Print Date: Feb 15th 2019

Certificate of Analysis

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Product Name: **Brequinar sodium** **Catalog No.: 6196** **Batch No.: 3**

CAS Number: 96201-88-6

IUPAC Name: 6-Fluoro-2-(2'-fluoro[1,1'-biphenyl]-4-yl)-3-methyl-4-quinolinecarboxylic acid sodium

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: $C_{23}H_{14}F_2NO_2Na.2H_2O$

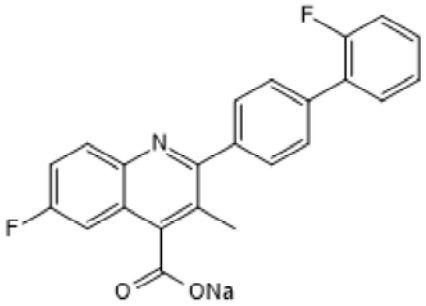
Batch Molecular Weight: 433.38

Physical Appearance: White solid

Solubility: water to 100 mM
DMSO to 100 mM

Storage: Store at +4°C

Batch Molecular Structure:



2. ANALYTICAL DATA

HPLC: Shows 99.2% purity

^{1}H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	63.74	4.19	3.23
Found	63.69	3.98	3.35

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Description:

Potent and selective dihydroorotate dehydrogenase (DHODH) inhibitor (IC_{50} = ~20 nM). Causes depletion of pyrimidine nucleotides. Exhibits minimal inhibition against a panel of >400 kinases. Triggers differentiation of AML cell lines (ED_{50} = ~ 1 µM. Note uridine concentration effects ED_{50} value). Causes differentiation and depletion of leukemia-initiating cells in vivo. Antimetabolite.

Physical and Chemical Properties:

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Minimum Purity: >99%

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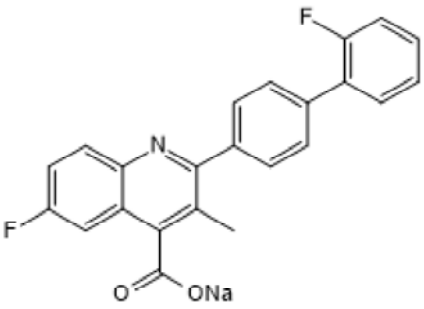

Storage: Store at +4°C

Solubility & Usage Info:

water to 100 mM
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:

Sykes *et al* (2016) Inhibition of dihydroorotate dehydrogenase overcomes differentiation blockade in acute myeloid leukemia. Cell ***167*** 171. PMID: 27641501.

Arteaga (1989) Phase I clinical and pharmacokinetic trial of Brequinar sodium (DuP 785; NSC 368390). Cancer Res. ***49*** 4648. PMID: 2743343.

Peters *et al* (1987) Inhibition of pyrimidine de novo synthesis by DUP-785 (NSC 368390). Invest.New Drugs ***5*** 235. PMID: 2822596.