Product Data Sheet

Product Name: YS-121
Cat. No.: GC17979

Chemical Properties

Cas. No.	916482-17-2		
Chemical Name	2-[[4-chloro-6-[(2,3-dimethylphenyl)amino]-2-pyrimidinyl]thio]-octanoic acid		
SMILES	CC1=C(NC2=CC(Cl)=NC(SC(C(O)=O)CCCCCC)=N2)C=CC=C1C		
Formula	$C_{20}H_{26}ClN_3O_2S$	M.Wt	408.0
Solubility	≤30mg/ml in ethanol;30mg/ml in DMSO;30mg/ml in dimethyl formamide	Storage	Store at -20°C
General tips	For obtaining a higher solubility , please warm the tube at 37 ℃ and shake it in the ultrasonic bath for a while.Stock solution can be stored below -20℃ 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	YS-121		

Background

YS-121 is a dual inhibitor of Microsomal prostaglandin E2 synthase-1 (mPGES-1) [1].

Cyclooxygenases (COX-1 and COX-2) have been involved in catalyzing the formation of prostaglandins and related eicosanoids and play an essential role in the pathogenesis of breast cancer. Actions of COX-2 are mediated by prostaglandin E2 (PGE2). Microsomal PGES-1 (mPGES-1), the inducible form of PGES, has a marked affinity for coupling with COX-2. Expression of mPGES-1 has been observed in inflammatory conditions and cancers of the stomach, colon, lung, endometrium, and skin [2].

YS-121 inhibited the activity of mPGES-1 with an IC50 of 3.9 μM [1]. YS-121 also inhibited the activity of 5-LO with the IC50 of 4.1 μM [3]. YS-121 effectively inhibited PGE2 and LT synthesis in both cell free and intact cell assays. Intraperitoneal administration of YS-121 (1.5 mg/kg) reduced pleural levels of PGE2 and LTB4 while blocking exudate formation and leukocyte infiltration in carrageenan-induced rat

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pleurisy [4]. YS-121 (10 μM) showed minor effects on COX-1 and COX-2, inhibiting these enzymes 24.8% and 38%, respectively [1].

References:

[1] Koeberle A, Zettl H, Greiner C, et al. Pirinixic acid derivatives as novel dual inhibitors of microsomal prostaglandin E2 synthase-1 and 5-lipoxygenase[J]. Journal of medicinal chemistry, 2008, 51(24): 8068-8076.

[2] Mehrotra S, Morimiya A, Agarwal B, et al. Microsomal prostaglandin E2 synthase-1 in breast cancer: a potential target for therapy[J]. The Journal of pathology, 2006, 208(3): 356-363.

Werz O, Greiner C, Koeberle A, et al. Novel and potent inhibitors of 5-lipoxygenase product synthesis based on the structure of pirinixic acid[J]. Journal of medicinal chemistry, 2008, 51(17): 5449-5453.

Koeberle A, Rossi A, Zettl H, et al. The molecular pharmacology and in vivo activity of 2-(4-chloro-6-(2, 3-dimethylphenylamino) pyrimidin-2-ylthio) octanoic acid (YS121), a dual inhibitor of microsomal prostaglandin E2 synthase-1 and 5-lipoxygenase[J]. Journal of Pharmacology and Experimental Therapeutics, 2010, 332(3): 840-848.