SMS2-IN-3

Cat. No.: HY-150559

CAS No.: 2414240-89-2

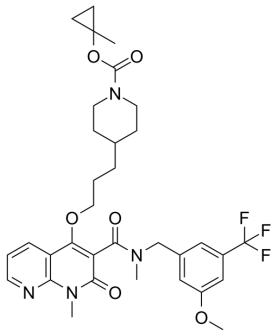
Molecular Formula: $C_{33}H_{39}F_3N_4O_6$

Molecular Weight: 644.68

Target: Others

Pathway: Others

Storage: Please store the product under the recommended conditions in the Certificate of Analysis.



BIOLOGICAL ACTIVITY

Description

SMS2-IN-3 is a potent and selective SMS2inhibitor (IC_{50}=2.2 nM), significantly reduces the hepatic SM (22:0) levels[1].

IC_{50} & Target

IC50: 2.2nM (SMS2)[1]

In Vitro

SMS2-IN-3 (37) is an excellent sphingomyelin synthase 2 inhibitor (SMS2). SMS2-IN-3 (37) has inhibition (IC_{50}= 2.2 nM) and good selectivity against SMS1[1].

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

Cell Viability Assay[1]

Cell Line:	FreeStyle293 cells
Concentration:	100mg/kg
Incubation Time:	60 min
Result:	Showed excellent SMS2 inhibition and good selectivity against SMS1 in biological evaluation.

In Vivo

SMS2-IN-3 (37) has excellent SMS2 activity and high selectivity against SMS1. SMS2-IN-3 also reduces the level of SM by subcutaneous treatment[1].

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

Animal Model:	KK-Ay/Ta mice[1]
Dosage:	100, 200 mg/kg
Administration:	SMS2-IN-3: s.c. (100, 200 mg/kg); p.o. (100, 200 mg/kg); once or twice per day for 7 days.
Result:	

cmpd	C_{max}, (μg/mL)	T_{max}, (h)	$C_{24\,h}$, (μg/mL)	AUC_{0-24}(μg•h/mL)	MRT(h)

37(p.o.)	6.5	0.83	0.007	18	3.0
37(s.c.)	0.70	8.0	0.23	12	9.4

REFERENCES

[1]. Takafumi Yukawa, et al. Discovery of 1,8-naphthyridin-2-one derivative as a potent and selective sphingomyelin synthase 2 inhibitor. Bioorg Med Chem. 2020 Apr 1;28(7):115376.

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