

Product Data Sheet

Product Name: TCS 2314

Cat. No.: GC18025

Chemical Properties

Cas. No. 317353-73-4

Chemical Name (S,Z)-2-(1-(4-(2-(4-((hydroxy(o-tolylimino)methyl)amino)phenyl)acetyl)morpholine-3-carbonyl)piperidin-4-yl)acetic acid

SMILES CC1=CC=CC=C1/N=C(O)/NC2=CC=C(CC(N3CCOC[C@@]3([H])C(N4CCC(CC(O)=O)CC4)=O)=O)C=C2

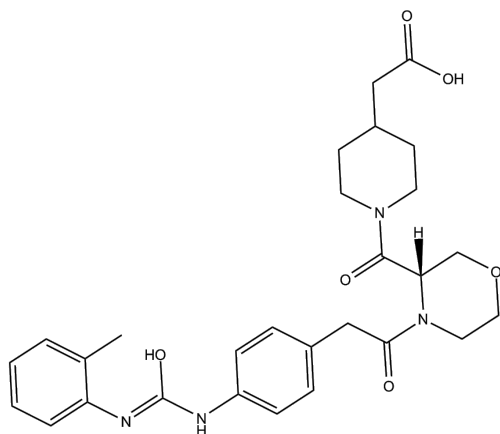
Formula $C_{28}H_{34}N_4O_6$ M.Wt 522.59

Solubility <52.26mg/ml in DMSO; <26.13mg/ml in ethanol Storage Store at RT

General tips For obtaining a higher solubility, please warm the tube at 37 °C and shake it in the ultrasonic bath for a while. Stock solution can be stored below -20°C for several months.

Shipping Condition Evaluation sample solution: ship with blue ice All other available size: ship with RT, or blue ice upon request.

Structure



Background

TCS 2314 (compound 3) is orally active and selective very late antigen-4 (VLA-4, $\alpha 4\beta 1$, CD49d/CD29) antagonist with an IC₅₀ of 4.4 nM[1].

References:

Caution: Product has not been fully validated for medical applications. For research use only.

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[1]. Muro F, et al. Discovery of trans-4-[1-[[2,5-Dichloro-4-(1-methyl-3-indolylcarboxamido)phenyl]acetyl]-(4S)-methoxy-(2S)-pyrrolidinylmethoxy]cyclohexanecarboxylic acid: an orally active, selective very late antigen-4 antagonist. J Med Chem. 2009 Dec 24;52(24):7974-92.

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