

PS (Pharmaceutical Substances)

Subject Coverage	<ul style="list-style-type: none"> Marketed Active Pharmaceutical Ingredients Preparation Methods for Pharmaceutical Substances 																
File Type	Substance (not structure searchable)																
Features	<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>CAS Registry Number® Identifiers</td> <td><input checked="" type="checkbox"/></td> <td>SLART</td> <td><input checked="" type="checkbox"/></td> </tr> <tr> <td>Keep & Share</td> <td><input checked="" type="checkbox"/></td> <td></td> <td></td> </tr> </table>	Thesaurus	None			Alerts (SDIs)	Not available			CAS Registry Number® Identifiers	<input checked="" type="checkbox"/>	SLART	<input checked="" type="checkbox"/>	Keep & Share	<input checked="" type="checkbox"/>		
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CAS Registry Number® Identifiers	<input checked="" type="checkbox"/>	SLART	<input checked="" type="checkbox"/>														
Keep & Share	<input checked="" type="checkbox"/>																
Record Content	<ul style="list-style-type: none"> 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	<ul style="list-style-type: none"> Pharmaceutical ingredients launched from 1957 – to date 2955 pharmaceutical substances 																
Coverage	1957 – to date																
Updates	Irregularly																
Language	English																
Database Producer	Georg Thieme Verlag Thieme Chemistry Rüdigerstr. 14 70469 Stuttgart Germany Phone: +49 711 8931-0 Email: marketing@thieme-chemistry.com 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), INCHI KEY (INKY) and CAS registry number (RN) fields)* (1)	None or /BI	S CODEINE/BI S 60-00-4 S C10H11NO3S S MBOMYENWWXQSNW	CN, DEF; INKY, RN
Accession Number Chemical Name (1)	/AN /CN	S 10006/AN S BETAMETHASONE ACETATE/CN S DIAZEPAM/CN	AN CN
Chemical Name Segment* (1) Definition (Compound Class) Entry Date (2) INCHI Key (2)	/CNS /DEF /ED /INKY (or INCHI)	S KETOPROFEN/CNS S TYROSINES/DEF S AUG 2022/ED S MBOMYENWWXQSNW-AWEZLNQCLSA- N/INKY	CNS DEF ED INKY
Molecular Formula Molecular Weight (2)	/MF /MW (or /FW)	S C22H30N6O4S/MF S MW>500	MF MW
CAS Registry Number Update Date (2)	/RN /UP	S 40054-69-1/RN S UP=2026	RN UP

(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	Entry Date	D ED
EIN	EINECS Number	D EIN
FRM	Formulation	D FRM
GI (PRE)	Graphical Image (Preparation(s))	D GI L9 1-5
INCH	INCHI Code	D INCHI
INKY (INCHI)	INCHI Key	D INKY
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
UP	Update Date	D UP

DISPLAY and PRINT Formats (cont'd)

ALL	AN, ED, CN, CC, THER, RN, MF, INCH, INKY, 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, INCH, INKY, 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
INCHI KEY	INKY (INCHI)	Y	Y
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: 10242 PS
 ENTRY DATE: Entered STN: 10 Apr 2026
 Last updated on STN: 10 Apr 2026
 CHEMICAL NAME: GENERIC: Avutometinib potassium
 SYNONYM: RO-5126766; CH-5126766; CKI-27; R-7304;
 RG-7304; VS-6766
 SYSTEMATIC: N-(3-fluoro-4-((4-methyl-2-oxo-7-(2-pyrimidinyl-2H-1-benzopyran-3-yl)methyl)-2-pyridinyl)-N'-methylsulfamide potassium salt
 THERAPEUTICS: dual MEK/RAF kinase inhibitor for the treatment of adult patients with KRAS-mutated recurrent low-grade serous ovarian cancer (LGSOC) in combination with the FAK inhibitor Fakzinja (defactinib)
 CAS REGISTRY NUMBER: 946128-90-1
 MOLECULAR FORMULA: C21H17FKN5O5S
 INCHI CODE: InChI=1S/C21H17FN5O5S.K/c1-12-15-5-4-14(31-21-25-7-3-8-26-21)11-17(15)32-20(28)16(12)10-13-6-9-24-19(18(13)22)27-33(29,30)23-2;/h3-9,11,23H,10H2,1-2H3;/q-1;+1
 INCHI KEY: KYKJFDDJHVJFIF-UHFFFAOYSA-N
 MOLECULAR WEIGHT: 509.55
 FORMULATION: Capsules containing 0.8 mg of avutometinib (corresponding to 0.864 mg of avutometinib potassium salt)
 DEFINITION: Pyridines; Pyrimidines; Sulfamides (Sulfuric diamides); Coumarins (2H-1-Benzopyran-2-ones)
 DERIVATIVES: CN.DRV Avutometinib (free base)
 LSF.DRV C21H18FN5O5S
 MW.DRV 471.46
 RN.DRV 946128-88-7

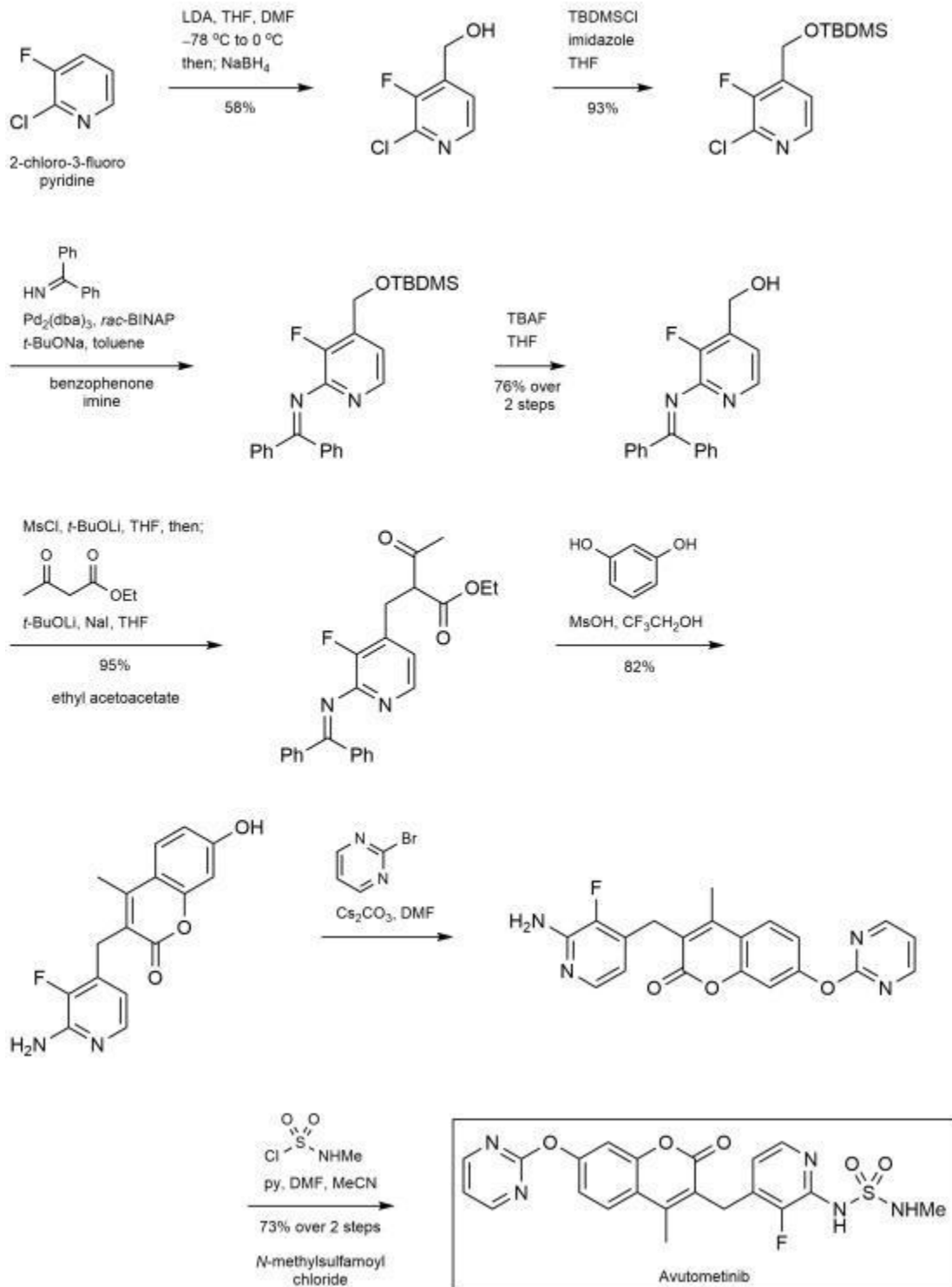
TRD

Trade Data

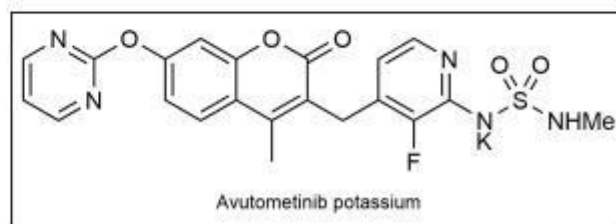
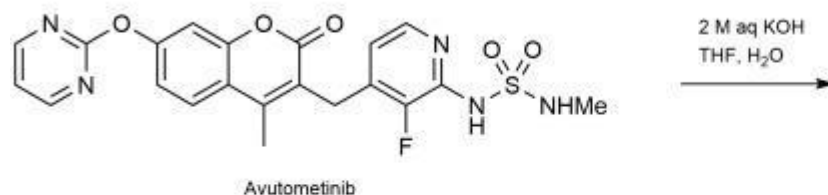
Launch	Trade Name	Company Name (Manufacturer)
Country		
=====+=====+=====		
USA	Avmapki	Verastem Oncology, 2025

PREPARATIONS:

a) Discovery synthesis:



b) Salt formation:



INT

Intermediate(s) in Substance Preparation

CAS RN	Molecular Formula	Chemical Name
1480-64-4	C5H3ClFN	2-chloro-3-fluoropyridine; - (CA Index Name)
1013-88-3	C13H11N	benzophenone imine; Benzophenone imine (CA Index Name)
141-97-9	C6H10O3	ethyl acetoacetate; Ethyl acetoacetate (CA Index Name)
108-46-3	C6H6O2	1,3-benzenediol; Resorcinol (CA Index Name)
4595-60-2	C4H3BrN2	2-bromopyrimidine; 2-Bromopyrimidine (CA Index Name)
10438-96-7	CH4ClNO2S	N-methylsulfamoyl chloride; N-Methylsulfamoyl chloride (CA Index Name)
4111-54-0	C6H14LiN	lithium diisopropylamide; - (CA Index Name)
109-99-9	C4H8O	tetrahydrofuran; Tetrahydrofuran (CA Index Name)
68-12-2	C3H7NO	N,N-dimethylformamide; Dimethylformamide (CA Index Name)
16940-66-2	NaBH4	sodium borohydride; Sodium borohydride (CA Index Name)
18162-48-6	C6H15ClSi	tert-butylchlorodimethylsilane; tert-Butyldimethylsilyl chloride (CA Index Name)
288-32-4	C3H4N2	imidazole; Imidazole (CA Index Name)
51364-51-3	C51H42O3Pd2	tris(dibenzylideneacetone)dipalladium(0); - (CA Index Name)
98327-87-8	C44H32P2	rac-BINAP; - (CA Index Name)
865-48-5	C4H9NaO	sodium tert-butoxide; Sodium tert-butoxide (CA Index Name)
108-88-3	C7H8	toluene; Toluene (CA Index Name)
429-41-4	C16H36FN	tetrabutylammonium fluoride; Tetrabutylammonium fluoride (CA Index Name)
124-63-0	CH3ClO2S	methanesulfonyl chloride; Methanesulfonyl chloride (CA Index Name)
1907-33-1	C4H9LiO	lithium tert-butoxide; - (CA Index Name)
7681-82-5	NaI	sodium iodide; - (CA Index Name)
75-75-2	CH4O3S	methanesulfonic acid; Methanesulfonic acid (CA Index Name)
75-89-8	C2H3F3O	2,2,2-trifluoroethanol; 2,2,2-Trifluoroethanol (CA Index Name)
534-17-8	Cs2CO3	cesium carbonate; - (CA Index Name)

110-86-1	C5H5N	pyridine; Pyridine (CA Index Name)
75-05-8	C2H3N	acetonitrile; Acetonitrile (CA Index Name)
1310-58-3	KOH	potassium hydroxide; Potassium hydroxide (CA Index Name)

REFERENCE:

WO2007091736A1 (Chugai; 16.08.2007; JP-prior. 09.02.2006).
US7897792B2 (Chugai; 01.03.2011; JP-prior. 09.02.2006).
a) Aoki, T. et al., ACS Med. Chem. Lett., (2014) 5, 309; DOI: 10.1021/ml400379x.
US11873296B2 (Verastem; 16.01.2024, US-prior. 07.06.2022).
US11517573B2 (Institute of Cancer Research; 06.12.2022, EP 13.09.2019).

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