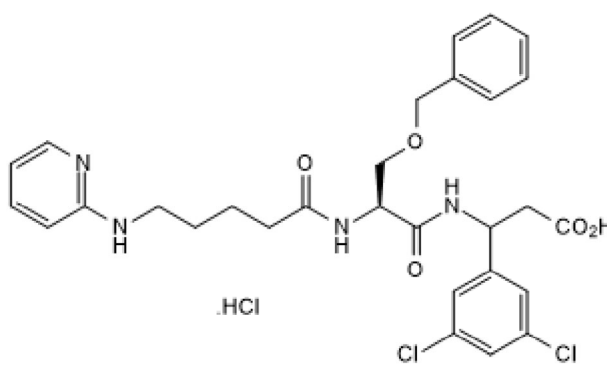


Product Name: EMD 527040 hydrochloride **Catalog No.:** 7508 **Batch No.:** 3
IUPAC Name: N-[1-Oxo-5-(2-pyridinylamino)pentyl]-O-(phenylmethyl)-L-seryl-3-(3,5-dichlorophenyl)-β-alanine hydrochloride

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₂₉H₃₂Cl₂N₄O₅.HCl.¼H₂O
Batch Molecular Weight: 628.46
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 98.8% purity
Chiral HPLC: Shows 98.5% purity
¹H NMR: Consistent with structure
Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen	Chlorine
Theoretical	55.42	5.37	8.92	16.92
Found	54.81	5.44	8.77	16.46

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Product Name: EMD 527040 hydrochloride

Catalog No.: 7508

3

IUPAC Name: N-[1-Oxo-5-(2-pyridinylamino)pentyl]-O-(phenylmethyl)-L-seryl-3-(3,5-dichlorophenyl)-β-alanine hydrochloride

Description:

EMD 527040 hydrochloride is an inhibitor of integrin $\alpha_v\beta_6$. EMD 527040 inhibits binding of $\alpha_v\beta_6$ to fibronectin and attachment of cells expressing $\alpha_v\beta_6$ to fibronectin (IC_{50} values = 6 nM and 1.6 μ M, respectively). EMD 527040 shows antifibrotic effects in an animal model of biliary fibrosis and is active in vivo.

Physical and Chemical Properties:

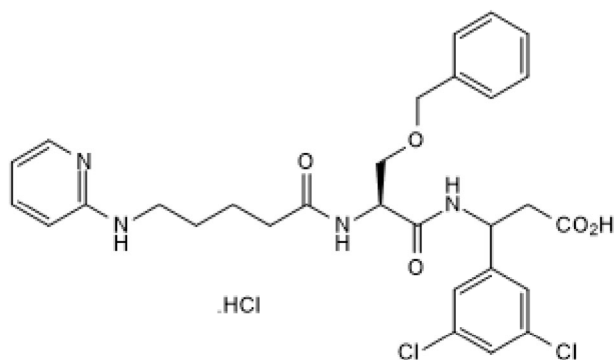
Batch Molecular Formula: $C_{29}H_{32}Cl_2N_4O_5 \cdot HCl \cdot \frac{1}{4}H_2O$

Batch Molecular Weight: 628.46

Physical Appearance: White solid

Minimum Purity: $\geq 98\%$

Batch Molecular Structure:



Storage: Store at $-20^{\circ}C$

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 $45-60^{\circ}C$ water bath).

Information concerning product stability, particularly in solution, has rarely been reported and in most cases we can only offer a general guide. *Unless contradicted by product-specific protocols or instructions, our standard recommendations apply:

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 $-20^{\circ}C$ or below and used within 1 month. Wherever possible solutions should be made up and used on the same day.

References:

Patsenker et al (2008) Inhibition of integrin $\alpha_v\beta_6$ on cholangiocytes blocks transforming growth factor- β activation and retards biliary fibrosis progression. *Gastroenterology* **135** 660. PMID: 18538673.

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