



# MATERIAL SAFETY DATA SHEET

Version 1.0, Feb 2014

## 1. IDENTIFICATION OF THE SUBSTANCE/MIXTURE AND OF THE COMPANY UNDERTAKING

### 1.1 Product identifiers

Product Name: LY411575  
Catalog Number: SM25  
CAS Number: 209984-57-6  
IUPAC Name: N-2-[(2S)-2-(3,5-difluorophenyl)-2-hydroxyethanoyl]-N1-[(7S)-5-methyl-6-oxo-6,7-dihydro-5H-dibenzo[b,d]azepin-7-yl]-L-alaninamide

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

Identified Uses: Laboratory chemicals, Manufacture of substances

### 1.3 Details of the supplier of the safety data sheet

Company: Cell Guidance Systems  
Moneta Building, Babraham Research Campus,  
Cambridge CB22 3AT, UK  
Web: [www.cellgs.com](http://www.cellgs.com)  
Email: [tech@cellgs.com](mailto:tech@cellgs.com)  
Telephone: + 44 (0)1223 850186

1.4 Emergency Telephone Emergency Tel: + 44 (0) 1223 850186 (09.00 - 17.00 GMT)

## 2. HAZARDS IDENTIFICATION

### 2.1 Classification of the substance or mixture

This substance does not meet the classification criteria of the EC Directives 67/548/EEC, 1999/45/EC or 1272/2008.

### 2.2 Label elements

The product does not need to be labeled in accordance with EC directives or respective national laws.

### 2.3 Other hazards

none

## 3. COMPOSITION/INFORMATION ON INGREDIENTS

### 3.1 Substances

Product Name: LY411575  
Synonyms: LSN-411575  
Formula:  $C_{26}H_{23}F_2N_3O_4$

Molecular Weight: 479.48  
CAS Number: 209984-57-6

#### 4. FIRST AID MEASURES

##### 4.1 Description of first aid measures

|                          |  |
|--------------------------|--|
| General advice.          | Consult a doctor and show this safety data sheet.  |
| If inhaled.              | Remove to fresh air and monitor breathing. If breathing becomes difficult, give oxygen. If breathing stops, give artificial respiration. Consult a doctor.             |
| In case of skin contact. | Immediately wash skin with copious amounts of soap and water for at least 15 minutes. Remove contaminated clothing and shoes and wash before reuse. Consult a doctor.  |
| In case of eye contact.  | Flush with copious amounts of water for at least 15 minutes. Consult a doctor.   |
| If swallowed.            | Rinse mouth with water. Do not induce vomiting unless directed to do so by medical personnel. Never give anything by mouth to an unconscious person. Consult a doctor. |

##### 4.2 Most important symptoms and effects, both acute and delayed

To the best of our knowledge, the chemical, physical and toxicological properties have not been thoroughly investigated.

##### 4.3 Indication of immediate medical attention and special treatment needed

Show this safety data sheet to the doctor in attendance. Immediate medical attention is required.

#### 5. FIRE-FIGHTING MEASURES

|   |   |
|---|---|
| 5.1 Suitable extinguishing media                          | Use water spray, alcohol-resistant foam, dry chemical or carbon dioxide.  |
| 5.2 Special hazards arising from the substance or mixture | Hazardous decomposition products formed under fire conditions. - Carbon oxides, nitrogen oxides (NOx), Hydrogen fluoride. |
| 5.3 Precautions for fire-fighters                         | Wear suitable protective clothing to prevent contact with skin and eyes and self-contained breathing apparatus.           |

#### 6. ACCIDENTAL RELEASE MEASURES

##### 6.1 Personal precautions, protective equipment and emergency procedures

Do not take action without suitable protective clothing - see section 8 of SDS. Evacuate personnel to safe areas. Ensure ventilation. Avoid breathing vapors, mist, dust or gas.

##### 6.2 Environmental precautions

Do not let product enter drains.

##### 6.3 Methods and materials for containment and cleaning up

Cover spillage with suitable absorbent material. Using non-spark tools, sweep up material and place in an appropriate container. Decontaminate spill site with 10% caustic solution and ventilate area until after disposal is complete. Hold all material for appropriate disposal as described under section 13 of SDS.

## 6.4 Reference to other sections

For required PPE see section 8. For disposal see section 13.

## 7. HANDLING AND STORAGE

### 7.1 Precautions for safe handling

Use in a chemical fume hood, with air supplied by an independent system. Avoid inhalation, contact with eyes, skin and clothing. Avoid the formation of dust and aerosols. Use in a well-ventilated area. Keep away from sources of ignition. Avoid prolonged or repeated exposure.

### 7.2 Conditions for safe storage, including any incompatibilities.

Store in cool, well-ventilated area. Keep away from direct sunlight. Keep container tightly sealed until ready for use.  
Recommended storage temperature: Store at -20°C

### 7.3 Specific end uses

Use in a laboratory fume hood where possible. Refer to employer's COSHH risk assessment.

## 8. EXPOSURE CONTROLS/PERSONAL PROTECTION

### 8.1 Control parameters

|  |   |
|--|---|
| Components with workplace control parameters | Contains no substances with occupational exposure limit values. |
|--|---|

### 8.2 Exposure controls

|                                  |   |
|----------------------------------|---|
| Appropriate engineering controls | Use in a fume hood where applicable. Ensure all engineering measures described under section 7 of SDS are in place.<br>Ensure laboratory is equipped with a safety shower and eye wash station. |
| Personal protective equipment    |   |
| Eye/face protection              | Use appropriate safety glasses.   |
| Skin protection                  | Use appropriate chemical resistant gloves (minimum requirement use standard BS EN 374:2003). Gloves should be inspected before use. Wash and dry hands thoroughly after handling.               |
| Body protection                  | Wear appropriate protective clothing.   |
| Respiratory protection           | If risk assessment indicates necessary, use a suitable respirator.  |

## 9. PHYSICAL AND CHEMICAL PROPERTIES

### 9.1 Information on basic physical and chemical properties

|                          |                            |
|--------------------------|----------------------------|
| Appearance               | Solid                      |
| Vapor pressure           | No data available          |
| Odor                     | No data available          |
| Vapor density            | No data available          |
| Odor threshold           | No data available          |
| Relative density         | No data available          |
| pH                       | No data available          |
| Solubility(ies)          | Soluble in DMSO >200 mg/ml |
| Melting / freezing point | No data available          |
| Partition coefficient    | No data available          |
| Boiling point / range    | No data available          |

|  |                   |
|--|-------------------|
| Auto-ignition temperature                      | No data available |
| Flash point                                    | No data available |
| Decomposition temperature                      | No data available |
| Evaporation rate                               | No data available |
| Viscosity                                      | No data available |
| Flammability (solid, gas)                      | No data available |
| Explosive properties                           | No data available |
| Upper / lower flammability or explosive limits | No data available |
| Oxidising properties                           | No data available |

## 9.2 Other safety information

No data available

## 10. STABILITY AND REACTIVITY

|  |  |
|--|--|
| <b>10.1 Reactivity</b>                         | Stable under recommended transport or storage conditions.  |
| <b>10.2 Chemical stability</b>                 | Stable under recommended storage conditions.   |
| <b>10.3 Possibility of hazardous reactions</b> | Hazardous reactions will not occur under normal transport or storage conditions. Decomposition may occur on exposure to conditions or materials listed below.                              |
| <b>10.4 Conditions to avoid</b>                | Heat, moisture.  |
| <b>10.5 Incompatible materials</b>             | Strong acids/alkalis, strong oxidising/reducing agents.  |
| <b>10.6 Hazardous decomposition products</b>   | Hazardous decomposition products formed under fire conditions. - Carbon oxides, nitrogen oxides (NO <sub>x</sub> ), Hydrogen fluoride<br>Other decomposition products - no data available. |

## 11. TOXICOLOGICAL INFORMATION

### 11.1 Information on toxicological effects

|   |   |
|---|---|
| Acute Toxicity  | No data available   |
| Skin corrosion/irritation   | Classification criteria are not met based on available data         |
| Serious eye damage/irritation   | Classification criteria are not met based on available data         |
| Respiratory or skin sensitization   | Classification criteria are not met based on available data         |
| Germ cell mutagenicity  | Classification criteria are not met based on available data         |
| Carcinogenicity   | Classification criteria are not met based on available data         |
| Reproductive toxicity   | Classification criteria are not met based on available data         |
| Specific target organ toxicity - single exposure  | Classification criteria are not met based on available data         |
| Specific target organ toxicity - repeated exposure  | Classification criteria are not met based on available data         |
| Aspiration hazard   | Classification criteria are not met based on available data         |
| Symptoms / Routes of exposure   |   |
| Inhalation:   | May be harmful if inhaled. May cause respiratory tract irritation.  |
| Ingestion:  | May be harmful if swallowed.  |
| Skin:   | May be harmful if absorbed through skin. May cause skin irritation. |
| Eyes:   | May cause eye irritation.   |
| Delayed / Immediate Effects:  | No known symptoms.  |
| Additional Information  | RTECS No: Not available   |
| Exposure may cause irritation to eyes, mucous membranes, upper respiratory tract and skin                           |   |
| To the best of our knowledge, the chemical, physical and toxicological properties have not been fully investigated. |   |

## 12. ECOLOGICAL INFORMATION

|   |  |
|---|--|
| 12.1 Toxicity                           | No data available                          |
| 12.2 Persistence and degradability      | No data available                          |
| 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              | May be harmful to the aquatic environment. |

## 13. DISPOSAL CONSIDERATIONS

### 13.1 Waste treatment methods

|                        |  |
|------------------------|--|
| Product                | Transfer to a suitable container and arrange for collection by specialized disposal company in accordance with National legislation. |
| Contaminated packaging | Dispose of in a regulated landfill site or other method for hazardous or toxic wastes in accordance with National legislation.       |

## 14. TRANSPORT INFORMATION

Classified according to the criteria of the UN Model Regulations as reflected in the IMDG Code, ADR, RID and IATA.

|                                    |   |
|------------------------------------|---|
| 14.1 UN-Number                     | Does not meet the criteria for classification as hazardous for transport.   |
| 14.2 UN proper shipping name       | Does not meet the criteria for classification as hazardous for transport.   |
| 14.3 Transport hazard class(es)    | Does not meet the criteria for classification as hazardous for transport.   |
| 14.4 Packaging group               | Does not meet the criteria for classification as hazardous for transport.   |
| 14.5 Environmental hazards         | This product is not classified as environmentally hazardous according to the UN Model Regulations, nor a marine pollutant according to the IMDG Code. |
| 14.6 Special precautions for users | No data available   |

## 15. REGULATORY INFORMATION

This safety datasheet complies with the requirements of Regulation (EC) No. 453/2010.

|   |  |
|---|--|
| 15.1 Safety, health and environmental regulations/legislation specific for the substance or mixture | No data available  |
| 15.2 Chemical safety assessment   | A Chemical Safety Assessment has not been made for this product. |

## 16. OTHER INFORMATION

Copyright 2013 Cell Guidance Systems. This company shall not be held liable for any damage resulting from handling or from contact with the above product. This material must only be handled by suitably qualified experienced scientists in appropriately equipped and authorized facilities. The above information is believed to be correct but does not purport to be all inclusive and should be used as a guide only for experienced personnel. Always consult your safety advisor and follow appropriate local and national safety legislature. The absence of warning must not, under any circumstance, be taken to mean that no hazard exists.

End of safety data sheet