

**Product Name:** BAY 805

**Catalog No.:** 7984

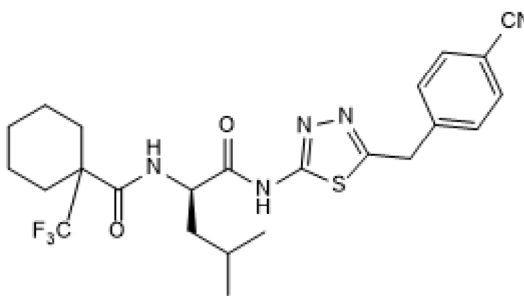
**Batch No.:** 1

CAS Number: 2925481-88-3

IUPAC Name: *N*-[(1*R*)-1-[[[5-[(4-Cyanophenyl)methyl]-1,3,4-thiadiazol-2-yl]amino]carbonyl]-3-methylbutyl]-1-(trifluoromethyl)cyclohexanecarboxamide

## 1. PHYSICAL AND CHEMICAL PROPERTIES

<b>Batch Molecular Formula:</b>	C <sub>24</sub> H <sub>28</sub> F <sub>3</sub> N <sub>5</sub> O <sub>2</sub> S.
<b>Batch Molecular Weight:</b>	507.58
<b>Physical Appearance:</b>	White solid
<b>Solubility:</b>	DMSO to 100 mM ethanol to 100 mM
<b>Storage:</b>	Store at -20°C
<b>Batch Molecular Structure:</b>	



## 2. ANALYTICAL DATA

<b>HPLC:</b>	Shows 99.6% purity
<b>Mass Spectrum:</b>	Consistent with structure
<b>Optical Rotation:</b>	[α] <sub>D</sub> = +52.6 (Concentration = 0.32, Solvent = Methanol)
<b>Microanalysis:</b>	

	Carbon	Hydrogen	Nitrogen
Theoretical	56.79	5.56	13.8
Found	56.82	5.48	13.61

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**Description:**

BAY 805 is a potent and selective inhibitor of USP21 (IC<sub>50</sub> = 6 nM, K<sub>d</sub> = 2.2 nM). BAY 805 induces NF-κB activation (EC<sub>50</sub> = 17 nM in a cell-based reporter assay).

**Physical and Chemical Properties:**

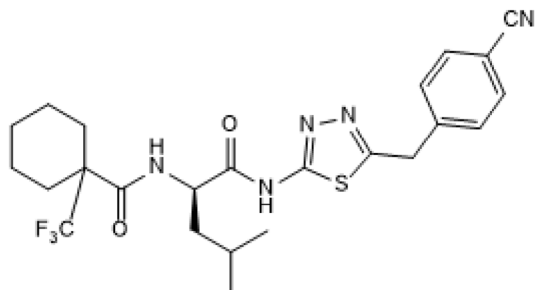
Batch Molecular Formula: C<sub>24</sub>H<sub>28</sub>F<sub>3</sub>N<sub>5</sub>O<sub>2</sub>S.

Batch Molecular Weight: 507.58

Physical Appearance: White solid

**Minimum Purity:** ≥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. \*Unless contradicted by product-specific protocols or instructions, our standard recommendations apply:

**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:**

Göricke *et al* (2023) Discovery and characterization of BAY-805, a potent and selective inhibitor of ubiquitin-specific protease USP21. *J.Med.Chem* **66** 3431. PMID: 36802665.

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