

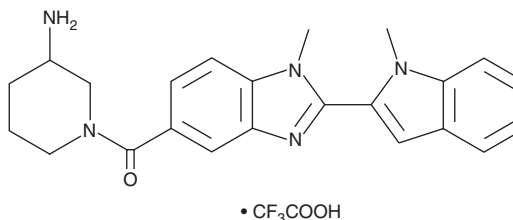
PRODUCT INFORMATION



GSK121 (trifluoroacetate salt)

Item No. 17491

CAS Registry No.: 1652591-80-4
Formal Name: (3-amino-1-piperidiny)[1-methyl-2-(1-methyl-1H-indol-2-yl)-1H-benzimidazol-5-yl]-methanone, 2,2,2-trifluoroacetate
MF: $C_{23}H_{25}N_5O \cdot CF_3COOH$
FW: 501.5
Purity: $\geq 98\%$
UV/Vis.: λ_{max} : 225, 319 nm
Supplied as: A crystalline solid
Storage: $-20^\circ C$
Stability: ≥ 4 years



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

Laboratory Procedures

GSK121 (trifluoroacetate salt) is supplied as a crystalline solid. A stock solution may be made by dissolving the GSK121 (trifluoroacetate salt) in the solvent of choice, which should be purged with an inert gas. GSK121 (trifluoroacetate salt) is soluble in organic solvents such as ethanol, DMSO, and dimethyl formamide. The solubility of GSK121 (trifluoroacetate salt) in these solvents is approximately 30 mg/ml.

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 GSK121 (trifluoroacetate salt) can be prepared by directly dissolving the crystalline solid in aqueous buffers. The solubility of GSK121 (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

Protein arginine deiminase 4 (PAD4) mediates the transformation of protein arginine into citrulline. Citrullination of proteins has normal roles in gene regulation and pathological roles in immunological and inflammatory diseases.¹ GSK121 is the initial compound identified in a screen for PAD4 inhibitors and was optimized to produce the more potent PAD4 inhibitors, GSK484 (Item No. 17488) and GSK199 (Item No. 17489).² GSK121 was shown to inhibit the citrullination of PAD4 target proteins in a functional assay with an IC_{50} value of 3.2 μM .²

References

1. Jones, J.E., Causey, C.P., Knuckley, B., *et al.* Protein arginine deiminase 4 (PAD4): Current understanding and future therapeutic potential. *Curr. Opin. Drug Discov. Devel.* **12**(5), 616-627 (2009).
2. Lewis, H.D., Liddle, J., Coote, J.E., *et al.* Inhibition of PAD4 activity is sufficient to disrupt mouse and human NET formation. *Nat. Chem. Biol.* **11**(3), 189-191 (2015).

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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