PS (Pharmaceutical Substances)

Subject Coverage

- Marketed Active Pharmaceutical Ingredients
- Preparation Methods for Pharmaceutical Substances

File Type

Substance (not structure searchable)

Features

Thesaurus	None		
Alerts (SDIs)	Not available		
CAS Registry Number® Identifiers	☑	SLART	☑
Keep & Share	☑		

Record Content

- Records contain essential information, trade data and preparation methods for active pharmaceutical ingredients.
- For indexed pharmaceutical substances ATC, therapeutic use, chemical name, molecular formula, CAS Registry Number, EINECS Number, lethal dose, information on derivatives, and substance class are given.
- Also provided are formulations, trade names and vendors, and an overview of the intermediates in the compound's preparation.
- Reaction schemes for industrial synthesis, can be displayed as images.

File Size

- Pharmaceutical ingredients launched from 1957 – to date
- 2807 pharmaceutical substances

Coverage

1957 – to date

Updates

Irregularly

Language

English

Database Producer

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Sources	• The U.S. Food and Drug Administration (FDA) • ATC Index from the WHO • Patents • Publications and databases in the field of organic chemistry
User Aids	• Online Helps (HELP DIRECTORY lists all help messages available) • STNGUIDE
Cluster	• BIOSCIENCE • CASRNS • PHARMACOLOGY • REACTIONS STN Database Cluster information: http://www.stn-international.com/en/customersupport/customer-support#cluster+%7C+subjects+%7C+features

Search and Display Field Codes

Fields that allow left truncation are indicated by an asterisk (*).

General Search Fields

Search Field Name	Search Code	Search Examples	Display Codes
Basic Index* (contains single words from the chemical name (CN), definition (DEF) and CAS registry number (RN) fields)* **(1)**	None or /BI	S CODEINE/BI S 60-00-4 S C10H11NO3S	CN, DEF;RN
Accession Number Chemical Name **(1)** Chemical Name Segment Definition (Compound Class) Entry Date **(2)** INCHI Key **(2)** Molecular Formula Molecular Weight **(2)** CAS Registry Number	/AN /CN /CNS /DEF /ED (or /UP) /INCHI /MF /MW (or /FW) /RN	S 10006/AN S BETAMETHASONE ACETATE/CN S DIAZEPAM/CN S KETOPROFEN/CNS S TYROSINES/DEF S AUG 2022/ED S MBOMYENWWXQSNW-AWEZNQCLSA-N/INCHI S C22H30N6O4S/MF S MW>500 S 40054-69-1/RN	AN CN CNS DEF ED INCHI MF MW RN

(1) CN search field contains Generic Names, Synonyms, Systematic Names, and Trade Names.
(2) Numeric search field which may be searched with numeric operators or ranges.

DISPLAY and PRINT Formats

Any combination of codes 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 in all searchable fields.
Highlighting must be ON during SEARCH to use the HIT, and OCC formats.

Format	Content	Examples
AN	Accession Number	DISPLAY L2 1-10 AN
CC	Classification Code (ATC Code)	D CC
CN	Chemical Name	DISPLAY CN 1-5
DEF	Definition (Compound Class)	D DEF
DRV	Derivatives (comprises CN.DRV, EIN.DRV, LD50.DRV, MF.DRV, RN.DRV)	D DRV
ED (UP)	Entry Date	D ED
EIN	EINECS Number	D EIN
FRM	Formulation	D FRM
GI (PRE)	Graphical Image (Preparation(s))	D GI L9 1-5
INCHI	INCHI Key	D INCHI
INT	Intermediate(s) Table	D INT
LD50	Lethal Dose	DIS LD50
MF	Molecular Formula	D MF
MW (FW)	Molecular Weight	D MW
RE	Reference	D REF L5 1
RN	CAS Registry Number	DIS RN
THER	Therapeutic Use	D THER
TRD	Trade Table	D TRD
ALL	AN, ED, CN, CC, THER, RN, MF, INCHI, MW, EIN, LD50, DEF, DRV, TRD, GI (PRE), INT, RE	D ALL
IALL	ALL, indented with text labels	D IALL
IDE	AN, ED, CN, CC, THER, RN, MF, INCHI, MW, EIN, DEF (default)	D IDE
TRIAL (TRI, SAMPLE, SAM, FREE)	AN, CN, CC	D TRIAL
SCAN **(1)**	CN, CC (random display, no answer number)	D SCAN
HIT	Hit term(s) and field(s)	D HIT
KWIC	Up to 50 words before and after hit term(s) (KeyWord-In-Context)	D KWIC
OCC	Number of occurrences of hit term(s) and field(s) in which they occur	D OCC

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

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
Chemical Name	CN	Y	N
Definition (Compound Class)	DEF	Y	N
Molecular Weight	MW (FW)	N	Y
CAS Registry Number	RN	Y	N

(1) Hit may be used to restrict extracted terms to terms that match the search expression used to create the answer set, e.g., SEL HIT CN.

Sample Record

DISPLAY IALL

```
ACCESSION NUMBER:       20190   PS
ENTRY DATE:             Entered STN: 24 Aug 2022
                        Last updated on STN: 24 Aug 2022
CHEMICAL NAME:          GENERIC: Belumosudil
                        SYNONYM: KD025, ME-3208
                        SYSTEMATIC: 2-(3-(4-((1H-Indazol-5-yl)amino)quinazolin-
                        2-yl)phenoxy)-N-(propan-2-yl)acetamide
CLASSIFICATION CODE:    L04AA48
THERAPEUTICS:           chronic graft versus host disease, rho-kinase 2
                        inhibitor
CAS REGISTRY NUMBER:    911417-87-3
MOLECULAR FORMULA:      C26H24N6O2
INCHI CODE:             GKHIVNAUVKXIIY-UHFFFAOYSA-N
MOLECULAR WEIGHT:       452.52
FORMULATION:            tbl. 200 mg
DEFINITION:             Indazoles; Quinazolines; Acetamides
DERIVATIVES:            CN.DRV    Mesylate
                        LSF.DRV   C26H24N6O2.CH3SO3H
                        MW.DRV    548.61
                        RN.DRV    2109704-99-4

TRD
Trade Data
Launch |Trade Name|Company Name (Manufacturer)
Country|          |
=======+==========+============================
USA    |Rezurock  |Kadmon Pharmaceuticals, 2021
       |          |
       |          |

PREPARATIONS:
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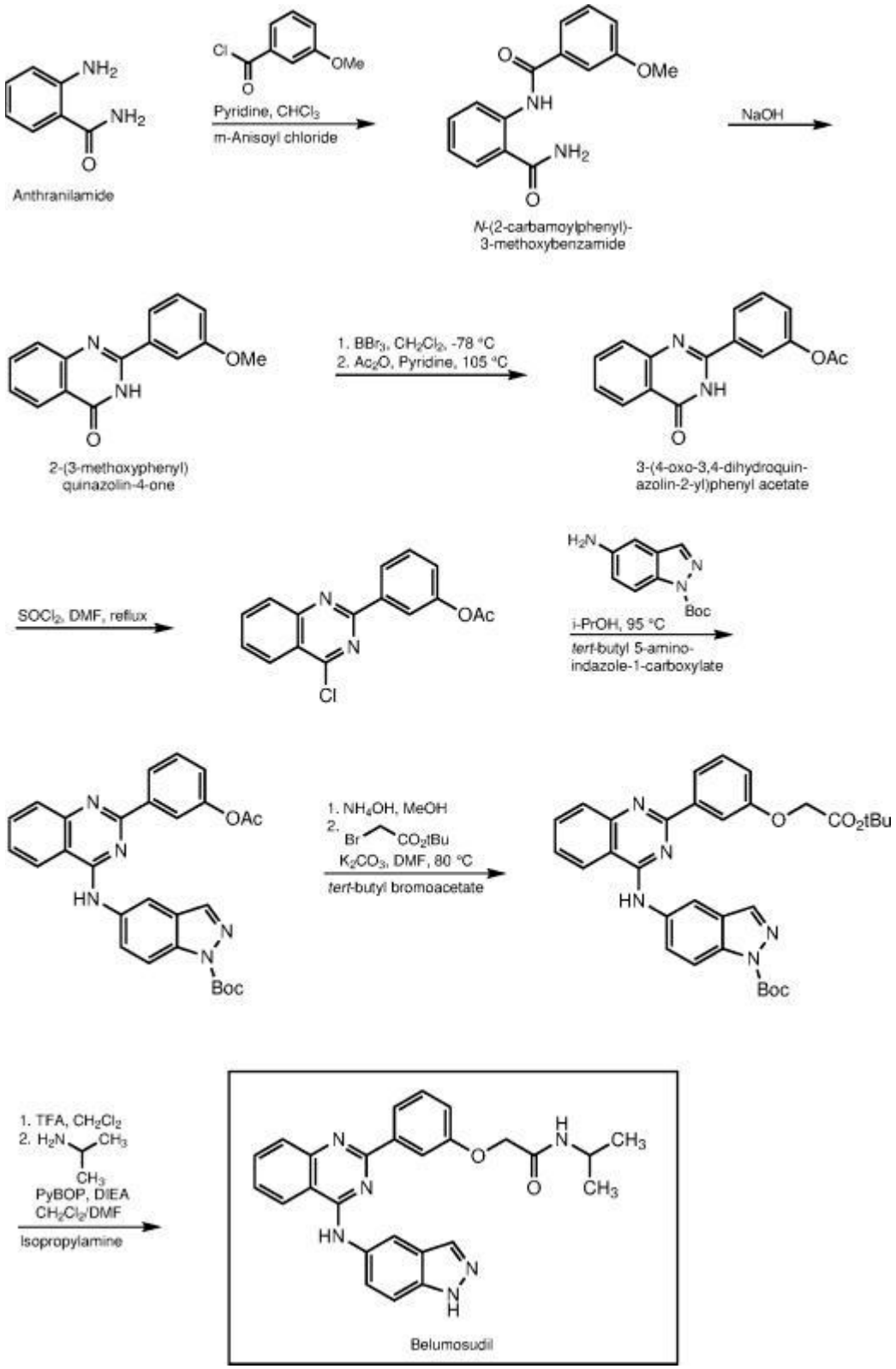

INT
Intermediate(s) in Substance Preparation

CAS RN	Molecular Formula	Chemical Name
88-68-6	C7H8N2O	Anthranilamide
1711-05-3	C8H7ClO2	m-Anisoyl chloride
330657-87-9	C15H14N2O3	N-(2-carbamoylphenyl)-3-methoxybenzamide

56071-04-6	C15H12N2O2	2-(3-methoxyphenyl)quinazolin-4-one
371947-93-2	C16H12N2O3	3-(4-oxo-3,4-dihydroquinazolin-2-yl)phenyl acetate
129488-10-4	C12H15N3O2	tert-butyl 5-amino-indazole-1-carboxylate
5292-43-3	C6H11BrO2	tert-butyl bromoacetate
75-31-0	C3H9N	Isopropylamine

REFERENCE:

WO 2006 105081 (Surface Logix; 05.10.2005; USA-prior. 25.05.2005).
US 8 357 693 (Surface Logix; 22.01.2013; USA-prior. 25.05.2005).
WO 2014 055996 (Kadmon Corp.; 10.04.2014; USA-prior. 05.10.2012).
US 9 815 820 (Kadmon Corp.; 14.11.2017; USA-prior. 05.10.2012).
US 10 183 931 (Kadmon Corp.; 22.01.2019; USA-prior. 05.10.2012).
US 10 696 660 (Kadmon Corp.; 30.06.2020; USA-prior. 05.10.2012).