

Product Name: TC-S 7010

Catalog No.: 5286

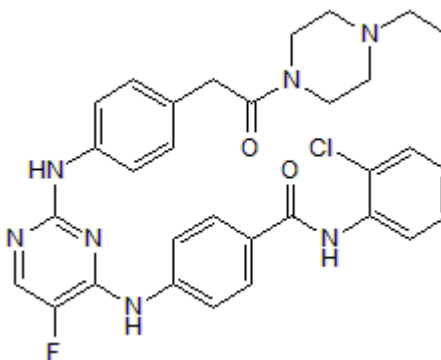
Batch No.: 1

CAS Number: 1158838-45-9

IUPAC Name: *N*-(2-Chlorophenyl)-4-[[2-[[4-[2-(4-ethyl-1-piperazinyl)-2-oxoethyl]phenyl]amino]-5-fluoro-4-pyrimidinyl]amino]-benzamide

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₃₁H₃₁ClFN₇O₂
Batch Molecular Weight: 588.07
Physical Appearance: White solid
Solubility: DMSO to 100 mM
Storage: Store at +4°C
Batch Molecular Structure:



2. ANALYTICAL DATA

HPLC: Shows 100% purity
¹H NMR: Consistent with structure
Mass Spectrum: Consistent with structure
Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	63.31	5.31	16.67
Found	62.94	5.45	16.57

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

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Description:

Potent and selective inhibitor of Aurora kinase A ($IC_{50} = 3.4$ nM); exhibits 1000-fold selectivity for Aurora kinase A over Aurora kinase B. Displays antiproliferative activity in HCT116 and HT29 cells (IC_{50} values are 0.19 and 2.9 μ M respectively).

Physical and Chemical Properties:

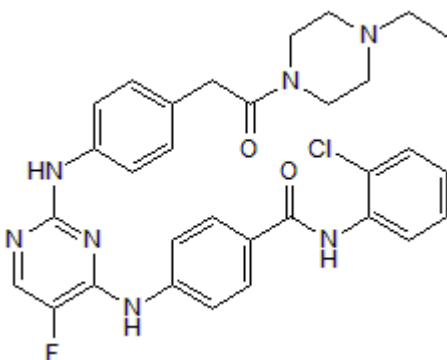
Batch Molecular Formula: $C_{31}H_{31}ClFN_7O_2$

Batch Molecular Weight: 588.07

Physical Appearance: White solid

Minimum Purity: >99%

Batch Molecular Structure:



Storage: Store at +4°C

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.

References:

Aliagas-Martin et al (2009) A class of 2,4-bis-anilinopyrimidine Aurora A inhibitors with unusually high selectivity against Aurora B. *J.Med.Chem.* **52** 3300. PMID: 19402633.

Yuan et al (2012) Overcoming CML acquired resistance by specific inhibition of Aurora A kinase in the KCL-22 cell model. *Carcinogenesis* **33** 285. PMID: 22116466.

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bio-techne.com

info@bio-techne.com

techsupport@bio-techne.com

North America

Tel: (800) 343 7475

China

info.cn@bio-techne.com

Tel: +86 (21) 52380373

Europe Middle East Africa

Tel: +44 (0)1235 529449

Rest of World

www.tocris.com/distributors

Tel: +1 612 379 2956