

**Product Name:** G6PDi 1

**Catalog No.:** 7561

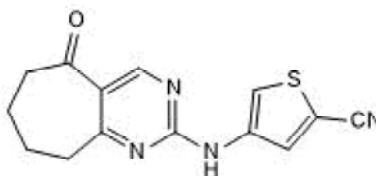
**Batch No.:** 1

CAS Number: 2457232-14-1

IUPAC Name: 4-((5-Oxo-6,7,8,9-tetrahydro-5H-cyclohepta[d]pyrimidin-2-yl)amino)thiophene-2-carbonitrile

**1. PHYSICAL AND CHEMICAL PROPERTIES**

**Batch Molecular Formula:** C<sub>14</sub>H<sub>12</sub>N<sub>4</sub>OS  
**Batch Molecular Weight:** 284.34  
**Physical Appearance:** Light orange solid  
**Solubility:** DMSO to 100 mM  
**Storage:** Store at -20°C  
**Batch Molecular Structure:**



**2. ANALYTICAL DATA**

**HPLC:** Shows 99.2% purity  
**<sup>1</sup>H NMR:** Consistent with structure  
**Mass Spectrum:** Consistent with structure

**Microanalysis:**

	Carbon	Hydrogen	Nitrogen
Theoretical	59.14	4.25	19.7
Found	58.45	4.23	19.48

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**Description:**

G6PDi 1 is a potent, reversible, nonsteroidal inhibitor of glucose-6-phosphate dehydrogenase (G6PD) ( $IC_{50} = 70$  nM). The compound dose-dependently and reversibly decreases 6-phosphogluconolactone (6-PG) levels in HCT116 and HepG2 cell lines in vitro. In activated T cells, G6PDi-1 inhibits flux through the pentose phosphate pathway and decreases NADPH generation. It also inhibits production of cytokines by activated T cells and oxidative burst in neutrophils.

**Physical and Chemical Properties:**

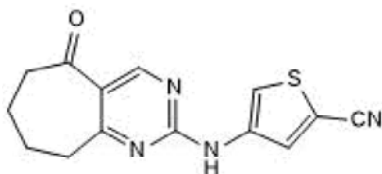
Batch Molecular Formula: C<sub>14</sub>H<sub>12</sub>N<sub>4</sub>O<sub>S</sub>

Batch Molecular Weight: 284.34

Physical Appearance: Light orange solid

**Minimum Purity:** ≥98%

**Batch Molecular Structure:**



**References:**

**Gherguson et al** (2020) A small molecule G6PD inhibitor reveals immune dependence on pentose phosphate pathway. *Nat.Chem.Biol.* **16** 731. PMID: 32393898.

**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. 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°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 Princeton University

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