# Technical Data Sheet

Small Molecules

# Emricasan

**Catalog Number(s)** SML21A, SML21B

**Synonyms** PF 03491390; IDN-6556

**Size** 5 mg or 10 mg

**Description**

Emricasan is a potent pan-caspase inhibitor, demonstrating irreversible inhibition and a significant first-pass effect. Emricasan acts in synergy with Chroman 1, a potent and selective ROCK inhibitor, to improve survival and viability of dissociated human pluripotent stem cells (hPSCs). When used in combination with Chroman 1, Trans-ISRIB, and polyamines (a small molecule combination known as CEPT), Emricasan's synergistic effects improves single-cell clonogenicity and gene editing, EB and organoid formation, and survival of pluripotent and differentiated cells following cryopreservation[1].

Emricasan has been found to directly improve hepatocyte phenotype in primary rat cirrhotic hepatocytes and has hepatoprotective effects in human liver cells[3], and has been used in clinical trials for the treatment of non-alcoholic steatohepatitis (NASH) with advanced fibrosis and cirrhosis. Emricasan, formerly known as IDN-6556, in combination with birinapant, has been used to treat acute myeloid leukemia[4]. It has also been shown to inhibit Zika virus (ZIKV)-induced increases in caspase-3 activity and protect infected astrocytes from ZIKV-induced cell death. Emricasan preserves cell viability after infection with several strains of Zika[5].

**Molecular Weight** 569.50

**Molecular Formula** $C_{26}H_{27}F_4N_3O_7$

**Chemical Name** (N-[2-(1,1-dimethylethyl)phenyl]-2-oxoglycyl-N-[(1S)-1-(carboxymethyl)-2-oxo-3-(2,3,5,6-tetrafluorophenoxy)propyl]-L-Alaninamide

**CAS Number** 254750-02-2

**Target** Caspase

**Appearance** White to off-white (solid)

**Purity** ≥98% by LCMS

**Solubility & Reconstitution**

| Stock Concentration | Compound Mass | | |
|---|---|---|---|
| | 1 mg | 5 mg | 10 mg |
| 1 mM | 1.7559 mL | 8.7796 mL | 17.5593 mL |
| 5 mM | 0.3512 mL | 1.7559 mL | 3.5119 mL |
| 10 mM | 0.1756 mL | 0.8780 mL | 1.7559 mL |
| 50 mM | 0.0351mL | 0.1756 mL | 0.3512 mL |

Solvent Volume



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**Solvent & Solubility**

**DMSO:** Soluble in DMSO to 100 mg/mL (175.59 mM)
**Ethanol:** Soluble in ethanol > 28.48 mg/mL (50 mM)
Ultrasonication may be required for complete solubilization at high concentrations.

**Storage**

| | | |
|---|---|---|
| **Powder:** | 20°C | 3 years |
| | 4°C | 2 years |
| **In solvent:** | -80°C | 6 months |
| | -20°C | 1 month |

Store as lyophilized powder or concentrated stock solutions.
Prepare working solutions in appropriate cell culture media just prior to use.

**Pathway**

Apoptosis, Cytoprotection, Anti-infection

**Reconstitution**

1. From the lyophilized compound, prepare a concentrated stock solution using the appropriate solvent (DMSO), according to the solubility table or custom calculations. Example: To generate a 5 mM concentrated stock solution of Emricasan, add 3.5119 mL of DMSO to 10 mg of Emricasan.
2. Ensure the compound is completely dissolved in the solvent. This may require gentle warming and/or vortexing/sonication to fully reconstitute the compound.
3. Aliquot the concentrated stock solution in single-use volumes, and either use immediately or freeze at -20°C or -80°C for later use. Avoid freeze/thaw cycles.
4. Concentrated stock solutions are designed to be diluted just prior to use (e.g. 1:1000 dilution in cell culture medium). For use in cell culture, warm the medium just prior to adding the reconstituted compound.

**References**


1. Y Chen, et al. (2021) A Versatile Polypharmacology Platform Promotes Cytoprotection and Viability of Human Pluripotent and Differentiated Cells. Nature Methods. May; 18(5): 528-514
2. J Tian et al. (2017) Combination of Emricasan with AP24534 Synergistically Reduces Ischemia/Reperfusion Injury in Rat Brain Through Simultaneous Prevention of Apoptosis and Necroptosis. Transl Stroke Res
3. FJ Barreyro et al. (2015) The pan-caspase inhibitor Emricasan (IDN-6556) decreases liver injury and fibrosis in a murine model of non-alcoholic steatohepatitis. Liver Int. Mar;35(3):953-66
4. G Brumatti et al. (2016) The caspase-8 inhibitor emricasan combines with the SMAC mimetic birinapant to induce necroptosis and treat acute myeloid leukemia. Science Translational Medicine, 8(339)339ra69
5. M Xu et al. (2016) Identification of small-molecule inhibitors of Zika virus infection and induced neural cell death via a drug repurposing screen. Nat Med. Oct;22(10):1101-1107


**Related Products**

| Description | Cat. No. | Application |
|---|---|---|
| Chroman 1 | SML20 | ROCK inhibitor, cell survival, CEPT |
| Trans-ISRIB | SML22 | Integrated stress response (ISR) inhibitor, CEPT |
| CET Cocktail | CET01 | Enhanced stem cell survival cocktail, CEPT |


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