

# SAFETY DATA SHEET

Forensic Toxicology Comprehensive Mix - Submix 6

## SECTION 1: Identification of the substance/mixture and of the company/undertaking

### 1.1 Product identifier

**Product name** : Forensic Toxicology Comprehensive Mix - Submix 6  
**Part no.** : 5190-0565

### 1.2 Relevant identified uses of the substance or mixture and uses advised against

**Identified uses** : For forensic use (FFU)  
 1 ml  
**Uses advised against** : None known.

### 1.3 Details of the supplier of the safety data sheet

Agilent Technologies LDA UK Ltd.  
 5500 Lakeside Cheadle Royal Business Park,  
 Cheadle, Cheshire, SK8 3GR  
 United Kingdom  
 Tel: +44 (0) 345 712 5292  
**e-mail address of person responsible for this SDS** : pdl-msds\_author@agilent.com

### 1.4 Emergency telephone number

**Emergency telephone number (with hours of operation)** : CHEMTREC®: +44 20 3807 3798

## SECTION 2: Hazards identification

### 2.1 Classification of the substance or mixture

**Product definition** : Mixture

#### Classification according to Regulation (EC) No. 1272/2008 [CLP/GHS]



<input checked="" type="checkbox"/> H225	FLAMMABLE LIQUIDS	Category 2
H302	ACUTE TOXICITY (oral)	Category 4
H312	ACUTE TOXICITY (dermal)	Category 4
H332	ACUTE TOXICITY (inhalation)	Category 4
H319	SERIOUS EYE DAMAGE/EYE IRRITATION	Category 2
H412	LONG-TERM (CHRONIC) AQUATIC HAZARD	Category 3

The product is classified as hazardous according to UK CLP Regulation SI 2019/720 as amended.

See Section 16 for the full text of the H statements declared above.

See Section 11 for more detailed information on health effects and symptoms.

### 2.2 Label elements

**Hazard pictograms** :  

**Signal word** :  Danger

**Hazard statements** :  H225 - Highly flammable liquid and vapour.  
 H302 + H312 + H332 - Harmful if swallowed, in contact with skin or if inhaled.  
 H319 - Causes serious eye irritation.  
 H412 - Harmful to aquatic life with long lasting effects.

## SECTION 2: Hazards identification

### 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.  
P273 - Avoid release to the environment.  
P261 - Avoid breathing vapour.
- Response** : P304 + P312 - IF INHALED: Call a POISON CENTER or doctor if you feel unwell.
- Storage** : Not applicable.
- Disposal** : P501 - Dispose of contents and container in accordance with all local, regional, national and international regulations.

**Hazardous ingredients** : acetonitrile

**Supplemental label elements** : Not applicable.

**Annex XVII - Restrictions on the manufacture, placing on the market and use of certain dangerous substances, mixtures and articles** : Not applicable.

### Special packaging requirements

- Containers to be fitted with child-resistant fastenings** : Not applicable.
- Tactile warning of danger** : Not applicable.

### 2.3 Other hazards

**Product meets the criteria for PBT or vPvB according to Regulation (EC) No. 1907/2006, Annex XIII** : This mixture does not contain any substances that are assessed to be a PBT or a vPvB.

**Other hazards which do not result in classification** : None known.

## SECTION 3: Composition/information on ingredients

**3.2 Mixtures** : Mixture

Product/ingredient name	Identifiers	%	Classification	Type
acetonitrile	EC: 200-835-2 CAS: 75-05-8 Index: 608-001-00-3	≥90	Flam. Liq. 2, H225 Acute Tox. 4, H302 Acute Tox. 4, H312 Acute Tox. 4, H332 Eye Irrit. 2, H319	[1] [2]
methyl[3-phenyl-3-[4-(trifluoromethyl)phenoxy]propyl] ammonium chloride	EC: 260-101-2 CAS: 56296-78-7	≤0.1	Acute Tox. 4, H302 Eye Dam. 1, H318 Aquatic Acute 1, H400 (M=10) Aquatic Chronic 1, H410 (M=10)	[1]
1-Pentanone, 5-methoxy-1-[4-(trifluoromethyl)phenyl]-, O-(2-aminoethyl)oxime, (1E)-, (2Z)-2-butenedioate (1:1)	CAS: 61718-82-9	≤0.1	Acute Tox. 4, H302 Acute Tox. 4, H332 Eye Dam. 1, H318 STOT SE 3, H335 Aquatic Chronic 1, H410 (M=10)	[1]

### SECTION 3: Composition/information on ingredients

See Section 16 for the full text of the H statements declared above.

There are no additional ingredients present which, within the current knowledge of the supplier and in the concentrations applicable, are classified as hazardous to health or the environment, are PBTs, vPvBs or Substances of equivalent concern, or have been assigned a workplace exposure limit and hence require reporting in this section.

Type

[1] Substance classified with a health or environmental hazard

[2] Substance with a workplace exposure limit

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

### SECTION 4: First aid measures

#### 4.1 Description of 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.
- 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.

#### 4.2 Most important symptoms and effects, both acute and delayed

##### Over-exposure signs/symptoms

- 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.

## SECTION 4: First aid measures

### 4.3 Indication of any immediate medical attention and special treatment needed

- 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.

## SECTION 5: Firefighting measures

### 5.1 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.

### 5.2 Special hazards arising from the substance or mixture

- Hazards from the substance or mixture** : Highly flammable liquid and vapour. 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. The vapour/gas is heavier than air and will spread along the ground. Vapours may accumulate in low or confined areas or travel a considerable distance to a source of ignition and flash back. This material is harmful to aquatic life with long lasting effects. Fire water contaminated with this material must be contained and prevented from being discharged to any waterway, sewer or drain.
- Hazardous combustion products** : Decomposition products may include the following materials:  
carbon dioxide  
carbon monoxide  
nitrogen oxides  
cyanides

### 5.3 Advice for firefighters

- 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. Clothing for fire-fighters (including helmets, protective boots and gloves) conforming to British standard BS EN 469 will provide a basic level of protection for chemical incidents.

## SECTION 6: Accidental release measures

### 6.1 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 spilt material. Shut off all ignition sources. No flares, smoking or flames in hazard area. Avoid breathing vapour or mist. Provide adequate ventilation. Wear appropriate respirator when ventilation is inadequate. Put on appropriate personal protective equipment.
- For emergency responders** : Specialised 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".

### 6.2 Environmental precautions

- : Avoid dispersal of spilt 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). Water polluting material. May be harmful to the environment if released in large quantities.

### 6.3 Methods and material for containment and cleaning up

**Forensic Toxicology Comprehensive Mix - Submix 6**

**SECTION 6: Accidental release measures**

**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.

**6.4 Reference to other sections** : See Section 1 for emergency contact information.  
See Section 8 for information on appropriate personal protective equipment.  
See Section 13 for additional waste treatment information.

**SECTION 7: Handling and storage**

**7.1 Precautions for safe handling**

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

**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.

**7.2 Conditions for safe storage, including any incompatibilities**

**Storage** : Store between the following temperatures: 18 to 25°C (64.4 to 77°F). 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 oxidising 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 unlabelled containers. Use appropriate containment to avoid environmental contamination. See Section 10 for incompatible materials before handling or use.

**Seveso Directive - Reporting thresholds**

**Danger criteria**

Category	Notification and MAPP threshold	Safety report threshold
P5c	5000 tonnes	50000 tonnes

**7.3 Specific end use(s)**

**Recommendations** : Industrial applications, Professional applications.

**Industrial sector specific solutions** : Not available.

**SECTION 8: Exposure controls/personal protection**

**8.1 Control parameters**

**Occupational exposure limits**

## SECTION 8: Exposure controls/personal protection

Product/ingredient name	Exposure limit values
acetonitrile	EH40/2005 WELs (United Kingdom (UK), 1/2020) STEL 15 minutes: 102 mg/m <sup>3</sup> . STEL 15 minutes: 60 ppm. TWA 8 hours: 40 ppm. TWA 8 hours: 68 mg/m <sup>3</sup> .

### Biological exposure indices

No exposure indices known.

### Recommended monitoring procedures

: Reference should be made to monitoring standards, such as the following: British Standard BS EN 689 (Workplace atmospheres - Guidance for the assessment of exposure by inhalation to chemical agents for comparison with limit values and measurement strategy) British Standard BS EN 14042 (Workplace atmospheres - Guide for the application and use of procedures for the assessment of exposure to chemical and biological agents) British Standard BS EN 482 (Workplace atmospheres - General requirements for the performance of procedures for the measurement of chemical agents) Reference to national guidance documents for methods for the determination of hazardous substances will also be required.

### DNELs/DMELs

Product/ingredient name	Result
acetonitrile	DNEL - General population - Long term - Oral 0.4 mg/kg bw/day
	DNEL - General population - Short term - Oral 0.6 mg/kg bw/day
	DNEL - General population - Long term - Dermal 1.2 mg/kg bw/day
	DNEL - General population - Long term - Inhalation 2.4 mg/m <sup>3</sup>

### PNECs

Not available.

## 8.2 Exposure controls

### 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, vapour or dust concentrations below any lower explosive limits. Use explosion-proof ventilation equipment.

### 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.

**SECTION 8: Exposure controls/personal protection**

- 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. Refer to British Standard BS EN 1149 for further information on material and design requirements and test methods.
- 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.
- 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.

**SECTION 9: Physical and chemical properties**

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

**9.1 Information on basic physical and chemical properties****Appearance**

- Physical state** : Liquid.
- Colour** : Colourless.
- Odour** : Ethereal.
- Odour threshold** : Not available.
- Melting point/freezing point** : -45.7°C
- Initial boiling point and boiling range** : 81.6°C
- Flammability** : Not applicable.
- Lower and upper explosion limit/flammability limit** : Lower: 3%  
Upper: 16%
- Flash point** : Closed cup: 12.8°C
- Auto-ignition temperature** :

Ingredient name	°C	Method
acetonitrile	524	-

- Decomposition temperature** : 120°C
- pH** : Not available.
- Viscosity** : Dynamic (room temperature): Not available.  
Kinematic (room temperature): Not available.  
Kinematic (40°C): Not available.

Media	Result
Water	Soluble

- Partition coefficient: n-octanol/water** : Not applicable.
- Vapour pressure** : 9.5 kPa (70.89 mm Hg)
- Relative density** : 0.8
- Density** : 0.79 g/cm<sup>3</sup> [20°C]
- Vapour density** : 1.4 [Air = 1]

**Particle characteristics**

**Forensic Toxicology Comprehensive Mix - Submix 6**

**SECTION 9: Physical and chemical properties**

**Median particle size** : Not applicable.

**9.2 Other information**

**9.2.1 Information with regard to physical hazard classes**

**Explosive properties** : Not available.

**Oxidising properties** : Not available.

**9.2.2 Other safety characteristics**

**Miscible with water** : Yes.

**Evaporation rate** : 2.33 (butyl acetate = 1)

**Physical/chemical properties comments** : Not available.

**SECTION 10: Stability and reactivity**

**10.1 Reactivity** : No specific test data related to reactivity available for this product or its ingredients.

**10.2 Chemical stability** : The product is stable.

**10.3 Possibility of hazardous reactions** : Under normal conditions of storage and use, hazardous reactions will not occur.

**10.4 Conditions to avoid** : Avoid all possible sources of ignition (spark or flame). Do not pressurise, cut, weld, braze, solder, drill, grind or expose containers to heat or sources of ignition. Do not allow vapour to accumulate in low or confined areas.

**10.5 Incompatible materials** : Reactive or incompatible with the following materials:  
oxidising materials  
Reactive or incompatible with the following materials: acids.

**10.6 Hazardous decomposition products** : Under normal conditions of storage and use, hazardous decomposition products should not be produced.

**SECTION 11: Toxicological information**

**11.1 Information on toxicological effects**

Acute toxicity

Product/ingredient name	Result	
acetonitrile	Rat - Oral - LD50	2460 mg/kg
	Rat - Inhalation - LC50 Vapour	17100 ppm [4 hours]
methyl[3-phenyl-3-[4-(trifluoromethyl)phenoxy]propyl]ammonium chloride	Rat - Oral - LD50	452 mg/kg

**Conclusion/Summary** : Not available.

[Product]

Acute toxicity estimates

Product/ingredient name	Oral (mg/kg)	Dermal (mg/kg)	Inhalation (gases) (ppm)	Inhalation (vapours) (mg/l)	Inhalation (dusts and mists) (mg/l)

**Forensic Toxicology Comprehensive Mix - Submix 6**

**SECTION 11: Toxicological information**

Forensic Toxicology Comprehensive Mix - Submix 6	501.3	1102.9	N/A	11.0	N/A
acetonitrile	500	1100	N/A	11	N/A
methyl[3-phenyl-3-[4-(trifluoromethyl)phenoxy]propyl]ammonium chloride	452	N/A	N/A	N/A	N/A
1-Pentanone, 5-methoxy-1-[4-(trifluoromethyl)phenyl]-, O-(2-aminoethyl)oxime, (1E)-, (2Z)-2-butenedioate (1:1)	500	N/A	N/A	N/A	1.5

**Skin corrosion/irritation**

**Conclusion/Summary** : Not available.

**[Product]**

**Serious eye damage/eye irritation**

**Product/ingredient name**

**Result**

acetonitrile

Rabbit - Eyes - Moderate irritant

Duration of treatment/  
exposure: 24 hours

**Conclusion/Summary** : Not available.

**[Product]**

**Respiratory corrosion/irritation**

**Conclusion/Summary** : May cause respiratory irritation.

**[Product]**

**Ingredient name**

**Conclusion/Summary**

acetonitrile

May cause respiratory irritation.

**Respiratory or skin sensitization**

**Skin**

**Conclusion/Summary** : Not available.

**[Product]**

**Respiratory**

**Conclusion/Summary** : Not available.

**[Product]**

**Germ cell mutagenicity**

**Conclusion/Summary** : Not available.

**[Product]**

**Carcinogenicity**

**Conclusion/Summary** : Not available.

**[Product]**

**Reproductive toxicity**

**Conclusion/Summary** : Not available.

**[Product]**

**Specific target organ toxicity (single exposure)**

**Product/ingredient name**

**Result**

Pentanone, 5-methoxy-1-[4-(trifluoromethyl)phenyl]-, O-(2-aminoethyl)oxime, (1E)-, (2Z)-2-butenedioate (1:1) STOT SE 3, H335 (Respiratory tract irritation)

**Specific target organ toxicity (repeated exposure)**

Not available.

**Aspiration hazard**

Not available.

**Information on likely routes of exposure**

Routes of entry anticipated: Oral, Dermal, Inhalation, Eyes.

**Potential acute health effects**

**Inhalation** : Harmful if inhaled.

**Ingestion** : Harmful if swallowed.

**Forensic Toxicology Comprehensive Mix - Submix 6**

**SECTION 11: Toxicological information**

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

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

Symptoms related to the physical, chemical and toxicological characteristics

**Inhalation** : No specific data.

**Ingestion** : No specific data.

**Skin contact** : No specific data.

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

Delayed and immediate effects as well as 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.

Potential chronic health effects

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

**General** : No known significant effects or critical hazards.

**Carcinogenicity** : No known significant effects or critical hazards.

**Mutagenicity** : No known significant effects or critical hazards.

**Reproductive toxicity** : No known significant effects or critical hazards.

**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**

**12.1 Toxicity**

**Product/ingredient name**

**Result**

acetonitrile	Acute - LC50 - Fresh water	-	-
	Daphnia - Water flea - <i>Daphnia magna</i>		
	Age: <24 hours		
	3600 mg/l [48 hours]		
	Effect: Mortality		
	Acute - IC50 - Fresh water	-	-
	Aquatic plants - Duckweed - <i>Lemna minor</i>		
	3685 mg/l [96 hours]		
	Effect: Population		
	Chronic - NOEC - Fresh water	-	-
	Daphnia - Water flea - <i>Daphnia magna</i>		
	Age: <24 hours		

**SECTION 12: Ecological information**

	160 mg/l [21 days] Effect: Reproduction		
	Chronic - NOEC - Fresh water Aquatic plants - Duckweed - <i>Lemna minor</i>	-	-
	1000 mg/l [96 hours] Effect: Population		
	Acute - LC50 - Fresh water Fish - Fathead minnow - <i>Pimephales promelas</i> Weight: 1.5 g 1000 mg/l [96 hours] Effect: Mortality	-	-
methy[3-phenyl-3-[4-(trifluoromethyl)phenoxy]propyl]ammonium chloride	Chronic - NOEC - Fresh water Fish - Western mosquitofish - <i>Gambusia affinis</i> - Neonate Age: 72 to 96 hours 5 ppb [88 days] Effect: Mortality	-	-
	Chronic - NOEC - Fresh water Daphnia - Water flea - <i>Daphnia magna</i> Age: 8 to 9 days 8.7 µg/l [21 days] Effect: Reproduction	-	-
	Acute - LC50 - Fresh water US EPA Fish - Fathead minnow - <i>Pimephales promelas</i> - Larvae Age: <24 hours 164 µg/l [96 hours] Effect: Mortality	-	-
	Acute - LC50 - Fresh water Crustaceans - Water flea - <i>Ceriodaphnia dubia</i> - Neonate Age: <24 hours 234 µg/l [48 hours] Effect: Mortality	-	-
	Chronic - IC10 - Fresh water US EPA Algae - Green algae - <i>Raphidocelis subcapitata</i> - Exponential growth phase 31.34 µg/l [96 hours]	-	-

Forensic Toxicology Comprehensive Mix - Submix 6

**SECTION 12: Ecological information**

Effect: Population

Acute - IC50 - Fresh water -  
 US EPA  
 Algae - Green algae - *Raphidocelis subcapitata*  
 - Exponential growth phase  
 44.99 µg/l [96 hours]  
 Effect: Population

1-Pentanone, 5-methoxy-1-[4-(trifluoromethyl)phenyl]-, O-(2-aminoethyl)oxime, (1E)-, (2Z)-2-butenedioate (1:1)  
 Chronic - NOEC - Fresh water -  
 Daphnia - Water flea - *Daphnia magna*  
 Age: 8 to 9 days  
 2.1 µg/l [21 days]  
 Effect: Reproduction

Acute - EC50 - Fresh water -  
 ISO, OECD  
 Daphnia - Water flea - *Daphnia magna*  
 Age: <24 hours  
 13 mg/l [48 hours]  
 Effect: Intoxication

**Conclusion/Summary** : Not available.

**[Product]**

**12.2 Persistence and degradability**

**Product/ingredient name**

**Result**

acetonitrile  
 OECD [Ready Biodegradability - CO2 in Sealed Vessels (Headspace Test)] 70% [21 days] - Readily -

**Conclusion/Summary** : Not available.

**[Product]**

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

**12.3 Bioaccumulative potential**

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

**12.4 Mobility in soil**

**Soil/water partition coefficient**

Product/ingredient name	logK <sub>oc</sub>	K <sub>oc</sub>
acetonitrile	0.42	2.62657
methyl[3-phenyl-3-[4-(trifluoromethyl)phenoxy]propyl]ammonium chloride	3.63	4259.22
1-Pentanone, 5-methoxy-1-[4-(trifluoromethyl)phenyl]-, O-(2-aminoethyl)oxime, (1E)-, (2Z)-2-butenedioate (1:1)	3.15	1407.22

**Results of PMT and vPvM assessment**

## SECTION 12: Ecological information

Product/ingredient name	PMT	P	M	T	vPvM	vP	vM
acetonitrile	No	No	Yes	No	No	No	Yes
methyl[3-phenyl-3-[4-(trifluoromethyl)phenoxy]propyl]ammonium chloride	No	No	No	Yes	No	No	No
1-Pentanone, 5-methoxy-1-[4-(trifluoromethyl)phenyl]-, O-(2-aminoethyl)oxime, (1E)-, (2Z)-2-butenedioate (1:1)	No	No	No	Yes	No	No	No

**Mobility** : Not available.

**Conclusion/Summary** : The product does not meet the criteria to be considered as a PMT or vPvM.

### 12.5 Results of PBT and vPvB assessment

#### Regulation (EC) No. 1907/2006 [REACH]

Product/ingredient name	PBT	P	B	T	vPvB	vP	vB
acetonitrile	No	No	No	No	No	No	No
methyl[3-phenyl-3-[4-(trifluoromethyl)phenoxy]propyl]ammonium chloride	No	No	No	Yes	No	No	No
1-Pentanone, 5-methoxy-1-[4-(trifluoromethyl)phenyl]-, O-(2-aminoethyl)oxime, (1E)-, (2Z)-2-butenedioate (1:1)	No	No	No	Yes	No	No	No

#### Regulation (EC) No. 1272/2008 [CLP]

Product/ingredient name	PBT	P	B	T	vPvB	vP	vB
acetonitrile	No	No	No	No	No	No	No
methyl[3-phenyl-3-[4-(trifluoromethyl)phenoxy]propyl]ammonium chloride	No	No	No	Yes	No	No	No
1-Pentanone, 5-methoxy-1-[4-(trifluoromethyl)phenyl]-, O-(2-aminoethyl)oxime, (1E)-, (2Z)-2-butenedioate (1:1)	No	No	No	Yes	No	No	No

**Conclusion/Summary** : The product does not meet the criteria to be considered as a PBT or vPvB.

**Regulation (EC) No. 1272/2008 [CLP]**

### 12.6 Endocrine disrupting properties

Not available.

**Conclusion/Summary [Product]** : The product does not meet the criteria to be considered as having endocrine disrupting properties according to the criteria set out in either Regulation (EC) No. 1907/2006 or Regulation (EC) No 1272/2008.

### 12.7 Other adverse effects

No known significant effects or critical hazards.

## SECTION 13: Disposal considerations

### 13.1 Waste treatment methods




#### Product

**Methods of disposal** : The generation of waste should be avoided or minimised 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.

## SECTION 13: Disposal considerations

- Hazardous waste** : The classification of the product may meet the criteria for a hazardous waste.
- Packaging**
- Methods of disposal** : The generation of waste should be avoided or minimised wherever possible. Waste packaging should be recycled. Incineration or landfill should only be considered when recycling is not feasible.
- Special precautions** : 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. Vapour 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 spilt material and runoff and contact with soil, waterways, drains and sewers.

## SECTION 14: Transport information

	ADR/RID	IMDG	IATA
14.1 UN number	UN1648	UN1648	UN1648
14.2 UN proper shipping name	ACETONITRILE solution	ACETONITRILE solution	Acetonitrile solution
14.3 Transport hazard class(es)	3 	3 	3 
14.4 Packing group	II	II	II
14.5 Environmental hazards	No.	No.	No.

### Additional information

Remarks: De minimis quantities

- ADR/RID** : **Hazard identification number** 33  
**Limited quantity** 1 L  
**Tunnel code** (D/E)
- IMDG** : **Emergency schedules** F-E, S-D
- 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.

**14.6 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.

**14.7 Transport in bulk according to IMO instruments** : Not available.

**SECTION 15: Regulatory information**

**15.1 Safety, health and environmental regulations/legislation specific for the substance or mixture**

**UK (GB)/REACH**

**Annex XIV - List of substances subject to authorisation**

**Annex XIV**

None of the components are listed.

**Substances of very high concern**

None of the components are listed.

**Ozone depleting substances**

Not listed.

**Prior Informed Consent (PIC)**

Not listed.

**Persistent Organic Pollutants**

Not listed.

**Annex XVII - Restrictions on the manufacture, placing on the market and use of certain dangerous substances, mixtures and articles**

Product / Ingredient name	Identifiers	Status
Forensic Toxicology Comprehensive Mix - Submix 6	-	3

**Labelling** :  Not applicable.

**Seveso Directive**

This product is controlled under the Seveso Directive.

**Danger criteria**

Category
P5c

**EU regulations**

**Industrial emissions (integrated pollution prevention and control) - Air** : Listed

**Industrial emissions (integrated pollution prevention and control) - Water** : Listed

**15.2 Chemical safety assessment** : This product contains substances for which Chemical Safety Assessments might still be required.

**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**

**Forensic Toxicology Comprehensive Mix - Submix 6**

**SECTION 15: Regulatory information**

Not listed.

Inventory list

**United States** : At least one component is inactive.

**SECTION 16: Other information**

Indicates information that has changed from previously issued version.

**Abbreviations and acronyms**

- : ATE = Acute Toxicity Estimate
- CLP = Classification, Labelling and Packaging Regulation [Regulation (EC) No. 1272/2008]
- DMEL = Derived Minimal Effect Level
- DNEL = Derived No Effect Level
- EUH statement = CLP-specific Hazard statement
- N/A = Not available
- PBT = Persistent, Bioaccumulative and Toxic
- PNEC = Predicted No Effect Concentration
- RRN = REACH Registration Number
- vPvB = Very Persistent and Very Bioaccumulative

Procedure used to derive the classification

Classification	Justification
Flam. Liq. 2, H225 Acute Tox. 4, H302 Acute Tox. 4, H312 Acute Tox. 4, H332 Eye Irrit. 2, H319 Aquatic Chronic 3, H412	On basis of test data Calculation method Calculation method Calculation method Calculation method Calculation method

Full text of abbreviated H statements

H225 H302 H312 H318 H319 H332 H335 H400 H410 H412	Highly flammable liquid and vapour. Harmful if swallowed. Harmful in contact with skin. Causes serious eye damage. Causes serious eye irritation. Harmful if inhaled. May cause respiratory irritation. Very toxic to aquatic life. Very toxic to aquatic life with long lasting effects. Harmful to aquatic life with long lasting effects.
--	---

Full text of classifications

Acute Tox. 4 Aquatic Acute 1 Aquatic Chronic 1 Aquatic Chronic 3 Eye Dam. 1 Eye Irrit. 2 Flam. Liq. 2 STOT SE 3	ACUTE TOXICITY - Category 4 SHORT-TERM (ACUTE) AQUATIC HAZARD - Category 1 LONG-TERM (CHRONIC) AQUATIC HAZARD - Category 1 LONG-TERM (CHRONIC) AQUATIC HAZARD - Category 3 SERIOUS EYE DAMAGE/EYE IRRITATION - Category 1 SERIOUS EYE DAMAGE/EYE IRRITATION - Category 2 FLAMMABLE LIQUIDS - Category 2 SPECIFIC TARGET ORGAN TOXICITY - SINGLE EXPOSURE - Category 3
--	--

**Date of issue/ Date of revision** : 26/12/2024

**Date of previous issue** : 31/01/2022

**Version** : 8

Notice to reader

**Disclaimer:** The information contained in this document is based on Agilent’s state of knowledge at the time of preparation. No warranty as to its accurateness, completeness or suitability for a particular purpose is expressed or implied.