

**Product Name:** FK 506

**Catalog No.:** 3631

**Batch No.:** 4

CAS Number: 104987-11-3

IUPAC Name: (3*S*,4*R*,5*S*,8*R*,9*E*,12*S*,14*S*,15*R*,16*S*,18*R*,19*R*,26*aS*)-5,6,8,11,12,13,14,15,16,17,18,19,24,25,26,26*a*-Hexadecahydro-5,19-dihydroxy-3-[(1*E*)-2-[(1*R*,3*R*,4*R*)-4-hydroxy-3-methoxycyclohexyl]-1-methylethenyl]-14,16-dimethoxy-4,10,12,18-tetramethyl-8-(2-propen-1-yl)-15,19-epoxy-3*H*-pyrido[2,1-*c*][1,4]oxaazacyclotricosine-1,7,20,21(4*H*,23*H*)tetrone

## 1. PHYSICAL AND CHEMICAL PROPERTIES

**Batch Molecular Formula:** C<sub>44</sub>H<sub>69</sub>NO<sub>12</sub>·H<sub>2</sub>O

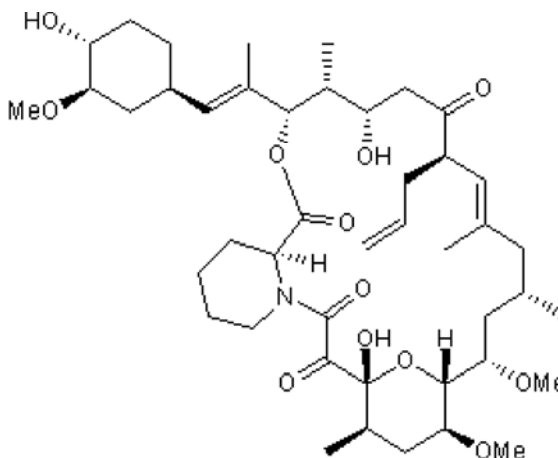
**Batch Molecular Weight:** 822.04

**Physical Appearance:** White solid

**Solubility:** DMSO to 100 mM  
ethanol to 100 mM

**Storage:** Store at -20°C

**Batch Molecular Structure:**



## 2. ANALYTICAL DATA

**HPLC:** Shows 99.1% purity

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

**Mass Spectrum:** Consistent with structure

**Microanalysis:**

	Carbon	Hydrogen	Nitrogen
Theoretical	64.29	8.71	1.7
Found	64.4	8.72	1.74

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**Description:**

Potent calcineurin (protein phosphatase 2B) inhibitor that requires FK 506-binding protein 12 (FKBP12) for activity (IC<sub>50</sub> = 3 nM). Inhibits secretion of IL-1, IL-2 (IC<sub>50</sub> = 1 nM), IL-3, IL-4, IL-6 (IC<sub>50</sub> = 35 nM), GM-CSF, TNFα (IC<sub>50</sub> = 10 nM), IFNγ and Myc from activated T cells in vitro. Exhibits potent immunosuppressive, neuroprotective and anticonvulsant activity in vivo. Identified as targeting human host cell proteins that interact with SARS-CoV-2. Analog also available.

**Physical and Chemical Properties:**

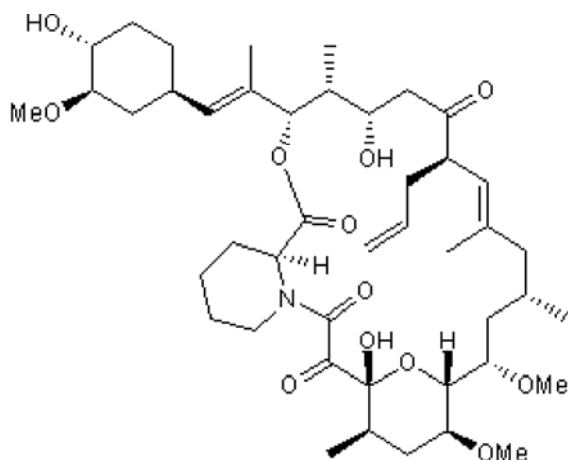
Batch Molecular Formula: C<sub>44</sub>H<sub>69</sub>NO<sub>12</sub>·H<sub>2</sub>O

Batch Molecular Weight: 822.04

Physical Appearance: White solid

**Minimum Purity:** ≥99%

**Batch Molecular Structure:**



**Storage:** Store at -20°C

**Solubility & Usage Info:**

DMSO to 100 mM

ethanol 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:**

**Gordon et al (2020)** A SARS-CoV-2-human protein-protein interaction map reveals drug targets and potential drug-repurposing. *BioRxiv* - Paper not yet peer reviewed.

**Sierra-Paredes and Sierra-Marcuno (2008)** Ascomycin and FK506: Pharmacology and therapeutic potential as anticonvulsants and neuroprotectants. *CNS Neurosci. Ther.* **14** 36. PMID: 18482098.

**Baughman et al (1997)** Tissue distribution and abundance of human FKBP51, and FK506-binding protein that can mediate calcineurin inhibition. *Biochem. Biophys. Res. Commun.* **232** 437. PMID: 9125197.

**Fruman et al (1995)** The complex of FK506-binding protein 12 and FK506 inhibits calcineurin phosphatase activity and IgE activation-induced cytokine transcripts, but not exocytosis, in mouse mast cells. *J. Immunol.* **154** 1846. PMID: 7530743.

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