Product Name: MI 192
Catalog No.: 5647
Batch No.: 1

CAS Number: 1415340-63-4
IUPAC Name: N-(2-Aminophenyl)-4-[(3,4-dihydro-4-methylene-1-oxo-2(1H)-isoquinolinyl)methyl]benzamide

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: \( \text{C}_{24}\text{H}_{21}\text{N}_{3}\text{O}_{2} \)
Batch Molecular Weight: 383.44
Physical Appearance: White solid
Solubility: DMSO to 100 mM
Storage: Store at -20°C
Batch Molecular Structure:

2. ANALYTICAL DATA

TLC: \( R_f = 0.35 \) (Dichloromethane:Methanol [9:1])
HPLC: Shows 98.7% purity
\(^1\text{H NMR:} \) 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>75.18</td>
<td>5.52</td>
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<td>75.28</td>
<td>5.61</td>
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</table>

Caution - Not Fully Tested • Research Use Only • Not For Human or Veterinary Use
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IUPAC Name: N-(2-Aminophenyl)-4-[(3,4-dihydro-4-methylene-1-oxo-2(1H)-isoquinolinyl)methyl]benzamide

Description:
Potent and selective HDAC2/3 inhibitor (IC₅₀ values are 16 and 30 nM, respectively). Exhibits >250-fold selectivity for HDAC2/3 over other HDAC isoforms. Promotes apoptosis of leukemia cell lines in vitro. Also attenuates IL-6 production in rheumatoid arthritis PBMCs in vitro.

Physical and Chemical Properties:
Batch Molecular Formula: C₂₆H₂₁N₃O₂
Batch Molecular Weight: 383.44
Physical Appearance: White solid
Minimum Purity: >98%

Storage: Store at -20°C
CAUTION - This product is light sensitive and we recommend that the solid material and any solutions obtained are protected from exposure to light.

Solubility & Usage Info:
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: