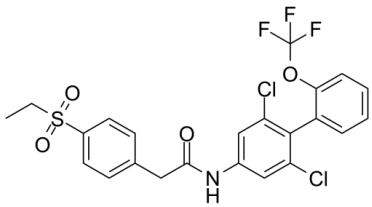
Data Sheet

Product Name:	GSK805
Cat. No.:	CS-5079
CAS No.:	1426802-50-7
Molecular Formula:	C23H18Cl2F3NO4S
Molecular Weight:	532.36
Target:	ROR
Pathway:	Metabolic Enzyme/Protease
Solubility:	DMSO : ≥ 100 mg/mL (187.84 mM); H2O : < 0.1 mg/mL (insoluble)



BIOLOGICAL ACTIVITY:

GSK805 is a potent, orally bioavailable, and CNS penetrant **RORγt** inhibitor with pIC_{50} of 8.4 and >8.2 for RORγ FRET assay and Th17 assay[1]. IC50 & Target: IC50: 8.4 (RORγt)[1]

PROTOCOL (Extracted from published papers and Only for reference)

Animal Administration: [1]Animal administration[1]

GSK805 are orally administered once daily at 3 doses (1, 3, and 10 mg/kg) to EAE mice from the day of immunization. Compared to the control, the treatment with 9a or 9g resulted in a delay and significant reduction in clinical severity of EAE in a dose-dependent manner. Compared to thiazole ketone amide 2, which only showed EAE efficacy up to day 20 at 100 mg/kg twice daily dosing,32 the biaryl amides 9a and 9g are much more efficacious. This could be attributed to their good in vitro activities as well as much improved oral exposure and CNS penetration. However, it should be noted that although 9g had more brain exposure than 9a, it exhibited less efficacy than 9a in EAE experiments, indicating that there might be additional factors such as "free" brain concentration affecting in vivo efficacy[1].

References:

[1]. Wang Y, et al. Discovery of Biaryl Amides as Potent, Orally Bioavailable, and CNS Penetrant RORγt Inhibitors. ACS Med Chem Lett. 2015 May 26;6(7):787-792.

CAIndexNames:

Benzeneacetamide, N-[2,6-dichloro-2'-(trifluoromethoxy)[1,1'-biphenyl]-4-yl]-4-(ethylsulfonyl)-

SMILES:

O=C(NC1=CC(Cl)=C(C2=CC=CC=C2OC(F)(F)F)C(Cl)=C1)CC3=CC=C(S(=O)(CC)=O)C=C3

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

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