

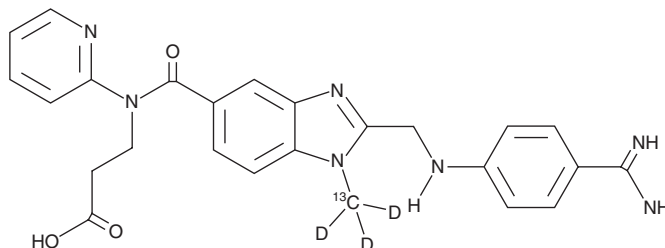
PRODUCT INFORMATION



Dabigatran-¹³C-d₃

Item No. 35705

CAS Registry No.: 2967480-55-1
Formal Name: N-[[2-[[[4-(aminoiminomethyl)phenyl]amino]methyl]-1-methyl-¹³C-d₃-1H-benzimidazol-5-yl]carbonyl]-N-2-pyridinyl-β-alanine
MF: C₂₄[¹³C]H₂₂D₃N₇O₃
FW: 475.5
Chemical Purity: ≥95% (Dabigatran)
Deuterium Incorporation: ≥99% deuterated forms (d₁-d₃); ≤1% d₀
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-¹³C-d₃ 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-¹³C-d₃ is supplied as a solid. A stock solution may be made by dissolving the dabigatran-¹³C-d₃ in the solvent of choice, which should be purged with an inert gas. Dabigatran-¹³C-d₃ is soluble in the organic solvent DMSO at a concentration of approximately 0.5 mg/ml. Dabigatran-¹³C-d₃ is soluble in an acidic solution.

Description

Dabigatran is an inhibitor of thrombin ($K_i = 0.0045 \mu\text{M}$) and an active metabolite of the thrombin inhibitor prodrug dabigatran etexilate (Item No. 17131).^{1,2} It also inhibits trypsin ($K_i = 0.0503 \mu\text{M}$) but is selective for thrombin and trypsin over plasmin, Factor Xa, activated protein C, and tissue plasminogen activator (tPA; $K_{iS} = 1.695, 3.76, 20.93, \text{ and } 45.36 \mu\text{M}$, respectively).¹

References

- Huel, 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).
- Eisert, W.G., Huel, N., Stangier, J., *et al.* Dabigatran: An oral novel potent reversible nonpeptide inhibitor of thrombin. *Arterioscler. Thromb. Vasc. Biol.* **30**(10), 1885-1889 (2010).

WARNING

THIS PRODUCT IS FOR RESEARCH ONLY - NOT FOR HUMAN OR VETERINARY DIAGNOSTIC OR THERAPEUTIC USE.

SAFETY DATA

This material should be considered hazardous until further information becomes available. Do not ingest, inhale, get in eyes, on skin, or on clothing. Wash thoroughly after handling. Before use, the user must review the complete Safety Data Sheet, which has been sent via email to your institution.

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