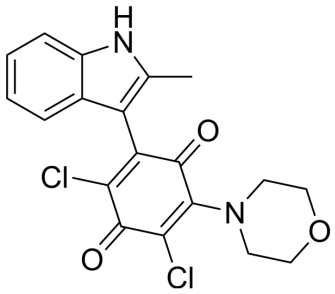
Anticancer agent 42

Cat. No.:	HY-146516
CAS No.:	2687265-18-3
Molecular Formula:	$C_{19}H_{16}Cl_2N_2O_3$
Molecular Weight:	391.25
Target:	MDM-2/p53; Apoptosis; Reactive Oxygen Species
Pathway:	Apoptosis; Immunology/Inflammation; Metabolic Enzyme/Protease; NF-κB
Storage:	Please store the product under the recommended conditions in the Certificate of Analysis.



BIOLOGICAL ACTIVITY

Description	Anticancer agent 42 (compound 10d) is an orally active anticancer agent, and shows a potent antitumor activity against MDA-MB-231 cell with an IC_{50} of 0.07 μM. Anticancer agent 42 can exert its anticancer activity by activating apoptotic pathway and p53 expression. Anticancer agent 42 can be used to study metastatic breast cancer[1].
IC_{50} & Target	IC_{50}: 0.07 μM (Anticancer in MDA-MB-231 cell)[1]

In Vitro

Anticancer agent 42 (compound 10d) (0-20 μM, 4 h) exhibits a potent antitumor activity against MDA-MB-231 cells[1].
Anticancer agent 42 (10 μM, 24 h) induces G2 and S phase arrest in MDA-MB-231 cells[1].
Anticancer agent 42 (10 μM, 24 h) induces cell apoptosis by regulating the expression of apoptosis related proteins in MDA-MB-231 cells[1].
Anticancer agent 42 (0-1 μM) depolarizes mitochondrial membrane and decreases the mitochondrial membrane potential leading to apoptosis[1].
Anticancer agent 42 (0-1 μM, 24 h) induces the cells to produce a large amount of ROS[1].

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

Cell Viability Assay

Cell Line:	A549, MDA-MB-231, HeLa[1]
Concentration:	0-20 μM
Incubation Time:	4 h
Result:	Exhibited a potent activity against MDA-MB-231 with an IC_{50} of 0.07 μM.

Cell Cycle Analysis

Cell Line:	MDA-MB-231 cells[1]
Concentration:	10 μM
Incubation Time:	24 h
Result:	Induced G2 and S phase arrest in MDA-MB-231 cells; caused the percentage of MDA-MB-231 cells in G1 phase to decrease significantly (from 74.44% to 16.48%), cells in G1 phase to increase (from 16.61% to 28.47%), and in G2 phase to significantly increase (from 8.95%

	to 55.05%).

Apoptosis Analysis

Cell Line:	MDA-MB-231 cells[1]
Concentration:	10 μM
Incubation Time:	24 h
Result:	Induced cell apoptosis, with apoptotic rate of 31.69%.

Western Blot Analysis

Cell Line:	MDA-MB-231 cells[1]
Concentration:	100 nM
Incubation Time:	48 h
Result:	Increased the level of human apoptosis-related proteins (pro-caspase 3, catalase, HTRA2/Omi and p53) in MDA-MB-231 cell.

Western Blot Analysis

Cell Line:	MDA-MB-231 cells[1]
Concentration:	0, 0.035, 0.07, 0.14, 0.21 μM
Incubation Time:	24 h
Result:	Increased caspase 9, caspase3, cytochrome C and Bax expression, but decreased Bal-2 expression with increasing concentration.

In Vivo

Anticancer agent 42 (compound 10d) (Kunming mice, 5000 mg/kg, Intragastric administration, once) has extremely low oral toxicity[1].

Anticancer agent 42 (Kunming mice, 238-600 mg/kg, IP, once) shows no obvious liver and kidney damage to mice, with an LD_{50} of 374 mg/kg[1].

Anticancer agent 42 (Kunming mice, 25 mg/kg, IP, once every two days) causes mild liver and kidney damage[1].

Anticancer agent 42 (BALB/c mice, suppresses breast cancer 4T1 tumor growth, the anti-tumor effect is better combined use with CA (Cyanoacrylates), and can cross through the skin to achieve anti-tumor effects.[1].

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

Animal Model:	Kunming mice (n=10, 5 male and 5 female)[1]
Dosage:	5000 mg/kg
Administration:	Intragastric administration, once
Result:	Had extremely low oral toxicity, did not cause death in mice at 5000 mg/kg.

Animal Model:	Kunming mice[1]
Dosage:	600, 476, 378, 300, 238 mg/kg

Administration:	IP, once
Result:	Showed no obvious liver and kidney damage to mice, with an LD_{50} of 374 mg/kg.

Animal Model:	Kunming mice (n=3)[1]
Dosage:	25 mg/kg
Administration:	IP, once every two days
Result:	Caused mild liver and kidney damage after administration, slightly increased ALT, AST and BUN of mice.

Animal Model:	BALB/c mice (4T1 tumor-bearing, female, eight groups, 6 mice per group)[1]
Dosage:	10d (50 mg/kg) + CA; 10d (50 mg/kg) + saline; 10d (200 mg/kg) + CA
Administration:	Intratumoral injection, every four days (50 mg/kg); smear, every two days (200 mg/kg), for 14 days.
Result:	Showed obvious antitumor effect from the 8th day; had protective effects on the spleens of tumor-bearing mice; the anti-tumor effect is better when combined use with CA; can cross through the skin to achieve anti-tumor effects.

REFERENCES

[1]. Jia J, Yin H, Chen C, et al. Design, synthesis, and evaluation of a novel series of mono-indolylbenzoquinones derivatives for the potential treatment of breast cancer. Eur J Med Chem. 2022 Apr 16;237:114375.

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