Tyrphostin AG 528

Cat. No.: HY-100499 CAS No.: 133550-49-9 Molecular Formula: $C_{18}H_{14}N_{2}O_{3}$ Molecular Weight: 306.32

EGFR Target:

Pathway: JAK/STAT Signaling; Protein Tyrosine Kinase/RTK

Storage: Powder

3 years 4°C 2 years

-80°C In solvent 6 months

-20°C

-20°C 1 month

Product Data Sheet

SOLVENT & SOLUBILITY

In Vitro

DMSO: 25 mg/mL (81.61 mM; Need ultrasonic)

Preparing Stock Solutions	Solvent Mass Concentration	1 mg	5 mg	10 mg
	1 mM	3.2646 mL	16.3228 mL	32.6456 mL
	5 mM	0.6529 mL	3.2646 mL	6.5291 mL
	10 mM	0.3265 mL	1.6323 mL	3.2646 mL

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

In Vivo

- 1. Add each solvent one by one: 10% DMSO >> 40% PEG300 >> 5% Tween-80 >> 45% saline Solubility: ≥ 2.5 mg/mL (8.16 mM); Clear solution
- 2. Add each solvent one by one: 10% DMSO >> 90% (20% SBE-β-CD in saline) Solubility: ≥ 2.5 mg/mL (8.16 mM); Clear solution

BIOLOGICAL ACTIVITY

Description Tyrphostin AG 528 is an inhibitor of EGFR and ErbB2 with IC₅₀s of 4.9 and 2.1 μM, respectively. Tyrphostin AG 528 (Tyrphostin B66) is a protein tyrosine kinase inhibitor, with IC₅₀s of 4.9 μM for epidermal growth factor receptors (EGFR) and 2.1 μM for ErbB2^[1]. Tyrphostin AG 528 is also an anticancer agent^[2].

IC₅₀ & Target **EGFR** ErbB2 $4.9 \, \mu M \, (IC_{50})$ $2.1 \, \mu M \, (IC_{50})$

In Vitro In the present study, the interaction between drug Tyrphostin AG528 and CNT(6,6-6) nanotube by Density Functional Theory (DFT) calculations in solvent water has been investigated for the first time. According to the calculations, intermolecular hydrogen bonds take place between an active position of the molecule Tyrphostin AG528 and hydrogen atoms of the

nanotube which play an important role in the stability of complex CNT(6,6-6)/Tyrphostin AG528. The non-bonded interaction effects of the molecule Tyrphostin AG528 with CNT(6,6-6) nanotube on the electronic properties, chemical shift tensors and natural charge have also been detected. The natural bond orbital (NBO) analysis suggested that the molecule Tyrphostin AG528 as an electron donor and the CNT(6,6-6) nanotube play the role of an electron acceptor at the complex CNT(6,6-6)/Tyrphostin AG528^[2].

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

REFERENCES

[1]. Naijue Zhu, et al. Tyrphostin Tumor Growth Inhibitors of EGFR and ErbB2 Tyrosine Kinase. J Chem Crystallogr. 2007, 37, 679–683.

[2]. Sheikhi M, et al. Investigation of Adsorption Tyrphostin AG528 Anticancer Drug Upon the CNT(6,6-6) Nanotube: A DFT Study. Curr Mol Med. 2019;19(2):91-104.

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

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