

## Certificate of Analysis

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**Product Name:** Ro 26-4550 trifluoroacetate

**Catalog No.:** 1794

**Batch No.:** 1

CAS Number: 1217448-66-2

IUPAC Name: *N*-[[[(3*R*)-1-(Aminoiminomethyl)-3-piperidinyl]acetyl]-4-(phenylethynyl)-L-phenylalanine methyl ester trifluoroacetate

### 1. PHYSICAL AND CHEMICAL PROPERTIES

**Batch Molecular Formula:** C<sub>26</sub>H<sub>30</sub>N<sub>4</sub>O<sub>3</sub>·CF<sub>3</sub>CO<sub>2</sub>H·¼H<sub>2</sub>O

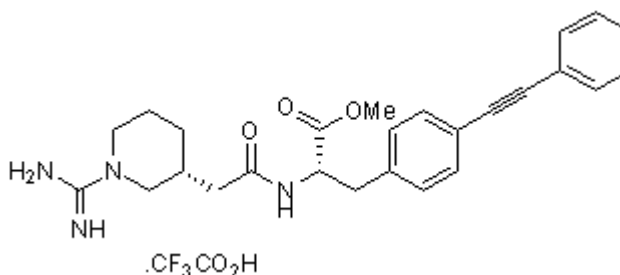
**Batch Molecular Weight:** 565.07

**Physical Appearance:** White solid

**Solubility:** DMSO to 50 mM  
ethanol to 5 mM

**Storage:** Desiccate at +4°C

**Batch Molecular Structure:**



### 2. ANALYTICAL DATA

**TLC:** R<sub>f</sub> = 0.27 (Dichloromethane:Methanol [1:10])

**HPLC:** Shows >98.71% purity

**<sup>1</sup>H NMR:** Consistent with structure

**Mass Spectrum:** Consistent with structure

**Microanalysis:**

	Carbon	Hydrogen	Nitrogen
Theoretical	59.52	5.62	9.91
Found	59.89	5.79	9.52

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**Description:**

Competitive reversible inhibitor of interleukin-2 (IL-2) binding to its receptor (IC<sub>50</sub> = 3 μM for inhibition of IL-2 interaction with IL-2R α-subunit). Appears to compete with IL-2Rα for its binding site on IL-2.

**Physical and Chemical Properties:**

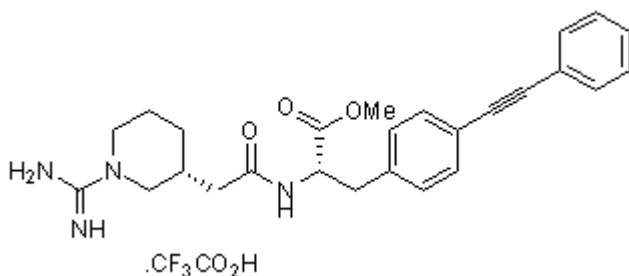
Batch Molecular Formula: C<sub>26</sub>H<sub>30</sub>N<sub>4</sub>O<sub>3</sub>.CF<sub>3</sub>CO<sub>2</sub>H.¼H<sub>2</sub>O

Batch Molecular Weight: 565.07

Physical Appearance: White solid

**Minimum Purity:** >98%

**Batch Molecular Structure:**



**Storage:** Desiccate at +4°C

**Solubility & Usage Info:**

DMSO to 50 mM

ethanol to 5 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:**

**Tilley *et al*** (1997) Identification of a small molecule inhibitor of the IL-2/IL-2Rα receptor interaction which binds to IL-2. *J.Am.Chem.Soc.* **119** 7589.

**Braisted *et al*** (2003) Discovery of a potent small molecule IL-2 inhibitor through fragment assembly. *J.Am.Chem.Soc.* **125** 3714. PMID: 12656598.

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