Product Name: GSK 6853
Catalog No.: 6198
Batch No.: 1
CAS Number: 1910124-24-1
IUPAC Name: \( N-[2,3\text{-dihydro}-1,3\text{-dimethyl}-6\text{-[(2R)-2-methyl-1-piperazinyl]-2-oxo-1H-benzimidazol-5-yl]-2-methoxybenzamide}\)

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: \( C_{22}H_{27}N_{5}O_{3} \cdot 1/4H_2O \)
Batch Molecular Weight: 413.98
Physical Appearance: Off White solid
Solubility:
- DMSO to 100 mM
- 1eq. HCl to 100 mM
Storage: Store at -20°C

2. ANALYTICAL DATA

HPLC: Shows 98.7% purity
Chiral HPLC: Shows 99.9% purity
\(^1\)H NMR: Consistent with structure
Mass Spectrum: Consistent with structure
Optical Rotation: \([\alpha]_D = -52.7\ (\text{Concentration} = 0.3, \text{Solvent} = \text{Methanol})\)

Microanalysis:

<table>
<thead>
<tr>
<th></th>
<th>Carbon</th>
<th>Hydrogen</th>
<th>Nitrogen</th>
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</thead>
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<tr>
<td>Theoretical</td>
<td>63.83</td>
<td>6.7</td>
<td>16.92</td>
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<td>Found</td>
<td>63.56</td>
<td>6.64</td>
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</tbody>
</table>

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

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Description: Potent and selective BRPF1 inhibitor. Exhibits >1600-fold selectivity for BRPF1 over other bromodomains (pIC_{50} values by TR-FRET are 8.1, 5.1/4.8 and 4.7/<4.3 for BRPF1, BRPF2/3 and BRD4 BD1/2, respectively). Negative Control also available.

Physical and Chemical Properties:
Batch Molecular Formula: C_{22}H_{27}N_{9}O_{3}·1/4H_{2}O
Batch Molecular Weight: 413.98
Physical Appearance: Off White solid

Minimum Purity: >98%

Batch Molecular Structure:

Storage: Store at -20°C

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

Licensing Information:
This probe is supplied in conjunction with the Structural Genomics Consortium. For further characterization details, please visit the GSK 6853 probe summary on the SGC website.

References: