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Under arrest: investigating factors that govern partial coalescence

Abigail Thiel, Patrick Spicer, and Richard Hartel

- **Arrested coalescence, also known as partial coalescence, occurs when fat globules begin to merge, but do not fully combine into a single spherical globule.**
- **Partially-coalesced fat networks are key in products like ice cream, whipped topping, and whipped cream for desired textural and rheological properties.**
- **Micromanipulation is the first technique that allows direct observation of fat globules undergoing coalescence instead of inferring results from indirect methods.**

Arrested coalescence occurs when fat globules come into contact with one another, begin to combine, but halt this fusion before total coalescence occurs. This phenomenon is controlled by two opposing forces: the Laplace driving force to minimize total interfacial area, and an elastic resistance that opposes deformation of the internal solid network. When interfacial forces dominate, it is favorable for two droplets to combine into one larger, spherical droplet, reducing the total interfacial free energy and resulting in full coalescence. Conversely, when a strong rheological resistance exists, such as the presence of a rigid internal solid fat network, or particles occupying the surface of fat globules (Pickering emulsions), the droplets may not coalesce at all. Arrested coalescence is seen when these two forces are nearly in balance, leading to the unique anisotropic structures **(see confocal scan of a doublet at https://youtu.be/ZwY37GGed2U).** This confocal image scans through a doublet found within an emulsion. The dark lances are solid fat crystals, which form a network within the droplets. The transmission electron micrograph shown in Figure 1a also captures crystalline fat entrapped within oil droplets in an ice cream sample. This solid matrix eventually arrests the structure, as it is energetically unfavorable to further compress or readjust the network, creating fat globule clusters as seen in Figure 1b.

The occurrence of partially-coalesced fat networks is critical to the stand-up properties of whipped toppings, but it can also stabilize air cells and prevent rapid melt-down in ice cream. Figure 2 shows two ice cream samples dispersed on a microscope slide. The sample on the left has almost no partially-coalesced networks (**see video of a low level of partial coalescence in ice cream at https://youtu.be/3udMzUKMMtE**). The sample on the right has a high amount of fat destabilization (**see video of a high level of partial coalescence in ice cream at https://youtu.be/Wo-6gGL3HZU**). Both samples are melting at room temperature. Most of the fat globules in the sample on the left are single and free flowing, and the two air cells labeled A and B, can be seen moving. Conversely, partially-coalesced networks in the sample on the right, marked as PC, are able to hold the air cells in place and stabilize the microstructure, as the ice cream melts over time. The ability of emulsion droplets to destabilize can be influenced by the type of fat, solid fat content, emulsifier, and co-surfactant used in the product, as well as, processing parameters like shear forces and temperature.

The most prevalent theory regarding arrested coalescence, described by Walstra in his book, *Physical Chemistry of Foods*, maintains that interfacial crystals protruding from fat globules are responsible for penetrating into neighboring droplets, initiating oil neck formation, and therefore promoting coalescence. This theory was not based on direct observation of such an event, but rather, experiments where the degree of destabilization within an emulsion appeared to correlate with the amount of interfacial crystals observed. Coalescence is also widely known to occur in emulsion droplets containing no solid particles, so the real explanation is likely some combination of phenomena.

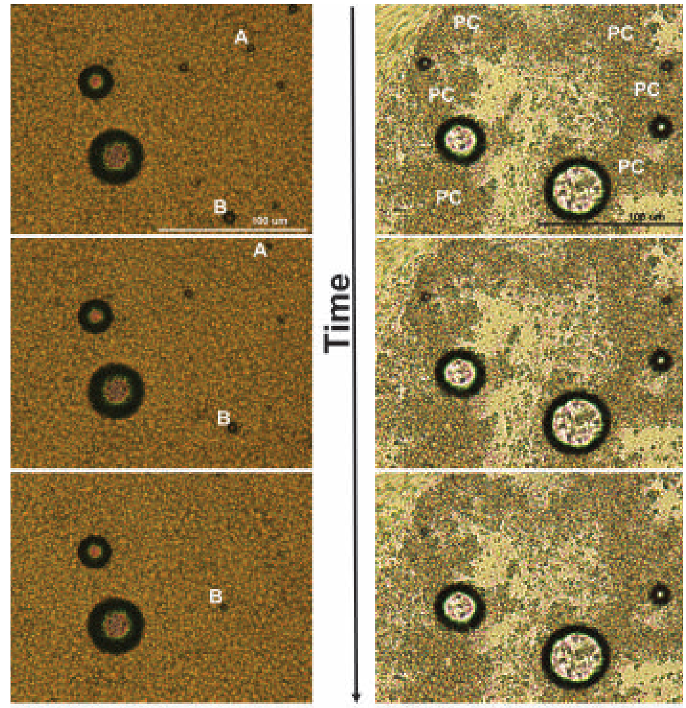
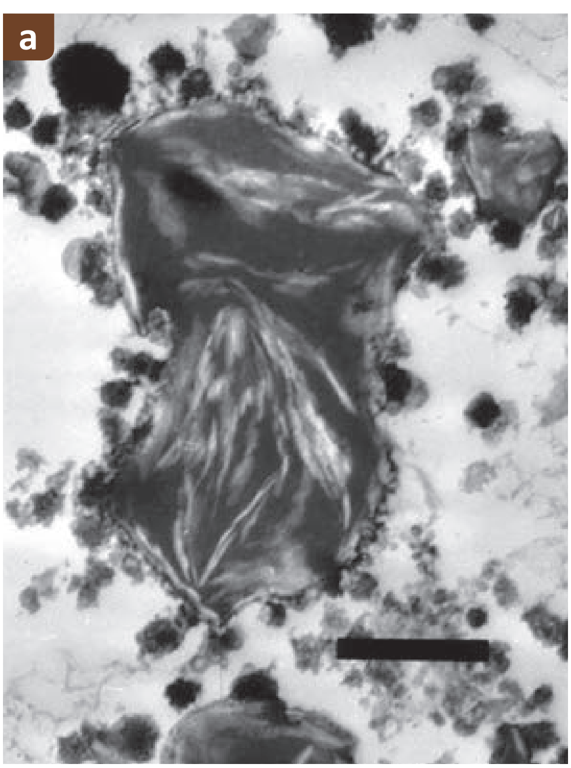


FIG. 2. (Left) Ice cream sample with very little partially coalesced structure (video at https://youtu.be/3udMzUKMMtE). Over time the free fat globules move as the ice cream melts, dragging the air cells with them. Two air cells are marked A and B to easily visualize the flow seen in this ice cream. By the third image, enough time has passed that air cell A has moved off the screen. (Right) Ice cream with a large amount of partially-coalesced fat networks, marked as PC, that maintain structural integrity even as the ice cream melts (video at https://youtu.be/Wo-6gGL3HZU). The lighter areas contain free fat globules that are flowing as the sample melts.



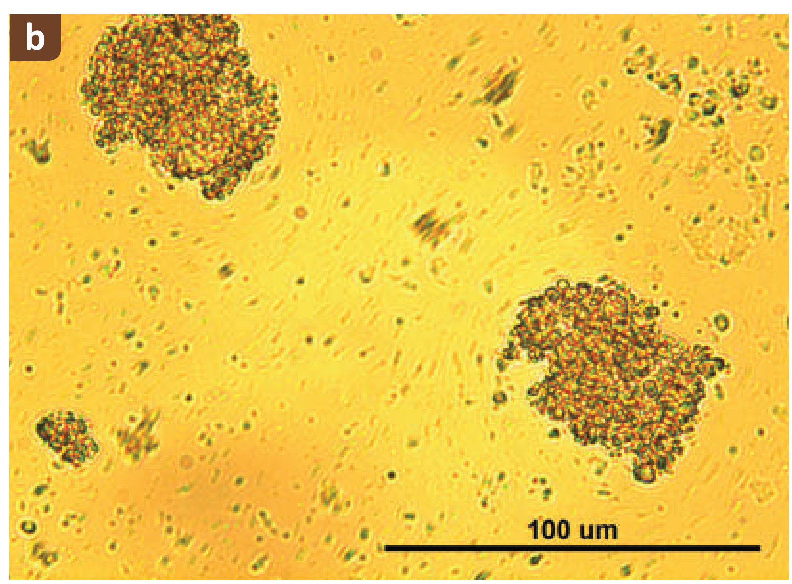


FIG. 1. (a) Transmission electron microscopy image of fat globules within ice cream. The white spears inside the fat globule make up the solid fat network. The crystalline fat network within fat globules provides an elastic resistance during coalescence. Scale Bar is 1 mm. Photo 1a courtesy of Doug Goff. (b) Optical microscopy image of fat globule clusters observed in a sample of melted ice cream.

Although Walstra's theory of arrested coalescence is widely cited, the lack of understanding surrounding the detailed mechanism of partial coalescence of fat globules remained. To further explore this area, a technique known as micromanipulation, used to precisely move microscopic objects during medical procedures like *in vitro* fertilization, was reapplied to study droplet arrest. Here two capillary tubes, which can apply a positive or negative pressure, are used to capture fat globules within an emulsion and direct them into contact. This setup is pictured in Figure 3a, where the two micromanipulators are each loaded with one fat globule. The manipulators are then manually moved to gently touch the globules together to evaluate coalescence status while observing through a microscope.

Utilizing the micromanipulation setup allows emulsions with different properties to be studied. Both Pickering emulsion droplets, where nanoparticles are contained at the interface, and partially crystalline emulsion droplets, where internal particles form a solid fat network, have been observed to undergo a wide range of coalescence behavior. In these studies, no interfacial fat crystals were observed, yet partial coalescence was achieved. Examples of the final structures created using two droplets composed of palm kernel oil and soybean oil can be seen in figure 3b-e. As the solid fat content (SFC) of the droplets is increased from 3b–e, the droplets arrest at an earlier stage of coalescence until total stability is achieved. Here structures range from full coalescence (3b) at the lowest SFC to no coalescence (3e) at the highest SFC. Figures 3c–d show structures that are partially coalesced. Further, Pawar *et al*. showed similarly that increasing surface coverage of nanoparticles on oil droplets also results in arrest at earlier stages of coalescence, eventually

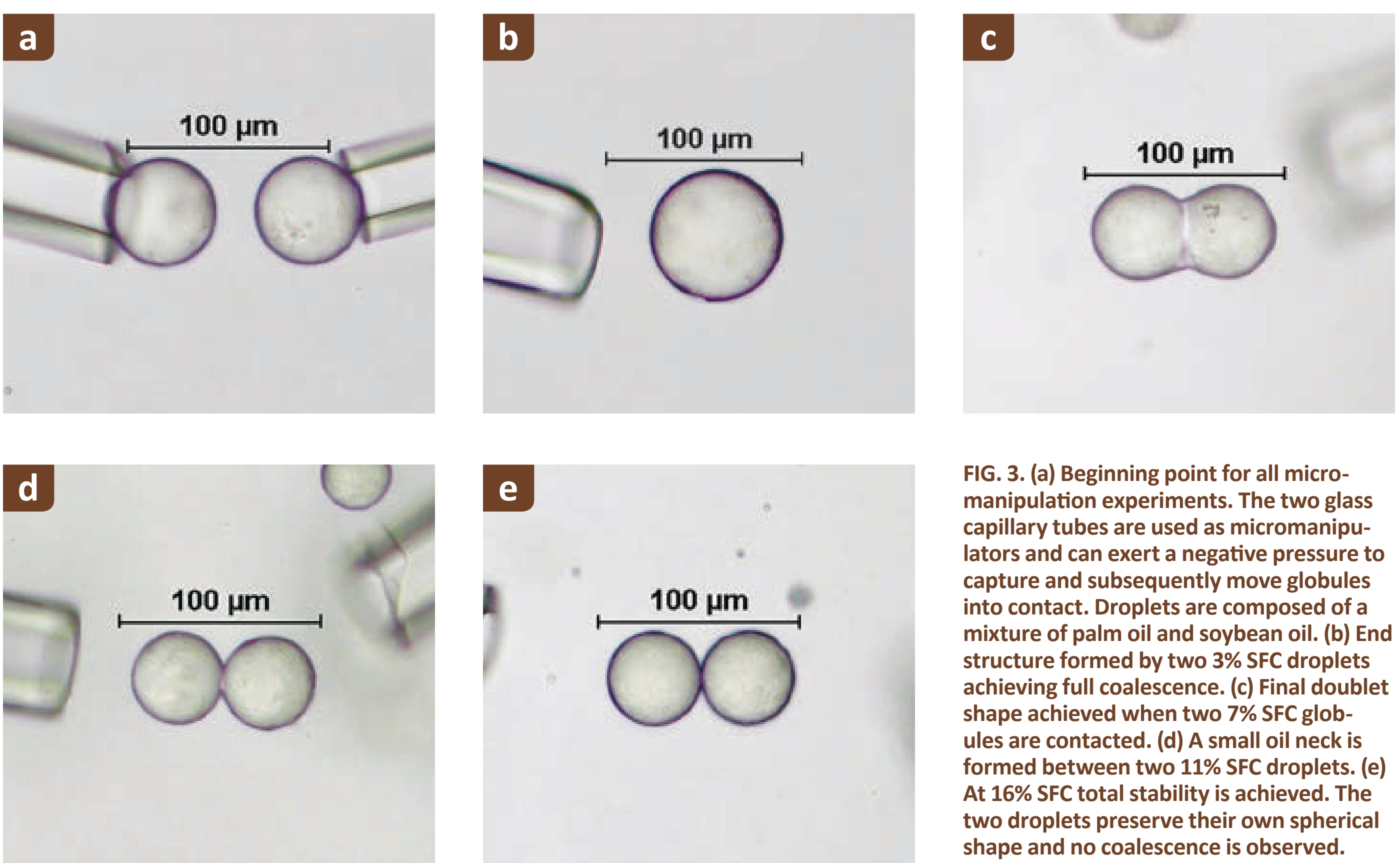


FIG. 3. (a) Beginning point for all micromanipulation experiments. The two glass capillary tubes are used as micromanipulators and can exert a negative pressure to capture and subsequently move globules into contact. Droplets are composed of a mixture of palm oil and soybean oil. (b) End structure formed by two 3% SFC droplets achieving full coalescence. (c) Final doublet shape achieved when two 7% SFC globules are contacted. (d) A small oil neck is formed between two 11% SFC droplets. (e) At 16% SFC total stability is achieved. The two droplets preserve their own spherical shape and no coalescence is observed.

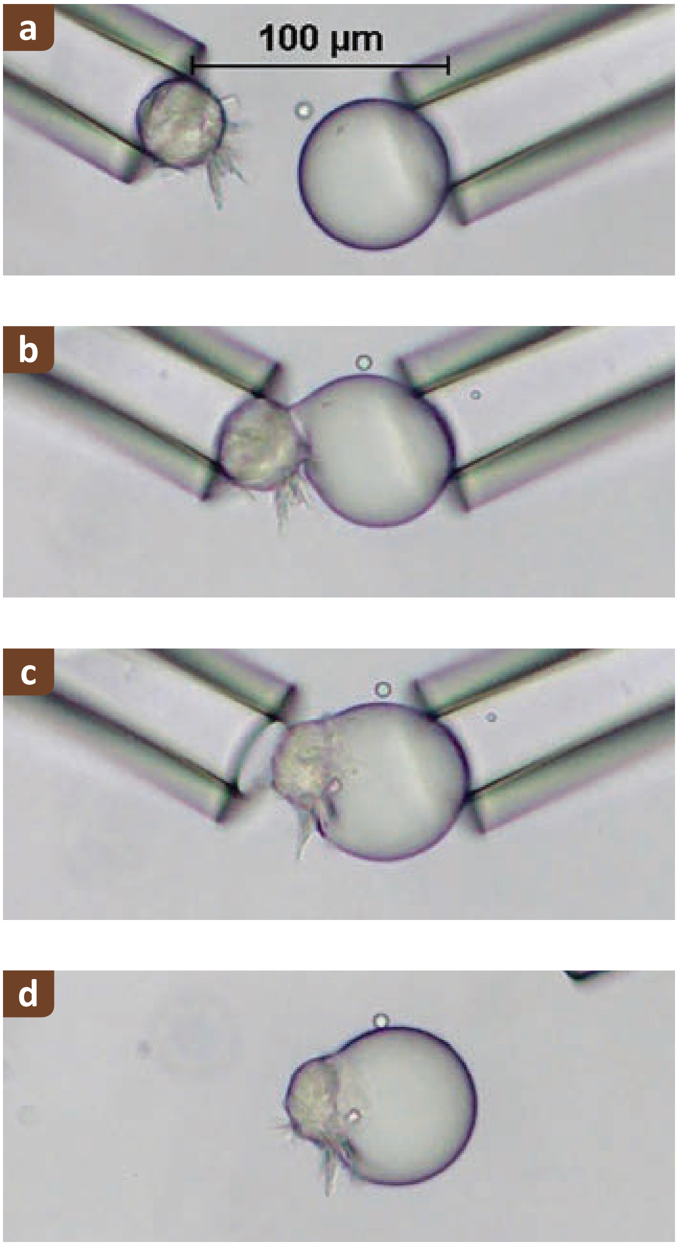


FIG. 4. (a) 100% Palm kernel oil droplet with interfacial crystals on the left manipulator and 4% SFC droplet composed of palm kernel oil and soybean oil on right the manipulator. (b) Interfacial crystals from left droplet are used to penetrate into right hand droplet. Oil begins to be shared between the two. (c) The oil being shared unites the droplets together. (d) Final structure showing the droplets arrested in a doublet configuration.

resulting in Pickering stabilization [1]. Nearly identical doublet assemblies to those in Figure 3 can also be seen by altering the surface coverage of nanoparticles situated at the interface of Pickering emulsion droplets. Note that no protruding, interfacial fat crystals are observed or needed for either Pickering emulsion droplets or partially crystalline emulsion droplets to initiate and undergo arrest.

This is not to say crystals at the interface of fat globule cannot initiate coalescence. Actually, such an event can be microscopically observed. Figure 4 shows one globule with crystals coaxed to the interface by adding a high amount

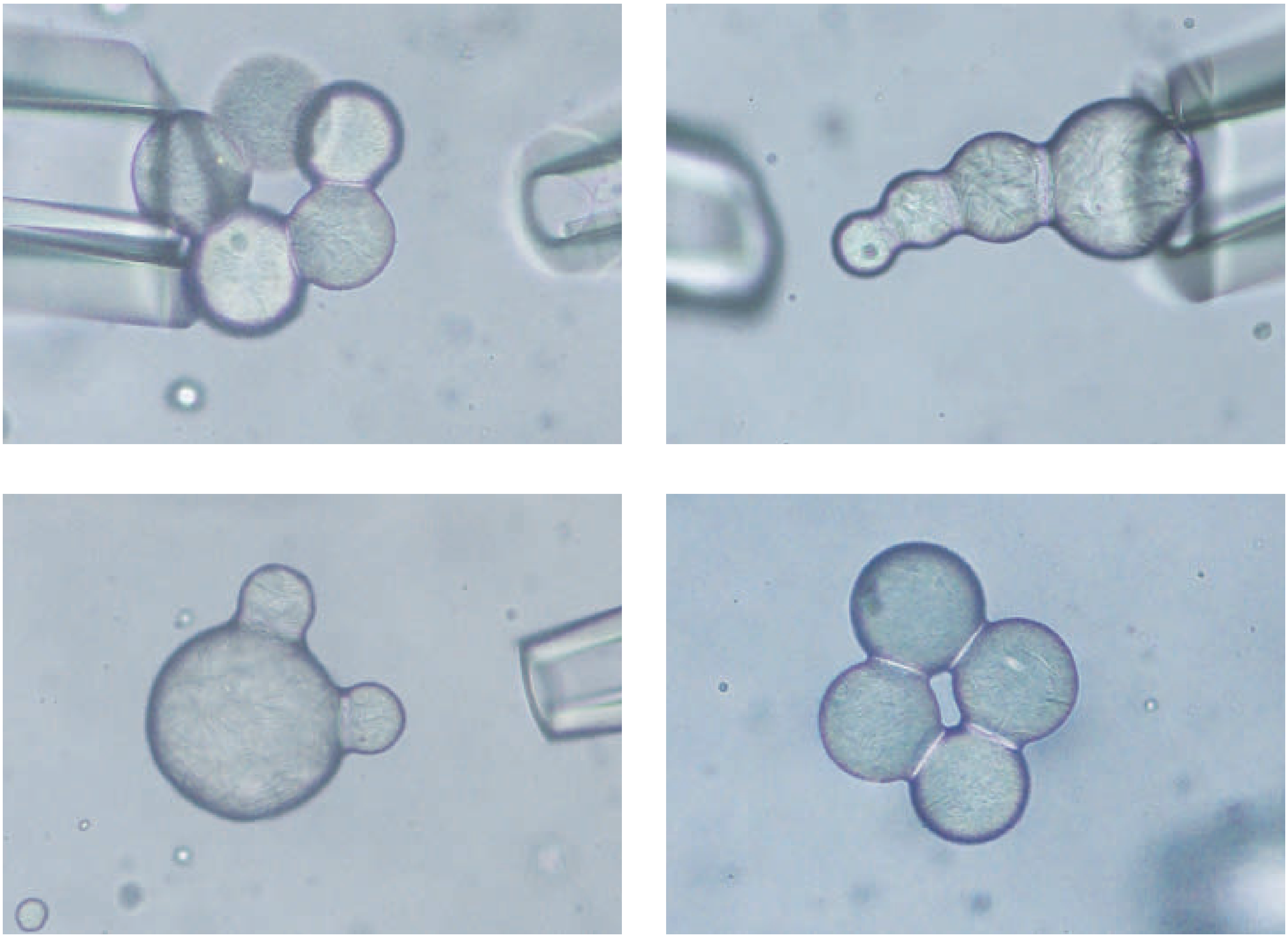


FIG. 5. Multiplets made by successively adding droplets to an existing arrested structure. Different anisotropic shapes can be attained depending on where the droplet is added.

of surfactant to the emulsion. The crystalline spears can be directed into the neighboring droplet and are seen to pierce through the interface. Oil begins to travel along the crystal, as if it were a bridge, merging the droplets. Therefore, crystalline fat at the interface can induce arrested coalescence, but is not a requirement.

Fabricating glass capillary tubes as micromanipulators allows great flexibility for working with different-sized droplets. Droplet diameters as small as 10 mm, and up to 100 mm, have been manipulated. Experimentally, as the diameter of same-sized droplets is increased, coalescence becomes arrested at earlier stages because of a reduction in the interfacial driving force.

Realistically, most emulsions have some variation in droplet size. To understand polydispersity, droplets of two different sizes have also been used to generate doublet structures. It was seen that the polydisperse pairs arrested earlier than monodisperse droplets. Additionally, as one droplet within the polydisperse pair was made smaller, doublets were seen to arrest earlier. As the total surface area of the monodisperse pair is larger than the polydisperse pair, these doublets underwent a greater degree of coalescence, at a given SFC, in attempts to minimize the total surface area exposed to the aqueous phase.

Moving beyond the shapes formed by two droplets, the next logical step is forming triplet structures. Here, two droplets are forced together and allowed to form a stable shape, then a third droplet is added to the existing doublet and its arrest studied. It was found that the orientation of the third droplet, relative to the first two, could change drastically from the original contact point, as the triplet underwent restructuring to lower its interfacial area. Conversely, the original positioning of the triplet can be preserved if droplets are composed of high solids. In this case, shape change would necessitate rearrangement or breakdown of the internal fat matrices, which is energetically unfavorable.

Investigating the fundamental behavior of doublets and triplets has led to numerous insights; however, in foods, partially-coalesced fat networks are likely to contain hundreds, if not thousands of individual droplets. Further studies into the mechanism of how these extensive, three-dimensional networks are created will be key to better controlling their occurrence in aerated foods. Additionally, investigating alternative shapes or assemblies of particles to achieve unique structures, as shown in Figure 5, could aid in drug delivery and provide enhanced functionality to consumer products, as these structures have higher surface area. Understanding how droplets can be used as building blocks to manipulate product microstructure will provide opportunities to optimize current food quality and to create new templates to design future food, consumer goods, and pharmaceuticals.

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Patrick Spicer is an associate professor of chemical engineering at the University of New South Wales in Sydney, Australia, where he studies microstructured fluids and their applications.

Abigail Thiel is a Ph.D. student at the University of Wisconsin–Madison, USA.

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Highlights from Minneapolis

Laura Cassiday

- The 2018 AOCS Annual Meeting & Expo, held in Minneapolis, Minnesota, USA, on May 6–9, offered many interesting and informative oral presentations.
- Those who attended could choose from more than 450 talks given during 67 technical sessions.
- Although complete coverage is not possible, this article highlights several talks that exemplify the high-quality science presented at the meeting.

Minneapolis, Minnesota, can still be wintry in May, but this year the weather was warm and spring-like for the 2018 AOCS Annual Meeting & Expo May 6–9. In addition to the stimulating science presented at the meeting, the 1,500+ attendees enjoyed the AOCS President's outdoor reception, a 5K fun run/walk, and, yes, bagpipers. This article highlights some of the interesting and informative oral presentations given during the meeting.

"DIETARY MONOUNSATURATED FATTY ACIDS AND CARDIOVASCULAR DISEASE PREVENTION: A SURPRISING STORY BEYOND OLEIC ACID"

Presented by Zhi-Hong Yang, National Heart, Lung and Blood Institute, National Institutes of Health
Health and Nutrition Division

Regular fish consumption has been demonstrated to benefit cardiovascular health. However, a recent meta-analysis showed no correlation between supplementation with omega-3 polyunsaturated fatty acids—commonly thought to underlie the cardioprotective effects of fish—and coronary heart disease or major vascular events (Aung, T, *et al.*, http://doi.org/10.1001/jamacardio.2017.5205, 2018). Therefore, some researchers have questioned whether other components besides omega-3 fatty acids may contribute to the cardioprotective effects of fish consumption. This presentation considered the possibility that the monounsaturated fatty acids (MUFAs) in fish might play a role.

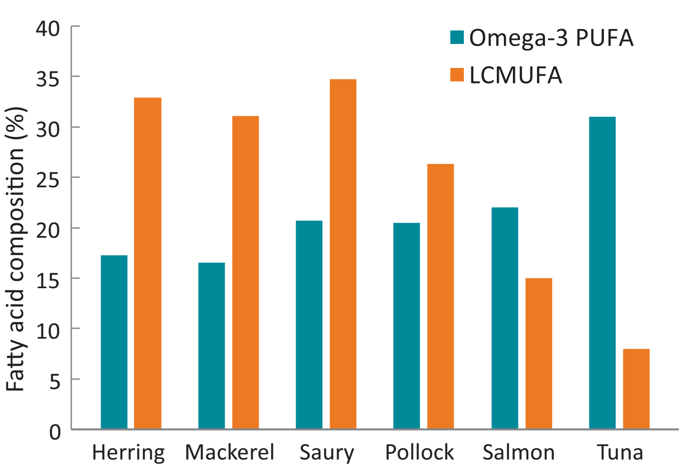

FIG. 1. Fatty acid composition of several edible fish. Omega-3 PUFA is the sum of ALA (C18:3 n-3), EPA (C20:5 n-3), DPA (C22:5 n-3), and DHA (C22:6 n-3). LCMUFA is the sum of C20:1 and C22:1 isomers.
Credit: Adapted from Yang, Z.H., *et al.*, http://doi.org/ 10.1186/s12944-016-0366-5, 2016.

MUFAs include palmitoleic acid (C16:1 n-7, found in macadamia nuts and some fish), oleic acid (C18:1 n-9, found in olives), and long-chain monounsaturated fatty acids (C20:1/ C22:1 n-11, found in fish). The heart-healthy effects of olive oil have been linked to oleic acid, with a carbon chain length of 18. However, much less is known about the cardiovascular effects of MUFAs with carbon chain lengths above or below 18. Epidemiological studies have indicated a cardioprotective effect of long-chain (LC) MUFAs (C > 18). Some fish species, such as herring, mackerel, saury, and salmon, are rich in C20:1 n-11 and C22:1 n-11 (Fig. 1).

Data from the Physician's Health Study have shown an inverse correlation between circulating LCMUFAs and incident coronary artery disease. In addition, several mouse studies have indicated that LCMUFA-rich oils reduce cardiovascular disease risk factors. In recent studies, Yang and colleagues conducted LCMUFA feeding trials on mouse models of atherosclerosis (Yang, Z.H., *et al.*, http://doi.org/10.1016/j.atherosclerosis.2017.04.017, 2017; Yang, Z.H., *et al.*, http://doi.org/10.1002/mnfr.201600142, 2016). They found that supplementing the mice's diets with 2–5% w/w of C20:1 and/or C22:1-rich fish oil suppressed the development of atherosclerotic lesions and improved high-density lipoprotein (HDL) cholesterol function, but did not change plasma low-density lipoprotein (LDL)-cholesterol levels. Proteomic analysis revealed that the LCMUFA supplementation altered the quality, but not quantity, of LDL-cholesterol subclasses, in particular, by shifting LDL-cholesterol to a larger, less atherogenic form.

In addition, Yang and colleagues investigated the relationship between short-chain (SC, C < 18) MUFAs and cardiovascular disease risk. In diabetic mice, palmitoleic acid (C16:1) reduced plasma triglyceride levels, increased insulin sensitivity, and favorably regulated the expression of genes involved in lipid metabolism (Yang, Z.H., et al., http://doi.org/10.1186/1476-511X-10-120, 2011). Furthermore, in rats C16:1 induced satiety to a greater extent than C18:1 (oleic acid), apparently by increasing secretion of the hunger-suppressing hormone cholecystokinin (CCK) from the small intestine (Yang, Z.H., et al., http://doi.org/10.1016/j.appet.2013.01.009, 2013).

Based on these promising results, Yang and her coworkers are now conducting two randomized, controlled clinical trials: one on the effects of LCMUFA fish oil supplements on lipoprotein metabolism (ClinicalTrials.gov, NCT03043365), and another on the effects of palmitoleic acid-rich oil on lipoprotein metabolism and satiety (NCT03372733). Thus, this research may contribute to improved dietary guidelines on MUFAs and to the formulation of new fatty acid supplements that improve cardiovascular health.

"SCREENING OF FATTY ACIDS SHOWING SELECTIVE ANTIBACTERIAL ACTIVITY AGAINST ACNE-ASSOCIATED *PROPIONIBACTERIUM ACNES*"

Presented by Toshihiro Nagao, Osaka Research Institute of Industrial Science and Technology, Japan
Biotechnology Division

Acne vulgaris is a common inflammatory skin disease that affects 85% of teenagers and 11% of adults. The condition has been linked to skin microorganisms, particularly the genus *Propionibacterium acnes* (Fig. 2, page 14), which was recently renamed *Cutibacterium acnes* to reflect its genetic differences from *Propionibacteria* that do not inhabit skin. However, the proportion of *C. acnes* in skin microbiota does not differ between healthy individuals and those who suffer from acne.

Previous research has shown that *C. acnes* can be separated into different strains on the basis of 16S rDNA sequence. Ribotypes (RT) 1, 2, and 3 are evenly distributed among healthy people and those who suffer from acne. RT4 and 5 are acne-associated strains, and RT6 is associated with healthy skin. Several differences have been identified between RT4 and 5 and other strains that may contribute to acne. For example, RT4 and RT5 produce higher levels of porphyrins, compounds that generate reactive oxygen species and cause inflammation in keratinocytes, and of the pro-inflammatory cytokines IFN-γ and IL-17.

Nagao and his collaborators, including Ayaka Uyama (Momotani Juntenkan Ltd., Japan), wanted to identify novel agents that selectively suppress the growth of the acne-associated strains RT4 and 5, but not of the harmless strain RT6. The researchers tested more than 40 common antibacterial agents, including salicylic acid, benzoyl peroxide, and triclosan, but all of these agents showed similar activities against the acne-associated (RT4 and 5) and non-acne-associated (RT6) strains. The researchers decided to test the activities of several saturated fatty acids and monoacylglycerols against the bacteria. They found that myristic (C14:0), pentadecylic (C15:0), palmitic (C16:0), and margaric (C17:0) acids inhibited the growth of RT4 and 5, but not RT6. In addition, monoacylglycerols containing pentadecylic acid or margaric acid selectively inhibited acne-associated strains. In contrast, five antibiotics used to treat acne killed RT6 more effectively than RT4 or 5. These results suggest a possible new strategy for treating acne that allows humans and harmless microorganisms to co-exist while killing disease-causing bacteria.

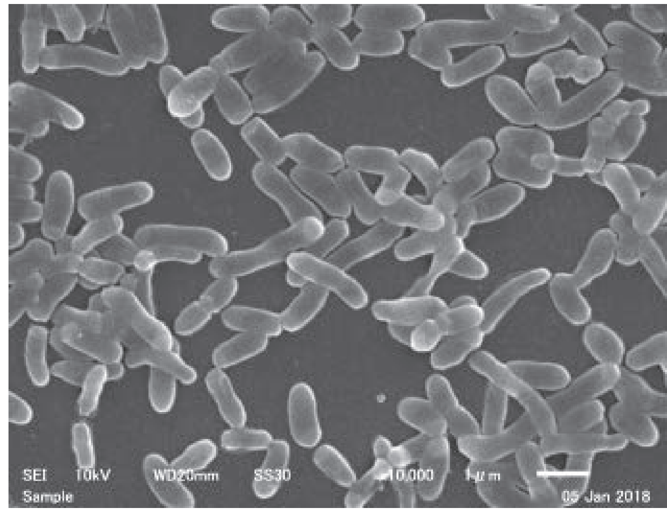

FIG. 2. *Cutibacterium acnes* (formerly *Propionibacterium acnes*).
Credit: Toshihiro Nagao

"MICROBES IN YOUR LAUNDRY: DOES WASHING ON 'COLD' MAKE A DIFFERENCE?"

Presented by Darci Ferrer, American Cleaning Institute
Surfactants & Detergents Division

Washing laundry in cold water extends clothing lifetime and reduces energy use. However, in a 2015 US consumer survey commissioned by the American Cleaning Institute (ACI), consumers said their main reason for not using cold water for laundry was that it "does not kill all germs" (reported by 21% of households). In light of this consumer concern, the ACI set out to examine whether washing laundry in cold water is less effective at removing microorganisms than washing at warmer temperatures.

In Europe, the International Association for Soaps, Detergents, and Maintenance Products (AISE) launched the "I Prefer 30°" campaign in 2013 to encourage people to wash laundry in cold water (30°C, or 86°F) for sustainability reasons. According to the AISE, the average wash temperature in Europe was 41°C (105.8°F). During the campaign, consumers voiced concerns to the AISE that laundering at 30°C was not hygienic. As a result, the AISE commissioned a weight of evidence review that assessed microbial inactivation at temperatures ranging from 15°C to 77°C (59°F to 170°F). The review determined that temperatures less than 40°C (104°F) had only a minor effect on microbial inactivation, which was attributed to the detergent and the physical motions of laundering.

In 2017, the ACI conducted a literature review of microbial inactivation at different wash temperatures, as the definition of "cold water" varies with location. For example, in Anchorage, Alaska, USA, the average cold water inlet temperature is about 4°C (39°F), whereas in Phoenix, Arizona, USA, the cold water inlet is 28°C (82°F). The US average is about 15°C (59°F). For hot water, the setting of US water heaters is 49°C (120°F). According to the ACI review, when no adjunct products such as bleach were used, microbial removal decreased with temperature. Viruses were more difficult to thermally inactivate than bacteria. Temperatures above 40°C (104°F) were required for removal of microbes due to thermal inactivation. The largest reduction in microbial load was observed at wash temperatures above 60°C (140°F). The review was unable to determine the effects of varying detergents due to insufficient data.

Because US water heaters are set to 49°C, even hot water washes are below the 60°C required for substantial microbial inactivation. "In the United States, the removal of germs at cold wash settings is similar to removals at even hot water settings," the ACI concluded. Opportunities for future research include examining how drying time, variations in wash cycles, water volume, and organic load affect microbial survival.

"RESULTS OF EXPERIMENTS TO REDUCE MCPD AND GLYCIDYL ESTERS IN EDIBLE FATS AND OILS BY IONIC LIQUID TREATMENT"

Presented by Frank Pudel, Pilot Pflanzenöltechnologie Magdeburg e.V., Magdeburg, Germany
Processing Division

MCPD and glycidyl esters are contaminants formed in edible oils during the refining process. Precursors for MCPD esters, found in crude vegetable oil, are chloride (organic and inorganic) and lipids (mono-, di-, triglycerides and phospholipids).

MCPD esters form at temperatures above 150°C, and their formation is influenced by time and pH. In contrast, glycidyl esters require only diacylglycerols (DAGs) as precursors and form at temperatures above 230°C. There are three major strategies to mitigate these process contaminants: 1) removal of precursors from the crude oil, 2) process changes, and 3) removal of MCPD and glycidyl esters from the refined oil.

3-MCPD esters and related compounds increase with increasing DAG content in edible oils. In palm oil, DAGs—and thus 3-MCPD esters—can be reduced by harvesting the palm fruit at the optimal ripeness, rejecting damaged fruits, and processing as quickly as possible (3–6 hours) after harvest. In addition, some palm fruit varieties have been identified that have reduced lipase activity, which can also lower DAGs. To reduce chloride precursors, the use of chloride-containing substances during cultivation, such as fertilizers, pesticides, and irrigation water, should be minimized. Also, avoiding cultivation on saline soils can reduce the chloride content of the crude oil.

During processing, acid degumming produces more 3-MCPD esters than water degumming. The pH and amount of bleaching clay can also affect 3-MCPD ester formation. A higher pH and greater amount of bleaching earth (3% versus 1%) reduces 3-MCPD esters in refined palm oil. Two-step deodorization processes have also been investigated. A short deodorization at a high temperature followed by a longer deodorization at a lower temperature produces remarkably lower levels of glycidyl esters. However, this process change does not significantly reduce 3-MCPD ester formation.

Instead of deodorization, short path distillation may be used to reduce 3-MCPD and glycidyl esters. This method uses a high vacuum and short heating time. Short path distillation does not produce 3-MCPD or glycidyl esters; however, sensory qualities of the oil are negatively affected. For example, palm oil refined by short path distillation is red in color because pigments are not destroyed during deodorization. A subsequent gentle deodorization at 160–180 °C eliminates the sensory disadvantages but forms a small amount of 3-MCPD esters.

After refining, 3-MCPD and glycidyl esters can be removed by post-bleaching with various adsorbents, followed by gentle deodorization. Other approaches include double bleaching and deodorization, or the use of short path distillation after deodorization.

Evonik (Marl, Germany) is developing a new approach for reducing 3-MCPD and glycidyl esters. In this process, crude palm oil is treated with ionic liquid, which reacts with free fatty acids, followed by removal of the ionic liquid-free fatty acid complex, bleaching of the oil, and modified deodorization at a reduced temperature. Importantly, the ionic liquid can be regenerated, avoiding the formation of soapstock and oil loss.

Ionic liquid-treated palm oil showed a much lower 3-MCPD ester content than conventionally refined palm oil (0.8 ppm versus 3.6 ppm). The treatment also greatly reduced glycidyl esters—from 6.1 ppm in physically refined palm oil to 1.5 ppm in ionic liquid-treated oil. Further optimization is ongoing.

"CAN HUMANS DETECT IF A CHOCOLATE IS IN THE Β' OR B_V FORM?"

Presented by Fernanda Peyronel, University of Guelph, Canada
Edible Applications Technology Division

Good chocolate is smooth, glossy, has snap, and melts just below body temperature. For fine artisanal chocolate that contains only cocoa butter as the fat, tempering is a fundamental step of production. During tempering, cocoa butter crystallization is carefully controlled to ensure that chocolate is in its most stable crystal form, β_V. However, given that the differences in atomic distances of the polymorphic forms are only a few angstroms, can consumers really tell the difference between two polymorphic forms, such as β' and β_V, or are they detecting larger structures in the chocolate?

Chocolate tempering involves cooling liquid chocolate from a temperature of about 50°C to about 27–29°C with constant stirring, and then increasing the temperature to

*Inform*ation

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Yang, Z.H., *et al.*, Chronic administration of palmitoleic acid reduces insulin resistance and hepatic lipid accumulation in KK-Ay mice with genetic type 2 diabetes, *Lipids Health Dis. 10*: 120, 2011, http://doi.org/10.1186/1476-511X-10-120.

Yang, Z.H., *et al.*, Oral administration of omega-7 palmitoleic acid induces satiety and the release of appetite-related hormones in male rats, *Appetite 65*: 1–7, 2013, http://doi.org/10.1016/j.appet.2013.01.009.

Yang, Z.H., *et al.*, Dietary marine-derived long-chain monounsaturated fatty acids and cardiovascular disease risk: a mini review, *Lipids Health Dis. 15:* 201, 2016, http://doi.org/ 10.1186/s12944-016-0366-5.

Yang, Z.H., *et al.*, Long-chain monounsaturated fatty acid-rich fish oil attenuates the development of atherosclerosis in mouse models, *Mol. Nutr. Food Res. 60*: 2208–2218, 2016, http://doi.org/10.1002/mnfr.201600142.

Yang, Z.H., *et al.*, Dietary supplementation with long-chain monounsaturated fatty acid isomers decreases atherosclerosis and alters lipoprotein proteomes in $LDLr^{-/-}$ mice, *Atherosclerosis 262*: 31–38, 2017, http://doi.org/10.1016/j.atherosclerosis.2017.04.017.

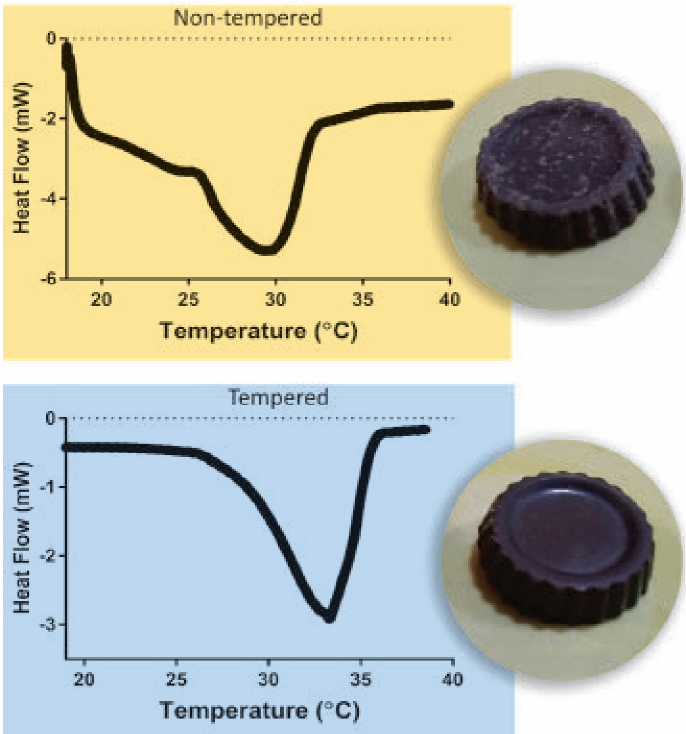


FIG. 3. A commercial chocolate bar was melted and recrystallized by different protocols to produce tempered and non-tempered chocolate. DSC curves showing that non-tempered chocolate (top) melts at a lower temperature than tempered chocolate (botoom). Credit: Fernanda Peyronel

30–32°C. The chocolate is maintained at each temperature for a particular amount of time. Next, the chocolate is poured into a mold and cooled to about 16°C. The first cooling step, when the chocolate is brought from 50°C to about 28°C, initiates nucleation of the cocoa butter. Typically, more β′ and α crystals than β_V crystals are formed at this step. Then, by raising the temperature slightly, the less stable crystals melt, leaving primarily β_V crystals. In the second cooling step, the β_V crystals act as seeds to drive further β_V crystallization. As a result, the molded chocolate will consist mainly of β_V crystals, which confer the desired textural and melting properties.

Routine checks of chocolate quality are conducted using x-ray diffraction, also referred to as wide-angle x-ray scattering (WAXS). This technique gives information about the polymorphic form present in the fat. Other x-ray scattering techniques used to study the structure are small-angle x-ray scattering (SAXS) and ultra-small-angle x-ray scattering (USAXS). SAXS provides information about the packing of the molecules into lamellae, whereas USAXS gives information regarding larger structures that can range from ~100 nm to ~30 µm. Peyronel used a combination of WAXS and USAXS to examine not only the cocoa butter structures formed, but also the cocoa powder and the sugar.

Peyronel investigated a commercial chocolate bar and compared the results with those obtained when the chocolate was melted and crystalized to produce tempered and non-tempered chocolate. WAXS results showed that the commercial and tempered chocolates were in the β_V form, whereas the non-tempered chocolate was in the less stable β′ form.

These results were confirmed using differential scanning calorimetry (DSC). The DSC results revealed that the melting point of the non-tempered chocolate was 29°C, compared with 33°C for the tempered chocolate and the commercial chocolate (Fig. 3). Using scanning electron microscopy of freeze-fractured chocolate, the researchers observed that the non-tempered chocolate appeared flakier. USAXS revealed that tempered and non-tempered chocolate present a different fractal structure in the 6 to 31-µm length scale. At this length scale, the tempering cycle seems to create a fractal dimension with a higher solid mass density than non-tempered chocolate.

When a panel of 10 volunteers was fed the chocolates, 7 identified that the non-tempered sample was different, and 5 agreed that the non-tempered chocolate melted faster. Six people found the non-tempered chocolate to be gritty. In foods, particles in the range between 11 to 80 µm could be perceived by the mouth as "gritty," depending on the matrix in which they are suspended. This work bridges the gap between sensory analysis and x-ray scattering by showing that the perceived mouth feel could be due to the differences in the fractal dimension in the length scale between 6 and 31 µm.

Laura Cassiday is a former associate editor of Inform.

2018 Annual Meeting & Expo: ingenuity, innovation, inspiration, imagination

The 2018 AOCS Annual Meeting & Expo provided 1,500+ professionals, scientists, researchers and students from the fats, oils, protein and surfactant industries with a forum to build their knowledge of today's market and learn about the latest scientific research. Attendees represented 580+ companies and 49 countries, and 1,179 people followed the meeting on social media.

The program featured 10 Hot Topic Symposia covering key issues such as olive oil quality and diversity and inclusion in the workplace, three special sessions, and XX+ oral presentions (42 of which were given by AOCS award winners and travel grant recipients), with topics ranging from food peptide behavior to dietary fats. Some of the highlights are covered on pages 12–16. Copies of presentations will be available to AOCS members in the AOCS Premium Content Library, subject to author/presenter permission.

The sold-out exhibition featured 98 suppliers in the international fats and oils trade in an engaging hands-on atmosphere that facilitated business and interaction among industry leaders and industry-related firms from around the world.

An outdoor President's Welcome Reception featuring foods and beverages from Minnesota, a dessert break, two complimentary lunches and happy hour receptions, and newcomer speed networking provided plenty of networking opportunities.

Members of the Student, Young Professional, and Professional Educator Common Interest Groups (CIGs) got up close and personal during the joint CIG luncheon, one of several CIG events, which included a meet-and-greet for each group at the President's Welcome Reception.

Participants engaged in the work of the Society at dozens of committee and leadership meetings, including this business meeting for the Young Professionals Group.

The meeting also featured about 120 poster presentations.

A morning 5K fun run/walk in a scenic park and a "Walk the Halls" pedometer got the blood moving and gave participants a chance to connect with one another on a different level.

Bagpipes led a procession from the Welcome Plenary to the President's Welcome Reception. The Welcome Plenary featured an ISF Kaufmann Memorial Lecture by award winner Dr. Kazuo Miyashita, Hokkaido University, Japan, and a plenary talk on positioning plant proteins to consumers by Dr. James House, University of Manitoba, Canada.

What a week! Looking forward to #AOCS2019 in St. Louis!

This has been such an awesome @aocs annual meeting... #AOCS2018 .. Thank you for all the great moments...

AOCS 2018 award recipients

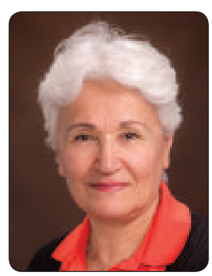
AOCS celebrates ingenuity and collaboration by honoring those individuals and teams who have taken the industry to the next level, who have advanced the quality and depth of the profession, and who have leveraged their knowledge for the benefit of the society. These individuals from around the world were recognized during the 2018 AOCS Annual Meeting & Expo held May 6-9. Scientific and Society Award nominations for 2019 are due October 1, 2018. **Nominations for all other awards are due November 1, 2018. To learn more, visit aocs.org/awards.**

SOCIETY AWARDS

FELLOW AWARD

Recognizes: Achievements in science or extraordinary service to the Society.

ROTIMI ALUKO is a professor in the Department of Food and Human Nutritional Sciences at the University of Manitoba, Winnipeg, where he directs the Richardson Centre for Functional Foods and Nutraceuticals. He earned a Ph.D. degree in Food Science from the University of Guelph, Ontario, Canada, in 1996. His work focuses on the structure-function properties of food proteins and peptides, with special focus on oilseeds and pulses. In addition to having more than 160 journal article publications, he also has 4 patents. Aluko has trained 12 doctoral and 8 master's degree students, 9 postdoctoral fellows, and several undergraduate summer research interns. In 2017, he was acknowledged as a Highly Cited Researcher in the Agricultural Sciences category by Thomson Reuter's Clarivate Analytics. The recognition is given to researchers who have distinguished themselves by publishing a high number of papers that rank in the top 1% most-cited in their respective fields over a recent 11-year period. For the past 13 years, Aluko has been involved with AOCS as a regular conference attendee as well as a technical session organizer and oral paper presenter in the Protein and Co-Products (PCP) Division. During that time, he also sponsored his staff and students to attend the AOCS annual meeting and make oral or poster presentations in PCP and Health and Nutrition Division sessions. His students have won several poster awards, and three are past recipients of the AOCS Honored Student Award. Aluko also served as Chair of the PCP Division from 2008 to 2010.



NURHAN DUNFORD is a professor in the Biosystems and Agricultural Engineering Department at Oklahoma State University, Stillwater, Oklahoma, where she has a joint appointment with the Robert M. Kerr Food and Agricultural Product Center as an oil and oilseed specialist. She contributes to all three missions of the university: teaching, research, and extension. Dunford's more than 25 years of experience as an engineer and scientist encompass positions in Turkey, Canada, and the United States. Her research focuses on optimization of sustainable processing technologies and advancing utilization of industrial by-products and waste streams for value-added product development, including biofuels, functional foods, and other industrial bioproducts. She is a two-time Fulbright Scholar who has mentored and hosted many students and scientists from Canada, Turkey, Mexico, China, Sweden, Columbia, South Korea, India, Iran, Iraq, Indonesia, and the United States. Dunford has been very active in several professional organizations, including AOCS. She served in many leadership positions on Division- and Society-level committees (member-at-large; secretary/treasurer; and chair of the AOCS Processing Division, AOCS Division Council, and the 2012 AOCS Annual Meeting & Expo). She has chaired many award committees, organized and chaired numerous annual meeting technical sessions, edited two books for the AOCS Press, and contributed scientific articles to the Society journals. She has received many national and international awards recognizing her contribution to the science and service to professional societies, including the AOCS Edible Applications Division Timothy L. Mounts Award (2011) and the Merit Award (2015).

DANIEL K.Y. SOLAIMAN, Research Molecular Biologist/Lead Scientist at the Eastern Regional Research Center of ARS, USDA, has made significant scientific contributions to the field of microbially produced lipid-based polymers and surfactants. He has authored or co-authored many publications and holds several patents as a result of his personal and team research on the characterization and applications of the genetic systems of the biosynthesis of polyhydroxyalkanoate biopolymers and the sophoro-/rhamno-lipid biosurfactants, and on the utilization of agricultural and industrial by-product waste-streams as low-cost fermentation feedstocks to produce these biobased products. His research team received AOCS' venerable ACI/NBB Glycerine Innovation Research Award in 2008, and the Philadelphia Federal Executive Board's Excellence in Government Gold Medal Award in 2016. Solaiman has been an active member and has served AOCS in many capacities since joining the Society in 2000. He is most active in the Biotechnology Division, serving on its Executive Steering Committee (2008–2012) as Secretary/Treasurer, Vice Chair, and Chair. Dan was also active in the Publication Steering Committee (2003–2012), serving as its first Vice Chair, and was assigned to chair a few important search committees. He also contributed to the Society's book publication efforts by co-editing *Biobased Surfactants and Detergents: Synthesis, Properties, and Application*s in 2010. Dan is grateful to be a part of the AOCS family that provides him with opportunities to grow and serve in his profession.

XUEBING XU, General Manager of Wilmar Global Research and Development Center, Shanghai, China, received his Ph.D. degree from the Technical University of Denmark, and is a former professor of Aarhus University, Denmark. Xu's areas of research include lipid technology, food/lipid/ingredients functionality, and enzyme technology. He has authored or co-authored more than peer-reviewed 270 papers, co-edited three books, and is inventor/co-inventor on 33 patents. Xu is the president of the International Sunflower Oil Association (2015–present). He is on the board of the International Association of Rice Bran Oil (2014–present). He is the recipient of the European Lipid Technology Award (2017), among many other awards. He is senior advisor to United Nations Office for Project Services (2015–present).

Xu has been involved in a number of activities in AOCS. He is the associate editor of *JAOCS* (2005–present) and was a member of student paper award evaluation committees (2003–2006) and evaluation committees for the Stephen S. Chang Award (2009–2010, 2013) and Young Scientist Award (2016–2017). He is currently chairman of the Phospholipids Division and deputy chairman of the AOCS China Section (2017–present). Xu has co-organized or served on the organizing committee for several AOCS-associated conferences, such as the AOCS–CCOA Joint Symposium on Functional Lipids (2014), and the first AOCS China Section Congress (2017). He has also served as a session chair or co-chair for numerous AOCS annual meetings.

SCIENTIFIC AWARDS

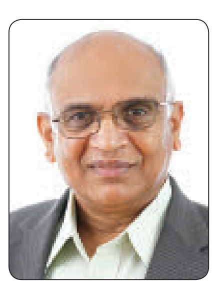
STEPHEN S. CHANG AWARD

Recognizes: A scientist or technologist who has made decisive accomplishments in research for the improvement or development of products related to lipids.
Endowed by: The late Stephen S. Chang and his wife, Lucy D. Chang.

N. A. MICHAEL ESKIN, a professor in the Department of Food and Human Nutritional Sciences at the University of Manitoba, Canada, has done extensive research on edible oils and was involved in the early development of canola oil. In 2016, he received the Order of Canada, the highest civilian honor, for his scientific contributions that led to the success of the Canadian canola oil industry. Michael has published over 130 research papers and 60 chapters, and is the author, co-author, and editor of 15 books—a number of which were translated into German, Japanese, Malay, and Portuguese. His current research focuses on the production and antioxidant properties of canolol from canola as well as improving the stability of hemp oil. He has been a member of AOCS for over 40 years, having served as Chair of the Lipid Oxidation and Quality Division, the first Chair of the newly formed Division Council, Associate Editor of *JAOCS*, as well as Chair of the Flavor Quality and Stability Committee. Michael has also been active on AOCS' Education Committee and is currently Associate Editor of Education for the AOCS Lipid Library®. He is the recipient of many awards and was made a Fellow of AOCS in 2004. This year marks his 50th year at the University of Manitoba, where he has served as Department Chair and Associate Dean. Last year, Michael was voted the Outstanding Professor by the students of his faculty. He is also known for his lipid rap songs, which are used in universities across North America as well as shown in a Nutrition Centre in Moscow.

ALTON E. BAILEY AWARD

Recognizes: Outstanding research and exceptional service in the field of lipids and associated products.
Sponsored by: Archer Daniels Midland Company

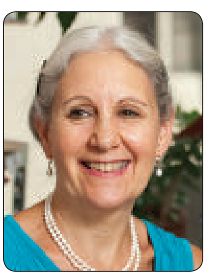


DHARMA R. KODALI is a research professor in Bioproducts and Biosystems Engineering at the University of Minnesota, Saint Paul, Minnesota, and a former professor of Boston University. He is a world-recognized expert in lipids and new product development, and has over 35 years of research experience in academia and industry. His industrial experience includes working as an R&D Manager at Cargill for 13 years, and as a Senior Principal Scientist at General Mills for one year. During that time, he developed several new products from concept to commercialization. His current areas of research continue to be developing value-added products from fats and oils for industrial applications.

Kodali has authored or co-authored over 75 publications and book chapters and edited two books on trans fats. He is an inventor/co-inventor on 30 patents. His accomplishments include Cargill's Chairman's Innovation Award (2001), the American Chemical Society's Industrial Innovation Award (2002), and the AOCS Edible Applications Technology Division's Timothy L. Mounts Award (2003). He is an elected Fellow of AOCS (2010) and the American Institute of Chemists. He has served AOCS in various capacities, including chairing the Industrial Oil Products Division, teaching short courses, serving as an Associate Editor and peer reviewer of *JAOCS*, as Session Chair at national meetings, and as a member of the Books and Publications and Recognition Program committees.

SUPELCO AOCS RESEARCH AWARD

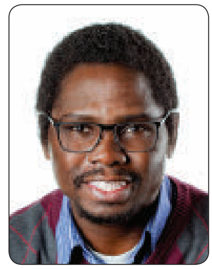
Recognizes: Outstanding original research in fats, oils, lipid chemistry, or biochemistry.
Sponsored by: MilliporeSigma, a subsidiary of Sigma-Aldrich Corp.



ALICE H. LICHTENSTEIN is the Stanley N. Gershoff Professor of Nutrition Science and Policy at the Friedman School, and Director of the Cardiovascular Nutrition Laboratory and Senior Scientist at the Jean Mayer USDA Human Nutrition Research Center on Aging at Tufts University. She holds secondary appointments as a professor of medicine at Tufts Medical Center, and an honorary doctoral degree from the University of Eastern Finland. Lichtenstein's research group focuses on assessing the interplay between diet and heart disease risk factors. Past and current work includes addressing issues related to trans fatty acids, soy protein and isoflavones, sterol/stanol esters, and novel vegetable oils differing in fatty acid profile and glycemic index. Additional work focuses on population-based studies to assess the relationship between nutrient biomarkers and cardiovascular disease risk, and application of systematic review methodology to the field of nutrition. Lichtenstein serves as an Associate Editor of the *Journal of Lipid Research* and Executive Editor of the Tufts Health and Nutrition Letter. She served on the 2000 (member) and 2015 (vice-chair) Dietary Guidelines Advisory Committee, and is a member of the American Heart Association's (AHA) Nutrition Committee, and Food and Nutrition Board of the National Academies of Sciences. She received the 2006 Robert H. Herman Memorial Award in Clinical Nutrition (ASN), 2008 Women's Mentoring Award (AHA), and 2010 Excellence in Dietary Guidance Award (American Public Health Association). In 2016, she received the David Kritchevsky Career Achievement Award in Nutrition (ASN), and in 2017 she was awarded the Ralph Holman Lifetime Achievement Award from AOCS.

AOCS YOUNG SCIENTIST RESEARCH AWARD

Recognizes: A young scientist that has made a significant and substantial research contributions in one of the areas represented by an AOCS Division.



CHIBUIKE UDENIGWE is an associate professor in Nutrition Sciences, with a cross-appointment in Chemistry and Biomolecular Sciences at the University of Ottawa, Canada. He earned a Ph.D. in Food and Nutritional Sciences from the University of Manitoba, Canada, and then joined the University of Guelph as a Natural Sciences and Engineering Research Council of Canada Postdoctoral Fellow (2011–2012). He joined Dalhousie University as an Assistant Professor (2012–2014), and was promoted to Associate Professor (2014–2016) before joining the University of Ottawa in 2016. His major areas of focus include chemistry, the role and mechanisms of food peptides in nutrition and health, molecular behavior in food and biological matrices, food protein allergens, and functionality of emerging (e.g., edible insect) proteins.

Chibuike joined AOCS as a student member and received the Honored Student Award during the centennial meeting in 2009. Since becoming a member, he has served as the PCP Division Secretary-Treasurer (2016–2018), Co-chair of Technical Sessions (2013–present), ADM Best Paper Award Committee Chair (2016–2018), Student Poster Award Judge, PCP Newsletter Editor (2013–2016), Mentor–Student Common Interest Group events, and Vice Chair–Canadian Section of AOCS (2017–present). He has published more than 95 articles in peer-reviewed journals and books, and presented invited papers at international conferences. In 2016, he was a visiting scientist at Wageningen University and Research, The Netherlands. He was a recipient of the International Union of Food Science and Technology Young Scientist Award (2012), and was elected into the Early Career Scientists Section of the International Academy of Food Science and Technology (2016).

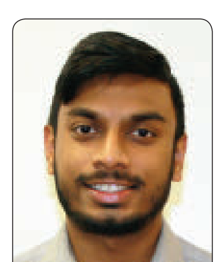
DIVISION AWARDS

ANALYTICAL

Herbert J. Dutton Award
WALTER VETTER, University of Hohenheim, Germany

Student Award
SUBIN R. C. K. RAJENDRAN, Dalhousie University, Canada

Vetter



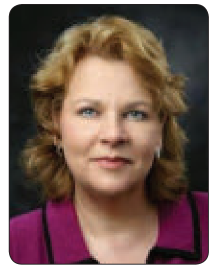
Rajendran

BIOTECHNOLOGY

Ching Hou Biotechnology Award
THOMAS McKEON, USDA-ARS, WRRC, USA

Student Award
First place: **S.M. MAHFUZUL ISLAM**, The University of Akron, USA
Second place: **SARAH A. WILLETT**, University of Georgia, USA
Third place: **CHEN HSU**, National Taiwan University, Taiwan


McKeon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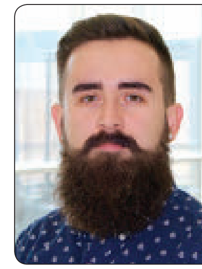
Yang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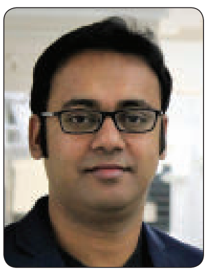
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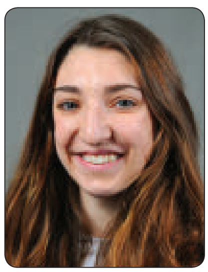
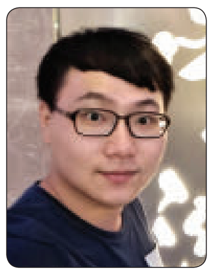
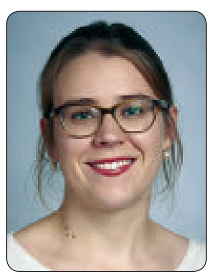

Willett


Hsu

EDIBLE APPLICATIONS TECHNOLOGY

Student Award
IRIS TAVERNIER, Ghent University, Belgium


Tavernier

HEALTH AND NUTRITION

Ralph Holman Lifetime Achievement Award
SUSAN K. RAATZ, USDA-ARS, USA

New Investigator Research Award
ZHI-HONG YANG, CPB-NHLBI-NHI, USA

Student Award
JUAN J. ARISTIZABAL HENAO, University of Waterloo, Canada

2018 AWARD SPONSORS

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Kemper


Aldana Rico

INDUSTRIAL OIL PRODUCTS
Student Award
LUCAS J. STOLP, University of Minnesota, USA

PROCESSING
Distinguished Service Award
TIMOTHY G. KEMPER, Desmet Ballestra Group, USA

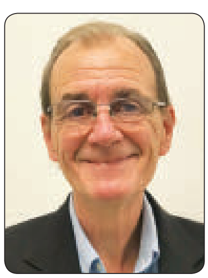
Student Award
ANDRÉS F. ALDANA RICO, Universidad del Norte, Columbia

SURFACTANTS AND DETERGENTS
Distinguished Service Award
JAN SHULMAN, Retired, USA

Samuel Rosen Memorial Award
DAVID SCHEUING, Clorox Services Co., USA

Student Award
LISA VAN RENTERGHEM, Ghent University, Belgium


Shulman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Van Renterghem

DIVISION POSTER AWARDS

EDIBLE APPLICATIONS TECHNOLOGY DIVISION (STUDENT)
First place: **RUOJIE ZHANG**, University of Massachusetts-Amherst, USA, for "Control of protein digestion under simulated gastrointestinal conditions using biopolymer microgels."

Second place: **DIANHUI WU**, North Dakota State University, USA, for "Electrostatic deposition of chitosan on lecithin stabilized emulsion inhibits mycotoxin production in *Fusarium graminearum*."

HEALTH AND NUTRITION DIVISION
Best overall: **RYOTA HOSOMI**, Kansai University, Japan, for "Dietary fat influences the composition of bacteria and its metabolites in cecum of rat."

First place student: **FABIEN SCHULTZ**, Technical University of Berlin, Neubrandenburg University of Applied Sciences, Germany, for "Investigation of bioactive lipids from African medicinal plants collected in the tropical rainforests of Uganda."

Second place student: **ADRIANA V. GAITÁN**, Louisiana State University, USA, for "Endocannabinoid metabolome in human breast milk—a Guatemalan cohort."

Third place student: **ZIPEI ZHANG**, University of Massachusetts-Amherst, USA, for "Edible hydrogel beads fabrication with self-regulating microclimate pH properties: retention of enzyme activity after exposure to gastric conditions."

LIPID OXIDATION AND QUALITY DIVISION (STUDENT)
JUNSI YANG, University of Nebraska-Lincoln, USA, for "Development of novel free-flowing fish oil-loaded hollow solid lipid micro- and nanoparticles to improve oxidative stability of fish oil."

PROTEIN AND CO-PRODUCTS DIVISION (STUDENT)
First place: **AYA HAMADA**, Nihon University, Japan, for "Physicochemical properties of rice albumin with a suppressive function against hyperglycemia."

Second place: **TEMITOLA O. AWOSIKA**, University of Manitoba, Canada, for "Inhibitory activities of yellow field pea protein-derived peptides against α-amylase and α-glucosidase."

Third place: **ADAM J. FRANCZYK**, University of Manitoba, Canada, for "Protein digestibility and quality determined using two *in vitro* methods in cooked, baked and extruded pulses."

SURFACTANTS AND DETERGENTS DIVISION (STUDENT)
TOMONE SASAYAMA, Tohoku University, Japan, for "Continuous production of sugar fatty acid ester from 100% biorenewable materials using heterogeneous resin catalyst."

STUDENT AWARDS

HANS KAUNITZ AWARD
ZIPEI ZHANG, University of Massachusetts-Amherst, USA

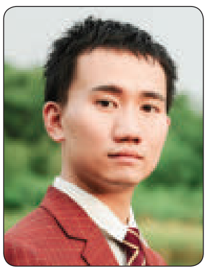
RALPH H. POTTS MEMORIAL FELLOWSHIP AWARD
THOMAS A. KWAN, Yale University, USA

LIPID CHEMISTRY AND NUTRITION AWARD
RUOJIE ZHANG, University of Massachusetts-Amherst, USA


Z. Zhang


Kwan


R. Zhang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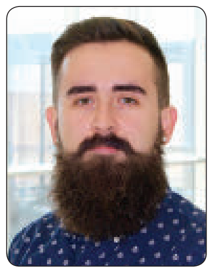
Henao

LIPID PROCESSING AND BIOTECHNOLOGY AWARD
JUN JIN, Jiangnan University, China

AOCS FOUNDATION
Manuchehr (Manny) Eijadi Award
ALI UBEYITOGULLARI, University of Nebraska-Lincoln, USA

Honored Student Award
JUAN J. ARISTIZABAL HENAO, University of Waterloo, Canada
THAIS L. T. da SILVA, University of Campinas, Brazil
JUN JIN, Jiangnan University, China
NAN SHANG, University of Alberta, Canada
ALI UBEYITOGULLARI, University of Nebraska-Lincoln, USA
RUOJIE ZHANG, University of Massachusetts-Amherst, USA
JuDONG YEO, Memorial University of Newfoundland, Canada

Peter and Clare Kalustian Award
JUAN J. ARISTIZABAL HENAO, University of Waterloo, Canada

Thomas H. Smouse Memorial Fellowship Award
RUOJIE ZHANG, University of Massachusetts-Amherst, USA


da Silva


Shang


Yeo

BEST PAPER AWARDS

ACI DISTINGUISHED PAPER
Optimized microemulsion systems for detergency of vegetable oils at low surfactant concentration and bath temperature (*JSD 20*(4):805–813).
Chodchanok Attaphong and David A. Sabatini

ARCHER DANIELS MIDLAND AWARD FOR BEST PAPER IN PROTEIN AND CO-PRODUCTS

Chemistry/Nutrition Category
Biologically active digests from pumpkin oil cake protein: effect of cross-linking by transglutaminase (*JAOCS 94*:1245–1251).
Ljiljana Popović, Žužana Stolić, Jelena Čakarević, Aleksandra Torbica, Jelena Tomić, and Mirjana Šijački

Engineering/Technology Category
Effects of steam distillation and screw-pressing on extraction, composition and functional properties of protein in dehulled coriander (*Coriandrum sativum* L.) (*JAOCS 94*:315–324).
Mila P. Hojilla-Evangelista and Roque L. Evangelista

EDWIN N. FRANKEL AWARD FOR BEST PAPER IN LIPID OXIDATION AND QUALITY
Application of differential pulse voltammetry to determine the efficiency of stripping tocopherols from commercial fish oil (*JAOCS 94*:527-536).
Rachele A. Lubeckyj, Jill K. Winkler-Moser, and Matthew J. Fhaner

PHOSPHOLIPID BEST PAPER AWARD
Food grade liposome systems: effect of solvent, homogenization types, and storage conditions on oxidative and physical stability (*Colloids and Surfaces A: Physicochem. Eng. Aspects 513*:468-478).
Selen Gruner and Mecit Halil Oztop

OTHER AWARDS

LABORATORY PROFICIENCY PROGRAM AWARDS
AOCS' Laboratory Proficiency Program is the world's most extensive and respected collaborative proficiency program for oil- and fat-related commodities, oilseeds, oilseed meals, and edible fats. A full listing of the Laboratory Program winners is available on aocs.org/series.

Challenges and opportunities to replace EDTA in the food industry

Lan Ban

Chelating agents such as ethylenediaminetetraacetic acid (EDTA) sequester metal ions are widely used in the food industry to help preserve freshness. EDTA is a very effective ingredient, and in many cases, the only preservative needed for maintaining the quality attributes of foods and beverages. It is cost effective and has little to no negative sensory impact on foods. However, its synthetic origin and non-biodegradable nature have put it on many manufacturers' list of ingredients to replace. To date, there has not been a one-to-one, clean label EDTA replacement identified that can provide equal performance, especially in acidic foods and beverages. Many highly effective chelators were designed and developed for other industry sectors [1]. However, most are still from synthetic routes, which makes it difficult to convince consumers that these are consumer-friendly food ingredients.

- **The mechanisms of the antioxidant ethylenediaminetetraacetic acid (EDTA) include more than just tight binding to heavy metal ions.**
- **Alternative approaches involving non-chelating agents have been tested for their potential to replace the antioxidant function that EDTA displays.**
- **A combination of three natural plant extracts has been found to greatly improve the oxidative stability of dressing and mayonnaise.**

EDTA's mechanisms of action to slow down lipid oxidation were proposed by multiple research groups. First, it is recognized that EDTA binds tightly to heavy metal ions including Fe (II) and Cu (I), which act as catalysts to accelerate lipid oxidation. Second, pH has less impact on the chelating capabilities of EDTA. The binding constant remains high even at the pH of most acidic foods and beverages (pH 3–5). In contrast, at this pH range, many organic acids would lose their chelating capabilities. For instance, phytic acid and citric acid are known chelators and antioxidants in fats and oils. However, in acidic foods, they lose electronegativity on their carboxylic or phosphate groups, resulting in diminishing chelating capabilities and lost antioxidant functions. Nielsen and colleagues tested various dosages of phytic acid in a milk beverage and in mayonnaise, where no improvements of oxidative stability were observed [2]. The pH effect could be overlooked, when either an *in-vitro* chelating assay is performed to screen for chelating agents, or chelators developed from biological studies are tested in acidic food systems. Third, the ability of EDTA to relocate metal ions away from the hot spots of oxidation (lipid phase or inter-facial area) might also play a role in slowing down the initiation of oxidation, at least in food emulsions as shown in the study by Cho and colleagues [3]. Last, the ability of EDTA to reduce the redox potential of Fe(II)/Fe(III) might play a key role in its excellent antioxidant potential. The redox property of the iron pairs, when they complex with EDTA, is remarkably different from its free state due to differences in the orders of magnitude of binding constants between EDTA-Fe (II) and EDTA-Fe (III) [4]. The redox potential change of Fe (II)/Fe(III) disables the metal ion

to actively participate in the initiation of lipid oxidation. This demonstrates that even though a chelator binds metal ions tightly, it is not necessarily going to reduce lipid oxidation, if the redox potential cannot be adjusted to reduce the catalytic activity of the metal ions.

While efforts continue to identify an effective and clean label chelator that may provide many functionalities of EDTA, alternative strategies are necessary to develop label-friendly ingredients to replace the individual functions found with EDTA. An internal study used a combinatorial approach to evaluate ingredients with different antioxidant mechanisms and polarities, as well as their interactions. This finally yielded a blend of three natural plant extracts to improve the oxidative stabilities of mayonnaise and dressing.

As previously stated, an *in-vitro* assay might produce false positives, because it is unable to take the matrix effect into account (e.g., the pH and ingredient interactions in a food system). A study was designed in which mayonnaise, a typical acidic food emulsion (pH lower than 4.3) was used as the model system for the development of the EDTA alternative

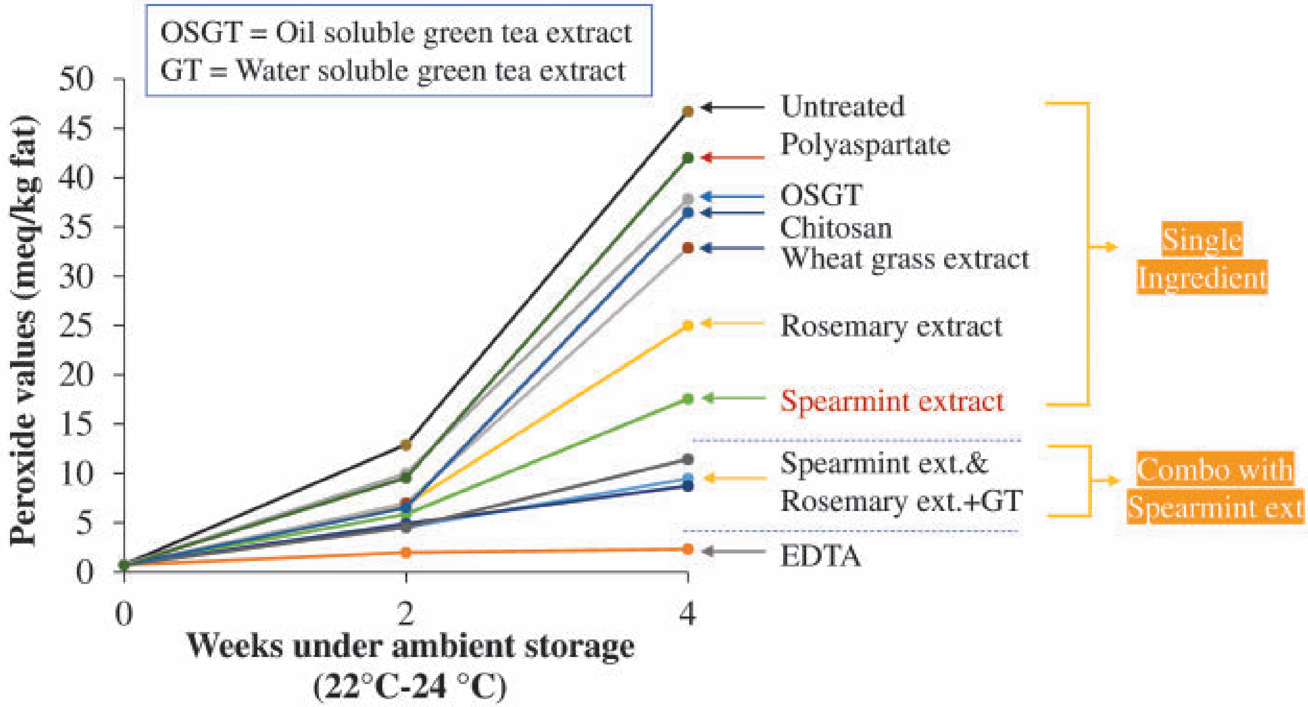

FIG. 1. Screening of various ingredients and ingredient combinations in mayonnaise model system

solution. The peroxide value was monitored during a 4-week storage period at ambient temperature (22–24°C) with daylight exposure that mimics a typical retail setting. Peroxide value was shown from previous internal studies to be one of the best chemical markers that correlates with the oxidative deterioration stage of mayonnaise. During the first stage of the study, various ingredients, both known chelating agents and plant extracts were treated individually in the mayonnaise. The dosage for plant extract was fixed to be the sensory threshold determined by informal consumer sensory panels. Among the six ingredients, spearmint water extract was shown to be most effective (Fig. 1 , page 27). The specific variety of spearmint plant was selected, through natural breeding processes, to minimize production of spearmint oil, while also producing more phenolic compounds. The medium polarity nature of this extract and its rich phenolic compounds may both have contributed to the efficacy of this ingredient. Rosemary extract has been accepted by the food industry for many years. The rosemary extract in this study is oil soluble, and most of its active compounds are non-polar. In acidic foods such as dressings and sauces, it showed improvement but may have further improved when combined with ingredients that contain different sets of active compounds, as these could be located to different phases in a complicated food emulsion system due to the inherent range of polarities. In addition to the screening, green tea extract was also picked as a candidate for a later combinatorial study, as it represents a polar ingredient with weak chelating potential in mayonnaise. The chelation function would not be enough for green tea extract to act as EDTA replacement by itself, but it might provide additional enhancement of antioxidant activities, if used in combination with other ingredients.

Finally, spearmint extract, rosemary extract, and green tea extract were subject to a Design of Experiments study. In this statistics-aided test, a total of 15 combinations containing various amounts of the three ingredients were treated in mayonnaise model systems, and the oxidation of each treated sample was also monitored over 4 weeks, at which point the peroxide values were analyzed. Mathematical algorithms were established to correlate the peroxide value with the dosage of each ingredient, which eventually gave an optimized ratio of each ingredient in a blended final product.

This approach yielded a blend that is composed of spearmint extract, rosemary extract, and green tea extract, in diminishing quantities, respectively. Formulation work was done to combine those three plant extracts with the help of carriers like maltodextrin. The formulation also resulted in rendering the product water-dispersible. The performance of this blend was tested in a larger-scale batch of mayonnaise, and in a generic ranch dressing matrix (Figs. 2 and 3).

In both cases, the product worked as expected by reducing oxidative byproducts. However, at the levels tested, there was no dose response observed in the ranch dressing study (Fig. 3). Compared to EDTA, higher dosages are needed to match the performance, and the level of improvement depended on the type of food emulsions. Nevertheless, the blend provided good protection against oxidation in acidic

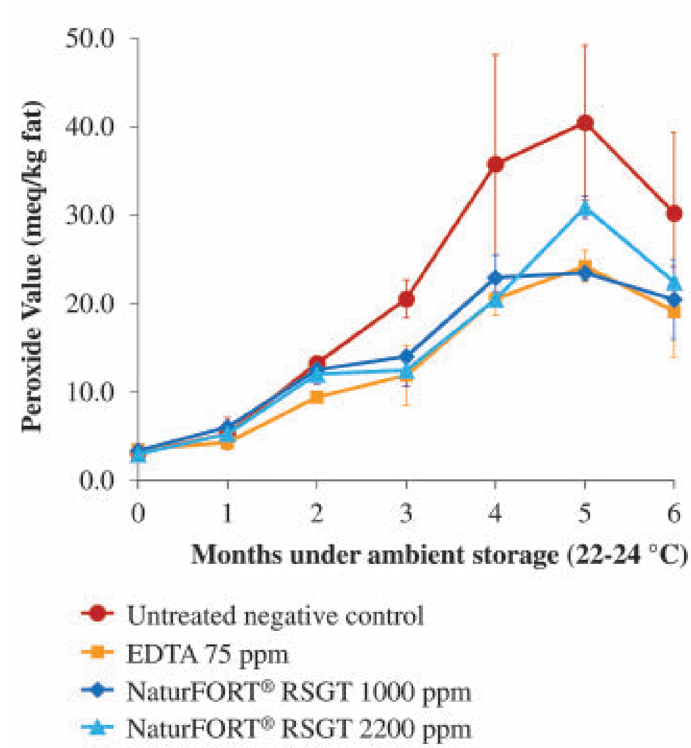

FIG. 2. Peroxide values in mayonnaise. NaturFORT RSGT = NaturFORT RSGT 101 Dry, the blend of spearmint extract, rosemary extract and green tea extract

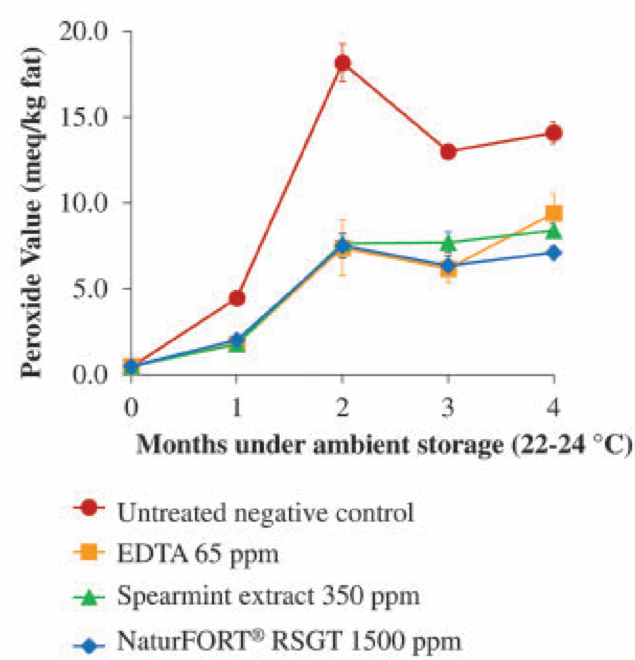

FIG. 3. Peroxide values in ranch dressing. NaturFORT RSGT = NaturFORT RSGT 101 Dry, the blend of spearmint extract, rosemary extract and green tea extract

food emulsions, and further formula optimization is ongoing. There is a vast array of different emulsion-based products on the market, with varying ranges of composition, flavor, and color. Consequently, the determination for the dosage rate is somewhat matrix-dependent, and should be evaluated when oxidative stability is tested in a new matrix.

In conclusion, it is still a challenge to identify label-friendly chelating agents that could replace all the functions of EDTA. Alternative approaches have been researched, with the objective of matching the antioxidant function of EDTA. This report has provided a method to quickly screen ingredients with reliable results to identify potential alternative candidates. Other emerging technologies are approaching EDTA replacement from different angles. For example, the incorporation of chelators in active packaging could be another delivery vehicle for the excellent chelating capabilities of synthetic chelators [5]. It is our belief that continued work will enrich the industry with more knowledge of how structures affect chelating capabilities, and could provide more insight into the relationship between chelating and antioxidant functions to provide the food industry with consumer-friendly options to replace EDTA.

Lan Ban received her Ph.D. in Bioorganic Chemistry from the University of Chicago, where she concentrated on the construction and application of carbohydrate microarrays for the discovery and biophysical characterization of carbohydrate modifying enzymes. After a brief postdoctoral appointment at California Institute of Technology, in 2012 she joined the research team in the Food Technologies unit at Kemin Industries, Inc. Lan has a wide interest in oxidation control and shelf-life extension in food systems, and has been focusing on using chemical and biophysical tools to facilitate the discovery and applications of ingredients from natural sources. She can be contacted at Lan.Ban@Kemin.com.

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The OLEUM Project: ensuring olive oil quality and authenticity

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

Laura Cassiday

Olive oil experts from Italy, Spain, Belgium, the United Kingdom, and the United States converged at the 2018 AOCS Annual Meeting & Expo in Minneapolis, Minnesota, May 6–9, to provide an update on the OLEUM project. The EU-financed project aims to better guarantee olive oil quality and authenticity. In a Hot Topics session entitled, "Olive Oil: Innovative Analytical Strategies to Guarantee Quality and Fight Food Fraud; Focus on the Advancements of the EU H2020 Project OLEUM," the speakers discussed progress made on several fronts since the project's inception in September 2016. The Hot Topics session was chaired by Tullia Gallina Toschi, professor of agricultural and food science at the University of Bologna, in Italy, and scientific coordinator for OLEUM, and Luisito Cercaci, vice president of quality and research development at Pompeian, Inc, an olive oil company that partially sponsored the session. AOCS has joined the project, and is planning an all-day olive oil seminar at the 2019 AOCS Annual Meeting & Expo in St. Louis, Missouri, USA, May 5-8.

According to Gallina Toschi, olive oil is one of the top foods subject to fraudulent activities. Authorities need analytical methods to detect illegal blends of extra virgin olive oil with soft-deodorized olive oil or vegetable oil, to verify olive oil freshness and quality, and to ascertain geographical origin. The OLEUM project has four main strategies: 1) improve existing analytical methods that are officially recognized, 2) develop novel analytical methods based on technological innovation, 3) develop an olive oil databank to ensure methods and data are widely available, and 4) establish a wide community of laboratories involved in olive oil quality control and fraud prevention.

Between February and October 2018, OLEUM plans to introduce three new validated methods and two revised and validated methods for olive oil analysis. A second wave of five new validated methods, two revised and validated methods, and two formulated and validated reference materials will be introduced at a later date.

Alessandra Bendini, assistant professor of agricultural and food sciences at the University of Bologna, discussed OLEUM's analysis and implementation of an olive oil regulatory framework. Currently, olive oil in the EU is subject to numerous international and national standards for quality, purity, and commercial category, such as the Codex Alimentarius, International Olive Council, the European Commission, and national governments. According to Bendini, the standards should be harmonized using International Organization for Standardization (ISO) methods. Bendini also discussed limitations of current EU methods for olive oil analysis, such as the determination of fatty acid ethyl esters and sterol composition, and some suggestions for improvements.

The next speaker at the session, Diego Luis Garcia Gonzalez, researcher at the Instituto de la Grasa, in Spain, discussed analytical solutions for olive oil quality issues. According to Garcia Gonzalez, two types of methods exist to assess olive oil quality: sensory panels and indirect measures. Improvements needed for sensory panels include better panelist training, reference materials, statistics, accreditation, and harmonization. For example, reference materials for sensory panels are not homogeneous from year to year, leading some to question whether synthetic reference materials would be more consistent. Standardized instrumental methods are also needed to support the panel work. Toward this end, OLEUM researchers are characterizing volatile markers associated with sensory defects identified by panelists.

Another aim of the OLEUM project is to develop an olive oil databank, said Alain Maquet, scientific project manager at the European Commission's Joint Research Centre in Belgium. This databank will be a web-access platform to store information about olive oil—either already existing or generated by OLEUM. The databank, which will facilitate data reanalysis, will be searchable and open access. Currently, about 15 olive oil databases exist throughout the world, with information on germplasm, genetics, and oil composition. Collectively, the databases use more than 35 analytical methods and variants, mostly spectroscopy and chromatography. Consolidating the databases requires conversion of data to an open format, as well as perusal of data quality and legal context. The final OLEUM database will be handed over to the European Commission for storage.

Tassos Koidis, lecturer in food science at Queen's University Belfast, in the United Kingdom, discussed networking and technology transfer for the OLEUM project. The project aims to enlarge expertise by assembling a wide user community of laboratories and stakeholders active in the analysis and authentication of olive oil, and to transfer technology to this group—the OLEUM Network—through a series of workshops. The network will have two platforms: 1) LinkedIn Groups for engaging the wider olive oil community, and 2) Basecamp platform for laboratories who have a direct interest in olive oil analysis.

Currently, the LinkedIn group has more than 50 members. The main feature is the "Question of the Month," in which a member of OLEUM answers common questions about olive oil from the wider community. The Basecamp platform was established for technology transfer, closed discussions, document sharing, and troubleshooting specific technical problems. Within Basecamp, there are private stakeholder groups, such as institutional and official authorities, research centers, olive oil producers, and consumer associations. More than 150 laboratories have been identified as candidates to join.

In addition to networking, the OLEUM project will provide training workshops to laboratories on at least four specialized analytical methods. Then, the laboratories will undergo proficiency testing to determine how well non-expert labs perform the method. At this stage, problems with the method can be identified, followed by formal method validation.

Finally, Selina Wang, assistant adjunct professor of food science and technology at the University of California, Davis, discussed how to communicate and implement the results of the OLEUM project in the United States. After the European Union, the United States is the second largest olive oil market, and olives are produced in the states of California, Texas, Georgia, and Florida. Several entities are involved with olive oil in the Unite States, including government agencies (Food and Drug Administration, US Department of Agriculture), trade groups (e.g., California Olive Oil Council and North American Olive Oil Association) and others (e.g., AOCS and UC Davis Olive Center). The OLEUM team can communicate their findings to these organizations through results sharing, method validation, and collaboration.

Walmart, Target push for sustainable cosmetics with industry scorecard

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

Vanessa Zainzinger

A group of organizations led by US retailers Walmart and Target has published a science-based scorecard (https://tinyurl.com/yaensro5) for the personal care industry, aimed at helping manufacturers create safer and more sustainable products.

The two rival retailers and NGO Forum for the Future (FFTF) began work on the project three years ago. Addressing chemicals of concern and ingredient transparency emerged as one of the main issues from actions agreed at the 2014 beauty and personal care (BPC) product sustainability summit.

A core group of 18 organizations across the BPC value chain—including Henkel, Johnson & Johnson, the Environmental Defense Fund (EDF), and the Sustainability Consortium—has since worked on the scorecard.

The final result is made up of 32 key performance indicators (KPIs) for sustainable personal care products. These KPIs are clustered into four areas:

- human health impact of ingredients and product formulations;
- resource usage and emissions during sourcing, manufacturing, and product use;
- ingredient disclosure to consumers; and
- environmental and health impacts of packaging.

The scorecard awards the highest number of points—130 out of 400—to the human health cluster, which focuses on aspects of chemicals in products.

The section includes a stewardship list of chemicals of concern. On it are all compounds on, among others, California's Prop 65 list of suspected carcinogens, the EU priority list of endocrine disruptors, and the list of carcinogens, mutagens and reprotoxicants (CMRs) under REACH Annex XVII.

Cosmetics manufacturers gather points on the scorecard by making sure their product does not include any chemicals on the stewardship list. Extra points are given to companies with a publicly stated policy not to include any of these substances in their formulations.

The stewardship list covers both intentionally and unintentionally added ingredients. For good practice, it says, companies should certify their product for safety by a third party, such as the Safer Choice or Cradle to Cradle Certified product standard.

Boma Brown-West, senior manager of consumer health at the Environmental Defense Fund, told *Chemical Watch* that through the scorecard major retailers are sending a joint signal to suppliers that it's time to improve product sustainability.

"This scorecard will incentivize a race to the top for safer, more sustainable products. While federal regulation continues to lag, this sets a clear, market-driven benchmark for sustainability performance," she said.

"There's a divide in the marketplace between companies who make safer product innovation a cornerstone of their business and those who do not. This scorecard will shed more light on the performance divide in the industry," Brown-West said.

However, in a blog post following the announcement. she said that despite major retailers' aligning on the stewardship list, the group could not reach consensus on how much the reduction of the use of chemicals on the lists should contribute to a product's sustainability score.

"This was disappointing to EDF; we hope that in the future, activity regarding the stewardship list will be sufficiently rewarded in practice," she said.

Other KPIs cover compliance with the International Fragrance Association (Ifra) standards for fragrance ingredients in final formulations; and a product's chemical footprint. Companies gain points by measuring their chemical footprint, according to the NGO Clean Production Action's initiative, and publicly disclosing it.

Several KPIs cover ingredient disclosure. To score the highest points, suppliers should provide information on all chemicals on the stewardship list that are reasonably expected to be present at detectable levels, whether they were intentionally or unintentionally added.

Lists of allergens, the function of each ingredient in the product, and names of any nanomaterials contained in it, should be publicly available, either on the pack or on online.

Vanessa Zainzinger is biocides editor of Chemical Watch.

AOCS MEETING WATCH

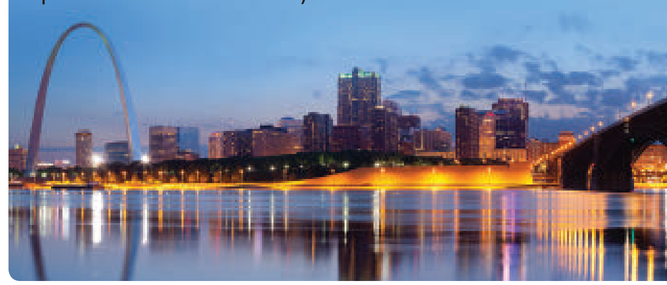
September 6, 2018. JOCS AOCS Joint Symposium, Kobe Gakuin University, Arise Campus, Kobe, Japan.

September 9–11, 2018. Canadian Section of the AOCS (CAOCS) to host 26th CAOCS Canadian Lipid & Bioresource Conference, Saskatoon, Saskatchewan, Canada.

October 28–31, 2018. Fabric and Home Care World Conference, Boca Raton Resort & Club, Boca Raton, Florida, USA.

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

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).



Cereal products for breakfast?

Leslie Kleiner

Latin America Update is a regular Inform *column that features information about fats, oils, and related materials in that region.*

In Argentina, where I grew up, it is common to start the day with "mate" and "facturas" (a type of tea and last ones being delicious, freshly baked pastries from the bakery store). This is a different breakfast than milk and cereal, or cereal bars, as we see in the United States. Therefore, I was curious to learn the role of cereals and cereal bars at the supermarket shelves in LATAM. I consulted Innova Market Insights [1], and this is what I found, in Q&A format:

Q: For the period January 2016 to April 2018, how many cereal products (cereal and cereal bars) can be found in the market in LATAM (this includes established, reformulated, repackaged and new products)?

The bar graph below shows the number of cereal products in the market for each country, for the period Jan-2016 to Apr-2018. From this graph, it is seen that cereal products are more popular in Brazil and Mexico than in other LATAM countries.

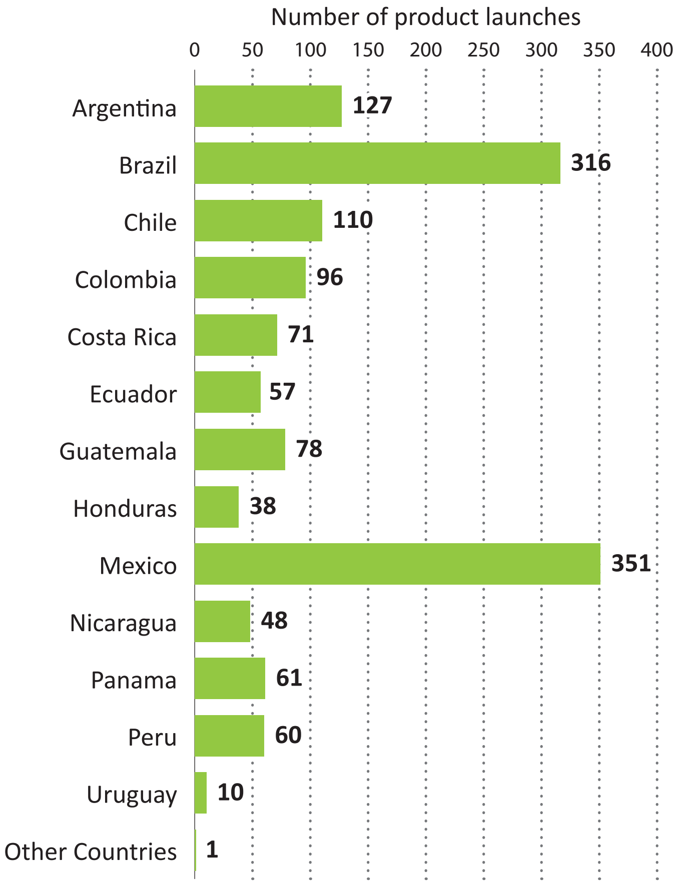


FIG. 1. Number of cereal products at the shelf in LATAM supermarkets, per country (Jan-2016 to Apr-2018)

Q: Considering all these products in the LATAM region, which are the top 10 brands and how many products do those brands carry? What are the most popular flavors?

Table 1 shows the top ten brands and number of cereal products. In terms of flavors, across the region, fruit leads with 689 products. This followed by brown flavors (582), nuts (338), dairy flavors (48), spices and seeds (40), dessert (28), cake-cookie-and pie (26), vanilla (26), vegetables (7), and ethnic flavors (4).

Q: What are the top 10 sources of fats and oils for cereal products, and what are examples of cereal products in the market for the region?

The top 10 sources of fats and oils (used alone or in combination) are vegetable oil (468 products), palm oil (306), vegetable fat (264), sunflower oil (231), canola oil (136), soy oil (127), palm kernel oil (1,120), sunflower oil (2,310), fractionated palm oil (61), coconut oil (56), and palm olein (49).

Examples of these products are:

- "Arcor Cereal Mix Yoghurt Frutilla Barras: Cereal Bar With Strawberry And Yogurt." This is a product that was re-launched with ecological packaging in Argentina, February 2018.
- "Fiber One 90 Calorie Barras De Avena Sabor A Chocolate Con Chispas De Chocolate: Chocolate Flavored Oatmeal Bars With Chocolate Chips," commercialized in Mexico—last report by Innova market Insights on February, 2018.
- "Nestle Nescau Cereal Matinal De Milho Sabor Chocolate: Corn Cereal Balls With Chocolate Flavor," commercialized in Brazil—last report by Innova market Insights on February, 2018.
- "Post Honey Bunches Of Oats Cereal With Yummy Vanilla Bunches And Whole Grains Flakes," commercialized in Ecuador—last report by Innova market Insights on November, 2017.

TABLE 1. Top ten brands of cereal in LATAM (Jan-2016 to Apr-2018)

Name	Count	Name	Count
Quaker	86	Nature Valley	31
Kelloggs	62	Great Value	24
Special K	50	Tosh	24
Fitness	32	Choco Krispis	23
Froot Loops	31	Nesquik	23

References

[1] www.innovadatabase.com

Latin America Update is produced by Leslie Kleiner, R&D Project Coordinator in Confectionery Applications at Roquette America, Geneva, Illinois, USA, and a contributing editor of *Inform*. She can be reached at LESLIE.KLEINER@roquette.com.

PATENTS

Oil-based foamable carriers and formulations

Tamarkin, D., *et al*., Foamix Pharmaceuticals Ltd., US9795564, October 24, 2017

A waterless foamable carrier and pharmaceutical composition which is suitable for external and internal administration is disclosed. The composition is single phase and includes at least one liquid oil; and a glyceride. Pharmaceutical compositions comprising active agents, methods for their preparation, propellants suitable for use with the carriers and uses thereof are further described.

Fertilizer and fertilizer additive compositions and methods comprising by-products from the manufacture of fatty acid alkyl esters and/or biodiesel

Lynch, J., et al., October 24, 2017

Fertilizers and fertilizer additive compositions and methods are provided. The compositions and methods comprise utilizing by-products from the manufacture of biodiesel and/or fatty alkyl esters, wherein the by-product comprises glycerin, mong, moisture, C6 -C24 saturated and unsaturated fatty acids, C6 -C24 saturated and unsaturated fatty acid salts, methyl esters, ethyl esters, and combinations thereof.

Fatty acid blends and uses therefor

Knuth, M., *et al*., Nucelis Inc., US9796938, October 24, 2017

Provided herein are blends oils or fatty acids comprising more than 50% medium-chain fatty acids, or the fatty acid alkyl esters thereof, and having low melting points. Such blends are useful as a fuel or as a starting material for the production of, for example, a biodiesel. Also provided genetically altered or modified plants, modified such that the amount of medium-chain fatty acids generated by the plant are increased. Further provided is a method of predicting the melting point of a blend of fatty acid methyl esters and the use of such a method for identifying blends suitable for use as, for example, a biodiesel.

Lauric ester compositions

Dummer, T., *et al*., Terravia Holdings, Inc., US9796949, October 24, 2017

Provided are compositions containing alkyl esters derived from triglyceride oils produced from genetically engineered microalgae. Specific embodiments relate to esters derived from oils with high C10-C12 fatty acid profile. Compositions comprising the esters include cleaning products, completion fluids, work-over fluids, drilling fluids, metal working fluids, lubricants, paints, and inks.

Biodegradable containers

Patel, V.C., US9797104, October 24, 2017

Biodegradable bags for disposing of an unwanted substance are formed from a bioplastic material made from a bio-based material in the form of a maize flour, and a biodegradable plasticizer selected from the group consisting of vegetable oil, polyesters made from glycerin, glycerin, derivatives of glycerin, and combinations thereof. The maize flour comprises a minor volume percent of the total volume of the bioplastic material. A biodegradable additive is used to provide a degree of stiffness to the material, a preferred additive being polylactic acid. A UV *et al* stabilizer may optionally be included. Biodegradable bags have an open end and a closed end with a sidewall extending between them. The bag includes a feature for enclosing a substance once placed into the bag. In an example, the feature comprises an opening through a sidewall. Alternatively, the feature may include an adhesive section.

Artificial tear emulsion

Claret, C., *et al*., Horus Pharma, US9801899, October 31, 2017

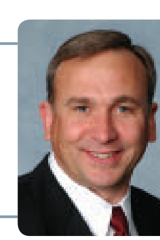
The present invention relates to an oil-in-water emulsion comprising at least one mucomimetic polymer, at least one lipid of phospholipid type, at least one lipid other than the phospholipid, at least one stabilizing polymer, and a hydrophilic liquid, to an emulsion comprising an aqueous phase that contains at least one stabilizing polymer and at least one mucomimetic polymer, and an oily phase that contains at least one lipid of phospholipid type and a lipid other than the phospholipid, to a medicament comprising one of these emulsions, and to the use of one of these emulsions as an agent for restoring and/or replacing the lachrimal film or as a carrier for an active compound.

Phospholipid composition and microbubbles and emulsions formed using same

Unger, E.C., Microvascuar Therapeutics LLC, US9801959, October 31, 2017

A composition for stabilizing a fluorocarbon emulsion. That composition includes phosphatidylcholine, phosphatidylethanolamine-PEG, and a cone-shaped lipid.

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.



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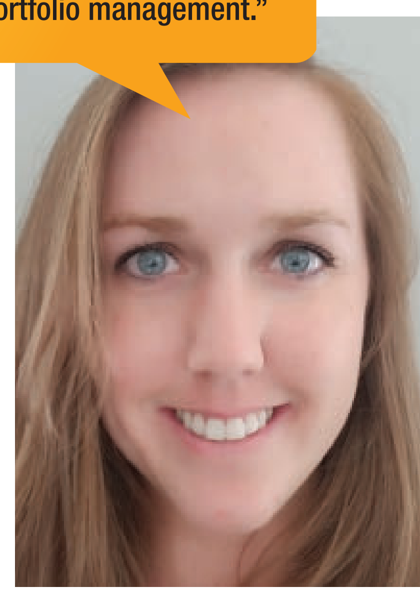

Sarah A. Echols, Head of Innovation of Sweet Ingredients, North America, at CSM Bakery Solutions and member of the Edible Applications Technology Division

- Student member in 2010–2011
- Member of inaugural leadership team of the Young Professional Common Interest Group, 2014–2018
- Secretary-Treasurer of the Edible Applications Technology Division, 2017–present

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Lipids and *JAOCS*: advancing research on medium-chain triglycerides

The following articles from *Lipids* and the *Journal of the American Oil Chemists' Society* (*JAOCS*) represent recent and varied studies related to medium-chain triglycerides (MCTs). MCTs are abundant in palm kernel and coconut oils. Over the last few decades, MCTs have come to be considered a source of healthy saturated oils, as they are readily metabolized for quick energy and have interesting physiological functions. The papers highlighted within *JAOCS* demonstrate how MCT oils can be blended with other edible oils and modified for use in applications such as edible films, confectionary products, margarines and spreads, or structured lipids for infant nutrition. In contrast, the papers from *Lipids* demonstrate how MCTs influence various metabolic pathways in mammals—from the ability of saturated fatty acids to enhance n-3 fatty acid metabolism in animals fed a high fat diet to the role of palmitic acid on cardiomyocyte function. The positive cardiovascular effects of MCT are detailed in several of the papers, and emerging data demonstrating the mechanisms underlying the positive impact of MCT in human health are also highlighted.

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JOURNAL OF THE AMERICAN OIL CHEMISTS' SOCIETY (JAOCS)

Biotechnological and novel approaches for designing structured lipids intended for infant nutrition
Şahin-Yeşilçubuk, N. and C.C. Akoh.

A review of the evidence supporting the taste of non-esterified fatty acids in humans
Running, C.A. and R.D. Mattes.

Crystallization behavior and kinetics of chocolate-lauric fat blends and model systems
Geary, M. and R. Hartel.

Enzymatic interesterification of coconut and high oleic sunflower oils for edible film application
Moore, M.A. and C.C. Akoh.

Feruloylated products from coconut oil and shea butter
Compton, D.L., *et al*.

Cocoa butter substitute (CBS) produced from palm mid-fraction/palm kernel oil/palm stearin for confectionery fillings
Biswas, N., Y.L. Cheow, C.P. Tan, S. Kanagaratnam, and L.F. Siow.

Enzymatic interesterification of lauric fat blends formulated by grouping triacylglycerol melting points
Nusantoro, B.P., M. Xanthina, S. Kadivar, N.A.M. Yanty, and K. Dewettinck.

Molecular finger printing of nutra-coconut oil with improved health protective phytoceuticals and its efficacy as frying medium
Faiza, S., Nasirullah, and S. Debnath.

Crystallization kinetics of coconut oil in the presence of sorbitan esters with different fatty acid moieties
Sonwai, S., P. Podchong, and D. Rousseau.

Preparation of infant formula fat analog containing capric acid and enriched with DHA and ARA at the sn-2 position
Ãlvarez, C.A. and C.C. Akoh.

LIPIDS

A high-fat, high-oleic diet, but not a high-fat, saturated diet, reduces hepatic α-linolenic acid and eicosapentaenoic acid content in mice
Picklo, M.J. and E.J. Murphy.

PAM, OLA, and LNA are differentially taken up and trafficked via different metabolic pathways in porcine adipocytes
Yu, C. , *et al*.

Myristic acid enhances diacylglycerol kinase δ-dependent glucose uptake in myotubes
Wada, Y. , S. Sakiyama, H. Sakai, and F. Sakane.

Olive oil-based lipid emulsions do not influence platelet receptor expression in comparison to medium- and long-chain triglycerides *In vitro*
Stoetzer, C. , *et al*.

Medium-chain enriched diacylglycerol (MCE-DAG) oil decreases body fat mass in mice by increasing lipolysis and thermogenesis in adipose tissue
Kim, H. , *et al*.

Lipid emulsions containing medium chain triacylglycerols blunt bradykinin-induced endothelium-dependent relaxation in porcine coronary artery rings
Amissi, S. , *et al*.

AMPK Prevents palmitic acid-induced apoptosis and lipid accumulation in cardiomyocytes
Adrian, L. , *et al*.

Fabric and Home Care World Conference aims to help attendees navigate future industry disruptions

From the role of robotics in home cleaning to understanding what consumers really want in natural and organic products, the 2018 Fabric and Home Care World Conference will provide attendees with a forum to discuss cutting-edge technologies and shifting trends affecting the future of the fabric and home care industry.

Over 600 industry leaders are expected to convene at the conference, which will be held at the Boca Raton Resort in Boca Raton, Florida, on October 28–31, 2018. This is the first time in its 40-year history the conference will be hosted in North America.

BOCA RATON RESORT IN BOCA RATON, FLORIDA

Not only will this year's conference take shape on a new continent, but it will also provide attendees with insights into how future industry innovations and disruptions will shape the global fabric and home care industry.

"The scale and pace of economic change over the past 30 years is historically unprecedented," according to Sree Ramaswamy, Partner at McKinsey & Company, who will be one of the keynote speakers at the conference. "Ongoing technological and demographic trends will accelerate the changes, and businesses need more external focus, greater agility, and a growth — not defense — strategy."

Including Ramaswamy, the conference program features four keynote speakers as part of three days of future-focused presentations:

- João Benjamin Parolin, CEO of Oxiteno, "New Technologies and Their Impact on the World of Cleaning"
- Sree Ramaswamy, Partner at McKinsey & Company, "No Ordinary Disruption: Global Business and Economic Trends"
- Stephan Füsti-Molnár, President of Henkel North America Consumer Goods, "Shaping the Future — How to Navigate the Global Transformation"
- Michitaka Sawada, President and CEO of Kao Corporation, Japan, "Connecting With Care: Human-Centric Innovation Across the Industry"

"The scale and pace of economic change over the past 30 years is historically unprecedented."

SREE RAMASWAMY

In addition to the keynote speakers, other industry leaders will provide insights into how businesses can adapt with agility and digitization to industry shifts while also making efforts to grow sustainably. For example, Zeynep Yalim Uzun, Chief Marketing Officer at Arcelik A.S., will discuss how the home of the future, a smart home filled with connected appliances, will propel the digital transformation of products and services to keep pace with an increasingly digitized living space.

However, consumers are not the only ones who can benefit from disruptions. Businesses can leverage digital transformation to streamline operations, and the conference program includes speakers who can help attendees see new ways to operate their business more efficiently. Yannis Skoufalos, Global Product Supply Officer at The Procter & Gamble Company, will present on how supply chains can leverage digital technologies. As part of his presentation, Skoufalos will discuss how, in the not too distant future, new digital supply systems will enable personalization, efficient distribution and true direct-to-consumer business models.

These shifts in technology reflect shifts in consumer demands and preferences — from how consumers access and use their products to the ingredients of which products are made. Anticipating what consumers want can be the most difficult aspect of researching and implementing new products. The content of the conference program, including several networking events, aims to help attendees navigate how changing preferences of consumers will necessitate changes in business plans and models.

For example, when it to comes to developing and marketing natural and organic products, appealing to consumer demands means understanding how consumers define "natural" and "organic," something consumers are not always sure of themselves. To help attendees better understand consumers in the natural and organic space, the program features Todd Wichmann, President, CEO, and Founder of HealthPro Brands Inc., who will discuss the drivers behind consumer demand for natural and organic products in home cleaning and what the implications are for the industry.

To connect attendees with the latest and upcoming products and services, the conference's Exhibition is expected to host over 50 companies and organizations, including key suppliers of equipment, chemicals and services from the industry. In addition, the Exhibition will also feature e-poster presentations, which will allow presenters to highlight new research and innovations.

Between insights offered by industry leaders, several networking events and the Exhibition, the 2018 Fabric and Home Care World Conference will help attendees ensure they are on course in a rapidly evolving industry.

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The full version of all AOCS journal articles are available online to members at www.aocs.org/journal. This column builds on that member benefit by primarily highlighting articles from other journals.

Assessment of the minor-component transformations in fat during the green Spanish-style table olive processing

López-López, A, *et al.*, *J. Agric. Food Chem. 66*: 4481–4489, 2018, https://doi.org/10.1021/acs.jafc.8b00927.

This work assesses the transformations that green Spanish-style processing of Manzanilla and Hojiblanca table olives produces on the minor components of their fat. Discriminant analysis showed that most of the variability was not due to processing (24.4%) but to differences between cultivars (59.2%). Therefore, the final products have a similar quality to the original olive fat; that is, the quality of the fat was scarcely affected. The only systematic trends observed were the decrease in hexacosanol, tetracosanol, and octacosanol (fatty alcohols) and C46 (wax), after lye treatment, and the high levels of alkyl esters in the packaged product. Thus, minor-component levels in green table olives are, in general, within the limits established for extra virgin olive oil since the alkyl esters should be considered habitual products of fermentation and not as an alteration as in olive oil.

Phytosterols and their derivatives: structural diversity, distribution, metabolism, analysis, and health-promoting uses

Moreau, R.A., *et al.*, *Prog. Lipid Res. 70*: 35–61, 2018, https://doi.org/10.1016/j.plipres.2018.04.001.

Phytosterols (plant sterols) occur in the cells of all plants. They are important structural components that stabilize the biological membranes of plants. Sterols can occur in the "free" unbound form or they can be covalently bound via an ester or glycosidic bond. Since our previous 2002 review on phytosterols and phytosterol conjugates, phytosterol glucosides have been found to be important structural components in the lipid rafts of the plasma membrane of plant cells, where they are thought to be essential to the function of plasma membrane enzymes and perhaps other proteins. Phytosterols also serve as precursors in the synthesis of important bioactive compounds such as steroidal saponins, steroidal glycoalkaloids, phytoecdysteroids, and brassinosteroids. Methods for the analysis of phytosterols range from traditional gas chromatography of free phytosterols to modern sophisticated forms of mass spectrometry which have been used for the new field of sterol lipidomics, sometimes called "sterolomics." Phytosterol-enriched functional foods first appeared about twenty years ago and many clinical studies have confirmed the low density lipoprotein (LDL) cholesterol-lowering properties of various types of phytosterols. In recent years additional clinical studies and more than ten important meta-analyses have provided insights to better understand the cholesterol-lowering and other biological effects of plant sterols.

Differences in the triacylglycerol and fatty acid compositions of human colostrum and mature milk

Zhao, P., *et al.*, *J. Agric. Food Chem. 66*: 4571–4579, 2018, https://doi.org/10.1021/acs.jafc.8b00868.

Human colostrum is important for immune system development and plays a protective role for infants. However, the comprehensive exploration of lipids, which account for 3–5% of milk, and their biological functions in human colostrum was limited. In present study, the triacylglycerol (TAG) and fatty acid (FA) compositions of human colostrum and mature milk were analyzed and compared. Variations were observed in both the TAG and FA compositions. The concentrations of 18:1/18:1/16:0 TAG, high-molecular-weight and unsaturated TAGs were significantly higher in colostrum, whereas mature milk contained more low/medium-molecular-weight TAGs and medium-chain FAs. Furthermore, there were also specific TAGs in both colostrum and mature milk. Our data highlighted targets for further investigation to elucidate the biological function of lipids in colostrum milk. In addition, the comprehensive analysis of TAGs in Chinese colostrum might help in designing infant formula for Chinese babies, especially the preterm ones.

Effects of medium-chain triacylglycerols on Maillard reaction in bread baking

Toyosaki, T., *et al.*, *J. Sci. Food Agric.* 98: 3169–3174, 2018, https://doi.org/10.1002/jsfa.8822.

Saturated fatty acids had a remarkable inhibitory effect on the amount of advanced glycation end products (AGEs) generated from the Maillard reaction in bread baking compared to unsaturated fatty acids. The amount of AGEs produced by each fatty acid (mg kg–1) was as follows: C18:0, 18.7; C12:0, 35.2; C16:0, 21.4; C18:0, 38.2; C18:1, 68.7; C18:2, 80.1; C20:4, 80.8; C22:4, 89.8. Saturated fatty acids were possibly involved in the Maillard reaction and, as a result, acted to inhibit it. In the case of unsaturated fatty acids, amounts of AGEs during the Maillard reaction in baking tended to increase as the degree of unsaturation increased. In other words, there was a positive correlation between the degree of unsaturation and the amount of AGEs. It was also confirmed that the air pore distribution in baked bread was closely related to

AGEs. These results led us to conclude that the fatty acid composition of the added lipids also influences properties that determine the tastiness of bread.

Postprandial metabolomics response to various cooking oils in humans

Wang, P.-S., *et al.*, *J. Agric. Food Chem. 66*: 4977–4984, 2018, https://doi.org/10.1021/acs.jafc.8b00530.

Lipids account for a high proportion of dietary calories, which greatly affect human health. As a result of differences in composition of fatty acid of individual cooking oils, certain biological effects of these oils may vary. This study aimed to compare postprandial metabolomic profiles of six commonly consumed cooking oils/fats. Adopting a switch-over experimental design ($n = 15$), we carried out a human feeding study with six groups (control without oils, soybean oil, olive oil, palm oil, camellia oil, and tallow) and collected fasting and postprandial serum samples. The metabolomic profile was measured by ultra-high-pressure liquid chromatography–quadrupole time of flight. We observed significant differences between the control group and experimental groups for 33 serum metabolites (false discovery rate; $p < 0.05$), which take part in lipid digestion, fatty acid metabolism, metabolism of pyrimidines and pyrimidine nucleosides, amino acid metabolism, neurobiology, and antioxidation. Sparse partial least squares discriminant analysis revealed distinct metabolomics patterns between monounsaturated fatty acid (MUFA) and saturated fatty acid oils, between soybean oil, olive oil, and palm oil, and between two MUFA-rich oils (olive and camellia oils). The present metabolomics study suggests shared and distinct metabolisms of various cooking oils/fats.

Enzymatic action mechanism of phenolic mobilization in oats (*Avena sativa* L.) during solid-state fermentation with *Monascus anka*

Bei, Q., *et al.*, *Food Chem. 245*: 297–304, 2018, https://doi.org/10.1016/j.foodchem.2017.10.086.

This work aims to investigate the effects of carbohydrate-hydrolyzing enzymes on the release of phenolics in oat fermentation with *Monascus anka*. There were good correlations between phenolic content and α-amylase, xylanase and FPase activities. A high level of α-amylase activity (141.07 U/g) was observed, while xylanase (2.40 U/g), total cellulase (0.52 U/g) and β-glucosidase activities (0.028 U/g) were relatively low in the fermentation system. The phenolic content of oat powder treated with crude enzyme from fermented oats significantly increased, especially that of the ferulic acid in the insoluble fraction and the vanillic acid in the soluble fraction. The surface SEM morphology of the oats showed that the cell wall structure was damaged by the crude enzyme treatment, which led to the release of phenolics. This study could provide metabolic understanding for optimization of phenolic compounds which could more efficiently increase the nutrition of oat intended for functional food ingredients.

Lipid Oxidation/Antioxidants

Impact of interfacial composition on lipid and protein co-oxidation in oil-in-water emulsions containing mixed emulisifers

Zhu, Z., *et al.*, *J. Agric. Food Chem. 66*: 4458–4468, 2018, https://doi.org/10.1021/acs.jafc.8b00590.

The impact of interfacial composition on lipid and protein co-oxidation in oil-in-water emulsions containing a mixture of proteins and surfactants was investigated. The emulsions consisted of 5% v/v walnut oil, 0.5% w/v whey protein isolate (WPI), and 0 to 0.4% w/v Tween 20 (pH 3 and pH 7). The protein surface load, magnitude of the ξ-potential, and mean particle diameter of the emulsions decreased as the Tween 20 concentration was increased, indicating the whey proteins were displaced by this nonionic surfactant. The whey proteins were displaced from the lipid droplet surfaces more readily at pH 3 than at pH 7, which may have been due to differences in the conformation or interactions of the proteins at the droplet surfaces at different pH values. Emulsions stabilized by whey proteins alone had relatively low lipid oxidation rates when incubated in the dark at 45°C for up to 8 days, as determined by measuring lipid hydroperoxides and 2-thiobarbituric acid-reactive substances (TBARS). Conversely, the whey proteins themselves were rapidly oxidized, as shown by carbonyl formation, intrinsic fluorescence, sulfhydryl group loss, and electrophoresis measurements. Displacement of whey proteins from the interface by Tween 20 reduced protein oxidation but promoted lipid oxidation. These results indicated that the adsorbed proteins were more prone to oxidation than the nonadsorbed proteins, and therefore, they could act as better antioxidants. Protein oxidation was faster, while lipid oxidation was slower at pH 3 than at pH 7, which was attributed to a higher antioxidant activity of whey proteins under acidic conditions. These results highlight the importance of interfacial composition and solution pH on the oxidative stability of emulsions containing mixed emulsifiers.

Relationship between the physiochemical properties of cocoa procyanidins and their ability to inhibit lipid oxidation in liposomes

Toro-Uribe, S., *et al.*, *J. Agric. Food Chem. 66*: 4490–4502, 2018, https://doi.org/10.1021/acs.jafc.8b01074.

The aim of this paper is to evaluate the effects of cocoa polyphenols and procyanidins with different degrees of polymerization that are encapsulated in liposome delivery systems on the inhibition of lipid oxidation at pH 3.0 and 5.0. In general, liposomes at pH 3.0 and 5.0 were physically stable in the presence of polyphenols and procyanidins with mean particle sizes of 56.56 ± 12.29 and 77.45 ± 8.67 nm and ζ-potentials of −33.50 ± 3.16 and −20.44 ± 1.98 mV at pH 3.0 and 5.0, respectively. At both pH 3.0 and pH

5.0, all the polyphenols and procyanidins inhibited lipid hydroperoxide and hexanal formation, and antioxidant activities increased with increasing polymer-chain sizes. The greater antioxidant activities of the isolated procyanidins were likely due to their increased metal-chelating capacities, as determined by ferric-reducing-ability (FRAP) assays, and their greater levels of partitioning into the lipids, as determined by their log Kow values and encapsulation efficiencies. The crude extract had the greatest antioxidant activity, which could be because other antioxidants were present, or combinations of the different polyphenols and procyanidins inhibited lipid oxidation synergistically.

Storage stability of DHA in enriched liquid eggs

Klensporf-Pawlik, D., *et al.*, *Eur. J. Lipid Sci. Technol. 120*: 1700164, 2018, https://doi.org/10.1002/ejlt.201700164.

The oxidative stability of liquid eggs enriched with very long-chain n-3 fatty acids and liquid regular eggs stored under refrigerated temperature, is investigated. Oxidized lipids can alter both nutritional and sensorial properties of foods. The extent of lipid oxidation is evaluated by quantification of total lipids, docosahexaenoic acid (DHA), and peroxide value (PV), but also by assessment of total tocopherols and γ-tocopherol losses. Additionally, the development of fishy off-flavor is evaluated. Results highlight significant differences between omega and regular liquid eggs stability. Although, the oxidative changes are observed in both types of liquid eggs, more susceptible to oxidation are omega liquid eggs.

Oxidation of fish oil oleogels formed by natural waxes in comparison with bulk oil

Hwang, H.-S., *et al.*, *Eur. J. Lipid Sci. Technol. 120*: 1700378, 2018, https://doi.org/10.1002/ejlt.201700378.

The aim of this study is to evaluate the oleogel (or organogel) technology as a new method to prevent oxidation of fish oil by immobilizing oil and to provide useful information on oxidation of oleogels for their application in actual food products. Four different natural waxes, rice bran wax, sunflower wax, candelilla wax, and beeswax are used to prepare fish oil oleogels. Peroxide value, conjugated diene value, eicosapentaenoic acid (EPA), and docosahexaenoic acid (DHA) are measured after storing oleogels at 35 and 50°C, respectively. All 3% wax-fish oil oleogels shows slower oxidation than the bulk fish oil at 35°C. Beeswax is not as effective as other waxes during storage at 50°C due to its lower melting point. The color penetration measurement method is developed as a convenient method to predict the oxidation rate of oleogel. Cooling oleogel at a faster rate can significantly reduce the oxidation rate of the oleogel. A larger amount of wax is not recommended to increase the protective effect, which can give a negative effect due to the prooxidant activity of wax. The oleogel technology may be applied to reduce oxidation of food products and nutritional supplements containing omega-3 oil.

Carotenoid stability during dry milling, storage, and extrusion processing of biofortified maize genotypes

Ortiz, D., *et al.*, *J. Agric. Food Chem. 66*: 4683–4691, 2018, https://doi.org/10.1021/acs.jafc.7b05706.

Translation of the breeding efforts designed to biofortify maize (Z. mays) genotypes with higher levels of provitamin A carotenoid (pVAC) content for sub-Saharan Africa is dependent in part on the stability of carotenoids during postharvest through industrial and in-home food processing operations. The purpose of this study was to simulate production of commercial milled products by determining the impact of dry milling and extrusion processing on carotenoid stability in three higher pVAC maize genotypes (C17xDE3, Orange ISO, Hi27xCML328). Pericarp and germ removal of biofortified maize kernels resulted in ~10% loss of total carotenoids. Separating out the maize flour fraction (<212 μm) resulted in an additional ~15% loss of total carotenoids. Carotenoid degradation was similar across milled maize fractions. Dry-milled products of Orange ISO and Hi27xCML328 genotypes showed ~28% pVAC loss after 90-days storage. Genotype C17xDE3, with highest levels of all-trans-β-carotene, showed a 68% pVAC loss after 90-day storage. Extrusion processing conditions were optimal at 35% extrusion moisture, producing fully cooked instant maize flours with high pVAC retention (70–93%). These results support the notion that postharvest losses in maize milled fractions may be dependent, in part, on genotype and that extrusion processing may provide an option for preserving biofortified maize products.

Designing antioxidant peptides based on the antioxidant properties of the amino acid side-chains

Matsui, R., *et al.*, Food Chem. *245*: 750–755, 2018, https://doi.org/10.1016/j.foodchem.2017.11.119.

Amino acids exert characteristic antioxidant activities depending on the properties of their side residues. The hydrophobic residues were effective against peroxyl radical, while acidic residues and their analogs were effective against peroxynitrite. Peptides containing tyrosine showed different activities against different reactive oxygen species (ROS) and/or reactive nitrogen species (RNS). The number and position of tyrosine did not affect the antioxidant activity against hypochlorite ion. Against the peroxyl radical, the number of tyrosine residues affected the antioxidant activity, while its position did not have a significant effect. The tyrosine position was an important factor for the antioxidant activity against peroxynitrite. The peptide GWWW showed higher antioxidant activity against peroxyl radical than tryptophan at concentrations below 25 μM, and high activity against peroxynitrite at 250 μM. Our results suggest that antioxidant peptides against a specific target ROS or RNS can be designed based on the characteristics of the amino acid side chains.

Antioxidant and anti-inflammatory activities of quercetin and its derivatives

Lesjak, M., *et al.*, *J. Funct. Foods 40*: 8–75, 2018, https://doi.org/10.1016/j.jff.2017.10.047.

Quercetin is hardly bioavailable and largely transformed to different metabolites. Although little is known about their biological activities, these metabolites are crucial for explanation of health benefits associated with quercetin dietary intake. In this study, the antioxidant and anti-inflammatory activities of six quercetin derivatives (quercetin-3-O-glucuronide, tamarixetin, isorhamnetin, isorhamnetin-3-O-glucoside, quercetin-3,4′-di-O-glucoside, quercetin-3,5,7,3′,4′-pentamethylether) were compared with the activity of common onion extract as the main source of dietary quercetin and standards (butylated hydroxytoluene and aspirin). The quercetin derivatives demonstrated notable bioactivities, similar to standards and onion. Derivatization of quercetin hydroxyl groups resulted in decrease of antioxidant potency. However, the number of quercetin free hydroxyl groups was not in direct correlation with its potential to inhibit inflammatory mediator production. To conclude, quercetin derivatives present in systemic circulation after consumption of quercetin may act as potent antioxidant and anti-inflammatory agents and can contribute to overall biological activity of quercetin-rich diet.

Role of quercetin in the physicochemical properties, antioxidant, and antiglycation activities of bread

Lin, J. and W. Zhou, *J. Funct. Foods 40*: 299–306, 2018, https://doi.org/10.1016/j.jff.2017.11.018.

As a natural glycation inhibitor, quercetin was incorporated into bread to develop antiglycative functional food. Quercetin added in the wheat bread flour at 0.05, 0.1, and 0.2% caused a loss of dough elasticity with lower resistance and higher extensibility. It further altered the quality of bread in terms of deceasing bread volume and increasing bread hardness. The antioxidant potential of the bread with quercetin was enhanced in a dose-dependent manner. The antiglycation capacity was assessed according to the ability of the bread to inhibit the formation of advanced glycation endproducts (AGEs) *in vitro*. Results showed that bread with 0.2% quercetin addition was able to inhibit 46–52% of total AGEs formed during protein glycation. Overall, the results support quercetin as a functional food ingredient in bread system, offering consumers a higher intake of antioxidant and a lower load of AGEs.

Yerba mate waste: a sustainable resource of antioxidant compounds

Gullón, B., *et al.*, *Ind. Crops Prod. 113*: 398–405, 2018, https://doi.org/10.1016/j.indcrop.2018.01.064.

The infusion of yerba mate (*Ilex paraguariensis* St. Hil.) is the most popular tea-like beverage of southern Latin American countries, and its health benefits such as stimulating effect and antioxidant activity are well known. The exhausted mate leaves are managed as waste and are not currently exploited or valorized as a bio-resource. In this work, a cost-effective alternative for extracting antioxidant compounds from this type of residue as a possible valorization route was investigated. Accordingly, different liquid/solid ratios, solvents and extraction times were evaluated with the aim of maximizing extraction performance, total phenolic (TPC) and flavonoid (TFC) content and antioxidant activity (AA) of the extracts. The optimal conditions allowed the recovery of high level of phenolics (TPC 63.13 mg gallic acid equivalents/g) and flavonoids (TFC 148.45 mg rutin equivalents/g) in the extract, with remarkable content in AA (111.18 mg Trolox equivalents/g). Pyrolysis-gas chromatography/mass spectrometry (Py-GC/MS) analysis identified that the main compounds in the extract were terpenes (phenol, guaiacol, 4-vinylguaicol and eugenol), caffeine, 4-ethyl-resorcinol, hydroquinone, palmitic acid, and stearic acid. Fourier transform infrared (FTIR) and thermogravimetric analysis (TGA) analyses provided the functional characteristics and thermal stability of the extract. From the results obtained, it can be concluded that the residue of yerba mate after the infusion of the original yerba mate still possesses high antioxidant potential, mainly associated with its phenolic and flavonoid composition. Furthermore, the content of antioxidant phenolic compounds reported here was higher than most of those reported for agro-industrial residues. Therefore, this type of waste, that is generally discarded, can be valorized as a source of high added-value compounds.

Effects of *in vitro* gastrointestinal digestion on phenolic compounds and antioxidant activity of different white winemaking byproducts extracts

José Jara-Palacios, M., *et al.*, *Food Res. Int. 109*: 433–439, 2018, https://doi.org/10.1016/j.foodres.2018.04.060.

The effect of *in vitro* gastrointestinal digestion on phenolic composition and antioxidant activity of different white winemaking byproducts extracts (grape pomace and its parts: seeds, skins, and stems) was evaluated. Fourteen individual phenolic compounds were evaluated by UHPLC. The antioxidant activity was measured by DPPH and ORAC assays. Differences on phenolic profile and antioxidant activity were observed depending on the digestion phase, the type of byproduct, the phenolic group and the antioxidant activity assay. In general, digestion had a reducing effect on TPC and antioxidant activity; however, ORAC values of seed and stem extracts increased after digestion and some recovery indexes of the phenolic groups were very high. Results indicate that extracts from white winemaking byproducts are a reliable source of bioaccessible antioxidant compounds, which could be used as functional food ingredients.

Industrial Applications

Lipid extraction from *Yarrowia lipolytica* biomass using high-pressure homogenization

Drévillon, L., *et al.*, *115*: 143–150, https://doi.org/10.1016/j.biombioe.2018.04.014.

This work aims at investigating the impact of high-pressure homogenization (HPH) for oil recovery from *Yarrowia lipolytica* yeast. First, HPH parameters (pressure and number of passes) were optimized, by measuring the disintegration index and the release of ions, proteins, and nucleic acids during the HPH pre-treatment. Results obtained showed that 1500 bar and 5 passes allowed the maximum cell disruption, and total oil recovery in dry route (lyophilization and *n*-hexane extraction). HPH-treated cells were then extracted in wet route by directly adding *n*-hexane (without drying) and mixing using a high-speed disperser. Different ratios and extraction times were tested in order to optimize the extraction parameters. Maximum oil recovery in wet route was ≈80%, obtained using 40 min extraction, a rotation speed of 10000 rpm, and a HPH-treated suspension:*n*-hexane ratio of 1:2. Microscopy pictures, granulometry, and Peleg's model exploitation supported the results obtained in this work.

Medical/Pharmaceutical Applications

Bioactivity-based molecular networking for the discovery of drug leads in natural product bioassay-guided fractionation

Nothias, L.-F., *et al.*, *J. Nat. Prod. 81*: 758–767, 2018, https://doi.org/10.1021/acs.jnatprod.7b00737.

It is a common problem in natural product therapeutic lead discovery programs that despite good bioassay results in the initial extract, the active compound(s) may not be isolated during subsequent bioassay-guided purification. Herein, we present the concept of bioactive molecular networking to find candidate active molecules directly from fractionated bioactive extracts. By employing tandem mass spectrometry, it is possible to accelerate the dereplication of molecules using molecular networking prior to subsequent isolation of the compounds, and it is also possible to expose potentially bioactive molecules using bioactivity score prediction. Indeed, bioactivity score prediction can be calculated with the relative abundance of a molecule in fractions and the bioactivity level of each fraction. For that reason, we have developed a bioinformatic workflow able to map bioactivity score in molecular networks and applied it for discovery of antiviral compounds from a previously investigated extract of Euphorbia dendroides where the bioactive candidate molecules were not discovered following a classical bioassay-guided fractionation procedure. It can be expected that this approach will be implemented as a systematic strategy, not only in current and future bioactive lead discovery from natural extract collections but also for the reinvestigation of the untapped reservoir of bioactive analogues in previous bioassay-guided fractionation efforts.

BACE1: Now we can see you

Bongarzone, S. and A.D. Gee, *J. Med. Chem. 61*: 3293–3295, 2018, https://doi.org/10.1021/acs.jmedchem.8b00474.

No *in vivo* imaging biomarker currently exists for BACE, a drug target for Alzheimer's disease (AD). A strategy aiming to find a novel brain-penetrant positron emission tomography (PET) radiotracer for BACE1 led to the discovery of a highly potent and selective aminothiazine inhibitor, PF-06684511. This scaffold has been now evaluated as BACE1 PET radiotracer ([18F] PF-06684511) after labeling with fluorine-18 (18F), allowing its evaluation in non-human primates (NHP) as the first a brain-penetrant PET radiotracer for imaging BACE1 *in vivo*.

Structural modification of natural product ganomycin I leading to discovery of a α-glucosidase and HMG-CoA reductase dual inhibitor improving obesity and metabolic dysfunction *in vivo*

Wang, K., *et al.*, *J. Med. Chem. 61*: 3609–3625, 2018, https://doi.org/10.1021/acs.jmedchem.8b00107.

It is a great challenge to develop drugs for treatment of metabolic syndrome. With ganomycin I as a leading compound, 14 meroterpene derivatives were synthesized and screened for their α-glucosidase and HMG-CoA reductase inhibitory activities. As a result, a α-glucosidase and HMG-CoA reductase dual inhibitor ((R,E)-5-(4-(tert-butyl)phenyl)-3-(4,8-dimethylnona-3,7-dien-1-yl) furan-2(5H)-one, 7d) with improved chemical stability and long-term safety was obtained. Compound 7d showed multiple and strong in vivo efficacies in reducing weight gain, lowering HbAlc level, and improving insulin resistance and lipid dysfunction in both ob/ob and diet-induced obesity (DIO) mice models. Compound 7d was also found to reduce hepatic steatosis in ob/ob model. 16S rRNA gene sequencing, SCFA, and intestinal mucosal barrier function analysis indicated that gut microbiota plays a central and causative role in mediating the multiple efficacies of 7d. Our results demonstrate that 7d is a promising drug candidate for metabolic syndrome.

Synthetic Biology

Enhanced biological fixation of methane for microbial lipid production by recombinant *Methylomicrobium buryatense*

Fei, Q., *et al.*, *Biotechnol. Biofuels 11*: 129, 2018, https://doi.org/10.1186/s13068-018-1128-6

Due to the success of shale gas development in the US, the production cost of natural gas has been reduced significantly, which in turn has made methane (CH_4), the major component of natural gas, a potential alternative substrate for bioconversion processes compared with other high-price raw material sources or edible feedstocks. Therefore, exploring effective ways to use CH_4 for the production of biofuels is attractive. Biological fixation of CH_4 by methanotrophic bacteria capable of using CH_4 as their sole carbon and energy source has obtained great attention for biofuel production from this resource.