

Product Data Sheet

Product Name: CAY10404

Cat. No.: GC43149

Chemical Properties

Cas. No. 340267-36-9

Chemical Name 3-[4-(methylsulfonyl)phenyl]-4-phenyl-5-(trifluoromethyl)-isoxazole

SMILES FC(F)(F)c1onc(c2ccc(cc2)S(=O)(=O)C)c1c1ccccc1

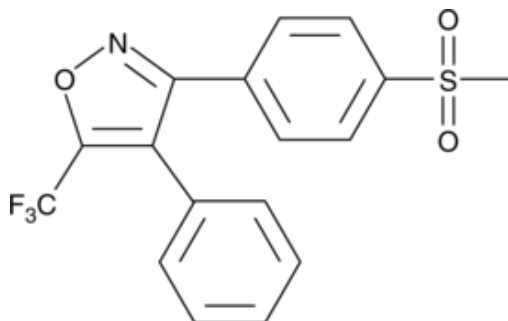
Formula $C_{17}H_{12}F_3NO_3S$ M.Wt 367.4

Solubility 17mg/mL in ethanol or DMSO, 21mg/mL in DMF Storage Store at -20°C

General tips For obtaining a higher solubility, please warm the tube at 37 °C and shake it in the ultrasonic bath for a while. Stock solution can be stored below -20°C for several months.

Shipping Condition Evaluation sample solution: ship with blue ice All other available size: ship with RT, or blue ice upon request.

Structure



Background

Many non-steroidal anti-inflammatory drugs (NSAIDs) are potent but non-selective inhibitors of both COX-1 and COX-2 in humans.[1] CAY10404 is one of the most selective inhibitors of COX-2 which has been reported to date, with a selectivity index (SI; SI = IC₅₀ COX-1/IC₅₀ COX-2) of >500,000. (The COX-1 IC₅₀ is >500 mM, and COX-2 IC₅₀ is <1 nM.)[2] As a reference point, the SI of celecoxib is about 400. Thus, CAY10404 has an SI which is several logs greater than the first generation of selective COX-2 inhibitors, and is comparable to the SI of second generation selective COX-2 inhibitors, such as valdecoxib and etoricoxib.[3]

Caution: Product has not been fully validated for medical applications. For research use only.

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Reference:

- [1.] Barnett, J., Chow, J., Ives, D., et al. Purification, characterization and selective inhibition of human prostaglandin G/H synthase 1 and 2 expressed in the baculovirus system. *Biochim Biophys. Acta.* 1209(1), 130-139 (1994).
- [2]. Habeeb, A.G., Rao, P.N.P., and Knaus, E.E. Design and syntheses of diarylisoxazoles: Novel inhibitors of cyclooxygenase-2 (COX-2) with analgesic-antiinflammatory activity. *Drug Development Research* 51, 273-286 (2000).
- [3]. Mardini, I.A., and Fitzgerald, G.A. Selective inhibitors of cyclooxygenase-2: A growing class of anti-inflammatory drugs. *Molecular Interventions* 1(1), 30-38 (2001).

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