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TOCRIS

Print Date: Sep 6th 2024

# Certificate of Analysis

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**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-dioxoisoindolin-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:** $C_{46}H_{39}F_2N_9O_7.2½H_2O$

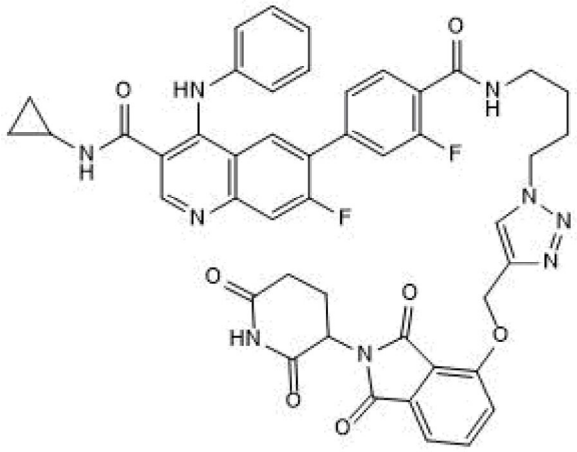
**Batch Molecular Weight:** 912.89

**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

**$^1$H 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. Please see product specific page on www.tocris.com for full description.

**Physical and Chemical Properties:**

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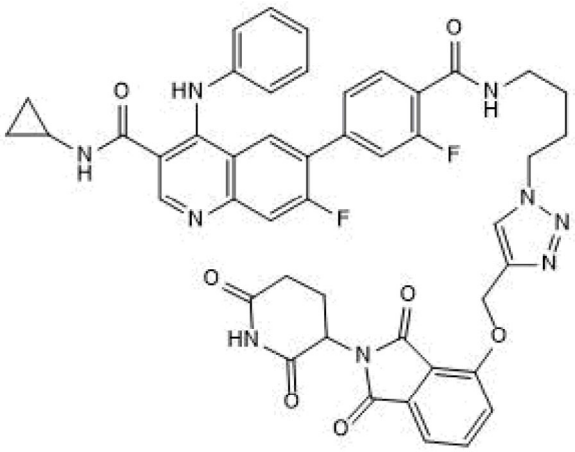
Batch Molecular Weight: 912.89

Physical Appearance: Yellow 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:**

Sold under license from C4 Therapeutics



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