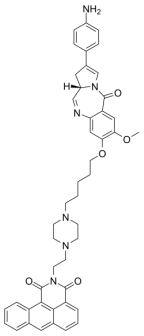
# Anticancer agent 81

| | |
|---|---|
| **Cat. No.:** | HY-151207 |
| **CAS No.:** | 2820286-56-2 |
| **Molecular Formula:** | $C_{46}H_{46}N_6O_5$ |
| **Molecular Weight:** | 762.89 |
| **Target:** | Apoptosis; ADC Cytotoxin |
| **Pathway:** | Apoptosis; Antibody-drug Conjugate/ADC Related |
| **Storage:** | Please store the product under the recommended conditions in the Certificate of Analysis. |



## BIOLOGICAL ACTIVITY

**Description**

Anticancer agent 81 (Compound 37b3) is an anticancer agent and can induce tumor cell cycle arrest and apoptosis. Anticancer agent 81 can be used as a payload to conjugate with Trastuzumab (HY-P9907) to obtain the antibody–agent conjugate (ADC) T-PBA. T-PBA maintained its mode of target and internalization ability of Trastuzumab[1].

**In Vitro**

Anticancer agent 81 (Compound 37b3) (72 h) shows cytotoxicity against SKOV3, MDA-MB-231 and NCI-N87 cells[1].
Anticancer agent 81 (0-5 μM) induces DNA interstrand cross-linking[1].
Anticancer agent 81 (0-3 nM; 24 h) arrests SKOV3 cell cycle at the S-phase[1].
Anticancer agent 81 (0-3 nM; 48 h) induces SKOV3 cell apoptosis[1].
Anticancer agent 81 (25 nM; 12 h) acts on DNA in the nucleus after entering SKOV3 cells and MDA-MB-231 cells[1].
Anticancer agent 81 induces DDR signaling pathways via cross-linking DNA and then activates the caspase cascade and PARP, finally leading to cell cycle arrest and apoptosis[1].
Anticancer agent 81 covalently binds to the DNA sequences and acts on the major groove of DNA[1].
MCE has not independently confirmed the accuracy of these methods. They are for reference only.

Cell Cytotoxicity Assay[1]

| | |
|---|---|
| Cell Line: | SKOV3, MDA-MB-231 and NCI-N87 |
| Concentration: | |
| Incubation Time: | 72 h |
| Result: | Showed cytotoxicity with $IC_{50}$s of 0.17 ± 0.07, 0.90 ± 0.11 and 0.94 ± 0.14 nM against SKOV3, MDA-MB-231 and NCI-N87 cells, respectively. |

Cell Cycle Analysis[1]

| | |
|---|---|
| Cell Line: | SKOV3 |
| Concentration: | 0.33, 1 and 3 nM |
| Incubation Time: | 24 h |
| Result: | Inhibited the cell cycle at the S-phase. |

Apoptosis Analysis[1]

| | |
|---|---|
| Cell Line: | SKOV3 |
| Concentration: | 0.33, 1 and 3 nM |
| Incubation Time: | 48 h |
| Result: | Induced cell apoptosis in a concentration-dependent manner. |

Western Blot Analysis[1]

| | |
|---|---|
| Cell Line: | SKOV3 and NCI-N87 |
| Concentration: | 0.02, 0.1, 0.5, 2.5 and 12.5 nM |
| Incubation Time: | 48 h |
| Result: | Induced the phosphorylation of histone 2AX (γ-H2AX) in a dose-dependent manner. Induced the cleavage of PARP (cPARP) and caspase 3 (cCas3) in a concentration-dependent manner. |

**In Vivo**

T-PBA (1-10 mg/kg; i.v.; every 3 days for 4 times) could significantly delay tumor growth in two Her2-positive xenograft models in mice without obvious toxicity and side effects, and the effect is better than Trastuzumab[1].

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

| | |
|---|---|
| Animal Model: | Female balb/c nude mice, SKOV3 and NCI-N87 tumor model[1] |
| Dosage: | 1, 5 and 10 mg/kg |
| Administration: | Tail vein injection on days 0, 3, 6, and 9 |
| Result: | Inhibited tumor growth in a dose-dependent manner (57.5% inhibition at 1 mg/kg, 70.0% inhibition at 5 mg/kg, and 91.5% inhibition at 10 mg/kg in SKOV3 tumor model; the tumor growth inhibitory rate was 50.2% for 1 mg/kg, 88.0% for 5 mg/kg, and 97.1% for 10 mg/kg in NCI-N87 tumor model) without obvious side effects. |

## REFERENCES

[1]. Lai W, et al. Design, Synthesis, and Bioevaluation of a Novel Hybrid Molecular Pyrrolobenzodiazepine-Anthracenecarboxyimide as a Payload for Antibody-Drug Conjugate. J Med Chem. 2022 Aug 18.



Tel: 609-228-6898 Fax: 609-228-5909 E-mail: tech@MedChemExpress.com

Address: 1 Deer Park Dr, Suite Q, Monmouth Junction, NJ 08852, USA