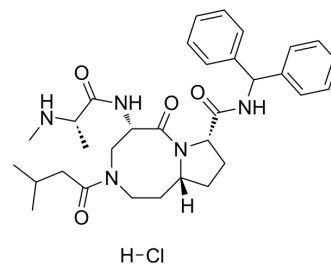


## Xevinapant hydrochloride

<b>Cat. No.:</b>	HY-13208
<b>CAS No.:</b>	1071992-57-8
<b>Molecular Formula:</b>	C <sub>32</sub> H <sub>44</sub> ClN <sub>5</sub> O <sub>4</sub>
<b>Molecular Weight:</b>	598.18
<b>Target:</b>	IAP; Apoptosis
<b>Pathway:</b>	Apoptosis
<b>Storage:</b>	-20°C, sealed storage, away from moisture and light * In solvent : -80°C, 6 months; -20°C, 1 month (sealed storage, away from moisture and light)



### SOLVENT & SOLUBILITY

<b>In Vitro</b>	DMSO : 175 mg/mL (292.55 mM; Need ultrasonic)				
		Solvent Concentration	Mass 1 mg	5 mg	10 mg
	<b>Preparing Stock Solutions</b>	1 mM	1.6717 mL	8.3587 mL	16.7174 mL
		5 mM	0.3343 mL	1.6717 mL	3.3435 mL
10 mM		0.1672 mL	0.8359 mL	1.6717 mL	
Please refer to the solubility information to select the appropriate solvent.					
<b>In Vivo</b>	<ol style="list-style-type: none"> <li>Add each solvent one by one: 10% DMSO &gt;&gt; 40% PEG300 &gt;&gt; 5% Tween-80 &gt;&gt; 45% saline Solubility: ≥ 8.75 mg/mL (14.63 mM); Clear solution</li> <li>Add each solvent one by one: 10% DMSO &gt;&gt; 90% (20% SBE-β-CD in saline) Solubility: ≥ 8.75 mg/mL (14.63 mM); Clear solution</li> <li>Add each solvent one by one: 10% DMSO &gt;&gt; 90% corn oil Solubility: ≥ 8.75 mg/mL (14.63 mM); Clear solution</li> </ol>				

### BIOLOGICAL ACTIVITY

<b>Description</b>	Xevinapant (AT-406) hydrochloride is a potent and orally bioavailable Smac mimetic and an antagonist of the inhibitor of apoptosis proteins (IAPs). Xevinapant hydrochloride binds to XIAP, cIAP1, and cIAP2 proteins with K <sub>i</sub> s of 66.4, 1.9, and 5.1 nM, respectively. Xevinapant hydrochloride effectively antagonizes XIAP BIR3 protein in a cell-free functional assay, induces rapid degradation of cellular cIAP1 protein, and inhibits cancer cell growth in various human cancer cell lines. Xevinapant hydrochloride is highly effective in induction of apoptosis in xenograft tumors <sup>[1][2]</sup> .		
<b>IC<sub>50</sub> &amp; Target</b>	cIAP1 1.9 nM (Ki)	cIAP2 5.1 nM (Ki)	XIAP 66.4 nM (Ki)

<b>In Vitro</b>	<p>Xevinapant (AT-406) hydrochloride potently inhibits cell growth in the MDA-MB-231 breast and SK-OV-3 ovarian cancer cell lines with <math>IC_{50}</math>=144 nM and 142 nM, respectively. Xevinapant (0-3 <math>\mu</math>M; 0-48 hours) hydrochloride effectively induces cell death in a time- and dose-dependent manner<sup>[1]</sup>.</p> <p>MCE has not independently confirmed the accuracy of these methods. They are for reference only.</p>								
<b>In Vivo</b>	<p>Xevinapant (AT-406) hydrochloride is very effective in inhibition of tumor growth in the MDA-MB-231 xenograft model, and has minimal toxicity to animals<sup>[1]</sup>. Xevinapant hydrochloride evaluated for its pharmacokinetic (PK) properties in mice, rats, non-human primates and dogs<sup>[1]</sup>.</p> <p>MCE has not independently confirmed the accuracy of these methods. They are for reference only.</p> <table border="1" data-bbox="347 449 1515 722"> <tr> <td data-bbox="347 449 618 512">Animal Model:</td> <td data-bbox="618 449 1515 512">SCID mice bearing MDA-MB-231 xenograft tumors<sup>[1]</sup></td> </tr> <tr> <td data-bbox="347 512 618 575">Dosage:</td> <td data-bbox="618 512 1515 575">30 and 100 mg/kg</td> </tr> <tr> <td data-bbox="347 575 618 638">Administration:</td> <td data-bbox="618 575 1515 638">p.o.; 5 days a week for 2 weeks</td> </tr> <tr> <td data-bbox="347 638 618 722">Result:</td> <td data-bbox="618 638 1515 722">Strongly inhibits tumor growth at 30 and 100 mg/kg and completely inhibits tumor growth during the treatment with 100 mg/kg.</td> </tr> </table>	Animal Model:	SCID mice bearing MDA-MB-231 xenograft tumors <sup>[1]</sup>	Dosage:	30 and 100 mg/kg	Administration:	p.o.; 5 days a week for 2 weeks	Result:	Strongly inhibits tumor growth at 30 and 100 mg/kg and completely inhibits tumor growth during the treatment with 100 mg/kg.
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## CUSTOMER VALIDATION

- J Med Chem. 2019 Oct 24;62(20):9188-9200.
- Biochim Biophys Acta Mol Basis Dis. 2019 Jun 26;1865(10):2618-2632.
- Viruses. 2021, 13(12), 2490.

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## REFERENCES

- [1]. Cai Q, Sun H, Peng Y, et al. A potent and orally active antagonist (SM-406/AT-406) of multiple inhibitor of apoptosis proteins (IAPs) in clinical development for cancer treatment. J Med Chem. 2011;54(8):2714-2726.
- [2]. Brunckhorst MK, et al. AT-406, an orally active antagonist of multiple inhibitor of apoptosis proteins, inhibits progression of human ovarian cancer. Cancer Biol Ther. 2012;13(9):804-811.

**Caution: Product has not been fully validated for medical applications. For research use only.**

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