Certificate of Analysis

Product Name: **Mirin** **Catalog No.: 3190** **Batch No.: 2**

CAS Number: 1198097-97-0

IUPAC Name: *Z*-5-(4-Hydroxybenzylidene)-2-imino-1,3-thiazolidin-4-one

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: $C_{10}H_8N_2O_2S.¾H_2O$

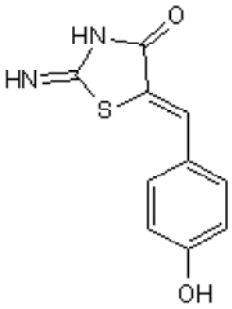
Batch Molecular Weight: 233.76

Physical Appearance: Pale yellow solid

Solubility: DMSO to 100 mM

Storage: Store at +4°C

Batch Molecular Structure:



2. ANALYTICAL DATA

HPLC: Shows 99.9% purity

^{1}H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	51.38	4.1	11.98
Found	51.36	3.79	11.97

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Description:

Mirin is a Mre11-Rad50-Nbs1 (MRN)-ATM pathway inhibitor that blocks the 3' and 5' exonuclease activity associated with Mre11. Prevents ATM activation in response to double strand breaks (IC_{50} = 12 µM) and induces G_2 cell cycle arrest. Also blocks homology-directed repair in vitro.

Physical and Chemical Properties:

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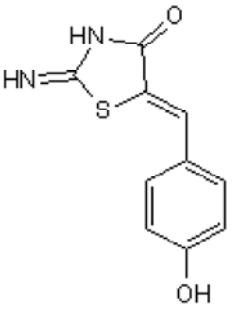
Batch Molecular Weight: 233.76

Physical Appearance: Pale yellow solid

Minimum Purity: ≥99%

Batch Molecular Structure:



Storage: Store at +4°C

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.

Other Information:

In the literature (**Garner** *et al* (2009) Nat.Chem.Biol. ***5*** 129) Mirin is reported as an orange solid. However, this coloration was found to have been caused by a brightly colored impurity. Upon further purification, Mirin was obtained as a pale yellow solid.

References:

Garner *et al* (2009) Corrected structure of mirin, a small-molecule inhibitor of the Mre11-Rad50-Nbs1 complex. Nat.Chem.Biol. ***5*** 129. PMID: 19219009.

Dupre *et al* (2008) A forward chemical genetic screen reveals an inhibitor of the Mre11-Rad50-Nbs1 complex. Nat.Chem.Biol. ***4*** 119. PMID: 18176557.

Stivers (2008) Small molecule versus DNA repair mechanisms. Nat.Chem.Biol. ***4*** 86. PMID: 18202674.