

화학물질 유해성 정보체계 및 이용방안

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1996 new substance registrations
indicate some interesting trends

- 1.3 million new substance registrations
 - 451,000 biosequences
 - 821,000 chemical substances
 - 639,000 organics
 - 182,000 others

In 1996 CAS registered 1.3 million new substances. (451,000 of which were biosequences.) This is an important number. Registry is an important file for biochemical and biotechnological information.

In order to look at trends, let's look at the 821,000 new non-sequence substance registrations in 1996. If we look at the 79% number, about 639,000 of these new substances are organic in nature. Where did these 639,000 substance registrations come from?

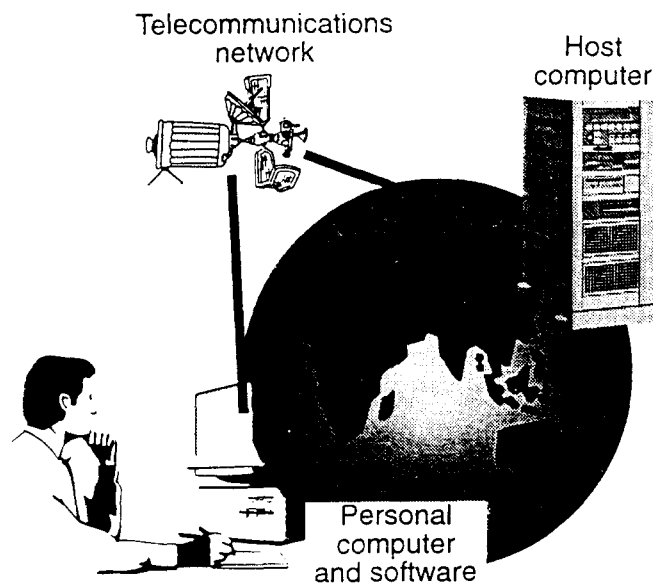


Figure 1 Components of the online connection

The searcher needs a computer and communications software with which to connect, via a communications network, to the host computer. To enter the system, a loginid and password are required.

Table 1 Clusters of databases^a

CLUSTER	NUMBER OF DATABASES	AREA COVERED
AGRICULTURE	22	Agriculture and related sciences
BIOSCIENCE	37	Biosciences
BUSINESS	21	Sci-Tech and business news
CHEMENG	16	Chemical engineering and applied chemistry
CHEMISTRY	37	Chemistry and related areas(excludes structure files)
COMPUTER	14	Computer sciences
CONSTRUCTION	9	Building and construction
ELECTRICAL	24	Electrical engineering sciences
ENGINEERING	46	Engineering and technology
ENVIRONMENT	37	Environment and environmental issues
FUELS	26	Energy sources
GEOSCIENCE	15	Earth and geosciences
GOVREGS	20	Governmental regulations
HEALTH	33	Health sciences
MATDATA	13	Numeric data for materials
MATERIALS	35	Materials sciences
MEDICINE	24	Medicine and medical sciences
METALS	14	Metals
METDATA	8	Numeric data for metals
NUMERIC	24	All files with numeric data
PATENTS	16	Patent files and bibliographic files with patent data
PETROLEUM	17	Petroleum and Petrochemicals
PHARMACOLOGY	31	Pharmacology and Pharmaceutical sciences
PHYSICS	16	Physics and Physical sciences
POLYMERS	15	Polymer sciences
SAFETY	16	Occupational health and safety
TOXICOLOGY	26	Toxicological information

^aAs more databases are being added to the networks, the numbers of databases in the various clusters increase. Searchers should check with the vendors on up-to-date numbers. This information is also available online (on STN: HELP CLUSTER), and in the annual catalogues produced by the vendor.

There are three primary access points to the finding information on substances :

- chemical names or name segments
- molecular formulas or element information
- structures

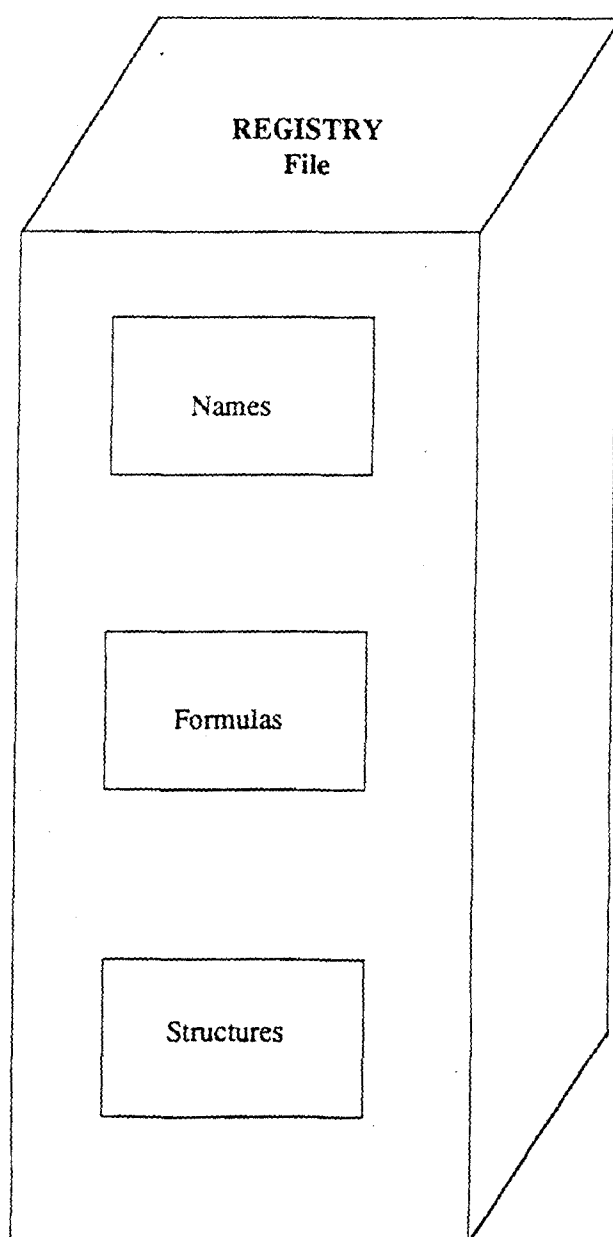


Table 2 Major substance based files on STN and the types of information they contain^a

FILE	NUMBER OF SUBSTANCES	TYPE OF INFORMATION
BEILSTEIN	6.6million	chemical and physical property information for organic substances
CHEMCATS	350,000	commercially available substances and their suppliers
CHEMLIST	170,000	EPA TSCA substances ^b and other regulatory information
CSCHEM	130,000	commercial chemicals and their suppliers
DRUGU	28,000	Registry segment contains information on drugs
GMELIN	700,000	chemical and physical property information for inorganic and organometallic substances
HODOC	26,000	chemical and physical data for the most common organic substances(CRC Handbook Data)
HSDB	4,500	toxicology and environmental effects of chemicals
MARPAT ^c	-	Markush structure (representing several million prophetic substances)
MRCK	10,000	drug descriptions
MSDS-CCOHS	96,000	Materials Safety Data Sheets
PHAR	17,000	information on pharmaceutical products
REGISTRY	14 mil.	CAS Registry Numbers; citations to files which have information on the substance
RTECS	120,000	factual toxicity data
SPECINFO	100,000	IR, ¹³ C NMR, and Mass Spectra

^aExcludes files which have numeric property information only, or which are based on chemical reactions

^bEPA=Environmental Protection Agency; TSCA= Toxic Substances and Chemicals Act

^cThe MARPAT File actually is a bibliographic file but it contains unique chemical substances(Markush structures)

Table 3 Substance search fields

FILES	NAME AND NAME SEG- MENTS	MF AND MF SEG- MENTS	STRUC -TURE	PRO- PERTY INF.	TOXI- COLO- GY INF.	CAS REGIST- RY NUM- BERS
BEILSTEIN	○	○	○	○	○	○
BIOBUSINESS						○
BIOSIS					○	○
CABA					○	○
CANCERLIT					○	○
CAPLUS					○	○
CHEMLIST	○			○	○	○
CSCHEM	○			○		○
DDFB					○	
DDFU					○	
DRUGB					○	
DRUGNL					○	○
DRUGU			○		○	
EMBAL					○	
EMBASE					○	○
ENERGY					○	
FSTA					○	
GMELIN	○	○	○	○		○
HEALSAFE					○	
HODOC	○	○		○		○
HSDB	○	○		○	○	○
IPA					○	○
JICST-EPLUS					○	
LIFESCI					○	
MARPAT			○			
MEDLINE					○	○
MSDS-OHS	○	○		○	○	○
NAPRALERT					○	
NLDB					○	
PROMT					○	○
REGISTRY	○	○	○			○
RTECS	○	○		○	○	○
SCISEARCH					○	
SPECINFO	○	○		○		○
TOXLINE				○	○	○
TOXLIT				○	○	○

(Note: Entry ○ means that the fields are present and searchable, but not all substances in the file may have information in the fields)

Search Question: Fumaric acid is a common reactant used in many reactions. Is fumaric acid listed on ECL or TSCA? Find toxicity information for fumaric acid.

* * * * * WELCOME TO STN International * * * * *

=> FILE REGISTRY REGISTRY 파일 선택

=> E FUMARIC ACID/CN 물질명 색인 열람

E1 1 FUMARATOCHROMIUM (III) NITRATE/CN

E2 1 FUMARIA OFFICINALIS, EXT./CN

E3 1 → FUMARIC ACID/CN

=> S E3 E3항 검색

L1 1 "FUMARIC ACID"/CN

=> D 검색결과 화면보기

L1 ANSWER 1 OF 1 REGISTRY COPYRIGHT 1995 ACS

RN 110-17-8 REGISTRY

CN 2-Butenedioic acid (E)- (9CI) (CA INDEX NAME)

OTHER CA INDEX NAMES:

CN **Fumaric acid** (8CI)

OTHER NAMES:

CN 2-Butenedioic acid, (E)-

CN Allomaleic acid

CN trans-2-Butenedioic acid

FS STEREOSEARCH

MF C4 H4 O4

CI COM

LC STN Files: ANABSTR, APILIT, APILIT2, APIPAT, APIPAT2, BEILSTEIN*, BIOBUSINESS, BIOSIS, CA, CABA, CANCERLIT, CAOLD, CAPLUS, CAPREVIEWS, CASREACT, CEN, CHEMCATS, CHEMINFORMRX, CHEMLIST, CBNB, CIN, CJACS, CSCHEM, CSNB, DETHERM*, DDFU, DIPPR*, DRUGU, EMBASE, GMELIN*, HODOC*, HSDB*, IFICDB, IFIPAT, IFIUDB, IPA, MEDLINE, MRCK*, MSDS-OHS, MSDS-SUM, NAPRALERT PDLCOM*, PIRA, PNI, PROMT, RTECS*, SPECINFO, TOXLINE, TOXLIT, TRCTHERMO*, USAN, USPATFULL, VETU, VTB

(*File contains numerically searchable property data)

Other Sources: DSL**, EINECS**, TSCA**

(*Enter CHEMLIST File for up-to-date regulatory information)

DES 2:E

Double bond geometry as shown.



```
=> FILE CHEMLIST ☞ CHEMLIST 파일 선택
=> S L1 ☞ REGISTRY 파일의 L1검색결과 검색
    L2 1 L1
=> D ☞ 검색결과 화면보기
L2 ANSWER 1 of 1 CHEMLIST COPYRIGHT (C) 1997 ACS
AN 2477 CHEMLIST
RN 110-17-8
CN 2-Butenedioic acid (E)- (TSCA, DSL)
FS CANADA: DSL; EEC: EINECS; KOREA: ECL; USA: SARA, STATE
    TSCA
CBI Public
RLN EINECS No. : 203-743-0
    ECL Serial No. : 2-886
INV On TSCA Inventory ☞ TSCA에 수록되어 있음
    June 1995 Inventory Tape.
    On DSL
    Supplement to Canada Gazette, Part I, January 26, 1991.
    On EINECS
    Annex to official Journal of the European Communities, 15 June
    1990.
    On ECL ☞ 화학유해물질조사집에 수록되어 있음
    Korean Existing Chemicals List, 1992 Ed.
FA RN CAS Registry Number ☞ FA 색인항의 내용 참조
    RLN Regulatory List Number
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=> FILE RTECS ☞ RTECS 파일 선택
=> S L1 ☞ REGISTRY 파일의 L1검색결과 검색
L3 1 L1
=> D ALL ☞ 검색결과 화면보기
L5 ANSWER 1 of 1 RTECS COPYRIGHT 1997 DOC
CAS Registry Number (RN): ***110-17-8*** RTECS
IRRITATION DATA (IRR):
Route |Organism | Dose |Duration | Effect | Source
RTE | ORGN | DOSE | DUR | EFF | SO
=====+=====+=====+=====+=====+=====
skin | rabbit |500 mg |24H |Mild | 85JCAE -,313,86
-----+-----+-----+-----+-----+-----
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MUTATION DATA (MUT):

System	Organism	Route	Dose	Source
SYS	ORGN	RTE	DOSE	SO
DNA inhibitor	rat	intravenous	40	JJCREP
		s	mg/kg	77,750,86

MUTATION DATA REFERENCES:

JJCREP Japanese Journal of Cancer Research (Elsevier Science Pub. BV, POB 211, 1000 AE Amsterdam, Netherlands) V.76- 1985-

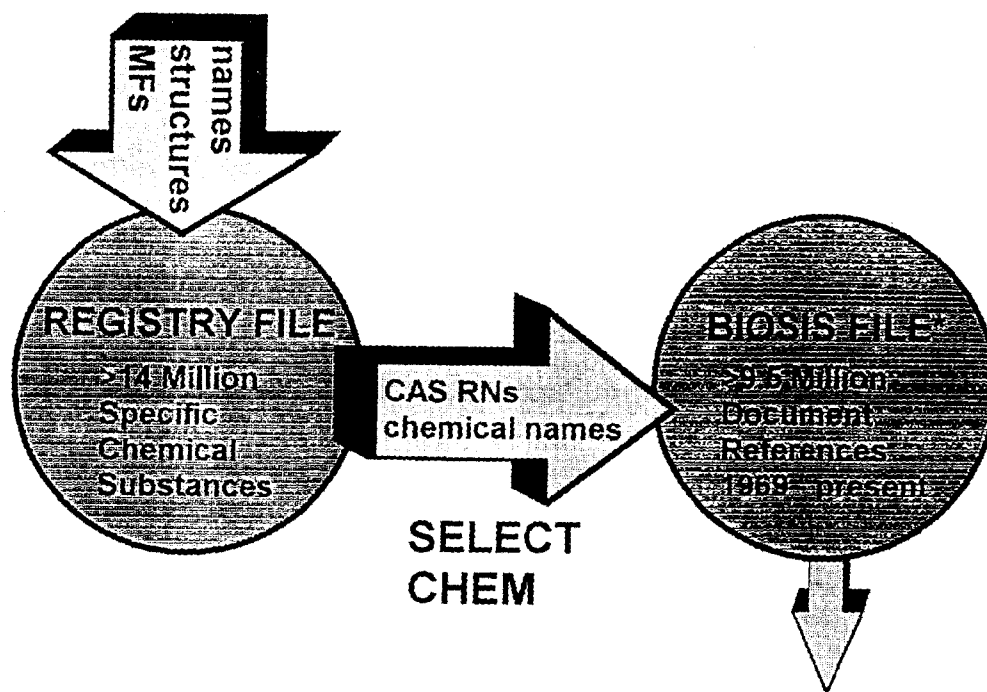
TOXICITY DATA (TOX):

Effect	Route	Organism	Dose	Source
EFF	RTE	ORGN	DOSE	SO
K30;L30;P01	intraperitoneal	rat	LDLo 587	JAPMA8
			mg/kg	35,298,46

TOXICITY DATA REFERENCES:

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

Crossing Over CAS RNs and Chemical Names to a Non-CAS Database



Answers - bibliographic citations

CAS RNs can be used as search terms in many non-CAS databases on STN.

*Type D CLUSTER CASRNS at an arrow prompt to see a list of RN-searchable files on STN.

(This list includes some files produced by CAS.)

=> D CLUSTER CASRNS

CLUSTER NAME CLUSTER DEFINITION

CASRNS	AAASD AIDSLINE ALFRAC ANABSTR APILIT APILIT2 APIPAT APIPAT2 ASMDATA BIOBUSINESS BIOSIS CABA CANCERLIT CAOLD CAPLUS CASREACT CBNB CEN CHEMCATS CHEMINFORMRX CHEMLIST CHEMSAFE CIN CJACS COPPERDATA CSCHEM CSNB DDFU DETHERM DIPPR DRUNGNL DRUGPAT DRUGU DRUGUPDATES EMBASE GENBANK GMELIN HODOC HSDB IFIPAT IPA IPS JANAF MEDLINE METALCREEP MRCK NAPRALERT NISTCERAM NISTTHERMO PDLCOM PIRA PLASPEC PNI PROMT REGISTRY RTECS SPECINFO TOXLINE TOXLIT TRCTHERMO USAN USPATFULL VTB CAS Registry Numbers Cluster
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Search question : Your fat-free lifestyle has prompted you to quit smoking.
To protect your investment in tobacco, however, you are interested in
smoking cessation methods using nicotine. Are such methods effective?

=> FILE REGISTRY

=> S NICOTINE/CN

L1 1 NICOTINE/CN

=> D

L1 ANSWER 1 OF 1 REGISTRY COPYRIGHT 1996 ACS

RN 54-11-5 REGISTRY

CN Pyridine, 3-(1-methyl-2-pyrrolidinyl)-, (S)- (9CI)
(CA INDEX NAME)

OTHER CA INDEX NAMES

CN NICOTINE(8CI)

OTHER NAMES;

CN (-)-3-(1-Methyl-2-pyrrolidyl)pyridine

CN (-)-Nicotine

CN (S)-(-)-Nicotine

CN (S)-3-(1-Methyl-2-pyrrolidinyl)pyridine

CN (S)-Nicotine

CN Flux Maag

CN 1-Nicotine

CN L-Nicotine

CN Nicoderm

CN Niconil

CN Nicotin

CN Nicotinell

CN XL All Insecticide

FS STEREOSEARCH

DR 551-13-3, 6912-85-2, 13890-18-8, 13890-82-9, 16760-37-5

MF C10 H14 N2

CI COM

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Using SELECT CHEM To Extract RNs and Chemical Names from REGISTRY Records

Use the SELECT CHEM command on STN to extract

- RNs
- chemical names(except the inverted CAS Index names)

from a REGISTRY L-number answer set for searching in non-CAS files containing RNs

=> D HIS L1

L1 1 S E3

=> FILE REGISTRY

=> SELECT CHEM

ENTER ANSWER SET OR SMARTSELECT L# OR (L1) : L1

ENTER ANSWER NUMBER OR RANGE (1) :1

=> D SEL E1-E19

E1	2	L-NICOTINE/BI
E2	1	(-)-NICOTINE/BI
E3	1	(-)-3-(1-METHYL-2-PYRROLIDYL)PYRIDINE/BI
E4	1	(S)-(-)-NICOTINE/BI
E5	1	(S)-NICOTINE/BI
E6	1	(S)-3-(1-METHYL-2-PYRROLIDINYL)PYRIDINE/BI
E7	1	FLUX MAAG/BI
E8	1	NICODERM/BI
E9	1	NICONIL/BI
E10	1	NICOTIN/BI
E11	1	NICOTINE/BI
E12	1	NICOTINELL/BI
E13	1	XL ALL INSECTICIDE/BI
E14	1	13890-81-8/BI
E15	1	13890-82-9/BI
E16	1	16760-37-5/BI
E17	1	54-11-5/BI
E18	1	551-13-3/BI
E19	1	6912-85-2/BI

=> FILE BIOSIS

=> S E1-E19

L2 11647 (L-NICOTINE/BI OR "(-)-NICOTINE"/BI OR
"(-)-3-(1-METHYL-2-PYRROLIDYL)PYRIDINE"/BI OR
"(S)-(-)-NICOTINE"/BI OR "(S)-NICOTINE"/BI OR
"(S)-3-(1-METHYL-2-PYRROLIDINYL)PYRIDINE"/BI OR
"FLUX MAAG"/BI OR NICODERM/BI OR NICOTINE/BI OR
NICOTINELL/BI OR "XL ALL INSECTICIDE"/BI OR 13890-81-8/BI OR
13890-82-9/BI OR 16760-37-5/BI OR 54-11-5/BI OR 551-13-3/BI OR
6912-85-2/BI

=> S SMOK? (S) CESSATION

44729 SMOK?

14546 CESSATION

L3 1959 SMOK? (S) CESSATION

=> S (TRANSDERM? OR GUM# OR SPRAY?)

2751 TRANSDERM

4917 GUM#

21655 SPRAY?

L4 29243 (TRANSDERM? OR GUM# OR SPRAY?)

=> S L2 AND L3 AND L4

=> D L5 1,20 BIB ABS RN

L5 ANSWER 1 OF 216 BIOSIS COPYRIGHT 1997 BIOSIS

AN 96:66751 BIOSIS

DN 98638886

TI Efficacy of a **nicotine** nasal **spray** in **smoking cessa**tion; A placebo-controlled, double-blind trial.

AU Schneider N G; Olmstead R; Mody F V; Doank ; Franzon M; Jarvik M E; Steinberg C

CS Nicotine Res. Unit, West LA VA Medical Cent., Brentwood Div., 691/B151D, Los Angeles, CA 90073, USA

SO Addiction 90 (12). 1995. 1671-1682. ISSN: 0965-2140

LA English

AB Laboratory trials have demonstrated the efficacy of **nicotine** replacement in **smoking cessation** but absolute success rates are low. For many, **nicotine gum** is hard to use and **transdermal nicotine** is

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peaked at day 1, day 5 and 3 weeks for strict abstinence. It is concluded NNS is safe, efficacious and a viable alternative treatment for **smoking cessation**

RN 54-11-5 (NICOTINE)

L5 ANSWER 20 OF 216 BIOSIS COPYRIGHT 1997 BIOSIS

AN 95:304114 BIOSIS

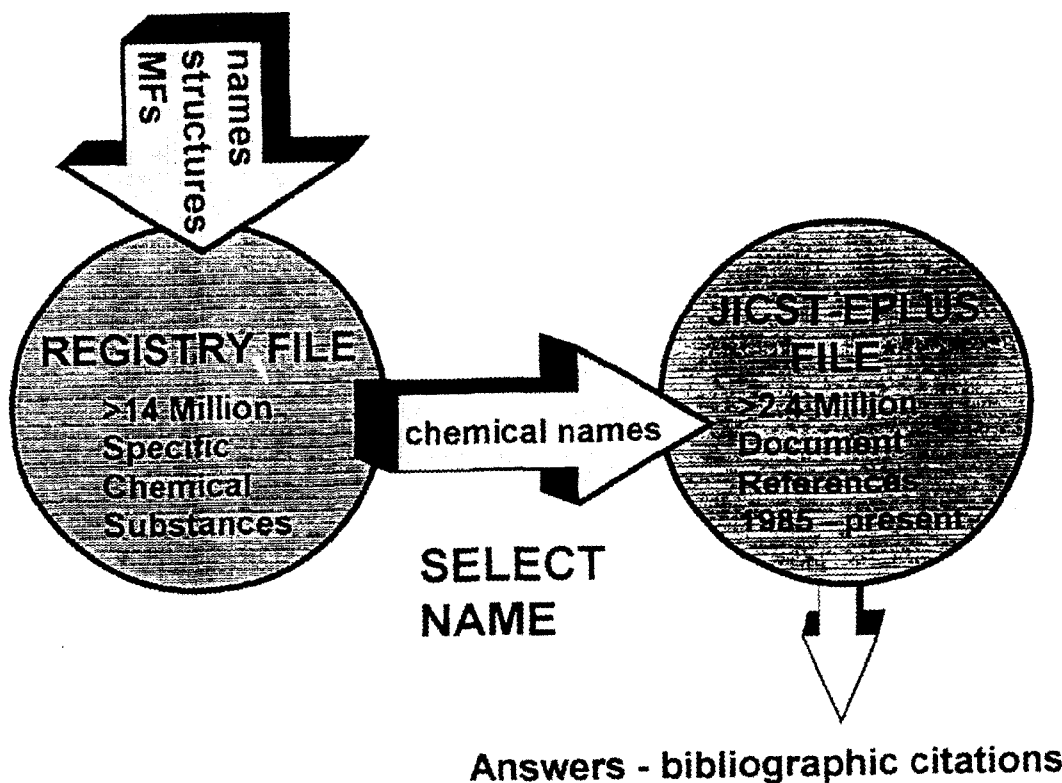
DN 98318414

TI Dose effects of **nicotine gum**

AU Gross J; Johnson J; Sigler L; Stitzer M L

CS Behavioral Pharmacol. Res. Unit, 5510 Nathan Shock Dr., Johns Hopkins Bayview Med. Cent., Baltimore, MD 21224

Crossing Over REGISTRY L-number Data to Files That
Lack CAS RNs



Not all files on STN are searchable by CAS RN. Does this mean that REGISTRY data cannot be crossed over to those files?

Not at all! The REGISTRY files is also an excellent source for chemical names to use in text searches.

SELECT NAME allows you to select only the chemical names from a REGISTRY answer set(excluding inverted CA Index Names) and leave the RNs behind.

The format for using the SELECT NAME command is identical with that for SELECT CHEM.

=> **FILE JICST-EPLUS**

=> **D HIS L1**

L1 1 S E3

=> **S L1**

L6 0 L1

=> **FILE REGISTRY**

=> **SELECT NAME**

ENTER ANSWER SET OR SMARTSELECT L# OR (L6) :L1

ENTR ANSWER NUMBER OR RANGE (1) :1

E1 THROUGH E13 ASSIGNED

=> **D SEL E1-E13**

E1	2	L-NICOTINE/BI
E2	1	(-)-NICOTINE/BI
E3	1	(-)-3-(1-METHYL-2-PYRROLIDYL)PYRIDINE/BI
E4	1	(S)-(-)-NICOTINE/BI
E5	1	(S)-NICOTINE/BI
E6	1	(S)-3-(1-METHYL-2-PYRROLIDYL)PYRIDINE/BI
E7	1	FLUS MAAG/BI
E8	1	NICODERM/BI
E9	1	NICONIL/BI
E10	1	NICOTIN/BI
E11	1	NICOTINE/BI
E12	1	NICOTINELL/BI
E13	1	XL ALL INSECTICIDE/BI

=> FILE JICST-EPLUS

=> SET POSTINGS OFF

SET COMMAND COMPLETED

=> S E7-E12

0 "FLUX MAAG"/BI
L7 625 ("FLUX MAAG"/BI OR NICOTERM/BI OR NICONIL/BI OR
NICOTIN/BI OR NOCOTINE/BI OR NICOTINELL/BI

=> D HIS L3-L4

L3 1959 S SMOK? (S) CESSATION
L4 29243 S (TRANSDERM? OR GUM# OR SPRAY?)

=> S L7 AND L3 AND L4

7806 SMOK?
1340 CESSATION
270 SMOK? (S) CESSATION
1024 TRANSDERM?
1359 GUM#
16862 SPRAY?
L8 25 L7 AND L3 AND L4

=> D L8 1 ALL

L8 ANSWER 1 OF 25 JICST-Eplus COPYRIGHT 1996 JICST
AN 950516082 JICST-Eplus
TI Practice of **smoking cessation** counseling with **nicotine gum**
AU SUZUKI YUKIE; YOHEHARA YASUKO; SHOJI SACHIKO; HAYASHI
TSUYOSHI
CS Hitachi, Ltd.
SO Sangyo Eiseigaku Zasshi (Journal of Occupational Health), (1995)
vol. 37, no. rinzo, pp. S287. Journal Code: F0261A
ISSN: 1341-0725
CY Japan
LA Japanese
STA New

화학물질정보 네트워크 구성도

