

Product Name: CRID3 sodium salt

Catalog No.: 5479

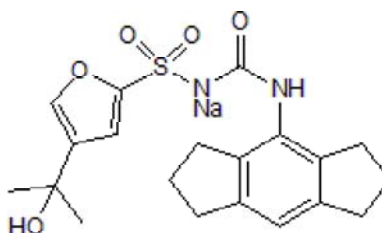
Batch No.: 1

CAS Number: 256373-96-3

IUPAC Name: *N*-[[[(1,2,3,5,6,7-Hexahydro-*s*-indacen-4-yl)amino]carbonyl]-4-(1-hydroxy-1-methylethyl)-2-furansulfonamide sodium salt

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula:	C ₂₀ H ₂₃ N ₂ NaO ₅ S
Batch Molecular Weight:	426.46
Physical Appearance:	Off White solid
Solubility:	water to 100 mM DMSO to 100 mM
Storage:	Store at +4°C
Batch Molecular Structure:	



2. ANALYTICAL DATA

HPLC:	Shows 98.4% purity
¹H NMR:	Consistent with structure
Mass Spectrum:	Consistent with structure

Microanalysis:	Carbon Hydrogen Nitrogen		
Theoretical	56.33	5.44	6.57
Found	56.18	5.42	6.53

Caution - Not Fully Tested • Research Use Only • Not For Human or Veterinary Use

bio-techne.com

info@bio-techne.com
techsupport@bio-techne.com

North America

Tel: (800) 343 7475

China

info.cn@bio-techne.com
Tel: +86 (21) 52380373

Europe Middle East Africa

Tel: +44 (0)1235 529449

Rest of World

www.tocris.com/distributors
Tel: +1 612 379 2956

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Description:

Potent NLRP3 inflammasome inhibitor; closes the active conformation of NLRP3 to the inactive state. Directly interacts with the Walker B motif within the NLRP3 NACHT domain. Inhibits IL-1 β , IL-18 and IL-1 α production (IC₅₀ values are 7.2, 10.3 and 12-18 nM, respectively). Selective for NLRP3 over NLRC4 inflammasome and Toll-like receptor signaling. Reduces severity of experimental autoimmune encephalomyelitis, skin inflammation and airway inflammation in mice. Also glutathione S-transferase omega 1 inhibitor. Orally bioavailable.

Physical and Chemical Properties:

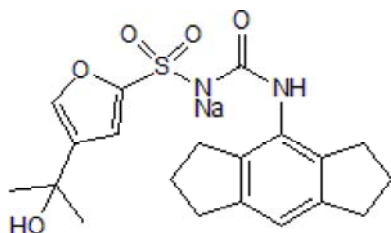
Batch Molecular Formula: C₂₀H₂₃N₂NaO₅S

Batch Molecular Weight: 426.46

Physical Appearance: Off White solid

Minimum Purity: >98%

Batch Molecular Structure:



References:

Coll et al (2019) MCC950 directly targets the NLRP3 ATP-hydrolysis motif for inflammasome inhibition. *Nat.Chem.Biol.* **15** 556. PMID: 31086327.

Tapia-Abellán et al (2019) MCC950 closes the active conformation of NLRP3 to an inactive state. *Nat.Chem.Biol.* **15** 560. PMID: 31086329.

Gordon et al (2018) Inflammasome inhibition prevents α -synuclein pathology and dopaminergic neurodegeneration in mice. *Sci.Transl.Med.* **10** eaah4066. PMID: 30381407.

Coll et al (2015) A small-molecule inhibitor of the NLRP3 inflammasome for the treatment of inflammatory diseases. *Nat.Med.* **21** 248. PMID: 25686105.

Laliberte et al (2003) Glutathione S-transferase omega 1-1 is a target of cytokine release inhibitory drugs and may be responsible for their effect on interleukin-1 β posttranslational processing. *J.Biol.Chem.* **278** 16567. PMID: 12624100.

Storage: Store at +4°C

Solubility & Usage Info:

water to 100 mM

DMSO to 100 mM

Stability and Solubility Advice:

Some solutions can be difficult to obtain and can be encouraged by rapid stirring, sonication or gentle warming (in a 45-60°C water bath).

Information concerning product stability, particularly in solution, has rarely been reported and in most cases we can only offer a general guide. Our standard recommendations are:

SOLIDS: Provided storage is as stated on the product label and the vial is kept tightly sealed, the product can be stored for up to 6 months from date of receipt.

SOLUTIONS: We recommend that stock solutions, once prepared, are stored aliquoted in tightly sealed vials at -20°C or below and used within 1 month. Wherever possible solutions should be made up and used on the same day.

Licensing Information:

Sold for research purposes under agreement from Pfizer Inc

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info@bio-techne.com

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North America

Tel: (800) 343 7475

China

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Tel: +86 (21) 52380373

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Tel: +44 (0)1235 529449

Rest of World

www.tocris.com/distributors

Tel:+1 612 379 2956