

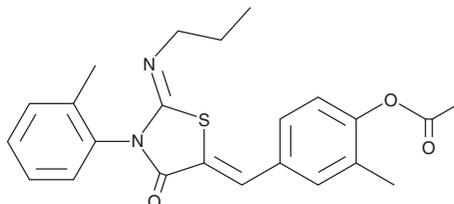
# PRODUCT INFORMATION



**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<sub>23</sub>H<sub>24</sub>N<sub>2</sub>O<sub>3</sub>S  
**FW:** 408.5  
**Purity:** ≥98%  
**UV/Vis.:** λ<sub>max</sub>: 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<sub>1</sub>; IC<sub>50</sub> = 25.12 nM in a β-arrestin recruitment assay) that was designed to prevent systemic effects following topical application.<sup>1</sup> It is selective for S1P<sub>1</sub> over S1P<sub>2</sub>, S1P<sub>3</sub>, and S1P<sub>4</sub> (IC<sub>50</sub>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).

### 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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