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PRODUCT INFORMATION



A-771726

Item No. 14404

CAS Registry No.: 163451-81-8

Formal Name: 2-cyano-3-hydroxy-N-[4-(trifluoromethyl)phenyl]-2Z-butenamide

Synonyms: Flucyamide, HMR 1726, SU 20, Teriflunomide

MF: C₁₂H₉F₃N₂O₂

FW: 270.2

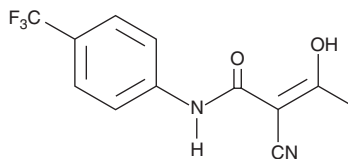
Purity: ≥98%

UV/Vis.: λ_{max}: 203, 251, 288 nm

Supplied as: A crystalline 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

A-771726 is supplied as a crystalline solid. A stock solution may be made by dissolving the A-771726 in the solvent of choice, which should be purged with an inert gas. A-771726 is soluble in organic solvents such as DMSO and dimethyl formamide (DMF). The solubility of A-771726 in these solvents is approximately 10.7 and 21.6 mg/ml, respectively.

A-771726 is sparingly soluble in aqueous buffers. For maximum solubility in aqueous buffers, A-771726 should first be dissolved in DMF and then diluted with the aqueous buffer of choice. A-771726 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

A-771726 is an active metabolite of the prodrug leflunomide (Item No. 14860) that inhibits dihydroorotate dehydrogenase (DHODH; IC₅₀ = 0.23 μM).¹ A-771726 inhibits the production of prostaglandin E₂ (PGE₂; Item No. 14010) in TNF-α- or IL-1α-stimulated isolated human synoviocytes (IC₅₀s = 7 and 3 μM, respectively).² It inhibits the proliferation of isolated human peripheral blood mononuclear cells (PBMCs) when used at concentrations of 25 and 100 μM.³ A-771726 (3 and 10 mg/kg) delays disease onset and decreases neurological deficits in a rat model of experimental autoimmune encephalomyelitis (EAE) induced by complete Freund's adjuvant (CFA) and *M. tuberculosis*.⁴ Formulations containing teriflunomide have been used in the treatment of multiple sclerosis.

References

1. Papageorgiou, C., Zurini, M., Weber, H.-P., *et al.* Leflunomide's bioactive metabolite has the minimal structural requirements for the efficient inhibition of human dihydroorotate dehydrogenase. *Bioorg. Chem.* **25**(4), 233-238 (1997).
2. Burger, D., Begué-Pastor, N., Benavent, S., *et al.* The active metabolite of leflunomide, A77 1726, inhibits the production of prostaglandin E₂, matrix metalloproteinase 1 and interleukin 6 in human fibroblast-like synoviocytes. *Rheumatology (Oxford)* **42**(1), 89-96 (2003).
3. Li, L., Liu, J., Delohery, T., *et al.* The effects of teriflunomide on lymphocyte subpopulations in human peripheral blood mononuclear cells in vitro. *J. Neuroimmunol.* **265**(1-2), 82-90 (2013).
4. Merrill, J.E., Hanak, S., Pu, S.-F., *et al.* Teriflunomide reduces behavioral, electrophysiological, and histopathological deficits in the Dark Agouti rat model of experimental autoimmune encephalomyelitis. *J. Neurol.* **256**(1), 89-103 (2009).

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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