

# Safety Data Sheet

## SAFETY DATA SHEET - LC LABORATORIES REVISION DATE: JULY 1, 2019

### SECTION 1. IDENTIFICATION:

Trade name: CHIR99021, Free Base  
Product Number: [C-6556](#)  
Manufacturer/Supplier:  
LC Laboratories  
165 New Boston Street  
Woburn, MA 01801 USA  
1-781-937-0777 Fax: 1-781-938-5420

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### SECTION 2. HAZARD(S) IDENTIFICATION:

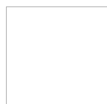
Hazard Description: pharmaceutically active substance that has not been fully tested  
Harmful if swallowed  
May be harmful if inhaled or absorbed through the skin  
Irritating to the skin and eyes  
May impair fertility or harm the unborn child  
Exposure may cause irritation of the respiratory tract and allergic respiratory and skin reaction  
Signal Word: Danger

#### GHS Hazard Statements:

H302+312+332 - Harmful if swallowed, in contact with skin or if inhaled

#### GHS Precautionary Statements:

P2562 - Do not get in eyes, on skin or on clothing  
WARNING: For Laboratory Research Use Only



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### SECTION 3. COMPOSITION/INFORMATION ON INGREDIENTS:

Chemical Name: 6-[[2-[[4-(2,4-Dichlorophenyl)-5-(5-methyl-1*H*-imidazol-2-yl)-2-pyrimidinyl]amino]ethyl]amino]-3-pyridinecarbonitrile  
Synonyms: CHIR 911, CT99021, GSK-3 Inhibitor XVI  
Hazardous Ingredient: CHIR99021, Free Base  
CAS Registry Number: 252917-06-9  
Molecular Weight: 465.34  
Molecular Formula: C<sub>22</sub>H<sub>18</sub>Cl<sub>2</sub>N<sub>8</sub>

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### SECTION 4. FIRST-AID MEASURES:

After Inhalation: If inhaled, remove to fresh air; if breathing is difficult, give oxygen; if breathing stops, give artificial respiration

After skin contact: flush with copious amounts of water; remove contaminated clothing and shoes; call a physician

After eye contact: check for and remove contact lenses; flush with copious amounts of water; assure adequate flushing by separating the eyelids with fingers; call a physician

After swallowing: if swallowed, wash out mouth with copious amounts of water; call a physician

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### **SECTION 5. FIRE-FIGHTING MEASURES:**

Suitable extinguishing agents: water spray, carbon dioxide, dry chemical powder or foam

Protective equipment: wear self-contained breathing apparatus and protective clothing to prevent contact with skin and eyes

Unusual fire hazard: may emit toxic fumes under fire conditions such as carbon monoxide, etc.

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### **SECTION 6. ACCIDENTAL RELEASE MEASURES:**

Person-related safety precautions: cordon off area of spill; wear self-contained breathing apparatus, protective clothing and heavy rubber gloves

Measures for cleaning/collecting: absorb solutions with finely- powdered liquid-binding material (diatomite, universal binders); decontaminate surfaces and equipment by scrubbing with alcohol; dispose of contaminated material according to Section 13

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### **SECTION 7. HANDLING AND STORAGE:**

Information for safe handling: avoid contact with skin, eyes and clothing; material may be an irritant

Storage: store solid and solutions at -20 °C

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### **SECTION 8. EXPOSURE CONTROLS/PERSONAL PROTECTION:**

Personal protective equipment as follows:

Breathing equipment: NIOSH/MSHA-approved respirator

Protection of hands: handle with Nitrile rubber gloves with minimum thickness of 0.11 mm (4.3 mil). This recommendation should not be interpreted as offering an approval for any specific use conditions. Please review this recommendation with a safety officer to evaluate if it is appropriate for the anticipated use.

Eye protection: chemical safety goggles

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### **SECTION 9. PHYSICAL AND CHEMICAL PROPERTIES:**

Form: crystalline solid; granular or powder

Color: off-white

Odor: none

Melting point/Melting range: 125-148 °C

Danger of explosion: none

Solubility in / Miscibility with water: very poorly soluble in water; maximum solubility in plain water is estimated to be about 20-40 µM; buffers, serum, or other additives may increase or decrease the aqueous solubility

Solvent content:

Organic solvents: soluble in DMSO at 25 mg/mL with warming; very poorly soluble in ethanol

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#### **SECTION 10. STABILITY AND REACTIVITY:**

Stability: avoid acids and bases

Thermal decomposition / conditions to be avoided: protect from light and heat

Dangerous products of decomposition: thermal decomposition may produce toxic gases such as carbon monoxide and carbon dioxide, and nitrogen oxides

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#### **SECTION 11. TOXICOLOGICAL INFORMATION:**

RTECS #: not available

Acute toxicity: not known; substance not fully tested

Primary irritant effect:

On the skin: causes skin irritation; may be harmful if absorbed through the skin

On the eye: causes serious eye irritation

Inhalation: may cause irritation of mucous membranes and upper respiratory tract; may be harmful if inhaled

Ingestion: harmful if swallowed

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#### **SECTION 12. ECOLOGICAL INFORMATION:**

General notes: no data available

Treat as potentially toxic if released into the environment

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#### **SECTION 13. DISPOSAL CONSIDERATIONS:**

Dispose of in accordance with prevailing country, federal, state and local regulations

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#### **SECTION 14. TRANSPORT INFORMATION:**

DOT:

Proper shipping name: none

Non-Hazardous for transport: this substance is considered to be non-hazardous for transport

IATA class:

Proper shipping name: none

Non-Hazardous for transport: this substance is considered to be non-hazardous for transport

**SECTION 15. REGULATORY INFORMATION:**

Code letter and hazard designation of product:

Hazard-determining components of labeling:

EU Risk And Safety phrases:

S22: Do not breathe dust

S24/25: Avoid contact with skin and eyes

S26: In case of contact with eyes, rinse immediately with plenty of water and seek medical advice

S28: After contact with skin, wash immediately with plenty of soap-suds

S36/37/39: Wear protective clothing, gloves and eye/face protection

R22: Harmful if swallowed

R38: Irritating to skin

R41: Risk of serious damage to eyes

R62: Possible risk of impaired fertility

R63: Possible risk of harm to the unborn child

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**SECTION 16. OTHER INFORMATION:**

The above information is believed to be correct based on our present knowledge but does not purport to be complete. For research use only by trained personnel. The burden of safe use of this material rests entirely with the user. LC Laboratories disclaims all liability

Reviewed: July 1, 2019