

Product Name: CHIR 99021 trihydrochloride

Catalog No.: 4953

Batch No.: 5

CAS Number: 1782235-14-6

IUPAC Name: 6-[[2-[[4-(2,4-Dichlorophenyl)-5-(5-methyl-1*H*-imidazol-2-yl)-2-pyrimidinyl]amino]ethyl]amino]-3-pyridinecarbonitrile trihydrochloride

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₂₂H₁₈Cl₂N₈·3HCl·½H₂O

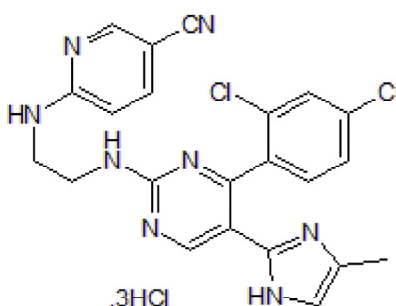
Batch Molecular Weight: 583.73

Physical Appearance: White solid

Solubility: water to 25 mM
DMSO to 50 mM

Storage: Store at -20°C

Batch Molecular Structure:



2. ANALYTICAL DATA

TLC: R_f = 0.4 (Dichloromethane:Methanol [9:1])

HPLC: Shows 99% purity

¹H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	45.27	3.8	19.2
Found	45.13	3.8	18.95

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Description:

CHIR 99021 trihydrochloride is a hydrochloride salt of CHIR 99021 (Cat. No. 4423), a highly selective GSK-3 inhibitor. CHIR 99021, CHIR 99021 in solution and CHIR 99021 synthesized to cGMP guidelines also available.

Physical and Chemical Properties:

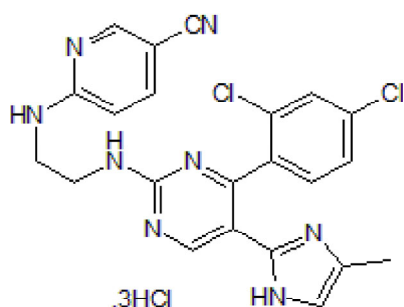
Batch Molecular Formula: C₂₂H₁₈Cl₂N₈.3HCl.½H₂O

Batch Molecular Weight: 583.73

Physical Appearance: White solid

Minimum Purity: ≥98%

Batch Molecular Structure:



Storage: Store at -20°C

Solubility & Usage Info:

water to 25 mM
DMSO 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. *Unless contradicted by product-specific protocols or instructions, our standard recommendations apply:

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:

Ye *et al* (2012) Pleiotropy of glycogen synthase kinase-3 inhibition by CHIR99021 promotes self-renewal of embryonic stem cells from refractory mouse strains. *PLoS One* **7** e35892. PMID: 22540008.

Pan *et al* (2011) AKT kinase activity is required for Li to modulate mood-related behaviors in mice. *Neuropsychopharmacology* **36** 1397. PMID: 21389981.

Ring *et al* (2003) Selective glycogen synthase kinase 3 inhibitors potentiate Ins activation of glucose transport and utilization in vitro and in vivo. *Diabetes* **52** 588. PMID: 12606497.

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