

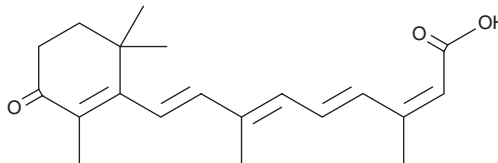
PRODUCT INFORMATION



4-oxo Isotretinoin

Item No. 34388

CAS Registry No.: 71748-58-8
Formal Name: 13-cis-4-oxo-retinoic acid
Synonym: Ro 22-6595
MF: C₂₀H₂₆O₃
FW: 314.4
Purity: ≥98%
UV/Vis.: λ_{max}: 285, 364 nm
Supplied as: A solid
Storage: -20°C
Stability: ≥4 years



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

Laboratory Procedures

4-oxo Isotretinoin is supplied as a solid. A stock solution may be made by dissolving the 4-oxo isotretinoin in the solvent of choice, which should be purged with an inert gas. 4-oxo Isotretinoin is soluble in organic solvents such as ethanol, DMSO, and dimethyl formamide (DMF). The solubility of 4-oxo isotretinoin in ethanol is approximately 15 mg/ml and approximately 30 mg/ml in DMSO and DMF.

4-oxo Isotretinoin is sparingly soluble in aqueous buffers. For maximum solubility in aqueous buffers, 4-oxo isotretinoin should first be dissolved in DMSO and then diluted with the aqueous buffer of choice. 4-oxo Isotretinoin has a solubility of approximately 0.2 mg/ml in a 1:4 solution of DMSO:PBS (pH 7.2) using this method. We do not recommend storing the aqueous solution for more than one day.

Description

4-oxo Isotretinoin is an active metabolite of the retinoid isotretinoin (Item No. 21648).¹ It is formed from isotretinoin by several cytochrome P450 (CYP450) isoforms, including CYP3A, CYP2B6, and CYP2C19.² 4-oxo Isotretinoin (10 μM) increases protein expression of cytokeratin 7 (CK7) and CK19 in normal human epidermal keratinocytes.³ It inhibits proliferation of retinoid-sensitive UM-SCC-22A and UM-SCC-35 head and neck squamous cell carcinoma (HNSCC) cells in a concentration-dependent manner.⁴ 4-oxo Isotretinoin has been found in influent and effluent wastewater.⁵ It is teratogenic to mouse embryos when administered to pregnant dams at a dose of 100 mg/kg on day 11 of gestation.⁶

References

1. Colburn, W.A., Vane, F.M., and Shorter, H.J. Pharmacokinetics of isotretinoin and its major blood metabolite following a single oral dose to man. *Eur. J. Clin. Pharmacol.* **24(5)**, 689-694 (1983).
2. Sonawane, P., Cho, H.E., Tagde, A., *et al.* Metabolic characteristics of 13-cis-retinoic acid (isotretinoin) and anti-tumour activity of the 13-cis-retinoic acid metabolite 4-oxo-13-cis-retinoic acid in neuroblastoma. *Br. J. Pharmacol.* **171(23)**, 5330-5344 (2014).
3. Baron, J.M., Heise, R., Blaner, W.S., *et al.* Retinoic acid and its 4-oxo metabolites are functionally active in human skin cells *in vitro*. *J. Invest. Dermatol.* **125(1)**, 143-153 (2005).
4. Klaassen, I., Brakenhoff, R.H., Smeets, S.J., *et al.* Metabolism and growth inhibition of four retinoids in head and neck squamous normal and malignant cells. *Br. J. Cancer* **85(4)**, 630-635 (2001).
5. Yeung, K.W.Y., Zhou, G.-J., Hilscherová, K., *et al.* Current understanding of potential ecological risks of retinoic acids and their metabolites in aquatic environments. *Environ. Int.* **136**, 105464 (2020).
6. Kochhar, D.M. and Penner, J.D. Developmental effects of isotretinoin and 4-oxo-isotretinoin: The role of metabolism in teratogenicity. *Teratology* **36(1)**, 67-75 (1987).

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.

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