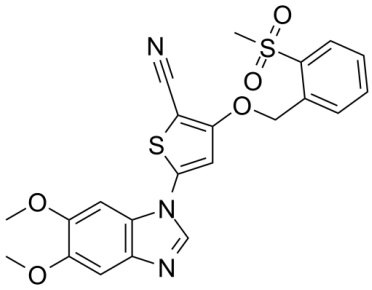
Data Sheet

Product Name:	GSK319347A
Cat. No.:	CS-0047
CAS No.:	862812-98-4
Molecular Formula:	$C_{22}H_{19}N_3O_5S_2$
Molecular Weight:	469.53
Target:	IKK
Pathway:	NF-κB
Solubility:	DMSO : 45 mg/mL (95.84 mM; Need ultrasonic)



BIOLOGICAL ACTIVITY:

GSK319347A is a dual inhibitor of **TBK1** and **IKKε** with **IC_{50}**s of 93 nM and 469 nM, respectively. GSK319347A also inhibits **IKK2** with an **IC_{50}** of 790 nM. IC50 & Target: IC50: 93 nM (TBK1), 469 nM (IKKε)[1]
IC50: 790 nM (IKK2)[2] **In Vitro:** GSK319347A (Compound 1) inhibits TBK1 enzyme with an IC_{50} of 93 nM, which also translates into good cell potency (72 nM). Moreover, IKK-3 Inhibitor exhibits excellent selectivity against cell-cycle kinases CDK2 and AurB[1]. IKK-3 Inhibitor (Compound 13) is a novel IκB kinase 2 (IKK2) inhibitor with an IC_{50} of 790 nM[2].

References:

[1]. Johannes JW, et al. Discovery of 6-aryl-azabenzimidazoles that inhibit the TBK1/IKK-ε kinases. Bioorg Med Chem Lett. 2014 Feb 15;24(4):1138-43.

[2]. Xie HZ, et al. Pharmacophore modeling and hybrid virtual screening for the discovery of novel IκB kinase 2 (IKK2) inhibitors. J Biomol Struct Dyn. 2011 Aug;29(1):165-79.

CAIndexNames:

2-Thiophenecarbonitrile, 5-(5,6-dimethoxy-1H-benzimidazol-1-yl)-3-[[2-(methylsulfonyl)phenyl]methoxy]-

SMILES:

COC1=CC2=C(C=C1OC)N(C3=CC(OCC4=CC=CC=C4S(=O)(C)=O)=C(C#N)S3)C=N2

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

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