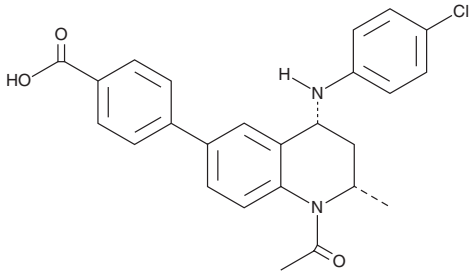
PRODUCT INFORMATION

I-BET726

Item No. 16872

CAS Registry No.:	1300031-52-0
Formal Name:	4-[(2S,4R)-1-acetyl-4-[(4-chlorophenyl) amino]-1,2,3,4-tetrahydro-2-methyl-6-quinolinyl]-benzoic acid
Synonym:	GSK1324726A
MF:	$C_{25}H_{23}ClN_2O_3$
FW:	435.0
Purity:	≥98%
UV/Vis.:	λ_{max}: 256, 291 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

I-BET726 is supplied as a crystalline solid. A stock solution may be made by dissolving the I-BET726 in the solvent of choice. I-BET726 is soluble in organic solvents such as ethanol, DMSO, and dimethyl formamide, which should be purged with an inert gas. The solubility of I-BET726 in these solvents is approximately 15, 25, and 30 mg/ml, respectively.

I-BET726 is sparingly soluble in aqueous buffers. For maximum solubility in aqueous buffers, I-BET726 should first be dissolved in DMSO and then diluted with the aqueous buffer of choice. I-BET726 has a solubility of approximately 0.2 mg/ml in a 1:4 solution of DMSO:PBS (pH 7.2) using this method. We do not recommend storing the aqueous solution for more than one day.

Description

I-BET726 is an inhibitor of BET family proteins that binds BRD2, BRD3, and BRD4 with high affinity (IC_{50}s = 41, 31, and 22 nM, respectively) and competes with tetra-acetylated histone 4 peptides for binding to the bromodomains of these proteins.[1,2] It exhibits >1,000-fold selectivity for these proteins over other bromodomain-containing homologs.[1] I-BET726 inhibits cell growth and induces cytotoxicity in neuroblastoma cell lines by modulating the expression of genes involved in apoptosis and Myc signaling.[1] I-BET726 can be administered orally to animals, and it reduces tumor growth in mouse xenograft models of human neuroblastoma.[1]

References

1. Gosmini, R., Nguyen, V.L., Toum, J., *et al.* The discovery of I-BET726 (GSK1324726A), a potent tetrahydroquinoline apoA1 up-regulator and selective BET bromodomain inhibitor. *J. Med. Chem.* **57**, 8111-8131 (2014).
2. Wyce, A., Ganji, G., Smitheman, K.N., *et al.* BET inhibition silences expression of MYCN and BCL2 and induces cytotoxicity in neuroblastoma tumor models. *PLoS One* **8(8)**, e72967 (2013).

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