

## PS (Pharmaceutical Substances)

<b>Subject Coverage</b>	<ul style="list-style-type: none"> <li>Marketed Active Pharmaceutical Ingredients</li> <li>Preparation Methods for Pharmaceutical Substances</li> </ul>																
<b>File Type</b>	Substance (not structure searchable)																
<b>Features</b>	<table border="0"> <tr> <td>Thesaurus</td> <td>None</td> <td></td> <td></td> </tr> <tr> <td>Alerts (SDIs)</td> <td>Not available</td> <td></td> <td></td> </tr> <tr> <td><a href="#">CAS Registry Number® Identifiers</a></td> <td><input checked="" type="checkbox"/></td> <td><a href="#">SLART</a></td> <td><input checked="" type="checkbox"/></td> </tr> <tr> <td><a href="#">Keep &amp; Share</a></td> <td><input checked="" type="checkbox"/></td> <td></td> <td></td> </tr> </table>	Thesaurus	None			Alerts (SDIs)	Not available			<a href="#">CAS Registry Number® Identifiers</a>	<input checked="" type="checkbox"/>	<a href="#">SLART</a>	<input checked="" type="checkbox"/>	<a href="#">Keep &amp; Share</a>	<input checked="" type="checkbox"/>		
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<b>Record Content</b>	<ul style="list-style-type: none"> <li>Records contain essential information, trade data and preparation methods for active pharmaceutical ingredients.</li> <li>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.</li> <li>Also provided are formulations, trade names and vendors, and an overview of the intermediates in the compound's preparation.</li> <li>Reaction schemes for industrial synthesis, can be displayed as images.</li> </ul>																
<b>File Size</b>	<ul style="list-style-type: none"> <li>Pharmaceutical ingredients launched from 1957 – to date</li> <li>2930 pharmaceutical substances</li> </ul>																
<b>Coverage</b>	1957 – to date																
<b>Updates</b>	Irregularly																
<b>Language</b>	English																
<b>Database Producer</b>	Georg Thieme Verlag Thieme Chemistry Rüdigerstr. 14 70469 Stuttgart Germany Phone: +49 711 8931-0 Email: <a href="mailto:marketing@thieme-chemistry.com">marketing@thieme-chemistry.com</a> Copyright Holder																

**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](#)
-

## 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)	/AN /CN	S 10006/AN S BETAMETHASONE ACETATE/CN S DIAZEPAM/CN	AN CN
Chemical Name Segment Definition (Compound Class)	/CNS /DEF	S KETOPROFEN/CNS S TYROSINES/DEF	CNS DEF
Entry Date (2) INCHI Key (2)	/ED (or /UP) /INCHI (or /INKY)	S AUG 2022/ED S MBOMYENWWXQSNW-AWEZLNQCLSA- N/INCHI	ED INCHI
Molecular Formula Molecular Weight (2)	/MF /MW (or /FW)	S C22H30N6O4S/MF S MW>500	MF MW
CAS Registry Number	/RN	S 40054-69-1/RN	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 CC CN DEF DRV  ED (UP) EIN FRM GI (PRE) INCHI (INKY) INT LD50 MF MW (FW) RE RN THER TRD	Accession Number Classification Code (ATC Code) Chemical Name Definition (Compound Class) Derivatives (comprises CN.DRV, EIN.DRV, LD50.DRV, MF.DRV, RN.DRV) Entry Date EINECS Number Formulation Graphical Image (Preparation(s)) INCHI Key Intermediate(s) Table Lethal Dose Molecular Formula Molecular Weight Reference CAS Registry Number Therapeutic Use Trade Table	DISPLAY L2 1-10 AN D CC DISPLAY CN 1-5 D DEF D DRV  D ED D EIN D FRM D GI L9 1-5 D INCHI D INT DIS LD50 D MF D MW D REF L5 1 DIS RN D THER D TRD
ALL  IALL IDE TRIAL (TRI, SAMPLE, SAM, FREE) SCAN (1)	AN, ED, CN, CC, THER, RN, MF, INCHI, MW, EIN, LD50, DEF, DRV, TRD, GI (PRE), INT, RE ALL, indented with text labels AN, ED, CN, CC, THER, RN, MF, INCHI, MW, EIN, DEF (default) AN, CN, CC  CN, CC (random display, no answer number)	D ALL  D IALL D IDE D TRIAL  D SCAN
HIT KWIC OCC	Hit term(s) and field(s) Up to 50 words before and after hit term(s) (KeyWord-In-Context) Number of occurrences of hit term(s) and field(s) in which they occur	D HIT D KWIC 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-
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

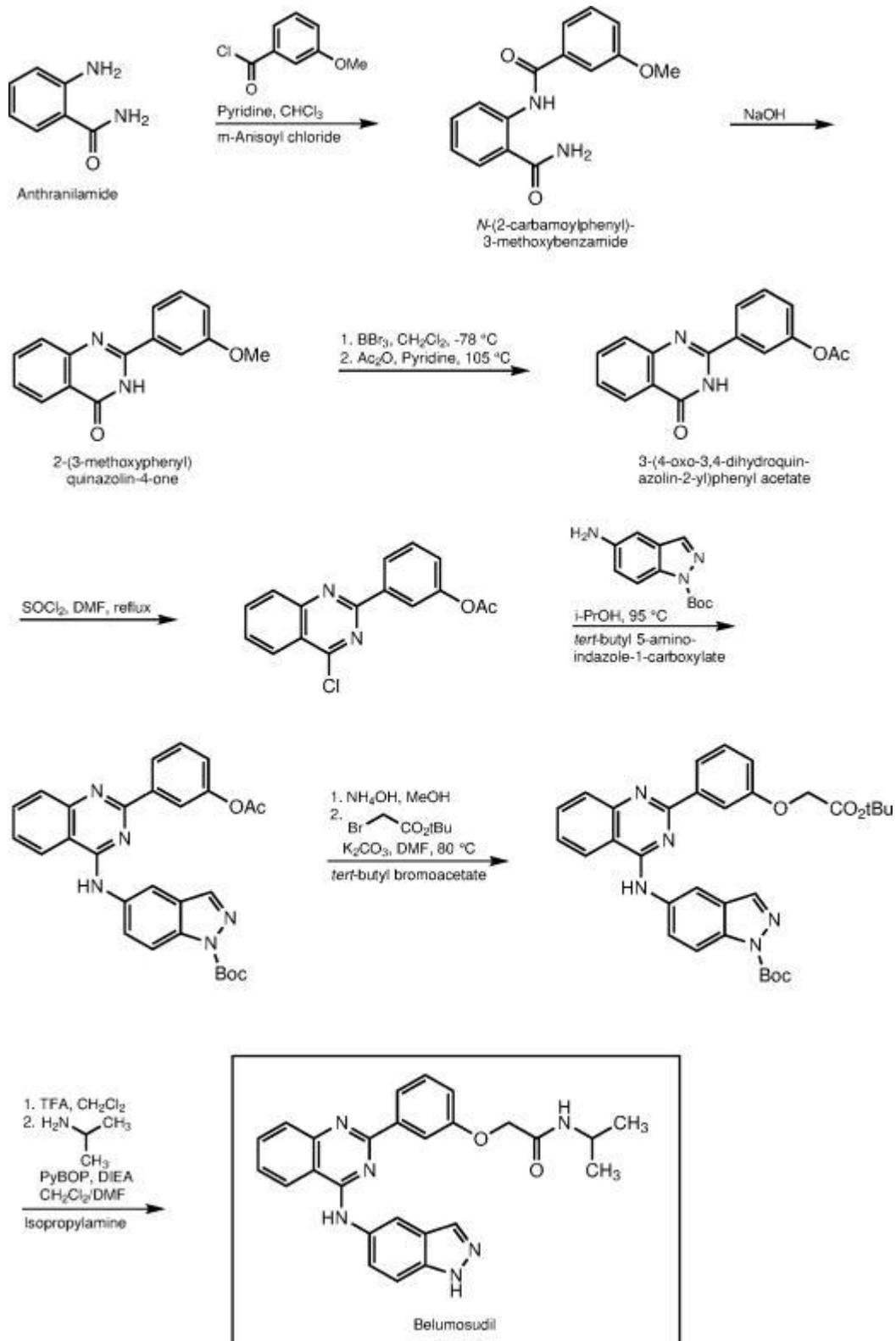
Trade Data

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

```

PREPARATIONS:



INT

Intermediate(s) in Substance Preparation

CAS RN |Molecular Formula|Chemical Name

88-68-6	C <sub>7</sub> H <sub>8</sub> N <sub>2</sub> O	Anthranilamide
1711-05-3	C <sub>8</sub> H <sub>7</sub> ClO <sub>2</sub>	m-Anisoyl chloride
330657-87-9	C <sub>15</sub> H <sub>14</sub> N <sub>2</sub> O <sub>3</sub>	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).

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