Print Date: Apr 24th 2014

Certificate of Analysis

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Product Name: XL 388 **Catalog No.: 4893** **Batch No.: 1**

CAS Number: 1251156-08-7

IUPAC Name: [7-(6-Amino-3-pyridinyl)-2,3-dihydro-1,4-benzoxazepin-4(5*H*)-yl][3-fluoro-2-methyl-4-(methylsulfonyl)phenyl]-methanone

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: $C_{23}H_{22}FN_3O_4S.½H_2O$

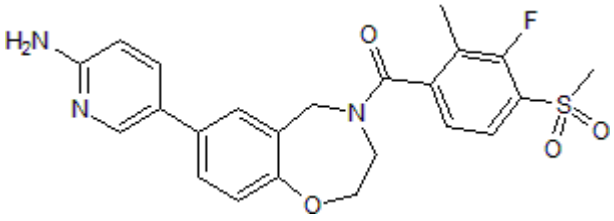
Batch Molecular Weight: 464.51

Physical Appearance: Pale yellow solid

Solubility: DMSO to 50 mM

Storage: Store at -20°C

Batch Molecular Structure:



2. ANALYTICAL DATA

TLC: R_f = 0.33 (Dichloromethane:Methanol [95:5])

HPLC: Shows >99.9% purity

^{1}H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	59.47	4.99	9.05
Found	59.42	4.91	8.88

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Description:

Potent and selective mTOR inhibitor (IC_{50} = 9.9 nM). Inhibits mTOR activity in an ATP-competitive manner. Exhibits >300-fold selectivity for mTOR over PI 3-K and a range of other kinases. Displays antitumor activity in athymic nude mice implanted with tumor xenografts.

Physical and Chemical Properties:

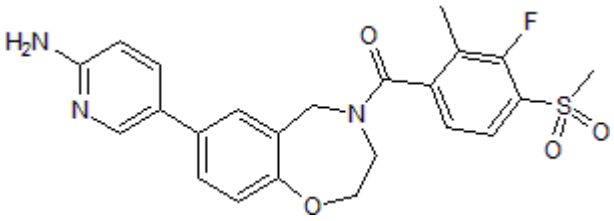
Batch Molecular Formula: $C_{23}H_{22}FN_3O_4S.½H_2O$

Batch Molecular Weight: 464.51

Physical Appearance: Pale yellow solid

Minimum Purity: >98%

Batch Molecular Structure:



Storage: Store at -20°C

Solubility & Usage Info:

DMSO to 50 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:

Takeuchi *et al* (2013) Discovery of a novel class of highly potent, selective, ATP-competitive, and orally bioavailable inhibitors of the mammalian target of rapamycin (mTOR). J.Med.Chem. ***56*** 2218. PMID: 23394126.