

**Product Name:** MS 436

**Catalog No.:** 5173

**Batch No.:** 1

CAS Number: 1395084-25-9

IUPAC Name: (E)-4-[2-(2-Amino-4-hydroxy-5-methylphenyl)diazenyl]-N-2-pyridinylbenzenesulfonamide

**1. PHYSICAL AND CHEMICAL PROPERTIES**

**Batch Molecular Formula:** C<sub>18</sub>H<sub>17</sub>N<sub>5</sub>O<sub>3</sub>S.1½H<sub>2</sub>O

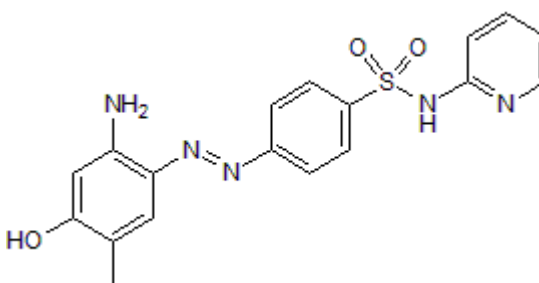
**Batch Molecular Weight:** 405.94

**Physical Appearance:** Red solid

**Solubility:** DMSO to 100 mM

**Storage:** Store at -20°C

**Batch Molecular Structure:**



**2. ANALYTICAL DATA**

**TLC:** R<sub>f</sub> = 0.48 (Dichloromethane:Methanol [9:1])

**HPLC:** Shows 99% purity

**<sup>1</sup>H NMR:** Consistent with structure

**Mass Spectrum:** Consistent with structure

**Microanalysis:**

	Carbon	Hydrogen	Nitrogen
Theoretical	53.26	4.84	17.25
Found	53.23	4.7	16.86

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

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**Description:**

Potent and selective BRD4 bromodomain inhibitor ( $K_i = 30 - 50$  nM for the first bromodomain (BRD4(1)). Exhibits 10-fold selectivity for BRD4(1) over BRD4(2). Blocks BRD4 transcriptional activity in lipopolysaccharide-induced production of both nitric oxide and IL-6 in mouse macrophages ( $IC_{50}$  values are 3.8 and 4.9  $\mu$ M, respectively). Attenuates melanoma cell proliferation in vitro.

**Physical and Chemical Properties:**

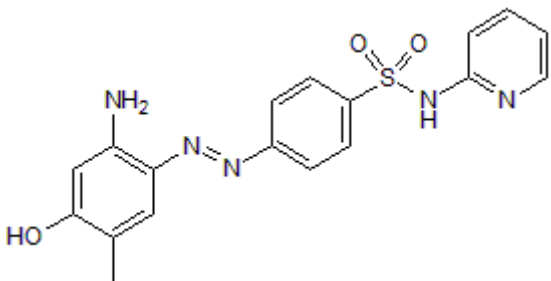
Batch Molecular Formula:  $C_{18}H_{17}N_5O_3S \cdot 1 \frac{1}{4}H_2O$

Batch Molecular Weight: 405.94

Physical Appearance: Red solid

**Minimum Purity:** >98%

**Batch Molecular Structure:**



**Storage:** Store at -20°C

CAUTION - This product is light sensitive and we recommend that the solid material and any solutions obtained are protected from exposure to light.

**Solubility & Usage Info:**

DMSO 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:**

**Zhang et al** (2013) Structure-guided design of potent diazobenzene inhibitors for the BET bromodomains. *J.Med.Chem.* **56** 9251. PMID: 24144283.

**Segura et al** (2013) BRD4 sustains melanoma proliferation and represents a new target for epigenetic therapy. *Cancer Res.* **73** 6264. PMID: 23950209.

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