

Product Name: CTA 056

Catalog No.: 4726

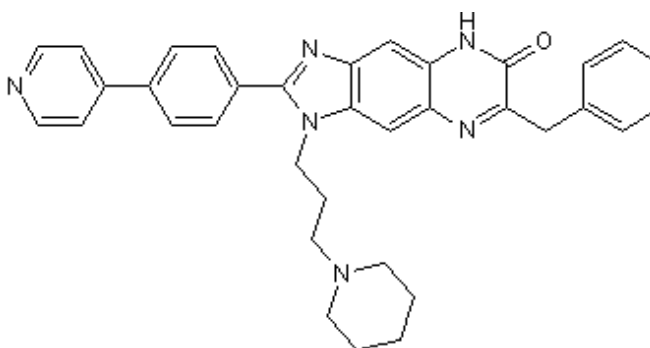
Batch No.: 1

CAS Number: 1265822-30-7

IUPAC Name: 1,5-Dihydro-7-(phenylmethyl)-1-[3-(1-piperidinyl)propyl]-2-[4-(4-pyridinyl)phenyl]-6*H*-imidazo[4,5-*g*]quinoxalin-6-one

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₃₅H₃₄N₆O.H₂O
Batch Molecular Weight: 572.7
Physical Appearance: Yellow solid
Solubility: DMSO to 10 mM with gentle warming
Storage: Store at -20°C
Batch Molecular Structure:



2. ANALYTICAL DATA

TLC: R_f = 0.4 (Dichloromethane:Methanol:Ammonia soln. [92:7:1])
HPLC: Shows 98.7% purity
¹H NMR: Consistent with structure
Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	73.4	6.34	14.67
Found	73.36	6.21	14.43

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

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Description:

Interleukin-2-inducible T-cell kinase (ITK) inhibitor (IC₅₀ values are 0.1, 0.4 and 5 μM for ITK, BTK and ETK, respectively). Inhibits growth of cancer cells expressing ITK, including MOLT-4 and Jurkat cells in vitro. Induces apoptosis in Jurkat cells. Inhibits MOLT-4 xenograft tumor growth in mice.

Physical and Chemical Properties:

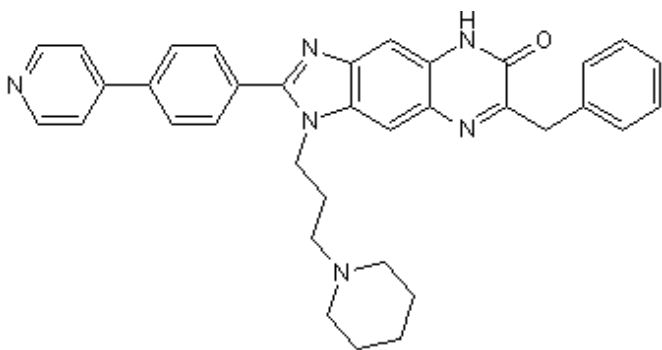
Batch Molecular Formula: C₃₅H₃₄N₆O.H₂O

Batch Molecular Weight: 572.7

Physical Appearance: Yellow solid

Minimum Purity: >98%

Batch Molecular Structure:



Storage: Store at -20°C

Solubility & Usage Info:

DMSO to 10 mM with gentle warming

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:

Guo et al (2012) Molecular characteristics of CTA056, a novel interleukin-2-inducible T-cell kinase inhibitor that selectively targets malignant T cells and modulates oncomirs. *Mol.Pharmacol.* **82** 938. PMID: 22899868.

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