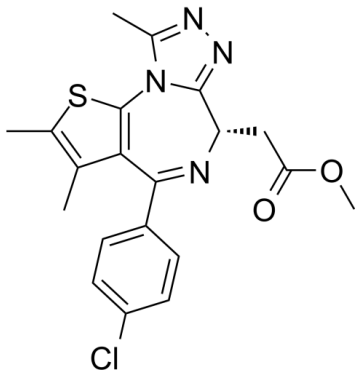
Data Sheet

Product Name:	MS417
Cat. No.:	CS-0034388
CAS No.:	916489-36-6
Molecular Formula:	C20H19ClN4O2S
Molecular Weight:	414.91
Target:	Epigenetic Reader Domain; HIV
Pathway:	Anti-infection; Epigenetics
Solubility:	Ethanol : 50 mg/mL (120.51 mM; Need ultrasonic)



BIOLOGICAL ACTIVITY:

MS417 is a BET-specific **BRD4** inhibitor, binds to BRD4-BD1 and BRD4-BD2 with **IC_{50}**s of 30, 46 nM and **K_d**s of 36.1, 25.4 nM, respectively, with weak selectivity at CBP BRD (**IC_{50}**, 32.7 μM). IC50 & Target: IC50: 30 nM (BRD4-BD1), 46 nM (BRD4-BD2), 32.7 μM (CBP BRD)[1]

Kd: 36.1 nM (BRD4-BD1), 25.4 nM (BRD4-BD2)[1] **In Vitro:** MS417 is a BET-specific BRD4 inhibitor, binds to BRD4-BD1 and BRD4-BD2 with IC_{50}s of 30, 46 nM and K_ds of 36.1, 25.4 nM, respectively, with less selectivity at CBP BrD (IC_{50}, 32.7 μM). MS417 effectively blocks BRD4 binding to NF-κB, almost completely suppresses TNFα-induced NF-κB transcription activation in human embryonic kidney 293T cells at 1 μM and also reduces NF-κB p65 acetylation in the HIV-infected RTECs. MS417 (1 μM) modulation of gene transcription in HIV-infected human primary renal tubular epithelial cells. In addition, MS417 suppresses NF-κB-targeted cytokines and chemokines[1]. **In Vivo:** MS417 (0.08 mg/kg) markedly improves renal function, reduces proteinuria and decreases glomerulosclerosis, tubular injury, and infiltration of inflammatory cells in the kidney of Tg26 mice[1].

References:

[1]. Zhang G, et al. Down-regulation of NF-κB transcriptional activity in HIV-associated kidney disease by BRD4 inhibition. J Biol Chem. 2012 Aug 17;287(34):28840-51.

CAIndexNames:

6H-Thieno[3,2-f][1,2,4]triazolo[4,3-a][1,4]diazepine-6-acetic acid, 4-(4-chlorophenyl)-2,3,9-trimethyl-, methyl ester, (6S)-

SMILES:

O=C(OC)C[C@H]1C2=NN=C(C)N2C3=C(C(C)=C(C)S3)C(C4=CC=C(Cl)C=C4)=N1

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

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