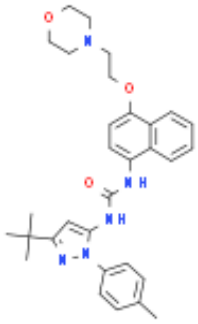
Product Data Sheet

Cas No.:	285983-48-4	Cat. No:	PC11764
Product Name:	BIRB 796 (Doramapimod)		
Product synonym:	1-[2-(4-甲基苯基)-5-叔丁基吡唑-3-基]-3-[4-(2-吗啉-4-基乙氧基)萘-1-基]脲;BIRB 796 (Doramapimod) 抑制剂;达马莫德;达马莫德杂质;多马莫德;肿瘤坏死因子-α(TNF-α)抑制剂;脲,N-[3-(1,1-二甲基乙基)-1-(4-甲基苯基)-1H-吡唑-5-基]-N'-[4-[2-(4-吗啉基)乙氧基]-1-萘基]		
Chemical name:	BIRB 796 (Doramapimod)		
MF:	C31H37N5O3	FW:	527.6572
Purity:	≥98%	Batch No.:	-
Storage:			
Structural formula:			
λmax:	-	Formulation:	-
Solubility :			
SMILES :	O1C([H])([H])C([H])([H])N(C([H])([H])C([H])([H])OC2=C([H])C([H])=C(C3=C([H])C([H])=C([H])C([H])=C23)N([H])C(N([H])C2=C([H])C(C(C([H])([H])[H])(C([H])([H])[H])C([H])([H])[H])=NN2C2C([H])=C([H])C(C([H])([H])[H])=C([H])C=2[H])=O)C([H])([H])C1([H])[H]		
InChI Code:	-		
InChI Key:			
WARNING This product is not for human or veterinary use.			

Product Description

具有细胞通透性的高选择性P38 MAPK抑制剂。Doramapimod 是一种高效的 p38α 抑制剂，IC50 为 4 nM，也抑制 B-Raf 和 Abl，IC50 分别为 83 nM 和 14.6 μM。

生物活性	Doramapimod (BIRB 796) is an orally active, highly potent **p38 MAPK** inhibitor, which has an **IC_{50}** for p38α=38 nM, for p38β=65 nM, for p38γ=200 nM, and for p38δ=520 nM. Doramapimod has picomolar affinity for p38 kinase (**K_d**=0.1 nM). Doramapimod also inhibits **B-Raf** with an **IC_{50}** of 83 nM.
IC50 & Target[1][2]	p38α: 38 nM (IC_{50}); p38β: 65 nM (IC_{50}); p38δ: 520 nM (IC_{50}); p38γ: 200 nM (IC_{50}); B-Raf: 83.4 nM (IC_{50}); Abl: 14600 nM (IC_{50}); p38 MAP kinase: 0.1 nM (Kd)

体外研究(In Vitro)	Doramapimod (BIRB 796) is usually associated with inflammation because of its role in T-cell proliferation and cytokine production. Doramapimod (BIRB 796) blocks the stress-induced phosphorylation of the scaffold protein SAP97, further establishing that this is a physiological substrate of SAPK3/p38γ. The binding of Doramapimod to the p38 MAPKs or JNK1/2 is impairing their phosphorylation by the upstream kinase MKK6 or MKK4. **Medlife has not independently confirmed the accuracy of these methods. They are for reference only.**
体内研究(In Vivo)	The mean xenograft weigh of Doramapimod (BIRB 796) is lighter than control. The inhibition rate of Doramapimod is 1.93%. The Doramapimod (BIRB 796) treatment slightly reduces blood pressure (166±7 mm Hg at week 7; P<0.05), whereas SD rats are normotensive (123±3 mm Hg). Despite the reduction in blood pressure, untreated and Doramapimod-treated dTGRs have similar heart weight and cardiac hypertrophy indices (heart-to-tibia ratio), which are significantly higher compare with nontransgenic SD rats (310±6 versus 307±6 versus 206±5 mg/cm, respectively; P<0.05). **Medlife has not independently confirmed the accuracy of these methods. They are for reference only.**
包装储存	Powder **-20°C** 3 years **4°C** 2 years In solvent **-80°C** 6 months **-20°C** 1 month
溶解度数据	*体外研究:* **DMSO : 125 mg/mL** (**236.89 mM;** Need ultrasonic) **Ethanol : 33.33 mg/mL** (**63.17 mM;** Need ultrasonic)

配制储备溶液	溶剂体积 质量 浓度	1 mg	5 mg	10 mg
	1 mM	1.8952 mL	9.4758 mL	18.9516 mL
	5 mM	0.3790 mL	1.8952 mL	3.7903 mL
	10 mM	0.1895 mL	0.9476 mL	1.8952 mL

* 产品不同，其溶解度不同。建议根据产品选择合适的溶剂配制储备溶液；配成溶液后，**建议分装保存，避免反复冻融造成的产品失效**。

储备液的保存方式和期限： -80°C, 6 months; -20°C, 1 month。-80°C 储存时，建议在 6 个月内使用，-20°C 储存时，建议在 1 个月内使用。

体内研究:

建议根据您的实验动物和给药方式选择适当的溶解方案。以下溶解方案都建议先按照 **体外研究** 方式配制澄清的储备液，再依次添加助溶剂：

——为保证实验结果的可靠性，**澄清的储备液可以根据储存条件，适当保存**；体内实验的工作液，**建议您现用现配，当天使用**； 以下溶剂前显示的百分比是指**该溶剂在您配制终溶液中的体积占比**；如在配制过程中出现沉淀、析出现象，可以通过**加热和/或超声的方式助溶**

1. 建议依照次序添加每种溶剂： 10% DMSO 90% corn oil

Solubility: ≥ 2.5 mg/mL (4.74 mM); Clear solution

此方案可获得 ≥ 2.5 mg/mL (4.74 mM，饱和度未知) 的澄清溶液，此方案不适用于实验周期在半个月以上的实验。

以 1 mL 工作液为例，取 100 μL 25.0 mg/mL 的澄清 DMSO 储备液加到 900 μL玉米油中，混合均匀。

2. 建议依照次序添加每种溶剂： 10% DMSO 40% PEG300 5% Tween-80 45% saline

Solubility: ≥ 2.08 mg/mL (3.94 mM); Clear solution

此方案可获得 ≥ 2.08 mg/mL (3.94 mM，饱和度未知) 的澄清溶液。

以 1 mL 工作液为例，取 100 μL 20.8 mg/mL 的澄清 DMSO 储备液加到 400 μL PEG300 中，混合均匀；向上述体系中加入50 μL Tween-80，混合均匀；然后继续加入 450 μL生理盐水定容至 1 mL。

将 0.9 g 氯化钠，完全溶解于 100 mL ddH?O 中，得到澄清透明的生理盐水溶液

3. 建议依照次序添加每种溶剂： 10% DMSO 90% (20% SBE-β-CD in saline)

Solubility: 2.08 mg/mL (3.94 mM); Suspended solution; Need ultrasonic

此方案可获得 2.08 mg/mL (3.94 mM) 的均匀悬浊液，悬浊液可用于口服和腹腔注射。

以 1 mL 工作液为例，取 100 μL 20.8 mg/mL 的澄清 DMSO 储备液加到 900 μL 20% 的 SBE-β-CD 生理盐水水溶液中，混合均匀。

将 2 g 磺丁基醚 β-环糊精加入 5 mL 生理盐水中，再用生理盐水定容至 10 mL，完全溶解，澄清透明

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