1. PHYSICAL AND CHEMICAL PROPERTIES

**Batch Molecular Formula:** $\text{C}_{17}\text{H}_{19}\text{N}_{7}\text{OCl}_{2};\frac{1}{4}\text{H}_{2}\text{O}$

**Batch Molecular Weight:** 412.79

**Physical Appearance:** White solid

**Solubility:** DMSO to 100 mM, ethanol to 100 mM

**Storage:** Store at +4°C

2. ANALYTICAL DATA

**TLC:** $R_f = 0.65$ (Chloroform:Methanol [9:1])

**HPLC:** Shows 99.5% purity

$^1\text{H NMR:}$ 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>49.46</td>
<td>49.71</td>
</tr>
<tr>
<td>Hydrogen</td>
<td>4.76</td>
<td>4.95</td>
</tr>
<tr>
<td>Nitrogen</td>
<td>23.75</td>
<td>23.22</td>
</tr>
</tbody>
</table>
Product Name: JTE 013
CATALOG NO.: 2392
BATCH NO.: 6

CAS Number: 383150-41-2
IUPAC Name: 1-[1,3-Dimethyl-4-(2-methyl-ethyl)-1H-pyrazolo[3,4-b]pyridin-6-yl]-4-(3,5-dichloro-4-pyridinyl)-semicarbazide

DESCRIPTION:
Sphingosine-1-phosphate (S1P) receptor antagonist, highly selective for S1P2 (EDG-5). Inhibits S1P binding to human S1P2 receptors with an IC50 value of 17.6 nM. At concentrations up to 10 μM, displays 4.2% inhibition of S1P3 and does not antagonize S1P1. Enhances S1P-induced angiogenesis in vivo.

PHYSICAL AND CHEMICAL PROPERTIES:
Batch Molecular Formula: C17H19N7OCl2.1/4H2O
Batch Molecular Weight: 412.79
Physical Appearance: White solid
Minimum Purity: >98%

STORAGE:
Store at +4°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.

REFERENCES: