# Inhibitors

# JAK2-IN-6

Cat. No.: HY-137756 CAS No.: 353512-04-6 Molecular Formula:  $C_{14}H_{10}CIN_3OS_2$ 

Molecular Weight: 335.83 JAK Target:

Pathway: Epigenetics; JAK/STAT Signaling; Protein Tyrosine Kinase/RTK; Stem Cell/Wnt

Powder Storage: -20°C 3 years 4°C 2 years

-80°C In solvent 6 months -20°C 1 month

**Product** Data Sheet

### **SOLVENT & SOLUBILITY**

In Vitro

DMSO: 60 mg/mL (178.66 mM; ultrasonic and adjust pH to 5 with HCl)

Preparing Stock Solutions	Solvent Mass Concentration	1 mg	5 mg	10 mg
	1 mM	2.9777 mL	14.8885 mL	29.7770 mL
	5 mM	0.5955 mL	2.9777 mL	5.9554 mL
	10 mM	0.2978 mL	1.4888 mL	2.9777 mL

Please refer to the solubility information to select the appropriate solvent.

# **BIOLOGICAL ACTIVITY**

Description  ${\sf JAK2\text{-}IN\text{-}6, a\ multiple-substituted\ aminothiazole\ derivative, is\ a\ potent\ and\ selective\ {\sf JAK2\ inhibitor\ with\ an\ IC_{50}\ of\ 22.86\ }\mu}$ g/mL, JAK2-IN-6 shows no activity against JAK1 and JAK3, JAK2-IN-6 has anti-proliferative effect against cancer cells<sup>[1]</sup>.

IC<sub>50</sub> & Target JAK2

 $22.86 \, \mu g/mL \, (IC_{50})$ 

In Vitro JAK2-IN-6 (Compound B2; 6.3-50 µg/mL; 48 hours; PC-9, H1975 and PANC-1 cells) treatment exhibits significantly

antiproliferative activity against all of these cancer cell lines, with IC50 values of 18.1 µg/mL, 58.3 µg/mL, 40.6 µg/mL against

PC-9, H1975 and PANC-1, respectively<sup>[1]</sup>.

JAK2-IN-6 (Compound B2), an intramolecular hydrogen bond is formed, holding the chlorothiophene substituent coplanar with the aminothiazole core. The chlorothiophene moiety is found to be located in the binding pocket adjacent to Val863 and Leu983, and extends towards the Asp994 of activation loop and the Gly993 of glycine-rich loop<sup>[1]</sup>.

MCE has not independently confirmed the accuracy of these methods. They are for reference only.

Cell Proliferation Assay<sup>[1]</sup>

Cell Line:	PC-9, H1975 and PANC-1 cells	
Concentration:	6.3 μg/mL, 12.5 μg/mL, 25 μg/mL, 50 μg/mL	
Incubation Time:	48 hours	
Result:	Exhibited significantly antiproliferative activity against all of these cancer cell lines.	

# **REFERENCES**

[1]. Ting-Ting Yao, et al. Integration of pharmacophore mapping and molecular docking in sequential virtual screening: towards the discovery of novel JAK2 inhibitors. RSC Adv., 2017, 7, 10353-10360.

Caution: Product has not been fully validated for medical applications. For research use only.

Tel: 609-228-6898 Fax: 609-228-5909 E-mail: tech@MedChemExpress.com

Address: 1 Deer Park Dr, Suite Q, Monmouth Junction, NJ 08852, USA

Page 2 of 2 www.MedChemExpress.com