

Data Sheet

Product Name: Tirabrutinib (hydrochloride)

Cat. No.: CS-5637

CAS No.: 1439901-97-9 **Molecular Formula:** C25H23CIN6O3

Molecular Weight: 490.94 Target: Btk

Pathway: Protein Tyrosine Kinase/RTK

Solubility: 10 mM in DMSO

BIOLOGICAL ACTIVITY:

Tirabrutinib (ONO-4059) hydrochloride is a selective and novel inhibitor of BTK with IC₅₀ 2.2 nm, Tirabrutinib binds to BTK within B cells, thereby preventing B-cell receptor signaling and impeding B-cell development. IC50 & Target: IC50: 2.2 nM (BTK)^[1].

References:

[1]. Akintunde Akinleye et al. Ibrutinib and novel BTK inhibitors in clinical development. J Hematol Oncol, 2013, 6: 59.

[2]. Harriet S et al. A phase 1 clinical trial of the selective BTK inhibitor ONO/GS-4059 in relapsed and refractory mature B-cell malignancies. Blood 2016, 127:411-419.

CAIndexNames:

8H-Purin-8-one, 6-amino-7,9-dihydro-9-[(3R)-1-(1-oxo-2-butyn-1-yl)-3-pyrrolidinyl]-7-(4-phenoxyphenyl)-, hydrochloride (1:1)

SMILES:

O = C1N(C2 = CC = C(OC3 = CC = C3)C = C2)C4 = C(N)N = CN = C4N1[C@H]5CN(C(C#CC) = O)CC5.[H]CICCO = C4N1[C@H]5CN(C(C#CC) = O)CC5.[H]5CN(C(C#CC) =

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

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

Page 1 of 1 www.ChemScene.com