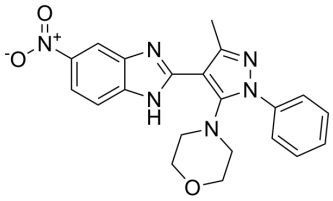
SphK1-IN-3

Cat. No.:	HY-148262
Molecular Formula:	$C_{21}H_{20}N_6O_3$
Molecular Weight:	404.42
Target:	SphK
Pathway:	Immunology/Inflammation
Storage:	Please store the product under the recommended conditions in the Certificate of Analysis.



BIOLOGICAL ACTIVITY

Description	SphK1-IN-3 is an effective sphingosine kinase-1 (SphK1) inhibitor. SphK1-IN-3 inhibits SphK1 kinase activity with an IC_{50} value of 2.48 μM. SphK1-IN-3 can be used for the research of many diseases such as cancer, rheumatoid arthritis, diabetes, asthma, and pulmonary fibrosis[1].
IC_{50} & Target	SphK1 2.48 μM (IC_{50})
In Vitro	SphK1-IN-3 (Compound 47) efficiently inhibits SphK1 kinase activity with an IC_{50} value of 2.48 μM[1]. SphK1-IN-3 (0-31.1 μM) exhibits significant decrease in the fluorescence intensity of SphK1 as well as formed stable protein-ligand complexes[1]. SphK1-IN-3 shows effective inhibitory potential toward SphK1 in enzyme inhibition assay[1]. SphK1-IN-3 (10 μM) demonstrates effective antitumor activity and growth inhibitory potential toward cancer cell lines[1]. SphK1-IN-3 fits well into the ATP-binding site of SphK1 and form significant hydrogen-bonding interactions with catalytically relevant residues as predicted by molecular docking[1]. MCE has not independently confirmed the accuracy of these methods. They are for reference only.

REFERENCES

[1]. Shadia A. Galal, et al. Design and synthesis of new pyrazolylbenzimidazoles as sphingosine kinase-1 inhibitors. Med Chem Res 30, 1614–1634 (2021).

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