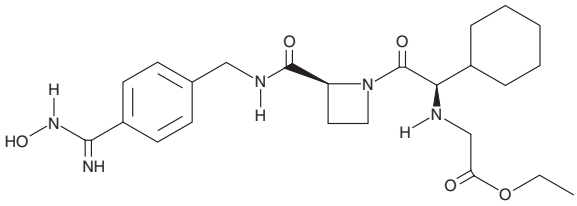
PRODUCT INFORMATION

Ximelagatran

Item No. 16862

CAS Registry No.: 192939-46-1
Formal Name: N-[(1R)-1-cyclohexyl-2-[(2S)-2-[[[[4-[(hydroxyamino)iminomethyl]phenyl]methyl]amino]carbonyl]-1-azetidinyl]-2-oxoethyl]-glycine, ethyl ester
Synonyms: Exanta, H 376/95
MF: $C_{24}H_{35}N_5O_5$
FW: 473.6
Purity: ≥98%
UV/Vis.: λ_{max}: 265 nm
Supplied as: A crystalline solid
Storage: -20°C
Stability: ≥4 years



Information represents the product specifications. Batch specific analytical results are provided on each certificate of analysis.

Laboratory Procedures

Ximelagatran is supplied as a crystalline solid. A stock solution may be made by dissolving the ximelagatran in the solvent of choice, which should be purged with an inert gas. Ximelagatran is soluble in organic solvents such as ethanol, DMSO, and dimethyl formamide (DMF). The solubility of ximelagatran in ethanol and DMF is approximately 1 mg/ml and approximately 5 mg/ml in DMSO.

Ximelagatran is sparingly soluble in aqueous buffers. For maximum solubility in aqueous buffers, ximelagatran should first be dissolved in DMSO and then diluted with the aqueous buffer of choice. Ximelagatran has a solubility of approximately 0.5 mg/ml in a 1:1 solution of DMSO:PBS (pH 7.2) using this method. We do not recommend storing the aqueous solution for more than one day.

Description

Ximelagatran is an ester prodrug of melagatran, a potent, direct, and reversible thrombin inhibitor (K_i = 1.2 nM).[1,2] While melagatran has poor oral bioavailability, ximelagatran displays good bioavailability resulting, in part, from rapid absorption at the gastrointestinal tract, as well as rapid onset of action.[2] Ximelagatran is converted to melagatran by reduction and hydrolysis at the liver and other tissues.[1,2] It is used as an anticoagulant in a variety of situations, including thromboembolic disorders, stroke prevention in atrial fibrillation, and therapy in vein thrombosis.[2,3]

References

1. Clement, B. and Lopian, K. Characterization of in vitro biotransformation of new, orally active, direct thrombin inhibitor ximelagatran, an amidoxime and ester prodrug. *Drug Metab. Dispos.* **31(5)**, 645-651 (2003).
2. Ho, S.J. and Brighton, T.A. Ximelagatran: Direct thrombin inhibitor. *Vasc. Health Risk Manag.* **2(1)**, 49-58 (2006).
3. Ufer, M. Comparative pharmacokinetics of vitamin K antagonists warfarin, phenprocoumon and acenocoumarol. *Clin. Pharmacokinet.* **44(12)**, 1227-1246 (2005).

CAYMAN CHEMICAL
1180 EAST ELLSWORTH RD
ANN ARBOR, MI 48108 · USA
PHONE: [800] 364-9897
[734] 971-3335
FAX: [734] 971-3640
CUSTSERV@CAYMANCHEM.COM
WWW.**CAYMANCHEM**.COM