

CAI/II-IN-12

Chemical Properties

CAS No. :

Formula:

Molecular Weight:

Storage: Powder: -20°C for 3 years | In solvent: -80°C for 1 year

Actual storage temperature shall be subject to the COA.

Biological Description

Description	CAI/II-IN-12 is a potent dual inhibitor of hCAI (IC ₅₀ = 7.12 μM, K _i = 9.26 μM) and hCAII (IC ₅₀ = 10.62 μM, K _i = 11.72 μM). It exhibits strong affinity for the active sites of CYP17A1, hCAI, and hCAII enzymes. CAI/II-IN-12 demonstrates rapid conformational stabilization, especially in the CYP17A1 complex, and is applicable in prostate cancer treatment and glaucoma research.
Targets(IC ₅₀)	Carbonic Anhydrase
In vitro	CAI/II-IN-12 (Compound 6d) demonstrates selective inhibitory activity against prostate cancer cells (DU145) with reduced toxicity to normal cells (PNT1a) at concentrations between 1-100 μM over 24 hours. When binding to CYP17A1, the compound forms a coordination bond between the carbonyl oxygen of its triazole moiety and the central iron atom in the enzyme's HEM group, indicating substantial potential. Cell Viability Assay was conducted with DU145 and PNT1a cells at concentrations of 1 μM, 10 μM, and 100 μM for 24 hours, showing dose-dependent inhibition of viability in DU145 cells. In PNT1a cells, the IC ₅₀ value was 113.44 μM, and the selectivity index (SI) was 2.28.

Inhibitor · Natural Compounds · Compound Libraries · Recombinant Proteins

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