PRODUCT INFORMATION

F-Amidine (trifluoroacetate salt)

Item No. 10610

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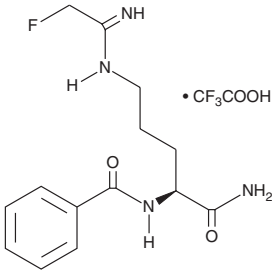

CAS Registry No.: 877617-46-4
Formal Name: N-[(1S)-1-(aminocarbonyl)-4-[(2-fluoro-1-iminoethyl) amino]butyl]-benzamide, 2,2,2-trifluoroacetate
MF: $C_{14}H_{19}FN_4O_2 \bullet CF_3COOH$
FW: 408.4
Purity: ≥95%
Supplied as: A solution in methanol
Storage: -20°C
Stability: ≥2 years

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

Laboratory Procedures

F-amidine (trifluoroacetate salt) is supplied as a solution in methanol. To change the solvent, simply evaporate the methanol under a gentle stream of nitrogen and immediately add the solvent of choice. Solvents such as ethanol, DMSO, and dimethyl formamide (DMF) purged with an inert gas can be used. The solubility of F-amidine (trifluoroacetate salt) in these solvents is 30 mg/ml in ethanol and approximately 20 mg/ml in DMF and DMSO.

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. If an organic solvent-free solution of F-amidine (trifluoroacetate salt) is needed, it can be prepared by evaporating the methanol and directly dissolving the neat oil in aqueous buffers. The solubility of F-amidine (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

F-amidine is an inhibitor of protein arginine deiminases (PAD) that is selective for PAD1 and PAD4 (IC_{50}s = 29.5, 350, and 21.6 µM for PAD1, PAD3, and PAD4 *in vitro*, respectively).[1,2] It irreversibly inactivates all four PAD subtypes (k_{inact}/K_I = 2,800, 380, 170, and 3,000 $M^{-1}min^{-1}$) by covalently modifying an active site cysteine that is important for its catalytic activity.[1,3] F-amidine is cytotoxic to HL-60, MCF-7, and HT-29 cancer cell lines (IC_{50}s = 0.5, 0.5, and 1 µM, respectively).[4]

References

1. Luo, Y., Arita, K., Bhatia, M., *et al.* Inhibitors and inactivators of protein arginine deiminase 4: Functional and structural characterization. *Biochem.* **45(39)**, 11727-11736 (2006).
2. Knuckley, B., Causey, C.P., Jones, J.E., *et al.* Substrate specificity and kinetic studies of PADs 1, 3, and 4 identify potent and selective inhibitors of protein arginine deiminase 3. *Biochem.* **49(23)**, 4852-4863 (2010).
3. 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).
4. Slack, J.L., Causey, C.P., and Thompson, P.R. Protein arginine deiminase 4: A target for an epigenetic cancer therapy. *Cell Mol. Life Sci.* **68(4)**, 709-720 (2011).

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