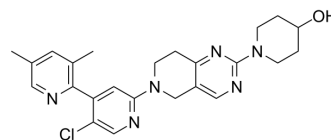


SMO-IN-4

Cat. No.:	HY-153499
CAS No.:	1567963-99-8
Molecular Formula:	C ₂₄ H ₂₇ ClN ₆ O
Molecular Weight:	450.96
Target:	Smo
Pathway:	Stem Cell/Wnt
Storage:	Please store the product under the recommended conditions in the Certificate of Analysis.



BIOLOGICAL ACTIVITY

Description	SMO-IN-4 (Compound 24) is a potent and orally active smoothed antagonist (IC ₅₀ : 24 nM). SMO-IN-4 has antitumor activity [1].																								
In Vitro	SMO-IN-4 (10 μM) shows minimal inhibition of all CYP isoforms, and also has low inhibition on hERG (IC ₅₀ = 38 μM) ^[1] . MCE has not independently confirmed the accuracy of these methods. They are for reference only.																								
In Vivo	<p>SMO-IN-4 (50 mg/kg, daily by oral gavage) leads to regression of subcutaneous tumor in a subcutaneous xenograft model of Ptch1^{+/-} mouse medulloblastoma^[2].</p> <p>PK properties of SMO-IN-4 (compound 24)^[2].</p> <table border="1"> <thead> <tr> <th>Species</th> <th>Dose (mg/kg)</th> <th>AUC_{0-24h} (ng·h/mL)</th> <th>C_{max} (ng/mL)</th> <th>t_{1/2} (h)</th> <th>F%</th> </tr> </thead> <tbody> <tr> <td>Mouse</td> <td>p.o. (10 mg/kg)</td> <td>4183</td> <td>4132</td> <td>1.0</td> <td>49</td> </tr> <tr> <td>Rat</td> <td>p.o. (10 mg/kg)</td> <td>5541</td> <td>2180</td> <td>2.3</td> <td>62</td> </tr> <tr> <td>Dog</td> <td>p.o. (5 mg/kg)</td> <td>7656</td> <td>1300</td> <td>5.4</td> <td>72</td> </tr> </tbody> </table> <p>MCE has not independently confirmed the accuracy of these methods. They are for reference only.</p>	Species	Dose (mg/kg)	AUC _{0-24h} (ng·h/mL)	C _{max} (ng/mL)	t _{1/2} (h)	F%	Mouse	p.o. (10 mg/kg)	4183	4132	1.0	49	Rat	p.o. (10 mg/kg)	5541	2180	2.3	62	Dog	p.o. (5 mg/kg)	7656	1300	5.4	72
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REFERENCES

[1]. Lu W, et al. Design, Synthesis, and Structure-Activity Relationship of Tetrahydropyrido[4,3-d]pyrimidine Derivatives as Potent Smoothed Antagonists with in Vivo Activity. ACS Chem Neurosci. 2017 Sep 20;8(9):1980-1994.

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

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