

(±)-Warfarin D5 (phenyl-D5) 100 μ g/mL in Acetonitrile Novachem Pty Ltd

Version No: 2.3

Safety Data Sheet according to WHS Regulations (Hazardous Chemicals) Amendment 2020 and ADG requirements

Chemwatch Hazard Alert Code: 4

Issue Date: **24/01/2023** Print Date: **24/01/2023** S.GHS.AUS.EN

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

Product Identifier	
Product name	(±)-Warfarin D5 (phenyl-D5) 100 μg/mL in Acetonitrile
Synonyms	Not Available
Proper shipping name	ACETONITRILE
Other means of identification	DRE-XA17940100AL

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

Relevant identified uses

Reference material for laboratory use only

Details of the manufacturer or supplier of the safety data sheet

Registered company name	Novachem Pty Ltd	Novachem Pty Ltd
Address	25 Crissane Road, Heidelberg West Victoria 3081 Australia	25 Crissane Road, Heidelberg West Victoria 3081 Australia
Telephone	+61384151255	+61384151255
Fax	+61386250088	+61386250088
Website	www.novachem.com.au	www.novachem.com.au
Email	novachem@novachem.com.au	novachem@novachem.com.au

Emergency telephone number

Association / Organisation	Victorian Poisons Information Centre	Victorian Poisons Information Centre
Emergency telephone numbers	13 11 26	13 11 26
Other emergency telephone numbers	Not Available	Not Available

SECTION 2 Hazards identification

Classification of the substance or mixture

Poisons Schedule	Not Applicable
Classification ^[1]	Serious Eye Damage/Eye Irritation Category 2A, Acute Toxicity (Dermal) Category 3, Flammable Liquids Category 2, Acute Toxicity (Inhalation) Category 3, Acute Toxicity (Oral) Category 3
Legend:	1. Classified by Chemwatch; 2. Classification drawn from HCIS; 3. Classification drawn from Regulation (EU) No 1272/2008 - Annex VI

Label elements

Hazard pictogram(s)





Signal word

Dange

Hazard statement(s)

. ,	
H319	Causes serious eye irritation.
H311	Toxic in contact with skin.
H225	Highly flammable liquid and vapour.
H331	Toxic if inhaled.
H301	Toxic if swallowed.

Version No: 2.3 Page 2 of 10 Issue Date: 24/01/2023

(±)-Warfarin D5 (phenyl-D5) 100 μg/mL in Acetonitrile

Print Date: 24/01/2023

Precautionary statement(s) Prevention

P210	P210 Keep away from heat, hot surfaces, sparks, open flames and other ignition sources. No smoking.	
P264	Wash all exposed external body areas thoroughly after handling.	
P270	Do not eat, drink or smoke when using this product.	
P271	Use only outdoors or in a well-ventilated area.	

Precautionary statement(s) Response

P301+P310	IF SWALLOWED: Immediately call a POISON CENTER/doctor/physician/first aider.	
P330	Rinse mouth.	
P370+P378	In case of fire: Use alcohol resistant foam or normal protein foam to extinguish.	
P302+P352	IF ON SKIN: Wash with plenty of water.	

Precautionary statement(s) Storage

P403+P235	Store in a well-ventilated place. Keep cool.
P405	Store locked up.

Precautionary statement(s) Disposal

P501 Dispose of contents/container to authorised hazardous or special waste collection point in accordance with any local regulation.

SECTION 3 Composition / information on ingredients

Substances

See section below for composition of Mixtures

Mixtures

CAS No	%[weight]	Name
75-05-8	>99	acetonitrile
75472-93-4*	<0.1	Warfarin-d5
Legend:	1. Classified by Chemwatch; 2. Classification drawn from HCIS; 3. Classification drawn from Regulation (EU) No 1272/2008 - Annex VI; 4. Classification drawn from C&L * EU IOELVs available	

SECTION 4 First aid measures

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Description of first aid measures		
Eye Contact	If this product comes in contact with the eyes: Immediately hold eyelids apart and flush the eye continuously with running water. Ensure complete irrigation of the eye by keeping eyelids apart and away from eye and moving the eyelids by occasionally lifting the upper and lower lids. Continue flushing until advised to stop by the Poisons Information Centre or a doctor, or for at least 15 minutes. Transport to hospital or doctor without delay. Removal of contact lenses after an eye injury should only be undertaken by skilled personnel.	
Skin Contact	If skin or hair contact occurs: Cuickly but gently, wipe material off skin with a dry, clean cloth. Immediately remove all contaminated clothing, including footwear. Wash skin and hair with running water. Continue flushing with water until advised to stop by the Poisons Information Centre. Transport to hospital, or doctor.	
Inhalation	 If fumes or combustion products are inhaled remove from contaminated area. Lay patient down. Keep warm and rested. Prostheses such as false teeth, which may block airway, should be removed, where possible, prior to initiating first aid procedures. Apply artificial respiration if not breathing, preferably with a demand valve resuscitator, bag-valve mask device, or pocket mask as trained. Perform CPR if necessary. Transport to hospital, or doctor, without delay. 	
	 If SWALLOWED, REFER FOR MEDICAL ATTENTION, WHERE POSSIBLE, WITHOUT DELAY. For advice, contact a Poisons Information Centre or a doctor. Urgent hospital treatment is likely to be needed. In the mean time, qualified first-aid personnel should treat the patient following observation and employing supportive measures as indicated by the patient's condition. If the services of a medical officer or medical doctor are readily available, the patient should be placed in his/her care and a copy of the SDS should be provided. Further action will be the responsibility of the medical specialist. 	

position, if possible) to maintain open airway and prevent aspiration. NOTE: Wear a protective glove when inducing vomiting by mechanical means.

If medical attention is not available on the worksite or surroundings send the patient to a hospital together with a copy of the SDS.

Where medical attention is not immediately available or where the patient is more than 15 minutes from a hospital or unless instructed

▶ INDUCE vomiting with fingers down the back of the throat, ONLY IF CONSCIOUS. Lean patient forward or place on left side (head-down

Indication of any immediate medical attention and special treatment needed

otherwise:

Ingestion

Version No: 2.3 Page 3 of 10 Issue Date: 24/01/2023

(±)-Warfarin D5 (phenyl-D5) 100 µg/mL in Acetonitrile

Print Date: 24/01/2023

For cyanide intoxication (and for certain nitriles which produce cyanide ion)

- Signs symptoms of acute cyanide poisoning reflect cellular hypoxia and are often non-specific.
- Cyanosis may be a late finding.
- A bradycardic, hypertensive and tachypneic patient suggests poisoning especially if CNS and cardiovascular depression subsequently occurs.
- Immediate attention should be directed towards assisted ventilation, administration of 100% oxygen, insertion of intravenous lines and institution of cardiac monitoring.
- Obtain an arterial blood gas immediately and correct any severe metabolic acidosis (pH below 7.15).
- Mildly symptomatic patients generally require supportive care alone. Nitrites should not be given indiscriminately in all cases of moderate to severe poisoning, they should be given in conjunction with thiosulfate. As a temporizing measure supply amyl nitrite perles (0.2ml inhaled 30 seconds every minute) until intravenous lines for sodium nitrite are established. 10 ml of a 3% solution is administered over 4 minutes to produce 20% methaemoglobin in adults. Follow directly with 50 ml of 25% sodium thiosulfate, at the same rate, IV. If symptoms reappear or persist within 1/2-1 hour, repeat nitrite and thiosulfate at 50% of initial dose. As the mode of action involves the metabolic conversion of the thiosulfate to thiocyanate, renal failure may enhance thiocyanate toxicity
- Methylene blue is not an antidote. [Ellenhorn and Barceloux: Medical Toxicology]

If amyl nitrite intervention is employed then Medical Treatment Kits should contain the following:

- One box containing one dozen amyl nitrite ampoules
- Two sterile ampoules of sodium nitrite solution (10 mL of a 3% solution in each)
- Two sterile ampoules of sodium thiosulfate solution (50 mL of a 25% solution in each)
- One 10 mL sterile syringe. One 50 mL sterile syringe. Two sterile intravenous needles. One tourniquet.
- One dozen gauze pads.
- Latex gloves
- A "Biohazard" bag for disposal of bloody/contaminated equipment.
- A set of cyanide instructions on first aid and medical treatment.
- Notes on the use of amvl nitrite:-
 - AN is highly volatile and flammable do not smoke or use around a source of ignition.
- If treating patient in a windy or draughty area provide some shelter or protection (shirt, wall, drum, cupped hand etc.) to prevent amyl nitrite vapour from being blown away. Keep ampoule upwind from the nose, the objective is to get amyl nitrite into the patients lungs.
- Rescuers should avoid AN inhalation to avoid becoming dizzy and losing competence.
- Lay the patient down. Since AN dilates blood vessels and lowers blood pressure, lying down will help keep patient conscious.
- DO NOT overuse excessive use might put the patient into shock. Experience at DuPont plants has not shown any serious after-effects from treatment with amyl nitrite.

ADDITIONAL NOTES:

Major medical treatment procedures may vary e.g. US (FDA method as recommended by DuPont) uses amyl nitrite as a methaemoglobin generator, followed by treatment with sodium nitrite and then sodium thiosulfate.

MODES OF ACTION: Amyl nitrite (AN) reacts with haemoglobin (HB) to form about 5% methaemoglobin (MHB). Sodium nitrite (NaNO2) reacts with haemoglobin to form approximately 20-30% methaemoglobin. Methaemoglobin attracts cyanide ions (CN) from tissue and binds with them to become cyanmethaemoglobin (CNMHB). Sodium thiosulfate (Na2S2O3) converts cyanmethaemoglobin to thiocyanate (HSCN) which is excreted by the kidneys. i.e. AN + HB = MHB NaNO2 + HB = MHB CN + MHB = CNMHB Na2S2O3 + CNMHB + O2 = HSCN

- ▶ The administration of the antidote salts is intravenous in normal saline, Ringers lactate or other available IV fluid.
- European practice may use 4-dimethylaminophenol (DMAP) as a methaemoglobin generator. Also hydroxycobalamin (Vitamin B12a) is used. Hydroxycobalamin works by reacting with cyanide to form cyanocobalamin (Vitamin B12) which is excreted in the urine.
- European and Australian NOHSC (ASCC) propose dicobalt edetate (Kelocyanor) as antidote. This acts by chelating cyanide to form stable cobalticyanide, which is excreted in the urine. In all cases hyperbaric therapy may increase the efficiency of a cyanide antidote kit.

SECTION 5 Firefighting measures

Extinguishing media

Special hazards arising from the substrate or mixture

Fire Incompatibility	▶ Avoid contamination with oxidising agents i.e. nitrates, oxidising acids, chlorine bleaches, pool chlorine etc. as ignition r
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Advice for firefighters		
Fire Fighting		
Fire/Explosion Hazard	Combustion products include: carbon dioxide (CO2) Liquid and vapour are highly flammable. Severe fire hazard when exposed to heat, flame and/or oxidisers. Vapour forms an explosive mixture with air. Severe explosion hazard, in the form of vapour, when exposed to flame or spark. nitrogen oxides (NOx) other pyrolysis products typical of burning organic material.	
HAZCHEM	•2YE	

SECTION 6 Accidental release measures

Personal precautions, protective equipment and emergency procedures

See section 8

Environmental precautions

See section 12

Methods and material for containment and cleaning up

Minor Spills

- Environmental hazard contain spillage.
- Remove all ignition sources
- Clean up all spills immediately. Avoid breathing vapours and contact with skin and eyes.
- Control personal contact with the substance, by using protective equipment.

may result

Version No: 2.3 Page 4 of 10 Issue Date: 24/01/2023

(±)-Warfarin D5 (phenyl-D5) 100 µg/mL in Acetonitrile

Print Date: 24/01/2023

For

Environmental hazard - contain spillage.

DO NOT touch the spill material

For alkyl nitriles:

Major Spills

For residue:

• Add alkaline hypochlorite solution to spill to produce cyanate

- Neutralise liquid, and absorb with sawdust.
- Collect solid residues and seal in drums for disposal.
- Wash spill area with large quantities of water.

Personal Protective Equipment advice is contained in Section 8 of the SDS.

SECTION 7 Handling and storage

Precautions for safe handling | Containers, even those that have been emptied, may contain explosive vapours. | Do NOT cut, drill, grind, weld or perform similar operations on or near containers. | Avoid all personal contact, including inhalation. | Wear protective clothing when risk of exposure occurs. | Use in a well-ventilated area. | Prevent concentration in hollows and sumps. | Store in original containers in approved flame-proof area. | No smoking, naked lights, heat or ignition sources. | DO NOT store in pits, depression, basement or areas where vapours may be trapped.

Conditions for safe storage, including any incompatibilities

Suitable container

 Glass container is suitable for laboratory quantities
Packing as supplied by manufacturer.

Keep containers securely sealed.

- Plastic containers may only be used if approved for flammable liquid.
 - ▶ Check that containers are clearly labelled and free from leaks.
 - For low viscosity materials (i): Drums and jerry cans must be of the non-removable head type. (ii): Where a can is to be used as an inner package, the can must have a screwed enclosure.
 - For materials with a viscosity of at least 2680 cSt. (23 deg. C)
 - For manufactured product having a viscosity of at least 250 cSt.

Acetonitrile

- ▶ forms cyanide gas on contact with steam
- reacts violently with oxidisers such as chlorine, bromine, fluorine; with chlorosulfonic acid, oleum or sulfuric acid
- is incompatible with water (especially if acid or alkaline), acids, caustics, nitrating agents, indium, nitrogen tetroxide, sulfur trioxide, iron(III) salts of perchlorate, nitrogen fluoride compounds
- attacks most rubber and plastics
- may accumulate electrical charges, causing ignition of vapours
- Contact with acids produces toxic fumes
- ▶ Nitriles may polymerise in the presence of metals and some metal compounds.
- ▶ They are incompatible with acids; mixing nitriles with strong oxidising acids can lead to extremely violent reactions.
- Nitriles are generally incompatible with other oxidising agents such as peroxides and epoxides.
- The combination of bases and nitriles can produce hydrogen cyanide.
 - The covalent cyano group is endothermic and many organic nitriles are reactive under certain conditions; N-cyano derivatives are reactive or unstable.
 - The majority of endothermic compounds are thermodynamically unstable and may decompose explosively under various circumstances of initiation.
 - Many but not all endothermic compounds have been involved in decompositions, reactions and explosions and, in general, compounds with significantly positive values of standard heats of formation, may be considered suspect on stability grounds.

BRETHERICK L.: Handbook of Reactive Chemical Hazards

WARNING

May decompose violently or explosively on contact with other substances.

- This substance, or one of its components, is one of the relatively few compounds which are described as "endothermic" i.e. heat is absorbed into the compound, rather than released from it, during its formation.
- The majority of endothermic compounds are thermodynamically unstable and may decompose explosively under various circumstances of initiation
- Many but not all endothermic compounds have been involved in decompositions, reactions and explosions and, in general, compounds with significantly positive values of standard heats of formation, may be considered suspect on stability grounds.
- Avoid reaction with oxidising agents

SECTION 8 Exposure controls / personal protection

Control parameters

Occupational Exposure Limits (OEL)

Storage incompatibility

INGREDIENT DATA

Source	Ingredient	Material name	TWA	STEL	Peak	Notes
Australia Exposure Standards	acetonitrile	Acetonitrile	40 ppm / 67 mg/m3	101 mg/m3 / 60 ppm	Not Available	Not Available

Emergency Limits

Ingredient	TEEL-1	TEEL-2	TEEL-3
acetonitrile	Not Available	Not Available	Not Available

Version No: 2.3 Page 5 of 10 Issue Date: 24/01/2023

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Print Date: 24/01/2023

(±)-Warfarin D5 (phenyl-D5) 100 µg/mL in Acetonitrile

Ingredient	Original IDLH	Revised IDLH
acetonitrile	500 ppm	137 ppm
Warfarin-d5	Not Available	Not Available

Exposure controls

Appropriate engineering controls

Engineering controls are used to remove a hazard or place a barrier between the worker and the hazard. Well-designed engineering controls can be highly effective in protecting workers and will typically be independent of worker interactions to provide this high level of protection.

The basic types of engineering controls are:

Process controls which involve changing the way a job activity or process is done to reduce the risk.

Enclosure and/or isolation of emission source which keeps a selected hazard "physically" away from the worker and ventilation that strategically "adds" and "removes" air in the work environment.

Personal protection









Eye and face protection

- Safety glasses with side shields.
- Chemical goggles.
- Contact lenses may pose a special hazard; soft contact lenses may absorb and concentrate irritants. A written policy document, describing the wearing of lenses or restrictions on use, should be created for each workplace or task.

Skin protection

See Hand protection below

Wear chemical protective gloves, e.g. PVC.

Wear safety footwear or safety gumboots, e.g. Rubber

Hands/feet protection

The selection of suitable gloves does not only depend on the material, but also on further marks of quality which vary from manufacturer to manufacturer. Where the chemical is a preparation of several substances, the resistance of the glove material can not be calculated in advance and has therefore to be checked prior to the application.

The exact break through time for substances has to be obtained from the manufacturer of the protective gloves and has to be observed when making a final choice.

Personal hygiene is a key element of effective hand care.

for acetonitrile:

Butyl rubber, PVAL, Teflon, Saranex, Silvershield, Viton/ chlorobutyl are all highly resistant to permeation

Body protection

See Other protection below

- ► Overalls.
 - PVC Apron.
 PVC protective suit may be required if exposure severe.
- ▶ Eyewash unit.

Other protection

- Some plastic personal protective equipment (PPE) (e.g. gloves, aprons, overshoes) are not recommended as they may produce static electricity.
- For large scale or continuous use wear tight-weave non-static clothing (no metallic fasteners, cuffs or pockets).
- Non sparking safety or conductive footwear should be considered. Conductive footwear describes a boot or shoe with a sole made from a conductive compound chemically bound to the bottom components, for permanent control to electrically ground the foot an shall dissipate static electricity from the body to reduce the possibility of ignition of volatile compounds.

Recommended material(s)

GLOVE SELECTION INDEX

Glove selection is based on a modified presentation of the:

"Forsberg Clothing Performance Index".

The effect(s) of the following substance(s) are taken into account in the *computer-generated* selection:

(±)-Warfarin D5 (phenyl-D5) 100 μ g/mL in Acetonitrile

Material	СРІ
BUTYL	Α
BUTYL/NEOPRENE	Α
CPE	Α
PE/EVAL/PE	Α
PVA	А
SARANEX-23	Α
NEOPRENE	В
TEFLON	В
NATURAL RUBBER	С
NATURAL+NEOPRENE	С
NITRILE	С
VITON/NEOPRENE	С

* CPI - Chemwatch Performance Index

A: Best Selection

B: Satisfactory; may degrade after 4 hours continuous immersion

C: Poor to Dangerous Choice for other than short term immersion

NOTE: As a series of factors will influence the actual performance of the glove, a final selection must be based on detailed observation. -

* Where the glove is to be used on a short term, casual or infrequent basis, factors such as "feel" or convenience (e.g. disposability), may dictate a choice of gloves which might

Respiratory protection

Type A Filter of sufficient capacity. (AS/NZS 1716 & 1715, EN 143:2000 & 149:2001, ANSI Z88 or national equivalent)

Where the concentration of gas/particulates in the breathing zone, approaches or exceeds the "Exposure Standard" (or ES), respiratory protection is required. Degree of protection varies with both face-piece and Class of filter; the nature of protection varies with Type of filter.

Required Minimum Protection Factor	Half-Face Respirator	Full-Face Respirator	Powered Air Respirator
up to 5 x ES	A-AUS / Class 1	-	A-PAPR-AUS / Class 1
up to 25 x ES	Air-line*	A-2	A-PAPR-2
up to 50 x ES	-	A-3	-
50+ x ES	-	Air-line**	-

^ - Full-face

A(All classes) = Organic vapours, B AUS or B1 = Acid gasses, B2 = Acid gas or hydrogen cyanide(HCN), B3 = Acid gas or hydrogen cyanide(HCN), E = Sulfur dioxide(SO2), G = Agricultural chemicals, K = Ammonia(NH3), Hg = Mercury, NO = Oxides of nitrogen, MB = Methyl bromide, AX = Low boiling point organic compounds(below 65 degC)

Version No: 2.3 Page 6 of 10

(±)-Warfarin D5 (phenyl-D5) 100 μg/mL in Acetonitrile

Issue Date: **24/01/2023**Print Date: **24/01/2023**

otherwise be unsuitable following long-term or frequent use. A qualified practitioner should be consulted.

- Cartridge respirators should never be used for emergency ingress or in areas of unknown vapour concentrations or oxygen content.
- The wearer must be warned to leave the contaminated area immediately on detecting any odours through the respirator. The odour may indicate that the mask is not functioning properly, that the vapour concentration is too high, or that the mask is not properly fitted. Because of these limitations, only restricted use of cartridge respirators is considered appropriate.
- Cartridge performance is affected by humidity. Cartridges should be changed after 2 hr of continuous use unless it is determined that the humidity is less than 75%, in which case, cartridges can be used for 4 hr. Used cartridges should be discarded daily, regardless of the length of time used

SECTION 9 Physical and chemical properties

Information on basic physical	and chemical properties		
Appearance	Colourless Liquid		
Physical state	Liquid	Relative density (Water = 1)	0.7822
Odour	Not Available	Partition coefficient n-octanol / water	Not Available
Odour threshold	Not Available	Auto-ignition temperature (°C)	525
pH (as supplied)	Not Available	Decomposition temperature (°C)	Not Available
Melting point / freezing point (°C)	-46	Viscosity (cSt)	Not Available
Initial boiling point and boiling range (°C)	81	Molecular weight (g/mol)	Not Available
Flash point (°C)	5	Taste	Not Available
Evaporation rate	Not Available	Explosive properties	Not Available
Flammability	HIGHLY FLAMMABLE.	Oxidising properties	Not Available
Upper Explosive Limit (%)	16	Surface Tension (dyn/cm or mN/m)	Not Available
Lower Explosive Limit (%)	4.4	Volatile Component (%vol)	Not Available
Vapour pressure (kPa)	9.70	Gas group	Not Available
Solubility in water	Partly miscible	pH as a solution (1%)	Not Available
Vapour density (Air = 1)	Not Available	VOC g/L	Not Available

SECTION 10 Stability and reactivity

Reactivity	See section 7
Chemical stability	 Presence of elevated temperatures. Unstable in the presence of incompatible materials. Product is considered stable. Hazardous polymerisation will not occur.
Possibility of hazardous reactions	See section 7
Conditions to avoid	See section 7
Incompatible materials	See section 7
Hazardous decomposition products	See section 5

SECTION 11 Toxicological information

single exposure by swallowing.

Information on toxicological effects

Inhaled	Inhalation of vapours or aerosols (mists, fumes), generated by the material during the course of normal handling, may produce toxic effects. The material is not thought to produce respiratory irritation (as classified by EC Directives using animal models). Nevertheless inhalation of vapours, fumes or aerosols, especially for prolonged periods, may produce respiratory discomfort and occasionally, distress. There is strong evidence to suggest that this material can cause, if inhaled once, serious, irreversible damage of organs. The smell of acetonitrile does not give enough warning of exposure. The gas is highly toxic, and inhaling it can cause loss of consciousness.
Inmention	Severely toxic effects may result from the accidental ingestion of the material; animal experiments indicate that ingestion of less than 5 gram may be fatal or may produce serious damage to the health of the individual.

Strong evidence exists that exposure to the material may cause irreversible damage (other than cancer, mutations and birth defects) following a

Version No: 2.3 Issue Date: 24/01/2023 Page 7 of 10 Print Date: 24/01/2023

(±)-Warfarin D5 (phenyl-D5) 100 µg/mL in Acetonitrile

Nitrile poisoning exhibits similar symptoms to poisoning due to hydrogen cyanide. The substances irritate the eyes and skin, and are absorbed quickly and completely through the skin. Cyanide poisoning can cause increased saliva output, nausea without vomiting, anxiety, confusion, vertigo, dizziness, stiffness of the lower jaw, convulsions, spasm, paralysis, coma and irregular heartbeat, and stimulation of breathing followed by failure. Often the skin becomes cyanosed (blue-grey), and this is often delayed. There is strong evidence to suggest that this material, on a single contact with skin, can cause serious, irreversible damage of organs. The material is not thought to be a skin irritant (as classified by EC Directives using animal models). Temporary discomfort, however, may result from prolonged dermal exposures. Skin Contact Open cuts, abraded or irritated skin should not be exposed to this material Entry into the blood-stream, through, for example, cuts, abrasions or lesions, may produce systemic injury with harmful effects. Examine the skin prior to the use of the material and ensure that any external damage is suitably protected. Skin contact with the material may produce toxic effects; systemic effects may result following absorption. There is evidence that material may produce eye irritation in some persons and produce eye damage 24 hours or more after instillation. Severe Eye inflammation may be expected with pain. Repeated or long-term occupational exposure is likely to produce cumulative health effects involving organs or biochemical systems. Chronic exposure to cyanides and certain nitriles may result in interference to iodine uptake by thyroid gland and its consequent enlargement. Chronic This occurs following metabolic conversion of the cyanide moiety to thiocyanate.

(±)-Warfarin D5 (phenyl-D5)	TOXICITY	IRRITATION
100 μg/mL in Acetonitrile	Not Available	Not Available
	TOXICITY	IRRITATION
	Dermal (rabbit) LD50: >2000 mg/kg ^[1]	Eye (rabbit):20 mg (open)-SEVERE
acetonitrile	Inhalation(Rabbit) LC50; 2828 ppm4h ^[2]	Skin (rabbit):500 mg (open)-mild
	Oral (Rabbit) LD50; 50 mg/kg ^[2]	
Markata In	TOXICITY	IRRITATION
Warfarin-d5	Not Available	Not Available
Legend:	Value obtained from Europe ECHA Registered Substance	res - Acute toxicity 2. Value obtained from manufacturer's SDS. Unless otherwise

specified data extracted from RTECS - Register of Toxic Effect of chemical Substances

ACETONITRILE (±)-Warfarin D5 (phenyl-D5)

ACETONITRILE

100 µg/mL in Acetonitrile &

The material may produce severe irritation to the eye causing pronounced inflammation. Repeated or prolonged exposure to irritants may produce conjunctivitis. The material may cause skin irritation after prolonged or repeated exposure and may produce on contact skin redness, swelling, the production of

vesicles, scaling and thickening of the skin Absorption of acetonitrile occurs after oral, skin, or inhalation exposure. The liquid or vapour is irritating to the skin, eyes, and airways. At high enough doses, death can occur quickly from respiratory failure. Lower doses cause typical symptoms of cyanide poisoning such as salivation, nausea, vomiting, anxiety, confusion, rapid and difficult breathing, rapid pulse, unconsciousness, and convulsions.

Acute Toxicity	✓	Carcinogenicity	X
Skin Irritation/Corrosion	×	Reproductivity	×
Serious Eye Damage/Irritation	✓	STOT - Single Exposure	X
Respiratory or Skin sensitisation	×	STOT - Repeated Exposure	×
Mutagenicity	×	Aspiration Hazard	×

Leaend:

★ - Data either not available or does not fill the criteria for classification - Data available to make classification

SECTION 12 Ecological information

	Endpoint	Test Duration (hr)	Species	Value	Source
±)-Warfarin D5 (phenyl-D5) 100 μg/mL in Acetonitrile	Not Available	Not Available	Not Available	Not Available	Not Available
	Endpoint	Test Duration (hr)	Species	Value	Source
acetonitrile	LC50	96h	Fish	>100mg/l	2
	EC50	48h	Crustacea	>1000mg/l	2
	NOEC(ECx)	24h	Crustacea	0.00001mg/l	4
	EC50	72h	Algae or other aquatic plants	>1000mg/l	2
	Endpoint	Test Duration (hr)	Species	Value	Source
Warfarin-d5	Not Available	Not Available	Not Available	Not Available	Not Available

- Bioconcentration Data 8. Vendor Data

Version No: 2.3 Page 8 of 10 Issue Date: 24/01/2023

(±)-Warfarin D5 (phenyl-D5) 100 μg/mL in Acetonitrile

On the basis of available evidence concerning either toxicity, persistence, potential to accumulate and or observed environmental fate and behaviour, the material may present a danger, immediate or long-term and /or delayed, to the structure and/ or functioning of natural ecosystems.

Soil Guidelines: Dutch Criteria: free cyanide: 1 mg/kg (target)

20 mg/kg (intervention)

complex cyanide (pH 5): 5 mg/kg (target)

50 mg/kg (intervention)

Air Quality Standards: no safe guidelines recommended due to carcinogenic properties.

Abiotic Effects: Acetonitrile is a volatile organic compound (VOC) substance, thus it is a contributor to the formation of photochemical smog in the presence of other VOCs.

Transport: Acetonitrile is primarily removed by volatilization and leaching into groundwater. It has low adsorption potential to soils. Air - Acetonitrile may persist in the troposphere and can be transported over long distances.

DO NOT discharge into sewer or waterways.

Persistence and degradability

Ingredient	Persistence: Water/Soil	Persistence: Air
acetonitrile	HIGH (Half-life = 360 days)	HIGH (Half-life = 541.29 days)

Bioaccumulative potential

Ingredient	Bioaccumulation
acetonitrile	LOW (BCF = 0.4)

Mobility in soil

Ingredient	Mobility
acetonitrile	LOW (KOC = 4.5)

SECTION 13 Disposal considerations

Waste treatment methods

Product / Packaging disposal

- ▶ Containers may still present a chemical hazard/ danger when empty.
- ▶ Return to supplier for reuse/ recycling if possible.

Otherwise:

- If container can not be cleaned sufficiently well to ensure that residuals do not remain or if the container cannot be used to store the same product, then puncture containers, to prevent re-use, and bury at an authorised landfill.
- ▶ Where possible retain label warnings and SDS and observe all notices pertaining to the product.

Legislation addressing waste disposal requirements may differ by country, state and/ or territory. Each user must refer to laws operating in their area. In some areas, certain wastes must be tracked.

A Hierarchy of Controls seems to be common - the user should investigate:

- ▶ Reduction
 - Reuse
 - Recycling
 - Disposal (if all else fails)

This material may be recycled if unused, or if it has not been contaminated so as to make it unsuitable for its intended use.

- DO NOT allow wash water from cleaning or process equipment to enter drains.
- It may be necessary to collect all wash water for treatment before disposal.
- In all cases disposal to sewer may be subject to local laws and regulations and these should be considered first.
- ▶ Where in doubt contact the responsible authority.
- Recycle wherever possible.
- Consult manufacturer for recycling options or consult local or regional waste management authority for disposal if no suitable treatment or disposal facility can be identified.
- Dispose of by: burial in a land-fill specifically licensed to accept chemical and / or pharmaceutical wastes or Incineration in a licensed apparatus (after admixture with suitable combustible material).
- Decontaminate empty containers.

SECTION 14 Transport information

Labels Required



Marine Pollutant	NO
HAZCHEM	•2YF

Land transport (ADG)

UN number	1648		
UN proper shipping name	ACETONITRILE		
Transport hazard class(es)	Class 3 Subrisk Not Applicable		
Packing group	II .		
Environmental hazard	Not Applicable		

Version No: 2.3 Page **9** of **10** Issue Date: 24/01/2023 Print Date: 24/01/2023

(±)-Warfarin D5 (phenyl-D5) 100 μg/mL in Acetonitrile

Special provisions Not Applicable Special precautions for user Limited quantity 1 L

Air transport (ICAO-IATA / DGR)

iii ii iiiiii ja	-7			
UN number	1648			
UN proper shipping name	Acetonitrile			
	ICAO/IATA Class	3		
Transport hazard class(es)	ICAO / IATA Subrisk	Not Applicable		
	ERG Code	3L		
Packing group	П			
Environmental hazard	Not Applicable			
	Special provisions		Not Applicable	
	Cargo Only Packing Instructions		364	
	Cargo Only Maximum	Qty / Pack	60 L	
Special precautions for user	Passenger and Cargo Packing Instructions		353	
	Passenger and Cargo Maximum Qty / Pack		5 L	
	Passenger and Cargo Limited Quantity Packing Instructions		Y341	
	Passenger and Cargo Limited Maximum Qty / Pack		1 L	

Sea transport (IMDG-Code / GGVSee)

UN number	1648		
UN proper shipping name	ACETONITRILE		
Transport hazard class(es)	IMDG Class 3 IMDG Subrisk Not Applicable		
Packing group			
Environmental hazard	Not Applicable		
Special precautions for user	EMS Number F-E, Special provisions Not A Limited Quantities 1 L	S-D pplicable	

Transport in bulk according to Annex II of MARPOL and the IBC code

Not Applicable

Transport in bulk in accordance with MARPOL Annex V and the IMSBC Code

Product name	Group
acetonitrile	Not Available
Warfarin-d5	Not Available

Transport in bulk in accordance with the ICG Code

Product name	Ship Type
acetonitrile	Not Available
Warfarin-d5	Not Available

SECTION 15 Regulatory information

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

acetonitrile is found on the following regulatory lists

Australia Hazardous Chemical Information System (HCIS) - Hazardous Chemicals Australian Inventory of Industrial Chemicals (AIIC)

Warfarin-d5 is found on the following regulatory lists

Not Applicable

National Inventory Status

National Inventory	Status
Australia - AIIC / Australia Non-Industrial Use	No (Warfarin-d5)
Canada - DSL	No (Warfarin-d5)
Canada - NDSL	No (acetonitrile; Warfarin-d5)
China - IECSC	No (Warfarin-d5)

Version No: 2.3 Issue Date: 24/01/2023 Page 10 of 10 Print Date: 24/01/2023

(±)-Warfarin D5 (phenyl-D5) 100 μg/mL in Acetonitrile

National Inventory Status Europe - EINEC / ELINCS / NLP No (Warfarin-d5) Japan - ENCS No (Warfarin-d5) Korea - KECI No (Warfarin-d5) New Zealand - NZIoC No (Warfarin-d5) Philippines - PICCS No (Warfarin-d5) USA - TSCA No (Warfarin-d5) Taiwan - TCSI No (Warfarin-d5) Mexico - INSQ No (Warfarin-d5) No (Warfarin-d5) Vietnam - NCI Russia - FBEPH No (Warfarin-d5) Yes = All CAS declared ingredients are on the inventory Legend:

SECTION 16 Other information

Revision Date	24/01/2023
Initial Date	30/11/2022

No = One or more of the CAS listed ingredients are not on the inventory. These ingredients may be exempt or will require registration.

SDS Version Summary

Version	Date of Update	Sections Updated
1.3	24/01/2023	Classification, Ingredients, Physical Properties

Other information

Classification of the preparation and its individual components has drawn on official and authoritative sources as well as independent review by the Chemwatch Classification committee using available literature references.

The SDS is a Hazard Communication tool and should be used to assist in the Risk Assessment. Many factors determine whether the reported Hazards are Risks in the workplace or other settings. Risks may be determined by reference to Exposures Scenarios. Scale of use, frequency of use and current or available engineering controls must be considered

Definitions and abbreviations

PC-TWA: Permissible Concentration-Time Weighted Average

PC-STEL: Permissible Concentration-Short Term Exposure Limit

IARC: International Agency for Research on Cancer

ACGIH: American Conference of Governmental Industrial Hygienists

STEL: Short Term Exposure Limit

TEEL: Temporary Emergency Exposure Limit。

IDLH: Immediately Dangerous to Life or Health Concentrations

ES: Exposure Standard OSF: Odour Safety Factor

NOAEL :No Observed Adverse Effect Level

LOAEL: Lowest Observed Adverse Effect Level

TLV: Threshold Limit Value LOD: Limit Of Detection

OTV: Odour Threshold Value BCF: BioConcentration Factors

BEI: Biological Exposure Index

AIIC: Australian Inventory of Industrial Chemicals

DSL: Domestic Substances List NDSL: Non-Domestic Substances List

IECSC: Inventory of Existing Chemical Substance in China

EINECS: European INventory of Existing Commercial chemical Substances

ELINCS: European List of Notified Chemical Substances

NLP: No-Longer Polymers

ENCS: Existing and New Chemical Substances Inventory

KECI: Korea Existing Chemicals Inventory

NZIoC: New Zealand Inventory of Chemicals

PICCS: Philippine Inventory of Chemicals and Chemical Substances

TSCA: Toxic Substances Control Act

TCSI: Taiwan Chemical Substance Inventory

INSQ: Inventario Nacional de Sustancias Químicas

NCI: National Chemical Inventory

FBEPH: Russian Register of Potentially Hazardous Chemical and Biological Substances

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