Print Date: Nov 22nd 2018

Certificate of Analysis

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Product Name: **AZD 5438** **Catalog No.: 3968** **Batch No.: 1**

CAS Number: 602306-29-6

IUPAC Name: 4-[2-Methyl-1-(1-methylethyl)-1*H*-imidazol-5-yl]-*N*-[4-(methylsulfonyl)phenyl]-2-pyrimidinamine

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: $C_{18}H_{21}N_5O_2S$

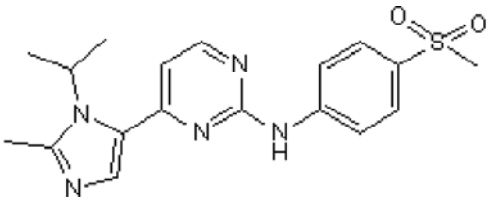
Batch Molecular Weight: 371.46

Physical Appearance: Off-white solid

Solubility: DMSO to 100 mM

Storage: Desiccate at RT

Batch Molecular Structure:



2. ANALYTICAL DATA

TLC: R_f = 0.15 (Dichloromethane:Methanol [95:5])

HPLC: Shows 99.9% purity

^{1}H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	58.2	5.7	18.85
Found	58.07	5.63	18.88

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Product Information

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Description:

Potent inhibitor of cyclin dependent kinases (cdks; reported IC_{50} values are 6 - 45, 14, 16 and 20 nM for cdk2, cdk5, cdk1 and cdk9 respectively). Also inhibits cdk4 and cdk7 in the sub micromolar range. Exhibits antiproliferative activity in human tumor cell lines. Blocks cell cycling at G2-M, S and G1 phases; reduces the proportion of actively cycling cells in vivo.

Physical and Chemical Properties:

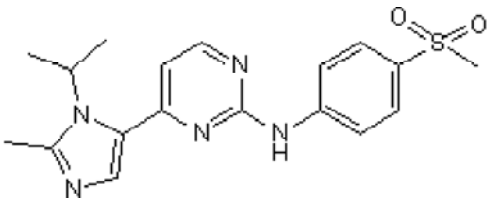
Batch Molecular Formula: $C_{18}H_{21}N_5O_2S$

Batch Molecular Weight: 371.46

Physical Appearance: Off-white solid

Minimum Purity: >99%

Batch Molecular Structure:



Storage: Desiccate at RT

Solubility & Usage Info:

DMSO 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:

Sold with the permission of AstraZeneca UK Ltd.

References:

Jorda *et al* (2018) How selective are pharmacological inhibitors of cell-cycle-regulating cyclin-dependent kinases? J.Med.Chem. ***61*** 9105. PMID: 30234987.

Byth *et al* (2009) AZD5438, a potent oral inhibitor of cyclin-dependent kinases 1, 2 and 9, leads to pharmacodynamic changes and potent antitumor effects in human tumor xenografts. Mol.Cancer Ther. ***8*** 1856. PMID: 19509270.