

## COX-2-IN-6

## Chemical Properties

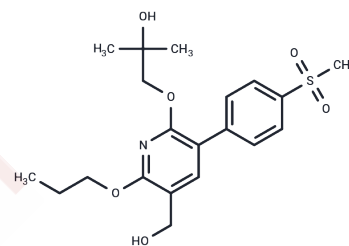
CAS No. : 2756347-91-6

Formula: C<sub>20</sub>H<sub>27</sub>N<sub>1</sub>O<sub>6</sub>S

Molecular Weight: 409.5

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	COX-2-IN-6 is a potent, selective, and orally available cyclooxygenase-2 (COX-2) inhibitor with an IC <sub>50</sub> of 0.84 μM and a K <sub>i</sub> of 69 nM. COX-2-IN-6 inhibits COX-2-driven PGE <sub>2</sub> synthesis with an IC <sub>50</sub> of 0.60 μM. COX-2-IN-6 is used to prevent colorectal cancer. COX-2-IN-6 can be used to prevent colorectal cancer.
Targets(IC <sub>50</sub> )	COX, Prostaglandin Receptor
In vitro	COX-2-IN-6 (Compound 10) inhibits human COX-2/COX-1 enzyme and COX-2/COX-1-driven PGE <sub>2</sub> synthesis in HEK293 cells, with IC <sub>50</sub> of 0.84 μM, >50 μM, 0.60 μM and, >50 μM, respectively.[1] COX-2-IN-6 exhibits stability in human or mouse liver microsomes and hepatocytes in vitro. The T <sub>1/2</sub> value of human hepatocytes is 3.1 min, and the T <sub>1/2</sub> value of mouse hepatocytes is 3.0 min.[1]
In vivo	COX-2-IN-6 (Compound 10) (30, 100, 300 mg/kg; oral; single dose; APC <sup>min</sup> /mouse model) inhibits adenoma progression and extends survival in the APC <sup>min</sup> /+ mouse model.[1] COX-2-IN-6 (10 mg/kg; oral; single dose; APC <sup>min</sup> /+ mouse model) exhibits high colonic exposure (>4300 ng/g) and low systemic exposure (6 ng/mL), C/P distribution ratio > 1200 in 4 hours.[1]

## Solubility Information

Solubility	DMSO: 60 mg/mL (146.52 mM), Sonication is recommended. (< 1 mg/ml refers to the product slightly soluble or insoluble)
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### Preparing Stock Solutions

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	<b>1mg</b>	<b>5mg</b>	<b>10mg</b>
1 mM	2.442 mL	12.210 mL	24.420 mL
5 mM	0.4884 mL	2.442 mL	4.884 mL
10 mM	0.2442 mL	1.221 mL	2.442 mL
50 mM	0.0488 mL	0.2442 mL	0.4884 mL

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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

Zhang Z, et al. Gut-Restricted Selective Cyclooxygenase-2 (COX-2) Inhibitors for Chemoprevention of Colorectal Cancer. *J Med Chem.* 2021 Aug 12;64(15):11570-11596.

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