

**Product Name:** Acetonitrile, LC-MS Grade, 99.8%, Thermo Scientific Chemicals

**Catalog Number:** 047138.K2

**CAS Number:** 75-05-8  
**IUPAC Name:** acetonitrile  
**Molecular Formula:** C<sub>2</sub>H<sub>3</sub>N  
**Molecular Weight:** 41.05  
**InChI Key:** WEVYAHXRMPXWCK-UHFFFAOYSA-N  
**SMILES:** CC#N  
**Synonym:** acetonitrile NCMc MeCN cyanure de methyl acetonitrile, 1-(14)c-labeled usaf EK-488  
 1-(14)c-labeled acetonitrile acetonitrile, 3H-labeled 1-(14)C-labeled acetonitrile  
 3h-labeled acetonitrile

## Product Specification

**Form:** Clear liquid

**Trace Metal:** ≤0.1 ppm each of: Barium (Ba), Calcium (Ca), Iron (Fe), Magnesium (Mg), Potassium (K), Silver (Ag), Sodium (Na), Tin (Sn), Zinc (Zn)

**Color (APHA):** ≤5

**Assay (unspecified):** Fluorescence at emission max for impurities ( at 254 nm): ≤1 ppb

**Assay (Titration):** Titrable acid ≤0.008 meq/g

**Assay (Titration):** Titrable base ≤0.0006 meq/g

**Assay (GC):** GC-ECD Responsive residue (single peak (as Heptachlorepoxyde):≤ 10 ppt

**Assay (GC):** GC-FID Responsive residue ( single peak) ( as 2-Octanol): ≤ 5 ppb

**Assay (HPLC):** LC gradient elution suitability at: 210nm:≤3 mAU and at 254nm: ≤0.5 mAU

**Comment:** Submicron filtered

**Water Content (Karl Fischer Titration):** ≤0.01%

**LCMS:** ≤50 ppb negative mode as Nitrophenol

**LCMS:** ≤50 ppb positive mode as Reserpine

**Optical Absorbance at:** 190 nm: ≤1.00 AU, 195 nm: ≤0.14 AU, 200 nm: ≤0.05 AU, 210 nm: ≤0.04 AU, 220 nm: ≤0.02 AU, 230 nm: ≤ 0.01 AU, 254 nm: ≤0.005 AU, 400 nm: ≤0.005 AU

**Residue on Evaporation:** ≤1 ppm

**Trace Metal:** ≤0.01 ppm each of: Copper (Cu), Manganese (Mn)

**Assay (GC):**  $\geq 99.8\%$  (corrected for water)  
**Trace Metal:**  $\leq 0.02$  ppm each of: Chromium (Cr), Cobalt (Co), Lead (Pb), Nickel (Ni)  
**Trace Metal:**  $\leq 0.5$  ppm each of: Aluminum (Al) and Cadmium (Cd):

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**Date Of Print:** 03/12/2025

*Product Specifications are subject to amendment and may change over time. Data contained is accurate as of the date printed.*