

**Product Name:** GSK 2830371

**Catalog No.:** 5140

**Batch No.:** 1

**CAS Number:** 1404456-53-6

**IUPAC Name:** 5-[[[(5-Chloro-2-methyl-3-pyridinyl)amino]methyl]-N-[(1S)-1-(cyclopentylmethyl)-2-(cyclopropylamino)-2-oxoethyl]-2-thiophenecarboxamide

## 1. PHYSICAL AND CHEMICAL PROPERTIES

**Batch Molecular Formula:** C<sub>23</sub>H<sub>29</sub>ClN<sub>4</sub>O<sub>2</sub>S.½H<sub>2</sub>O

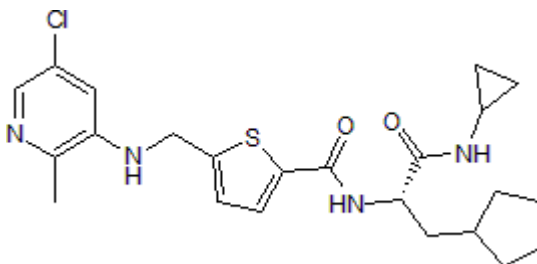
**Batch Molecular Weight:** 465.52

**Physical Appearance:** Off White powder

**Solubility:** DMSO to 100 mM  
ethanol to 50 mM

**Storage:** Store at -20°C

**Batch Molecular Structure:**



## 2. ANALYTICAL DATA

**TLC:** R<sub>f</sub> = 0.22 (Ethyl acetate:Petroleum ether [3:7])

**HPLC:** Shows 99.2% purity

**Chiral HPLC:** Shows 100% purity

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

**Mass Spectrum:** Consistent with structure

**Microanalysis:**

Carbon Hydrogen Nitrogen

Theoretical 59.34 6.39 12.04

Found 59.19 6.35 11.81

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**Description:**

Potent and selective allosteric inhibitor of Wip1 phosphatase ( $IC_{50} = 6$  nM). Exhibits selectivity for Wip1 over 21 other phosphatases. Increases phosphorylation of Wip1 substrates, including p53, Chk2, H2AX and ATM. Attenuates tumor cell growth in a variety of lymphoid cell lines. Also inhibits lymphoma xenograft growth in vivo. Orally bioavailable.

**Physical and Chemical Properties:**

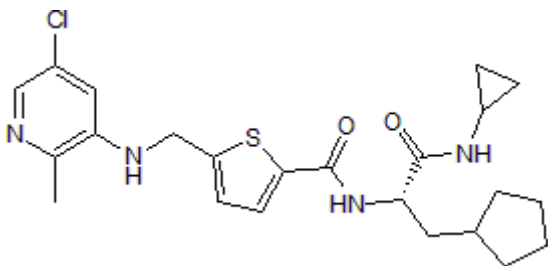
Batch Molecular Formula:  $C_{23}H_{29}ClN_4O_2S \cdot \frac{1}{4}H_2O$

Batch Molecular Weight: 465.52

Physical Appearance: Off White powder

**Minimum Purity:** >98%

**Batch Molecular Structure:**



**Storage:** Store at -20°C

**Solubility & Usage Info:**

DMSO to 100 mM

ethanol 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°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.

**References:**

**Gilmartin et al** (2014) Allosteric Wip1 phosphatase inhibition through flap-subdomain interaction. *Nat.Chem.Biol.* **10** 181. PMID: 24390428.

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