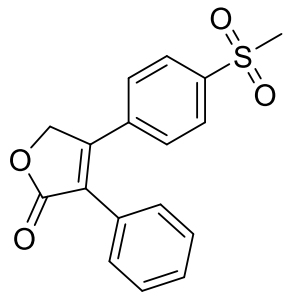
Product data sheet

MedKoo Cat#: 314273 Name: Rofecoxib CAS#: 162011-90-7 Chemical Formula: $C_{17}H_{14}O_4S$ Exact Mass: 314.06128 Molecular Weight: 314.36	
Product supplied as:	Powder
Purity (by HPLC):	≥ 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:
Rofecoxib is a nonsteroidal anti-inflammatory drug (NSAID) that has now been withdrawn over safety concerns. Rofecoxib exhibits anti-inflammatory, analgesic, and antipyretic activities in animal models. The mechanism of action of rofecoxib is believed to be due to inhibition of prostaglandin synthesis, via inhibition of cyclooxygenase-2 (COX-2). At therapeutic concentrations in humans, rofecoxib does not inhibit the cyclooxygenase-1 (COX-1) isoenzyme. Studies to elucidate the mechanism of action of fofecoxib in the acute treatment of migraine have not been conducted.

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
DMF	25.0	79.53
DMSO	40.44	128.65
Ethanol	0.1	0.32

4. Stock solution preparation table:

Concentration / Solvent Volume / Mass	1 mg	5 mg	10 mg
1 mM	3.18 mL	15.91 mL	31.81 mL
5 mM	0.64 mL	3.18 mL	6.36 mL
10 mM	0.32 mL	1.59 mL	3.18 mL
50 mM	0.06 mL	0.32 mL	0.64 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. Al-Nimer MS, Al-Deen SM, Abdul Lateef ZW. Rofecoxib prevents ctdsDNA against damage induced by copper sulfate and ultraviolet B radiation in vitro study. J Basic Clin Pharm. 2010 Dec;2(1):21-5. Epub 2011 Feb 15. PMID: 24825998; PMCID: PMC3979209.
2. Chan CC, Boyce S, Brideau C, Charleson S, Cromlish W, Ethier D, Evans J, Ford-Hutchinson AW, Forrest MJ, Gauthier JY, Gordon R, Gresser M, Guay J, Kargman S, Kennedy B, Leblanc Y, Leger S, Mancini J, O'Neill GP, Ouellet M, Patrick D, Percival MD, Perrier H, Prasit P, Rodger I, et al. Rofecoxib [Vioxx, MK-0966; 4-(4'-methylsulfonylphenyl)-3-phenyl-2-(5H)-furanone]: a potent and orally active cyclooxygenase-2 inhibitor. Pharmacological and biochemical profiles. J Pharmacol Exp Ther. 1999 Aug;290(2):551-60. PMID: 10411562.

In vivo study

Product data sheet

1. Zou YH, Guan PP, Zhang SQ, Guo YS, Wang P. Rofecoxib Attenuates the Pathogenesis of Amyotrophic Lateral Sclerosis by Alleviating Cyclooxygenase-2-Mediated Mechanisms. Front Neurosci. 2020 Aug 13;14:817. doi: 10.3389/fnins.2020.00817. PMID: 32903591; PMCID: PMC7438558.
2. Liu NN, Sun YZ, Zhao N, Chen L. Rofecoxib inhibits retinal neovascularization via down regulation of cyclooxygenase-2 and vascular endothelial growth factor expression. Clin Exp Ophthalmol. 2015 Jul;43(5):458-65. doi: 10.1111/ceo.12473. Epub 2015 Jan 15. PMID: 25472856.

7. Bioactivity

Biological target:

Rofecoxib is a potent, specific and orally active COX-2 inhibitor, with IC50s of 26 and 18 nM for human COX-2 in human osteosarcoma cells and Chinese hamster ovary cells, with a 1000-fold selectivity for COX-2 over human COX-1 (IC50 > 50 μM in U937 cells and > 15 μM in Chinese hamster ovary cells).

In vitro activity

Rofecoxib significantly attenuated the separation of double strands of DNA (detected by increase the absorbance of DNA at 260 nm) induced by Cu ions. Rofecoxib significantly offered protection against UVB-induced DNA damage. It is concluded that rofecoxib offered protection against copper ions or UVB inducedDNA damage via different mechanisms not related to the inhibition COX-2.

Reference: J Basic Clin Pharm. 2010 Dec;2(1):21-5. https://pubmed.ncbi.nlm.nih.gov/24825998/

In vivo activity

To this end, Western blot analysis was carried out to measure the expression of COX-2, IL-1β, and TNF-α in the spinal cords of SOD1G93A mice. The results demonstrated that rofecoxib treatment clearly inhibited the expression of IL-1β and TNF-α by decreasing the protein expression of COX-2 in the spinal cords of SOD1G93A mice (Figures 6A,B). Taken together, our findings reveal that rofecoxib shows neuroprotective effects by targeting COX-2 proinflammatory signaling cascades in ALS mice.

Reference: Front Neurosci. 2020 Aug 13;14:817. https://pubmed.ncbi.nlm.nih.gov/32903591/

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.