TOCRIS
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Print Date: Jan 13th 2016

Certificate of Analysis

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Product Name: **WIN 55,212-3 mesylate** **Catalog No.: 2327** **Batch No.: 3**

CAS Number: 131543-25-4

IUPAC Name: [(3*S*)-2,3-Dihydro-5-methyl-3-(4-morpholinylmethyl)pyrrolo[1,2,3-*de*]-1,4-benzoxazin-6-yl]-1-naphthalenyl-methanone monomethanesulfonate

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: $C_{27}H_{26}N_2O_3.CH_3SO_3H.¼H_2O$

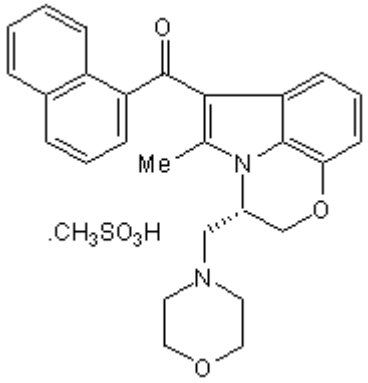
Batch Molecular Weight: 527.11

Physical Appearance: Off-white solid

Solubility: DMSO to 100 mM with gentle warming

Storage: Store at +4°C

Batch Molecular Structure:



2. ANALYTICAL DATA

HPLC: Shows 99.2% purity

Chiral HPLC: Shows 100% purity

^{1}H NMR: Consistent with structure

Optical Rotation: $[\alpha]_D$ = -35 (Concentration = 1, Solvent = DMF)

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	63.8	5.83	5.31
Found	63.72	5.98	5.18

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Description:

Novel, low potency CB_2 receptor silent antagonist and CB_1 receptor partial inverse agonist. Competitively antagonizes effects of CP 55,940 (pA_2 = 6.1) and SR 144528 (pEC_{50} = 5.3) at CB_2 receptors and acts as a partial inverse agonist at CB_1 receptors (pIC_{50} = 5.5). Displays modest activity at human melatonin MT_1 and muscarinic M_4 receptors, but is selective over several other GPCRs.

Physical and Chemical Properties:

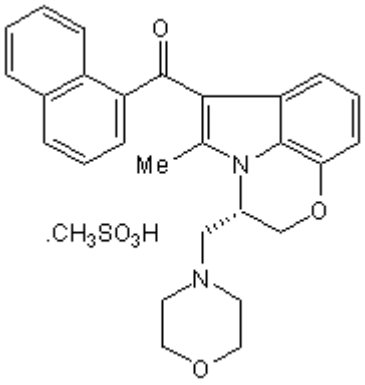
Batch Molecular Formula: $C_{27}H_{26}N_2O_3.CH_3SO_3H.¼H_2O$

Batch Molecular Weight: 527.11

Physical Appearance: Off-white solid

Minimum Purity: >98%

Batch Molecular Structure:



Storage: Store at +4°C

Solubility & Usage Info:

DMSO to 100 mM with gentle warming

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 relevent licence or be exempt from restrictions in order to purchase and posess this material.

References:

Savinainen *et al* (2005) Identification of WIN55212-3 as a competitive neutral antagonist of the human cannabinoid CB_2 receptor. Br.J.Pharmacol. ***145*** 636. PMID: 15852035.

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