TOCRIS
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Print Date: Mar 25th 2020

Certificate of Analysis

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Product Name: **CH 223191** **Catalog No.: 3858** **Batch No.: 2**

CAS Number: 301326-22-7

IUPAC Name: 1-Methyl-*N*-[2-methyl-4-[2-(2-methylphenyl)diazenyl]phenyl-1*H*-pyrazole-5-carboxamide

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: $C_{19}H_{19}N_5O$

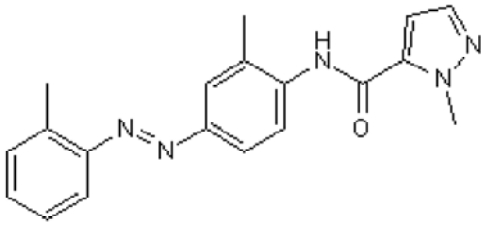
Batch Molecular Weight: 333.39

Physical Appearance: Orange solid

Solubility: DMSO to 100 mM
ethanol to 10 mM

Storage: Store at +4°C

Batch Molecular Structure:



2. ANALYTICAL DATA

TLC: R_f = 0.38 (Chloroform:Methanol [9:1])

HPLC: Shows 98.5% purity

^{1}H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	68.45	5.74	21.01
Found	68.44	5.78	21.03

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Product Information

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IUPAC Name: 1-Methyl-*N*-[2-methyl-4-[2-(2-methylphenyl)diazenyl]phenyl-1*H*-pyrazole-5-carboxamide

Description:

Potent aryl hydrocarbon receptor (AhR) antagonist (IC_{50} = 30 nM). Exhibits no AhR agonist-like activity (at concentrations up to 100 µM). Inhibits 2,3,7,8-Tetrachlorodibenzo-p-dioxin (TCDD) -induced AhR-dependent transcription in vitro and reduces TCDD-induced toxicity in vivo. Attenuates Th17 differentiation of naive CD4 T cells and promotes expansion of hematopoietic stem cells in vitro.

Physical and Chemical Properties:

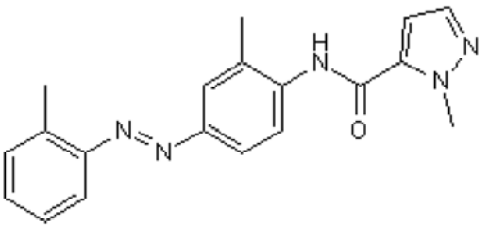
Batch Molecular Formula: $C_{19}H_{19}N_5O$

Batch Molecular Weight: 333.39

Physical Appearance: Orange solid

Minimum Purity: ≥98%

Batch Molecular Structure:



Storage: Store at +4°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
ethanol to 10 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:

Dubrovska *et al* (2012) CXCR4 activation maintains a stem cell population in tamoxifen-resistant breast cancer cells through AhR signalling. Br.J.Cancer. ***107*** 43. PMID: 22644306.

Boitano *et al* (2010) Aryl hydrocarbon receptor antagonists promote the expansion of human hematopoietic stem cells. Science ***329*** 1345. PMID: 20688981.

Veldhoen *et al* (2009) Natural agonists for aryl hydrocarbon receptor in culture medium are essential for optimal differentiation of TH17 T cells. J.Exp.Med. ***206*** 43. PMID: 19114668.

Kim *et al* (2006) Novel compound 2-methyl-2*H*-pyrazole-3-carboxylic acid (2-methyl-4-*o*-tolylazo-phenyl)-amide (CH-223191) prevents 2,3,7,8-TCDD-induced toxicity by antagonizing the aryl hydrocarbon receptor. Mol.Pharmacol. ***69*** 1871. PMID: 16540597.

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