

PRODUCT INFORMATION



COX Inhibitor Pack

Item No. 10186

Laboratory Procedures

For long term storage, we suggest that COX Inhibitor Pack be stored as supplied at -20°C. It should be stable for at least one year.

The Cayman COX Inhibitor Pack contains a combination of frequently used cyclooxygenase (COX) inhibitors. Each kit contains aspirin, the archetype nonselective, irreversible COX inhibitor.¹ A series of COX-2 selective inhibitors are available in the COX Inhibitor Pack, including NS-398, one of the first reported and most widely used.² Another COX-2-selective inhibitor included is CAY10404, with nearly 500,000-fold COX-2 selectivity.³

The potent COX-1-selective inhibitor SC-560 is an example of a reversible, diaryl heterocycle COX-1 inhibitor with low nM activity.⁴ Also included is valeroyl salicylate, an irreversible alkylator of COX enzymes with some selectivity toward COX-1.⁵ *trans*-Resveratrol is also included in the COX Inhibitor Pack due to its complex activities, which include COX inhibition, peroxidase inhibition, antioxidant activity, and gene regulation.^{6,7}

Component	Amount	Solubility
CAY10404	5 mg	>0.5 mg/ml in DMF:PBS (pH 7.2) (1:1)
Aspirin	50 mg	>2.7 mg/ml in PBS (pH 7.2)
APHS	5 mg	N/A
SC-560	5 mg	>1.2 mg/ml in DMF:PBS (pH 7.2) (1:1)
NS-398	5 mg	>0.4 mg/ml in DMSO:PBS (pH 7.2) (1:3)
SC-58125	5 mg	>0.25 mg/ml in DMF:PBS (pH 7.2) (1:3)
Valeroyl Salicylate	50 mg	>6 mg/ml in PBS (pH 7.2)
<i>trans</i> -Resveratrol	10 mg	>0.1 mg/ml in PBS (pH 7.2)
Valdecoxib	5 mg	>0.5 mg/ml in DMSO:PBS (pH 7.2) (1:8)
Licofelone	5 mg	>0.5 mg/ml in DMSO:PBS (pH 7.2) (1:8)

References

1. Vane, J.R. and Botting, R. Inflammation and the mechanism of action of anti-inflammatory drugs. *FASEB J.* **1**, 89-96 (1987).
2. Futaki, N., Takahashi, S., Yokoyama, M., *et al.* NS-398, A new anti-inflammatory agent, selectively inhibits prostaglandin G/H synthase/cyclooxygenase (COX-2) activity *in vitro*. *Prostaglandins* **47**, 55-59 (1994).
3. Habeeb, A.G., Rao, P.N.P., and Knaus, E.E. Design and syntheses of diarylisoxazoles: Novel inhibitors of cyclooxygenase-2 (COX-2) with analgesic-antiinflammatory activity. *Drug Dev. Res.* **51(4)**, 273-286 (2000).
4. Smith, C.J., Zhang, Y., Koboldt, C.M., *et al.* Pharmacological analysis of cyclooxygenase-1 in inflammation. *Proc. Natl. Acad. Sci. USA* **95**, 13313-13318 (1998).
5. Bhattacharyya, D.K., Lecomte, M., Dunn, J., *et al.* Selective inhibition of prostaglandin endoperoxide synthase-1 (cyclooxygenase-1) by valeryl salicylic acid. *Arch. Biochem. Biophys.* **317**, 19-24 (1995).
6. Johnson, J.L. and Maddipati, K.R. Paradoxical effects of resveratrol on the two prostaglandin H synthases. *Prostaglandins and Other Lipid Mediators* **56**, 131-143 (1998).
7. Jang, M., Cai, L., Udeani, G.O., *et al.* Cancer chemopreventive activity of resveratrol, a natural product derived from grapes. *Science* **275**, 218-220 (1997).

WARNING

THIS PRODUCT IS FOR RESEARCH ONLY - NOT FOR HUMAN OR VETERINARY DIAGNOSTIC OR THERAPEUTIC USE.

SAFETY DATA

This material should be considered hazardous until further information becomes available. Do not ingest, inhale, get in eyes, on skin, or on clothing. Wash thoroughly after handling. Before use, the user must review the complete Safety Data Sheet, which has been sent via email to your institution.

WARRANTY AND LIMITATION OF REMEDY

Buyer agrees to purchase the material subject to Cayman's Terms and Conditions. Complete Terms and Conditions including Warranty and Limitation of Liability information can be found on our website.

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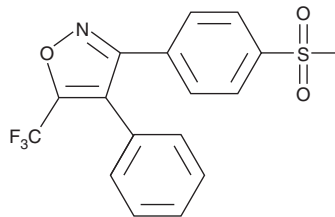
PRODUCT INFORMATION



CAY10404

Item No. 70210

CAS Registry No.: 340267-36-9
Formal Name: 3-[4-(methylsulfonyl)phenyl]-4-phenyl-5-(trifluoromethyl)-isoxazole
MF: C₁₇H₁₂F₃NO₃S
FW: 367.4
Purity: ≥98%
UV/Vis.: λ_{max}: 239 nm
Supplied as: A crystalline solid
Storage: -20°C
Stability: ≥2 years



Information represents the product specifications. Batch specific analytical results are provided on each certificate of analysis.

Laboratory Procedures

CAY10404 is supplied as a crystalline solid. A stock solution may be made by dissolving the CAY10404 in the solvent of choice, which should be purged with an inert gas. CAY10404 is soluble in organic solvents such as ethanol, DMSO, and dimethyl formamide (DMF). The solubility of CAY10404 in DMF is approximately 21 mg/ml and approximately 17 mg/ml in ethanol and DMSO.

CAY10404 is sparingly soluble in aqueous buffers. For maximum solubility in aqueous buffers, CAY10404 should first be dissolved in DMF and then diluted with the aqueous buffer of choice. CAY10404 has a solubility of approximately 0.5 mg/ml in a 1:1 solution of DMF:PBS (pH 7.2) using this method. We do not recommend storing the aqueous solution for more than one day.

Description

CAY10404 is an inhibitor of COX-2 (IC₅₀ = <1 nM).¹ It is selective for COX-2 over COX-1 (IC₅₀ = >500 μM). CAY10404 inhibits the proliferation of SH-EP and SH-SY5Y neuroblastoma cells (IC₅₀s = ~60 μM for both), and induces apoptosis and cell cycle arrest at the G₂/M phase in the same cells.² It inhibits carrageenan-induced paw edema in rats when administered at a dose of 10 mg/kg.¹

References

1. Habeeb, A.G., Rao, P.N.P., and Knaus, E.E. Design and syntheses of diarylisoxazoles: Novel inhibitors of cyclooxygenase-2 (COX-2) with analgesic-antiinflammatory activity. *Drug Dev. Res.* **51(4)**, 273-286 (2000).
2. Parashar, B., Shankar, S.L., O'Guin, K., *et al.* Inhibition of human neuroblastoma cell growth by CAY10404, a highly selective Cox-2 inhibitor. *J. Neurooncol.* **71(2)**, 141-148 (2005).

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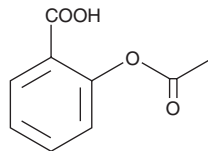
PRODUCT INFORMATION



Aspirin

Item No. 70260

CAS Registry No.: 50-78-2
Formal Name: 2-(acetyloxy)-benzoic acid
Synonym: Acetylsalicylic Acid
MF: C₉H₈O₄
FW: 180.2
Purity: ≥99%
UV/Vis.: λ_{max}: 226, 275 nm
Supplied as: A crystalline solid
Storage: Room temperature
Stability: ≥2 years



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Laboratory Procedures

Aspirin is supplied as a crystalline solid. A stock solution may be made by dissolving the aspirin in the solvent of choice. Aspirin is soluble in organic solvents such as ethanol, DMSO, and dimethyl formamide, which should be purged with an inert gas. The solubility of aspirin in these solvents is approximately 80, 41, and 30 mg/ml, respectively.

Further dilutions of the stock solution into aqueous buffers or isotonic saline should be made prior to performing biological experiments. Ensure that the residual amount of organic solvent is insignificant, since organic solvents may have physiological effects at low concentrations. Organic solvent-free aqueous solutions of aspirin can be prepared by directly dissolving the crystalline solid in aqueous buffers. The solubility of aspirin in PBS, pH 7.2, is approximately 2.7 mg/ml. Avoid adding aspirin to basic solutions (pH > 7.4), since base treatment will hydrolyze aspirin to salicylic acid. Store aqueous solutions of aspirin on ice and use within 30 minutes of preparation.

Description

Aspirin is a non-selective, irreversible COX inhibitor. The IC₅₀ values for ovine COX-1 and -2 are 0.75 and 1.25 mM, respectively.¹ Aspirin acetylates COX-1 at Ser⁵³⁰ and COX-2 at Ser⁵¹⁶ resulting in irreversible enzyme inhibition.

Reference

1. Johnson, J.L., Wimsatt, J., Buckel, S.D., *et al.* Purification and characterization of prostaglandin H synthase-2 from sheep placental cotyledons. *Arch. Biochem. Biophys.* **324**, 26-34 (1995).

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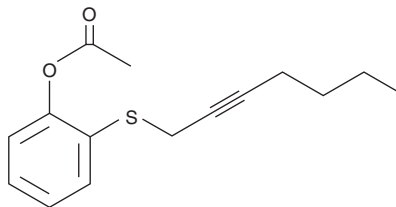
PRODUCT INFORMATION



APHS

Item No. 70330

CAS Registry No.: 209125-28-0
Formal Name: 2-(2-heptynylthio)-phenol acetate
MF: C₁₅H₁₈O₂S
FW: 262.4
Purity: ≥98%
UV/Vis.: λ_{max}: 249 nm
Supplied as: A solution in methyl acetate
Storage: -20°C
Stability: ≥1 year



Information represents the product specifications. Batch specific analytical results are provided on each certificate of analysis.

Laboratory Procedures

APHS is supplied as a solution in methyl acetate. To change the solvent, simply evaporate the methyl acetate under a gentle stream of nitrogen and immediately add the solvent of choice. Solvents such as ethanol, DMSO, and dimethyl formamide purged with an inert gas can be used. The solubility of APHS in these solvents is approximately 12.5, 11.1, and 14.3 mg/ml, respectively.

Further dilutions of the stock solution into aqueous buffers or isotonic saline should be made prior to performing biological experiments. Ensure that the residual amount of organic solvent is insignificant, since organic solvents may have physiological effects at low concentrations. If an organic solvent-free solution of APHS is needed, it can be prepared by evaporating the methyl acetate and directly dissolving the neat oil in aqueous buffers. The solubility of APHS in PBS, pH 7.2, is approximately 0.02 mg/ml. We do not recommend storing the aqueous solution for more than one day.

Description

APHS is an O-acetyl, S-alkyl ether of 2-thio phenol and a selective, irreversible inhibitor of COX-2. APHS is a potent inhibitor of both COX-1 and COX-2, with IC₅₀ values of 17 and 0.8 μM for human recombinant COX-1 and COX-2, respectively.¹ APHS exhibits 20-fold selectivity toward the inhibition of COX-2, yet it is still more potent than aspirin in the inhibition of COX-1. APHS acetylates COX-1 at Ser⁵³⁰ and COX-2 at Ser⁵¹⁶ resulting in irreversible enzyme inhibition.¹

Reference

1. Kalgutkar, A.S., Crews, B.C., Rowlinson, S.W., *et al.* Aspirin-like molecules that covalently inactivate cyclooxygenase-2. *Science* **280**, 1268-1270 (1998).

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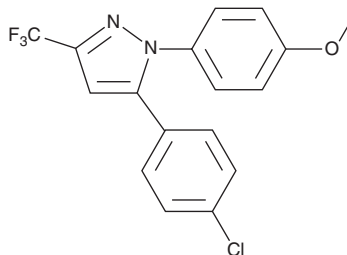
PRODUCT INFORMATION



SC-560

Item No. 70340

CAS Registry No.: 188817-13-2
Formal Name: 5-(4-chlorophenyl)-1-(4-methoxyphenyl)-3-(trifluoromethyl)-1H-pyrazole
MF: C₁₇H₁₂ClF₃N₂O
FW: 352.7
Purity: ≥98%
UV/Vis.: λ_{max}: 232, 251 nm
Supplied as: A crystalline solid
Storage: -20°C
Stability: ≥2 years



Information represents the product specifications. Batch specific analytical results are provided on each certificate of analysis.

Laboratory Procedures

SC-560 is supplied as a crystalline solid. A stock solution may be made by dissolving the SC-560 in the solvent of choice. SC-560 is soluble in organic solvents such as ethanol, DMSO, and dimethyl formamide (DMF), which should be purged with an inert gas. The solubility of SC-560 in these solvents is approximately 22, 24, and 150 mg/ml, respectively.

SC-560 is sparingly soluble in aqueous buffers. For maximum solubility in aqueous buffers, SC-560 should first be dissolved in DMF and then diluted with the aqueous buffer of choice. SC-560 has a solubility of approximately 1.2 mg/ml in a 1:1 solution of DMF:PBS (pH 7.2) using this method. We do not recommend storing the aqueous solution for more than one day.

Description

SC-560 is a member of the diaryl heterocycle class of cyclooxygenase (COX) inhibitors which includes celecoxib (Celebrex™) and rofecoxib (Vioxx™). However, unlike these selective COX-2 inhibitors, SC-560 is a selective inhibitor of COX-1. Using human recombinant enzymes, the IC₅₀ value for SC-560 with respect to COX-1 is 9 nM, while the corresponding IC₅₀ value for COX-2 is 6.3 μM.¹ Thus, SC-560 shows 700-fold selectivity for the COX-1 enzyme. SC-560 is orally active in the rat, where 10 mg/kg completely abolishes the ionophore-induced production of thromboxane B₂ in whole blood. However, SC-560 is ineffective in the treatment of inflammation in models, such as the LPS-induced rat air-pouch model, in which COX-2-generated prostaglandins play a significant role in the inflammatory process.² In whole cells, however, SC-560 appears to act as a non-selective COX inhibitor.³ The mechanism of the selective versus non-selective effects of SC-560 in a cell-free environment compared whole cells has not been elucidated.

References

1. Smith, C.J., Zhang, Y., Koboldt, C.M., *et al.* Pharmacological analysis of cyclooxygenase-1 in inflammation. *Proc. Natl. Acad. Sci. USA* **95**, 13313-13318 (1998).
2. Masferrer, J.L., Zweifel, B.S., Manning, P.T., *et al.* Selective inhibition of inducible cyclooxygenase 2 *in vivo* is antiinflammatory and nonulcerogenic. *Proc. Natl. Acad. Sci. USA* **91**, 3228-3232 (1994).
3. Brenneis, C., Maier, T.J., Schmidt, R., *et al.* Inhibition of prostaglandin E₂ synthesis by SC-560 is independent of cyclooxygenase 1 inhibition. *FASEB J.* **20**, 1352-1360 (2006).

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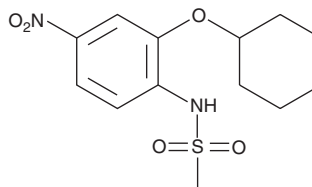
PRODUCT INFORMATION



NS-398

Item No. 70590

CAS Registry No.: 123653-11-2
Formal Name: N-[2-(cyclohexyloxy)-4-nitrophenyl]-methanesulfonamide
MF: C₁₃H₁₈N₂O₅S
FW: 314.4
Purity: ≥98%
UV/Vis.: λ_{max}: 238, 296, 337 nm
Supplied as: A crystalline solid
Storage: Room temperature
Stability: ≥2 years



Information represents the product specifications. Batch specific analytical results are provided on each certificate of analysis.

Laboratory Procedures

NS-398 is supplied as a crystalline solid. A stock solution may be made by dissolving the NS-398 in the solvent of choice. NS-398 is soluble in organic solvents such as ethanol, DMSO, and dimethyl formamide, which should be purged with an inert gas. The solubility of NS-398 in these solvents is approximately 0.5, 25, and 30 mg/ml, respectively.

NS-398 is sparingly soluble in aqueous buffers. For maximum solubility in aqueous buffers, NS-398 should first be dissolved in DMSO and then diluted with the aqueous buffer of choice. NS-398 has a solubility of approximately 0.4 mg/ml in a 1:3 solution of DMSO:PBS (pH 7.2) using this method. We do not recommend storing the aqueous solution for more than one day.

Description

NS-398 is a selective inhibitor of cyclooxygenase-2 (COX-2). The IC₅₀ values for human recombinant COX-1 and -2 are 75 and 1.77 μM, respectively.¹ The IC₅₀ values for ovine COX-1 and -2 are 220 and 0.15 μM, respectively.²

References

1. Barnett, J., Chow, J., Ives, D., *et al.* Purification, characterization and selective inhibition of human prostaglandin G/H synthase 1 and 2 expressed in the baculovirus system. *Biochim. Biophys. Acta* **1209**, 130-139 (1994).
2. Johnson, J.L., Wimsatt, J., Buckel, S.D., *et al.* Purification and characterization of prostaglandin H synthase-2 from sheep placental cotyledons. *Arch. Biochem. Biophys.* **324**, 26-34 (1995).

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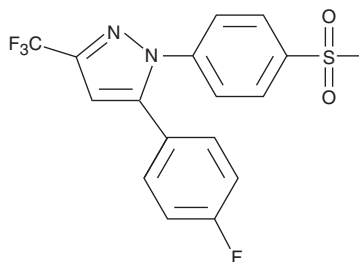
PRODUCT INFORMATION



SC-58125

Item No. 70655

CAS Registry No.: 162054-19-5
Formal Name: 5-(4-fluorophenyl)-1-[4-(methylsulfonyl)phenyl]-3-(trifluoromethyl)-1H-pyrazole
MF: C₁₇H₁₂N₂SO₂F₄
FW: 384.3
Purity: ≥98%
UV/Vis.: λ_{max}: 255 nm
Supplied as: A crystalline solid
Storage: -20°C
Stability: ≥1 year



Information represents the product specifications. Batch specific analytical results are provided on each certificate of analysis.

Laboratory Procedures

SC-58125 is supplied as a crystalline solid. A stock solution may be made by dissolving the SC-58125 in the solvent of choice. SC-58125 is soluble in organic solvents such as ethanol, DMSO, and dimethyl formamide (DMF), which should be purged with an inert gas. The solubility of SC-58125 in ethanol and DMSO is approximately 10 mg/ml and approximately 30 mg/ml in DMF.

SC-58125 is sparingly soluble in aqueous buffers. For maximum solubility in aqueous buffers, SC-58125 should first be dissolved in DMF and then diluted with the aqueous buffer of choice. SC-58125 has a solubility of approximately 0.25 mg/ml in a 1:3 solution of DMF:PBS (pH 7.2) using this method. We do not recommend storing the aqueous solution for more than one day.

Description

SC-58125 is a member of the diaryl heterocycle group of selective COX-2 inhibitors which includes MK 966 (rofecoxib), DUP-697, and celecoxib. SC-58125 is a potent and time-dependent inhibitor of COX-2.¹ When tested on the isolated recombinant enzymes, SC-58125 is at least 150 times more potent in the inhibition of COX-2 as COX-1.² In cultured HUVEC cells, SC-58125 inhibits COX-2 with an IC₅₀ value of 70 nM.³ It also inhibits the growth of the COX-2 expressing cell line HCA-7 in nude mice at 5-10 mg/kg when given intraperitoneally.⁴

References

1. Seibert, K., Zhang, Y., Leahy, K., *et al.* Pharmacological and biochemical demonstration of the role of cyclooxygenase 2 in inflammation and pain. *Proc. Natl. Acad. Sci. USA* **91**, 12013-12017 (1994).
2. Anderson, G.D., Hauser, S.D., McGarity, K.L., *et al.* Selective inhibition of cyclooxygenase (COX)-2 reverses inflammation and expression of COX-2 and interleukin 6 in rat adjuvant arthritis. *J. Clin. Invest.* **97**, 2672-2679 (1996).
3. Miralpeix, M., Camacho, M., López-Belmonte, J., *et al.* Selective induction of cyclo-oxygenase-2 activity in the permanent human endothelial cell line HUV-EC-C: Biochemical and pharmacological characterization. *Br. J. Pharmacol.* **121**, 171-180 (1997).
4. Sheng, H., Shao, J., Kirkland, S.C., *et al.* Inhibition of human colon cancer cell growth by selective inhibition of cyclooxygenase-2. *J. Clin. Invest.* **99**, 2254-2259 (1997).

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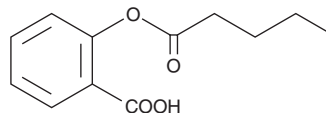
PRODUCT INFORMATION



Valeroyl Salicylate

Item No. 70670

CAS Registry No.: 64206-54-8
Formal Name: 2-[(1-oxopentyl)oxy]-benzoic acid
Synonym: 2-Valeryloxybenzoic Acid
MF: C₁₂H₁₄O₄
FW: 222.2
Purity: ≥99%
Supplied as: A crystalline solid
Storage: Room temperature
Stability: ≥2 years



Information represents the product specifications. Batch specific analytical results are provided on each certificate of analysis.

Laboratory Procedures

Valeroyl salicylate is supplied as a crystalline solid. A stock solution may be made by dissolving the valeroyl salicylate in the solvent of choice. Valeroyl salicylate is soluble in organic solvents such as ethanol, DMSO, and dimethyl formamide, which should be purged with an inert gas. The solubility of valeroyl salicylate in these solvents is approximately 95, 43, and 70 mg/ml, respectively.

Further dilutions of the stock solution into aqueous buffers or isotonic saline should be made prior to performing biological experiments. Ensure that the residual amount of organic solvent is insignificant, since organic solvents may have physiological effects at low concentrations. Organic solvent-free aqueous solutions of valeroyl salicylate can be prepared by directly dissolving the crystalline solid in aqueous buffers. The solubility of valeroyl salicylate in PBS, pH 7.2, is approximately 6 mg/ml. We do not recommend storing the aqueous solution for more than one day.

Description

Valeroyl salicylate is a selective, irreversible inhibitor of COX-1. The IC₅₀ values for ovine COX-1 and -2 are 0.8 mM and 15 mM, respectively.¹ The half-lives for inactivation of human recombinant and ovine COX-1 in the presence of 500 μM valeroyl salicylate are 12 and 45 minutes, respectively.^{1,2}

References

1. Johnson, J.L., Wimsatt, J., Buckel, S.D., *et al.* Purification and characterization of prostaglandin H synthase-2 from sheep placental cotyledons. *Arch. Biochem. Biophys.* **324**, 26-34 (1995).
2. Bhattacharyya, D.K., Lecomte, M., Dunn, J., *et al.* Selective inhibition of prostaglandin endoperoxide synthase-1 (cyclooxygenase-1) by valerylsalicylic acid. *Arch. Biochem. Biophys.* **317**, 19-24 (1995).

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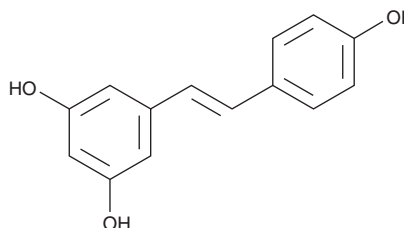
PRODUCT INFORMATION



trans-Resveratrol

Item No. 70675

CAS Registry No.: 501-36-0
Formal Name: 5-[(1E)-2-(4-hydroxyphenyl)ethenyl]-1,3-benzenediol
Synonym: (E)-Resveratrol
MF: C₁₄H₁₂O₃
FW: 228.2
Purity: ≥98%
UV/Vis.: λ_{max}: 218, 307, 321 nm
Supplied as: A crystalline solid
Storage: -20°C
Stability: ≥2 years
Special Conditions: Light and pH sensitive



Information represents the product specifications. Batch specific analytical results are provided on each certificate of analysis.

Laboratory Procedures

trans-Resveratrol is supplied as a crystalline solid. A stock solution may be made by dissolving the *trans*-resveratrol in the solvent of choice, which should be purged with an inert gas. *trans*-Resveratrol is soluble in organic solvents such as ethanol, DMSO, and dimethyl formamide (DMF). The solubility of *trans*-resveratrol in ethanol and DMSO is approximately 50 mg/ml and approximately 100 mg/ml in DMF.

Further dilutions of the stock solution into aqueous buffers or isotonic saline should be made prior to performing biological experiments. Ensure that the residual amount of organic solvent is insignificant, since organic solvents may have physiological effects at low concentrations. Organic solvent-free aqueous solutions of *trans*-resveratrol can be prepared by directly dissolving the crystalline solid in aqueous buffers. The solubility of *trans*-resveratrol in PBS, pH 7.2, is approximately 0.1 mg/ml. We do not recommend storing the aqueous solution for more than one day.

Description

trans-Resveratrol is a polyphenol that has been found in grapes and has diverse biological activities.^{1,2} It inhibits the cyclooxygenase and hydroperoxidase activities of COX-1 (EC₅₀s = 15 and 3.7 μM, respectively) but not COX-2 (EC₅₀s = >100 μM and 85 μM, respectively).¹ *trans*-Resveratrol (200 μM) also activates sirtuin 1 (SIRT1), as well as inhibits a variety of targets including ERK1, JNK1, Src, PKCα, aromatase/CYP19, and DNA polymerases α and δ (IC₅₀s = 37, 50, 20, <10, 25, 3.3, and 5 μM, respectively) *in vitro*.^{2,3} It inhibits free radical formation induced by phorbol 12-myristate 13-acetate (TPA; Item No. 10008014) in HL-60 cells and reduces the tumor incidence and number of tumors in a two-stage mouse model of skin cancer induced by TPA and 7,12-dimethyl-benz[a]anthracene (DMBA). *trans*-Resveratrol (3 and 8 mg/kg) inhibits carrageenan-induced paw edema in mice. Intravaginal administration of *trans*-resveratrol (12.5% v/v) inhibits herpes simplex virus 1 (HSV-1) and HSV-2 replication and delays the development of extrvaginal disease in mouse models of vaginal HSV infection.⁴ It also prolongs lifespan in model organisms including *C. elegans*, *D. melanogaster*, and mice.²

References

1. Jang, M., Cai, L., Udeani, G.O., *et al.* *Science* **275**(5297), 218-220 (1997).
2. Pirola, L. and Fröjdö, S. *IUBMB Life* **60**(5), 323-332 (2008).
3. Borra, M.T., Smith, B.C., and Denu, J.M. *J. Biol. Chem.* **280**(17), 17187-17195 (2005).
4. Docherty, J.J., Fu, M.M., Hah, J.M., *et al.* *Antiviral Res.* **67**(3), 155-162 (2005).

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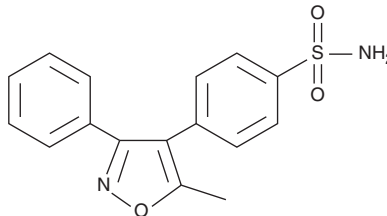
PRODUCT INFORMATION



Valdecoxib

Item No. 10006120

CAS Registry No.: 181695-72-7
Formal Name: 4-(5-methyl-3-phenyl-4-isoxazolyl)-benzenesulfonamide
Synonym: SC-65872
MF: C₁₆H₁₄N₂O₃S
FW: 314.4
Purity: ≥98%
UV/Vis.: λ_{max}: 202, 235 nm
Supplied as: A crystalline solid
Storage: -20°C
Stability: ≥2 years



Information represents the product specifications. Batch specific analytical results are provided on each certificate of analysis.

Laboratory Procedures

Valdecoxib is supplied as a crystalline solid. A stock solution may be made by dissolving the valdecoxib in the solvent of choice. Valdecoxib is soluble in organic solvents such as ethanol, DMSO, and dimethyl formamide (DMF), which should be purged with an inert gas. The solubility of valdecoxib in ethanol is approximately 5 mg/ml and approximately 20 mg/ml in DMSO and DMF.

Valdecoxib is sparingly soluble in aqueous buffers. For maximum solubility in aqueous buffers, valdecoxib should first be dissolved in DMSO and then diluted with the aqueous buffer of choice. Valdecoxib has a solubility of approximately 0.5 mg/ml in a 1:8 solution of DMSO:PBS (pH 7.2) using this method. We do not recommend storing the aqueous solution for more than one day.

Description

Valdecoxib is a selective inhibitor of COX-2 (IC₅₀s = 0.005 and 140 μM for human recombinant COX-2 and COX-1, respectively).¹ It decreases LPS-induced production of prostaglandin E₂ (PGE₂; Item No. 14010) in isolated human whole blood (IC₅₀ = 0.89 μM). Valdecoxib reduces carrageenan-induced paw edema and adjuvant-induced arthritis in rats (ED₅₀s = 10.2 and 0.032 mg/kg, respectively).

Reference

1. Talley, J.J., Brown, D.L., Carter, J.S., *et al.* 4-[5-Methyl-3-phenylisoxazol-4-yl]-benzenesulfonamide, valdecoxib: A potent and selective inhibitor of COX-2. *J. Med. Chem.* **43**(5), 775-777 (2000).

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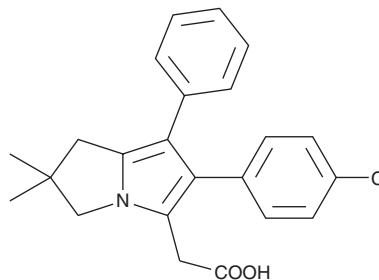
PRODUCT INFORMATION



Licofelone

Item No. 10007692

CAS No.:	156897-06-2
Formal Name:	6-(4-chlorophenyl)-2,3-dihydro-2,2-dimethyl-7-phenyl-1H-pyrrolizine-5-acetic acid
Synonym:	ML 3000
MF:	C ₂₃ H ₂₂ ClNO ₂
FW:	379.9
Purity:	≥98%
UV/Vis.:	λ _{max} : 248, 278 nm
Supplied as:	A crystalline solid
Storage:	-20°C
Stability:	≥2 years



Information represents the product specifications. Batch specific analytical results are provided on each certificate of analysis.

Laboratory Procedures

Licofelone is supplied as a crystalline solid. A stock solution may be made by dissolving the licofelone in the solvent of choice. Licofelone is soluble in organic solvents such as ethanol, DMSO, and dimethyl formamide (DMF), which should be purged with an inert gas. The solubility of licofelone in ethanol is approximately 5 mg/ml and approximately 20 mg/ml in DMSO and DMF.

Licofelone is sparingly soluble in aqueous buffers. For maximum solubility in aqueous buffers, licofelone should first be dissolved in DMSO and then diluted with the aqueous buffer of choice. Licofelone has a solubility of approximately 0.5 mg/ml in a 1:8 solution of DMSO:PBS (pH 7.2) using this method. We do not recommend storing the aqueous solution for more than one day.

Description

Cross-talk between lipoxygenase (LO) and cyclooxygenase (COX) pathways has been observed in human osteoarthritic synovial explants which creates an arachidonic acid shunting phenomenon, stimulating interleukin-1 β (IL-1 β) synthesis. Licofelone is a dual inhibitor of COX and LO pathways, that decreases levels of prostaglandin E₂, leukotriene B₄, and lipoxins and prevents lipopolysaccharide-stimulated IL-1 β expression.¹ The IC₅₀ values for inhibition of human thrombocyte COX and human 5-LO are 0.16 μ M and 0.23 μ M, respectively.² Unlike other non-steroidal anti-inflammatory drugs, licofelone causes little or no damage to the gastric mucosa in rabbit parietal cells. This is presumably the result of licofelone's effects on acid-secretory mechanisms, mediated by the inhibition of 5-LO activity.³

References

1. Marcouiller, P., Pelletier, J.-P., Guévremont, M., *et al.* Leukotriene and prostaglandin synthesis pathways in osteoarthritic synovial membranes: Regulating factors for interleukin 1 β synthesis. *J. Rheumatol.* **32**(4), 704-712 (2005).
2. Laufer, S.A., Augustin, J., Dannhardt, G., *et al.* (6,7-Diaryldihydropyrrolizin-5-yl)acetic acids, a novel class of potent dual inhibitors of both cyclooxygenase and 5-lipoxygenase. *J. Med. Chem.* **37**, 1894-1897 (1994).
3. Smolka, A.J., Goldenring, J.R., Gupta, S., *et al.* Inhibition of gastric H,K-ATPase activity and gastric epithelial cell IL-8 secretion by the pyrrolizine derivative ML 3000. *BMC Gastroenterology* **4**(4), 1-11 (2004).

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