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The complexity of clean-label cosmetics

Rebecca Guenard

Market research shows consumers now rank natural ingredients and environmental impact ahead of brand recognition and product descriptions. They expect personalized products from a company whose values align with their own. Food containing nothing artificial once qualified as acceptable, but according to a 2017 survey, shoppers now look for labels with less sugar, more protein, and fewer ingredients with recognizable names (https://tinyurl.com/y9xysyjy).

- **It started with food. Now the clean-label movement is influencing the development of personal care formulations.**
- **Providing a clean label for personal care items requires formulators to consider new ways of making safer, sustainable ingredients.**
- **Cosmetics companies adhere to an international set of guidelines on ingredient names, but they are less confident about the definition of the term "natural."**

A survey of social media outlets reveals a spike in the use of the term "clean label" over the past two years (https://tinyurl.com/y8sr2jfo). This consumer-driven movement has now crept into the personal care industry, where it has the potential to have a major impact. The skin care market is predicted to grow annually by 6% globally until 2022, and according to a recent analysis, much of this growth will be driven by increased consumer interest in natural, plant-based ingredients (https://tinyurl.com/ycrj87zw).

"Clean beauty from our perspective is the next frontier for people who are looking to create a healthy home," says Lindsay Dahl, vice president of social and environmental responsibility at Beautycounter, a clean label personal care company headquartered in Santa Monica, California, USA, that launched in Spring of 2013.

Founder and CEO Gregg Renfrew conceived of creating a personal care line that was all natural and free from ingredients that advocacy groups or regulatory agencies outside the United States deemed unsafe. In a recent *New York Times* article, Renfrew explained that achieving a clean-label personal care line was more complicated than she imagined—a truth many personal care companies face as natural sources for essential ingredients do not exist yet, and consumers require routine education on a label's nomenclature. However, the industry is finding ways to satisfy the growing demand for cleaner products. Ingredient manufacturers are developing greener ways to create their products, and cosmetics companies are signaling that the term "natural" needs a clearer definition in a mutual effort to achieve clean-label cosmetics.

INNOVATING INGREDIENTS

Damien Perriman is senior vice president of specialty chemicals at Genomatica, a bioengineering company in San Diego, California, USA, that develops bio-based technologies. In 2018, his company introduced its first personal care product, a natural butylene glycol (Brontide™) used

by formulators as a moisturizing ingredient. Since the 1960s, the ingredient has only been made by starting with crude oil and producing the intermediate acetaldehyde, a known Group 1 carcinogen.

Using biological processes to produce cosmetic ingredients has become increasingly popular over the past five years. Biology is more selective than chemistry and can be tuned to result in a pure compound instead of the racemic mixtures that often result from chemical synthesis. In addition, the technology bypasses petrochemicals. Genomatica harnessed biology to make butylene glycol a new way, through a fermentation process with genetically engineered E-coli that feed on plant sugars.

Perriman says Genomatica's natural diol product offers equivalent antimicrobial and humectant properties to petrochemical counterparts. More importantly for clean-label clients, using microorganisms instead of petrochemicals is sustainable and environmentally friendly. "Our mission, as custodians of technology, is to help people understand why change can be better," says Perriman. "In this example of butylene glycol, change is better because now we can use sugar instead of acetaldehyde to make an ingredient that is widely used in personal care formulations, satisfying that natural need and moving away from a bad raw material."

Personal care formulators are also considering natural solutions for low-molecular-weight emulsifiers and surfactants that can cause irritation in topical creams. Researchers are considering natural ingredients like clay, alumina, or starch that are less irritating and not harmful to the environment. The aquatic fate of currently used surfactants is unknown.

To fill this natural ingredient void, an international team of researchers studied emulsifiers made from modified starch granules. The starches were isolated from quinoa, rice, and amaranth, then chemically altered to increase hydrophobicity and enhance their emulsifying properties. The result, according to the researchers, is a tasteless, colorless, odorless, inexpensive, non-allergic cosmetic ingredient that is also an approved food additive (http://dx.doi.org/10.1016/j.carbpol.2017.07.044). They plan to continue their research by investigating how protein content in these natural ingredients will affect their performance in formulations.

Of all the formulating challenges the personal care industry faces, a lack of clean-label friendly preservatives prevails. Consumers store food in refrigerators or dry pantries, but personal care items reside on bathroom shelves where the environment is prime for microbial growth. Preservatives are essential for the safety and durability of these products, but antimicrobial compounds exhibit bioactivity that is often toxic to humans. The toxicological effects of preservatives like paraben and chromated copper arsenate have left consumers fearful of the very ingredients that were designed to protect them from microbes and preserve the quality of their products.

Personal care needs new preservatives. Dahl says, "It is one of the top priorities for the entire industry, but certainly for us at Beautycounter. We have made some progress but,

given the nature of preservatives and the function they perform in a product it's not an easy nut to crack."

A research team at the Berkeley Center for Green Chemistry (BCGC) at the University of California, Berkeley, USA, is looking at ways to exploit the differences between human and microbial biochemical processes or cell structures to improve antimicrobial potency without adverse effects to human health. The team, led by Heather Buckley, currently an assistant professor at the University of Victoria, British Columbia, Canada, focused on the redox activity of phenolic compounds, homing in on the esters and amides of hydroxyl-substituted benzoic acids like gallic acid (https://doi.org/10.1021/acssuschemeng.7b00374).

Using a systematic analysis of several different functionalities, the BCGC team showed how they could explore a phenol's substituent chain length or location to optimize antimicrobial properties. Their comprehensive approach led to a first-place prize from the Green Chemistry and Commerce Council's Preservative Challenge for a molecule that functions as a preservative during use but decomposes upon disposal (https://tinyurl.com/yb9eu2st).

Beautycounter has partnered with BCGC to bring new preservatives to market in the next few years. Until such time, her company focuses on educating their customers. "We spend a lot of time letting people know why preserving their personal care product is important, and whether the preservation is taking place through a synthetic preservative or a naturally derived preservative," says Dahl. "People are starting to understand that preservation is important, but not all preservatives are created equal."

As these efforts to innovate show, no matter how clean the personal care industry tries to make their labels they will need to be in constant communication with their customers to relay accurate science. Beautycounter maintains a blog to educate its online shoppers about aspects of human and environmental health. "The consumer is often asking for the source of the ingredient, in other words, is it natural or is it synthetic. We want to screen ingredients for safety regardless of their source," says Dahl. "We know that just because something is an essential oil does not mean that it is automatically safe."

Presumably, shoppers gravitate to essential oils because they are composed of recognizable substances like orange, lavender, or mint. Recognizable names are harder to come by in the beauty industry than in the food industry. One reason is internationally agreed upon nomenclature, an Achille's heel for clean-label cosmetics.

SETTING STANDARDS

In 1970, the Personal Care Products Council established the International Nomenclature of Cosmetics Ingredients (INCI) (https://tinyurl.com/yaoem4sy). Lists of ingredients on cosmetics labels around the world follow the INCI (pronounced inky) system. Standardized labels that use the same name globally are beneficial, but not always to a consumer who cannot recognize them.

"We have an article on our blog about how a hard-to-pronounce or unpronounceable ingredient doesn't automatically mean that an ingredient is unsafe," says Dahl. She says that through the blog Beautycounter explains that INCI is an internationally standardized ingredient list, and though the INCI name for shea butter may look scary, it is still just shea butter.

When Genomatica found a greener way to make a popular moisturizing ingredient, they had few options for what to name it. "The name is interesting, 1,3 butane diol, which in the INCI classification is called butylene glycol. We can't really call it anything different," say Perriman. "People in the industry are familiar with butylene glycol, but a lot of people don't like it because it sounds petrochemical." Perriman says he respects that, but he counters that a company like his should not be determining the market definition of natural.

"We don't see ourselves as evangelists of natural products. We see ourselves as an innovator that is bringing a natural solution to a market that wants it. From that perspective the word "natural" seems to have different definitions to a lot of different people," says Perriman.

Which brings up the ultimate issue surrounding clean label beauty, a lack of regulation. "There is the ISO 16128 standard for determining if an ingredient is natural," says Perriman. "Using this standard, we can say that butylene glycol made by a fermentation process from a renewable resource like sugar is a natural ingredient." But he acknowledges that there are customers out there who are not familiar with that standard and will define natural in a different way.

The International Organization for Standards (ISO) provides guidelines for how to define natural and organic cosmetics. However, it does not address product claims and labeling or human and environmental safety. Other NGOs, such as the Environmental Working Group, do address safety, and many beauty companies include the EWG seal on their label. However, there is no federal oversight for personal care product ingredients and labeling in the United States.

Dahl says her company would like to see more US government involvement. "Beautycounter has been working since we started for a more health-protective federal regulatory system," she says. "If you look at the European Union and Canada, they are far ahead of the US." Beautycounter's CEO has spent time convincing US law makers to regulate her industry.

Dahl says there are a few things they are looking for in cosmetics regulation. They are asking US Congress to give the US Food and Drug Administration (FDA) the ability to study and make determinations about ingredient safety. "Right now, there is no system for the FDA to be able to say a paraben is unsafe, safe if used in certain ways, or should be removed from the market. There is no green, yellow, red light system," she says. Beautycounter is also advocating for the FDA to have the ability to recall harmful products from the market. She laments that recall authority is a basic consumer protection that currently does not exist in the personal care space. Dahl says lawmakers have shown bipartisan support for change to the industry. "There has been indication from leaders from both the US House and Senate that cosmetic reform is something that they want to take on in 2019," she says.

Were US regulations imposed on the industry, questions about what natural means and how to supply a clean label could be simplified. For now, that responsibility rests with companies within the industry. "We try to use our websites and interactions with our care team to help people understand how we define safety at Beautycounter. Without any federal oversight of safety, it is really up to companies to define safety for themselves."

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AOCS MEETING WATCH

May 5–8, 2019. AOCS Annual Meeting & Expo, America's Center Convention Complex, St. Louis, Missouri, USA.

April 26–29, 2020. AOCS Annual Meeting & Expo, Palais des congrès de Montréal, Montréal, Québec, Canada.

May 2–5, 2021. AOCS Annual Meeting & Expo, Oregon Convention Center, Portland, Oregon, USA.

October 8–11, 2019. 18th AOCS Latin American Congress and Exhibition on Fats, Oils and Lipids, Bourbon Cataratas Convention & Spa Resort, Foz do Iguaçu, Brazil.

November 8–10, 2019. 2nd AOCS China Section Conference: Health, Advanced Processing, and Value-Added Utilization, Zhujiang (Pearl River) Hotel, Guangzhou (Canton), China.

For in-depth details on these and other upcoming meetings, visit http://aocs.org/meetings or contact the AOCS Meetings Department (email: meetings@aocs.org; phone: +1 217-693-4843).

Revised Toxic Substances Control Act (TSCA)—Challenges for "new" and "existing" substances

Jeffrey Hafer

- The Frank R. Lautenberg Chemical Safety for the 21st Century Act (LCSA) changes many components of the original US Toxic Substances Control Act (TSCA). These include the addition of systematic evaluation of existing chemicals, introduction of new concepts to the assessment of new chemicals, and altering how confidential business information (CBI) is reviewed and maintained.
- The effects of the existing chemicals prioritization and risk evaluation process on industry have yet to be realized. Changes to the new chemical process continue to evolve. However, it is clear that the use of "insufficient information" findings and the inclusion of "reasonably foreseeable uses" in the new chemical review process have had a profound effect on the outcomes of assessments, resulting in a reduction in the number of new chemicals that are commercialized.
- Changes to the procedure for protection of CBI make requirements for substantiation more frequent and more challenging.

The main driver for amending the United States Toxic Substances Control Act (TSCA) was the perception that little was known about the risk to human health and the environment from the majority of chemicals in commerce. While that perception underestimates the actual extent of knowledge about chemicals, it was based on the fact that ~62,000 of the greater than 85,000 substances on the TSCA inventory were added during the original inventory compilation in 1978–79 without a risk evaluation (known as "existing substances"). A major flaw in "old TSCA" was that it was extremely difficult for the US Environmental Protection Agency (EPA) to take substantive action on existing substances, even those with well-known risks, such as asbestos.

The Frank R. Lautenberg Chemical Safety for the 21st Century Act (LCSA) corrected this deficiency, directing the US EPA to systematically prioritize existing chemicals for evaluation and, if necessary, apply risk-management measures up to and including an outright ban. Initially, it seemed that this component of LCSA would have the most significant effect on the chemical industry. It turns out that changes to the process that addresses how "new" substances are added to the Inventory have had a much more immediate impact. This article focuses on the regulatory treatment of new and existing chemicals under the revised TSCA, as well as some other components of the LCSA that are affecting chemicals in commerce.

NEW SUBSTANCES: THE PREMANUFACTURE NOTICE (PMN) PROCESS UNDER LCSA

For a new substance to be added to the inventory, a PMN must be submitted to the US EPA. The Agency then conducts a risk assessment based on 1) the information provided by the submitter; 2) toxicology data for the substance and/or "read-across" data on structurally similar substances provided by the submitter, already in the Agency's possession or available in the open literature; and 3) data generated by models. Within 90 days, the Agency must make one of three findings. The new substance:

- presents an unreasonable risk ("A" determination);
- may present an unreasonable risk, and/or there is insufficient information to permit a reasoned evaluation, and/or there are significant exposures/releases ("B" determination); or
- is not likely to present an unreasonable risk ("C" determination).

If an "A" determination is made, US EPA is required to issue an order to either limit the amount allowed in commerce or to impose other restrictions on the substance designed to mitigate the risk up to complete prohibition.

If a "B" determination is made, US EPA is required to issue a Consent Order (CO). A CO is a legally binding agreement between the Agency and the PMN submitter that places requirements on the manufacture, processing, distribution, use, or disposal of the new chemical substance to reduce the risk. The CO may also require the manufacturer to submit testing to the Agency before exceeding a specified production volume. The CO is followed with a Significant New Use Rule (SNUR) that extends the CO restrictions to all manufacturers/importers/users.

If a "C" determination is made, the rationale for this decision must be published. Once notified by the US EPA that the chemical substance is not likely to present an unreasonable risk, the PMN submitter may immediately begin commercial activity (need not wait for the statutory 90-day review period to expire).

LCSA has not changed the process for new chemical risk assessment, but it has incorporated several new concepts that have radically changed the outcome of the process.

- If the substance "may present unreasonable risk" and/or there is "insufficient information to make a determination," the Agency must regulate the substance or ban commercialization. Previously "insufficient information" was used to justify regulation only if unreasonable risk was also indicated. Now, "insufficient information" in and of itself may be used as the basis for regulation. The additional information that might be required to meet the "sufficient" standard could involve testing to better define the hazard, more detailed information on human exposure and environmental releases, or both.
- The use(s) of the PMN substance identified in the submission remain the focus of the risk assessment. However, other "reasonably foreseen" uses not intended by the submitter may now be included in the assessment and can result in a finding of unreasonable risk.
- In addition, any "potentially exposed susceptible subpopulation" that may be at greater risk than the general population from exposure must be considered (e.g., infants, children, pregnant women, workers, and the elderly). While consumer uses always received more rigorous scrutiny than industrial uses, the lower acceptable exposure limits for infants and the elderly can greatly increase the possibility that potential exposures might result in a finding of unreasonable risk.

Incorporation of these concepts into the new chemical review has resulted in a radical shift in the results of the assessments. The percentage of submissions regulated or withdrawn has increased from an average of approximately 10% prior to LCSA enactment to more than 80% (Fig. 1)

In addition, findings of insufficient information have resulted in an order of magnitude increase in COs and the number of tests needed to address the concerns identified in the assessment.

PMN STRATEGY

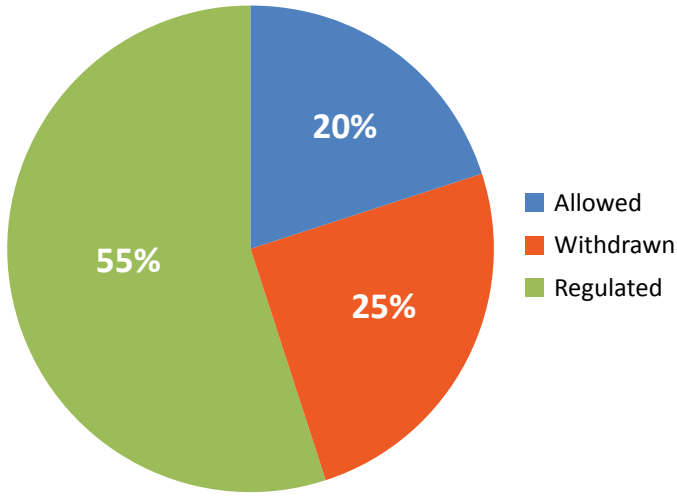
To maximize the chances of a successful PMN submission, it is essential to inform the risk assessment by critically evaluating the hazard and exposure (including environmental release) data that are supplied. One important resource is the US EPA "chemical categories" document that specifies the minimum data that the Agency suggests are needed to address hazard concerns for groups of substances [2]. For instance, anionic, cationic, and nonionic surfactants are categories that each have a suggested testing protocol to address ecotoxicity.

Unfortunately, the weakest component of a PMN submission is frequently the information supplied on human exposures and environmental releases. This is generally not an issue when all manufacture and use sites are under the control of the submitter, but if the substance is supplied to downstream customers not under the control of the submitter, specific exposure and release information is typically not available. In the absence of sufficient exposure and release data or to supplement the information provided by the submitter, the Agency uses exposure models and generic-use scenarios that incorporate conservative assumptions. This increases the probability of a "may present unreasonable risk" determination. It is also important to consider "reasonably foreseen" uses other than those submitted in the PMN itself, including those with "potentially exposed susceptible subpopulations."

Recently, the US EPA developed new categories that address concerns with impaired lung function from exposure to surfactants and other substances by inhalation. As opposed to the existing anionic, cationic, and nonionic surfactant categories that focus on potential ecotoxicity from environmental releases, this new category addresses potential risk from a specific human exposure pathway during end use. Even if a PMN does not include a use with potential inhalation exposure, and none are intended, if the Agency has reason to believe that inhalation exposure is possible, the testing requirements and risk management measures specified in these categories may be applied to the submission.

For any PMN, it is essential to document not only how the substance is intended to be used, but, if possible, how it cannot be used, along with the degree of control you have over the use(s). For instance, if a substance cannot possibly generate an aerosol due to its vapor pressure or viscosity, consideration of exposure by inhalation can be eliminated. A statement in a safety data sheet (SDS) simply warning against potential inhalation exposure would likely not be sufficient to substantiate control.

FIG. 1. The percentage of new chemical submissions allowed, regulated, and withdrawn [1]



EXISTING CHEMICALS

LCSA mandates that the Agency systematically prioritize the inventory to conduct risk evaluations on high priority existing substances. If risk is identified in the evaluation phase, then risk management measures up to and including an outright ban may be applied. Note that costs or other non-risk factors may be considered in the development of risk management measures, but they may not be considered in the risk-evaluation phase. The statute requires that each risk evaluation last no longer than 3 years with one possible 6-month extension, and that the Agency allow for at least one 30-day public comment period on the draft prior to publishing a final risk evaluation.

The risk evaluation will initially encompass the following:

- Ten chemical substances from the 2014 update to the TSCA Work Plan [3];
- Substances designated as high priority by the US EPA prioritization process; and
- Substances nominated by industry that meet the criteria for US EPA to conduct an evaluation.

All manufacturers and importers of substances that are subject to a US EPA-mandated risk evaluation will be required to generate and submit data and to contribute to the $1,230,000 fee for each evaluation ($270,000 for small businesses). Since this represents a significant potential liability, it would be prudent to evaluate all purchased and manufactured substances to determine if any may be subject to this process now or in the future. Preference for high-priority designation is given to the following:

- Remaining substances listed in the 2014 TSCA Work Plan;
- Substances that have persistence and bioaccumulation scores of 3 (Persistence 3 = Half-life > 6 months, Bioaccumulation 3 = BCF or BAF ≥ 5000); and
- Substances that are known human carcinogens and have high acute and chronic toxicity.

CONFIDENTIAL BUSINESS INFORMATION (CBI)

Under "old" TSCA, there was no time limit for CBI protection. In addition to adding a 10-year statutory time limit, LCSA has drastically changed how the USEPA handles CBI [4].

- There are currently more than 17,000 chemicals on the confidential portion of the TSCA inventory. Until now, there has been no mandate to review these CBI claims. Within 1 year of final active substance inventory designation (outcome of the TSCA Inventory Notification (Active-Inactive) Rule, expected by January 2019), US EPA must promulgate a rule to review all of these claims. They must also review all other existing CBI claims within 5–7 years.
- Prior to LCSA, substantiation for CBI claims was not required with the PMN submission, only at commencement (the required notice to the USEPA of the date commercial activity began). Now, substantiation for non-exempt information is required with the submission. US EPA must review all non-exempt claims and 25% of exempt claims.
- Prior to LCSA, CBI claims did not sunset. Now, all claims must be re-substantiated every 10 years. In July 2018, US EPA sent a number of "Final Deficiency Notices" for some existing CBI claims. Recipients of these notices are given 30 days to provide the information required to dispute the deficiency or the information is immediately made public.

LCSA poses many challenges, but forewarned is forearmed. For new substances to avoid extensive delays or the potential for an undesirable outcome in the PMN process, prior to submission it is essential to determine whether sufficient information is included with the notice for the Agency to make a determination of risk (especially exposure and release during the substance lifecycle). For existing substances, it makes sense to identify those that may be prioritized for review, and prepare for future action. For all substances, it is essential to assure that all existing and future confidentiality claims are supported by robust documentation.

During a 36-year career in industry, Jeffrey Hafer has held a variety of positions, including global regulatory specialist, global product stewardship manager for the Dow Chemical coatings business, and most recently, corporate TSCA manager for Dow Chemical. After retiring in 2016, he joined knoell USA, LLC as a senior regulatory scientist.

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Vegetable oil-based removal of harmful metals from water

Kenneth M. Doll, Robert O. Dunn, Kim L. Ascherl, and Grigor B. Bantchev

- The thiolene reaction is an atom-efficient and convenient way to produce thioether-functionalized vegetable oils.
- Thioether-functionalized vegetable oils can take metal ions out of aqueous solutions.
- Different vegetable oils can be used to create different sulfur environments in these water remediation agents.
- The binding of mercury ions to thioether-functionalized corn oil is stronger than the binding of silver ions to the same oil.

The variety of techniques by which metals or metal ions can be removed from water have been reviewed in detail elsewhere [1], and include: chemical precipitation, ion exchange, adsorption, membrane filtration, flotation, electro-dialysis, coagulation, and flocculation. These techniques all rely on the interaction of the metal with the remediant through means such as ion pairing, covalent binding, or adsorption. The metal is then removed from the system, leaving uncontaminated water as the product. Therefore, to be effective, a remediant for water must balance two important properties: selective binding, or similar interaction, with the metal, and formation of a phase which is easily separated from water.

Simple materials, such as activated carbon and pillared clay, to more sophisticated materials, such as graphene, zeolites, and carbon nanotubes, have been used in remediation applications [1]. Such materials can be separated from water by filtration methods, but they lack selectivity—especially for heavy-metal species, such as mercury. Some chelating agents, such as 1,3-benzenediamidoethanethiol, show selectivity in binding due to the specific chemical interactions of the sulfur groups with the soft metal species. However, the problem then arises in removing the bound metal from the aqueous solution. This type of system generally requires specific conditions which favor the formation of fine precipitates to be effective.

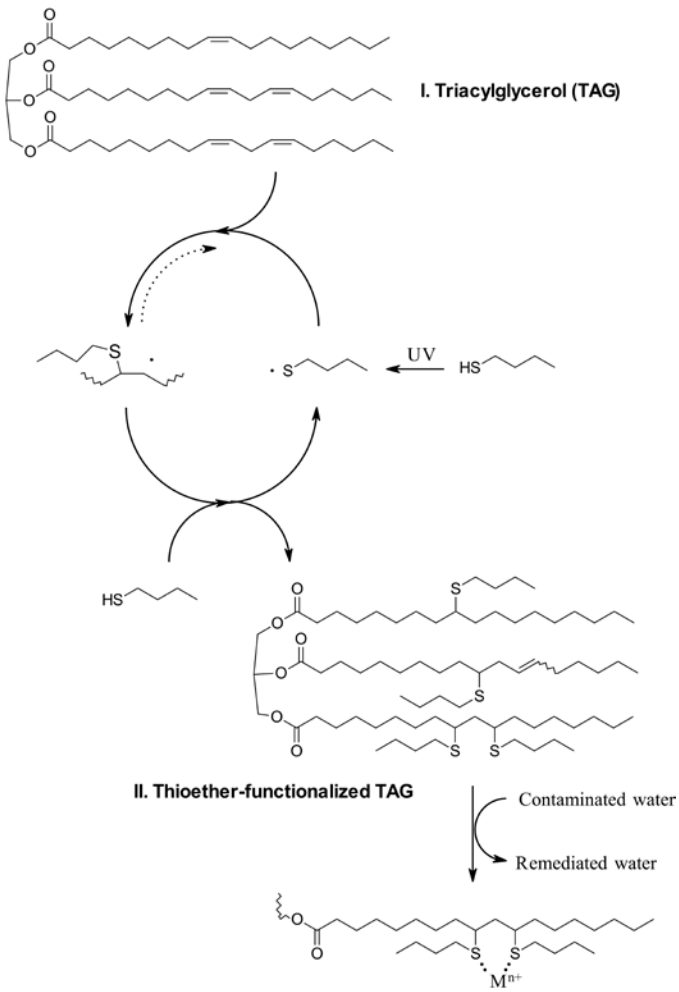
The approach detailed in this article [2–5] uses materials that possess specific interactions, such as those between sulfur and metal ions,

yet the materials that are used are also easily separated from water without precipitation. Vegetable oils are an ideal starting point for such a material, as they are used in food applications and have more recently demonstrated their utility in a variety of industrial applications [6]. They also satisfy the two most important properties for the water remediation application. They have almost no water solubility, allowing easy separation by a variety of engineering methods, and they have chemical functionality useful for the attachment of metal binding ligands. The triacylglycerol (TAG) structure of unsaturated oils, such as corn oil or canola oil, make them ideal selections.

The chemistry involved in transforming ordinary vegetable oils into highly effective remediation agents is the well-known photocatalyzed thiolene reaction [7]. In this theoretically 100% atom-efficient reaction, a thiol is added to the unsaturated group through a radical reaction (Fig. 1). The radical is generated through ultraviolet irradiation, which selectively forms an alkylthiyl radical. The key to this selectivity is the relatively weak S–H bond, ~ 360 kJ mol^{-1}, compared to ~ 413 kJ mol^{-1} for a typical C–H bond. Because other radicals are not formed in significant amounts, the alkylthiyl radical is free to react with the unsaturated groups in the vegetable oil. Virtually any thiol could be used in this method, where butane thiol was chosen in the effort to create the most effective aqueous remediation oil.

The structure of the remediation oil was studied by a variety of methods. The most direct was ^{1}H NMR spectroscopy, where up to 90% reaction of the double bonds initially present in the oil are removed as manifested by the decrease in signals corresponding to vinylic and allylic hydrogens. Similar results were also obtained using infrared ^{13}C NMR spectroscopy. The later of those techniques also displayed new signals corresponding to sulfur environments, confirming the attachment of the

FIG. 1. The synthetic route used to produce thioether-functionalized oils using the thiolene reaction



binding ligand to the TAG oil. For further information on the nature of the sulfur environments, the triacylglycrol was converted to methyl esters via base-catalyzed methanolysis (Fig. 2), and those products were analyzed by GC-mass spectrometry. The high reaction conversion, greater than 90%, was confirmed, where butylthio fatty esters, bis-butylthio fatty esters, and a small concentration of tris-butylthiofatty esters, were all identified in the chromatograms with their identities confirmed by the mass spectrometer. This is evidence that even though only one ordinary thiol was used as starting material, a variety of different metal-binding environments was produced. It also shows the versatility of the route where initial vegetable oil selection can be used to select specific metal-binding environments.

Although these new materials were initially tested as a lubricant additive [8], the versatility of the synthetic method opens up applications of real value, such as those discussed here. Because they have both the selectivity of a variety of thioether binding groups, and the low solubility imparted by the vegetable oil structure, their use in aqueous remediation is a natural application (Fig. 3).

In the first model study [4], the species chosen for study was the Ag^+ ion (Fig. 4), a convenient model for a variety of metals which are known to contaminate water. The results were quite impressive. Starting from a solution of silver nitrate at over 600 ppm, nearly complete removal of the metal ions was achieved in about an hour using a small quantity of oil. The remediation oil made from corn oil had greater efficacy than a similar oil made from canola oil, despite the overall similar sulfur contents of the two oils. This efficacy variance was due to differences in the profiles of the parent oils, which carried over into the remediation oils and resulted in different metal-binding environments. The increased amount of linoleic acid in corn oil compared to canola oil, ~56% vs ~19%, leads to an increase in the population of chains with 2 or more thiol groups (Fig. 2), hence stronger binding to the target ligand. This stronger binding results in a remarkable capacity of this oil to remove up to 2 wt% Ag^+ ions.

Next, the relative selectivity of the oil for binding mercury, even in the presence of silver, was demonstrated in a competitive experiment. A solution containing both metals, 326 mg kg^{-1} Ag^+ and 410 mg kg^{-1} Hg^{2+}, was treated with the corn oil version of the remediation oil. The results (Fig. 5) show rapid decreases of both metal species. However, only 88.9% of the silver was removed whereas mercury uptake was 99.6%. Additionally, the mercury was taken up at ~ twice the rate of the silver.

The simplest analysis of the data requires the creation of an adsorption model [5], where a useful partition coefficient (K_D) can be calculated as the ratio of metal in the oil divided

FIG. 2. The methanolysis of thioether-functionalized oils used for analytical purposes. The product, thioether-functionalized fatty acid methyl esters (FAME), can also be used as a remediant, although it is less effective due to lower insolubility.

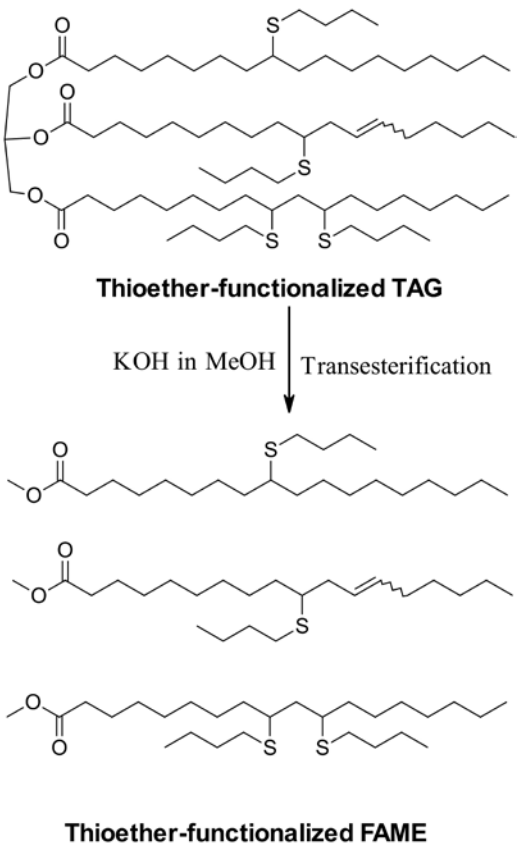


FIG. 3. A useful application of thioether-functionalized vegetable oil in aqueous remediation. The data in this graph were obtained with traditional chemical stirring, although this method is thought to produce similar or even better results.

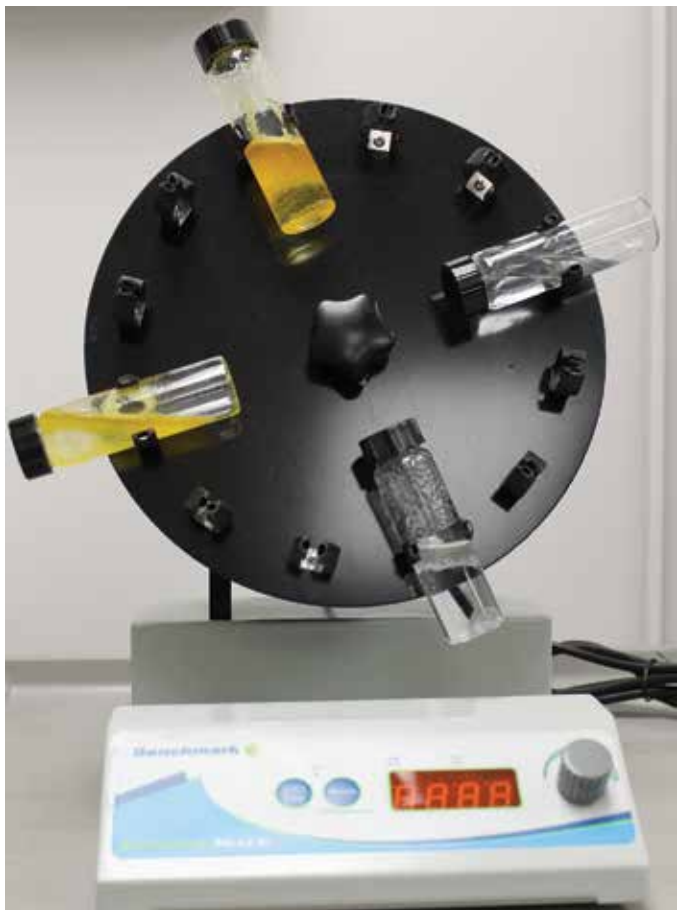


FIG. 4. The concentration of silver metal ions in a water brought in contact with different oils: unmodified corn oil (red rhombuses), thioether-functionalized canola oil (red open circles), or thioether-functionalized corn oil (blue open circles with x)

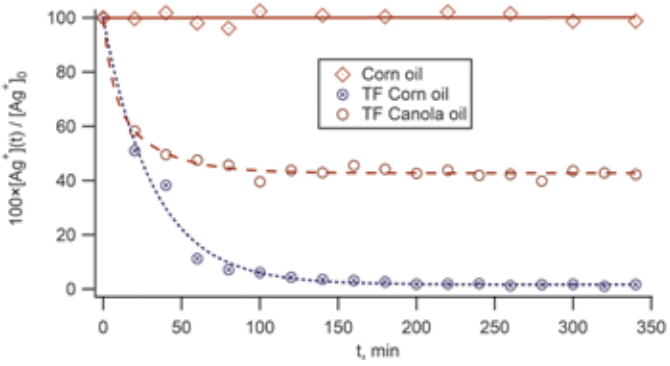
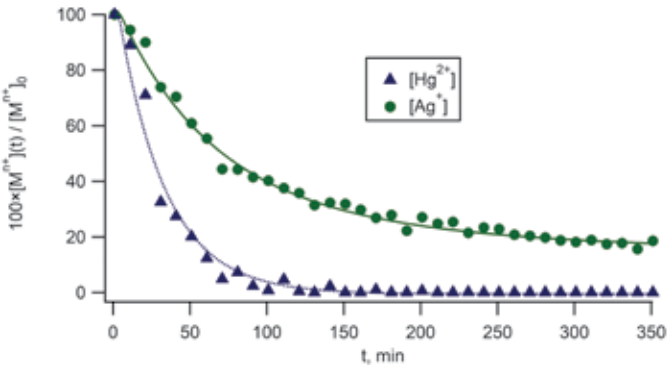


FIG. 5. The competition binding of heavy metal ions in a water brought in contact with thioether-functionalized corn oil: silver ions (green solid circles) and mercury ions (blue solid triangles)



by the metal in the aqueous phase. A higher value indicates stronger adsorption, and from data where only silver is present, a $K_{D\,Ag+}$ of 195 can be calculated. When mercury is added into the system, the competition for the binding sites causes the calculated $K_{D\,Ag+}$ value to drop to 158. The value for mercury, $K_{D\,Hg2+}$, is 200, and demonstrates the significant selectivity of this system for the mercury species. A more rigorous treatment of the data using either a Langmuir or a Freundlich isotherm is also available [5], and also shows the comparison of this remediation oil versus many other adsorbents including: bentonite clay, sulfur-chlorinated jojoba, and cellulose-grafted calix(4)arenes. From this data, it can be seen that these relatively simple remediation oils have extremely good adsorption characteristics, which is even more emphasized by their comparatively low surface area.

Chemical modification of vegetable oils is a promising way to solve some of the problems of heavy metal contamination in aqueous solutions. The advantages of a convenient liquid remediation agent are obvious, where the low water solubility of vegetable oil makes for easy separation. Different starting materials give different amounts and types of sulfur functionality, allowing this method to produce altered selectivity, simply by selecting a different parent oil. The thiolene

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reaction used in this work reaction is selective, can be performed commercially, and is amicable to scale-up or flow-reactor methodologies.

Further work on increasing the variety of thiol groups available in these remediation oils is a currently underdeveloped area. Multifunctional and even crosslinking groups could be used, assuming the end user is willing to give up the convenient liquid format.

Kenneth Doll received a B.S. in chemistry in 1995 from the University of Wyoming, and a Ph.D. from Colorado State University in 2003, the same year that he joined the US Department of Agriculture (USDA) in Peoria Illinois, USDA. Doll currently works in the Bio-Oils research unit with the objective to evaluate biologically derived oils for direct use in industrial applications or for the synthesis of chemical building blocks from those biologically based materials. He can be contacted at Kenneth.Doll@usda.gov.

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Wild about oats: detecting unlabeled oats in breakfast cereals using LC-MS

Michelle Colgrave

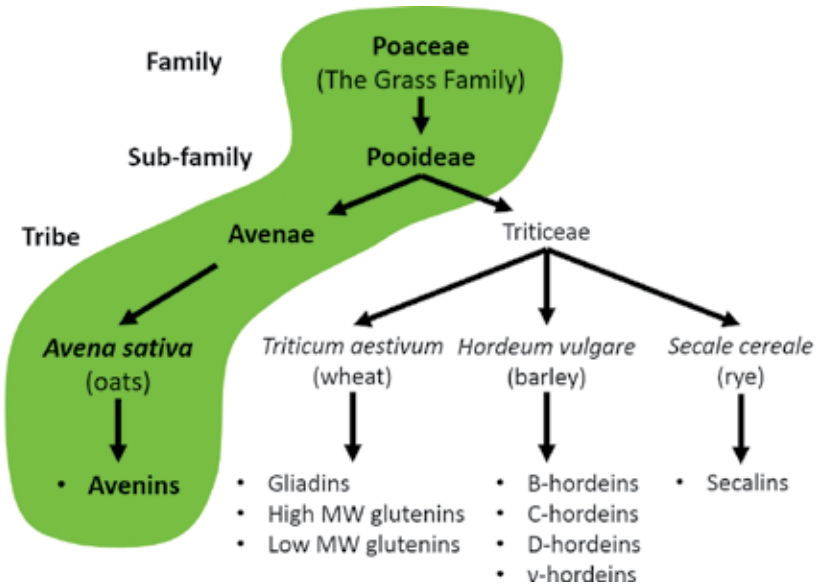
Oats have high nutritional quality, being rich in lipids, vitamins, minerals, and insoluble fiber. They also offer health benefits, with β-glucan acting to lower "bad" (low-density lipoprotein) cholesterol levels. Despite these benefits, oats are avoided by a significant portion of people who have the autoimmune disorder Coeliac disease (CD). CD is one of the most common lifelong disorders, affecting about 1% of the population worldwide. CD involves an immune response to partially digested gluten proteins, causing inflammation of the small intestine and villous atrophy. The damage results in the malabsorption of nutrients which,, in turn, triggers clinical symptoms including tiredness, abdominal pain, and diarrhea. The only treatment for CD is total avoidance of grains containing gluten in a lifelong elimination diet.

- **In North America and Europe, oats are considered "safe" for people with Coeliac disease (CD), but in Australia, oats are not recommended for consumption by people with CD, unless they do so under medical guidance.**
- **The safety of oats in CD is controversial, because oats contain proteins (avenins) that are similar to the gluten proteins in wheat, barley, and rye.**
- **Because there is no current method for detecting avenins (or oats) in food, our lab in Australia began development of an accurate method that complements those previously developed for detecting wheat and barley in oats.**

Gluten refers to storage proteins found in some grains (Fig. 1): the gliadins and glutenins in wheat, the hordeins in barley, and the secalins in rye. Similar proteins, termed the avenins, exist in oats, but they do not contain the same immunotoxic sequences (epitopes) reported in wheat, rye, and barley, and they are present at lower levels.

Oats have been identified as a candidate for a nutritious grain that could be introduced into the gluten-free (GF) diet [2]. Controversy exists over the safety of oats as part of a GF diet [3]. Typical CD symptoms,

FIG. 1. Phylogenetic relationship between oats and wheat, barley and rye (reproduced from [1])



"REPEAT EXPERIMENTS CONDUCTED ON NEWLY SOURCED FLOUR CONFIRMED THAT OAT CONTAMINATION, ALBEIT AT LOW LEVELS (<0.2%), WAS FREQUENTLY NOTED IN SPELT, RYE, BUCKWHEAT, AND RICE, WHILE TEF AND QUINOA WERE FREE OF CONTAMINATION."

including mucosal inflammation and villous atrophy, were observed in sensitive patients consuming oats in early studies [4–5], while more recently oats were shown to activate an avenin-specific immune response but lower than that noted for barley [6]. An opposing view exists wherein oats are considered safe, but contamination (by barley or wheat) as is commonly observed in the commercial oat supply [7–8] may be the source of adverse reactions. In a study of the Canadian oats supply, 88% were found to be contaminated above the 20 mg/kg threshold deemed safe for consumption [8].

In North America and Europe, oats are considered safe for people with CD, allowing pure oat products to bear a "gluten free" claim. In Australia, oats are not recommended for consumption by people with CD unless they do so under medical guidance. Part of the challenge is that there is no current test for avenins (or oats) in food. Given the widespread contamination of oats and possible intolerance of some Coeliacs to pure oats, our laboratory in Australia began development of an accurate method for testing commercial food products for contamination with oats. This method will complement the methods previously developed for detecting wheat [9] and barley [10] in oats.

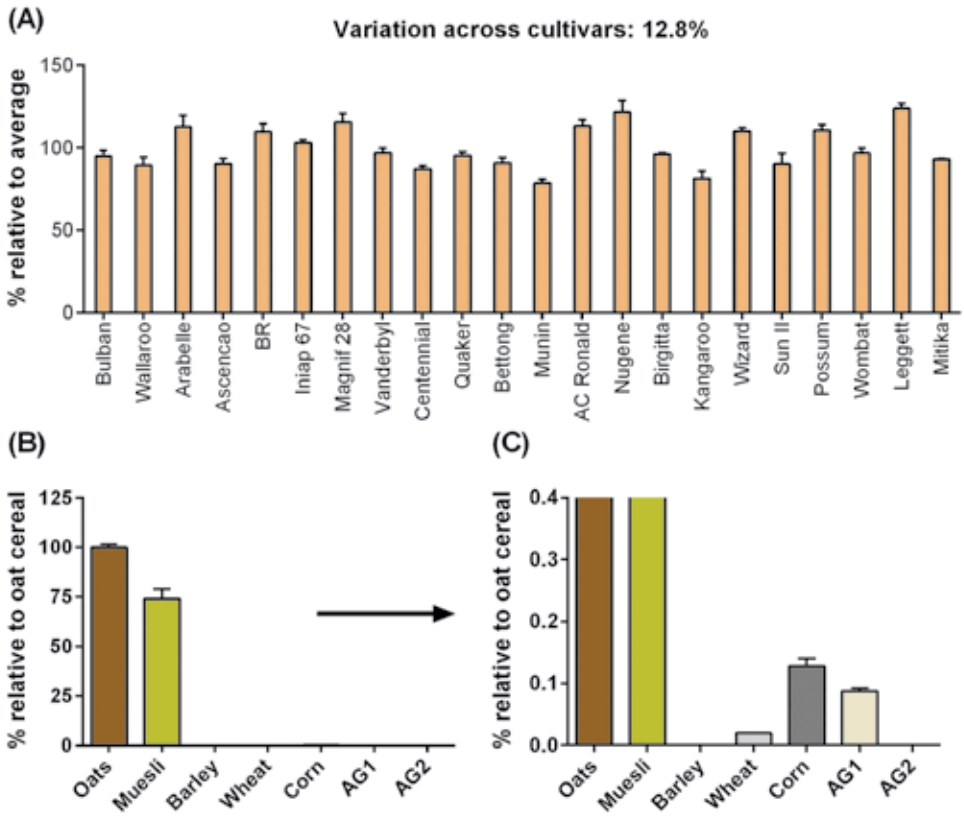
The current method endorsed by the World Health Organisation (WHO) is the ELISA R5 Mendez method, but the R5 ELISA kits do not detect oat avenins [11]. Mass spectrometry (MS) has emerged as an alternative technology for gluten detection, and our laboratory has used it as a tool to detect

wheat [9] and barley [10] contamination in commercial food products. The challenge was to develop a method to detect oats and apply this to both raw and processed food products.

In this study [1], 22 different oat cultivars that were selected based on their geographical (growing region) and temporal diversity (year of release) were explored. The range of avenin proteins that existed (19 in total), as well as many

non-gluten proteins, were identified using discovery proteomics. An average of 11 avenins (range 5–17) were detected in each of the cultivars tested. To achieve this, the proteins from the grain were extracted. Then, using enzymes as molecular scissors, the proteins were cut into smaller fragments, known as peptides. These peptides act as markers representing the proteins from which they were derived. These peptides were then analyzed by liquid chromatography (LC), a separation technique, coupled to mass spectrometry, a detection method (together known as LC-MS). Each peptide marker was assessed to ensure it was present in all oat cultivars tested (Fig. 2), and would therefore be useful no matter which oat variety was used in food manufacture. In the next round of verification experiments, the peptide markers were tested against a range of common food ingredients. This stage ensured that the peptide markers were specific to oats, but not present in pure wheat, barley, or any of the 15 common grains tested.

FIG. 2. Detection of an oat peptide marker across 22 oat cultivars; (A) in breakfast cereals relative to pure oats (B), and zoomed in to show detection of oats as an unlabelled ingredient (C). The cultivar (A) or grain species (B–C) is listed on the x-axis, where AG refers to ancient grain.



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One of the concerning results in the preliminary screen was the detection of low-level oat contamination in three of the "pure" flours purchased from health food stores. Two of the contaminated flours were rye and spelt, both gluten-containing species that would not be suitable for people with CD, thus not presenting a risk. Yet, the detection of oat contamination in the third sample (rice) was an unexpected result and warranted further investigation. Repeat experiments conducted on newly sourced flour confirmed that oat contamination, albeit at low levels (<0.2%), was frequently noted in spelt, rye, buckwheat, and rice, while tef and quinoa were free of contamination.

The peptide markers were then used to analyze seven breakfast cereals to demonstrate their ability to detect oats in processed food products. Breakfast cereals are typically produced using thermal and/or pressure treatments, commonly in the presence of sugars. These processes can lead to modification of the proteins, potentially altering both their physical and chemical properties. Despite these possible challenges, the peptide markers were found to be useful for detecting the presence of unlabelled oats in several breakfast cereals (Figs. 2B–C). The zoomed graphs (y-axis expanded) show the detection of oat contamination in three of the five breakfast cereals that were not labelled as containing oats: wheat-based cereal, corn-based cereal, and one made with ancient grains (AG1).

Overall, the newly developed analytical method for detecting oats was rapid, sensitive, and selective. LC-MS represents a suitable technology for detecting gluten contamination, which is critical for transparency in food labelling and, in turn, ensuring the wellbeing of people with CD or gluten sensitivity.

Michelle Colgrave is the Molecular Analysis Team Leader at CSIRO Agriculture and Food, based at the Queensland Bioscience Precinct in Brisbane, Australia, where she uses mass spectrometry (MS) and proteomics (the study of proteins using mass spectrometry) to help identify and characterize the functions and post-translational modifications of key proteins that will benefit Australia's livestock and plant industries and improve human health.

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Eight reasons to attend the 2019 AOCS Annual Meeting & Expo

Dan Klen

Like the St. Louis Arch that celebrates the city as "the gateway to the west," the 2019 AOCS Annual Meeting & Expo is the gateway to understanding the future technical and business challenges—and solutions—for those working in fats, oils, surfactants, proteins, and related materials. The meeting will be held May 5–8 in St. Louis, Missouri, USA, and is expected to host more than 1,500 professionals representing more than 40 countries. Here are eight reasons you should join your colleagues at the 2019 meeting.

1 GAIN INSIGHT INTO HOW EMERGING TECHNOLOGIES, INNOVATIVE RESEARCH, AND CHANGING REGULATIONS MAY AFFECT YOUR BUSINESS.

Hot Topic Symposia convene a panel of experts to provide attendees with a better understanding of the challenges and questions related to current, critical issues in the industry of fats and oils. "Ingredient Transparency" and "Healthy Oils at the Heart of Personalized Medicine" are among this year's symposia.

Attendees at a 2018 Hot topic symposium on "Healthy Oils: The New Functional Ingredient?"

2 DISCOVER HOW TO TELL GREAT SCIENCE STORIES WITH KEYNOTE SPEAKER AINISSA RAMIREZ.

Communicating the impact, benefit, and challenges of scientific research to the public is often challenging. But effectively communicating how science can "enrich the lives of people everywhere" (part of the mission of AOCS) is crucial to improving the public's understanding of science. Ainissa G. Ramirez, who earned her PhD in materials science and engineering from Stanford University, will discuss the elements of a great story and how storytelling can be used to bridge the gap between scientists and those unfamiliar with science. She will speak at the Opening Celebration on Sunday, May 5.

Ainissa Ramirez will discuss how to explain the impact, benefit, and challenges of science in an accessible manner using strong storytelling.

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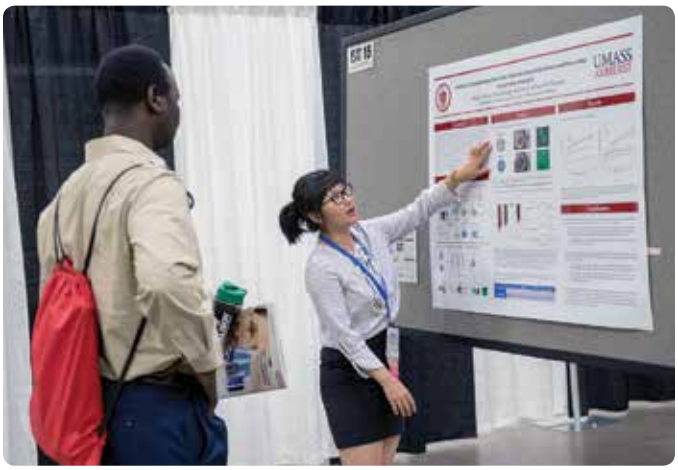


Engage with presenters at the one of the 10 interest-area poster sessions.

3 LEARN ABOUT THE LATEST RESEARCH AND DEVELOPMENTS FROM EXPERTS ACROSS THE INDUSTRY.

Like last year, this year's technical program consists of more than 650 oral and poster presentations across 10 interest areas. The strong technical program provides ample sessions to learn about both broad and niche advancements in the science and technology of fats, oils, surfactants, lipids, and proteins. AOCS offers *The App*, released about two weeks before the meeting, for you to plan your schedule and maximize your time at the meeting.

4 DEVELOP SPECIFIC EXPERTISE WITH A PRE-MEETING COURSE.

Whether you need a crash course in the fundamentals of edible oils processing or need to expand your knowledge of lipids and skin health, AOCS pre-meeting courses and workshops provide essential knowledge in a condensed format. Speakers represent academia, industry, and government. The following pre-meeting courses and workshops are being offered this year:

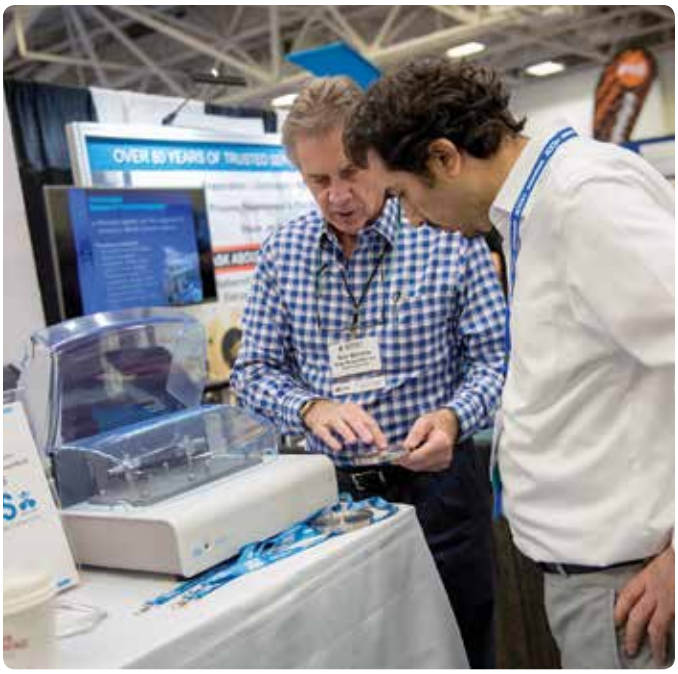
- Fundamentals of Edible Oil Processing
- New Techniques in Edible Oil Processing and Refinery Optimization
- 2019 AOCS Lipids School on Lipids and Skin Health
- Olive Oil Workshop and Tasting Luncheon

5 CREATE NEW PROFESSIONAL BONDS THROUGH CAREER CATALYST AND OTHER NETWORKING EVENTS.

The Annual Meeting hosts many networking events where you can create lifelong professional bonds that go beyond the lab. Before the Opening Celebration on Sunday, AOCS interest-focused and career-based communities will host "Career Catalyst" for all registrants at the convention center, where you can meet new colleagues in a structured yet casual setting. After the Opening Celebration, attendees can reconnect with colleagues, and continue to meet new ones, at the President's Reception—Welcome to St. Louis!

Divisions and Common Interest Groups also host receptions, luncheons, and dinners during the meeting, where colleagues with similar technical interests or at similar career stages can meet and talk about the latest in their fields. You can buy tickets in advance during registration for specific luncheons and dinners. Receptions are free.

The Young Professional Common Interest Group at their reception last year.



The number of companies attending the 2019 Annual Meeting Expo is expected to grow from 2018.

6 FIND SOLUTIONS TO A BUSINESS CHALLENGE AND THE NEWEST PRODUCTS AT THE EXPO.

Are you looking for solutions to a business challenge, or curious about the newest products from top suppliers? More than 95 companies from across the world are expected to attend the Expo, where you can learn about their newest products and services. In addition, the Technology Fast Track is a special session hosted Monday through Wednesday in the Exhibition Hall; companies highlight their technological innovations in 5-minute presentations.

7 JOIN US FOR A CELEBRATION OF OUR MEMBERS AND VOLUNTEERS AND LEARN WHAT THE AOCS FAMILY IS ALL ABOUT.

It takes a village, as the saying goes. To celebrate the more than 500 volunteers who help make the AOCS Family what it is, AOCS is hosting a member and volunteer appreciation luncheon on Wednesday afternoon. Even if you are not a member, you are welcome and encouraged to join us at the luncheon and discover what makes our membership like no other.

8 EXPLORE ST. LOUIS THROUGH AN AOCS-ORGANIZED TOUR OR THE 5K FUN RUN/WALK.

Start off Tuesday morning by walking or running around Gateway Arch National Park in Downtown St. Louis. The Park, situated along the shore of the Mississippi River, provides a scenic view of the historic Eads Bridge, in addition to the Arch. There is also a full-day excursion that includes a stop at the Anheuser-Bush Brewery, and an afternoon excursion that includes the Science Center and Planetarium and "The Loop," a historic district of restaurants, shopping, and entertainment on the National Register of Places. Pre-registration is required for these events and space is limited, so be sure to sign up early.

As the gateway to the future of our industry, the 2019 AOCS Annual Meeting will equip attendees with the knowledge, tools, and network to adapt to the technical and business challenges of the future. Register by February 22 at annualmeeting.aocs.org/2019 to save up to US $200. We'll meet you in St. Louis.

Dan Klen is a communication specialist at AOCS. He can be reached at dklen@aocs.org.

Gateway Arch National Park.

Plants for pets? Can cats and dogs be vegetarian?

Olio is an Inform *column that highlights research, issues, trends, and technologies of interest to the oils and fats community.*

Rebecca Guenard

A lynx and a wolf prowl through pet food commercials, persuading pet owners that cats and dogs need meat due to the savage origins of their domestic descendants. Over the past decade, such marketing campaigns have been successful, and sales of high-meat pet foods increased. Today, population growth and global warming are causing some pet owners to question the sustainability of meat production. As humans shift to meat-free diets they want their pets to do the same. Is a plant-based diet healthy for companion animals?

Pet food advertisements with wild animals are evolutionarily accurate. Cats and dogs belong to the order Carnivora; their ancestors existed on a diet of captured prey. The sharp teeth these predecessors used to rip flesh are still evident in modern animals. However, dogs no longer need as much protein as their wolf ancestors due to biological adaptations for better carbohydrate metabolism (https://www.nature.com/articles/nature11837). Scientists estimate that dogs became dependent on table scraps about 30,000 years ago, when humans domesticated them from wolves. As they began to rely on humans, they evolved behaviorally and physiologically to incorporate more plant-based foods into their diet.

Cats, on the other hand, are believed to have adapted to companionship 20,000 years later than dogs. In addition, cats initially served a very different companion role than dogs; they were essentially exterminators (https://doi:10.3390/ani6090057). Though they came to rely more on humans, they did not abandon their hunting instincts as significantly as dogs did. Less human interaction resulted in less biological adaptation. Consequently, modern cats, like their wild ancestors, need to get half of their metabolizable energy from protein (by comparison, dogs require a third).

Andrew Knight, veterinarian and professor of animal welfare and ethics at the University of Winchester in Hampshire, England, says the origin of pet behavior may be interesting, but it has little basis for how we should feed animals for the way they live today. Routine feeding intervals over longer lifespans require that pets receive species-specific nutritional profiles which can be achieved on a meat-free diet.

"No animals—or humans, for that matter—have a biological requirement for any particular ingredient, but we all have requirements for a set of nutrients," says Knight. "And there is no scientific reason why we can't provide all the nutrients required in formulations that are entirely plant-, mineral-, and synthetic-based."

The pet food company Wild Earth is taking this to heart by using fermentation to synthesize proteins for dog treats. "There is still a lot of unscientific thinking about nutrition, that there is something about meat that cats need." says Ron Ghiseta, chief science officer for the company. He says he respects why people have this misunderstanding, but it means

a vegan pet food company like his must navigate such social bias. For now, Wild Earth caters to dogs.

Currently, Wild Earth is focused on the fungus *Aspergillus oryzae*, better known as koji, the same microorganism used to make soy sauce and sake. The fungi make proteins for pet food through a fermentation process which Ghiseta says may eventually be used to make the amino acids taurine and carnitine that cat physiology cannot produce. Wild Earth has also developed lab-grown mouse meat cultured from mouse cells. Once their dog food is established in the market they plan to launch this lab-grown meat product for cats.

The mission of a company like Wild Earth follows a trend among consumers to be more socially conscious. Pet owners want to feed their animals vegan or vegetarian diets because they are aware of the issues surrounding the ecological costs of industrial farming.

"We are reaching the limit of the earth to bear produce to feed people and the population has not stopped growing yet," says Ghiseta. "The demand for protein is growing globally." He says the pressure to mass produce livestock to meet this demand means the quality of food suffers.

"There are a lot of wonderful people who produce meat and they have great intentions, but the demands of that scale are going to create all kinds of quality pressure," says Ghiseta. "It is much easier to scale protein production in a fermentation plant with media and tanks rather than use more land to grow grass and convert that to animal protein." He says Wild Earth wants to leverage their knowledge of microbiology and the chemical engineering of fermentation to create more scalable food.

Research shows there is a market for it. Estimates indicate there are 1.5 billion vegetarians globally. In the developing world, many are vegetarians by necessity, which leaves 75 million people who are vegetarians by choice. In nearly a decade since that data was collected, the number of voluntary vegetarians has grown along with education and affluence.

Affluent individuals tend to be pet owners. According to the European Pet Food Industry Federation (FEDIAF), 80 million households in Europe own a minimum of one pet (http://www.fediaf.org/who-we-are/european-statistics.html). In 2016, FEDIAF estimated €19.5 billion ($21.5 billion) was spent on pet food in Europe. A study published last year estimates that there are 163 million dogs and cats in the United States and calculated that 25–30% of the land, water, and fossil fuel used in the country can be attributed to the manufacture of protein for pet food (https://doi.org/10.1371/journal.pone.0181301).

With more and more pet owners concerned about the health, welfare, and environmental impact of agricultural animals, the number of vegetarian cats and dogs is likely to increase. Unfortunately, not all vegetarian pet food brands are reliably nutritious.

Knight performed a review of several studies evaluating whether the nutritional content of commercial plant-based diets matched the claims on their labels (https://www.mdpi.com/2076-2615/6/9/57). Such nutritional claims must meet a set of guidelines decided on by the Association of American Feed Control Officers in the United States and the European Pet Food Industry in the European Union.

Analysis of several different brands found that about 25% of commercial vegetarian pet foods are nutritionally deficient. Typical deficiencies existed in the amount of protein, fat, and fiber. Knight points out that these deficiencies say more about the quality control of the processes used by the manufacturers than the viability of a meatless diet for pets. He does do not feel that these findings should discourage owners from plant-based pet food. Many high-meat commercial pet foods were also nutritionally lacking.

Studies comparing meat-free diets to routine commercial diets found that, in either case, animals were in good physical condition with normal blood tests after four months (https://doi.org/10.2527/jas.2014-7789). Knight says most commercial plant-based diets are formulated to meet the nutritional needs of a specific species while also achieving palatability and bioavailability. Meeting these needs on a homemade diet is more of a challenge.

"I would advise people if they are going on a plant-based diet to ensure the diet is nutritionally complete and reasonably balanced," says Knight. "You are more likely to be successful with a high-quality diet, such as a veterinary prescription diet."

To limit deficiencies Knight recommends a gradual transition to a plant-based diet while closely monitoring a pet's health. In addition, owners should check urine alkalinity regularly throughout the transition. High alkalinity could lead to health problems. Aside from these precautions, evidence indicates pets can live healthy, active lives on a diet devoid of meat.

Olio is produced by Inform*'s associate editor, Rebecca Guenard. She can be contacted at rebecca.guenard@aocs.org.*

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"AOCS and my volunteer experience have helped me network and remain connected with new research in the industry, which in turn helped me with product development and fats and oils portfolio management."

Sarah A. Echols, R&D Manager—Nut Butters at Golden Boy Foods and member of the Edible Applications Technology Division

- Student member in 2010–2011
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Characterization of industrial polymers for regulatory submission

Regulatory Review is a regular column featuring updates on regulatory matters concerning oils- and fats-related industries.

Yawei Zhang

Polymers are widely used in a vast range of industries. For this reason, many countries have updated their chemical regulations and integrated the concept of polymers into them. Most regulatory systems apply the OECD definition of a polymer, which must meet three criteria:

- the substance consists of molecules characterized by a sequence of one or more types of monomer units distributed over a range of molecular weights (MWs), in which differences in MW are primarily attributable to differences in the number of monomer units;
- >50% w/w of the molecules must consist of at least three monomer units, which are covalently bound to at least one other monomer unit or "other reactant." This is defined as a molecule covalently bound to one or more sequences of monomer units but which, under the relevant reaction conditions used for the particular process, cannot become a repeating unit in the polymer structure. Examples include capping agents, chain transfer agents and initiators; and
- the content of polymer species with the same MW represents <50% w/w of the total distribution.

It is also important to note that polymer nomenclature can be very complex, and different regulatory systems have adopted different conventions. If there is doubt over the correct name for the substance, the inventory expert service of Cas (https://www.cas.org/services/knowledge/inventory-expert) may be able to help.

Although the same definition has been adopted, different countries have their own ideas of how to regulate polymers, which leads to differing regulatory requirements worldwide. For instance, the notification of a polymer itself might be required in Australia, Canada, South Korea, China, and the United States, whereas in the European Union, polymers are exempted from registration and evaluation under REACH, but are still are subject to authorization and restriction. Manufacturers and importers of polymers in the EU are required to register the monomers and/or other substances used as building blocks if they are present at amounts of >2% in the polymer, as these are generally recognized as being of higher concern than the polymer molecule itself.

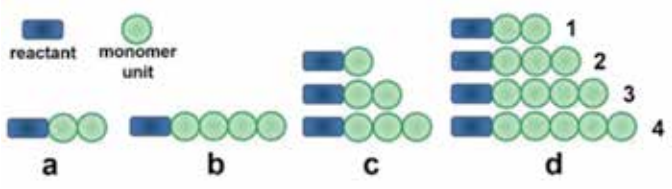
Due to the variations in global regulatory requirements, a complete analytical characterization of polymers would be essential to establish all the obligations under different regulations. This is a short overview of the most common. In general, physico-chemical characterization of discrete substances (molecules) is straightforward. Polymers introduce complexity, as the "substance" to be characterized is a mixture of molecules that vary widely in MW, composition or both.

MOLECULAR WEIGHT

To understand the properties of a polymer that are relevant to a risk assessment, such as the potential for diffusion through biological membranes or bioavailability, it is necessary to know the length of the polymer chains. Chain length is often expressed in terms of the MW of the polymer chain, which is related to the relative molecular mass of the monomers and the number of these in the chain.

However, synthetic polymers exist as a distribution of different chain lengths and thus, MWs. So unlike for discrete molecules, the MW is not a single value. This must instead be described as an average derived from the MWs of all the chains in the sample. Several different averages can be calculated, but the two most commonly cited are "weight average MW" (Mw) and "number average MW" (Mn).

The Mw considers the total weight of all molecules, but not the number at each individual weight. Therefore, it can be skewed by a small percentage of large molecules, providing a false low estimate of the mass of the majority. The Mn takes into account the number of molecules at all of the various MWs in the sample and is thus representative of the average weight of the typical components.



For this reason, the Mn is the average value used in regulatory submissions and risk assessments. MW analysis methods fall into three categories:

- absolute, where measurement is directly related to the MW, without assumptions about the chemical and/or physical properties of the polymer;
- equivalent, where the chemical structure of the polymer must be known to obtain the MW; and
- relative, where the quantity measured depends on the physical structure of the polymer being tested. A calibration curve relating detector response and MW values must be known, and is typically established by measurements on a series of standards of the analyte polymer, or a surrogate with a very similar chemical and physical structure.

RELATIVE ANALYSIS

The most common method of analysis is gel permeation chromatography (GPC), also known as size exclusion chromatography (SEC). In this, the separation of the polymer molecules is ideally governed by the hydrodynamic volume (HV) of each molecular species as it passes through a column filled with porous material. Smaller molecules penetrate the pores and thereby travel a longer path through the column, eluting after larger molecules.

One limitation with GPC is that the polymer must be soluble in one of the solvents commonly used. High-temperature GPC can address polymers insoluble at standard temperatures, like polyolefins. Detection techniques used for GPC include refractive index (RI), UV absorption and light scattering (LS).

GPC may be absolute or relative, depending on the method of calibration. Though the linear polystyrenes (PSs) are used extensively as internal standards, they may not always provide a reliable calibration as a function of the structure and functionality of the polymer being analysed. For instance, linear PS has a relatively high surface area/MW ratio and therefore possesses a large HV, because it can sweep out a large volume. A highly branched polymer has a lower surface area-to-MW ratio, as it is more spherical in shape and thus has a smaller HV. Polymer functionality for example, ionic or reactive, also affects molecular mobility, limiting the value of linear PS standards for calibration.

Despite these drawbacks, GPC has been established as the method of choice for polymer characterization. Accurate GPC for complex polymers requires using the standards related to the polymer or a suitable analogue and these would require absolute analysis to establish the MW values prior to use in the subsequent relative analysis.

ABSOLUTE ANALYSIS

Matrix-assisted laser desorption/ionisation and time-of-flight mass spectrometry (Maldi-ToF MS) is a technique comprising two sequential steps that was originally used to determine the composition of biomolecules. It is also used for complex industrial polymers, especially those insoluble in common GPC solvents or that incorporate bio-based or other complex reactants.

In Maldi, the sample is mixed in a matrix that absorbs the laser light and converts it to heat energy. A small part of the matrix is vaporized together with the sample. In ToF MS, charged ions of various sizes are generated, a potential difference between the sample ground attracts the ions and the velocity of the these is determined by the law of conservation of energy. Ions with smaller mass-to-charge ratio (m/z) value and more highly charged ions move faster until they reach the detector. Consequently, the time of ion flight differs according its m/z value.

Maldi-ToF MS provides information not only on the MW distribution, but also on the composition of the individual oligomer and polymer units detected. There is one drawback, however. Although the determination of the MW distribution via Maldi-ToF MS works quite well with polymers of very low polydispersity, it is possible for conflict to arise with the third element of the common definition of a polymer.

COMPOSITION AND IDENTITY

Polymer composition is typically defined by the relative weight percent of the monomers and other reactants used in its manufacture, taking into account also the excess charges and residuals due to incomplete reaction. Infrared (IR) spectroscopy is useful for confirming the presence of functional groups like acids and alcohols. Nuclear magnetic resonance (NMR) spectroscopy provides more compositional details and is commonly used in end group analysis, as well as in the determination of copolymer compositions.

While physico-chemical characterization of polymers can be challenging, it is essential to understand their structure and composition, so that the information provided in any regulatory submission represents the actual substance that is intended to be distributed in commerce. Many other factors can affect the risk assessment, for instance the presence of certain heavy metals, the existence of, and potential for, crosslinking or the ready degradation by, or transformation of, the polymer in the environment.

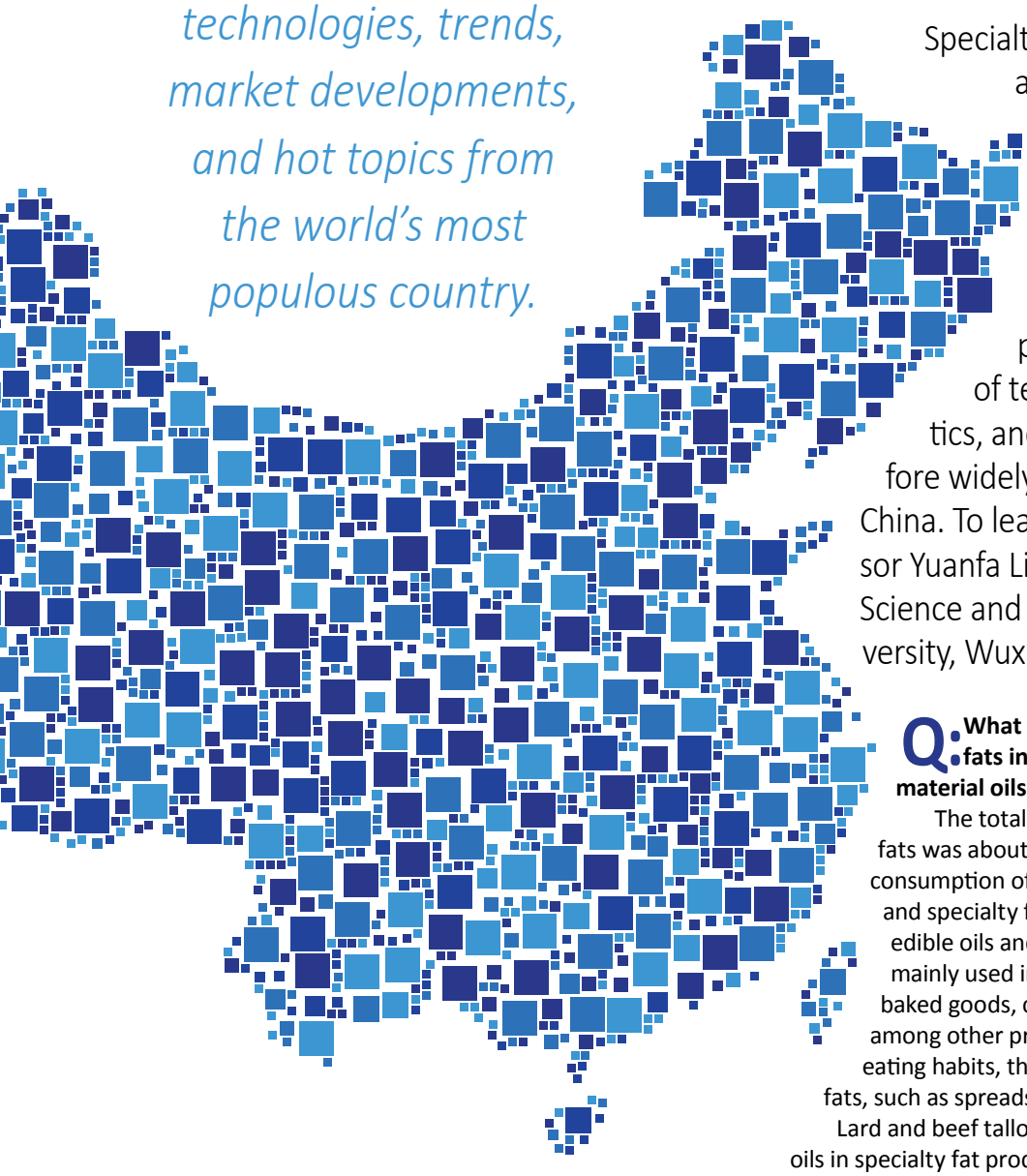
A detailed presentation of the basic physico-chemical characterization data, including sufficient supporting documentation, reduces the likelihood of conservative assumptions being used, thus facilitating an accurate assessment of risk. Information about the data collection method would typically include the instrument details and running conditions, identification of standards and calibration curve (if any) and the "slice table," showing the number of "slices" within the peak of interest for which the MW is calculated.

Yawei Zhang is a professional in chemistry and analytics, Knoell Germany. Antje Britze, Radu Adrian Gropeanu and Jeffrey Hafer also contributed to this article.

The development of specialty fat industries in China

China Update highlights new technologies, trends, market developments, and hot topics from the world's most populous country.

Zong Meng



Specialty fats made of vegetable oils and animal fats, such as shortenings, margarines, chocolate fats, filling fats, coating fats, ice cream fats, non-dairy creamer fats, and so on, have a positive influence on product performance in terms of texture, sensory characteristics, and shelf-life. They are therefore widely used in the food industry in China. To learn more, I interviewed Professor Yuanfa Liu, Dean of the School of Food Science and Technology at Jiangnan University, Wuxi, Jiangsu, China.

Q: What is the annual consumption of specialty fats in China, and what are the main raw material oils and fats used to make them?

The total annual consumption of edible oils and fats was about 34.3 million tons in 2017. The annual consumption of specialty fats was 2.81 million tons, and specialty fats accounted for about 8.2% of total edible oils and fats consumption. Specialty fats are mainly used in the food industry and consumed as baked goods, chocolate, fried foods, whipped topping, among other products. Unlike European and American eating habits, there are fewer direct uses of specialty fats, such as spreads, in Chinese households.

Lard and beef tallow are the two animal fats used as base oils in specialty fat production, and large quantities of beef tallow are imported from Australia and New Zealand. Palm oil,

palm kernel oil, and coconut oil are three tropical oils that are largely used as base oils for food specialty fats. The consumption of palm oil is much higher than that of palm kernel oil and coconut oil, and has exceeded 5 million tons annually for nearly 10 years now.

Q: What are the main production areas of specialty fat products in China?

More than half of the specialty fats in China are produced in three areas: the Circum-Bohai Sea Economic Zone, Yangtze River Delta, and the Pearl River Delta, which respectively account for 19%, 23%, and 22% of total production. These three areas are also the most economically developed areas of China, and important hubs for the Chinese food industry.

Q: What are the development trends and challenges of specialty fats in China?

In 2004, the annual consumption of specialty fats was about 0.50 million tons. It is estimated that the consumption of specialty fats from 2004 to 2017 increased at an annual rate of 15%–40%, and forecasts predict that specialty fat consumption will increase by more than 15% in the near future. Meanwhile, application and development trends have shifted from trans/low-trans products to non/zero-trans or non-hydrogenated products, and consumers are becoming increasingly interested in low-saturated and low-energy products. The Chinese National Standard, namely GB 28050-2011 (National Food Safety Standard, General Rules for Nutrition Labeling of Prepackaged Food) includes two rules for trans-fatty acids: (1) the label claim "non-trans-fatty acid" can only be made if the content of trans fatty acid is lower than 0.3g per 100g (solid) or 100mL (liquid) and (2) the trans fatty acid intake should not exceed 2.2g/day or more than 1% of total energy intake for the whole day.

The challenges encountered by the Chinese specialty fat industry are enormous. Research and development is weak for Chinese enterprises, especially for small businesses. National standards for products are scarce and dated. For example, the product standard for shortening that has been implemented since 1992 cannot keep pace with the rapid development of the Chinese food industry and the demand for specialty fats.

Zong Meng is an associate professor in the School of Food Science and Technology, Jiangnan University, 1800 Lihu Road, Wuxi 214122, Jiangsu, China, and a contributing editor of Inform. *He can be contacted at mengzong@jiangnan.edu.cn.*

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Learn more about oils, fats, and proteins in China and nearby regions

The best way to get up to speed on specialty fats and dozens of other topics in China and nearby regions is to attend the second **AOCS China Section Conference: Health, Advanced Processing, and Value-Added Utilization, November 8–10, 2019, https://www.aocschina.com/.**

This special two-day conference will be held in **Zhujiang (Pearl River) Hotel,** Guangzhou (Canton), China, a city in Southern China, not far from Hong Kong, Shenzhen, and many South Asian countries. The conference features a half day plenary session that will cover raw material production and supply; marketing trends and consumer perceptions; special oilseed crops and lipids; health and nutrition; and advanced processing and applications for lipids, proteins and co-products. A full day of technical sessions will cover various topics, including analytics, safety, lipid oxidation, quality, biocatalysis, processing, edible and industrial application, health benefits, biopeptides, and proteins. Young scientist forums and site visits to two nearby universities are also on the agenda.

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Volunteering as a networking tool

Member Spotlight is a regular column that features members who play critical roles in AOCS.

"I've been involved with AOCS since 2011," said Cynthia Srigley, a research chemist with the US Food and Drug Administration's (FDA) Center for Food Safety and Applied Nutrition. "From day one, I felt welcomed by the community and that my research was valued and appreciated."

Srigley joined FDA in 2011 as a postdoctoral research fellow working on analytical methods for trans fat. Her current research focuses on analytical methods development and validation for the analysis of fatty acids, sterols, and other lipids in foods and dietary supplements. "Marine oils are my favorite matrix," she noted, "because of their complexity."

Srigley is serving her second term as secretary/treasurer of the AOCS Analytical Division. As such, she works with AOCS staff to develop the division budget, to plan the annual luncheon, and to record the minutes from the Executive Committee and Analytical Division Session Planning Roundtable meetings. "I felt that this role would be a great opportunity to contribute my technical and leadership skills in serving AOCS," Srigley added.

"I find that one of the best ways that my work supports both FDA and AOCS is by participating in multi-laboratory studies," she remarked. This has allowed her to develop a strong network within the Analytical Division. "The Division members are an exceptionally talented group of individuals, and I am comfortable reaching out to them for technical assistance or recommendations."

Srigley has a suggestion for students and others, like herself, who are early in their careers. "I highly recommend attending the short courses offered each year prior to the start of the Annual Meeting. These courses provide a basic technical background and introduce the various areas of the research within industry, academia, and government. More importantly, they offer the opportunity to network with experts in the field and other AOCS members. It's great way to kick off the Annual Meeting," she concluded.

Fast facts

Name	Cynthia Srigley (pronounced SRIG-lee)
Joined AOCS	2013
Education	Ph.D. in nutritional sciences with a concentration in molecular nutrition from Cornell University (2011)
Job title	Research chemist
Employer	US Food and Drug Administration's Center for Food Safety and Applied Nutrition (College Park, Maryland, USA)
Role in AOCS	Secretary/treasurer, AOCS Analytical Division
High-fat indulgence	Beer-battered French fries: I rarely order them, but when I do, I'll eat them all before even touching the rest of my meal.
Fat-related nickname	In grad school, my labmates and I would call ourselves the "Fat Girls."
Most memorable AOCS experience	I love attending the Uniform Methods Committee meetings each year because they highlight some of the most important methods that are currently being developed and validated. I leave those meetings feeling inspired and motivated to pursue new research activities that support the needs of government and industry.
Other involvement	Examination Board chair, Annual Meeting session chair, Analytical Division Executive Steering Committee

PATENTS

Lipid-based nanoparticles

Annapragada, A.V., *et al.*, University of Houston and Alzeca Biosciences, LLC, US10124078, November 13, 2018

Lipid-based nanoparticle compositions are provided. The compositions generally comprise lipid-hydrophilic polymer-amyloid binding ligand conjugates, and may be liposomal compositions. The compositions, including the liposomal compositions, may be useful for imaging and/or the treatment of amyloid-beta. plaque deposits characteristic of Alzheimer's disease.

Renewable oil refining processes

Morgan, T.G., *et al.*, Advanced Energy Development, US10125331, November 13, 2018

Processes are described for refining a renewable oil. The processes may include the steps of adding one or more compounds to the renewable oil to produce a soap stock in the renewable oil, and separating at least a portion of the soap stock from the renewable oil. The processes may further include adding a polymer to the separated renewable oil to produce a refined renewable oil.

Oral compositions containing gel networks

Deckner, G.E., *et al.*, The Procter & Gamble Co., US10130567, November 20, 2018

The present invention is directed to an oral composition containing a gel network phase comprising: (i) one or more fatty amphiphiles, (ii) one or more surfactants, and (iii) one or more solvents; and an oral carrier phase. In certain embodiments, the gel network is used to structure the oral composition. The present invention is also directed to a method of forming an oral composition containing a gel network.

Concentrated therapeutic phospholipid compositions

Sampalis, F., *et al.*, Acasti Pharma Inc., US10130644, November 20, 2018

The invention relates to concentrated therapeutic phospholipid compositions; methods for treating or preventing diseases associated with cardiovascular disease, metabolic syndrome, inflammation and diseases associated therewith, neurodevelopmental diseases, and neurodegenerative diseases, comprising administering an effective amount of a concentrated therapeutic phospholipid composition.

Lubricant composition of matter and methods of preparation

Benecke, H.P., *et al.*, Petroliam Nasional Berhad, US10131616, November 20, 2018

Ester polyol esters are a unique class of lubricants that have adjustable molecular weights, viscosities, and pour points based on the character of their reaction materials and relative ratios. There is provided a method for preparing at least one ester polyol ester, the method comprising esterifying an ester polyol reaction mixture to produce ester polyol, the reaction mixture comprising an ozone acid mixture and at least one primary polyol, wherein the ozone acid mixture comprises at least one dicarboxylic acid and at least one monocarboxylic acid; and capping the ester polyol with at least one capping carboxylic acid to produce ester polyol ester.

Chocolate wax composition for candles

Steiner, J., US10136659, November 27, 2018

A candle or candle composition is provided made from only edible materials and is formed from palatably desirable compositions. Cocoa butter and chocolate at a ratio of between approximately three parts to approximately five parts cocoa butter to one-part chocolate provides a composition that is moldable and capable of being formed into a self-supporting candle structure that is capable of being lit and maintaining a flame. At the same time, the unignited portions, when melted, creates a pool of melted, edible chocolate flavor material. Inclusion of trace amounts of sugar and vanilla improve the palatability and gastronomic effect of the melted material.

Cosmetic composition and methods of use thereof

Collier, J., *et al.*, Mary Kay Inc**.**, US10137074, November 27, 2018

The present invention relates generally to the field of cosmetics. More particularly, it concerns compositions that can be used to exfoliate, moisturize, or prepare skin for moisturization. In another aspect, the composition can be used as a cleanser to remove dirt, oil, grease, tars, etc. from surfaces.

Water-in-oil polyacrylamide-based microemulsions and related methods

Sexton, F.E., *et al.*, Exacto, Inc., US10138366, November 27, 2018

A water-in-oil microemulsion, including a polyacrylamide, a fatty acid, a surfactant, an oil continuous phase, and an aqueous discontinuous phase in the oil continuous phase. The fatty acid includes a tall oil fatty acid, oleic acid, or a combination of a tall oil fatty acid and oleic acid. The water-in-oil microemulsion contains 6 to 48 parts by weight of the polyacrylamide, 30 to 62 parts by weight of the fatty acid, and 20 to 44 parts by weight of the surfactant per 100 parts by weight of the polyacrylamide, the fatty acid, and the surfactant combined.

Low energy, cold process formulation aid

Mateu, J.R., *et al*., Jeen International Corp., US10138374, November 27, 2018

Provided are cold process formulation aids (CPFAs), methods for their manufacture, and personal care products made using them. CPFAs include (i) a polymer having an aliphatic backbone and a plurality of pendant groups thereon that are pendant ionic or ionizable groups, or pendant groups having at least one permanent dipole that includes an acid, alcohol, thiol, ester, amine, amide, imide, imine, or nitrile moiety, and (ii) a wax selected from natural waxes and synthetic waxes, wherein if the wax is not micronized and is not self-emulsifying, the ratio, by weight, of the non-micronized wax to the polymer having an aliphatic backbone is from about 60:40 to 80:20, and if the wax is a micronized wax or a self-emulsifying wax, the ratio, by weight, of wax to polymer backbone is 70:30 to 98:2.

Conversion of lipids into olefins

Ullah, A., *et al*., University of Alberta, US10138430, November 27, 2018

A method of converting lipids to useful olefins includes reacting a mixture of lipids and a reactant olefin with microwave irradiation in the presence of ruthenium metathesis catalysts. The lipids may be unsaturated triacylglycerols or alkyl esters of fatty acids. The lipids may be sourced from renewable sources such as vegetable oil, waste cooking oil, or waste animal products.

Blown and stripped blend of soybean oil and corn stillage oil

Hora, M.J., *et al*., Cargill, Inc., US10144902, December 4, 2018

A method for producing a high-viscosity, low-volatiles blown-stripped oil blend is provided. The method may include the steps of: (i) obtaining an oil blend of corn stillage oil and soybean oil having a weight ratio of corn stillage oil to soybean oil of from about 1:2 to 3:1; (ii) heating the oil blend to at least 90°C.; (iii) passing air through the heated oil blend to produce a blown oil having a viscosity of at least 50 cSt at 40°C.; and (iv) stripping the blown oil from step (iii) to reduce an acid value of the blown oil to less than 5.0 mg KOH/gram.

Semi-continuous process for the production of rhamnolipids at high yield and titer

Lohitharn, N., Logos Technologies, LLC, US10144943, December 4, 2018

Provided is a semi-continuous fermentation method of a rhamnolipid producing microorganism to produce rhamnolipids. The fermentation may be run as a batch process but at the end of the fermentation, at least about 70% of the fermentation medium comprising one or more rhamnolipids is drawn out and the new culture medium (feedstock) is fed in as a replacement. This process may be repeated for at least about one month without having to sacrifice RL yield and titer. It allows the fermenter to be utilized at a higher capacity with less downtime for clean-up compared to batch and fed batch fermentation strategies.

Method for preparing diglyceride using bubble column reactor

Wang, Y., *et al*., Jinan University, US10138501, November 27, 2018

Disclosed is a method for synthesizing diglyceride using a bubble column reactor. The method comprises the steps of: an immobilized enzyme is placed on the bearing mechanism of the bubble column reactor; a hot bath mechanism is actuated to heat the reactor body to 55–75° C; glycerol, fatty acid, and water are added into a feed chute, preheated to 55–75°C, and then transferred into the reactor body to initiate the reaction; a bubbling mechanism is actuated so that the inert gas is continuously blown into the reactor body via a sieve plate, forming boiling-like bubbles which promotes the mixing and hence to facilitate the reaction; after the reaction, the water bath mechanism and the bubbling mechanism are turned off, the heating and the inert gas circulation are stopped, a compacting mechanism is actuated, and the reaction mixture is settled and layered, thus obtaining an upper layer which is the crude glyceride layer, and a lower layer which is the glycerol layer; and the crude glyceride layer is subjected to two-stage molecular distillation so as to obtain high-purity diglyceride.

Method for producing oil containing polyunsaturated fatty acid using lipase

Ikemoto, H., *et al*., Nippon Suisan Kaisha, Ltd., US10138502, November 27, 2018

A method for lowering saturated fatty acid content, the method comprising concentrating polyunsaturated fatty acid using a lipase having low reactivity for the polyunsaturated fatty acid to react with a glyceride containing a polyunsaturated fatty acid; wherein the lipase reaction is performed at a temperature of not more than 25°C.

Probiotic confection and lipid compositions

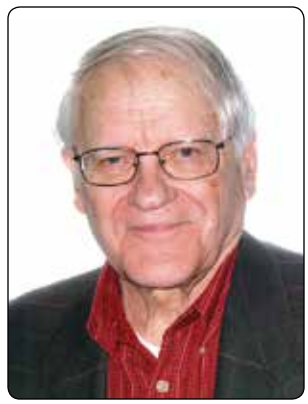
Lefkowitz, A.R., Ganeden Biotech, Inc., US10143649, December 4, 2018

The present application relates to probiotic confection-based compositions comprising lactic acid-producing bacteria and oil-based compositions comprising the same.

Patent information was compiled by Scott Bloomer, a registered US patent agent and Director, Technical Services at AOCS. Contact him at scott.bloomer@aocs.org.

Q & A with AOCS journal reviewer Arnis Kuksis

Arnold Kuksis is a Senior Associate Editor of ***Lipids*** and a professor emeritus at the University of Toronto in Ontario, Canada. His research has ranged from separations of amino acids by paper to oligo-nucleotides of DNA by ion exchange column-chromatography; TLC and column chromatography of lipid classes; high-temperature GLC of triacylglycerols; profiling of total lipids of lipoproteins by GC-MS and LC-MS; stereospecific analyses of lipids, lipases, and phospholipases; and isolation of monoacylglycerol acyltransferase.



1. HOW DID YOU GET A START AS A PEER REVIEWER?

I had published previously, but my report on an unexpected high-temperature gas liquid chromatographic resolution of natural triacylglycerols (1962) caught the attention and imagination of readers and editors. Soon invitations for reviewing related papers started arriving from journals on lipid chromatography and analytical lipid chemistry.

2. HOW LONG HAVE YOU BEEN A REVIEWER?

I started reviewing in 1963, and have continued it until today. Requests for reviews have come from the *Journal of American Oil Chemists' Society, Journal of Lipid Research, Journal of Chromatography, Biochimica et Biophysica Acta*, and, after 1966, from *Lipids*.

3. HOW MANY YEARS HAVE YOU BEEN AN AUTHOR/EDITOR/REVIEWER FOR *LIPIDS*?

I have been an author for *Lipids* since its first volume in 1966, and have published 66 papers in the journal up to 2017. I became a Senior Associate Editor of *Lipids* in 2006, when Eric Murphy became Editor-in-Chief. I have since lost count of the number of reviews performed on articles submitted for publication in *Lipids*.

4. HOW HAS LIPID RESEARCH CHANGED SINCE YOU FIRST ENTERED THE FIELD?

Since 1958, when I started, lipid research has progressed from adsorption chromatography (columns and thin-layers) of lipid classes to gas liquid chromatography of fatty acids (packed and capillary columns), followed by high-temperature gas-liquid chromatography of triacylglycerols and glycerophospholipids (packed and capillary columns) with flame ionization detection. Later, liquid chromatography (normal and reversed phase, and chiral) was developed with evaporative light scattering and flame ionization detection. Eventually, most chromatographic detectors became replaced by mass spectrometry and tandem mass spectrometry (with multiple reaction monitoring) as detectors. As a result of the increased certainty of peak identification, a meaningful application of lipid analyses to specific biological fluids and tissues of both normal and disease states became possible. New terminology, such as lipidomic and shot-gun lipidomic analyses replaced the older references to analysis of molecular species and total lipid profiling. Shotgun lipidomics is now a global lipid analysis in absence of chromatographic separation. Modern lipid analyses have revealed a bewildering complexity of minor lipid components arising from enzymatic oxidation and autoxidation of lipids, a rigorous analysis of which requires the application of the complete repertoire of analytical tricks and sound reasoning.

5. CAN YOU RECALL A TIME WHEN A REVIEW SHAPED AN AUTHOR'S PROFESSIONAL DEVELOPMENT?

I have no knowledge of a specific review shaping an author's professional development. However, an accumulation of scientific publications in prestigious journals leads to grant awards, promotions, and job security. It reflects upon and shapes the author's development. It was true in the past and is true today. However, an occasional bad review and rejection of a manuscript may also benefit professional development. I believe that everything eventually becomes published after corrections in *Lipids* or elsewhere.

6. WHAT DO YOU FIND MOST REWARDING ABOUT YOUR INVOLVEMENT WITH LIPIDS?

There are clearly benefits to be derived from being a reviewer, such as expanding one's knowledge, staying up to date on the latest literature, and having advance access to new research. I must admit that I cannot separate the rewards gained from involvement with *Lipids* from those picked up by involvement with other lipid journals. However, I have found *Lipids* more appropriate to the research of my group because its Associate Editors included leaders in both lipid separations and applications, while other lipid journals tended to emphasize either analytical work or applications.

7. HOW HAS YOUR WORK ON THE JOURNAL ADVANCED YOUR PROFESSIONAL DEVELOPMENT/CAREER OVER THE YEARS?

Based on my own experience, including publication and editing for *Lipids*, I can say that it has advanced my professional career along with academic promotion. It helped me maintain my Medical Research Associateship (Career Investigator-ship) for a total of 37 years. It was essential in acquiring adequate grant support to operate a well-equipped and active research laboratory. It helped to attract graduate students and postdoctoral fellows. It led to professorships and eventually to an Emeritus professorship.

8. WHAT QUALITIES MAKE A GOOD REVIEWER?

Competence, objectivity, and willingness to thoroughly research the submitted manuscripts as well as the submitters. The reviewer must know the subject area and the methodologies available to be able to provide well-founded criticisms and suggestions for improvement to authors, and a comprehensive report and clear recommendation for editors. This takes time, and a quick turn-around is usually impossible. A good reviewer must review previous publications in the subject area and watch out for such red flags as unjustified assumptions, over optimism, and potential oversell. A simple reality check involves an assessment of the appropriateness of the equipment and methodology for the study, and for the delivery of sound conclusions. Are the authors experienced in using the equipment or merely listing it? Are there severe overlaps with their own earlier publications? Do they have vested interests in the outcome of the study?

9. WHAT ADVICE WOULD YOU GIVE SOMEONE WHO WANTS TO BECOME A REVIEWER?

Reviewing requires time and skill, sometimes as much time as writing a paper. Usually editors of journals select reviewers who are experts in the area of the paper. A prospective reviewer can write to the editor of a journal and identify the area of interest and qualifications for reviewing there. Some publishers are offering webinars and training courses for would-be reviewers.

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Dark chocolate with a high-oleic peanut oil microcapsule content

Agibert, S.A.C. and S. C. da S. Lannes, *J. Sci. Food Ag. 98*: 5591–5597, 2018, https://doi.org/10.1002/jsfa.9102.

The present study aimed to determine the viability of the industrial production of dark chocolate with microcapsules of high-oleic peanut oil content. Microcapsules of high-oleic peanut oil were added to a control formulation using variations of mixing time. The chocolates presented a rheology characterized by a pseudoplastic behavior adjusted to the Casson model ($r > 0.98$) and calorimetric behavior indicating melting onset (21°C), peak melting (32°C), and melting end (41°C); caramelization peak (183°C); and carbonization peak (237°C), being considered thermal stable. The mixing time and the amount of microcapsules added to the control chocolate did not significantly influence the flow limit (11.09 ± 1.73 Pa) or the physical characteristics of the chocolate: pH (6.74 ± 0.14), maximum particle size (0.019 ± 0.001 mm), water activity (0.358 ± 0.023), and brittleness (18.61 ± 3.74 N). However, the addition of microcapsules with a high-oleic peanut oil content significantly increased the chocolate whiteness index, thixotropy, and Casson's plastic viscosity, although it did not have a significant influence on the mixing time. The products obtained have a desirable quality and physical properties, being suitable for industrial production.

Relationship between dietary sterols and gut microbiota: a review

Cuevas-Tena, M., *et al.*, *Eur. J. Lipid Sci. Technol. 120*: 1800054, 2018, https://doi.org/10.1002/ejlt.201800054.

Cholesterol intestinal absorption differs markedly from that of plant sterols; whereas the cholesterol absorption rate is high (30–60%), for total plant sterols it is low (2–3%). Non-absorbed sterols reach the colon, where the microbiota interacts with them. Non-absorbed cholesterol biotransformation has been widely studied by *in vitro* fermentation assays using gut microbiota from human feces and pure cultures of enteric microorganisms. A great variety of sterols and its metabolites have been detected, which allows establishing two pathways for cholesterol microbial degradation to coprostanol. However, biotransformation studies of plant sterols are scarce and its microbial transformation pathway remains to be fully clarified. Furthermore, the sterol contents in feces are highly variable among individuals, due to specific microbiota and especially dietary factors. However, no standardized methodology has been developed for sterols and their metabolites determination in feces. Studies on sterol excretion values, microbial transformation, and sterol determination methodology have been reviewed. Given that cholesterol metabolites can contribute to the development of colon cancer and that information about plant sterols biotransformation is scarce, this review contributes to improve the knowledge of the sterol implication in the gut microbiota and of PS impact in the colonic microbiota metabolization of cholesterol.

Comparison of green and conventional extraction methods on lipid yield and fatty-acid profiles of fish species

Ozogul, Y., *et al.*, *Eur. J. Lipid Sci. Technol. 120*: 1800107, 2018, https://doi.org/10.1002/ejlt.201800107.

The efficiency of the green extraction methods ultrasound-assisted extraction (UAE) and microwave-assisted extraction (MAE), and conventional methods (Soxhlet and Bligh and Dyer), on lipid content and fatty-acid profiles of six fish species (*Mullus barbatus*, red mullet; *Upeneus moluccensis*, goldband goatfish; *Mullus surmuletus*, surmullet; *Anguilla anguilla,* European eel; *Pagellus erythrinus*, common pandora, and *Saurida undosquamis*, brushtooth lizardfish) are evaluated. The results of lipid content of fish species show that the Bligh and Dyer method and UAE in general are more efficient than other methods. There are statistical differences in the fatty-acid composition of fish oil by four extraction methods ($p < 0.05$). Saturated (SFA), monounsaturated (MUFA), and polyunsaturated fatty acid (PUFA) contents of fish species range from 29.51 mg 100 g^{-1} fish (Soxhlet)–1400 mg 100 g^{-1} (UAE), 15.52 mg 100 g^{-1} (UAE)–2237.18 mg 100 g^{-1} (Bligh and Dyer), and 14.36% (Soxhlet)–646 mg 100 g^{-1} (Bligh and Dyer), respectively. Generally, Bligh and Dyer give the higher values in surmullet, red mullett, and common pandora in terms of SFA, MUFA, PUFA, and the dominant fatty acids (C16:0, C18:0, C16:1, C18:1n9, C18:1n7, C22:1n9, EPA, DHA), whereas MAE and UAE methods give better results in goldband goldfish and European eel, respectively. Thus, extraction methods affect the lipid yield and fatty acid profiles of extracted oil of different fish species.

Tocols and oil content in whole grain, brewer's spent grain, and pearling fractions of malting, feed, and food barley genotypes

Badea, A., *et al.*, *Cereal Chem. 95*: 779–789, 2018, https://doi.org/10.1002/cche.10093.

Vitamin E is an important dietary component found mainly in plants and is a group of compounds including tocopherols and tocotrienols, collectively known as tocols. In this study, tocols and

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oil content were evaluated in whole grain, brewer's spent grain, and pearling fractions from various barley genotypes grown at two sites in 2014, and at three sites in 2015 in Manitoba, Canada. Mean tocols and oil content were much higher in brewer's spent grain than in whole grain of malting genotypes. Pearling fractions had higher tocols and oil content than whole grain of six distinct feed/food genotypes, with the highest tocols and oil content observed in the 5%–10% pearling fraction. Brewer's spent grain and the 5%–10% pearling fraction could be used as novel functional food ingredients or be valuable sources for extraction of health-promoting tocols and/or oil. Using barley processing by-products like brewer's spent grain and pearling fractions in value-added products with beneficial health properties may offer unique economic and waste management opportunities. A relatively large number of malting and feed/food barley genotypes were screened for all eight tocol vitamers and oil content. This study serves as a valuable resource for barley research scientists and the barley industry as a whole.

Alkyl ferulate esters as multifunctional food additives: antibacterial activity and mode of action against *Escherichia coli in vitro*

Shi, Y-G., *et al., J. Agric. Food Chem. 66*: 12088–12101, 2018, https://doi.org/10.1021/acs.jafc.8b04429.

This work aims to prepare ferulic acid alkyl esters (FAEs) through the lipase-catalyzed reaction between methyl ferulate and various fatty alcohols in deep eutectic solvents and ascertain their antibacterial activities and mechanisms. Screens of antibacterial effects of FAEs against *Escherichia coli* ATCC 25922 (*E. coli*) and *Listeria monocytogenes* ATCC 19115 (*L. monocytogenes*) revealed that hexyl ferulate (FAC6) exerted excellent bacteriostatic and bactericidal effects on *E. coli* and *L. monocytogenes* (minimum inhibitory concentration (MIC): 1.6 and 0.1 mM, minimum bactericidal concentration (MBC): 25.6 and 0.2 mM, respectively). The antibacterial mechanism of FAC6 against *E. coli* was systematically studied to facilitate its practical use as a food additive with multifunctionalities. The growth and time-kill curves implied the partial cell lysis and inhibition of the growth of *E. coli* caused by FAC6. The result related to propidium iodide uptake and cell constituents' leakage (K^+, proteins, nucleotides, and beta-galactosidase) implied that bacterial cytomembranes were substantially compromised by FAC6. Variations on morphology and cardiolipin microdomains and membrane hyperpolarization of cells visually verified that FAC6 induced cell elongation and destructed the cell membrane with cell wall perforation. SDS-PAGE analysis and alterations of fluorescence spectra of bacterial membrane proteins manifested that FAC6 caused significant changes in constitutions and conformation of membrane proteins. Furthermore, it also could bind to minor grooves of *E. coli* DNA to form complexes. Meanwhile, FAC6 exhibited antibiofilm formation activity. These findings indicated that that FAC6 has promising potential to be developed as a multifunctional food additive.

Determination of key active components in different edible oils affecting lipid accumulation and reactive oxygen species production in HepG2 cells

Li, X., *et al., J. Agric. Food Chem. 66*: 11943–11956, https://doi.org/10.1021/acs.jafc.8b04429.

Owing to the poor ability of cells to decompose triglycerides, most studies of edible oil have depended on animal or clinical trials. However, such trials are expensive and time-consuming, and the results are limited to considerable individual differences. This is the first study to comprehensively investigate the effect of different oils on the lipid accumulation and reactive oxygen species (ROS) production in HepG2 cells by hydrolyzing oil to fatty acids with integrated fat content. In addition, the key components of fatty acid composition, phytosterol, polyphenols, and tocopherol/tocotrienol in different oils, contributing to a decrease in content of lipid accumulation, cholesterol, ROS, and malondialdehyde (MDA), were analyzed using multivariate analysis. The results showed that the lipid accumulation content of coconut oil, Pu'er tea oil, olive oil, and flaxseed oil at a concentration of 200 mM decreased by 45.98 ± 0.75, 50.35 ± 1.37, 40.43 ± 2.44, and 42.76 ± 1.88%, respectively, compared with the lard. In addition, the ROS contents of Pu'er tea oil, olive oil, and flaxseed oil had no significant difference from that of control cells ($p < 0.05$). In the results, (3-beta,5-alpha)-stigmastan-3-yl, cholane-5,20(22)-diene-3b-ph, and beta-sitosterol were determined to be the key components in edible oils associated with lipid accumulation and ROS production.

Dose-dependent increases in liver cholesterol but not plasma cholesterol from consumption of one to five whole eggs and no effects from egg whites on liver or plasma cholesterol in hamsters

Zhu, H., *et al., J. Agric. Food Chem.66*: 12805–12814, 2018, https://doi.org/10.1021/acs.jafc.8b04730.

The dose-dependent effect of egg consumption on plasma cholesterol in humans remains inconclusive. It is unknown if egg white consumed in a normal amount can reduce plasma cholesterol. We used hamsters as a model to (i) investigate the dose-dependent effect of consuming zero to five whole eggs on plasma total cholesterol (TC) and (ii) examine if egg white, equivalent to one to five eggs, possessed any reducing effects on plasma TC. In experiment 1, hamsters were divided into six groups ($n = 8$ each) and fed either a control diet or one of five experimental diets supplemented with whole-egg powder equivalent to one to five eggs per 2000 kcal. Results showed that supplementation with one egg increased plasma TC by 25% compared with that of the control (226 ± 16 versus 282 ± 56 mg/dL, $p < 0.05$), whereas supplementation with two

to five eggs did not significantly produce any additional effects on plasma cholesterol. However, supplementation with one to five eggs in diets caused a dose-dependent accumulation of cholesterol in the liver from 21.5 ± 4.4 to 71.3 ± 7.3 mg/g ($p < 0.01$). In the second experiment, hamsters were divided into six groups and fed either a high-cholesterol control diet or one of five experimental diets supplemented with egg-white powder from one to five eggs. Results showed that egg-white powder affected neither plasma nor liver cholesterol levels. The egg-white powder did not affect fecal sterol excretion, suggesting it had no effect on cholesterol absorption. It was therefore concluded that consumption of two to five eggs did not significantly produce any additional effects on plasma cholesterol, whereas egg white did not possess a plasma-cholesterol-lowering activity if it was consumed at amounts similar to those in a normal human diet.

Does pregnancy alter life-course lipid trajectories? Evidence from the HUNT Study in Norway

Markovitz, A.R., *et al., J. Lipid Res. 59*: 2403–2412, https://doi.org/10.1194/jlr.P085720.

We examined the association between pregnancy and life-course lipid trajectories. Linked data from the Nord-Trøndelag Health Study and the Medical Birth Registry of Norway yielded 19,987 parous and 1,625 nulliparous women. Using mixed-effects spline models, we estimated differences in nonfasting lipid levels from before to after first birth in parous women and between parous and nulliparous women. HDL cholesterol (HDL-C) dropped by −4.2 mg/dl (95% CI: −5.0, −3.3) from before to after first birth in adjusted models, a 7% change, and the total cholesterol (TC) to HDL-C ratio increased by 0.18 (95% CI: 0.11, 0.25), with no change in non-HDL-C or triglycerides. Changes in HDL-C and the TC/HDL-C ratio associated with pregnancy persisted for decades, leading to altered life-course lipid trajectories. For example, parous women had a lower HDL-C than nulliparous women at the age of 50 years (−1.4 mg/dl; 95% CI: −2.3, −0.4). Adverse changes in lipids were greatest after first birth, with small changes after subsequent births, and were larger in women who did not breastfeed. Findings suggest that pregnancy is associated with long-lasting adverse changes in HDL-C, potentially setting parous women on a more atherogenic trajectory than prior to pregnancy.

Structural variants of a liver fluke derived granulin peptide potently stimulate wound healing

Dastpeyman, M., *et al., J. Med. Chem. 61*: 8746–8753, 2018, https://doi.org/10.1021/acs.jmedchem.8b00898.

Granulins and progarnulins are not only involved in wound and inflammation but also important for other diseases like cancer and metabolic diseases. Therefore, finding natural ligands that inhibit the expressions of such proteins can be very useful in maintaining health and wellness of the human body.

Granulins are a family of growth factors involved in cell proliferation. The liver-fluke granulin, Ov-GRN-1, isolated from a carcinogenic liver fluke *Opisthorchis viverrini*, can significantly accelerate wound repair *in vivo* and *in vitro*. However, it is difficult to express Ov-GRN-1 in recombinant form at high yield, impeding its utility as a drug lead. Previously we reported that a truncated analogue (Ov-GRN12–35_3s) promotes healing of cutaneous wounds in mice. NMR analysis of this analogue indicates the presence of multiple conformations, most likely as a result of proline cis/trans isomerization. To further investigate whether the proline residues are involved in adopting the multiple confirmations, we have synthesized analogues involving mutation of the proline residues. We have shown that the proline residues have a significant influence on the structure, activity, and folding of Ov-GRN12–35_3s. These results provide insight into improving the oxidative folding yield and bioactivity of Ov-GRN12–35_3s and might facilitate the development of a novel wound healing agent.

Validation of matrix metalloproteinase-9 (MMP-9) as a novel target for treatment of diabetic foot ulcers in humans and discovery of a potent and selective small-molecule MMP-9 inhibitor that accelerates healing

Trung, T., *et al., J. Med. Chem. 61*: 8825–8837, 2018, https://doi.org/ 10.1021/acs.jmedchem.8b01005.

MMP9 enzymes may be a novel target for diabetic foot ulcers but they are part of other MMPs known to be important for extracellular matrix. MMps are involved in inflammatory diseases. Cannabis extract is one natural composition known to have MMP9 inhibitory activity.

Diabetic foot ulcers (DFUs) are a significant health problem. A single existing FDA-approved drug for this ailment, becaplermin, is not standard-of-care. We previously demonstrated that upregulation of active matrix metalloproteinase (MMP)-9 is the reason that the diabetic wound in mice is recalcitrant to healing and that MMP-8 participates in wound repair. In the present study, we validate the target MMP-9 by identifying and quantifying active MMP-8 and MMP-9 in human diabetic wounds using an affinity resin that binds exclusively to the active forms of MMPs coupled with proteomics. Furthermore, we synthesize and evaluate enantiomerically pure (R)- and (S)-ND-336, as inhibitors of the detrimental MMP-9, and show that the (R)-enantiomer has superior efficacy in wound healing over becaplermin. Our results reveal that the mechanisms of pathology and repair are similar in diabetic mice and diabetic humans and that (R)-ND-336 holds promise for the treatment of DFUs as a first-in-class therapeutic.


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Bioavailability of quercetin from onion extracts after intraruminal application in cows

Wein, S., *et al.*, *J. Agric. Food Chem.* *66*: 10188–10192, 2018, https://doi.org/10.1021/acs.jafc.8b03049.

Bioavailability of micro and macro nutrients with low solubility is a significant hurdle in an effort to deploy them as natural therapies. This report concludes with data that the use of biomass, such as onions, is a better way to deliver such nutrients. The study is not a human study but still suggests that, not surprisingly, consuming natural materials as food has advantages over using food supplements.

The aim of the present study was to investigate the bioavailability of quercetin from onion bulb (OB) and onion skin (OS) extracts in ruminants. Three non-lactating cows equipped with a permanent rumen fistula intraruminally received equimolar amounts of quercetin as either aglycone, rutin, or OB or OS extract, respectively, at a dose of 50 mg of quercetin equivalents/kg of body weight. Blood samples were drawn before and frequently within the 24 h period after application of the respective substance. Quercetin and quercetin metabolites with an intact flavonol structure (kaempferol, isorhamnetin, and tamarixetin) were analyzed in plasma samples by high-performance liquid chromatography with fluorescence detection. All quercetin sources administered resulted in a fast increase of the plasma concentrations of quercetin and total flavonols (sum of quercetin and its metabolites), followed by a rapid decline, whereby significant higher concentrations occurred with OB extract and rutin compared to quercetin aglycone and OS extract, respectively. The results clearly demonstrate a higher systemic availability of quercetin from OB extract and rutin. Taken together, OB extract with a high content of quercetin glucosides is an interesting source for the application of quercetin to ruminants.

Effect of food thermal processing on the composition of the gut microbiota

Pérez-Burillo, S., *et al.*, *J. Agric. Food Chem.* *66*: 11500–11509, 2018, https://doi.org/10.1021/acs.jafc.8b04077.

Heating and cooking food helps to balance the microbiota in favor of beneficial bacteria, but not all foods are to be cooked in the same way for a maximum benefit.

Cooking modifies food composition due to chemical reactions. Additionally, food composition shapes the human gut microbiota. Thus, the objective of this research was to unravel the effect of different food cooking methods on the structure and functionality of the gut microbiota. Common culinary techniques were applied to five foods, which were submitted to *in vitro* digestion–fermentation. Furosine, 5-(hydroxymethyl)furfural, and furfural were used as Maillard reaction indicators to control the heat treatment. Short-chain fatty acids production was quantified as indicator of healthy metabolic output. Gut microbial community

structure was analyzed through 16S rRNA. Both food composition and cooking methods modified the microbiota composition and released short-chain fatty acids. In general, intense cooking technologies (roasting and grilling) increased the abundance of beneficial bacteria like *Ruminococcus* spp. or *Bifidobacterium* spp. compared to milder treatments (boiling). However, for some foods (banana or bread), intense cooking decreased the levels of healthy bacteria.

Nutraceutical potential of hemp (*Cannabis sativa* L.) seeds and sprouts

Frassinetti, S., *et al.*, *Food Chem. 262*: 56–66, 2018, https://doi.org/10.1016/j.foodchem.2018.04.078

This timely review may help to reduce the confusion between cannabis and hemp.

In this study, the antioxidant effect of *Cannabis sativa* L. seeds and sprouts (3 and 5 days of germination) was evaluated. Total polyphenols, flavonoids, and flavonols content, when expressed on dry weight basis, were highest in sprouts; ORAC and DPPH (*in vitro* assays), CAA-RBC (cellular antioxidant activity in red blood cells) and hemolysis test (*ex vivo* assays) evidenced a good antioxidant activity higher in sprouts than in seeds. Untargeted analysis by high resolution mass spectrometry in negative ion mode allowed the identification of main polyphenols (caffeoyltyramine, cannabisin A, B, C) in seeds and of ω-6 (linoleic acid) in sprouts. Antimutagenic effect of seeds and sprouts extracts evidenced a significant decrease of mutagenesis induced by hydrogen peroxide in Saccharomyces cerevisiae D7 strain. Our results show that *C. sativa* seeds and sprouts exert beneficial effects on yeast and human cells and should be further investigated as a potential functional food.

Activity-based protein profiling delivers selective drug candidate ABX-1431, a monoacylglycerol lipase inhibitor, to control lipid metabolism in neurological disorders

Jiang, M., and M. van der Stelt, *J. Med. Chem. 61*: 9059–9061, 2018, https://doi.org/10.1021/acs.jmedchem.8b01405.

Monoacylglycerol lipase (MGLL or MAGL) is a critical point of regulation of both endocannabinoid and eicosanoid signaling pathways in the brain, thereby providing novel therapeutic opportunities for neurological and neurodegenerative diseases. In this issue Cisar disclose the discovery, optimization, and initial preclinical profiling of ABX-1431, a covalent, irreversible MGLL inhibitor. Activity-based protein profiling was key to the discovery of ABX-1431. ABX-1431 is a first-in-class experimental drug that was well-tolerated and safe in phase 1 clinical studies. Data from an exploratory phase 1b study indicate that it has the potential to treat symptoms of adult patients with syndrome of Gilles de la Tourette. ABX-1431 is currently entering clinical phase 2 studies for this neurological disorder as well as for other indications, such as neuromyeltis optica and multiple sclerosis.

Oleanolic acid inhibits liver X receptor alpha and pregnane X receptor to attenuate ligand-induced lipogenesis

Lin, Y.-N., *et al.*, *J. Agric. Food Chem. 66*: 10964–10976, 2018, https://doi.org/ 10.1021/acs.jafc.8b03372.

Liver X receptor alpha (LXRα) controls important biological and pathophysiological processes such as lipid homeostasis. Inhibiting LXRα transactivation may beneficial in the treatment of nonalcoholic fatty liver disease (NAFLD), which is one of the main causes of liver diseases and hyperlipidemia. Oleanolic acid (OA) is a naturally occurring triterpenoid found in many plants. It has several beneficial effects on biological pathways; however, the mechanisms underlying its effects on LXRα are unclear. Therefore, we evaluated the effects of OA on T0901317-induced LXRα activation and explored whether OA can attenuate hepatic lipogenesis. The results showed that OA significantly decreased the promoter activities of LXR response element and sterol regulatory element binding protein-1c (SREBP-1c). It also decreased the mRNA and protein expression of LXRα target genes. These resulted in reduced hepatocellular lipid content. Our results also revealed that the overall binding pose of OA is similar to the X-ray pose of T0901317. Furthermore, OA stimulated AMP-activated protein kinase phosphorylation in hepatic cells. Additionally, it increased small heterodimer partner-interacting leucine zipper protein (SMILE) but decreased steroid receptor coactivator-1 (SRC-1) recruitment to the SREBP-1c promoter region. OA also enhanced LXRα-mediated induction of reverse cholesterol transport (RCT)-related gene, ATP-binding cassette transporter (ABC) A1, and ABCG1 expression in intestinal cells. It was found that OA increased the binding of SRC-1 but decreased SMILE recruitment to the ABCG1 gene promoter region. Furthermore, it reduced valproate- and rifampin-induced LXRα- and pregnane X receptor-mediated lipogenesis, respectively, which indicates its potential benefit in treating drug-induced hepatic steatosis. The results also show that OA is liver-specific and can be selectively repressed of lipogenesis. Moreover, it preserves and enhances LXRα-induced RCT stimulation. The results show that OA may be a promising treatment for NAFLD. Additionally, it can be used in the development of LXRα agonists to prevent atherosclerosis.

Polymorphism, textural, and crystallization properties of winged bean (*Psophocarpus tetragonolobus*, DC.) oil-based trans-fatty acids-free ternary margarine blends

Makeri, M., *et al.*, *LWT–Food Sci. Technol. 100*: 158–166, 2019, https://doi.org/10.1016/j.lwt.2018.09.012.

Most margarine and bakery fats are produced from hydrogenated oils making the ingestion of large amounts of trans-fatty acids inevitable with consequential health hazards. Taking advantage of its high solid fat content (15%), winged bean oil-based margarine blends (F320 & F322) were prepared from wing bean oil (WBO), palm stearin (PS), and palm olein (PO) as follows (w/w):

F320 (48.5%PS:1.5%PO:50%WBO) and F322 (1.5%PS:48.5%PO:50%WBO). The blends were tested for textural, thermal properties and crystal growth pattern and polymorphic characteristics. Results showed F320 exhibited harder texture, had crystal morphology with size ranges of 1.0–1.60 micrometer (50%), 1.61–2.20 micrometer (23.38%), 2.21–3.40 micrometer (16.50%), and 3.41–5.20 micrometer (6.18%), evenly distributed resembling beta polymorphs, whereas F322 exhibited soft texture, and polymorphs with protruding needle-like crystals with size ranges of 1–1.60 micrometer (48.25%), 1.61–2.20 micrometer (23.96%), 2.21–3.40 micrometer (16.84%), and 3.41–5.20 micrometer (6.39%), unevenly distributed. Blend F320 thus showed good physicochemical properties as multi-purpose for use as table and bakery margarine especially in tropical climates. Both blends showed low atherogenic and thrombogenic indexes and thus low risk of CHD. This study further offer insight into the potential use of underutilized oilseed crop resources for making specialty and structured fats for the betterment of human life.

Oxidative stability of burgers containing chia oil microparticles enriched with rosemary by green-extraction techniques.

Heck, R.T., *et al*., *Meat Sci. 146*: 147–153, 2018, https://doi.org/10.1016/j.meatsci.2018.08.009.

In the first part of this study, the oxidative stability of chia oils enriched with rosemary by ultrasound-assisted extraction (UAE) and by a conventional maceration extraction (CME) was evaluated. In the second part, chia oil enriched with rosemary by UAE or CME was microencapsulated and used to replace 50% fat in burgers. The oxidative and sensory quality of burgers were evaluated during 120 days of storage at –18°C. Chia oil enriched with rosemary by UAE presented a higher oxidative stability compared to CME. Higher Eh and TBARS values were found in burgers containing chia oil microparticles without rosemary. The burgers produced with chia oil microparticles enriched with rosemary by UAE showed greater oxidative stability than other treatments, mainly after cooking. Furthermore, the incorporation of rosemary antioxidants to chia oil reduced the sensory defects caused by the lipid reformulation.

Antioxidant properties, phenolic and mineral composition of germinated chia, golden flax, evening primrose, phacelia and fenugreek

Pająk, P., *et al*., *Food Chem. 275*: 69–76, 2019, https://doi.org/10.1016/j.foodchem.2018.09.081.

Seeds and sprouts are of considerable interest due to their numerous pro-health benefits. The aim of this study was to investigate the effect of germination on the mineral composition (performed by flame absorption atomic spectroscopy), total phenolic content, antioxidant activity, as well as phenolic profiles (before and after alkaline hydrolysis by high-performance liquid chromatography) of chia, golden flax, evening primrose, phacelia, and fenugreek seeds. Generally, significant ($p < 0.05$) changes in the individual minerals composition of the seeds, improvement of their antioxidant properties, as well as increase in levels of individual phenolic compounds was found after seeds germination. Alkaline hydrolysis allowed to release free forms of phenolics and to confirm (chromatographically) their significantly higher amounts when compared to the nonhydrolyzed fraction. Gallic, protocatechuic, caffeic, p-coumaric, ferulic, and sinapic acids, as well as quercetin and kaempferol were identified in analyzed seeds and sprouts. Sprouts exhibited better nutritional values than their un-germinated forms.

Effect of the solvent composition on the profile of phenolic compounds extracted from chia seeds

Alcântara, M., A., *et al*., *Food Chem. 275*: 489–496, 2019, https://doi.org/10.1016/j.foodchem.2018.09.133.

This study investigated the efficiency of the extraction of phenolic compounds from seeds of chia, *Salvia hispanica* L. utilizing the statistical tool of mixture planning, simplex-lattice design. The solvents used were acetone, ethanol and water and the responses analyzed were total phenolic content (TPC), antioxidant activity by the capture of the free radical DPPH and ferric reduction ability (FRAP). Moderately polar mixtures were highly efficient to extract the antioxidant phenolic compounds. The best results were obtained for the water-acetone (1/3–2/3) binary mixture, presenting TPC, DPPP, and FRAP values of 58.44 mg GAE/g, 250.20 micromol TE/g, and 720.15 micromol TE/g, respectively. The best ternary mixture was water-ethanol-acetone (1/6–1/6–2/3), with 60.96 mg GAE/g, 380.53 micromol TE/g, and 990.15 micromol TE/g, respectively. The phenolic profile showed that the acids rosmarinic, caffeic, salicylic, and the flavonoids myricetin and quercetin are the compounds that most contribute to the elevated antioxidant activity.

Kinetics of lipid oxidation in omega fatty acids-rich blends of sunflower and sesame oils using Rancimat

Ghosh, M., et al., *Food Chem. 272*: 471–77, 2019, https://doi.org/10.1016/j.foodchem.2018.08.072.

Blended sunflower (SO) (50–80%) and sesame oils (SEO) (20–50%) were evaluated for thermo-oxidative stability (induction period, IP), oxidation kinetics (rate constant, *k*), synergy and shelf-life (25°C) (IP_{25}) using Rancimat (100, 110, 120, and 130°C). The Arrhenius equation (ln *k vs.* 1/T) and activated complex theory (ln *k*/*T vs.* 1/T) were used to estimate activation energies, activation enthalpies and entropies, which varied from 92.05 to 99.17 kJ/mol, 88.83 to 95.94 kJ/mol, –35.58 to –4.81 J/mol K, respectively ($R^2 > 0.90$, $p < 0.05$). Oil blend (OB) with 1:1 SO to SEO exhibited greatest synergy (115%), highest IP (100°C) (13.2 *vs.* 6.1 h) and most extended IP_{25}(193 *vs.* 110 days) with a nutritionally stable composition of ω-fatty acids (ω9, 34.5 *vs.*28.7%; ω6, 49 *vs.* 52%) compared with SO. Better retention of lignans (6205 *vs.*3951 mg/kg) and tocopherols (332 *vs.*189 mg/kg) were also noted in OB compared with SO alone.

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