

**Product Name:** CU-76

**Catalog No.:** 7820

**Batch No.:** 1

CAS Number: 2400954-58-5

IUPAC Name: Methyl 4-amino-6-[(3,5-difluoro-4-iodophenyl)amino]-1,3,5-triazine-2-carboxylate

**1. PHYSICAL AND CHEMICAL PROPERTIES**

**Batch Molecular Formula:** C<sub>11</sub>H<sub>8</sub>F<sub>2</sub>IN<sub>5</sub>O<sub>2</sub>·¾H<sub>2</sub>O

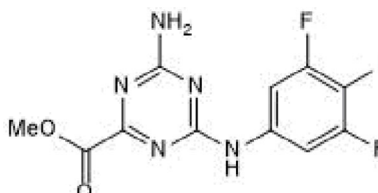
**Batch Molecular Weight:** 420.63

**Physical Appearance:** White solid

**Solubility:** DMSO to 100 mM  
ethanol to 10 mM

**Storage:** Store at -20°C

**Batch Molecular Structure:**



**2. ANALYTICAL DATA**

**HPLC:** Shows 99.7% purity

**<sup>1</sup>H NMR:** Consistent with structure

**Mass Spectrum:** Consistent with structure

**Microanalysis:**

	Carbon	Hydrogen	Nitrogen
Theoretical	31.41	2.28	16.65
Found	32.01	2.41	16.04

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**Description:**

CU-76 is a selective inhibitor of cyclic GMP-AMP synthase (cGAS) with  $IC_{50} = 0.24 \mu\text{M}$ . It specifically inhibits cGAS-STING pathway and has no effect on other nucleic acid sensing pathways such as the RIG-I-MAVS or Toll-like receptor pathways. CU-76 reduces DNA-induced IFN regulatory factor 3 (IRF3) dimerization in a dose-dependent manner, and it decreases production of IFN- $\beta$  in THP-1 cells stimulated with interferon-stimulatory DNA.

**Physical and Chemical Properties:**

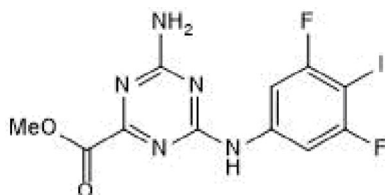
Batch Molecular Formula:  $\text{C}_{11}\text{H}_8\text{F}_2\text{IN}_5\text{O}_2 \cdot \frac{3}{4}\text{H}_2\text{O}$

Batch Molecular Weight: 420.63

Physical Appearance: White solid

**Minimum Purity:**  $\geq 98\%$

**Batch Molecular Structure:**



**References:**

Li *et al* (2021) Therapeutic development by targeting the cGAS-STING pathway in autoimmune disease and cancer. *Front Pharmacol* **12** 779425. PMID: 34867409.

Wang *et al* (2021) Small molecule approaches to treat autoimmune and inflammatory diseases (Part II): Nucleic acid sensing antagonists and inhibitors. *Bioorg.Med.Chem.Lett* **44** 128101. PMID: 33984476.

Salinas *et al* (2020) Discovery of small-molecule cyclic GMP-AMP synthase inhibitors. *J.Org.Chem* **85** 1579. PMID: 31829590.

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

**Solubility & Usage Info:**

DMSO to 100 mM

ethanol to 10 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  $45\text{-}60^\circ\text{C}$  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  $-20^\circ\text{C}$  or below and used within 1 month. Wherever possible solutions should be made up and used on the same day.

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