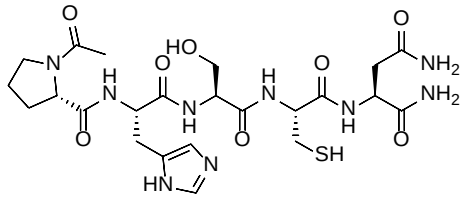
Product data sheet

MedKoo Cat#: 200350 Name: ATN-161 free base CAS#: 262438-43-7 (free base) Chemical Formula: $C_{23}H_{35}N_9O_8S$ Molecular Weight: 597.64	
Product supplied as:	Powder
Purity (by HPLC):	≥ 98%
Shipping conditions	Ambient temperature
Storage conditions:	Powder: -20°C 3 years; 4°C 2 years.
	In solvent: -80°C 3 months; -20°C 2 weeks.

1. Product description:

ATN-161 is a small peptide antagonist of integrin α5β1 with potential antineoplastic activity. ATN-161 selectively binds to and blocks the receptor for integrin α5β1, thereby preventing integrin α5β1 binding. This receptor blockade may result in inhibition of endothelial cell-cell interactions, endothelial cell-matrix interactions, angiogenesis, and tumor progression. Integrin α5β1 is expressed on endothelial cells and plays a crucial role in endothelial cell adhesion and migration.

2. CoA, QC data, SDS, and handling instruction

SDS and handling instruction, CoA with copies of QC data (NMR, HPLC and MS analytical spectra) can be downloaded from the product web page under "QC And Documents" section. Note: copies of analytical spectra may not be available if the product is being supplied by MedKoo partners. Whether the product was made by MedKoo or provided by its partners, the quality is 100% guaranteed.

3. Solubility data

Solvent	Max Conc. mg/mL	Max Conc. mM
Water	7.50	12.56

4. Stock solution preparation table:

Concentration / Solvent Volume / Mass	1 mg	5 mg	10 mg
1 mM	1.67 mL	8.37 mL	16.73 mL
5 mM	0.33 mL	1.67 mL	3.35 mL
10 mM	0.17 mL	0.84 mL	1.67 mL
50 mM	0.03 mL	0.17 mL	0.33 mL

5. Molarity Calculator, Reconstitution Calculator, Dilution Calculator

Please refer the product web page under section of "Calculator"

6. Recommended literature which reported protocols for in vitro and in vivo study

In vitro study

1. Beddingfield BJ, Iwanaga N, Chapagain PP, Zheng W, Roy CJ, Hu TY, Kolls JK, Bix GJ. The Integrin Binding Peptide, ATN-161, as a Novel Therapy for SARS-CoV-2 Infection. JACC Basic Transl Sci. 2021 Jan;6(1):1-8. doi: 10.1016/j.jacbts.2020.10.003. Epub 2020 Oct 16. PMID: 33102950; PMCID: PMC7566794.
2. Wang W, Wang F, Lu F, Xu S, Hu W, Huang J, Gu Q, Sun X. The antiangiogenic effects of integrin alpha5beta1 inhibitor (ATN-161) in vitro and in vivo. Invest Ophthalmol Vis Sci. 2011 Sep 14;52(10):7213-20. doi: 10.1167/iovs.10-7097. PMID: 21813636.

In vivo study

1. Edwards DN, Salmeron K, Lukins DE, Trout AL, Fraser JF, Bix GJ. Integrin α5β1 inhibition by ATN-161 reduces neuroinflammation and is neuroprotective in ischemic stroke. J Cereb Blood Flow Metab. 2020 Aug;40(8):1695-1708. doi: 10.1177/0271678X19880161. Epub 2019 Oct 1. PMID: 31575337; PMCID: PMC7370357.
2. Lv X, Li Z, Guan J, Zhang J, Xu B, He W, Lan Y, Zhao K, Lu H, Song D, Gao F. ATN-161 reduces virus proliferation in PHEV-infected mice by inhibiting the integrin α5β1-FAK signaling pathway. Vet Microbiol. 2019 Jun;233:147-153. doi: 10.1016/j.vetmic.2019.04.029. Epub 2019 Apr 26. PMID: 31176401.

7. Bioactivity

Biological target: Integrin α5β1 antagonist.

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In vitro activity

The binding of the SARS-CoV-2 spike protein with ACE2 and α5β1 was explored using ELISA-based methods. To determine the spike protein's ability to bind α5β1, plates were coated with α5β1 and incubated with a mixture of ATN-161 and a trimeric version of the spike protein. The SARS-CoV-2 spike protein was bound to α5β1 with an affinity that was roughly equivalent to α5β1's native ligand, fibronectin, and inhibited binding with a U-shaped, dose-dependent manner, with maximum effect at 100 nM (Figure 1A). This U-shaped response was not surprising because it was consistent with previous in vitro and in vivo studies on ATN-161 in the context of blocking angiogenesis and solid tumor growth. This might be due to the ability of ATN-161, at saturating concentrations, to affect the expression of α5β1 integrin, which was demonstrated to occur in experimental stroke.

Reference: JACC Basic Transl Sci. 2021 Jan;6(1):1-8. https://www.ncbi.nlm.nih.gov/pmc/articles/PMC7566794/

In vivo activity

Following tandem transient common carotid artery/middle cerebral artery occlusion on wild-type mice, the integrin a5b1 inhibitor, ATN-161, was administered by intraperitoneal (IP) injection at 1 mg/kg acutely after reperfusion, on post-stroke day (PSD)1 and PSD2. Systemic changes (heart rate, pulse distension, and body temperature) were determined. Additionally, infarct volume and edema were determined by 2,3-triphenyltetrazolium chloride and magnetic resonance imaging, while neurological changes were evaluated using an 11-point Neuroscore. Brain immunohistochemistry was performed for claudin-5, α5β1, IgG, and CD45 + cells, and quantitative polymerase chain reaction (qPCR) was performed for matrix metalloproteinase-9 (MMP-9), interleukin (IL)-1β, collagen IV, and CXCL12. ATN-161 significantly reduced integrin α5β1 expression in the surrounding peri-infarct region with no systemic changes. Infarct volume, edema, and functional deficit were significantly reduced in ATN-161-treated mice. Furthermore, ATN-161 treatment reduced IgG extravasation into the parenchyma through conserved claudin-5, collagen IV, CXCL12 while reducing MMP-9 transcription. Additionally, IL-1β and CD45 + cells were reduced in the ipsilateral cortex following ATN-161 administration.

Reference: J Cereb Blood Flow Metab. 2020 Aug;40(8):1695-1708. https://pubmed.ncbi.nlm.nih.gov/33102950/

Note: The information listed here was extracted from literature. MedKoo has not independently retested and confirmed the accuracy of these methods. Customer should use it just for a reference only.