Product Data Sheet

Product Name: 1-Naphthyl 3,5-dinitrobenzoate
Cat. No.: GC13379

Chemical Properties

Cas. No.	93261-39-3		
Chemical Name	1-(3,5-dinitrobenzoate) 1-naphthalenol		
SMILES	O=C(C1=CC([N+]([O-])=O)=CC([N+]([O-])=O)=C1)OC2=CC=CC3=C2C=CC=C3		
Formula	$C_{17}H_{10}N_2O_6$	M.Wt	338.3
Solubility	≤0.1mg/ml in methanol;0.5mg/ml in DMSO	Storage	Store at -20°C
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			

Background

IC50: 1 and 3.6 μM for 5-lipoxygenase and microsomal prostaglandin E synthase-1, respectively

1-Naphthyl 3,5-dinitrobenzoate is a dual 5-lipoxygenase and microsomal prostaglandin E synthase-1 inhibitor.

Human 5-lipoxygenase (5-LOX), a target for antiinflammation drug design, catalyzes the first two reactions in the production of leukotrienes from arachidonic acid (AA): oxygenation of AA to 5-HPETE and further dehydration to leukotriene A4 (LTA4). Then LTA4 is metabolized to other leukotrienes. Furthermore, 5-LOX is also found to play key roles in tumor formation and cancer metastasis and thus is considered as a potential target for anticancer drugs.

In vitro: A previous study built a comparative model for the human 5-LOX closed

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

conformation and successfully used it in virtual screening. Out of around 200 000 compounds, 105 compounds were selected for experimental test. In cell-free assay, 30 compounds were found to have IC50 values less than 100 μM and 11 with IC50 values less than 10 μM. Eventually, 1-Naphthyl 3,5-dinitrobenzoate was screened out to have inhibition activity in the human whole blood assay with IC50 values less than 10 μM. 1-Naphthyl 3,5-dinitrobenzoate was also identified as efficient dualfunctional inhibitors of 5-LOX and mPGES-1 in both cell-free assay and cell-based assay. In addition, 1-Naphthyl 3,5-dinitrobenzoate was able to simultaneously suppress the production of LTB4 and PGE2 in human whole blood, and its targets was verified as 5-LOX and mPGES-1, not LTA4H, COX-1, COX-2 [1].

In vivo: Up to now, there is no animal in vivo data reported.

Clinical trial: So far, no clinical study has been conducted.

Reference:
[1] Wu, Y. ,He, C.,Gao, Y., et al. Dynamic modeling of human 5-lipoxygenase-inhibitor interactions helps to discover novel inhibitors. Journal of Medicinal Chemistry 55, 2597-2605 (2012).

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