

# SAFETY DATA SHEET



iTRAQ REAGENT - 8 PLEX -116 (25U)

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

### 1.1 Product identifier

**Product name** : iTRAQ REAGENT - 8 PLEX -116 (25U)  
**Product type** : Liquid.  
**Other means of identification** : Not available.  
**Product part number** : 4389942  
**Kit name** : iTRAQ Reagent 8 Plex 25 U Kit  
**Kit part number** : 4390733

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

**Product use** :  Research and Development  
**Area of application** : Professional applications.

#### Uses advised against

None identified.

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

AB Sciex UK Limited  
21F18, 21 Mereside, Alderley Park  
Macclesfield, Cheshire  
SK10 4TG  
United Kingdom  
Telephone no.: 00800 2255 2279

**e-mail address of person responsible for this SDS** : msds.inquiry@sciex.com

### 1.4 Emergency telephone number

#### National advisory body/Poison Centre

**Telephone number** : CHEMTREC: +44 20 3807 3798

#### Supplier

**Telephone number** : 1-877-740-2129 (8:30A PT - 5:00P PT)

## 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]

Flam. Liq. 2, H225  
Acute Tox. 4, H302  
Acute Tox. 4, H312  
Acute Tox. 4, H332  
Skin Corr. 1, H314  
Eye Dam. 1, H318

## SECTION 2: Hazards identification

The product is classified as hazardous according to Regulation (EC) 1272/2008 as amended.


**Ingredients of unknown toxicity** : 7.6 percent of the mixture consists of component(s) of unknown acute oral toxicity  
7.6 percent of the mixture consists of component(s) of unknown acute dermal toxicity  
7.6 percent of the mixture consists of component(s) of unknown acute inhalation toxicity

**Ingredients of unknown ecotoxicity** : Contains 7.6% of components with unknown hazards to the aquatic environment

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.  
H314 - Causes severe skin burns and eye damage.

#### Precautionary statements

**Prevention** : P280 - Wear protective gloves, protective clothing and eye or face protection.  
P210 - Keep away from heat, hot surfaces, sparks, open flames and other ignition sources. No smoking.

**Response** : P304 + P310 - IF INHALED: Immediately call a POISON CENTER or doctor.  
P301 + P310 - IF SWALLOWED: Immediately call a POISON CENTER or doctor.  
P303 + P361 + P353 - IF ON SKIN (or hair): Take off immediately all contaminated clothing. Rinse skin with water.

**Storage** : Not applicable.

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

**Hazardous ingredients** : acetonitrile  
Butanoic-1,2,3,4-13C4 acid, 4-[methyl[2-[[2-(4-methyl-1-piperazinyl)-2,3-13C2-1-15N)acetyl-1-13C]amino]ethyl]amino]-4-oxo-, 2,5-dioxo-1-pyrrolidinyl ester, ditrifluoroacetate

**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

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## SECTION 2: Hazards identification

**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	%	Regulation (EC) No. 1272/2008 [CLP]	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 Skin Irrit. 2, H315 Eye Irrit. 2, H319 STOT SE 3, H335	[1] [2]
Butanoic-1,2,3,4-13C4 acid, 4-[methyl[2-[[2-(4-methyl-1-piperazinyl-2,3-13C2-1-15N)acetyl-1-13C]amino]ethyl]amino]-4-oxo-, 2,5-dioxo-1-pyrrolidinyl ester, ditrifluoroacetate	CAS: 945218-46-2	≤10	See Section 16 for the full text of the H statements declared above.	[1]

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
- [3] Substance meets the criteria for PBT according to Regulation (EC) No. 1907/2006, Annex XIII
- [4] Substance meets the criteria for vPvB according to Regulation (EC) No. 1907/2006, Annex XIII
- [5] Substance of equivalent concern
- [6] Additional disclosure due to company policy

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

## SECTION 4: First aid measures

### 4.1 Description of first aid measures

**Eye contact** :  Get medical attention immediately. Call a poison center or physician. 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. Chemical burns must be treated promptly by a physician.

**Inhalation** :  Get medical attention immediately. Call a poison center or physician. 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. 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

## SECTION 4: First aid measures

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** :  Get medical attention immediately. Call a poison center or physician. 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. Chemical burns must be treated promptly by a physician. Wash clothing before reuse. Clean shoes thoroughly before reuse.
- Ingestion** :  Get medical attention immediately. Call a poison center or physician. 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. Chemical burns must be treated promptly by a 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  
watering  
redness
- Inhalation** : No specific data.
- Skin contact** :  Adverse symptoms may include the following:  
pain or irritation  
redness  
blistering may occur
- Ingestion** :  Adverse symptoms may include the following:  
stomach pains

### 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

## SECTION 5: Firefighting measures

- 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.
- Hazardous thermal decomposition products** : Decomposition products may include the following materials:  
 carbon dioxide  
 carbon monoxide  
 nitrogen oxides  
 halogenated compounds  
 cyanides  
 hydrogen fluoride

### 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 European standard 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. Do not breathe 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".

### 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).

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

- Small spill** : 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.
- Large spill** : Stop leak if without risk. Move containers from spill area. Use spark-proof tools and explosion-proof equipment. Approach the release from upwind. Prevent entry into sewers, water courses, basements or confined areas. Wash spillages into an effluent treatment plant or proceed as follows. Contain and collect spillage with non-combustible, absorbent material e.g. sand, earth, vermiculite or diatomaceous earth and place in container for disposal according to local regulations. The spilled material may be neutralized with sodium carbonate, sodium bicarbonate or sodium hydroxide. Dispose of via a licensed waste disposal contractor. Contaminated absorbent material may pose the same hazard as the spilt product.

## SECTION 6: Accidental release measures

- 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). Do not get in eyes or on skin or clothing. Do not breathe vapour or mist. Do not ingest. 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. Keep away from alkalis. 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.

### 7.2 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. Store locked up. Eliminate all ignition sources. Separate from alkalis. 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 (in tonnes)

##### Danger criteria

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

### 7.3 Specific end use(s)

- Recommendations** : Not available.  
**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	<p><b>EH40/2005 WELs (United Kingdom (UK), 1/2020).</b>                      STEL: 102 mg/m<sup>3</sup> 15 minutes.                      STEL: 60 ppm 15 minutes.                      TWA: 40 ppm 8 hours.                      TWA: 68 mg/m<sup>3</sup> 8 hours.</p> <p><b>EU OEL (Europe, 10/2019). Absorbed through skin. Notes: list of indicative occupational exposure limit values</b>                      TWA: 40 ppm 8 hours.                      TWA: 70 mg/m<sup>3</sup> 8 hours.</p>

**Recommended monitoring procedures** : If this product contains ingredients with exposure limits, personal, workplace atmosphere or biological monitoring may be required to determine the effectiveness of the ventilation or other control measures and/or the necessity to use respiratory protective equipment. Reference should be made to monitoring standards, such as the following: European Standard EN 689 (Workplace atmospheres - Guidance for the assessment of exposure by inhalation to chemical agents for comparison with limit values and measurement strategy) European Standard EN 14042 (Workplace atmospheres - Guide for the application and use of procedures for the assessment of exposure to chemical and biological agents) European Standard 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	Type	Exposure	Value	Population	Effects
acetonitrile	DNEL	Short term Oral	0.6 mg/kg bw/day	General population	Systemic
	DNEL	Long term Inhalation	4.8 mg/m <sup>3</sup>	General population	Local
	DNEL	Long term Inhalation	4.8 mg/m <sup>3</sup>	General population	Systemic
	DNEL	Short term Inhalation	22 mg/m <sup>3</sup>	General population	Local
	DNEL	Long term Dermal	32.2 mg/kg bw/day	Workers	Systemic
	DNEL	Short term Inhalation	68 mg/m <sup>3</sup>	Workers	Local
	DNEL	Long term Inhalation	68 mg/m <sup>3</sup>	Workers	Local
	DNEL	Short term Inhalation	68 mg/m <sup>3</sup>	Workers	Systemic
	DNEL	Long term Inhalation	68 mg/m <sup>3</sup>	Workers	Systemic
	DNEL	Short term Inhalation	220 mg/m <sup>3</sup>	General population	Systemic

### PNECs

No PNECs available

## 8.2 Exposure controls



## SECTION 8: Exposure controls/personal protection

- 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 and/or face shield. If inhalation hazards exist, a full-face respirator may be required instead.
- 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. Refer to European Standard 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

### 9.1 Information on basic physical and chemical properties

#### Appearance

- Physical state** : Liquid.
- Colour** :  Yellow./Pink
- Odour** : Not available.
- Odour threshold** : Not available.
- pH** :



## SECTION 9: Physical and chemical properties

<b>Melting point/freezing point</b>	: Not available.
<b>Initial boiling point and boiling range</b>	: >36°C
<b>Flash point</b>	: Closed cup: <23°C
<b>Evaporation rate</b>	: Not available.
<b>Flammability (solid, gas)</b>	: Not applicable.
<b>Upper/lower flammability or explosive limits</b>	: Not available.
<b>Vapour pressure</b>	: Not available.
<b>Vapour density</b>	: Not available.
<b>Relative density</b>	: Not available.
<b>Solubility(ies)</b>	: Not available.
<b>Partition coefficient: n-octanol/water</b>	: Not applicable.
<b>Auto-ignition temperature</b>	: Not available.
<b>Decomposition temperature</b>	: Not available.
<b>Viscosity</b>	: Not available.
<b>Explosive properties</b>	: Not available.
<b>Oxidising properties</b>	: Not available.

### 9.2 Other information

<b>Physical/chemical properties comments</b>	: No additional information.
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## SECTION 10: Stability and reactivity

<b>10.1 Reactivity</b>	: No specific test data related to reactivity available for this product or its ingredients.
<b>10.2 Chemical stability</b>	: The product is stable.
<b>10.3 Possibility of hazardous reactions</b>	: Under normal conditions of storage and use, hazardous reactions will not occur. Under normal conditions of storage and use, hazardous polymerisation will not occur.
<b>10.4 Conditions to avoid</b>	: 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. Protect from moisture.
<b>10.5 Incompatible materials</b>	: Attacks many metals producing extremely flammable hydrogen gas which can form explosive mixtures with air. Reactive or incompatible with the following materials: alkalis oxidising materials Reactive or incompatible with the following materials: reducing materials and metals. aluminium
<b>10.6 Hazardous decomposition products</b>	: Under normal conditions of storage and use, hazardous decomposition products should not be produced.

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## SECTION 11: Toxicological information

### 11.1 Information on toxicological effects

#### Acute toxicity

Product/ingredient name	Result	Species	Dose	Exposure
acetonitrile	LC50 Inhalation Gas. LD50 Oral	Rat Rat	17100 ppm 2460 mg/kg	4 hours -

**Conclusion/Summary** : Not available.

#### 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)
iTRAQ REAGENT - 8 PLEX -116 (25U) acetonitrile	546.2 500	1201.7 1100	18681 17100	N/A N/A	N/A N/A

#### Irritation/Corrosion

Product/ingredient name	Result	Species	Score	Exposure	Observation
acetonitrile	Eyes - Moderate irritant	Rabbit	-	24 hours 100 uL	-

**Conclusion/Summary** : Not available.

#### Sensitisation

**Conclusion/Summary** : Not available.

#### Mutagenicity

**Conclusion/Summary** : Not available.

#### Carcinogenicity

**Conclusion/Summary** : Not available.

#### Reproductive toxicity

**Conclusion/Summary** : Not available.

#### Teratogenicity

**Conclusion/Summary** : Not available.

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

Product/ingredient name	Category	Route of exposure	Target organs
Butanoic-1,2,3,4-13C4 acid, 4-[methyl[2-[[2-(4-methyl-1-piperazinyl-2,3-13C2-1-15N)acetyl-1-13C]amino]ethyl]amino]-4-oxo-, 2,5-dioxo-1-pyrrolidinyl ester, ditrifluoroacetate	Category 3	-	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.

#### Potential acute health effects

## SECTION 11: Toxicological information

- Eye contact** : Causes serious eye damage.
- Inhalation** : Harmful if inhaled.
- Skin contact** : Causes severe burns. 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  
watering  
redness
- Inhalation** : No specific data.
- Skin contact** : Adverse symptoms may include the following:  
pain or irritation  
redness  
blistering may occur
- Ingestion** : Adverse symptoms may include the following:  
stomach pains

### 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

- 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** : Not available.

## SECTION 12: Ecological information

### 12.1 Toxicity

Product/ingredient name	Result	Species	Exposure
acetonitrile	Acute IC50 3685000 µg/l Fresh water	Aquatic plants - Lemna minor	96 hours
	Acute LC50 3600000 µg/l Fresh water	Daphnia - Daphnia magna	48 hours
	Acute LC50 1000000 µg/l Fresh water	Fish - Pimephales promelas	96 hours
	Chronic NOEC 1000000 µg/l Fresh water	Aquatic plants - Lemna minor	96 hours
	Chronic NOEC 160000 µg/l Fresh water	Daphnia - Daphnia magna	21 days

**Conclusion/Summary** : Not available.

### 12.2 Persistence and degradability

## SECTION 12: Ecological information

Product/ingredient name	Test	Result	Dose	Inoculum
acetonitrile	OECD 301C Ready Biodegradability - Modified MITI Test (I)	65 % - Readily - 28 days	-	Activated sludge

**Conclusion/Summary** : Not available.

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	-	low

### 12.4 Mobility in soil

**Soil/water partition coefficient (K<sub>oc</sub>)** : Not available.

**Mobility** : Not available.

### 12.5 Results of PBT and vPvB assessment

This mixture does not contain any substances that are assessed to be a PBT or a vPvB.

**12.6 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.

**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.

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## SECTION 14: Transport information

	ADR/RID	ADN	IMDG	IATA
14.1 UN number	UN2924	UN2924	UN2924	UN2924
14.2 UN proper shipping name	FLAMMABLE LIQUID, CORROSIVE, N.O.S. (acetonitrile, trifluoroacetic acid)	FLAMMABLE LIQUID, CORROSIVE, N.O.S. (acetonitrile, trifluoroacetic acid)	FLAMMABLE LIQUID, CORROSIVE, N.O.S. (acetonitrile, trifluoroacetic acid)	Flammable liquid, corrosive, n.o.s. (acetonitrile, trifluoroacetic acid)
14.3 Transport hazard class(es)	3 (8) 	3 (8) 	3 (8) 	3 (8) 
14.4 Packing group	II	II	II	II
14.5 Environmental hazards	No.	No.	No.	No.

### Additional information

- ADR/RID** : **Hazard identification number** 338  
**Limited quantity** 1 L  
**Special provisions** 274  
**Tunnel code** (D/E)
- ADN** : **Special provisions** 274
- IMDG** : **Emergency schedules** F-E, S-C  
**Special provisions** 274
- IATA** : **Quantity limitation** Passenger and Cargo Aircraft: 1 L. Packaging instructions: 352. Cargo Aircraft Only: 5 L. Packaging instructions: 363. Limited Quantities - Passenger Aircraft: 0.5 L. Packaging instructions: Y340.  
**Special provisions** A3, A803

**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

#### EU Regulation (EC) No. 1907/2006 (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.

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

iTRAQ REAGENT - 8 PLEX -116 (25U)

## SECTION 15: Regulatory information

**Substances requiring labelling** : Not applicable.

### Other EU regulations

**Europe inventory** : All components are listed or exempted.

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

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

### Ozone depleting substances (1005/2009/EU)

Not listed.

### Prior Informed Consent (PIC) (649/2012/EU)

Not listed.

### Seveso Directive

This product is controlled under the Seveso Directive.

### Danger criteria

#### Category

P5c

### 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.

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

**15.3 Registration status** : Mixture. Information concerning the substance : Contact local supplier or distributor.



## 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

**Key literature references and sources for data** : Regulation (EC) No. 1272/2008 [CLP]; European Agreement concerning the International Carriage of Dangerous Goods by Road (ADR), concluded in Geneva on 30 September 1957 plus amendments (Uniform text: Journal of Laws 27/2009 pos. 162 plus amendments); European Agreement concerning the International Carriage of Dangerous Goods by Inland Waterways (ADN); Occupational exposure limits; International regulations

### Procedure used to derive the classification according to Regulation (EC) No. 1272/2008 [CLP/GHS]

Classification	Justification
Flam. Liq. 2, H225 Acute Tox. 4, H302 Acute Tox. 4, H312 Acute Tox. 4, H332 Skin Corr. 1, H314 Eye Dam. 1, H318	On basis of test data Calculation method Calculation method Calculation method On basis of test data On basis of test data

### Full text of abbreviated H statements

H225 H302 H312 H314 H315 H318 H319 H332 H335	Highly flammable liquid and vapour. Harmful if swallowed. Harmful in contact with skin. Causes severe skin burns and eye damage. Causes skin irritation. Causes serious eye damage. Causes serious eye irritation. Harmful if inhaled. May cause respiratory irritation.
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### Full text of classifications [CLP/GHS]

Acute Tox. 4 Eye Dam. 1 Eye Irrit. 2 Flam. Liq. 2 Skin Corr. 1 Skin Irrit. 2 STOT SE 3	ACUTE TOXICITY - Category 4 SERIOUS EYE DAMAGE/EYE IRRITATION - Category 1 SERIOUS EYE DAMAGE/EYE IRRITATION - Category 2 FLAMMABLE LIQUIDS - Category 2 SKIN CORROSION/IRRITATION - Category 1 SKIN CORROSION/IRRITATION - Category 2 SPECIFIC TARGET ORGAN TOXICITY - SINGLE EXPOSURE - Category 3
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**Training advice** : Ensure operatives are trained to minimise exposures. Training staff on good practice.

**Date of issue/ Date of revision** : 15/03/2022

**Date of previous issue** : 19/06/2012

**Version** : 3

## SECTION 16: Other information

### Notice to reader

To the best of our knowledge, the information contained herein is accurate. However, neither the above-named supplier, nor any of its subsidiaries, assumes any liability whatsoever for the accuracy or completeness of the information contained herein.

Final determination of suitability of any material is the sole responsibility of the user. All materials may present unknown hazards and should be used with caution. Although certain hazards are described herein, we cannot guarantee that these are the only hazards that exist.