

SAFETY DATA SHEET

3mm sample kit - cold probe 13C, Part Number 190350511

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

This product is considered an article. This Safety Data Sheet is written based on the encapsulated substance or mixture in this article.

1.1 Product identifier

Product name	: 3mm sample kit - cold probe 13C, Part Number 190350511		
Part No. (Kit)	: 190350511		
Part No.	: 1H S/N		190350670
	4Hz 0.1% H ₂ O/D ₂ O		190350609
	Temp Grad		190350611
	1H Lineshape		190350689
	13C S/N ASTM doped		190350691
	ID 1		190350696
	ID 2		190350697
	Sucrose, NMR tested		190350612

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

Identified uses		
Analytical chemistry.		
1H S/N	250	µl
4Hz 0.1% H ₂ O/D ₂ O	250	µl
Temp Grad	250	µl
1H Lineshape	250	µl
13C S/N ASTM doped	250	µl
ID 1	250	µl
ID 2	250	µl
Sucrose, NMR tested	250	µl

1.3 Details of the supplier of the safety data sheet

Agilent Technologies Manufacturing GmbH & Co. KG
Hewlett-Packard-Str. 8
76337 Waldbronn
Germany
0800 603 1000

e-mail address of person responsible for this SDS : pdl-msds_author@agilent.com

1.4 Emergency telephone number

Emergency telephone number (with hours of operation) : CHEMTREC®: +(44)-870-8200418

SECTION 2: Hazards identification

This article, when used under reasonable conditions and in accordance with the directions for use, should not present a health hazard. The substance or mixture is encapsulated in the article. Only if released due to use or processing of the article in a manner not in accordance with the product's directions for use it may present potential health and safety hazards.

2.1 Classification of the substance or mixture

SECTION 2: Hazards identification

Product definition	:	1H S/N	Mixture (encapsulated in article)
		4Hz 0.1% H2O/D2O	Mixture (encapsulated in article)
		Temp Grad	Mixture (encapsulated in article)
		1H Lineshape	Mixture (encapsulated in article)
		13C S/N ASTM doped	Mixture (encapsulated in article)
		ID 1	Mixture (encapsulated in article)
		ID 2	Mixture (encapsulated in article)
		Sucrose, NMR tested	Mixture (encapsulated in article)

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

1H S/N

H302	ACUTE TOXICITY (oral) - Category 4
H315	SKIN CORROSION/IRRITATION - Category 2
H351	CARCINOGENICITY - Category 2
H373	SPECIFIC TARGET ORGAN TOXICITY (REPEATED EXPOSURE) - Category 2
H412	LONG-TERM AQUATIC HAZARD - Category 3

1H Lineshape

H225	FLAMMABLE LIQUIDS - Category 2
H319	SERIOUS EYE DAMAGE/ EYE IRRITATION - Category 2
H351	CARCINOGENICITY - Category 2
H336	SPECIFIC TARGET ORGAN TOXICITY (SINGLE EXPOSURE) (Narcotic effects) - Category 3
H412	LONG-TERM AQUATIC HAZARD - Category 3

13C S/N ASTM doped

H225	FLAMMABLE LIQUIDS - Category 2
H315	SKIN CORROSION/IRRITATION - Category 2
H319	SERIOUS EYE DAMAGE/ EYE IRRITATION - Category 2
H340	GERM CELL MUTAGENICITY - Category 1B
H350	CARCINOGENICITY - Category 1A
H335	SPECIFIC TARGET ORGAN TOXICITY (SINGLE EXPOSURE) (Respiratory tract irritation) - Category 3
H372	SPECIFIC TARGET ORGAN TOXICITY (REPEATED EXPOSURE) - Category 1
H412	LONG-TERM AQUATIC HAZARD - Category 3

ID 1

H302	ACUTE TOXICITY (oral) - Category 4
H315	SKIN CORROSION/IRRITATION - Category 2
H351	CARCINOGENICITY - Category 2
H373	SPECIFIC TARGET ORGAN TOXICITY (REPEATED EXPOSURE) - Category 2
H412	LONG-TERM AQUATIC HAZARD - Category 3

ID 2

H319	SERIOUS EYE DAMAGE/ EYE IRRITATION - Category 2
H373	SPECIFIC TARGET ORGAN TOXICITY (REPEATED EXPOSURE) - Category 2

Ingredients of unknown ecotoxicity

:	1H S/N	Not applicable.
	4Hz 0.1% H2O/D2O	Not applicable.
	Temp Grad	Not applicable.
	1H Lineshape	Not applicable.
	13C S/N ASTM doped	Not applicable.
	ID 1	Percentage of the mixture consisting of ingredient(s) of unknown hazards to the aquatic environment: 1%
	ID 2	Not applicable.
	Sucrose, NMR tested	Not applicable.

Classification according to Directive 1999/45/EC [DPD]

1H S/N	The product is classified as dangerous according to Directive 1999/45/EC and its amendments.
4Hz 0.1% H2O/D2O	The product is not classified as dangerous according to Directive 1999/45/EC and its amendments.
Temp Grad	The product is not classified as dangerous according to Directive 1999/45/EC and its amendments.
1H Lineshape	The product is classified as dangerous according to Directive 1999/45/EC and its amendments.

SECTION 2: Hazards identification

13C S/N ASTM doped	The product is classified as dangerous according to Directive 1999/45/EC and its amendments.
ID 1	The product is classified as dangerous according to Directive 1999/45/EC and its amendments.
ID 2	The product is not classified as dangerous according to Directive 1999/45/EC and its amendments.
Sucrose, NMR tested	The product is not classified as dangerous according to Directive 1999/45/EC and its amendments.

Classification	:	1H S/N	Carc. Cat. 3; R40 Xn; R22, R48/20/22 Xi; R38
		4Hz 0.1% H2O/D2O	Not classified.
		Temp Grad	Not classified.
		1H Lineshape	F; R11
			Carc. Cat. 3; R40 Xi; R36 R66, R67
		13C S/N ASTM doped	R10 Carc. Cat. 1; R45 Muta. Cat. 2; R46 T; R48/23/24/25 Xn; R65 Xi; R36/37/38
		ID 1	Carc. Cat. 3; R40 Xn; R22, R48/20/22 Xi; R38
		ID 2	Not classified.
		Sucrose, NMR tested	Not classified.

Physical/chemical hazards	:	1H S/N	Not applicable.
		4Hz 0.1% H2O/D2O	Not applicable.
		Temp Grad	Not applicable.
		1H Lineshape	Highly flammable.
		13C S/N ASTM doped	Flammable.
		ID 1	Not applicable.
		ID 2	Not applicable.
		Sucrose, NMR tested	Not applicable.

Human health hazards	:	1H S/N	Limited evidence of a carcinogenic effect. Harmful if swallowed. Harmful: danger of serious damage to health in case of prolonged exposure through inhalation and if swallowed. Irritating to skin.
		4Hz 0.1% H2O/D2O	Not applicable.
		Temp Grad	Not applicable.
		1H Lineshape	Limited evidence of a carcinogenic effect. Irritating to eyes. Repeated exposure may cause skin dryness or cracking. Vapours may cause drowsiness and dizziness.
		13C S/N ASTM doped	May cause cancer. May cause heritable genetic damage. Also toxic: danger of serious damage to health by prolonged exposure through inhalation, in contact with skin and if swallowed. Also harmful: may cause lung damage if swallowed. Irritating to eyes, respiratory system and skin.
		ID 1	Limited evidence of a carcinogenic effect. Harmful if swallowed. Harmful: danger of serious damage to health in case of prolonged exposure through inhalation and if swallowed. Irritating to skin.
		ID 2	Not applicable.
		Sucrose, NMR tested	Not applicable.

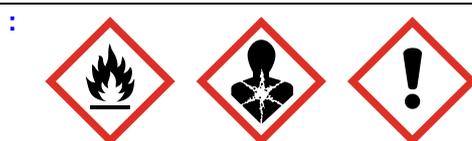
See Section 16 for the full text of the R phrases or H statements declared above.

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

2.2 Label elements

SECTION 2: Hazards identification

Hazard pictograms



Signal word

: 1H S/N
 4Hz 0.1% H2O/D2O
 Temp Grad
 1H Lineshape
 13C S/N ASTM doped
 ID 1
 ID 2
 Sucrose, NMR tested

Warning
 No signal word.
 No signal word.
 Danger
 Danger
 Warning
 Warning
 No signal word.

Hazard statements

: 1H S/N
 4Hz 0.1% H2O/D2O
 Temp Grad
 1H Lineshape
 13C S/N ASTM doped
 ID 1
 ID 2
 Sucrose, NMR tested

GHS07 -
 Harmful if swallowed.
 Causes skin irritation.
GHS08 -
 Suspected of causing cancer.
 May cause damage to organs through prolonged or repeated exposure.
 Harmful to aquatic life with long lasting effects.
GHS02 -
 No known significant effects or critical hazards.
 No known significant effects or critical hazards.
GHS02 -
 Highly flammable liquid and vapour.
GHS07 -
 Causes serious eye irritation.
 May cause drowsiness or dizziness.
GHS08 -
 Suspected of causing cancer.
 Harmful to aquatic life with long lasting effects.
GHS02 -
 Highly flammable liquid and vapour.
GHS07 -
 Causes skin irritation.
 May cause respiratory irritation.
 Causes serious eye irritation.
GHS08 -
 May cause genetic defects.
 May cause cancer.
 Causes damage to organs through prolonged or repeated exposure.
 Harmful to aquatic life with long lasting effects.
GHS07 -
 Harmful if swallowed.
 Causes skin irritation.
GHS08 -
 Suspected of causing cancer.
 May cause damage to organs through prolonged or repeated exposure.
 Harmful to aquatic life with long lasting effects.
GHS07 -
 Causes serious eye irritation.
GHS08 -
 May cause damage to organs through prolonged or repeated exposure.
 No known significant effects or critical hazards.

Precautionary statements

SECTION 2: Hazards identification

Prevention	: 1H S/N	P201 - Obtain special instructions before use. P280 - Wear protective gloves. P273 - Avoid release to the environment. P260 - Do not breathe vapour.	
	4Hz 0.1% H2O/D2O Temp Grad 1H Lineshape	Not applicable. Not applicable. P201 - Obtain special instructions before use. P280 - Wear protective gloves. Wear eye or face protection. P210 - Keep away from heat, sparks, open flames and hot surfaces. - No smoking. P241 - Use explosion-proof electrical, ventilating, lighting and all material-handling equipment. P273 - Avoid release to the environment.	
	13C S/N ASTM doped	P201 - Obtain special instructions before use. P280 - Wear protective gloves. Wear eye or face protection. P210 - Keep away from heat, sparks, open flames and hot surfaces. - No smoking. P241 - Use explosion-proof electrical, ventilating, lighting and all material-handling equipment. P273 - Avoid release to the environment.	
	ID 1	P201 - Obtain special instructions before use. P280 - Wear protective gloves. P273 - Avoid release to the environment. P260 - Do not breathe vapour.	
	ID 2	P280 - Wear eye or face protection. P260 - Do not breathe vapour. P264 - Wash hands thoroughly after handling.	
	Sucrose, NMR tested	Not applicable.	
	Response	: 1H S/N	P314 - Get medical attention if you feel unwell. P301 + P312 - IF SWALLOWED: Call a POISON CENTER or physician if you feel unwell.
		4Hz 0.1% H2O/D2O Temp Grad 1H Lineshape	Not applicable. Not applicable. P304 + P340 - IF INHALED: Remove victim to fresh air and keep at rest in a position comfortable for breathing. P303 + P361 + P353 - IF ON SKIN (or hair): Take off immediately all contaminated clothing. Rinse skin with water or shower.
		13C S/N ASTM doped	P304 + P340 - IF INHALED: Remove victim to fresh air and keep at rest in a position comfortable for breathing. P303 + P361 + P353 - IF ON SKIN (or hair): Take off immediately all contaminated clothing. Rinse skin with water or shower.
		ID 1	P314 - Get medical attention if you feel unwell. P301 + P312 - IF SWALLOWED: Call a POISON CENTER or physician if you feel unwell.
ID 2		P314 - Get medical attention if you feel unwell. P305 + P351 - IF IN EYES: Rinse cautiously with water for several minutes.	
Sucrose, NMR tested		Not applicable.	
Storage		: 1H S/N	P405 - Store locked up.
		4Hz 0.1% H2O/D2O Temp Grad 1H Lineshape	Not applicable. Not applicable. P235 - Keep cool.
		13C S/N ASTM doped	P235 - Keep cool.
		ID 1	P405 - Store locked up.
	ID 2	Not applicable.	
	Sucrose, NMR tested	Not applicable.	

SECTION 2: Hazards identification

Disposal	: 1H S/N 4Hz 0.1% H2O/D2O Temp Grad 1H Lineshape 13C S/N ASTM doped ID 1 ID 2 Sucrose, NMR tested	P501 - Dispose of contents and container in accordance with all local, regional, national and international regulations. Not applicable. Not applicable. P501 - Dispose of contents and container in accordance with all local, regional, national and international regulations. P501 - Dispose of contents and container in accordance with all local, regional, national and international regulations. P501 - Dispose of contents and container in accordance with all local, regional, national and international regulations. P501 - Dispose of contents and container in accordance with all local, regional, national and international regulations. Not applicable.
Hazardous ingredients	: 1H S/N (² H)Chloroform 1H Lineshape (² H ₆)Acetone Trichloromethane 13C S/N ASTM doped (² H ₆)Benzene 1,4-Dioxane ID 1 (² H)Chloroform ID 2 di[(² H ₃)Methyl] sulphoxide	
Supplemental label elements	: 1H S/N 4Hz 0.1% H2O/D2O Temp Grad 1H Lineshape 13C S/N ASTM doped ID 1 ID 2 Sucrose, NMR tested	Not applicable. Not applicable. Not applicable. Not applicable. Not applicable. Not applicable. Not applicable.
<u>Special packaging requirements</u>		
Tactile warning of danger	: 1H S/N 4Hz 0.1% H2O/D2O Temp Grad 1H Lineshape 13C S/N ASTM doped ID 1 ID 2 Sucrose, NMR tested	Not applicable. Not applicable. Not applicable. Not applicable. Not applicable. Not applicable. Not applicable.
2.3 Other hazards		
Other hazards which do not result in classification	: 1H S/N 4Hz 0.1% H2O/D2O Temp Grad 1H Lineshape 13C S/N ASTM doped ID 1 ID 2 Sucrose, NMR tested	None known. None known. None known. Defatting to the skin. Prolonged or repeated contact may dry skin and cause irritation. Defatting to the skin. Prolonged or repeated contact may dry skin and cause irritation. None known. None known. None known.

SECTION 3: Composition/information on ingredients

This article, when used under reasonable conditions and in accordance with the directions for use, should not present a health hazard. The substance or mixture is encapsulated in the article. Only if released due to use or processing of the article in a manner not in accordance with the product's directions for use it may present potential health and safety hazards.

Substance/mixture	: 1H S/N 4Hz 0.1% H2O/D2O Temp Grad 1H Lineshape 13C S/N ASTM doped ID 1 ID 2 Sucrose, NMR tested	Mixture (encapsulated in article) Mixture (encapsulated in article)
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Product/ingredient name	Identifiers	%	Classification		Type
			67/548/EEC	Regulation (EC) No. 1272/2008 [CLP]	
1H S/N (² H)Chloroform	EC: 200-663-8 CAS: 865-49-6 Index: 602-006-00-4	>=90	Carc. Cat. 3; R40 Xn; R22, R48/20/22 Xi; R38	Acute Tox. 4, H302 Skin Irrit. 2, H315 Carc. 2, H351 STOT RE 2, H373	[1] [2]
1H Lineshape (² H ₆)Acetone	EC: 200-662-2 CAS: 666-52-4 Index: 606-001-00-8	>=90	F; R11 Xi; R36 R66, R67	Flam. Liq. 2, H225 Eye Irrit. 2, H319 STOT SE 3, H336 (Narcotic effects)	[1] [2]
Trichloromethane	EC: 200-663-8 CAS: 67-66-3 Index: 602-006-00-4	>=1 - <5	Carc. Cat. 3; R40 Xn; R22, R48/20/22 Xi; R38	Acute Tox. 4, H302 Skin Irrit. 2, H315 Carc. 2, H351 STOT RE 2, H373	[1] [2]
13C S/N ASTM doped (² H ₆)Benzene	EC: 200-753-7 CAS: 1076-43-3 Index: 601-020-00-8	>=50 - <75	F; R11 Carc. Cat. 1; R45 Muta. Cat. 2; R46 T; R48/23/24/25 Xn; R65 Xi; R36/38	Flam. Liq. 2, H225 Skin Irrit. 2, H315 Eye Irrit. 2, H319 Muta. 1B, H340 Carc. 1A, H350 STOT RE 1, H372 Asp. Tox. 1, H304	[1] [2]
1,4-Dioxane	EC: 204-661-8 CAS: 123-91-1 Index: 603-024-00-5	>=35 - <50	F; R11 R19 Carc. Cat. 3; R40 Xi; R36/37 R66	Flam. Liq. 2, H225 Eye Irrit. 2, H319 Carc. 2, H351 STOT SE 3, H335 (Respiratory tract irritation)	[1] [2]
ID 1 (² H)Chloroform	EC: 200-663-8 CAS: 865-49-6 Index: 602-006-00-4	>=90	Carc. Cat. 3; R40 Xn; R22, R48/20/22 Xi; R38	Acute Tox. 4, H302 Skin Irrit. 2, H315 Carc. 2, H351 STOT RE 2, H373	[1] [2]
Iodomethane (¹³ C)	EC: 200-819-5 CAS: 4227-95-6 Index: 602-005-00-9	>=1 - <3	Carc. Cat. 3; R40 T; R23/25 Xn; R21 Xi; R37/38	Acute Tox. 3, H301 Acute Tox. 4, H312 Acute Tox. 3, H331 Skin Irrit. 2, H315 Carc. 2, H351 STOT SE 3, H335 (Respiratory tract irritation)	[1]
Trimethyl phosphite	EC: 204-471-5 CAS: 121-45-9	>=1 - <3	R10 Xn; R21/22 Xi; R36/37/38	Flam. Liq. 3, H226 Acute Tox. 4, H302 Acute Tox. 3, H311	[1]

SECTION 3: Composition/information on ingredients

<p>ID 2 di[(²H₃)Methyl] sulphoxide</p> <p>Benzamide (¹⁵N)</p>	<p>EC: 200-664-3 CAS: 2206-27-1</p> <p>CAS: 31656-62-9</p>	<p>>=90</p> <p>>=1 - <3</p>	<p>Not classified.</p> <p>Xn; R22</p> <p>See Section 16 for the full text of the R-phrases declared above.</p>	<p>Skin Irrit. 2, H315 Eye Irrit. 2, H319 STOT SE 3, H335 (Respiratory tract irritation)</p> <p>Eye Irrit. 2, H319 STOT RE 2, H373 (kidneys and liver) (oral) Acute Tox. 4, H302</p> <p>See Section 16 for the full text of the H statements declared above.</p>	<p>[1]</p> <p>[1]</p>
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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 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

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

SECTION 4: First aid measures

4.1 Description of first aid measures

<p>Eye contact : 1H S/N</p>	<p>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.</p>
<p>4Hz 0.1% H2O/D2O</p>	<p>Immediately flush eyes with plenty of water, occasionally lifting the upper and lower eyelids. Check for and remove any contact lenses. Get medical attention if irritation occurs.</p>
<p>Temp Grad</p>	<p>Immediately flush eyes with plenty of water, occasionally lifting the upper and lower eyelids. Check for and remove any contact lenses. Get medical attention if irritation occurs.</p>
<p>1H Lineshape</p>	<p>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.</p>
<p>13C S/N ASTM doped</p>	<p>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.</p>
<p>ID 1</p>	<p>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.</p>
<p>ID 2</p>	<p>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 following exposure or if feeling unwell.</p>
<p>Sucrose, NMR tested</p>	<p>Immediately flush eyes with plenty of water, occasionally lifting the upper and lower eyelids. Check for and remove any contact lenses. Get medical attention if irritation occurs.</p>

SECTION 4: First aid measures

Inhalation	: 1H S/N	Remove victim to fresh air and keep at rest in a position comfortable for breathing. 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 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.
	4Hz 0.1% H2O/D2O	Remove victim to fresh air and keep at rest in a position comfortable for breathing. Get medical attention if symptoms occur.
	Temp Grad	Remove victim to fresh air and keep at rest in a position comfortable for breathing. Get medical attention if symptoms occur.
	1H Lineshape	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 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.
	13C S/N ASTM doped	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 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.
	ID 1	Remove victim to fresh air and keep at rest in a position comfortable for breathing. 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 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.
	ID 2	Remove victim to fresh air and keep at rest in a position comfortable for breathing. 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 following exposure or if feeling unwell. If unconscious, place in recovery position and get medical attention immediately.

SECTION 4: First aid measures

		Maintain an open airway. Loosen tight clothing such as a collar, tie, belt or waistband.
	Sucrose, NMR tested	Remove victim to fresh air and keep at rest in a position comfortable for breathing. Get medical attention if symptoms occur.
Skin contact	: 1H S/N	Flush contaminated skin with plenty of water. Remove contaminated clothing and shoes. Continue to rinse for at least 10 minutes. Get medical attention. Wash clothing before reuse. Clean shoes thoroughly before reuse.
	4Hz 0.1% H2O/D2O	Flush contaminated skin with plenty of water. Remove contaminated clothing and shoes. Get medical attention if symptoms occur.
	Temp Grad	Flush contaminated skin with plenty of water. Remove contaminated clothing and shoes. Get medical attention if symptoms occur.
	1H Lineshape	Wash skin thoroughly with soap and water or use recognised skin cleanser. Remove contaminated clothing and shoes. Continue to rinse for at least 10 minutes. Get medical attention. Wash clothing before reuse. Clean shoes thoroughly before reuse.
	13C S/N ASTM doped	Wash skin thoroughly with soap and water or use recognised skin cleanser. 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. Wash clothing before reuse. Clean shoes thoroughly before reuse.
	ID 1	Flush contaminated skin with plenty of water. Remove contaminated clothing and shoes. Continue to rinse for at least 10 minutes. Get medical attention. Wash clothing before reuse. Clean shoes thoroughly before reuse.
	ID 2	Flush contaminated skin with plenty of water. Remove contaminated clothing and shoes. Continue to rinse for at least 10 minutes. Get medical attention following exposure or if feeling unwell. Wash clothing before reuse. Clean shoes thoroughly before reuse.
	Sucrose, NMR tested	Flush contaminated skin with plenty of water. Remove contaminated clothing and shoes. Get medical attention if symptoms occur.
Ingestion	: 1H S/N	Wash out mouth with water. Remove dentures if any. Remove victim to fresh air and keep at rest in a position comfortable for breathing. 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.
	4Hz 0.1% H2O/D2O	Wash out mouth with water. Remove victim to fresh air and keep at rest in a position comfortable for breathing. If material has been swallowed and the exposed person is conscious, give small quantities of water to drink. Do not induce vomiting unless directed to do so by medical personnel. Get medical attention if symptoms occur.
	Temp Grad	Wash out mouth with water. Remove victim to fresh air and keep at rest in a position comfortable for breathing. If material has been swallowed and the exposed person is conscious, give small quantities of water to drink. Do not induce vomiting unless directed to do so by medical personnel. Get medical attention if symptoms occur.
	1H Lineshape	Wash out mouth with water. Remove dentures if any.

SECTION 4: First aid measures

	Remove victim to fresh air and keep at rest in a position comfortable for breathing. 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.
13C S/N ASTM doped	Wash out mouth with water. Remove dentures if any. Remove victim to fresh air and keep at rest in a position comfortable for breathing. 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. 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.
ID 1	Wash out mouth with water. Remove dentures if any. Remove victim to fresh air and keep at rest in a position comfortable for breathing. 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.
ID 2	Wash out mouth with water. Remove dentures if any. Remove victim to fresh air and keep at rest in a position comfortable for breathing. 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 following exposure or if feeling unwell. 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.
Sucrose, NMR tested	Wash out mouth with water. Remove victim to fresh air and keep at rest in a position comfortable for breathing. If material has been swallowed and the exposed person is conscious, give small quantities of water to drink. Do not induce vomiting unless directed to do so by medical personnel. Get medical attention if symptoms occur.

SECTION 4: First aid measures

Protection of first-aiders	: 1H S/N	No action shall be taken involving any personal risk or without suitable training. It may be dangerous to the person providing aid to give mouth-to-mouth resuscitation.
	4Hz 0.1% H2O/D2O	No action shall be taken involving any personal risk or without suitable training.
	Temp Grad	No action shall be taken involving any personal risk or without suitable training.
	1H Lineshape	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.
	13C S/N ASTM doped	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.
	ID 1	No action shall be taken involving any personal risk or without suitable training. It may be dangerous to the person providing aid to give mouth-to-mouth resuscitation.
	ID 2	No action shall be taken involving any personal risk or without suitable training. It may be dangerous to the person providing aid to give mouth-to-mouth resuscitation.
	Sucrose, NMR tested	No action shall be taken involving any personal risk or without suitable training.

4.2 Most important symptoms and effects, both acute and delayed

Potential acute health effects

Eye contact	: 1H S/N	Causes serious eye irritation.
	4Hz 0.1% H2O/D2O	No known significant effects or critical hazards.
	Temp Grad	No known significant effects or critical hazards.
	1H Lineshape	Causes serious eye irritation.
	13C S/N ASTM doped	Causes serious eye irritation.
	ID 1	Causes serious eye irritation.
	ID 2	Causes eye irritation.
	Sucrose, NMR tested	No known significant effects or critical hazards.
Inhalation	: 1H S/N	Exposure to decomposition products may cause a health hazard. Serious effects may be delayed following exposure.
	4Hz 0.1% H2O/D2O	No known significant effects or critical hazards.
	Temp Grad	No known significant effects or critical hazards.
	1H Lineshape	Can cause central nervous system (CNS) depression. May cause drowsiness or dizziness. Exposure to decomposition products may cause a health hazard. Serious effects may be delayed following exposure.
	13C S/N ASTM doped	May cause respiratory irritation.
	ID 1	Exposure to decomposition products may cause a health hazard. Serious effects may be delayed following exposure.
	ID 2	No known significant effects or critical hazards.
	Sucrose, NMR tested	No known significant effects or critical hazards.
Skin contact	: 1H S/N	Causes skin irritation.
	4Hz 0.1% H2O/D2O	No known significant effects or critical hazards.
	Temp Grad	No known significant effects or critical hazards.
	1H Lineshape	Defatting to the skin. May cause skin dryness and irritation.
	13C S/N ASTM doped	Causes skin irritation. Defatting to the skin.
	ID 1	Causes skin irritation.
	ID 2	No known significant effects or critical hazards.
	Sucrose, NMR tested	No known significant effects or critical hazards.

SECTION 4: First aid measures

Ingestion	: 1H S/N 4Hz 0.1% H2O/D2O Temp Grad 1H Lineshape 13C S/N ASTM doped ID 1 ID 2 Sucrose, NMR tested	Harmful if swallowed. Irritating to mouth, throat and stomach. No known significant effects or critical hazards. No known significant effects or critical hazards. Can cause central nervous system (CNS) depression. Irritating to mouth, throat and stomach. Irritating to mouth, throat and stomach. Harmful if swallowed. Irritating to mouth, throat and stomach. May be irritating to mouth, throat and stomach. No known significant effects or critical hazards.
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Over-exposure signs/symptoms

Eye contact	: 1H S/N 4Hz 0.1% H2O/D2O Temp Grad 1H Lineshape 13C S/N ASTM doped ID 1 ID 2 Sucrose, NMR tested	Adverse symptoms may include the following: pain or irritation watering redness No specific data. No specific data. Adverse symptoms may include the following: pain or irritation watering redness Adverse symptoms may include the following: pain or irritation watering redness Adverse symptoms may include the following: pain or irritation watering redness Adverse symptoms may include the following: irritation watering redness No specific data.
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Inhalation	: 1H S/N 4Hz 0.1% H2O/D2O Temp Grad 1H Lineshape 13C S/N ASTM doped ID 1 ID 2 Sucrose, NMR tested	No specific data. No specific data. No specific data. Adverse symptoms may include the following: nausea or vomiting headache drowsiness/fatigue dizziness/vertigo unconsciousness Adverse symptoms may include the following: respiratory tract irritation coughing No specific data. No specific data. No specific data.
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Skin contact	: 1H S/N 4Hz 0.1% H2O/D2O Temp Grad 1H Lineshape 13C S/N ASTM doped	Adverse symptoms may include the following: irritation redness No specific data. No specific data. Adverse symptoms may include the following: irritation dryness cracking Adverse symptoms may include the following: irritation redness dryness cracking
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SECTION 4: First aid measures

	ID 1	Adverse symptoms may include the following: irritation redness
	ID 2	No specific data.
Ingestion	Sucrose, NMR tested	No specific data.
	: 1H S/N	No specific data.
	4Hz 0.1% H ₂ O/D ₂ O	No specific data.
	Temp Grad	No specific data.
	1H Lineshape	No specific data.
	13C S/N ASTM doped	No specific data.
	ID 1	No specific data.
	ID 2	No specific data.
	Sucrose, NMR tested	No specific data.

4.3 Indication of any immediate medical attention and special treatment needed

Notes to physician	: 1H S/N	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.	
	4Hz 0.1% H ₂ O/D ₂ O	Treat symptomatically. Contact poison treatment specialist immediately if large quantities have been ingested or inhaled.	
	Temp Grad	Treat symptomatically. Contact poison treatment specialist immediately if large quantities have been ingested or inhaled.	
	1H Lineshape	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.	
	13C S/N ASTM doped	Treat symptomatically. Contact poison treatment specialist immediately if large quantities have been ingested or inhaled.	
	ID 1	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.	
	ID 2	Treat symptomatically. Contact poison treatment specialist immediately if large quantities have been ingested or inhaled.	
	Sucrose, NMR tested	Treat symptomatically. Contact poison treatment specialist immediately if large quantities have been ingested or inhaled.	
	Specific treatments	: 1H S/N	No specific treatment.
		4Hz 0.1% H ₂ O/D ₂ O	No specific treatment.
Temp Grad		No specific treatment.	
1H Lineshape		No specific treatment.	
13C S/N ASTM doped		No specific treatment.	
ID 1		No specific treatment.	
ID 2		No specific treatment.	
Sucrose, NMR tested	No specific treatment.		

SECTION 5: Firefighting measures

5.1 Extinguishing media

Suitable extinguishing media	: 1H S/N	Use an extinguishing agent suitable for the surrounding fire.	
	4Hz 0.1% H ₂ O/D ₂ O	Use an extinguishing agent suitable for the surrounding fire.	
	Temp Grad	Use an extinguishing agent suitable for the surrounding fire.	
	1H Lineshape	Use dry chemical, CO ₂ , water spray (fog) or foam.	
	13C S/N ASTM doped	Use dry chemical, CO ₂ , water spray (fog) or foam.	
	ID 1	Use an extinguishing agent suitable for the surrounding fire.	
	ID 2	Use an extinguishing agent suitable for the surrounding fire.	
	Sucrose, NMR tested	Use an extinguishing agent suitable for the surrounding fire.	
	Unsuitable extinguishing media	: 1H S/N	None known.
		4Hz 0.1% H ₂ O/D ₂ O	None known.
Temp Grad		None known.	
1H Lineshape		Do not use water jet.	
13C S/N ASTM doped		Do not use water jet.	
ID 1		None known.	
ID 2		None known.	
Sucrose, NMR tested	None known.		

SECTION 5: Firefighting measures

5.2 Special hazards arising from the substance or mixture

Hazards from the substance or mixture	: 1H S/N	In a fire or if heated, a pressure increase will occur and the container may burst. 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.
	4Hz 0.1% H2O/D2O	In a fire or if heated, a pressure increase will occur and the container may burst.
	Temp Grad	In a fire or if heated, a pressure increase will occur and the container may burst.
	1H Lineshape	Highly flammable liquid and vapour. In a fire or if heated, a pressure increase will occur and the container may burst, with the risk of a subsequent explosion. Runoff to sewer may create fire or explosion hazard. 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.
	13C S/N ASTM doped	Highly flammable liquid and vapour. In a fire or if heated, a pressure increase will occur and the container may burst, with the risk of a subsequent explosion. Runoff to sewer may create fire or explosion hazard. 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.
	ID 1	In a fire or if heated, a pressure increase will occur and the container may burst. 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.
	ID 2	In a fire or if heated, a pressure increase will occur and the container may burst.
	Sucrose, NMR tested	In a fire or if heated, a pressure increase will occur and the container may burst.
Hazardous combustion products	: 1H S/N	Decomposition products may include the following materials: carbon dioxide carbon monoxide halogenated compounds carbonyl halides
	4Hz 0.1% H2O/D2O	No specific data.
	Temp Grad	No specific data.
	1H Lineshape	Decomposition products may include the following materials: carbon dioxide carbon monoxide halogenated compounds carbonyl halides
	13C S/N ASTM doped	Decomposition products may include the following materials: carbon dioxide carbon monoxide
	ID 1	Decomposition products may include the following materials: carbon dioxide carbon monoxide phosphorus oxides halogenated compounds carbonyl halides
	ID 2	Decomposition products may include the following materials: carbon dioxide carbon monoxide sulfur oxides
	Sucrose, NMR tested	No specific data.

5.3 Advice for firefighters

SECTION 5: Firefighting measures

Special precautions for fire-fighters	: 1H S/N	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.
	4Hz 0.1% H2O/D2O	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.
	Temp Grad	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.
	1H Lineshape	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.
	13C S/N ASTM doped	Move containers from fire area if this can be done without risk. Use water spray to keep fire-exposed containers cool. 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.
	ID 1	Move containers from fire area if this can be done without risk. Use water spray to keep fire-exposed containers cool. 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.
	ID 2	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.
	Sucrose, NMR tested	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.

Special protective equipment for fire-fighters	: 1H S/N	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.
	4Hz 0.1% H2O/D2O	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.
	Temp Grad	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.
	1H Lineshape	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.
	13C S/N ASTM doped	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.
	ID 1	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.
	ID 2	Fire-fighters should wear appropriate protective equipment

SECTION 5: Firefighting measures

Sucrose, NMR tested

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.

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

: 1H S/N

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. Avoid breathing vapour or mist. Provide adequate ventilation. Wear appropriate respirator when ventilation is inadequate. Put on appropriate personal protective equipment.

4Hz 0.1% H2O/D2O

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. Put on appropriate personal protective equipment.

Temp Grad

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. Put on appropriate personal protective equipment.

1H Lineshape

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.

13C S/N ASTM doped

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.

ID 1

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. Avoid breathing vapour or mist. Provide adequate ventilation. Wear appropriate respirator when ventilation is inadequate. Put on appropriate personal protective equipment.

ID 2

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. Avoid breathing vapour or mist. Provide adequate ventilation. Wear appropriate respirator when ventilation is inadequate. Put on appropriate personal protective equipment.

Sucrose, NMR tested

No action shall be taken involving any personal risk or

SECTION 6: Accidental release measures

For emergency responders	: 1H S/N	without suitable training. Evacuate surrounding areas. Keep unnecessary and unprotected personnel from entering. Do not touch or walk through spilt material. Put on appropriate personal protective equipment.
	4Hz 0.1% H2O/D2O	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".
	Temp Grad	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".
	1H Lineshape	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".
	13C S/N ASTM doped	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".
	ID 1	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".
	ID 2	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".
	Sucrose, NMR tested	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	: 1H S/N	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.
	4Hz 0.1% H2O/D2O	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).
	Temp Grad	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).
	1H Lineshape	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.
	13C S/N ASTM doped	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.
	ID 1	Avoid dispersal of spilt material and runoff and contact with soil, waterways, drains and sewers. Inform the relevant

SECTION 6: Accidental release measures

	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.
ID 2	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).
Sucrose, NMR tested	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 materials for containment and cleaning up

Methods for cleaning up	: 1H S/N	Stop leak if without risk. Move containers from spill area. 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.
	4Hz 0.1% H2O/D2O	Stop leak if without risk. Move containers from spill area. 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.
	Temp Grad	Stop leak if without risk. Move containers from spill area. 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.
	1H Lineshape	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.
	13C S/N ASTM doped	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.
	ID 1	Stop leak if without risk. Move containers from spill area. 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.
	ID 2	Stop leak if without risk. Move containers from spill area. 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.
	Sucrose, NMR tested	Stop leak if without risk. Move containers from spill area. Dilute with water and mop up if water-soluble. Alternatively, or if water-insoluble, absorb with an inert dry material and place in an appropriate waste disposal container. Dispose of via a licensed waste disposal contractor.

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

SECTION 7: Handling and storage**7.1 Precautions for safe handling**

Protective measures : 1H S/N

	Put on appropriate personal protective equipment (see Section 8). Avoid exposure - obtain special instructions before use. Do not handle until all safety precautions have been read and understood. Do not get in eyes or on skin or clothing. Do not breathe vapour or mist. Do not ingest. Avoid release to the environment. If during normal use the material presents a respiratory hazard, use only with adequate ventilation or wear appropriate respirator. Keep in the original container or an approved alternative made from a compatible material, kept tightly closed when not in use. Empty containers retain product residue and can be hazardous. Do not reuse container.
4Hz 0.1% H2O/D2O	Put on appropriate personal protective equipment (see Section 8).
Temp Grad	Put on appropriate personal protective equipment (see Section 8).
1H Lineshape	Put on appropriate personal protective equipment (see Section 8). Avoid exposure - obtain special instructions before use. Do not handle until all safety precautions have been read and understood. Do not get in eyes or on skin or clothing. Do not ingest. 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.
13C S/N ASTM doped	Put on appropriate personal protective equipment (see Section 8). Avoid exposure - obtain special instructions before use. Do not handle until all safety precautions have been read and understood. Do not get in eyes or on skin or clothing. Do not breathe vapour or mist. Do not ingest. 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.
ID 1	Put on appropriate personal protective equipment (see Section 8). Avoid exposure - obtain special instructions before use. Do not handle until all safety precautions have been read and understood. Do not get in eyes or on skin or clothing. Do not breathe vapour or mist. Do not ingest. Avoid release to the environment. If during normal use the material presents a respiratory hazard, use only with adequate ventilation or wear appropriate respirator. Keep in the original container or an approved alternative made from a compatible material, kept tightly closed when not in use. Empty containers retain product residue and can be hazardous. Do not reuse container.

SECTION 7: Handling and storage**Advice on general occupational hygiene**

ID 2	Put on appropriate personal protective equipment (see Section 8). Do not breathe vapour or mist. Do not ingest. Avoid contact with eyes, skin and clothing. Keep in the original container or an approved alternative made from a compatible material, kept tightly closed when not in use. Empty containers retain product residue and can be hazardous. Do not reuse container.
Sucrose, NMR tested	Put on appropriate personal protective equipment (see Section 8).
: 1H S/N	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.
4Hz 0.1% H2O/D2O	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.
Temp Grad	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.
1H Lineshape	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.
13C S/N ASTM doped	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.
ID 1	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.
ID 2	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.
Sucrose, NMR tested	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.

SECTION 7: Handling and storage**7.2 Conditions for safe storage, including any incompatibilities**

: 1H S/N

Store in accordance with local regulations. 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. 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.

4Hz 0.1% H2O/D2O

Store in accordance with local regulations. 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. 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.

Temp Grad

Store in accordance with local regulations. 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. 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.

1H Lineshape

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 oxidizing materials. Keep container tightly closed and sealed until ready for use. Containers that have been opened must be carefully resealed and kept upright to prevent leakage. Do not store in unlabelled containers. Use appropriate containment to avoid environmental contamination.

13C S/N ASTM doped

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 oxidizing materials. Keep container tightly closed and sealed until ready for use. Containers that have been opened must be carefully resealed and kept upright to prevent leakage. Do not store in unlabelled containers. Use appropriate containment to avoid environmental contamination.

ID 1

Store in accordance with local regulations. 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. 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.

ID 2

Store in accordance with local regulations. 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. 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

SECTION 7: Handling and storage

Sucrose, NMR tested

appropriate containment to avoid environmental contamination.

Store in accordance with local regulations. 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. 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.

7.3 Specific end use(s)

Recommendations :

1H S/N	Industrial applications, Professional applications.
4Hz 0.1% H ₂ O/D ₂ O	Industrial applications, Professional applications.
Temp Grad	Industrial applications, Professional applications.
1H Lineshape	Industrial applications, Professional applications.
13C S/N ASTM doped	Industrial applications, Professional applications.
ID 1	Industrial applications, Professional applications.
ID 2	Industrial applications, Professional applications.
Sucrose, NMR tested	Industrial applications, Professional applications.

Industrial sector specific solutions : Not applicable.

SECTION 8: Exposure controls/personal protection

Since the hazardous ingredient in this article is encapsulated, the risk of exposure by inhalation, ingestion, skin contact and eyes contact is minimum.

8.1 Control parameters

Occupational exposure limits

Product/ingredient name	Exposure limit values
1H S/N (² H)Chloroform	EU OEL (Europe, 12/2009). Absorbed through skin. Notes: list of indicative occupational exposure limit values TWA: 2 ppm 8 hours. TWA: 10 mg/m ³ 8 hours.
1H Lineshape (² H ₆)Acetone Trichloromethane	EU OEL (Europe, 12/2009). Notes: list of indicative occupational exposure limit values TWA: 500 ppm 8 hours. TWA: 1210 mg/m ³ 8 hours. EU OEL (Europe, 12/2009). Absorbed through skin. Notes: list of indicative occupational exposure limit values TWA: 10 mg/m ³ 8 hours. TWA: 2 ppm 8 hours.
13C S/N ASTM doped (² H ₆)Benzene 1,4-Dioxane	EU OEL (Europe, 12/2009). Absorbed through skin. TWA: 1 ppm 8 hours. TWA: 3.25 mg/m ³ 8 hours. EU OEL (Europe, 12/2009). Notes: list of indicative occupational exposure limit values TWA: 73 mg/m ³ 8 hours. TWA: 20 ppm 8 hours.
ID 1 (² H)Chloroform	EU OEL (Europe, 12/2009). Absorbed through skin. Notes: list of indicative occupational exposure limit values TWA: 2 ppm 8 hours. TWA: 10 mg/m ³ 8 hours.

SECTION 8: Exposure controls/personal protection

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.

Derived effect levels

No DNELs available.

Predicted effect concentrations

No PNECs available.

8.2 Exposure controls

Appropriate engineering controls : Use only with adequate ventilation. Use process enclosures, local exhaust ventilation or other engineering controls to keep worker exposure to airborne contaminants below any recommended or statutory limits. The engineering controls also need to keep gas, vapour or dust concentrations below any lower explosive limits. Use explosion-proof ventilation equipment.

Individual protection measures

Hygiene measures : Wash hands, forearms and face thoroughly after handling chemical products, before eating, smoking and using the lavatory and at the end of the working period. Appropriate techniques should be used to remove potentially contaminated clothing. Wash contaminated clothing before reusing. Ensure that eyewash stations and safety showers are close to the workstation location.

Eye/face protection : Safety eyewear complying with an approved standard should be used when a risk assessment indicates this is necessary to avoid exposure to liquid splashes, mists, gases or dusts. If contact is possible, the following protection should be worn, unless the assessment indicates a higher degree of protection: chemical splash goggles.

Skin protection

Hand protection : Chemical-resistant, impervious gloves complying with an approved standard should be worn at all times when handling chemical products if a risk assessment indicates this is necessary. Considering the parameters specified by the glove manufacturer, check during use that the gloves are still retaining their protective properties. It should be noted that the time to breakthrough for any glove material may be different for different glove manufacturers. In the case of mixtures, consisting of several substances, the protection time of the gloves cannot be accurately estimated.

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 : Use a properly fitted, air-purifying or air-fed respirator complying with an approved standard if a risk assessment indicates this is necessary. Respirator selection must be based on known or anticipated exposure levels, the hazards of the product and the safe working limits of the selected respirator.

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	: 1H S/N	Liquid.
	4Hz 0.1% H2O/D2O	Liquid.
	Temp Grad	Liquid.
	1H Lineshape	Liquid.
	13C S/N ASTM doped	Liquid.
	ID 1	Liquid.
	ID 2	Liquid. [Clear.]
Colour	Sucrose, NMR tested	Liquid. [Clear.]
	: 1H S/N	Not available.
	4Hz 0.1% H2O/D2O	Colourless.
	Temp Grad	Colourless.
	1H Lineshape	Not available.
	13C S/N ASTM doped	Not available.
	ID 1	Not available.
Odour	ID 2	Colourless.
	Sucrose, NMR tested	Not available.
	: 1H S/N	Not available.
	4Hz 0.1% H2O/D2O	Not available.
	Temp Grad	Not available.
	1H Lineshape	Not available.
	13C S/N ASTM doped	Not available.
Odour threshold	ID 1	Not available.
	ID 2	Ripe olive.
	Sucrose, NMR tested	Not available.
	: 1H S/N	Not available.
	4Hz 0.1% H2O/D2O	Not available.
	Temp Grad	Not available.
	1H Lineshape	Not available.
pH	13C S/N ASTM doped	Not available.
	ID 1	Not available.
	ID 2	Not available.
	Sucrose, NMR tested	Not available.
	: 1H S/N	Not available.
	4Hz 0.1% H2O/D2O	7
	Temp Grad	Not available.
Melting point/freezing point	1H Lineshape	Not available.
	13C S/N ASTM doped	Not available.
	ID 1	Not available.
	ID 2	Not available.
	Sucrose, NMR tested	Not available.
	: 1H S/N	-64°C
	4Hz 0.1% H2O/D2O	3.81°C
Initial boiling point and boiling range	Temp Grad	3.81°C
	1H Lineshape	-95°C
	13C S/N ASTM doped	Not available.
	ID 1	-64°C
	ID 2	18 to 18.54°C
	Sucrose, NMR tested	0°C
	: 1H S/N	60.9°C
4Hz 0.1% H2O/D2O	101.42°C	
	Temp Grad	101.42°C
	1H Lineshape	55.5°C
	13C S/N ASTM doped	90°C
	ID 1	60.9°C
	ID 2	189°C
	Sucrose, NMR tested	100°C

SECTION 9: Physical and chemical properties

Flash point	: 1H S/N 4Hz 0.1% H2O/D2O Temp Grad 1H Lineshape 13C S/N ASTM doped ID 1 ID 2 Sucrose, NMR tested	Not available. Not available. Not available. Closed cup: -17°C Closed cup: 21.1°C Not available. Closed cup: 88°C Not available.
Evaporation rate	: 1H S/N 4Hz 0.1% H2O/D2O Temp Grad 1H Lineshape 13C S/N ASTM doped ID 1 ID 2 Sucrose, NMR tested	Not available. Not available. Not available. Not available. Not available. Not available. Not available. Not available.
Flammability (solid, gas)	: 1H S/N 4Hz 0.1% H2O/D2O Temp Grad 1H Lineshape 13C S/N ASTM doped ID 1 ID 2 Sucrose, NMR tested	Not available. Not available. Not available. Not available. Not available. Not available. Not available. Not available.
Upper/lower flammability or explosive limits	: 1H S/N 4Hz 0.1% H2O/D2O Temp Grad 1H Lineshape 13C S/N ASTM doped ID 1 ID 2 Sucrose, NMR tested	Not available. Not available. Not available. Not available. Not available. Not available. Lower: 3% Not available.
Vapour pressure	: 1H S/N 4Hz 0.1% H2O/D2O Temp Grad 1H Lineshape 13C S/N ASTM doped ID 1 ID 2 Sucrose, NMR tested	Not available. Not available. Not available. Not available. Not available. Not available. 0.061 kPa [room temperature] Not available.
Vapour density	: 1H S/N 4Hz 0.1% H2O/D2O Temp Grad 1H Lineshape 13C S/N ASTM doped ID 1 ID 2 Sucrose, NMR tested	Not available. Not available. Not available. Not available. Not available. Not available. 1.04 [Air = 1] Not available.
Relative density	: 1H S/N 4Hz 0.1% H2O/D2O Temp Grad 1H Lineshape 13C S/N ASTM doped ID 1 ID 2 Sucrose, NMR tested	1.5 1.1 1.1 0.872 0.98 1500 1.18 Not available.
Solubility(ies)	: 1H S/N 4Hz 0.1% H2O/D2O Temp Grad 1H Lineshape	Very slightly soluble in the following materials: cold water and hot water. Easily soluble in the following materials: cold water and hot water. Easily soluble in the following materials: cold water and hot water. Easily soluble in the following materials: cold water, hot water and acetone.

SECTION 9: Physical and chemical properties

	13C S/N ASTM doped	Easily soluble in the following materials: cold water and hot water.
	ID 1	Very slightly soluble in the following materials: cold water and hot water.
	ID 2	Soluble in the following materials: cold water and hot water.
	Sucrose, NMR tested	Easily soluble in the following materials: cold water and hot water.
Partition coefficient: n-octanol/water	: 1H S/N	Not available.
	4Hz 0.1% H2O/D2O	Not available.
	Temp Grad	Not available.
	1H Lineshape	Not available.
	13C S/N ASTM doped	Not available.
	ID 1	Not available.
	ID 2	Not available.
	Sucrose, NMR tested	Not available.
Auto-ignition temperature	: 1H S/N	Not available.
	4Hz 0.1% H2O/D2O	Not available.
	Temp Grad	Not available.
	1H Lineshape	Not available.
	13C S/N ASTM doped	Not available.
	ID 1	Not available.
	ID 2	215°C
	Sucrose, NMR tested	Not available.
Decomposition temperature	: 1H S/N	Not available.
	4Hz 0.1% H2O/D2O	Not available.
	Temp Grad	Not available.
	1H Lineshape	Not available.
	13C S/N ASTM doped	Not available.
	ID 1	Not available.
	ID 2	Not available.
	Sucrose, NMR tested	Not available.
Viscosity	: 1H S/N	Not available.
	4Hz 0.1% H2O/D2O	Not available.
	Temp Grad	Not available.
	1H Lineshape	Not available.
	13C S/N ASTM doped	Not available.
	ID 1	Not available.
	ID 2	Not available.
	Sucrose, NMR tested	Not available.
Explosive properties	: 1H S/N	Not available.
	4Hz 0.1% H2O/D2O	Not available.
	Temp Grad	Not available.
	1H Lineshape	Vapours may form explosive mixtures with air.
	13C S/N ASTM doped	Slightly explosive in the presence of the following materials or conditions: acids.
	ID 1	Not available.
	ID 2	Not available.
	Sucrose, NMR tested	Not available.

9.2 Other information

No additional information.

SECTION 10: Stability and reactivity

10.1 Reactivity	: 1H S/N	No specific test data related to reactivity available for this product or its ingredients.
	4Hz 0.1% H2O/D2O	No specific test data related to reactivity available for this product or its ingredients.
	Temp Grad	No specific test data related to reactivity available for this product or its ingredients.
	1H Lineshape	No specific test data related to reactivity available for this product or its ingredients.
	13C S/N ASTM doped	No specific test data related to reactivity available for this

SECTION 10: Stability and reactivity

ID 1	product or its ingredients. No specific test data related to reactivity available for this product or its ingredients.
ID 2	No specific test data related to reactivity available for this product or its ingredients.
Sucrose, NMR tested	No specific test data related to reactivity available for this product or its ingredients.

10.2 Chemical stability : 1H S/N The product is stable.
 4Hz 0.1% H2O/D2O The product is stable.
 Temp Grad The product is stable.
 1H Lineshape The product is stable.
 13C S/N ASTM doped The product is stable.
 ID 1 The product is stable.
 ID 2 The product is stable.
 Sucrose, NMR tested The product is stable.

10.3 Possibility of hazardous reactions : 1H S/N Under normal conditions of storage and use, hazardous reactions will not occur.
 4Hz 0.1% H2O/D2O Under normal conditions of storage and use, hazardous reactions will not occur.
 Temp Grad Under normal conditions of storage and use, hazardous reactions will not occur.
 1H Lineshape Under normal conditions of storage and use, hazardous reactions will not occur.
 13C S/N ASTM doped Under normal conditions of storage and use, hazardous reactions will not occur.
 ID 1 Under normal conditions of storage and use, hazardous reactions will not occur.
 ID 2 Under normal conditions of storage and use, hazardous reactions will not occur.
 Sucrose, NMR tested Under normal conditions of storage and use, hazardous reactions will not occur.

10.4 Conditions to avoid : 1H S/N No specific data.
 4Hz 0.1% H2O/D2O No specific data.
 Temp Grad No specific data.
 1H Lineshape 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.
 13C S/N ASTM doped 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.
 ID 1 No specific data.
 ID 2 No specific data.
 Sucrose, NMR tested No specific data.

10.5 Incompatible materials : 1H S/N No specific data.
 4Hz 0.1% H2O/D2O No specific data.
 Temp Grad No specific data.
 1H Lineshape Reactive or incompatible with the following materials: oxidizing materials
 13C S/N ASTM doped Reactive or incompatible with the following materials: oxidizing materials
 ID 1 No specific data.
 ID 2 No specific data.
 Sucrose, NMR tested No specific data.

SECTION 10: Stability and reactivity

10.6 Hazardous decomposition products	: 1H S/N 4Hz 0.1% H2O/D2O Temp Grad 1H Lineshape 13C S/N ASTM doped ID 1 ID 2 Sucrose, NMR tested	Under normal conditions of storage and use, hazardous decomposition products should not be produced. Under normal conditions of storage and use, hazardous decomposition products should not be produced. Under normal conditions of storage and use, hazardous decomposition products should not be produced. Under normal conditions of storage and use, hazardous decomposition products should not be produced. Under normal conditions of storage and use, hazardous decomposition products should not be produced. Under normal conditions of storage and use, hazardous decomposition products should not be produced. 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
1H S/N (² H)Chloroform	LC50 Inhalation Vapour	Rat	47702 mg/m ³	4 hours
	LD50 Dermal	Rabbit	>20 g/kg	-
	LD50 Oral	Rat	300 mg/kg	-
1H Lineshape (² H ₆)Acetone Trichloromethane	LD50 Oral	Rat	5800 mg/kg	-
	LC50 Inhalation Vapour	Rat	47702 mg/m ³	4 hours
	LD50 Dermal	Rabbit	>20 g/kg	-
	LD50 Oral	Rat	300 mg/kg	-
13C S/N ASTM doped (² H ₆)Benzene 1,4-Dioxane	LD50 Oral	Rat	930 mg/kg	-
	LD50 Oral	Rat	4200 mg/kg	-
ID 1 (² H)Chloroform Iodomethane (¹³ C) Trimethyl phosphite	LC50 Inhalation Vapour	Rat	47702 mg/m ³	4 hours
	LD50 Dermal	Rabbit	>20 g/kg	-
	LD50 Oral	Rat	300 mg/kg	-
	LC50 Inhalation Vapour	Rat	1300 mg/m ³	4 hours
	LD50 Oral	Rat	76 mg/kg	-
	LC50 Inhalation Vapour	Rat	182000 mg/m ³	1 hours
	LD50 Dermal	Rabbit	933.8 mg/kg	-
LD50 Oral	Rat	1350 mg/kg	-	
ID 2 di[(² H ₃)Methyl] sulphoxide	LD50 Dermal	Rat	40000 mg/kg	-
	LD50 Oral	Rat	14500 mg/kg	-

Acute toxicity estimates

Route	ATE value
1H S/N Oral	500.5 mg/kg
1H Lineshape Oral	50000 mg/kg
ID 1 Oral Dermal Inhalation (vapours)	477.3 mg/kg
	50505.5 mg/kg
	300 mg/l

SECTION 11: Toxicological information

ID 2
Oral

25000 mg/kg

Irritation/Corrosion

Product/ingredient name	Result	Species	Score	Exposure	Observation
1H S/N (² H)Chloroform	Eyes - Moderate irritant	Rabbit	-	24 hours 20 milligrams	-
	Skin - Mild irritant	Rabbit	-	24 hours 500 milligrams	-
1H Lineshape (² H ₆)Acetone	Eyes - Mild irritant	Human	-	186300 parts per million	-
	Eyes - Mild irritant	Rabbit	-	10 microliters	-
	Eyes - Moderate irritant	Rabbit	-	24 hours 20 milligrams	-
	Eyes - Severe irritant	Rabbit	-	20 milligrams	-
	Skin - Mild irritant	Rabbit	-	24 hours 500 milligrams	-
	Skin - Mild irritant	Rabbit	-	395 milligrams	-
Trichloromethane	Eyes - Moderate irritant	Rabbit	-	24 hours 20 milligrams	-
	Skin - Mild irritant	Rabbit	-	24 hours 500 milligrams	-
13C S/N ASTM doped (² H ₆)Benzene	Eyes - Moderate irritant	Rabbit	-	88 milligrams	-
	Eyes - Severe irritant	Rabbit	-	24 hours 2 milligrams	-
	Skin - Mild irritant	Rat	-	8 hours 60 microliters	-
	Skin - Mild irritant	Rabbit	-	24 hours 15 milligrams	-
	Skin - Moderate irritant	Rabbit	-	24 hours 20 milligrams	-
1,4-Dioxane	Eyes - Moderate irritant	Rabbit	-	24 hours 100 milligrams	-
	Skin - Mild irritant	Rabbit	-	515 milligrams	-
ID 1 (² H)Chloroform	Eyes - Moderate irritant	Rabbit	-	24 hours 20 milligrams	-
	Skin - Mild irritant	Rabbit	-	24 hours 500 milligrams	-
Iodomethane (¹³ C)	Eyes - Severe irritant	Rabbit	-	100 milligrams	-
	Skin - Mild irritant	Rat	-	30 minutes 1 Grams	-
	Skin - Severe irritant	Rabbit	-	500 milligrams	-
	Skin - Mild irritant	Human	-	10 minutes 1 Grams	-
Trimethyl phosphite	Eyes - Mild irritant	Rabbit	-	0.1 Mililiters	-
	Skin - Severe irritant	Rabbit	-	500 milligrams	-
ID 2 di[(² H ₃)Methyl] sulphoxide	Eyes - Mild irritant	Rabbit	-	24 hours 500 milligrams	-
	Eyes - Mild irritant	Rabbit	-	100	-

SECTION 11: Toxicological information

	Skin - Mild irritant	Rabbit	-	milligrams 24 hours 500	-
	Skin - Mild irritant	Rabbit	-	milligrams 100 milligrams	-

Sensitiser

Conclusion/Summary : Not available.

Chronic toxicity / Carcinogenicity / Mutagenicity / Teratogenicity / Reproductive toxicity

Not available.

Specific target organ toxicity (single exposure)

Product/ingredient name	Category	Route of exposure	Target organs
1H Lineshape (² H ₆)Acetone	Category 3	Not applicable.	Narcotic effects
13C S/N ASTM doped 1,4-Dioxane	Category 3	Not applicable.	Respiratory tract irritation
ID 1 Iodomethane (¹³ C)	Category 3	Not applicable.	Respiratory tract irritation
Trimethyl phosphite	Category 3	Not applicable.	Respiratory tract irritation

Specific target organ toxicity (repeated exposure)

Product/ingredient name	Category	Route of exposure	Target organs
1H S/N (² H)Chloroform	Category 2	Not determined	Not determined
1H Lineshape Trichloromethane	Category 2	Not determined	Not determined
13C S/N ASTM doped (² H ₆)Benzene	Category 1	Not determined	Not determined
ID 1 (² H)Chloroform	Category 2	Not determined	Not determined
ID 2 di[(² H ₃)Methyl] sulphoxide	Category 2	Oral	kidneys and liver

Aspiration hazard

Product/ingredient name	Result
13C S/N ASTM doped (² H ₆)Benzene	ASPIRATION HAZARD - Category 1

Information on the likely routes of exposure : Not available.

Potential acute health effects

Inhalation	: 1H S/N	Exposure to decomposition products may cause a health hazard. Serious effects may be delayed following exposure.
	4Hz 0.1% H ₂ O/D ₂ O	No known significant effects or critical hazards.
	Temp Grad	No known significant effects or critical hazards.
	1H Lineshape	Can cause central nervous system (CNS) depression. May cause drowsiness or dizziness. Exposure to decomposition products may cause a health hazard. Serious effects may be delayed following exposure.
	13C S/N ASTM doped	May cause respiratory irritation.
	ID 1	Exposure to decomposition products may cause a health

SECTION 11: Toxicological information

	ID 2	hazard. Serious effects may be delayed following exposure.
	Sucrose, NMR tested	No known significant effects or critical hazards.
Ingestion	: 1H S/N	No known significant effects or critical hazards.
	4Hz 0.1% H2O/D2O	Harmful if swallowed. Irritating to mouth, throat and stomach.
	Temp Grad	No known significant effects or critical hazards.
	1H Lineshape	No known significant effects or critical hazards.
	13C S/N ASTM doped	Can cause central nervous system (CNS) depression.
	ID 1	Irritating to mouth, throat and stomach.
	ID 2	Harmful if swallowed. Irritating to mouth, throat and stomach.
	Sucrose, NMR tested	May be irritating to mouth, throat and stomach.
Skin contact	: 1H S/N	No known significant effects or critical hazards.
	4Hz 0.1% H2O/D2O	Causes skin irritation.
	Temp Grad	No known significant effects or critical hazards.
	1H Lineshape	No known significant effects or critical hazards.
	13C S/N ASTM doped	Defatting to the skin. May cause skin dryness and irritation.
	ID 1	Causes skin irritation. Defatting to the skin.
	ID 2	Causes skin irritation.
	Sucrose, NMR tested	No known significant effects or critical hazards.
Eye contact	: 1H S/N	No known significant effects or critical hazards.
	4Hz 0.1% H2O/D2O	Causes serious eye irritation.
	Temp Grad	No known significant effects or critical hazards.
	1H Lineshape	No known significant effects or critical hazards.
	13C S/N ASTM doped	Causes serious eye irritation.
	ID 1	Causes serious eye irritation.
	ID 2	Causes eye irritation.
	Sucrose, NMR tested	No known significant effects or critical hazards.

Symptoms related to the physical, chemical and toxicological characteristics

Inhalation	: 1H S/N	No specific data.
	4Hz 0.1% H2O/D2O	No specific data.
	Temp Grad	No specific data.
	1H Lineshape	Adverse symptoms may include the following: nausea or vomiting headache drowsiness/fatigue dizziness/vertigo unconsciousness
	13C S/N ASTM doped	Adverse symptoms may include the following: respiratory tract irritation coughing
	ID 1	No specific data.
	ID 2	No specific data.
	Sucrose, NMR tested	No specific data.
Ingestion	: 1H S/N	No specific data.
	4Hz 0.1% H2O/D2O	No specific data.
	Temp Grad	No specific data.
	1H Lineshape	No specific data.
	13C S/N ASTM doped	No specific data.
	ID 1	No specific data.
	ID 2	No specific data.
	Sucrose, NMR tested	No specific data.
Skin contact	: 1H S/N	Adverse symptoms may include the following: irritation redness
	4Hz 0.1% H2O/D2O	No specific data.
	Temp Grad	No specific data.
	1H Lineshape	Adverse symptoms may include the following: irritation dryness cracking

SECTION 11: Toxicological information

	13C S/N ASTM doped	Adverse symptoms may include the following: irritation redness dryness cracking
	ID 1	Adverse symptoms may include the following: irritation redness
	ID 2	No specific data.
	Sucrose, NMR tested	No specific data.
Eye contact	: 1H S/N	Adverse symptoms may include the following: pain or irritation watering redness
	4Hz 0.1% H2O/D2O	No specific data.
	Temp Grad	No specific data.
	1H Lineshape	Adverse symptoms may include the following: pain or irritation watering redness
	13C S/N ASTM doped	Adverse symptoms may include the following: pain or irritation watering redness
	ID 1	Adverse symptoms may include the following: pain or irritation watering redness
	ID 2	Adverse symptoms may include the following: irritation watering redness
	Sucrose, NMR tested	No specific data.

Delayed and immediate effects and also chronic effects from short and long term exposure**Short term exposure****Potential immediate effects** : Not available.**Potential delayed effects** : Not available.**Long term exposure****Potential immediate effects** : Not available.**Potential delayed effects** : Not available.**Potential chronic health effects**

General	: 1H S/N	May cause damage to organs through prolonged or repeated exposure.
	4Hz 0.1% H2O/D2O	No known significant effects or critical hazards.
	Temp Grad	No known significant effects or critical hazards.
	1H Lineshape	Prolonged or repeated contact can defat the skin and lead to irritation, cracking and/or dermatitis.
	13C S/N ASTM doped	Causes damage to organs through prolonged or repeated exposure. Prolonged or repeated contact can defat the skin and lead to irritation, cracking and/or dermatitis.
	ID 1	May cause damage to organs through prolonged or repeated exposure.
	ID 2	May cause damage to organs through prolonged or repeated exposure.
	Sucrose, NMR tested	No known significant effects or critical hazards.

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Carcinogenicity	: 1H S/N	Suspected of causing cancer. Risk of cancer depends on duration and level of exposure.
	4Hz 0.1% H2O/D2O	No known significant effects or critical hazards.
	Temp Grad	No known significant effects or critical hazards.
	1H Lineshape	Suspected of causing cancer. Risk of cancer depends on duration and level of exposure.
	13C S/N ASTM doped	May cause cancer. Risk of cancer depends on duration and level of exposure.
	ID 1	Suspected of causing cancer. Risk of cancer depends on duration and level of exposure.
Mutagenicity	ID 2	No known significant effects or critical hazards.
	Sucrose, NMR tested	No known significant effects or critical hazards.
	: 1H S/N	No known significant effects or critical hazards.
	4Hz 0.1% H2O/D2O	No known significant effects or critical hazards.
	Temp Grad	No known significant effects or critical hazards.
	1H Lineshape	No known significant effects or critical hazards.
Teratogenicity	13C S/N ASTM doped	May cause genetic defects.
	ID 1	No known significant effects or critical hazards.
	ID 2	No known significant effects or critical hazards.
	Sucrose, NMR tested	No known significant effects or critical hazards.
	: 1H S/N	No known significant effects or critical hazards.
	4Hz 0.1% H2O/D2O	No known significant effects or critical hazards.
Developmental effects	Temp Grad	No known significant effects or critical hazards.
	1H Lineshape	No known significant effects or critical hazards.
	13C S/N ASTM doped	No known significant effects or critical hazards.
	ID 1	No known significant effects or critical hazards.
	ID 2	No known significant effects or critical hazards.
	Sucrose, NMR tested	No known significant effects or critical hazards.
Fertility effects	: 1H S/N	No known significant effects or critical hazards.
	4Hz 0.1% H2O/D2O	No known significant effects or critical hazards.
	Temp Grad	No known significant effects or critical hazards.
	1H Lineshape	No known significant effects or critical hazards.
	13C S/N ASTM doped	No known significant effects or critical hazards.
	ID 1	No known significant effects or critical hazards.
Toxicokinetics	ID 2	No known significant effects or critical hazards.
	Sucrose, NMR tested	No known significant effects or critical hazards.
	Absorption	
	: 1H S/N	Not available.
	4Hz 0.1% H2O/D2O	Not available.
	Temp Grad	Not available.
Distribution	1H Lineshape	Not available.
	13C S/N ASTM doped	Not available.
	ID 1	Not available.
	ID 2	Not available.
	Sucrose, NMR tested	Not available.
	: 1H S/N	Not available.
4Hz 0.1% H2O/D2O	Not available.	
Temp Grad	Not available.	
1H Lineshape	Not available.	
13C S/N ASTM doped	Not available.	
ID 1	Not available.	
ID 2	Not available.	
Sucrose, NMR tested	Not available.	

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Metabolism : 1H S/N Not available.
 4Hz 0.1% H2O/D2O Not available.
 Temp Grad Not available.
 1H Lineshape Not available.
 13C S/N ASTM doped Not available.
 ID 1 Not available.
 ID 2 Not available.
 Sucrose, NMR tested Not available.

Elimination : 1H S/N Not available.
 4Hz 0.1% H2O/D2O Not available.
 Temp Grad Not available.
 1H Lineshape Not available.
 13C S/N ASTM doped Not available.
 ID 1 Not available.
 ID 2 Not available.
 Sucrose, NMR tested Not available.

Other information : Not available.

SECTION 12: Ecological information

12.1 Toxicity

Product/ingredient name	Result	Species	Exposure
1H S/N (² H)Chloroform	Acute EC50 13.3 mg/l Fresh water	Algae - Chlamydomonas reinhardtii - Exponential growth phase	72 hours
	Acute LC50 81.5 mg/l Marine water	Crustaceans - Penaeus duorarum	48 hours
	Acute LC50 29000 µg/l Fresh water	Daphnia - Daphnia magna	48 hours
	Acute LC50 13300 µg/l Fresh water	Fish - Lepomis macrochirus	96 hours
	Chronic EC10 3.61 mg/l Fresh water	Algae - Chlamydomonas reinhardtii - Exponential growth phase	72 hours
	Chronic NOEC 6300 µg/l Fresh water	Daphnia - Daphnia magna	21 days
1H Lineshape (² H ₆)Acetone	Acute EC50 20.565 mg/l Marine water	Algae - Ulva pertusa	96 hours
	Acute LC50 6000000 µg/l Fresh water	Crustaceans - Gammarus pulex	48 hours
	Acute LC50 10000 µg/l Fresh water	Daphnia - Daphnia magna	48 hours
	Acute LC50 100000 µg/l Fresh water	Fish - Pimephales promelas - Juvenile (Fledgling, Hatchling, Weanling)	96 hours
	Chronic NOEC 4.95 mg/l Marine water	Algae - Ulva pertusa	96 hours
	Chronic NOEC 0.1 ml/L Fresh water	Daphnia - Daphnia magna - Neonate	21 days
Trichloromethane	Acute EC50 13.3 mg/l Fresh water	Algae - Chlamydomonas reinhardtii - Exponential growth phase	72 hours
	Acute EC50 2.803 mg/l Fresh water	Crustaceans - Cypris subglobosa	48 hours
	Acute LC50 63800 µg/l Fresh water	Daphnia - Daphnia magna - Neonate	48 hours
	Acute LC50 13.3 ppm Fresh water	Fish - Lepomis macrochirus	96 hours
	Chronic EC10 3.61 mg/l Fresh water	Algae - Chlamydomonas reinhardtii - Exponential growth phase	72 hours
	Chronic NOEC 6300 µg/l Fresh water	Daphnia - Daphnia magna	21 days
13C S/N ASTM doped (² H ₆)Benzene	Acute EC50 29000 µg/l Fresh water	Algae - Pseudokirchneriella subcapitata	72 hours
	Acute EC50 1360000 µg/l Fresh water	Algae - Scenedesmus abundans	96 hours
	Acute EC50 9230 µg/l Fresh water	Daphnia - Daphnia magna - Neonate	48 hours

SECTION 12: Ecological information

1,4-Dioxane	Acute LC50 21000 µg/l Marine water	Crustaceans - Artemia salina - Nauplii	48 hours
	Acute LC50 5.28 ul/L Fresh water	Fish - Oncorhynchus gorboscha - Fry	96 hours
	Chronic NOEC 1.5 to 5.4 ul/L Marine water	Fish - Morone saxatilis - Juvenile (Fledgling, Hatchling, Weanling)	4 weeks
	Acute LC50 6700000 µg/l Marine water	Fish - Menidia beryllina	96 hours
ID 1 (² H)Chloroform	Acute EC50 13.3 mg/l Fresh water	Algae - Chlamydomonas reinhardtii - Exponential growth phase	72 hours
	Acute LC50 81.5 mg/l Marine water	Crustaceans - Penaeus duorarum	48 hours
	Acute LC50 29000 µg/l Fresh water	Daphnia - Daphnia magna	48 hours
	Acute LC50 13300 µg/l Fresh water	Fish - Lepomis macrochirus	96 hours
	Chronic EC10 3.61 mg/l Fresh water	Algae - Chlamydomonas reinhardtii - Exponential growth phase	72 hours
	Chronic NOEC 6300 µg/l Fresh water	Daphnia - Daphnia magna	21 days
ID 2 di[(² H ₃)Methyl] sulphoxide	Acute LC50 25000 ppm Fresh water	Daphnia - Daphnia magna - Neonate	48 hours
	Acute LC50 34000000 µg/l Fresh water	Fish - Pimephales promelas	96 hours
Benzamide (¹⁵ N)	Acute LC50 661000 µg/l Fresh water	Fish - Pimephales promelas	96 hours

12.2 Persistence and degradability

Conclusion/Summary : Not available.

12.3 Bioaccumulative potential

Product/ingredient name	LogP _{ow}	BCF	Potential
1H S/N (² H)Chloroform	1.97	690	high
1H Lineshape (² H ₆)Acetone Trichloromethane	-0.23	-	low
	1.97	690	high
13C S/N ASTM doped (² H ₆)Benzene 1,4-Dioxane	2.13	11	low
	-0.42	0.3 to 0.7	low
ID 1 (² H)Chloroform Iodomethane (¹³ C) Trimethyl phosphite	1.97	690	high
	1.57	-	low
	-0.73	-	low
ID 2 di[(² H ₃)Methyl] sulphoxide	-1.35	3.16	low

12.4 Mobility in soil

Soil/water partition coefficient (K_{oc}) : Not available.

Mobility : Not available.

12.5 Results of PBT and vPvB assessment

PBT : Not applicable.

vPvB : Not applicable.

SECTION 12: Ecological information

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. Vapor from product residues may create a highly flammable or explosive atmosphere inside the container. Do not cut, weld or grind used containers unless they have been cleaned thoroughly internally. Avoid dispersal of spilt material and runoff and contact with soil, waterways, drains and sewers.

SECTION 14: Transport information

This Safety Data Sheet (EU_English) is written based on the encapsulated substance or mixture in this article. Since the hazardous ingredient is encapsulated, the risk of exposure by inhalation, ingestion, skin contact and eyes contact is minimum.

Regulatory information

ADR/RID / IMDG / IATA : Not regulated.

Additional information : **Remarks**
De minimis quantities

14.7 Transport in bulk according to Annex II of MARPOL 73/78 and the IBC Code : 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

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 : For use in industrial installations only.

Other EU regulations

Europe inventory : Not determined.

Black List Chemicals : Not listed

Priority List Chemicals : Listed

SECTION 15: Regulatory information

Integrated pollution prevention and control list (IPPC) - Air : Listed

Integrated pollution prevention and control list (IPPC) - Water : Not listed

Product/ingredient name	Carcinogenic effects	Mutagenic effects	Developmental effects	Fertility effects
1H S/N (² H)Chloroform	Carc. 2, H351	-	-	-
1H Lineshape Trichloromethane	Carc. 2, H351	-	-	-
13C S/N ASTM doped (² H ₆)Benzene 1,4-Dioxane	Carc. 1A, H350 Carc. 2, H351	Muta. 1B, H340 -	- -	- -
ID 1 (² H)Chloroform Iodomethane (¹³ C)	Carc. 2, H351 Carc. 2, H351	- -	- -	- -

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

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]
 DNEL = Derived No Effect Level
 EUH statement = CLP-specific Hazard statement
 PNEC = Predicted No Effect Concentration
 RRN = REACH Registration Number

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

Classification	Justification
1H S/N Acute Tox. 4, H302 Skin Irrit. 2, H315 Carc. 2, H351 STOT RE 2, H373 Aquatic Chronic 3, H412	Calculation method Calculation method Calculation method Calculation method Calculation method
1H Lineshape Flam. Liq. 2, H225 Eye Irrit. 2, H319 Carc. 2, H351 STOT SE 3, H336 (Narcotic effects) Aquatic Chronic 3, H412	On basis of test data Calculation method Calculation method Calculation method Calculation method
13C S/N ASTM doped Flam. Liq. 2, H225 Skin Irrit. 2, H315 Eye Irrit. 2, H319 Muta. 1B, H340 Carc. 1A, H350 STOT SE 3, H335 (Respiratory tract irritation) STOT RE 1, H372 Aquatic Chronic 3, H412	On basis of test data Calculation method Calculation method Calculation method Calculation method Calculation method Calculation method Calculation method

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SECTION 16: Other information

<p>ID 1 Acute Tox. 4, H302 Skin Irrit. 2, H315 Carc. 2, H351 STOT RE 2, H373 Aquatic Chronic 3, H412</p> <p>ID 2 Eye Irrit. 2, H319 STOT RE 2, H373</p>	<p>Calculation method Calculation method Calculation method Calculation method Calculation method</p> <p>Calculation method Calculation method</p>
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Full text of abbreviated H statements : 1H S/N

H302	Harmful if swallowed.
H315	Causes skin irritation.
H351	Suspected of causing cancer.
H373	May cause damage to organs through prolonged or repeated exposure.
H412	Harmful to aquatic life with long lasting effects.

1H Lineshape

H225	Highly flammable liquid and vapour.
H302	Harmful if swallowed.
H315	Causes skin irritation.
H319	Causes serious eye irritation.
H336 (Narcotic effects)	May cause drowsiness or dizziness. (Narcotic effects)
H351	Suspected of causing cancer.
H373	May cause damage to organs through prolonged or repeated exposure.
H412	Harmful to aquatic life with long lasting effects.

13C S/N ASTM doped

H225	Highly flammable liquid and vapour.
H304	May be fatal if swallowed and enters airways.
H315	Causes skin irritation.
H319	Causes serious eye irritation.
H335 (Respiratory tract irritation)	May cause respiratory irritation. (Respiratory tract irritation)
H340	May cause genetic defects.
H350	May cause cancer.
H351	Suspected of causing cancer.
H372	Causes damage to organs through prolonged or repeated exposure.
H412	Harmful to aquatic life with long lasting effects.

ID 1

H226	Flammable liquid and vapour.
H301	Toxic if swallowed.
H302	Harmful if swallowed.
H302 (oral)	Harmful if swallowed.
H311 (dermal)	Toxic in contact with skin.
H312	Harmful in contact with skin.
H315	Causes skin irritation.
H319	Causes serious eye irritation.
H331	Toxic if inhaled.
H335 (Respiratory tract irritation)	May cause respiratory irritation. (Respiratory tract irritation)
H351	Suspected of causing cancer.
H373	May cause damage to organs through prolonged or repeated exposure.
H412	Harmful to aquatic life with long lasting effects.

ID 2

H302	Harmful if swallowed.
H319	Causes serious eye irritation.
H373	May cause damage to organs through prolonged or repeated exposure.

SECTION 16: Other information

	H373 (kidneys and liver) (oral)	May cause damage to organs through prolonged or repeated exposure if swallowed. (kidneys and liver)
Full text of classifications [CLP/GHS]	1H S/N	
	Acute Tox. 4, H302	ACUTE TOXICITY (oral) - Category 4
	Aquatic Chronic 3, H412	LONG-TERM AQUATIC HAZARD - Category 3
	Carc. 2, H351	CARCINOGENICITY - Category 2
	Skin Irrit. 2, H315	SKIN CORROSION/IRRITATION - Category 2
	STOT RE 2, H373	SPECIFIC TARGET ORGAN TOXICITY (REPEATED EXPOSURE) - Category 2
	1H Lineshape	
	Acute Tox. 4, H302	ACUTE TOXICITY (oral) - Category 4
	Aquatic Chronic 3, H412	LONG-TERM AQUATIC HAZARD - Category 3
	Carc. 2, H351	CARCINOGENICITY - Category 2
	Eye Irrit. 2, H319	SERIOUS EYE DAMAGE/ EYE IRRITATION - Category 2
	Flam. Liq. 2, H225	FLAMMABLE LIQUIDS - Category 2
	Skin Irrit. 2, H315	SKIN CORROSION/IRRITATION - Category 2
	STOT RE 2, H373	SPECIFIC TARGET ORGAN TOXICITY (REPEATED EXPOSURE) - Category 2
	STOT SE 3, H336 (Narcotic effects)	SPECIFIC TARGET ORGAN TOXICITY (SINGLE EXPOSURE) (Narcotic effects) - Category 3
	13C S/N ASTM doped	
	Aquatic Chronic 3, H412	LONG-TERM AQUATIC HAZARD - Category 3
	Asp. Tox. 1, H304	ASPIRATION HAZARD - Category 1
	Carc. 1A, H350	CARCINOGENICITY - Category 1A
	Carc. 2, H351	CARCINOGENICITY - Category 2
	Eye Irrit. 2, H319	SERIOUS EYE DAMAGE/ EYE IRRITATION - Category 2
	Flam. Liq. 2, H225	FLAMMABLE LIQUIDS - Category 2
	Muta. 1B, H340	GERM CELL MUTAGENICITY - Category 1B
	Skin Irrit. 2, H315	SKIN CORROSION/IRRITATION - Category 2
	STOT RE 1, H372	SPECIFIC TARGET ORGAN TOXICITY (REPEATED EXPOSURE) - Category 1
	STOT SE 3, H335 (Respiratory tract irritation)	SPECIFIC TARGET ORGAN TOXICITY (SINGLE EXPOSURE) (Respiratory tract irritation) - Category 3
	ID 1	
	Acute Tox. 3, H301	ACUTE TOXICITY (oral) - Category 3
	Acute Tox. 3, H311	ACUTE TOXICITY (dermal) - Category 3
	Acute Tox. 3, H331	ACUTE TOXICITY (inhalation) - Category 3
	Acute Tox. 4, H302	ACUTE TOXICITY (oral) - Category 4
	Acute Tox. 4, H312	ACUTE TOXICITY (dermal) - Category 4
	Aquatic Chronic 3, H412	LONG-TERM AQUATIC HAZARD - Category 3
	Carc. 2, H351	CARCINOGENICITY - Category 2
	Eye Irrit. 2, H319	SERIOUS EYE DAMAGE/ EYE IRRITATION - Category 2
	Flam. Liq. 3, H226	FLAMMABLE LIQUIDS - Category 3
	Skin Irrit. 2, H315	SKIN CORROSION/IRRITATION - Category 2
	STOT RE 2, H373	SPECIFIC TARGET ORGAN TOXICITY (REPEATED EXPOSURE) - Category 2
	STOT SE 3, H335 (Respiratory tract irritation)	SPECIFIC TARGET ORGAN TOXICITY (SINGLE EXPOSURE) (Respiratory tract irritation) - Category 3
	ID 2	
	Acute Tox. 4, H302	ACUTE TOXICITY (oral) - Category 4
	Eye Irrit. 2, H319	SERIOUS EYE DAMAGE/ EYE IRRITATION - Category 2
	STOT RE 2, H373	SPECIFIC TARGET ORGAN TOXICITY (REPEATED EXPOSURE) - Category 2
	STOT RE 2, H373 (kidneys and liver) (oral)	SPECIFIC TARGET ORGAN TOXICITY (REPEATED EXPOSURE) (kidneys and liver) (oral) - Category 2

SECTION 16: Other information

<p>Full text of abbreviated R phrases</p>	<p>: 1H S/N</p> <p>4Hz 0.1% H2O/D2O Temp Grad 1H Lineshape</p> <p>13C S/N ASTM doped</p> <p>ID 1</p> <p>ID 2 Sucrose, NMR tested</p> <p>Full text of classifications [DSD/DPD] : 1H S/N</p> <p>4Hz 0.1% H2O/D2O Temp Grad 1H Lineshape</p> <p>13C S/N ASTM doped</p> <p>ID 1</p>	<p>R40- Limited evidence of a carcinogenic effect. R22- Harmful if swallowed. R48/20/22- Harmful: danger of serious damage to health in case of prolonged exposure through inhalation and if swallowed. R38- Irritating to skin. Not applicable. Not applicable. R11- Highly flammable. R40- Limited evidence of a carcinogenic effect. R22- Harmful if swallowed. R48/20/22- Harmful: danger of serious damage to health in case of prolonged exposure through inhalation and if swallowed. R36- Irritating to eyes. R38- Irritating to skin. R66- Repeated exposure may cause skin dryness or cracking. R67- Vapours may cause drowsiness and dizziness. R11- Highly flammable. R10- Flammable. R19- May form explosive peroxides. R45- May cause cancer. R40- Limited evidence of a carcinogenic effect. R46- May cause heritable genetic damage. R48/23/24/25- Also toxic: danger of serious damage to health by prolonged exposure through inhalation, in contact with skin and if swallowed. R65- Also harmful: may cause lung damage if swallowed. R36/37- Irritating to eyes and respiratory system. R36/38- Irritating to eyes and skin. R36/37/38- Irritating to eyes, respiratory system and skin. R66- Repeated exposure may cause skin dryness or cracking. R10- Flammable. R40- Limited evidence of a carcinogenic effect. R23/25- Toxic by inhalation and if swallowed. R21- Harmful in contact with skin. R22- Harmful if swallowed. R21/22- Harmful in contact with skin and if swallowed. R48/20/22- Harmful: danger of serious damage to health in case of prolonged exposure through inhalation and if swallowed. R38- Irritating to skin. R37/38- Irritating to respiratory system and skin. R36/37/38- Irritating to eyes, respiratory system and skin. R22- Harmful if swallowed. Not applicable. Carc. Cat. 3 - Carcinogen category 3 Xn - Harmful Xi - Irritant Not applicable. Not applicable. F - Highly flammable Carc. Cat. 3 - Carcinogen category 3 Xn - Harmful Xi - Irritant F - Highly flammable Carc. Cat. 1 - Carcinogen category 1 Carc. Cat. 3 - Carcinogen category 3 Muta. Cat. 2 - Mutagen category 2 T - Toxic Xn - Harmful Xi - Irritant Carc. Cat. 3 - Carcinogen category 3</p>
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SECTION 16: Other information

		T - Toxic
		Xn - Harmful
		Xi - Irritant
	ID 2	Xn - Harmful
	Sucrose, NMR tested	Not applicable.
Date of issue/ Date of revision	: 29/01/2014	
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Version	: 3	

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