Safety Data Sheet

Simpinicline

Catalog No. **BP-06859** · CAS **753015-44-0** · Physical form **Oil** · Version **1.1** · Revision **2026-11-16**

FOR RESEARCH USE ONLY. NOT FOR HUMAN OR VETERINARY USE.

SECTION 1 — IDENTIFICATION

Product name	**Simpinicline**
Catalog number	**BP-06859**
CAS number	**753015-44-0**
Recommended use	**Laboratory research chemical**
Restrictions on use	**Not for drug, household, or other uses**
Supplier	**Guangzhou Yuyuan Biotech Co., Ltd. (BiochemProbe)**
Address	**Baiyun District, Guangzhou, Guangdong, China**
Telephone / Fax	**+86 20 31130026 / +86 20 36822386**
Email / Web	**tech@biochemprobe.com · www.biochemprobe.com**
Emergency phone	**+86 20 31130026 (business hours) · local poison control as applicable**

SECTION 2 — HAZARD(S) IDENTIFICATION

GHS classification

- Not classified based on available data, or data are insufficient for classification.

Signal word: None

Hazard statements: No hazard statements assigned based on available data.

Precautionary statements: P261 Avoid breathing dust/fume/gas/mist/vapours/spray. P280 Wear protective gloves/eye protection. P501 Dispose of contents/container in accordance with local regulations. Handle as a research chemical; avoid dust/mist inhalation and skin/eye contact.

Additional notes: This SDS does not imply the substance is non-hazardous. Update when classification data become available.

SECTION 3 — COMPOSITION / INFORMATION ON INGREDIENTS

Chemical name	**Simpinicline**
Synonyms	**OC-02**
Molecular formula	**$C_{10}H_{13}N_3$**
Molecular weight	**175.2303**
CAS number	**753015-44-0**

SECTION 4 — FIRST-AID MEASURES

Inhalation: Move to fresh air. If breathing is difficult, give oxygen. Seek medical attention if symptoms persist.

Skin contact: Wash with plenty of soap and water. Remove contaminated clothing. Seek medical advice if irritation develops.

Eye contact: Rinse cautiously with water for several minutes. Remove contact lenses if present and easy to do. Continue rinsing.

Ingestion: Rinse mouth. Do NOT induce vomiting. Call a poison center or physician if you feel unwell.

Most important symptoms / medical attention: Treat symptomatically. Provide this SDS to medical personnel.

SECTION 5 — FIRE-FIGHTING MEASURES

Suitable extinguishing media	**Water spray, dry chemical, carbon dioxide, or alcohol-resistant foam**
Unsuitable media	**No data available**
Specific hazards	**May emit toxic fumes under fire conditions**
Protective equipment	**Self-contained breathing apparatus and full protective gear**

SECTION 6 — ACCIDENTAL RELEASE MEASURES

Personal precautions: Wear suitable PPE (Section 8). Ensure adequate ventilation.

Environmental precautions: Prevent entry into drains and surface water.

Cleanup: Absorb with inert material. Place in a suitable closed container for disposal.

SECTION 7 — HANDLING AND STORAGE

Handling: Handle in a well-ventilated area or fume hood. Avoid contact with skin and eyes. Do not eat, drink, or smoke when using this product.

Storage: Powder -20℃, 3 years; 4℃, 2 years; In solvent -20℃, 1 month;

Incompatibilities: Strong oxidizing agents (general guidance). Keep away from food and feed.

SECTION 8 — EXPOSURE CONTROLS / PERSONAL PROTECTION

Occupational exposure limits	**No specific OELs established for this substance**
Engineering controls	**Local exhaust / laboratory fume hood**
Eye / face protection	**Safety glasses with side shields or chemical goggles**
Skin protection	**Chemical-resistant gloves (e.g. nitrile); lab coat**
Respiratory protection	**If vapors/mists are generated, use approved respirator**

SECTION 9 — PHYSICAL AND CHEMICAL PROPERTIES

Appearance	**Yellow to brown oil**
Physical state	**Oil**
Color	**Yellow to brown**
Odor	**No data available**
Melting / freezing point	**No data available**
Boiling point	**No data available**
Flash point	**No data available**
Solubility	**soluble in DMSO**
Viscosity	**No data available**

SECTION 10 — STABILITY AND REACTIVITY

Chemical stability	**Stable under recommended storage conditions**
Conditions to avoid	**Excessive heat, ignition sources (if flammable)**
Incompatible materials	**Strong oxidizers**
Hazardous decomposition products	**Carbon / nitrogen / sulfur / halogen oxides may form under fire conditions**

SECTION 11 — TOXICOLOGICAL INFORMATION

Likely routes of exposure: Skin and eye contact, inhalation of vapors/mists, ingestion.

Acute toxicity	**See Section 2. Substance-specific LD50/LC50 data not available.**
Skin corrosion / irritation	**See Section 2.**
Serious eye damage / irritation	**See Section 2.**
Respiratory or skin sensitization	**No data available.**
Germ cell mutagenicity	**No data available.**
Carcinogenicity	**No data available. No component present at ≥0.1% is identified as a probable, possible, or confirmed human carcinogen by IARC, NTP, or OSHA based on available data.**
Reproductive toxicity	**No data available.**
STOT — single exposure	**See Section 2.**
STOT — repeated exposure	**No data available.**
Aspiration hazard	**No data available.**

Additional information: To the best of our knowledge, the chemical, physical, and toxicological properties have not been thoroughly investigated. Treat as a research chemical.

SECTION 12 — ECOLOGICAL INFORMATION

No specific ecotoxicity data available. Do not release to the environment. Avoid discharge to sewer and waterways.

SECTION 13 — DISPOSAL CONSIDERATIONS

Dispose of contents/container in accordance with local, regional, and national regulations. Offer surplus and non-recyclable material to a licensed disposal company.

SECTION 14 — TRANSPORT INFORMATION

DOT (US)	**Not dangerous goods**
IMDG	**Not dangerous goods**
IATA	**Not dangerous goods**
Special precautions	**Transport in sealed containers; protect from moisture / leakage**

SECTION 15 — REGULATORY INFORMATION

Intended for research use only. The user must determine applicability of local chemical inventory listings and workplace regulations before use.

SECTION 16 — OTHER INFORMATION

SDS version	**1.1**
Revision date	**2026-11-16**

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