Acetaminophen-d_4

Cat. No.: HY-66005S

CAS No.: 64315-36-2

Molecular Formula: $C_8H_5D_4NO_2$

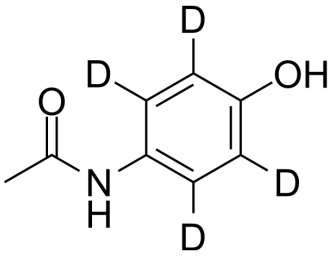
Molecular Weight: 155.19

Target: COX; Histone Acetyltransferase; Endogenous Metabolite

Pathway: Immunology/Inflammation; Epigenetics; Metabolic Enzyme/Protease

Storage:

Powder	-20°C	3 years
	4°C	2 years
In solvent	-80°C	6 months
	-20°C	1 month



SOLVENT & SOLUBILITY

In Vitro

DMSO : ≥ 100 mg/mL (644.37 mM)

* "≥" means soluble, but saturation unknown.

Preparing Stock Solutions

Solvent / Mass / Concentration	1 mg	5 mg	10 mg
1 mM	6.4437 mL	32.2186 mL	64.4371 mL
5 mM	1.2887 mL	6.4437 mL	12.8874 mL
10 mM	0.6444 mL	3.2219 mL	6.4437 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 (16.11 mM); Clear solution
2. Add each solvent one by one: 10% DMSO >> 90% (20% SBE-β-CD in saline)
   Solubility: ≥ 2.5 mg/mL (16.11 mM); Clear solution
3. Add each solvent one by one: 10% DMSO >> 90% corn oil
   Solubility: ≥ 2.5 mg/mL (16.11 mM); Clear solution

BIOLOGICAL ACTIVITY

Description

Acetaminophen-d_4 is the deuterium labeled Acetaminophen. Acetaminophen (Paracetamol) is a selective cyclooxygenase-2 (COX-2) inhibitor with an IC50 of 25.8 μM; is a widely used antipyretic and analgesic agent[1][2][3]. Acetaminophen is a potent hepatic N-acetyltransferase 2 (NAT2) inhibitor[4].

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[1].

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]. Hinz, B, et al. Acetaminophen (paracetamol) is a selective cyclooxygenase-2 inhibitor in man. FASEB J, 2008. 22(2): p. 383-90.

[3]. Miroslav Dinić, et al. Lactobacillus fermentum Postbiotic-induced Autophagy as Potential Approach for Treatment ofAcetaminophen Hepatotoxicity. Front Microbiol. 2017 Apr 6;8:594.

[4]. Uchida NS, et al. Hepatoprotective Effect of Citral on Acetaminophen-Induced Liver Toxicity in Mice. Evid Based Complement Alternat Med. 2017;2017:1796209.

[5]. Rothen JP, et al. Acetaminophen is an inhibitor of hepatic N-acetyltransferase 2 in vitro and in vivo. Pharmacogenetics. 1998 Dec;8(6):553-9.

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