# PRODUCT INFORMATION

## Daclatasvir-$d_6$

*Item No. 29077*

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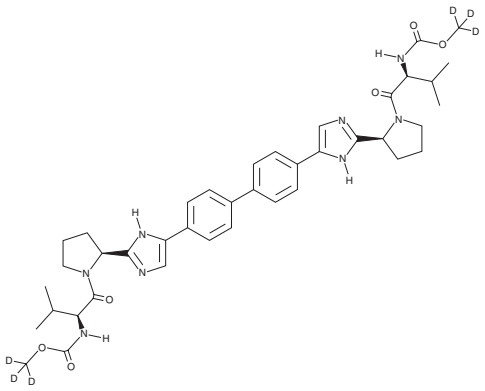
|---|---|
| **CAS Registry No.:** | 1801709-41-0 |
| **Formal Name:** | N,N′-[[1,1′-biphenyl]-4,4′-diylbis[1H-imidazole-5,2-diyl-(2S)-2,1-pyrrolidinediyl[(1S)-1-(1-methylethyl)-2-oxo-2,1-ethanediyl]]]*bis*-carbamic acid, C,C′-di(methyl-$d_3$) ester |
| **MF:** | $C_{40}H_{44}D_6N_8O_6$ |
| **FW:** | 744.9 |
| **Chemical Purity:** | ≥95% (Daclatasvir) |
| **Deuterium Incorporation:** | ≥99% deuterated forms ($d_1$-$d_6$); ≤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

Daclatasvir-$d_6$ is intended for use as an internal standard for the quantification of daclatasvir (Item No. 23730) 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).

Daclatasvir-$d_6$ is supplied as a solid. A stock solution may be made by dissolving the daclatasvir-$d_6$ in the solvent of choice, which should be purged with an inert gas. Daclatasvir-$d_6$ is soluble in organic solvents such as methanol and DMSO.

### Description

Daclatasvir is a first generation direct-acting inhibitor of hepatitis C virus (HCV) non-structural protein 5A (NS5A; $K_d$s = 8 and 210 nM for the $NS5A^{33-202}$ and $NS5A^{26-202}$ residues of HCV genotype 1b, respectively).[1,2] It potently inhibits HCV replication in multiple HCV replicon genotypes ($EC_{50}$s = 9-146 pM) with the highest potency in genotypes 1b and 4a ($EC_{50}$s = 9 and 12 pM, respectively).[1] Daclatasvir disrupts the subcellular localization of NS5A in Huh7.5 cells and inhibits viral RNA synthesis and virion assembly and secretion when used at a concentration of 1 nM in HCV-infected Huh7 cells.[3,4] Daclatasvir also inhibits organic anion transport polypeptides 1B1 (OAT1B1) and OAT1B3 ($IC_{50}$s = 1.5 and 3.27 µM, respectively).[5] Formulations containing daclatasvir have been used alone and in combination with NS3/4A and NS5B inhibitors in the treatment of HCV.

### References


1. Gao, M., Nettles, R.E., Belema, M., *et al. Nature* **465(7294)**, 96-100 (2010).
2. Ascher, D.B., Wielens, J., Nero, T.L., *et al. Sci. Rep.* **4**, 4765 (2014).
3. Lee, C., Ma, H., Hang, J.Q., *et al. Virology* **414(1)**, 10-18 (2011).
4. Guedj, J., Dahari, H., Rong, L., *et al. Proc. Nat. Acad. Sci. USA* **110(10)**, 3991-3996 (2013).
5. Furihata, T., Matsumoto, S., Fu, Z., *et al. Antimicrob. Agents Chemother.* **58(8)**, 4555-4565 (2014).





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