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"Transformative Role of Artificial Intelligence (AI) and Machine Learning (ML) in the field of Surfactant Science: A Short Review"

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Abstract:*In This paper I attempt to highlight the budding and transformative role of Artificial Intelligence (AI) and Machine Learning (ML) in the field of Surfactant Science and its associated domains. Surfactant Science, an integral aspect of the Fast-Moving Consumer Goods (FMCG) sector, has evolved into a mature and knowledge-rich discipline. In the contemporary era of rapid Information Technology advancement, there exists a compelling need to re-envision the utilization of revolutionary IT tools and interfaces to expedite the assessment of Physico-chemical properties of Surfactants and their derivatives. By embracing the capabilities of AI, researchers are empowered to innovate novel surfactant molecules through the fusion of Machine Learning and computational modeling. This infusion of AI catalyzes a paradigm shift in surfactant production and applications, amplifying efficiency, efficacy, and sustainability benchmarks. The forefront of this transformation lies in the ability to prognosticate surfactant attributes and behaviors, thereby curtailing the temporal and financial expenses associated with traditional synthesis methods. The spotlight is cast on AI/ML-driven investigations into phase behaviors, wherein these technologies significantly contribute. By cultivating predictive models, AI underpins the assessment of surfactant performance within specific applications like emulsions, foams, and coatings. This augments the profound comprehension of the intricate interplay between surfactant properties and application proficiency, subsequently culminating in the formulation of solutions that seamlessly integrate effectiveness with ecological conscientiousness.*

Keywords: Surfactants, Artificial Intelligence, AI, ML, CMC, Phase, Synthesis, Surface Tension.

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1. **Introduction:** Surfactant Science occupies a pivotal role in the realm of Fast-Moving Consumer Goods (FMCG) companies, being a mature and knowledge-intensive discipline [1]. Surfactants are widely applied in industry as detergents, foaming agents or dispersants, amongst others. They play a critical role in the personal and home care segment. Market studies presented a growth of the global production to over 19 million tons by 2023. By 2028 production is predicted as 21.53 mn ton, corresponding to an annual revenue of around 45.5 billion US-dollars [2]. Companies face not only business competition, but also increasingly more stringent regulations regarding environmental compatibility, toxicity, and sustainability. For product design and development, machine learning-based techniques can be exploited for virtual screening and prediction of key properties, like the critical micelle concentration. In this way, raw material costs and development time can be reduced by focusing experimental testing on the most promising candidates. As the landscape of Information Technology advances at an unprecedented pace, it becomes imperative to revisit the methodologies employed for the evaluation of Physico-chemical properties of Surfactants and their derivatives [3]. This paper delves into the synergy between Artificial Intelligence (AI), Machine Learning (ML), and Surfactant Science, accentuating their collaborative potential. By harnessing AI, researchers can embark on the creation of novel surfactant molecules through a symbiotic blend of Machine Learning techniques and computational modeling [4]. The result is a paradigmatic shift in how surfactants are produced and applied, ushering in heightened levels of efficiency, efficacy, and sustainability. The core of this transformation lies in AI's ability to predict surfactant traits and behaviors, thus minimizing the temporal and financial costs linked with conventional synthesis routes. Particularly noteworthy is the application of AI and ML in studying phase behaviors, contributing significantly to the understanding of these intricate phenomena. This technological synergy fosters the development of predictive models that enable the evaluation of surfactant performance across diverse applications, including emulsions, foams, and coatings. Through such advancements, a deeper comprehension of the intricate relationship between surfactant properties and application efficacy is unveiled, paving the way for more tailored and efficient solutions in various industries.

2. Artificial Intelligence and machine learning:

2.1 Artificial Intelligence (AI)-

Artificial Intelligence (AI) has emerged as a transformative force in various scientific and industrial, academic and government domains [4,5,6]. Over the past few decades, the concept of artificial intelligence (AI) has garnered diverse definitions. Among them, John McCarthy's definition from his 2004 paper emphasizes AI as the science and engineering behind intelligent machines and computer programs [7]. This perspective broadens the scope beyond mirroring human intelligence, allowing for methods not bound by biological observation.

However, the origins of AI discourse trace back to Alan Turing's influential work, "Computing Machinery and Intelligence," published in 1950 [8]. Turing, a pivotal figure in computer science, posed the pivotal question, "Can machines think?" His renowned "Turing Test" proposed that a human evaluator discern between computer and human responses. While this test has faced scrutiny, it holds historical significance and maintains philosophical relevance through its linguistic foundations.

Stuart Russell and Peter Norvig's seminal textbook, "Artificial Intelligence: A Modern Approach," introduced multiple definitions of AI, delineating systems that emulate human thought or action, as well as those prioritizing rationality. Turing's concept aligns with the "systems that act like humans" category [9].

In simple one statement- “Artificial intelligence is a field, which combines computer science and robust datasets, to enable problem-solving.”

2.2 Machine Learning (ML)-

Machine Learning (ML) techniques have become invaluable tools in the advancement of Surfactant Science and its applications. By leveraging ML algorithms, researchers can uncover intricate relationships between surfactant properties, molecular structures, and performance characteristics. Through the analysis of large datasets, ML models can predict phase behaviors, stability profiles, and surface interactions, enhancing the understanding of surfactant systems. For instance, ML-driven investigations into the dynamics of emulsions and foams have yielded insights that were previously elusive through traditional methods. Additionally, ML-enabled optimization approaches have streamlined the formulation of surfactant-based products, leading to enhanced efficiency, and reduced environmental impact. The integration of ML in Surfactant Science not only expedites research processes

but also paves the way for the development of novel applications across industries, ranging from personal care to materials science.

2.3 Differences between AI and ML-

as per google web page and an online tutorial below is the simple differences between AI and ML. though the technical depth may show lighter on it, for sake of simplicity in this paper we will limit to the key differences only.

a. Artificial intelligence-AI

- AI allows a machine to simulate human intelligence to solve problems.
- The goal is to develop an intelligent system that can perform complex tasks.
- We build systems that can solve complex tasks like a human.
- AI has a wide scope of applications.
- AI uses technologies in a system so that it mimics human decision-making.
- AI works with all types of data: structured, semi-structured, and unstructured.
- AI systems use logic and decision trees to learn, reason, and self-correct.

b. Machine learning-ML

ML allows a machine to learn autonomously from past data.

The goal is to build machines that can learn from data to increase the accuracy of the output.

- Machine learning has a limited scope of applications.
- ML uses self-learning algorithms to produce predictive models.
- ML can only use structured and semi-structured data.
- ML systems rely on statistical models to learn and can self-correct when provided with new data.

in this paper. For the sake of simplicity, we will frequently use AI/ML as combined key world for describing different contexts.

3. AI and ML in Surfactant Science:

The use of AI/ML the context of Surfactant Science and related fields in emerging at a very fast pace. As we can see from number of literatures published graph by using lense.org [9] with a search query," artificial intelligence" AND "Surfactants".

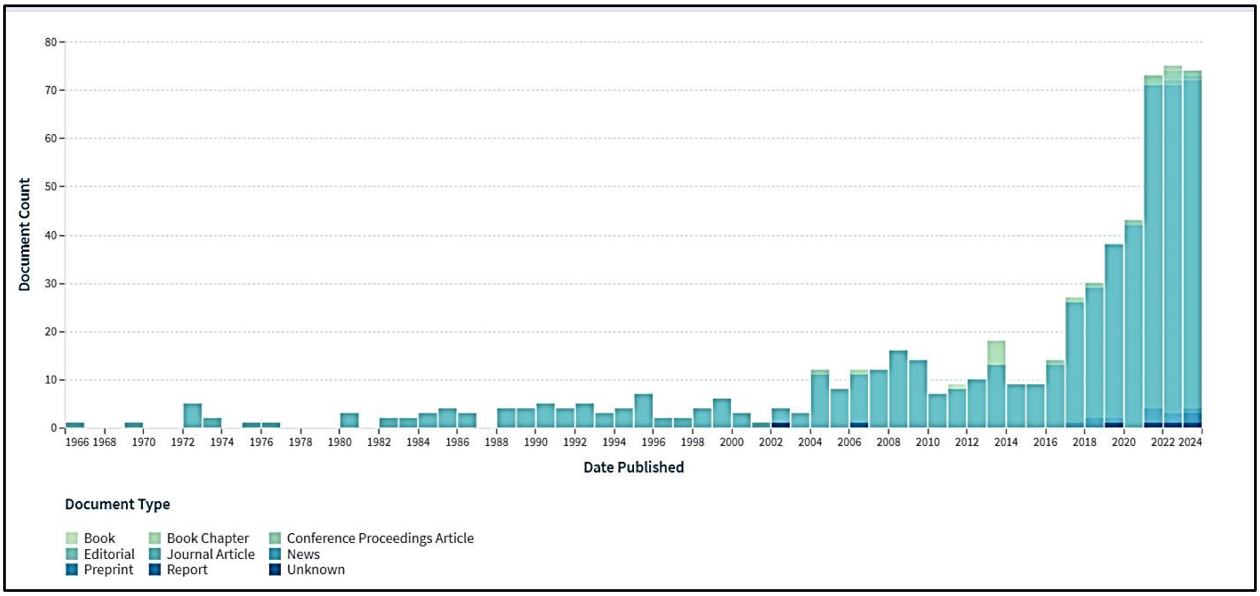

Figure:1*Literature published graph by using lense.org with a search query,"Artificial intelligence" AND "Surfactants".[9]*

The integration of AI/ML into the realm of Surfactant Science and its allied disciplines is rapidly gaining momentum. A compelling illustration of this trend emerges from the extensive literature on the subject, as observed in a comprehensive search through lense.org [10] for the intersection of "artificial intelligence" AND "surfactants."

This surge in publications showcases the evolving synergy between artificial intelligence and surfactant-related research. While not all studies exclusively focus on AI's role in surfactant properties, they collectively underscore the dynamic convergence of these two fields, bolstering scientific understanding.

For instance, in an article titled "Approach of Different Properties of Alkylammonium Surfactants using Artificial Intelligence and Response Surface Methodology," authors Gonzalo Astray and Juan C. Mejuto ingeniously employed AI to predict essential physical and chemical attributes of alkylammonium surfactants. This encompassed characteristics like density, speed of sound, kinematic viscosity, and surface tension in aqueous solutions [11].

Another notable contribution by Roy Setiawan, Reza Daneshfar, Omid Rezvanjou, and SiavashAshoori delved into the surface tension prediction of environmentally friendly ionic liquids. Their work harnessed artificial neural networks (ANN) to draw insights from a diverse dataset of 748 data points, effectively identifying influential factors [12].

Takuya Inokuchi, Na Li, Kei Morohosh, and Noriyoshi Ara explored how AI and ML can unveil a treasure trove of physical properties based on molecular structures. Their study

advocates the potential of machine learning and AI in deciphering multiscale systems encompassing surfactant molecules, micelle structures, and solution properties [13].

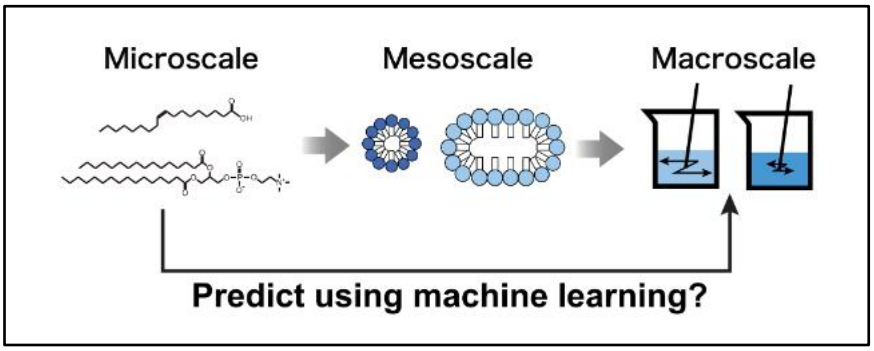

FIGURE 2: *From,"Multiscale prediction of functional self-assembled materials using machine learning: high-performance surfactant molecules.Takuya Inokuchi et al [12]*

Dale Seddon, Erich A. Müller, and João T. Cabral present a novel hybrid approach employing machine learning for predicting surface tension profiles of hydrocarbon surfactants in aqueous solutions. Their method correlates molecular properties to surface excess concentration and Langmuir constants, unveiling new insights [14].

In this ongoing era of scientific exploration, the fusion of AI and ML with Surfactant Science promises innovative avenues for predictive modeling and enhanced understanding.

In a recent publication titled "Can Machine Learning Predict the Phase Behavior of Surfactants?" [15], authored by Joseph C. R. Thacker, David J. Bray, Patrick B. Warren, and Richard L. Anderson, an exceptional exploration of surfactant phase behavior prediction emerges. This unique study, published in J. Phys. Chem. B in April 2023, sets out to conquer the intricate challenge of forecasting surfactant phase behaviors, defying conventional linearity. The authors skillfully wield Machine Learning (ML) as a potent tool to extrapolate from limited data, specifically addressing nonionic surfactants.

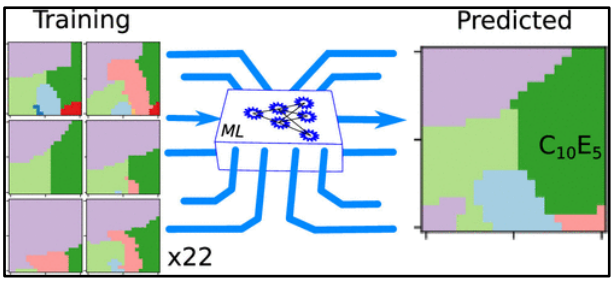

Figure 3: *A general graphics showing the phase diagram of nonionic surfactants in relation to process of training and then predicted. [J. Phys. Chem. B 2023, 127, 16, 3711-3727]*

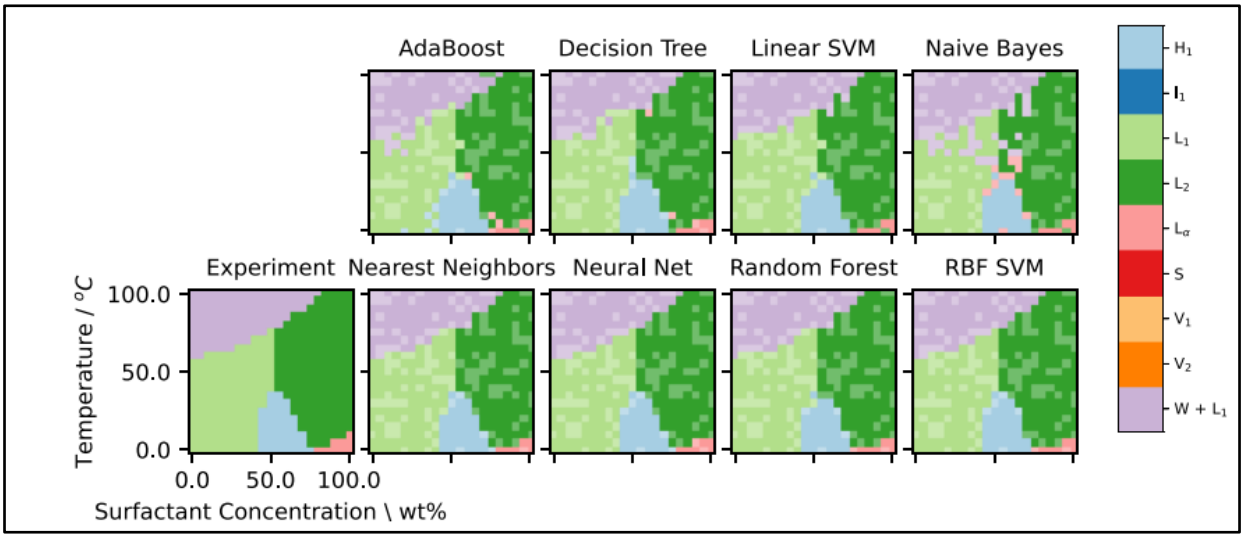

Figure 4: *An actual graphics comparing the phase diagram of nonionic surfactants using ML based on different models. [J. Phys. Chem. B 2023, 127, 16, 3711-3727]*

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Traditionally elusive due to their non-linear characteristics, surfactant phase behaviors are poised to be deciphered through this pioneering approach. The authors, to great extent, navigate this complex landscape, as showcased by a comprehensive graphical representation of nonionic surfactant phase diagrams [15]. However, in this journey, the authors also identify avenues for further refinement. They propose an evolution in three critical areas to enhance predictive accuracy and scope. First, they advocate for a more balanced representation of surfactant phases observed in the training dataset. Second, they highlight the necessity to expand the training dataset's chemical space to encompass a broader spectrum of surfactants. Lastly, they emphasize the value of a comprehensive feature space that encapsulates pertinent chemical attributes [15].

This study paves toward conquering the complexities of surfactant phase behavior prediction. By synergizing Machine Learning with surfactant science, this publication reshapes our understanding and abilities in a field marked by intricacy and innovation.

4. Surfactant molecular design by using AI/ML:

Molecular design by modeling and based on QPSR is not new. In the past and in current scientific community, companies are using the different methods to design molecules with specific properties. With evolution of AI and ML this task has become more efficient, and accuracy has improved. Although specifically there is not much said about, designing of a

surfactant molecule, by using AL/ML, for commercialization. But there a plenty of indirect information and data available in literature which can be utilized to design hypothetical a desired surfactant and then commercialize it later. Unveiling a New Era. The art of molecular design, guided by AI/ML prowess and underpinned by QPSR principles, is a realm not unfamiliar. Across epochs, within the scientific tapestry, diverse methodologies have been harnessed to architect molecules of precise attributes. Yet, today's AI and ML surge has wrought a transformation, imbuing this endeavor with unprecedented efficiency and heightened precision. Albeit the discourse around surfactant molecule crafting via AI/ML for commercial ends may be hushed, the literature resonates with covert revelations. Buried within, a trove of data beckons - a reservoir from which to conjure the blueprint of a coveted surfactant, destined for eventual commercial glory."

5. Efficient Synthesis routes of surfactants by suing AI/ML:

In general, surfactants are mostly derived from organic synthesis routes. Any use of AI and ML in organic chemistry synthesis will directly impact the surfactant synthesis. It's important to highlight the use of AL and ML in the field of organic synthesis.

A review paper published byFranck Petretti and Jean Michel Brunel in 2018 [16], describe the use of Machine learning for finding a synthesis route and efficiently utilize the process to obtain a desired molecule.

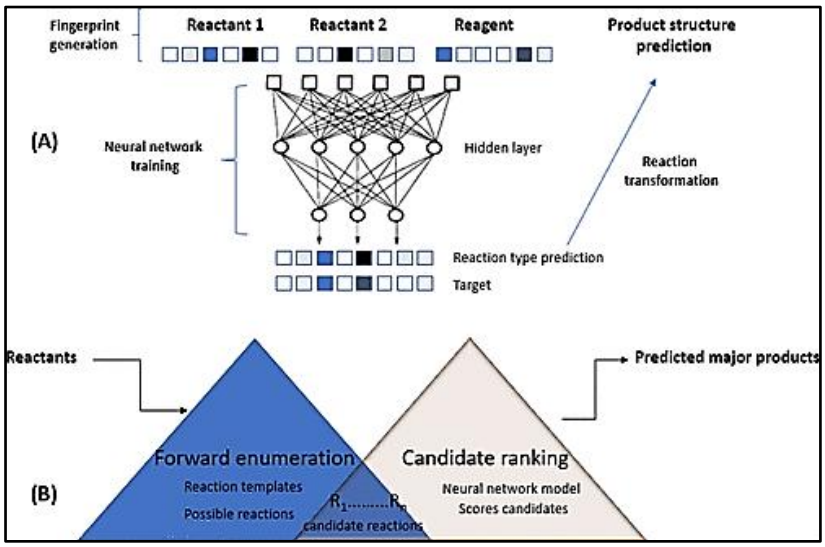

Figure 5:*A detail general description of using the ML models for designing and predicting the organic synthesis. ACS Omega 2018, 3, 10, 13263–13266 Publication "Artificial Intelligence: The Future for Organic Chemistry?" (Reproduced from permission from ACS)*

Another paper published in 2017[17] describes the use of machine learning for organic synthesis - where 15,000 experimental reaction records from granted United States patents, where the true product was found by applying the 1689 most popular templates were taken from the USPTO literature and augmented by adding the non-recorded products to create a set of 5,335,669 examples. The model was trained and tested. In a 5-fold cross-validation, the trained model assigns the major product rank 1 in 71.8% of cases, rank≤3 in 86.7% of cases, and rank≤5 in 90.8% of cases.

Below is the list of publication trend over the years using key worlds "Organic Synthesis" AND "Artificial Intelligence" OR Machine Learning" using lens.org data base.

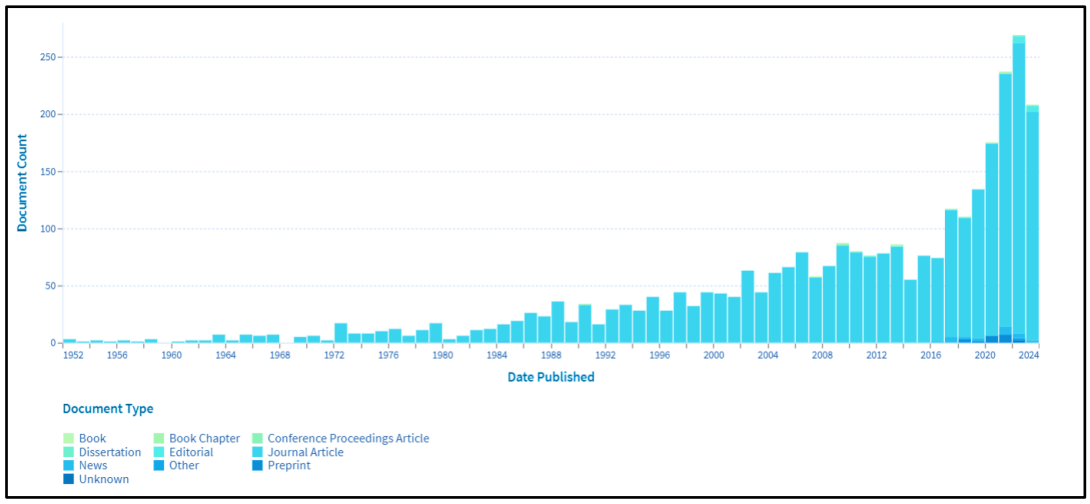

Figure 4:*List of publication trend over the years using key worlds "OrganicSynthesis" AND "Artificial Intelligence" OR Machine Learning" using lens.org database.*

6. A summary of literature published about use of AI/ML in surfactant science.

Table-1 (next page) summarizes a few notable research articles about how Artificial Intelligence (AI) and Machine Learning (ML) are being used in the field of surfactant science.

The table includes references, methods used, data sources, and important findings, highlighting how these advanced computer techniques are helping researchers understand surfactants better. These studies use different AI and ML methods like neural networks and clustering to analyze surfactant behavior and molecular dynamics. The table showcases the growing relationship between AI, ML, and surfactant research, giving readers an overview of how these technologies are changing the way we study surfactants and their applications in various industries.

Author Name	Year	Article Full Name	Topic
Thacker, J. C. R., et al.	2023	Can Machine Learning Predict the Phase Behavior of Surfactants? J. Phys. Chem. B, 127(16), 3711–3727.	Predicting phase behavior of surfactants using machine learning.
Seddon, D., Müller, E. A., et al.	2022	Machine learning hybrid approach for the prediction of surface tension profiles of hydrocarbon surfactants	Predicting surface tension profiles of hydrocarbon surfactants using machine learning.
Setiawan, R., Daneshfar, R., et al.	2021	Surface tension of binary mixtures containing environmentally friendly ionic liquids: Insights from AI	Studying surface tension of mixtures with ionic liquids using artificial intelligence.
Inokuchi, T., Li, N., Morohoshi, K., & Ara, N.	2018	Multiscale prediction of functional self-assembled materials using machine learning	Predicting properties of self-assembled materials through machine learning.
ACS Omega	2018	Artificial Intelligence: The Future for Organic Chemistry?	Discussing the role of AI in the future of organic chemistry.
Coley, C. W., et al.	2017	Prediction of organic reaction outcomes using machine learning	Using machine learning to predict organic reaction outcomes.
Astray, G., & Mejuto, J. C.	2017	Approach of Different Properties of Alkylammonium Surfactants using AI and Response Surface Methodology	Using AI and response surface methodology to analyze surfactant properties.

Table 1: *Summary of few Literatures on AI/ML Applications in Surfactant Science.*

7. **Conclusion:** This paper attempts topresent a short review about the pivotal role of Artificial Intelligence (AI) and Machine Learning (ML) in Surfactant Science, a mature and knowledge-rich domain within the Fast-Moving Consumer Goods (FMCG) sector. The integration of AI and ML offers a transformative pathway towards reimagining the assessment and development of surfactants and their derivatives. By leveraging AI, researchers can expedite the creation of novel surfactant molecules, leading to enhanced efficiency, efficacy, and sustainability in their production and application. The predictive capabilities of AI revolutionize the understanding of surfactant properties and behaviors, reducing the time and cost associated with traditional synthesis approaches. Notably, AI-driven investigations into phase behaviors provide crucial insights, further augmenting the comprehension of complex phenomena. These advancements culminate in the development of predictive models that enable accurate assessment of surfactant performance across diverse applications. Ultimately, this

synergy between AI, ML, and Surfactant Science propels the formulation of solutions that seamlessly combine effectiveness with environmental conscientiousness, shaping the future of surfactant research and industry.

Disclaimer- *Author claims no conflict of interest and the data /work presented in this paper is not the data/work the author has done in Affiliated companies. These companies are cited only as to show a professional affiliation/Experience of the author.*

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