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

1.1. Product identifier
NMR-SAMPLE 0,1 mg GdCl3/ml D2O + 1% H2O +0,1% CH3OH 13C (DOPED WATER)

Further trade names
NMR-SAMPLE 0,1 mg GdCl3/ml D2O + 1% H2O +0,1% CH3OH 13C (DOPED WATER):
Z100933, Z10727, Z10046, Z10083, Z10906, Z10085
Z10082, Z10084, Z10916
NMR-SAMPLE 0,1 mg GdCl3/ml D2O + 1% H2O (DOPED WATER):
Z10047, Z10088, Z10090
Z10087, Z10089

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
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
This mixture is not classified as hazardous according to Regulation (EC) No. 1272/2008.

2.2. Label elements
Special labelling of certain mixtures
EUH210 Safety data sheet available on request.

2.3. Other hazards
Not known.

SECTION 3: Composition/information on ingredients

3.2. Mixtures
Chemical characterization
CPID 288920-33
The product contains: 98.99% vol. Deuterium oxide (D2O), CAS-No. 7789-20-0, 0.9% vol. H2O.
Hazardous components

<table>
<thead>
<tr>
<th>CAS No</th>
<th>Chemical name</th>
<th>Quantity</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>EC No</td>
<td>Index No</td>
</tr>
<tr>
<td></td>
<td>Classification according to Regulation (EC) No. 1272/2008 [CLP]</td>
<td></td>
</tr>
<tr>
<td>14742-26-8</td>
<td>methanol-13C</td>
<td>0.100 %</td>
</tr>
<tr>
<td></td>
<td>603-001-00-X</td>
<td></td>
</tr>
<tr>
<td>13450-84-5</td>
<td>Gadolinium chloride, hexahydrate</td>
<td>&lt;1 %</td>
</tr>
<tr>
<td></td>
<td>Skin Irrit. 2, Eye Irrit. 2, STOT SE 3; H315 H319 H335</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
No specific precautions required.

After inhalation
No specific precautions required.

After contact with skin
No specific precautions required.

After contact with eyes
No specific precautions required.

After ingestion
No specific precautions required.

4.2. Most important symptoms and effects, both acute and delayed
Health injuries are not known or expected under normal use.

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
The product is not combustible.

Unsuitable extinguishing media
Fire-extinguishing activities according to surrounding.

5.2. Special hazards arising from the substance or mixture
None

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

Additional information
Closed NMR sample tubes may rupture when heated and may cause severe injury of eyes and skin. Fire residues and contaminated firefighting water must be disposed of in accordance with the local regulations.

SECTION 6: Accidental release measures

6.1. Personal precautions, protective equipment and emergency procedures
No specific precautions required.

6.2. Environmental precautions
No specific precautions required.

6.3. Methods and material for containment and cleaning up
No specific precautions required.
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
Handling should only be allowed by trained personnel.

Further information on handling
Do not open the glass tube. Avoid contact with skin, eyes and clothing. Use only in a chemical fume hood. 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. Keep under inert gas. The product is hygroscopic.

Advice on storage compatibility
Store separately from other hazardous and incompatible substances. See also chapter: 10

Further information on storage conditions
Protect from moisture.

7.3. Specific end use(s)
NMR Sample

SECTION 8: Exposure controls/personal protection

8.1. Control parameters

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). PVA gloves (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
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

<table>
<thead>
<tr>
<th>Physical state:</th>
<th>Liquid</th>
</tr>
</thead>
<tbody>
<tr>
<td>Colour:</td>
<td>Colourless, clear</td>
</tr>
<tr>
<td>Odour:</td>
<td>n.a.</td>
</tr>
</tbody>
</table>
pH-Value: 7.43 (Deuterium oxide (D2O))

**Changes in the physical state**

<table>
<thead>
<tr>
<th>Property</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Melting point</td>
<td>(Deuterium oxide (D2O)) 3.82 °C</td>
</tr>
<tr>
<td>Initial boiling point and boiling range</td>
<td>(Deuterium oxide (D2O)) 101.42 °C</td>
</tr>
<tr>
<td>Flash point</td>
<td>n.a.</td>
</tr>
<tr>
<td>Ignition temperature</td>
<td>n.a.</td>
</tr>
<tr>
<td>Vapour pressure</td>
<td>n.a.</td>
</tr>
<tr>
<td>Density (at 25 °C)</td>
<td>(Deuterium oxide (D2O)) 1.107 g/cm³ Value from literature</td>
</tr>
<tr>
<td>Water solubility</td>
<td>n.a.</td>
</tr>
<tr>
<td>Viscosity / dynamic</td>
<td>n.a.</td>
</tr>
</tbody>
</table>

**9.2. Other information**

No data available.

**SECTION 10: Stability and reactivity**

**10.1. Reactivity**

Not known.

**10.2. Chemical stability**

Stable under normal conditions.

**10.3. Possibility of hazardous reactions**

Not known.

**10.4. Conditions to avoid**

Protect from moisture.

**10.5. Incompatible materials**

Keep under inert gas. The product is hygroscopic.

**10.6. Hazardous decomposition products**

No data available.

**SECTION 11: Toxicological information**

**11.1. Information on toxicological effects**

Toxicokinetics, metabolism and distribution

No data available.

**Acute toxicity**

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

**Irritation and corrosivity**

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

**Sensitising effects**

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

**STOT-single exposure**

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

**Severe effects after repeated or prolonged exposure**

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

**Carcinogenic/mutagenic/toxic effects for reproduction**

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

**Aspiration hazard**

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

**SECTION 12: Ecological information**

**12.1. Toxicity**

No data available.

**12.2. Persistence and degradability**
NMR-SAMPLE  0.1 mg GdCl3/ml D2O + 1% H2O +0.1% CH3OH 13C (DOPED WATER)

12.3. Bioaccumulative potential
No data available.

12.4. Mobility in soil
No data available.

12.5. Results of PBT and vPvB assessment
No data available.

12.6. Other adverse effects
No data available.

SECTION 13: Disposal considerations

13.1. Waste treatment methods
Advice on disposal
Treat by state-of-the-art technology before discharging into drains. 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, WIPING 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); Marine transport (IMDG); Air transport (ICAO); Inland waterways transport (ADN):

14.1. UN number:
Not applicable. No hazardous material as defined by the transport regulations.

14.2. UN proper shipping name:
Not applicable. No hazardous material as defined by the transport regulations.

14.3. Transport hazard class(es):
Not applicable. No hazardous material as defined by the transport regulations.

14.4. Packing group:
Not applicable. No hazardous material as defined by the transport regulations.

14.5. Environmental hazards
Not applicable. No hazardous material as defined by the transport regulations.

14.6. Special precautions for user
Not applicable. No hazardous material as defined by the transport regulations.

14.7. Transport in bulk according to Annex II of MARPOL73/78 and the IBC Code
Not applicable. No hazardous material as defined by the transport regulations.

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.
H301 Toxic if swallowed.
H311 Toxic in contact with skin.
H315 Causes skin irritation.
H319 Causes serious eye irritation.
H331 Toxic if inhaled.
H335 May cause respiratory irritation.
H370 Causes damage to organs.
EUH210 Safety data sheet available on request.

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.)