

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: C₁₈H₁₇N₅O₃S.1¼H₂O

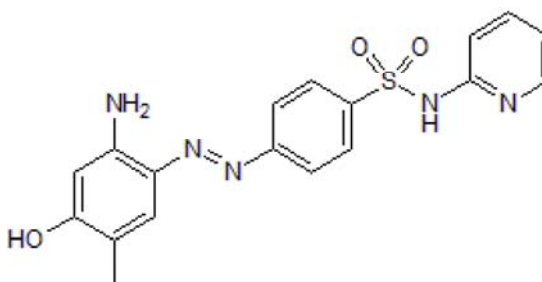
Batch Molecular Weight: 405.94

Physical Appearance: Red solid

Solubility: DMSO to 100 mM

Storage: Store at -20°C

Batch Molecular Structure:



2. ANALYTICAL DATA

TLC: R_f = 0.48 (Dichloromethane:Methanol [9:1])

HPLC: Shows 99.0% purity

¹H 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 μ M, respectively). Attenuates melanoma cell proliferation in vitro.

Physical and Chemical Properties:

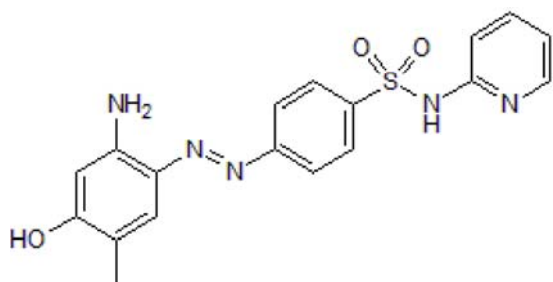
Batch Molecular Formula: $C_{18}H_{17}N_5O_3S \cdot 1\frac{1}{4}H_2O$

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.

Licensing Information:

Sold under license from Icahn School of Medicine at Mount Sinai.

References:

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

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

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