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Analytical Chemistry's Experimental Methods: A Semantic Analysis

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Abstract

Finding the data that is most relevant to a given context is a major obstacle to reusing and integrating existing data. The scientific literature that provides descriptions of the experiments that led to the data is the primary source of metadata. We manually annotated 100 recent open access publications in Analytical Chemistry as semantic graphs to encourage the development of natural language processing techniques for extracting this data from articles. Because we are particularly interested in the subject, which also falls under the purview of a number of ontologies and controlled vocabularies, we concentrated our efforts on articles that included a mention of mass spectrometry in their experimental sections. The resulting gold standard dataset is accessible to the general public and can be used to verify automated methods for locating this metadata in the literature. We also made a few observations regarding the experiment structure, description, and open access publication in this journal.

Keywords: Bio sensing • Analytical applications • Covalent-organic frameworks

Introduction

The jag genes were examined to determine which threonine residue was involved in cyclization. The thioesterase domain, which is responsible for cyclization-mediated release from biosynthetic machinery to form ester bonds in cyclic peptides, was compared to other thioesterase domains whose genes and ring sizes had previously been identified. The jag thioesterase is similar to a group of thioesterases that make cyclooctapeptides, according to an analysis of the genes' similarities and differences. Peracylation and NMR spectroscopy of peracylated-jagaricin confirmed this structure and position of cyclization. When the knockout mutant was grown on mushroom tissue and examined with IMS, no jagaricin was found. This was done in order to provide additional evidence that the jag genes were the ones responsible for the production of jagaricin.

By applying the pure compound to mushroom tissue, we were able to examine the native biological function of Jagaricin. According to these tests, it causes lesions similar to those found in mushrooms that have soft rot. Further antimicrobial testing revealed that jagaricin is effective against Candida albicans, Aspergillus fumigatus, and A. terreus, common human fungal pathogens.

Despite the fact that the history of science is frequently viewed as a list of bearded old men, many amazing and inspiring women have made a difference in the field. This special ABC issue is therefore dedicated to presenting research conducted by a select list of early and advanced career female scientists with a great deal of optimism and the general belief that these female pioneers are inspiring not only women but also men. This issue unquestionably demonstrates that women are present in all areas of analytical science, with the extremely rich and varied scientific articles of the sixty chosen female researchers contributing to classical analytical fields like mass spectrometry, chromatography, electrochemistry, and spectroscopy as well as more nanoscience-oriented approaches like molecular nanosensors, microchip analysis, and nanoparticles for sensing. It is still our responsibility to ensure the visibility of their outstanding research, which is connected to their ongoing efforts to uphold the highest scientific standards. It seems like centuries ago when there were only a few female chemists available. This special issue makes it abundantly clear that analytical chemists of the present and future will have access to numerous role models in 2020.

Methods

The purpose of the social program was to provide an opportunity for casual conversation and to strengthen friendships with analytical chemistry societies. The following were the main points: gathering on Sunday evening in the main building of the Warsaw University of Technology to welcome friends to Warsaw; Beer barbecue party in Heritage Park outside of Warsaw called "Gociniec Wiecha," which is a great way to try Mazovian village fare on Monday night; On the stage of the renowned "Teatr Polski," beautiful costumes, live folk music, and dance performed by dancers provided the opportunity for a music-and-dance journey through various regions of Poland on Tuesday evening; Last but not least was the conference Gala Dinner, which was held on Wednesday in the Main Hall of the Warsaw University of Technology. For this event, the hall was transformed into a one-of-a-kind ballroom, and a spectacular arrangement of light and music added to the experience.

Metabolomics emerged at the end of the 1990s, shortly after proteomics. The detection, identification, and quantification of compounds with a low molecular weight that are present in a particular biological medium are the subject of this research. The metabolome does not include biological polymers like proteins or nucleic acids. Instead, it includes all compounds with a low molecular weight (1000 Da or 1500 Da, depending on the definition). These metabolites can be molecules like amino acids, sugars, nucleotides, or fatty acids that are involved in the numerous reactions that the cells of an organism use to produce and use energy. Any biological species has the ability to synthesize other types of metabolites for specific biological functions, such as glucocorticoids or neurotransmitters in mammals or alkaloids in plants. Because they are present in biological media and can be detected by the analytical chemistry tools that are utilized for metabolomics, xenobiotics, also known as chemicals that are found in living organisms but are not produced by them, such as drugs and pollutants, as well as their metabolites, are also included in the metabolome. This demonstrates that metabolites come from a variety of sources, including the microbiota, food and beverages, drugs, the environment,

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and cellular metabolism. Because of this, metabolomics is an effective method for observing how a living organism and its environment interact. Due to their large chemical diversity and a lack of metabolic knowledge, many metabolites remain uncharacterized. In fact, less than 5% of the features found in biological media by mass spectrometry-based metabolomics techniques are thought to be annotated.

Miniaturization has been a major focus in recent years, with formats like chips, 3D-printed objects, and paper-based devices emerging. The low cost, portability, and waste reduction of these systems have been utilized in chemical and biological processes. To meet the current analytical challenges, it is necessary to continue developing devices that are simpler to use and have improved performance. In this sense, reticular porous materials like metal- (MOFs) and covalent- (COFs) organic frameworks have attracted a lot of attention in a variety of fields. These materials have unique characteristics like tailorable porous architectures and tunable chemistry. However, very little research has been done on the combination of these materials with emerging and miniaturized formats. This review aims to fill this void and highlight these materials' most recent contributions in these analytical formats. As a result, the purpose of this work is to provide a comprehensive overview of the field by focusing on the incorporation strategies that have been incorporated into the functional supports that have been made available to date and the applications of the systems that have resulted in both on-site analysis and off-site laboratory studies that are mostly dedicated to (micro) extraction. Last but not least, issues and directions for the future in this field are discussed.

Discussion

The sudden shift from working with students in person to working with them remotely in March 2020 was jarring for David Harvey, who works at DePauw University. The transition for lecture classes was relatively simple, despite being challenging. For laboratory work, this was not the case. Harvey stated, "Making measurements takes time, but if we cannot be in the lab right now, we can capture that time and use it in a variety of ways." We can, for instance, have students approach a brand-new subject virtually by employing an instrument simulator. They can then work in class to comprehend the connection between the settings of an instrument and the data they collect. "Come Fall, the big challenge will be finding a way to meaningfully train and reinforce the lab skills that we expect for students in analytical chemistry," stated Chris Harrison of San Diego State University. I want to teach my students the most important analytical lab skills in less than half the time, utilizing take-home kits and simulated lab data to make up for missed typical labs. "I think we can safely say that lecture and recitation can be replaced with an online experience," stated Augustus Way Fountain of the University of South Carolina. However, my greatest concern is in the laboratory. This spring, Fountain discovered that the best strategy was to record himself working in the labs, giving students the data they needed to analyze and write about. "Chemistry is as much hands-on laboratory skill as it is book knowledge," Fountain added. The entire laboratory experience cannot be replicated remotely. For the labs in the fall, we really need to focus on addressing this gap.

Unfortunately, our pharmacy curriculum only provides a limited number of hours for practical work: The number of hours spent on analytical chemistry by pharmaceutical sciences students is lower than that of chemistry students because chemistry is part of a comprehensive, multidisciplinary curriculum. It should be noted that courses must be taken within the first three years of the curriculum in the French pharmacy system, so there is little room for error. Up until the third year, the courses aim to establish a common foundation of knowledge relevant to pharmacy careers [1-5].

Conclusion

Additionally, our institution's analytical chemistry classes are primarily concentrated in the second year of the curriculum (whereas those at other French universities sometimes span the second and third years). In this intensive program, the students have limited time to manipulate each technique because of the high number of students and limited number of instruments in our laboratory. There is a correlation between the limited budget and the limited number of instruments, which reduces student experimentation opportunities and duration.

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Conflict of Interest

None.

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