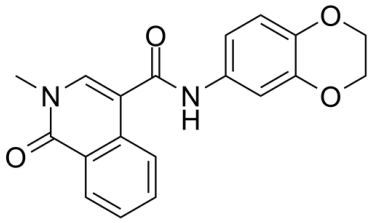
Data Sheet

Product Name:	CeMMEC1
Cat. No.:	CS-0040872
CAS No.:	440662-09-9
Molecular Formula:	C19H16N2O4
Molecular Weight:	336.34
Target:	DNA/RNA Synthesis; Epigenetic Reader Domain
Pathway:	Cell Cycle/DNA Damage; Epigenetics
Solubility:	DMSO : 100 mg/mL (297.32 mM; Need ultrasonic)



BIOLOGICAL ACTIVITY:

CeMMEC1 is an inhibitor of **BRD4**, and also has high affinity for **TAF1**, with an **IC_{50}** of 0.9 μM for TAF1, and a **K_d** of 1.8 μM for TAF1 (2). IC50 & Target: Kd: 1.8 μM (TAF1 (2))[1]

IC50: 0.9 μM (TAF1)[1] **In Vitro:** CeMMEC1 is an inhibitor of BRD4, and also has high affinity for TAF1, with an IC_{50} of 0.9 μM for TAF1, and a K_d of 1.8 μM for TAF1 (2) and slso shows high affinity for the bromodomains of CREBBP, EP300, BRD9. CeMMEC1 (1, 10, 20 μM) decreases the number of THP1 cells in S phase in a dose manner. CeMMEC1 also induces apoptosis. CeMMEC1 in combination with (S)-JQ1 displays potently impaired cell viability than treatment alone[1].

PROTOCOL (Extracted from published papers and Only for reference)

Kinase Assay: [1]**TAF1** binding assays are conducted using the EPIgeneous Binding Domain kit B. Binding is determined by the displacement of an acetylated biotin peptide from a GST-tagged TAF1 protein using HTRF with a Eu^{3+}-conjugated GST antibody donor and streptavidin-conjugated acceptor. Compounds (**CeMMEC1**) are dispensed into assay plates, ProxiPlate-384 Plus using an Echo 525 Liquid Handler. Binding assays are conducted in a final volume of 20 μL with 5 nM TAF1-GST, 50 nM peptide (SGRGK (ac)GGK (ac)GLGK (ac)GGAK (ac)RHRK (biotin)-acid), 6.25 nM Streptavidin-XL665, 1:200 Anti-GST-Eu^{3+} cryptate and 0.1% DMSO. Assay reagents are dispensed into plates using a Multidrop combi and incubated at room temperature for 3 h. Fluorescence is measured using a PHERAstar microplate reader using the HTRF module with dual emission protocol (A = excitation of 320 nm, emmission of 665 nm, and B = excitation of 320 nm, emission of 620 nm). Raw data are processed to give an HTRF ratio (channel A/B × 10,000), which is used to generate IC_{50} curves[1]. **Cell Assay:** [1]Cells are seeded on clear flat-bottom 96-well or 384-well plates and treated with the indicated compounds (**CeMMEC1**) for the specified conditions. Live-cell imaging pictures are taken with the Operetta High Content Screening System, 20× objective and nonconfocal mode[1].

References:

[1]. Sdelci S, et al. Mapping the chemical chromatin reactivation landscape identifies BRD4-TAF1 cross-talk. Nat Chem Biol. 2016 Jul;12(7):504-10.

CAIndexNames:

4-Isoquinolinecarboxamide, N-(2,3-dihydro-1,4-benzodioxin-6-yl)-1,2-dihydro-2-methyl-1-oxo-

SMILES:

O=C(C(C1=C2C=CC=C1)=CN(C)C2=O)NC3=CC=C(OCCO4)C4=C3

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

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