TOCRIS
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Print Date: Apr 9th 2020

Certificate of Analysis

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Product Name: **SR 144528** **Catalog No.: 5039** **Batch No.: 1**

CAS Number: 192703-06-3

IUPAC Name: 5-(4-Chloro-3-methylphenyl)-1-[(4-methylphenyl)methyl]-*N*-[(1*S*,2*S*,4*R*)-1,3,3-trimethylbicyclo[2.2.1]hept-2-yl]-1*H*-pyrazole-3-carboxamide

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: $C_{29}H_{34}ClN_3O.¼H_2O$

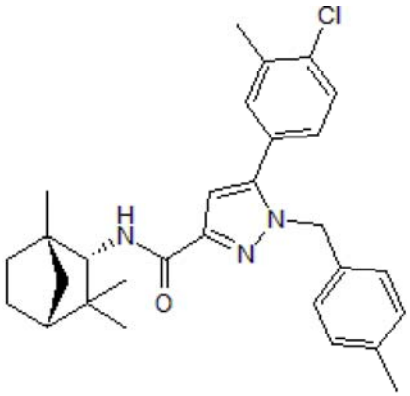
Batch Molecular Weight: 480.55

Physical Appearance: White solid

Solubility: DMSO to 100 mM
ethanol to 100 mM

Storage: Store at -20°C

Batch Molecular Structure:



2. ANALYTICAL DATA

TLC: R_f = 0.5 (Ethyl acetate:Petroleum ether [9:1])

HPLC: Shows 99.3% purity

Chiral HPLC: Shows 100% purity

^{1}H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	72.48	7.24	8.74
Found	72.69	7.27	8.72

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Description:

High affinity and selective CB_2 inverse agonist (K_i = 0.6 nM). Exhibits >700-fold selectivity for CB_2 over CB_1 receptors. Blocks the effects of CP 55,940 (Cat. No. 0949) on forskolin-sensitive adenylyl cyclase activity and MAPK in CHO cells expressing CB_2 receptors. Also blocks CP 55,940-induced B-cell activation. Orally bioavailable.

Physical and Chemical Properties:

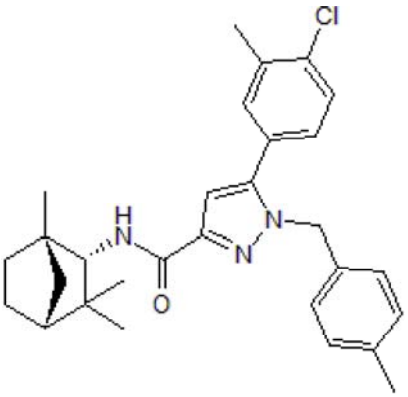
Batch Molecular Formula: $C_{29}H_{34}ClN_3O.¼H_2O$

Batch Molecular Weight: 480.55

Physical Appearance: White solid

Minimum Purity: ≥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.

Other Information:

INFORMATION FOR CUSTOMERS IN THE UK ONLY

This product is a Schedule 1 Home Office controlled substance and customers in the UK are required to hold the relevant licence or be exempt from restrictions in order to purchase and possess this material.

References:

Kotsikorou *et al* (2013) The importance of hydrogen bonding and aromatic stacking to the affinity and efficacy of cannabinoid receptor CB_2 antagonist, 5-(4-chloro-3-methylphenyl)-1-[(4-methylphenyl)methyl]-*N*-[(1*S*,2*S*,4*R*)-1,3,3-trimeth J.Med.Chem. ***56*** 6593. PMID: 23855811.

Bouaboula *et al* (1999) G_i protein modulation induced by a selective inverse agonist for the peripheral cannabinoid receptor CB_2: implication for intracellular signalization cross-regulation. Mol.Pharmacol. ***55*** 473. PMID: 10051530.

Rinaldi-Carmona *et al* (1998) SR 144528, the first potent and selective antagonist of the CB_2 cannabinoid receptor. J.Pharmacol.Exp.Ther. ***284*** 644. PMID: 9454810.

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