

# Certificate of Analysis

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**Product Name:** Y 11

**Catalog No.:** 4498

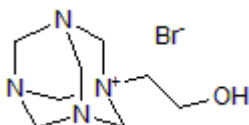
**Batch No.:** 1

**CAS Number:** 1086639-59-9

**IUPAC Name:** 1-(2-Hydroxyethyl)-3,5,7-triaza-1-azaniatricyclo[3.3.1.1<sup>3,7</sup>]decane bromide

## 1. PHYSICAL AND CHEMICAL PROPERTIES

**Batch Molecular Formula:** C<sub>8</sub>H<sub>17</sub>N<sub>4</sub>OBr  
**Batch Molecular Weight:** 265.15  
**Physical Appearance:** White solid  
**Solubility:** water to 100 mM  
DMSO to 100 mM  
**Storage:** Store at -20°C  
**Batch Molecular Structure:**



## 2. ANALYTICAL DATA

**Melting Point:** Between 140 - 143°C  
**<sup>1</sup>H NMR:** Consistent with structure  
**<sup>13</sup>C NMR:** Consistent with structure  
**Mass Spectrum:** Consistent with structure

**Microanalysis:**

	Carbon	Hydrogen	Nitrogen
Theoretical	36.24	6.46	21.13
Found	36.29	6.46	21.09

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

## Product Information

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### Description:

Potent inhibitor of focal adhesion kinase (FAK); prevents FAK autophosphorylation at the Y397 site (IC<sub>50</sub> ~ 50 nM in an in vitro kinase assay). Displays selectivity for FAK over a panel of other kinases (concentration used in assay = 1 µM). Decreases cell viability in a number of cancer cell lines; blocks colony formation in SW620 and BT474 cell lines.

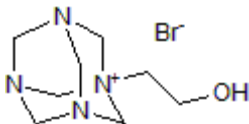
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Batch Molecular Weight: 265.15

Physical Appearance: White solid

### Batch Molecular Structure:



**Storage:** Store at -20°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:

**Golubovskaya et al** (2008) A small molecule inhibitor, 1,2,4,5-benzenetetraamine tetrahydrochloride, targeting the Y397 site of focal adhesion kinase decreases tumor growth. *J.Med.Chem.* **51** 7405. PMID: 18989950.

**Golubovskaya et al** (2012) A small molecule focal adhesion kinase (FAK) inhibitor, targeting Y397 site: 1-(2-hydroxyethyl) -3, 5, 7-triaza-1-azoniatricyclo [3.3.1.13,7]decane; bromide effectively inhibits FAK autophosphorylation activity and decreases cancer cell viability, clonogenicity and tumor growth *in vivo*. *Carcinogenesis*. PMID: 22402131.

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