

# Certificate of Analysis

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**Product Name:** Ticagrelor

**Catalog No.:** 6864

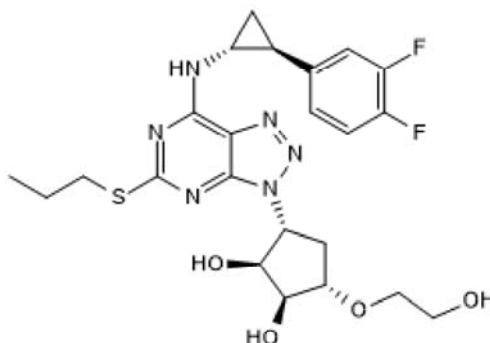
**Batch No.:** 1

**CAS Number:** 274693-27-5

**IUPAC Name:** (1*S*,2*S*,3*R*,5*S*)-3-[7-[[[(1*R*,2*S*)-2-(3,4-Difluorophenyl)cyclopropyl]amino]-5-(propylthio)-3*H*-1,2,3-triazolo[4,5-*d*]pyrimidin-3-yl]-5-(2-hydroxyethoxy)-1,2-cyclopentanediol

## 1. PHYSICAL AND CHEMICAL PROPERTIES

**Batch Molecular Formula:** C<sub>23</sub>H<sub>28</sub>F<sub>2</sub>N<sub>6</sub>O<sub>4</sub>S  
**Batch Molecular Weight:** 522.57  
**Physical Appearance:** White solid  
**Solubility:** DMSO to 100 mM  
 ethanol to 50 mM  
**Storage:** Store at -20°C  
**Batch Molecular Structure:**



## 2. ANALYTICAL DATA

**HPLC:** Shows 100% purity  
**<sup>1</sup>H NMR:** Consistent with structure  
**Mass Spectrum:** Consistent with structure  
**Microanalysis:**

	Carbon Hydrogen Nitrogen		
Theoretical	52.86	5.4	16.08
Found	52.91	5.41	16.18

Caution - Not Fully Tested • Research Use Only • Not For Human or Veterinary Use

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**Description:**

High affinity and reversible P2Y<sub>12</sub> antagonist (pK<sub>i</sub> = 8.7) that displays inverse agonism in 1321N1 cells. Also high affinity inhibitor of equilibrative nucleoside transporter 1 (ENT1; K<sub>i</sub> = 41 nM). Inhibits ADP-induced platelet aggregation.

**Physical and Chemical Properties:**

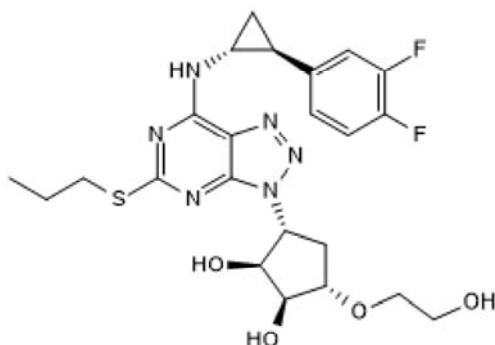
Batch Molecular Formula: C<sub>23</sub>H<sub>28</sub>F<sub>2</sub>N<sub>6</sub>O<sub>4</sub>S

Batch Molecular Weight: 522.57

Physical Appearance: White solid

**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:**

**Aungraheeta et al** (2016) Inverse agonism at the P2Y<sub>12</sub> receptor and ENT1 transporter blockade contribute to platelet inhibition by ticagrelor. *Blood*. **128** 2717. PMID: 27694321.

**Armstrong et al** (2014) Characterization of the adenosine pharmacology of ticagrelor reveals therapeutically relevant inhibition of equilibrative nucleoside transporter 1. *J.Cardiovasc.Pharmacol.Ther.* **19** 209. PMID: 24414167.

**Springthorpe et al** (2007) From ATP to AZD6140: the discovery of an orally active reversible P2Y<sub>12</sub> receptor antagonist for the prevention of thrombosis. *Bioorg.Med.Chem.Letts.* **17** 6013. PMID: 17827008.

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