1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C_{17}H_{20}N_{4}S
Batch Molecular Weight: 312.43
Physical Appearance: Yellow solid
Solubility: DMSO to 100 mM
1eq. HCl to 100 mM
ethanol to 10 mM
Storage: Store at +4°C

2. ANALYTICAL DATA

Melting Point: Between 192 - 196°C
HPLC: Shows 99.9% purity
\(^1\)H NMR: Consistent with structure
Mass Spectrum: Consistent with structure
Microanalysis:

<table>
<thead>
<tr>
<th>Element</th>
<th>Theoretical</th>
<th>Found</th>
</tr>
</thead>
<tbody>
<tr>
<td>Carbon</td>
<td>65.35</td>
<td>65.13</td>
</tr>
<tr>
<td>Hydrogen</td>
<td>6.45</td>
<td>6.64</td>
</tr>
<tr>
<td>Nitrogen</td>
<td>17.92</td>
<td>18.25</td>
</tr>
</tbody>
</table>
**Description:**
Antagonist of 5-HT\textsubscript{2A} and dopamine D\textsubscript{2} receptors (K\textsubscript{i} values are 4 and 11 nM respectively). Also displays affinity for a range of other receptors including D\textsubscript{1} and D\textsubscript{4}, 5-HT\textsubscript{2C}, \(\alpha_1\), H\textsubscript{1} and M\textsubscript{1-4} receptors (K\textsubscript{i} values range between 1.9 and 31 nM). Atypical antipsychotic. Displays anticholinergic properties. Also a highly potent activator of hM\textsubscript{3}D\textsubscript{2} DREADDs (EC\textsubscript{50} values are 5 nM in vitro and 7 nM in vivo).

**Physical and Chemical Properties:**
Batch Molecular Formula: C\textsubscript{17}H\textsubscript{20}N\textsubscript{4}S  
Batch Molecular Weight: 312.43  
Physical Appearance: Yellow solid  
Minimum Purity: \textgreater 99%

**Storage:** Store at +4°C

**Solubility & Usage Info:**
DMSO to 100 mM  
1eq. HCl to 100 mM  
ethanol to 10 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:**