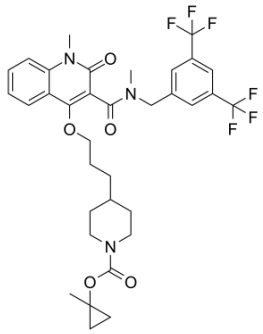
SMS2-IN-1

Cat. No.:	HY-102041
CAS No.:	2098890-15-2
Molecular Formula:	$C_{34}H_{37}F_6N_3O_5$
Molecular Weight:	681.67
Target:	Others
Pathway:	Others
Storage:	Please store the product under the recommended conditions in the Certificate of Analysis.



BIOLOGICAL ACTIVITY

Description	SMS2-IN-1 is a potent and highly selective sphingomyelin synthase 2 (SMS2) inhibitor with an IC_{50} of 6.5 nM and a K_d of 37 nM. SMS2-IN-1 shows 150-fold selectivity for SMS2 over SMS1 (IC_{50} of 1000 nM)[1].
IC_{50} & Target	IC50: 6.5 nM (SMS2), 1000 nM (SMS1)[1] Kd: 37 nM (SMS2)[1]
In Vitro	AS/MS binding experiments are conducted using these SMS2-mutant membrane fractions, SMS2-IN-1 (compound 2) binds to the S217A, H272A, and D276A mutants. S227 and H229 are pivotal amino acid residues for the binding of SMS2-IN-1 to SMS2 [1]. MCE has not independently confirmed the accuracy of these methods. They are for reference only.

REFERENCES

[1]. Adachi R, et al. Discovery and characterization of selective human sphingomyelin synthase 2 inhibitors. Eur J Med Chem. 2017 Aug 18;136:283-293.

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

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