Invention: Chemical molecule and synthesis route

Applicant: QuantiVEX

Inventors: Nithin D H

Chemical Formula: C15H28NNaO3

Chemical Name: Sodium Lauroyl Sarcosinate

Chemical synthesis routes:

The production of **Sodium Lauroyl Sarcosinate ($C_{15}H_{28}NNaO_3$)** is a well-established process that involves the reaction of **Lauric Acid ($C_{12}H_{24}O_2$)** with **Sarcosine ($C_3H_7NO_2$)**, followed by neutralization with **Sodium Hydroxide (NaOH)**. This surfactant is widely used in personal care products such as shampoos and facial cleansers due to its mild cleansing properties, foaming ability, and biodegradability. The most efficient and environmentally friendly method for its production is the **direct amidation process**, which eliminates the need for hazardous chemicals while ensuring high yield and purity.

Chemical Information

- **Chemical Name:** Sodium N-Lauroyl Sarcosinate
- **Molecular Formula:** C15H28NNaO3
- **Molecular Weight:** ~293.38 g/mol
- **Structural Formula:** CH3-(CH2)10-C(=O)-N(CH3)-CH2-COO^- Na^+
- **Physical Properties:**
- Appearance: White to off-white powder or liquid (depending on formulation)
- Solubility: Soluble in water, forms a clear solution
- pH (5% Solution): 7.0 - 8.5
- Biodegradability: Readily biodegradable

Primary Mode of Synthesis: Direct Amidation Process Route

Raw Materials and Chemicals Required

a. **Lauric Acid (C12H24O2) –** Main fatty acid precursor
b. **Sodium Hydroxide (NaOH) –** Used to neutralize the acid
c. **Sarcosine (C3H7NO2) –** An amino acid derivative
d. **Solvent (Water/Alcohol mixture) –** For reaction medium
e. **Catalyst (Enzymatic/Base Catalyst) –** For improving efficiency

Utilities and Equipment Required:

1. **Reactor System** – Stainless steel, high-pressure batch/semi-batch reactor with agitation for amidation reaction.

2. **Steam Generation** – Provides heat for reactor and distillation units.

3. **Feedstock Preheating & Mixing** – Ensures homogeneous mixing of Lauric Acid and Sarcosine before reaction.

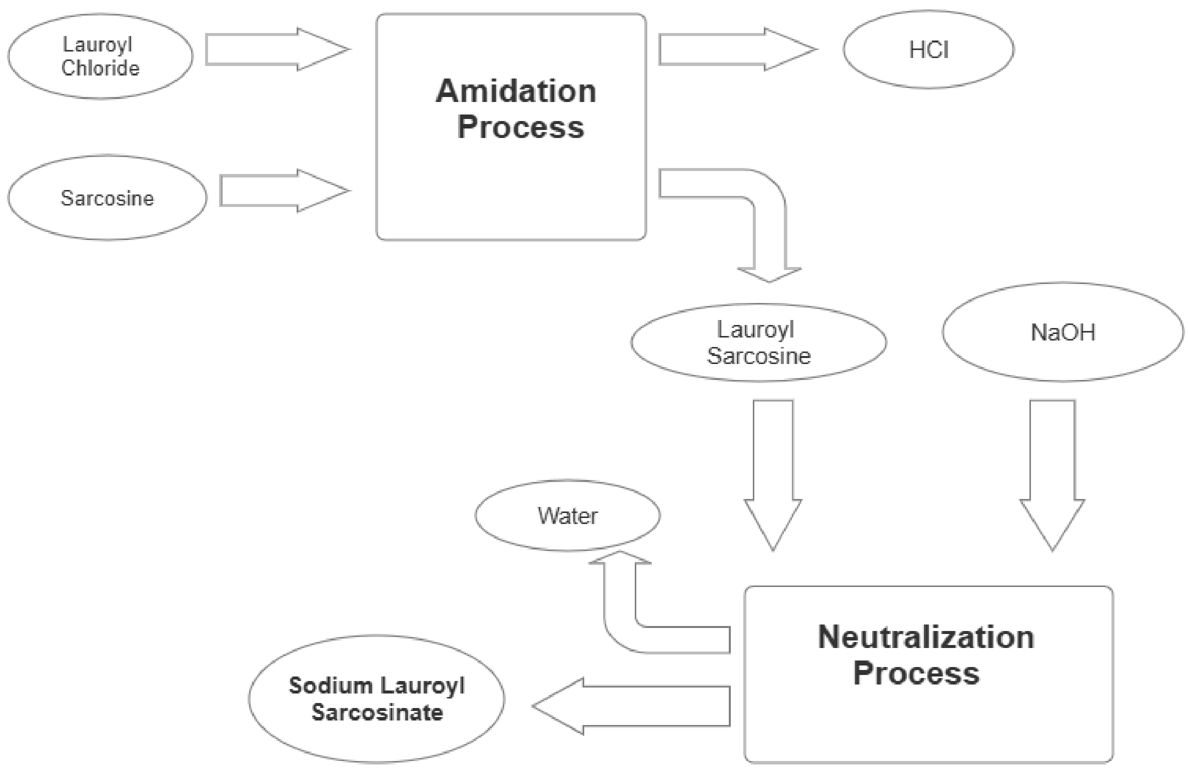
4. **Cooling System** – Chillers and heat exchangers to control reaction and neutralization temperatures.

5. **Stripping & Purification –** Removes unreacted reactants and impurities for high-purity products.

6. **Neutralization & Storage** – NaOH addition, filtration, drying, and final product storage.

7. **Automation & Safety** – DCS/PLC control, gas scrubbers, wastewater treatment, and fire suppression

Stepwise Production Process of Sodium Lauroyl Sarcosinate(Direct Amidation Process)

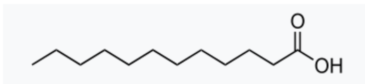


Chemical Reaction and Process Mechanism

The production of Sodium Lauroyl Sarcosinate occurs in two key steps:

Step 1: Amidation of Lauric Acid with Sarcosine

The reaction is carried out in an **aqueous or alcohol-based medium** at a temperature of **80-120°C** under **alkaline conditions (pH 8-9)**. The reaction proceeds as follows:



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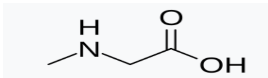

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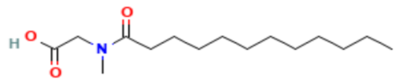


+H2O

C12H24O2 + C3H7NO2 → C15H29NO3 + H2O

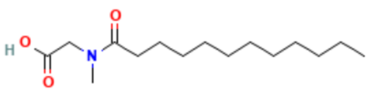
(Lauric Acid) + (Sarcosine) → (Lauroyl Sarcosine) + (Water)

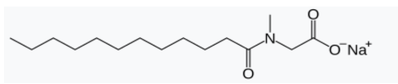
Lauric Acid and Sarcosine are mixed in a **1:1.05 molar ratio** to ensure complete reaction.

- A **base catalyst (NaOH/KOH)** or an **enzymatic catalyst** (lipase) is added to improve the reaction rate and selectivity.
- The reaction mixture is **heated at 80-120°C** for several hours to allow the formation of **lauroyl sarcosine (amide intermediate)**.
- Water formed as a by-product is **removed by controlled evaporation** to drive the reaction toward completion.

Step 2: Neutralization with Sodium Hydroxide

To convert **lauroyl sarcosine** into its sodium salt form (**Sodium Lauroyl Sarcosinate**), a **neutralization step** is performed:



+ NaOH =>


+ H2O

C15H29NO3 + NaOH → C15H28NNaO3 + H2O

(Lauroyl Sarcosine) + (Sodium Hydroxide) → (Sodium Lauroyl Sarcosinate) + (Water)

- A **stoichiometric amount of NaOH** is added to the reaction mixture under gentle stirring at room temperature.
- The **pH is adjusted to ~8.5-9** to ensure complete conversion into the sodium salt.
- Excess water is removed through **vacuum evaporation** to concentrate the product.

Separation and Purification process

To achieve **high purity (>99%)** and remove impurities such as unreacted fatty acids and by-products, the following **separation and purification steps** are undertaken:

f. **Filtration**: Insoluble by-products and impurities (unreacted fatty acids) are removed by filtration.
g. **Liquid-Liquid Extraction**: A non-polar solvent such as hexane is used to separate unwanted organic residues.
h. **Crystallization**: The solution is cooled to precipitate pure Sodium Lauroyl Sarcosinate.
i. **Spray Drying**: The final product is dried using a spray dryer to obtain a **fine powder or granules**, suitable for commercial applications.

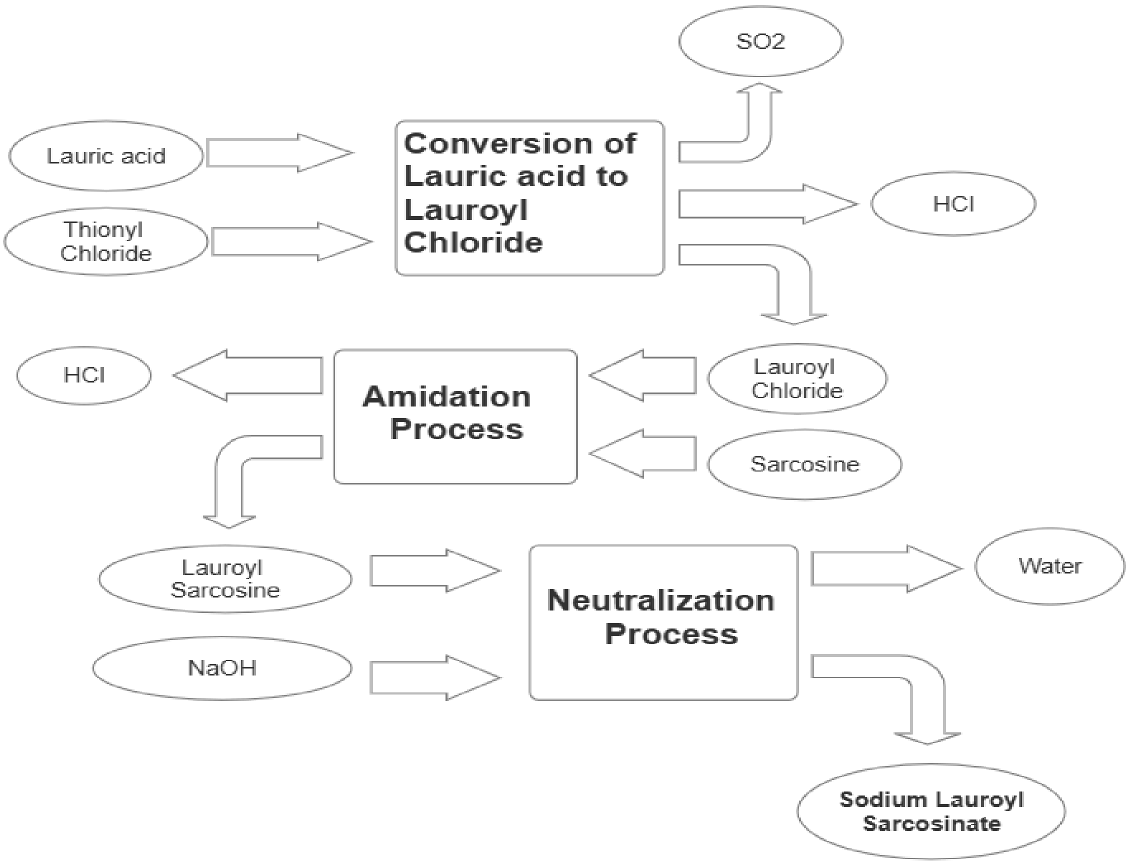
Alternate Synthesis Route : Acid Chloride Route

Raw materials and Chemicals required

The key raw materials involved in this process include:

- **Lauric Acid ($C_{12}H_{24}O_2$)** – A fatty acid derived from coconut oil or palm kernel oil.
- **Thionyl Chloride ($SOCl_2$)** – A **reactive chlorinating agent** used to convert Lauric Acid into Lauroyl Chloride.
- **Sarcosine ($C_3H_7NO_2$)** – An amino acid derivative that reacts with Lauroyl Chloride to form Lauroyl Sarcosine.
- **Sodium Hydroxide (NaOH)** – Used to neutralize the product and convert it into **Sodium Lauroyl Sarcosinate**.
- **Solvent (Dichloromethane/Toluene)** – Provides a medium for the reaction and helps in separation.

Production Process of Sodium Lauroyl Sarcosinate(Acid Chloride Process)



Chemical Reaction and Process Mechanism

The **Acid Chloride Route** consists of **three main reaction steps**:

Step 1: Conversion of Lauric Acid to Lauroyl Chloride

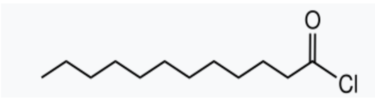
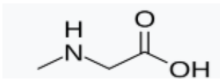
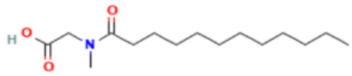
Lauric Acid is reacted with **Thionyl Chloride ($SOCl_2$)** to produce **Lauroyl Chloride ($C_{12}H_{23}ClO$)** and gaseous byproducts **HCl and SO_2**.

C12H24O2 + SOCl2 → C12H23ClO + SO2 + HCl

- This reaction is carried out in a **dry solvent (Dichloromethane/Toluene)** at **room temperature (~25-30°C)** under **anhydrous conditions**.
- As the reaction proceeds, **HCl and SO_2 gases are released**, requiring a **scrubber system** to safely remove toxic fumes.

Step 2: Amidation with Sarcosine

The **Lauroyl Chloride** reacts with **Sarcosine** to form **Lauroyl Sarcosine** and **HCl**.

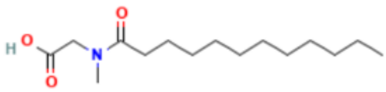
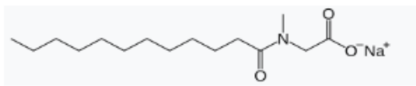
 +  =>  +HCl

$C_{12}H_{23}ClO + C_3H_7NO_2 \rightarrow C_{15}H_{29}NO_3 + HCl$

- The reaction occurs in a **basic aqueous medium (pH ~8-9)** to **neutralize the HCl formed**.
- A slight excess of **Sarcosine** is used to **drive the reaction to completion** and avoid excess acid chloride.

Step 3: Neutralization to Form Sodium Lauroyl Sarcosinate

The **Lauroyl Sarcosine** is then neutralized with **Sodium Hydroxide (NaOH)** to form **Sodium Lauroyl Sarcosinate**.

 + NaOH =>  + H2O

$C_{15}H_{29}NO_3 + NaOH \rightarrow C_{15}H_{28}NNaO_3 + H_2O$

- This step is **critical for surfactant properties**, as the **sodium salt form** is **more water-soluble**.
- The reaction is carried out under **stirring at room temperature**, with **pH adjustment (~8.5-9)** to avoid unwanted hydrolysis.

After the main reaction steps, the product must be purified to **remove unreacted reagents, organic solvents, and impurities**. The **separation process includes the following steps**:

1. **Solvent Removal**:
   Vacuum distillation is used to remove residual organic solvents such as **Dichloromethane or Toluene**.

2. **Filtration**:
   The mixture is filtered to **remove any insoluble byproducts**.
3. **Liquid-Liquid Extraction**:
   The product is extracted using a **polar solvent (water/ethanol mixture)** to **separate organic residues**.
4. **Crystallization**:
   The extracted solution is cooled to **precipitate pure Sodium Lauroyl Sarcosinate**.
5. **Spray Drying**:
   The purified product is spray-dried to obtain a **fine powder** suitable for commercial applications.

Two synthesis routes for producing Sodium Lauroyl Sarcosinate are identified: **The Direct Amidation Process**, which is eco-friendly, highly efficient with a **yield of 95%** and **purity exceeding 99%**, and cost-effective, albeit requiring careful pH control; and **The Acid Chloride Route**, which involves converting Lauric Acid to Lauroyl Chloride using toxic Thionyl Chloride, resulting in **lower yields(~85%)**and **complex purification**. Ultimately, the Direct Amidation Process is favored due to its superior yield, cost-effectiveness, and environmental safety.

References:

1. https://patents.google.com/patent/CN111333531A/en

2. https://pubchem.ncbi.nlm.nih.gov/compound/Sodium-lauroyl-sarcosinate

3. https://en.wikipedia.org/wiki/Sodium_lauroyl_sarcosinate

List the contributions of each author:

1. Nithin D H worked on selection of the chemical and selection of the manufacturing process and studying the process in detail, doing its feasibility analysis and other factors.

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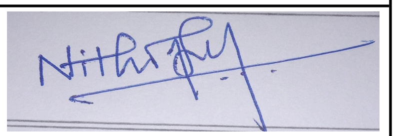
Nithin T M(CEO)	230709	
Nithin D H	230708