

## **Certificate of Analysis**

MedKoo Cat#:	Product Name:	Lot#:
206450	Selonsertib (GS-4997	SSC60722

Chemical name		
5-(4-cyclopropyl-1H-imidazol-1-yl)-2-fluoro-N-(6-(4-isopropyl-4H-1,2,4-triazol-3-yl)pyridin-		
2-yl)-4-methylbenzamide		
Synonyms		
GS-4997; GS4997; GS 4997; Selonsertib		
Chemical structure	CAS# and Theoretical analysis	
	MedKoo Cat#: 206450	
	Name: Selonsertib (GS-4997)	
	CAS#: 1448428-04-3	
	Lot#SSC60722	
	Chemical Formula: C <sub>24</sub> H <sub>24</sub> FN <sub>7</sub> O	
	Exact Mass: 445.20264	
	Molecular Weight: 445.5	

Analysis item	Specifications / Results
Appearance	White to off-white solid powder
Structure	<sup>1</sup> H-NMR analysis matches the structure. MS analysis gives the correct molecule weight. Both NMR and MS data are consistent with those reported in the literature.
Purity (HPLC)	>95.0%
Solubility	Soluble in DMSO
Conclusion	This product conforms with MedKoo's quality standards
Shipping condition	Shipped under ambient temperature as non-hazardous chemical. This product is stable for a few weeks during ordinary shipping and time spent in customs.
Storage condition	Short term storage (weeks): $0 - 4$ °C under dry condition Long term storage (months): -20 °C under dry condition
Shelf life	At least 5 years if properly stored.

## CAUTION: NOT FULLY TESTED. FOR RESEARCH ONLY, NOT FOR HUMAN USE



## Statement of possible tautomerization in selonsertib

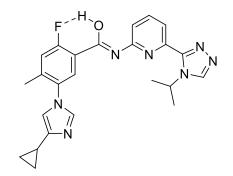
We followed literature (WO2013112741 A1) to synthesize selonsertib (GS4977).

NMR analysis in CDCl3 and DMSO-d6 confirmed the correct structure with excellent purity.

Depending on methods/conditions used, HPLC and LC/MS analysis may show two peaks in a ratio of  $\sim$  95: 5. Both peaks showed the same molecule weight.

Based on the QC test results, we believe that selonsertib (GS4977) may exist two tautomers through amide bond tautomerization. The major isomer is ~ 95%, the minor isomer is ~ 5%. Total purity is > 99%. In general, amide bond tautomerization is not detectable using regularly analytic methods. However, in selonsertib (GS4977) molecule, the amide bond tautomerization may be stabilized by intramolecularly hydrogen bonding (F---H—O) see the scheme below.

Selonsertib (GS-4997) (major)



Selonsertib (GS-4997) tautomer (minor) This isomer can be stabilized by intramolecularly hydrogen bonding