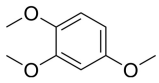
Product Datasheet

Physicochemical Properties

Product Name	1,2,4-Trimethoxybenzene
Cat No.	V111332
Molecular Formula	C9H12O3
Molecular Weight	168.19
CAS #	135-77-3
Appearance	Liquid
Synonyms	trimethyl hydroxyhydroquinone
HS Tariff Code	2934.99.9001
Storage	Powder -20°C 3 years 4°C 2 years In solvent -80°C 6 months -20°C 1 month
Shipping Condition	Room temperature (This product is stable at ambient temperature for a few days during ordinary shipping and time spent in Customs)



Solubility Data

Solubility (In Vitro)	May dissolve in DMSO (in most cases), if not, try other solvents such as H2O, Ethanol, or DMF with a minute amount of products to avoid loss of samples
Solubility (In Vivo)	**Note:** Listed below are some common formulations that may be used to formulate products with low water solubility (e.g. < 1 mg/mL), you may test these formulations using a minute amount of products to avoid loss of samples. **Injection Formulations** **(e.g. IP/IV/IM/SC)** **Injection Formulation 1:** DMSO : Tween 80 Saline = 10 : 5 : 85 (i.e. **100 μL** DMSO stock solution → **50 μL** Tween 80 → **850 μL** Saline) *Preparation of saline: Dissolve 0.9 g of sodium chloride in 100 mL ddH ₂ O to obtain a clear solution. **Injection Formulation 2:** DMSO : PEG300 Tween 80 : Saline = 10 : 40 : 5 : 45 (i.e. **100 μL** DMSO → **400 μL**PEG300 → **50 μL** Tween 80 → **450 μL** Saline) **Injection Formulation 3:** DMSO : Corn oil = 10 : 90 (i.e. **100 μL** DMSO → **900 μL** Corn oil) Example: Take the **Injection Formulation 3** (DMSO : Corn oil = 10 : 90) as an example, if **1 mL** of 2.5 mg/mL working solution is to be prepared, you can take **100 μL 25 mg/mL DMSO stock solution** and add to **900 μL corn oil**, mix well to obtain a clear or suspension solution (2.5 mg/mL, ready for use in animals). ▶ View More **Oral Formulations** **Oral Formulation 1:** Suspend in 0.5% CMC Na (carboxymethylcellulose sodium) **Oral Formulation 2:** Suspend in 0.5% Carboxymethyl cellulose Example: Take the **Oral Formulation 1** (Suspend in 0.5% CMC Na) as an example, if **100 mL** of 2.5 mg/mL working solution is to be prepared, you can first prepare 0.5% CMC Na solution by measuring **0.5 g CMC Na** and dissolve it in **100 mL ddH2O** to obtain a clear solution; then add 250 mg of the product to 100 mL 0.5% CMC Na solution, to make the suspension solution (2.5 mg/mL, ready for use in animals).

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Preparing Stock Solutions	Solvent Volume / Mass / Concentration	1 mg	5 mg	10 mg
	1 mM	5.9457 mL	29.7283 mL	59.4566 mL
	5 mM	1.1891 mL	5.9457 mL	11.8913 mL
	10 mM	0.5946 mL	2.9728 mL	5.9457 mL

*Note: Please select an appropriate solvent for the preparation of stock solution based on your experiment needs. For most products, DMSO can be used for preparing stock solutions (e.g. 5 mM, 10 mM, or 20 mM concentration); some products with high aqueous solubility may be dissolved in water directly. Solubility information is available at the above Solubility Data section. Once the stock solution is prepared, aliquot it to routine usage volumes and store at -20°C or -80°C. Avoid repeated freeze and thaw cycles.

Biological Activity I Assay Protocols (From Reference)

In Vitro	1,2,4-Trimethoxybenzene (0.5–1 mM, 1.5 h) significantly inhibited the activation of the NLRP3 inflammasome in Nigericin and Lipopolysaccharides (LPS)-induced immortalized mouse bone marrow-derived macrophages (iBMDM), manifested as caspase-1 (Casp-1) lysis and decreased IL-1β secretion [1]. 1,2,4-Trimethoxybenzene (1 mM, 75–90 min) inhibited LPS and ATP-induced activation of NLRP3 in iBMDM, primary microglia, and primary macrophages [1]. 1,2,4-Trimethoxybenzene (45 min–2 h) did not inhibit the activation of the AIM2 inflammasome in primary peritoneal macrophages and lbmdm induced by LPS and poly(dA:dT) [1]. 1,2,4-Trimethoxybenzene (1 hour) reduced the formation of ASC spots in LPS and Nigericin-induced iBMDM and primary microglia: immunofluorescence showed a significant reduction in the number of ASC spots; DSS crosslinking assays showed an increase in soluble ASC and a decrease in insoluble ASC [1]. 1,2,4-Trimethoxybenzene (1 hour) blocked the protein-protein interaction between NLRP3 and ASC in LPS-induced iBMDM [1]. 1,2,4-Trimethoxybenzene (1 hour) inhibited LPS and Nigericin-induced NLRP3 oligomerization in iBMDM and primary macrophages: DSS crosslinking assays showed a reduction in the formation of NLRP3 monomers, dimers and higher oligomers [1].
In vivo	1,2,4-Trimethoxybenzene (200 mg/kg, face, once daily for 17 days) significantly alleviated clinical symptoms, weight loss and demyelinating pathology in the EAE model [1]. 1,2,4-Trimethoxybenzene (50-100 mg/kg, face, once daily for 3 days) enhanced daily extinction of fear in the model by traction on NLRP3 neurosomes and relieved subsequent PTSD. 1,2,4-Trimethoxybenzene (50-200 mg/kg, lateral wall, once daily for 8 weeks) improved related cognitive dysfunction by inhibiting the activation of NLRP3 pathway neurosomes and regulating the damaged microbiota in type 2 diabetes [3].
Cell Assay	Western Blot Analysis[1] **Cell Types:** Immortalized murine bone marrow-derived macrophages (iBMDMs) **Tested Concentrations:** 0.5 mM, 1 mM **Incubation Duration:** 1.5 h **Experimental Results:** Caspase-1 (Casp-1) cleavage and IL-1β secretion are reduced.
	Animal/Disease Models: Female C57BL/6 mice (6-8 weeks old) were subcutaneously injected with 150 μg of MOG35-55 peptide, and intraperitoneally injected with 200 ng of pertussis toxin on the day of immunization (day 0) and day 2, to simulate EAE[1]. **Doses:** 200 mg/kg **Route of Administration:** P.o., once daily for 17 days **Experimental Results:** The incidence of end-stage renal disease (ESRD) decreased, and clinical symptoms were significantly alleviated. Significantly reduced weight loss indicates a reduction in systemic inflammatory response. The area of myelin basic protein (MBP)

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	reduction in systemic inflammatory response. The area of myelin basic protein (MBP) positive in spinal cord sections was significantly larger than in the control group, indicating a reduced degree of demyelination. The percentage of demyelinated area was significantly lower than in the control group, confirming the protection of myelin structure. ASC specks were significantly reduced in spinal cord sections, suggesting that NLRP3 inflammasome activation was inhibited. The expression of NLRP3, ASC, and cleaved caspase-1 proteins was downregulated in spinal cord tissue. The mRNA expression of pro-inflammatory cytokines IFN-γ and IL-17a and the chemokine CCL-5 was decreased in the spinal cord, while the expression of the anti-inflammatory cytokine IL-4 was upregulated.
Animal Protocol	**Animal/Disease Models:** Male C57BL/6 mice (8 weeks old) were intraperitoneally injected with lipopolysaccharide (LPS, 2 mg/kg/d) for 3 consecutive days to induce depressive-like behavior[2]. **Doses:** 50 mg/kg, 100 mg/kg **Route of Administration:** P.o., once daily for 3 days **Experimental Results:** Sucrose preference was significantly increased (with improved depressive-like behavior), and immobility time in the tail suspension test (TST) and forced swimming test (FST) was significantly reduced. Activation of the hippocampal NLRP3 inflammasome was inhibited (e.g., reduced expression of cleaved IL-1β, cleaved caspase-1, and ASC spot formation). **Animal/Disease Models:** Male Sprague-Dawley rats (8 weeks old, 200 g) were first given a high-sugar, high-fat diet for 5 weeks, and then type 2 diabetes (T2DM) was induced by intraperitoneal injection of streptozotocin (STZ, 30 mg/kg)[3]. **Doses:** 50 mg/kg, 100 mg/kg, 200 mg/kg **Route of Administration:** P.o., once daily for 8 weeks **Experimental Results:** Significant improvements were observed in blood glucose levels (FBG, OGTT-AUC), insulin resistance index (HOMA-IR), and blood lipids (TC, TG, LDL-C) in rats, along with a decrease in oxidative stress markers (MDA). Shortened escape latency and increased target quadrant time indicate enhanced learning and memory abilities. Improved neuronal structure was observed in the hippocampal CA1 region, with ELISA detecting elevated BDNF levels and decreased AChE levels in the hippocampus. Inhibition of the hippocampal NLRP3 inflammasome pathway (e.g., reduced expression of NLRP3, ASC, caspase-1, GSDMD, and IL-1β).
References	[1]. https://pubmed.ncbi.nlm.nih.gov/33627802/ [2]. https://pubmed.ncbi.nlm.nih.gov/40031427/ [3]. https://pubmed.ncbi.nlm.nih.gov/41067284/

These protocols are for reference only. InvivoChem does not independently validate these methods.