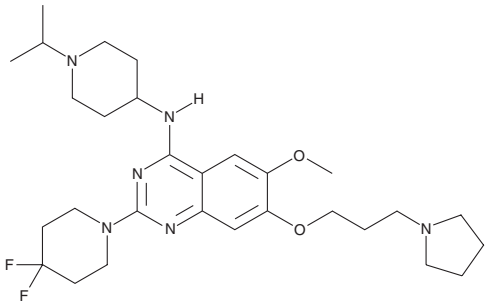
PRODUCT INFORMATION

UNC0642

Item No. 14604

CAS Registry No.:	1481677-78-4
Formal Name:	2-(4,4-difluoropiperidin-1-yl)-N-(1-isopropylpiperidin-4-yl)-6-methoxy-7-(3-(pyrrolidin-1-yl) propoxy)quinazolin-4-amine
MF:	$C_{29}H_{44}F_2N_6O_2$
FW:	546.7
Purity:	≥95%
UV/Vis.:	λ_{max}: 214, 250, 276, 343 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

UNC0642 is supplied as a crystalline solid. A stock solution may be made by dissolving the UNC0642 in the solvent of choice, which should be purged with an inert gas. UNC0642 is soluble in organic solvents such as ethanol, DMSO, and dimethyl formamide (DMF). The solubility of UNC0642 in these solvents is approximately 2, 20, and 30 mg/ml, respectively.

UNC0642 is sparingly soluble in aqueous buffers. For maximum solubility in aqueous buffers, UNC0642 should first be dissolved in DMF and then diluted with the aqueous buffer of choice. UNC0642 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

The methylation of lysine residues on histones plays a central role in determining euchromatin structure and gene expression. The histone methyltransferases G9a and G9a-like protein (GLP) can mono- or dimethylate lysine 9 on histone 3, contributing to early embryogenesis, genomic imprinting, and lymphocyte development.[1-3] UNC0642 is a selective inhibitor of G9a and GLP that competitively inhibits binding of H3K9 substrates with a K_i = 3.7 nM. It exhibits >2,000-fold selectivity over the lysine methyltransferase EZH2 and >20,000-fold selectivity over other methyltransferases.[4] UNC0642 has been shown to reduce H3K9 dimethylation levels in MDA-MB-231 and PANC-1 cells with IC_{50} values of 110 and 40 nM, respectively.[4] Furthermore, it displays improved pharmacokinetic properties relative to UNC0638 (Item No. 10734).[4] See the Structural Genomics Consortium (SGC) website for more information.

References

1. Tachibana, M., Sugimoto, K., Nozaki, M., *et al.* G9a histone methyltransferase plays a dominant role in euchromatic histone H3 lysine 9 methylation and is essential for early embryogenesis. *Genes Dev.* **16(14)**, 1779-1791 (2002).
2. Wagschal, A., Sutherland, H.G., Woodfine, K., *et al.* G9a histone methyltransferase contributes to imprinting in the mouse placenta. *Mol. Cell Biol.* **28(3)**, 1104-1113 (2008).
3. Thomas, L.R., Miyashita, H., Cobb, R.M., *et al.* Functional analysis of histone methyltransferase G9a in B and T lymphocytes. *J. Immunol.* **181(1)**, 485-493 (2008).
4. Liu, F., Barsyte-Lovejoy, D., Li, F., *et al.* Discovery of an in vivo chemical probe of the lysine methyltransferases G9a and GLP. *J. Med. Chem.* **56(21)**, 8931-8942 (2013).

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