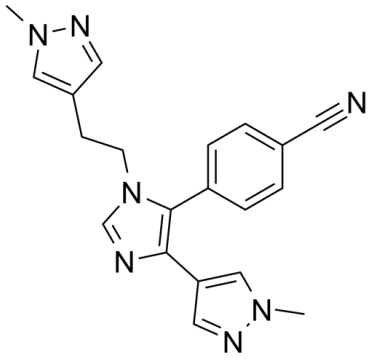
Data Sheet

Product Name:	BAZ2-ICR
Cat. No.:	CS-0015282
CAS No.:	1665195-94-7
Molecular Formula:	$C_{20}H_{19}N_7$
Molecular Weight:	357.41
Target:	Epigenetic Reader Domain
Pathway:	Epigenetics
Solubility:	DMSO : 10 mg/mL (27.98 mM; Need ultrasonic and warming); DMF : 20 mg/mL (55.96 mM; Need ultrasonic and warming)



BIOLOGICAL ACTIVITY:

BAZ2-ICR is a potent, selective, cell active and orally active **BAZ2A/B bromodomains** inhibitor with **IC_{50}**s of 130 nM and 180 nM, and **K_d**s of 109 nM and 170 nM, respectively. BAZ2-ICR shows 10-15-fold selectivity for binding **BAZ2A/B** over CECR2 and >100-fold selectivity over all other bromodomains. BAZ2-ICR is an epigenetic chemical probe[1]. IC50 & Target: IC50: 130 nM (BAZ2A) and 180 nM (BAZ2B); Kd: 109 nM (BAZ2A) and 170 nM (BAZ2A)[1] **In Vitro:** To investigate whether BAZ2-ICR (Compound 13) can displace BAZ2 bromodomains from chromatin in living cells, a fluorescence recovery after photobleaching (FRAP) assay utilizing GFP-tagged BAZ2A full length protein transfected into human osteosarcoma cells (U2OS) are tested. 1 μM BAZ2-ICR reduces the recovery time of the wild-type (wt) construct to a level similar to the dominant negative mutant, confirming that BAZ2-ICR inhibits BAZ2A in cells[1]. **In Vivo:** BAZ2-ICR (Compound 13) shows very high solubility (25 mM in D2O), a measured log D of 1.05, high stability in mouse microsomes, and permeation in the CaCo-2 model and thus a suitable profile for oral and intravenous gavage. BAZ2-ICR (5 mg/kg) shows 70% bioavailability and moderate clearance (□50% of mouse liver blood flow) and volume of distribution [1].

References:

[1]. Drouin L, et al. Structure enabled design of BAZ2-ICR, a chemical probe targeting the bromodomains of BAZ2A and BAZ2B. J Med Chem. 2015 Mar 12;58(5):2553-9.

CAIndexNames:

Benzonitrile, 4-[4-(1-methyl-1H-pyrazol-4-yl)-1-[2-(1-methyl-1H-pyrazol-4-yl)ethyl]-1H-imidazol-5-yl]-

SMILES:

N#CC1=CC=C(C2=C(C3=CN(C)N=C3)N=CN2CCC4=CN(C)N=C4)C=C1

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

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