

Product Name: MRK 740

Catalog No.: 6803

Batch No.: 1

CAS Number: 2387510-80-5

IUPAC Name: 3-(3,5-Dimethoxyphenyl)-5-(1-methyl-9-(2-methylpyridin-4-yl)-1,4,9-triazaspiro[5.5]undecan-4-yl)-1,2,4-oxadiazole

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₂₅H₃₂N₆O₃·¾H₂O

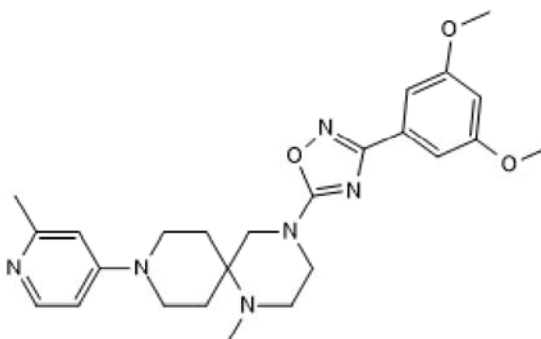
Batch Molecular Weight: 478.07

Physical Appearance: Pale yellow solid

Solubility: DMSO to 100 mM
1eq. HCl to 100 mM
ethanol to 100 mM

Storage: Store at -20°C

Batch Molecular Structure:



2. ANALYTICAL DATA

HPLC: Shows 99.3% purity

¹H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	62.81	7.06	17.58
Found	62.91	6.93	17.43

Caution - Not Fully Tested • Research Use Only • Not For Human or Veterinary Use

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Description:

MRK 740 is a potent PRDM9 histone methyltransferase inhibitor (IC_{50} = 85 nM for in vitro methylation of H3K4), which displays >100-fold selectivity over other histone methyltransferases. MRK 740 inhibits H3K4 methylation in cells (IC_{50} = 0.8 μ M).

Physical and Chemical Properties:

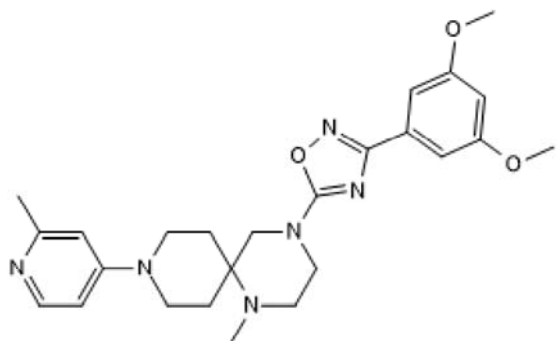
Batch Molecular Formula: $C_{25}H_{32}N_6O_3 \cdot \frac{3}{4}H_2O$

Batch Molecular Weight: 478.07

Physical Appearance: Pale yellow solid

Minimum Purity: $\geq 98\%$

Batch Molecular Structure:



Storage: Store at -20°C

Solubility & Usage Info:

DMSO to 100 mM
1eq. HCl 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 MRK-740 probe summary on the SGC website.

References:

Allali-Hassani *et al* (2019) Discovery of a chemical probe for PRDM9. *Nat. Commun.* **10** 5759. PMID: 31848333 .

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