

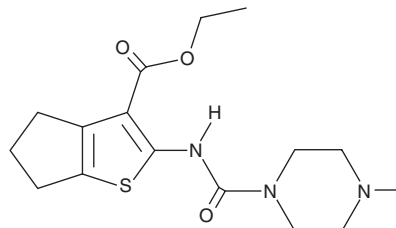
PRODUCT INFORMATION



SMU127

Item No. 33147

CAS Registry No.: 903864-87-9
Formal Name: 5,6-dihydro-2-[[[4-methyl-1-piperazinyl) carbonyl]amino]-4H-cyclopenta[b]thiophene-3-carboxylic acid, ethyl ester
Synonym: ZINC666243
MF: C₁₆H₂₃N₃O₃S
FW: 337.4
Purity: ≥98%
UV/Vis.: λ_{max}: 230, 251, 322 nm
Supplied as: A crystalline solid
Storage: -20°C
Stability: ≥2 years



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

Laboratory Procedures

SMU127 is supplied as a crystalline solid. A stock solution may be made by dissolving the SMU127 in the solvent of choice, which should be purged with an inert gas. SMU127 is soluble in the organic solvent dimethyl formamide (DMF) at a concentration of approximately 1 mg/ml. SMU127 is also slightly soluble in DMSO.

SMU127 is sparingly soluble in aqueous buffers. For maximum solubility in aqueous buffers, SMU127 should first be dissolved in DMF and then diluted with the aqueous buffer of choice. SMU127 has a solubility of approximately 0.2 mg/ml in a 1:4 solution of DMF:PBS (pH 7.2) using this method. We do not recommend storing the aqueous solution for more than one day.

Description

SMU127 is an agonist of the toll-like receptor 1/2 (TLR1/2) heterodimer.¹ It induces NF-κB signaling in cells expressing human TLR2 (EC₅₀ = 0.55 μM) but not cells expressing human TLR3, -4, -5, -7, or -8 when used at concentrations ranging from 0.1 to 100 μM. SMU127 induces the production of TNF-α in isolated human peripheral blood mononuclear cells (PBMCs) when used at concentrations ranging from 0.01 to 1 μM. *In vivo*, SMU127 (0.1 mg/animal) reduces tumor volume in a 4T1 murine mammary carcinoma model.

Reference

1. Chen, Z., Cen, X., Yang, J., *et al.* Structure-based discovery of a specific TLR1-TLR2 small molecule agonist from the ZINC drug library database. *Chem. Commun. (Camb.)* **54(81)**, 11411-11414 (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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