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

- **Product identifier**

- **Trade name:** Hexahydro-1,3,5-trinitro-1,3,5-triazine (RDX) Metabolite Standard (1X1 mL)

- **Part number:** NAIM-245-1

- **Relevant identified uses of the substance or mixture and uses advised against**
  Reagents and Standards for Analytical Chemical Laboratory Use

- **Details of the supplier of the safety data sheet**

- **Manufacturer/Supplier:**
  Agilent Technologies Manufacturing GmbH & Co. KG
  Hewlett-Packard-Str.8
  76337 Waldbronn
  Germany

- **Further information obtainable from:**
  Telephone: 0800 603 1000
  pdl-msds_author@agilent.com
  **Emergency telephone number:** CHEMTREC®: +(44)-870-8200418

2 Hazards identification

- **Classification of the substance or mixture**

- **Classification according to Regulation (EC) No 1272/2008**

  - GHS02 flame
  - Flam. Liq. 2 H225 Highly flammable liquid and vapour.

  - GHS07
  - Acute Tox. 4 H302 Harmful if swallowed.
  - Eye Irrit. 2 H319 Causes serious eye irritation.

- **Label elements**

- **Labelling according to Regulation (EC) No 1272/2008**
  The product is classified and labelled according to the CLP regulation.

- **Hazard pictograms**

  - GHS02
  - GHS07

- **Signal word** Danger

- **Hazard-determining components of labelling:**
  acetonitrile
  1,3,5-trinitroso-1,3,5-triazacyclohexane

- **Hazard statements**
  H225 Highly flammable liquid and vapour.
  H302 Harmful if swallowed.
  H319 Causes serious eye irritation.

(Contd. on page 2)
## 3 Composition/information on ingredients

### Chemical characterisation: Mixtures

### Description: Mixture of substances listed below with nonhazardous additions.

### Dangerous components:

<table>
<thead>
<tr>
<th>CAS: 75-05-8</th>
<th>Acetonitrile</th>
<th>99.618%</th>
</tr>
</thead>
<tbody>
<tr>
<td>EINECS: 200-835-2</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>CAS: 23374-70-1</th>
<th>1,3,5-trinitroso-1,3,5-triazacyclohexane</th>
<th>0.127%</th>
</tr>
</thead>
</table>

### Additional information: For the wording of the listed hazard phrases refer to section 16.

## 4 First aid measures

### Description of first aid measures

### General information:

Immediately remove any clothing soiled by the product.

Symptoms of poisoning may even occur after several hours; therefore medical observation for at least 48 hours after the accident.

### After inhalation: Supply fresh air; consult doctor in case of complaints.

(Contd. on page 3)
48.1.26 · After skin contact: Immediately rinse with water.
· After eye contact: Rinse opened eye for several minutes under running water. If symptoms persist, consult a doctor.
· After swallowing: Call for a doctor immediately.
· Information for doctor:
· Most important symptoms and effects, both acute and delayed No further relevant information available.
· Indication of any immediate medical attention and special treatment needed No further relevant information available.

5 Firefighting measures

· Extinguishing media
· Suitable extinguishing agents: CO2, powder or water spray. Fight larger fires with water spray or alcohol resistant foam.
· For safety reasons unsuitable extinguishing agents: Water with full jet
· Special hazards arising from the substance or mixture No further relevant information available.
· Advice for firefighters
· Protective equipment: No special measures required.

6 Accidental release measures

· Personal precautions, protective equipment and emergency procedures
  Wear protective equipment. Keep unprotected persons away.
· Environmental precautions: Do not allow to enter sewers/ surface or ground water.
· Methods and material for containment and cleaning up:
  Absorb with liquid-binding material (sand, diatomite, acid binders, universal binders, sawdust).
  Dispose contaminated material as waste according to item 13.
  Ensure adequate ventilation.
· Reference to other sections
  See Section 7 for information on safe handling.
  See Section 8 for information on personal protection equipment.
  See Section 13 for disposal information.

7 Handling and storage

· Handling:
· Precautions for safe handling No special precautions are necessary if used correctly.
· Information about fire - and explosion protection:
  Keep ignition sources away - Do not smoke.
  Protect against electrostatic charges.
· Conditions for safe storage, including any incompatibilities
· Storage:
  Requirements to be met by storerooms and receptacles: Store in a cool location.
  Information about storage in one common storage facility: Not required.
  Further information about storage conditions:
  Keep container tightly sealed.
  Store in cool, dry conditions in well sealed receptacles.
Safety data sheet
according to 1907/2006/EC, Article 31

Trade name: Hexahydro-1,3,5-trinitro-1,3,5-triazine (RDX) Metabolite Standard (1X1 mL)

- Specific end use(s) No further relevant information available.

8 Exposure controls/personal protection

- Additional information about design of technical facilities: No further data; see item 7.

- Control parameters

| Ingredients with limit values that require monitoring at the workplace: |
|------------------|------------------|
| 75-05-8 acetonitrile |
| WEL | Short-term value: 102 mg/m³, 60 ppm | Long-term value: 68 mg/m³, 40 ppm |

- Additional information: The lists valid during the making were used as basis.

- Exposure controls

- Personal protective equipment:
  - General protective and hygienic measures:
    - Keep away from foodstuffs, beverages and feed.
    - Immediately remove all soiled and contaminated clothing.
    - Wash hands before breaks and at the end of work.
    - Avoid contact with the eyes.
    - Avoid contact with the eyes and skin.

- Respiratory protection:
  - When used as intended with Agilent instruments the use of the product under normal laboratory conditions and with standard practices does not result in significant airborne exposures and therefore respiratory protection is not needed.
  - Under an emergency condition where a respirator is deemed necessary, use a NIOSH or equivalent approved device equipment with appropriate organic or acid gas cartridge.

- Protection of hands:
  - Although not recommended for constant contact with the chemicals or for clean up, nitrile gloves 11-13mil thickness are recommended for normal use. The breakthrough time is 1hr. For cleaning a spill where there is direct contact of the chemical, butyl rubber gloves are recommended 12-15mil thickness with breakthrough times exceeding 4 hrs. Supplier recommendations should be followed.

- Material of gloves
  - For normal use: nitrile rubber, 11-13 mil thickness
  - For direct contact with the chemical: butyl rubber, 12-15 mil thickness

- Penetration time of glove material
  - For normal use: nitrile rubber: 1 hour
  - For direct contact with the chemical: butyl rubber: > 4 hours

- Eye protection:
  - Tightly sealed goggles
### 9 Physical and chemical properties

<table>
<thead>
<tr>
<th>Property</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Appearance</strong></td>
<td></td>
</tr>
<tr>
<td>Form</td>
<td>Fluid</td>
</tr>
<tr>
<td>Colour</td>
<td>Colourless</td>
</tr>
<tr>
<td>Odour</td>
<td>Aromatic</td>
</tr>
<tr>
<td>Odour threshold</td>
<td>Not determined</td>
</tr>
<tr>
<td><strong>pH-value</strong></td>
<td>Not determined</td>
</tr>
<tr>
<td><strong>Change in condition</strong></td>
<td></td>
</tr>
<tr>
<td>Melting point/freezing point</td>
<td>-46 °C</td>
</tr>
<tr>
<td>Initial boiling point and boiling range</td>
<td>81 °C</td>
</tr>
<tr>
<td><strong>Flash point</strong></td>
<td>2 °C</td>
</tr>
<tr>
<td><strong>Flammability (solid, gas)</strong></td>
<td>Not applicable</td>
</tr>
<tr>
<td><strong>Ignition temperature</strong></td>
<td>525 °C</td>
</tr>
<tr>
<td><strong>Decomposition temperature</strong></td>
<td>Not determined</td>
</tr>
<tr>
<td><strong>Auto-ignition temperature</strong></td>
<td>Product is not selfigniting</td>
</tr>
<tr>
<td><strong>Explosive properties</strong></td>
<td>Product is not explosive. However, formation of explosive air/vapour mixtures are possible.</td>
</tr>
<tr>
<td><strong>Explosion limits</strong></td>
<td></td>
</tr>
<tr>
<td>Lower</td>
<td>4.4 Vol %</td>
</tr>
<tr>
<td>Upper</td>
<td>16 Vol %</td>
</tr>
<tr>
<td><strong>Vapour pressure at 20 °C</strong></td>
<td>0 hPa</td>
</tr>
<tr>
<td><strong>Density at 20 °C</strong></td>
<td>0.786 g/cm³</td>
</tr>
<tr>
<td><strong>Relative density</strong></td>
<td>Not determined</td>
</tr>
<tr>
<td><strong>Vapour density</strong></td>
<td>Not determined</td>
</tr>
<tr>
<td><strong>Evaporation rate</strong></td>
<td>Not determined</td>
</tr>
<tr>
<td><strong>Solubility in / Miscibility with water</strong></td>
<td>Not miscible or difficult to mix</td>
</tr>
<tr>
<td><strong>Partition coefficient: n-octanol/water</strong></td>
<td>Not determined</td>
</tr>
<tr>
<td><strong>Viscosity</strong></td>
<td></td>
</tr>
<tr>
<td>Dynamic at 20 °C</td>
<td>0.39 mPas</td>
</tr>
<tr>
<td>Kinematic</td>
<td>Not determined</td>
</tr>
<tr>
<td><strong>Solvent content</strong></td>
<td></td>
</tr>
<tr>
<td>VOC (EC)</td>
<td>0.00 %</td>
</tr>
<tr>
<td><strong>Solids content</strong></td>
<td></td>
</tr>
<tr>
<td><strong>Other information</strong></td>
<td></td>
</tr>
<tr>
<td><strong>Not determined</strong></td>
<td></td>
</tr>
</tbody>
</table>

### 10 Stability and reactivity

- **Reactivity** No further relevant information available.
48.1.26

· Chemical stability
  · Thermal decomposition / conditions to be avoided: No decomposition if used according to specifications.
  · Possibility of hazardous reactions No dangerous reactions known.
  · Conditions to avoid No further relevant information available.
  · Incompatible materials: No further relevant information available.
  · Hazardous decomposition products: No dangerous decomposition products known.

11 Toxicological information

· Information on toxicological effects
  · Acute toxicity
    Harmful if swallowed.

· LD/LC50 values relevant for classification:

<table>
<thead>
<tr>
<th>ATE (Acute Toxicity Estimates)</th>
<th>Oral LD50</th>
<th>1,303 mg/kg</th>
</tr>
</thead>
<tbody>
<tr>
<td>75-05-8 acetonitrile</td>
<td>Oral LD50</td>
<td>1,320 mg/kg (rat)</td>
</tr>
<tr>
<td></td>
<td>Dermal LD50</td>
<td>&gt;2,000 mg/kg (rabbit)</td>
</tr>
<tr>
<td></td>
<td>Inhalative LC50/4 h</td>
<td>3,587 mg/L (mouse)</td>
</tr>
</tbody>
</table>

· Primary irritant effect:
  · Skin corrosion/irritation Based on available data, the classification criteria are not met.
  · Serious eye damage/irritation
    Causes serious eye irritation.
  · Respiratory or skin sensitisation Based on available data, the classification criteria are not met.
  · CMR effects (carcinogenity, mutagenicity and toxicity for reproduction)
  · Germ cell mutagenicity Based on available data, the classification criteria are not met.
  · Carcinogenicity Based on available data, the classification criteria are not met.
  · Reproductive toxicity Based on available data, the classification criteria are not met.
  · STOT-single exposure Based on available data, the classification criteria are not met.
  · STOT-repeated exposure Based on available data, the classification criteria are not met.
  · Aspiration hazard Based on available data, the classification criteria are not met.

12 Ecological information

· Toxicity
  · Aquatic toxicity: No further relevant information available.
  · Persistence and degradability: No further relevant information available.

· Behaviour in environmental systems:
  · Bioaccumulative potential: No further relevant information available.

· Mobility in soil: No further relevant information available.

· Additional ecological information:
  · General notes:
    Water hazard class 2 (German Regulation) (Self-assessment): hazardous for water
    Do not allow product to reach ground water, water course or sewage system.
    Danger to drinking water if even small quantities leak into the ground.

· Results of PBT and vPvB assessment
  · PBT: Not applicable.
  · vPvB: Not applicable.
13 Disposal considerations

- Waste treatment methods
  - Recommendation
    Must not be disposed together with household garbage. Do not allow product to reach sewage system.

- European waste catalogue
  - HP 3 Flammable
  - HP 4 Irritant - skin irritation and eye damage
  - HP 6 Acute Toxicity

- Uncleaned packaging:
  - Recommendation: Disposal must be made according to official regulations.

*14 Transport information

- Not Regulated, De minimus Quantities

- UN-Number
  - ADR, IMDG, IATA
  - UN1648

- UN proper shipping name
  - ADR
  - IMDG, IATA
  - 1648 ACETONITRILE mixture
  - ACETONITRILE mixture

- Transport hazard class(es)
  - ADR, IMDG, IATA

- Class
  - 3 Flammable liquids.
- Label
  - 3

- Packing group
  - ADR, IMDG, IATA
  - II

- Environmental hazards:
  - Not applicable.

- Special precautions for user
  - Warning: Flammable liquids.
- Danger code (Kemler):
  - 33
- EMS Number:
  - F-E,S-D
- Stowage Category
  - B
- Stowage Code
  - SW2 Clear of living quarters.

- Transport in bulk according to Annex II of Marpol and the IBC Code
  - Not applicable.
### Transport/Additional information:

- **ADR**
  - **Limited quantities (LQ)**: 1L
  - **Excepted quantities (EQ)**: Code: E2
    - Maximum net quantity per inner packaging: 30 ml
    - Maximum net quantity per outer packaging: 500 ml
- **Transport category**: 2
- **Tunnel restriction code**: D/E
- **IMDG**
  - **Limited quantities (LQ)**: 1L
  - **Excepted quantities (EQ)**: Code: E2
    - Maximum net quantity per inner packaging: 30 ml
    - Maximum net quantity per outer packaging: 500 ml
- **UN "Model Regulation":** UN 1648 ACETONITRILE MIXTURE, 3, II

### 15 Regulatory information

- **Safety, health and environmental regulations/legislation specific for the substance or mixture**
  - **Directive 2012/18/EU**
  - **Named dangerous substances - ANNEX I** None of the ingredients is listed.
  - **Seveso category** P5c FLAMMABLE LIQUIDS
  - **Qualifying quantity (tonnes) for the application of lower-tier requirements**: 5,000 t
  - **Qualifying quantity (tonnes) for the application of upper-tier requirements**: 50,000 t
- **REGULATION (EC) No 1907/2006 ANNEX XVII** Conditions of restriction: 3
- **Chemical safety assessment**: A Chemical Safety Assessment has not been carried out.

### 16 Other information

The information contained in this document is based on Agilent’s state of knowledge at the time of preparation. No warranty as to its accurateness, completeness or suitability for a particular purpose is expressed or implied.

- **Relevant phrases**
  - H225 Highly flammable liquid and vapour.
  - H301 Toxic if swallowed.
  - H302 Harmful if swallowed.
  - H312 Harmful in contact with skin.
  - H319 Causes serious eye irritation.
  - H332 Harmful if inhaled.
- **Abbreviations and acronyms:**
  - ADR: Accord européen sur le transport des marchandises dangereuses par Route (European Agreement concerning the International Carriage of Dangerous Goods by Road)
  - IMDG: International Maritime Code for Dangerous Goods
  - IATA: International Air Transport Association
  - GHS: Globally Harmonised System of Classification and Labelling of Chemicals
  - EINECS: European Inventory of Existing Commercial Chemical Substances
  - ELINCS: European List of Notified Chemical Substances
  - CAS: Chemical Abstracts Service (division of the American Chemical Society)
  - VOC: Volatile Organic Compounds (USA, EU)
  - LC50: Lethal concentration, 50 percent
  - LD50: Lethal dose, 50 percent
Trade name: Hexahydro-1,3,5-trinitro-1,3,5-triazine (RDX) Metabolite Standard (1X1 mL)

<table>
<thead>
<tr>
<th>Classification</th>
<th>Category</th>
</tr>
</thead>
<tbody>
<tr>
<td>PBT: Persistent, Bioaccumulative and Toxic</td>
<td></td>
</tr>
<tr>
<td>vPvB: very Persistent and very Bioaccumulative</td>
<td></td>
</tr>
<tr>
<td>Flam. Liq. 2: Flammable liquids</td>
<td>Category 2</td>
</tr>
<tr>
<td>Acute Tox. 3: Acute toxicity</td>
<td>Category 3</td>
</tr>
<tr>
<td>Acute Tox. 4: Acute toxicity</td>
<td>Category 4</td>
</tr>
<tr>
<td>Eye Irrit. 2: Serious eye damage/eye irritation</td>
<td>Category 2</td>
</tr>
</tbody>
</table>

- * Data compared to the previous version altered.