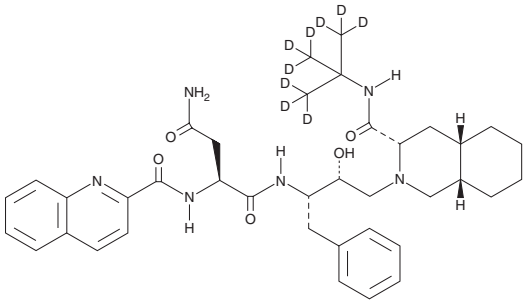
PRODUCT INFORMATION

Saquinavir-d_9

Item No. 28906

CAS Registry No.:	1356355-11-7
Formal Name:	(2S)-N^1-[(1S,2R)-3-[(3S,4aS,8aS)-3-[[(1,1-di(methyl-d_3)ethyl-2,2,2-d_3)amino]carbonyl]octahydro-2(1H)-isoquinolinyl]-2-hydroxy-1-(phenylmethyl)propyl]-2-[(2-quinolinylcarbonyl)amino]-butanediamide
MF:	$C_{38}H_{41}D_9N_6O_5$
FW:	679.9
Chemical Purity:	≥95% (Saquinavir)
Deuterium Incorporation:	≥99% deuterated forms (d_1-d_9); ≤1% d_0
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.

Laboratory Procedures

Saquinavir-d_9 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_9 is supplied as a solid. A stock solution may be made by dissolving the saquinavir-d_9 in the solvent of choice, which should be purged with an inert gas. Saquinavir-d_9 is soluble in organic solvents such as chloroform and methanol.

Description

Saquinavir is an HIV protease inhibitor (K_is = 0.12 and <0.1 nM for HIV-1 and HIV-2 protease, respectively).[1] 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_{50} = 2 nM).[1,2] It also inhibits the activity of the severe acute respiratory coronavirus 2 (SARS-CoV-2) main protease (M^{pro}), also known as 3C-like protease ($3CL^{pro}$), with an IC_{50} value of 9.92 µM.[3]

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).

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