1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: \( \text{C}_{14}\text{H}_{13}\text{N}_{3}\text{O}_{2}\text{S} \)
Batch Molecular Weight: 287.34
Physical Appearance: Off-white solid
Solubility: DMSO to 100 mM
ethanol to 10 mM
Storage: Store at +4°C

2. ANALYTICAL DATA

HPLC: Shows 100% 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>58.52</td>
<td>4.56</td>
<td>14.62</td>
</tr>
<tr>
<td>Found</td>
<td>58.52</td>
<td>4.58</td>
<td>14.61</td>
</tr>
</tbody>
</table>
Product Name: ML 130
CAS Number: 799264-47-4
IUPAC Name: 1-{(4-Methylphenyl)sulfonyl}-1H-benzimidazol-2-amine

Description:
Potent and selective inhibitor of NOD1; displays 36-fold selectivity for NOD1 over NOD2 (IC\textsubscript{50} values are 0.56 and >20 μM for NOD1 and NOD2 respectively). Inhibits NOD1-induced NF-κB activation in HEK293 cells with no cytotoxicity. Shown to alter subcellular targeting of NOD1; also thought to alter the conformation of NOD1 protein in vitro.

Physical and Chemical Properties:
Batch Molecular Formula: C\textsubscript{14}H\textsubscript{13}N\textsubscript{2}O\textsubscript{2}S
Batch Molecular Weight: 287.34
Physical Appearance: Off-white solid
Minimum Purity: >99%

Storage: Store at +4°C

Solubility & Usage Info:
DMSO 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: