

Product Name: VE 821

Catalog No.: 6160

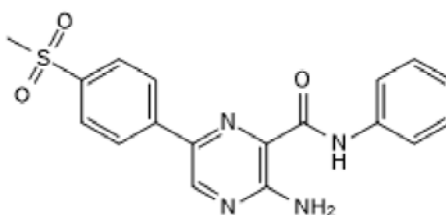
Batch No.: 1

CAS Number: 1232410-49-9

IUPAC Name: 3-Amino-6-[4-(methylsulfonyl)phenyl]-N-phenyl-2-pyrazinecarboxamide

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₁₈H₁₆N₄O₃S
Batch Molecular Weight: 368.41
Physical Appearance: Yellow solid
Solubility: DMSO to 100 mM
Storage: Store at -20°C
Batch Molecular Structure:



2. ANALYTICAL DATA

TLC: R_f = 0.3 (Ethyl acetate:Petroleum ether [1:1])
HPLC: Shows 99% purity
¹H NMR: Consistent with structure
Mass Spectrum: Consistent with structure
Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	58.68	4.38	15.21
Found	58.48	4.32	15.28

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

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CAS Number: 1232410-49-9

IUPAC Name: 3-Amino-6-[4-(methylsulfonyl)phenyl]-N-phenyl-2-pyrazinecarboxamide

Description:

High affinity and selective ATP-competitive ATR inhibitor ($K_i = 13$ nM). Exhibits >75-fold selectivity for ATR over related kinases mTOR, DNA-PK, PI 3-Ky and PIKKs (K_i values are >1, 2.2, 3.9 and 16 μ M, respectively) and a panel of other kinases. Induces cell death in colon cancer cell lines in vitro and sensitizes tumor cells to treatment with DNA damaging anticancer agents.

Physical and Chemical Properties:

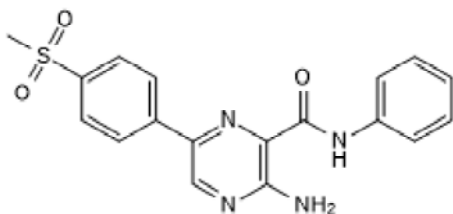
Batch Molecular Formula: C₁₈H₁₆N₄O₃S

Batch Molecular Weight: 368.41

Physical Appearance: Yellow solid

Minimum Purity: >98%

Batch Molecular Structure:



Storage: Store at -20°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:

Williamson et al (2016) ATR inhibitors as a synthetic lethal therapy for tumours deficient in ARID1A. *Nat.Commun.* **7** 13837. PMID: 27958275.

Reaper et al (2011) Selective killing of ATM- or p53-deficient cancer cells through inhibition of ATR. *Nat.Chem.Biol.* **7** 428. PMID: 21490603.

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