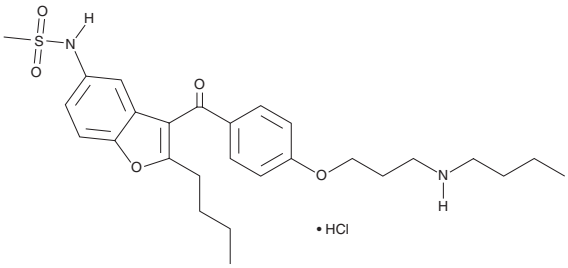
PRODUCT INFORMATION

N-Desbutyl Dronedarone (hydrochloride)

Item No. 34888



CAS Registry No.:	197431-02-0
Formal Name:	N-[2-butyl-3-[4-[3-(butylamino)propoxy]benzoyl]-5-benzofuranyl]-methanesulfonamide, monohydrochloride
MF:	$C_{27}H_{36}N_2O_5S \bullet HCl$
FW:	537.1
Purity:	≥95%
UV/Vis.:	λ_{max}: 218, 250, 291 nm
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

N-Desbutyl dronedarone (hydrochloride) is supplied as a solid. A stock solution may be made by dissolving the N-desbutyl dronedarone (hydrochloride) in the solvent of choice, which should be purged with an inert gas. N-Desbutyl dronedarone (hydrochloride) is soluble in organic solvents such as ethanol, DMSO, and dimethyl formamide (DMF). The solubility of N-desbutyl dronedarone (hydrochloride) in ethanol is approximately 1 mg/ml and approximately 30 mg/ml in DMSO and DMF.

N-Desbutyl dronedarone (hydrochloride) is sparingly soluble in aqueous buffers. For maximum solubility in aqueous buffers, N-desbutyl dronedarone (hydrochloride) should first be dissolved in DMSO and then diluted with the aqueous buffer of choice. N-Desbutyl dronedarone (hydrochloride) has a solubility of approximately 0.14 mg/ml in a 1:6 solution of DMSO:PBS (pH 7.2) using this method. We do not recommend storing the aqueous solution for more than one day.

Description

N-Desbutyl dronedarone is an active metabolite of the antiarrhythmic agent dronedarone (Item No. 9000543).[1-3] It is formed from dronedarone by cytochrome P450s (CYPs) and monoamine oxidase (MAO) in human hepatocyte preparations.[4] N-Desbutyl dronedarone inhibits the binding of 3,3',5-triiodo-L-thyronine (T3; Item No. 16028) to the thyroid hormone receptors $TR\alpha_1$ and $TR\beta_1$ (IC_{50}s = 59 and 280 µM for the chicken and human receptors, respectively).[1] It inhibits CYP2J2-mediated formation of 14,15-EET from arachidonic acid and soluble epoxide hydrolase-mediated formation of 14,15-DHET from 14,15-EET (IC_{50}s = 1.59 and 2.73 µM, respectively, in cell-free assays).[2] N-Desbutyl dronedarone decreases intracellular ATP levels in H9c2 rat cardiomyocytes (IC_{50} = 1.07 µM) and inhibits mitochondrial complex I, also known as NADH dehydrogenase, and mitochondrial complex II, also known as succinate dehydrogenase, activities in isolated rat heart mitochondria (IC_{50}s = 11.94 and 24.54 µM, respectively).[3]

References

1. Van Beeren, H.C., Jong, W.M.C., Kaptein, E., *et al*. *Endocrinology* **144(2)**, 552-558 (2003).
2. Karkhanis, A., Tram, N.D.T., and Chan, E.C.Y. *Biochem. Pharmacol.* **146**, 188-198 (2017).
3. Karkhanis, A., Leow, J.W.H., Hagen, T., *et al*. *Toxicol. Sci.* **163(1)**, 79-91 (2018).
4. Klieber, S., Arabeyre-Fabre, C., Moliner, P., *et al*. *Pharmacol. Res. Perspec.* **2(3)**, e00044 (2014).

CAYMAN CHEMICAL
1180 EAST ELLSWORTH RD
ANN ARBOR, MI 48108 · USA
PHONE: [800] 364-9897
[734] 971-3335
FAX: [734] 971-3640
CUSTSERV@CAYMANCHEM.COM
WWW.**CAYMANCHEM**.COM