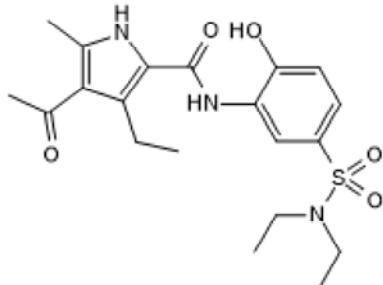


Certificate of Analysiswww.tocris.com**Product Name:** XD 14**Catalog No.:** 5489**Batch No.:** 1

CAS Number: 1370888-71-3

IUPAC Name: 4-Acetyl-N-[5-[(diethylamino)sulfonyl]-2-hydroxyphenyl]-3-ethyl-5-methyl-1*H*-pyrrole-2-carboxamide**1. PHYSICAL AND CHEMICAL PROPERTIES****Batch Molecular Formula:** C₂₀H₂₇N₃O₅S·¾H₂O**Batch Molecular Weight:** 435.02**Physical Appearance:** Off White solid**Solubility:** DMSO to 100 mM
ethanol to 100 mM**Storage:** Store at -20°C**Batch Molecular Structure:****2. ANALYTICAL DATA****HPLC:** Shows 99.7% purity**¹H NMR:** Consistent with structure**Mass Spectrum:** Consistent with structure**Microanalysis:** Carbon Hydrogen Nitrogen

Theoretical 55.22 6.6 9.66

Found 55.19 6.57 9.53

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

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Product Information

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Catalog No.: 5489

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IUPAC Name: 4-Acetyl-N-[5-[(diethylamino)sulfonyl]-2-hydroxyphenyl]-3-ethyl-5-methyl-1*H*-pyrrole-2-carboxamide

Description:

BET bromodomain inhibitor (K_d values are 160, 170, 380, 490, 830 and 850 nM for BRD4(1), BRD2(1), BRD3(1), BRD3(2), BRD2(2) and BRD4(2) respectively). Also inhibits BRDT(1), CBP, p300 and BRDT(2) (K_d values are 1.2, 1.6, 2.6 and 3.7 μ M respectively). Attenuates proliferation of HL-60 leukemia cells in vitro.

Physical and Chemical Properties:

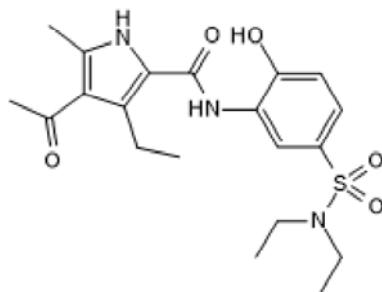
Batch Molecular Formula: $C_{20}H_{27}N_3O_5S \cdot \frac{3}{4}H_2O$

Batch Molecular Weight: 435.02

Physical Appearance: Off White solid

Minimum Purity: $\geq 98\%$

Batch Molecular Structure:



Storage: Store at -20°C

Solubility & Usage Info:

DMSO to 100 mM
ethanol to 100 mM

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.

References:

Lucas *et al* (2013) 4-Acyl pyrroles: mimicking acetylated lysines in histone code reading. *Angew.Chem.Int.Ed. Engl.* **52** 14055. PMID: 24272870.

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