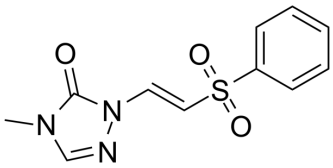
R079

Cat. No.:	HY-163027
CAS No.:	2115659-62-4
Molecular Formula:	$C_{11}H_{11}N_3O_3S$
Molecular Weight:	265.29
Target:	Keap1-Nrf2
Pathway:	NF-κB
Storage:	Please store the product under the recommended conditions in the Certificate of Analysis.



BIOLOGICAL ACTIVITY

Description

R079 (compound 17) is a selective, orally active Nrf2 activator. R079 increases Nrf2 translocation activity (EC_{50} = 32.41 μM). R079 can neutralize excess levels of reactive oxygen species through activating Nrf2. R079 has anti-inflammatory properties and can be used in multiple sclerosis research [1].

In Vitro

R079 (2-10 μM) increases expression of Nrf2 and HO-1 in THP-1 cells[1].
R079 shows microsomal stability, with $t_{1/2}$s of >60 min in mouse, rat, dog, monkey and human microsomes [1].
MCE has not independently confirmed the accuracy of these methods. They are for reference only.

In Vivo

R079 (30-90 mg/kg, p.o., b.i.d for 28 days) demonstrates a robust dose-dependent reduction in disease severity in mouse EAE model[1].

PK Parameters for R079 in Balb/c Mice[1]

Parameter	Balb/c Mice (p.o., 5mg/kg)
clearance (mL/min/kg)	2.01
half-life (h)	1.0
V_{ss} (L/kg)	0.14
oral AUC (ng·h/mL)	22900
oral C_{max} (ng/mL)	19600 (73.96 μM)
bioavailability (%F)	56

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Animal Model:	mouse experimental autoimmune encephalomyelitis (EAE) model[1]

Dosage:	30, 60, and 90 mg/kg
Administration:	Oral gavage (p.o.), b.i.d for 28 days
Result:	Demonstrated a robust dose-dependent reduction in disease severity (41% reduction in clinical score at 30 mg/kg to 89% at 60 mg/kg), p.o. (60, 90 mg/kg) increased levels of Nrf2 for an 8 h period in mouse thymus.

REFERENCES

[1]. Simon J. Shaw, et al. Tuning the Reactivity of Nuclear Factor Erythroid 2 Related Factor 2 (Nrf2) Activators for Optimal in Vivo Efficacy. ACS Medicinal Chemistry Letters . 2023Article ASAP.

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