MOLNOVA
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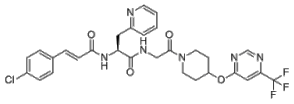
Datasheet (Version 1.0)

Product Name	:	ASP 9853
Synonyms	:	ASP9853;ASP-9853;FR 260330 dehydrate
Cat No.	:	M14503
CAS Number	:	442198-67-6
Molecular Formula	:	C29H28ClF3N6O4
Formula Weight	:	617.03
Chemical Name	:	(S,E)-3-(4-chlorophenyl)-N-(1-oxo-1-((2-oxo-2-(4-((6-(trifluoromethyl)pyrimidin-4-yl)oxy)piperidin-1-yl)ethyl)amino)-3-(pyridin-2-yl)propan-2-yl)acrylamide
Description	:	A potent, orally active iNOS inhibitor (IC50=10 nM, NO release DLD-1 cells) that prevents dimerization of iNOS, but has no effect on the expression or enzyme activity of iNOS; reduces NOx production in plasma from rats exposed to LPS (IC50=1.6 mg/kg), without effect on mean arterial blood pressure; also shows greater tumor growth inhibition than docetaxel alone against non-small lung cancer xenografts in combination with docetaxe.Blood Cancer Phase 1 Discontinued
Pathway	:	Immunology/Inflammation
Target	:	NOS
Receptor	:	NOS
Solubility	:	——
SMILES	:	C1CN(CCC1OC2=NC=NC(=C2)C(F)(F)F)C(=O)CNC(=O)C(CC3=CC=CC=N3)NC(=O)C=CC4=CC=C(C=C4)Cl
Storage	:	(-20℃)
Stability	:	≥ 2 years
Reference	:	



1. Luke JJ, et al. Cancer Chemother Pharmacol. 2016 Mar;77(3):549-58.| 2. Chida N, et al. Eur J Pharmacol. 2005 Feb 10;509(1):71-6.

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