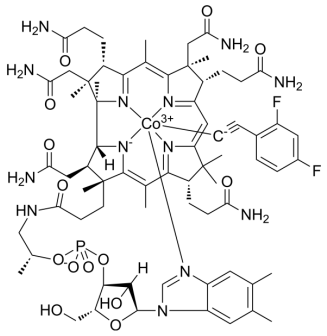
2,4-Difluorophenylethynylcobalamin

Cat. No.:	HY-154992
CAS No.:	2101750-19-8
Molecular Formula:	$C_{70}H_{91}CoF_2N_{13}O_{14}P$
Molecular Weight:	1466.45
Target:	Others
Pathway:	Others
Storage:	4°C, protect from light * In solvent : -80°C, 6 months; -20°C, 1 month (protect from light)



SOLVENT & SOLUBILITY

In Vitro

DMSO : 100 mg/mL (68.19 mM; Need ultrasonic)

Preparing Stock Solutions	Solvent / Mass / Concentration	1 mg	5 mg	10 mg
	1 mM	0.6819 mL	3.4096 mL	6.8192 mL
	5 mM	0.1364 mL	0.6819 mL	1.3638 mL
	10 mM	0.0682 mL	0.3410 mL	0.6819 mL

Please refer to the solubility information to select the appropriate solvent.

BIOLOGICAL ACTIVITY

Description

2,4-Difluorophenylethynylcobalamin is a potential B12 antivitamin via binding to human B12 -processing enzyme CblC with high affinity (KD=130 nm). 2,4-Difluorophenylethynylcobalamin withstood tailoring by CblC, and stabilizes the ternary complex with the cosubstrate glutathione (GSH)[1]. 2,4-Difluorophenylethynylcobalamin is a click chemistry reagent, it contains an Alkyne group and can undergo copper-catalyzed azide-alkyne cycloaddition (CuAAc) with molecules containing Azide groups.

IC_{50} & Target

B12 -processing enzyme CblC[1]

REFERENCES

[1]. Ruetz M, et al. Antivitamin B12 Inhibition of the Human B12 -Processing Enzyme CblC: Crystal Structure of an Inactive Ternary Complex with Glutathione as the Cosubstrate. Angew Chem Int Ed Engl. 2017 Jun 19;56(26):7387-7392.

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

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