

**Product Name:** I 432

**Catalog No.:** 7292

**Batch No.:** 1

CAS Number: 1268874-09-4

IUPAC Name: 3-[(2S)-3-[4-(2-Aminoethyl)-1-piperidiny]-2-[[[(2',4'-dichloro[1,1'-biphenyl]-3-yl)sulfonyl]amino]-3-oxopropyl]benzenecarboximidamide ditrifluoroacetate

## 1. PHYSICAL AND CHEMICAL PROPERTIES

**Batch Molecular Formula:** C<sub>29</sub>H<sub>33</sub>Cl<sub>2</sub>N<sub>5</sub>O<sub>3</sub>S.2CF<sub>3</sub>CO<sub>2</sub>H.2½H<sub>2</sub>O

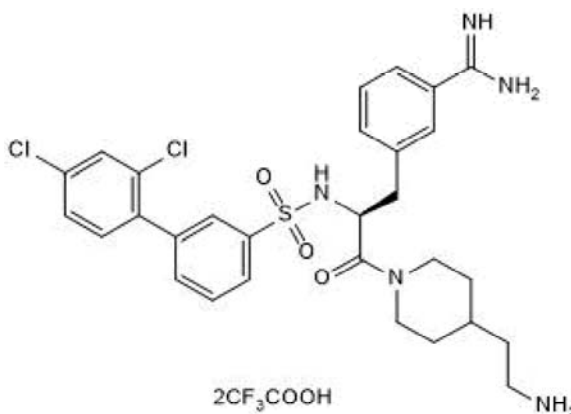
**Batch Molecular Weight:** 871.15

**Physical Appearance:** White solid

**Solubility:** DMSO to 100 mM  
ethanol to 100 mM

**Storage:** Store at -20°C

**Batch Molecular Structure:**



## 2. ANALYTICAL DATA

**HPLC:** Shows 98.6% purity

**Chiral HPLC:** Shows 98.6% purity

**<sup>1</sup>H NMR:** Consistent with structure

**Mass Spectrum:** Consistent with structure

**Microanalysis:**

	Carbon	Hydrogen	Nitrogen
Theoretical	45.5	4.57	8.04
Found	45.14	4.21	7.71

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**Description:**

I 432 is a TMPRSS2 (transmembrane serine proteinase 2) inhibitor ( $K_i = 0.9$  nM). It blocks influenza virus propagation in airway epithelial cells. In IPEC-J2 pig jejunal epithelial cells, I 432 (50  $\mu$ M) inhibits TMPRSS2 without affecting cell viability after 48 h treatment.

**Physical and Chemical Properties:**

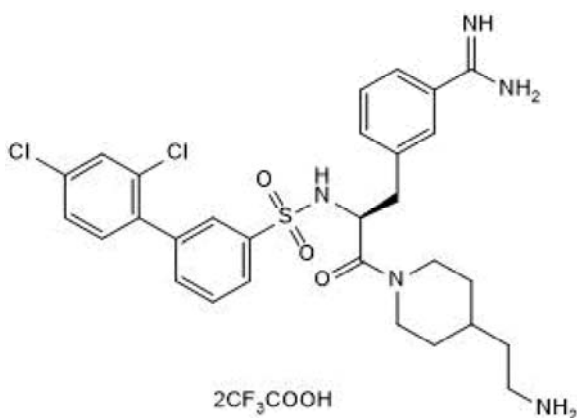
Batch Molecular Formula:  $C_{29}H_{33}Cl_2N_5O_3S \cdot 2CF_3CO_2H \cdot \frac{1}{4}H_2O$

Batch Molecular Weight: 871.15

Physical Appearance: White solid

**Minimum Purity:**  $\geq 98\%$

**Batch Molecular Structure:**



**Storage:** Store at -20°C

**Solubility & Usage Info:**

DMSO to 100 mM  
ethanol to 100 mM

**Stability and Solubility Advice:**

Some solutions can be difficult to obtain and can be encouraged by rapid stirring, sonication or gentle warming (in a 45-60°C water bath).

Information concerning product stability, particularly in solution, has rarely been reported and in most cases we can only offer a general guide. Our standard recommendations are:

**SOLIDS:** Provided storage is as stated on the product label and the vial is kept tightly sealed, the product can be stored for up to 6 months from date of receipt.

**SOLUTIONS:** We recommend that stock solutions, once prepared, are stored aliquoted in tightly sealed vials at -20°C or below and used within 1 month. Wherever possible solutions should be made up and used on the same day.

**References:**

**Alexander et al (2020)** A rational roadmap for SARS-CoV-2/COVID-19 pharmacotherapeutic research and development: IUPHAR Review 29. Br.J.Pharmacol. **177** 4942. PMID: 32358833.

**Pászti-Gere et al (2016)** *In vitro* characterization of TMPRSS2 inhibition in IPEC-J2 cells. J.Enzyme Inhib.Med.Chem. **31** 123. PMID: 27277342.

**Meyer et al (2013)** Identification of the first synthetic inhibitors of the type II transmembrane serine protease TMPRSS2 suitable for inhibition of influenza virus activation. Biochem J. **452** 331. PMID: 23527573.

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**bio-techne.com**

info@bio-techne.com  
techsupport@bio-techne.com

**North America**

Tel: (800) 343 7475

**China**

info.cn@bio-techne.com  
Tel: +86 (21) 52380373

**Europe Middle East Africa**

Tel: +44 (0)1235 529449

**Rest of World**

www.tocris.com/distributors  
Tel:+1 612 379 2956