# **Product data sheet**



MedKoo Cat#: 527888				
Name: CAY10404				
CAS#: 340267-36-9				
Chemical Formula: C <sub>17</sub> H <sub>12</sub> F <sub>3</sub> NO <sub>3</sub> S				
Exact Mass: 367.049				
Molecular Weight: 367.3422				
Product supplied as:	Powder			
Purity (by HPLC):	$\geq 98\%$			
Shipping conditions	Ambient temperature			
Storage conditions:	Powder: -20°C 3 years; 4°C 2 years.			
	In solvent: -80°C 3 months; -20°C 2 weeks.			



## 1. Product description:

CAY10404 is one of the most selective inhibitors of COX-2 over COX-1.

## 2. CoA, QC data, SDS, and handling instruction

SDS and handling instruction, CoA with copies of QC data (NMR, HPLC and MS analytical spectra) can be downloaded from the product web page under "QC And Documents" section. Note: copies of analytical spectra may not be available if the product is being supplied by MedKoo partners. Whether the product was made by MedKoo or provided by its partners, the quality is 100% guaranteed.

#### 3. Solubility data

Solvent	Max Conc. mg/mL	Max Conc. mM
DMSO	100	272.23

## 4. Stock solution preparation table:

Concentration / Solvent Volume / Mass	1 mg	5 mg	10 mg
1 mM	2.72 mL	13.61 mL	27.22 mL
5 mM	0.54 mL	2.72 mL	5.44 mL
10 mM	0.27 mL	1.36 mL	2.72 mL
50 mM	0.05 mL	0.27 mL	0.54 mL

## 5. Molarity Calculator, Reconstitution Calculator, Dilution Calculator

Please refer the product web page under section of "Calculator"

## 6. Recommended literature which reported protocols for in vitro and in vivo study

#### In vitro study

1. Cho Y, Park MJ, Park M, Min SS, Yee J, Kim C, Han MS, Han SH. Effects of CAY10404 on the PKB/Akt and MAPK pathway and apoptosis in non-small cell lung cancer cells. Respirology. 2009 Aug;14(6):850-8. doi: 10.1111/j.1440-1843.2009.01563.x. PMID: 19703066.

#### In vivo study

1. Robertson JA, Sauer D, Gold JA, Nonas SA. The role of cyclooxygenase-2 in mechanical ventilation-induced lung injury. Am J Respir Cell Mol Biol. 2012 Sep;47(3):387-94. doi: 10.1165/rcmb.2011-0005OC. Epub 2012 May 3. PMID: 22556158; PMCID: PMC3488687.

## 7. Bioactivity

## Biological target:

CAY10404 is a potent and selective cyclooxygenase-2 (COX-2) inhibitor with an IC50 of 1 nM and a selectivity index (SI; COX-1 IC50/COX-2 IC50) of >500000.

## In vitro activity

Treatment with CAY10404 in the range of 10-100 microM caused dose-dependent growth inhibition, with an average 50% inhibitory concentration (IC(50)) of 60-100 micromol/L, depending on the cell line. Western blot analysis of CAY10404-treated cells showed cleavage of poly (ADP-ribose) polymerase (PARP) and procaspase-3, signifying caspase activity and apoptotic cell death. CAY10404

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treatment inhibited the phosphorylation of Akt, glycogen synthase kinase-3beta and extracellular signal-regulated kinases 1/2 in H460 and H358 cells.

Reference: Respirology. 2009 Aug;14(6):850-8. https://doi.org/10.1111/j.1440-1843.2009.01563.x

## In vivo activity

The objective was to determine the role of cyclooxygenase-2 in mechanical ventilation-induced lung injury and the effects of cyclooxygenase-2 inhibition on lung inflammation and barrier disruption. Mice were mechanically ventilated at low and high tidal volumes, in the presence or absence of pharmacologic cyclooxygenase-2-specific inhibition with 3-(4-methylsulphonylphenyl)-4-phenyl-5-trifluoromethylisoxazole (CAY10404). Lung injury was assessed using markers of alveolar-capillary leakage and lung inflammation. Cyclooxygenase-2 expression and activity were measured by Western blotting, real-time PCR, and lung/plasma prostanoid analysis, and tissue sections were analyzed for cyclooxygenase-2 staining by immunohistochemistry. High tidal volume ventilation induced lung injury, significantly increasing both lung leakage and lung inflammation relative to control and low tidal volume ventilation. High tidal volume mechanical ventilation significantly induced cyclooxygenase-2 expression and activity, both in the lungs and systemically, compared with control mice and low tidal volume mice. The immunohistochemical analysis of lung sections localized cyclooxygenase-2 expression to monocytes and macrophages in the alveoli. The pharmacologic inhibition of cyclooxygenase-2 with CAY10404 significantly decreased cyclooxygenase activity and attenuated lung injury in mice ventilated at high tidal volume, attenuating barrier disruption, tissue inflammation, and inflammatory cell signaling. This study demonstrates the induction of cyclooxygenase-2 by mechanical ventilation, and suggests that the therapeutic inhibition of cyclooxygenase-2 may attenuate ventilator-induced acute lung injury.

Reference: Am J Respir Cell Mol Biol. 2012 Sep;47(3):387-94. https://www.ncbi.nlm.nih.gov/pmc/articles/pmid/22556158/

Note: The information listed here was extracted from literature. MedKoo has not independently retested and confirmed the accuracy of these methods. Customer should use it just for a reference only.