

**Product Name:** AZ 13705339

**Catalog No.:** 6177

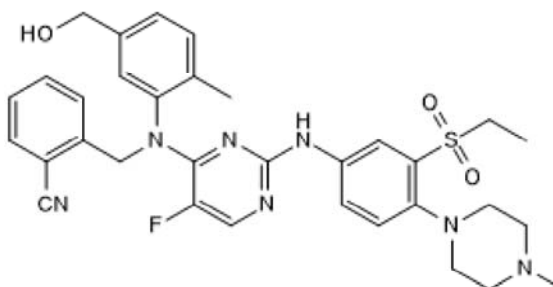
**Batch No.:** 1

CAS Number: 2016806-57-6

IUPAC Name: 2-[[[2-[[3-(Ethylsulfonyl)-4-(4-methyl-1-piperazinyl)phenyl]amino]-5-fluoro-4-pyrimidinyl]][5-(hydroxymethyl)-2-methylphenyl]amino]methyl]benzotrile

## 1. PHYSICAL AND CHEMICAL PROPERTIES

<b>Batch Molecular Formula:</b>	C <sub>33</sub> H <sub>36</sub> FN <sub>7</sub> O <sub>3</sub> S.½H <sub>2</sub> O
<b>Batch Molecular Weight:</b>	638.76
<b>Physical Appearance:</b>	White solid
<b>Solubility:</b>	DMSO to 100 mM ethanol to 20 mM with gentle warming
<b>Storage:</b>	Store at -20°C
<b>Batch Molecular Structure:</b>	



## 2. ANALYTICAL DATA

<b>HPLC:</b>	Shows 98.5% purity
<b><sup>1</sup>H NMR:</b>	Consistent with structure
<b>Mass Spectrum:</b>	Consistent with structure
<b>Microanalysis:</b>	

	Carbon	Hydrogen	Nitrogen
Theoretical	62.05	5.84	15.35
Found	61.72	5.85	15.27

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

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**Description:**

Highly potent PAK1 and PAK2 inhibitor (IC<sub>50</sub> values are 0.33 and 6 nM for PAK1 and PAK2, respectively). Displays >7500-fold selectivity for PAK1 over PAK4 (IC<sub>50</sub> = 2.6 μM).

**Physical and Chemical Properties:**

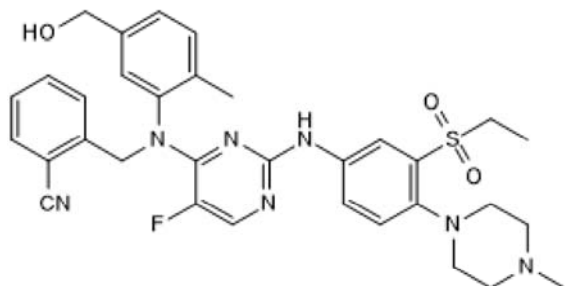
Batch Molecular Formula: C<sub>33</sub>H<sub>36</sub>FN<sub>7</sub>O<sub>3</sub>S.½H<sub>2</sub>O

Batch Molecular Weight: 638.76

Physical Appearance: White solid

**Minimum Purity:** >98%

**Batch Molecular Structure:**



**Storage:** Store at -20°C

**Solubility & Usage Info:**

DMSO to 100 mM

ethanol to 20 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:**

**McCoull et al** (2016) Optimization of highly kinase selective bis-anilino pyrimidine PAK1 inhibitors. ACS.Med.Chem.Lett. **7** 1118. PMID: 27994749.

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