# Product Data Sheet

Product Name: N-acetyl-2-carboxy Benzenesulfonamide
Cat. No.: GC16440

## Chemical Properties

| | | | |
|---|---|---|---|
| Cas. No. | 849067-18-1 | | |
| Chemical Name | 2-[(acetylamino)sulfonyl]-benzoic acid | | |
| SMILES | CC(=O)NS(=O)(=O)c1ccccc1C(=O)O | | |
| Formula | $C_9H_9NO_5S$ | M.Wt | 243.2 |
| Solubility | ≤30mg/ml in ethanol;30mg/ml in DMSO;30mg/ml in dimethyl formamide | 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 | | | |

## Background

IC50: 0.06 and 0.25 μM for COX-1 and COX-2, respectively

N-acetyl-2-carboxy Benzenesulfonamide is a non-selective inhibitor of COX.

Pharmaceutical inhibition of COX is able to provide relief from the symptoms of inflammation and pain. Nonsteroidal anti-inflammatory drugs, such as aspirin, exert its effect via inhibition of COX.

In vitro: Previous in-vitro COX-1/COX-2 inhibition studies showed that N-acetyl-2-carboxy benzenesulfonamide was a more potent inhibitor than aspirin, and like aspirin. Moreover, N-acetyl-2-carboxy benzenesulfonamide was found to be a nonselective COX-2 inhibitor. In addition, the molecular modeling (docking) study demonstrated that the SO2NHCOCH3 substituent present in N-acetyl-2-carboxy benzenesulfonamide, like the acetoxy substituent in aspirin, was suitably positioned to acetylate the Ser530 hydroxyl


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group in the COX-2 primary binding site [1].

In vivo: Animal study showed that N-acetyl-2-carboxy benzenesulfonamide and its C-4 2,4-difluorophenyl derivative had superior antiinflammatory activity (oral dosing) in a carrageenan-induced rat paw edema assay compared to aspirin. In addition, N-acetyl-2-carboxy benzenesulfonamide and its C-4 2,4-difluorophenyl derivative exhibited comparable analgesic activity to iflunisal, and superior analgesic activity compared to aspirin [1].

Clinical trial: So far, no clinical study has been conducted.

Reference:
[1] Chen, Q. H.,Rao, P.N.P., and Knaus, E.E. Design, synthesis, and biological evaluation of N-acetyl-2-carboxybenzenesulfonamides: A novel class of cyclooxygenase-2 (COX-2) inhibitors. Bioorganic & Medicinal Chemistry 13, 2459-2468 (2005).