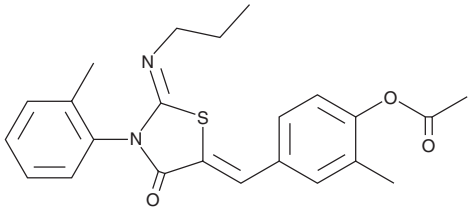
PRODUCT INFORMATION

CAY10739

Item No. 27837

CAS Registry No.:	2328109-05-1
Formal Name:	(2Z,5Z)-5-[[4-(acetyloxy)-3-methylphenyl] methylene]-3-(2-methylphenyl)-2-(propylimino)-4-thiazolidinone
MF:	$C_{23}H_{24}N_2O_3S$
FW:	408.5
Purity:	≥98%
UV/Vis.:	λ_{max}: 333 nm
Supplied as:	A crystalline solid
Storage:	-20°C
Stability:	≥2 years



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

Laboratory Procedures

CAY10739 is supplied as a crystalline solid. A stock solution may be made by dissolving the CAY10739 in the solvent of choice, which should be purged with an inert gas. CAY10739 is soluble in organic solvents such as ethanol, DMSO, and dimethyl formamide (DMF). The solubility of CAY10739 in these solvents is approximately 0.3, 5, and 10 mg/ml, respectively.

CAY10739 is sparingly soluble in aqueous buffers. For maximum solubility in aqueous buffers, CAY10739 should first be dissolved in DMF and then diluted with the aqueous buffer of choice. CAY10739 has a solubility of approximately 0.3 mg/ml in a 1:2 solution of DMF:PBS (pH 7.2) using this method. We do not recommend storing the aqueous solution for more than one day.

Description

CAY10739 is a soft-drug agonist of the sphingosine-1-phosphate receptor 1 ($S1P_1$; IC_{50} = 25.12 nM in a β-arrestin recruitment assay) that was designed to prevent systemic effects following topical application.[1] It is selective for $S1P_1$ over $S1P_2$, $S1P_3$, and $S1P_4$ (IC_{50}s = 1,000, >10,000, >10,000 nM, respectively, in a β-arrestin recruitment assay). In human S9 skin subcellular fractions, an ester group that protects an unstable phenol group is cleaved to release the active soft drug. The active soft drug and its nonenzymatically formed isomers are rapidly metabolized in isolated human hepatocytes.

Reference

1. Bell, M., Foley, D., Naylor, C., *et al.* Discovery of soft-drug topical tool modulators of sphingosine-1-phosphate receptor 1 (S1PR1). *ACS Med. Chem. Lett.* **10(3)**, 341-347 (2019).

CAYMAN CHEMICAL
1180 EAST ELLSWORTH RD
ANN ARBOR, MI 48108 · USA
PHONE: [800] 364-9897
[734] 971-3335
FAX: [734] 971-3640
CUSTSERV@CAYMANCHEM.COM
WWW.**CAYMANCHEM**.COM