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Sodium Tetradecyl Sulfate Molecule: Patent Analysis Based on Chemical Compounds Search †

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Abstract: Sodium tetradecyl sulfate is the most common and widely utilized type of synthetic surfactant used in medicine. It is an organic compound prepared by the aldol condensation followed by sulfonation of the alcohol. This work of patent analysis summarizes the current state of the art by describing what has been invented and patented concerning sodium tetradecyl sulfate. Furthermore, a detailed analysis of patents has been provided using the Patentscope database's "Chemical Compounds Search" feature in terms of publication years, jurisdictions, inventors, applicants, and patent classifications.

Keywords: sodium tetradecyl sulfate; anionic surfactant; chemical compounds search; patent data; innovation.

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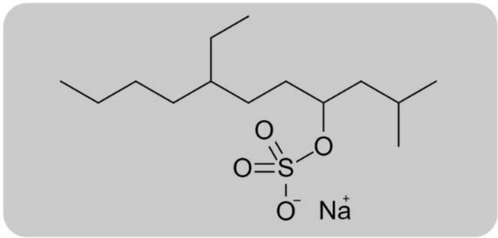
1. Introduction

Sodium tetradecyl sulfate (STS) is an anionic surfactant developed in the 1940s [1]. Due mainly to their relatively low cost of manufacture, anionic surfactants are the most widely used class of surfactants in industrial applications [2]. STS is one of the sulfate surfactants; they are usually molecules that have a lipophilic head (sulfate group) attached at the end of a hydrophobic chain (linear alkyl group). These are generally produced by the reaction of an alcohol with chlorosulfonic acid or sulfur dioxide/air mixtures to sulfate the alcohol. The properties of the sulfate surfactants depend on the nature of the alkyl chain and the sulfate group. A general formula may be ascribed as: $C_nH_{2n+1}\ SO_3^-\ X^+$, where n represents the chain length and it is in the range of 8-16 atoms, and the counterion X^+ is usually Na^+ [3].

Sometimes also referred to as [4-undecanol,7-ethyl-2-methyl-, 4-(hydrogen sulfate), sodium salt], STS is a synthetic organic compound with the formula $C_{14}H_{29}NaO_4S$ (Figure 1). It is made by combining methyl isobutyl ketone and 2-ethylhexanal in an aldol reaction at 90-110°C, then sulfonating the resultant alcohol [3-6].

STS is extensively used not only for fundamental studies but also for many applications in industry, including detergency and cosmetics [7], as well as pharmaceutics and medicine [8-12]. It is used throughout the world as a remarkable active ingredient (or additive) for foaming [13,14] and wetting agents [15], stabilizers for dispersion [16], emulsifying agents for emulsions [17], antiseptics [18], and detergents [19]. Furthermore, it is characterized by good detergent power and abundant foam. However, it is irritating to the skin. However, to overcome this last suitable property for detergency and cosmetics, the STS is commonly used in hand-dishwashing liquids, in soaps, and in shampoos, in combination with other amphoteric (i.e., zwitterionic) surfactants [3].



Element	Composition (%)
C	53.14
H	9.24
Na	7.27
S	10.13
O	20.22

Figure 1. Chemical structure and elementary analysis of sodium tetradecyl sulfate ($C_{14}H_{29}NaO_4S$).

Although the STS was developed in the 1940s and has been utilized for several years, the first patent application for this anionic surfactant was filed in 1974, and granted in 1976 [20]. In this patent, Thiele has invented the first liquefied composition containing a non-necrotic vascular sclerosing fatty acid compound to treat demineralization resulting from screws, pins, and other metal inserts that have been inserted into fractured bones. Comprising STS, benzyl alcohol, disodium phosphate, and sodium dihydrogen or sodium hydroxide, the liquefied composition has shown that the demineralized region is caused to “heal” in that healthy bone results upon the injecting. This proof of concept has confirmed that fractures, breaks, and nonunions of bones are more easily healed without muscle atrophy by injecting the liquefied composition containing STS [20]. Since this first patent, several patent applications concerning STS-based formulations, preparation methods, and applications are filed each year. Furthermore, there are several organizations that are now engaged in research and development of this anionic surfactant around the world [21].

According to the World Intellectual Property Organization (WIPO), a patent application for an invention must be filed in each country where the inventor wishes to get patent protection. Furthermore, an applicant may consider filing an international application under the Patent Cooperation Treaty (PCT) if patent protection is needed in a number of countries throughout the world [22].

This study concerns only the international patent applications on the STS molecule through the PCT global system. More specifically, this overview presents the patentability study of the STS molecule by presenting what has been invented and patented. Specifically, the “Chemical Compounds Search” feature of the Patentscope database is used to provide a detailed analysis of publication years, jurisdictions, inventors, applicants, and patent classifications.

2. Materials and Methods

The study of the STS molecule patents presented hereinafter was conducted on the Patentscope's "Chemical Compounds Search", which is a provided service by the WIPO [21,23]. The chemical structure search, according to the WIPO, identifies chemical compound names in patent texts as well as structures, which may be embedded illustrations. In a nutshell, this utility converts all of the numerous chemical structure representations to the InChI textual identification (i.e., International Chemical Identifier). This is a textual identification created to make web searches for chemical structures easier. Furthermore, InChIKey is a second parameter for the chemical structure that might be employed. It is a reduced digital representation of an InChI with a defined length (27 characters). It gives a chemical compound a precise, reliable, and authorized structure-derived tag [23]. The STS molecule's information used in this study is shown in Table 1.

Table 1. The queries used in this study: InChI, InChiKey, molecular formula, and molecular weight.

Molecule	Sodium tetradecyl sulfate
InChI	1S/C14H30O4S.Na/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-18-19(15,16)17;/h2-14H2,1H3,(H,15,16,17);/q;+1/p-1
InChiKey	UPUIQOIQVMNQAP-UHFFFAOYSA-M
Molecular formula	$C_{14}H_{29}NaO_4S$
Molecular weight	316.4367 g.mol^{-1}

3. Results and Discussion

Through the chemical structure search, 5821 patents concerning STS molecules were found. The publication year is the year in which a patent document is published [24-26]. For the STS molecule, 2331 patents have been published between 2012 and 2021. The year 2012 saw the publication of 224 patents. However, the year 2018 was the year with the maximum number of 324 patents (Figure 2).

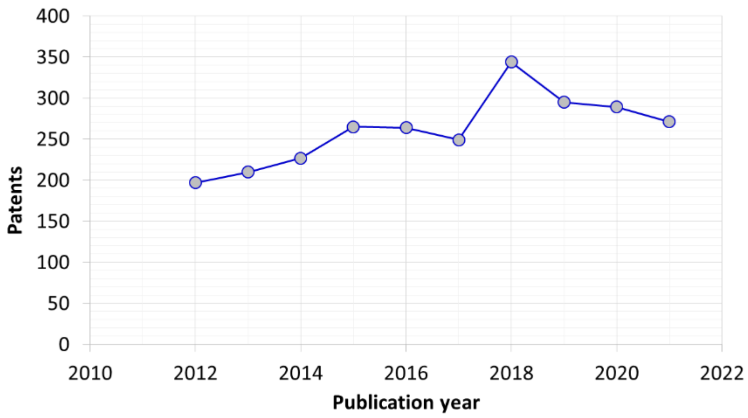


Figure 2. Evolution of the resultant patents for the STS molecule as a function of the published date between 2012 and 2021.

A jurisdiction is a territory or region in which the applicant normally resides, has a place of business, has his domicile, or from where the invention originated [24-26]. For the STS molecule, the jurisdictions (top 10) for patent filings are shown in Figure 3. The Japan Patent Office (JPO) has recorded 2040 patents, with a patent contribution of around 30% of the total. However, the United States Patent and Trademark Office (USPTO) has recorded 1755 patents, with a patent contribution of around 26% of the total. Finally, the China National Intellectual Property Administration (CNIPA) has recorded 1033 patents, with a patent contribution of around 15% of the total. The global system for filing patent applications (i.e., PCT), which is administered by WIPO, has recorded 747 patents with a patent contribution of around 11% of the total, and the EPO (i.e., European Patent Office), through which patents are filed in Europe, has recorded 384 patents with a patent contribution of around 6% of the total.

An inventor is a person who has been assigned to a patent application [24-26]. For the STS molecule, the top 10 inventors are presented in Figure 4.

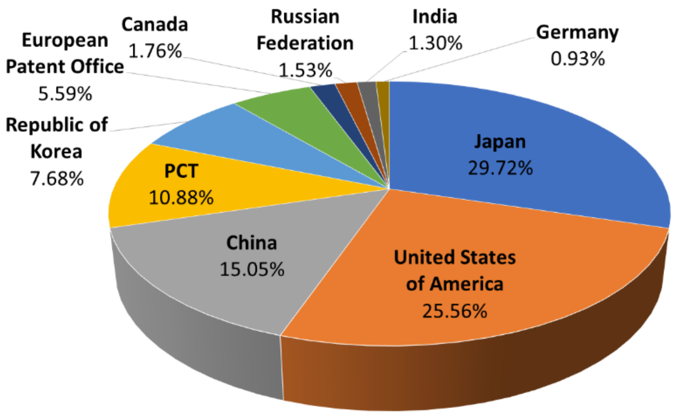


Figure 3. Patent contribution (%) as a function of the top 10 jurisdictions of filed patents for the STS molecule under the PCT global system (between 2012 and 2021).

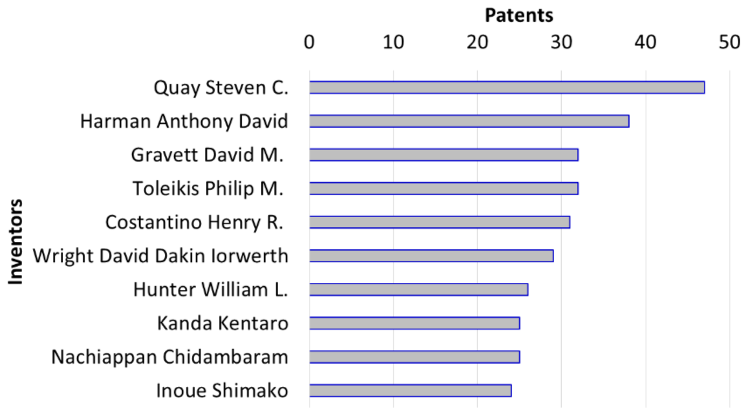


Figure 4. Inventors (top 10) of the resultant patents for the STS molecule between 2012 and 2021.

A natural person or a legal entity that has filed a patent application is referred to as an applicant [24-26]. For the STS molecule, the top 10 applicants are presented in Figure 5.

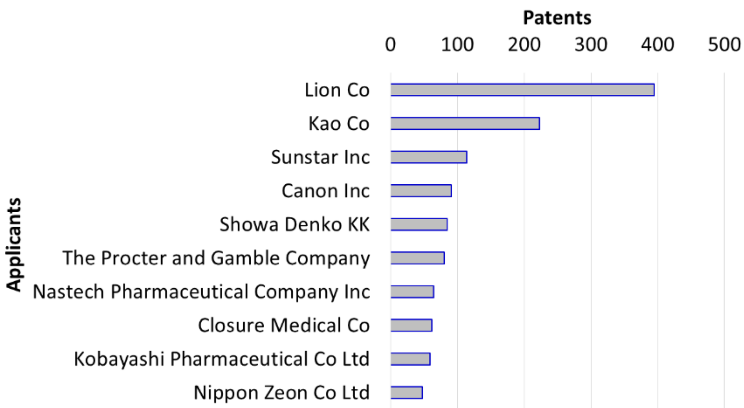


Figure 5. Applicants (top 10) of the resultant patents of the STS molecule between 2012 and 2021.

The International Patent Classification (IPC) is a code-based hierarchical system that classifies all technological domains. It provides standardized data for categorizing inventions and assessing their technological distinctiveness [27].

The top 10 IPC codes for the STS molecule are listed in Table 2. Only patent applications filed under the PCT worldwide system are covered by these IPC codes. The most common IPC code for STS molecule patents corresponds to A61K, which is a subclass meaning the preparations for medical, dental, or toilet purposes. This subclass has recorded 3397 patents alone. Secondly, the subclass A61Q, which defines the specific use of cosmetics or similar toilet preparations, has recorded 1301 patents. Thirdly, the subclass A61P, which means the specific therapeutic activity of chemical compounds or medicinal preparations, has recorded 720 patents. For more details concerning these top 10, a description of each IPC code is shown in Table 2.

Table 2. Patent classifications concerning the resultant patents for STS molecules between 2012 and 2021 [27].

IPC	Description	Patents
A61K	Preparations for medical, dental, or toilet purposes.	3397
A61Q	Specific use of cosmetics or similar toilet preparations.	1301
A61P	Specific therapeutic activities of chemical compounds or medicinal preparations.	720
C11D	Detergent compositions; use of single substances as detergents; soap or soap-making; resin soaps; recovery of glycerol.	548
C08F	Macromolecular compounds obtained by reactions only involving carbon-to-carbon unsaturated bonds.	390
C08L	Compositions of macromolecular compounds.	327
A61L	Methods or apparatus for sterilizing materials or objects in general; disinfection, sterilization, or deodorization of air; chemical aspects of bandages, dressings, absorbent pads, or surgical articles; materials for bandages, dressings, absorbent pads, or surgical articles.	310
G03G	Electrography; electrophotography; magnetography.	292
A01N	Preservation of bodies of humans, animals, plants, or parts thereof.	266
G01N	Investigating or analyzing materials by determining their chemical or physical properties.	244

4. Conclusions

This study provides a comprehensive overview of the patent situation for the STS molecule. It was established according to standards of patent analysis. In patent literature, the chemical structure search detected the STS molecule's name as well as its structures from the embedded illustrations. Thanks to the two used queries (i.e., InChI and InChiKey), 2331 patents concerning STS molecules were found and published between 2012 and 2021. Japan leads the patent race in the STS molecule sector. Chemical synthesis, preparation procedures, formulations, and fabrication processes, as well as applications, were all areas where STS innovated and improved. Based on the patent classifications, all filed patents concerned preparations for medical, dental, or toilet purposes, and chemical substances or pharmaceutical preparations with unique therapeutic properties. Moreover, according to this study, the patents' inventions concern specific uses of cosmetics or similar toilet preparations and detergent formulations, as well as techniques or apparatus for sterilizing materials.

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Data Availability Statement: The data presented in this study are available within this article content.

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Conflicts of Interest: The author declares that the content of this article has no conflict of interest. The author is a co-inventor on a patent family pertaining to chitosan–sodium tetradecyl sulfate hydrogel (Granted Patents: CA2704971C, US9731043B2, and US8840867B2; Patent Applications: US20140377187A1, US20110286925A1, and CA2704971A1).

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