substances to find related literature or vice versa.

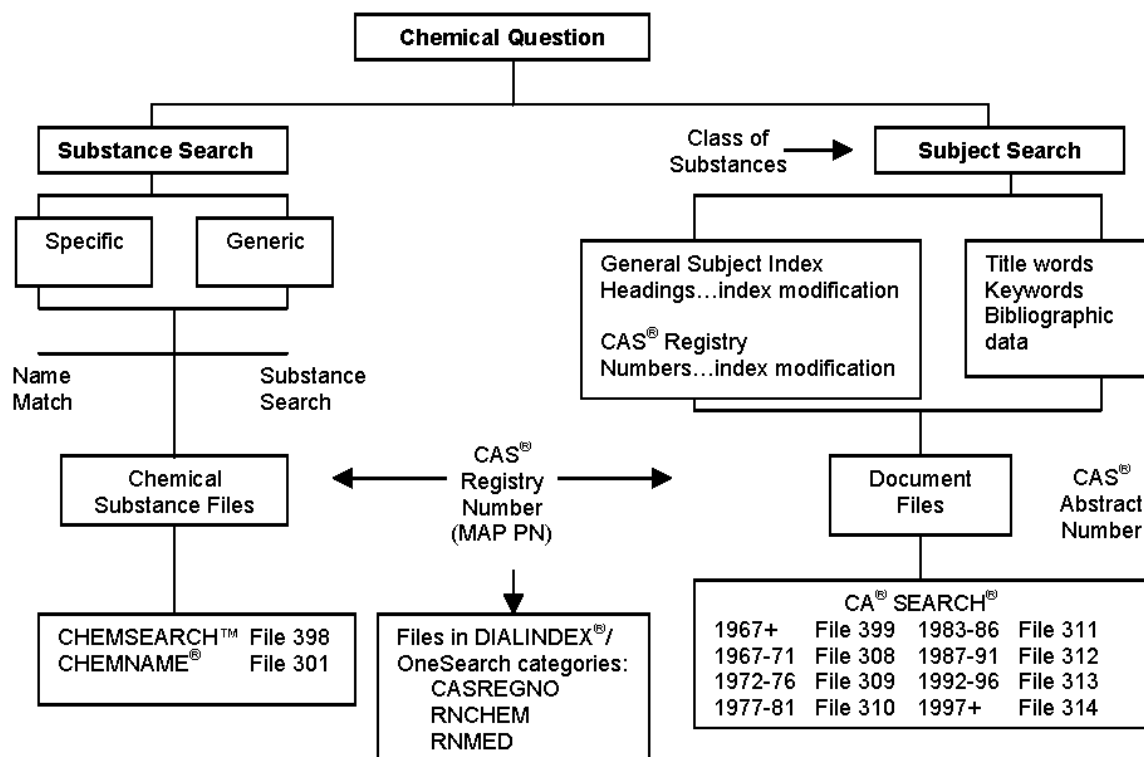


Figure 1. Chemical Search Strategies Chart

The subsequent sections of this seminar will present examples for searching both by substance and by subject. With comprehensive chemical information from Chemical Abstracts Service, Royal Society of Chemistry, Beilstein, Merck, patent granting authorities, and many other providers, Dialog offers an ideal solution for both chemical science and business research. Consult the *Dialog Database Catalog* or the *Smart Tool: Chemistry* for details about specific databases.

Section 2: Chemical Substance Searching

In this section you will learn:

- To locate and identify a CAS Registry Number
- A general strategy for chemical name searching
- To use the molecular formula for chemical name searching

Chemical Substance Names

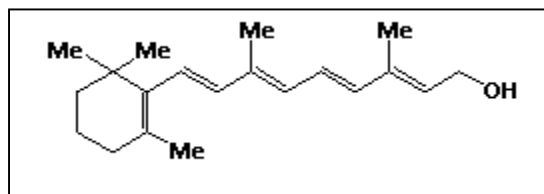
The most common search in the chemistry files on Dialog is for information about a particular substance or compound. Most chemical compounds are known by several different names or **synonyms**.

Examples of synonyms for **borozon** include:

boron nitride	geksanit R
boron mononitride	hexanite R
elboron	super mighty M
bzn 550	elbor RM
wurzin	

Examples of synonyms for Vitamin A include:

Afavin
prepalin
beta retinal
testavol
vitpex



So, how does one perform a comprehensive search for a compound given the variety of names/synonyms that can appear in the chemical literature? CAS Registry Numbers offer a convenient solution to this challenge.

Chemical Abstracts Service CAS Registry Numbers

Most chemicals are assigned a number called a CAS Registry Number.

Example:

<u>Common Name</u>	<u>CAS Registry Number</u>
Borozon	10043-11-5
Vitamin A	68-26-8

Each number is unique and represents the chemical regardless of which synonym is used (i.e., vitamin A, beta-retinol, vitpex).

CAS Registry Numbers are analogous to fingerprints. No matter where you go, no matter what name you use, even if you legally change your name, your fingerprints remain the same. Fingerprints are a unique identification throughout most of the world. The same is true of chemicals, only *their* identification key is the CAS Registry Number. Each CAS Registry Number is a unique numeric identifier, designates only one substance, has no chemical significance and provides a link to a wealth of information about a specific chemical substance. These identification numbers are searchable in many Dialog files using the RN= prefix (hyphens included). For example: S RN=10043-11-5 retrieves references to borozon, regardless of the name used in the record.

Locating a CAS Registry Number

The most comprehensive and most precise strategy for finding information on a particular substance is to search the CAS Registry Number of that substance. CHEMNAME[®] (File 301) and CHEMSEARCH[™] (File 398) are the starting points for most chemical substance searches.

CHEMSEARCH (File 398) is the world's largest substance database with over 25 million chemical names. This database mostly covers substances identified from the scientific literature from 1957 to the present. CHEMSEARCH contains a wide variety of substances including the world's largest collection of organic compounds, inorganic compounds, metals, alloys, minerals, coordination compounds, organometallics, elements, isotopes, nuclear particles, proteins and nucleic acids, polymers, nonstructurable materials (VCBs), etc.

CHEMNAME includes chemical substances cited in Chemical Abstracts two or more times from 1967 through the most recent monthly update. Records for substances in CHEMNAME are also contained in CHEMSEARCH.

Each substance in CHEMSEARCH and CHEMNAME is identified by a unique numeric identifier called a CAS Registry Number.

The following is a general strategy for chemical name searching:

- BEGIN in File 301 or File 398 or another chemical substance file
- EXPAND NA= (NA=Name of Substance, Synonym etc.)
- SELECT from EXPAND list
- TYPE the record to view Registry Number
- Note Registry Number (first entry of record)
- BEGIN literature databases (files that contain Registry Numbers like File 314)
- SELECT RN= to search for references to a compound
- SELECT and combine other concepts to focus search

Note: Other databases to use for substance identification in addition to CHEMSEARCH (File 398) or CHEMNAME (File 301) are: BEILSTEIN (File 390), Chapman & Hall (File 303), Merck Index OnlineSM (File 304), and Pesticide Fact File (File 306).

► **Topic** ◀ Robert Henry Wentorf, Jr., a physical chemist at General Electric, invented a new form of boron nitride that was not found in nature. GE announced Wentorf's invention on February 12, 1957. The company began to sell it under the trademark "Borazon." Borazon has a crystalline molecular structure similar to diamond with a hardness second only to diamond. In some ways it was even better than diamond due to its much higher temperature tolerance. The new boron nitride with a crystalline molecular structure has many uses, but its main application today is in industrial tools for drilling, grinding, cutting, scraping and polishing. (Source : www.tecsoc.org/pubs/history/2002/feb12.htm)

What is the registry number and molecular formula of this compound? Does this compound have any synonyms?

*BEGIN the
RNLOOKUP
OneSearch
category. All
databases have
registry numbers.*

***Note:** Use the
BEST technique
(Begin, Expand,
Select, Type)*

*EXPAND using the
NA= prefix and the
compound name.*

```
?b rnlookup
File 304:THE MERCK INDEX ONLINE(SM)/2001Q1(c)2001 MERCK&CO.
File 336:RTECS 2001/Q1 Comp & dist by NIOSH, Intl
File 390:Beilstein Online (c) Beilstein Chemiedaten und
Software
File 398:CHEMSEARCH(TM)1957-2002/SEP(c) 2002 AMER.CHEM.SOC.

      Set  Items  Description
      ---  -
?e na=borazon
Ref  Items  Index-term
E1   2      NA=BORAZOLE
E2   1      NA=BORAZOLE-1,3,5-TRIMETHYLBORAZINE POLYMER
E3   2      *NA=BORAZON
E4   1      NA=BORAZYNE,CYCLIC TETRAMER
E5   1      NA=BORAZYNE,CYCLIC TRIMER
E6   1      NA=BORBENZOYLACETONDIPLUORID

Enter P or PAGE for more
```

SELECT the appropriate E number.

DISPLAY SETS--
DS FROM EACH
--shows which files contain the compound.

TYPE the two records using Format 9 to see the entire record.

Note the CAS Registry Number and molecular formula.

```
?s e3
      S1      2  NA='BORAZON'
?ds s1 from each

Set   File      Items  Description
-----
      304         0
      336         1
      390         0
      398         1
S1    2          NA='BORAZON'

?t s1/9/all
1/9/1      (Item 1 from file: 336)
DIALOG(R)File 336:RTECS
Comp & dist by NIOSH, Intl Copyright All Rights Res. All
rts. reserv.

?t s1/9/all
037722      RTECS Number: ED7800000
Substance Name: Boron nitride
CAS Registry Number: 10043-11-5   Molecular Formula: BN
Molecular Weight:24.82
Synonyms: BN 40SHP ; Borazon ; Boron mononitride ; BZN 550
; Denka boron nitride GP ; Denka GP ; Elbor ; Elbor LO 10B1-
100 ; Elboron ; Elbor R ; Elbor RM ; Geksanit R ; Hexanite R
; Hexanit R ; KBN-H10 ; Kubonit ; Kubonit KR ; Sho BN ; Sho
BN HPS ; SP 1 ; SP 1 (Nitride) ; Super mighty M ; UHP-Ex ;
Wurzin
Record Date: 199701

TOXICITY EFFECTS DATA:
* Oral Rat LD >50 gm/kg UCDS** 7/20/1965
* Skin Rabbit LD >20 mL/kg UCDS** 7/20/1965

NIOSH CRITERIA DOCUMENTS:
NOES 1983:HZD X6983;NIS 1;TNF 26;NOS 2;TNE 492;TFE 130
NOES 1983: HZD X9689; NIS 6; TNF 82; NOS 8; TNE 5857; TFE
1478
NOES 1983: HZD 81731; NIS 16;TNF 208; NOS 15; TNE 3277;
TFE 1005

NTP, NIOSH, EPA STATUS:
EPA TSCA Section 8(b) CHEMICAL INVENTORY

TOXICITY EFFECTS JOURNAL REFERENCES:
UCDS** Union Carbide Data Sheet. Union Carbide Corp., 39
Old Ridgebury Rd., Danbury, CT 06817

NIOSH CRITERIA DOCUMENTS JOURNAL REFERENCES:

NTP, NIOSH, EPA STATUS JOURNAL REFERENCES:

DATA PRESENT: Toxicity Effects; NIOSH Criteria Documents;
NTP, NIOSH, EPA Status

1/9/2      (Item 1 from file: 398)
DIALOG(R)File 398:CHEMSEARCH(TM)
(c) 2002 AMER.CHEM.SOC. All rts. reserv.

CAS REGISTRY NUMBER: 10043-11-5
MOLECULAR FORMULA: BN
REPLACED CAS REGISTRY NUMBER(S) : 54824-38-3 56939-87-8
```

58799-13-660569-72-4 69071-29-0 69495-08-5 78666-05-4
165390-92-1

CA NAME(S):

HP=Boron nitride(BN) (8CI 9CI)

SYNONYMS: Belbor; BN 40SHP; BN-GP; BN-MOD; Borazon; Boron mononitride; Boron nitride; Boronate FS 1; BZN 550; Cerac B 1084; CTF 5; CTH 40; CTL 40; CTUF; Cubonite; Denka Boron Nitride GP; Denka Boron Nitride HGP; Denka Boron Nitride SGP; Denka Boron Nitride SP 2; Elbor; Elbor LO 10B1-100; Elbor R; Elbor RM; Elboron; FS 1; FS 1(nitride); Geksanit R; GP; HCJ 48; Hexanit R; Hexanite R; High Flow FMX 1; HP 1; HP 1(nitride); HP 2; HP 2(nitride); HP 6; HP 6(nitride); HP-P 1; HP-P 1(nitride); HTP-FK; KBN(h)-SR; KBN-H 10; KBN-H-S; KBN-H-SP; Kubonit; Kubonit KR; Kubonite; Lubien LBN 5026; MBN 010; MBN 010T; MBN 050; MBN 250; Orpac Boron Nitride Releasecoat-Conc 25; PolarTherm PT 110; PolarTherm PT 120; PolarTherm PT 160; PolarTherm PT 670; PolarTherm 180; PT 160; PT 350; Releasecoat Conc 25; Sandvik CB 50; SBN-T 325-400; SGP; Sho BN; Sho BN HPS; Sho BN-UHP; Sho BN-UHP 10; Sho BS; SHP 325; SHP 6; SP 1; SP 1(nitride); Super Mighty M; Svetlanit; TRES-BN XP 3002; TRES-BN XP 3004; TRES-BN XP 3008; UBN-A; UBN-X; UHP-EX; UHPS 1; Wurzin

SUBFILE: CHEMNAME **17691 LITERATURE REFERENCE(S) IN
FILE 399.**

LAST UPDATE: 200204

398,301

CHEMSEARCH™ CHEMNAME® ONTAP® CHEMSEARCH™ (FILE 231)

FILE DESCRIPTION

The chemical substance files on DIALOG, CHEMSEARCH™, File 398, and CHEMNAME®, File 301, are non-bibliographic files of chemical substances registered through Chemical Abstracts Service. Each record describes a single chemical entity, and contains the CAS® Registry Numbers, molecular formula, CA Substance Index Name(s), available synonyms, complete ring data, and other chemical substance information. The primary purpose of these files is to support specific substance searching and various forms of substructure searching in the DIALOG chemical files. The CAS® Registry Number can be very effectively used to search for information about specific chemicals in several DIALOG databases (see DIALINDEX® categories RNCHEM, and CASREGNO).

ONTAP® CHEMSEARCH™, File 231, is available for **ON**line **T**raining **A**nd **P**ractice. It contains 52,951 records. The substances in File 231 correspond to many of those covered in the bibliographic records in File 204, ONTAP® CA SEARCH, as well as other ONTAP® files containing CAS Registry Numbers.

SUBJECT COVERAGE

CHEMSEARCH, File 398, contains all chemical substances registered since 1957, including substances that have been cited in the CAS literature since 1967.

CHEMNAME, File 301, presently includes those chemical substances in the CAS Registry System cited in Chemical Abstracts two or more times from 1967 through the most recent monthly update. Records for substances in CHEMNAME are also contained in CHEMSEARCH.

SOURCES

Chemical substance data in these files are derived from the CAS Registry Nomenclature Service and the CAS Component and Ring Analysis Service provided by Chemical Abstracts Service. Also included are value added enhancements such as the number of records in File 399 CA SEARCH, chemical name segmentation, the ability to MAP CAS Registry Numbers and chemical names between files, and added fields such as Element Count, Periodic Index Terms, and Number of Components.

DIALOG FILE DATA

Inclusive Dates: 1967 forward (File 301)
1957 forward (File 398)
Selected records (File 231)
Update Frequency: Closed (File 231)
Monthly (Files 301, 398)
File Size: 2,992,583 records as of July 2000 (File 301)
25,180,294 records as of July 2000 (File 398)
52,951 records (File 231)

CONTACT

The chemical substance files are produced by The Dialog Corporation using data provided by Chemical Abstracts Service. Questions concerning search strategies, file content, or data integrity should be directed to DIALOG or CAS.

Chemical Abstracts Service
Attn: Customer Service
P.O. Box 3012
Columbus, OH 43210
Phone: 614-447-3731
Toll Free: 800-753-4227
E-Mail: help@cas.org

Search Strategy and File Content:
The Dialog Corporation
The Knowledge Center
11000 Regency Parkway, Suite 10
Cary, NC 27511
Phone: 919-462-8600
Toll Free: 800-334-2564
Fax: 919-468-9890
E-Mail: customer@dialog.com

Files 398,301
SAMPLE RECORD

CHEMSEARCH™

RN=
 /EC, EC=, ME=, MF=
 AR=, FR=, IR=, NR=, SR=
 RN=, RD=
 CN=, NA=, /NA
 HP=
 SB=
 NM=
 ST=
 HP=
 SB=
 CN=, NA=, /NA
 HP=
 SB=
 HP=
 SB=
 NM=
 HP=
 NM=
 SY=, /SY, NA=, /NA
 UD=

DIALOG(R)File 398:CHEMSEARCH(TM)
 (c) 1996 Amer.Chem.Soc. All rts. reserv.
 CAS REGISTRY NUMBER: 14325-03-2 (COORD-COMPD)
 MOLECULAR FORMULA: C34H30CoN4O4.2H
 RING SYSTEM DATA:
 (01) (nr=08; sr=5,5,5,5,6,6,6,6; ar=C4N.04-C3CoN2.04;
 fr=NC4.04-CoNC3N.04; ir=9832-11-7)
 REPLACED CAS REGISTRY NUMBER(S) : 7097-74-7 13965-24-7
 CA NAME(S):
 HP=Cobaltate(2-) (9CI)
 SB=(7,12-diethenyl-3,8,13,17-tetramethyl-21H,23H-porphine-
 2,18-dipropanoato(4-)-N21,N22,N23,N24)-
 NM=dihydrogen
 ST=(SP-4-2)-
 HP=Cobalt (8CI)
 SB=(dihydrogen 3,7,12,17-tetramethyl-8,13-divinyl-2,18-
 porphinedipropionato(2-))-
 OTHER CA NAMES:
 HP=Cobalt (7CI)
 SB=(dihydrogen protoporphyrin IX-ato(2-))-
 HP=21H,23H-Porphine-2,18-dipropanoic acid
 SB=7,12-diethenyl-3,8,13,17-tetramethyl-
 NM=cobalt complex
 HP=21H,23H-Porphine
 NM=cobalt complex
 SYNONYMS: Cobalt protoporphyrin IX; Cobalt(II) protoporphyrin IX;
 Cobalt-heme
 SUBFILE: CHEMNAME 143 LITERATURE REFERENCE(S) IN FILE 399.
 LAST UPDATE: 199301

RN=
 /EC, EC=, ME=, MF=
 AF=, MF=
 CN=, AC=, NA=, /NA
 HP=
 NM=
 CN=, AC=, NA=, /NA
 HP=
 NM=
 HP=
 NM=
 HP=
 NM=
 SY=, NA=, /NA
 RC=
 UD=

DIALOG(R)File 398:CHEMSEARCH(TM)
 (c) 1996 Amer.Chem.Soc. All rts. reserv.
 CAS REGISTRY NUMBER: 73064-67-2 (ALLOY)
 MOLECULAR FORMULA: Ag.Au.Cu.Si
 ALTERNATE FORMULA: Unknown
 CA NAME(S):
 HP=Silver alloy(base) (9CI)
 NM=Ag 82,Au 10,Si 4.9,Cu 3.3
 OTHER CA NAMES:
 HP=Gold alloy(nonbase)
 NM=Ag 82,Au 10,Si 4.9,Cu 3.3
 HP=Silicon alloy(nonbase)
 NM=Ag 82,Au 10,Si 4.9,Cu 3.3
 HP=Copper alloy(nonbase)
 NM=Ag 82,Au 10,Si 4.9,Cu 3.3
 SYNONYMS: Copper 5, gold 5, silicon 17, silver 73 (atomic)
 COMPONENT CAS REGISTRY NUMBER(S):
 (7440-21-3 7440-22-4 7440-50-8 7440-57-5)
 Component RN Component Molecular Formula
 =====
 1) 7440-21-3 Si
 2) 7440-22-4 Ag
 3) 7440-50-8 Cu
 4) 7440-57-5 Au
 SUBFILE: CHEMSIS 10CI 1 LITERATURE REFERENCE(S) IN FILE 399.
 LAST UPDATE: 199203

SEARCH OPTIONS

BASIC INDEX

SEARCH SUFFIX	DISPLAY CODE	FIELD NAME	INDEXING	SELECT EXAMPLES
— —	— —	All Basic Index Fields ¹ Substance Class Descriptor	Word Phrase	S DIHYDROGEN(W)PROTOPORPHYRIN S COORD-COMPD S ALLOY
/EC /NA	— NA	Element Count ² Chemical Names (includes CA Name and Synonyms) ^{2,3,4}	Word Segment & Word & Phrase	S N4/EC S PORPHINE/NA S DIHYDROGEN(W)PROTOPORPHYRIN/NA S COBALTATE(2-)/NA
/SY	SY	Synonym ^{2,3,5}	Segment & Word & Phrase	S PROTO(W)PORPHYRIN/SY S COBALT(W)PROTOPORPHYRIN/SY S COBALT PROTOPORPHYRIN IX/SY

¹ All words are indexed, including the standard Dialog stop words.

² Searchable in the Basic Index and in the Additional Indexes.

³ All chemical names are indexed as complete phrases, individual words, and chemically significant segments of words. Words such as PROTOPORPHYRIN may be searched by either segment, e.g., PROTO or PORPHYRIN; for segments that are also complete words, use /FF, e.g., S PORPHYRIN/FF. Locants, i.e., numbers indicating the position of a chemical group within the structure, are searched as words, e.g., S 21. Locant strings, i.e., multiple positions for a recurring group such as 7,12-DIETHENYL, are searched as a single word, e.g., S 7,12 rather than using proximity operators.

⁴ CA Name field contains terms and segments from CA Index Names also indexed in HP=, SB=, and NM= fields; CA Name also may be searched using CN=, NA= and /NA.

⁵ Synonym, /SY, field contains complete synonyms and segments of synonyms; SY= and NA= fields contain only the complete synonym name.

ADDITIONAL INDEXES

SEARCH PREFIX	DISPLAY CODE	FIELD NAME	INDEXING	SELECT EXAMPLES
AC= CN= HP=	— CN —	Alloy Component CA Name ^{2,6} Heading Parent ^{2,4,7}	Phrase Phrase Segment & Word & Phrase	S AC=AG 82 S CN=COBALTATE(2-),(7,12-DIETHENYL? S HP=(DI(W)PROPAN(W)OIC) S HP=(DIPROPANOIC(W)ACID) S HP=21H,23H-PORPHINE-2,18?
NA= NM=	NA —	Chemical Names (CA Name and Synonyms) ^{2,4} Name Modification ^{2,4,7}	Phrase Segment & Word & Phrase	S NA=COBALT-HEME S NM=(DI(W)HYDROGEN) S NM=(COBALT(W)COMPLEX) S NM=COBALT COMPLEX
— SB=	OC —	Other CA Index Names Substituent ^{2,4}	Segment & Word & Phrase	S SB=(TETRA(W)METHYL) S SB=(DIETHENYL(S)TETRAMETHYL) S SB=7,12-DIETHENYL-3,8,13,17-TETRA?
ST=	—	Stereochemical Descriptor ⁴	Word & Phrase	S ST=SP S ST=(SP-4-2)-
SY=	SY	Synonym ^{2,5}	Phrase	S SY=COBALT-HEME

MOLECULAR FORMULA DATA

AF= EC= GN= ME= MF=	AF — — — MF	Alternate MF Element Count ² Group Number Molecular Element Molecular Formula ⁸	Phrase Phrase Phrase Phrase Phrase	S AF=UNKNOWN S EC=C0034(S)EC=O0004 S GN=A5 S ME=CHCONO S MF=C34H30CON4O4.2H S MF=C34H30CON4O4 S MF=UNKNOWN
NC= NE= PI=	— — —	Number of Components Number of Elements Periodic Index Term	Phrase Phrase Phrase	S NC=02 S NE=05 S PI=A56 S PI=A56B8
PT=	—	Periodic Transition Row	Phrase	S PT=T1

RING DATA

— AR=	— —	Ring System Multiplier Analysis of Rings	Word Phrase	S 01(S)AR=C4N.04-C3CON2.04 S AR=C4N.04-C3CON2.04
CR= ER= FR= IR=	— — — —	Component of Rings Elements of Rings Formula of Rings Identity of Rings	Phrase Phrase Phrase Phrase	S CR=CCON S ER=N0004 S FR=NC4.04-CONC3N.04 S IR=9832-11-7 S IR=9832
NR= — SR=	— RS —	Number of Rings Ring System Data ⁹ Size of Rings	Phrase Phrase	S NR=08 S SR=5,5,5,5,6,6,6,6

ADDITIONAL INDEXES (cont'd)

SEARCH PREFIX	DISPLAY CODE	FIELD NAME	INDEXING	SELECT EXAMPLES
TR=	—	Total Number of Rings	Phrase	S TR=08
CAS REGISTRY NUMBER DATA				
ON=	ON	Other Registry Number ¹³	Phrase	S ON=7097-74-7
RA=	RA	Alternate Registry Number	Phrase	S RA=10031-75-1
RC=	RC	Component Registry Number ¹²	Phrase	S RC=7440-21-3
RD=	RD	Replaced Registry Number	Phrase	S RD=7097-74-7
RF=	RF	Fragment Registry Number	Phrase	S RF=20683-82-3
RG=	RG	Replacing Registry Number	Phrase	S RG=14325-03-2
—	RM	Main Registry Number		
RN=	RN	CAS(R) Registry Number ^{10,11,13,14}	Phrase	S RN=73064-67-2 S RN=14325-03-2
RP=	RP	Preferred Registry Number	Phrase	S RP=10045-95-1
OTHER DATA				
—	RE	Number of References		
—	SF	Subfile (Collective Index)		
UD=	UD	Update	Phrase	S UD=199301

⁶ CA Name is CA Index Names HP=, SB=, and NM= terms separated by commas.

⁷ Chemical names are indexed as complete phrases, individual words, and chemically significant segments of words. Use /FW, Full Word, to limit to the unsegmented term. Note, use of /FW is valid only for HP=, SB=, and NM=; for all other fields use /FF to limit to unsegmented chemical terms. Locant strings, such as 7,12 in 7,12-DIETHENYL, are searched as a single word, e.g., SELECT 7,12(W)DIETHENYL.

⁸ Includes AF=.

⁹ Use the RS display code to display ALL Ring System data.

¹⁰ RN= searches all Registry Numbers except RC= or RF=; RN display Code displays all Registry Numbers except RC or RF.

¹¹ Use /FF to limit the search to the main CAS Registry Number, e.g., S RN=14325-03-2/FF.

¹² Includes RF=.

¹³ Includes RA=, RD=, RG=, and RP=.

¹⁴ MAP RN maps all Registry Numbers in a record except RC (Component Registry) and RF (Fragment Registry) Numbers.

SPECIAL FEATURES

For command descriptions, enter HELP LIMIT, HELP SORT, HELP RANK, HELP MAP online.

LIMIT	/PLM -- Polymers /STE -- Stereochemical Descriptors	SELECT S4/PLM SELECT S2/STE
SORT	MF, RN, TR	SORT S4/ALL/TR PRINT S4/5/1-31/MF/RN
RANK	All phrase- and numeric-indexed fields in the Additional Indexes can be ranked. Other RANK codes include: IR, RC, RN, SY	RANK NA RANK MF S4
MAP	IR, RC, RN, SY, SYRN	MAP SY TEMP S2

PREDEFINED FORMAT OPTIONS

NO.	DIALOGWEB FORMAT	RECORD CONTENT
1	--	DIALOG Accession Number (not meaningful)
2	--	CAS Registry Number, Other CAS Registry Numbers (except Component or Fragment Registry Numbers), Molecular Formula, Ring System Data, CA Index Name(s) (excluding other CA Names), all Synonyms, Subfile, and Number of References in File 399
3	Medium	CAS Registry Number, Other CAS Registry Numbers (except Component or Fragment Registry Numbers), Molecular Formula, Ring System Data, CA Index Name(s) (excluding other CA Names), all Synonyms, Subfile, and Number of References in File 399
5	--	Full Record
6	--	CAS Registry Number, Molecular Formula, CA Index Name(s), Subfile, and Number of References in CA SEARCH (File 399)
7	Long	CA Index Name(s) (excluding other CA Names) and Ring System Data
8	Short	CA Index Name(s) (excluding other CA Names)
9	Full	Full Record

OTHER OUTPUT OPTIONS

For an explanation, enter HELP TYPE, HELP UDF, HELP TAG online.

USER DEFINED FORMATS	Display codes listed in the Search Options tables can be used to customize output.	TYPE S3/RN,MF,SY/1-5
TAG	Output can be displayed with tags identifying each display field.	TYPE S2/5/1-6 TAG
DIRECT RECORD ACCESS	Direct Record Access is not applicable in Files 398, 301, and 231.	

FOR ONLINE HELP:

See HELP FIELDS 398 for searchable fields; HELP FORMAT 398 for output formats; HELP LIMIT 398 for limits; HELP RATES 398 for cost information; HELP SORT 398 for sorts.

Locating a CAS Registry Number (cont.)

► **Topic** ◀ Locate the CAS Registry Number for ethylene glycol. Use the Registry Number in RTECS® (File 336) to track the reproductive review of ethylene glycol.

*TYPE the record to
view the CAS®
Registry Number,
synonyms, and
molecular formula
for ethylene glycol.*

```
?B 301
File 301:CHEMNAME(R) 1967-2002/Oct
(c) 2002 Amer.Chem.Soc.

Set Items Description
---
?e na=ethylene glycol

Ref Items Index-term
E1 1 NA=ETHYLENE GERMANATE(IV)
E2 1 NA=ETHYLENE GLYCOL-MAGNESIUM BIS(2-HYDROXYETHYL P
E3 1 *NA=ETHYLENE GLYCOL
E4 1 NA=ETHYLENE GLYCOL .ALPHA.-D-GLUCOPYRANOSIDE
E5 2 NA=ETHYLENE GLYCOL .ALPHA.,.ALPHA.-DIHYDROPERFLUO
E6 1 NA=ETHYLENE GLYCOL (13C2H6O2)
E7 1 NA=ETHYLENE GLYCOL ACETAL OF 2,2,2-TRIS-CYANOETHY
E8 1 NA=ETHYLENE GLYCOL ACETATE
E9 1 NA=ETHYLENE GLYCOL ACETATE BUTYRATE
E10 1 NA=ETHYLENE GLYCOL ACETATE HEXANOATE
E11 1 NA=ETHYLENE GLYCOL ACETATE MONOETHYL ETHER
E12 1 NA=ETHYLENE GLYCOL ACETATE MONOMETHYL ETHER

Enter P or PAGE for more

?S E3
S1 1 NA='ETHYLENE GLYCOL'

?T S1/9
1/9/1
DIALOG(R)File 301:CHEMNAME(R)
(c) 2002 Amer.Chem.Soc. All rts. reserv.

CAS REGISTRY NUMBER: 107-21-1
MOLECULAR FORMULA: C2H6O2
REPLACED CAS REGISTRY NUMBER(S) : 37221-95-7 71767-64-1
CA NAME(S):
HP=1,2-Ethenediol (9CI)
HP=Glycol (6CI 7CI)
OTHER CA NAMES:
HP=Ethylene glycol (8CI)
SYNONYMS: Dowtherm SR 1; Ethylene alcohol; Ethylene
dihydrate; Fridex; Glycol alcohol; Macrogol 400 BPC;
Monoethylene glycol; Norkool; Ramp; Tescol; Ucar 17; Union
Carbide XL 54 Type I De-icing Fluid; Zerex; 1,2-
```

Search using the CAS Registry Number in File 336. In this file you can track the toxicity of ethylene glycol. The record also contains mutation effects, reproductive effects, reviews and more.

```

Dihydroxyethane; 1,2-Ethylene glycol; 146AR; 2-
Hydroxyethanol
  SUBFILE: CHEMNAME      33125 LITERATURE REFERENCE(S) IN
FILE 399.
  LAST UPDATE: 200210

?B 336; S RN=107-21-1

File 336:RTECS 2001/Q1
  Comp & dist by NIOSH, Intl Copyright All Rights Res
Set  Items  Description
---  ----  -
S1      1  RN=107-21-1

?T S1/9

  1/9/1
DIALOG(R)File 336:RTECS
Comp & dist by NIOSH, Intl Copyright All Rights Res. All
rts. reserv.

060935      RTECS Number: KW2975000
Substance Name: Ethylene glycol
CAS Registry Number: 107-21-1; 71767-64-1  Molecular
Formula: C2H6O2
Molecular Weight: 62.08
Synonyms: Athylenglykol (German) ; 1,2-Dihydroxyethane ;
1,2-Ethandiol ; 1,2-Ethanediol ; Ethane-1,2-diol ; Ethylene
alcohol ; Ethylene dihydrate ; Ethylene glycol (ACGIH) ;
Glycol alcohol ; Lutrol-9 ; Macrogol 400 BPC ; M.E.G. ;
Monoethylene glycol ; NCI-C00920 ; Norkool; Tescol ;
Dowtherm SR 1 ; Ucar 17
Compound Class: Agricultural Chemical; Tumorigen; Mutagen;
Reproductive Effector; Human Data; Primary Irritant
Wiswesser Line Notation: Q2Q
Record Date: 200012
. . . . .
REPRODUCTIVE EFFECTS DATA:
  Developmental Abnormalities: Skin and skin appendages
;Developmental Abnormalities: Musculoskeletal system
;Developmental Abnormalities: Blood and lymphatic systems
Oral Rat TDLo 50 gm/kg 6-15D preg TXAPA9 81,113,1985
. . . . .
TOXICITY EFFECTS DATA:
  Recordings from specific areas of CNS ;Mydriasis
(pupillary dilation) ;Lungs, Thorax, or Respiration--Other
changes Oral Man TDLo 24 gm/kg JTCTDW 38,445,2000
  Sensory change involving peripheral nerve ;Ulceration or
bleeding from small intestine ;Renal function tests
depressed Oral Man TDLo 15 gm/kg AEMED3 20,208,1991.
. . . . .

```

Experimental data and toxicological references are available in this database.

Note the journal references for reproductive effects.

Note: The above long record has been abbreviated; however, the final segment indicates the types of data present.

REVIEWS:

ACGIH TLV-Not classifiable as a human carcinogen DTLVS* TLV/BEI,1999

ACGIH TLV-CL 100 mg/m3 DTLVS* TLV/BEI,1999

TOXICOLOGY REVIEW AJMEAZ 38,409,1965

TOXICOLOGY REVIEW FAATDF 13,747,1989

TOXICOLOGY REVIEW REPTED 8,99,1994

STANDARDS AND REGULATIONS:

EPA FIFRA 1988 PESTICIDE SUBJECT TO REGISTRATION OR RE REGISTRATION FEREAC 54,7740,1989

MSHA STANDARD-air TWA 10 mg/m3 (particulate) DTLWS* 3,19,1973

OEL-AUSTRALIA TWA 60 mg/m3, STEL 120 mg/m3, JAN1993

OEL-AUSTRIA MAK 10 ppm (26 mg/m3), Skin, JAN1999

REPRODUCTIVE EFFECTS JOURNAL REFERENCES:

CHYCDW Zhonghua Yufangyixue Zazhi. Chinese Journal of Preventive Medicine. China International Book Trading Corp., POB 2820, Beijing, Peop. Rep. China Beginning history not known.

EVHPAZ EHP, Environmental Health Perspectives. U.S. Government Printing Office, Supt of Documents, Washington, DC 20402 No.1- 1972-FAATDF Fundamental and Applied Toxicology. Academic Press, Inc., 1 E. First St., Duluth, MN 55802 V.1-40, 1981-97. For publisher information, see TOSCF2

NTIS** National Technical Information Service. Springfield, VA 22161 Formerly U.S. Clearinghouse for Scientific & Technical Information.

TJADAB Teratology, The International Journal of Abnormal Development. Alan R. Liss, Inc., 41 E. 11th St., New York, NY 10003 V.1- 1968-

TOXID9 Toxicologist. Soc. of Toxicology, Inc., 475 Wolf Ledge Parkway, Akron, OH 44311 V.1- 1981-

TXAPA9 Toxicology and Applied Pharmacology. Academic Press, Inc., 1 E. First St., Duluth, MN 55802 V.1- 1959-

WDZAEK Weisheng Dulixue Zazhi. Journal of Health Toxicology. Weisheng Dulixue Zazhi Bianjibu, Dongdaqiao, Chaoyang Menwai, Beijing, Peop. Rep. China V.1- 1987

TOXICITY EFFECTS JOURNAL REFERENCES:

AEMED3 Annals of Emergency Medicine. American College of Emergency Physicians, 1125 Executive Circle, Irving, TX 75038

AGGHAR Archiv fuer Gewerbepathologie und Gewerbehygiene. Berlin, Ger. V.1-18, 1930-61. For publisher information, see IAEDHW.

DATA PRESENT: Irritation Effects; Mutation Effects; Reproductive Effects; Toxicity Effects; Human Toxicity Effects; Other Multiple Dose Effects; Reviews; Standards and Regulations; NIOSH Criteria Documents; NTP, NIOSH, EPA Status

► **Topic** ◀ Sometimes you can use the chemical name to retrieve a record, but it is not clear which record in your results is the one you want. In the sample search below, the requester has asked for information on acetone-carbonyl oxide.

```
?B 301

File 301:CHEMNAME(R) 1967-2002/Oct
      (c) 2002 Amer.Chem.Soc.

      Set  Items  Description
      ---  -
?e na=acetone carbonyl oxide

Ref  Items  Index-term
E1   1      NA=ACETONE BISULFITE
E2   1      NA=ACETONE BUTYLHYDRAZONE
E3   2      *NA=ACETONE CARBONYL OXIDE
E4   1      NA=ACETONE CARBOXYLASE
E5   1      NA=ACETONE CATION
E6   1      NA=ACETONE CATION RADICAL
E7   1      NA=ACETONE CHLOROFORM
E8   1      NA=ACETONE COMPOUND WITH IODINE (1:1)
E9   1      NA=ACETONE COMPOUND WITH M-NITROPHENOL (1:1)
E10  1      NA=ACETONE COMPOUND WITH S-TRINITROBENZENE
E11  1      NA=ACETONE COMPOUND WITH WATER (1:1)
E12  1      NA=ACETONE CONJUGATE ACID

      Enter P or PAGE for more

?S E3
      S1          2  NA='ACETONE CARBONYL OXIDE'

?T S1/9/ALL

      1/9/1
DIALOG(R)File 301:CHEMNAME(R)
(c) 2002 Amer.Chem.Soc. All rts. reserv.

CAS REGISTRY NUMBER: 126463-77-2
MOLECULAR FORMULA: C3H6O2
CA NAME(S):
  HP=Ethyl (9CI)
  SB=1-dioxy-1-methyl-  SYNONYMS: Acetone carbonyl
oxide; Acetone oxide; Dimethylcarbonyl oxide
  SUBFILE: CHEMNAME 14 LITERATURE REFERENCE(S) IN FILE 399.
  LAST UPDATE: 199811
1/9/2
DIALOG(R)File 301:CHEMNAME(R)
(c) 2002 Amer.Chem.Soc. All rts. reserv.

CAS REGISTRY NUMBER: 65339-02-8
MOLECULAR FORMULA: C3H6O2
REPLACED CAS REGISTRY NUMBER(S) : 68941-71-9 138434-16-9
CA NAME(S):
  HP=Oxonium (9CI)
  SB=hydroxy(1-methylethylidene)-
  NM=inner salt
  SYNONYMS: Acetone carbonyl oxide; Acetone oxide
  SUBFILE: CHEMNAME 9 LITERATURE REFERENCE(S) IN FILE
399.
  LAST UPDATE: 199310
```

In these records both synonyms and molecular formulas are identical. Consult with the requester/chemist to choose the most appropriate record.

Using the Molecular Formula Technique

You can conduct a substance search online using the molecular formula technique by using MF= (Molecular Formula) field. A molecular formula is a precise representation of the atoms contained in a molecule. A molecular formula can be searched in the Chapman & Hall Chemical Database (File 303), CHEMSEARCH™ (File 398), CHEMNAME® (File 301), RTECS (File 336), The Merck Index OnlineSM (File 304), The Pesticide Fact File (File 306), Beilstein Online (File 390), CHEMTOX® Online (File 337), and in many pharmaceutical databases.

Molecular formula shorthand must be listed in a specific order (Hill Order), with carbon (C) always being first, followed by hydrogen (H) second, and then all other elements listed in alphabetical order. For compounds that do not contain carbon, simply arrange the elements in alphabetical order.

► **Topic** ◀ Locate the CAS Registry Number for malachite $\text{CH}_2\text{CU}_2\text{O}_5$, a rich green mineral used for ornaments or in making jewelry. Hint: use the MF= field and the Hill Order.

SELECT the molecular formula using MF=. Note that carbon is listed first, hydrogen second and the other elements are listed in alphabetical order.

```
?B 398
File 398:CHEMSEARCH(TM) 1957-2002/Oct
(c) 2002 Amer.Chem.Soc.

      Set  Items  Description
      ---  -
?S MF=CH2CU2O5
      S1      12  MF=CH2CU2O5

?s s1 and malachite
              12  S1
              68  MALACHITE
      S2      1  S1 AND MALACHITE

?T S1/9

1/9/1
DIALOG(R)File 398:CHEMSEARCH(TM)
(c) 2002 Amer.Chem.Soc. All rts. reserv.

CAS REGISTRY NUMBER: 1319-53-5 (MINERAL)
MOLECULAR FORMULA: CH2Cu2O5
REPLACED CAS REGISTRY NUMBER(S) : 12424-14-5
CA NAME(S) :
      HP=Malachite (Cu2(CO3)(OH)2) (9CI)
SYNONYMS: Malachite; Rivotite; Rokusyo
SUBFILE: CHEMNAME          644 LITERATURE REFERENCE(S) IN FILE
399.
LAST UPDATE: 200005
```

Chemical Segmentation

You may need to find information about a compound with a longer, more complicated chemical name. For example:

2,4-dichloro-2,4-dimethylhexane

► **Topic** ◀ Find the CAS Registry Number for the compound: 2,4-dichloro-2,4-dimethylhexane.

Note that this name is not found in the EXPANDED list of chemical names.

E4 shows a hit for a similar pentane derivative.

```
?B 398
File 398:CHEMSEARCH(TM) 1957-2002/Oct
(c) 2002 Amer.Chem.Soc.

Set Items Description
---
?e na=2,4-DICHLORO-2,4-DIMETHYLHEXANE

Ref Items Index-term
E1 1 NA=2,4-DICHLORO-2,4-DI(CHLOROMETHYL)-1,1,1,3,3,5,
E2 1 NA=2,4-DICHLORO-2,4-DIMETHYL-2,4-DISILAPENTANE
E3 0 *NA=2,4-DICHLORO-2,4-DIMETHYLHEXANE
E4 1 NA=2,4-DICHLORO-2,4-DIMETHYLPENTANE
E5 1 NA=2,4-DICHLORO-2,4-DINITROSOPENTANE
E6 1 NA=2,4-DICHLORO-2,4-DISILAPENTANE
E7 2 NA=2,4-DICHLORO-2,4,6,6-TETRAKIS(DIMETHYLAMINO)-1
E8 1 NA=2,4-DICHLORO-2,4,6,6-TETRAKIS(ETHYL(2-HYDROXYE
E9 1 NA=2,4-DICHLORO-2,4,6,6-TETRAKIS(ISOPROPYLAMINO)-
E10 1 NA=2,4-DICHLORO-2,4,6,6-TETRAKIS(2,2-DIHYDROPERFL
E11 1 NA=2,4-DICHLORO-2'-FLUORO-4'-NITRODIPHENYL ETHER
E12 1 NA=2,4-DICHLORO-2'-HYDROXYCHALCONE

Enter P or PAGE for more
```

Chemical Name Search Techniques

Technique 1: Select segments of the chemical name in the basic index.

Note: 2,4 are known as locants or locant strings.

Locant strings containing commas and periods are retained as searchable terms in Files 398, 301, 303, 304, 316 and 306.

```
?S DICHLORO AND DIMETHYL AND HEXANE
333979 DICHLORO
1748639 DIMETHYL
261617 HEXANE
S1 377 DICHLORO AND DIMETHYL AND HEXANE

?S DICHLORO AND DIMETHYLHEXANE
333979 DICHLORO
229 DIMETHYLHEXANE
S2 6 DICHLORO AND DIMETHYLHEXANE

?S 2,4(D)DICHLORO AND 2,4(D)DIMETHYL AND HEXANE
939929 2,4
333979 DICHLORO
32118 2,4(W)DICHLORO
939929 2,4
1748639 DIMETHYL
35955 2,4(W)DIMETHYL
261617 HEXANE
```

```

S3      1  2,4()DICHLORO AND 2,4()DIMETHYL AND HEXANE
?T S3/9/1

3/9/1
DIALOG(R) File 398:CHEMSEARCH(TM)
(c) 2002 Amer.Chem.Soc. All rts. reserv.

CAS REGISTRY NUMBER: 76637-61-1
MOLECULAR FORMULA: C8H16Cl2
CA NAME(S):
  HP=Hexane (9CI)
  SB=2,4-dichloro-2,4-dimethyl-
SUBFILE: CHEMNAME      2 LITERATURE REFERENCE(S) IN FILE
399.
LAST UPDATE: 199104

```

Technique 2: Check the CAS naming conventions of a similar compound, noting any unique spelling or punctuation characteristics.

Note that hexane was listed before 2,4-dichloro-2,4-dimethyl-.

To find this compound, use HP=Heading Parent, SB=Substituent

Or, invert the name and use the comma.

```

?s hp=hexane and sb=2,4-dichloro-2,4-dimethyl-
      246107  HP=HEXANE
      12     SB=2,4-DICHLORO-2,4-DIMETHYL-
S2      1     HP=HEXANE AND SB=2,4-DICHLORO-2,4-DIMETHYL-

?s na=hexane,2,4-dichloro-2,4-dimethyl-
S5      1     NA=HEXANE,2,4-DICHLORO-2,4-DIMETHYL-

```

Segmentation of chemical names enhances searching because any single segment will retrieve all compound names that contain that segment either as a complete word or as part of a longer compound word. It can be very useful for classes of substances or for targets that have not been synthesized.

A large number of records contain the segment AMINO alone or in combination with other segments.

Note: /FF stands for Full Field. It allows you to search for a term as a full word (a word that begins and ends with a space and not as a segment of a longer word. Punctuation (-) is treated as a space on Dialog.

See Table 2-1 for Dialog Files with Chemical Segmentation.

See the difference in number of records when the search is limited using /FF.

?B 399

File 399:CA SEARCH(R) 1967-2002/UD=13719
(c) 2002 American Chemical Society

Set	Items	Description
---	-----	-----
?S OPIOID?()PEPTIDE?/TI AND AMINO/TI		
	13309	OPIOID?/TI
	138883	PEPTIDE?/TI
	2061	OPIOID?/TI (W) PEPTIDE?/TI
	272249	AMINO/TI
S1	28	OPIOID?()PEPTIDE?/TI AND AMINO/TI
?T S1/TI/1-3		
	1/TI/1	
DIALOG(R)File 399:(c) 2002 American Chemical Society. All		
rts. reserv.		
Opioid peptide receptor studies. 15. Relative efficacy of		
4-((N-allyl-3-methyl-4-piperidinyl)phenylamino)-N,N-		
diethylbenzamide and related compounds at the cloned human		
.delta.-opioid receptor		
	1/TI/2	
DIALOG(R)File 399:(c) 2002 American Chemical Society. All		
rts. reserv.		
Stereochemical requirements for receptor recognition of the		
.mu.-opioid peptide endomorphin-1: biological activity, NMR		
and conformational analysis of D-amino acid substituted		
analogs		
	1/TI/3	
DIALOG(R)File 399:(c) 2002 American Chemical Society. All		
rts. reserv.		
Synthesis, conformational analysis, and biological activity		
of opioid peptide analogs containing side chain fluorinated		
amino acids		
?S OPIOID?()PEPTIDE?/TI AND AMINO/FF, TI		
	13309	OPIOID?/TI
	138883	PEPTIDE?/TI
	2061	OPIOID?/TI (W) PEPTIDE?/TI
	137197	AMINO/FF, TI
S2	19	OPIOID?()PEPTIDE?/TI AND AMINO/FF, TI

?T S2/TI/ALL

2/TI/1

DIALOG(R)File 399:(c) 2002 American Chemical Society. All
rts. reserv.

Stereochemical requirements for receptor recognition of
the .mu.-opioid peptide endomorphin-1: biological activity,
NMR and conformational analysis of **D-amino acid** substituted
analogs

2/TI/2

DIALOG(R)File 399:(c) 2002 American Chemical Society. All
rts. reserv.

Synthesis, conformational analysis, and biological
activity of opioid peptide analogs containing side chain
fluorinated **amino acids**

2/TI/3

DIALOG(R)File 399:(c) 2002 American Chemical Society. All
rts. reserv.

Influence of hippocampal excitatory **amino acid** receptors
on biosynthesis of endogenous opioid peptides during
penicillin- induced seizure

Table 2-1: Dialog Files with Chemical Segmentation

File Number	File Name	Non-Segment Limit	Locants as one word	Segments recombined	(T) operator active
5,55	BIOSIS Previews®	/FW	NO	YES	YES
23-25,340,123,125,223-225,341	CLAIMS®/U.S. Patent Abstracts, UNITERM, and Reassignment & Reexamination	/FW	NO	YES	YES
124,242	CLAIMS® Reference and Compound Registry	/FF	YES	YES	YES
156	TOXFILE	/FF	NO	YES	YES
301,398	CHEMNAME® CHEMSEARCH™	/FF	YES	NO	NO
303	Chapman & Hall Chemical Database Online (CHCD)	/FF	YES	NO	NO
304	The Merck Index Online SM	/FF	YES	YES	YES
305	Analytical Abstracts	/FW	NO	YES	YES
306	The Pesticide Fact File	/FW	YES	NO	NO
308-313,399	CA SEARCH®	/FF	NO	YES	YES
315	Chemical Engineering and Biotechnology Abstracts	/FW	NO	YES	YES
317	Chemical Safety Newsbase	/FW	NO	YES	YES
336	Registry of Toxic Effects of Chemical Substances (RTECS®)	/FW	NO	YES	YES
337	CHEMTOX®	/FW	NO	YES	YES

Table 2-1: Dialog Files with Chemical Segmentation (Continued)

344	Chinese Patent Abstracts in English	/FF	NO	YES	YES
350,351	Derwent World Patents Index	/FW	NO	YES	YES
353	Ei EnCompassPat™	/FW	NO	YES	YES
354	Ei EnCompassLit™	/FW	NO	YES	YES
357	Derwent Biotechnology Abstracts	/FW	NO	YES	YES
358	Current Biotechnology Abstracts	/FW	NO	YES	YES`
377	Derwent Drug File	/FW	NO	YES	YES
390	Beilstein Online	/FW	NO	YES	YES

+Not defined

Table 2-2: Files for Locating CAS Registry Numbers

Databases File Number	CHEMSEARCH CHEMNAME (Files 398/301)	BEILSTEIN ONLINE (File 390)	RTECS (File 336)	MERCK INDEX (File 304)
Number of Substances	Over 25,180,294	Over 7,169,374	Over 152,000	Over 10,430
Kinds of Substances	File 398 includes all chemical substances registered by Chemical Abstracts Service (CAS) since 1957. File 301 includes registered substances cited two or more times in the literature and abstracted by CAS since 1967.	Acyclic, isocyclic, and heterocyclic organic compounds reported in the literature since 1779.	Drugs, food additives, pesticides, fungicides, herbicides, solvents, dilutants, and chemical wastes.	Chemicals, drugs and biologicals

Using Element Count

► **Topic** ◀ Find representative lethal dose data for mercury containing compounds with 1-10 Hg atoms.

*EC=Element Count
Zeroes precede
numerical values.*

DP= Data Present

*Note: Enter HELP
FIELDS 304 for an
updated list of the
fields available on
The Merck Index
Online (File 304).*

*Note: Historical
information,
published prior to
online databases, is
included and
provides older
journal/patent
information as part
of the record.*

```
?B 304
File 304:THE MERCK INDEX ONLINE(SM) /2001Q1
      (c) 2001 MERCK & CO. INC.

      Set  Items  Description
      ---  ----  -
?S EC=HG0001:HG0010
   S1      65  EC=HG0001:HG0010

?S S1 AND DP=LETHAL DOSE
           65  S1
          2645 DP=LETHAL DOSE
   S2      9  S1 AND DP=LETHAL DOSE

?T S2/9/1
2/9/1
DIALOG(R)File 304:THE MERCK INDEX ONLINE(SM)
(c) 2001 MERCK & CO. INC. All rts. reserv.

09451  Monograph Name: Thimerosal
CAS REGISTRY NUMBER: 54-64-8
MOLECULAR FORMULA: C9H9HgNaO2S  MOLECULAR WEIGHT: 404.82
MOLECULAR COMPOSITION:  C 26.70%, H 2.24%, Hg 49.55%, Na
5.68%, O 7.90%, S 7.92%
C.A.  CHEMICAL NAME(s):  Ethyl(2-mercaptobenzoato(2-)-
O,S)mercurate(1-) sodium; ((o-
carboxyphenyl)thio)ethylmercury sodium salt
SYNONYMS:
sodium ethylmercurithiosalicylate; thiomersalate;
mercurothiolate
BRAND NAME (and COMPANY):
Merthiolate (Lilly); Merzonin (Takeda); Vitaseptol
(Faure)
LITERATURE REFERENCES:
Prepd by reacting ethylmercuric chloride (or ethylmercuric
hydroxide) with thiosalicylic acid: Kharasch, U.S. pat.
1,672,615 (1928); Trikojus, Nature 158, 472 (1946); Swirska
et al., Przemysl Chem. 39, 371 (1960), C.A. 55, 3507a
(1961). Toxicity: Mason et al., Clin. Toxicol. 4, 185
(1971).
PATENT INFORMATION:
US 1672615
```

File 304 is a very valuable resource for "composition of matter" patents.

LD = Lethal Dose Data

Note: Refer also to RTECS (File 336), CHEMTOX® (File 337) and DIALINDEX category TOXICOL.

PHYSICAL DATA:

Cream-colored, crystalline powder. Stable in air, but not in sunlight. One gram dissolves in about 1 ml water, in about 8 ml alcohol. Practically insol in ether and benzene. Stabilization of solns with EDTA: Davisson, U.S. pat. 2,864,844 (1958 to Lilly). pH of 1% aq soln: 6.7. LD50 s.c. in rats: 98 mg/kg (Mason).

PHYSICAL DATA:

LD50: LD50 s.c. in rats: 98 mg/kg (Mason)
USE: Pharmaceutic aid (preservative).
THERAPEUTIC CATEGORY: Anti-infective.
THERAPEUTIC CATEGORY VET: Antibacterial, antifungal (topical).
REFERENCE KEYS PRESENT: Patent number; Prepd; Toxicity
DATA KEYS PRESENT: Molecular weight; Patent number; Uses; Therap. Cat.; Therap. Cat. Vet.; Lethal dose

Using Component Registry Numbers (RC=)

► **Topic** ◀ Locate all chemical substances containing only two components resulting from a reaction of substances with CAS Registry numbers 124-09-4 and 141-82-2.

Note: File 301 is a subfile of File 398.

Number of Components field label is NC. You can also use parentheses with one field label.

Use **SAVE TEMP** to save search results for seven days at no charge.

BEGIN in File 398 and **EXS** to execute the SearchSave.

?B 301

File 301:CHEMNAME(R) 1967-2002/Oct
 (c) 2002 Amer.Chem.Soc.

Set	Items	Description
---	----	-----
?S	RC=124-09-4 AND RC=141-82-2 AND NC=02	
	1449	RC=124-09-4
	167	RC=141-82-2
	525860	NC=02
S1	1	RC=124-09-4 AND RC=141-82-2 AND NC=02
?S	RC=(124-09-4 AND 141-82-2) AND NC=02	
	1449	RC=124-09-4
	167	RC=141-82-2
	525860	NC=02
S2	1	RC=(124-09-4 AND 141-82-2) AND NC=02

?SAVE TEMP

Temp SearchSave "TD411" stored

?B 398;EXS

Note: Compare search results for identical searches conducted in CHEMNAME® (File 301) [1 result] and CHEMSEARCH™ (File 398) [2 results].

```
File 398:CHEMSEARCH(TM) 1957-2002/Oct
(c) 2002 Amer.Chem.Soc.

      Set  Items  Description
      ---  -
Executing TD411
          7343  RC=124-09-4
          942  RC=141-82-2
        2648821  NC=02
      S1          2  RC=124-09-4 AND RC=141-82-2 AND NC=02
          7343  RC=124-09-4
          942  RC=141-82-2
        2648821  NC=02
      S2          2  RC=(124-09-4 AND 141-82-2) AND NC=02
?T S1/9/ALL
```

```
1/9/1
DIALOG(R)File 398:CHEMSEARCH(TM)
(c) 2002 Amer.Chem.Soc. All rts. reserv.
```

```
CAS REGISTRY NUMBER: 76958-88-8
MOLECULAR FORMULA: C6H16N2.xC3H4O4
CA NAME(S):
  HP=Propanedioic acid (9CI)
  NM=compd. with 1,6-hexanediamine
OTHER CA NAMES:
  HP=1,6-Hexanediamine
  NM=propanedioate
SYNONYMS: Malonic acid hexamethylenediamine salt
COMPONENT CAS REGISTRY NUMBER(S):
(124-09-4 141-82-2)
```

Component	RN	Component	Molecular Formula
1)	124-09-4	C6H16N2	
2)	141-82-2	C3H4O4	

```
SUBFILE: CHEMSIS 10CI 1 LITERATURE REFERENCE(S) IN FILE
399. LAST UPDATE: 199104
```

```
1/9/2
DIALOG(R)File 398:CHEMSEARCH(TM)
(c) 2002 Amer.Chem.Soc. All rts. reserv.
```

```
CAS REGISTRY NUMBER: 36863-61-3 (POLYMER)
MOLECULAR FORMULA: (C6H16N2.C3H4O4)x
CA NAME(S):
  HP=Propanedioic acid (9CI)
  NM=polymer with 1,6-hexanediamine
OTHER CA NAMES:
  HP=1,6-Hexanediamine
  NM=polymer with propanedioic acid
```

```

SYNONYMS: Nylon 63; 1,6-Hexanediamine-malonic acid
copolymer
COMPONENT CAS REGISTRY NUMBER(S) :
(124-09-4 141-82-2)

Component RN      Component Molecular Formula
=====
1)      124-09-4   C6H16N2
2)      141-82-2   C3H4O4

SUBFILE: CHEMNAME      19 LITERATURE REFERENCE(S) IN FILE
399.
LAST UPDATE: 199309

```

Ring System Data

Chemical structure and molecular formula provided by the requester.

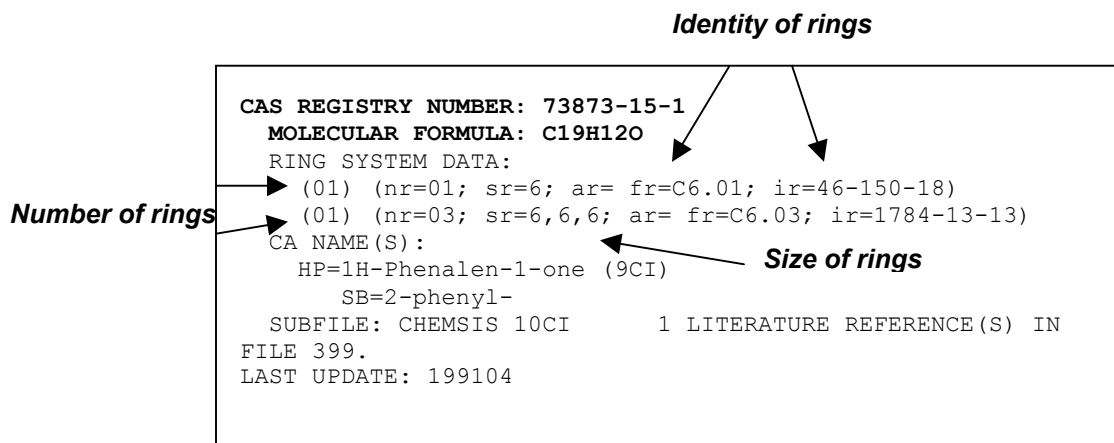


Figure 2-1. Record from CHEMSEARCH (File 398)

TR= Total number of rings: (NR=01 + NR=03: TR=04

SR= Size of rings: SR=6 and SR=6,6,6

IR= Identity of rings: IR= 46-150-18 (Phenyl Ring System)

IR= Identity of rings: IR= 1784-13-13

Ring System Data for Cyclic Substances: IR=, SR=, TR=

- Rings are defined as three or more atoms cyclically bonded together.
- Over 80% of the compounds in the CAS Registry Number system contain at least one ring system.
- Dialog's ring data indexing of elements allows searchers to:
 - Check the presence of any specific ring or rings, organic or inorganic, in a substance.
 - Identify all compounds having the same ring or ring systems.
- Use the ring data indexing elements with nomenclature, locant string points-of-attachment, molecular formulae, etc. to search the Registry system as extensively as desired.

Example of Use of Ring System Data fields in CHEMSEARCH (File 398)

Note: There are 36 structural isomers.

TYPE out the record in the following User-Defined Formats (UDF):

NA= Complete Name and Synonyms

RN= CAS Registry Number

MF= Molecular Formula

RS= Ring System Data

```
?B 398
File 398:CHEMSEARCH(TM) 1957-2002/Oct
(c) 2002 Amer.Chem.Soc.

Set Items Description
---
?S MF=C18H11N3O4S/FF
S1 36 MF=C18H11N3O4S/FF

?S S1 AND SR=6,6,6 AND TR=04 AND IR=46-150-18
36 S1
511243 SR=6,6,6
2886561 TR=04
10817766 IR=46-150-18
S2 1 S1 AND SR=6,6,6 AND TR=04 AND IR=46-150-18

?T S2/NA,RN,MF,RS/1
2/NA,RN,MF,RS/1
DIALOG(R)File 398:(c) 2002 Amer.Chem.Soc. All rts. reserv.

CAS REGISTRY NUMBER: 73883-68-8
MOLECULAR FORMULA: C18H11N3O4S
RING SYSTEM DATA:
(01) (nr=01; sr=6; ar= fr=C6.01; ir=46-150-18)
(01) (nr=03; sr=6,6,6; ar=C4NS.01-C6.02; fr=NC2SC2.01-
C6.02; ir=2508-272-18)
CA NAME(S):
HP=10H-Phenothiazine (9CI)
SB=1,3-dinitro-10-phenyl-
```

Online Practice Exercises

Check your knowledge with online practice.

1. What is the CAS Registry Number for L-3-keto-threo-hexuronic acid lactone? What is its common name?
2. What is a popular trade name for methyldiazepinone and what is its molecular formula using the Hill Order?
3. What drug is diphenhydramine hydrochloride and what is its Registry Number?
4. What is the Registry Number for this everyday product, methylaspartylphenylalanate?
5. What is the Registry Number and street name for this illicit drug, d-lysergic acid diethylamide?

Section 3: Using the MAP Command

In this section you will learn:

- What the MAP command is
- Where to use the MAP command
- Why the MAP command is useful
- How to use the MAP command to save CAS Registry Numbers
- How to use the MAP command to save chemical name synonyms

What is the MAP Command?

The MAP command extracts search terms from a specific field in a record or group of records and creates a SearchSave. MAP eliminates the chore of scanning records for search terms of interest, and then re-keying those terms online. The SearchSave created by MAP can be permanent or temporary, and can be executed in the same or different Dialog files. MAP can also be incorporated into another SearchSave or into a Dialog AlertSM strategy. Two fields in the chemical files where the MAP command is regularly used are:

CAS Registry Numbers (RN)

Command: MAP RN TEMP

Synonym names (SY)

Command: MAP SY TEMP

Note: *The TEMP at the end of the MAP command indicates that the SearchSave is temporary and will be saved for seven days at no charge.*

You can also MAP both synonym names and the CAS Registry Numbers at the same time:

Synonym names + CAS Registry Numbers (SYRN)

Command: MAP SYRN TEMP

Dialog DIALINDEX[®]/OneSearch[®] categories in which Registry Numbers can be searched using RN= include:

CASREGNO	all files where CAS Registry Numbers can be searched
RNCHEM	chemical information
RNMED	medical information
RNLOOKUIP	file to look up registry numbers

The benefits of using the MAP command are:

- Saves time by automatically keying in all the selected search terms, rather than requiring you to do it manually.
- Provides more thorough results by searching more search terms than you might initially have considered.

The specific data fields available for MAP in each database are listed on the database Bluesheet as well as online under the command HELP MAPn, where n is the file number of the database. For example: HELP MAP 301 discussed the MAP command in CHEMNAME.

Locating the CAS Registry Number to MAP

►Topic◀ Use the MAP command to locate references on ethylene glycol in CA SEARCH[®] (File 314).

```
?B 301
File 301:CHEMNAME(R) 1967-2002/Oct
(c) 2002 Amer.Chem.Soc.

Set  Items  Description
---  -
?e na=ethylene gylcol

Ref  Items  Index-term
E1   1  NA=ETHYLENE  GERMANATE (IV)
E2   1  NA=ETHYLENE  GLCYOL-MAGNESIUM BIS(2-HYDROXYETHYL P
E3   1  *NA=ETHYLENE  GLYCOL
E4   1  NA=ETHYLENE  GLYCOL .ALPHA.-D-GLUCOPYRANOSIDE
E5   2  NA=ETHYLENE  GLYCOL .ALPHA.,.ALPHA.-DIHYDROPERFLUO
E6   1  NA=ETHYLENE  GLYCOL (13C2H6O2)
E7   1  NA=ETHYLENE  GLYCOL ACETAL OF 2,2,2-TRIS-CYANOETHY
E8   1  NA=ETHYLENE  GLYCOL ACETATE
E9   1  NA=ETHYLENE  GLYCOL ACETATE BUTYRATE
E10  1  NA=ETHYLENE  GLYCOL ACETATE HEXANOATE
E11  1  NA=ETHYLENE  GLYCOL ACETATE MONOETHYL ETHER
E12  1  NA=ETHYLENE  GLYCOL ACETATE MONOMETHYL ETHER

Enter P or PAGE for more

?S E3
      S1          1  NA='ETHYLENE GLYCOL'
?T S1/9
```

Note the CAS Registry Number.

The current CAS Registry Number and replaced CAS Registry Numbers are stored in the computer to be used in other databases containing the RN= field.

Use the MAP command to extract CAS registry Numbers and create a temporary Search Save of the numbers.

File 314 contains the newest records available in CA Search[®] (File 399).

EXS entered alone executes the most recently created SearchSave of the current search (TD417).

Note you can use the semicolon to stack the commands

```

1/9/1
DIALOG(R)File 301:CHEMNAME(R)
(c) 2002 Amer.Chem.Soc. All rts. reserv.

CAS REGISTRY NUMBER: 107-21-1
MOLECULAR FORMULA: C2H6O2
REPLACED CAS REGISTRY NUMBER(S) : 37221-95-7 71767-64-1
CA NAME(S):
  HP=1,2-Ethanediol (9CI)
  HP=Glycol (6CI 7CI)
OTHER CA NAMES:
  HP=Ethylene glycol (8CI)
SYNONYMS: Dowtherm SR 1; Ethylene alcohol; Ethylene
dihydrate; Fridex; Glycol alcohol; Macrogol 400 BPC;
Monoethylene glycol; Norkool; Ramp; Tescol; Ucar 17; Union
Carbide XL 54 Type I De-icing Fluid; Zerex; 1,2-
Dihydroxyethane; 1,2-Ethylene glycol; 146AR; 2-
Hydroxyethanol
SUBFILE: CHEMNAME      33125 LITERATURE REFERENCE(S) IN
FILE 399.
LAST UPDATE: 200210

?MAP RN TEMP

1 Select Statement(s), 3 Search Term(s)
Serial#TD417

1 SearchSaves, 3 Search Term(s)

?B 314;EXS

File 314:CA SEARCH(R) 1997-2002/UD=13719
(c) 2002 American Chemical Society

Set  Items  Description
---  -
Executing TD417
      9273  RN=107-21-1 (SEE ?IGNOTE)
      0    RN=37221-95-7
      0    RN=71767-64-1
S1   9273  RN=107-21-1 + RN=37221-95-7 + RN=71767-64-1

```

There are also Replaced CAS Registry Numbers listed. Use both for comprehensive results.

User-defined formats (UDFs) can be specified using the display codes that are listed on the database Bluesheet. As in this example, a predefined format (Format 3) can be combined with one or more display codes (RN for Registry Numbers).

?T S1/3,RN/1-2

1/3,RN/1

DIALOG(R)File 314:CA SEARCH(R)

(c) 2002 American Chemical Society. All rts. reserv.

137284457 CA: 137(19)284457z **PATENT**

Methods and apparatus for the inactivation of viruses

INVENTOR(AUTHOR): Castor, Trevor P.; Lander, Arthur D.

LOCATION: USA

PATENT: United States ; US 6465168 B1 DATE: 20021015

APPLICATION: US 474475 (19991229) *US 844513 (19920302)

PAGES: 10 pp., Cont.-in-part of U.S. Ser. No. 844,513, abandoned.

CODEN: USXXAM LANGUAGE: English CLASS: 435002000; A01N-001/02A; C12N-007/06B; C12M-001/36B

CAS REGISTRY NUMBERS:

64-17-5 67-56-1 67-64-1 74-98-6 **107-21-1** 10024-97-2

biological studies, methods and app. for inactivation of viruses

124-38-9 biological studies, supercrit.; methods and app. for inactivation of viruses

75-45-6 593-70-4 methods and app. for inactivation of viruses

1/3,K/6

DIALOG(R)File 314:CA SEARCH(R)

(c) 2002 American Chemical Society. All rts. reserv.

137281001 CA: 137(19)281001k **JOURNAL**

Catalytic synthesis of acetals or ketals with vitamin C

AUTHOR(S): Wen, Rui-ming; You, Pei-qing; Luo, Xin-xiang; Yu, Shan-xin

LOCATION: Department of Chemistry, Yiyang Teachers

College, Yiyang, Peop. Rep. China, 413049

JOURNAL: Shiyou Huagong (Shiyou Huagong) DATE: 2002

VOLUME: 31

NUMBER: 5 PAGES: 373-375 CODEN: SHHUE8 ISSN: 1000-8144

LANGUAGE: Chinese PUBLISHER: Shiyou Huagong Bianjibu

Locating Synonyms to MAP

Synonyms are another field that is easy to MAP. If you are searching a database where the CAS Registry Number field (RN=) is not present, create a temporary SearchSave by using the MAP command with the synonym field (SY=). Synonyms are then searched in the Basic Index.

► **Topic** ◀ Locate fulltext articles on the use of temozolomide in the treatment of brain metastases. Use the MAP command for the most comprehensive retrieval.

Retrieve the
chemical name
using NA=.

```
?B 398

File 398:CHEMSEARCH(TM) 1957-2002/Oct
      (c) 2002 Amer.Chem.Soc.

      Set  Items  Description
      ---  -
?e na=temozolomide

Ref  Items  Index-term
E1   1      NA=TEMORINE
E2   1      NA=TEMOVATE
E3   1      *NA=TEMOZOLOMIDE
E4   1      NA=TEMP
E5   1      NA=TEMP BOND NE
E6   1      NA=TEMP PLUS
E7   1      NA=TEMP 1
E8   1      NA=TEMP 100
E9   1      NA=TEMP 100D
E10  1      NA=TEMP-BOND
E11  1      NA=TEMPACE
E12  1      NA=TEMPACID

      Enter P or PAGE for more

?S E3
      S1          1  NA='TEMOZOLOMIDE'

?T S1/9

1/9/1
DIALOG(R) File 398:CHEMSEARCH(TM)
(c) 2002 Amer.Chem.Soc. All rts. reserv.

CAS REGISTRY NUMBER: 85622-93-1
MOLECULAR FORMULA: C6H6N6O2
RING SYSTEM DATA:
(01) (nr=02; sr=5,6; ar=C3N2.01-C2N4.01; fr=NCNC2.01-
N3CNC.01; ir=333-1738-1)
REPLACED CAS REGISTRY NUMBER(S) : 97716-75-1

CA NAME(S) :
HP=Imidazo(5,1-d)-1,2,3,5-tetrazine-8-carboxamide (9CI)
SB=3,4-dihydro-3-methyl-4-oxo-
```

MAP the synonyms using SY.

BEGIN in File 444 to retrieve fulltext articles.

EXECUTE the last SearchSave.

```

SYNONYMS: CCRG 81045; M and B 39831; MB 39831;
Methazolastone; NSC 362856; Sch 52365; Temodal;
Temozolomide
SUBFILE: CHEMNAME          255 LITERATURE REFERENCE(S) IN
FILE 399.
LAST UPDATE: 200104

?MAP SY TEMP

1 Select Statement(s), 8 Search Term(s)
Serial#TD419

1 SearchSaves, 8 Search Term(s)

?B 444;EXS

File 444:New England Journal of Med. 1985-2002/Nov W2
(c) 2002 Mass. Med. Soc.

Set  Items  Description
---  -
Executing TD419
      0  CCRG
      0  81045
      0  CCRG(W)81045
21639  M
      0  AND
13150  B
      0  39831
      0  M(W)AND(W)B(W)39831
1962  MB
      0  39831
      0  MB(W)39831
      0  METHAZOLASTONE
25    NSC
      0  362856
      0  NSC(W)362856
39    SCH
      0  52365
      0  SCH(W)52365
      0  TEMODAL
      3  TEMOZOLOMIDE
S1    3  CCRG()81045 + M()'AND'()B()39831 +
      MB()39831 + METHAZOLASTONE + NSC()362856
      + SCH()52365 + TEMODAL + TEMOZOLOMIDE

?T S1/3,K/ALL

```

The KWIC (Key Word in Context) format option displays only those portions of your records containing the search terms SELECTed. It shows the search terms in the context in which they occur, allowing you to judge the relevance of the search results.

1/3,K/1

DIALOG(R)File 444:New England Journal of Med.
(c) 2002 Mass. Med. Soc. All rts. reserv.

00121703

Copyright 2001 by the Massachusetts Medical Society

Treatment of Brain Metastases of Malignant Melanoma with Temozolomide (Correspondence)

Biasco, Guido; Pantaleo, Maria A.; Casadei, Simona.
The New England Journal of Medicine
Aug 23, 2001; 345 (8),pp 621-622
LINE COUNT: 00034 WORD COUNT: 00470

(Correspondence)

TEXT

...a finding confirmed by magnetic resonance imaging (Figure 1A). The patient was treated with oral temozolomide at a dose of 200 mg per square meter of body-surface area for five...

...that the brain lesions had disappeared (Figure 1B). The patient is still receiving therapy with temozolomide. He is in good health, without signs or symptoms of relapse. |*Figure 1.-Magnetic Resonance Images of the Brain. There are multiple bilateral metastases before therapy with temozolomide (Panel A). After six cycles of temozolomide, the lesions detectable by magnetic resonance imaging have disappeared (Panel B)
*.*FIGURE OMITTED...

... Temozolomide, a new oral alkylating agent, is as active as dacarbazine in malignant melanoma. (Ref. 1) Temozolomide can cross the blood-brain barrier, and its concentration in the central nervous system is...
...percent of its concentration in plasma. (Ref. 2) Another report has suggested the efficacy of temozolomide plus radiotherapy for the treatment of brain metastases of malignant melanoma. (Ref. 3) Our case shows that temozolomide alone can be effective in the treatment of such lesions. |Guido Biasco, M.D.Maria

CITED REFERENCES 001|

1. Middleton MR, Grob JJ, Aaronson N, et al. Randomized phase III study of temozolomide versus dacarbazine in the treatment of patients with advanced metastatic malignant melanoma. J Clin Oncol...
...2351.]

Reference 002

2. Agarwala SS, Reyderman L, Statkevich P, et al. Pharmacokinetic study of temozolomide penetration into CSF in a patient with dural melanoma.
Ann Oncol 1998;9:Suppl 4:138. abstract.

Reference 003

3. Franke W, Neumann N, Richter-Hintz D, et al.
Temozolomide -- a promising agent in the therapy of brain
metastases in malignant
melanoma. In: American Society...

1/3,K/2

DIALOG(R)File 444:New England Journal of Med.
(c) 2002 Mass. Med. Soc. All rts. reserv.

00121182

Copyright 2001 by the Massachusetts Medical Society

**The DNA-Repair Gene MGMT and the Clinical Response of
Gliomas to Alkylating Agents (Correspondence)**

Buckner, Jan C.; Moynihan, Timothy J.; Quinn, David I.;
Schlegel, Uwe; Ali-Osman, Francis; Srivenugopal, Kalkunte;
Sawaya, Raymond; Esteller, Manel; Herman, James G.;
Weinstein, John N.

The New England Journal of Medicine

Mar 1, 2001; 344 (9),pp 686-688

LINE COUNT: 00149 WORD COUNT: 02066

TEXT

...of DNA base alkylation by monofunctional and
bifunctional nitrosoureas and related alkylating agents,
such as temozolomide and procarbazine, is not the O(sup
6)-position of guanine but rather the N...

1/3,K/3

DIALOG(R)File 444:New England Journal of Med.
(c) 2002 Mass. Med. Soc. All rts. reserv.

00121026

Copyright 2001 by the Massachusetts Medical Society

Medical Progress: Brain Tumors (Review Articles)

DeAngelis, Lisa M.

The New England Journal of Medicine

Jan 11, 2001; 344 (2),pp 114-123

LINE COUNT: 00506 WORD COUNT: 06989

TEXT

...Traditional agents have included nitrosourea drugs, if
not used initially, and procarbazine. The efficacy of
temozolomide in the treatment of recurrent malignant
gliomas has been demonstrated. (Ref. 50) Temozolomide ,
which is administered orally, has a favorable side-effect
profile and thus is well tolerated...tumor. Agents that
appear to have some efficacy against recurrent
oligodendroglial tumors include melphalan, thiotepa,
temozolomide , carboplatin, cisplatin, and etoposide...

CITED REFERENCES

...50. Yung WK, Prados MD, Yaya-Tur R, et al. Multicenter phase II trial of temozolomide in patients with anaplastic astrocytoma or anaplastic oligoastrocytoma at first relapse. J Clin Oncol 1999...

Locating Synonyms and CAS Registry Numbers to MAP

You can MAP both Registry Numbers and synonyms at the same time. **Note:** In addition to the command mode, the MAP feature is available in an easy-to-use menu mode. You can enter the command MAP alone to receive a series of database-specific menus for parameters you wish to apply.

► **Topic** ◀ Use the MAP command to locate current information concerning the pesticide diflubenzuron.

```
?B 304
File 304:THE MERCK INDEX ONLINE(SM) /2001Q1
(c) 2001 MERCK & CO. INC.

Set Items Description
--- ----
?e na=diflubenzuron

Ref Items Index-term
E1 1 NA=DIFLOXACIN
E2 1 NA=DIFLOXACIN MONOHYDROCHLORIDE
E3 1 *NA=DIFLUBENZURON
E4 1 NA=DIFLUCAN
E5 1 NA=DIFLUCORTOLONE
E6 1 NA=DIFLUCORTOLONE 21-VALERATE
E7 1 NA=DIFLUDOL
E8 1 NA=DIFLUFENICAN
E9 1 NA=DIFLUFENZOPYR
E10 1 NA=DIFLUFENZOPYR MIXTURE WITH DICAMBA
E11 1 NA=DIFLUNISAL
E12 1 NA=DIFLUORODICHLOROMETHANE

Enter P or PAGE for more

?S E3
S1 1 NA='DIFLUBENZURON'

?T S1/3,SY
1/3,SY/1
DIALOG(R)File 304:THE MERCK INDEX ONLINE(SM)
(c) 2001 MERCK & CO. INC. All rts. reserv.

03188 Monograph Name: Diflubenzuron
CAS REGISTRY NUMBER: 35367-38-5
MOLECULAR FORMULA: C14H9ClF2N2O2 MOLECULAR WEIGHT: 310.69
```

```

MOLECULAR COMPOSITION: C 54.12%, H 2.92%, Cl 11.41%, F
12.23%, N 9.02%, O 10.30%
C.A. CHEMICAL NAME(s): N-(((4-Chlorophenyl)amino)carbonyl)-
2,6-difluorobenz amide
SYNONYMS:
1-(4-chlorophenyl)-3-(2,6-difluorobenzoyl)urea; difluron
DRUG CODES: DU-112307; PH-60-40; TH-6040; ENT-29054;
OMS-1804
BRAND NAME (and COMPANY):
Dimilin (Duphar); Duphacid (Duphar); Micromite
(Uniroyal)
LITERATURE REFERENCES:
Substituted benzoylphenylurea, inhibits chitin deposition
in insect cuticle. Prepn: K. Wellinga, R. Mulder, Ger. pat.
2,123,236; eidem, U.S. pat. 3,748,356 (1971, 1973 both to
Philips). Insecticidal activity: K. Wellinga et al., J.
Agr. Food Chem. 21, 993 (1973); R. Mulder, M. J. Gijswijt,
Pestic. Sci. 4, 737 (1973). Mode of action: E. Hunter, J.
F. V. Vincent, Experientia 30, 1432 (1974); S. M. Meola, R.
T. Mayer, Science
207, 985 (1980). Field trials against locusts and
grasshoppers: A. Bouaichi et al., Crop Protect. 13, 53, 60
(1994). Brief review: J. L. Marx, Science 197, 1170-1172
(1977). Review of activity, environmental fate, mode of
action: A. Verloop, C. D. Ferrell, ACS Symposium Series 37,
237-270 (1977); of chemistry and analyses: B. Rabenort et
al., Anal. Methods Pestic. Plant Growth Regul. 10, 57-72
(1978).
PATENT INFORMATION:
DE 2123236; US 3748356
USE: Insecticide.
REFERENCE KEYS PRESENT: Activity; Mode of action; Patent
number; Prepn; Review
DATA KEYS PRESENT: Molecular weight; Patent number; Uses;
Melting point; Lethal dose
?MAP SYRN TEMP

1 Select Statement(s), 10 Search Term(s)
Serial#TD418

1 SearchSaves, 10 Search Term(s)

```

Select synonyms
(SY) and CAS
Registry Numbers
(RN) to MAP.

BEGIN in File 399, a chemical literature database, and EXECUTE the most recent SearchSave.

?B 399;EXS

File 399:CA SEARCH(R) 1967-2002/UD=13719
(c) 2002 American Chemical Society

Set	Items	Description
---	-----	-----
Executing TD418		
	5	DIFLURON
	251	DIMILIN
	1398	DU
	0	112307
	0	DU(W)112307
	0	DUPHACID
	891	ENT
	1	29054
	0	ENT(W)29054
	2	MICROMITE
	48	OMS
	23	1804
	0	OMS(W)1804
	111528	PH (SEE ?GENERAL)
	20067	60
	23823	40
	5	PH(W)60(W)40
	4726	TH
	73	6040
	40	TH(W)6040
	1735	RN=35367-38-5
S1	1740	DIFLURON + DIMILIN + DU()112307 + DUPHACID + ENT()29054 + MICROMITE + OMS()1804 + PH()60()40 + TH()6040 + RN=35367-38-5

?T S1/3/1-4

1/3/1

DIALOG(R)File 399:CA SEARCH(R)
(c) 2002 American Chemical Society. All rts. reserv.

137243403 CA: 137(17)243403k JOURNAL
Preventative treatments for control of fungus gnats and shore flies

AUTHOR(S): Van Epenhuijsen, C. W.;Page,B. B. C.;
Koolaard, J. P.

LOCATION: New Zealand Institute for Crop & Food Research
Limited, Palmerston North, N. Z.,

JOURNAL: Proc. N. Z. Plant Prot. Conf. (Proceedings of
the New Zealand Plant Protection Conference) DATE: 2001
VOLUME: 54th, PAGES: 42-46

CODEN: PNZCEJ ISSN: 1172-0719 LANGUAGE: English
PUBLISHER: New Zealand Plant Protection Society

TYPE several records to see the types of records you will retrieve.

1/3/2

DIALOG(R)File 399:CA SEARCH(R)
(c) 2002 American Chemical Society. All rts. reserv.

137231593 CA: 137(16)231593j JOURNAL
Objections to tolerances established for certain pesticide chemicals

CORPORATE AUTHOR(S): Environmental Protection Agency
(EPA)
LOCATION: USA
JOURNAL: Fed. Regist. (Federal Register) DATE: 2002
VOLUME: 67
NUMBER: 118 PAGES: 41628-41635 CODEN: FERECAC ISSN:
0097-6326
LANGUAGE: English PUBLISHER: Superintendent of Documents

1/3/3

DIALOG(R)File 399:CA SEARCH(R)
(c) 2002 American Chemical Society. All rts. reserv.

137196872 CA: 137(14)196872a JOURNAL
**Responses of water bug *Diplonychus rusticus* (=indicus)
Venk. and Rao and fish *Gambusia affinis* to diflubenzuron,
BHC and deltamethrin in mosquito breeding site**

AUTHOR(S): Venkatesan, P.
LOCATION: Aquatic Entomology and Biocontrol Research
Laboratory,
Department of Zoology, Loyola College, Chennai, 600 034,
India
JOURNAL: J. Entomol. Res. (Journal of Entomological
Research) DATE: 2002
VOLUME: 26 NUMBER: 1 PAGES: 55-61 CODEN: JEREDP ISSN:
0378-9519
LANGUAGE: English PUBLISHER: Malhotra Publishing House

1/3/4

DIALOG(R)File 399:CA SEARCH(R)
(c) 2002 American Chemical Society. All rts. reserv.

137151337 CA: 137(11)151337p PATENT
**Synergistic insecticidal compositions for genetically-
modified legumes expressing delta-endotoxins**

INVENTOR(AUTHOR): Kern, Manfred
LOCATION: Germany,
ASSIGNEE: Aventis Cropscience G.m.b.H.
PATENT: Germany Offen. ; DE 10104871 A1 DATE: 20020808
APPLICATION: DE 10104871 (20010203)

Using the MAP Command with Number of Components

You can MAP parts of sets and convert Registry numbers to component Registry numbers as shown in the following example.

► **Topic** ◀ Locate co-polymers of 2-Butene containing three chemical components.

*NA= Complete
name and
Synonyms*

*HP= Heading
Parent*

SB= Substituent

NM= Name Modifier

*ST=
Stereochemistry*

```
?B 398
File 398:CHEMSEARCH(TM) 1957-2002/Oct
(c) 2002 Amer.Chem.Soc.

Set Items Description
--- -----
?e na=2-butene

Ref Items Index-term
E1 1 NA=2-BUTENAMIDE,4,4'-((1,1,3,3-TETRAKIS(PHENYLMET
E2 1 NA=2-BUTENAMIDE,4,4',4''-(OCTYLSTANNYLIDYNE)TRIS
E3 3 *NA=2-BUTENE
E4 1 NA=2-BUTENE DICATION
E5 1 NA=2-BUTENE EPOXIDE
E6 1 NA=2-BUTENE NITRILE, 2-CHLORO 3((1,1-DIMETHYL ETH
E7 1 NA=2-BUTENE OXIDE
E8 1 NA=2-BUTENE OXIDE-4-VINYL-7-OXABICYCLO(4.1.0)HEPT
E9 1 NA=2-BUTENE RADICAL CATION
E10 1 NA=2-BUTENE SECONDARY OZONIDE
E11 2 NA=2-BUTENE (DITHIOIC) ACID,METHYL ESTER
E12 1 NA=2-BUTENE (DITHIOIC) ACID,2-ACETYL-3-HYDROXY-,ME

Enter P or PAGE for more

?S E3
S1 3 NA='2-BUTENE'

?S S1/FF
S2 3 S1/FF

?T S2/NA/ALL
2/NA/1
DIALOG(R)File 398:(c) 2002 Amer.Chem.Soc. All rts. reserv.

CA NAME(S):
HP=2-Butene (9CI)
ST=(2E) -
HP=2-Butene (8CI)
ST=(E) -
```

MAP RN T S2/1
MAP Registry
numbers for only
one record of a set if
only (E)-2-Butene is
to be searched.

RC= Component
Registry Number

MAP Registry
numbers for all
possible 2-Butenes.

MAP RN T S1/RC=
to convert all RNs to
RCs for searching
on chemicals as
components or
building blocks of
larger chemicals.

NC= Number of
Components

```

SYNONYMS: .beta.-trans-Butylene; (E)-2-Butene; (E)-2-
Butene; trans-Butene ; trans-butene-2; trans-1,2-
Dimethylethylene; trans-2-Butene; trans-2-Butylene; 2-trans-
Butene; 2-trans-Butylene

2/NA/2
DIALOG(R)File 398:(c) 2002 Amer.Chem.Soc. All rts. reserv.

CA NAME(S) :
  HP=2-Butene (9CI)
  ST=(2Z) -
  HP=2-Butene (8CI)
  ST=(Z) -
SYNONYMS: .beta.-cis-Butylene; (Z)-2-Butene; cis-Butene;
cis-1,2-Dimethylethylene; cis-2-Butene; cis-2-Butylene

2/NA/3
DIALOG(R)File 398:(c) 2002 Amer.Chem.Soc. All rts. reserv.

CA NAME(S) :
  HP=2-Butene (8CI 9CI)
SYNONYMS: .beta.-Butene; .beta.-Butylene; Pseudobutylene

?MAP RN T S2/1

1 Select Statement(s), 1 Search Term(s)
Serial#TD409

1 SearchSaves, 1 Search Term(s)

?MAP RN T S1/RC=

1 Select Statement(s), 4 Search Term(s)
Serial#TD410

1 SearchSaves, 4 Search Term(s)

?EXS TD410
          91  RC=107-01-7
          73  RC=590-18-1
          77  RC=624-64-6
           0  RC=1735-76-8
S4       208  RC=107-01-7 + RC=590-18-1 + RC=624-64-6 +
          RC=1735-76-8

?S S4 AND NC=03
          208  S4
        614831 NC=03
S5       46   S4 AND NC=03

```

?T S5/9/1,2

5/9/1

DIALOG(R) File 398:CHEMSEARCH(TM)
(c) 2002 Amer.Chem.Soc. All rts. reserv.

CAS REGISTRY NUMBER: 360556-65-6

MOLECULAR FORMULA: C8H7NO2.C4H8.1/2Zn

RING SYSTEM DATA:

(01) (nr=01; sr=6; ar=C5N.01; fr=NC5.01; ir=46-156-30)

CA NAME(S):

HP=2-Propenoic acid (9CI)

SB=3-(4-pyridinyl)-

NM=zinc salt, (2E)-, compd. with (2E)-2-butene (1:2)

OTHER CA NAMES:

HP=2-Butene

NM=(2E)-, compd. with zinc bis((2E)-3-(4-pyridinyl)-
2-propenate) (2:1)

COMPONENT CAS REGISTRY NUMBER(S):

(624-64-6 84228-93-3)

1) 624-64-6 C4H8

2) 84228-93-3 C8H7NO2

SUBFILE: CHEMSIS 14CI 1 LITERATURE REFERENCE(S) IN
FILE 399.

LAST UPDATE: 200111

5/9/2

DIALOG(R) File 398:CHEMSEARCH(TM)
(c) 2002 Amer.Chem.Soc. All rts. reserv.

CAS REGISTRY NUMBER: 313216-99-8 (POLYMER)

MOLECULAR FORMULA: (C10H10.C4H8.C4H6)x

RING SYSTEM DATA:

(01) (nr=01; sr=6; ar= fr=C6.01; ir=46-150-18)

CA NAME(S):

HP=Benzene (9CI)

SB=diethenyl-

NM=polymer with 1,3-butadiene and 2-butene

OTHER CA NAMES:

HP=1,3-Butadiene

NM=polymer with 2-butene and diethenylbenzene

HP=2-Butene

NM=polymer with 1,3-butadiene and diethenylbenzene

COMPONENT CAS REGISTRY NUMBER(S):

(106-99-0 107-01-7 1321-74-0)

Note: Component Registry Number(s) RC=) and Component Molecular Formula present in records.

Component RN	Component Molecular Formula
1) 106-99-0	C4H6
2) 107-01-7	C4H8
3) 1321-74-0	C10H10

SUBFILE: CHEMSIS 14CI 1 LITERATURE REFERENCE(S) IN
FILE 399.
LAST UPDATE: 200101

The MAP Command Summary

The MAP command can be used to find chemical or physical properties, using the CAS Registry Number for chemical substances (MAP RN). Refer to the individual Dialog Bluesheets to determine whether a database offers MAP. Enter MAP to obtain the menu options.

Two fields where you can regularly use MAP in chemical files are:

- CAS Registry Numbers (RN=)
Command: MAP RN TEMP
- Synonym Names (SY=)
Command: MAP SY TEMP

You can use the MAP command with Synonym names and the CAS Registry Numbers at the same time. For example: MAP SYRN

Use the following Dialog DIALINDEX/OneSearch categories to search CAS Registry Numbers using RN=.

- CASREGNO: all files where CAS Registry Numbers can be searched
- RNCHEM: all chemical information
- RNMED: medical information

The MAP feature is available in two formats:

- Command mode
- Menu mode

Online Practice Exercises

Try some searches online to practice what you have learned.

1. What does the latest medical literature reveal about the therapeutic effect of CAS Registry Number 59-30-3 in the treatment of coronary heart disease? Hint: MAP all synonyms and include the HP= field. Use MEDTEXT to access fulltext medical journals.
2. Use the MAP command to locate fulltext medical articles that concern the use of Vitamin A with cancer.
3. Use the MAP command to find the latest information in New Scientist (File 369) concerning CAS RN 68-26-8 and eye sight.

Section 4: Applications

In this section you will learn to search for:

- Toxicity information
- Environmental information
- Patent information
- Analytical methods

Sometimes, the object of a search is simply to obtain the CAS Registry Number for a chemical substance, as discussed in Section 2. Usually, however, the object is to obtain information about a substance, such as toxicological information or environmental impact or a certain use of a chemical that has been patented.

Scientific and patent databases, available on Dialog, provide a virtual online library far exceeding any collection of information available in most academic or corporate libraries.

This section guides you through some sample searches in which the goal is to obtain information for chemical substances in the literature files on Dialog.

Application 1: Locating Toxicity Information

► **Topic** ◀ Where would you find information or any studies on the toxicological effects of hexamethonium?

Start in the DIALINDEX category RNLOOKUP to locate CAS Registry Numbers. RN LOOKUP contains the following files.

304	The Merck Index Online
336	Registry of Toxic Effects of Chemical Substances (RTECS)
390	Beilstein Online
398	CHEMSEARCH

Note: Files in the DIALINDEX category TOXICOL are good choices to find toxicity information.

*Using the
RNLOOKUP
OneSearch category
is an easy way to
find CAS Registry
Numbers and view
records in the
databases from this
category.*

*EXPAND on the
chemical name.*

*DISPLAY SETS
FROM EACH shows
the number of
records in each
database from the
RNLOOKUP
category.*

*TYPE the record
from File 336 by
appending the file
number to the TYPE
command.*

?B RNLOOKUP

SYSTEM:OS - DIALOG OneSearch

File 304:THE MERCK INDEX ONLINE(SM) /2001Q1
(c) 2001 MERCK & CO. INC.
File 336:RTECS 2001/Q1
Comp & dist by NIOSH,Intl Copyright All Rights Res
File 390:Beilstein Online
(c) Beilstein Chemiedaten und Software GmbH
File 398:CHEMSEARCH(TM) 1957-2002/Oct
(c) 2002 Amer.Chem.Soc.

Set Items Description
--- ----

?e na=hexamethonium

Ref	Items	Index-term
E1	1	NA=HEXAMETHONIUM CHLORIDE
E2	1	NA=HEXAMETHONE
E3	3	*NA=HEXAMETHONIUM
E4	1	NA=HEXAMETHONIUM ACETATE
E5	1	NA=HEXAMETHONIUM BENZOSULFONATE
E6	1	NA=HEXAMETHONIUM BIS(TRIBROMIDE)
E7	2	NA=HEXAMETHONIUM BITARTRATE
E8	5	NA=HEXAMETHONIUM BROMIDE
E9	1	NA=HEXAMETHONIUM BUTYRATE
E10	5	NA=HEXAMETHONIUM CHLORIDE
E11	1	NA=HEXAMETHONIUM CHLORIDE DIHYDRATE
E12	2	NA=HEXAMETHONIUM DIBROMIDE

Enter P or PAGE for more

?S E3

S1 3 NA='HEXAMETHONIUM'

?display sets from each

Set	File	Items	Description
	304	1	
	336	1	
	390	0	
	398	1	
S1		3	NA='HEXAMETHONIUM'

?T S1/9/1 FROM 336

1/9/2 (Item 1 from file: 336)
DIALOG(R)File 336:RTECS
Comp & dist by NIOSH, Intl Copyright All Rights Res. All
rts. reserv.

011326 RTECS Number: BQ8385000
Substance Name: Ammonium, hexamethylenebis(trimethyl-
CAS Registry Number: 60-26-4 Molecular Formula: C12H30N2
Molecular Weight: 202.44 Beilstein Registry Number: 1760389
Synonyms: Benzoexamethonium ; Bistrum ; Esametonio
(Italian) ;
Hexamethonium ; Hexane-1,6-bis(trimethylammonium) ;
1,6-Hexanediaminium, N,N,N,N',N',N'-hexamethyl- ;
Hexanium ; Hexon ; Hexonium

```

Compound Class: Drug
Wiswesser Line Notation: 1K1&1&6K1&1&1
Record Date: 199612

TOXICITY EFFECTS DATA:
* Oral Rat LD50 500 mg/kg ARZNAD 7,123,1957
* Intraperitoneal Rat LD50 230 mg/kg ARZNAD
7,123,1957
* Subcutaneous Rat LD50 165 mg/kg ARZNAD 7,123,1957
* Intravenous Rat LD50 35 mg/kg ARZNAD 7,123,1957
* Oral Mouse LD50 490 mg/kg PHTXA6 21,110,1958
Somnolence (general depressed activity) ;Antipsychotic
Intraperitoneal
Mouse LD50 137 mg/kg FRPSAX 8,317,1953
Somnolence (general depressed activity) ;Excitement
;Dyspnea
Subcutaneous Mouse LD50 83 mg/kg SIZSAR
6,362,1954
* Intravenous Mouse LD50 49 mg/kg PHTXA6
21,110,1958

TOXICITY EFFECTS JOURNAL REFERENCES:
ARZNAD Arzneimittel-Forschung. Drug Research. Editio
Cantor Verlag, Postfach 1255, W-7960 Aulendorf, Fed. Rep.
Ger. V.1- 1951-
FRPSAX Farmaco, Edizione Scientifica. Casella Postale
227, 27100 Pavia, Italy V.8-43]1953-88 For publisher
information, see FRMCE8
PHTXA6 Pharmacology and Toxicology. English translation
of FATOAO. New York, NY V.20-22, 1957-59. Discontinued.
SIZSAR Sapporo Igaku Zasshi. Sapporo Medical Journal.
Sapporo Igaku Daigaku, Nishi-17-chome, Minami-1-jo, Chuo-ku,
Sapporo 060, Japan V.3- 1952-

DATA PRESENT: Toxicity Effects

?MAP RN TEMP

1 Select Statement(s), 3 Search Term(s)
Serial#TD421

1 SearchSaves, 3 Search Term(s)

?BEGIN 156;EXS

File 156:ToxFile 1965-2002/Oct W4
(c) format only 2002 The Dialog Corporation

Set Items Description
--- ----
Executing TD421
0 RN=55-97-0
194 RN=60-26-4 (HEXAMETHONIUM)
0 RN=3343-60-0
S1 194 RN=55-97-0 + RN=60-26-4 + RN=3343-60-0

?S ((ADVERSE OR SIDE OR UNTOWARD)(1W)(REACTION? OR EFFECT?
OR EVENT? OR EXPERIENCE?) OR TOXIC? OR CONTRAINDICAT? OR
CONTRA(W)INDICAT? OR POISON? OR
CHEMICALLY(W)INDUC?)/TI,DE,ID

426997 ADVERSE/TI,DE,ID
6519 SIDE/TI,DE,ID

```

Use the MAP
command to extract
the CAS Registry
Number and save it
as a temporary
SearchSave.

BEGIN in ToxFile
(File 156) and
execute the
SearchSave to
retrieve all CAS
Registry Numbers.

Limit the search to
adverse effects
using keywords and
restrict to the
descriptor, title, and
identifier fields.

```

    99 UNTOWARD/TI,DE, ID
    45790 REACTION?/TI,DE, ID
    836627 EFFECT?/TI,DE, ID
    3312 EVENT?/TI,DE, ID
    9473 EXPERIENCE?/TI,DE, ID
    427185 ...
    212831 TOXIC?/TI,DE, ID
    1969 CONTRAINDICAT?/TI,DE, ID
    133 CONTRA/TI,DE, ID
    9085 INDICAT?/TI,DE, ID
    31 CONTRA/TI,DE, ID(W) INDICAT?/TI,DE, ID
    75095 POISON?/TI,DE, ID
    283000 CHEMICALLY/TI,DE, ID
    386366 INDUC?/TI,DE, ID
    282368 CHEMICALLY/TI,DE, ID(W) INDUC?/TI,DE, ID
S2 746914 ((ADVERSE OR SIDE OR UNTOWARD) (1W)
    (REACTION? OR EFFECT? OR EVENT? OR
    EXPERIENCE?) OR TOXIC? OR
    CONTRAINDICAT? OR CONTRA(W) INDICAT? OR
    POISON? OR CHEMICALLY(W) INDUC?)/TI,DE, ID
?S S1 AND S2
    194 S1
    746914 S2
S3 114 S1 AND S2

```

?T S3/6,K/1-10

3/6,K/1

DIALOG(R)File 156:(c) format only 2002 The Dialog Corporation. All rts. reserv.

03063745 21995413 PMID: 11998397

[Action of regulators of peripheral cholinergic processes on development of early arrhythmia in myocardial ischemic rats]

Vliianie regulatorov perifericheskikh kholinergicheskikh protsessov na razvitie rannikh aritmii u krys pri ishemii miokarda.
Jan-Mar 2002

Descriptors: Arrhythmia-- chemically induced -- CI; *Arrhythmia--prevention and control--PC; *Cholinergic Agents--pharmacology--PD; *Myocardial Ischemia--complications--CO...; Myocardial Ischemia--physiopathology--PP; Neostigmine--pharmacology--PD; Nicotine--pharmacology--PD; Oxyphenonium--pharmacology--PD; Rats; Tachycardia-- chemically induced --CI; Ventricular Fibrillation-- chemically induced --CI
...CAS Registry No.: 84-7 (Oxyphenonium); 51-84-3 (Acetylcholine); 54-11-5 (Nicotine); 59-99-4 (Neostigmine); 60-26-4 (Hexamethonium) ; 60-30-0 (pentamine)

3/6,K/2

DIALOG(R)File 156:(c) format only 2002 The Dialog Corporation. All rts. reserv.

03058420 21859739 PMID: 11870258

Protecting research subjects--the crisis at Johns Hopkins.
Feb 28 2002

Descriptors: Asthma--physiopathology--PP; *Clinical Trials--standards--ST ; *Ganglionic Blockers-- adverse effects --AE; *Hexamethonium-- adverse effects --AE; *Human Experimentation
CAS Registry No.: 0 (Ganglionic Blockers); 60-26-4 (Hexamethonium)

?T S3/9/2

TYPE a record in
FULL format
(Format 9).

Note the article was a publicized case resulting in the death of a research subject.

```

3/9/2
DIALOG(R)File 156:ToxFile
(c) format only 2002 The Dialog Corporation. All rts.
reserv.

03058420 21859739 PMID: 11870258
Protecting research subjects--the crisis at Johns Hopkins.
Steinbrook Robert
New England journal of medicine (United States) Feb 28
2002, 346 (9) p716-20, ISSN 1533-4406 Journal Code:
0255562
Comment in N Engl J Med. 2002 Jun 27;346(26) 2093-5;
discussion 2093-5; Comment in PMID 12088026; Comment
in N Engl J Med. 2002 Jun 27;346(26):2093-5;
discussion 2093-5; Comment in PMID 12088027; Comment in N
Engl J Med. 2002 Jun 27;346(26):2093-5; discussion 2093-
5; Comment in PMID 12087152; Erratum in N Engl J Med 2002
May 23;346(21):1678
Document type: Journal Article
Languages: ENGLISH
Main Citation Owner: NLM
Record type: Completed
Subfile: Toxbib ; AIM; INDEX MEDICUS
Tags: Case Report; Female; Human
Descriptors: *Asthma--physiopathology--PP; *Clinical
Trials--standards --ST; *Ganglionic Blockers--adverse
effects--AE; *Hexamethonium--adverse effects--AE; *Human
Experimentation; Academic Medical Centers; Adult;
Baltimore; Ethics Committees, Research; Fatal
Outcome; Financing,
Government; Ganglionic Blockers--pharmacology--PD;
Hexamethonium --pharmacology--PD; Human
Experimentation--economics--EC; Human Experimentation--
legislation and jurisprudence--LJ; National Institutes of
Health (U.S.); Research Support; United States; United
States Food and Drug Administration
CAS Registry No.: 0 (Ganglionic Blockers); 60-26-4
(Hexamethonium)
Record Date Created: 20020228
    
```

Application 2: Finding Environmental Information

The RANK Command

The RANK command allows you to perform trend or statistical analysis on an existing search set. To use this command, simply enter RANK <field> (RANK PA (Patent Assignee). The Dialog system then extracts terms from the specified field in a set of records and lists them in ranked order, with the most highly posted term appearing first. Once a term is ranked, the top eight terms are automatically listed—you can use this unique Dialog browse feature to view additional terms. Each ranked term is also assigned a “Rank number” that can be used to save a term for later use, thus providing assistance in exploring your search topic fully.

Applications

The RANK command is designed to work in most phrase-indexed Additional Index fields, most numeric additional Index fields, and with phrase-indexed Descriptor (DE) and Identifier (ID) Basic Index fields. Plus, RANK works with all MAP fields. Some of the many key applications for RANK include:

- Competitive analysis
- Market analysis
- Expert identification
- Patent analysis
- Search improvement

► **Topic** ◀ Find articles discussing ozone depletion and the stratosphere.

EXPAND on the chemical name in order to retrieve the registry numbers.

```
?B 398
File 398:CHEMSEARCH(TM) 1957-2002/Oct
(c) 2002 Amer.Chem.Soc.

Set  Items  Description
---  ----  -
?e na=ozone

Ref  Items  Index-term
E1   1      NA=OZOLAN BROWN 7RL
E2   3      NA=OZOLINONE
E3   1      *NA=OZONE
E4   1      NA=OZONE (O2170)
E5   1      NA=OZONE (O2180)
E6   1      NA=OZONE (O3)
E7   1      NA=OZONE (160160170)
E8   1      NA=OZONE (160160180)
E9   1      NA=OZONE (160170160)
E10  1      NA=OZONE (160170180)
E11  1      NA=OZONE (160180160)
E12  1      NA=OZONE (170180180)

Enter P or PAGE for more

?S E3
```

MAP the registry numbers for ozone.

Execute the SearchSave containing the registry numbers

Add keywords to limit the search and combine sets.

To narrow the search further, use the (L) connector to link the registry numbers to the stratosphere descriptor.

```

      S1      1  NA='OZONE'
?MAP RN T

1 Select Statement(s), 3 Search Term(s)
Serial#TD436

1 SearchSaves, 3 Search Term(s)
?B 314;EXS

File 314:CA SEARCH(R) 1997-2002/UD=13720
(c) 2002 American Chemical Society

      Set  Items  Description
      ---  -
Executing TD436
      16263  RN=10028-15-6
           0  RN=74087-86-8
           0  RN=412908-40-8
      S1  16263  RN=10028-15-6 + RN=74087-86-8 + RN=412908-
40-8

?S STRATOSPHERE?
      S2      2086  STRATOSPHERE?

?S S1 AND S2
           16263  S1
           2086  S2
      S3      1150  S1 AND S2

?S S1(L)S2 AND DEPLET?/TI,DE
           16263  S1/DE
           2025  S2/DE
           354  S1/DE(L)S2/DE
           5987  DEPLET?/TI,DE
      S4      145  S1(L)S2 AND DEPLET?/TI,DE

?T S4/3/1-2

4/3/1
DIALOG(R)File 314:CA SEARCH(R)
(c) 2002 American Chemical Society. All rts. reserv.

137297665  CA: 137(20)297665r  JOURNAL
Phase diagram of the nitric acid/water system: Implications
for polar stratospheric clouds
AUTHOR(S): Beyer, Keith D.; Hansen, Anne R.
LOCATION: Department of Chemistry, Wisconsin Lutheran
College, Milwaukee, WI, 53226, USA
JOURNAL: J. Phys. Chem. A (Journal of Physical Chemistry
A) DATE: 2002
VOLUME: 106 NUMBER: 43 PAGES: 10275-10284 CODEN: JPCAFH
ISSN: 1089-5639 PUBLISHER ITEM IDENTIFIER: 1089-
5639(02)05535-4 LANGUAGE: English PUBLISHER: American
Chemical Society

4/3/2
DIALOG(R)File 314:CA SEARCH(R)
(c) 2002 American Chemical Society. All rts. reserv.

```

The command
RANK DE
instructs the
system to count
the individual
occurrences of
each descriptor,
and then sort by
the number of
times each occurs
in the last set.

Number 4 in the
ranked list is about
ozone in the
atmosphere.
Choose the item
number(s) of
interest; then EXIT
the RANK menu,
making sure to
save all items you
want.

```
137297664 CA: 137(20)297664q JOURNAL
Laboratory Evidence for Surface Nucleation of Solid Polar
Stratospheric Cloud Particles
AUTHOR(S): Tabazadeh, A.; Djikaev, Y. S.; Hamill, P.;
Reiss, H.
LOCATION: NASA Ames Research Center, Moffett Field, CA,
94035, USA
JOURNAL: J. Phys. Chem. A (Journal of Physical Chemistry
A) DATE: 2002
VOLUME: 106 NUMBER: 43 PAGES: 10238-10246 CODEN: JPCAFH
ISSN: 1089-5639 PUBLISHER ITEM IDENTIFIER: 1089-
5639(02)01045-9 LANGUAGE: English PUBLISHER: American
Chemical Society
```

?RANK DE

```
Started processing RANK
..Ranking 100 of 145 records
Completed Ranking 145 records
DIALOG RANK Results
```

```
-----
RANK: S4/1-145 Field: /DE File(s): 314
(Rank fields found in 145 records -- 103 unique terms)Page 1
of 13
```

RANK No.	Items	Term
1	138	STRATOSPHERE
2	70	ATMOSPHERIC AEROSOLS
3	44	ICE
4	43	ATMOSPHERIC OZONE
5	39	CLOUDS
6	31	ATMOSPHERE (EARTH)
7	26	TROPOSPHERE
8	24	AIR POLLUTION

```
P = next page Pn = Jump to page n
P- = previous page M = More Options Exit = Leave RANK
```

To view records from RANK, enter VIEW followed by RANK
number, format, and item(s) to display, e.g., VIEW 2/9/ALL.

Enter desired option(s) or enter RANK number(s) to save
terms.

?4

```
RANK numbers saved: 4
```

```
DIALOG RANK Results
```

```
-----
RANK: S4/1-145 Field: /DE File(s): 314
(Rank fields found in 145 records -- 103 unique terms)Page 1
of 13
```

RANK No.	Items	Term
1	138	STRATOSPHERE
2	70	ATMOSPHERIC AEROSOLS
3	44	ICE
4	43	ATMOSPHERIC OZONE
5	39	CLOUDS
6	31	ATMOSPHERE (EARTH)
7	26	TROPOSPHERE
8	24	AIR POLLUTION

```
P = next page Pn = Jump to page n
```

EXECUTE the search saved with RANK; then type out a few titles to determine the relevance of the search.

```
P- = previous page  M = More Options      Exit = Leave RANK

To view records from RANK, enter VIEW followed by RANK
number,
format, and item(s) to display, e.g., VIEW 2/9/ALL.

Enter desired option(s) or enter RANK number(s) to save
terms.
?exit

RANK results will be erased; have you saved all the terms of
interest?
(YES/NO)
?Y

Creating temporary SearchSave ... TD437

Enter EXS to execute the SearchSave

?EXS
Executing TD437
   S5      662  "ATMOSPHERIC OZONE"/DE

?T S5/6/1-3

   5/6/1
DIALOG(R)File 314:(c) 2002 American Chemical Society. All
rts. reserv.

   Indoor ozone/terpene reactions as a source of indoor
particles

   5/6/2
DIALOG(R)File 314:(c) 2002 American Chemical Society. All
rts. reserv.
   Influence of biomass combustion emissions on the
distribution of acidic trace gases over the Southern Pacific
basin during austral springtime

   5/6/3
DIALOG(R)File 314:(c) 2002 American Chemical Society. All
rts. reserv.

   Assimilation of total ozone satellite measurements in a
three-dimensional tracer transport model
```

The RANK command in this example provides additional search terms and identifies the ones that are used most for given concepts.

Application 3: Locating Patent Information

To augment scientific literature searches, researchers also search and review patents, a rich source of technical information, since approximately 75% of all technical discoveries are published as patents rather than in peer-reviewed scientific literature.

Many of the records in CA SEARCH reference patents from up to 40 countries. It is a simple matter to search using Registry Numbers and then use the Dialog limit capability to restrict the retrieval to patents. Only the first publication of the patent is referenced. The MAP command enables you to extract the patent number from a set of records. Then, it is easy to find the same patents in a file that gives more information such as CLAIMS[®]/U.S. Patents Abstracts or Derwent World Patents Index.

► **Topic** ◀ Locate patents that involve Zestril. Name the companies that own these patents. Create a tabular report.

```
?B 398

File 398:CHEMSEARCH(TM) 1957-2002/Oct
      (c) 2002 Amer.Chem.Soc.

      Set  Items  Description
      ---  ----  -
?e na=zestril

Ref  Items  Index-term
E1   1      NA=ZESTORETIC
E2   1      NA=ZESTOVER
E3   1      *NA=ZESTRIL
E4   1      NA=ZESTRON
E5   1      NA=ZESTRON LP
E6   1      NA=ZESTRON VD 200
E7   1      NA=ZESTY PC 24219
E8   1      NA=ZET-GE KOAG H 312W
E9   1      NA=ZET-GE KOAG H 525
E10  1      NA=ZETA B
E11  1      NA=ZETA HC
E12  1      NA=ZETA HLC BOND

      Enter P or PAGE for more

?S E3
      S1          1  NA='ZESTRIL'

?MAP SYRN T

3 Select Statement(s), 28 Search Term(s)
Serial#TD423

1 SearchSaves, 28 Search Term(s)

?B 399

File 399:CA SEARCH(R) 1967-2002/UD=13720
      (c) 2002 American Chemical Society

      Set  Items  Description
      ---  ----  -
```

*MAP synonyms
and registry
numbers to create
a temporary
SearchSave.*

*Execute the
SearchSave in CA
Search (File 399)
to retrieve
chemical literature
records.*

Limit the search to patent records only using /PAT.

Now, MAP patent numbers from the last set.

BEGIN in Derwent World Patents Index (File 351) to find equivalents to the patents found in the SearchSave. You will find comprehensive, well-written abstracts.

```
?EXS
Executing TD423
. . . . .
          0  LINVAS
          0  LIPRIL
         425 LISINOPRIL
          0  LISIPRIL
          0  LISORIL
          0  LISPRIL
          0  LISTRIL
        3048 MK
         139 521
           7 MK(W)521
        3048 MK
         130 522
          0  MK(W)522
          0  NOPERTEN
         207 NOVATEC
          0  PRESITEN
          0  PRINIL
           1 PRINIVIL
          0  PRINVIL
        S1   636 ACERBON + ALAPRIL + CARACE + CIPRAL +
                CIPRIL + CORIC + INOPRIL + LINOPRIL +
                LINVAS + LIPRIL + LISINOPRIL + LISIPRIL
                + LISORIL + LISPRIL + LISTRIL + MK()521 +
                MK()522 + NOPERTEN + NOVATEC + PRESITEN +
                PRINIL + PRINIVIL + PRINVIL
          0  TENSOPRIL
          0  TENSYN
          0  VIVATEC
          0  ZESTRIL
         897 RN=76547-98-3
        S2   897 TENSOPRIL + TENSYN + VIVATEC + ZESTRIL +
                RN=76547-98-3
        S3  1116 S1:S2

?S S3/PAT
        S4   445 S3/PAT

?MAP PN T
Processing MAP
Processing MAP
Processing MAP
. . . . .

46 Select Statement(s), 605 Search Term(s)
Serial#TD424

1 SearchSaves, 605 Search Term(s)

?B 351;EXS
File 351:Derwent WPI 1963-2002/UD,UM &UP=200272
          (c) 2002 Thomson Derwent

          Set  Items  Description
          ---  ----  -
Executing TD424
          0  PN=JP 86127743
          1  PN=JP 61127743
          0  PN=JP 86205127
          1  PN=JP 61205127
```

Use the RANK command to identify who owns the most patents involving Zestril. The PANAME field includes only patent assignee names.

The RANK command will sort the records by patent assignee name and count the number of records for each owner.

```

0 PN=JP 87127351
1 PN=JP 62127351
0 PN=JP 8899253
0 PN=JP 88099253
1 PN=JP 63099253
0 PN=JP 89121297
1 PN=JP 1121297
0 PN=JP 89121298
1 PN=JP 1121298
S1      6 PN=(JP 86127743 + JP 61127743) +
          PN=(JP 86205127 + JP 61205127) + PN=(JP
          87127351 + JP 62127351) + PN=(JP
          8899253 + JP 88099253 + JP 63099253)
          + PN=(JP 89121297 + JP 1121297) +
          PN=(JP 89121298 + JP 1121298)
0 PN=JP 89126375
1 PN=JP 1126375
0 PN=JP 8982931
0 PN=JP 89082931
1 PN=JP 1082931
0 PN=JP 8982932
0 PN=JP 89082932
1 PN=JP 1082932
0 PN=JP 94287401
1 PN=JP 6287401
0 PN=JP 94287814
1 PN=JP 6287814
1 PN=JP 9503525
0 PN=JP 95003525
1 PN=JP 7003525
S2      7 PN=(JP 89126375 + JP 1126375) + PN=(JP
          8982931 + JP 89082931 + JP 1082931) +
          PN=(JP 8982932 + JP 89082932 + JP
          1082932) + PN=(JP 94287401 +
          JP 6287401) + PN=(JP 94287814 + JP
          6287814) + PN=(JP 9503525 + JP 95003525
          + JP 7003525)
. . . . .
1 PN=WO 9936062
1 PN=WO 9937290
1 PN=WO 9965500
S45     1 PN=ZA 8303161
        10 PN=WO 9915643 + PN=WO 9920260 + PN=WO
           9923064 + PN=WO 9925374 + PN=WO 9930690 +
           PN=WO 9932150 + PN=WO 9936062 + PN=WO
           9937290 + PN=WO 9965500 + PN=ZA 8303161
S46     368 S1:S45
?RANK S46 PANAME
Started processing RANK
...Ranking 100 of 368 records
...Ranking 200 of 368 records
..Ranking 300 of 368 records
Completed Ranking 368 records
DIALOG RANK Results
-----
RANK: S46/1-368 Field: PANAME= File(s): 351
(Rank fields found in 368 records -- 308 unique terms)Page 1
of 39

RANK No.  Items  Term
-----  -

```

EXIT from the RANK menu to continue searching.

```
1      23  SQUIBB & SONS INC E R
2      22  MERCK & CO INC
3      16  SEKISUI CHEM IND CO LTD
4      15  MITSUBISHI CHEM CORP
5      15  NIPPON POLYCHEM KK
6      11  JAPAN POLYCHEM CORP
7      9   ALZA CORP
8      8   BRISTOL-MYERS SQUIBB CO
P = next page      Pn = Jump to page n
P- = previous page M = More Options      Exit = Leave RANK

To view records from RANK, enter VIEW followed by RANK
number, format, and item(s) to display, e.g., VIEW 2/9/ALL.

Enter desired option(s) or enter RANK number(s) to save
terms.
?exit
```

Patents as Technical Documents

► **Topic** ◀ What is the US patent classification code for a primary alkaline battery utilizing manganese dioxide as its cathode? Who has the most patents in the area of alkaline MnO_2 ?

Conduct the search in File 304 for the chemical manganese dioxide.

TYPE out the record to verify its contents.

```
?b 304
File 304:THE MERCK INDEX ONLINE(SM) /2001Q1
(c) 2001 MERCK & CO. INC.

Set  Items  Description
---  -
?e na=manganese dioxide

Ref  Items  Index-term
E1      1  NA=MANGANESE DIFLUORIDE TETRAHYDRATE
E2      1  NA=MANGANESE DIIODIDE
E3      1  *NA=MANGANESE DIOXIDE
E4      1  NA=MANGANESE DIPYRIDOXAL DIPHOSPHATE
E5      1  NA=MANGANESE ETHYLENEBIS (DITHIOCARBAMATE)
(POLYME
E6      1  NA=MANGANESE FLUORIDE
E7      1  NA=MANGANESE GREEN
E8      1  NA=MANGANESE HYPOPHOSPHITE
E9      1  NA=MANGANESE HYPOPHOSPHITE MONOHYDRATE
E10     1  NA=MANGANESE IODIDE
E11     1  NA=MANGANESE IODIDE TETRAHYDRATE
E12     1  NA=MANGANESE MONOSULFIDE

Enter P or PAGE for more
?S E3
      S1      1  NA='MANGANESE DIOXIDE'
?T S1/9

1/9/1
DIALOG(R)File 304:THE MERCK INDEX ONLINE(SM)
(c) 2001 MERCK & CO. INC. All rts. reserv.
05770 Monograph Name: Manganese Dioxide
CAS REGISTRY NUMBER: 1313-13-9
MOLECULAR FORMULA: MnO2 MOLECULAR WEIGHT: 86.94
MOLECULAR COMPOSITION: Mn 63.19%, O 36.81%
SYNONYMS:
Manganese binoxide; manganese peroxide; manganese
superoxide; black manganese oxide
LITERATURE REFERENCES:
Occurs in nature as the mineral pyrolusite, or made
artificially (pptd). The native product is heavy, steel-gray
when in lumps, black when powdered; the pptd product is a
brownish-black, fine powder. Both usually contain some Mn3O4
and some water. When ignited evolves oxygen, leaving Mn3O4.
Lab prepn: Moore et al., J. Am. Chem. Soc. 72, 856 (1950);
Covington et al., Trans. Faraday Soc. 58, 1975
```

Use the MAP command to extract the registry numbers (RN) from the previous record.

Execute the SearchSave in CA SEARCH (File 399).

Limit the search to patent documents only using /PAT.

Limit the search using keywords in the Identifier, Descriptor and/or Title fields.

Note limited truncation to pick up one extra letter (e.g., cell?).

(1962). Toxicity study: D. J. Holbrook, Jr. et al., Environ. Health Perspect. 10, 95 (1975). Review of use as reagent: J. S. Pizey, Synthetic Reagents vol. 2 (John Wiley, New York, 1974) pp 143-174.

PHYSICAL DATA:

Tetragonal crystals (rutile structure). Insol in water, nitric or cold sulfuric acid. Slowly dissolves in cold HCl with evolution of Cl₂; in presence of hydrogen peroxide or oxalic acid it dissolves in dil H₂SO₄ or HNO₃. Strong oxidizer; should not be heated or rubbed with organic matter or other oxidizable substances, e.g., sulfur, sulfides, phosphides, hypophosphites, etc. LD50 orally in rats: > 40 mmole/kg (Holbrook).

PHYSICAL DATA:

LD50: LD50 orally in rats: > 40 mmole/kg (Holbrook)
 USE: The mineral is the source of manganese and all its compds; largely used in manuf manganese steel; oxidizer; in alkaline batteries (dry cells); for making amethyst glass, decolorizing glass; painting on porcelain, faience and majolica. The ppt is used in electrotechnics, pigments, browning gun barrels, drier for paints and varnishes, printing and dyeing textiles.

REFERENCE KEYS PRESENT: Prepn; Review; Toxicity; Use
 DATA KEYS PRESENT: Molecular weight; Uses; Lethal dose

?MAP RN T

1 Select Statement(s), 1 Search Term(s)
 Serial#TD425

1 SearchSaves, 1 Search Term(s)

?B 399

File 399:CA SEARCH(R) 1967-2002/UD=13720
 (c) 2002 American Chemical Society

Set	Items	Description
---	-----	-----

?EXS

Executing	TD425	
S1	17414	RN=1313-13-9 (SEE ?IGNOTE)

?S S1/PAT

S2	9309	S1/PAT
----	------	--------

?S S2 AND CATHODE/ID,DE AND (BATTER? OR CELL? ?)/ID,DE

	9309	S2
	47689	CATHODE/ID,DE
	78999	BATTER?/ID,DE
	921107	CELL? ?/ID,DE
S3	1592	S2 AND CATHODE/ID,DE AND (BATTER? OR CELL? ?)/ID,DE

?s S3 AND (primary OR nonrecharg? OR non()recharg?)/ti,de,id

	1592	S3
	77396	PRIMARY/TI,DE, ID
	0	NONRECHARG?/TI,DE, ID
	163844	NON/TI,DE, ID
	4324	RECHARG?/TI,DE, ID
	1	NON/TI,DE, ID (W) RECHARG?/TI,DE, ID
S4	456	S3 AND (PRIMARY OR NONRECHARG? OR NON() RECHARG?)/TI,DE, ID

When you have a manageable number of records, RANK by U.S. classification code (CL).

Note that the main class code is HO1M-004.

EXIT the RANK menu and save any terms of interest.

RANK the patent assignee name to retrieve a list of companies involved with this type of battery.

```
?RANK CL
Started processing RANK
...Ranking 100 of 456 records
...Ranking 200 of 456 records
...Ranking 300 of 456 records
...Ranking 400 of 456 records
Completed Ranking 456 records
DIALOG RANK Results
-----
RANK: S4/1-456   Field: CL=   File(s): 399
(Rank fields found in 455 records -- 181 unique terms) Page 1
of 23

RANK No.  Items  Term
-----  -
      1      75  H01M-004/06
      2      48  H01M-004/50
      3      39  H01M-006/16
      4      36  H01M-004/50A
      5      35  H01M-004/62
      6      34  H01M-004/06B
      7      27  H01M-004/08
      8      24  H01M-004/50B
P = next page          Pn = Jump to page n
P- = previous page    M = More Options          Exit = Leave RANK

To view records from RANK, enter VIEW followed by RANK
number, format, and item(s) to display, e.g., VIEW 2/9/ALL.

Enter desired option(s) or enter RANK number(s) to save
terms.
?exit
RANK results will be erased; have you saved all the terms of
interest?
(YES/NO)

?Y
Exiting rank... (no terms were saved)

?RANK PA
Started processing RANK
...Ranking 100 of 456 records
...Ranking 200 of 456 records
...Ranking 300 of 456 records
...Ranking 400 of 456 records
Completed Ranking 456 records
DIALOG RANK Results
-----
RANK: S4/1-456   Field: PA=   File(s): 399
(Rank fields found in 448 records -- 98 unique terms) Page 1
of 13
```

RANK No.	Items	Term
1	88	MATSUSHITA ELECTRIC INDUSTRIAL CO., LTD.
2	45	TOSHIBA BATTERY CO., LTD.
3	44	SANYO ELECTRIC CO., LTD.
4	25	HITACHI MAXELL, LTD.
5	19	DAINI SEIKOSHA CO., LTD.
6	19	SEIKO INSTRUMENTS AND ELECTRONICS, LTD.
7	15	FUJI ELECTROCHEMICAL CO., LTD.
8	11	DURACELL INC.

Section 4: Applications

Files	Freq Update	Abs-tracts	Claims	Full text	Images	Countries	Early Dates	Fam. Data	Legal Status	Cited Pat/Ref	Citing Info	Class Codes	CAS RNs	Alerts
Derwent World Patents Index (Files 351/352)	W	•	• (1)		•	41	1963	•		• (2)		IPC		W
Derwent Patents Citation Index (File 342)	W					6	1973	•		•	•	IPC		W
CLAIMS/U.S. Patents (File 340)	W	•	•			U.S.	1950	•		•		US, IPC	• (3)	
U.S. Patents Fulltext (Files 652, 654)	W	•	•	•	•	U.S.	1971 (4)	•	•	•	•	US, IPC		W (5)
European Patents Fulltext (File 348)	W	•	• (6)	• (7)	•	EPO (8)	1978		•	•		IPC		W
WIPO/PCT Patents Fulltext (File 349)	1-2 d	•	•	• (14)	•	115	1983		•			IPC		W
INPADOC/Family and Legal Status (File 345)	W					71	1968	•	•			IPC, US		W & M
JAPIO (File 347)	M	•				Japan	1976	•	•			IPC		M
Chinese Patent Abstracts (File 344)	M	•				China	1985	•				IPC		M
CLAIMS/Current Patent Legal Status (File 123)	W		• (9)			U.S.	1980	•						W & M
Claims/citation (Files 220-222)	Q					U.S.	1790			• (12)	• (12)			
CLAIMS/Compound Registry (File 242)	A													
CLAIMS/Reference (File 124)	Q					U.S.						US		
Ei EnCompassPat™ (File 353)	M	• (10)				31	1964					IPC	•	
IMS Patents Focus (File 447)	M	•				64	1955	• (11)					•	M
CA Search:Chemical Abstracts (File 399)	W	•			•		1967						•	M (13)
French Patents (File 371)	W				• (15)	France	1966		•			IPC		W
LitAlert (File 670)	W			•		U.S.	1970							W

1 US_IP_Derwent adds as abstracts the examined

2 WO and IP only; 1978-1997

3 Updated through 1978

4 Selective coverage from 1971 to 1973 only

5 File 654 only

6 Beginning in 1986 for A documents

7 Beginning in 1991 for B documents

8 Member countries to the EPO

9 Reexamination claims only

10 Searchable, but displayable to subscribers

11 Limited patent family information

12 Not searchable

13 Biweekly

14 Fulltext in English (71%), French (5%), German (15%), Spanish (.05%)

15 Images from 1978 forward

Application 4: Analytical Methods

Analytical methods have to be developed to separate and characterize the target molecule and to monitor the quality control of its production.

► **Topic** ◀ Use CHEMSEARCH (File 398) to locate the CAS Registry number for Taxol. Use the MAP command for subsequent searches.

*SELECT Taxol,
Taxol A and Taxol
B from the
expanded list.*

*Page down (P) to
see further entries.*

*Combine sets
using the OR
operator.*

```
?B 398

File 398:CHEMSEARCH(TM) 1957-2002/Oct
      (c) 2002 Amer.Chem.Soc.

Set  Items  Description
---  -
?e na=taxol

Ref  Items  Index-term
E1   2      NA=TAXODONE
E2   1      NA=TAXODONE, (+) -
E3   1      *NA=TAXOL
E4   1      NA=TAXOL A
E5   1      NA=TAXOL A .ALPHA.-(CHLOROMETHYL CARBONATE), 4-ET
E6   1      NA=TAXOL A TRIHYDRATE
E7   1      NA=TAXOL A 2'-(CHLOROACETATE)
E8   1      NA=TAXOL A 7-BENZOATE
E9   1      NA=TAXOL A 7-BENZOATE 2'-(CHLOROACETATE)
E10  1      NA=TAXOL A-CINCHONINE MIXT.
E11  1      NA=TAXOL A, .ALPHA.-ETHER WITH .ALPHA.-HYDRO-.OME
E12  1      NA=TAXOL A, .ALPHA.,4-DIETHER WITH .ALPHA.-HYDRO-

Enter P or PAGE for more

?S E3:E4
S1           1  NA='TAXOL':NA='TAXOL A'

?P
Ref  Items  Index-term
E13  1      NA=TAXOL A, 4-ETHER WITH .ALPHA.-HYDRO-.OMEGA.-HY
E14  1      NA=TAXOL B
E15  1      NA=TAXOL C
E16  1      NA=TAXOL C 7-XYLOSIDE
E17  1      NA=TAXOL D
E18  1      NA=TAXOL 2'-(2-HYDROXYETHYL SUCCINATE)
E19  1      NA=TAXOL 2'-CARBAMATE
E20  1      NA=TAXOL 7-CARBAZATE
E21  1      NA=TAXOL-3'-14C
E22  1      NA=TAXOL-7-XYLOSIDE
E23  1      NA=TAXOLEIC ACID
E24  1      NA=TAXOLENE

Enter P or PAGE for more

?S E14
S2           1  NA='TAXOL B'

?S S1 OR S2
           1  S1
```

Note: /FF is used here to combine records to the minimal number since some CAS Replaced Registry Numbers have their own records. This is particularly useful for Polymer records.

```

          1  S2
S3        2  S1 OR S2

?S S3/FF
          2  S3/FF
S4

?T S4/9/ALL

4/9/1
DIALOG(R) File 398:CHEMSEARCH(TM)
(c) 2002 Amer.Chem.Soc. All rts. reserv.

CAS REGISTRY NUMBER: 71610-00-9
MOLECULAR FORMULA: C45H53NO14
RING SYSTEM DATA:
(02) (nr=01; sr=6; ar= fr=C6.01; ir=46-150-18)
(01) (nr=04; sr=4,6,6,8; ar=C30.01-C6.02-C8.01;
fr=OC3.01-C6.02-C8.01; ir=4462-1-1)
CA NAME(S):
HP=Benzenepropanoic acid (9CI)
SB=.alpha.-hydroxy-.beta.-((2E)-2-methyl-1-oxo-2-
butenyl)amino)-
NM=(2aR,4S,4aS,6R,9S,11S,12S,12aR,12bS)-6,12b-
bis(acetyloxy)-12-
(benzoyloxy)2a,3,4,4a,5,6,9,10,11,
12,12a,12b-dodecahydro-4,11-dihydroxy-4a,8,13,13-
tetramethyl-5-oxo-7,11-methano-1H-cyclodeca(3,4)
benz(1,2-b)oxet-9-yl ester
ST=(.alpha.R,.beta.S)-
HP=Benzenepropanoic acid
SB=.alpha.-hydroxy-.beta.-((2-methyl-1-oxo-2-
butenyl)amino)-
NM=6,12b-bis(acetyloxy)-12-(benzoyloxy)-
2a,3,4,4a,5,6,9,10,11,12,12a,12b-dodecahydro-4,11-dihydroxy-
4a,8,13,13-tetramethyl-5-oxo-7,11-methano-1H cyclodeca(3,4)
benz(1,2-b)oxet-9-yl ester
ST=(2aR-(2a.alpha.,4.beta.,4a.beta.,6.beta.,9.alpha.
(.alpha.R*,.beta
.S*(E)),11.alpha.,12.alpha.,12a.alpha.,12b.alpha.))-
OTHER CA NAMES:
HP=7,11-Methano-1H-cyclodeca(3,4)benz(1,2-b)oxete
NM=benzenepropanoic acid deriv.
SYNONYMS: Cephalomannine; Taxol B
SUBFILE: CHEMNAME          275 LITERATURE REFERENCE(S) IN FILE
399.
LAST UPDATE: 199808

4/9/2
DIALOG(R) File 398:CHEMSEARCH(TM)
(c) 2002 Amer.Chem.Soc. All rts. reserv.

CAS REGISTRY NUMBER: 33069-62-4
MOLECULAR FORMULA: C47H51NO14
RING SYSTEM DATA:
(03) (nr=01; sr=6; ar= fr=C6.01; ir=46-150-18)
(nr=04; sr=4,6,6,8; ar=C30.01-C6.02-C8.01; fr=OC3.01-
C6.02-C8.01; ir=4462-1-1)
CA NAME(S):
HP=Benzenepropanoic acid (9CI)
SB=.beta.-(benzoylamino)-.alpha.-hydroxy-
NM=(2aR,4S,4aS,6R,9S,11S,12S,12aR,12bS)-6,12b-bis
(acetyloxy)-12-(benzoyloxy)-2a,3,4,4a,5,6,9,10,

```

Note: This is an example of mapping CAS Registry Numbers and synonyms from an entire set.

Use RECALL and the SearchSave number to view a list of the MAPed registry numbers and synonyms.

You can append "P" (for Preparative) in CA SEARCH, File 399, only.

```

11,12,12a,12b-dodecahydro-4,11-dihydroxy-
4a,8,13,13-tetramethyl-5-oxo-7,11-methano-1H-
cyclodeca(3,4)benz (1,2-b)oxet-9-yl ester
ST=(.alpha.R,.beta.S)-
HP=Tax-11-en-9-one (8CI)
SB=5.beta.,20-epoxy-1,2.alpha.,4,7.beta.,10.beta.,
13.alpha.-hexahydroxy-
NM=4,10-diacetate 2-benzoate 13-ester with
(2R,3S)-N-benzoyl-3-phenylisoserine

OTHER CA NAMES:
HP=Benzenepropanoic acid
SB=.beta.-(benzoylamino)-.alpha.-hydroxy-
NM=6,12b-bis(acetyloxy)-12-(benzoyloxy)-
2a,3,4,4a,5,6,9,10,11,12,12a,12b-dodecahydro-4,11-dihydroxy-
4a,8,13,13-tetramethyl-5-oxo-7,11-methano-1H-
cyclodeca(3,4)benz (1,2-b)oxet-9-yl ester
ST=(2aR-(2a.alpha.,4.beta.,4a.beta.,6.beta.,9.alpha.
(.alpha.R*,.beta.S*)),11.alpha.,12.alpha.,12a.alpha.,
12b.alpha.))-
HP=7,11-Methano-1H-cyclodeca(3,4)benz(1,2-b)oxete
NM=benzenepropanoic acid deriv.
SYNONYMS: ABI 007; BMS 181339-01; NSC 125973; Paclitaxel;
Plaxicel; Taxol; Taxol A; Yewtaxan
SUBFILE: CHEMNAME 6485 LITERATURE REFERENCE(S) IN
FILE 399.
LAST UPDATE: 200208

?MAP RN T S4

1 Select Statement(s), 2 Search Term(s)
Serial#TD429

1 SearchSaves, 2 Search Term(s)

?RECALL TD429

Line Command
-----
1. S RN=33069-62-4 + RN=71610-00-9
Note: To view an address, enter RECALL ADDRESS <name>

?MAP SY T S4

1 Select Statement(s), 10 Search Term(s)
Serial#TD430

1 SearchSaves, 10 Search Term(s)

?RECALL TD430

Line Command
-----
1. S ABI()007 + BMS()181339()01 + CEPHALOMANNINE +
NSC()125973 +
PACLITAXEL + PLAXICEL + TAXOL + TAXOL()A + TAXOL()B +
YEW TAXAN
Note: To view an address, enter RECALL ADDRESS <name>

?MAP RN T S4/"P"

1 Select Statement(s), 2 Search Term(s)
Serial#TD435

```

EXECUTE
mapped data from
the previous
search to retrieve
the registry

Use the (S)
proximity operator.
The (L) proximity
operator may also
be used since
Registry Numbers
are only found in
the Descriptor
fields in this
database.

TYPE a few
records to check
relevancy.

```

1 SearchSaves, 2 Search Term(s)

?RECALL TD435

Line Command
-----
1. S RN=33069-62-4P + RN=71610-00-9P
Note: To view an address, enter RECALL ADDRESS <name>

?B 399;EXS TD429

File 399:CA SEARCH(R) 1967-2002/UD=13720
(c) 2002 American Chemical Society

Set Items Description
---
          92 RN=33069-62-4
          10 RN=71610-00-9
S1       93 RN=33069-62-4 + RN=71610-00-9

?S S1 (S) (ANAL OR DETN OR SEPN)
          6550 S1
          373345 ANAL (ANALYSIS, ANALYTICAL (LY))
          871563 DETN (DETERMINATION)
          170525 SEPN (SEPARATION)
S2       225 S1 (S) (ANAL OR DETN OR SEPN)

?S S2(S)(HPLC OR HIGH()PRESSURE()LIQUID OR HIGH()PERFORMANCE
()LIQUID)
          225 S2
          63915 HPLC
1133715 HIGH
249132 PRESSURE (SEE ?GENERAL)
852065 LIQUID
          3403 HIGH(W) PRESSURE(W) LIQUID
1133715 HIGH
143364 PERFORMANCE
852065 LIQUID
          32661 HIGH(W) PERFORMANCE(W) LIQUID
S3       63 S2(S)(HPLC OR HIGH()PRESSURE()LIQUID OR
HIGH() PERFORMANCE() LIQUID)

?T S3/8/1

3/8/1
DIALOG(R)File 399:(c) 2002 American Chemical Society. All
rts. reserv.

Determination of taxol in extracts of Chinese by high-
performance liquid chromatography
SECTION:
CA264002 Pharmaceutical Analysis
IDENTIFIERS: taxol detn ext Taxus HPLC, liq chromatog
taxol detn ext Taxus
DESCRIPTORS:
HPLC... Yew(Taxus)...
detn. of taxol in exts. of Chinese Taxus by HPLC
CAS REGISTRY NUMBERS:
33069-62-4 detn. of taxol in exts. of Chinese Taxus by HPLC

```

Limit the search to non-patent documents (/NPT).

Use parentheses around the ORed terms when you use the AND and OR operators in the same search statement.

```
?S S3/NPT
      S4      63  S3/NPT

?T S4/3/1-3

  4/3/1
DIALOG(R)File 399:CA SEARCH(R)
(c) 2002 American Chemical Society. All rts. reserv.

137237841  CA: 137(16)237841k  JOURNAL
Determination of taxol in extracts of Chinese by high-
performance liquid chromatography
AUTHOR(S): Zhou, Hao-ran; Wang, Jia-xiang; Liang, Shu-min;
Peng, Li-ping
LOCATION: Analysis and Test Centre of Heilongjiang
Province, Harbin, Peop. Rep. China, 150050
JOURNAL: Huaxue Yu Nianhe (Huaxue Yu Nianhe)  DATE: 2002
NUMBER: 4  PAGES: 188-189  CODEN: HYZHEN  ISSN: 1001-0017
LANGUAGE: Chinese
PUBLISHER: Huaxue Yu Nianhe Bianji Weiyuanhui

  4/3/2
DIALOG(R)File 399:CA SEARCH(R)
(c) 2002 American Chemical Society. All rts. reserv.

137024397  CA: 137(2)24397h  JOURNAL
A novel prepurification for paclitaxel from plant cell
cultures
AUTHOR(S): Kim, J. H.; Kang, I. S.; Choi, H. K.; Hong, S.
S.; Lee, H. S.
LOCATION: Department of Chemical Engineering, Kongju
National University, Kongju, Chungnam, 314-701, S. Korea
JOURNAL: Process Biochem. (Oxford, U. K.) (Process
Biochemistry (Oxford, United Kingdom))  DATE: 2002  VOLUME:
37  NUMBER: 7  PAGES: 679-682
CODEN: PBCHE5  ISSN: 1359-5113  PUBLISHER ITEM IDENTIFIER:
0032-9592(01)00247-3  LANGUAGE: English  PUBLISHER: Elsevier
Science Ltd.

  4/3/3
DIALOG(R)File 399:CA SEARCH(R)
(c) 2002 American Chemical Society. All rts. reserv.

136252591  CA: 136(16)252591b  JOURNAL
Determination of paclitaxel and related substances by HPLC
AUTHOR(S): Yang, Xuemei; Xu, Jiangping
LOCATION: Department of Chemistry, The First Military
Medical University, Canton, Peop. Rep. China, 510515
JOURNAL: Zhongguo Yaoxue Zazhi (Beijing, China)  DATE:
2001  VOLUME: 36  NUMBER: 12  PAGES: 840-842  CODEN: ZYZAEU
ISSN: 1001-2494  LANGUAGE: Chinese  PUBLISHER: Zhongguo
Yaoxue Zazhishe

?S S1 AND (HPLC OR HIGH()PRESSURE()LIQUID OR
HIGH()PERFORMANCE ()LIQUID)

      6550  S1
      63915  HPLC
      1133715  HIGH
      249132  PRESSURE (SEE ?GENERAL)
      852065  LIQUID
      3403  HIGH(W) PRESSURE(W) LIQUID
```

Use the NOT operator to eliminate the non-patent records.

```
1133715 HIGH
143364 PERFORMANCE
852065 LIQUID
32661 HIGH (W) PERFORMANCE (W) LIQUID
S5 127 S1 AND (HPLC OR HIGH () PRESSURE () LIQUID OR
HIGH () PERFORMANCE () LIQUID)

?S S5 NOT S4
127 S5
63 S4
S6 64 S5 NOT S4

?T S6/6/1,2

6/6/1
DIALOG(R) File 399:(c) 2002 American Chemical Society. All
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Comparison of LC-UV and LC-MS-MS for the determination of
taxol

6/6/2
DIALOG(R) File 399:(c) 2002 American Chemical Society. All
rts. reserv.

Isolation of a kind of endophytic fungus which can produce
taxol compounds
```

Table 4-1: *Abbreviations and Symbols Used in CAS Publications

A	ampere (unit)	cond.	conductivity
abs.	absolute	cor.	corrected
abstr.	abstract	crit.	critical
addn.	addition	cryst.	crystalline
ADP	adenosine 5'-diphosphate	crystd.	crystallized
alc.	alcoholic	cwt	hundredweight (unit)
alk.	alkaline (not alkali)	d.	density
alky.	alkalinity	detn.	determination
amt.	amount	distn.	distillation
anal.	analysis (analytically)	d.p.	degree of polymerization
approx.	approximate(ly)	ED	effective dose
aq.	aqueous	emu	electromagnetic unit
arom.	aromatic	equil.	equilibrium(s)
assoc.	associate	esp.	especially
at.	atomic	est.	estimate
atm.	atmosphere (unit)	Et	ethyl
av.	Average	eV	electron volt (unit)
b.p.	Boiling point	evap.	evaporate
Btu	British thermal unit	examd.	examined
Bu	Butyl (normal)	expt.	experiment
bu	Bushel (unit)	ext.	extract
uB	Bohr magneton (unit)	F	farad
C	Colomb (unit)	*F	degree Fahrenheit (unit)
*C	Degree Celsius (centigrade) (unit)	fermn.	fermentation
cal	Calorie (unit)	f.p.	freezing point
calc	Calculate	ft	Foot (unit)
cGMP	Cyclic GMP	ft-lb	foot-pound (unit)
chem.	chemical(ly), chemistry	g	gram (unit)
Ci	Curie (unit)	g	gravitational constant
coeff.	Coefficient	gal	gallon (unit)
compd.	Compound	prepn.	preparation
conc.	concentrate	sepn.	separation

*An excerpt from the "CAS Standard Abbreviations" sheets produced by Chemical Abstracts

Online Practice Exercises

1. Find recent, technical articles about the adverse effects of caffeine.

Database _____

Search Statement _____

2. Find patents on Nylon 66.

Database _____

Search Statement _____

3. Determine who has published the most articles on Taxol.

Database _____

Search Statement _____

4. Using the MAP command, find medical information on the effects of lead on children.

Database _____

Search Statement _____

Section 5: Seminar Wrap Up

Summary

In this seminar we reviewed techniques to retrieve CAS Registry numbers and synonyms for chemical names. We also searched using molecular formulae, element count, and ring data.

We also practiced with the Dialog MAP and RANK commands to make obtaining comprehensive search results easier.

Examples in Section 4 illustrated how to use the strategies to locate chemical information to retrieve references to chemical literature in areas such as toxicology, environmental data, and patents.

Other Training Options

Enhance your Dialog search skills by taking advantage of additional training opportunities. At the Dialog Training Center on the Web (training.dialog.com/sem_info/calendar), you can find training schedules, seminar workbooks, and subject-specific short training aids.

1. Of particular interest to the chemical searcher may be:

Searching MEDLINE[®] Using Dialog Classic

Biomedical Information on Dialog, Part 2

Chemical Search Solutions at: training.dialog.com/quick/solutions/#scitech

Pharmaceutical Seminar workbooks at training.dialog.com/sem_info/courses

2. Also, check the Dialog training schedule worldwide for upcoming offerings in your area at training.dialog.com/seminfo/calendar

3. Check with the Alerts Bureau to have Alerts set up for you by experienced Dialog staff at ***www.dialog.com/info/support/alerts***
4. For information on any of the Dialog products or services, contact the Knowledge Center nearest you or search the Dialog Knowledge Center SolutionsBase on the Web at ***www.dialog.com/info/support:***

North America: 1-800-334-2564

Europe, Middle East, Africa: 0800.690.000

Asia Pacific: Australia – 1-800-65 45 25

Outside Australia – 61 2 8587 7719

Appendixes

Appendix A: Dialog Commands (Review)

Appendix B: Chemical Names and Definitions

Appendix C: Chemical Elements

Appendix D: Answers to Exercises

Appendix A: Dialog Commands (Review)

Throughout this seminar the following Dialog commands are featured:

BEGIN (B)	SORT
EXPAND (E)	RANK
SELECT (S)	SHOW FILES
TYPE (T)	HELP RATES <i>n</i>
PRINT (PR)	SET DETAIL ON/OFF
DISPLAY SETS (DS)	REMOVE DUPLICATES (RD)
MAP	COST
EXECUTE STEPS (EXS)	HELP
SAVE TEMP	RECALL

Dialog OneSearch Categories

The following subject categories (DIALINDEX or OneSearch search acronyms) are available on Dialog and are especially helpful for chemical searching:

CASREGNO	PATFULL
CEHMLIT	PATENTS
CHEMBUS, BIOBUS	PHARMIND
CHEMSUBS	RNCHEM, RNMED
CHEMPROP	SAFETY
ENVIRON, POLLUT	TOXICOL
ENG	WATER

Dialog Proximity Operators

- The (W) operator specifies that two terms must occur next to each other and in the order specified. For example, SELECT LUNAR (W) ECLIPSE retrieves the phrase “lunar eclipse.”
- The (N) operator specifies that two terms must occur next to each other in any order. For example, SELECT ECONOM? (N) RECOVERY retrieves “economic recovery” or “recovery of the economy.”
- **The (L) operator** specifies that terms must occur in the same descriptor. For example, GOLD(L)ADVERSE EFFECTS retrieves the descriptor “Gold—Adverse Effects.”
- **The (S) operator** specifies that terms must occur in the same subfield. For example, SELECT WATER(S)RATION? retrieves records in which the term “water” and variations of the term “ration” appear in the same subfield. (In complete text databases, each paragraph of the text is commonly treated as a subfield.)
- **The (F) operator** specifies that terms must occur in the same field. For example, SELECT POLLUTION(F)CONTROL retrieves records in which the terms “pollution” and “control” appear in the same field (e.g., the title, descriptor, abstract, etc.).

- **The (T) operator** is a special operator used in the chemistry databases. The (T) operator specifies what two chemical segments must be present in the same single term. For example, SELECT BUTYL(T)AMINE retrieves occurrences of these two segments in a single term such as "dibutylamine." Both the (W) operator and, with these enhancements, the (N) operator include (T) proximity, i.e., (W) and (N) retrieve the same records retrieved by (T) plus additional records in which the terms occur in adjacent words. Chemical searchers use (T) to add precision to their searches.

Dialog Direct-Record Access

If the Dialog accession number is known, a specific chemical substance may be retrieved by entering the following:

T <Accession Number>/<Format>

Example:

To retrieve CA citation: CA: 121(18)208516x in Format 3,

Enter:

T 121208516/3

The Abstract Number must be 6 digits in CA SEARCH (File 399). If it is less than 6 digits, TYPE the access numbers as a zero-filled to the left value:

Example:

To retrieve CA citation: CA: 121(1)33e in Format 3

Enter:

T 121000033/3

Note: In File 399 the Dialog accession number is composed of the Chemical Abstract Volume (121) and Abstract Number (208516); the issue number (18) is omitted.

Appendix B: Chemical Names and Definitions

CAS Registry number – a unique number given to each chemical by the American Chemical Society to identify the particular substance.

Chemical element – a pure substance that is made of only one kind of atom. It is a substance that cannot be further decomposed by ordinary chemical means. Some examples of common elements and their symbols are aluminum (AL), gold (Au), and silver (Ag). A Table of all elements is found in Appendix C.

Chemical compound – a pure substance that contains two or more elements, chemically combined together in definite, well-defined ratios to each other. It is a substance that can be decomposed into two or more simpler substances by ordinary chemical means. Some common examples are: table salt and sugar.

Hill order – using Hill order, if carbon is present, it is listed first, followed by hydrogen (if present), followed by all other elements listed alphabetically. If carbon is not present, then all elements are listed alphabetically.

Molecular formula – a precise representation of the atoms contained in a molecule. Elements in a molecular formula are listed in Hill order.

Substance – a homogeneous material consisting of one particular kind of matter. A substance has a definite chemical composition. Substances include compounds and elements.

Appendix C: Chemical Elements

Each Chemical Element is represented by a unique one or two letter symbol. Elements and their symbols appear below.

Element	Symbol	Element	Symbol	Element	Symbol
Actinium	Ac	Gallium	Ga	Polonium	Po
Aluminum	Al	Germanium	Ge	Potassium	K
Americium	Am	Gold	Au	Praseodymium	Pr
Antimony	Sb	Hafnium	Hf	Promethium	Pm
Argon	Ar	Helium	He	Protactinium	Pa
Arsenic	As	Holmium	Ho	Radium	Ra
Astatine	At	Hydrogen	H	Radon	Rn
Barium	Ba	Indium	In	Rhenium	Re
Berkelium	Bk	Iodine	I	Rhodium	Rh
Beryllium	Be	Iridium	Ir	Rubidium	Rb
Bismuth	Bi	Iron	Fe	Ruthenium	Ru
Boron	B	Krypton	Kr	Samarium	Sm
Bromine	Br	Lanthanum	La	Scandium	Sc
Cadmium	Cd	Lawrencium	Lr	Selenium	Se
Calcium	Ca	Lead	Pb	Silicon	Si
Californium	Cf	Lithium	Li	Silver	Ag
Carbon	C	Lutetium	Lu	Sodium	Na
Cerium	Ce	Magnesium	Mg	Strontium	Sr
Cesium	Cs	Manganese	Mn	Sulfur	S
Chlorine	Cl	Mendelevium	Md	Tantalum	Ta
Chromium	Cr	Mercury	Hg	Technitium	Tc
Cobalt	Co	Molybdenum	Mo	Tellurium	Te
Copper	Cu	Neodymium	Nd	Terbium	Tb
Curium	Cm	Neon	Ne	Thallium	Tl
Dysprosium	Dy	Neptunium	Np	Thorium	Th
Einsteinium	Es	Nickel	Ni	Thulium	Tm
Element 104		Niobium	Nb	Tin	Sn
Element 105		Nitrogen	N	Titanium	Ti
Element 106		Nobelium	No	Tungsten	W
Erbium	Er	Osmium	Os	Uranium	U
Europium	Eu	Oxygen	O	Vanadium	V
Fermium	Fm	Palladium	Pd	Xenon	Xe
Fluorine	F	Phosphorus	P	Ytterbium	Yb
Francium	Fr	Platinum	Pt	Yttrium	Y
Gadolinium	Gd	Plutonium	Pu	Zinc	Zn
				Zirconium	Zr

CA also routinely uses symbols for the two isotopes of Hydrogen:

Deuterium (Hydrogen mass=2) D

Tritium (Hydrogen mass=3) T

For elements 104 and above CAS has adopted IUPAC nomenclature and their associated 3 character element symbols.

Appendix D: Answers to Exercises

p. Section 2: p. 36

1. What is the Registry Number for L-3-keto-threo-hexuronic acid lactone? What is its common name? How many hydrogen atoms are present in the molecular formula?

Registry Number is 50-81-7
Common Name is Vitamin C
The molecular formula is C₆H₉O₆

2. What is a popular trade name for methyldiazepinone and what is its molecular formula using the Hill Order? (File 398)

Trade Name is Allergin
Molecular Formula: C₁₆H₁₃CIN₂O

3. What drug is diphenhydramine hydrochloride and what is its Registry Number? (File 301)

Drug Name: Benadryl
Registry Number: 147-24-0

4. What is the Registry Number for this everyday product, methylaspartylphenylalanate? (File 301)

Drug Name: NutraSweet
Registry Number 22839-47-0

5. What is the Registry Number and street name for this illicit drug, d-lysergic acid diethylamide? (File 301)

Drug Name: LSD
Registry Number: 50-37-3

Section 3: p. 53

1. What does the latest medical literature reveal about the therapeutic effect of CAS Registry Number 59-30-3 in the treatment of coronary heart disease? Hint: MAP all synonyms and include the HP= field. Use MEDTEXT to access fulltext medical journals.

B 301
S m=59-30-3
Map sy t
B medtext;exs
S s3 and coronary(2n)heart
B 398

[continued from previous page]

S RN= 68-26-8
T s1/3/all [continues on next page]

MAP SY T s1/2
B 369
EXS
S s5(S)eye?
T s1/3,k/all

- Use the MAP command to locate fulltext medical articles that concern the use of Vitamin A with cancer.
B 398
E na= vitamin a
S e3
T s1/3/all
Map sy temp s1/2
B 444 (New England Journal of Medicine)
Exs
S s5(s)cancer
Set hi on
t s6/3,k/1-2

Section 4: p. 81

- Find recent, technical articles about the adverse effect of caffeine. (File 301)
E na=caffeine
S e number(s)
Map rn temp
B 72;exs
S adverse/de and s1
Rank de
S caffeine(L)adverse drug reaction
- Find patents on Nylon 66.
B 411; sf chembus
S na=nylon 66
Save temp

Map rn t
B 314; exs
S s1/pat
- Determine who published the most articles on Taxol.
B 398
E na=taxol
Map rn t
B rnmed

[continued from previous page]

Exs
Rank au

4. Using the MAP command, find medical information on the effects of lead on children.

B 304

E na=lead

S e3

T s1/9

Map rn t

B 155

Exs

S s1 and child?/ti and effect?/de

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11000 Regency Parkway
Suite 10
Cary, NC 27511
United States
+(1) 919 462 8600
+(1) 800 3 DIALOG

DIALOG
EUROPE
MIDDLE EAST & AFRICA

Palace House
3 Cathedral Street
London SE1 9DE
United Kingdom
+44 (20) 7940 6900

DIALOG
ASIA PACIFIC
20/F Sunning Plaza
10 Hysan Avenue
Causeway Bay
Hong Kong
+(852) 2530 5778

GSM-03-30013

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