

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 ₂₄ H ₂₄ FN ₇ O	
	Exact Mass: 445.20264	
	Molecular Weight: 445.5	

Analysis item	Specifications / Results
Appearance	White to off-white solid powder
Structure	¹ 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

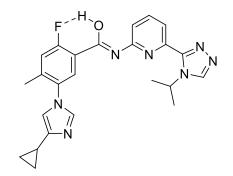
We followed literature (WO2013112741 A1) to synthesize selonsertib (GS4977).

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