# G4/HDAC-IN-1

**Cat. No.:** HY-151263

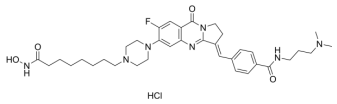
**Molecular Formula:** $C_{36}H_{49}ClFN_7O_4$

**Molecular Weight:** 698.27

**Target:** HDAC; G-quadruplex

**Pathway:** Cell Cycle/DNA Damage; Epigenetics

**Storage:** Please store the product under the recommended conditions in the Certificate of Analysis.



## BIOLOGICAL ACTIVITY

**Description**

G4/HDAC-IN-1 (compound a6) is a G4/HDAC dual-targeting compound. G4/HDAC-IN-1 inhibits intracellular HDAC activity with an $IC_{50}$ value of 1.1 μM, and induces G4 formation. G4/HDAC-IN-1 inhibits TNBC proliferation and tumor growth in TNBC xenograft model. G4/HDAC-IN-1 can be used for the research of cancer[1].

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

| | | | |
|---|---|---|---|
| HDAC8<br>0.03 μM ($IC_{50}$) | HDAC6<br>0.65 μM ($IC_{50}$) | HDAC1<br>1.26 μM ($IC_{50}$) | HDAC11<br>1.38 μM ($IC_{50}$) |
| HDAC4<br>2.64 μM ($IC_{50}$) | | | |

**In Vitro**

G4/HDAC-IN-1 (0-10 μM; 1.5 h) shows HDAC inhibitory activity with an $IC_{50}$ of 1.9 μM by determining nuclear extract and exhibits inhibitory activity on intracellular HDAC activity in MDA-MB-231 cells with an $IC_{50}$ value of 1.1 μM[1].

G4/HDAC-IN-1 (0-50 μM) shows G4 binding activity with an $IC_{50}$ of 0.4 μM[1].

G4/HDAC-IN-1 (0-10 μM; 1.5 h) inhibits HDAC1, HDAC8, HDAC4, HDAC6 and HDAC11 activities with $IC_{50}$s of 1.26, 0.03, 2.64, 0.65 and 1.38 μM, respectively[1].

G4/HDAC-IN-1 (0-50 μM) binds with Pu22, HRAS and HTG21 sequences with $K_D$ values of 1.8, 3.6 and ⊠10 μM, respectively[1].

G4/HDAC-IN-1 (1.25-5.0 μM; 48 h) dose-dependently increases DNA G4 level[1].

G4/HDAC-IN-1 (0-50 μM; overnight) inhibits cytotoxic activities of TNBC cell lines[1].

MCE has not independently confirmed the accuracy of these methods. They are for reference only.

Western Blot Analysis[1]

| | |
|---|---|
| Cell Line: | MDA-MB-231 cell line |
| Concentration: | 1.25, 2.5 and 5.0 μM |
| Incubation Time: | 48 hours |
| Result: | Increased the acetylation levels of HDAC1/2/3/8 substrate acetyl histone H3 (ac-H3), acetyl-histone H4 (ac-H4), and the HDAC6 substrate acetyl-α-tubulin (ac-Tub). |

Cell Cytotoxicity Assay[1]

| | |
|---|---|
| Cell Line: | TNBC cell lines |

| | |
|---|---|
| Concentration: | 0-50 μM |
| Incubation Time: | Overnight |
| Result: | Showed cytotoxic activities to MDA-MB-231, MDA-MB-468, SUM159PT and BT549 with $IC_{50}$s of 4.1, 3.3, 7.4 and 6.5 μM, respectively. |

**In Vivo**

G4/HDAC-IN-1 (2.5 mg/kg; i.p. once daily for 31 days) shows antitumor activity[1].

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| | |
|---|---|
| Animal Model: | Five week-old female BALB/C mice with TNBC xenografts[1] |
| Dosage: | 2.5 mg/kg |
| Administration: | Intraperitoneal injection; 2.5 mg/kg once daily; for 31 days |
| Result: | Showed well tolerance in vivo and exhibited potent antitumor activity. |

## REFERENCES

[1]. Jiang XC, et al. Discovery of a Novel G-Quadruplex and Histone Deacetylase (HDAC) Dual-Targeting Agent for the Treatment of Triple-Negative Breast Cancer. J Med Chem. 2022 Sep 2.



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