# CF53

**Cat. No.:** HY-112610

**CAS No.:** 1808160-52-2

**Molecular Formula:** $C_{24}H_{25}N_7O_2$

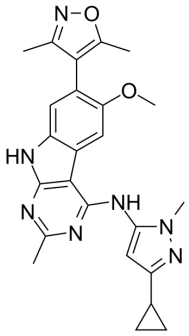
**Molecular Weight:** 443.5

**Target:** Epigenetic Reader Domain; Histone Acetyltransferase

**Pathway:** Epigenetics

**Storage:** -20°C, stored under nitrogen

* In solvent : -80°C, 6 months; -20°C, 1 month (stored under nitrogen)



## SOLVENT & SOLUBILITY

**In Vitro**

DMSO : 110 mg/mL (248.03 mM; Need ultrasonic)

**Preparing Stock Solutions**

| Solvent / Mass / Concentration | 1 mg | 5 mg | 10 mg |
|---|---|---|---|
| 1 mM | 2.2548 mL | 11.2740 mL | 22.5479 mL |
| 5 mM | 0.4510 mL | 2.2548 mL | 4.5096 mL |
| 10 mM | 0.2255 mL | 1.1274 mL | 2.2548 mL |

Please refer to the solubility information to select the appropriate solvent.

**In Vivo**

1. Add each solvent one by one: 10% DMSO >> 40% PEG300 >> 5% Tween-80 >> 45% saline
   Solubility: ≥ 1.83 mg/mL (4.13 mM); Clear solution
2. Add each solvent one by one: 10% DMSO >> 90% corn oil
   Solubility: ≥ 1.83 mg/mL (4.13 mM); Clear solution

## BIOLOGICAL ACTIVITY

**Description**

CF53 is a highly potent, selective and orally active inhibitor of BET protein, with a $K_i$ of <1 nM, $K_d$ of 2.2 nM and an $IC_{50}$ of 2 nM for BRD4 BD1. CF53 binds to both the BD1 and BD2 domains of BRD2, BRD3, BRD4, and BRDT BET proteins with high affinities, very selective over non-BET bromodomain-containing proteins. CF53 shows potent anti-tumor activity both in vitro and in vivo[1].

**$IC_{50}$ & Target**

| | | | |
|---|---|---|---|
| BRD4 (BD1)<br><1 nM (Ki) | BRD4 (BD1)<br>2 nM ($IC_{50}$) | BRD4 (BD1)<br>2.2 nM (Kd) | BRD4 (BD2)<br>0.8 nM (Kd) |
| BRD2 (BD2)<br>0.6 nM (Kd) | BRD2 (BD1)<br>1.1 nM (Kd) | BRD3 (BD2)<br>0.49 nM (Kd) | BRD3 (BD1)<br>0.52 nM (Kd) |
| BRDT (BD2) | BRDT (BD1) | CECR2 | |

| | | | |
|---|---|---|---|
| | 1 nM (Kd) | 2 nM (Kd) | 570 nM (Kd) |
| **In Vitro** | CF53 (Compound 28) binds to both the BD1 and BD2 domains of BRD2, BRD3, BRD4, and BRDT BET proteins with high affinities, $K_d$s are 1.1 nM (BRD2 BD1), 0.6 nM (BRD2 BD2), 0.52 nM (BRD3 BD1), 0.49 nM (BRD3 BD2), 0.8 nM (BRD4 BD2), 2 nM (BRDT BD1), 2.1 nM (BRDT BD2), 47 nM (CREBBP), 570 nM (CECR2), 110 nM (EP300), respectively[1].<br>CF53 exhibits $IC_{50}$s of 7, 85 nM against MOLM-13 acute leukemia and MDA-MB-231 breast cancer cell lines, respectively[1].<br>MCE has not independently confirmed the accuracy of these methods. They are for reference only. | | |
| **In Vivo** | CF53 (25, 50 mg/kg, p.o.) exhibits potent anti-tumor activity both in MDA-MB-231 xenograft tumor model and in RS4;11 model in mice[1].<br>MCE has not independently confirmed the accuracy of these methods. They are for reference only. | | |

## REFERENCES

[1]. Zhao Y, et al. Structure-Based Discovery of CF53 as a Potent and Orally Bioavailable Bromodomain and Extra-Terminal (BET) Bromodomain Inhibitor. J Med Chem. 2018 Jul 26;61(14):6110-6120.



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