

Product Name: MRTX 849

Catalog No.: 7488

Batch No.: 1

CAS Number: 2326521-71-3

IUPAC Name: 4-[7-(8-Chloro-1-naphthalenyl)-5,6,7,8-tetrahydro-2-[[[(2S)-1-methyl-2-pyrrolidinyl]methoxy]pyrido[3,4-d]pyrimidin-4-yl]-1-(2-fluoro-1-oxo-2-propen-1-yl)-(2S)-2-piperazineacetonitrile

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₃₂H₃₅ClFN₇O₂·¼H₂O

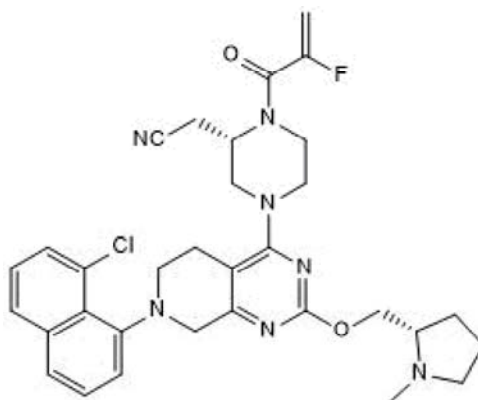
Batch Molecular Weight: 608.63

Physical Appearance: Cream solid

Solubility: DMSO to 100 mM
ethanol to 100 mM

Storage: Store at -20°C

Batch Molecular Structure:



2. ANALYTICAL DATA

HPLC: Shows 98.8% purity

¹H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	63.15	5.88	16.11
Found	62.83	5.88	15.95

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Description:

MRTX 849 is a mutant-selective inhibitor of KRAS^{G12C} (IC₅₀ = 142 nM). MRTX 849 covalently binds to KRAS^{G12C} at the cysteine 12 residue and inhibits KRAS-dependent signal transduction by locking the protein in its inactive GDP-bound state. MRTX 849 induces pronounced tumor regression in 17 of 26 (65%) KRAS^{G12C} -positive cell lines and patient-derived xenograft models from multiple tumor types. It is orally bioavailable.

Physical and Chemical Properties:

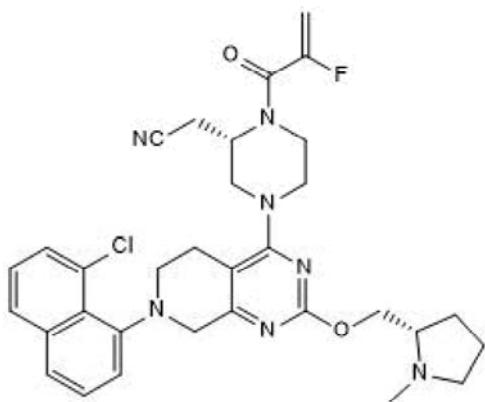
Batch Molecular Formula: C₃₂H₃₅ClFN₇O₂·½H₂O

Batch Molecular Weight: 608.63

Physical Appearance: Cream solid

Minimum Purity: ≥98%

Batch Molecular Structure:



Storage: Store at -20°C

Solubility & Usage Info:

DMSO to 100 mM
ethanol to 100 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:

Fell et al (2020) Identification of the clinical development candidate MRTX849, a covalent KRAS^{G12C} inhibitor for the treatment of cancer. *J.Med.Chem.* **63** 6679. PMID: 32250617.

Hallin et al (2020) The KRAS G12C inhibitor MRTX849 provides insight toward therapeutic susceptibility of KRAS-mutant cancers in mouse models and patients. *Cancer Discov.* **10** 54. PMID: 31658955.

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