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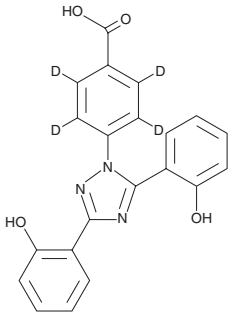
PRODUCT INFORMATION

Deferasirox-d_4

Item No. 25430

CAS Registry No.:	1133425-75-8
Formal Name:	4-[3,5-*bis*(2-hydroxyphenyl)-1H-1,2,4-triazol-1-yl]-benzoic-2,3,5,6-d_4 acid
MF:	$C_{21}H_{11}D_4N_3O_4$
FW:	377.4
Chemical Purity:	≥98% (Deferasirox)
Deuterium Incorporation:	≥99% deuterated forms (d_1-d_4); ≤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

Deferasirox-d_4 is intended for use as an internal standard for the quantification of deferasirox (Item No. 16753) 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).

Deferasirox-d_4 is supplied as a solid. A stock solution may be made by dissolving the deferasirox-d_4 in the solvent of choice, which should be purged with an inert gas. Deferasirox-d_4 is soluble in organic solvents such as ethanol, DMSO, and dimethyl formamide. The solubility of deferasirox-d_4 in these solvents is approximately 2, 20, and 30 mg/ml, respectively.

Description

Deferasirox is a synthetic, tridentate iron chelator that binds iron at a 2:1 ratio.[1] It is selective for iron (Fe(III)) over Cu(II), Zn(II), Mg(II), and Ca(II) but does bind to Al(III). Deferasirox decreases iron levels in iron-loaded rat heart cells *in vitro* by 45.8 and 55.6% compared to control levels when used at concentrations of 160 and 320 µM, respectively.[2] In hypertransfused rats, deferasirox (200 mg/kg) decreases radiolabeled liver iron levels from 41 to 21.7% and blood iron levels from 8.2 to 3.4%.[2] It is primarily excreted *via* the fecal route, in contrast to the iron chelator deferoxamine (Item No. 14595).[2] Deferasirox also inhibits proliferation of SAS human oral squamous carcinoma cells (EC_{50} = 21 µM), decreases cyclin D1 protein levels, and increases protein levels of N-Myc downregulated gene 1 (NDRG1) and NDRG3.[3] It acts in a synergistic manner when used in combination with gemcitabine (Item Nos. 11690 | 22080 | 9003096) to reduce proliferation of BxPC-3 pancreatic cancer cells *in vitro* and reduce tumor growth in a BxPC-3 mouse xenograft model when administered at a dose of 200 mg/kg.[4] Formulations containing deferasirox have been used in the treatment of β-thalassemia and chronic iron overload.

References

1. Heinz, U., Hegetschweiler, K., Acklin, P., *et al. Angew. Chem. Int. Ed.* **38(17)**, 2568-2570 (1999).
2. Hershko, C., Konijn, A.M., Nick, H.P., *et al. Blood* **97(4)**, 1115-1122 (2001).
3. Lee, J.-C., Chiang, K.-C., Feng, T.-H., *et al. Int. J. Mol. Sci.* **17(9)**, pii: E1435 (2016).
4. Shinoda, S., Kaino, S., Amano, S., *et al. Oncotarget* **9(47)**, 28434-28444 (2018).

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