

Product Name: SGC SMARCA-BRDVIII

Catalog No.: 7460

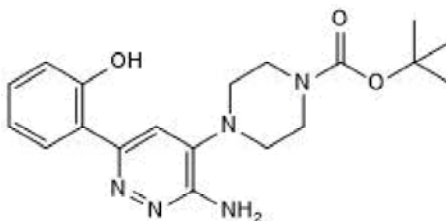
Batch No.: 1

CAS Number: 1997319-84-2

IUPAC Name: 1,1-Dimethylethyl 4-[3-amino-6-(2-hydroxyphenyl)-4-pyridazinyl]-1-piperazinecarboxylate

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₁₉H₂₅N₅O₃.
Batch Molecular Weight: 371.44
Physical Appearance: Off-white solid
Solubility: DMSO to 100 mM
 ethanol to 10 mM
Storage: Store at -20°C
Batch Molecular Structure:



2. ANALYTICAL DATA

HPLC: Shows 99.1% purity
¹H NMR: Consistent with structure
Mass Spectrum: Consistent with structure

Microanalysis:

| | Carbon | Hydrogen | Nitrogen |
|-------------|--------|----------|----------|
| Theoretical | 61.44 | 6.78 | 18.85 |
| Found | 61.43 | 6.83 | 18.93 |

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

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Description:

SGC-SMARCA-BRDVIII is a selective and high affinity SMARCA2/4 and PB1(bromo 5)-selective SWI/SNF bromodomains (K_d (ITC) values are 35, 36 and 13 nM, respectively). SGC-SMARCA-BRDVIII exhibits selectivity over 25 other bromodomain families and shows no off-target activity on 85 protein kinases screened using temperature-shift binding assays. SGC-SMARCA-BRDVIII suppresses formation of 3T3-L1 mouse fibroblasts into adipocytes ($EC_{50} < 1.0 \mu\text{M}$).

Physical and Chemical Properties:

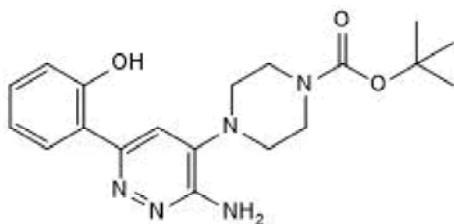
Batch Molecular Formula: $C_{19}H_{25}N_5O_3$.

Batch Molecular Weight: 371.44

Physical Appearance: Off-white solid

Minimum Purity: $\geq 98\%$

Batch Molecular Structure:



Storage: Store at -20°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 $45-60^\circ\text{C}$ 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 SGC SMARCA-BRDVIII probe summary on the SGC website.

References:

Wanior et al (2020) Pan-SMARCA/PB1 Bromodomain Inhibitors and Their Role in Regulating Adipogenesis. *J. Med. Chem.* **63** 14680. PMID: 33216538.

Farnaby et al (2019) BAF complex vulnerabilities in cancer demonstrated via structure-based PROTAC design. *Nat. Chem. Biol.* **15** 672. PMID: 31178587.

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