

Product Name: GSK 6853

Catalog No.: 6198

Batch No.: 1

CAS Number: 1910124-24-1

IUPAC Name: *N*-[2,3-dihydro-1,3-dimethyl-6-[(2*R*)-2-methyl-1-piperazinyl]-2-oxo-1*H*-benzimidazol-5-yl]-2-methoxybenzamide

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₂₂H₂₇N₅O₃·¼H₂O

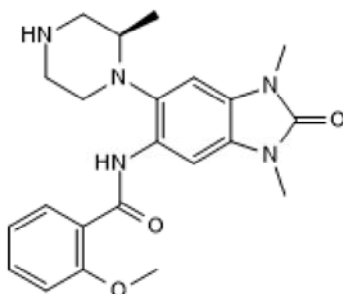
Batch Molecular Weight: 413.98

Physical Appearance: Off White solid

Solubility: DMSO to 100 mM
1eq. HCl to 100 mM

Storage: Store at -20°C

Batch Molecular Structure:



2. ANALYTICAL DATA

HPLC: Shows 98.7% purity

Chiral HPLC: Shows 99.9% purity

¹H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Optical Rotation: [α]_D = -52.7 (Concentration = 0.3, Solvent = Methanol)

Microanalysis:

| | Carbon | Hydrogen | Nitrogen |
|-------------|--------|----------|----------|
| Theoretical | 63.83 | 6.7 | 16.92 |
| Found | 63.56 | 6.64 | 16.75 |

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

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Description:

Potent and selective BRPF1 inhibitor. Exhibits >1600-fold selectivity for BRPF1 over other bromodomains (pIC₅₀ 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:

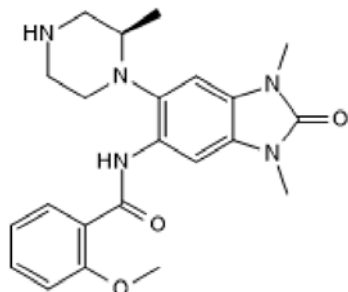
Batch Molecular Formula: C₂₂H₂₇N₅O₃·¼H₂O

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:

Bamborough et al (2016) GSK6853, a chemical probe for inhibition of the BRPF1 bromodomain. *ACS Med.Chem.Lett.* **7** 552. PMID: 27326325.

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