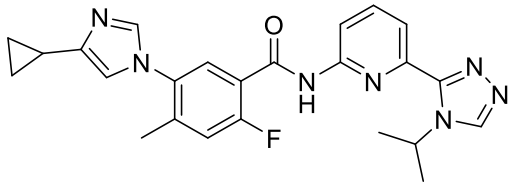
MedKoo Biosciences

Certificate of Analysis

MedKoo Cat#:	Product Name:	Lot#:
206450	Selonsertib (GS-4997)	EOS70210

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#: EOS70210 Chemical Formula: $C_{24}H_{24}FN_7O$ 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)	>98.0%
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

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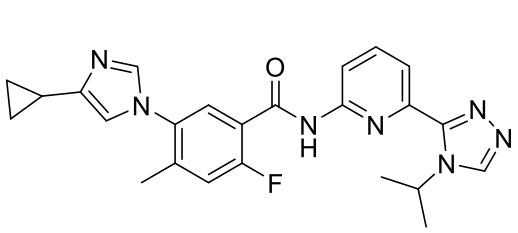
Statement of possible tautomerization in selonsertib

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

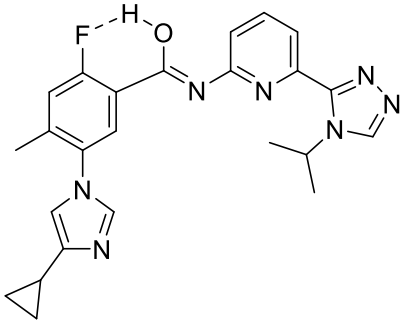
NMR analysis in CDCl3 and DMSO-d6 confirmed the correct structure with excellent purity.

Depending on methods/conditions used, HPLC and LC/MS analysis may show two peaks in a ratio of ~ 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

MedKoo Biosciences, Inc., 2500 Gateway Centre Blvd. Suite#400, Morrisville, NC27560, USA
Tel: 919-636-5577, Fax: 919-9804831, http://www.medkoo.com, sales@medkoo.com.