Product Name: YM 202074 sesquifumarate
Catalog No.: 3413
Batch No.: 1
CAS Number: 299900-84-8

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C_{22}H_{30}N_{4}O_{2}S.1.5C_{4}H_{4}O_{4}.1\frac{1}{2}H_{2}O
Batch Molecular Weight: 593.17
Physical Appearance: White solid
Solubility: water to 20 mM
DMSO to 100 mM
Storage: Store at +4°C

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:

<table>
<thead>
<tr>
<th></th>
<th>Carbon</th>
<th>Hydrogen</th>
<th>Nitrogen</th>
</tr>
</thead>
<tbody>
<tr>
<td>Theoretical</td>
<td>56.7</td>
<td>6.2</td>
<td>9.45</td>
</tr>
<tr>
<td>Found</td>
<td>56.65</td>
<td>6.36</td>
<td>9.05</td>
</tr>
</tbody>
</table>

Caution - Not Fully Tested • Research Use Only • Not For Human or Veterinary Use
**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

**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: \(C_{22}H_{32}N_6O_5S.1.5C_4H_9O_4.\frac{1}{4}H_2O\)  
Batch Molecular Weight: 593.17  
Physical Appearance: White solid  
Minimum Purity: >99%

**Batch Molecular Structure:**

```
\[
\text{MeO} \quad \begin{array}{c}
\text{N} \\
\text{C2H3O4}
\end{array} \quad \begin{array}{c}
\text{N} \\
\text{C6H9O4}
\end{array} \quad \begin{array}{c}
\text{N} \\
\text{C6H4}
\end{array} \quad \begin{array}{c}
\text{N} \\
\text{C6H9O4}
\end{array}
\]
```

**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:**  