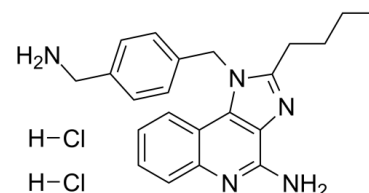


Data Sheet

Product Name:	TLR7/8 agonist 1 (dihydrochloride)
Cat. No.:	CS-0032947
CAS No.:	1620278-72-9
Molecular Formula:	C ₂₂ H ₂₇ Cl ₂ N ₅
Molecular Weight:	432.39
Target:	Toll-like Receptor (TLR)
Pathway:	Immunology/Inflammation
Solubility:	DMSO : 83.33 mg/mL (192.72 mM; Need ultrasonic)



BIOLOGICAL ACTIVITY:

TLR7/8 agonist 1 dihydrochloride is a toll-like receptor (TLR7)/TLR8 dual-agonistic imidazoquinoline. IC₅₀ & Target: TLR7/TLR8^[1] **In Vitro:** TLR7/8 agonist 1 (Compound 5d) shows prominent immunostimulatory activities. TLR7/8 agonist 1 serves as a convenient precursor for the covalent attachment of fluorophores without significant loss of activity. TLR7/8 agonist 1 retains TLR7-agonistic activity with an EC₅₀ of 20 nM^[1]. TLR7/8 agonist 1 (Compound 1) shows substantially different agonistic potencies in human TLR7 (50 nM) and TLR8 (55 nM) primary screens^[2].

PROTOCOL (Extracted from published papers and Only for reference)

Cell Assay: ^[2]Fresh human peripheral blood mononuclear cells (hPBMC) are used. Aliquots of PBMCs (10⁵ cells in 100 μL/well) are stimulated for 12 h with graded concentrations of test compounds (e.g., TLR7/8 agonist 1; 0.1, 1, 10, and 100 μg/mL). Supernatants are isolated by centrifugation and are assayed in duplicates using analyte-specific multiplexed cytokine/chemokine bead array assays ^[2].

References:

[1]. Shukla NM, et al. Syntheses of fluorescent imidazoquinoline conjugates as probes of Toll-like receptor 7. *Bioorg Med Chem Lett.* 2010 Nov 15;20(22):6384-6.

[2]. Beesu M, et al. Structure-Based Design of Human TLR8-Specific Agonists with Augmented Potency and Adjuvanticity. *J Med Chem.* 2015 Oct 8;58(19):7833-49.

CAIndexNames:

1H-Imidazo[4,5-c]quinolin-4-amine, 1-[[4-(aminomethyl)phenyl]methyl]-2-butyl-, hydrochloride (1:2)

SMILES:

NC1=NC2=CC=CC=C2C3=C1N=C(CCCC)N3CC4=CC=C(CN)C=C4.[H]Cl.[H]Cl

Caution: Product has not been fully validated for medical applications. For research use only.

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