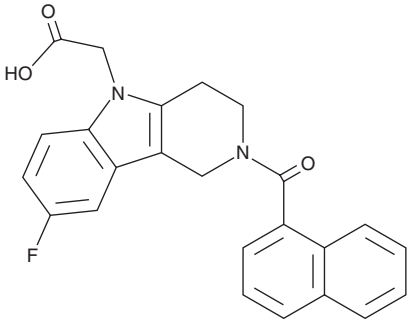
PRODUCT INFORMATION

Setipiprant

Item No. 28291

CAS Registry No.:	866460-33-5
Formal Name:	8-fluoro-1,2,3,4-tetrahydro-2-(1-naphthalenylcarbonyl)-5H-pyrido[4,3-b]indole-5-acetic acid
Synonym:	ACT-129968
MF:	$C_{24}H_{19}FN_2O_3$
FW:	402.4
Purity:	≥98%
UV/Vis.:	λ_{max}: 224, 283 nm
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

Setipiprant is supplied as a solid. A stock solution may be made by dissolving the setipiprant in the solvent of choice, which should be purged with an inert gas. Setipiprant is soluble in organic solvents such as ethanol, DMSO, and dimethyl formamide (DMF). The solubility of setipiprant in these solvents is approximately 3, 30, and 50 mg/ml, respectively.

Setipiprant is sparingly soluble in aqueous buffers. For maximum solubility in aqueous buffers, setipiprant should first be dissolved in DMF and then diluted with the aqueous buffer of choice. Setipiprant has a solubility of approximately 0.5 mg/ml in a 1:1 solution of DMF:PBS (pH 7.2) using this method. We do not recommend storing the aqueous solution for more than one day.

Description

Setipiprant is an orally bioavailable antagonist of the prostaglandin D_2 (PGD_2; Item No. 12010) receptor $CRTH_2/DP_2$ (IC_{50} = 6 nM for the human receptor).[1] It is selective for $CRTH_2/DP_2$ over DP_1 in a radioligand binding assay (IC_{50} = 1,290 nM) and the prostaglandin E_2 (PGE_2; Item No. 14010) receptor subtypes EP_2 and EP_4 in a β-arrestin assay (IC_{50}s = 2,600 and >10,000 nM, respectively). Setipiprant inhibits PGD_2-induced calcium flux in HEK293 cells expressing human $CRTH_2/DP_2$ (IC_{50} = 30 nM) and PGD_2-induced shape change in human eosinophils (IC_{50} = 235 nM).

Reference

1. Fretz, H., Valdenaire, A., Pothier, J., *et al.* Identification of 2-(2-(1-naphthoyl)-8-fluoro-3,4-dihydro-1*H*-pyrido[4,3-*b*]indol-5(2*H*)-yl)acetic acid (setipiprant/ACT-129968), a potent, selective, and orally bioavailable chemoattractant receptor-homologous molecule expressed on Th2 cells (CRTH2) antagonist. *J. Med. Chem.* **56(12)**, 4899-4911 (2013).

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