Product Data Sheet

Product Name: NS3694
Cat. No.: GC12639

Chemical Properties

Cas. No.	426834-38-0		
Chemical Name	4-chloro-2-[[[[3-(trifluoromethyl)phenyl]amino]carbonyl]amino]-benzoic acid		
SMILES	ClC1=CC=C(C(O)=O)C(NC(NC2=CC=CC(C(F)(F)F)=C2)=O)=C1		
Formula	$C_{15}H_{10}ClF_3N_2O_3$	M.Wt	358.7
Solubility	≤14mg/ml in ethanol;20mg/ml in DMSO;25mg/ml in dimethyl formamide	Storage	Store at -20°C
General tips	For obtaining a higher solubility , please warm the tube at 37 ℃ and shake it in the ultrasonic bath for a while.Stock solution can be stored below -20℃ for several months.		
Shipping Condition	Evaluation sample solution : ship with blue ice All other available size: ship with RT , or blue ice upon request.		
Structure	NS3694		

Background

IC50: approximately 50 μM for cytochrome c-induced caspase activation in HeLa cell cytosolic extracts

NS3694 inhibits apoptosome formation and caspase activation.

The release of mitochondrial proapoptotic proteins into the cytosol is a critical event in apoptosis signaling, resulting in the activation of caspases. Once in the cytosol, cytochrome c triggers the formation of a caspase-activating protein complex called the apoptosome, while Smac/Diablo and Omi/htra2 antagonize the caspase inhibitory effect.

In vitro: Previous study found that NS3694, and its two analogs (NS1764 and NS1784) were well-tolerated by MCF-7S1 breast cancer cells at concentrations up to 100, 50, and 25 μM, respectively. Moreove, all three compounds could not inhibit recombinant caspase 9 and caspase 3 at concentrations ranging from 25 to 100 μM. In addition,

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NS3694 was able to inhibit the co-immunoprecipitation of caspase 9 and Apaf-1 from HeLa cell cytosol stimulated by cytochrome c and dATP. NS3694 could also inhibit the formation of the active 700-kDa apoptosome complex, but had no effect on TNF-induced caspase-independent death of WEHI-S cells. NS3694 did not inhibit FasL-induced caspase activation or death in type I cells neither [1].

In vivo: Up to now, there is no animal in vivo study reported.

Clinical trial: So far, no clinical study has been conducted.

Reference:
[1] Lademann, U. ,Cain, K.,Gyrd-Hansen, M., et al. Diarylurea compounds inhibit caspase activation by preventing the formation of the active 700-kilodalton apoptosome complex. Mol.Cell Biol. 23(21), 7829-7837 (2003).

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