

**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:** C<sub>20</sub>H<sub>27</sub>N<sub>3</sub>O<sub>5</sub>S·<sup>3</sup>/<sub>4</sub>H<sub>2</sub>O

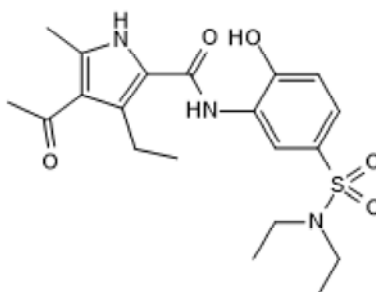
**Batch Molecular Weight:** 435.02

**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

**<sup>1</sup>H 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

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**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  $\mu$ M respectively). Attenuates proliferation of HL-60 leukemia cells in vitro.

**Physical and Chemical Properties:**

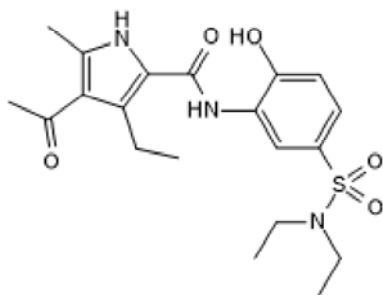
Batch Molecular Formula:  $C_{20}H_{27}N_3O_5S \cdot \frac{3}{4}H_2O$

Batch Molecular Weight: 435.02

Physical Appearance: Off White solid

**Minimum Purity:**  $\geq 98\%$

**Batch Molecular Structure:**



**Storage:** Store at  $-20^{\circ}C$

**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  $45-60^{\circ}C$  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  $-20^{\circ}C$  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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