

NMS-P118

## Chemical Properties

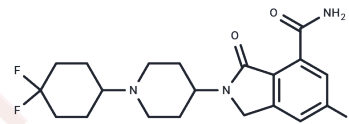
CAS No. : 1262417-51-5

Formula: C<sub>20</sub>H<sub>24</sub>F<sub>3</sub>N<sub>3</sub>O<sub>2</sub>

Molecular Weight: 395.42

Storage: Powder: -20°C for 3 years | In solvent: -80°C for 1 year

Actual storage temperature shall be subject to the COA.



## Biological Description

Description	NMS-P118 is a potent, selective and orally available Inhibitor of PARP-1 for cancer therapy.
Targets(IC50)	PARP
In vitro	NMS-P118 proved to be a potent, orally available, and highly selective PARP-1 inhibitor endowed with excellent ADME and pharmacokinetic profiles and high efficacy in vivo both as a single agent and in combination with Temozolomide in MDA-MB-436 and Capan-1 xenograft models, respectively. Cocrystal structures of 20by with both PARP-1 and PARP-2 catalytic domain proteins allowed rationalization of the observed selectivity.

## Solubility Information

Solubility	DMSO: 16 mg/mL (40.46 mM), Sonication and heating are recommended. (< 1 mg/ml refers to the product slightly soluble or insoluble)
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## Preparing Stock Solutions

	1mg	5mg	10mg
1 mM	2.529 mL	12.6448 mL	25.2896 mL
5 mM	0.5058 mL	2.529 mL	5.0579 mL
10 mM	0.2529 mL	1.2645 mL	2.529 mL
50 mM	0.0506 mL	0.2529 mL	0.5058 mL

Please select the appropriate solvent to prepare the stock solution, according to the solubility of the product in different solvents. Please use it as soon as possible.

Note: The dilution table applies only to solid products. For liquid products, please calculate the stock solution based on the stated concentration and/or density.

Reference

Papeo G, et al. Discovery of 2-[1-(4,4-Difluorocyclohexyl)piperidin-4-yl]-6-fluoro-3-oxo-2,3-dihydro-1H-isoindole-4-carboxamide (NMS-P118): A Potent, Orally Available, and Highly Selective PARP-1 Inhibitor for Cancer Therapy. J Med Chem. 2015 Sep 10;58(17):6875-98.

**Inhibitor · Natural Compounds · Compound Libraries · Recombinant Proteins**

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