CASBIOACTIVITY™ (File label CASBIOACTIVI)

Subject Coverage	• Pharmaceuticals (area of focus) • Drug Discovery • Structure-Activity Relationship Properties • ADME Properties • Toxicological Properties
File Type	Substances, Bibliographic
Features	Thesaurus — None Alerts (SDIs) — ☑ CAS Registry Number® Identifiers — ☑
Record Content	• Bibliographic information for patents and journal articles reporting bioactivity assays. • Information about reported bioactivity assays 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 5.9 million records (3/2026)
Coverage	• Over 7,000 peer reviewed scientific journals monitored for relevant content • Includes global key patent offices from 1902-present
Updates	Twice per week
Language	English
Database Producer	CAS 2540 Olentangy River Road P.O. Box 3012 Columbus, Ohio 43210-0012 USA Phone: 800-753-4227 (North America) Phone: 614-447-3731 (worldwide) Email: help@cas.org Copyright Holder
Sources	• Patents • Journals
User Aids	• Online Helps (HELP DIRECTORY lists all help messages available)
Cluster	• BIOSCIENCE • CASRNS • MEDICINE • PHARMACOLOGY • TOXICOLOGY STN Database Cluster information
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
Basic Index (contains single words from available general fields below noted with *)	None (or /BI)	S CHLORO S 1214899-18-9 S ICATIBANT	CN, RN
General Record Fields			
Chemical Name*	/CN	S CYCLOHEXENE/CN (XW) FLUOROCARB?	CN
Ligand Entry Date **(3)**	/ED	S 20250908/ED	ED
Ligand Update Date **(3)**	/UP	S 20251124/UP	UP
Field Availability	/FA	S AAOR/FA	FA
Ligand InChi Key	/INKY	S QURWXBZNHXJZBE-MCDGZUPGSA-N/INKY S QURWXBZNHXJZB?/INKY	INKY
Property Files	/PF	S ADMEPROP/PF	PF
Ligand RN*	/RN	S 2410424-26-7/RN	RN
Source Entry Date **(3)**	/SED	S 20250908/SED	SED
Source Update Date **(3)**	/SUP	S 20250908/SUP	SUP
Property File Type General Fields			
ADME Fields:			
ADME Assay Count **(1, 3)**	/AABT	S 13/ACNT	AABT
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 Assay Type *	/AATP	S NON-CLINICAL TRIAL ADME STUDY/AATP	AATP
ADME Bio Type *	/AABT	S IN VITRO/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 Ligand Dose *	/ALDS	S 0.1 µM/ALDS	ALDS
ADME Organ *	/AORG	S LIVER/AORG	AORG
ADME Organism *	/AAOR	S RATTUS?/AAOR	AAOR
ADME Parameter *	/APAM	S METABOLIC STABILITY/APAM	APAM
ADME Reference + Locator *	/AREF	S COMPOUND/AREF	AREF
ADME Route of Administration *	/ARTE	S INTRAVENOUS/ARTE	ARTE
ADME Target Name *	/ATNM	S ESTROGEN RECEPTOR ALPHA/ATNM	ATNM
ADME Target RN	/ATRN	S 329978-01-0/ATRN	ATRN
ADME Value * **(2)**	/AAVL	S 260/AAVL	AAVL
Structure Activity Relationship Fields:			
SAR Assay Count **(1,3)**	/SCNT	S 2911640-21-4/RN AND 22/SCNT	SCNT
SAR Assay Name *	/SANM	S ERBB2/SANM	SANM
SAR Assay Procedure *	/SAPR	S "[3H]KAINIC ACID"/SAPR	SAPR
SAR Assay Type *	/SATP	S BINDING/SATP	SATP
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 Organism *	/SAOR	S RATTUS NORVEGICUS/SAOR	SAOR
SAR Parameter *	/SPAM	S (PROTEIN (S) EXPRESSION)/SPAM S DIABETES AND "FOOD INTAKE"/SPAM	SPAM
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
SAR Value * **(2)**	/SAVL	S 10.5/SAVL	SAVL

General Search Fields (cont.)

Search Field Name	Search Code	Search Examples	Display Code
Property File Type General Fields (cont.)			
TOX Fields:			
TOX Assay Count **(1,3)**	/TCNT	S 5/TCNT	TCNT
TOX Assay Locator *	/TALC	S TABLE 2/TALC	TALC
TOX Assay Name *	/TANM	S AMES TEST/TANM	TANM
TOX Assay Procedure *	/TAPR	S MTT ASSAY/TAPR	TAPR
TOX Assay Type *	/TATP	S FUNCTIONAL/TATP	TATP
TOX Bio Type *	/TABT	S IN VITRO/TABT S IN VIVO/TABT	TABT
TOX Cell *	/TACL	S HEPATOCYTES/TACL	TACL
TOX Disease *	/TADS	S PNEUMONIA/TADS	TADS
TOX Function *	/TAFN	S ANTITUMOR AGENT/TAFN	TAFN
TOX Ligand Dose *	/TLDS	S 0.1 µM/TLDS	TLDS
TOX Organism *	/TAOR	S HUMAN/TAOR	TAOR
TOX Parameter *	/TPAM	S ADVERSE EFFECT/TPAM	TPAM
TOX Reference + Locator *	/TREF	S 2017(W)861685/TREF	TREF
TOX Route of Administration *	/TRTE	S CUTANEOUS/TRTE	TRTE
TOX Target Name *	/TTNM	S RABBIT/TTNM	TTNM
TOX Target RN	/TTRN	S 330196-93-5/TTRN	TTRN
TOX Toxicity Type*	/TXTP	S CYTOTOXICITY/TXTP	TXTP
TOX Value * **(2)**	/TAVL	S 30/TAVL	TAVL

(1) No highlighting is supported for ACNT, SCNT, TCNT, and ED fields when they are individually searched and displayed.
(2) AAVL, SAVL, and TAVL fields are searched as text only.
(3) Numeric search field that may be searched with numeric operators or ranges.

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 Property File field> a table display is presented. RN, CN**, ED, INCH**, and INKY** will be displayed as a header to the table (***when available).*

Format	Content	Examples
ACNT	ADME Assay Count	D ACNT
AALC	ADME Assay Locator	D AALC
AANM	ADME Assay Name	D AANM
AAPR	ADME Assay Procedure	D AAPR
AATP	ADME Assay Type	D AATP
AABT	ADME Bio Type	D AABT
AACL	ADME Cell	D AACL
AADS	ADME Disease	D AADS
AAFN	ADME Function	D AAFN
ALDS	ADME Ligand Dose	D ALDS
AORG	ADME Organ	D AORG
AAOR	ADME Organism	D AAOR
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
AAVL	ADME Value	D AAVL
CN	Chemical Name (CA INDEX NAME)	D CN

DISPLAY and PRINT Formats (cont.)

Format	Content	Examples
INCH	InChI Code	D INCH
INKY	Ligand InChI Key	D INKY
ED	Ligand Entry Date	D ED
RN	Ligand RN	D RN
PF	Property File	D PF
SCNT	SAR Assay Count	D SCNT
SANM	SAR Assay Name	D SANM
SAPR	SAR Assay Procedure	D SAPR
SATP	SAR Assay Type	D SATP
SABT	SAR Bio Type	D SABT
SACL	SAR Cell	D SACL
SADS	SAR Disease	D SADS
SAFN	SAR Function	D SAFN
SAOR	SAR Organism	D SAOR
SPAM	SAR Parameter	D SPAM
SREF	SAR Reference + Locator	D SREF
STNM	SAR Target Name	D STNM
STRN	SAR Target RN	D STRN
SAVL	SAR Value	D SAVL
SED	Source Entry Date	D SED
SUP	Source Update Date	D SUP
TCNT	TOX Assay Count	D TCNT
TALC	TOX Assay Locator	D TALC
TANM	TOX Assay Name	D TANM
TAPR	TOX Assay Procedure	D TAPR
TATP	TOX Assay Type	D TATP
TABT	TOX Bio Type	D TABT
TACL	TOX Cell	D TACL
TADS	TOX Disease	D TADS
TAFN	TOX Function	D TAFN
TLDS	TOX Ligand Dose	D TLDS
TAOR	TOX Organism	D TAOR
TPAM	TOX Parameter	D TPAM
TREF	TOX Reference + Locator	D TREF
TRTE	TOX Route of Administration	D TRTE
TTNM	TOX Target Name	D TTNM
TTRN	TOX Target RN	D TTRN
TXTP	TOX Toxicity Type	D TXTP
TAVL	TOX Value	D TAVL
UP	Update Date	D UP

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 HIT 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 Assay Count	/ACNT	Y	Y
ADME Assay Locator	/AALC	Y	Y
ADME Assay Name	/AANM	Y	Y
ADME Assay Procedure	/AAPR	Y	Y
ADME Assay Type	/AATP	Y	Y
ADME Bio Type	/AABT	Y	Y
ADME Cell	/AACL	Y	Y
ADME Disease	/AADS	Y	Y
ADME Function	/AAFN	Y	Y
ADME Ligand Dose	/ALDS	Y	Y
ADME Organ	/AORG	Y	Y
ADME Organism	/AAOR	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
ADME Value	/AAVL	Y	Y
Chemical Name	/CN	Y	Y
Field Availability	/FA	N	Y
Ligand InChI Key	/INKY	Y	Y
Ligand Entry Date	/ED	Y	Y
Ligand RN	/RN	Y	Y
SAR Assay Count	/SCNT	Y	Y
SAR Assay Name	/SANM	Y	Y
SAR Assay Procedure	/SAPR	Y	Y
SAR Assay Type	/SATP	Y	Y
SAR Bio Type	/SABT	Y	Y
SAR Cell	/SACL	Y	Y
SAR Disease	/SADS	Y	Y
SAR Function	/SAFN	Y	Y
SAR Organism	/SAOR	Y	Y
SAR Parameter	/SPAM	Y	Y
SAR Reference + Locator	/SREF	Y	Y
SAR Target Name	/STNM	Y	Y
SAR Target RN	/STRN	Y	Y
SAR Value	/SAVL	Y	Y
Source Entry Date	/SED	Y	Y
Source Update Date	/SUP	Y	Y
TOX Assay Count	/TCNT	Y	Y
TOX Assay Locator	/TALC	Y	Y
TOX Assay Name	/TANM	Y	Y
TOX Assay Procedure	/TAPR	Y	Y
TOX Assay Type	/TATP	Y	Y
TOX Bio Type	/TABT	Y	Y
TOX Cell	/TACL	Y	Y
TOX Disease	/TADS	Y	Y
TOX Function	/TAFN	Y	Y
TOX Ligand Dose	/TLDS	Y	Y
TOX Organism	/TAOR	Y	Y

SELECT and ANALYZE Fields (cont.)

Field Name	Field Code	Analyze	Select
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 Toxicity Type	/TXTP	Y	Y
TOX Value	/TAVL	Y	Y
Update Date	/UP	Y	Y

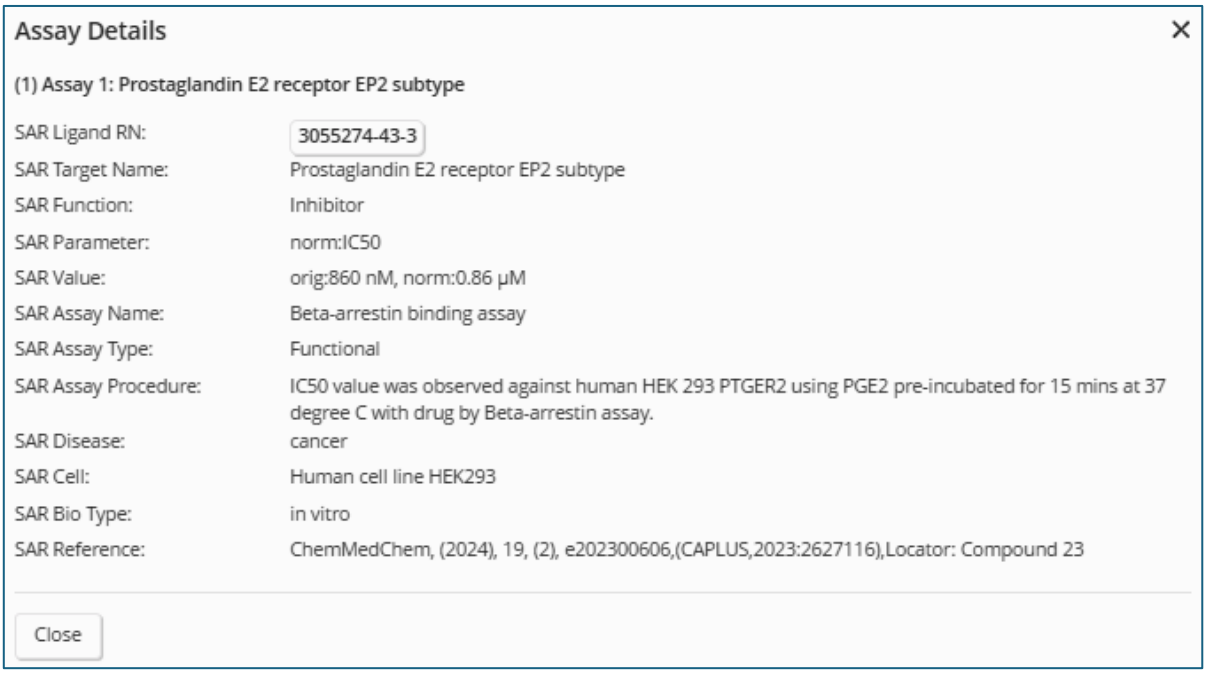
Sample Records

DISPLAY SARPROP

```
=> s 3055274-43-3/rn; d sarprop

L1           1 3055274-43-3/RN


L1   ANSWER 1 OF 1  CASBIOACTIVI  COPYRIGHT 2025 ACS on STN
Ligand RN: 3055274-43-3
Ligand Entry Date: 04 Aug 2025
Chemical Name: Benzoic acid, 4-[[[(5-benzo[b]thien-3-yl-2,3-dimethoxyphenyl)methyl]amino]methyl]-   (CA Index Name)
Ligand InChI String: InChI=1S/C25H23NO4S/c1-29-22-12-18(21-15-31-23-6-4-3-5-20(21)23)11-19(24(22)30-2)14-26-13-16-7-
9-17(10-8-16)25(27)28/h3-12,15,26H,13-14H2,1-2H3,(H,27,28)
Ligand InChI Key: AFGYXLCJSJFJMZ-UHFFFAOYSA-N
Property Files: SARPROP

SAR PROPERTIES
SARPROP Assay Count: 2
(1) ChemMedChem, (2024), 19, (2), e202300606,(CAPLUS,2023:2627116),Locator: Compound 23
```

TARGET NAME	TARGET RN	FUNCTION	PARAMETER	VALUE	DISEASE	ORGANISM	ASSAY
Prostaglandin E2 receptor EP2 subtype		Inhibitor	norm:IC50	orig:860 nM, norm:0.86 µM	cancer		Assay
Prostaglandin E2 receptor EP4 subtype		Inhibitor	norm:IC50	orig:190 nM, norm:0.19 µM	cancer		Assay

Additional data presented in popup display window when Assay button presented in table is clicked:



DISPLAY HIT

```
=> s 3059393-11-9/rn and antimicrobial; d hit

             1 3059393-11-9/RN
         31260 ANTIMICROBIAL
           127 ANTIMICROBIALS
         31275 ANTIMICROBIAL
                (ANTIMICROBIAL OR ANTIMICROBIALS)
L1           1 3059393-11-9/RN AND ANTIMICROBIAL

L1   ANSWER 1 OF 1  CASBIOACTIVI  COPYRIGHT 2025 ACS on STN
RN   3059393-11-9  CASBIOACTIVI
Ligand RN: 3059393-11-9
Ligand Entry Date: 08 Sep 2025
Ligand InChI String: InChI=1S/2C4H6N2.2C3H4O2.Cu/c2*1-4-5-2-3-6-4;2*1-2-3(4)5;/h2*2-3H,1H3,(H,5,6);2*2H,1H2,
(H,4,5);/q;;;;+2/p-2
Ligand InChI Key: RXQULRVNFPWCDD-UHFFFAOYSA-L
Property Files: SARPROP
```

SAR PROPERTIES

SARPROP Assay Count: 5
(1) Molecules, (2018), 23, (12), 3253/1-3253/17,(CAPLUS,2019:697186),Locator: Complex 1

TARGET NAME	TARGET RN	FUNCTION	PARAMETER	VALUE	DISEASE	ORGANISM	ASSAY
Bacillus subtilis		Inhibitor	orig:Antimicrobial activity, norm:Zone of inhibition	norm:Improved	disease by infectious agent		Assay
Pseudomonas aeruginosa ATCC 27853		Inhibitor	orig:Antimicrobial activity, norm:Zone of inhibition	norm:Exhibited	disease by infectious agent		Assay
Staphylococcus aureus ATCC 25923		Inhibitor	orig:Antimicrobial activity, norm:Zone of inhibition	norm:Improved	disease by infectious agent		Assay
Escherichia coli ATCC 25922		Inhibitor	orig:Antimicrobial activity, norm:Zone of inhibition	norm:Exhibited	disease by infectious agent		Assay

DISPLAY SADS (Custom Display)

Ligand RN: 1579961-75-3
Ligand Entry Date: 26 Jun 2025
Ligand InChI String: InChI=1S/C24H24N4/c1-2-8-21(9-3-1)27-16-14-26(15-17-27)18-20-19-28(24-12-6-7-13-25-24)23-11-5-4-10-22(20)23/h1-13,19H,14-18H2

SAR PROPERTIES

SARPROP Assay Count: 2
(1) Eur. J. Med. Chem., 2014, 75 (), 159-168,(CAPLUS,2014:367503),MEDLINE,24531229,Locator: Compound 3v (Page No: 160, Table No: 2)

DISEASE	ASSAY
sleeping sickness; schizophrenia; depression; memory deficit; circadian rhythm disorder	Assay
sleeping sickness; schizophrenia; depression; memory deficit; circadian rhythm disorder	Assay

APPEARANCE OF PROPERTY TABLE IN TRANSCRIPT

SARPROP example

```
L7   ANSWER 1 OF 1  CASBIOACTIVI  COPYRIGHT 2025 ACS on STN

Ligand RN: 3037142-87-0
Ligand Entry Date: 26 Jun 2025
Chemical Name: Imidazo[1,2-a]pyridine-2-carboxamide,
3-ethyl-N-(tetrahydro-4-methyl-1,1-dioxido-2H-thiopyran-4-yl)-6-[[3-(2,2,2-trifluoroeth
oxy)-2-pyridinyl]oxy]-   (CA Index Name)
Ligand InChI String:
InChI=1S/C23H25F3N4O5S/c1-3-16-19(20(31)29-22(2)8-11-36(32,33)12-9-22)28-18-7-6-15(13-3
0(16)18)35-21-17(5-4-10-27-21)34-14-23(24,25)26/h4-7,10,13H,3,8-9,11-12,14H2,1-2H3,(H,2
9,31)
Ligand InChI Key: SISQNLSFTTXFSY-UHFFFAOYSA-N
Property Files: SARPROP
SARPROP Assay Count: 1

(1) Assay 1: Diacylglycerol O-acyltransferase 2
SAR Ligand RN: 3037142-87-0
SAR Target Name: Diacylglycerol O-acyltransferase 2
SAR Target RN: 1776102-82-9
SAR Function: Inhibitor
SAR Parameter: norm:IC50
SAR Value: orig:44 nM, norm:0.044 µM
SAR Assay Name: Enzyme inhibition assay
SAR Assay Type: Functional
SAR Cell: Spodoptera frugiperda cell line SF9
SAR Bio Type: in vitro
SAR Reference: PCT Int. Appl., 173pp.,CAPLUS,2024:1012387,Locator: Example 115
SAR Assay Procedure: IC50 was determined against human diacylglyceride O-acyltransferase
2 in Spodoptera frugiperda cell line SF9.
```

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