

Product Name: Selpercatinib

Catalog No.: 7696

Batch No.: 1

CAS Number: 2152628-33-4

IUPAC Name: 6-(2-Hydroxy-2-methylpropoxy)-4-[6-[(6-methoxy-3-pyridinyl)methyl]-3,6-diazabicyclo[3.1.1]hept-3-yl]-3-pyridinyl]pyrazolo[1,5-a]pyridine-3-carbonitrile

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₂₉H₃₁N₇O₃·1/4H₂O

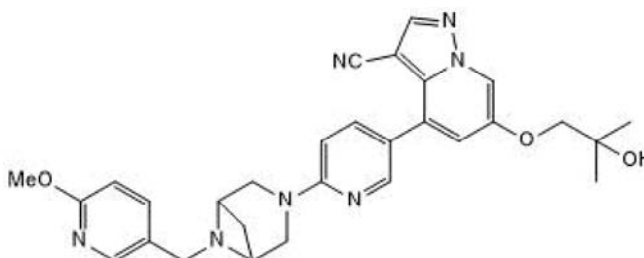
Batch Molecular Weight: 530.1

Physical Appearance: Off White solid

Solubility: DMSO to 20 mM

Storage: Store at -20°C

Batch Molecular Structure:



2. ANALYTICAL DATA

HPLC: Shows 99.4% purity

¹H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	65.71	5.99	18.5
Found	65.46	5.96	18.4

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Description:

Selpercatinib, is a potent and selective receptor tyrosine kinase RET inhibitor ($EC_{50} = 4$ nM). It shows > 100-fold selectivity for > 95% of 228 purified kinase domains in radiometric assays. In vitro, it inhibits proliferation of cancer cell lines containing RET mutations or gene fusions. In vivo, it inhibits tumor growth in diverse RET mouse models. Selpercatinib is orally bioavailable.

Physical and Chemical Properties:

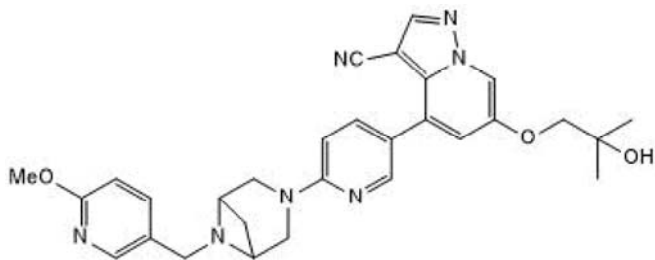
Batch Molecular Formula: $C_{29}H_{31}N_7O_3 \cdot \frac{1}{4}H_2O$

Batch Molecular Weight: 530.1

Physical Appearance: Off White solid

Minimum Purity: ≥98%

Batch Molecular Structure:



Storage: Store at -20°C

Solubility & Usage Info:

DMSO to 20 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:

Subbiah et al (2018) Selective RET kinase inhibition for patients with RET-altered cancers. *Ann.Oncol.* **29** 1869. PMID: 29912274.

Brandhuber et al (2016) The development of LOXO-292, a potent, KDR/VEGFR2-sparing RET kinase inhibitor for treating patients with RET-dependent cancers. *International Conference on Molecular Targets and Cancer Therapeutics.*

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