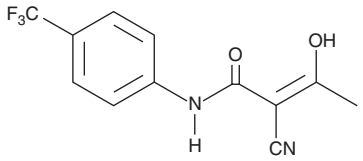
PRODUCT INFORMATION

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:	$C_{12}H_9F_3N_2O_2$
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; IC_{50} = 0.23 µM).[1] A-771726 inhibits the production of prostaglandin E_2 (PGE_2; Item No. 14010) in TNF-α- or IL-1α-stimulated isolated human synoviocytes (IC_{50}s = 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 E_2, 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).

CAYMAN CHEMICAL
1180 EAST ELLSWORTH RD
ANN ARBOR, MI 48108 · USA
PHONE: [800] 364-9897
[734] 971-3335
FAX: [734] 971-3640
CUSTSERV@CAYMANCHEM.COM
WWW.**CAYMANCHEM**.COM