

Product Name: EC 144

Catalog No.: 4701

Batch No.: 3

CAS Number: 911397-80-3

IUPAC Name: 5-[2-Amino-4-chloro-7-[(4-methoxy-3,5-dimethyl-2-pyridinyl)methyl]-7H-pyrrolo[2,3-d]pyrimidin-5-yl]-2-methyl-4-pentyn-2-ol

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₂₁H₂₄ClN₅O₂·¼H₂O

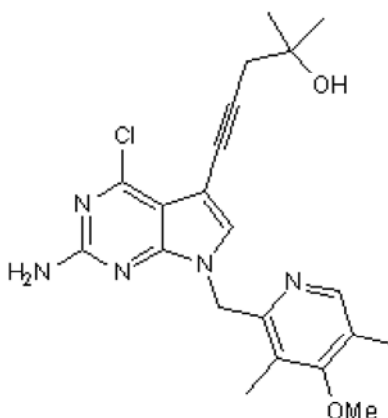
Batch Molecular Weight: 418.4

Physical Appearance: Beige solid

Solubility: DMSO to 100 mM
ethanol to 5 mM

Storage: Store at -20°C

Batch Molecular Structure:



2. ANALYTICAL DATA

HPLC: Shows 99.0% purity

¹H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	60.28	5.9	16.74
Found	59.96	5.95	16.63

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

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Description:

High affinity, potent and selective Hsp90 inhibitor ($K_i = 0.2$ nM and $IC_{50} = 1.1$ nM). Exhibits selectivity for Hsp90 over Grp94 and TRAP1 (K_i values are 61 and 255 nM respectively) and has no effect ($IC_{50} >10$ μ M) against a panel of 285 kinases. Degrades Her-2 in MCF-7 breast cancer cells ($EC_{50} = 14$ nM). Blocks tumor growth and induces partial tumor regression in an N87 gastric tumor mouse model. Also inhibits LPS-induced TNF α release in an LPS shock mouse model and suppresses disease development in a rat model of collagen-induced arthritis. Exhibits <20-fold efficacy over BIIB 021 (Cat. No. 4608) in mice. Orally available a... Please see product datasheet on www.tocris.com for full description.

Physical and Chemical Properties:

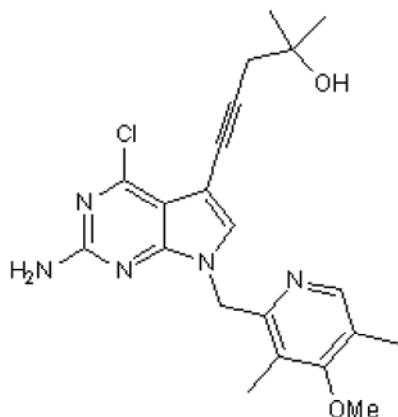
Batch Molecular Formula: C₂₁H₂₄ClN₅O₂. $\frac{1}{4}$ H₂O

Batch Molecular Weight: 418.4

Physical Appearance: Beige solid

Minimum Purity: $\geq 98\%$

Batch Molecular Structure:



References:

Shi et al (2012) EC144 is a potent inhibitor of the heat shock protein 90. *J.Med.Chem.* **55** 7786. PMID: 22938030.

Yun et al (2011) EC144, a synthetic inhibitor of heat shock protein 90, blocks innate and adaptive immune responses in models of inflammation and autoimmunity. *J.Immunol.* **186** 563. PMID: 21131419.

Storage: Store at -20°C

Solubility & Usage Info:

DMSO to 100 mM
ethanol to 5 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.

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