

# Product data sheet



MedKoo Cat#: 562353 Name: TLR2-IN-C29 CAS#: 363600-92-4 Chemical Formula: C <sub>16</sub> H <sub>15</sub> NO <sub>4</sub> Exact Mass: 285.1001 Molecular Weight: 285.29		
Product supplied as:	Powder	
Purity (by HPLC):	≥ 98%	
Shipping conditions:	Ambient temperature	
Storage conditions:	Powder: -20°C 3 years; 4°C 2 years. In solvent: -80°C 3 months; -20°C 2 weeks.	

## 1. Product description:

TLR2-IN-C29 is an inhibitor of TLR2/1 and TLR2/6 signaling. It is induced by synthetic and bacterial TLR2 agonists in human HEK-TLR2 and THP-1 cells, but only TLR2/1 signaling in murine macrophages.

## 2. CoA, QC data, SDS, and handling instruction

SDS and handling instruction, CoA with copies of QC data (NMR, HPLC and MS analytical spectra) can be downloaded from the product web page under “QC And Documents” section. Note: copies of analytical spectra may not be available if the product is being supplied by MedKoo partners. Whether the product was made by MedKoo or provided by its partners, the quality is 100% guaranteed.

## 3. Solubility data

Solvent	Max Conc. mg/mL	Max Conc. mM
DMF	10.0	35.05
DMSO	32.67	114.50
Ethanol	3.25	11.39
PBS (pH 7.2)	0.3	1.05

## 4. Stock solution preparation table:

Concentration / Solvent Volume / Mass	1 mg	5 mg	10 mg
1 mM	3.51 mL	17.53 mL	35.05 mL
5 mM	0.70 mL	3.51 mL	7.01 mL
10 mM	0.35 mL	1.75 mL	3.51 mL
50 mM	0.07 mL	0.35 mL	0.70 mL

## 5. Molarity Calculator, Reconstitution Calculator, Dilution Calculator

Please refer the product web page under section of “Calculator”

## 6. Recommended literature which reported protocols for in vitro and in vivo study

### In vitro study

1. Mistry P, Laird MH, Schwarz RS, Greene S, Dyson T, Snyder GA, Xiao TS, Chauhan J, Fletcher S, Toshchakov VY, MacKerell AD Jr, Vogel SN. Inhibition of TLR2 signaling by small molecule inhibitors targeting a pocket within the TLR2 TIR domain. Proc Natl Acad Sci U S A. 2015 Apr 28;112(17):5455-60. doi: 10.1073/pnas.1422576112. Epub 2015 Apr 13. PMID: 25870276; PMCID: PMC4418912.

### In vivo study

1. Mistry P, Laird MH, Schwarz RS, Greene S, Dyson T, Snyder GA, Xiao TS, Chauhan J, Fletcher S, Toshchakov VY, MacKerell AD Jr, Vogel SN. Inhibition of TLR2 signaling by small molecule inhibitors targeting a pocket within the TLR2 TIR domain. Proc Natl Acad Sci U S A. 2015 Apr 28;112(17):5455-60. doi: 10.1073/pnas.1422576112. Epub 2015 Apr 13. PMID: 25870276; PMCID: PMC4418912.

## 7. Bioactivity

Biological target:

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C29 is a Toll-like receptor 2 (TLR2) inhibitor. C29 blocks hTLR2/1 and hTLR2/6 signaling with IC<sub>50</sub>s of 19.7 and 37.6  $\mu$ M, respectively.

## In vitro activity

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Compound C29 (Fig. 1A) blocked P3C- and P2C-induced IL-8 mRNA dose-dependently in HEK-TLR2 stable transfectants, although it had no effect on TNF- $\alpha$ -induced signaling or on cytotoxicity (Fig. 1B and Fig. S3). C29 also inhibited P3C- and P2C-induced IL-1 $\beta$  gene expression significantly at both 1 h and 4 h following stimulation (Fig. 1C), as well as both P3C- and P2C-induced NF- $\kappa$ B-luciferase activity in transiently transfected HEK293T cells expressing hTLR2 and an NF- $\kappa$ B-sensitive luciferase reporter construct (Fig. S4). Thus, C29 inhibits both TLR2/1 and TLR2/6 signaling in human cell lines.

Reference: Proc Natl Acad Sci U S A. 2015 Apr 28;112(17):5455-60. <https://pubmed.ncbi.nlm.nih.gov/25870276/>

## In vivo activity

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Mice treated twice with C29L before administration of P3C significantly blocked IL-12 p40 and TNF- $\alpha$  liver cytokine mRNA and serum protein (Fig. 4). Importantly, C29L had a significant inhibitory effect at the later time point for IL-12 p40. Collectively, C29L blocks TLR2/1 signaling both in vitro and in vivo.

Reference: Proc Natl Acad Sci U S A. 2015 Apr 28;112(17):5455-60. <https://pubmed.ncbi.nlm.nih.gov/25870276/>

*Note: The information listed here was extracted from literature. MedKoo has not independently retested and confirmed the accuracy of these methods. Customer should use it just for a reference only.*