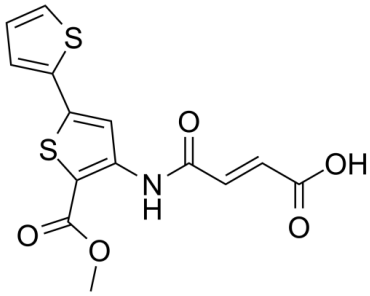
Data Sheet

Product Name:	HTS01037
Cat. No.:	CS-6858
CAS No.:	682741-29-3
Molecular Formula:	C14H11NO5S2
Molecular Weight:	337.37
Target:	FABP
Pathway:	Metabolic Enzyme/Protease
Solubility:	DMSO : ≥ 150 mg/mL (444.62 mM); H2O : < 0.1 mg/mL (insoluble)



BIOLOGICAL ACTIVITY:

HTS01037 is an inhibitor of **fatty acid** binding; and a competitive antagonist of **protein-protein** interactions mediated by AFABP/aP2 with a K_i of 0.67 μM. IC50 & Target: IC50: 0.67 μM (AFABP/aP2)[1] **In Vitro:** HTS01037 functions as a high affinity ligand of AFABP/aP2 with an apparent K_i of 0.67 μM. HTS01037 is somewhat selective for AFABP/aP2, but at higher concentrations is a pan-specific FABP inhibitor. HTS01037 inhibits lipolysis in 3T3-L1 adipocytes and reduces LPS-stimulated inflammation in cultured macrophages. HTS01037 acts as an antagonist of the protein-protein interaction between AFABP/aP2 and hormone sensitive lipase but does not activate PPARγ in macrophage or CV-1 cells[1]. Treatment of microglial cells with HTS01037 increases expression of Ucp2 and arginase in the presence or absence of palmitic acid. Moreover, cells exposed to HTS01037 exhibits attenuated expression of inducible nitric oxide synthase (iNOS) compared to palmitic acid alone indicating reduced NFκB signaling[2]. Treatment of macrophages with HTS01037results in a marked decrease in both basal and fatty acid-stimulated LTC4 secretion but no change in 5-HETE production or 5-lipoxygenase expression[3].

PROTOCOL (Extracted from published papers and Only for reference)

Kinase Assay: [1]To analyze the ligand (HTS01037) binding properties of the FABPs, the fluorescent ligand 1-anilinonapthalene 8-sulfonic acid (1,8-ANS) is utilized. 1,8 ANS is dissolved in absolute ethanol and diluted with 25 mM Tris-HCl (pH 7.4) to a final concentration of 5 μM (final EtOH concentration of 0.05%). Protein is titrated into 500 μL 1,8-ANS and the fluorescence enhancement is measured using a Perkin Elmer 650-10S fluorescence spectrophotometer with 4 nm excitation and emission slit widths. Quantitative analysis of ligand binding is evaluated using non-linear regression using PRISM software[1]. **Cell Assay:** HTS01037 is suspended in DMSO and diluted to 30 μM in DMEM.[2]Cells are pretreated with HTS01037 or vehicle for 3 h and then challenged with or without palmitic acid for 1 h. Cells are then exposed to the ROS Deep Red Dye for 1 h in 5% CO_2 at 37°C. Intracellular superoxide and hydroxyl radicals react with the deep red dye, producing a fluorescent signal which is measured using a spectrophotometer at 650Ex/675Em[2].

References:

[1]. Hertzel AV, et al. Identification and characterization of a small molecule inhibitor of Fatty Acid binding proteins. J Med Chem. 2009 Oct 8;52(19):6024-31.

[2]. Duffy CM, et al. Identification of a fatty acid binding protein4-UCP2 axis regulating microglial mediated neuroinflammation. Mol Cell Neurosci. 2017 Apr;80:52-57.

[3]. Long EK, et al. Fatty acids induce leukotriene C4 synthesis in macrophages in a fatty acid binding protein-dependent manner. Biochim Biophys Acta. 2013 Jul;1831(7):1199-207.

CAIndexNames:

[2,2'-Bithiophene]-5-carboxylic acid, 4-[(3-carboxy-1-oxo-2-propen-1-yl)amino]-, 5-methyl ester

SMILES:

O=C(C1=C(NC(/C=C/C(O)=O)=O)C=C(C2=CC=CS2)S1)OC

Tel: 732-484-9848 Fax: 888-484-5008 E-mail: sales@ChemScene.com

Address: 1 Deer Park Dr, Suite Q, Monmouth Junction, NJ 08852, USA