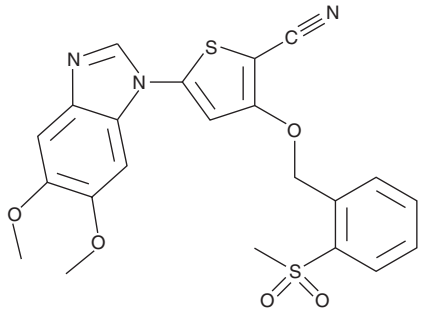
PRODUCT INFORMATION

CAY10576

Item No. 10011249

CAS Registry No.:	862812-98-4
Formal Name:	5-(5,6-dimethoxy-1H-benzimidazol-1-yl)-3-[[2-(methylsulfonyl)phenyl]methoxy]-2-thiophenecarbonitrile
MF:	$C_{22}H_{19}N_3O_5S_2$
FW:	469.5
Purity:	≥95%
UV/Vis.:	λ_{max}: 276, 294 nm
Supplied as:	A crystalline solid
Storage:	-20°C
Stability:	≥4 years



Information represents the product specifications. Batch specific analytical results are provided on each certificate of analysis.

Laboratory Procedures

CAY10576 is supplied as a crystalline solid. A stock solution may be made by dissolving the CAY10576 in the solvent of choice, which should be purged with an inert gas. CAY10576 is soluble in organic solvents such as DMSO and dimethyl formamide. The solubility of CAY10576 in these solvents is approximately 20 and 12.5 mg/ml, respectively.

CAY10576 is sparingly soluble in aqueous buffers. For maximum solubility in aqueous buffers, CAY10576 should first be dissolved in DMSO and then diluted with the aqueous buffer of choice. CAY10576 has a solubility of approximately 0.25 mg/ml in a 1:3 solution of DMSO:PBS (pH 7.2) using this method. We do not recommend storing the aqueous solution for more than one day.

Description

CAY10576 is a multi-kinase inhibitor.[1-3] It inhibits TANK-binding kinase 1 (TBK1), polo-like kinase 1 (Plk1), and IKKβ (IC_{50}s =0.093, 0.63, and 0.79 µM, respectively) and is selective for these kinases over IKKε, Aurora B kinase, and cyclin-dependent kinase 2 (Cdk2; IC_{50}s = 5, >5.32 and >30 µM, respectively).[1-3] CAY10576 also inhibits Rho-associated kinase1 (ROCK1) and ROCK2 (IC_{50}s = 1.8 and 0.04 µM, respectively).[4]

Reference

1. Bamborough, P., Christopher, J.A., Cutler, G.J., *et al.* 5-(1*H*-benzimidazol-1-yl)-3-alkoxy-2-thiophenecarbonitriles as potent, selective, inhibitors of IKK-ε kinase. *Bioorg. Med. Chem. Lett.* **16(24)**, 6236-6240 (2006).
2. Johannes, J.W., Chuaqui, C., Cowen, S., *et al.* Discovery of 6-aryl-azabenzimidazoles that inhibit the TBK1/IKK-ε kinases. *Bioorg. Med. Chem. Lett.* **24(4)**, 1138-1143 (2014).
3. Xie, H.-Z., Liu, L.-Y., Ren, J.-X., *et al.* Pharmacophore modeling and hybrid virtual screening for the discovery of novel IκB kinase 2 (IKK2) inhibitors. *J. Biomol. Struct. Dyn.* **29(1)**, 165-179 (2011).
4. Wang, P., Yang, Y., Shao, Q., *et al.* Selective inhibition of ROCK kinase isoforms to promote neuroregeneration after brain surgery. *Med. Chem. Res.* **25**, 40-50 (2016).

CAYMAN CHEMICAL
1180 EAST ELLSWORTH RD
ANN ARBOR, MI 48108 · USA
PHONE: [800] 364-9897
[734] 971-3335
FAX: [734] 971-3640
CUSTSERV@CAYMANCHEM.COM
WWW.CAYMANCHEM.COM