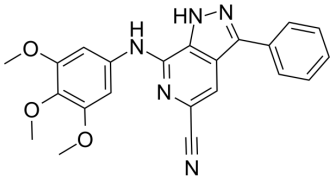
A1/A3 AR antagonist 3

Cat. No.:	HY-153333
CAS No.:	2665804-57-7
Molecular Formula:	$C_{22}H_{19}N_5O_3$
Molecular Weight:	401.42
Target:	Adenosine Receptor
Pathway:	GPCR/G Protein
Storage:	Please store the product under the recommended conditions in the Certificate of Analysis.



BIOLOGICAL ACTIVITY

Description	A1/A3 AR antagonist 3 is an A_1R/A_3R dual antagonist with high affinity at low-micromolar to low-nanomolar. A1/A3 AR antagonist 3 can be used for the research of chronic heart diseases[1].
IC_{50} & Target	pKd: 8.25 (A1R); 7.87 (A3R)[1]. pKi: 8.36 (A1R); 8.01 (A3R)[1].
In Vitro	A1/A3 AR antagonist 3 (A17) has binding affinity for A_1R and A_3R with pK_d values of 8.25 and 7.87, respectively[1]. A1/A3 AR antagonist 3 has binding affinity for A_1R and A_3R with pK_i values of 8.36 and 8.01, respectively[1]. MCE has not independently confirmed the accuracy of these methods. They are for reference only.

REFERENCES

[1]. Stampelou M, et al. Dual A1/A3 Adenosine Receptor Antagonists: Binding Kinetics and Structure-Activity Relationship Studies Using Mutagenesis and Alchemical Binding Free Energy Calculations. J Med Chem. 2022;65(19):13305-13327.

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