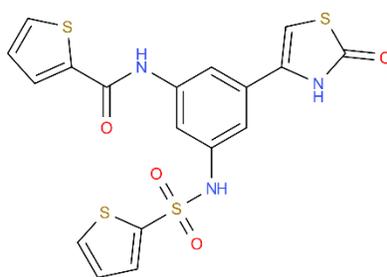


Technical Product Information

EPIGENETICS

Bromodomain Inhibitor

ASIS-P017



AsisChem Inc.
ADVANCING SCIENCE

Product: ASIS-P017

Quantities: 20 mg - 1 g

Custom Batch Orders Produced

Product Properties

Names:	2-thiazolidinone bromodomain inhibitor for BRD3 and BRD4, Compound 40a (Zhao et al. 2013)
SMILES:	<chem>c1(cccs1)C(=O)Nc1cc(cc(c1)NS(=O)(=O)c1cccs1)c1[nH]c(=O)sc1</chem>
Formal name:	N-(3-(2-oxo-2,3-dihydrothiazol-4-yl)-5-(thiophene-2-ulfonamido)phenyl)thiophene-2-carboxamide
MW:	367.42
Formula:	C₁₈H₁₇N₅O₂S
CAS#:	1355554-28-7
Purity:	>95%
Appearance:	White to Yellow Crystalline Powder
Short Term Storage:	Room Temperature (25 °C)
Long Term Storage:	+ 4 °C
Solubility:	Soluble in anhydrous solvents
Handling:	No toxicity known

Biological Description

ASIS-P017, published as Compound 40a (Zhao et al. 2013), is a 2-thiazolidinone bromodomain inhibitor with high affinity for BRD3 and BRD4 (IC₅₀ of 0.23 ± 0.04 μM, ALPHAScreen®) as well as lesser affinity for BRD2, and a short half-life of approximately 5 minutes in liver microsomes (Sharp et al. 2014). Histone modification plays a vital role in epigenetic regulation and is increasingly being studied as a mechanism and potential drug target for a variety of diseases including some carcinomas, leukemia, various inflammatory diseases and HIV. Lysine acetylation of histones is mediated by proteins containing a bromodomain, an approximately 110 amino acid conserved domain. Many of these bromodomain proteins, including BRD3, BRD4, CREBBP, TIF1α, ATAD2, and SMARCA4 are studied for their roles in disease and pathology.

References

Bamborough, P., H. Diallo, J. D. Goodacre, L. Gordon, A. Lewis, J. T. Seal, D. M. Wilson, M. D. Woodrow and C. W. Chung (2012). "Fragment-based discovery of bromodomain inhibitors part 2: optimization of phenylisoxazole sulfonamides." *J Med Chem* 55(2): 587-596. <http://1.usa.gov/1hjKivY>

James, L. I., D. Barysyt-Lovejoy, N. Zhong, L. Krichevsky, V. K. Korboukh, J. M. Herold, C. J. MacNevin, J. L. Norris, C. A. Sagum, W. Tempel, E. Marcon, H. Guo, C. Gao, X. P. Huang, S. Duan, A. Emili, J. F. Greenblatt, D. B. Kireev, J. Jin, W. P. Janzen, P. J. Brown, M. T. Bedford, C. H. Arrowsmith and S. V. Frye (2013). "Discovery of a chemical probe for the L3MBTL3 methyllysine reader domain." *Nat Chem Biol* 9(3): 184-191
<http://www.ncbi.nlm.nih.gov/pubmed/23292653>

James, L. I., V. K. Korboukh, L. Krichevsky, B. M. Baughman, J. M. Herold, J. L. Norris, J. Jin, D. B. Kireev, W. P. Janzen, C. H. Arrowsmith and S. V. Frye (2013). "Small-molecule ligands of methyl-lysine binding proteins: optimization of selectivity for L3MBTL3." *J Med Chem* 56(18): 7358-7371. <http://www.ncbi.nlm.nih.gov/pubmed/24040942>

Sharp, P. P., J.-M. Garnier, D. C. S. Huang and C. J. Burns (2014). "Evaluation of functional groups as acetyl-lysine mimetics for BET bromodomain inhibition." *MedChemComm* 5(12): 1834-1842.
<http://pubs.rsc.org/en/Content/ArticleLanding/2014/MD/C4MD00182F>

Zhao, L., D. Cao, T. Chen, Y. Wang, Z. Miao, Y. Xu, W. Chen, X. Wang, Y. Li, Z. Du, B. Xiong, J. Li, C. Xu, N. Zhang, J. He and J. Shen (2013). "Fragment-based drug discovery of 2-thiazolidinones as inhibitors of the histone reader BRD4 bromodomain." *J Med Chem* 56(10): 3833-3851. <http://1.usa.gov/1FRboX1>

Customer Service:
support@asischem.com

Sales and Custom Synthesis:
Sales@asischem.com

Toll Free: 866-609-8657