# **PRODUCT** INFORMATION



## Saquinavir-d<sub>9</sub>

Item No. 28906

CAS Registry No.: Formal Name:	1356355-11-7 (2S)-N <sup>1</sup> -[(1S,2R)-3-[(3S,4aS,8aS)-3- [[(1,1-di(methyl-d <sub>3</sub> )ethyl-2,2,2-d <sub>3</sub> )amino] carbonyl]octahydro-2(1H)-isoquinolinyl]-		
	2-hydroxy-1-(phenylmethyl)propyl]-2-[(2- quinolinylcarbonyl)amino]-butanediamide	NI	
MF:	$C_{38}H_{41}D_9N_6O_5$	04	
FW:	679.9	∧ N ∐	
Chemical Purity:	≥95% (Saquinavir)		
Deuterium		L L I	0
Incorporation:	≥99% deuterated forms (d <sub>1</sub> -d <sub>9</sub> ); ≤1% d <sub>0</sub>	$\checkmark$ $\checkmark$	
Supplied as:	A solid		
Storage:	-20°C		
Stability:	≥4 years		
Information represents the product specifications. Batch specific analytical results are provided on each certificate of analysis			

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#### Laboratory Procedures

Saquinavir-do is intended for use as an internal standard for the quantification of saquinavir (Item No. 9001893) by GC- or LC-MS. The accuracy of the sample weight in this vial is between 5% over and 2% under the amount shown on the vial. If better precision is required, the deuterated standard should be quantitated against a more precisely weighed unlabeled standard by constructing a standard curve of peak intensity ratios (deuterated versus unlabeled).

Saquinavir-d<sub>q</sub> is supplied as a solid. A stock solution may be made by dissolving the saquinavir-d<sub>q</sub> in the</sub></sub>solvent of choice, which should be purged with an inert gas. Saquinavir- $d_o$  is soluble in organic solvents such as chloroform and methanol.

#### Description

Saquinavir is an HIV protease inhibitor (K<sub>i</sub>s = 0.12 and <0.1 nM for HIV-1 and HIV-2 protease, respectively).<sup>1</sup> It is selective for HIV-1 and HIV-2 protease over human aspartic proteases, renin, pepsin, pepsinogen C, cathepsin D, and cathepsin E at 10 µM. Saquinavir inhibits replication of clinical isolates of HIV-1 in a variety of cell-based assays and has antiviral activity against HIV-1 in infected C8166 cells (IC<sub>50</sub> = 2 nM).<sup>1,2</sup> It also inhibits the activity of the severe acute respiratory coronavirus 2 (SARS-CoV-2) main protease (M<sup>pro</sup>), also known as 3C-like protease (3CL<sup>pro</sup>), with an IC<sub>50</sub> value of 9.92 µM.<sup>3</sup>

#### References

- 1. Roberts, N.A., Martin, J.A., Kinchington, D., et al. Rational design of peptide-based HIV proteinase inhibitors. Science 248(4953), 358-361 (1990).
- 2. Stefanidou, M., Herrera, C., Armanasco, N., et al. Saquinavir inhibits early events associated with establishment of HIV-1 infection: Potential role for protease inhibitors in prevention. Antimicrob. Agents Chemother. 56(8), 4381-4390 (2012).
- 3. Chiou, W.-C., Hsu, M.-S., Chen, Y.-T., et al. Repurposing existing drugs: Identification of SARS-CoV-2 3C-like protease inhibitors. J. Enzyme Inhib. Med. Chem. 36(1), 147-153 (2021).

WARNING THIS PRODUCT IS FOR RESEARCH ONLY - NOT FOR HUMAN OR VETERINARY DIAGNOSTIC OR THERAPEUTIC USE.

#### SAFETY DATA

This material should be considered hazardous until further information becomes available. Do not ingest, inhale, get in eyes, on skin, or on clothing. Wash thoroughly after handling. Before use, the user must review the complete Safety Data Sheet, which has been sent via email to your institution.

#### WARRANTY AND LIMITATION OF REMEDY

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