Product Name: CHIR 99021
Catalog No.: 4423
Batch No.: 13
CAS Number: 252917-06-9
IUPAC Name: 6-[[2-[[4-(2,4-Dichlorophenyl)-5-(5-methyl-1H-imidazol-2-yl)-2-pyrimidinyl]amino]ethyl]amino]-3-pyridinecarbonitrile

1. PHYSICAL AND CHEMICAL PROPERTIES

- Batch Molecular Formula: C_{22}H_{18}Cl_{2}N_{8}
- Batch Molecular Weight: 465.34
- Physical Appearance: Cream solid
- Solubility: DMSO to 20 mM
- Storage: Store at -20°C
- Batch Molecular Structure:

2. ANALYTICAL DATA

- HPLC: Shows 99.8% purity
- \(^1\)H NMR: Consistent with structure
- Mass Spectrum: Consistent with structure
- Microanalysis: Carbon Hydrogen Nitrogen
  - Theoretical: 56.78 3.9 24.08
  - Found: 56.58 3.89 23.75

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

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**Product Name:** CHIR 99021  
**Catalog No.:** 4423  
**Batch No.:** 13

### Description:
Potent and highly selective inhibitor of glycogen synthase kinase 3 (GSK-3) (IC\textsubscript{50} values are 6.7 and 10 nM for GSK-3\(\beta\) and GSK-3\(\alpha\) respectively). Exhibits >500-fold selectivity for GSK-3 over closely related kinases; also displays >800-fold selectivity against 45 additional enzymes and receptors. In combination with tranylcypromine (Cat. No. 3852), enables reprogramming of mouse embryonic fibroblasts, transduced by Oct4 and Klf4 only, into iPSCs. Enhances mouse and human ESC self-renewal when used in combination with PD 0325901 (Cat. No. 4192). Allows formation of extended pluripotent stem (EPS) cells in combination with (S)-(... Please see product datasheet on www.tocris.com for full description.

### Physical and Chemical Properties:
- **Batch Molecular Formula:** C\textsubscript{22}H\textsubscript{18}Cl\textsubscript{2}N\textsubscript{5}
- **Batch Molecular Weight:** 465.34
- **Physical Appearance:** Cream solid
- **Minimum Purity:** >98%
- **Storage:** Store at -20°C

### Solubility & Usage Info:
- DMSO to 20 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: