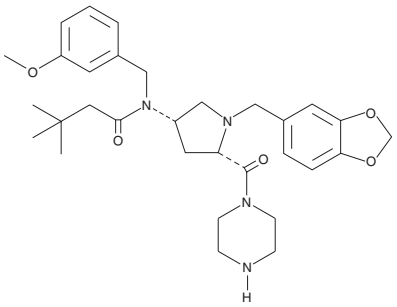
PRODUCT INFORMATION

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:	$C_{31}H_{42}N_4O_5$
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

1. 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).
2. 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).
3. 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).
4. 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).

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