

PRODUCT INFORMATION



CUR 61414

Item No. 14931

CAS Registry No.: 334998-36-6
Formal Name: N-[(3S,5S)-1-(1,3-benzodioxol-5-ylmethyl)-5-(1-piperazinylcarbonyl)-3-pyrrolidinyl]-N-[(3-methoxyphenyl)methyl]-3,3-dimethyl-butanamide

Synonym: G-856

MF: C₃₁H₄₂N₄O₅

FW: 550.7

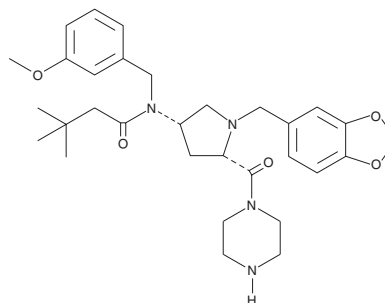
Purity: ≥98%

UV/Vis.: λ_{max}: 281 nm

Supplied as: A crystalline 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

CUR 61414 is supplied as a crystalline solid. A stock solution may be made by dissolving the CUR 61414 in the solvent of choice. CUR 61414 is soluble in organic solvents such as ethanol, DMSO, and dimethyl formamide, which should be purged with an inert gas. The solubility of CUR 61414 in these solvents is approximately 10 mg/ml.

CUR 61414 is sparingly soluble in aqueous buffers. For maximum solubility in aqueous buffers, CUR 61414 should first be dissolved in ethanol and then diluted with the aqueous buffer of choice. CUR 61414 has a solubility of approximately 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

CUR 61414 is a potent inhibitor of hedgehog-induced cellular activity (IC₅₀ = 100-200 nM).^{1,2} It binds directly with the pathway activator Smoothened (K_i = 44 nM).³ CUR 61414 blocks proliferation and induces apoptosis in mouse basal cell carcinoma and causes regression of basaloid lesions triggered by ultraviolet light in mouse skin.^{1,4}

References

- Williams, J.A., Guicherit, O.M., Zaharian, B.I., *et al.* Identification of a small molecule inhibitor of the hedgehog signaling pathway: Effects on basal cell carcinoma-like lesions. *Proc. Natl. Acad. Sci. USA* **100**(8), 4616-4621 (2003).
- Manetti, F., Faure, H., Roudaut, H., *et al.* Virtual screening-based discovery and mechanistic characterization of the acylthiourea MRT-10 family as smoothened antagonists. *Mol. Pharmacol.* **78**(4), 658-665 (2010).
- Frank-Kamenetsky, M., Zhang, X.M., Bottega, S., *et al.* Small-molecule modulators of Hedgehog signaling: Identification and characterization of smoothened agonists and antagonists. *J. Biol.* **1**(2), (2002).
- Tang, T., Tang, J.Y., Li, D., *et al.* Targeting superficial or nodular basal cell carcinoma with topically formulated small molecule inhibitor of smoothened. *Clin. Cancer Res.* **17**(10), 3378-3387 (2011).

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.

WARRANTY AND LIMITATION OF REMEDY

Buyer agrees to purchase the material subject to Cayman's Terms and Conditions. Complete Terms and Conditions including Warranty and Limitation of Liability information can be found on our website.

Copyright Cayman Chemical Company, 12/15/2022

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