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STN Database Summary Sheet

PROUSDDR (Prous Drug Data Report Database) contains preliminary drug research results from patents for bioactive compounds. PROUSDDR is a pipeline database that selects top candidate drugs. The file contains information on bioactive compounds and associated structures. More than 13,700 records contain CAS Registry Numbers®.

The records contain the chemical names, drug names, generic names, brand names, CAS Registry Number, molecular formula, physical properties, highest development phase, originator, licensee, classification code, mechanism of action, other sources and entry date into the file, structure diagram, Prous References, reference text, patent references, and other references.

The structure diagrams are TIFF images. Any program that handles TIFF images compressed in Group 4 fax format, e.g., STN Express®, may be used to capture images from DISPLAY or viewed directly with DISPLAY when using STN® on the WebSM.

The FOCUS command may be used with answer sets created in this file to rearrange the search results to place the more relevant answers at the start of a new L-number.

Subject Coverage

- Essential drug information from patents
- Validated and classified by mechanism of action

Sources

- Drug Data Report
- Patents
- Journals

File Data

- 1988 to the present
- More than 190,914 records (4/07)
- Updated monthly
- Automatic current-awareness searches (SDIs) may be run monthly

User Aids

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

Database Producer

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PROUSDDR

Search and Display Field Codes

The field that allows left truncation (/CNS) is marked with an asterisk (*).

Search Field Name	Search Code	Search Examples	Display Codes
Basic Index (contains single words from the chemical name (CN), company name (CO), reference text (RTX), title (TI), molecular formula (MF), and CAS Registry Number fields)	None (/BI)	S INHIBITOR S ACP-ALA S TAXOL AND BRISTOL S C7H9CLN4OS S 137073-91-7	CN, CO, MF, RN, RTX, TI
Accession Number	/AN	S 2003:514/AN	AN
Chemical Name (includes generic, brand, or drug names)	/CN (/TN)	S PALA/CN S RETINOIC ACID?/CN S AU-2?/CN	CN
Chemical Name Segment *	/CNS	S THIOXANTHEN/CNS S ?CARBONYL?/CNS	CN
Classification Code	/CC	S HIV/CC S DEMENTIA/CC	CC
Company Name (originator)	/CO	S GEORGIA TECH?/CO S SYNAPTIC/CO	CO
Document Number (Prous Entry Number)	/DN	S 288846/DN	DN
Entry Date (1)	/ED (/UP)	S L1 AND ED>=20040500	ED
Field Availability (code and text)	/FA	S L7 AND CC/FA	Not displayed
Highest Development Phase	/HDP (/DSTA)	S LAUNCHED?/HDP	HDP
Inventor	/IN	S WINTERS C?/IN	IN
Mechanism of Action	/ACTN	S COLONY STIMULATING FACTORS/ACTN	ACTN
Molecular Formula (3)	/MF	S GA N3 O9/MF S C23H25NO.CLH/MF	MF
Number of Components (1,3)	/NC	S 1/NC	MF
Other Sources (2)	/OS	S SYNTHLINE/OS	OS
Patent Assignee	/PA	S ABBOTT/PA	PA
Patent Date (1)	/PPD	S 19870916/PPD	PI
Patent Number	/PN (/PATS)	S US2616927/PN S DE10041574/PATS	PATS, PI, PN
Periodic Group	/PG	S T3/PG	MF
Physical Property	/PHP	S SALT/PHP	PHP
Priority Country	/PRC	S AU/PRC	PRAI, PRN
Priority Date (1)	/PRD	S 20040106/PRD	PRAI, PRN
Priority Information	/PRN	S US2002-391813/PRN	PRAI, PRN
Priority Year (1)	/PRY	S 1999/PRY	PRAI, PRN
Reference Text	/RTX	S (SILYLAT? (L) KETONE#)/RTX	RTX
Specific Element Count (1)	/Element symbol	S 2-5/NA S 7/O	MF
Status	/STA	S ACTIVELY INVESTIGATED/STA	STA
Title	/TI	S CONFORMATION?/TI S PROTEIN KINASE/TI S (INHIBITOR# (P) PYRROLE#)/TI	TI
Update Date (1)	/UP	S L5 AND UP>=20050100	ED

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

(2) The OS field includes related PROUSDDR references and corresponding SYNTHLINE references.

(3) All molecular formulas are single component. For example, the MF of Amifostine hydrate is C5 H17 N2 O4 P S not C5 H15 N2 O3 P S . H2 O.

Display and Print Formats

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

Hit-term highlighting is available for all fields except STR, which is not searchable. Highlighting must be ON during SEARCH in order to use the HIT, KWIC, and OCC formats.

Format	Content	Examples
AN ACTN CC CN (TN) CO DN DSTA ED HDP IN MF OS PA PHP PI (PATS, PN) PRAI (PRN) RE RN RTX STA STR (1) TI TN	Accession Number Mechanism of Action Classification Code Chemical Name, Brand Name, Drug Name, and Generic Name Company Name (Originator) Document Number (Prous Entry Number) Development Status (Highest Development Phase) Entry Date Highest Development Phase Inventor Molecular Formula of the End Product Other Sources Patent Assignee Physical Property Patent Information (Patent Number) Priority Information Prous References CAS Registry Number Reference Text Status Structure Image Title Trade Name	D AN D ACTN D CC 1,3-5 D CN D CO 5-10 D DN D DSTA D ED D HDP 2 7 D IN D MF 6,9 D OS D PA D PHP D 1,4 PI D PRAI D RE D RN D L3 4 RTX D L3 STA D STR 2 L5 D TI 2 D TN
ALL (1) BIB DALL (1) IALL (1) IBIB IDE (1) IIDE (1) QRD SCAN (2) TRIAL (1) (TRI, SAM, FREE) XML (1)	AN, DN, CN, RN, MF, STA, HDP, CO, CC, ED, ACTN, OS, ED, STR, RE, RTX, TI, IN, PA, PI, PRAI AN, RE, RTX, TI, IN, PA, PI, PRAI ALL, delimited for post-processing ALL, indented with text labels BIB, indented with text labels AN, DN, CN, RN, MF, STA, HDP, CO, OS, ED, STR IDE, indented with text labels Query Related Data (AN, DN, CN, RN, MF, STA, HDP, CO, CC, ED, STR), plus fields containing hit terms (QRD is the default) CN (Chemical Name only), CC (random display, no answer number) AN, CN, CO, CC, ACTN ALL, in XML format	D ALL D BIB D DALL 1-3 D IALL D IBIB D IDE D IIDE D L3 9 D SCAN D TRIAL TOTAL D XML
HIT KWIC OCC	Fields containing hit terms Hit term with 20 words on either side (KeyWord-In-Context) Number of occurrences of hit terms and fields in which they occur	D HIT D KWIC NOH D OCC 1-6

(1) Any program that handles TIFF images compressed in Group 4 fax format, e.g., STN Express[®], may be used to capture graphic images from DISPLAY, or they may be viewed directly on the screen during an STN[®] on the WebSM session.

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

PROUSDDR

SELECT, ANALYZE, and SORT Fields

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

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

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

Field Name	Field Code	ANALYZE/ SELECT (1)	SORT
Accession Number	AN	Y	N
CAS Registry Number and Chemical Name of End Product	CHEM	Y (default)	N
CAS Registry Number	RN	Y	Y
Chemical Name of End Product	CN	Y	N
	NAME	Y	N
Classification Code	CC	Y	Y
Company Name (Originator)	CO	Y	Y
Development Status (Highest Phase)	DSTA	Y	Y
Document Number	DN	Y	Y
Entry Date	ED	Y	Y
Highest Development Phase	HDP	Y	Y
Inventor	IN	Y	Y
Mechanism of Action	ACTN	Y	N
Molecular Formula	MF	Y	Y
Occurrence Count of Hit Terms	OCC	N	Y
Other Sources	OS	Y (2,3)	N
Patent Assignee	PA	N	Y
Patent Date	PPD	Y	N
Patent Information	PI	Y	N
	PATS	Y	N
Patent Number	PN	Y	N
Physical Property	PHP	N	N
Priority Date	PRD	Y	Y
Priority Information	PRAI (PRN)	Y	N
Reference Text	RTX	Y	N
Status	STA	Y	Y
SYNTHLINE references in OS	SYN	Y (3)	N
Title	TI	Y	Y
Trade Name	TN	Y	N

(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 CC.

(2) SELECT HIT and ANALYZE HIT are not valid in the OS field.

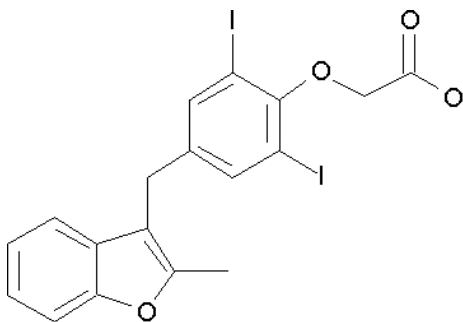
(3) SELECT OS or ANALYZE OS extracts only PROUSDDR references for searching related references in the PROUSDDR file. SELECT SYN or ANALYZE SYN extracts only SYNTHLINE references for searching in the SYNTHLINE file.

Sample Records

DISPLAY IALL

ACCESSION NUMBER: 2002:28 PROUSSDR
DOCUMENT NUMBER: 279038
CHEMICAL NAME: 2-(2,6-Diiodo-4-(2-methyl-1-benzofuran-3-ylmethyl)phenoxy)acetic acid
DRUG NAME: KB-130015
CAS REGISTRY NUMBER: 147030-48-6
MOLECULAR FORMULA: C18 H14 I2 O4
STATUS: Actively Investigated
HIGHEST DEV. PHASE: PRECLINICAL
ORIGINATOR: Karo Bio
CLASSIFICATION CODE: Antiarrhythmic Drugs
ACTION MECHANISM: Antithyroid Drugs
OTHER SOURCE: SYNTHLINE 2003000041
ENTRY DATE: Entered STN: 9 May 2004
Last Updated on STN: 9 May 2004

STRUCTURE:



PROUS REFERENCES:

RefID: 651349 (Text Available)
Drug Data Report, Vol. 24, No. 2, pp 131, 2002

REFERENCE TEXT:

RefID: 651349
ACTION - Class III antiarrhythmic agent, a benzofuran benzyl derivative with high affinity for human thyroid hormone receptors hThR alpha and hThR beta1 (IC50 = 4.5 and 5.1 mcM, respectively) and functional antagonist activity at these receptors (IC50 = 2.2 and 4.1 mcM, respectively, in a reporter cell assay in CHO cells stably transfected with hThRalpha and hThRbeta1, respectively). Transmembrane electrophysiological experiments in guinea pig papillary muscle showed that compound at a dose of 40 mg/kg/day i.p. for 20 days prolonged the action potential duration at 50% and 90% repolarization (ADP50 and ADP90) in the absence of reverse rate dependency. In rats after chronic oral administration, the effects of compound on lipid metabolism and liver function appeared to be less severe than those of amiodarone, without producing the reduction in weight gain seen with amiodarone.

PROUSSDR**DISPLAY IALL (cont'd)**

PATENT REFERENCES:

TITLE: Receptor ligands
INVENTOR(S): Norinder, U.; Bajorath, J.; Stearns, J.F.
PATENT ASSIGNEE(S): Karo Bio
PATENT INFORMATION: WO 9220331 19921126
PRIORITY INFORMATION: SE 1509 19910517

REFERENCES:

- (1) RefID: 649686, Periodic Publication
"Synthesis and preliminary characterization of a novel antiarrhythmic compound (KB130015) with an improved toxicity profile compared with amiodarone"
Carlsson, B.; Singh, B.N.; Temciuc, M.; Nilsson, S.; Li, Y.-L.; Mellin, C.; Malm, J., J Med Chem, Vol. 45, No. 3, pp 623, 2002
- (2) RefID: 728807, Periodic Publication
"KB130015: Antiarrhythmic treatment of the fibrillating atrium without ventricular proarrhythmia?"
Brandts, B.; et al., PACE - Pacing Clin Electrophysiol, Vol. 26, No. 4, Part 2, (Abst 710), 2003
- (3) RefID: 747869, Periodic Publication
"Antiarrhythmic therapy of atrial fibrillation without ventricular proarrhythmia? Unique profile of the novel class III drug KR130015"
Brandts, B.; Borchard, R.; Dirkmann, D.; et al., Eur Heart J, Vol. 24, No. Suppl., (Abst P2753), 2003
- (4) RefID: 755565, Periodic Publication
"Action potential changes associated with a slowed inactivation of cardiac voltage-gated sodium channels by KB130015"
Macianskiene, R.; et al., Br J Pharmacol, Vol. 139, No. 8, pp 1469, 2003
- (5) RefID: 767674, Periodic Publication
"KB130015, a new amiodarone derivative with multiple effects on cardiac ion channels"
Mubagwa, K.; Macianskiene, R.; Viappiani, S.; Gendviliene, V.; Carlsson, B.; Brandts, B., Cardiovasc Drug Rev, Vol. 21, No. 3, pp 216, 2003
- (6) RefID: 781193, Periodic Publication
"Inhibition of G protein-coupled and ATP-sensitive potassium currents by 2-methyl-3-(3,5-diiodo-4-carboxymethoxybenzyl)benzofuran (KB130015), an amiodarone derivative"
Brandts, B.; et al., J Pharmacol Exp Ther, Vol. 308, No. 1, pp 134, 2004