# Ivacaftor-$d_{19}$

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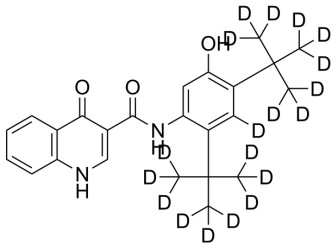
| **Cat. No.:** | HY-13017S1 |
| **CAS No.:** | 1413431-22-7 |
| **Molecular Formula:** | $C_{24}H_9D_{19}N_2O_3$ |
| **Molecular Weight:** | 411.61 |
| **Target:** | Autophagy; CFTR |
| **Pathway:** | Autophagy; Membrane Transporter/Ion Channel |
| **Storage:** | Please store the product under the recommended conditions in the Certificate of Analysis. |



## BIOLOGICAL ACTIVITY

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| **Description** | Ivacaftor-$d_9$ is a potent CFTR modulator and exhibits an $EC_{50}$ value of 255 nM for CFTR potentiation in G551D/F508del HBE Cells. Ivacaftor-D9 acts as an orally active and improved deuterated Ivacaftor analog for cystic fibrosis research[1]. |
| **In Vitro** | "Stable heavy isotopes of hydrogen, carbon, and other elements have been incorporated into drug molecules, largely as tracers for quantitation during the drug development process. Deuteration has gained attention because of its potential to affect the pharmacokinetic and metabolic profiles of drugs[1].<br>Potential advantages of deuterated compounds:<br>(1) Extend the half-life in vivo. Deuterated compounds may be able to prolong the pharmacokinetic characteristics of the compound, that is, prolong the half-life in vivo. This can improve compound safety, efficacy and tolerability, and increase ease of administration.<br>(2) Improve oral bioavailability. Deuterated compounds may reduce the degree of unwanted metabolism (first-pass metabolism) in the gut wall and liver, allowing a greater proportion of the unmetabolized drug to reach its target site of action. High bioavailability determines its activity at low doses and better tolerance.<br>(3) Improve metabolic characteristics. Deuterated compounds may reduce the formation of toxic or reactive metabolites and improve drug metabolism.<br>(4) Improve drug safety. Deuterated compounds may reduce or eliminate adverse side effects of pharmaceutical compounds and are safe.<br>(5) Preserve the therapeutic properties. Deuterated compounds are expected to retain similar biochemical potency and selectivity to hydrogen analogs in previous studies.<br>"<br>MCE has not independently confirmed the accuracy of these methods. They are for reference only. |

## REFERENCES


[1]. Russak EM, et al. Impact of Deuterium Substitution on the Pharmacokinetics of Pharmaceuticals. Ann Pharmacother. 2019;53(2):211-216.

[2]. Delaunay JL, et al. Functional defect of variants in the adenosine triphosphate-binding sites of ABCB4 and their rescue by the cystic fibrosis transmembrane conductance regulator potentiator, ivacaftor (VX-770). Hepatology. 2017 Feb;65(2):560-570

[3]. Hadida S, et al. Discovery of N-(2,4-di-tert-butyl-5-hydroxyphenyl)-4-oxo-1,4-dihydroquinoline-3-carboxamide (VX-770, ivacaftor), a potent and orally bioavailable CFTR potentiator. J Med Chem. 2014 Dec 11;57(23):9776-9

[4]. Van Goor F, et al. Rescue of CF airway epithelial cell function in vitro by a CFTR potentiator, VX-770. Proc Natl Acad Sci U S A. 2009 Nov 3;106(44):18825-30.

[5]. Mutyam V, et al. Therapeutic benefit observed with the CFTR potentiator, ivacaftor, in a CF patient homozygous for the W1282X CFTR nonsense mutation. J Cyst Fibros. 2017 Jan;16(1):24-29



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