

Product Name: TC-S 7003

Catalog No.: 3567

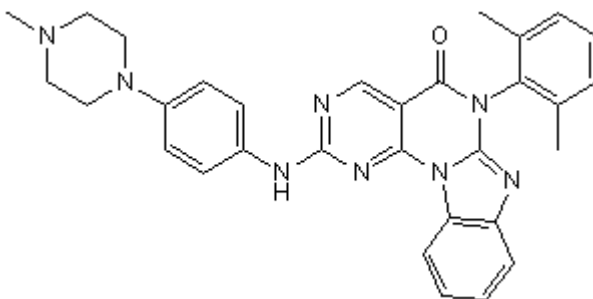
Batch No.: 1

CAS Number: 847950-09-8

IUPAC Name: 6-(2,6-Dimethylphenyl)-2-[[4-(4-methyl-1-pyrimido[5',4':5,6]pyrimido[1,2-a]benzimidazol-5(6H)-one

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₃₁H₃₀N₈O.½H₂O
Batch Molecular Weight: 539.63
Physical Appearance: Yellow solid
Solubility: DMSO to 100 mM
 ethanol to 10 mM with gentle warming
Storage: Store at -20°C
Batch Molecular Structure:



2. ANALYTICAL DATA

HPLC: Shows 99.2% purity
¹H NMR: Consistent with structure
Mass Spectrum: Consistent with structure
Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	69	5.79	20.76
Found	69	5.58	20.78

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

Product Name: TC-S 7003

Catalog No.: 3567

Batch No.: 1

CAS Number: 847950-09-8

IUPAC Name: 6-(2,6-Dimethylphenyl)-2-[[4-(4-methyl-1-pyrimido[5',4':5,6]pyrimido[1,2-a]benzimidazol-5(6H)-one

Description:

Potent inhibitor of lymphocyte specific kinase (Lck). IC₅₀ values are 0.007, 0.021, 0.042 and 0.20 μM for Lck, Lyn, Src and Syk kinases respectively. Displays >1000-fold selectivity for Lck over MAPK, CDK and RSK family representatives. Inhibits T-cell proliferation in vitro and inhibits arthritis in two in vivo models. Orally active.

Physical and Chemical Properties:

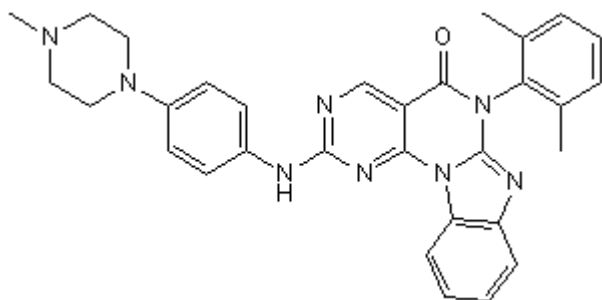
Batch Molecular Formula: C₃₁H₃₀N₈O.½H₂O

Batch Molecular Weight: 539.63

Physical Appearance: Yellow solid

Minimum Purity: >98%

Batch Molecular Structure:



Storage: Store at -20°C

Solubility & Usage Info:

DMSO to 100 mM

ethanol to 10 mM with gentle warming

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:

Martin et al (2008) Structure-based design of novel 2-amino-6-phenyl-pyrimido[5',4':5,6]pyrimido[1,2-a]benzimidazol-5(6H)-ones as potent and orally active inhibitors of lymphocyte specific kinase (Lck): synthesis, SAR, and in vivo anti-inflammatory activity. *J.Med.Chem.* **51** 1637. PMID: 18278858.

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

————— Tocris Bioscience is an R&D Systems company —————
USA & CANADA Tel: (800) 343-7475 EUROPE Tel: +44 (0)1235 529449 CHINA Tel: +86 (21) 52380373
www.RnDSystems.com

R&D
SYSTEMS®