

PRODUCT INFORMATION



KI-696

Item No. 42039

CAS Registry No.: 1799974-70-1

Formal Name: β S-[3-[[[(4R)-3,4-dihydro-4-methyl-1,1-dioxido-2H-5,1,2-benzoxathiazepin-2-yl]methyl]-4-methylphenyl]-7-methoxy-1-methyl-1H-benzotriazole-5-propanoic acid

MF: $C_{28}H_{30}N_4O_6S$

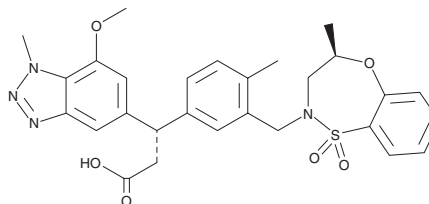
FW: 550.6

Purity: $\geq 98\%$

Supplied as: A solid

Storage: -20°C

Stability: ≥ 4 years



Information represents the product specifications. Batch specific analytical results are provided on each certificate of analysis.

Laboratory Procedures

KI-696 is supplied as a solid. A stock solution may be made by dissolving the KI-696 in the solvent of choice, which should be purged with an inert gas. KI-696 is soluble (≥ 10 mg/ml) in ethanol and DMSO.

Description

KI-696 is an inhibitor of the protein-protein interaction between Kelch-like ECH-associated protein 1 (Keap1) and nuclear factor erythroid 2-related factor 2 (Nrf2).¹ It binds to the Keap1 Kelch domain ($K_d = 1.3$ nM) and increases the accumulation of Nrf2 in isolated human bronchial epithelial cells in a concentration-dependent manner. KI-696 increases the expression of the Nrf2 target genes *NQO1*, *GCLM*, *HMOX1*, and *TXNRD1* in bronchial epithelial cells isolated from patients with chronic obstructive pulmonary disease (COPD; EC_{50} s = 22, 36, 16, and 27 nM, respectively). *In vivo*, KI-696 (50 $\mu\text{mol/kg}$) increases lung expression of *Nqo1*, *Hmox1*, and *Txnrd1* in rats.

Reference

1. Davies, T.G., Wixted, W.E., Coyle, J.E., *et al.* Monoacidic inhibitors of the Kelch-like ECH-associated protein 1: Nuclear factor erythroid 2-related factor 2 (KEAP1:NRF2) Protein-protein interaction with high cell potency identified by fragment-based discovery. *J. Med. Chem.* **59**(8), 3991-4006 (2016).

WARNING

THIS PRODUCT IS FOR RESEARCH ONLY - NOT FOR HUMAN OR VETERINARY DIAGNOSTIC OR THERAPEUTIC USE.

SAFETY DATA

This material should be considered hazardous until further information becomes available. Do not ingest, inhale, get in eyes, on skin, or on clothing. Wash thoroughly after handling. Before use, the user must review the [complete](#) Safety Data Sheet, which has been sent via email to your institution.

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