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Print Date: Feb 28th 2020

Certificate of Analysis

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Product Name: **BAY 293** **Catalog No.: 6857** **Batch No.: 1**

CAS Number: 2244904-70-7

IUPAC Name: (*R*)-6,7-Dimethoxy-2-methyl-*N*-[1-[4-[2-[(methylamino)methyl]phenyl]thiophene-2-yl]ethyl]quinazolin-4-amine

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: $C_{25}H_{28}N_4O_2S.½H_2O$

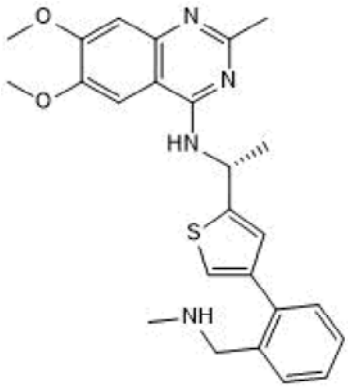
Batch Molecular Weight: 457.6

Physical Appearance: Light Beige solid

Solubility: DMSO to 100 mM
ethanol to 100 mM

Storage: Store at -20°C

Batch Molecular Structure:



2. ANALYTICAL DATA

TLC: R_f = 0.5 (Dichloromethane:Methanol:Ammonia soln. [90:9:1])

HPLC: Shows 99% purity

Chiral HPLC: Shows 98.8% purity

^{1}H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Optical Rotation: $[\alpha]_D$ = -103.8 (Concentration = 1, Solvent = DMSO)

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	65.62	6.39	12.24
Found	65.62	6.24	12.12

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Description:

Potent KRas/son of sevenless 1 (SOS1) interaction inhibitor (IC_{50} = 21 nM); active R-enantiomer. Downregulates active RAS in tumor cells. Inhibits RAS-RAF-MEK-ERK pathway. Exhibits synergistic effects with $KRAS^{G12C}$ inhibitor ARS-853. Negative control also available.

Physical and Chemical Properties:

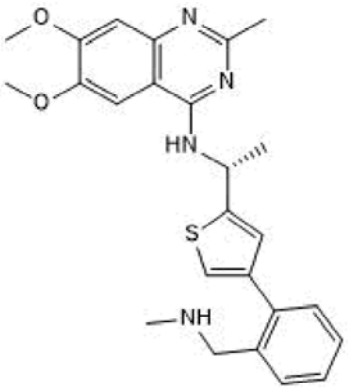
Batch Molecular Formula: $C_{25}H_{28}N_4O_2S.½H_2O$

Batch Molecular Weight: 457.6

Physical Appearance: Light Beige 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.

Licensing Information:

This probe is supplied in conjunction with the Structural Genomics Consortium. For further characterization details, please visit the BAY 293 probe summary on the SGC website.

References:

Hillig *et al* (2019) Discovery of potent SOS1 inhibitors that block RAS activation via disruption of the RAS-SOS1 interaction. Proc.Natl.Acad.Sci.USA. ***116*** 2551. PMID: 30683722.