Product Data Sheet

Product Name: Tyrphostin AG 528
Cat. No.: GC19364

Chemical Properties

Cas. No.	133550-49-9		
SMILES	O=C(/C(C#N)=C/C1=CC=C(O)C(O)=C1)N2CCC3=CC=CC=C32		
Formula	$C_{18}H_{14}N_2O_3$	M.Wt	306.32
Solubility	DMSO : 25 mg/mL (81.61 mM)	Storage	Store at -20°C
General tips	For obtaining a higher solubility , please warm the tube at 37 °C and shake it in the ultrasonic bath for a while.Stock solution can be stored below -20°C for several months.		
Shipping Condition	Evaluation sample solution : ship with blue ice All other available size: ship with RT , or blue ice upon request.		

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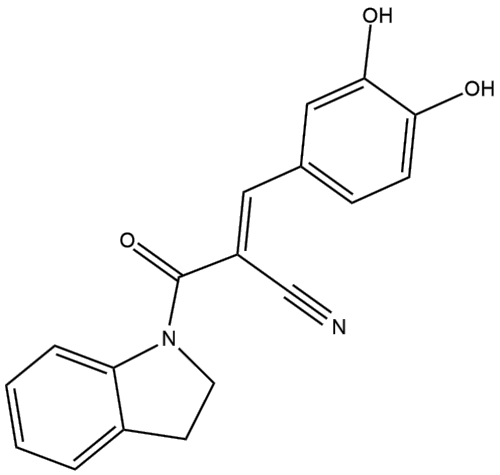
Product Data Sheet

Structure



Background

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].

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].

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.

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