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STN Database Summary Sheet

PS (Pharmaceutical Substances) is a substance-based, structure-searchable file that contains essential substance information, trade data, and preparation methods for active pharmaceutical ingredients. The database includes pharmaceutical compounds of significance currently on the market. The database covers compounds launched from 1957 to the present.

PS corresponds to the printed Pharmaceutical Substances - Synthesis, Patents, Applications.

For indexed pharmaceutical substances, the ATC code, therapeutic use, chemical name, molecular formula, CAS Registry Number, EINECS Number, lethal dose, information on derivatives, and substance class are given. In addition, formulations, trade names, and vendors, as well as an overview of intermediates from the preparations, are also included. Reaction schemes for industrial synthesis can be displayed as TIFF images. The reactants and products are structure-searchable with a single reaction query including reaction roles. Citations, predominantly patents, are given for all indexed pharmaceutical compounds.

Subject Coverage

- Marketed active pharmaceutical ingredients
- Preparation methods for pharmaceutical substances

Sources

- The U.S. Food and Drug Administration (FDA)
- ATC Index from the WHO
- Patents
- Publications and databases in the field of organic chemistry

File Data

- Pharmaceutical ingredients launched from 1957 to the present
- 2352 pharmaceutical substances (08/04)
- About 8200 reactions (08/04)
- Updated twice a year
- Automatic current-awareness searches (SDIs) are not available in this file

User Aids

- Online Helps (HELP DIRECTORY lists all file-specific help messages available)
- STNGUIDE

Database Producer

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Search and Display Field Codes

The fields that allow left truncation (/BI, /CNS) are marked with an asterisk (*).

Search Field Name	Search Code	Search Examples	Display Codes
Basic Index * (contains single words from the CN, DEF, DRV, EIN, INT, MF, RN, and TRD fields)	None (or (BI)	S CODEINE/BI S 60-00-4 S C10H11NO3 S ?GLUCO?	CN, DRV, INT, TRD, DEF, EIN, CN.INT, CO
Accession Number	/AN	S 265009/AN	AN
Application Date (1)	/AD	S 19990101-20001231/AD	RE
ATC Code	/CC	S A01?/CC	CC
Author	/AU	S SHAPIRO E L/AU	RE
CAS Registry Number	/RN	S 40054-69-1/RN	RN
Chemical Name (2)	/CN	S DIAZEPAM/CN	CN
Chemical Name Segment *	/CNS	S KETOPROFEN/CNS	CNS
Corporate Name (Manufacturer) (3)	/CO	S KNOLL ?/CO	TRD
Data Entry Date (1)	/DED	S DED>2000	DED
Definition (Compound Class)	/DEF	S TYROSINES/DEF	DEF
Derivative CAS Registry Number	/RN.DRV	S 50832-74-1/RN.DRV	DRV
Derivative Chemical Name	/CN.DRV	S CALCIUM SALT/CN.DRV	DRV
Derivative EINECS Number	/EIN.DRV	S 200-055-2/EIN.DRV	DRV
Derivative Lethal Dose	/LD50.DRV	S 100 MG/KG ?/LD50.DRV	DRV
Derivative Molecular Formula	/MF.DRV	S C5H8NNAO3S/MF.DRV	DRV
Derivative Molecular Weight (1)	/MW.DRV	S 150-160/MW.DRV	DRV
Document Type	/DT	S PATENT/DT	Not displayed
EINECS Number	/EIN	S 200-014-9/EIN	EIN
Entry Date (1)	/ED	S 2003?/ED	ED
Field Availability (4)	/FA	S FORMULATION/FA	Not displayed
Formulation	/FRM	S AEROSOL/FRM	FRM
Intermediate CAS Registry Number	/RN.INT	S 104-85-8/RN.INT	INT
Intermediate Chemical Name	/CN.INT	S ABIETIC ACID/CN.INT	INT
Intermediate Chemical Name Segment	/CNS.INT	S ACETALDEHYDE/CNS.INT	INT
Intermediate Molecular Formula	/MF.INT	S C20H12O8/MF.INT	INT
International Standard (Document Number [CODEN])	/ISN	S JACSAT/ISN	RE
Journal Title	/JT	S J BIOL CHEM/JT	RE
Launch Country Code (ISO Code and text)	/LNC	S GB/LNC	TRD
Launch Year (1)	/LNY	S 2000-2001/LNY	TRD
Lethal Dose	/LD50	S G/KG ?/LD50	LD50
Molecular Formula	/MF	S C22H30N6O4S/MF	MF
Molecular Weight (1)	/MW (/FW)	S MW>500	MW
Patent Assignee (3)	/PA (/CS)	S HOECHST?/PA	RE
Patent Country (WIPO Code and Text)	/PC	S DE/PC	RE
Patent Number	/PN	S DE2004686/PN	RE
Preparation Conditions	/PRE.COND	S STREPTOMYCES/PRE.COND	Not displayed
Priority Country (WIPO Code and Text)	/PRC	S WO/PRC	RE
Priority Date (1)	/PRD	S PRD>20010000	RE
Publication Date (1)	/PD	S 20020000-20021231/PD	RE
Publication Year (1)	/PY	S 2000-2001/PY	RE
Reference (contains single terms from the Author, CODEN, Journal Title, Patent Assignee, Patent Country, Publication Date, Patent Number, Priority Country, Priority Date, and Publication Year fields)	/RE	S BASF/RE	RE
Status	/STA	S WFM/STA	TRD
Therapeutic Use	/THER	S ANTIALLERGIC/THER	THER
Trade Name	/TN	S DIANE 25/TN	TRD

(1) Numeric search field that may be searched with numeric operators or ranges.

(2) CN search field contains generic names, synonyms, systematic names, and trade names.

(3) Search with implied (S) proximity is available in this field.

(4) Searching for all information available in each display field.

Structure Search Terms

Terms	Search Examples
L-numbers of structures built using the STRUCTURE command or uploaded from STN Express® or STN® on the Web SM (Boolean logic allowed between the L-numbers)	S L1 SSS
L-numbers of a structure built using the STRUCTURE command or uploaded from STN Express or STN on the Web combined with L-numbers of the screen sets created using the SCREEN command (Boolean logic allowed between the L-numbers)	S L1 AND L2 NOT L3

(1) The L-number answer set from a structure search may be combined with text terms, e.g., S L6 AND ANTIALLERGIC/THER.

Types of Structure Searching

Type	Definition	Search Code	Search Examples
Closed Substructure	Search for substances that match the query exactly. Substitution is allowed at positions opened by CONNECT. Additional components may be retrieved.	CSS	S L1 CSS FULL
Substructure (default)	Search for substances that match the query. Substitution is allowed at all open positions. Additional components be retrieved.	SSS	S L1 SSS FULL

Scopes of Structure Searches

To create an L-number answer set containing candidate structures that have passed the screening step of your structure search, enter EXTEND on the search command line or enter SET EXTEND ON or SET EXTEND ON PERM at an arrow prompt (=>). For details, enter HELP SET EXTEND at an arrow prompt.

Scope	Definition	Search Code	Search Examples
Full (default)	Search 100% of the file.	FUL	S L2 SSS FUL
SUBSET FULL	Search 100% of an answer set created by a search in PS.	SUB FUL	S L8 SUB=L6 CSS FUL

PS

Display and Print Formats

Any combination of formats or fields may be used to display or print answers. Multiple codes must be separated by spaces or commas, e.g., D L1 1-5 FRM TRD. The fields are displayed or printed in the order requested.

Hit-term highlighting is available for AN, CC, CN, DED, DEF, DRV, EIN, ED, FRM, LD50, MF, MW, RN, and THER. Highlighting must be on during SEARCH in order to use the HIT, KWIC, and OCC display formats.

Format	Content	Examples
AN CC CN DED DEF DRV (CN.DRV, EIN.DRV, LD50.DRV, MF.DRV, MW.DRV, RN.DRV) EIN ED (1) FRM GI (PRE) (2) INT (CN.INT, MF.INT, RN.INT) LD50 MF MW RE RN THER TRD (CO, LNC, LNY, STA, TN)	Accession Number ATC Code Chemical Name Data Entry Date Definition, Compound Class Derivative EINECS Number Entry Date Formulation Graphic Image (Preparation(s)) Intermediate(s) Lethal Dose Molecular Formula Molecular Weight Reference CAS Registry Number Therapeutic Use Trade Data	D L2 1-12 AN D CC DISPLAY CN 1-5 D DED D DEF DIS DRV L2 1 D EIN D ED D FRM D GI L9 1-5 D INT DIS LD50 D MF D MW D REF L5 1 DIS RN D THER DISPLAY TRD L3 1
ALL IALL IDE IIDE IPRED ISTD PRED (GID) STD SCAN (3)	AN, IDE, DRV, TRD, FRM, PRED ALL, indented with text labels AN, DED, CN, TN, CC, THER, RN, MF, MW, EIN, LD50, TN, DEF IDE, indented with text labels PRED, indented with text labels STD, indented with text labels GI, INT, RE IDE, DRV, TRD, RE CN (Generic Name), CC (display with no answer number)	DISPLAY L2 1 ALL D IALL DIS IDE L2 1-10 D IIDE DIS IPRED DISPLAY ISTD L8 1 DIS PRED L4 DISPLAY L1 STD 1-5 D SCAN
HIT (4) KWIC OCC QRD (default)	GI for all HIT reactions All fields containing hit terms Hit term with 20 words on either side (KeyWord-In-Context) Number of occurrences of hit terms and the fields in which they occur IDE, HIT	D HIT D KWIC D OCC D L1 1 5 QRD

(1) Custom display only.

(2) You can use the GI format in the DISPLAY command for the images of all available synthesis paths for a title substance. Any program that handles TIFF images compressed in Group 4 FAX format, e.g., STN Express[®], may be used to capture the graphic image.

(3) SCAN must be specified on the command line, i.e., D SCAN or DISPLAY SCAN.

(4) The HIT display format cannot be used after a structure search. To display reactions after a structure search, use the GI (alias PRE) display format.

SELECT, ANALYZE, and SORT Fields

The SELECT command is used to create E-numbers containing terms taken from the specified field(s) in an answer set.

The ANALYZE command is used to create an L-number containing terms taken from the specified field(s) in an answer set.

The SORT command is used to rearrange the search results in either alphabetic (A) or numeric (N) order of the specified field(s).

Field Name	Field Code	ANALYZE/ SELECT (1)	SORT
Accession Number	AN	Y	-
ATC Code	CC	Y	A
Author	AU	Y (2)	-
CAS Registry Number	RN	Y	A
Chemical Name	CN	Y (3)	-
Corporate Name (Manufacturer)	CO	Y (2)	-
Data Entry Date	DED	Y	N
Definition (Compound Class)	DEF	Y	-
Derivative CAS Registry Number	RN.DRV	Y (5)	-
EINECS Number	EIN	Y	A
Intermediate CAS Registry Number	RN.INT	Y (2,5)	-
Intermediate Chemical Name	CN.INT	Y (2,4)	-
Molecular Formula	MF	Y	A
Molecular Weight	MW	Y	N
Patent Assignee	PA	Y (2)	-
Patent Number	PN	Y (2)	-
Therapeutic Use	THER	Y	A
Trade Name	TN	Y (2)	-

- (1) HIT may be used to restrict terms extracted to terms that match the search expression used to create the answer set, e.g., SEL HIT AU.
- (2) SELECT HIT and ANALYZE HIT are not valid with this field.
- (3) Selects or analyzes the generic names, synonyms, systematic names, and trade names of the title compounds with /CN appended to the terms created by SELECT.
- (4) Appends /CN to the terms created by SELECT.
- (5) Appends /RN to the terms created by SELECT.

PS**Sample Records****DISPLAY IALL**

L2 ANSWER 1 OF 1 PS COPYRIGHT 2004 THIEME on STN
 Accession Number 265011
 Data Entry Date 20030618
 Chemical Name GENERIC: Fluconazole
 Chemical Name SYNONYM: UK-49858
 Chemical Name SYSTEMATIC: .alpha.-(2,4-difluorophenyl)-
 .alpha.-(1H-1,2,4-triazol-1-ylmethyl)-1H-1,2,4-
 triazole-1-ethanol
 Trade Name Diflucan; Fungafa; Beagyne; Triflucan;
 Diflucan; Biozolene; Diflucan; Elazor;
 Diflucan; Diflucan
 ATC Code J02AC01; J02AX
 Therapeutic Use(s) antifungal (treatment of vaginal,
 oropharyngeal and atrophic oral candidiasis)
 CAS Registry Number 86386-73-4
 Molecular Formula C13H12F2N6O
 Molecular Weight 306.28
 LD50 >200 mg/kg (M, i.v.); 1408 mg/kg (M,
 p.o.); >200 mg/kg (R, i.v.); 1271 mg/kg (R,
 p.o.); >100 mg/kg (dog, i.v.); >300 mg/kg (dog,
 p.o.)
 Definition (Compound Class) .beta.-Amino alcohols, N-(2-hydroxyethyl)
 substituted N-heterocyclic Systems
 Definition (Compound Class) Fluorine compounds
 Definition (Compound Class) 1,2,4-Triazoles

Trade Data

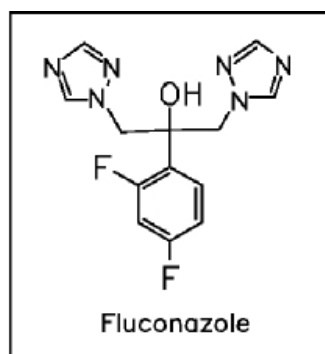
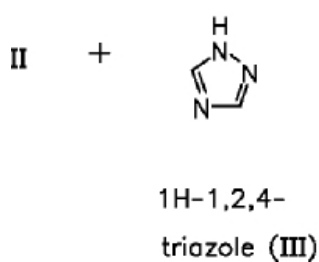
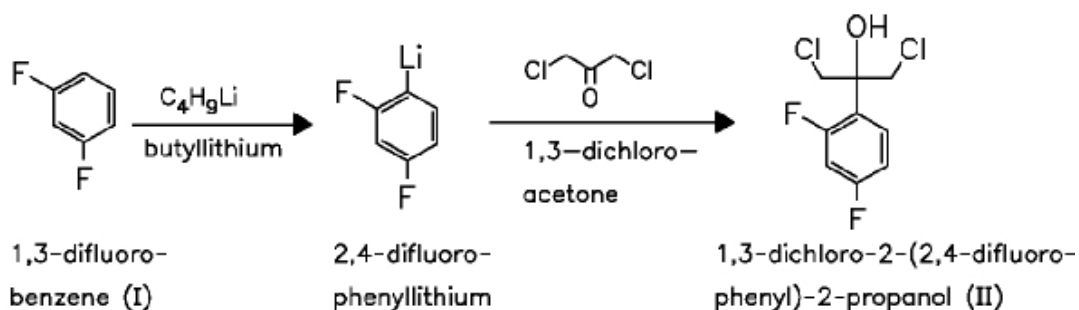
Launch Year	Launch Country	Trade Name	Company Name (Manufacturer)
	DE	Diflucan	Pfizer
	DE	Fungafa	Mack, Illert.
	FR	Beagyne	Effik
1989	FR	Triflucan	Pfizer
1988	GB	Diflucan	Pfizer
1989	IT	Biozolene	Bioindustria
	IT	Diflucan	Roerig
	IT	Elazor	Sigma-Tau
	JP	Diflucan	Pfizer
1990	US	Diflucan	Pfizer

Formulation(s) cps. 50 mg, 100 mg, 150 mg, 200 mg; susp. 50 mg/5 ml; syrup 50
 mg/10ml; tabl. 50 mg, 100 mg, 150 mg, 200 mg; vial 50 mg/50 ml,
 100 mg/50 ml, 200 mg/100 ml, 400 mg

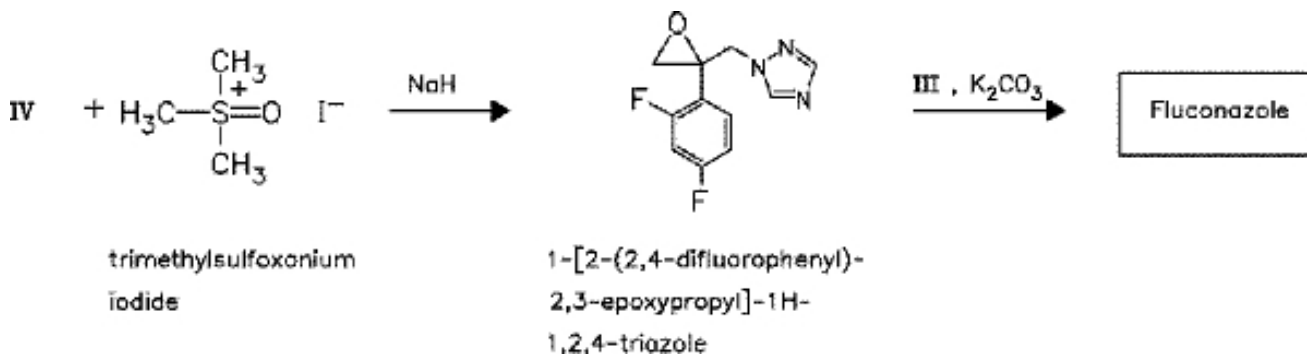
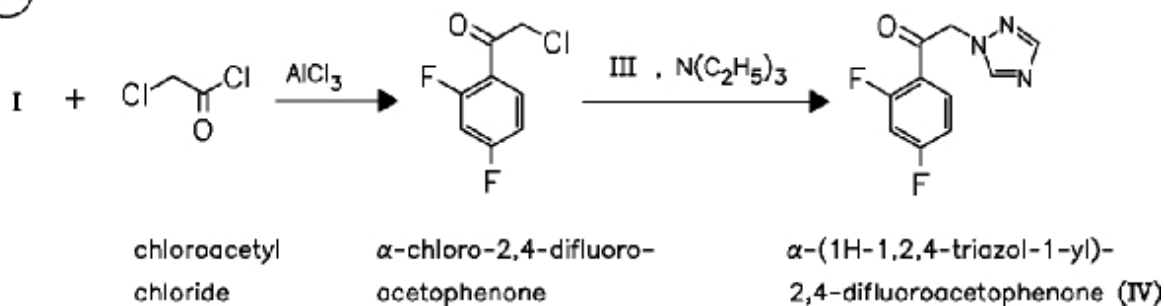
DISPLAY IALL (cont'd)

Preparation(s)

a



b



DISPLAY IALL (cont'd)

Intermediate(s) in Substance Preparation

CAS Reg. No.	Molecular Formula	Chemical Name
79-04-9	C2H2Cl2O	chloroacetyl chloride; Acetyl chloride, chloro-
51336-94-8	C8H5ClF2O	.alpha.-chloro-2,4-difluoroacetophenone; Ethanone, 2-chloro-1-(2,4-difluorophenyl)-
534-07-6	C3H4Cl2O	1,3-dichloroacetone; 2-Propanone, 1,3-dichloro-
86386-74-5	C9H8Cl2F2O	1,3-dichloro-2-(2,4-difluorophenyl)-2-propanol; Benzenemethanol, ?, .alpha.-bis(chloromethyl)-2,4-difluoro-
372-18-9	C6H4F2	1,3-difluorobenzene; Benzene, 1,3-difluoro-
86386-76-7	C11H9F2N3O	1-[2-(2,4-difluorophenyl)-2,3-epoxypropyl]-1H-1,2,4-triazole; 1H-1,2,4-Triazole, 1-[[2-(2,4-difluorophenyl)oxiranyl]methyl]-
87820-35-7	C6H3F2Li	(2,4-difluorophenyl)lithium; Lithium, (2,4-difluorophenyl)-
288-88-0	C2H3N3	1H-1,2,4-triazole; 1H-1,2,4-Triazole
86404-63-9	C10H7F2N3O	.alpha.-(1H-1,2,4-triazol-1-yl)-2,4-difluoroacetophenone; Ethanone, 1-(2,4-difluorophenyl)-2-(1H-1,2,4-triazol-1-yl)-
1774-47-6	C3H9IOS	trimethylsulfoxonium iodide; Sulfoxonium, trimethyl-, iodide

Reference(s)

- (1) US 4 404 216 (Pfizer; 13.9.1983; GB-prior. 6.6.1981, 17.10.1981, 4.3.1982).
 - (2) US 4 416 682 (Pfizer; 22.11.1983; GB-prior. 2.6.1980, 30.1.1981).
 - (3) GB 2 099 818 (Pfizer; appl. 22.4.1982; prior. 6.6.1981, 4.3.1982).
 - (4) EP 69 442 (Pfizer; GB-prior. 6.6.1981).
- process for preparing fluconazole and its crystal modifications:
- (5) EP 96 569 (Pfizer; appl. 6.6.1983; GB-prior. 9.6.1982, 30.7.1982) tablet formulation:
 - (6) WO 2 002 076 955 (Richter Gideon; 3.10.2002; appl. 23.3.2001). controlled -release compositions :
 - (7) EP 178 682 (Schering Corp.; appl. 23.4.1986; USA-prior. 19.10.1984) formulation for external application :
 - (8) WO 2 001 062 195 (Advanced Pharma; 30.8.2001; appl. 23.2.2001; USA-prior. 24.2.2000) alternative synthesis:
 - (9) WO 2 002 062 336 (Boryung Pharma; 15.8.2002; appl. 7.2.2002; KR-prior. 7.2.2001).
 - (10) ES 549 684 (Lazlo Int.; appl. 6.12.1985).
 - (11) ES 5 490 202 (Inke S. A.; appl. 19.11.1985).
 - (12) US 5 710 280 (Dev. Center Biotech. Taiwan; 20.1.1998; appl. 9.7.1996).
 - (13) WO 9 703 971 (Apotex; appl. 17.7.1996; NZ-prior. 17.7.1995).