# **Product data sheet**



MedKoo Cat#: 562110				
Name: NSC-109555 Ditosylate				
CAS: 66748-43-4				
Chemical Formula: $C_{33}H_{40}N_{10}O_7S_2$				
Molecular Weight: 752.866				
Product supplied as:	Powder			
Purity (by HPLC):	$\geq 98\%$			
Shipping conditions	Ambient temperature			
Storage conditions:	Powder: -20°C 3 years; 4°C 2 years.			
	In solvent: -80°C 3 months; -20°C 2 weeks.			



# 1. Product description:

NSC-109555 Ditosylate is a potent, selective, reversible, ATP-competitive Chk2 inhibitor. It acts by inhibiting histone H1 phosphorylation and attenuating mitochondrial ATP synthesis.

# 2. CoA, QC data, SDS, and handling instruction

SDS and handling instruction, CoA with copies of QC data (NMR, HPLC and MS analytical spectra) can be downloaded from the product web page under "QC And Documents" section. Note: copies of analytical spectra may not be available if the product is being supplied by MedKoo partners. Whether the product was made by MedKoo or provided by its partners, the quality is 100% guaranteed.

#### 3. Solubility data

Solvent	Max Conc. mg/mL	Max Conc. mM
DMSO	7.53	10.0

#### 4. Stock solution preparation table:

Concentration / Solvent Volume / Mass	1 mg	5 mg	10 mg
1 mM	1.33 mL	6.64 mL	13.28 mL
5 mM	0.27 mL	1.33 mL	2.66 mL
10 mM	0.13 mL	0.66 mL	1.33 mL
50 mM	0.03 mL	0.13 mL	0.27 mL

# 5. Molarity Calculator, Reconstitution Calculator, Dilution Calculator

Please refer the product web page under section of "Calculator"

# 6. Recommended literature which reported protocols for in vitro and in vivo study

#### In vitro study

1. Zhu L, Zhao L, Wang H, Wang Y, Pan D, Yao J, Li Z, Wu G, Guo Q. Oroxylin A reverses P-glycoprotein-mediated multidrug resistance of MCF7/ADR cells by G2/M arrest. Toxicol Lett. 2013 May 23;219(2):107-15. doi: 10.1016/j.toxlet.2013.01.019. Epub 2013 Mar 5. PMID: 23470866.

2. Jobson AG, Cardellina JH 2nd, Scudiero D, Kondapaka S, Zhang H, Kim H, Shoemaker R, Pommier Y. Identification of a Bisguanylhydrazone [4,4'-Diacetyldiphenylurea-bis(guanylhydrazone); NSC 109555] as a novel chemotype for inhibition of Chk2 kinase. Mol Pharmacol. 2007 Oct;72(4):876-84. doi: 10.1124/mol.107.035832. Epub 2007 Jul 6. Erratum in: Mol Pharmacol. 2008 Oct;74(4):1170. PMID: 17616632.

#### In vivo study

TBD

# 7. Bioactivity

Biological target:

NSC-109555 Ditosylate is a potent, selective, reversible, ATP-competitive Chk2 inhibitor.

# In vitro activity

In vitro data show the specific inhibition of Chk2 kinase activity by NSC 109555 using in vitro kinase assays and kinase-profiling experiments. NSC 109555 was shown to be a competitive inhibitor of Chk2 with respect to ATP, which was supported by docking of

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NSC 109555 into the ATP binding pocket of the Chk2 catalytic domain. The potency of NSC 109555 was comparable with that of other known Chk2 inhibitors, such as debromohymenialdisine and 2-arylbenzimidazole.

Reference: Mol Pharmacol. 2007 Oct;72(4):876-84. https://pubmed.ncbi.nlm.nih.gov/17616632/

In vivo activity

TBD

Note: The information listed here was extracted from literature. MedKoo has not independently retested and confirmed the accuracy of these methods. Customer should use it just for a reference only.