Print Date: Nov 5th 2019

Certificate of Analysis

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Product Name: **YM 202074 sesquifumarate** **Catalog No.: 3413** **Batch No.: 1**

CAS Number: 299900-84-8

IUPAC Name: *N*-Cyclohexyl-6-[[*N*-(2-methoxyethyl)-*N*-methylamino]methyl]-*N*-methylthiazolo[3,2-a]benzoimidazole-2-carboxamide sesquifumarate

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: $C_{22}H_{30}N_4O_2S.1.5C_4H_4O_4.¼H_2O$

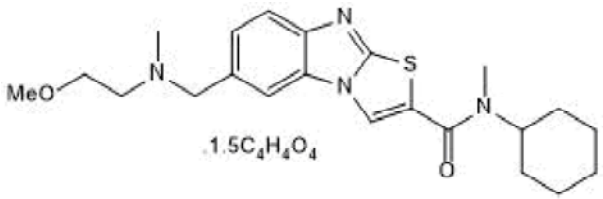
Batch Molecular Weight: 593.17

Physical Appearance: White solid

Solubility: water to 20 mM
DMSO to 100 mM

Storage: Store at +4°C

Batch Molecular Structure:



2. ANALYTICAL DATA

TLC: R_f = 0.12 (Ethyl acetate:Methanol [95:5])

HPLC: Shows 98.8% purity

^{1}H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	56.7	6.2	9.45
Found	56.65	6.36	9.05

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Description:

High affinity, selective metabotropic glutamate receptor type 1 ($mGlu_1$) antagonist. Binds an allosteric site of the rat $mGlu_1$ receptor with a K_i of 4.8 nM. Inhibits $mGlu_1$-mediated inositol phosphates production (IC_{50} = 8.6 nM in rat cerebellar granule cells). Neuroprotective in vivo.

Physical and Chemical Properties:

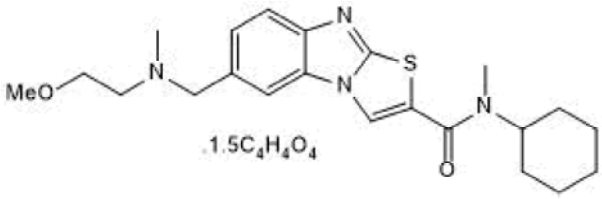
Batch Molecular Formula: $C_{22}H_{30}N_4O_2S.1.5C_4H_4O_4.¼H_2O$

Batch Molecular Weight: 593.17

Physical Appearance: White solid

Minimum Purity: >99%

Batch Molecular Structure:



Storage: Store at +4°C

Solubility & Usage Info:

water to 20 mM
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.

References:

Yanamoto *et al* (2010) Radiosynthesis and evaluation of [^{11}C]YM-202074 as a PET ligand for imaging the metabotropic glutamate receptor type 1. Nucl.Med.Biol. ***37*** 615. PMID: 20610166.

Ferraguti *et al* (2008) Metabotropic glutamate 1 receptor: current concepts and perspectives. Pharmacol.Rev. ***60*** 536. PMID: 19112153.

Kohara *et al* (2008) Neuroprotective effects of the selective type 1 metabotropic glutamate receptor antagonist YM-202074 in rat stroke models. Brain Res. ***1191*** 168. PMID: 18164695.

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