# ATR-IN-20

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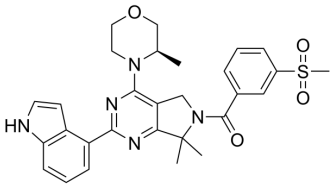
|---|---|
| **Cat. No.:** | HY-151915 |
| **Molecular Formula:** | $C_{29}H_{31}N_5O_4S$ |
| **Molecular Weight:** | 545.65 |
| **Target:** | ATM/ATR; mTOR |
| **Pathway:** | Cell Cycle/DNA Damage; PI3K/Akt/mTOR |
| **Storage:** | Please store the product under the recommended conditions in the Certificate of Analysis. |



## BIOLOGICAL ACTIVITY

**Description**

ATR-IN-20 is a potent ATR (ATM/ATR) inhibitor with an $IC_{50}$ of 3 nM. ATR-IN-20 possess an inhibitory effect on mTOR ($IC_{50}$ of 18 nM) while displaying good selectivity against PI3Kα (100 nM), ATM (100 nM), and DNA-PK (662 nM). ATR-IN-20 exhibits excellent pharmacokinetic profile (F = 30%), and has anticancer effects[1].

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

| ATR | mTOR | ATM | PI3Kα |
|---|---|---|---|
| 3 nM ($IC_{50}$) | 18 nM ($IC_{50}$) | 100 nM ($IC_{50}$) | 100 nM ($IC_{50}$) |

DNA-PK
662 nM ($IC_{50}$)

**In Vitro**

ATR-IN-20 (compound 48f; 0.03-3 μM; 24 hours) significantly inhibits migrating in a concentration-dependent manner in LoVo cells[1].
ATR-IN-20 (compound 48f) displays strong monotherapy efficacy in ATM kinase-deficient tumor cells LoVo, SW620, OVCAR-3 cell lines with IC50 values of 0.040 μM, 0.095 μM, 0.098 μM, respectively[1].
ATR-IN-20 (compound 48f; 0.03-3 μM) decreases the colony-forming ability in a dose-dependent manner in LoVo cells[1].
ATR-IN-20 (compound 48f) shows no significant inhibition against CYP1A2, CYP2C9, and CYP2D6. However, ATR-IN-20 exhibits a weak inhibitory potency against CYP2C19 and CYP3A4 with $IC_{50}$ values of 1 μM[1].
MCE has not independently confirmed the accuracy of these methods. They are for reference only.

Cell Migration Assay [1]

| | |
|---|---|
| Cell Line: | LoVo cells |
| Concentration: | 0.03 μM, 0.1 μM, 0.3 μM, 1 μM, 3 μM |
| Incubation Time: | 24 hours |
| Result: | Significantly inhibited migrating in a concentration-dependent manner. |

**In Vivo**

ATR-IN-20 (compound 48f) shows a favorable pharmacokinetic profile with a bioavailability of 30.0% in SD rats, acceptable plasma protein binding (PPB), high permeability, and low risk of drug-drug interactions[1].
Mean values of pharmacokinetic parameters of ATR-IN-20 (compound 48f) after an i.v. at 1 mg/kg in Sprague-Dawley Rats[1].

| Parameters | ATR-IN-20 (compound 48f) |
|---|---|
| $T_{1/2}$ (h) | 1.32 |
| $MRT_{0-inf}$ (h) | 1.45 |
| $MRT_{0-t}$ (h) | 1.36 |
| $AUC_{0-inf}$ (ng·h·mL$^{-1}$) | 1170 |
| $AUC_{0-t}$ (ng·h·mL$^{-1}$) | 1160 |
| CL (mL·kg$^{-1}$·min$^{-1}$) | 14.2 |
| Vdss (L·kg$^{-1}$) | 1.24 |

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

## REFERENCES

[1]. Yinliang Qi, et al. Discovery of novel 7,7-dimethyl-6,7-dihydro-5H-pyrrolo[3,4-d]pyrimidines as ATR inhibitors based on structure-based drug design. Eur J Med Chem. 2022 Nov 26;246:114945.



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