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## Product Data Sheet

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Product Name: CC-90005

Cat. No.: GC62612

### Chemical Properties

Cas. No. 1799574-70-1

Formula  $C_{21}H_{27}F_2N_7O_2$

M.Wt 447.48

Solubility DMSO : 62.5 mg/mL (139.67 mM; Need ultrasonic) Storage Store at -20°C

General tips For obtaining a higher solubility , please warm the tube at 37 °C and shake it in the ultrasonic bath for a while. Stock solution can be stored below -20°C for several months.

Shipping Condition Evaluation sample solution : ship with blue ice All other available size: ship with RT , or blue ice upon request.

Structure

### Background

CC-90005 is a potent, selective and orally active inhibitor of protein kinase C- $\theta$  (PKC- $\theta$ ), with an IC<sub>50</sub> of 8 nM. CC-90005 shows selectivity for PKC- $\theta$  over PKC- $\delta$  (IC<sub>50</sub>=4440 nM). CC-90005 can inhibit T cell activation by IL-2 expression[1].

CC-90005 shows the exquisite selectivity of CC-90005, with IC<sub>50</sub>s for all other family members of >3  $\mu$ M[1]. CC-90005 is a moderate inhibitor of both CYP2C9 (IC<sub>50</sub>=8  $\mu$ M) and CYP2C19 (IC<sub>50</sub>=5.9  $\mu$ M) in human liver microsomes[1]. CC-90005 inhibits IL-2 expression in LRS\_WBC human PBMCs, with an IC<sub>50</sub> of 0.15  $\mu$ M[1]. CC-90005 (1-10  $\mu$ M; 24 h) inhibits T cell proliferation in PBMCs by 51% at 1  $\mu$ M and 88% at 3  $\mu$ M[1].

CC-90005 (3-30 mg/kg; p.o. twice daily for 4 days) significantly reduces the popliteal lymph node (PLN) size in a model of chronic T cell activation[1]. CC-90005 (100 mg/kg; a single p.o.) significantly inhibits plasma and spleen IL-2 release by 51 and 54%, respectively[1]. CC-90005 exhibits reasonable oral bioavailability (66 and 46%) and C<sub>max</sub> (1.18 and 1.2  $\mu$ M) following oral administration (10 and 3 mg/kg) in rat and dog, respectively[1]. CC-90005 exhibits the mean residence time (0.52 and 2.0 h), CL (69.1 and 20.5 mL/min/kg) and V<sub>ss</sub> (2.11 and 2.44 L/kg) following intravenous administration (2 and 1 mg/kg) in rat and dog, respectively[1].

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

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[1]. Papa P, et, al. Discovery of the Selective Protein Kinase C- $\theta$  Kinase Inhibitor, CC-90005. J Med Chem. 2021 Aug 26;64(16):11886-11903.

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