1. PHYSICAL AND CHEMICAL PROPERTIES

**Batch Molecular Formula:** \( \text{C}_{13}\text{H}_{13}\text{NO}_{2} \)

**Batch Molecular Weight:** 215.25

**Physical Appearance:** Pale yellow solid

**Solubility:**
- DMSO to 100 mM
- Ethanol to 100 mM

**Storage:** Store at +4°C

**Batch Molecular Structure:**

![Molecular Structure Image]

2. ANALYTICAL DATA

**TLC:** \( R_f = 0.35 \) (Dichloromethane:Methanol [95:5])

**\(^1\)H NMR:** Consistent with structure

**Mass Spectrum:** Consistent with structure

**Microanalysis:**

<table>
<thead>
<tr>
<th></th>
<th>Theoretical</th>
<th>Found</th>
</tr>
</thead>
<tbody>
<tr>
<td>Carbon</td>
<td>72.54</td>
<td>72.64</td>
</tr>
<tr>
<td>Hydrogen</td>
<td>6.09</td>
<td>6.12</td>
</tr>
<tr>
<td>Nitrogen</td>
<td>6.51</td>
<td>6.61</td>
</tr>
</tbody>
</table>

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

Product Name: TC-E 5008
Catalog No.: 5244
Batch No.: 1

CAS Number: 50405-58-8
IUPAC Name: 1-Hydroxy-4-methyl-6-(phenylmethyl)-2-(1H)pyridinone

Description:
Selective mutant isocitrate dehydrogenase 1 (mIDH1) inhibitor ($K_i = 120-190$ nM). Displays >60-fold selectivity for mIDH1 (found in ~75% of gliomas) over wild type IDH1. Also inhibits D-2-hydroxyglutaric acid in cells expressing mIDH1 ($EC_{50} = 2.4 \mu M$). Does not display cytotoxicity towards non-cancerous human cells. Phenotypically lethal.

Physical and Chemical Properties:
- **Storage:** Store at +4°C
- **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).

**References:**