ACS Webinars
CLICK • WATCH • LEARN • DISCUSS

ACS Chemistry for Life®

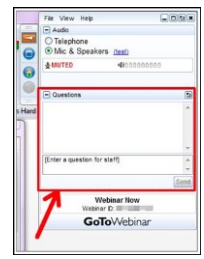
We will begin momentarily at 2pm ET

Slides available now! Recordings available as an exclusive ACS member benefit.

www.acs.org/acswebinars

Have Questions?

ACS Chemistry for Life®



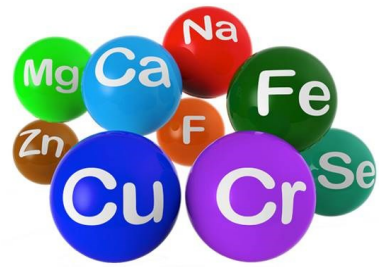
Type them into questions box!

"Why am I muted?"
Don't worry. Everyone is muted except the presenter and host. Thank you and enjoy the show.

ACS Webinars
CLICK • WATCH • LEARN • DISCUSS

ACS Chemistry for Life

Have you discovered the missing element?



http://bit.ly/benefitsACS

Find the many benefits of ACS membership!

3

ACS Webinars
CLICK • WATCH • LEARN • DISCUSS

ACS Chemistry for Life

Benefits of ACS Membership

c&en CHEMICAL & ENGINEERING NEWS

Chemical & Engineering News (C&EN)
The preeminent weekly news source.

ACS Presentations on Demand™
YOUR SOURCE FOR RECORDED MEETING CONTENT

NEW! Free Access to ACS Presentations on Demand®
ACS Member only access to over 1,000 presentation recordings from recent ACS meetings and select events.

NEW! ACS Career Navigator
Your source for leadership development, professional education, career services, and much more.

http://bit.ly/benefitsACS

4

Let's get Social…post, tweet, and link to ACS Webinars during today's broadcast!

facebook.com/acswebinars

@acswebinars

Search for "acswebinars" and connect!

5

How has ACS Webinars® benefited you?

"Fabulous, Fabulous webinar; a terrific presentation and perfect example of basic and translational science working together -- the discoveries that evolve from funding basic science and the benefits of basic science staying tuned into its potential for translational applications."

Quote in reference to: http://bit.ly/STFTechnology

Fan of the Week

Shirley Stiver, MD, PhD
ACS member for 39 years strong!

Be a featured fan on an upcoming webinar! Write to us @ acswebinars@acs.org

6

ACS Webinars®
CLICK • WATCH • LEARN • DISCUSS

ACS Chemistry for Life®

7

ACS Webinars®
CLICK • WATCH • LEARN • DISCUSS

ACS Chemistry for Life®

Learn from the best and brightest minds in chemistry! Hundreds of webinars presented by subject matter experts in the chemical enterprise.

Recordings are available to current ACS members one week after the Live broadcast date. **www.acs.org/acswebinars**

Broadcasts of ACS Webinars® continue to be available to the general public LIVE every Thursday at 2pm ET!

www.acs.org/acswebinars

8

ChemIDP.org

Upcoming ACS Webinars

www.acs.org/acswebinars

Thursday, October 27, 2016

Rational Design of Small Molecules Targeting RNA

Session 10 of the 2016 Drug Design and Delivery Symposium

Matthew Disney, The Scripps Research Institute

Amanda Garner, University of Michigan

Thursday, November 3, 2016

Chemistry of Life: *Instantly Treating Wounds with Hemostatic Gel*

Session 11 of the 2016 Material Science Series

Joe Landolina, Cresilon

Mark Jones, Dow Chemical

Contact ACS Webinars ® at acswebinars@acs.org

ACS Chemistry for Life™

ACS Green Chemistry Institute®

ACS Green Chemistry Institute®

Engaging you to reimagine chemistry and engineering for a sustainable future.

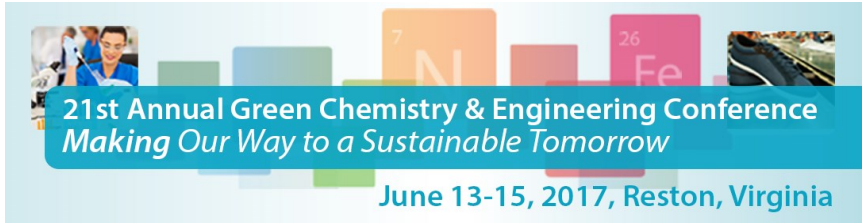
We believe sustainable and green chemistry innovation holds the key to solving most environmental and human health issues facing our world today.

- Advancing Science
- Advocating for Education
- Accelerating Industry

www.acs.org/greenchemistry

ACS Chemistry for Life™

ACS Green Chemistry Institute®



- Sustainable Chemicals
- Flexible Chemical Manufacturing
- More Efficient Processes
- Green Chemistry Curricula
- Circular Economy Considerations
- Sustainable Materials
- Academic-Industry Collaborations
- Chemicals Policy
- Cosmetics
- And More!

Submit to the GC&E 2017 Call for Papers!
Open From January 4th to February 13th, 2017

gcande.org

ACS Chemistry for Life™

ACS Green Chemistry Institute®

ACS GCI Industrial Roundtables

Catalyzing the integration of sustainable and green chemistry and engineering throughout the global chemistry enterprise.

PR Pharmaceutical Roundtable
Bringing global industry leaders together to catalyze the beneficial implementation of green chemistry and engineering.

FR Formulators' Roundtable
Driving the use of green chemistry and engineering to make innovative products that are safer for consumers to use.

Including companies in the cosmetics industry.

ChMR Chemical Manufacturers Roundtable
Defining and applying green chemistry and engineering for the chemical manufacturing industry.

HFR Hydraulic Fracturing Roundtable
Integrating the principles of green chemistry and engineering into the chemical supply chain for hydraulic fracturing.

BTLR Biochemical Technology Leadership Rountable
Catalyzing and enabling the bio-based and renewable chemicals economy.

We convene 40 companies from across the world to focus on the science of sustainable and green chemistry and its implementation.

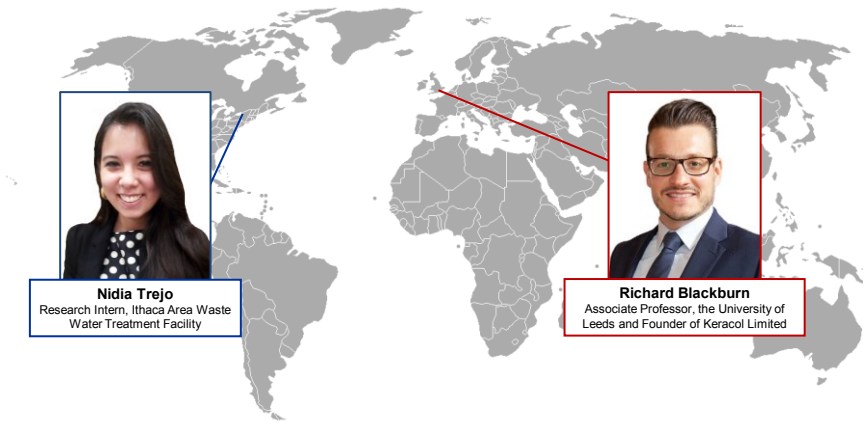
American Chemical Society

ACS Green Chemistry Institute®

ACS Webinars® CLICK • WATCH • LEARN • DISCUSS

ACS Chemistry for Life®

"Cosmetic Chemistry:
Novel Approaches using Natural and Renewable Ingredients"



Nidia Trejo
Research Intern, Ithaca Area Waste Water Treatment Facility

Richard Blackburn
Associate Professor, the University of Leeds and Founder of Keracol Limited

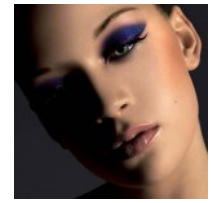
Slides available now! Recordings are an exclusive ACS member benefit.

www.acs.org/acswebinars

This ACS Webinar is being co-produced by the ACS Green Chemistry Institute

14

Cosmetics industry and natural ingredients



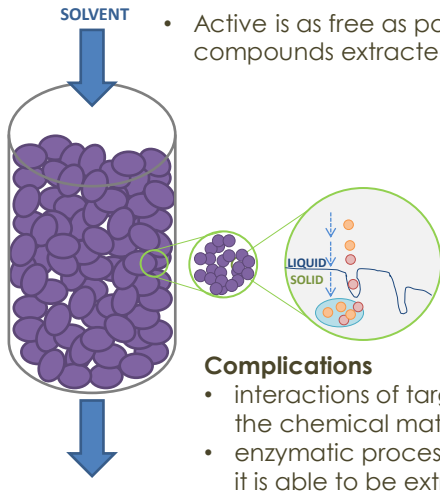
- Cosmetics products include **deodorants**, **hair dyes**, **hair styling products**, **make-up**, **sunscreens**, **nail colorants**, **skin & hair care products**, and **skin & hair cleansing products**, amongst others
- Global beauty care products industry forecast to reach around **$265 billion in 2017** (Mintel)
- Interest in natural ingredients is significantly increasing among cosmetic consumers in general
- **Naturally-derived** personal care market is expected to reach **$16 billion by 2020** (Grand View Research)
- Potentially reduces reliance on petroleum-based products


15

Extraction of active ingredients from plant matter

Idealised extraction from plant material

- Target compound (active) exhaustively removed from source
- Active is as free as possible from interfering or undesirable compounds extracted from the same source



1) **Mass transfer process**: solvent is transferred into the solid phase
2) **Molecular diffusion**: solvent penetrates the solid matrix
3) **Solvation of soluble material** and return to the surface of the solid
4) **Transfer of solvated active** to bulk solution *via* natural/coerced convection

Complications

- interactions of target active with other compounds within the chemical matrix
- enzymatic processes that may degrade target active before it is able to be extracted


16

Extraction & Purification

Clean extraction

- Polar metabolites such as anthocyanins can be extracted using water, superheated water, ethanol, or solvent blends

Non-toxic solvents that allow efficient extractions in optimised conditions
Acceptable solvents for food or personal care and cosmetic applications
No-regulatory limitations

Non-selective solvents
Free sugars, proteins and low-polarity metabolites are extracted too

Solid-Phase Extraction (SPE): strategy for extract purification

- Anthocyanins interact with solid phase *via* H-bonding and hydrophobic interactions
- Resin allows for removal of interferents *via* preferential sorption of active
  Free sugars removed with acidified water
- Anthocyanins subsequently eluted with acidified ethanol

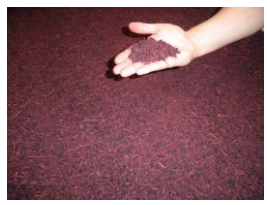
Simple, safe and low cost
Allows high recovery of active
Reduces consumption of solvents

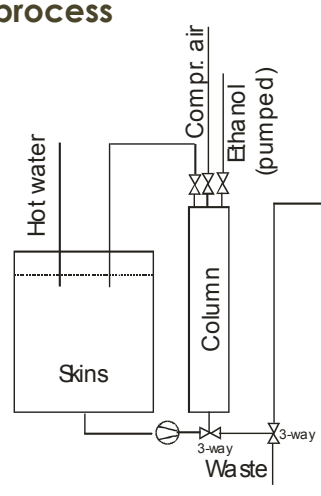
Source needs to be loaded in water
Scale-up limitation?


17

Extraction-Purification

Industrial-scale process






18

Audience Survey Question

ANSWER THE QUESTION ON BLUE SCREEN IN ONE MOMENT

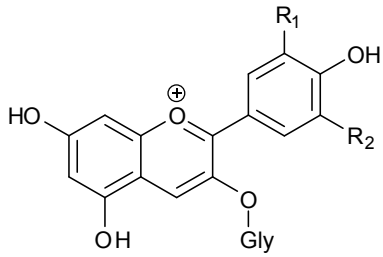
Which is the most difficult color to obtain from nature for application in cosmetics, food and textiles?

- Red
- Yellow
- Blue
- Purple

19

Anthocyanins

- Found in fruits, vegetables, flowers



Anthocyanin	R_1	R_2	λ_{max} @ pH3
pelargonidin	– H	– H	503
cyanidin	– OH	– H	517
peonidin	– OCH_3	– H	517
delphinidin	– OH	– OH	526
petunidin	– OCH_3	– OH	526
malvidin	– OCH_3	– OCH_3	529

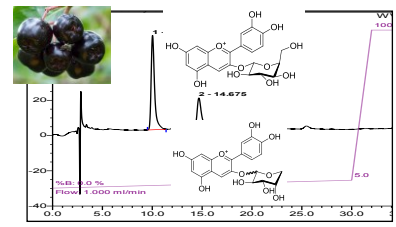
- Glycosylation typically at 3-O position
- In fruits, typically various mono- and disaccharides
- More complex glycosylation observed in other plants

20

- Need to work with fruits where there is a sustainable supply of waste material

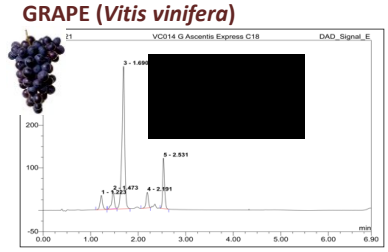
STRAWBE… (*Fragari… ananassa*)
BLACKBERRY (*…bu… uticosus*)
BLUEBERRY (*Va… m corymbosum*)
BLACK MUL… RY (*…us nigra*)

ARONIA (*Aronia melanocarpa*)



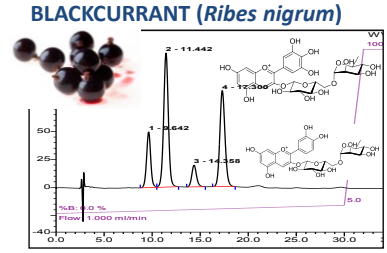
1. cyanidin-3-*O*-galactoside (68%)
2. cyanidin-3-*O*-arabinoside (30%)

GRAPE (*Vitis vinifera*)



1. Cyanidin-3-*O*-glucoside (5.84%)
2. Delphinidin-3-*O*-glucoside (7.27%)
3. Malvidin-3-*O*-glucoside (65.30%)
4. Peonidin-3-*O*-glucoside (5.95%)
5. Petunidin-3-*O*-glucoside (15.64%)

BLACKCURRANT (*Ribes nigrum*)



1. delphinidin-3-*O*-glucoside (15.71%)
2. delphinidin-3-*O*-rutinoside (43.25%)
3. cyanidin-3-*O*-glucoside (7.03%)
4. cyanidin-3-*O*-rutinoside (34.00%)

21

Case Study 1: Natural hair dyes

Extract from blackcurrants (*Ribes nigrum*)

grown in UK and sustainably sourced

waste from blackcurrant juice process (Ribena)

Extracted and purified using SPE to give high levels anthocyanins

Formulated to give optimum hair dyeing performance

- Patented semi-permanent hair colorants and coloration process[1]
- Range of shades, fast to 12+ washes

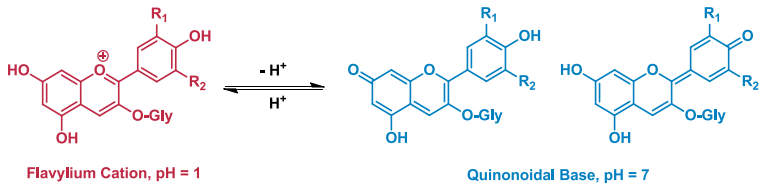
1. US8361167

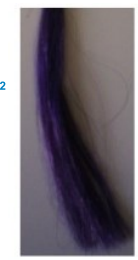
22

Case Study 1: Natural hair dyes

Dyeing from acidic medium (pH 3-4)

- λ_{max} in aqueous solution at pH 3.0: cyanidin 517 nm; delphinidin 526 nm
  - purple/violet colour consistent with flavylium cation

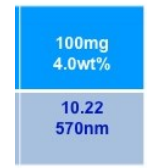




- λ_{max} when adsorbed onto hair from aqueous medium:

  570-580 nm

  - Blue colour consistent with quinonoidal base
  - *in situ* neutralisation by basic sites on hair surface leading to formation of anhydrobase
  - Stable over 12+ washes, minimal colour loss, no colour change

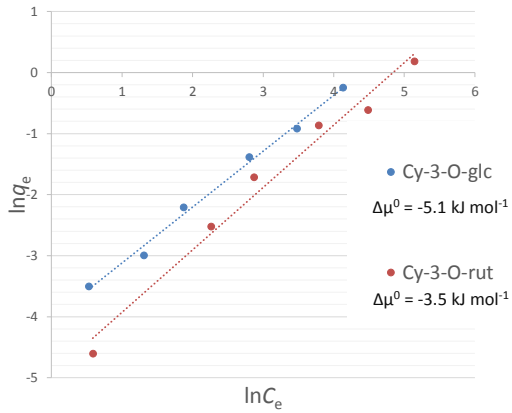


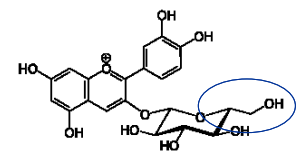
23

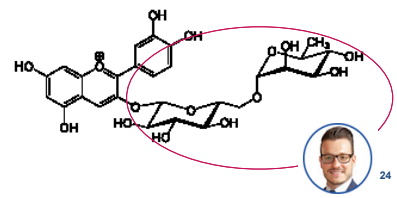
Case Study 1: Natural hair dyes

Blackcurrant glycoside sorption

- HPLC study revealed apparent preferential adsorption in favour of monosaccharides (glucosides): two-fold over disaccharides (rutinosides)
- Isotherm study: cyanidin-3-*O*-glucoside higher adsorption energy in comparison with cyanidin-3-*O*-rutinoside
- Superior H-bonding through primary hydroxyl? Steric effects?





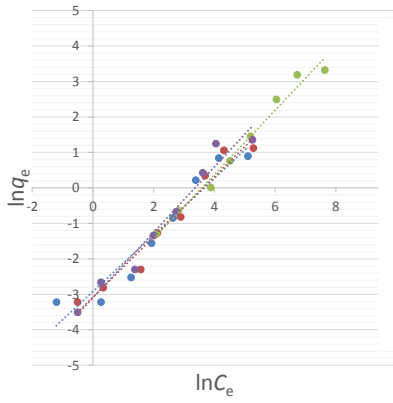


24

Case Study 1: Natural hair dyes

Grape glucoside sorption

- Isotherm study: Glucosides show consistent sorption properties
- Anthocyanin parent structure does not have significant effect on sorption – glycosylation more important



$\Delta\mu^0$ = -7.8 kJ mol^{-1}
Cy-3-O-glc

$\Delta\mu^0$ = -7.5 kJ mol^{-1}
Del-3-O-glc

$\Delta\mu^0$ = -7.2 kJ mol^{-1}
Mal-3-O-glc

$\Delta\mu^0$ = -7.4 kJ mol^{-1}
Peo-3-O-glc

25

What is the French Paradox?

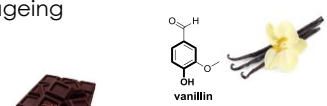
- French was the official language of England from 1066 to 1362
- Despite a diet of cheese, croissants, and crème brûlée, the French have low levels of CVD
- French toast isn't French and was actually invented by a man called Joseph French
- The croissant was actually invented in Austria

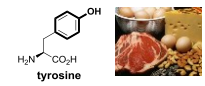
26

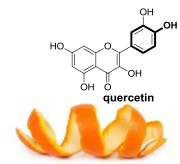
Antioxidants for skin care

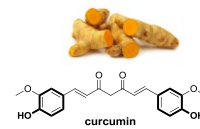
- Radicals cause skin damage and skin ageing, originating from:
  - our own metabolism
  - external factors: UV radiation, tobacco smoke, pollution, etc…
- Antioxidants provide cell protection so they can regenerate and repair themselves
- Reduces skin damage and ageing

Naturally occurring antioxidants
plant phenolics: carotenoids & flavonoids

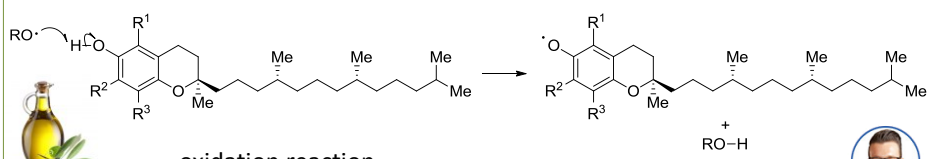








Vitamin E (tocopherol)



oxidation reaction

27

Case Study 2: Pure Super Grape

- Expanding portfolio of M&S cosmetic products
- Want a range of skincare products that fit in with **Plan A**
- Extraction of antioxidants from M&S waste

M&S SIMPLY FOOD

Plan A
Because there is no Plan B

M&S BEAUTY
Science & Nature. *Beautifully.*

ACTIVE INGREDIENT
Resveratrol

28

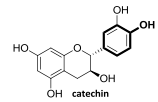
Case Study 2: Pure Super Grape

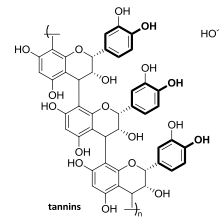
world's largest fruit crop
>60 million tonnes/year

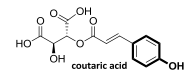
~10 million tonnes/year

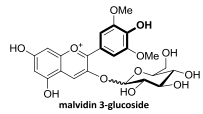
>250 billion litres of wine

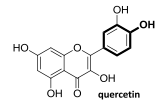
- Opportunity with Pinot noir pressed for champagne and sparkling wine
- Waste pomace rich in polyphenols

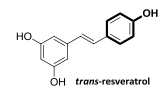








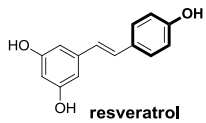


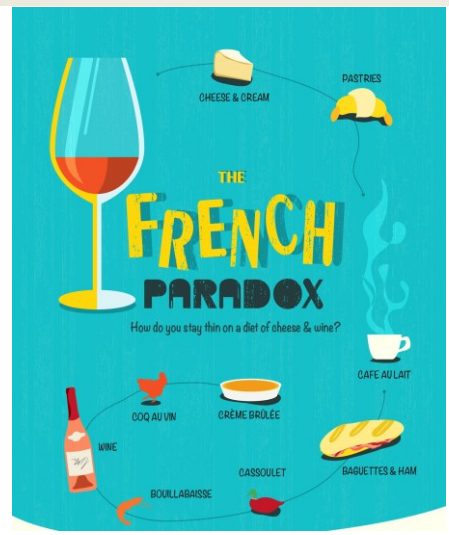



29

Resveratrol

- ***Phytoalexin*** - a protective compound produced by plants in response to environmental stresses (dehydration, nutrient deprivation, attack by pathogenic organisms)
- Present in nuts and berries, in particular in grape (skin and seeds) ⟶ wine
- Discovered in 1940
- 1992 - credited with a key role in the cardiovascular health benefits of red wine ➡ the *French Paradox*
- Biological properties: antioxidant, anti-inflammatory, antithrombotic, anticancer






30

Case Study 2: Pure Super Grape

Pinot Noir grape pomace harvested in October 2012
stored at -20°C

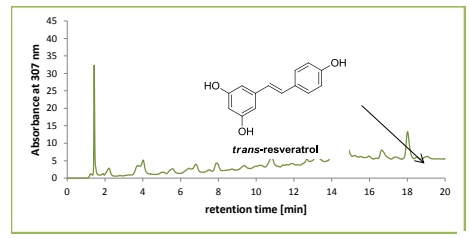
1) Optimization of the extraction procedure
   optimum extraction time for highest extract yield and activity
   optimum solvent-feed ratio for highest extract yield and activity

2) Quantification of actives

Total phenolic content

Folin-Ciocalteu Assay

High Pressure Liquid Chromatography
trans-resveratrol content in grape extract



3) Process scale-up

31

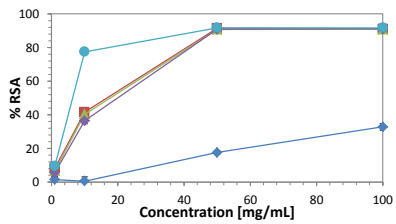
Case Study 2: Pure Super Grape

4) Range of products developed

Face serum, Day Cream, Night Cream, Eye Cream, Overnight oil treatment, Clay mask

- Formulations developed to maximise antioxidant activity
- Full formulation based on sustainable and naturally-derived ingredients as much as possible

Radical Scavenging Activity of formulations



Launched in July 2014

32

the best of science and nature

33

Audience Survey Question

ANSWER THE QUESTION ON BLUE SCREEN IN ONE MOMENT

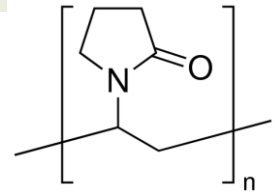
What are some fastest growing organisms on the planet, which come in several colors, rich in trace elements, have vitamins, carotenoids and other antioxidants, and contain polymers that are gelling and emulsifying?

- Berries
- Cruciferous Vegetables
- Whole Grains
- Seaweeds

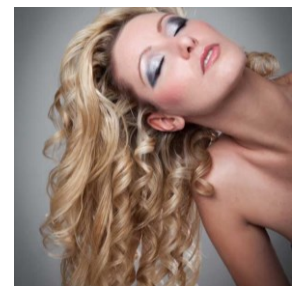
34

Case Study 3: Haircare Naturally

- Hair sprays and hair gels typically utilise film-forming polymers (*e.g.* polyvinyl pyrrolidone) to provide hold
- Industry desire to move to natural polymers to provide this activity
- Some natural polymer systems have been developed, but mainly aqueous systems
- Need to use ethanol-water mixtures for effective delivery and rapid drying of styling product
- Natural polymers incompatible with significant levels of ethanol



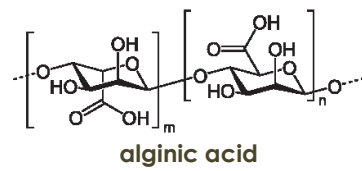
PVP



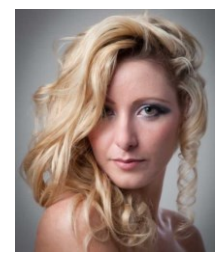
35

Case Study 3: Haircare Naturally

- KeraStyle natural styling polymers
- Extracted from seaweed or waste fruit skins
- Patented formulation combining alginic acid or pectin with an amine to make amine salt[2]
- **Soluble in up to 80% ethanol**
- Performance as good as (if not better than) current PVP/VA copolymer systems
  - Strong hold
  - Natural feel
  - High shine
  - Good sprayability
  - Excellent film forming
  - High curl retention in both dry and humid conditions



alginic acid



36

2. WO2014102545

Case Study 3: Haircare Naturally

Hair Gels

- Citrus fruit peel – converted waste from food and drink industry
- Pectin amine derivative – gives both hold and gels the system
- Pectin much more viscous than alginate

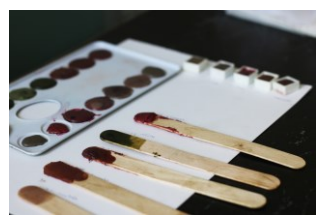
Hair Sprays

- Seaweed – produced from sustainable seaweed sources growing naturally on British coastline
- Alginic acid derivative – gives both hold and gels the system
- Less viscous, so can be delivered in a spray


37

The future of our research…

- Semi-permanent hair colorant products to be launched commercially in 2017
- Applications of anthocyanins in make-up and other skin applications being developed
- New actives for both skin care and hair care from waste food/plant material being developed
- **Interested in working with large companies, SMEs and other academic groups to work collaboratively on novel approaches in using natural and renewable ingredients in cosmetics**




38

Things to consider…

- Does the use of naturally-derived ingredients represent true sustainability or marketing greenwash?
- Does the use of natural extracts and the perception of their inherent safety, present toxicology concerns?
- Plant-based materials often produced either by cultivation or from wild harvesting - should this land be used to grow food?
- Cosmetics industry needs to consider alternative sources of green materials such as marine ingredients, microalgae, bacteria, and food waste
- Extraction of naturally-derived extracts must involve green chemical processes
- Can we use biotechnology to make even better naturally-derived ingredients
- Majority of cosmetic formulation is a vehicle to deliver an active ingredient (typically present at levels of under 5% by weight)
- Use of green chemistry to produce more sustainable cosmetic formulations, including green surfactants, emulsifiers, conditioning agents, emollients, *etc*.

Contacts

r.s.blackburn@leeds.ac.uk

design.leeds.ac.uk/people/richard-blackburn/

@RichardBlackb18

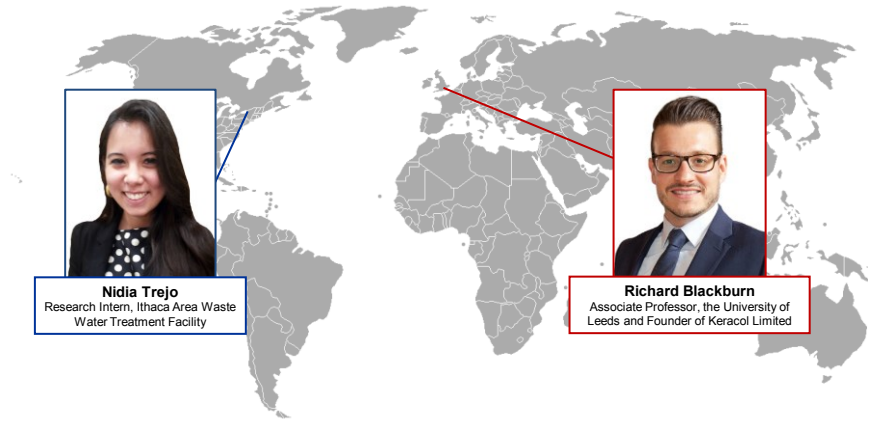
keracol.co.uk

@keracol

ACS Webinars
CLICK • WATCH • LEARN • DISCUSS

ACS Chemistry for Life

"Cosmetic Chemistry:
Novel Approaches using Natural and Renewable Ingredients"



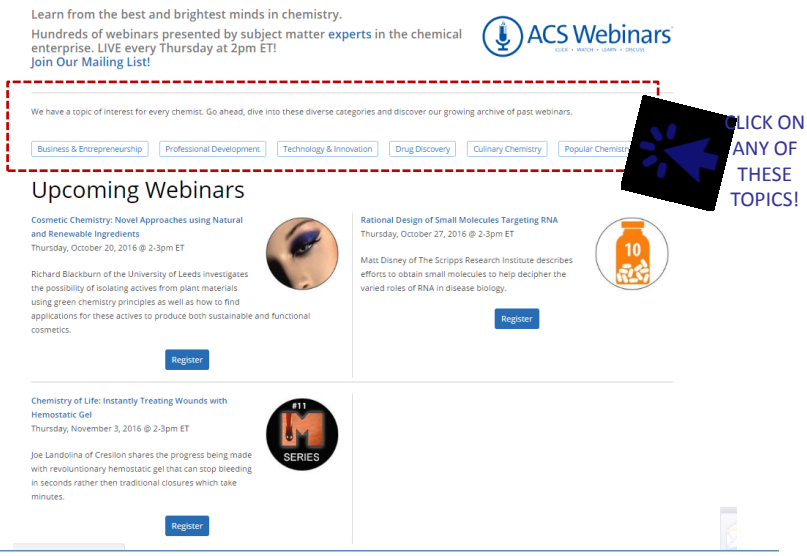
Slides available now! Recordings are an exclusive ACS member benefit.
www.acs.org/acswebinars

This ACS Webinar is being co-produced by the ACS Green Chemistry Institute

41

Celebrate National Chemistry Week with our Open Archive to the Public!

ACS Chemistry for Life



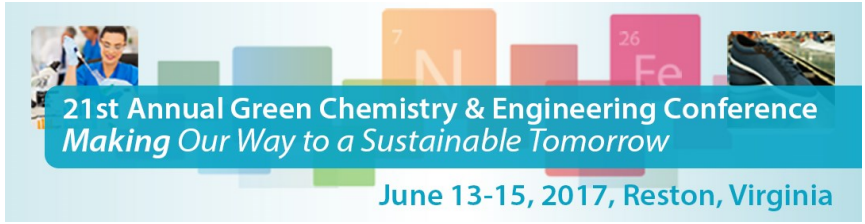
CLICK ON ANY OF THESE TOPICS!

42

www.acs.org/acswebinars

ACS Chemistry for Life™

ACS Green Chemistry Institute®



- Sustainable Chemicals
- Flexible Chemical Manufacturing
- More Efficient Processes
- Green Chemistry Curricula
- Circular Economy Considerations
- Sustainable Materials
- Academic-Industry Collaborations
- Chemicals Policy
- Cosmetics
- And More!

Submit to the GC&E 2017 Call for Papers!
Open From January 4th to February 13th, 2017

gcande.org

Upcoming ACS Webinars

www.acs.org/acswebinars

ACS Chemistry for Life®

Thursday, October 27, 2016

Rational Design of Small Molecules Targeting RNA

Session 10 of the 2016 Drug Design and Delivery Symposium

Matthew Disney, The Scripps Research Institute

Amanda Garner, University of Michigan

Thursday, November 3, 2016

Chemistry of Life: *Instantly Treating Wounds with Hemostatic Gel*

Session 11 of the 2016 Material Science Series

Joe Landolina, Cresilon

Mark Jones, Dow Chemical

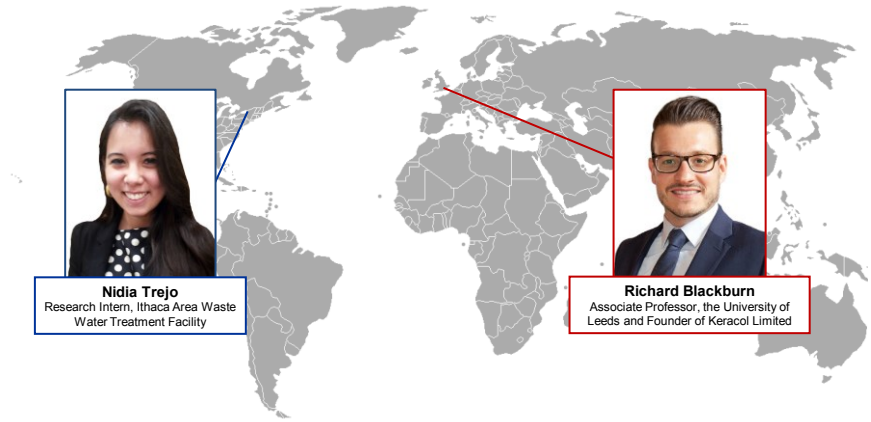
Contact ACS Webinars ® at acswebinars@acs.org

44

ACS Webinars®
CLICK • WATCH • LEARN • DISCUSS

ACS Chemistry for Life®

"Cosmetic Chemistry:
Novel Approaches using Natural and Renewable Ingredients"



Slides available now! Recordings are an exclusive ACS member benefit.
www.acs.org/acswebinars

This ACS Webinar is being co-produced by the ACS Green Chemistry Institute

45

How has ACS Webinars® benefited you?

ACS Chemistry for Life®

"Fabulous, Fabulous webinar; a terrific presentation and perfect example of basic and translational science working together -- the discoveries that evolve from funding basic science and the benefits of basic science staying tuned into its potential for translational applications."

Quote in reference to: http://bit.ly/STFTechnology

Fan of the Week

Shirley Stiver, MD, PhD
ACS member for 39 years strong!

Be a featured fan on an upcoming webinar! Write to us @ acswebinars@acs.org

46

ACS Webinars
CLICK • WATCH • LEARN • DISCUSS

ACS Chemistry for Life

47

ACS Webinars
CLICK • WATCH • LEARN • DISCUSS

ACS Chemistry for Life

Benefits of ACS Membership

c&en CHEMICAL & ENGINEERING NEWS

Chemical & Engineering News (C&EN)
The preeminent weekly news source.

ACS Presentations on Demand
YOUR SOURCE FOR RECORDED MEETING CONTENT

NEW! Free Access to ACS Presentations on Demand®
ACS Member only access to over 1,000 presentation recordings from recent ACS meetings and select events.

NEW! ACS Career Navigator
Your source for leadership development, professional education, career services, and much more.

http://bit.ly/benefitsACS

48

ACS Webinars® does not endorse any products or services. The views expressed in this presentation are those of the presenter and do not necessarily reflect the views or policies of the American Chemical Society.

Upcoming ACS Webinars

www.acs.org/acswebinars

Thursday, October 27, 2016

Rational Design of Small Molecules Targeting RNA

Session 10 of the 2016 Drug Design and Delivery Symposium

Matthew Disney, The Scripps Research Institute

Amanda Garner, University of Michigan

Thursday, November 3, 2016

Chemistry of Life: *Instantly Treating Wounds with Hemostatic Gel*

Session 11 of the 2016 Material Science Series

Joe Landolina, Cresilon

Mark Jones, Dow Chemical