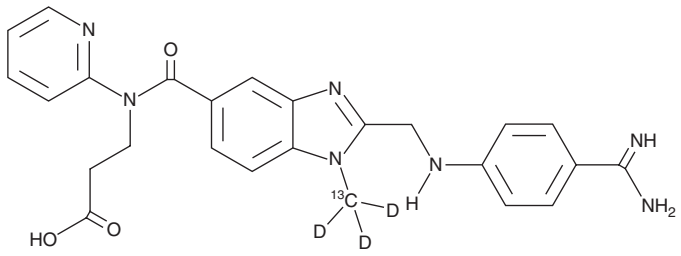
PRODUCT INFORMATION

Dabigatran-^{13}C-d$_3$

Item No. 35705

CAS Registry No.: 2967480-55-1
Formal Name: N-[[2-[[[4-(aminoiminomethyl)phenyl]amino]methyl]-1-methyl-^{13}C-d$_3$-1H-benzimidazol-5-yl]carbonyl]-N-2-pyridinyl-β-alanine
MF: $C_{24}[^{13}C]H_{22}D_3N_7O_3$
FW: 475.5
Chemical Purity: ≥95% (Dabigatran)
Deuterium Incorporation: ≥99% deuterated forms (d_1-d_3); ≤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

Dabigatran-^{13}C-d$_3$ is intended for use as an internal standard for the quantification of dabigatran (Item No. 17133) 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).

Dabigatran-^{13}C-d$_3$ is supplied as a solid. A stock solution may be made by dissolving the dabigatran-^{13}C-d$_3$ in the solvent of choice, which should be purged with an inert gas. Dabigatran-^{13}C-d$_3$ is soluble in the organic solvent DMSO at a concentration of approximately 0.5 mg/ml. Dabigatran-^{13}C-d$_3$ is soluble in an acidic solution.

Description

Dabigatran is an inhibitor of thrombin (K_i = 0.0045 µM) and an active metabolite of the thrombin inhibitor prodrug dabigatran etexilate (Item No. 17131).[1,2] It also inhibits trypsin (K_i = 0.0503 µM) but is selective for thrombin and trypsin over plasmin, Factor Xa, activated protein C, and tissue plasminogen activator (tPA; K_is = 1.695, 3.76, 20.93, and 45.36 µM, respectively).[1]

References

1. Hauel, N.H., Nar, H., Priepke, H., *et al.* Structure-based design of novel potent nonpeptide thrombin inhibitors. *J. Med. Chem.* **45(9)**, 1757-1766 (2002).
2. Eisert, W.G., Hauel, N., Stangier, J., *et al.* Dabigatran: An oral novel potent reversible nonpeptide inhibitor of thrombin. *Arterioscler. Thromb. Vasc. Biol.* **30(10)**, 1885-1889 (2010).

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