



Product Information

Heptafluorobutyric acid

Product Number **H 7133**
Storage Temperature 2-8 °C

Product Description

Molecular Formula: C₄HF₇O₂
Molecular Weight: 214.0
CAS Number: 375-22-4
Boiling Point: 120 °C
Density: 1.645 g/ml
Molarity: 7.69 M (based on density)
pK_a: approximately 0.4
Synonyms: HFBA, perfluorobutyric acid

Heptafluorobutyric acid (HFBA) is a strong acid and ion-pairing agent that is used in analytical chemistry, notably in HPLC and in gas chromatography/mass spectrometry (GC/MS), in a similar manner to trifluoroacetic acid (TFA). The strong acidity of HFBA ensures that other acidic groups such as carboxylic acid moieties on biomolecules remain protonated, and thus the biomolecule samples are able to interact with organic solvents in such processes as reverse phase chromatography. The longer alkyl chain of HFBA makes it more hydrophobic than TFA, and thus HFBA can be utilized with more hydrophobic samples.¹

HFBA (0.1%) has been used in the mobile phase of an HPLC/LC-MS protocol for the detection of marine bacterioplankton siderophores.² A study of the effects of various acids, including HFBA, on the resolution of intact proteins by reversed-phase LC/ESI-MS has been published.³ A modified version of the peptide ladder sequencing technique that incorporates allyl isothiocyanate and HFBA has been reported.⁴

The use of HFBA in a method for the chiral LC analysis of (+)- and (-)-epibatidine has been reported.⁵ The analysis of selenium containing compounds using

Precautions and Disclaimer

For Laboratory Use Only. Not for drug, household or other uses.

Preparation Instructions

This product is miscible in ethanol (0.1 ml/ml, v/v), yielding a clear, colorless solution.

References

1. Serwe, M., et al., in *Microcharacterization of Proteins*, 2nd ed., Kellner, R. et al., ed. Wiley-VCH (Weinheim, Germany: 1999), pp. 69-70.
2. McCormack, P., et al., Separation and detection of siderophores produced by marine bacterioplankton using high-performance liquid chromatography with electrospray ionization mass spectrometry. *Anal. Chem.*, **75(11)**, 2647-2652 (2003).
3. Garcia, M. C., et al., Effect of the mobile phase composition on the separation and detection of intact proteins by reversed-phase liquid chromatography-electrospray mass spectrometry. *J. Chromatogr. A*, **957(2)**, 187-199 (2002).
4. Gu, Q. M., and Prestwich, G. D., Efficient peptide ladder sequencing by MALDI-TOF mass spectrometry using allyl isothiocyanate. *J. Pept. Res.*, **49(6)**, 484-491 (1997).
5. Watt, A. P., et al., Determination of the *in vitro* metabolism of (+)- and (-)-epibatidine. *J. Chromatogr. A*, **896(1-2)**, 229-238 (2000).
6. Lindemann, T., and Hintelmann, H., Selenium speciation by HPLC with tandem mass spectrometric detection. *Anal. Bioanal. Chem.*, **372(3)**, 486-490 (2002).

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HFBA in the MS matrix has been described.⁶

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