Product Data Sheet

Product Name: WAY 170523
Cat. No.: GC13707

Chemical Properties

Cas. No.	307002-73-9		
Chemical Name	N-(2-(4-(N-benzyl-N-(2-(hydroxycarbamoyl)-4,6-dimethylphenyl)sulfamoyl)phenoxy)ethyl)benzofuran-2-carboxamide		
SMILES	O=C(C1=CC2=CC=CC=C2O1)NCCOC3=CC=C(S(=O)(N(C4=C(C)C=C(C)C=C4C(NO)=O)CC5=CC=CC=C5)=O)C=C3		
Formula	$C_{33}H_{31}N_3O_7S$	M.Wt	613.68
Solubility	<61.37mg/ml in DMSO; <61.37mg/ml in ethanol	Storage	Desiccate at RT
General tips	For obtaining a higher solubility , please warm the tube at 37 ℃ and shake it in the ultrasonic bath for a while.Stock solution can be stored below -20℃ 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	WAY 170523		

Background

Description:IC50: 17 nm (MMP-13)
Collagenase 3 is an enzyme that in humans is encoded by the MMP13 gene. Proteins of the matrix metalloproteinase (MMP) family are involved in the breakdown of extracellular matrix in normal physiological processes, such as embryonic development, reproduction, and tissue remodeling, as well as in disease processes, such as arthritis and metastasis .
In vitro: The combination of NMR spectroscopy with molecular modeling techniques and HTS data resulted in the design of a novel, potent, and selective MMP-13 inhibitor (WAY-170523) which has an IC50 of 17 nM for MMP-13 and showed >5800-, 56-, and >500-fold selectivity against MMP-1, MMP-9, and TACE, respectively. To the best of our knowledge, this represents the first example of a potent MMP-13 inhibitor that has been shown to be selective against MMP-9 [1].
In vivo: In order to investigate a putative role of MMP-13 in ISO-dependent cardiac

Tel: (909) 407-4943 Fax: (626) 353-8530 E-mail: tech@glpbio.com
Address: 10292 Central Ave. #205, Montclair, CA, USA

dysfunction, the authors infused WT mice with ISO for 7 days and concurrently delivered the specific MMP-13 inhibitor WAY170523 daily by i.p injection. Remarkably, they found that WAY170523 completely abolished ISO-dependent increase of the left ventricular systolic diameter and preserved cardiac function in ISO-infused animals without modifying the hypertrophic response similar to the PAR1 KO animals. [2].
Clinical trial: WAY-170523 is currently in the preclinical development and no clinical trial is ongoing.

References:

[1] James M. Chen, Frances C. Nelson, Jeremy I. Levin, Dominick Mobilio, Franklin J. Moy, Ramaswamy Nilakantan, Arie Zask, and Robert Powers. Structure-Based Design of a Novel, Potent, and Selective Inhibitor for MMP-13 Utilizing NMR Spectroscopy and Computer-Aided Molecular Design. J. Am. Chem. Soc. 2000, 122, 9648-9654

[2] Jaffré F, Friedman AE, Hu Z, Mackman N, Blaxall BC. β-adrenergic receptor stimulation transactivates protease-activated receptor 1 via matrix metalloproteinase 13 in cardiac cells. Circulation. 2012;125(24):2993-3003.

Tel: (909) 407-4943 Fax: (626) 353-8530 E-mail: tech@glpbio.com
Address: 10292 Central Ave. #205, Montclair, CA, USA