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Print Date: Apr 23rd 2020

Certificate of Analysis

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Product Name: **AP 24534** **Catalog No.: 4274** **Batch No.: 2**

CAS Number: 943319-70-8

IUPAC Name: 3-(2-Imidazo[1,2-*b*]pyridazin-3-ylethynyl)-4-methyl-*N*-[4-[(4-methyl-1-piperazinyl)methyl]-3-(trifluoromethyl)phenyl] -benzamide

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: $C_{29}H_{27}F_3N_6O.¼H_2O$

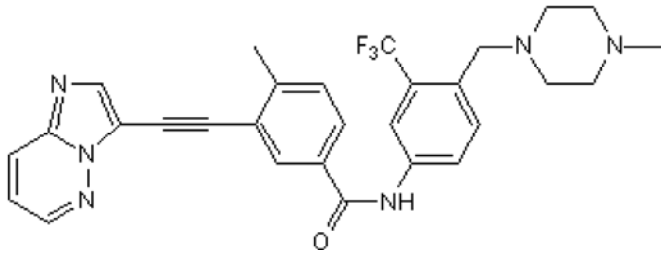
Batch Molecular Weight: 537.06

Physical Appearance: Yellow solid

Solubility: DMSO to 100 mM
ethanol to 50 mM

Storage: Store at -20°C

Batch Molecular Structure:



2. ANALYTICAL DATA

HPLC: Shows 98.7% purity

^{1}H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	64.86	5.16	15.65
Found	64.96	5.15	15.84

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Product Information

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Description:

Potent multi-kinase and pan-Bcr-Abl inhibitor. Displays potent activity against cell lines expressing native Bcr-Abl or Bcr-Abl^{T3151} (IC_{50} values are 0.37 and 2.0 nM respectively); also inhibits other Abl kinase domain mutants at nanomolar potencies. Exhibits inhibitory activity against PDGFRα, c-Src and c-Kit (IC_{50} values are 1.1, 5.4 and 12.5 nM respectively); potently inhibits FGFR and VEGFR family kinases. Orally active. Identified as targeting human host proteins that interact with SARS-CoV-2.

Physical and Chemical Properties:

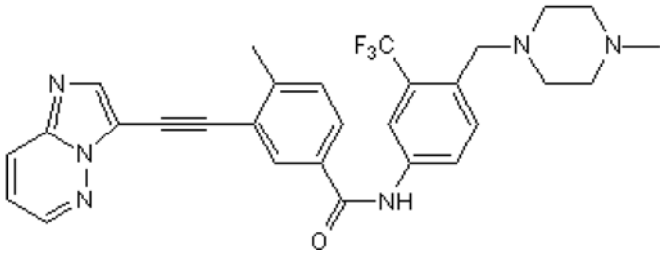
Batch Molecular Formula: $C_{29}H_{27}F_3N_6O.¼H_2O$

Batch Molecular Weight: 537.06

Physical Appearance: Yellow solid

Minimum Purity: ≥98%

Batch Molecular Structure:



Storage: Store at -20°C

Solubility & Usage Info:

DMSO to 100 mM
ethanol to 50 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:

Gordon *et al* (2020) A SARS-CoV-2-human protein-protein interaction map reveals drug targets and potential drug-repurposing. BioRxiv - Paper not yet peer reviewed.

Gozgit *et al* (2011) Potent activity of ponatinib (AP24534) in models of FLT3-driven acute myeloid leukemia and other hematologic malignancies. Mol.Cancer Ther. ***10*** 1028. PMID: 21482694.

Huang *et al* (2010) Discovery of 3-[2-(imidazo[1,2-*b*]pyridazin-3-yl)ethynyl]-4-methyl-*N*-{4-[(4-methylpiperazin-1-yl)-methyl] -3-(trifluoromethyl)phenyl}benzamide (AP24534), a potent, orally active pan-inhibitor of breakpoint cluster region-Abelson (BCR-ABL) J.Med.Chem. ***53*** 4701. PMID: 20513156.

O'Hare *et al* (2009) AP24534, a pan-BCR-ABL inhibitor for chronic myeloid leukemia, potently inhibits the T315I mutant and overcomes mutation-based resistance. Cancer Cell ***16*** 401. PMID: 19878872.