

Product Name: GNE 2861

Catalog No.: 6490

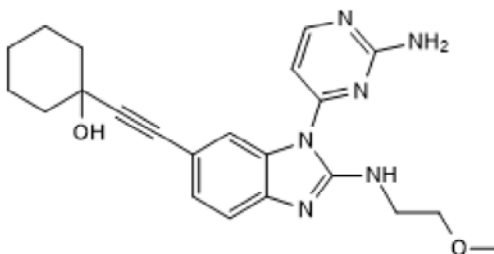
Batch No.: 1

CAS Number: 1394121-05-1

IUPAC Name: 1-[2-[1-(2-Amino-4-pyrimidinyl)-2-[(2-methoxyethyl)amino]-1*H*-benzimidazol-6-yl]ethynyl]cyclohexanol

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₂₂H₂₆N₆O₂
Batch Molecular Weight: 406.48
Physical Appearance: Cream solid
Solubility: DMSO to 100 mM
 ethanol to 100 mM
Storage: Store at -20°C
Batch Molecular Structure:



2. ANALYTICAL DATA

TLC: R_f = 0.4 (Dichloromethane:Methanol [9:1])
HPLC: Shows 99.8% purity
¹H NMR: Consistent with structure
Mass Spectrum: Consistent with structure
Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	65.01	6.45	20.68
Found	64.92	6.53	20.42

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

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Description:

Inhibitor of group II p21 activated kinases (PAK; IC₅₀ values are 7.5, 126 and 36 nM for PAK4, PAK5 and PAK6, respectively). Displays selectivity for group II PAK over a panel of 222 kinases. Inhibits tumor cell proliferation, migration and invasion in two breast cancer cell lines. Also sensitizes tamoxifen-resistant breast cancer cell lines to tamoxifen (Cat. No. 6342) via PAK4-dependent regulation of estrogen receptor α (ERα) target gene expression.

Physical and Chemical Properties:

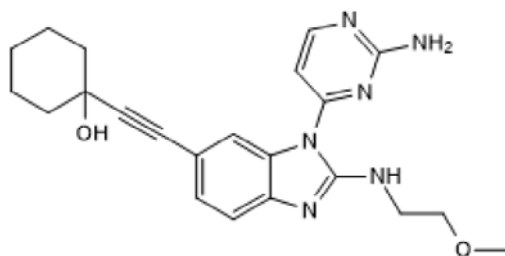
Batch Molecular Formula: C₂₂H₂₆N₆O₂

Batch Molecular Weight: 406.48

Physical Appearance: Cream solid

Minimum Purity: >98%

Batch Molecular Structure:



Storage: Store at -20°C

Solubility & Usage Info:

DMSO to 100 mM
ethanol 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:

Zhuang *et al* (2015) p21-activated kinase group II small compound inhibitor GNE-2861 perturbs estrogen receptor alpha signaling and restores tamoxifen-sensitivity in breast cancer cells. *Oncotarget*. **6** 43853. PMID: 26554417.

Staben *et al* (2014) Back pocket flexibility provides group II p21-activated kinase (PAK) selectivity for type I 1/2 kinase inhibitors. *J.Med.Chem.* **57** 1033. PMID: 24432870.

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