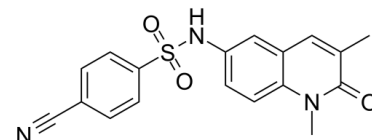


Data Sheet

Product Name:	NI-42
Cat. No.:	CS-0020882
CAS No.:	1884640-99-6
Molecular Formula:	C ₁₈ H ₁₅ N ₃ O ₃ S
Molecular Weight:	353.40
Target:	Epigenetic Reader Domain
Pathway:	Epigenetics
Solubility:	DMSO : 100 mg/mL (282.97 mM; Need ultrasonic)



BIOLOGICAL ACTIVITY:

NI-42 (compound 13-d), a structurally orthogonal chemical probe for the BRPFs, is a biased, potent inhibitor of the **BRD of the BRPFs** (IC₅₀s of BRPF1/2/3=7.9/48/260 nM; K_ds of BRPF1/2/3=40/210/940 nM) with excellent selectivity over nonclass IV BRD proteins^[1]. IC₅₀ & Target: IC₅₀: 7.9/48/260 nM (BRPF1/2/3), 82/310 nM (BRD7/9), 4500 nM (BRD4 (BD1))^[1]
K_d: 40/210/940 nM (BRPF1/2/3), 1130 nM (BRD9)^[1] **In Vitro**: NI-42 shows IC₅₀s of 82, 310, and 4500 nM for BRD7, BRD9, and BRD4 (BD1), respectively, and has a K_d of 1130 nM for BRD9^[1].

References:

[1]. Igoe N, et al. Design of a Biased Potent Small Molecule Inhibitor of the Bromodomain and PHD Finger-Containing (BRPF) Proteins Suitable for Cellular and in Vivo Studies. J Med Chem. 2017 Jan 26;60(2):668-680.

CAIndexNames:

Benzenesulfonamide, 4-cyano-N-(1,2-dihydro-1,3-dimethyl-2-oxo-6-quinolinyl)-

SMILES:

O=S(C1=CC=C(C#N)C=C1)(NC2=CC=C(N(C)C(C)=C3)O)C3=C2)=O

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

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