

PRODUCT INFORMATION



CAY10723 (hydrochloride)

Item No. 38018

Formal Name: N-[(1S)-4-[(2-fluoro-1-iminoethyl)amino]-1-(4-methoxy-1-methyl-1H-benzimidazol-2-yl)butyl]-2,3-dihydro-3-oxo-1H-isoindole-4-carboxamide, monohydrochloride

Synonyms: AFM30a, AMF30a

MF: C₂₄H₂₇N₆O₃ • HCl

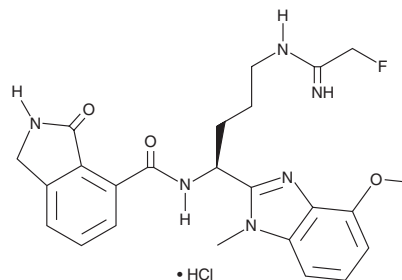
FW: 503.0

Purity: ≥95%

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

CAY10723 (hydrochloride) is supplied as a solid. A stock solution may be made by dissolving the CAY10723 (hydrochloride) in the solvent of choice, which should be purged with an inert gas. CAY10723 (hydrochloride) is soluble in organic solvents such as ethanol, DMSO, and dimethyl formamide (DMF). The solubility of CAY10723 (hydrochloride) in ethanol is approximately 5 mg/ml and approximately 30 mg/ml in DMSO and 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 CAY10723 (hydrochloride) can be prepared by directly dissolving the solid in aqueous buffers. The solubility of CAY10723 (hydrochloride) in PBS (pH 7.2) is approximately 10 mg/ml. We do not recommend storing the aqueous solution for more than one day.

Description

CAY10723 is an inhibitor of peptidyl arginine deiminase 2 (PAD2; EC₅₀ = 9.5 μM in a cellular target engagement assay).¹ It is approximately 1.6-, 47-, and 15-fold selective for PAD2 over PAD1, PAD3, and PAD4, respectively. CAY10723 inhibits histone H3 citrullination in HEK293T cells expressing human PAD2 (EC₅₀ = 0.4 μM). It also inhibits fibrinogen citrullination in the presence of isolated human polymorphonuclear leukocytes (PMNs) or synovial fluid from patients with rheumatoid arthritis when used at a concentration of 20 μM.² CAY10723 (25 μM) decreases IFN-γ production in isolated human CD4⁺ T cells.³

References

1. Muth, A., Subramanian, V., Beaumont, E., *et al.* Development of a selective inhibitor of protein arginine deiminase 2. *J. Med. Chem.* **60**(7), 3198-3211 (2017).
2. Monreal, M.T.M., Rebak, A.S., Massarenti, L., *et al.* Applicability of small-molecule inhibitors in the study of peptidyl arginine deiminase 2 (PAD2) and PAD4. *Front. Immunol.* **12**, 716250 (2021).
3. Liu, Y., Lightfoot, Y.L., Seto, N., *et al.* Peptidylarginine deiminases 2 and 4 modulate innate and adaptive immune responses in TLR-7-dependent lupus. *JCI Insight* **3**(23), e124729 (2018).

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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