

Product Name: aTAG 2139

Catalog No.: 6970

Batch No.: 2

CAS Number: 2387510-81-6

IUPAC Name: 6-(6-((4-(2-((2-(2,6-Dioxopiperidin-3-yl)-1,3-dioxoisindolin-4-yl)oxy)acetamido)butyl)carbamoyl)pyridin-3-yl)-N-methyl-4-(phenylamino)quinoline-3-carboxamide

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₄₂H₃₈N₈O₈·³/₄H₂O

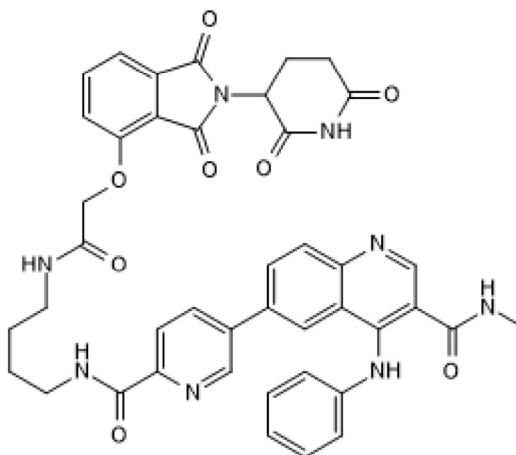
Batch Molecular Weight: 796.32

Physical Appearance: Yellow solid

Solubility: DMSO to 50 mM

Storage: Store at -20°C

Batch Molecular Structure:



2. ANALYTICAL DATA

HPLC: Shows 98.2% purity

¹H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	63.35	5	14.07
Found	63.25	4.9	14.02

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Description:

aTAG 2139 is a degrader of MTH1 fusion proteins for use within the aTAG system. Comprises a ligand selective for MTH1, a linker and the cereblon-binding ligand Thalidomide (Cat. No. 0652). Induces highly potent and selective degradation of fusion proteins after a 4 h incubation ($DC_{50} = 0.27$ nM; $D_{max} = 92.1\%$). Cell-permeable. Suitable for in vitro and in vivo applications. Negative control aTAG 2139-NEG (Cat. No. 7575) also available. Mouse DMPK properties are provided in the supplementary file (see below). MTH1 can be expressed as a fusion with a target protein of interest using genome engineering techniques via CRISPR-mediated locus-s... Please see product specific page on www.tocris.com for full description.

Physical and Chemical Properties:

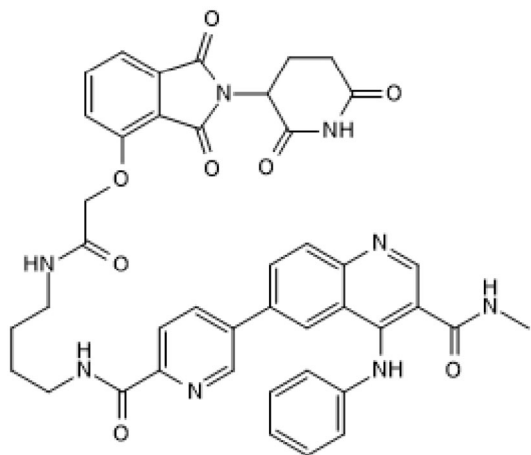
Batch Molecular Formula: $C_{42}H_{38}N_8O_8 \cdot \frac{3}{4}H_2O$

Batch Molecular Weight: 796.32

Physical Appearance: Yellow solid

Minimum Purity: ≥98%

Batch Molecular Structure:



References:

Veits *et al* (2021) Development of an AchillesTAG degradation system and its application to control CAR-T activity. *Curr.Res.Chem.Biol.* **1** 100010.

Storage: Store at -20°C

Solubility & Usage Info:

DMSO to 50 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:

Sold under exclusive license from C4 Therapeutics

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