# Product Data Sheet

Product Name: NCT-505
Cat. No.: GC33219

## Chemical Properties

| | | | |
|---|---|---|---|
| Cas. No. | 2231079-74-4 | | |
| SMILES | N#CC1(C2=CC=CC=C2)CCN(C3=C(C(N4CCN(S(=O)(C)=O)CC4)=O)C=NC5=CC=C(F)C=C35)CC1 | | |
| Formula | $C_{27}H_{28}FN_5O_3S$ | M.Wt | 521.61 |
| Solubility | Soluble in DMSO | Storage | Store at -20°C |
| General tips | For obtaining a higher solubility , please warm the tube at 37 ℃ and shake it in the ultrasonic bath for a while.Stock solution can be stored below -20℃ 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 | NCT-505 | | |

## Protocol


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**Cell experiment:**

Cells are harvested, and an equal volume of first compound (NCT-505 or paclitaxel (Taxol)) at the indicated concentration or vehicle DMSO (final DMSO concentration is the same in all conditions) is added to the cell suspension before dispensing. Cells are dispensed into 384-well, white, TC-treated plates at a density of 3000 cells/well in a volume of 30 µL of growth media/well using a Multidrop Combi dispenser. Immediately after dispensing, the second compound (ALDH1A1 inhibitor or paclitaxel) and control solutions (92 nL) are transferred using a pintool. Plates are covered with a breathable seal and incubated for 4 days at 37°C, 5% CO2, 85% RH followed by addition of 20 µL of CellTiter-Glo. After a ~30 min incubation at rt, samples are analyzed for luminescence intensity using a ViewLux high-throughput CCD imager equipped with clear filters. Pinned compounds are tested as 16-point dilution series, with concentrations ranging from 30.7 µM to 70.1 nM for ALDH1A1 inhibitors (NCT-505, etc.) or 31.7 µM to 0.034 nM for paclitaxel, in triplicate. Data are normalized to positive control bortezomib (1 µM final) and neutral control DMSO[1].


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References:

[1]. Yang SM, et al. Discovery of Orally Bioavailable, Quinoline-Based Aldehyde Dehydrogenase 1A1 (ALDH1A1) Inhibitors with Potent Cellular Activity. J Med Chem. 2018 Jun 14;61(11):4883-4903.

## Background

NCT-505 is a potent and selective aldehyde dehydrogenase (ALDH1A1) inhibitor, with an IC50 of 7 nM, and weakly inhibits hALDH1A2, hALDH1A3, hALDH2, hALDH3A1 (IC50s, >57, 22.8, 20.1, >57 μM).

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[1]. Yang SM, et al. Discovery of Orally Bioavailable, Quinoline-Based Aldehyde Dehydrogenase 1A1 (ALDH1A1) Inhibitors with Potent Cellular Activity. J Med Chem. 2018 Jun 14;61(11):4883-4903.


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