

Certificate of Analysis

Print Date: Sep 1st 2021

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Product Name: dTAG^V-1 hydrochloride Catalog No.: 7374 Batch No.: 1

CAS Number: 2624313-16-0

IUPAC Name: (R)-3-(3,4-Dimethoxyphenyl)-1-(2-(2-(((S)-1-(((S)-4-hydroxy-2-(((S)-1-(4-(4-methylthiazol-5-yl)phenyl)ethyl)

carbamoyl)pyrrolidin-1-yl)-3,3-dimethyl-1-oxobutan-2-yl)amino)-7-oxoheptyl)amino)-2-oxoethoxy)phenyl)propyl (S)

-1-((S)-2-(3,4,5-trimethoxyphenyl)butanoyl)piperidine-2-carboxylate hydrochloride

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: $C_{68}H_{90}N_6O_{14}S.HCl.H_2O$

Batch Molecular Weight: 1302.03 **Physical Appearance:** White solid

Solubility: DMSO to 100 mM Storage: Store at -20°C

Batch Molecular Structure:

2. ANALYTICAL DATA

HPLC: Shows 98.0% purity

¹H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis: Carbon Hydrogen Nitrogen Chlorine

Theoretical 62.73 7.2 6.45 2.72 Found 63.33 7.32 6.39 1.6

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Product Information

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Batch No.: 1

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carbamoyl)pyrrolidin-1-yl)-3,3-dimethyl-1-oxobutan-2-yl)amino)-7-oxoheptyl)amino)-2-oxoethoxy)phenyl)propyl (S)

-1-((S)-2-(3,4,5-trimethoxyphenyl)butanoyl)piperidine-2-carboxylate hydrochloride

Description:

dTAGV-1 hydrochloride is a hydrochloride salt of dTAGV-1 (Cat. No. 6914). Suitable for use in vivo. Following ip administration of 10 mg/kg in mice: $T_{1/2}=4.43$ h; $C_{\text{max}}=2123$ ng mL-1; AUC $_{\text{inf}}=18517$ hr*ng mL-1 and CL = 9.05 mL min-1 kg-1 Negative control dTAGV-1-NEG (Cat. No. 6915) also available. Important: It is recommended that DMSO stock solutions of this compound are made and used on the same day and are not subjected to freeze/thaw.

Physical and Chemical Properties:

Batch Molecular Formula: $C_{68}H_{90}N_6O_{14}S.HCI.H_2O$

Batch Molecular Weight: 1302.03 Physical Appearance: White solid

Minimum Purity: ≥98%

Batch Molecular Structure:

Storage: Store at -20°C

Solubility & Usage Info:

DMSO to 100 mM

It is recommended that DMSO stock solutions of this compound are made and used on the same day and are not subjected to freeze/thaw.

Catalog No.: 7374

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.

Licensing Information:

Sold under license from Dana-Farber Cancer Institute

References:

Nabet et al (2020) Rapid and direct control of target protein levels with VHL-recruiting dTAG molecules. Nat.Commun. 11 4687. PMID: 32948771.

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