

## CASBIOACTIVITY™ (File label CASBIOACTIVI)

This file is exclusive to STNext

- Subject Coverage**
- Pharmaceuticals\* (area of focus)
  - Drug Discovery
  - Materials
  - Structure-Activity Relationship Properties
  - ADME Properties
  - Toxicological Properties

**File Type** Substances, Bibliographic

- Features**
- |  |                                     |                       |                          |
|--|-------------------------------------|-----------------------|--------------------------|
| Thesaurus  | None                                |                       |                          |
| <a href="#">Alerts (SDIs)</a>                    | <input type="checkbox"/>            |                       |                          |
| <a href="#">CAS Registry Number® Identifiers</a> | <input checked="" type="checkbox"/> | <a href="#">SLART</a> | <input type="checkbox"/> |
| <a href="#">Keep &amp; Share</a>                 | <input type="checkbox"/>            | Structures            | <input type="checkbox"/> |

- Record Content**
- Bibliographic information and abstracts for patents and journal articles reporting bioactivity assay properties.
  - Information about the bioactivity assay properties including CAS Registry Numbers
  - Information about the Structure-Activity Relationship (SAR) Properties, ADME and TOXICITY Properties.
  - Designed to find relationships between chemical structure (or structural-related properties) and biological activity (or target property) of studied compounds.

- File Size**
- More than 4.99 million records (08/2023)

- Coverage**
- Includes 7245 peer reviewed scientific journals with continued expansion.
  - Includes global key patent offices from 1902-present
  - Total of 61M bioactivity measurements with ~20M normalized values from 37M document references.
  - Connect 24M ligand records and >7M unique substances to the CAS Registry

**Updates** Quarterly

**Language** English

**Database Producer**

CAS  
2540 Olentangy River Road  
P.O. Box 3012  
Columbus, Ohio 43210-0012 USA  
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Phone: 614-447-3731 (worldwide)  
Email: [help@cas.org](mailto:help@cas.org)  
Copyright Holder

**Sources**

- Patents
  - Journals
  - Linceptor, etc.
- 

**User Aids**

- Training materials are available on the CAS website at [www.cas.org](http://www.cas.org)
  - Online Helps (HELP DIRECTORY lists all help messages available)
- 

**Cluster**

- BIOSCIENCE
- MEDICINE
- PHARMACOLOGY
- STRUCTURE
- TOXICOLOGY

STN Database Cluster information:

<https://www.cas.org/support/training/stn/database-clusters>

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**Related  
Databases**

- CAplus
  - CAS Registry
-

## Search and Display Field Codes

All searchable text fields allow right truncation. The minimum stem length for right truncation is one (1) character.

### General Search Fields

Search Field Name	Search Code	Search Examples	Display Code
ADME Bio Type	/AABT	S IN VITRO CELL/AABT	AABT
ADME Cell	/AACL	S MDR1-MDCK CELLS/AACL	AACL
ADME Disease	/AADS	S (DEPRESSION (S) ANXIETY)/AADS	AADS
ADME Function	/AAFN	S ANTITUMOR AGENT/AAFN	AAFN
ADME Assay Locator	/AALC	S TABLE 1/AALC	AALC
ADME Assay Name	/AANM	S HALF LIFE/AANM	AANM
ADME Assay Procedure	/AAPR	S "t1/2 WAS ASSESSED"/AAPR	AAPR
ADME Species	/AASP	S RAT/AASP	AASP
ADME Assay Type	/AATP	S NON-CLINICAL TRIAL ADME STUDY/AATP	AATP
ADME Value	/AAVL	S "ORIG:0.31"/AAVL	AAVL
ADME Assay Count <sup>(1)</sup>	/ACNT	S 13/ACNT	ACNT
ADME Ligand Dose	/ALDS	S 0.1 µM/ALDS	ALDS
ADME Ligand RN	/ALRN	S 50-00-0/ALRN	ALRN
ADME Organ	/AORG	S LIVER/AORG	AORG
ADME Parameter	/APAM	S METABOLIC STABILITY/APAM	APAM
ADME Reference + Locator	/AREF	S COMPOUND/AREF	AREF
ADME Route of Administration	/ARTE	S I.V./ARTE	ARTE
ADME Target Name	/ATNM	S ESTROGEN RECEPTOR ALPHA/ATNM	ATNM
ADME Target RN	/ATRN	S 329978-01-0/ATRN	ATRN
Chemical Name	/CN	S CYCLOHEXENE/CN (XW) FLUOROCARB?	CN
Ligand Entry Date	/ED	S 2023//ED	ED
Field Availability	/FA	S SLOC/FA S SREF/FA	FA
Ligand InChI Key	/INKY	S QURWXBZNXHJZBE-MCDGZUPGSA?/INKY	INKY
Ligand RN	/RN	S 2410424-26-7/RN	RN
SAR Bio Type	/SABT	S IN VIVO/SABT	SABT
SAR Cell	/SACL	S CHO (S) CELL LINE/SACL S CHO CELL LINE/SACL	SACL
SAR Disease	/SADS	S CANCER/SADS S (OVARIAN (S) KIDNEY)/SADS S (OVARIAN (NOTS) KIDNEY)/SADS	SADS
SAR Function	/SAFN	S INHIBITOR/SAFN	SAFN
SAR Assay Name	/SANM	S ERBB2/SANM	SANM
SAR Parameter	/SPAM	S (IC50 (S) ORIG)SPAM NOT NORM(S)SPAM	SPAM
SAR Assay Procedure	/SAPR	S "[3H]KAINIC ACID"/SAPR	SAPR
SAR Species	/SASP	S HEPATI?/SASP	SASP
SAR Assay Type	/SATP	S "TISSUE/ORGAN BUT NOT ON WHOLE ANIMAL"/SATP	SATP
SAR Value <sup>(3)</sup>	/SAVL	S "10.5+/-0.25"/SAVL	SAVL
SARPROP Assay Count <sup>(1)</sup>	/SCNT	S 2911640-21-4/RN AND 22/SCNT	SCNT
SAR Ligand RN	/SLRN	S 2911640-21-4/SLRN	SLRN
SAR Reference + Locator	/SREF	S US?/SREF AND WO?/SREF	SREF
SAR Target Name	/STNM	S PLASMA KALLIKREIN/STNM	STNM
SAR Target RN	/STRN	S 345967-15-9/STRN	STRN
TOX Bio Type	/TABT	S IN VITRO CELL/TABT	TABT

## CASBIOACTIVITY

Search Field Name	Search Code	Search Examples	Display Code
TOX Cell	/TACL	S HEPATOCYTES/TACL	TACL
TOX Disease	/TADS	S PNEUMONIA/TADS	TADS
TOX Function	/TAFN	S ANTITUMOR AGENT/TAFN	TAFN
TOX Assay Locator	/TALC	S TABLE 2/TALC	TALC
TOX Assay Name	/TANM	S AMES TEST/TANM	TANM
TOX Assay Procedure	/TAPR	S COMPOUND/SAPR	SAPR
TOX Species	/TASP	S HUMAN/TASP	TASP
TOX Assay Type	/TATP	S FUNCTIONAL/TATP	TATP
TOX Value	/TAVL	S 30/TAVL	TAVL
TOX Assay Count <sup>(1)</sup>	/TCNT	S 5/TCNT	TCNT
TOX Ligand Dose	/TLDS	S 0.1 µM/TLDS	TLDS
TOX Ligand RN	/TLRN	S 50-0-0/TLRN	TLRN
TOX Parameter	/TPAM	S VIABLE CELLS/TPAM	TPAM
TOX Reference + Locator	/TREF	S 2017:861685/TREF	TREF
TOX Route of Administration	/TRTE	S P.O./TRTE	TRTE
TOX Target Name	/TTNM	S RABBIT/TTNM	TTNM
TOX Target RN	/TTRN	S 329967-85-3/TTRN	TTRN
TOX Type	/TXTP	S CYTOTOXICITY/TXTP	TXTP

- (1) No highlighting is supported for ACNT, SCNT, TCNT and ED fields when they are individually searched and displayed.
- (2) SAVL field is searched as TEXT only.
- (3) EXPANDs with the individual field codes are supported.

## DISPLAY and PRINT Formats

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

Hit term highlighting is available in most fields. With D SARPROP/ D HIT/ D <individual Field> Table view is presented. RN, CN, ED, INCH, INKY will be displayed as a header to the table.

Format	Content	Examples
AABT	ADME Bio Type	D AABT
AACL	ADME Cell	D AACL
AADS	ADME Disease	D AADS
AAFN	ADME Function	D AAFN
AALC	ADME Assay Locator	D AALC
AANM	ADME Assay Name	D AANM
AAPR	ADME Assay Procedure	D AAPR
AASP	ADME Species	D AASP
AATP	ADME Assay Type	D AATP
AAVL	ADME Value	D AAVL
ACNT	ADME Assay Count	D ACNT
ALDS	ADME Ligand Dose	D ALDS
ALRN	ADME Ligand RN	D ALRN
AORG	ADME Organ	D AORG
APAM	ADME Parameter	D APAM
AREF	ADME Reference + Locator	D AREF
ARTE	ADME Route of Administration	D ARTE
ATNM	ADME Target Name	D ATNM
ATRN	ADME Target RN	D ATRN
CN	Chemical Name (CA INDEX NAME)	D CN
ED	Ligand Entry Date	D ED
INCH	Ligand InChI String	D INCH
INKY	Ligand InChI Key	D INKY

Format	Content	Examples
RN	Ligand RN	D RN
SABT	SAR Bio Type	D SABT
SACL	SAR Cell	D SACL
SADS	SAR Disease	D SADS
SAFN	SAR Function	D SAFN
SANM	SAR Assay Name	D SANM
SPAM	SAR Parameter	D SPAM
SAPR	SAR Assay Procedure	D SAPR
SASP	SAR Species	D SASP
SATP	SAR Assay Type	D SATP
SAVL	SAR Value	D SAVL
SCNT	SARPROP Assay Count	D SCNT
SLRN	SAR Ligand RN	D SLRN
SREF	SAR Reference + Locator	D SREF
STNM	SAR Target Name	D STNM
STRN	SAR Target RN	D STRN
TABT	TOX Bio Type	D TABT
TACL	TOX Cell	D TACL
TADS	TOX Disease	D TADS
TAFN	TOX Function	D TAFN
TALC	TOX Assay Locator	D TALC
TANM	TOX Assay Name	D TANM
TPAM	TOX Parameter	D TPAM
TAPR	TOX Assay Procedure	D TAPR
TASP	TOX Species	D TASP
TATP	TOX Assay Type	D TATP
TXTP	TOX Toxicity Type	D TXTP
TAVL	TOX Value	D TAVL
TLDS	TOX Ligand Dose	D TLDS
TLRN	TOX Ligand RN	D TLRN
TREF	TOX Reference + Locator	D TREF
TRTE	TOX Route of Administration	D TRTE
TTNM	TOX Target Name	D TTNM
TCNT	TOX Assay Count	D TCNT
TTRN	TOX Target RN	D TTRN

## Predefined DISPLAY and PRINT Formats

Format	Content	Examples
ADMEPROP	RN, CN, ED, INCH, INKY, available ADME properties table	D ADMEPROP
SARPROP	RN, CN, ED, INCH, INKY, available SAR properties table	D SARPROP
TOXPROP	RN, CN, ED, INCH, INKY, available TOX properties table	D TOXPROP
HIT	RN, CN, ED, INCH, INKY, Fields containing IT terms	D HIT

## SELECT and ANALYZE 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.

Field Name	Field Code	Analyze	Select
ADME Bio Type	/AABT	Y	Y
ADME Cell	/AACL	Y	Y
ADME Disease	/AADS	Y	Y
ADME Function	/AAFN	Y	Y
ADME Assay Locator	/AALC	Y	Y
ADME Assay Name	/AANM	Y	Y
ADME Assay Procedure	/AAPR	Y	Y
ADME Species	/AASP	Y	Y
ADME Assay Type	/AATP	Y	Y
ADME Value	/AAVL	Y	Y
ADME Assay Count *	/ACNT	Y	Y
ADME Ligand Dose	/ALDS	Y	Y
ADME Ligand RN	/ALRN	Y	Y
ADME Organ	/AORG	Y	Y
ADME Parameter	/APAM	Y	Y
ADME Reference + Locator	/AREF	Y	Y
ADME Route of Administration	/ARTE	Y	Y
ADME Target Name	/ATNM	Y	Y
ADME Target RN	/ATRN	Y	Y
Chemical Name	/CN	Y	Y
Ligand Entry Date	/ED	Y	Y
Field Availability	/FA	Y	Y
Ligand InChI Key	/INKY	Y	Y
Ligand RN	/RN	Y	Y
SAR Bio Type	/SABT	Y	Y
SAR Cell	/SACL	Y	Y
SAR Disease	/SADS	Y	Y
SAR Function	/SAFN	Y	Y
SAR Assay Name	/SANM	Y	Y
SAR Parameter	/SPAM	Y	Y
SAR Assay Procedure	/SAPR	Y	Y
SAR Species	/SASP	Y	Y
SAR Assay Type	/SATP	Y	Y
SAR Value	/SAVL	Y	Y
SARPROP Assay Count	/SCNT	Y	Y
SAR Ligand RN	/SLRN	Y	Y
SAR Reference + Locator	/SREF	Y	Y
SAR Target Name	/STNM	Y	Y
SAR Target RN	/STRN	Y	Y
TOX Bio Type	/TABT	Y	Y
TOX Cell	/TACL	Y	Y
TOX Disease	/TADS	Y	Y
TOX Function	/TAFN	Y	Y
TOX Assay Locator	/TALC	Y	Y
TOX Assay Name	/TANM	Y	Y
TOX Assay Procedure	/TAPR	Y	Y
TOX Species	/TASP	Y	Y
TOX Assay Type	/TATP	Y	Y
TOX Value	/TAVL	Y	Y
TOX Assay count *	/TCNT	Y	Y

Field Name	Field Code	Analyze	Select
TOX Ligand Dose	/TLDS	Y	Y
TOX Ligand RN	/TLRN	Y	Y
TOX Parameter	/TPAM	Y	Y
TOX Reference + Locator	/TREF	Y	Y
TOX Route of Administration	/TRTE	Y	Y
TOX Target Name	/TTNM	Y	Y
TOX Target RN	/TTRN	Y	Y
TOX Type	/TXTP	Y	Y

## Sample Records

### DISPLAY SARPROP

⏪=> s 1214899-18-9; d sarprop

L1 1 1214899-18-9  
(1214899-18-9/RN)

L1 ANSWER 1 OF 1 CASBIOACTIVI COPYRIGHT 2023 ACS on STN

Ligand RN: **1214899-18-9**

Ligand Entry Date: 17 Jan 2023

Chemical Name: [1,2,4]Triazolo[1,5-a]pyridin-2-amine, N-phenyl-5-(1,2,3,6-tetrahydro-4-pyridinyl)- (CA Index Name)

Ligand InChI String: InChI=1S/C17H17N5/c1-2-5-14(6-3-1)19-17-20-16-8-4-7-15(22(16)21-17)13-9-11-18-12-10-13/h1-9,18H,10-12H2,(H,19,21)

Ligand InChI Key: DRIVGUZTNJAGIB-UHFFFAOYSA-N

#### SAR PROPERTIES

SARPROP Assay Count: 10

(1) Bahmanyar (Signal Pharmaceuticals, LLC), EP 2344494 B1,CAPLUS,2010:305749,EP 2344494 B1,Locator: compd 513(page 326)

TARGET NAME	TARGET RN	FUNCTION	PARAMETER	VALUE	DISEASE	SPECIES	ASSAY
Tyrosine kinase Syk	<b>138674-26-7</b>	Inhibitor	orig:IC50, norm:IC50	orig:1-10 uM, norm:1- 10 μM	Crohn's disease; Grave's disease; ulcerative colitis; multiple sclerosis; rheumatoid arthritis		<b>Assay</b>

(2) Bahmanyar, US Patent Application 2013/0005707 A1,CAPLUS,2010:305749,US 20130005707 A1,Locator: compd 513(page 295)

TARGET NAME	TARGET RN	FUNCTION	PARAMETER	VALUE	DISEASE	SPECIES	ASSAY
Tyrosine kinase Syk	<b>138674-26-7</b>	Inhibitor	orig:IC50, norm:IC50	orig:1-10 uM, norm:1- 10 μM	throat cancer; prostate cancer; breast cancer; blood cancer; osteoarthritis; Alzheimer's disease		<b>Assay</b>



## DISPLAY HIT

L2 1 1214899-18-9 AND THROAT CANCER/SADS

L2 ANSWER 1 OF 1 CASBIOACTIVI COPYRIGHT 2023 ACS on STN

RN 1214899-18-9 CASBIOACTIVI

Ligand RN: 1214899-18-9

Ligand Entry Date: 17 Jan 2023

Chemical Name: [1,2,4]Triazolo[1,5-a]pyridin-2-amine, N-phenyl-5-(1,2,3,6-tetrahydro-4-pyridinyl)- (CA Index Name)

Ligand InChI String: InChI=1S/C17H17N5/c1-2-5-14(6-3-1)19-17-20-16-8-4-7-15(22(16)21-17)13-9-11-18-12-10-13/h1-9,18H,10-12H2,(H,19,21)

Ligand InChI Key: DRIVGUZTNJAGIB-UHFFFAOYSA-N

## SAR PROPERTIES

SARPROP Assay Count: 10

(1) Bahmanyar, US Patent Application 2013/0005707 A1,CAPLUS,2010:305749,US 20130005707 A1,Locator: compd 513(page 295)

TARGET NAME	TARGET RN	FUNCTION	PARAMETER	VALUE	DISEASE	SPECIES	ASSAY
Tyrosine kinase Syk	138674-26-7	Inhibitor	orig:IC50, norm:IC50	orig:1-10 uM, norm:1- 10 µM	throat cancer; prostate cancer; breast cancer; blood cancer; osteoarthritis; Alzheimer's disease		Assay
Polo-like kinase PLK1	165245-99-8	Inhibitor	orig:IC50, norm:IC50	orig:<10 uM, norm:< 10 µM	throat cancer; prostate cancer; breast cancer; blood cancer; osteoarthritis; Alzheimer's disease		Assay
Tyrosine kinase FLT3		Inhibitor	orig:IC50, norm:IC50	orig:<10 uM, norm:< 10 µM	throat cancer; prostate cancer; breast cancer; blood cancer; osteoarthritis; Alzheimer's disease		Assay
					throat cancer; prostate cancer;		

DISPLAY SADS

Ligand RN:

Ligand Entry Date: 17 Jan 2023

Chemical Name: [1,2,4]Triazolo[1,5-a]pyridin-2-amine, N-phenyl-5-(1,2,3,6-tetrahydro-4-pyridinyl)- (CA Index Name)

Ligand InChI String: InChI=1S/C17H17N5/c1-2-5-14(6-3-1)19-17-20-16-8-4-7-15(22(16)21-17)13-9-11-18-12-10-13/h1-9,18H,10-12H2,(H,19,21)

Ligand InChI Key: DRIVGUZTNJAGIB-UHFFFAOYSA-N

SAR PROPERTIES

SARPROP Assay Count: 10

(1) Bahmanyar (Signal Pharmaceuticals, LLC), EP 2344494 B1,CAPLUS,2010:305749,EP 2344494 B1,Locator: compd 513(page 326)

DISEASE

ASSAY

Crohn's disease; Grave's disease; ulcerative colitis; multiple sclerosis; rheumatoid arthritis

(2) Bahmanyar, US Patent Application 2013/0005707 A1,CAPLUS,2010:305749,US 20130005707 A1,Locator: compd 513(page 295)

DISEASE

ASSAY

throat cancer; prostate cancer; breast cancer; blood cancer; osteoarthritis; Alzheimer's disease

throat cancer; prostate cancer; breast cancer; blood cancer; osteoarthritis; Alzheimer's disease

throat cancer; prostate cancer; breast cancer; blood cancer; osteoarthritis; Alzheimer's disease

throat cancer; prostate cancer; breast cancer; blood cancer; osteoarthritis; Alzheimer's disease

throat cancer; prostate cancer; breast cancer; blood cancer; osteoarthritis; Alzheimer's disease

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