# **Product** Data Sheet

## **IPAG**

Cat. No.: HY-100985 CAS No.: 193527-91-2 Molecular Formula:  $C_{17}H_{22}IN_3$ Molecular Weight: 395.28

Target: Sigma Receptor

Pathway: Neuronal Signaling

Storage: 4°C, protect from light

\* In solvent: -80°C, 6 months; -20°C, 1 month (protect from light)

# **SOLVENT & SOLUBILITY**

In Vitro

DMSO : 8.33 mg/mL (21.07 mM; ultrasonic and adjust pH to 3 with 1M HCl and heat to 60°C)

Preparing Stock Solutions	Solvent Mass Concentration	1 mg	5 mg	10 mg
	1 mM	2.5299 mL	12.6493 mL	25.2985 mL
	5 mM	0.5060 mL	2.5299 mL	5.0597 mL
	10 mM	0.2530 mL	1.2649 mL	2.5299 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: ≥ 0.83 mg/mL (2.10 mM); Suspended solution
- 2. Add each solvent one by one: 10% DMSO >> 90% (20% SBE-β-CD in saline) Solubility: ≥ 0.83 mg/mL (2.10 mM); Clear solution
- 3. Add each solvent one by one: 10% DMSO >> 90% corn oil Solubility: ≥ 0.83 mg/mL (2.10 mM); Clear solution

### **BIOLOGICAL ACTIVITY**

Description

IPAG is a potent sigma-1 receptor antagonist with a  $pK_i$  of 4.3<sup>[1]</sup>. IPAG induces apoptosis<sup>[2]</sup>.

In Vitro

Sigma1 inhibition by IPAG causes the autolysosomal degradation of PD-L1 in PC3 (hormone-insensitive prostate cancer) and MDA-MB-231 (triple-negative breast cancer) cell lines and reduces the levels of functional PD-L1 on the surface of the cells<sup>[2]</sup>. IPAG treatment produces a mean of  $100\pm8~\mu g$  per  $10^6$  cells. IPAG can inhibit cell proliferation. Treatment with IPAG decreases cell mass<sup>[3]</sup>.

IPAG treatment suppresses phosphorylation of translational regulator proteins p70S6K, S6, and 4E-BP1<sup>[3]</sup>. MCE has not independently confirmed the accuracy of these methods. They are for reference only.

Cell Viability Assay<sup>[3]</sup>

Cell Line:	T47D cells		
Concentration:	10 μΜ		
Incubation Time:	24 hours		
Result:	The mean forward scatter height (FSC-H) of DMSO (control) measured 412±5, whereas the mean FSC-H of IPAG treated cells was 390±4.		
Western Blot Analysis <sup>[3]</sup>			
Cell Line:	T47D cells		
Concentration:	10 μΜ		
Incubation Time:			
Result:	Decreased levels of phospho-threonine 389-p70S6Kinase (P-S6K), phospho-serine 235/236-ribosomal S6 (P-S6), and phospho-serine 65-4E-BP1 (P-4E-BP1).		

#### **REFERENCES**

[1]. James M Brimson, et al. Simple ammonium salts acting on sigma-1 receptors yield potential treatments for cancer and depression. Sci Rep. 2020 Jun 8;10(1):9251.

[2]. Halley M Oyer, et al. Small-Molecule Modulators of Sigma1 and Sigma2/TMEM97 in the Context of Cancer: Foundational Concepts and Emerging Themes. Front Pharmacol. 2019 Oct 21;10:1141.

[3]. Felix J Kim, et al. Inhibition of tumor cell growth by Sigma1 ligand mediated translational repression. Biochem Biophys Res Commun. 2012 Sep 21;426(2):177-82.

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

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