

Product Name: aTAG 4531

Catalog No.: 6971

Batch No.: 2

CAS Number: 2412985-00-1

IUPAC Name: *N*-Cyclopropyl-6-(4-((4-(4-(((2-(2,6-dioxopiperidin-3-yl)-1,3-dioxoisindolin-4-yl)oxy)methyl)-1*H*-1,2,3-triazol-1-yl)butyl)carbamoyl)-3-fluorophenyl)-7-fluoro-4-(phenylamino)quinoline-3-carboxamide

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₄₆H₃₉F₂N₉O₇·2½H₂O

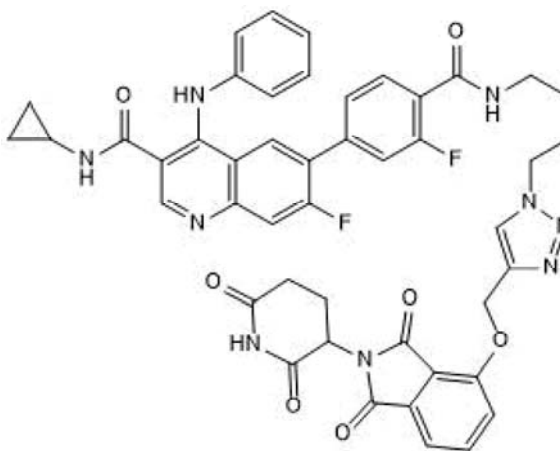
Batch Molecular Weight: 912.89

Physical Appearance: Yellow solid

Solubility: DMSO to 100 mM

Storage: Store at -20°C

Batch Molecular Structure:



2. ANALYTICAL DATA

HPLC: Shows 99.1% purity

¹H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	60.52	4.86	13.81
Found	60.3	4.46	13.64

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Description:

aTAG 4531 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 ($DC_{50} = 0.34$ nM; $D_{max} = 93.14\%$). 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-... Please see product specific page on www.tocris.com for full description.

Physical and Chemical Properties:

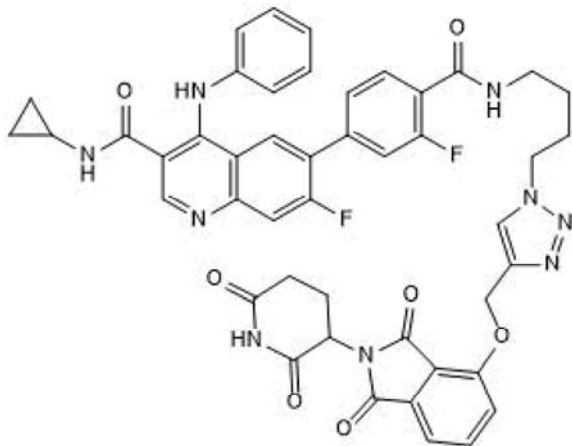
Batch Molecular Formula: $C_{46}H_{39}F_2N_9O_7 \cdot 2\frac{1}{2}H_2O$

Batch Molecular Weight: 912.89

Physical Appearance: Yellow solid

Minimum Purity: $\geq 98\%$

Batch Molecular Structure:



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

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 $45-60^{\circ}C$ 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 license from C4 Therapeutics

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