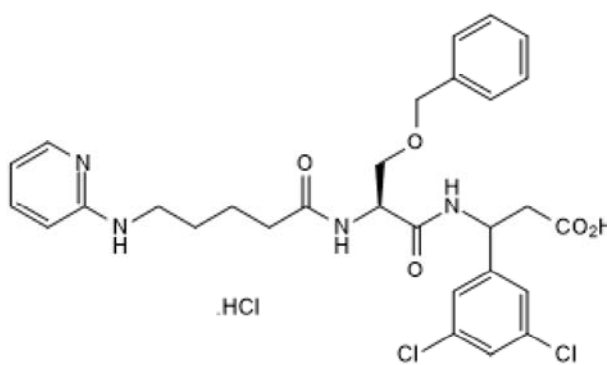


Product Name: EMD 527040 hydrochloride **Catalog No.:** 7508 **Batch No.:** 2
IUPAC Name: N-[1-Oxo-5-(2-pyridinylamino)pentyl]-O-(phenylmethyl)-L-seryl-3-(3,5-dichlorophenyl)-β-alanine hydrochloride

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₂₉H₃₂Cl₂N₄O₅.HCl.½H₂O
Batch Molecular Weight: 632.97
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 99.4% purity
Chiral HPLC: Shows 96.8% purity
¹H NMR: Consistent with structure
Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen	Chlorine
Theoretical	55.03	5.41	8.85	16.8
Found	54.8	5.32	8.79	15.99

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Description:

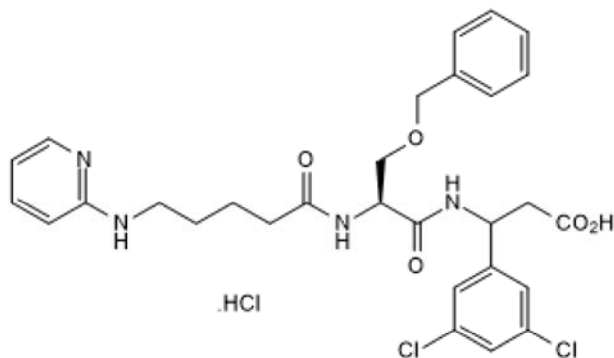
EMD 527040 hydrochloride is an inhibitor of integrin α_vβ₆. EMD 527040 inhibits binding of α_vβ₆ to fibronectin and attachment of cells expressing α_vβ₆ to fibronectin (IC₅₀ values = 6 nM and 1.6 μM, respectively). EMD 527040 shows antifibrotic effects in an animal model of biliary fibrosis and is active in vivo.

Physical and Chemical Properties:

Batch Molecular Formula: C₂₉H₃₂Cl₂N₄O₅·HCl·½H₂O
 Batch Molecular Weight: 632.97
 Physical Appearance: White solid

Minimum Purity: ≥98%

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:

Patsenker et al (2008) Inhibition of integrin α_vβ₆ on cholangiocytes blocks transforming growth factor-β activation and retards biliary fibrosis progression. *Gastroenterology* **135** 660. PMID: 18538673.

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