# Product Data Sheet

## Phenylephrine-2,4,6-d<sub>3</sub> hydrochloride

Cat. No.:	HY-B0471S1	
CAS No.:	1276197-50-2	D, , D
Molecular Formula:	C <sub>9</sub> H <sub>11</sub> D <sub>3</sub> CINO <sub>2</sub>	Ϋ́ Ϋ́
Molecular Weight:	206.68	
Target:	Adrenergic Receptor; Endogenous Metabolite	
Pathway:	GPCR/G Protein; Neuronal Signaling; Metabolic Enzyme/Protease	
Storage:	4°C, sealed storage, away from moisture	H-CI
	* In solvent : -80°C, 6 months; -20°C, 1 month (sealed storage, away from moisture)	

### SOLVENT & SOLUBILITY

In Vitro	DMSO : 50 mg/mL (241.92 mM; Need ultrasonic)					
	Preparing Stock Solutions	Solvent Mass Concentration	1 mg	5 mg	10 mg	
		1 mM	4.8384 mL	24.1920 mL	48.3840 mL	
		5 mM	0.9677 mL	4.8384 mL	9.6768 mL	
		10 mM	0.4838 mL	2.4192 mL	4.8384 mL	
	Please refer to the sol	ubility information to select the ap	propriate solvent.			
In Vivo	1. Add each solvent one by one: 10% DMSO >> 40% PEG300 >> 5% Tween-80 >> 45% saline Solubility: ≥ 1.25 mg/mL (6.05 mM); Clear solution					
	2. Add each solvent one by one: 10% DMSO >> 90% (20% SBE-β-CD in saline) Solubility: ≥ 1.25 mg/mL (6.05 mM); Clear solution					
	3. Add each solvent o Solubility: ≥ 1.25 m	one by one: 10% DMSO >> 90% cor ng/mL (6.05 mM); Clear solution	n oil			

Description       Phenylephrine-2,4,6-d <sub>3</sub> (hydrochloride) is the deuterium labeled Phenylephrine hydrochloride. (R)-(-)-Phenylephrine hydrochloride is a selective α1-adrenoceptor agonist with pKis of 5.86, 4.87 and 4.70 for α1D, α1B and α1A receptors respectively.					
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In Vitro Stable heavy isotopes of hydrogen, carbon, and other elements have been incorporated into drug molecules, largely as tracers for quantitation during the drug development process. Deuteration has gained attention because of its potential to affect the pharmacokinetic and metabolic profiles of drugs <sup>[1]</sup> . MCE has not independently confirmed the accuracy of these methods. They are for reference only.	In Vitro	Stable heavy isotopes of hydrogen, carbon, and other elements have been incorporated into drug molecules, largely as tracers for quantitation during the drug development process. Deuteration has gained attention because of its potential to affect the pharmacokinetic and metabolic profiles of drugs <sup>[1]</sup> . MCE has not independently confirmed the accuracy of these methods. They are for reference only.			

### REFERENCES

[1]. Russak EM, et al. Impact of Deuterium Substitution on the Pharmacokinetics of Pharmaceuticals. Ann Pharmacother. 2019;53(2):211-216.

[2]. Ford AP, et al. Pharmacological pleiotropism of the human recombinant alpha1A-adrenoceptor: implications for alpha1-adrenoceptor classification. Br J Pharmacol. 1997 Jul;121(6):1127-35.

[3]. Minneman KP, et al. Selectivity of agonists for cloned alpha 1-adrenergic receptor subtypes. Mol Pharmacol. 1994 Nov;46(5):929-36.

[4]. Wang J, et al. Phenylephrine promotes cardiac fibroblast proliferation through calcineurin-NFAT pathway. Front Biosci (Landmark Ed). 2016 Jan 1;21:502-13.

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[6]. Li NJ, et al. Effect of phenylephrine on alveolar fluid clearance in ventilator-induced lung injury. Chin Med Sci J. 2013 Mar;28(1):1-6.

#### Caution: Product has not been fully validated for medical applications. For research use only.

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