# PRODUCT INFORMATION

## TDFA (trifluoroacetate salt)

*Item No. 22484*

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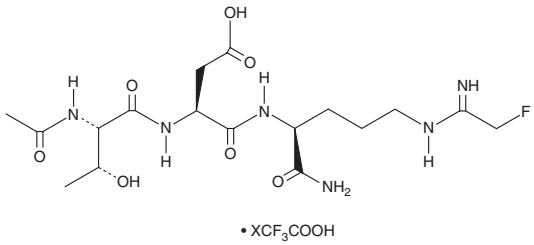
| **Formal Name:** | N-acetyl-L-threonyl-L-α-aspartyl-$N^5$-(2-fluoro-1-iminoethyl)-L-ornithinamide, trifluoroacetate salt |
| **Synonym:** | Thr-Asp-F-amidine |
| **MF:** | $C_{17}H_{29}FN_6O_7 \bullet XCF_3COOH$ |
| **FW:** | 448.5 |
| **Purity:** | ≥98% |
| **Supplied as:** | A solid |
| **Storage:** | -20°C |
| **Stability:** | ≥4 years |




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

### Laboratory Procedures

TDFA (trifluoroacetate salt) is supplied as a solid. A stock solution may be made by dissolving the TDFA (trifluoroacetate salt) in the solvent of choice, which should be purged with an inert gas. TDFA (trifluoroacetate salt) is soluble in organic solvents such as ethanol, DMSO, and dimethyl formamide (DMF). The solubility of TDFA (trifluoroacetate salt) in ethanol is approximately 16 mg/ml and approximately 33 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 TDFA (trifluoroacetate salt) can be prepared by directly dissolving the solid in aqueous buffers. The solubility of TDFA (trifluoroacetate salt) in PBS, pH 7.2, is approximately 10 mg/ml. We do not recommend storing the aqueous solution for more than one day.

### Description

TDFA is an irreversible inhibitor of protein arginine deiminase 4 (PAD4; $IC_{50}$ = 2.3 µM).[1] It is selective for PAD4 over PAD1, PAD2, and PAD3 ($IC_{50}$s = 8.5, 71, and 26 µM, respectively). TDFA (1, 10, and 100 nM) reduces global citrullination in HL-60 granulocytes and reduces citrullination of histone 3 arginine 2, 8, and 17 (H3R2Cit/R8Cit/R17Cit) in MCF-7 cells when used at concentrations of 1 and 10 µM.

### Reference


1. Jones, J.E., Slack, J.L., Fang, P., *et al.* Synthesis and screening of a haloacetamidine containing library to identify PAD4 selective inhibitors. *ACS Chem. Biol.* **7(1)**, 160-165 (2012).





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