

Product Name: aTAG 2139

Catalog No.: 6970

Batch No.: 1

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: C₄₂H₃₈N₈O₈·¾H₂O

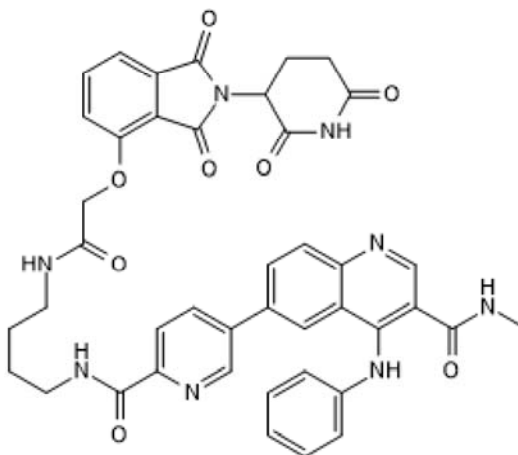
Batch Molecular Weight: 796.32

Physical Appearance: Yellow solid

Solubility: DMSO to 50 mM

Storage: Store at -20°C

Batch Molecular Structure:



2. ANALYTICAL DATA

TLC: R_f = 0.37 (Dichloromethane:Methanol [37:3])

HPLC: Shows 98.0% purity

¹H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	63.35	5	14.07
Found	63.29	4.92	13.83

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

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

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Description:

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. 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-specific knock-in. See protocol for more information. Custom knock-in cell l... Please see product datasheet on www.tocris.com for full description.

Physical and Chemical Properties:

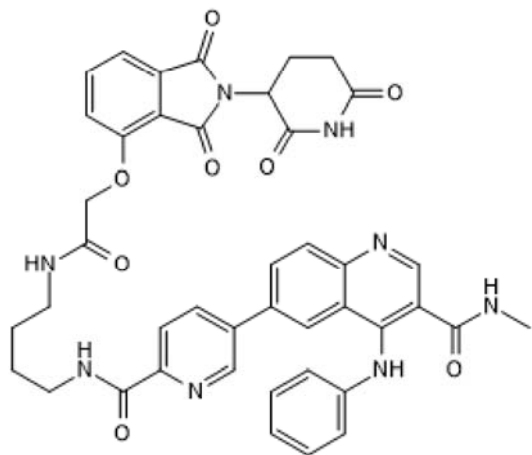
Batch Molecular Formula: $C_{42}H_{38}N_8O_8 \cdot \frac{3}{4}H_2O$

Batch Molecular Weight: 796.32

Physical Appearance: Yellow solid

Minimum Purity: $\geq 98\%$

Batch Molecular Structure:



Storage: Store at $-20^{\circ}C$

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 $45-60^{\circ}C$ 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 $-20^{\circ}C$ 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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North America

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