1. PHYSICAL AND CHEMICAL PROPERTIES

**Batch Molecular Formula:** \( C_{29}H_{34}ClN_3O \)

**Batch Molecular Weight:** 476.05

**Physical Appearance:** White solid

**Solubility:** DMSO to 100 mM

**Storage:** Store at -20°C

2. ANALYTICAL DATA

**HPLC:** Shows 99.4% purity

**Chiral HPLC:** Shows 99.9% purity

**\(^1\text{H} \text{NMR}:** Consistent with structure

**Mass Spectrum:** Consistent with structure
Product Name: SR 144528
Catalog No.: 5039
Batch No.: 2

CAS Number: 192703-06-3

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

Description:
High affinity and selective CB₂ inverse agonist (Kᵢ = 0.6 nM). Exhibits >700-fold selectivity for CB₂ over CB₁ receptors. Blocks the effects of CP 55,940 (Cat. No. 0949) on forskolin-sensitive adenyl cyclase activity and MAPK in CHO cells expressing CB₂ receptors. Also blocks CP 55,940-induced B-cell activation. Orally bioavailable.

Physical and Chemical Properties:
Batch Molecular Formula: C₂₉H₃₄ClN₃O
Batch Molecular Weight: 476.05
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 CB2 antagonist, 5-(4-chloro-3-methylphenyl)-1-[(4-methylphenyl)methyl]-N-[(1S,2S,4R)-1,3,3-trimethylbicyclo[2.2.1]hept-2-yl]-1H-pyrazole-3-carboxamide J.Med.Chem. 56 6593. PMID: 23855811.
