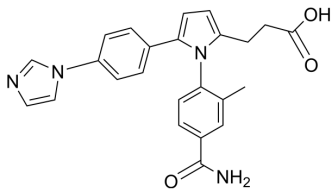
N6022

Cat. No.:	HY-14984
CAS No.:	1208315-24-5
Molecular Formula:	$C_{24}H_{22}N_4O_3$
Molecular Weight:	414.46
Target:	GSNOR
Pathway:	Metabolic Enzyme/Protease
Storage:	Powder -20°C 3 years 4°C 2 years In solvent -80°C 2 years -20°C 1 year



SOLVENT & SOLUBILITY

In Vitro

DMSO : 25 mg/mL (60.32 mM; Need ultrasonic)
H_2O : < 0.1 mg/mL (insoluble)

Preparing Stock Solutions

Solvent / Mass / Concentration	1 mg	5 mg	10 mg
1 mM	2.4128 mL	12.0639 mL	24.1278 mL
5 mM	0.4826 mL	2.4128 mL	4.8256 mL
10 mM	0.2413 mL	1.2064 mL	2.4128 mL

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

In Vivo

1. Add each solvent one by one: 10% DMSO >> 40% PEG300 >> 5% Tween-80 >> 45% saline
   Solubility: ≥ 2.5 mg/mL (6.03 mM); Clear solution
2. Add each solvent one by one: 10% DMSO >> 90% (20% SBE-β-CD in saline)
   Solubility: ≥ 2.5 mg/mL (6.03 mM); Clear solution

BIOLOGICAL ACTIVITY

Description

N6022 is a potent, selective, reversible, and efficacious S-Nitrosoglutathione reductase(GSNOR) inhibitor with IC_{50} of 8 nM.

IC_{50} & Target

IC50: 8 nM (GSNOR)[2]

In Vitro

N6022 shows concentration-dependent binding to rat plasma proteins. N6022 has more effect on ATP at lower drug concentrations (20 μM) than on GSH[1]. N6022 binds in the GSNO substrate binding pocket like a competitive inhibitor with an IC_{50} of 8 nM and a K_i of 2.5 nM. N6022 is uncompetitive with cofactors NAD^+ and NADH[2].

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

In Vivo	N6022 (50 mg/kg)-treated rats show a slight increase in the incidence of granulomas. In serum, N6022 remains in solution up to 5 mg/mL[1]. MCE has not independently confirmed the accuracy of these methods. They are for reference only.

PROTOCOL

Cell Assay [1]	N6022 is tested using a rat hepatoma (H4IIE) cell line whereby cells are seeded into 96-well plates and cultured in medium containing 20% bovine serum. Following an equilibration period of 48 h, the cells are treated with N6022 (5% DMSO vehicle) at concentrations of 0, 1, 5, 10, 20, 50, 100, and 300 μM for 24 h at 37°C in 5% CO_2. Camptothecin and rotenone are included as positive controls. The cell supernatant or the cells themselves are harvested for biochemical analysis. MCE has not independently confirmed the accuracy of these methods. They are for reference only.

CUSTOMER VALIDATION

- Cell Death Dis. 2019 May; 10(5): 329.
- Food Chem. 2022 May 24;392:133299.
- Free Radic Biol Med. 2017 Apr 15;108:445-451.
- Mol Pharmacol. 2016 Oct;90(4):418-26.
- Pediatr Pulm. 2019 Dec;54(12):1989-1996.

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REFERENCES

[1]. Sun X, et al. Structure-activity relationships of pyrrole based S-nitrosoglutathione reductase inhibitors: pyrrole regioisomers and propionic acid replacement. Bioorg Med Chem Lett. 2011 Jun 15;21(12):3671-5.

[2]. Colagiovanni DB, et al. A nonclinical safety and pharmacokinetic evaluation of N6022: a first-in-class S-nitrosoglutathione reductase inhibitor for the treatment of asthma. Regul Toxicol Pharmacol. 2012 Feb;62(1):115-24.

[3]. Green LS, et al. Mechanism of inhibition for N6022, a first-in-class drug targeting S-nitrosoglutathione reductase. Biochemistry. 2012 Mar 13;51(10):2157-68.

[4]. Thomas M. Raffay, et al. Methods of treating respiratory disorders. Patent. US 20170209419 A1.

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