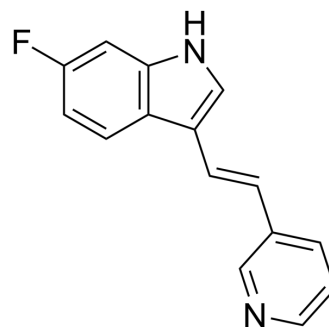


## 680C91

Cat. No.:	HY-108681		
CAS No.:	163239-22-3		
Molecular Formula:	C <sub>15</sub> H <sub>11</sub> FN <sub>2</sub>		
Molecular Weight:	238.26		
Target:	Others		
Pathway:	Others		
Storage:	Powder	-20°C	3 years
		4°C	2 years
	In solvent	-80°C	6 months
		-20°C	1 month



### SOLVENT & SOLUBILITY

#### In Vitro

DMSO : 125 mg/mL (524.64 mM; Need ultrasonic)

Concentration	Solvent	Mass		
		1 mg	5 mg	10 mg
Preparing Stock Solutions	1 mM	4.1971 mL	20.9855 mL	41.9710 mL
	5 mM	0.8394 mL	4.1971 mL	8.3942 mL
	10 mM	0.4197 mL	2.0985 mL	4.1971 mL

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

### BIOLOGICAL ACTIVITY

#### Description

680C91 is an orally active, selective tryptophan 2,3-dioxygenase (TDO) inhibitor with a K<sub>i</sub> of 51 nM. TDO is the key enzyme of tryptophan catabolism. 680C91 can be used for the research of cancer immunotherapy and Alzheimer's Disease<sup>[1][2][3][4]</sup>.

#### In Vitro

680C91 is a potent (K<sub>i</sub>=51 nM) and selective TDO inhibitor with no inhibitory activity against indoleamine 2,3-dioxygenase, monoamine oxidase A and B, 5-HT uptake and 5-HT<sub>1A</sub>,1D,2A and 2C receptors at a concentration of 10 μM<sup>[2]</sup>. 680C91 inhibits the catabolism of tryptophan by rat liver cells and rat liver perfused in situ<sup>[2]</sup>. Tdo2 could regulate cell proliferation and stimulate the expression of decidual marker Dtprp in the uterine stromal cells and decidual cells. Tdo2 inhibitor 680C91 also inhibits the proliferation activity of uterine decidual cells at 24 h<sup>[3]</sup>. Treatment of leiomyoma smooth muscle cell (LSMC) and myometrial smooth muscle cell (MSMC) spheroids with 680C91 (25 and 50 μM) significantly represses the expression of collagen type I (COL1A1) and type III (COL3A1) in a dose-dependent manner<sup>[4]</sup>. MCE has not independently confirmed the accuracy of these methods. They are for reference only. Cell Proliferation Assay<sup>[3]</sup>

Cell Line:	Uterine stromal cells
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	<table border="1"> <tr> <td>Concentration:</td> <td>0.01, 0.05, 0.1, 0.5, 1, 5, and 10 <math>\mu</math>M</td> </tr> <tr> <td>Incubation Time:</td> <td>24 hours</td> </tr> <tr> <td>Result:</td> <td>The proliferation activity of stromal cells was significantly decreased at 5 and 10 <math>\mu</math>M.</td> </tr> </table>	Concentration:	0.01, 0.05, 0.1, 0.5, 1, 5, and 10 $\mu$ M	Incubation Time:	24 hours	Result:	The proliferation activity of stromal cells was significantly decreased at 5 and 10 $\mu$ M.		
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	<p>Western Blot Analysis<sup>[4]</sup></p> <table border="1"> <tr> <td>Cell Line:</td> <td>MSMC and LSMC</td> </tr> <tr> <td>Concentration:</td> <td>25 and 50 <math>\mu</math>M</td> </tr> <tr> <td>Incubation Time:</td> <td>48 hours</td> </tr> <tr> <td>Result:</td> <td>Significantly reduced the expression of COL1A1 and COL3A1 in LSMC spheroids with no significant effect on expression of these proteins in MSMC spheroids.</td> </tr> </table>	Cell Line:	MSMC and LSMC	Concentration:	25 and 50 $\mu$ M	Incubation Time:	48 hours	Result:	Significantly reduced the expression of COL1A1 and COL3A1 in LSMC spheroids with no significant effect on expression of these proteins in MSMC spheroids.
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<b>In Vivo</b>	<p>680C91 (a dose of 15 mg/kg for acute treatment ) elevates tryptophan in brain<sup>[5]</sup>. MCE has not independently confirmed the accuracy of these methods. They are for reference only.</p> <table border="1"> <tr> <td>Animal Model:</td> <td>Male C57Bl6/NCrI mice aged 13-18 weeks<sup>[5]</sup></td> </tr> <tr> <td>Dosage:</td> <td>15 mg/kg</td> </tr> <tr> <td>Administration:</td> <td>Administered per os</td> </tr> <tr> <td>Result:</td> <td>Caused a significant increase in brain tryptophan.</td> </tr> </table>	Animal Model:	Male C57Bl6/NCrI mice aged 13-18 weeks <sup>[5]</sup>	Dosage:	15 mg/kg	Administration:	Administered per os	Result:	Caused a significant increase in brain tryptophan.
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## REFERENCES

- [1]. M Salter, et al. The effects of an inhibitor of tryptophan 2,3-dioxygenase and a combined inhibitor of tryptophan 2,3-dioxygenase and 5-HT reuptake in the rat. *Neuropharmacology*. 1995 Feb;34(2):217-27.
- [2]. M Salter, et al. The effects of a novel and selective inhibitor of tryptophan 2,3-dioxygenase on tryptophan and serotonin metabolism in the rat. *Biochem Pharmacol*. 1995 May 17;49(10):1435-42.
- [3]. Dang-Dang Li, et al. Differential expression and regulation of Tdo2 during mouse decidualization. *J Endocrinol*. 2013 Dec 2;220(1):73-83.
- [4]. Tsai-Der Chuang, et al. Tryptophan catabolism is dysregulated in leiomyomas. *Fertil Steril*. 2021 Oct;116(4):1160-1171.
- [5]. Sophie Imbeault, et al. Effects of IDO1 and TDO2 inhibition on cognitive deficits and anxiety following LPS-induced neuroinflammation. *Acta Neuropsychiatr*. 2020 Feb;32(1):43-53.
- [6]. Li DD, et al. Differential expression and regulation of Tdo2 during mouse decidualization. *J Endocrinol*. 2013 Dec 2;220(1):73-83.

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

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