

CAS SciFinder®

ライフサイエンスデータの検索

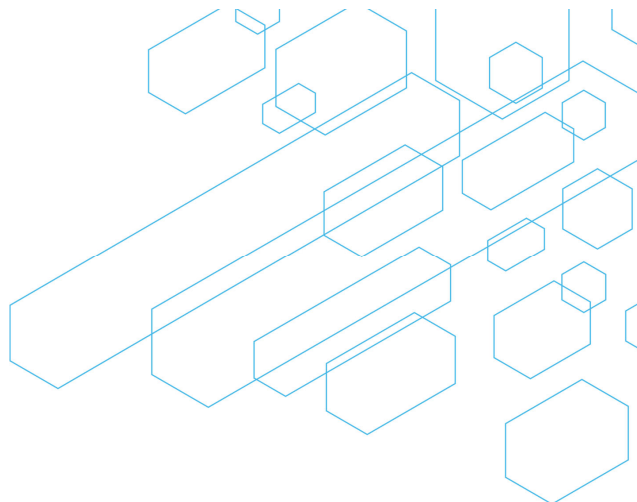
化学情報協会 情報事業部
2026/6

© 2026 American Chemical Society. All rights reserved.



本日の内容

- CAS SciFinder のライフサイエンスデータ
- ライフサイエンスデータの検索



CAS SciFinder のライフサイエンスデータ

3

© 2026 American Chemical Society. All rights reserved.



CAS Life Sciences Data

- **Pharmacological Data**

薬理学的データ (IC 50、EC 50 など)

- **ADME**

ADME (吸収・分布・代謝・排泄) データ ($C_{\max}$ 、 $t_{1/2}$ 、AUC など)

- **Toxicity**

毒性 (LD50、NOAEL など)

- **Biomarkers**

ターゲットと疾患の関連性を示す分子指標 (文献情報に収録)

4

© 2026 American Chemical Society. All rights reserved.



CAS Life Sciences Data

ライフサイエンスデータは物質と文献情報に収録されている

CAS Registry Number: 2647530-73-0

物質の詳細情報

C22H17ClF3N9O2

Patents Containing Substance in Claims

Substituted pyrazolo[3,4-b]pyridine compounds as SARS-CoV-2 papain-like protease inhibitors and methods of their use

Role: Pharmacological Activity, Therapeutic Use

Patent Number: US20200152399

Publication Date: 2020-05-07

Method for treating coronavirus infection in patient with obeliskvir

Role: Adverse Effect, Including Toxicity, Pharmacological Activity, Therapeutic Use

Patent Number: WO2020060034

この物質に対して報告されている薬理学的データ

Pharmacological Data

Target	Function	Parameter	Value	Disease	Organism	Assay	Source
Replicase polyprotein 1ab	Inhibitor	EC50	0.17 μM	COVID-19	Severe acute respiratory syndrome coronavirus 2	View Detail	(1) CAS
Replicase polyprotein 1ab	Inhibitor	EC50	0.27 μM	COVID-19	Severe acute respiratory syndrome coronavirus 2	View Detail	(1) CAS
Replicase polyprotein 1ab	Inhibitor	EC50	0.22 μM	COVID-19	Severe acute respiratory syndrome coronavirus 2	View Detail	(1) CAS
Replicase polyprotein 1ab	Inhibitor	EC50 ratio	1.59	COVID-19	Severe acute respiratory syndrome coronavirus 2	View Detail	(1) CAS

(1) Eltayb, Wafa A.; ACS Omega (2023), 8(6), 5234-5246, Caplus and MEDLINE
(2) Sasaki, Michihito; Science Translational Medicine (2023), 15(679), eabq064, Caplus and MEDLINE

Novel Investigational Anti-SARS-CoV-2 Agent Ensitrivir "S-217622"
Broad-Spectrum Antiviral at the Therapeutic Frontline of COVID-19

文献の詳細情報

By: Eltayb, Wafa A.; Abdellah, Mohamed; Rabie, Amgad M.

DOI: 10.1021/acscomega.2c03881

Lately, nitrogenous heterocyclic antivirals, such as nucleoside-like compounds, oxadiazoles, thiazidiazoles, triazoles, quinolines, and isoxanthenes, topped the therapeutic scene as promising agents of choice for the treatment of the severe acute respiratory syndrome coronavirus 2 (SARS-CoV-2) infections and their accompanying ailments, the coronavirus disease 2019 (COVID-19). At the same time, the continuous emergence of new strains of SARS-CoV-2, like the Omicron variant and its multiple sublineages, resulted in a new defence in the enduring COVID-19 battle. Ensitrivir (S-217622) is a newly discovered orally active nonnucleoside nonpeptidic agent with potential strong broad-spectrum anticonvulsant activities, exhibiting promising nanomolar potencies against the different SARS-CoV-2 variants. S-217622 effectively and nonspecifically hits the main protease (M^{pro}) enzyme of a broad scope of coronaviruses. Herein, in the present computational study, we tried to extend these previous findings to prove the universal activities of this investigational agent against any coronavirus, irrespectively of its type, through synchronously acting on most of its main unchanged replication enzymes/proteins, including (in addition to the M^{pro}), e.g., the highly conserved RNA-dependent RNA polymerase (RdRp) and 3'-5' exonuclease (ExoN). Biochem. evaluation proved, using the in vitro anti-RdRp bioassay, that S-217622 can potentially inhibit the replication of coronaviruses, including the new virulent strains of SARS-CoV-2, with extremely minute in vitro anti-RdRp and anti-RdRp/ExoN half-maximal effective concentration (EC₅₀) values of 0.17 and 0.27 μM, resp., transcending the anti-COVID-19 drug molinivir. The preliminary in silico results greatly supported these biochem. results, proposing that the S-217622 mol. strongly and stably binds to the key catalytic pockets of the SARS-CoV-2 RdRp and ExoN's principal active sites predictably via the nucleoside analog mode of anti-RNA action (once the S-217622 mol. can be considered as a uridine analog). Moreover, the specific drug-likeness and pharmacokinetic characteristics of S-217622 make it ready for pharmaceutical formulation with the expected very good clin. behavior as a drug for the infections caused by coronaviruses, e.g., COVID-19. To cut it short, the current critical findings of this extension work significantly potentiate and extend the S-217622's previous in vitro/in vivo (preclin.) results since they showed that the striking inhibitory activities of this novel anti-SARS-CoV-2 agent on the M^{pro} could be extended to other replication enzymes like RdRp and ExoN, unveiling the possible universal use of this compound against the next versions of the virus (i.e., disclosing the nonspecific anticonvulsant properties of this compound against almost any coronavirus strain, e.g., SARS-CoV-3, and encouraging us to rapidly start the compound's vast clin. anti-COVID-19 evaluations.

この文献に記載の薬理学的データ

Pharmacological Data

Ligand	Target	Function	Parameter	Value	Disease	Organism	Assay
2647530-73-0	Replicase polyprotein 1ab	Inhibitor	EC50 ratio	1.59	COVID-19	Severe acute respiratory syndrome coronavirus 2	View Detail

相互にリンク

5 © 2026 American Chemical Society. All rights reserved.

ライフサイエンスデータの検索

6 © 2026 American Chemical Society. All rights reserved.

Advanced Search

物質/文献の切り替え

184475-35-2

情報を組み合わせての検索が可能

AND Target EGFR

Molecular Formula

CAS Registry Number

Chemical Identifier

Document Identifier

Patent Identifier

Experimental Spectra

Life Science Data

Biological

Chemical Properties

Target

Ligand

Disease

ライフサイエンスデータはターゲット、リガンド、疾患の情報から検索できる

Proton nmr spectral data for C13H13Br

Featured Search

Prior Art Discovery

Patent Markush

Advanced Search

Retrosynthetic Analysis

7 © 2026 American Chemical Society. All rights reserved.



ライフサイエンスデータを持つ物質の絞り込み

Life Science Data フィルター

Life Science Data フィルター

ライフサイエンスデータが収録されている文献に限定できる
(報告されているパラメータでは限定できない)

▼ Reference Role

▲ Life Science Data

☐ Pharmacological Data (2)

☐ ADME (1)

☐ Toxicity (1)

▼ Commercial Availability

▼ Number of Components

8 © 2026 American Chemical Society. All rights reserved.



ライフサイエンスデータの確認 (1/2)

Substances Advanced search 検索結果画面

View Related Results

Filter Results

Analyze Results

Structure Match

As Drawn (0)

Substructure (119)

Similarity (22)

Analyze Structure Precision

Behavior

Filter by Exclude

Search Within Results

Search for up to 3 structures within the result set.

Draw

Search

Reaction Role

Product (114)

Reactant (9)

Reagent (1)

CAS Registry Number: 184475-35-2 物質の詳細

16K 898 109 View in CAS BioFinder

C22H24ClFN4O3
4-Quinazolinamine, N-(3-chloro-4-fluorophenyl)-7-methoxy-6-[3-(4-morpholinyl)propoxy]- (9CI, ACI)

Properties

Properties	Value	Condition
Molecular Weight	446.90	-
Melting Point (Experimental)	196 °C	-
Boiling Point (Predicted)	586.755±50.00 °C	Press: 760.00 Torr
Density (Predicted)	1.323±0.06 g/cm³	Temp: 25 °C; Press: 760 Torr
pKa (Experimental)	7.20	-

Experimental Properties | Spectra

Other Names

Experimental Spectra

Pharmacological Data

ADME

Toxicity

Predicted Properties

Patents Containing Substance in Claims

Startrace: multiplex drug testing platform for personalized medicine

Patent Number: US20260139320

Publication Date: 2026-05-21

Combination of RAS inhibitor and EGFR inhibitor and use thereof

Patent Number: WO2026103823

Publication Date: 2026-05-21

RAS and EGFR inhibitors combination therapy for cancer treatment

Patent Number: WO2026107237

Publication Date: 2026-05-21

View All Patents

ライフサイエンスデータは物質/文献の詳細情報にあるCAS LIFE SCIENCESのタブから確認ができる (→ p.10)

ライフサイエンスデータの確認 (2/2)

Pharmacological Data

アッセイ情報の詳細

Target	Function	Parameter
WT : L858R/T790M	Inhibitor	IC50
Wi-38 cell	Inhibitor	IC50
Vascular endothelial growth factor receptor 2	Inhibitor	IC50
Vascular endothelial growth factor receptor 2	Inhibitor	IC50

Assay Data CAS LIFE SCIENCES

← Prev (2 of 1,348) Next →

Ligand: 184475-35-2

Target: Wi-38 cell

Assay Name: MTT assay

Procedure: IC50 of gefitinib was measured on human cell line Wi-38 incubated for 24 h using MTT assay.

Assay Comment: -

Condition: -

Parameter: IC50

Value: 35.1 µM

Measurement Remarks: -

Ligand Dose: -

Biological System: In vitro: Homo sapiens: Human cell line Wi-38; Lung fibroblast cell line: Homo sapiens

Source: Discovery of novel thiazolyl-pyrazolines as dual EGFR and VEGFR-2 inhibitors endowed with in vitro antitumor activity towards non-small lung cancer
By: Abdelsalam, Esraa A.; Abd El-Hafeez, Amer Ali; Eldehna, Wagdy M.; El Hassab, Mahmoud A.; Marzouk, Hala Mohamed M.; Elasser, Mahmoud M.; Abou Taleb, Nageh A.; Amin, Kamilla M.; Abdel-Aziz, Hatem A.; Ghosh, Pradipta; et al

Knowledge Graph → p.12

CAS LIFE SCIENCES

Knowledge Graph

Assay Source

ダウンロード

View Detail (2) CAS

View Detail (3) CAS

View Detail (4) CAS

出典文献へのリンク

(1) Yi, Yuanyuan; Chemical Biology & Drug Design (2018), 92(6), 1988-1997, Cplup and MEDLINE

(2) Abdelsalam, Esraa A.; Journal of Enzyme Inhibition and Medicinal Chemistry (2022), 37(1), 2265-2282, Cplup and MEDLINE

(3) Hasan Alshammari, Aya; Biochemical Pharmacology (Amsterdam, Netherlands) (2022), 197114914, Cplup and MEDLINE

(4) Jing, Tongfei; Bioorganic & Medicinal Chemistry (2018), 26(8), 1784-1796, Cplup and MEDLINE

表示するパラメータ等の指定

Pharmacological Data

昇順/降順の設定

ライフサイエンスデータの表に表示する項目はフィルターで選択できる

Filter Parameter

☒ IC50 (642)
☐ Protein expression (267)
☐ Protein phosphorylation (139)
☐ Cell viability (75)
☐ Gene expression (67)
☐ Combination index (60)

Clear Apply

Target	Function	Parameter	Value	Disease	Organism	Assay	Source
Epidermal growth factor receptor	Inhibitor	IC50		inhibition of cellular proliferation	Homo sapiens	View Detail	(1) CAS
Epidermal growth factor receptor	Inhibitor	IC50		lung cancer	-	View Detail	(2) CAS
Epidermal growth factor receptor	Inhibitor	IC50		lung cancer	-	View Detail	(2) CAS
Epidermal growth factor receptor	-	IC50		lung non-small cell carcinoma	-	View Detail	(3) CAS
Epidermal growth factor receptor	-	IC50	0.056 μM	-	-	View Detail	(4) CAS
Epidermal growth factor receptor	Inhibitor	IC50	0.011 μM	-	Homo sapiens	View Detail	(5) CAS



Knowledge Graph

Knowledge Graph

リガンド、疾患、ターゲットの関連性を可視化

View Detail (1) CAS

Knowledge Graph for Pharmacological Data

Filter Behavior

Filter by Exclude

Target

☒ Epidermal growth factor receptor (64)
☐ Receptor tyrosine-protein kinase erbB-2 (15)
☐ GTPase KRas (13)
☐ Phosphatidylinositol 3,4,5-trisphosphate 3-phosphatase and dual-specificity protein phosphatase PTEN (11)
☐ Human cell line PC-9 (10)

View All

Function

☒ Inhibitor (64)

View All

Parameter

☒ IC50 (64)
☐ Combination index (24)
☐ Protein expression (21)
☐ Cell viability (18)
☐ Apoptosis rate (10)

View All

疾患とターゲットの表示を設定できる

Key Ligands Targets Diseases

Search the graph...

Epidermal growth factor receptor

colon cancer lung carcinoma skin cancer breast cancer lung non-small cell carcinoma

lung cancer

Gefitinib



Biomarkers

Biomarkers の情報は文献情報の詳細に収録されている

Novel 4-anilinoquinazoline derivatives featuring an 1-adamantyl moiety as potent EGFR inhibitors with enhanced activity against NSCLC cell lines

Details for "EGFR (DNA)"

52 98

In This Reference

- Concepts
- Substances
- Reactions
- Life Science Data
- Cited Documents

Biomarker	EGFR (DNA)
Category	Gene-disease association linked with altered gene expression
Biomarker Type	Molecular
Disease	lung non-small cell carcinoma

Biological State	Biological System	Method	Measurement	Biochemical Agent	Value
Disease	Human	-	Association score	-	1.0

Novel 4-anilinoquinazoline derivatives featuring an 1-adamantyl moiety as potent EGFR inhibitors with enhanced activity against NSCLC cell lines.

Pharmacological Data

Biomarkers

Biomarker	Biomarker Type	Disease	Category	Measurement	Details
EGFR (DNA)	Molecular	lung non-small cell carcinoma	Gene-disease association linked with altered gene expression	Association score	View Detail

CAS LIFE SCIENCES

13

© 2026 American Chemical Society. All rights reserved.



JAICI ヘルプデスク

0120-003-462 (平日 9:00-17:00)

support@jaici.or.jp

14

© 2026 American Chemical Society. All rights reserved.

