



107th AOCS Annual Meeting & Expo

May 1–4, 2016 | Salt Palace Convention Center | Salt Lake City, Utah, USA

Imaging Techniques Interest Area Technical Program Abstracts

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The presenter is the first author or otherwise indicated with an asterisk ().
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IMG 1/EAT 1.1: Structure Effects on Oil Binding

This session developed in conjunction with the Edible Applications Division.

Chairs: G. Cherian, Kellogg North America Co., USA; and M. Willson, LipoLogic Consultancy LLC, USA

Palm Based Structured Oils for Trans-free and Reduced Sat Solution. G. Wang, L. Liu, and G.P. McNeill, IOI Loders Croklaan LLC, USA.

Structured fats and oils provide the desirable physicochemical and sensory attributes to food items. With FDA's announcement to ban PHO last year, formulation strategies based on palm are becoming commercially viable because they are capable of delivering the structure without altering sensory and shelf life stability. Three types of structured technologies are reviewed for different food applications, e.g. fractionation, oil blending, and fat modification. Fractionated palm oils satisfy clean label requirement for variety applications, such as peanut butter stabilizer, microwave popcorn with no wick issue. Oil blending is another way to create structured oils with reduced saturated fat content. These trans-free, no hydro, reduced Sat formulations are important to industry with clean label demand. Reduced saturation can also be achieved through fat modification. This approach creates new fats with fast set-up crystallization profile. Customers can apply these approaches to replace pho but still maintain current shelf life stability and sensory acceptance.

Effect of High Intensity Ultrasound, Agitation, and Crystallization Temperature on the Crystallization Behavior of Interesterified Soybean Oil. J.V. Kadamne and S. Martini, Utah State University, USA.

Interesterified soybean oil (M.P. 41.9±0.5°C) was crystallized at 29 and 34°C without and with the application of high intensity ultrasound (HIU). Two crystallization set-ups were studied: (i) continued agitation for entire crystallization process (60min) (CA), and (ii) agitation for 10min (A10). Sonication and agitation did not affect induction times of nucleation while crystal morphology, crystallization kinetics, and viscoelasticity were all affected by these processing variables. For e.g., HIU reduced crystal sizes and increased viscosity (5.7±1.9 to 3,057.5±318.5Pa.s) and elasticity (86.7±4.0 to 95,955±2735Pa) of crystalline networks obtained at 29°C under A10 condition. Similar increases in viscosity and elasticity were observed when samples were crystallized at 34°C under A10 condition. However, this effect was not as significant for samples crystallized under the CA condition. HIU also increased crystallization rates for all conditions tested. Kinetic constants obtained from an Avrami fit increased from 1.73 x10⁻⁵ to 7.28 x10⁻⁵ min⁻ⁿ for samples crystallized at 29°C A10 without and with sonication, respectively, and up to 7.9 10⁻⁹ to 2.1 10⁻⁷ for samples crystallized at 34°C A10 without and with sonication, respectively. This rise in crystallization rate was also observed for samples crystallized under the CA condition.

Effect of Sugars on the Crystallization Behavior of Confectionery Fat-hydrogenated Palm Kernel Oil.

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The effects of different sugars on the isothermal crystallization rate, thermal properties, hardness, and viscosity of hydrogenated palm kernel oil were studied. The results showed that the crystallization rate of hydrogenated palm kernel oil was promoted by sugars. The crystallization rate of sample added with lactitol was the fastest, followed by isomaltulose, sucrose, and maltitol. After adding sugars, the products density was increased, which led to the increase of hardness, especially for adding lactitol, which had the highest value. For the product viscosity, the highest viscosity was observed by adding isomaltulose, followed by the maltitol, isomaltulose, and sucrose gave the lowest viscosity. Overall, maltitol may act as one of the sugar substitutes for chocolate.

Arrested Coalescence of Droplets Containing Crystalline Fat Networks. A. Thiel, University of Wisconsin-Madison, USA.

In oil-and-water emulsions, a phenomenon known as arrested coalescence, can occur when two fat globules begin to coalesce but are stopped from fully merging. Micromanipulation techniques were used to bring two oil droplets into contact to gain a more microscopic view of coalescence. Here, four different combinations of fats were investigated microscopically to map full coalescence to total stability. Increasing amounts of a high melting fat (higher solid fat content), with larger elastic modulus of the fat crystalline networks, decreased extent of coalescence. To achieve the same degree of coalescence, emulsions prepared using anhydrous milk fat (AMF) or palm oil (PO) required a larger elastic modulus than emulsions made using coconut stearin (CS) or palm kernel oil (PKO). Extent of coalescence of AMF or PO droplets changed linearly with log G' while samples containing PKO or CS had an exponential relationship with log G'. Droplet diameter also was shown to affect coalescence. The degree of coalescence decreased for all fats investigated as diameter increased from 10 to 90µm. Understanding when oil droplets undergo full coalescence, arrested coalescence, or total stability microscopically allows for predictions of their behavior in foods like ice cream and whipped topping.

Surfactant-mediated Interfacial Crystallization of Solid Fat-encapsulated Water-in-Oil Emulsions.

N.L. Green, T. Tran, and D. Rousseau, Ryerson University, Canada.

We have previously shown that shear-crystallized fat/oil mixtures will produce spheroidal fat crystals. The addition of 10% (w/w) water to these systems can form encapsulated droplets surrounded by Pickering crystal shells. Encapsulation efficiency was dependent on emulsifier type, with the molecular complementary of the nonpolar moiety and the polar head group size together seeming to dictate which emulsifiers were most capable. The emulsifiers studied were glycerol monostearate (GMS), glycerol monopalmitate (GMP), glycerol monooleate (GMO), sorbitan monostearate (SMS), sorbitan tristearate (STS), and polyglycerol polyricinoleate (PGPR). Emulsions were prepared using a rotor-stator and then further shear-crystallized using a rheometer with parallel plate geometry. Analysis of viscosity profiles, thermal behaviour, and resulting polymorphic forms revealed that the addition of emulsified water did not significantly affect crystal polymorphism compared to bulk systems. However, the glycerol-based emulsifiers (GMS, GMP, and GMO) produced smooth-surfaced crystal spheroid shells while the sorbitan-based emulsifiers produced irregularly-shaped shells and droplet cores (SMS) or incomplete crystal shell formation (STS). The propensity for interfacial crystallization was explored using a temperature-controlled tensiometer to observe the onset and progress of crystallization over time.

Effect of Hydrocolloids and Crystal Promoter on the SFC of a Palm Oil Based Fat Reduced W/O Solid Emulsion.

M. Cordova-Barragan and E. Dibildox-Alvarado, Universidad de Autónoma de San Luis Potosí, Mexico.

The effect of the addition of hydrocolloids and crystal promoter on the solid fat content (SFC) of a palm oil based fat reduced water-in-oil (w/o) emulsion was studied. In this line, a palm oil based w/o emulsion (w/o 35/65) was prepared dispersing hydrocolloids [xanthan gum, K-carrageenan, carboxymethyl cellulose (CMC), sodium alginate and citric pectin] in the aqueous or the oil phase adding or not a crystal promoter. After the preparation, the emulsion was crystallized in two water baths at 8 and -4°C, looking for an emulsion temperature of 22 and 12°C, respectively; the emulsion was stored at 18°C. These emulsions were analyzed after 72 hours by SFC and the results were statistically analyzed. The outcomes obtained reflected that the addition of a crystal promoter and the dispersion of hydrocolloids in the water phase significantly increased ($p < 0.05$) the SFC. In this way, citric pectin, K-carrageenan, xanthan gum, CMC and sodium alginate dispersed in water phase increased the SFC of the emulsions added with a crystal promoter in 1.12, 1.09, 1.04, 1.04 and 1.04%, respectively. These results suggest an increase in stability in fat reduced w/o solid emulsions that can be used in the food industry (i.e., margarines).

Algae Butter, a Novel Structuring Lipid, Its Similarities and Differences in Composition, and Observed Functionality When Compared to a Conventional Stearin Butter.

A.G. Marangoni¹, W.G. Rakitsky², E. Blum², and L. Zou³, ¹Dept. of Food Science, University of Guelph, Canada, ²Solazyme Inc., USA, ³Bunge North America, Inc., USA.

The focus of this research is to evaluate algae butter properties and composition, their differences and similarities when compared with Shea stearin. In particular, their fatty acid profiles, triglyceride structures, melting properties, crystallization kinetics, and crystal structures are evaluated. Also, areas of compositional differences that leads to functionality differences in food products will be highlighted.

In addition, application results of this study revealed that this unique technology can be used in many different food product applications such as confectionery, bakery, etc. However, these functional products confer superior performance without affecting taste, texture, and mouthfeel of the finish products.

Conclusion: The study demonstrates unique novelty of Algae butter as a structuring agent when compared to conventional Shea stearin.

A Materials Science Approach to Understanding the Functionality of Low Saturated Emulsion Systems. P. Smith¹, F. Davoli², S. Metin², and D. Karleskind³, ¹Cargill R&D Centre Europe, Belgium, ²Cargill Inc, USA, ³Cargill Malt, Belgium.

To provide function in bakery fat systems provide more than triglycerides. Solids are needed to develop structures for products. This is provided by hard saturated fat. Therefore it is not simple to reduce saturated fat. However there is a drive to reduce saturated and total fat in foods. Consequently its structural behavior must be replicated by other components.

Emulsion systems allow the opportunity to create structure at lower amounts of fat and so can be used to replace higher saturated systems. In this work we demonstrate how by understanding the performance of the original and low-saturated systems novel solutions are created that can allow for improved behavior of reduced fat systems.

The work focuses on relating the physical and rheological properties of structured systems and the structure and performance of pastries. This is used to create models that allow prediction of performance with composition. Careful manufacture creating shells around droplets allows control of the behavior and good performance with low saturate systems.

The work demonstrates how shells are built and structured. Effects of composition/ emulsifiers and processing on shells are shown.

The combination of shell building and materials science approach gives capability to design low saturated emulsions for varied applications.

Oil Structuring Using Particle Stabilized Systems. S. Metin¹, P. Smith², F. Davoli¹, D. Karleskind³, and B. Wainwright⁴,
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There is a drive to reduce the saturated fat in foods to improve nutritional content. Many foods are structured and stabilized by solid fat. Traditionally, solid fat was contributed by trans-fat and by saturated fat. Today, the vast majority of trans-fat has been eliminated from the food supply thereby relegating structuring capacity more or less exclusively to saturates. Consequently, there is widespread interest in developing alternative structuring elements. Many researchers are active in this area, but it is a challenge to commercialize low-saturated fats with desired functionality

and cost with label friendly ingredients that is acceptable to consumers.

Our approach starts with understanding the functionality of a particular fat in a high fat food product. This work focused on reduction of saturated fat using label friendly porous edible particles. Processing, characterization and application of particle stabilized fat systems in bakery and confectionery products will be demonstrated.

Low-saturated particle stabilized fat systems were developed by coupling particle stabilization technology with fat crystal optimization. Interactions between the lipid and the particles must be controlled so that the lipid forms a continuous, phase wherein the particles are distributed. The particles act as network builders structuring the lipid phase, providing a structured system.

IMG 2/EAT 2.1: Nano-, Micro-, Macrostructure

This session developed in conjunction with the Edible Applications Technology Division.

Chairs: A.G. Marangoni, University of Guelph, Canada; and P.R.R. Ramel, Jr., University of Guelph, Canada

Formation and Microstructures of Whipped Oils Composed of Vegetable Oils and High-melting Fat Crystals.

K. Sato, S. Mishima, and S. Ueno, Hiroshima University, Japan.

In food materials, foams have significant advantages of shape retention, soft texture, thermal barrier, and low calorie content. We reports the experimental results of formation processes of whipped oils composed of vegetable oils (salad oil) and high-melting fat crystals of fully hydrogenated rapeseed oil rich in behenic acid (FHR-B). No emulsifier was added to form this whipped oil. Micro-probe FT-IR spectroscopy, synchrotron radiation microbeam X-ray diffraction, polarized optical microscopy, and DSC were employed to observe fine fat crystal particles of the most stable beta polymorph of FHR-B, and their adsorption at the air-oil surfaces before, during, and after the formation of the whipped oil. The following results were obtained. (1) Preparation of organogel composed of salad oil and small fibrous beta fat crystals by special tempering procedure is a prerequisite for forming whipped oil. (2) The beta fat crystals are adsorbed at air-oil surfaces to encapsulate the air bubbles during the formation process of whipped oil. (3) The values of overrun of the whipped oil reached >200% after an aeration time of 30min at 20°C. (4) The microbeam X-ray diffraction experiments demonstrated that the lamellar planes of the beta fat crystals near the air-oil surfaces were arranged almost parallel to the air-oil surface plane.

Acoustic Cavitation and Bubble Dynamics in Edible Oils.

P.R. Birkin¹, T. Foley¹, S. Martini*², and T. Truscott²,
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The objective of this research is to detect, quantify, and exploit cavitation events generated by high intensity ultrasound (HIU, 20kHz) in edible lipids. In this study lipids, such as soybean and sunflower oil, were sonicated and the dynamics of the bubbles produced in these systems characterized using high-speed imaging, laser scattering, and a hydrophone. The results from this research show, for the first time, that the cavitation field in these lipids is significantly different from that observed in water. Cavitation clusters were generated in these oils even though the viscosity of this media was significantly higher than water. In addition, a 'streamer' of bubbles was also formed during sonication. This dense and opaque streamer appears more axially defined compared to water and was composed of many small bubbles that traveled rapidly vertically away from the tip at velocities greater than 5m s⁻¹. In addition long-lasting bubbles can be observed in the bulk of the oils. Lastly, a significant increase in temperature was observed in the stream of bubbles. The knowledge gained from this research could be exploited to optimize sonication conditions in the processing of lipids in order to change their final physical

properties.

Effect of Interfacial Crystallization on the Rheological Behavior and Droplet Localization of a Fat Crystal Network-stabilized Emulsion.

R.R. Rafanan and D. Rousseau, Ryerson University, Canada.

Physical properties of water-in-oil (w/o) emulsions, such as tablesreads, depend on the presence of interfacial fat (Pickering, PK) crystals and/or a 3D fat crystal network in the continuous oil phase. How the droplet interface interacts with the surrounding fat crystal network is not widely understood. Investigating these interactions is of great importance to control textural properties of the final product, such as fracture, spreadability, or flow. It is hypothesized that interfacially adsorbed solids will alter viscoelastic properties, namely by reinforcing the network than droplets without adsorbed solids. To test this, fat crystal network emulsions comprised of hydrogenated soy oil were constructed containing 0-20wt% water. Water droplets were stabilized by either monoglycerides (PK) or polyglycerol polyricinoleate (liquid surfactant, LS) at a constant water:surfactant ratio. PK emulsions displayed better storage stability, exhibited higher storage moduli (G') than their LS counterparts and resisted time-dependent shear deformation above 10%_{w/w} water content. Light microscopy showed that LS droplets adsorbed to the fat crystal surface, while PK droplets localized within individual crystals. This indicates that surfactant structure mediates droplets localization within the network which is a contributing factor in viscoelastic behaviour.

Freeze-thaw Stability of O/W Emulsions: Influence of Crystallization Behavior of Fats.

C. Ishibashi, H. Hondoh, and S. Ueno, Graduate School of Biosphere Science, Hiroshima University, Japan.

O/W emulsions are highly unstable in freezing, and it is demulsified rapidly after thawing. It is well known that partial coalescence of fat crystals is one of the factors affecting freeze-thaw stability. The morphology, the size, and the amount of fat crystals influence the freeze-thaw stability of O/W emulsion. However, there are few reports which focus on the crystal growth of fats in O/W emulsion during freezing. In this study, we observe the crystallization behavior of O/W emulsion which used rapeseed oil or soybean oil as an oil phase. In addition, the influence of fat crystals on the freeze-thaw stability of O/W emulsion are reported.

The main results are as follows: (i) the soybean oil emulsion showed higher freeze-thaw stability than the rapeseed oil emulsion. (ii) In the rapeseed oil emulsion, partial coalescence was clearly observed during a storage. Finally, the microscopic images were almost covered with fat crystals. (iii) In contrast, in the soybean oil emulsion, fat

crystals only appeared at the interface of the oil droplet. From these results, we conclude that the rapeseed oil emulsion were destabilized by partial coalescence, whereas, the soybean oil emulsion were not.

Effect of Oil Type on Fat Crystallization Thermodynamics.

N.L. Green¹, G. Marinoni², and D. Rousseau¹, ¹Ryerson University, Canada, ²University of Udine, Italy.

Much of the exploration into fat crystallization has neglected to focus on the effect of oil type in a fat-oil mixture. The fats studied are an industrially-relevant blend with high tristearin content and also pure tristearin. We used a variety of oils, including triacylglycerols with varying degrees of unsaturation, their corresponding unsaturated fatty acids, as well as both pure and blends of aliphatic compounds. Crystallization at both slow and fast cooling rates revealed the relative stability of the mixtures. Concurrent x-ray diffraction revealed the polymorphic form(s) upon crystallization onset as well as their evolution. Further, microscopic observation of the resulting crystals revealed large differences in crystal morphology. Reduced molecular complementarity of fat and oil led to earlier crystallization onset, as well as the formation of lesser polymorphs. We explain our results using solubility parameters that are typically utilized for a polymer-solvent system. These account for a range of interactions (dispersion, polar, and hydrogen bonding) to quantify the complementarity of solute (fat) and solvent (oil).

Structural and Physical Characteristics of Fats Crystallized Under High Pressure.

M. Zulkurnain¹, V.M. Balasubramaniam^{1,2}, and F. Maleky¹, ¹Dept. of Food Science & Technology, Ohio State University, USA, ²Dept. of Food, Agricultural, & Biological Engineering, Ohio State University, USA.

Different processing conditions have been introduced to modify lipid crystalline network. Limited effort is placed in evaluating effects of high pressure processing. However, application of pressure during crystallization have shown texture improvement. We plan to understand how pressure influences lipid crystallization mechanism and its ultimate functional properties. Binary mixtures of hard fats (5-30%) and oil were crystallized under pressure (0.1-600MPa) using a laboratory scale high pressure kinetic tester with thermally controlled condition. Crystallized sample's structural and physical properties were characterized using X-ray diffraction, polarized light microscopy, rheometer, differential scanning calorimetry, and analyzed for binding capacity. Samples crystallized at 0.1MPa were used as control. The presence of smaller nano- and microscale of spherical β crystals were documented in samples crystallized under high pressure. However, when initial temperature fell below sample's crystallization temperature, nucleation prior to compression produced mixture of β' and β spherulitic crystals. These observations propose different mechanisms of lipid

crystallization under the influence of quasi-instantaneous volume reduction during compression. Substantial increment in storage modulus and oil binding capacity suggested improvement in plasticity and network stability towards oil migration.

Microviscosity of Liquid Oils in Confined Colloidal Fat Crystal Networks.

M.A. Rogers¹ and M.G. Corradini², ¹University of Guelph, Canada, ²Rutgers University, USA.

Molecular rotors may be utilized as non-invasive, non-disruptive, and highly sensitive alternatives to conventional measures of bulk viscosity when the oil is entrained in a colloidal fat crystal network. Oil viscosity changes based on the molecular confinement of the oil, which is dependent on its molecular volume. Changes in micro-viscosity were not dependent on the solids content, but instead were strongly dependent on the box-counting fractal dimension in high-space filling colloidal fat crystal networks (i.e., $D > 1.89$). A bulk oil viscosity is often an overestimation of the actual viscosity of the entrained oil and may not be appropriate when predicting diffusion in multi-phase materials.

Mechanisms of Retardation Effects of Polyglycerine Fatty Acid Esters on Crystallization of Diacylglycerols Examined with Small-angle X-ray Diffraction.

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Edible oil containing high concentration (>80%) of diacylglycerols (DAG-rich oil) have beneficial healthy effects on obesity and obesity-related diseases. The DAG-rich oil, however, causes precipitation of 1,3-positional isomers of DAGs containing high-melting saturated fatty acid chains at chilled temperatures, which is undesired for real applications. We examined the effects of polyglycerine fatty acid esters (PGFEs) on retardation of the crystallization of the DAG-rich oil by using SFC, DSC, polarized optical microscopy, and X-ray diffraction (XRD) techniques. We found that, prior to the crystallization of high-melting DAG fractions, the cooled DAG-rich oil containing the PGFE additives showed birefringence under polarized light. In addition, small angle XRD patterns revealed the formation of supramolecular assembly composed of DAG and PGFEs, which are quite different from those of DAG crystals. From these results, it can be considered that the retardation of crystallization of DAG-rich oil is caused by the formation of liquid crystal-like supramolecular complex structures in which high-melting fractions of DAGs is incorporated.

Structure-function Relationship of Puff-pastry Shortenings.

B.A. Macias-Rodriguez, F. Peyronel, and A.G. Marangoni, University of Guelph, Canada.

Puff-pastry shortenings are specialty fats rich in saturated (SFA) and trans fatty acids (TFA). We studied different commercial systems to identify key parameters underlying their functionality. We characterized the solid

structure by ultra small angle (USAXS), small angle (SAXS), and wide angle (WAXS) X-ray scattering. We used small and large deformation rheology to obtain rheological parameters in the linear and non-linear regime. All shortenings have similar polymorphism (β , β' , or both) while the domain sizes are in the range of 300-400Å. USAXS indicate that the aggregation of crystalline nanoparticles (CNPs) for laminating shortenings is either via diffusion limited-cluster aggregation or reaction limited cluster aggregation, while for the multipurpose shortening, CNPs remain un-aggregated. Creep-recovery parameters show lower retarded compliance values

and higher zero-shear viscosity for laminating shortenings compared to multipurpose shortening. The viscoelastic moduli (G' and G''): 1-3MPa) and yield stresses (350-750Pa) remain unremarkable. Lissajous curves (stress versus strain) and Fourier-transform rheology in the nonlinear region suggest less strain-stiffening behavior in laminating shortenings compared to the multipurpose one. This study provides novel insight on the structural and rheological signatures of laminating fats, and opens up the possibility for the design of healthier shortenings.

IMG 3/EAT 4.1: Length Scales and Lipids

This session developed in conjunction with the Edible Applications Technology Division.

Chairs: K.B. Koch, North Dakota State University, USA; and C. Rogers-Kelly, Mississippi State Chemical Lab, USA

Influence of Maillard Conjugation on the Stability of Emulsion-based Delivery Systems: Lutein-enriched Corn Oil Emulsions at Different pH and Temperature Conditions.

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Lutein may be utilized in foods as a natural pigment to replace synthetic colorants, or as a nutraceutical ingredient to improve eye health. However, due to its poor water-solubility and chemical instability the incorporation into foods needs further research. In this study, we evaluated the effect of storage temperature and pH on the physical and chemical stability of lutein-enriched emulsion-based delivery systems prepared using caseinate and Maillard conjugates as the emulsifier. Also, we compared the fate of the emulsions stabilized by casein alone versus casein-dextran conjugates in the gastrointestinal tract as well as the lutein bioaccessibility. The emulsions stabilized with both emulsifiers remained physically stable at all temperatures (5-70°C); however the rate of chemical degradation of lutein increased with increasing temperature ($E_a = 38\text{kJ/mol}$). The samples stabilized with protein alone irreversibly aggregated at pH 4 and 5; however, the samples at the same pH values stayed stable when the protein was replaced by protein-polysaccharide conjugates. The emulsion stabilized by casein alone was not stable in the gastric phase of the digestion, whereas the samples made with Maillard conjugates were still stable after the same step. The emulsifier type did not influence the lutein bioaccessibility.

Surfactant-free Solid Lipid Nanoparticles Prepared with Novel Synthetic Ultra-long Chain Fatty Acyl Based Amphiphilic Lipids. W. Wei^{1,2}, F. Feng², B.C. Pérez¹, M. Dong¹, H. Mu³, X. Xu¹, and Z. Guo¹, ¹Aarhus University, Denmark, ²Zhejiang University, China, ³University of Copenhagen, Denmark.

Recently, scientific and technological interest in nanocarrier system arises from the possibility of making surfactant-free system. However, most of the studies reported are focusing on surfactant-free emulsions which are liquid. The surfactant-free "solid" lipid nanoparticles (SF-SLN) are of great interest yet rarely reported. A major challenge is developing structurally simple amphiphilic lipids that are solid state at physiological temperature. In our recent study, we have design and synthesized an array of amphiphilic lipids based of behenic acid (22:0) as ultra-long acyl hydrophobic tail with varied hydrophilic heads *via* enzymatic approach. The synthetic compounds were examined as novel excipients for developing SF-SLN. Results revealed that the headgroup

has a dramatic influence on the forming of the SF-SLN. Small size and narrow distribution SF-SLNs were made with some of the synthetic compounds. The SF-SLNs show high loading efficiency of lipophilic model drug, Fenofibrate and long term *in vitro* drug release. Moreover, the structures of the particles were investigated using Atomic force microscopy and Transmission electron microscopy which revealed that SF-SLNs were vesicles with drug incorporate into the lipid bilayer. The SF-SLNs is a safe and versatile system for drug and active delivery, which are suitable for different administration routes.

Shear-induced Aggregate Creation or Destruction in Edible Oils: Models and Computer Simulation. B. Townsend¹, N. Callaghan-Patrarachar², F. Peyronel¹, K. Ramadurai³, A.G. Marangoni¹, and D.A. Pink^{*2,1}, ¹Dept. of Food Science, University of Guelph, Canada, ²Physics Dept., St. Francis Xavier University, Canada, ³Dept. of Mathematics, College of the North Atlantic, Canada.

Edible Oils are Complex Fluids possessing many components some of which are in a non-liquid state. Flowing Edible Oils generally experience shear: In processing and consumption a non-shear flow is generally not realized due to the presence of surfaces with which the fluid interacts. In order to understand experimental data it is advantageous to possess models which predict observable effects. These models must correctly represent both the system of interest and the flow. Modeling the flow involves the Navier-Stokes equation(s) while the boundary conditions involve defining fluid flow at surfaces which themselves might undergo change as the flow proceeds. We shall present simple models of aggregates in order to identify aspects relevant to Edible Oil flow. We used Dissipative Particle Dynamics to model a sheared system and computed structure functions, $S(q)$, to interpret the results, approaches not hitherto used. We found that a critical shear gradient exists which distinguishes between shear which destroys aggregates and shear which accelerates aggregation compared to aggregation under static conditions. This critical value is system-dependent. We shall exhibit examples for isotropic (spheres) and anisotropic (cylinders) objects, and compare them to USAXS measurements on sheared and non-sheared samples.

Organogels of Comprised of a Cyclic Peptide from Flaxseed Oil. M.A. Rogers¹ and M.J.T. Reaney², ¹University of Guelph, Canada, ²University of Saskatchewan, Canada.

To the best of our knowledge, this is the first report on an orbitide, capable of self-assembling from 0D objects to 1D nano-fibers and resulting in 3D molecular gel networks. LOB3 (a.k.a. cyclolinopeptide A), extracted from *Linum usitatissimum* L. (flaxseed), forms molecular gels in

acetonitrile. Molecular gels, comprised of cyclic peptides, allow for much more complex amino acid sequences than have been currently reported. It appears that cyclization to form orbitides imparts conformational aspects to the molecule that drives self-organization into fibrillar objects with very large aspect ratios. These nanoscale fibers, ~300nm in diameter and >100mm in length, seem to aggregate into bundles of fibers that reach micron dimensions. Within the nano-fibers, the orbitides adopt an antiparallel β -sheet-like conformation with very high periodicity, as illustrated by NMR and XRD giving rise to the very high aspect ratio fibers.

Which Length Scales are Affected in Sheared Edible Fat Systems? F. Peyronel¹, D.A. Pink^{2,1}, and A.G. Marangoni¹,
¹University of Guelph, Canada, ²St. Francis Xavier University, Canada.

The food industry must eliminate trans fats and reduce saturated fats in food products. By understanding how solid fat structures respond to shear, one can seek alternatives with similar characteristics.

We combined ultra small angle X-ray scattering (USAXS) with wide and small angle scattering (WAXS, SAXS) to investigate structures on length scales from angstroms to ~6 micrometres. Static and sheared systems containing up to 20% SSS in OOO, 20% FHSO in HOSO and 20% SSS in OOO + cotton seed oil, were studied employing cooling rates of 30 and 0.5deg/min. Theoretical prediction indicate that structures arising from crystalline nanoplatelet (CNP) aggregation can be formed: (1) cylinders (TAGwoods) with fractal dimension $D_m \sim 1$, (2) DLCA structures ($D_m \sim 1.7-1.8$); (3) RLCA structures ($D_m \sim 2.0-2.1$); (4) aggregates with $D_m \sim 2.2-3$, all of which were confirmed by USAXS. Sheared fats exhibited CNP morphologies that were similar to those of static systems but with different average sizes: (1) 70% larger for the sheared systems and (2) 40% larger for samples using a 0.5°C/min ramp. Sheared samples did not form fractal structures on length scales from ~0.8 μ m to ~3 μ m as indicated by an absent of a constant slope in the double logarithmic plot of scattering intensity vs scattering vector.

CLA-rich Chocolate Bar and Chocolate Paste Production and Characterization. S.E. Mayfield¹, D. Van de Walle², C. Delbaere², S.E. Shinn¹, A. Proctor¹, K. Dewettinck², and A.R. Patel², ¹University of Arkansas, USA, ²University of Ghent, Belgium.

Conjugated linoleic acid (CLA) is an 18-carbon fatty acid with multiple health benefits, including anti-obesity and anti-carcinogenic properties. CLA-rich soy oil (CLARSO) can be produced through a heterogeneous catalysis process, and this oil was previously used to produce CLA-rich margarines and shortenings. The objectives of this study were to produce CLA-rich chocolate bars and pastes by replacing a portion of the fat with CLARSO and compare the rheological, textural, and thermal properties of these pastes/bars to controls made with either soy oil or traditional fats. CLARSO was used to

prepare bars/pastes. Rheology, firmness, and thermal behavior of the pastes and fracturability, hardness, and thermal behavior of the bars were determined. The CLARSO chocolate pastes/bars contained no additional saturated fat relative to soy oil controls but the pastes had more solid-like rheology and were firmer and the bars had a higher fracture force relative to soy oil controls. Relative to non-soy controls, CLARSO pastes had similar rheology and CLARSO bars had similar fracturability, despite containing less saturated fat. The fat crystals of all samples were in the same polymorphic form. Therefore, it was successfully demonstrated that CLARSO has the ability to produce chocolate pastes/bars with similar physical properties as traditional products containing more saturated fat.

Physical Properties of Shea Butter and Its Blends with Cocoa Butter. M.L. Herrera¹ and R.J. Candal², ¹Inst. de Tecnologia en Polimeros y Nanotecnologia, University of Buenos Aires, National Research Council of Argentina, Argentina, ²Inst. de Investigacion e Ingenieria Ambiental, University of San Martín, Argentina.

Shea butter is an off-white or ivory-colored fat extracted from the nut of Shea tree. Shea butter is known for its use in cosmetic industry and as it is an edible fat is also used in food formulation. Shea butter is solid and a good alternative to replace *trans*-fat in food or use as cocoa butter alternative. The objective of this study was to investigate the physical properties of Shea butter and its blends with cocoa butter. Blends with different amounts of cocoa butter, from 10 to 90% were prepared. Thermal behavior and melting points were studied by DSC. Fatty acid and TAG compositions were analyzed by capillary GC. Polymorphism was described by X-ray diffraction. Compatibility with cocoa butter was analyzed from iso-solid diagrams built from NMR experiments. Thermal behavior and polymorphism of Shea butter were similar to the ones of cocoa butter. Up to 20% Shea butter may be added to cocoa butter without changing SFC values. However, iso-solid diagrams showed eutectic formation above this percentage. Shea butter may be used as cocoa butter extender or in applications where solid fats are required.

Holistic Control of Fish Oils Based on NMR Spectroscopy. B.W.K. Diehl, E. Zailer*, and Y.B. Monakhova, Spectral Service AG, Germany.

The assessment of quality of fish oils is traditionally performed based on several separate analytical methods, which were developed and standardized several decades ago being very time-consuming and sometimes even erroneous.

A proton nuclear magnetic resonance (¹H NMR) spectroscopic method was developed and validated for targeted control of oil quality parameters (e.g., peroxide value, anisidine value, acidic value, iodine value, hydroxyl value, and fatty acid composition) and tocopherols (a, b, g, d) within short time and in only one analytical run.

Additional information about glyceride composition and free fatty acids can be obtained using ¹³C NMR spectroscopy. Furthermore, DHA, EPA, and total Omega-3 content are quantitative determined.

Furthermore, multivariate models (principal component analysis and classification methods) based on the NMR distribution of major and minor components were developed for type screening of fish, especially of salmon oils. An important point is the distinction between natural and synthesized fish oil in general.

Thus, NMR spectroscopy combining with targeted and non-targeted approaches is a versatile technique, which can be applied for the quality and authenticity control of fish oils. The developed NMR method can replace multiple tedious conventional techniques for routine fish oil analysis.

Extraction and Characterization of Montmorency Sour Cherry (*Prunus cerasus* L.) Pit Oil. N. Korlesky¹, L.J. Stolp*¹, D.R. Kodali¹, W.C. Byrdwell², and R.J. Goldschmidt²,
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Montmorency sour cherry (*Prunus cerasus* L.) pit oil (CPO) was extracted and characterized by various methods including: GC, LC-MS, NMR, TGA, DSC, and XRD. The cherry kernels were 22.4% of the weight of the pits and contained 30.9% oil. The oil had an acid value of 1.45mg KOH/g, saponification value of 193mg KOH/g and unsaponifiable matter content of 0.72%. The total tocopherols and sterols were 525 and 3766ppm respectively. The major fatty acids of CPO were oleic (47.6%) and linoleic acids (34.5%) along with smaller concentrations of saturates (11.6%) and a nutritionally important fatty acid, α -eleostearic acid (EI, 5.6%). The CPO contained six major triacylglycerols (TAG), OOO (16.91%), OLO (16.72%), LLO (13.27%), PLO (7.29%), OOP (6.52%), and LEIL (6.19%) plus a number of other minor TAGs. The TAGs containing at least one saturated fatty acid constitute 32% of the total. The polymorphic behavior of CPO as studied by DSC and XRD confirmed the presence of α , β' and β crystal forms. The CPO has moderate oxidative stability and high thermal stability with oxidative induction time of 30.3 minutes at 130°C and a thermal decomposition temperature of 352°C.