

# PRODUCT INFORMATION



## YS-121

Item No. 13665

CAS Registry No.: 916482-17-2

Formal Name: 2-[[4-chloro-6-[(2,3-dimethylphenyl)amino]-2-pyrimidinyl]thio]octanoic acid

MF:  $C_{20}H_{26}ClN_3O_2S$

FW: 408.0

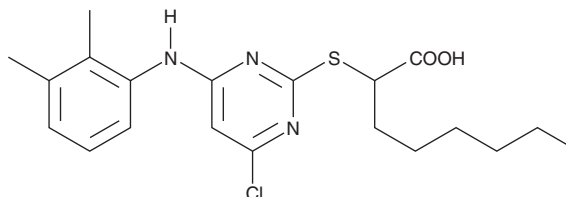
Purity:  $\geq 98\%$

UV/Vis.:  $\lambda_{max}$ : 203, 246, 292 nm

Supplied as: A solution in methyl acetate

Storage:  $-20^{\circ}C$

Stability:  $\geq 1$  year



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

### Laboratory Procedures

YS-121 is supplied as a solution in methyl acetate. To change the solvent, simply evaporate the methyl acetate under a gentle stream of nitrogen and immediately add the solvent of choice. Solvents such as ethanol, DMSO, and dimethyl formamide purged with an inert gas can be used. The solubility of YS-121 in these solvents is approximately 30 mg/ml.

YS-121 is sparingly soluble in aqueous buffers. For maximum solubility in aqueous buffers, the methyl acetate solution of YS-121 should be diluted with the aqueous buffer of choice. YS-121 has a solubility of 0.5 mg/ml in a 1:1 solution of ethanol:PBS (pH 7.2) using this method. We do not recommend storing the aqueous solution for more than one day.

### Description

Microsomal prostaglandin  $E_2$  synthase-1 (mPGES-1), with cyclooxygenase-2 (COX-2), synthesizes  $PGE_2$ , which is directly involved in signaling during inflammation, fever, and pain. 5-Lipoxygenase (5-LO) initiates the synthesis of leukotrienes (LTs), which are pro-inflammatory mediators. YS-121 is a dual inhibitor of mPGES-1 ( $IC_{50} = 3.9 \mu M$ )<sup>1</sup> and 5-LO ( $IC_{50} = 4.1 \mu M$ )<sup>2</sup>. It effectively inhibits  $PGE_2$  and LT synthesis in both cell free and intact cell assays. Moreover, YS-121 (1.5 mg/kg, intraperitoneal) reduced pleural levels of  $PGE_2$  and  $LTB_4$  while blocking exudate formation and leukocyte infiltration in carrageenan-induced rat pleurisy.<sup>2</sup> YS-121 has minor effects on COX-1 and COX-2, inhibiting these enzymes 24.8% and 38%, respectively, at  $10 \mu M$ .<sup>1</sup>

### References

1. Koeberle, A., Zettl, H., Greiner, C., et al. Pirinixic acid derivatives as novel dual inhibitors of microsomal prostaglandin  $E_2$  synthase-1 and 5-lipoxygenase. *J. Med. Chem.* **51**(24), 8068-8076 (2008).
2. Werz, O., Greiner, C., Koeberle, A., et al. Novel and potent inhibitors of 5-lipoxygenase product synthesis based on the structures of pirinixic acid. *J. Med. Chem.* **51**(17), 5449-5453 (2008).
3. 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  $E_2$  synthase-1 and 5-lipoxygenase. *J. Pharmacol. Exp. Ther.* **332**(3), 840-848 (2010).

#### 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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