

Certificate of Analysis

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Product Name: BAY 9835

Catalog No.: 8826

Batch No.: 1

CAS Number: 3032487-31-0

IUPAC Name: 5,6-Difluoro-N-[[[(4S)-4-(1-methyl-1H-pyrazol-5-yl)-2,5-dioxo-4-imidazolidinyl)methyl]-4'-(trifluoromethyl)-[1,1'-biphenyl]-2-carboxamide

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₂₂H₁₆F₅N₅O₃·½H₂O

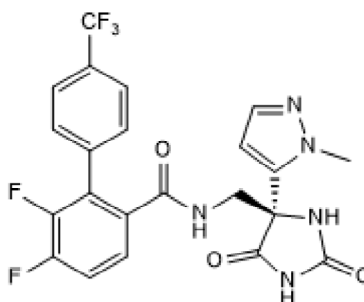
Batch Molecular Weight: 502.4

Physical Appearance: White solid

Solubility: DMSO to 100 mM

Storage: Store at -20°C

Batch Molecular Structure:



2. ANALYTICAL DATA

HPLC: Shows 99.8% purity

Chiral HPLC: Shows 99.9% purity

¹H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis:

Carbon Hydrogen Nitrogen

Theoretical 52.6 3.41 13.94

Found 51.86 3.11 13.45

Caution - Not Fully Tested • Research Use Only • Not For Human or Veterinary Use

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Description:

BAY 9835 is a potent ADAMTS7 and ADAMTS12 inhibitor (IC₅₀ values are 6 nM and 30 nM, respectively). BAY 9835 is selective over other metalloproteases (ADAMTS4, ADAMTS5, ADAM8, ADAM10, ADAM17, MMP2, MMP12, MMP14, MMP15). BAY 9835 is the first orally bioavailable ADAMTS7 inhibitor.

Physical and Chemical Properties:

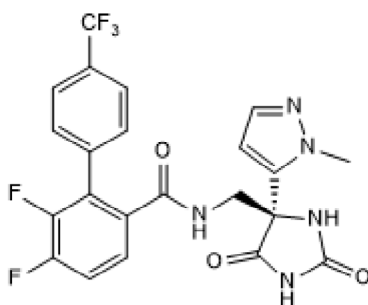
Batch Molecular Formula: C₂₂H₁₆F₅N₅O₃·½H₂O

Batch Molecular Weight: 502.4

Physical Appearance: White solid

Minimum Purity: ≥98%

Batch Molecular Structure:



Storage: Store at -20°C

Solubility & Usage Info:

DMSO 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.

Licensing Information:

This probe is supplied in conjunction with the Structural Genomics Consortium. For further characterization details, please visit the ... page on the SGC website.

References:

Meibom et al (2024) BAY-9835: Discovery of the first orally bioavailable ADAMTS7 inhibitor. *J.Med.Chem.* **67** 2907. PMID: 38348661.

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