Product Datasheet

Technical Data

Formula	$C_{22}H_{30}F_3N_5O_4S_2$					
Molecular Weight	549.63	**CAS No.**	2920904-06-7			
Solubility (25°C)*	In vitro	DMSO	100 mg/mL (181.94 mM)			
		Ethanol	100 mg/mL (181.94 mM)			
		Water	Insoluble			
	In vivo (Add solvents to the product individually and in order)	Oral Administration	Homogeneous suspension	CMC-NA	≥5mg/ml	Taking the 1 mL working solution as an example, add 5 mg of this product to 1 ml of CMC-Na solution, mix evenly to obtain a homogeneous suspension with a final concentration of 5 mg/ml.
		Injection	Clear solution	5%DMSO [1] → 40%PEG300 [2] → 5%Tween80 [3] → 50%ddH2O Validated by Capsid Bio labs. Should you need adjustments to this formulation, contact our sales team for custom testing.	5.000mg/ml (9.10mM)	Taking the 1 mL working solution as an example, add 50 μL of 100 mg/ml clarified DMSO stock solution to 400 μL of PEG300, mix evenly to clarify it; add 50 μL of Tween80 to the above system, mix evenly to clarify; then continue to add 500 μL of ddH2O to adjust the volume to 1 mL. The mixed solution should be used immediately for optimal results.
			Clear solution	5% DMSO [1] → 95% Corn oil Validated by Capsid Bio labs. Should you need adjustments to this formulation, contact our sales team for custom testing.	1.250mg/ml (2.27mM)	Taking the 1 mL working solution as an example, add 50 μL of 25 mg/ml clear DMSO stock solution to 950 μL of corn oil and mix evenly. The mixed solution should be used immediately for optimal results.

* <1 mg/ml means slightly soluble or insoluble.
* Please note that Capsid Bio tests the solubility of all compounds in-house, and the actual solubility may differ slightly from published values. This is normal and is due to slight batch-to-batch variations.
* Room temperature shipping (Stability testing shows this product can be shipped at 2-8°C for storage purposes.)

Preparing Stock Solutions

Biological Activity

Description	Simnotrelvir(SIM0417, SARS-CoV-2-IN-41) is an inhibitor of **coronavirus main proteinase (3CLpro) (SARS-CoV-2 3CLpro)** with an IC50 of 24 nM. It has a potential anti-SARS-CoV-2 activity.
Targets	SARS-CoV-2 3CL protease [1] 24 nM

References

https://pubmed.ncbi.nlm.nih.gov/37833261/

RETURN POLICY

Capsid Bio's Unconditional Return Policy ensures a smooth online shopping experience for our customers. If you are in any way unsatisfied with your purchase, you may return any item(s) within 7 days of receiving it. In the event of product quality issues, either protocol related or product related problems, you may return any item(s) within 365 days from the original purchase date. Please follow the instructions below when returning products.

SHIPPING & STORAGE

Capsid Bio products are transported at room temperature. If you receive the product at room temperature, please rest assured, the Capsid Bio Quality Inspection Department has conducted experiments to verify that the normal temperature placement of one month will not affect the biological activity of powder products. After collecting, please store the product according to the requirements described in the datasheet. Most Capsid Bio products are stable under the recommended conditions.

NOT FOR HUMAN, VETERINARY DIAGNOSTIC OR THERAPEUTIC USE.

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