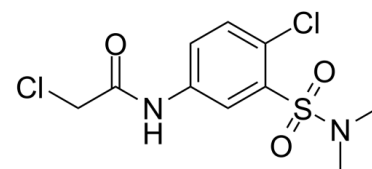


Data Sheet

Product Name:	GSTO1-IN-1
Cat. No.:	CS-0042397
CAS No.:	568544-03-6
Molecular Formula:	C ₁₀ H ₁₂ Cl ₂ N ₂ O ₃ S
Molecular Weight:	311.18
Target:	Gutathione S-transferase
Pathway:	Metabolic Enzyme/Protease
Solubility:	DMSO : ≥ 300 mg/mL (964.07 mM)



BIOLOGICAL ACTIVITY:

GSTO1-IN-1 is a potent **glutathione S-transferase omega 1 (GSTO1)** inhibitor with an **IC₅₀** of 31 nM. **IC₅₀ & Target: IC₅₀: 31 nM (GSTO1)**^[1] **In Vitro:** GSTO1-IN-1 (C1-27) potently inhibits GSTO1 enzyme activity with an **IC₅₀** value of 31 nM. GSTO1-IN-1 also potently competes with 5-chloromethylfluorescein diacetate (CMFDA) for binding to recombinant protein, as well as endogenous GSTO1 in the milieu of a soluble proteome. HCT116 cells treated with GSTO1-IN-1 also show a decrease in cell viability in a dose-dependent manner. GSTO1-IN-1 inhibits the clonogenic survival of HCT116 cells at sub-micromolar concentrations^[1]. **In Vivo:** To test whether GSTO1-IN-1 had in vivo efficacy, its effects are evaluated in a human colon cancer cell line xenograft model. GSTO1-IN-1 (20-45 mg/kg) is administered as a single agent to nude mice bearing HCT116 xenografts. After 5 weeks of treatment, tumor growth is significantly inhibited in GSTO1-IN-1-treated mice compared with the vehicle-treated group ($P < 0.05$). GSTO1-IN-1 treatment is generally well tolerated by mice up to 45 mg/kg, with no overt signs of toxicity and no significant variations in average body weights throughout the duration of the study^[1].

PROTOCOL (Extracted from published papers and Only for reference)

Cell Assay: ^[1]Cell proliferation is assessed by a MTT assay. **Cancer cells H630, HT29 and HCT116** are seeded in 96-well microtitre plates and, after overnight attachment, treated with GSTO1 inhibitors (e.g., **GSTO1-IN-1; 0.1, 1, 10 and 100 μM**). After 72 h, MTT solution (3 mg/mL; 20mL) is added to each well and cells are incubated for 3 h at 37°C. After incubation, media from each well is removed and the dark blue formazan crystals formed by live cells are dissolved in DMSO (150 mL per well). The absorbance intensity is measured at 570 nm on a microplate reader. Cell viability after 24 h treatment is assessed using ApoTox-Glo triplex assay. At least three independent dose-response experiments with each concentration tested in triplicate are performed for each cell line^[1].

Animal Administration: In the HCT116 xenograft study, GSTO1-IN-1 (C1-27) is diluted using peanut oil^[1],^[1]Mice^[1] In the pilot study, HCT116 cells (1×10^6) in exponential phase are injected subcutaneously into the left flank of **8- to 10-week-old female nude mice (25-30 g)**. The perpendicular diameters of the tumors are measured three times weekly using standard calipers and tumour volumes are calculated. Tumors are allowed to grow to a volume of 50 mm³ and mice are randomized into control (n=5) and GSTO1-IN-1 (n=3) treatment groups. **GSTO1-IN-1 is administered intraperitoneally (20 mg/kg per day) for the first 2 weeks** on a 5 days on/2 days off schedule. The dose is then increased to 25 mg/kg per day for the next 23 days and further escalated by 5 mg/kg per day to a final dose of 45 mg/kg for the remaining duration of treatment. Tumor volumes and body weights are measured three times weekly to monitor tumor burden and weight loss during treatment. At the end of the experiment, animals are killed and tumor, kidney and liver are collected, fixed and paraffin embedded for histology^[1].

References:

[1]. Ramkumar K, et al. Mechanistic evaluation and transcriptional signature of a glutathione S-transferase omega 1 inhibitor. Nat Commun. 2016 Oct 5;7:13084.

CAIndexNames:

Acetamide, 2-chloro-N-[4-chloro-3-[(dimethylamino)sulfonyl]phenyl]-

SMILES:

O=C(NC1=CC=C(Cl)C(S(=O)(N(C)C)=O)=C1)CCl

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

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