Integrin Inhibitors
(inhibitors, agonists and modulators)

Integrins are cell adhesion receptors that are evolutionary old and that play important roles during developmental and pathological processes. The integrin family is composed of 24 αβ heterodimeric members that mediate the attachment of cells to the extracellular matrix (ECM) but that also take part in specialized cell-cell interactions.
**Tirofiban hydrochloride monohydrate - CAS 150915-40-5**

**Catalog Number:** B0084-084608  
**Price:** $298/100 mg  
**Molecular Weight:** 495.07  
**Molecular Formula:** C22H39ClN2O6S  
**Description:** Tirofiban is a specific nonpeptide platelet fibrinogen receptor (GPIIb/IIIa) antagonist. Tirofiban is an antithrombotic used in the treatment of unstable angina.

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**CWHM-12 - CAS 1564286-55-0**

**Catalog Number:** B0084-463546  
**Price:** $598/100 mg  
**Molecular Weight:** 590.47  
**Molecular Formula:** C26H32BrN5O6  
**Description:** CWHM 12 demonstrated high potency against all of the five possible β subunit binding partners (αvβ1, αvβ3, αvβ5, αvβ6 and αvβ8) in in vitro ligand-binding assays, with somewhat less potency against αvβ5 than against the other αv integrins. Treated mice with CCl4 for 3 weeks to establish fibrotic disease and then treated with CWHM 12 or vehicle for the final 3 weeks of CCl4. CWHM12 significantly reduced liver fibrosis even after fibrotic disease had been established. Similar to our findings in the liver, administration of CWHM 12 significantly inhibited progression of pulmonary fibrosis.

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**GLPG-0187 - CAS 1320346-97-1**

**Catalog Number:** B0084-484680  
**Price:** $149/10 mg  
**Molecular Weight:** 595.719  
**Molecular Formula:** C29H37N7O5S  
**Description:** GLPG-0187 is a small molecule integrin receptor antagonist (IRA) with nanomolar affinity for the RGD-integrin receptors αvβ1, αvβ3, αvβ5, αvβ6 and α5β1 (IC50s = 1.2–3.7 nM). Integrin receptors are expressed on the surface of tumor vessel endothelial cells and some types of cancer cells, and play a crucial role in endothelial cell adhesion and migration. This compound shows an inhibitory activity of angiogenesis, bone-resorption and tumor, which is hopefully used as an anticancer drug.

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**SR121566A - CAS 180144-61-0**

**Catalog Number:**  
**Molecular Weight:** 431.51  
**Molecular Formula:** C20H25N5O4S  
**Description:** SR121566A, a non-peptide Glycoprotein IIb/IIIa (GP IIb-IIIa) antagonist, has been shown to block platelet aggregation induced by a wide variety of agonists including HIT serum/heparin, reduced in a dose-dependent manner the HIT serum/heparin-induced, platelet mediated expression and release of the above mentioned proteins.
**GRGDSP**

Catalog Number: S87.59  
Molecular Weight: 587.59  
Molecular Formula: C22H37N9O10  
Description: GRGDSP, a synthetic linear RGD peptide, is an integrin inhibitor which can be used to modify the surface of cardiovascular implants such as vascular grafts to promote endothelialization.

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**ALG1001 - CAS 1307293-62-4**

Catalog Number:  
Molecular Weight: 637.66  
Molecular Formula: C22H39N9O11S  
Description: ALG1001, also known as Luminate, a first-in-class integrin peptide therapy, is an angiogenesis inhibitors and Integrin alpha 5 beta 1 modulator. A study from Johns Hopkins University also showed that ALG-1001 reduced vascular leakage.

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**Leukadherin-1 - CAS 344897-95-6**

Catalog Number:  
Molecular Weight: 421.48  
Molecular Formula: C22H15NO4S2  
Description: Leukadherin-1, also known as LA1, is a small molecule agonist that enhances CD11b/CD18-dependent cell adhesion to its ligand ICAM-1. Leukadherin-1 suppresses human innate inflammatory signalling. leukadherin-1 increases CD11b/CD18-dependent adhesion via membrane tethers. It also competitively inhibits YopH (Ki = 1.94 µM), a tyrosine phosphorylase secreted by Y. pestis into immune cells to block signal transduction, and anthrax lethal factor metalloproteinase, a component of anthrax toxin (IC50 = 6 µM).

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**Echistatin, α1 isoform - CAS 154303-05-6**

Catalog Number:  
Molecular Weight: 5417.1  
Molecular Formula: C217H341N71O74S9  
Description: Echistatin, α1 isoform is a potent and irreversible αVβ3 integrin antagonist (Ki = 0.27 nM). It exhibits inhibitory activity for bone reabsorption (IC50 = 0.1 nM) and prevents ADP-induced platelet aggregation by inhibiting glycoprotein IIb/IIIa (GpIIb/IIIa, αIIbβ3) receptors (IC50 = 30 nM) in vitro.
Cilengitide (TFA salt) - CAS 188968-51-6

Catalog Number:  
Molecular Weight: 588.666  Molecular Formula: C27H40N8O7

Description: Cilengitide is a cyclic Arg-Gly-Asp peptide with potential antineoplastic activity. Cilengitide binds to and inhibits the activities of the alpha(v)beta(3) and alpha(v)beta(5) integrins, thereby inhibiting endothelial cell-cell interactions, endothelial cell-matrix interactions, and angiogenesis. It is being studied for the treatment of glioblastoma.

Zaurategrast - CAS 455264-31-0

Catalog Number: 455264-31-0  
Molecular Weight: 521.41  Molecular Formula: C26H25BrN4O3

Description: Zaurategrast is an oral α4-integrin inhibitor. It significantly decreased the capacity of lymphocytes to bind vascular adhesion molecule-1 (VCAM-1) and the expression of α4-integrin on VCAM-1-binding cells.

BTT 3033 - CAS 1259028-99-3

Catalog Number:  
Molecular Weight: 465.5  Molecular Formula: C23H20FN5O3S

Description: BTT 3033 is a selective inhibitor of α2β1 integrin (EC50 = 130 nM for α2β1 binding to collagen I) that binds to the α2I domain. BTT 3033 inhibits platelet aggregation to collagen I coated capillaries under flow, and also inhibits binding of α2-expressing CHO cells to collagen I under shear stress conditions.

BOP sodium salt - CAS 1947348-42-6

Catalog Number:  
Molecular Weight: 537.56  Molecular Formula: C25H28N3O7SNa

Description: BOP is a dual α9β1/α4β1 integrin inhibitor preferentially mobilizes HSCs and progenitors.
**BIO 5192 - CAS 327613-57-0**

**Catalog Number:**

**Molecular Weight:** 817.78  
**Molecular Formula:** C38H46Cl2N6O8S

**Description:** BIO 5192 is a selective and potent inhibitor of integrin $\alpha_4\beta_1$ (Very Late Antigen-4; VLA-4) (Kd < 10 pM) with selectivity for $\alpha_4\beta_1$ over a range of other integrins (IC50 values are 1.8, 138, 1053, > 500 and > 10,000 nM for $\alpha_4\beta_1$, $\alpha_9\beta_1$, $\alpha_2\beta_1$, $\alpha_4\beta_7$ and $\alpha_{IIb}\beta_3$, respectively). BIO 5192 causes a 30-fold increase in mobilization of murine hematopoietic stem and progenitors (HSPCs) over basal levels.

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**RWJ 50271 - CAS 162112-37-0**

**Catalog Number:**

**Molecular Weight:** 410.41  
**Molecular Formula:** C18H17F3N4O2S

**Description:** RWJ 50271 is a selective inhibitor of LFA-1/ICAM-1 mediated cell adhesion (sICAM) (IC50= 5 μM in HL60 cells).

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**TCS 2314 - CAS 317353-73-4**

**Catalog Number:**

**Molecular Weight:** 522.59  
**Molecular Formula:** C28H34N4O6

**Description:** TCS 2314 is an integrin very late antigen-4 (VLA-4; $\alpha_4\beta_1$) antagonist (IC50 = 4.4 nM) that inhibits the activation of inflammatory cells.

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**P11 - CAS 848644-86-0**

**Catalog Number:**

**Molecular Weight:** 720.78  
**Molecular Formula:** C30H48N12O9

**Description:** P11 is a potent antagonist of the integrin $\alpha_v\beta_3$-vitronectin interaction with IC50 value of 25.72 nM.
**Obtustatin**

**Catalog Number:**

**Molecular Weight:** 4393.07  
**Molecular Formula:** C184H284N52O57S8

**Description:** Obtustatin is an integrin α1β1 inhibitor with IC50 value of 0.8 nM for α1β1 binding to type IV collagen. Some research shows that it has antitumor efficacy in a synergistic mouse model of Lewis lung carcinoma.

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**LDV FITC - CAS 1207610-07-8**

**Catalog Number:**

**Molecular Weight:** 1368.54  
**Molecular Formula:** C69H81N11O17S

**Description:** LDV FITC is a fluorescent ligand. It can bind to the α4β1 integrin (VLA-4) with high affinity. It can be used to detect VLA-4 affinity and conformational changes.

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**R-BC154**

**Catalog Number:**

**Molecular Weight:** 1212.37  
**Molecular Formula:** C55H61N9O13S3.CH3CO2H

**Description:** R-BC154, a high affinity fluorescent α4β1/α9β1 integrin antagonist (Kd= 12.7 and 38 nM, respectively), was based on a series of N-phenylsulfonyl proline dipeptides and assembled using the Cu(I)-catalyzed azide alkyne cycloaddition (CuAAC) reaction. R-BC154 represents a useful multi-purpose fluorescent integrin probe that can be used for screening small molecule inhibitors of α9β1 and α4β1 integrins, investigating the biochemical properties of α9β1 and α4β1 integrin binding and investigating integrin expression and activation on defined cell phenotypes in vivo.

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**TC-I 15 - CAS 916734-43-5**

**Catalog Number:**

**Molecular Weight:** 520.62  
**Molecular Formula:** C23H28N4O6S2

**Description:** TC-I 15 is a potent α2β1 integrin inhibitor (IC50 = 12 and 715 nM for the inhibition of human platelet adhesion to type I collagen and for platelets under static conditions and under flow, respectively), displaying selectivity for α2β1 over αvβ3, α5β1, α6β1 and αIIbβ3 at concentrations exceeding 1000 nM. TC-I 15 was shown to reduce collagen IV production in mesangial cells.
Vedolizumab - CAS 943609-66-3

Catalog Number: B0084-185641
Molecular Weight: 146836.67  Molecular Formula: C6528H10072N1732O2042S42
Description: Vedolizumab is a monoclonal antibody developed by Millennium Pharmaceuticals for the treatment of ulcerative colitis and Crohn’s disease under the trade name Entyvio. Vedolizumab binds to integrin α4β7 (LPAM-1) and blocks α4β7, displaying anti-inflammatory activity.

Firategrast - CAS 402567-16-2

Catalog Number: 402567-16-2
Molecular Weight: 499.5  Molecular Formula: C27H27F2NO6
Description: Firategrast is an orally bioavailable alpha4 beta1/alpha4 beta7 integrin antagonist designed to reduce trafficking of lymphocytes into the central nervous system (CNS).

Arg-Gly-Asp-Ser - CAS 91037-65-9

Catalog Number: 91037-65-9
Molecular Weight: 433.42  Molecular Formula: C15H27N7O8
Description: Arg-Gly-Asp-Ser is an integrin binding sequence that inhibits integrin receptor function. It is a tetrapeptide found on fibronectin, fibrinogen α, and von Willebrand factor, but not vitronectin or collagen. It decreases systemic inflammation via inhibition of collagen-triggered activation of leukocytes and attenuates expression of inflammatory cytokines, iNOS and MMP-9. It inhibits thrombin-induced binding of platelets to fibronectin, fibrinogen α, and von Willebrand factor. It promotes cell attachment and abrogates apoptosis via the mitochondrial pathway in osteoblasts in vitro. It also blocks the attachment of certain pathogens to cells.

BIO 1211 - CAS 187735-94-0

Catalog Number:
Molecular Weight: 708.8  Molecular Formula: C36H48N6O9
Description: BIO 1211 is a selective and high affinity integrin α4β1 (Very Late Antigen 4; VLA-4) inhibitor with 200-fold selectivity for the activated form of α4β1 (KD = 70 pM; IC50 = 0.004 μM).
### ATN-161 - CAS 262438-43-7

**Catalog Number:** 262438-43-7  
**Molecular Weight:** 597.648  
**Molecular Formula:** C23H35N9O8S  
**Description:** ATN-161 is a small peptide antagonist of integrin alpha5beta1 with potential antineoplastic activity. ATN-161 selectively binds to and blocks the receptor for integrin alpha5beta1, thereby preventing integrin alpha5beta1 binding.

### TR-14035 - CAS 232271-19-1

**Catalog Number:** 232271-19-1  
**Molecular Weight:** 474.33  
**Molecular Formula:** C24H21Cl2NO5  
**Description:** TR14035 blocked the binding of human alpha(4)beta(7) to an (125)I-MAdCAM-Ig fusion protein with IC(50) values of 0.75 nM. TR14035 blocked binding of human alpha(4)beta(7)-expressing RPMI-8866 cells or murine mesenteric lymph node lymphocytes to MAdCAM-Ig with IC(50) values of 0.1 microM. TR14035 blocked adhesion to HEVs [ED(50) of 0.01-0.1 mpk i.v.]. TR-14035 was taken up by rat and human hepatocytes by an apparently single saturable mechanism with K(m) of 6.7 and 2.1 microM, respectively, and taurocholate and digoxin reduced this uptake.

### ATN-161 trifluoroacetate salt - CAS 904763-27-5

**Catalog Number:** 904763-27-5  
**Molecular Weight:** 711.67  
**Molecular Formula:** C25H36F3N9O10S  
**Description:** ATN-161 trifluoroacetate salt is a beta integrin antagonist with antitumor activity. It is a five-amino-acid peptide derived from the synergy region of fibronectin. It inhibited VEGF-induced migration and capillary tube formation in hCECs, but did not inhibit proliferation.

### Cyclo (-RGDFK) - CAS 161552-03-0

**Catalog Number:** 161552-03-0  
**Molecular Weight:** 717.69  
**Molecular Formula:** C29H42F3N9O9  
**Description:** Cyclo (-RGDFK) is a potent and selective avβ3 integrin inhibitor.
**Integrin Antagonists 27 - CAS 593274-97-6**

**Catalog Number:** 593274-97-6  
**Molecular Weight:** 444.44  
**Molecular Formula:** C24H20N4O5  
**Description:** Integrin Antagonists 27, as a novel anticancer agent, is a small molecule integrin αvβ3 antagonist.

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**ILK-IN-1 - CAS 1333146-24-9**

**Catalog Number:** 1333146-24-9  
**Molecular Weight:** 533.59  
**Molecular Formula:** C30H30F3N5O  
**Description:** ILK-IN-1, an ILK inhibitor, has been found to restrain the tumor cell growth through regulating signaling pathways related to oncogenesis and tumor progression. IC50: 0.6 μM.

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**Cilengitide TFA salt - CAS 199807-35-7**

**Catalog Number:** 199807-35-7  
**Molecular Weight:** 702.68  
**Molecular Formula:** C29H41F3N8O9  
**Description:** Cilengitide TFA salt, is a cyclic Arg-Gly-Asp acid pentapeptide that induces anoikis in angiogenic blood vessels and brain tumor, selectively and potently blocks the ligation of the αvβ3 and αvβ5 integrins to provisional matrix proteins such as vitronectin, fibrinectin, fibrinogen, von Willebrand factor, osteopontin, and others.

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**JNJ26076713 - CAS 669076-03-3**

**Catalog Number:** 669076-03-3  
**Molecular Weight:** 490.65  
**Molecular Formula:** C29H38N4O3  
**Description:** JNJ26076713 is an orally active alpha V integrin antagonist. It may be a potential therapeutic candidate for the treatment of age-related macular degeneration, proliferative diabetic retinopathy and macular edema.