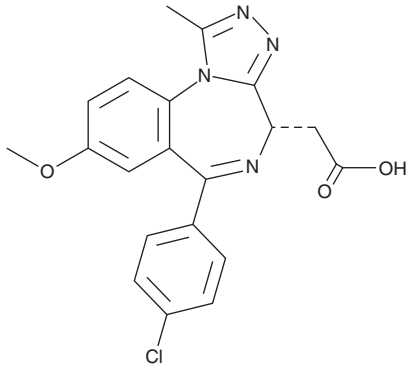
PRODUCT INFORMATION

I-BET762 Carboxylic Acid

Item No. 45717



CAS Registry No.:	1300019-38-8
Formal Name:	(4S)-6-(4-chlorophenyl)-8-methoxy-1-methyl-4H-[1,2,4]triazolo[4,3-a][1,4]benzodiazepine-4-acetic acid
MF:	$C_{20}H_{17}ClN_4O_3$
FW:	396.8
Purity:	≥98%
Supplied as:	A 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

I-BET762 carboxylic acid is supplied as a solid. A stock solution may be made by dissolving the I-BET762 carboxylic acid in the solvent of choice, which should be purged with an inert gas. I-BET762 carboxylic acid is soluble (≥10 mg/ml) in DMSO.

Further dilutions of the stock solution into aqueous buffers or isotonic saline should be made prior to performing biological experiments. Ensure that the residual amount of organic solvent is insignificant, since organic solvents may have physiological effects at low concentrations. Organic solvent-free aqueous solutions of I-BET762 carboxylic acid can be prepared by directly dissolving the solid in aqueous buffers. I-BET762 carboxylic acid is slightly soluble (0.1-1 mg/ml) in PBS (pH 7.2). We do not recommend storing the aqueous solution for more than one day.

Description

I-BET762 carboxylic acid is a derivative of I-BET762 (Item No. 10676), a bromodomain and extra terminal domain (BET) family of proteins inhibitor.[1] I-BET762 carboxylic acid inhibits BET-containing proteins to a lesser extent than I-BET762 and does not inhibit LPS-induced IL-6 production in isolated human peripheral blood mononuclear cells (PBMCs; IC_{50} = >100 µM). It has been used in the synthesis of synthetic genome reader/regulator 3 (SynGR3), which restores frataxin expression in Friedreich's ataxia patient-derived GM15850 cells.[2] It has also been used in the synthesis of CEM202, a bifunctional synthetic ligand of mutant FKBP (FKBP*) activating chemical epigenetic modifier (SLF*-CEMa) that recruits BET bromodomains.[3]

References

1. Mirguet, O., Gosmini, R., Toum, J., *et al*. Discovery of epigenetic regulator I-BET762: Lead optimization to afford a clinical candidate inhibitor of the BET bromodomains. *J. Med. Chem.* **56(19)**, 7501-7515 (2013).
2. Mohammed, A., Waddell, M.B., Sutkeviciute, I., *et al.* Domain-selective BET ligands yield next-generation synthetic genome readers/regulators with nonidentical cellular functions. *J. Am. Chem. Soc.* (2025).
3. Lu, D., Foley, C.A., Birla, S.V., *et al.* Bioorthogonal chemical epigenetic modifiers enable dose-dependent CRISPR targeted gene activation in mammalian cells. *ACS Synth. Biol.* **11(4)**, 1397-1407 (2022).

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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