

PRODUCT INFORMATION

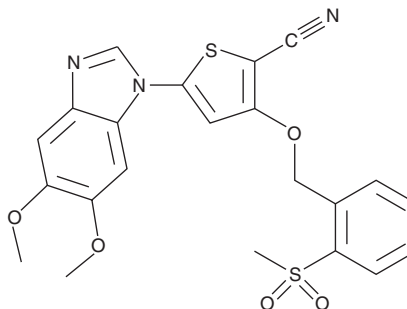


CAY10576

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: C₂₂H₁₉N₃O₅S₂
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 (IC₅₀s = 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; IC₅₀s = 5, >5.32 and >30 μM, respectively).¹⁻³ CAY10576 also inhibits Rho-associated kinase1 (ROCK1) and ROCK2 (IC₅₀s = 1.8 and 0.04 μM, respectively).⁴

Reference

1. Bamborough, P., Christopher, J.A., Cutler, G.J., et al. 5-(1H-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).

WARNING

THIS PRODUCT IS FOR RESEARCH ONLY - NOT FOR HUMAN OR VETERINARY DIAGNOSTIC OR THERAPEUTIC USE.

SAFETY DATA

This material should be considered hazardous until further information becomes available. Do not ingest, inhale, get in eyes, on skin, or on clothing. Wash thoroughly after handling. Before use, the user must review the complete Safety Data Sheet, which has been sent via email to your institution.

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