Conforms to Code of Practice for the Preparation of Safety Data Sheets for Hazardous Chemicals

SAFETY DATA SHEET

Agilent Technologies

Forensic Toxicology Comprehensive Mix - Submix 6

Section 1. Identification

Product identifier : Forensic Toxicology Comprehensive Mix - Submix 6

Part no. : 5190-0565

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

Identified uses : For forensic use (FFU)
1 ml

Supplier/Manufacturer : Agilent Technologies Australia Pty Ltd
679 Springvale Road
Mulgrave
Victoria 3170, Australia
1800 802 402

Emergency telephone number (with hours of operation) : CHEMTREC®: +(61)-290372994

Section 2. Hazard(s) 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	SERIOUS EYE DAMAGE/EYE IRRITATION - Category 2A
H412	LONG-TERM (CHRONIC) AQUATIC HAZARD - Category 3

GHS 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.

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.

Supplemental label elements

Additional warning phrases : Not applicable.

Section 2. Hazard(s) identification

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

Section 3. Composition and ingredient information

Substance/mixture : Mixture

Ingredient name	% (w/w)	Identifiers
Acetonitrile	≥90	CAS: 75-05-8 EC: 200-835-2
methyl[3-phenyl-3-[4-(trifluoromethyl)phenoxy]propyl]ammonium chloride	<0.1	CAS: 56296-78-7 EC: 260-101-2
1-Pentanone, 5-methoxy-1-[4-(trifluoromethyl)phenyl]-, O-(2-aminoethyl) oxime, (1E)-, (2Z)-2-butenedioate (1:1)	≤0.1	CAS: 61718-82-9

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.

The total concentration of ingredients in this product, reported or not in this section, is 100%.

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.

Section 4. First aid measures

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.

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. Firefighting measures

Extinguishing media

Suitable extinguishing media : Use dry chemical, CO_2, water spray (fog) or foam.

Unsuitable extinguishing media : Do not use water jet.

Specific hazards arising from the chemical : 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 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.

Hazchem code : •2YE

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 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 : If 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".

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.

Methods and material 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 vapour or mist. Avoid release to the environment. 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 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.

Section 8. Exposure controls and personal protection

Control parameters

Occupational exposure limits

Ingredient name	Exposure limits
Acetonitrile	**Safe Work Australia (Australia, 1/2024)** Absorbed through skin. STEL 15 minutes: 101 mg/m³. STEL 15 minutes: 60 ppm. TWA 8 hours: 67 mg/m³. TWA 8 hours: 40 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, vapour 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 and safety characteristics

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

Appearance

Physical state : Liquid.

Colour : Colourless.

Odour : Ethereal.

Odour threshold : Not available.

pH : Not available.

Melting point/freezing point : -45.7°C (-50.3°F)

Boiling point or initial boiling point and boiling range : 81.6°C (178.9°F)

Flash point : Closed cup: 12.8°C (55°F)

Evaporation rate : 2.33 (butyl acetate = 1)

Flammability : Not applicable.

Lower and upper explosion limit/flammability limit : Lower: 3%
Upper: 16%

Vapour pressure : 9.5 kPa (70.89 mm Hg)

Relative vapour density : 1.4 [Air = 1]

Relative density : 0.8

Density : 0.79 g/cm³ [20°C (68°F)]

Solubility(ies) :

Media	Result
water	Soluble

Miscible with water : Yes.

Partition coefficient: n-octanol/water : Not applicable.

Auto-ignition temperature : Not available.

Ingredient name	°C	°F	Method
Acetonitrile	524	975.2	-

Decomposition temperature : 120°C (248°F)

Viscosity : Dynamic (room temperature): Not available.
Kinematic (room temperature): Not available.
Kinematic (40°C (104°F)): Not available.

Particle characteristics

Median particle size : Not applicable.

Section 10. Stability and reactivity

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

Chemical stability : The product is stable.

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

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.

Section 10. Stability and reactivity

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

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

Section 11. Toxicological information

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 [Product] : Not available.

Skin corrosion/irritation

Conclusion/Summary [Product] : Not available.

Serious eye damage/eye irritation

Product/ingredient name	Result	
Acetonitrile	Rabbit - Eyes - Moderate irritant	Duration of treatment/ exposure: 24 hours

Conclusion/Summary [Product] : Not available.

Respiratory corrosion/irritation

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

Ingredient name	Conclusion/Summary
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.

Carcinogenicity

Conclusion/Summary [Product] : Not available.

Reproductive toxicity

Conclusion/Summary [Product] : Not available.

Specific target organ toxicity (single exposure)

Product/ingredient name	Result
1-Pentanone, 5-methoxy-1-[4-(trifluoromethyl)phenyl]-, O-(2-aminoethyl)oxime, (1E)-, (2Z) -2-butenedioate (1:1)	SPECIFIC TARGET ORGAN TOXICITY - SINGLE EXPOSURE (Respiratory tract irritation) - Category 3

Section 11. Toxicological information

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

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 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.

Numerical measures of toxicity

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	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

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 - *Daphnia magna*
	Acute - IC50 - Fresh water	3685 mg/l [96 hours]	Aquatic plants - Duckweed - *Lemna minor*
	Chronic - NOEC - Fresh water	160 mg/l [21 days]	Daphnia - Water flea - *Daphnia magna*
	Chronic - NOEC - Fresh water	1000 mg/l [96 hours]	Aquatic plants - Duckweed - *Lemna minor*
	Acute - LC50 - Fresh water	1000 mg/l [96 hours]	Fish - Fathead minnow - *Pimephales promelas*
methyl[3-phenyl-3-[4-(trifluoromethyl)phenoxy]propyl] ammonium chloride	Chronic - NOEC - Fresh water	5 ppb [88 days]	Fish - Western mosquitofish - *Gambusia affinis* - Neonate
	Chronic - NOEC - Fresh water	8.7 µg/l [21 days]	Daphnia - Water flea - *Daphnia magna*
	Acute - LC50 - Fresh water	164 µg/l [96 hours]	Fish - Fathead minnow - *Pimephales promelas* - Larvae
	Acute - LC50 - Fresh water	234 µg/l [48 hours]	Crustaceans - Water flea - *Ceriodaphnia dubia* - Neonate
	Chronic - IC10 - Fresh water	31.34 µg/l [96 hours]	Algae - Green algae - *Raphidocelis subcapitata* - Exponential growth phase
	Acute - IC50 - Fresh water	44.99 µg/l [96 hours]	Algae - Green algae - *Raphidocelis subcapitata* - Exponential growth phase
1-Pentanone, 5-methoxy-1-[4-(trifluoromethyl)phenyl]-, O-(2-aminoethyl)oxime, (1E)-, (2Z)-2-butenedioate (1:1)	Chronic - NOEC - Fresh water	2.1 µg/l [21 days]	Daphnia - Water flea - *Daphnia magna*
	Acute - EC50 - Fresh water	13 mg/l [48 hours]	Daphnia - Water flea - *Daphnia magna*

Conclusion/Summary [Product] : Not available.

Persistence and degradability

Product/ingredient name	Result		
Acetonitrile	OECD [Ready Biodegradability - CO2 in Sealed Vessels (Headspace Test)]	70% [21 days] - Readily	-

Conclusion/Summary [Product] : Not available.

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

Bioaccumulative potential

Product/ingredient name	$LogP_{ow}$	BCF	Potential
Acetonitrile	-0.34	3	Low

Section 12. Ecological information

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 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. 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. 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

ADG / IMDG / IATA : Not regulated as Dangerous Goods according to the ADG Code .

Additional information

Remarks: De minimis quantities

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.

Transport in bulk according to IMO instruments : Not available.

Section 15. Regulatory information

Standard for the Uniform Scheduling of Medicines and Poisons

Not regulated.

Model Work Health and Safety Regulations - Scheduled Substances

No listed substance

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

Section 15. Regulatory information

Australia : Not determined.

New Zealand : Not determined.

United States : At least one component is inactive.

Section 16. Any other relevant information

History

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

Date of previous issue : 31/01/2022

Version : 8

Key to abbreviations : ADG = Australian Dangerous Goods
ADR = The European Agreement concerning the International Carriage of Dangerous Goods by Road
ATE = Acute Toxicity Estimate
BCF = Bioconcentration Factor
GHS = Globally Harmonized System of Classification and Labelling of Chemicals
IATA = International Air Transport Association
IBC = Intermediate Bulk Container
IMDG = International Maritime Dangerous Goods
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
SUSMP = Standard Uniform Schedule of Medicine and Poisons
UN = United Nations

Procedure used to derive the classification

Classification	Justification
FLAMMABLE LIQUIDS - Category 2	On basis of test data
ACUTE TOXICITY (oral) - Category 4	Calculation method
ACUTE TOXICITY (dermal) - Category 4	Calculation method
ACUTE TOXICITY (inhalation) - Category 4	Calculation method
SERIOUS EYE DAMAGE/EYE IRRITATION - Category 2A	Calculation method
LONG-TERM (CHRONIC) AQUATIC HAZARD - Category 3	Expert judgment

Indicates information that has changed from previously issued version.

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.