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Section Chemical and Molecular Sciences

A vertical strip on the left side of the page features a blue-tinted microscopic image of cells, showing various cellular structures and membranes.

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The Chemical and Molecular Sciences section of the *Applied Sciences* journal is the ideal forum for publication of significant original and high-quality research, as well as reviews in all branches of chemistry and its sub-disciplines. These also include research on how chemistry is used for various applications in modern society. All manuscripts submitted for publication under this section will undergo the high quality peer review process of the *Applied Sciences* journal and, if accepted, will be published rapidly online.

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Selected Papers



Application of Quantum-Chemical Methods in the Forensic Prediction of Psychedelic Drugs' Spectra (IR, NMR, UV-VIS, and MS): A Case Study of LSD and Its Analogs

Authors: Jelica Džodić, Dejan Milenković, Milica Marković, Zoran Marković and Dušan Dimić

Abstract: Lysergic acid diethylamide (LSD) and its analogs are commonly encountered substances at crime scenes due to their misuse as hallucinogenic compounds. Modern methods have led to synthesizing different LSD analogs with pronounced physiological effects. Theoretical methods can be a valuable tool for predicting the spectra and stability of novel substances, especially when experimental data are partially available. The current work describes the application of theoretical methods in predicting IR, NMR, UV-VIS, and MS spectra of LSD based on the optimized structure at the M05-2X/6-311++G(d,p) level of theory. A suitable functional has been determined by comparison of the theoretically obtained geometrical parameters with the experimental ones based on the crystallographic structure. The MAE values for the structure optimized at M05-2X/6-311++G(d,p) level of theory were 0.0436 Å (bond lengths) and 2.70° (bond angles). The IR spectra of LSD and LSD tartrate have been described in detail, with the prominent bands being well reproduced (the difference between experimental and theoretical C=O stretching vibration wavenumbers was lower than 11 cm⁻¹). Detailed assignment of ¹³C NMR spectra led to a high correlation factor (0.999) and low mean absolute error (2.0 ppm) between experimental and theoretical chemical shifts. Optimizing the ground and excited states allowed for the calculation of the energy difference of 330 nm, which reproduced the observed band position in the UV-VIS spectrum of LSD. The most abundant fragments in the experimental mass spectrum (at 323, 221, 207, 181, and 72 m/z) have been optimized, and their stability has been discussed from the structural point of view. This methodology has been validated by comparison with the experimental GC-MS spectra of sample seized at the crime screen and by structure optimization and computation of NMR spectra of common LSD analogs. The theoretical methods for the structure determination and prediction of spectra show great potential in the fast-developing world of new psychedelics.

<https://doi.org/10.3390/app13052984>



Toxicity of Different Chemical Components in Sun Cream Filters and Their Impact on Human Health: A Review

Authors: Sonia Santander Ballestín and María José Luesma Bartolomé

Abstract: Some chemical components in sun cream filters have endocrine-disrupting activity or can be carcinogenic, neurotoxic, bioaccumulative, allergens, or be toxic for human reproduction. It is important that sunscreens have safety requirements. The objective of this work is to compare sun cream filters used in conventional commercial sunscreens and those that are considered natural products, especially focused on endocrine-disrupting effects. In order to achieve the above objective, the compositions of different conventional and natural sun cream filters were evaluated and compared, taking into account the presence of the different sun cream filters whose effects were evaluated on the website specialized in safety and cosmetics, Environmental Working Group (EWG), and in the Register of chemical substances and mixtures in the EU Registration, Evaluation, Authorization and Restriction of Chemicals (REACH) Regulation. The currently available evidence of each sun cream filter and their degree of safety has been summarized. Several organic sun cream filters present a potential risk to health and the environment; however, inorganic sun cream filters such as titanium dioxide and zinc oxide (ZnO and TiO₂) show a very low risk in humans as they are not absorbed through intact or damaged tissues. The legislation does not oblige manufacturers to specify the concentration of each substance, which provides qualitative but not quantitative information for the consumer.

<https://doi.org/10.3390/app13020712>



Strategic Development of Piezoelectric Nanogenerator and Biomedical Applications

Authors: Omkar Y. Pawar, Snehal L. Patil, Rahul S. Redekar, Sharad B. Patil, Sooman Lim and Nilesh L. Tarwal

Abstract: Nanogenerators are the backbone of self-powered systems and they have been explored for application in miniaturized biomedical devices, such as pacemakers. Piezoelectric nanogenerators (PENGs) have several advantages, including their high efficiency, low cost, and facile fabrication processes, which have made them one of the most promising nano power sources for converting mechanical energy into electrical energy. In this study, we review the recent major progress in the field of PENGs. Various approaches, such as morphology tuning, doping, and compositing active materials, which have been explored to improve the efficiency of PENGs, are discussed in depth. Major emphasis is given to material tailoring strategies and PENG fabrication approaches, such as 3D printing, and their applications in the biomedical field. Moreover, hybrid nanogenerators (HNG), which have evolved over the last few years, are discussed. Finally, the current key challenges and future directions in this field are presented.

<https://doi.org/10.3390/app13052891>

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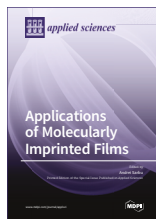
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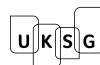
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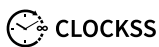
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