

Product Name: MRS 5698

Catalog No.: 5428

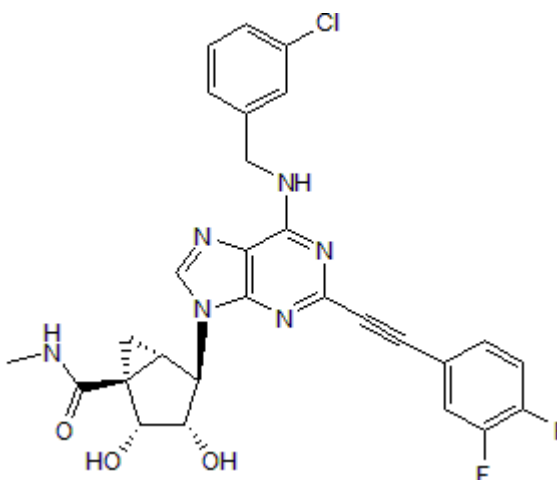
Batch No.: 1

CAS Number: 1377273-00-1

IUPAC Name: (1*S*,2*R*,3*S*,4*R*,5*S*)-4-[6-[[[(3-Chlorophenyl)methyl]amino]-2-[2-(3,4-difluorophenyl)ethynyl]-9*H*-purin-9-yl]-2,3-dihydroxy-*N*-methylbicyclo[3.1.0]hexane-1-carboxamide

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula:	C ₂₈ H ₂₃ ClF ₂ N ₆ O ₃
Batch Molecular Weight:	564.97
Physical Appearance:	White solid
Solubility:	DMSO to 10 mM
Storage:	Store at -20°C
Batch Molecular Structure:	



2. ANALYTICAL DATA

HPLC:	Shows 96.1% purity
¹H NMR:	Consistent with structure
Mass Spectrum:	Consistent with structure

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

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Description:

High affinity and selective A₃ adenosine receptor agonist (K_i ~ 3 nM); displays >1000-fold selectivity over A₁ and A_{2A} adenosine receptors. Reverses mechanoallodynia in several neuropathic pain models in vivo. Orally bioavailable.

Physical and Chemical Properties:

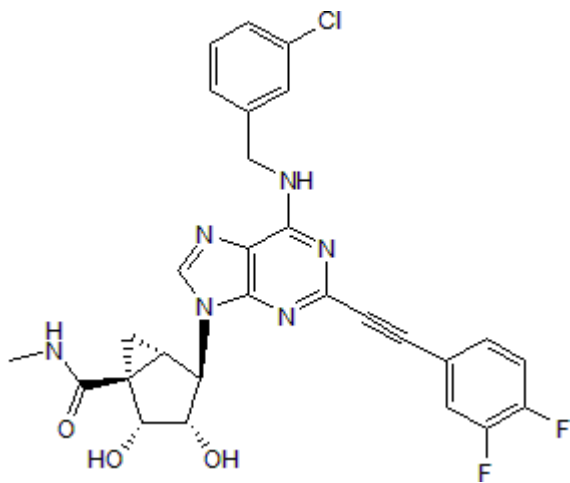
Batch Molecular Formula: C₂₈H₂₃ClF₂N₆O₃

Batch Molecular Weight: 564.97

Physical Appearance: White solid

Minimum Purity: >96%

Batch Molecular Structure:



References:

Tosh et al (2012) Structure-guided design of A₃ adenosine receptor-selective nucleosides: combination of 2-arylethynyl and bicyclo [3.1.0]hexane substitutions. *J.Med.Chem.* **55** 4847. PMID: 22559880.

Tosh et al (2015) Efficient, large-scale synthesis and preclinical studies of MRS5698, a highly selective A₃ adenosine receptor agonist that protects against chronic neuropathic pain. *Purinergic Signal.* **11** 371. PMID: 26111639.

Little et al (2015) Endogenous adenosine A₃ receptor activation selectively alleviates persistent pain states. *Brain* **138** 28. PMID: 25414036.

Storage: Store at -20°C

Solubility & Usage Info:

DMSO to 10 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.

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