

Product Name: TC AC 28

Catalog No.: 6105

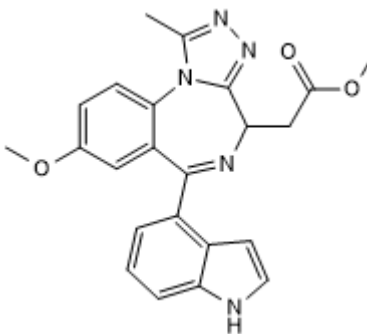
Batch No.: 1

CAS Number: 1809296-92-1

IUPAC Name: 6-(1*H*-Indol-4-yl)-8-methoxy-1-methyl-4*H*-[1,2,4]triazolo[4,3-*a*][1,4]benzodiazepine-4-acetic acid methyl ester

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₂₃H₂₁N₅O₃·³/₄H₂O
Batch Molecular Weight: 428.95
Physical Appearance: White solid
Solubility: DMSO to 5 mM with gentle warming
 ethanol to 5 mM with gentle warming
Storage: Store at -20°C
Batch Molecular Structure:



2. ANALYTICAL DATA

TLC: R_f = 0.35 (Dichloromethane:Methanol [95:5])
HPLC: Shows 100% purity
¹H NMR: Consistent with structure
Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	64.4	5.29	16.33
Found	64.73	5.12	16.07

Caution - Not Fully Tested • Research Use Only • Not For Human or Veterinary Use

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Description:

High affinity BET bromodomain ligand (K_d values are 40 and 800 nM for Brd2(2) and Brd2(1), respectively). Exhibits 20-fold selectivity for the second over the first bromodomain.

Physical and Chemical Properties:

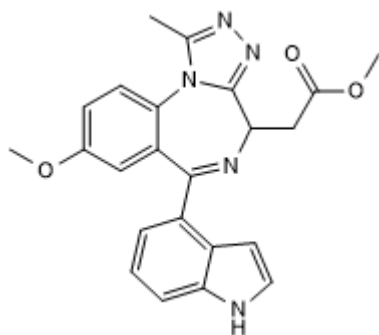
Batch Molecular Formula: $C_{23}H_{21}N_5O_3 \cdot \frac{3}{4}H_2O$

Batch Molecular Weight: 428.95

Physical Appearance: White solid

Minimum Purity: >98%

Batch Molecular Structure:



Storage: Store at -20°C

Solubility & Usage Info:

DMSO to 5 mM with gentle warming
ethanol to 5 mM with gentle warming

Stability and Solubility Advice:

Some solutions can be difficult to obtain and can be encouraged by rapid stirring, sonication or gentle warming (in a 45-60°C water bath).

Information concerning product stability, particularly in solution, has rarely been reported and in most cases we can only offer a general guide. Our standard recommendations are:

SOLIDS: Provided storage is as stated on the product label and the vial is kept tightly sealed, the product can be stored for up to 6 months from date of receipt.

SOLUTIONS: We recommend that stock solutions, once prepared, are stored aliquoted in tightly sealed vials at -20°C or below and used within 1 month. Wherever possible solutions should be made up and used on the same day.

Licensing Information:

Sold under licence from the University of Dundee.

References:

Baud et al (2016) New synthetic routes to triazolo-benzodiazepine analogues: expanding the scope of the bump-and-hole approach for selective bromo and extra-terminal (BET) bromodomain inhibition. *J.Med.Chem.* **59** 1492. PMID: 26367539.

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