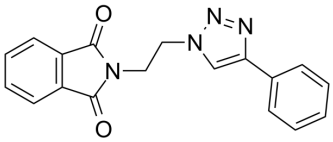
PT4

Cat. No.:	HY-146166
CAS No.:	1280738-47-7
Molecular Formula:	$C_{18}H_{14}N_4O_2$
Molecular Weight:	318.33
Target:	Parasite; Reactive Oxygen Species
Pathway:	Anti-infection; Immunology/Inflammation; Metabolic Enzyme/Protease; NF-κB
Storage:	Please store the product under the recommended conditions in the Certificate of Analysis.



BIOLOGICAL ACTIVITY

Description

PT4 is a therapeutic agent against Cutaneous leishmaniasis (CL). PT4 is effective against both species of Leishmania, with IC_{50}s of 125.18 and 233.18 μM for L. amazonensis and L. braziliensis, respectively. PT4 decreases of mitochondrial membrane potential and increases production of reactive oxygen species, which leads to parasite death. PT4 has a potent in vivo anti-inflammatory activity[1].

In Vitro

PT4 (0-1256.5 μM, 48 hours) can inhibit mammalian cells viability[1].
PT4 (314.1-19.6 μM, 48 hours) inhibits the growth of promastigote and amastigote of L. amazonensis and L. braziliensis promastigotes[1].
PT4 causes depolarization of the mitochondrial membrane of L. amazonensis and L. braziliensis promastigotes and increasing ROS in mitochondria[1].
MCE has not independently confirmed the accuracy of these methods. They are for reference only.

Cell Cytotoxicity Assay[1]

Cell Line:	Balb/c mice peritoneal exudate (mPEC), J774A.1 macrophages, Fibroblasts
Concentration:	0-1256.5 μM
Incubation Time:	48 hours
Result:	Inhibited mPEC, J774A.1 and fibroblasts with CC_{50} value of 981.37 μM, 521.47 μM and 895.17 μM, respectively.

Cell Proliferation Assay[1]

Cell Line:	L. amazonensis, L. braziliensis promastigotes
Concentration:	314.1-19.6 μM
Incubation Time:	48 hours
Result:	Inhibited promastigote of L. amazonensis and L. braziliensis promastigotes with IC_{50} value of 70.46 μM and 181.73 μM, respectively. Inhibited amastigote of them with IC_{50} value of 125.18 μM and 233.18 μM, respectively.

In Vivo

The pharmacokinetic and toxicological parameters of PT4

Parameter	
HBA (≤10)	4
HBD (≤5)	0
LogP (≤5)	2.23
MW (≤500) g/mol	318.33
n-ROTB (≤10)	4
TPSA (A2)	68.09
BBB	Yes
GIA	High
P-GP substrate	No
Skin permeability (cm/s)	-6.85
CYP450 2C9 inhibitor	Yes
CYP450 2D6 inhibitor	No
CYP450 2C19 inhibitor	Yes
CYP450 3A4 inhibitor	No
CYP450 1A2 inhibitor	Yes
Total Clearance (log ml/min/kg)	0.117
Renal OCT2 substrate	No
LD50 (mg/Kg)	4700

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

REFERENCES

[1]. Vanderlan Nogueira Holanda, et al. Antileishmanial activity of 4-phenyl-1-[2-(phthalimido-2-yl)ethyl]-1H-1,2,3-triazole (PT4) derivative on Leishmania amazonensis and Leishmania braziliensis: In silico ADMET, in vitro activity, docking and m

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

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