3050 Spruce Street
Saint Louis, Missouri 63103 USA
Telephone 800-325-5832 • (314) 771-5765
Fax (314) 286-7828
email: techserv@sial.com
sigma-aldrich.com

# ProductInformation

**Acetonitrile**

Product Number **A 3396**
Store at Room Temperature

**Product Description**
Molecular Formula: $C_2H_3N$
Molecular Weight: 41.05
CAS Number: 75-05-8
Boiling Point: 81.6 °C[1]
Density: 0.787 g/ml (15 °C)[1]
Surface tension: 29.04 dynes/cm (20 °C)[1]
Synonyms: methyl cyanide, cyanomethane, ethanenitrile[1]

Acetonitrile is a widely used, polar aprotic organic solvent. Acetonitrile is utilized as a starting material for the production of such compounds as acetophenone, α-naphthaleneacetic acid, thiamine, and acetamidine. It can be used in the recrystallization of steroids and as a solvent for non-aqueous titrations, as well as a non-aqueous solvent for inorganic salts.[1] In analytical chemistry, acetonitrile is utilized in such areas as biopartitioning studies, in the HPLC analysis of small organic compounds, and enantiomer resolution by LC on polysaccharide type chiral stationary phases.[2,3,4]

A method for the pre-fractionation of lysates of cells and tissue for proteomics analysis that incorporates a five-step gradient of increasing acetonitrile concentrations has been published.[5] A protocol has been reported for the enrichment of low-abundance peptides for proteomic analysis that uses acetonitrile as part of the elution-modified displacement chromatography method.[6] A method that incorporates acetonitrile in the mobile phase for the LC/ESI-MS analysis of flavonoid glycosides has been described.[7] The use of acetonitrile and other organic solvents in mixed organic/aqueous solvents in the digestion of proteins on immobilized trypsin columns has been reported.[8]

Acetonitrile has been used in the synthesis of such organic compounds as functionalized pyrrolo[3,2-*d*]pyrimidines, methanesulfonyl carbonates, and arylzinc compounds.[9,10,11]

Inorganic compounds which have been synthesized in acetonitrile include dimorphic copper(I) coordination polymers, osmium phosphiniminato complexes, and vanadium iron sulfur clusters as structural analogs to the PN cluster of nitrogenase.[12,13,14]

**Precautions and Disclaimer**
For Laboratory Use Only. Not for drug, household or other uses.

**Preparation Instructions**
This product is miscible in water, methanol, ethyl acetate, acetone, ether, chloroform, and many unsaturated hydrocarbons.[1]

**References**
1. The Merck Index, 12th ed., Entry# 68.
2. Cimpean, D. M., and Poole, C. F., Systematic search for surrogate chromatographic models of biopartitioning processes. Analyst, **127(6)**, 724-729 (2002).
3. Loregian, A., et al., Separation methods for acyclovir and related antiviral compounds. J. Chromatogr. B Biomed. Sci. Appl., **764(1-2)**, 289-311 (2001).
4. Tachibana, K., and Ohnishi, A., Reversed-phase liquid chromatographic separation of enantiomers on polysaccharide type chiral stationary phases. J. Chromatogr. A, **906(1-2)**, 127-154 (2001).
5. Badock, V., et al., Prefractionation of protein samples for proteome analysis using reversed-phase high-performance liquid chromatography. Electrophoresis, **22(14)**, 2856-2864 (2001).
6. Wilkins, J. A., et al., Selective enrichment of low-abundance peptides in complex mixtures by elution-modified displacement chromatography and their identification by electrospray ionization mass spectrometry. Anal. Chem., **74(16)**, 3933-3941 (2002).

7. Cuyckens, F., and Claeys, M., Optimization of a liquid chromatography method based on simultaneous electrospray ionization mass spectrometric and ultraviolet photodiode array detection for analysis of flavonoid glycosides. Rapid Commun. Mass Spectrom., **16(24)**, 2341-2348 (2002).
8. Slysz, G. W., and Schriemer, D. C., On-column digestion of proteins in aqueous-organic solvents. Rapid Commun. Mass. Spectrom., **17(10)**, 1044-1050 (2003).
9. Marcotte, F. A., et al., Diversity-oriented synthesis of functionalized pyrrolo[3,2-*d*]pyrimidines with variation of the pyrimidine ring nitrogen substituents. J. Org. Chem., **68(18)**, 6984-6987 (2003).
10. Bratt, M. O., and Taylor, P. C., Synthesis of carbonates and related compounds from carbon dioxide via methanesulfonyl carbonates. J. Org. Chem., **68(14)**, 5439-5444 (2003).
11. Fillon, H., et al., New chemical synthesis of functionalized arylzinc compounds from aromatic or thienyl bromides under mild conditions using a simple cobalt catalyst and zinc dust. J. Am. Chem. Soc., **125(13)**, 3867-3870 (2003).
12. Nather, C., and Jess, I., Synthesis, crystal structures, and thermal and thermodynamic properties of dimorphic copper(I) coordination polymers. Inorg. Chem., **42(9)**, 2968-2976 (2003).
13. Bennett, B. K., et al., Osmium phosphiniminato complexes: synthesis, protonation, structure, and redox-coupled hydrolytic scission of N-p bonds. Inorg. Chem., **42(13)**, 4127-4134 (2003).
14. Zuo, J. L., et al., Vanadium-iron-sulfur clusters containing the cubane-type [$VFe_3S_4$] core unit: synthesis of a cluster with the topology of the PN cluster of nitrogenase. Inorg. Chem., **42(15)**, 4624-4631 (2003).

GCY/RXR 11/03