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

1.1. Product identifier
NMR-SAMPLE 0,3% CHCl3 in Acetone-d6 (LINESHAPE)

Further trade names
Z10701, Z10702, Z10903, Z10029
Z10913

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

Use of the substance/mixture
For R&D use only.

Uses advised against
Not for drug, household or other uses.

1.3. Details of the supplier of the safety data sheet

Company name: Bruker BioSpin AG
Street: Industriestrasse 26
Place: CH-8117 Fällanden
Telephone: +41 44 825 9111 / 9622
Telefax: +41 44 825 96 96
Internet: www.bruker.com
Responsible Department: Responsible for the safety data sheet: sds@gbk-ingelheim.de
(001) 352 323 3500 - Transport, EMTEL ID: 94135
Responsible for the safety data sheet: sds@gbk-ingelheim.de

1.4. Emergency telephone number:
Emergency telephone: +49 (0) 6132 / 84463 (GBK GmbH, Ingelheim)
+41 44 251 51 51 - Swiss Toxicological Information Center (24 h)

SECTION 2: Hazards identification

2.1. Classification of the substance or mixture according to 1272/2008/EC
Hazard categories:
Flammable liquid: Flam. Liq. 2
Serious eye damage/eye irritation: Eye Irrit. 2
Specific target organ toxicity - single exposure: STOT SE 3

Hazard Statements:
Highly flammable liquid and vapour.
Causes serious eye irritation.
May cause drowsiness or dizziness.

2.2. Label elements

Hazard components for labelling
Acetone-d6

Signal word: Danger

Pictograms:

H225 Highly flammable liquid and vapour.
H319 Causes serious eye irritation.
H336 May cause drowsiness or dizziness.

Precautionary statements
P210 Keep away from heat, hot surfaces, sparks, open flames and other ignition sources. No smoking.
P233 Keep container tightly closed.
P235 Keep cool.
P280 Wear protective gloves/protective clothing/eye protection/face protection.
P305+P351+P338 IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if

NMR-SAMPLE  0.3% CHCl3 in Acetone-d6 (LINSHAPE)

present and easy to do. Continue rinsing.
P337+P313 If eye irritation persists: Get medical advice/attention.
P501 Disposal in accordance with local regulations.

Special labelling of certain mixtures
EUH066 Repeated exposure may cause skin dryness or cracking.

2.3. Other hazards
Not known.

SECTION 3: Composition/information on ingredients

3.2. Mixtures
Chemical characterization
CPID 259576-86

Hazardous components

<table>
<thead>
<tr>
<th>CAS No</th>
<th>Chemical name</th>
<th>Quantity</th>
</tr>
</thead>
<tbody>
<tr>
<td>EC No</td>
<td>Index No</td>
<td>REACH No</td>
</tr>
<tr>
<td></td>
<td>Classification according to Regulation (EC) No. 1272/2008 [CLP]</td>
<td></td>
</tr>
<tr>
<td>666-52-4</td>
<td>Acetone-d6</td>
<td>99.7 %</td>
</tr>
<tr>
<td>211-563-9</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Flam. Liq. 2, Eye Irrit. 2, STOT SE 3; H225 H319 H336 EUH066</td>
<td></td>
<td></td>
</tr>
<tr>
<td>67-66-3</td>
<td>chloroform; trichloromethane</td>
<td>0.3 %</td>
</tr>
<tr>
<td>200-663-8</td>
<td></td>
<td>602-006-00-4 01-2119486657-20</td>
</tr>
<tr>
<td>Carc. 2, Repr. 2, Acute Tox. 3, Acute Tox. 4, Skin Irrit. 2, Eye Irrit. 2, STOT RE 1; H351 H361d H331 H302 H315 H319 H372</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Full text of H and EUH statements: see section 16.

SECTION 4: First aid measures

4.1. Description of first aid measures

General information
Harmful if swallowed. Ensure adequate ventilation. If patient is not breathing, apply artificial respiration. Do not breathe vapour. May cause cancer. May cause heritable genetic damage. May cause liver injury and blood disorders.

After inhalation
Take affected person into fresh air. Consult a physician.

After contact with skin
Wash off immediately with plenty of water for at least 15 minutes. Remove contaminated clothing immediately and dispose of safely.

After contact with eyes
Rinse immediately with plenty of water, also under the eyelids. If eye irritation persists consult a physician.

After ingestion

4.2. Most important symptoms and effects, both acute and delayed
Irritating to eyes. Limited evidence of a carcinogenic effect. Repeated exposure may cause skin dryness or cracking. Vapours may cause drowsiness and dizziness.

4.3. Indication of any immediate medical attention and special treatment needed
Treat symptoms.

SECTION 5: Firefighting measures

5.1. Extinguishing media

Suitable extinguishing media
Foam, carbon dioxide (CO2), dry chemical, water-spray

Unsuitable extinguishing media
Full water jet.
5.2. Special hazards arising from the substance or mixture

Burning may release the following flue gases such as: Phosgene, carbon dioxide (CO2), Hydrogen chloride (HCl).

5.3. Advice for firefighters

In case of fire, wear suitable respiratory equipment with positive air supply. Use personal protective clothing.

Additional information

Vapours are heavier than air. In use formation of flammable/explosive vapour-air mixtures possible. Danger of backfiring. Contain escaping vapours with water. Collect contaminated fire-fighting water, avoid any release into the sewerage. Closed NMR sample tubes may rupture when heated and may cause severe injury of eyes and skin.

SECTION 6: Accidental release measures

6.1. Personal precautions, protective equipment and emergency procedures

The appropriate action is to be taken immediately if the product is spilled or leaks. Take affected person away from danger area. Ensure adequate ventilation. Avoid contact with the skin and the eyes. Do not breathe vapour. Wear self-contained breathing apparatus and protective suit.

6.2. Environmental precautions

Do not discharge into the drains/surface waters/ground water. Inform competent authority about release into the sewage, ground or into waters.

6.3. Methods and material for containment and cleaning up

Soak up with inert absorbent material (e.g. sand, silica gel, acid binder, universal binder). Shovel into suitable container for disposal. Ensure adequate ventilation.

6.4. Reference to other sections

Information for disposal see section 13.

SECTION 7: Handling and storage

7.1. Precautions for safe handling

Advice on safe handling

Highly flammable. Take measures against electrostatic charging. Keep away from heat and sources of ignition.

Further information on handling

Do not open the glass tube. Avoid contact with skin, eyes and clothing. Do not breathe vapour. Heating will cause pressure rise with risk of bursting. See also chapter: 10

7.2. Conditions for safe storage, including any incompatibilities

Requirements for storage rooms and vessels

To be kept tightly closed, in a cool and dry place. Protect from light. Keep away from heat and sources of ignition.

Advice on storage compatibility

Store separately from other hazardous and incompatible substances. See also chapter: 10

Further information on storage conditions

Do not discharge into the drains/surface waters/ground water.

7.3. Specific end use(s)

NMR Sample

SECTION 8: Exposure controls/personal protection

8.1. Control parameters

Exposure limits (EH40)

<table>
<thead>
<tr>
<th>CAS No</th>
<th>Substance</th>
<th>ppm</th>
<th>mg/m³</th>
<th>fibres/ml</th>
<th>Category</th>
<th>Origin</th>
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</thead>
<tbody>
<tr>
<td>67-64-1</td>
<td>Acetone</td>
<td>500</td>
<td>1210</td>
<td></td>
<td>TWA (8 h)</td>
<td>WEL</td>
</tr>
<tr>
<td></td>
<td></td>
<td>1500</td>
<td>3620</td>
<td></td>
<td>STEL (15 min)</td>
<td>WEL</td>
</tr>
<tr>
<td>67-66-3</td>
<td>Chloroform</td>
<td>2</td>
<td>9.9</td>
<td></td>
<td>TWA (8 h)</td>
<td>WEL</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td>STEL (15 min)</td>
<td>WEL</td>
</tr>
</tbody>
</table>

8.2. Exposure controls
Appropriate engineering controls
Ensure adequate ventilation, especially in confined areas. Use only in a chemical fume hood.

Protective and hygiene measures
Take the usual precautions when handling with chemicals. Wash hands before breaks and at the end of workday. When using do not eat, drink or smoke. Avoid contact with skin, eyes and clothing. Do not breathe vapour. If you feel unwell, seek medical advice. Workers should be trained on good working practices and informed on applicable local regulations.

Eye/face protection
In case of eye contact wear safety goggles or face protection (EN 166). Eye wash bottle with pure water (EN 15154).

Hand protection
Chemical-resistant gloves (EN 374). Impervious butyl rubber gloves, Natural rubber (recommended: minimum protection index 2, corresponding to a permeation rate > 30 minutes according to EN 374). Follow the recommendations of the glove manufacturer for breakthrough properties especially for workplace conditions involving mechanical stress and contact duration.

Skin protection
Use only in a chemical fume hood. Protective clothing

Respiratory protection
In case of vapour / mist formation use respirator.

SECTION 9: Physical and chemical properties

9.1. Information on basic physical and chemical properties

| Physical state:                      | Liquid                  |
| Colour:                              | Colourless, clear       |
| Odour:                               | characteristic          |

pH-Value: 5-6 (365 g/l water) *)

Changes in the physical state

| Melting point:                      | -95.4 °C *)             |
| Initial boiling point and boiling range: | 56 °C *)             |
| Flash point:                        | -20 °C *)               |

Explosive properties
Formation of explosive gas/air mixtures.

| Lower explosion limits:            | 2.6 vol. %             |
| Upper explosion limits:            | 13 vol. %              |
| Ignition temperature:             | 465 °C *)              |
| Vapour pressure:                  | 233 hPa *)             |
| Density:                           | 0.79 g/cm³ *)          |
| Water solubility:                 | 1000 g/L *)            |

Solubility in other solvents
fats: Soluble
Organic solvent: Soluble

| Partition coefficient:            | Log Pow: -0.24 *)       |

9.2. Other information

*) All data refer to the solution

SECTION 10: Stability and reactivity

10.1. Reactivity
No data available.
10.2. Chemical stability
Stable under normal conditions.

10.3. Possibility of hazardous reactions
Reactions with light. (Hydrogen chloride (HCl))

10.4. Conditions to avoid
To avoid thermal decomposition, do not overheat.

10.5. Incompatible materials
Metals, strong bases, amines, oxidizing agents, halogenated compounds, nitrosyl compounds.

10.6. Hazardous decomposition products
Phosgene, carbon monoxide (CO), carbon dioxide (CO2), Hydrogen chloride (HCl), chlorine (Cl2).

SECTION 11: Toxicological information

11.1. Information on toxicological effects

Acute toxicity
Based on available data, the classification criteria are not met.
Chloroform, CAS-No.: 67-66-3
LD50/oral/rat: 908 mg/kg
LC50/inhalation/rat: 47.7 mg/m3/4h
LC0/Inhalation/Human: 25000 ppm/5 min
Acetone-d6, CAS-No.: 666-52-4
LD50/oral/rat: 5800 mg/kg
LD50/dermal/rabbit: 20 mg/kg
LC0/inhalation/rat: 76 mg/m3/4h

Irritation and corrosivity
Causes serious eye irritation.
Chloroform, CAS-No.: 67-66-3:
Skin irritation (rabbit): Slightly irritating.
Eyes irritation (rabbit): Slightly irritating.
Acetone-d6, CAS-No.: 666-52-4
Skin irritation (rabbit): Irritant
Eyes irritation (rabbit): Irritant

Sensitising effects
Based on available data, the classification criteria are not met.
Chloroform, CAS-No.: 67-66-3: No data available.
Acetone-d6, CAS-No.: 666-52-4: No data available.

STOT-single exposure
May cause drowsiness or dizziness. (Acetone-d6)

Severe effects after repeated or prolonged exposure
Repeated exposure may cause skin dryness or cracking.

Carcinogenic/mutagenic/toxic effects for reproduction
Based on available data, the classification criteria are not met.
Acetone-d6, CAS-No.: 666-52-4: No data available.

Aspiration hazard
Based on available data, the classification criteria are not met.

SECTION 12: Ecological information

12.1. Toxicity
The product has not been tested. The information is derived from the properties of the individual components.
Chloroform, CAS-No.: 67-66-3
LC50/fish: 18 mg/l (96 h, Lepomis macrochirus)
EC50: 79 mg/l (48 h, Daphnia magna)
IC5/Algae: 1100 mg/l (8 d, Scenedesmus quadricauda)
Acetone-d6, CAS-No.: 666-52-4
LC50/fish: 8300 mg/l (96 h, Lepomis macrochirus)
**NMR-SAMPLE  0.3% CHCl3 in Acetone-d6 (LINESHAPE)**

EC50: 12600 - 12700 mg/l (48 h, Daphnia magna)
IC50/Algae: 7500 mg/l (8 d, Scenedesmus quadricauda)

### 12.2. Persistence and degradability

**Acetone-d6, CAS-No.: 666-52-4:** Biodegradation: 91% / 28 d (Readily biodegradable.)

### 12.3. Bioaccumulative potential

There is no indication of bioaccumulation potential.

### 12.4. Mobility in soil

**Chloroform, CAS-No.: 67-66-3:** Log Pow: 2 (20°C)
**Acetone-d6, CAS-No.: 666-52-4:** Log Pow: -0.24

### 12.5. Results of PBT and vPvB assessment

Not determined.

### 12.6. Other adverse effects

Do not flush into surface water or sanitary sewer system.

### Further information

Do not flush into surface water or sanitary sewer system.

### SECTION 13: Disposal considerations

#### 13.1. Waste treatment methods

**Advice on disposal**

Do not flush into surface water or sanitary sewer system. This product is to be brought to a properly certified waste site approved to handle energy wastes.

**Waste disposal number of waste from residues/unused products**

160506 WASTES NOT OTHERWISE SPECIFIED IN THE LIST; gases in pressure containers and discarded chemicals; laboratory chemicals, consisting of or containing hazardous substances, including mixtures of laboratory chemicals

Classified as hazardous waste.

**Waste disposal number of contaminated packaging**

150107 WASTE PACKAGING; ABSORBENTS, WIPIING CLOTHS, FILTER MATERIALS AND PROTECTIVE CLOTHING NOT OTHERWISE SPECIFIED; packaging (including separately collected municipal packaging waste); glass packaging

Contaminated packaging

Disposal in accordance with local regulations.

### SECTION 14: Transport information

**Land transport (ADR/RID)**

14.1. UN number: UN 1090
14.2. UN proper shipping name: ACETONE
14.3. Transport hazard class(es): II
14.4. Packing group: 3

**Hazard label:**

Classification code: F1
Limited quantity: 1 L
Excepted quantity: E2
Transport category: 2
Hazard No: 33
Tunnel restriction code: D/E

**Inland waterways transport (ADN)**

14.1. UN number: UN 1090
14.2. UN proper shipping name: ACETONE
14.3. Transport hazard class(es): 3
14.4. Packing group: II
Hazard label: 3

Classification code: F1
Limited quantity: 1 L
Excepted quantity: E2

Marine transport (IMDG)
14.1. UN number: UN 1090
14.2. UN proper shipping name: ACETONE
14.3. Transport hazard class(es): 3
14.4. Packing group: II
Hazard label: 3

Special Provisions: -
Limited quantity: 1 L
Excepted quantity: E2
EmS: F-E, S-D

Air transport (ICAO)
14.1. UN number: UN 1090
14.2. UN proper shipping name: ACETONE
14.3. Transport hazard class(es): 3
14.4. Packing group: II
Hazard label: 3

Limited quantity Passenger: 1 L
Passenger LQ: Y341
Excepted quantity: E2
IATA-packing instructions - Passenger: 353
IATA-max. quantity - Passenger: 5 L
IATA-packing instructions - Cargo: 364
IATA-max. quantity - Cargo: 60 L

14.5. Environmental hazards
ENVIRONMENTALLY HAZARDOUS: no

14.6. Special precautions for user
Handle in accordance with good industrial hygiene and safety practice.

14.7. Transport in bulk according to Annex II of MARPOL73/78 and the IBC Code
The transport takes place only in approved and appropriate packaging.

SECTION 15: Regulatory information

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

EU regulatory information

Additional information
The product is labeled in accordance with Regulation (EC) no. 1272/2008 (GHS).
National regulatory information

15.2. Chemical safety assessment
For this substance a chemical safety assessment has not been carried out.

SECTION 16: Other information

Changes
Section 8, 13, 14, 15.

Abbreviations and acronyms
ADR = Accord européen relatif au transport international des marchandises Dangereuses par Route
RID = Règlement concernant le transport international ferroviaire de marchandises dangereuses
ADN = Accord européen relatif au transport international des marchandises dangereuses par voie de navigation intérieure
IMDG = International Maritime Code for Dangerous Goods
IATA/ICAO = International Air Transport Association / International Civil Aviation Organization
MARPOL = International Convention for the Prevention of Pollution from Ships
IBC-Code = International Code for the Construction and Equipment of Ships Carrying Dangerous Chemicals in Bulk
GHS = Globally Harmonized System of Classification and Labelling of Chemicals
REACH = Registration, Evaluation, Authorization and Restriction of Chemicals
CAS = Chemical Abstract Service
EN = European norm
ISO = International Organization for Standardization
DIN = Deutsche Industrie Norm
PBT = Persistent Bioaccumulative and Toxic
vPvB = Very Persistent and very Bio-accumulative
LD = Lethal dose
LC = Lethal concentration
EC = Effect concentration
IC = Median immobilisation concentration or median inhibitory concentration

Relevant H and EUH statements (number and full text)
H225 Highly flammable liquid and vapour.
H302 Harmful if swallowed.
H315 Causes skin irritation.
H319 Causes serious eye irritation.
H331 Toxic if inhaled.
H336 May cause drowsiness or dizziness.
H351 Suspected of causing cancer.
H361d Suspected of damaging the unborn child.
H372 Causes damage to organs through prolonged or repeated exposure.
EUH066 Repeated exposure may cause skin dryness or cracking.

Further Information
Data of items 4 to 8, as well as 10 to 12, do partly not refer to the use and the regular employing of the product (in this sense consult information on use and on product), but to liberation of major amounts in case of accidents and irregularities.
The information describes exclusively the safety requirements for the product(s) and is based on the present level of our knowledge.
The delivery specifications are contained in the corresponding product sheet.
This data does not constitute a guarantee for the characteristics of the product(s) as defined by the legal warranty regulations.
(n.a. = not applicable; n.d. = not determined)

(Information about the composition are based on information from the sub-contractor)

(The data for the hazardous ingredients were taken respectively from the last version of the sub-contractor's safety data sheet.)