

# SAFETY DATA SHEET

## LC/MS ESI-X Tuning Mix

### Section 1. Identification

**Product identifier** : LC/MS ESI-X Tuning Mix

**Part no.** : 5191-6449

**Relevant identified uses of the substance or mixture and uses advised against**

**Identified uses** : Reagents and Standards for Analytical Chemistry Laboratory Use  
Bottle  
100 ml

**Supplier/Manufacturer** : Agilent Technologies, Inc.  
5301 Stevens Creek Blvd  
Santa Clara, CA 95051, USA  
800-227-9770

**Emergency telephone number (with hours of operation)** : CHEMTREC®: 1-800-424-9300

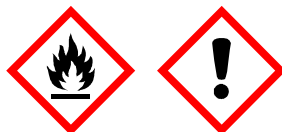
### Section 2. Hazard identification

**Classification of the substance or mixture**

H225 FLAMMABLE LIQUIDS - Category 2  
H302 ACUTE TOXICITY (oral) - Category 4  
H312 ACUTE TOXICITY (dermal) - Category 4  
H332 ACUTE TOXICITY (inhalation) - Category 4  
H319 EYE IRRITATION - Category 2A

**GHS label elements**

**Hazard pictograms** :



**Signal word** : Danger

**Hazard statements** : H225 - Highly flammable liquid and vapor.  
H302 + H312 + H332 - Harmful if swallowed, in contact with skin or if inhaled.  
H319 - Causes serious eye irritation.

**Precautionary statements**

**Prevention** : P280 - Wear protective gloves and protective clothing. Wear eye or face protection.  
P210 - Keep away from heat, hot surfaces, sparks, open flames and other ignition sources. No smoking.  
P261 - Avoid breathing vapor.  
P270 - Do not eat, drink or smoke when using this product.  
P264 - Wash thoroughly after handling.

**Response** : P304 + P312 - IF INHALED: Call a POISON CENTER or doctor if you feel unwell.  
P302 + P312 - IF ON SKIN: Call a POISON CENTER or doctor if you feel unwell.  
P305 + P351 + P338 - IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing.  
P337 + P313 - If eye irritation persists: Get medical advice or attention.

**Storage** : Not applicable.

**Disposal** : P501 - Dispose of contents and container in accordance with all local, regional, national and international regulations.

## Section 3. Composition/information on ingredients

**Substance/mixture** : Mixture

Ingredient name	Synonyms	% (w/w)	Identifiers	
Acetonitrile	Acetonitrile	≥80	CAS: 75-05-8	-

Ranges if listed above for hazardous ingredient(s) are prescribed ranges. The actual concentration(s) or actual concentration range(s) are being withheld as a trade secret.

There are no additional ingredients present which, within the current knowledge of the supplier and in the concentrations applicable, are classified and hence require reporting in this section.

Occupational exposure limits, if available, are listed in Section 8.

## Section 4. First-aid measures

### Description of necessary first aid measures

- Eye contact** : Immediately flush eyes with plenty of water, occasionally lifting the upper and lower eyelids. Check for and remove any contact lenses. Continue to rinse for at least 10 minutes. Get medical attention.
- Inhalation** : Remove victim to fresh air and keep at rest in a position comfortable for breathing. If it is suspected that fumes are still present, the rescuer should wear an appropriate mask or self-contained breathing apparatus. If not breathing, if breathing is irregular or if respiratory arrest occurs, provide artificial respiration or oxygen by trained personnel. It may be dangerous to the person providing aid to give mouth-to-mouth resuscitation. Get medical attention if adverse health effects persist or are severe. If necessary, call a poison center or physician. If unconscious, place in recovery position and get medical attention immediately. Maintain an open airway. Loosen tight clothing such as a collar, tie, belt or waistband. In case of inhalation of decomposition products in a fire, symptoms may be delayed. The exposed person may need to be kept under medical surveillance for 48 hours.
- Skin contact** : Wash with plenty of soap and water. Remove contaminated clothing and shoes. Wash contaminated clothing thoroughly with water before removing it, or wear gloves. Continue to rinse for at least 10 minutes. Get medical attention if adverse health effects persist or are severe. If necessary, call a poison center or physician. Wash clothing before reuse. Clean shoes thoroughly before reuse.
- Ingestion** : Wash out mouth with water. Remove dentures if any. If material has been swallowed and the exposed person is conscious, give small quantities of water to drink. Stop if the exposed person feels sick as vomiting may be dangerous. Do not induce vomiting unless directed to do so by medical personnel. If vomiting occurs, the head should be kept low so that vomit does not enter the lungs. Get medical attention. If necessary, call a poison center or physician. Never give anything by mouth to an unconscious person. If unconscious, place in recovery position and get medical attention immediately. Maintain an open airway. Loosen tight clothing such as a collar, tie, belt or waistband.

### Most important symptoms/effects, acute and delayed

#### Potential acute health effects

- Eye contact** : Causes serious eye irritation.
- Inhalation** : Harmful if inhaled.
- Skin contact** : Harmful in contact with skin.
- Ingestion** : Harmful if swallowed.

#### Over-exposure signs/symptoms

- Eye contact** : Adverse symptoms may include the following:  
pain or irritation  
watering  
redness
- Inhalation** : No specific data.

## Section 4. First-aid measures

- Skin contact** : No specific data.
- Ingestion** : No specific data.

### Indication of immediate medical attention and special treatment needed, if necessary

- Notes to physician** : In case of inhalation of decomposition products in a fire, symptoms may be delayed. The exposed person may need to be kept under medical surveillance for 48 hours.
- Specific treatments** : No specific treatment.
- Protection of first-aiders** : No action shall be taken involving any personal risk or without suitable training. If it is suspected that fumes are still present, the rescuer should wear an appropriate mask or self-contained breathing apparatus. It may be dangerous to the person providing aid to give mouth-to-mouth resuscitation. Wash contaminated clothing thoroughly with water before removing it, or wear gloves.

See toxicological information (Section 11)

## Section 5. Fire-fighting measures

### Extinguishing media

- Suitable extinguishing media** : Use dry chemical, CO<sub>2</sub>, water spray (fog) or foam.
- Unsuitable extinguishing media** : Do not use water jet.

**Specific hazards arising from the chemical** : Highly flammable liquid and vapor. Runoff to sewer may create fire or explosion hazard. In a fire or if heated, a pressure increase will occur and the container may burst, with the risk of a subsequent explosion.

**Hazardous thermal decomposition products** : Decomposition products may include the following materials:  
carbon dioxide  
carbon monoxide  
nitrogen oxides  
cyanides

**Special protective actions for fire-fighters** : Promptly isolate the scene by removing all persons from the vicinity of the incident if there is a fire. No action shall be taken involving any personal risk or without suitable training. Move containers from fire area if this can be done without risk. Use water spray to keep fire-exposed containers cool.

**Special protective equipment for fire-fighters** : Fire-fighters should wear appropriate protective equipment and self-contained breathing apparatus (SCBA) with a full face-piece operated in positive pressure mode.

## Section 6. Accidental release measures

### Personal precautions, protective equipment and emergency procedures

- For non-emergency personnel** :  No action shall be taken involving any personal risk or without suitable training. Evacuate surrounding areas. Keep unnecessary and unprotected personnel from entering. Do not touch or walk through spilled material. Shut off all ignition sources. No flares, smoking or flames in hazard area. Avoid breathing vapor. Put on appropriate personal protective equipment.
- For emergency responders** : If specialized clothing is required to deal with the spillage, take note of any information in Section 8 on suitable and unsuitable materials. See also the information in "For non-emergency personnel".

**Environmental precautions** : Avoid dispersal of spilled material and runoff and contact with soil, waterways, drains and sewers. Inform the relevant authorities if the product has caused environmental pollution (sewers, waterways, soil or air).

## Section 6. Accidental release measures

### Methods and materials for containment and cleaning up

- Methods for cleaning up** : Stop leak if without risk. Move containers from spill area. Use spark-proof tools and explosion-proof equipment. Dilute with water and mop up if water-soluble. Alternatively, or if water-insoluble, absorb with an inert dry material and place in an appropriate waste disposal container. Dispose of via a licensed waste disposal contractor.

## Section 7. Handling and storage

### Precautions for safe handling

- Protective measures** : Put on appropriate personal protective equipment (see Section 8). Do not ingest. Avoid contact with eyes, skin and clothing. Avoid breathing vapor or mist. Use only with adequate ventilation. Wear appropriate respirator when ventilation is inadequate. Do not enter storage areas and confined spaces unless adequately ventilated. Keep in the original container or an approved alternative made from a compatible material, kept tightly closed when not in use. Store and use away from heat, sparks, open flame or any other ignition source. Use explosion-proof electrical (ventilating, lighting and material handling) equipment. Use only non-sparking tools. Take precautionary measures against electrostatic discharges. Empty containers retain product residue and can be hazardous. Do not reuse container.

- Advice on general occupational hygiene** : Eating, drinking and smoking should be prohibited in areas where this material is handled, stored and processed. Workers should wash hands and face before eating, drinking and smoking. Remove contaminated clothing and protective equipment before entering eating areas. See also Section 8 for additional information on hygiene measures.

- Conditions for safe storage, including any incompatibilities** : Store in accordance with local regulations. Store in a segregated and approved area. Store in original container protected from direct sunlight in a dry, cool and well-ventilated area, away from incompatible materials (see Section 10) and food and drink. Eliminate all ignition sources. Separate from oxidizing materials. Keep container tightly closed and sealed until ready for use. Containers that have been opened must be carefully resealed and kept upright to prevent leakage. Do not store in unlabeled containers. Use appropriate containment to avoid environmental contamination. See Section 10 for incompatible materials before handling or use.

## Section 8. Exposure controls/personal protection

### Control parameters

### Occupational exposure limits

Ingredient name	Exposure limits
Acetonitrile	<p><b>CA Saskatchewan Provincial (Canada, 4/2021)</b> Absorbed through skin.            STEL 15 minutes: 30 ppm.            TWA 8 hours: 20 ppm.</p> <p><b>CA British Columbia Provincial (Canada, 8/2025)</b> Absorbed through skin.            TWA 8 hours: 20 ppm.</p> <p><b>CA Ontario Provincial (Canada, 6/2019)</b> Absorbed through skin.            TWA 8 hours: 20 ppm.</p> <p><b>CA Quebec Provincial (Canada, 2/2024)</b> Absorbed through skin.            TWAEV 8 hours: 20 ppm.</p> <p><b>CA Alberta Provincial (Canada, 3/2023)</b> OEL 8 hours: 34 mg/m<sup>3</sup>.</p>

## Section 8. Exposure controls/personal protection

OEL 8 hours: 20 ppm.

### Biological exposure indices

No exposure indices known.

- Appropriate engineering controls** : Use only with adequate ventilation. Use process enclosures, local exhaust ventilation or other engineering controls to keep worker exposure to airborne contaminants below any recommended or statutory limits. The engineering controls also need to keep gas, vapor or dust concentrations below any lower explosive limits. Use explosion-proof ventilation equipment.
- Environmental exposure controls** : Emissions from ventilation or work process equipment should be checked to ensure they comply with the requirements of environmental protection legislation. In some cases, fume scrubbers, filters or engineering modifications to the process equipment will be necessary to reduce emissions to acceptable levels.

### Individual protection measures

- Hygiene measures** : Wash hands, forearms and face thoroughly after handling chemical products, before eating, smoking and using the lavatory and at the end of the working period. Appropriate techniques should be used to remove potentially contaminated clothing. Wash contaminated clothing before reusing. Ensure that eyewash stations and safety showers are close to the workstation location.
- Eye/face protection** : Safety eyewear complying with an approved standard should be used when a risk assessment indicates this is necessary to avoid exposure to liquid splashes, mists, gases or dusts. If contact is possible, the following protection should be worn, unless the assessment indicates a higher degree of protection: chemical splash goggles.
- Skin protection**
- Hand protection** : Chemical-resistant, impervious gloves complying with an approved standard should be worn at all times when handling chemical products if a risk assessment indicates this is necessary. Considering the parameters specified by the glove manufacturer, check during use that the gloves are still retaining their protective properties. It should be noted that the time to breakthrough for any glove material may be different for different glove manufacturers. In the case of mixtures, consisting of several substances, the protection time of the gloves cannot be accurately estimated.
- Body protection** : Personal protective equipment for the body should be selected based on the task being performed and the risks involved and should be approved by a specialist before handling this product. When there is a risk of ignition from static electricity, wear anti-static protective clothing. For the greatest protection from static discharges, clothing should include anti-static overalls, boots and gloves.
- Other skin protection** : Appropriate footwear and any additional skin protection measures should be selected based on the task being performed and the risks involved and should be approved by a specialist before handling this product.
- Respiratory protection** : Based on the hazard and potential for exposure, select a respirator that meets the appropriate standard or certification. Respirators must be used according to a respiratory protection program to ensure proper fitting, training, and other important aspects of use.

## Section 9. Physical and chemical properties

The conditions of measurement of all properties are at standard temperature and pressure unless otherwise indicated.

### Appearance

- Physical state** : Liquid. [Clear.]
- Color** : Colorless.
- Odor** : Ether-like.

## Section 9. Physical and chemical properties

<b>Odor threshold</b>	: Not available.
<b>pH</b>	: Not available.
<b>Melting point/freezing point</b>	: Not available.
<b>Initial boiling point and boiling range</b>	: 81.6°C (178.9°F)
<b>Flash point</b>	: Closed cup: 12.8°C (55°F)
<b>Evaporation rate</b>	: Not available.
<b>Flammability (solid, gas)</b>	: Not applicable.
<b>Upper/lower flammability or explosive limits</b>	: Lower: 4.4% Upper: 16%
<b>Vapor pressure</b>	: 11.6 kPa (87.0071427 mm Hg)
<b>Vapor density</b>	: Not available.
<b>Relative density</b>	: Not available.

<b>Solubility</b>	: <b>Media</b>	<b>Result</b>
	water	Soluble

<b>Miscible with water</b>	: Yes.
<b>Partition coefficient: n-octanol/water</b>	: Not applicable.
<b>Auto-ignition temperature</b>	: 524°C (975.2°F)
<b>Decomposition temperature</b>	: Not available.
<b>Viscosity</b>	: Dynamic (room temperature): Not available. Kinematic (room temperature): Not available. Kinematic (40°C (104°F)): Not available.

### Particle characteristics

<b>Median particle size</b>	: Not applicable.
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## Section 10. Stability and reactivity

<b>Reactivity</b>	: No specific test data related to reactivity available for this product or its ingredients.
<b>Chemical stability</b>	: The product is stable.
<b>Possibility of hazardous reactions</b>	: Under normal conditions of storage and use, hazardous reactions will not occur.
<b>Conditions to avoid</b>	: Avoid all possible sources of ignition (spark or flame). Do not pressurize, cut, weld, braze, solder, drill, grind or expose containers to heat or sources of ignition.
<b>Incompatible materials</b>	: Reactive or incompatible with the following materials: oxidizing materials
<b>Hazardous decomposition products</b>	: Under normal conditions of storage and use, hazardous decomposition products should not be produced.

## Section 11. Toxicological information

### Information on toxicological effects

#### Acute toxicity

<b>Product/ingredient name</b>	<b>Result</b>	
Acetonitrile	Rat - Oral - LD50	2460 mg/kg
	Rat - Inhalation - LC50 Vapor	17100 ppm [4 hours]

**Conclusion/Summary [Product]** : Not available.

#### Skin corrosion/irritation

**Conclusion/Summary [Product]** : Not available.

#### Serious eye damage/eye irritation

<b>Product/ingredient name</b>	<b>Result</b>	
Acetonitrile	Rabbit - Eyes - Moderate irritant	Duration of treatment/ exposure: 24 hours Amount/concentration applied: 100 uL

**Conclusion/Summary [Product]** : Not available.

#### Respiratory corrosion/irritation

**Conclusion/Summary [Product]** : May cause respiratory irritation.

<b>Ingredient name</b>	<b>Conclusion/Summary</b>
Acetonitrile	May cause respiratory irritation.

#### Respiratory corrosion/irritation

Not available.

**Conclusion/Summary [Product]** : May cause respiratory irritation.

<b>Ingredient name</b>	<b>Conclusion/Summary</b>
acetonitrile	May cause respiratory irritation.

#### Respiratory or skin sensitization

##### **Skin**

**Conclusion/Summary [Product]** : Not available.

##### **Respiratory**

**Conclusion/Summary [Product]** : Not available.

#### Germ cell mutagenicity

**Conclusion/Summary [Product]** : Not available.

## Section 11. Toxicological information

### Carcinogenicity

**Conclusion/Summary** : Not available.

[Product]

### Classification

Product/ingredient name	IARC	NTP	ACGIH
Acetonitrile	-	-	A4

### Reproductive toxicity

**Conclusion/Summary** : Not available.

[Product]

### Specific target organ toxicity (single exposure)

Not available.

### Specific target organ toxicity (repeated exposure)

Not available.

### Aspiration hazard

Not available.

**Information on the likely routes of exposure** : Routes of entry anticipated: Oral, Dermal, Inhalation, Eyes.

### Potential acute health effects

**Eye contact** : Causes serious eye irritation.

**Inhalation** : Harmful if inhaled.

**Skin contact** : Harmful in contact with skin.

**Ingestion** : Harmful if swallowed.

### Symptoms related to the physical, chemical and toxicological characteristics

**Eye contact** : Adverse symptoms may include the following:  
pain or irritation  
watering  
redness

**Inhalation** : No specific data.

**Skin contact** : No specific data.

**Ingestion** : No specific data.

### Delayed and immediate effects and also chronic effects from short and long term exposure

#### Short term exposure

**Potential immediate effects** : Not available.

**Potential delayed effects** : Not available.

#### Long term exposure

**Potential immediate effects** : Not available.

**Potential delayed effects** : Not available.

## Section 11. Toxicological information

### Potential chronic health effects

<b>Conclusion/Summary [Product]</b>	: Not available.
<b>General</b>	: No known significant effects or critical hazards.
<b>Carcinogenicity</b>	: No known significant effects or critical hazards.
<b>Mutagenicity</b>	: No known significant effects or critical hazards.
<b>Reproductive toxicity</b>	: No known significant effects or critical hazards.

### Numerical measures of toxicity

#### Acute toxicity estimates

Product/ingredient name	Oral (mg/kg)	Dermal (mg/kg)	Inhalation (gases) (ppm)	Inhalation (vapors) (mg/l)	Inhalation (dusts and mists) (mg/l)
LC/MS ESI-X Tuning Mix Acetonitrile	533.5 500	1173.7 1100	N/A N/A	11.7 11	N/A N/A

**Other information** : Adverse symptoms may include the following: May cause headache, weakness, dizziness, shortness of breath, cyanosis, rapid heart beat, unconsciousness and possible death.

## Section 12. Ecological information

### Toxicity

Product/ingredient name	Result
Acetonitrile	Acute - LC50 - Fresh water 3600 mg/l [48 hours] Daphnia - Water flea - <i>Daphnia magna</i>
	Acute - IC50 - Fresh water 3685 mg/l [96 hours] Aquatic plants - Duckweed - <i>Lemna minor</i>
	Chronic - NOEC - Fresh water 160 mg/l [21 days] Daphnia - Water flea - <i>Daphnia magna</i>
	Chronic - NOEC - Fresh water 1000 mg/l [96 hours] Aquatic plants - Duckweed - <i>Lemna minor</i>
	Acute - LC50 - Fresh water 1000 mg/l [96 hours] Fish - Fathead minnow - <i>Pimephales promelas</i>

**Conclusion/Summary [Product]** : Not available.

### Persistence and degradability

Product/ingredient name	Result
Acetonitrile	OECD [Ready Biodegradability - CO <sub>2</sub> in Sealed Vessels (Headspace Test)] 70% [21 days] - Readily -

**Conclusion/Summary [Product]** : Not available.

Product/ingredient name	Aquatic half-life	Photolysis	Biodegradability
Acetonitrile	-	-	Readily

## Section 12. Ecological information

### Bioaccumulative potential

Product/ingredient name	LogP <sub>ow</sub>	BCF	Potential
Acetonitrile	-0.34	3	Low

### Mobility in soil




Soil/Water partition coefficient : Not available.

Other adverse effects : No known significant effects or critical hazards.

## Section 13. Disposal considerations

**Disposal methods** : The generation of waste should be avoided or minimized wherever possible. Disposal of this product, solutions and any by-products should at all times comply with the requirements of environmental protection and waste disposal legislation and any regional local authority requirements. Dispose of surplus and non-recyclable products via a licensed waste disposal contractor. Waste should not be disposed of untreated to the sewer unless fully compliant with the requirements of all authorities with jurisdiction. Waste packaging should be recycled. Incineration or landfill should only be considered when recycling is not feasible. This material and its container must be disposed of in a safe way. Care should be taken when handling emptied containers that have not been cleaned or rinsed out. Empty containers or liners may retain some product residues. Vapor from product residues may create a highly flammable or explosive atmosphere inside the container. Do not cut, weld or grind used containers unless they have been cleaned thoroughly internally. Avoid dispersal of spilled material and runoff and contact with soil, waterways, drains and sewers.

## Section 14. Transport information

	TDG Classification	IMDG	IATA
UN number	UN1648	UN1648	UN1648
UN proper shipping name	ACETONITRILE solution	ACETONITRILE solution	Acetonitrile solution
Transport hazard class(es)	3 	3 	3 
Packing group	II	II	II
Environmental hazards	No.	No.	No.

**Proof of classification statement** : Product classified as per the following sections of the Transportation of Dangerous Goods Regulations: 2.18-2.19 (Class 3).

### Additional information

**TDG Classification** : Product classified as per the following sections of the Transportation of Dangerous Goods Regulations: 2.18-2.19 (Class 3).  
**Explosive Limit and Limited Quantity Index 1**  
**Passenger Carrying Road or Rail Index 5**

**IMDG** : **Emergency schedules** F-E, S-D

## Section 14. Transport information

**IATA** : **Quantity limitation** Passenger and Cargo Aircraft: 5 L. Packaging instructions: 353. Cargo Aircraft Only: 60 L. Packaging instructions: 364. Limited Quantities - Passenger Aircraft: 1 L. Packaging instructions: Y341.

**Special precautions for user** : **Transport within user's premises:** always transport in closed containers that are upright and secure. Ensure that persons transporting the product know what to do in the event of an accident or spillage.

## Section 15. Regulatory information

### Canadian lists

**Canadian NPRI** : The following components are listed: acetonitrile

**CEPA Toxic substances** : None of the components are listed.

### International regulations

#### Chemical Weapon Convention List Schedules I, II & III Chemicals

Not listed.

#### Montreal Protocol

Not listed.

#### Stockholm Convention on Persistent Organic Pollutants

Not listed.

#### Rotterdam Convention on Prior Informed Consent (PIC)

Not listed.

#### UNECE Aarhus Protocol on POPs and Heavy Metals

Not listed.

### Inventory list

**Canada** : Not determined.

**United States** : Not determined.

## Section 16. Other information

### History

**Date of issue/Date of revision** : 06/10/2026

**Date of previous issue** : 12/23/2025

**Version** : 3

### Key to abbreviations

: ATE = Acute Toxicity Estimate  
 BCF = Bioconcentration Factor  
 DOT = Department of Transportation  
 GHS = Globally Harmonized System of Classification and Labelling of Chemicals  
 HPR = Hazardous Products Regulations  
 IATA = International Air Transport Association  
 IBC = Intermediate Bulk Container  
 IMDG = International Maritime Dangerous Goods  
 IMO = International Maritime Organization  
 LogPow = logarithm of the octanol/water partition coefficient  
 MARPOL = International Convention for the Prevention of Pollution From Ships, 1973 as modified by the Protocol of 1978. ("Marpol" = marine pollution)  
 N/A = Not available  
 SGG = Segregation Group  
 TDG = Transportation of Dangerous Goods  
 UN = United Nations

## Section 16. Other information

### Procedure used to derive the classification

<b>Classification</b>	<b>Justification</b>
FLAMMABLE LIQUIDS - Category 2 ACUTE TOXICITY (oral) - Category 4 ACUTE TOXICITY (dermal) - Category 4 ACUTE TOXICITY (inhalation) - Category 4 EYE IRRITATION - Category 2A	On basis of test data Calculation method Calculation method Calculation method Calculation method

✔ Indicates information that has changed from previously issued version.

### Notice to reader

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