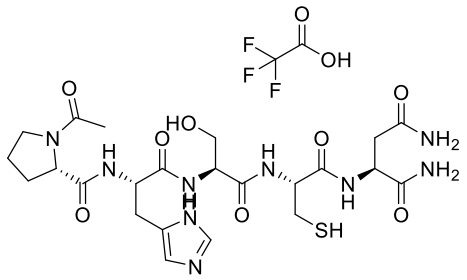
Product data sheet

MedKoo Cat#: 206976 Name: ATN-161 TFA salt CAS#: 904763-27-5 (TFA) Chemical Formula: $C_{25}H_{36}F_3N_9O_{10}S$ Molecular Weight: 711.67	
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 alpha$_5$beta$_1$ with potential antineoplastic activity. ATN-161 selectively binds to and blocks the receptor for integrin alpha$_5$beta$_1$, thereby preventing integrin alpha$_5$beta$_1$ binding. This receptor blockade may result in inhibition of endothelial cell-cell interactions, endothelial cell-matrix interactions, angiogenesis, and tumor progression. Integrin alpha$_5$beta$_1$ is expressed on endothelial cells and plays a crucial role in endothelial cell adhesion and migration. Note: The Catalog number of ATN-161 TFA salt was changed from 200350B to 206976.

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
DMSO	1.0	1.41
Water	8.33	11.70

4. Stock solution preparation table:

Concentration / Solvent Volume / Mass	1 mg	5 mg	10 mg
1 mM	1.41 mL	7.03 mL	14.05 mL
5 mM	0.28 mL	1.41 mL	2.81 mL
10 mM	0.14 mL	0.70 mL	1.41 mL
50 mM	0.03 mL	0.14 mL	0.28 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. Chen YC, Chuang TY, Liu CW, Liu CW, Lee TL, Lai TC, Chen YL. Particulate matters increase epithelial-mesenchymal transition and lung fibrosis through the ETS-1/NF-κB-dependent pathway in lung epithelial cells. Part Fibre Toxicol. 2020 Aug 14;17(1):41. doi: 10.1186/s12989-020-00373-z. PMID: 32799885; PMCID: PMC7429884.

In vivo study

1. Sui A, Zhong Y, Demetriades AM, Shen J, Su T, Yao Y, Gao Y, Zhu Y, Shen X, Xie B. ATN-161 as an Integrin α5β1 Antagonist Depresses Ocular Neovascularization by Promoting New Vascular Endothelial Cell Apoptosis. Med Sci Monit. 2018 Aug 22;24:5860-5873. doi: 10.12659/MSM.907446. PMID: 30133427; PMCID: PMC6116638.
2. Doñate F, Parry GC, Shaked Y, Hensley H, Guan X, Beck I, Tel-Tsur Z, Plunkett ML, Manuia M, Shaw DE, Kerbel RS, Mazar AP. Pharmacology of the novel antiangiogenic peptide ATN-161 (Ac-PHSCN-NH2): observation of a U-shaped dose-response curve in

several preclinical models of angiogenesis and tumor growth. Clin Cancer Res. 2008 Apr 1;14(7):2137-44. doi: 10.1158/1078-0432.CCR-07-4530. PMID: 18381955.

7. Bioactivity

Biological target:

ATN-161 trifluoroacetate salt is a novel integrin α5β1 antagonist.

In vitro activity

This study performed similar assays to investigate ACE2 binding to α5β1, using a mixture of ATN-161 and hACE2. Clear inhibition of ACE2/α5β1 binding by ATN-161 was apparent and dose-dependent (Figure 1B). Furthermore, application of ATN-161 reduced binding of the trimeric spike protein to hACE2, either alone or in combination with α5β1, the latter of which trended to support greater spike binding than to hACE2 alone (Figure 1C). Application of ATN-161 also reduced binding of the monomeric spike to hACE2 (Supplemental Figure S1).

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

In vivo activity

In the present study, 2 mouse models of ocular NV (neurovascularization) were used to investigate the potential role and underlying mechanism of action of ATN-161. The protein levels of integrin α5β1 increased in the CNV (choroidal neovascularization) and OIR (oxygen-induced retinopathy) mice, indicating a close relationship between integrin α5β1 and ocular NV. Next, this study explored the inhibition of integrin α5β1 by ATN-161 and demonstrated that ATN-161 inhibited the protein expression of integrin α5β1 in a dose-dependent manner. The NV areas were reduced in OIR and CNV mice after treatment with ATN-161 compared with PBS groups.

Reference: Med Sci Monit. 2018 Aug 22;24:5860-5873. https://www.ncbi.nlm.nih.gov/pmc/articles/PMC6116638/