20th Annual Green Chemistry & Engineering Conference

Portland, Oregon

June 14-16, 2016

Jim Hutchison and Adelina Voutchkova

Program Chairs

TUESDAY MORNING

Hilton Portland & Executive Tower
Plaza Level

7:00pm-5:00pm
Registration

7:30am-5:00pm
Networking Breakfast

7:30am-5:00pm
Exhibits

Hilton Portland & Executive Tower
Pavilion Ballroom East

Keynote presented by Paul Anastas
8:30am-9:30am

Hilton Portland & Executive Tower
Broadway III/IV

2016 Presidential Green Chemistry Challenge Award Winners

B. A. Drake, Organizer, Presiding
Hilton Portland & Executive Tower
Studio Suite

**Advances in Continuous Chemistry: Back to the Future**

M. E. Kopach, *Organizer, Presiding*

**9:50** 1. Flow chemistry for sustainable chemical manufacturing. **M.G. Organ**

**10:30** 2. Merging catalysis and continuous for greener processes. **S.A. May**

**11:10** 3. Synthetic transformations employing continuous flow technologies. **C.L. Liotta**


Hilton Portland & Executive Tower
Forum Suite

**Challenges, Tools, & Innovation in the Apparel & Footwear Sector**

J. D. Frazier, *Organizer, Presiding*

**9:50** Introductory Remarks.


**10:50** 6. How to use the alternatives assessment process to green your products using the EcoValuate tool. **J. Malaczynski**


**11:30** 8. INSQIN Waterborne PU: Addressing the sustainability challenges of PU coated textiles. **R. Saunders**

**11:50** 9. Innovations in denim finishing: Comparative savings in chemical, energy and water use. **S.F. Echols**

Hilton Portland & Executive Tower
Broadway I/II
CO2 Utilization by Design: From Molecular Catalysts to Surface Chemistry

G. Li, Organizer, Presiding

9:50 10. Designing catalysts for the reduction of CO2 using an energy-based approach. A.M. Appel

10:10 11. Electrocatalytic conversion of CO2 using manganese-centered molecular catalysts. J. Agarwal

10:30 12. Differences in carbon isotope discrimination during the photocatalytic reduction of CO2. A.M. Angeles Boza


12:10 17. Enhanced interfacial actions between oil and CO2 by oil-CO2 amphiphilic compounds. Q. Shi, W. Qiao

Hilton Portland & Executive Tower
Directors Suite

General Advances in Green Chemistry

J. E. Hutchison, A. Voutchkova, Organizers, Presiding

9:50 18. Green design for substitution with no regrets. P.T. Anastas


10:30 20. DOZN: A quantitative green chemistry evaluator. E. Ponnusamy

11:10 22. Harnessing the power of drug design for safer environmental chemicals. C. Ng

11:30 23. The role of recycled materials. R. Peoples

11:50 190. Integrated fermentation and catalytic processing of biomass derived pyrones and lactones to produce fuels and chemicals. S. Gupta, M. Alam, N. Sinha, M. Haider

11:50 24. Withdrawn

Hilton Portland & Executive Tower
Council Suite

Green Chemistry in Consumer Products: From Demand to Supply

A. Nestler, Organizer
L. Heine, A. M. Noce, Organizers, Presiding

9:50 26. What are the odds? A journalist’s take on ingredients for “green” products. M. Bomgardner

10:10 27. Rivertop renewables: “Rising to the demand for green chemistry”. B. T. Furey

10:30 28. Systematic transition to safer consumer products. R. McFadden

10:50 29. U.S. market pressures and the battle between hazard and risk. R. Engler


11:30 31. Accelerating green chemistry innovation through collaborative partnerships: Examples and lessons from the GC3. L. Hoch, M. Becker

11:50 32. EPA’s Safer Choice Program: Meeting consumer demand and offering green chemistry solutions. B. Williams

12:10 33. Government policy drivers for the adoption of green and sustainable chemistry. R. J. Garant

TUESDAY AFTERNOON

12:30pm-2:00pm
Lunch on your own
Challenges, Tools, & Innovation in the Apparel & Footwear Sector

J. D. Frazier, Organizer, Presiding

1:30 34. Learnings from the commercial introduction of a renewably sourced durable water repellent. G. Brown, R.C. Buck, J.C. Sworen

1:50 35. The route to fluorine-free repellent coatings in outdoor apparel: Consumer use, maintenance and physiological comfort. P. Hill, M. Taylor, P. Goswami, R.S. Blackburn

2:10 36. Permanent, perfluorocarbon-free, water-free finishing of textiles and footwear. G.S. Selwyn

2:30 37. Alternatives assessment of 11 non-fluorinated DWR products utilizing the GHS-column model. K. Schubert, R.C. Buck

2:50 Panel Discussion: DWR/Repellency.

3:10 Intermission.

3:30 38. Eco-friendly dyeing of electrospun cellulose nanofibers with reactive dye. S. Hajahmadi


4:10 40. The collision of comfort and sustainable design. J. Zwillinger

4:25 Concluding Remarks.

CO2 Utilization by Design: From Molecular Catalysis to Surface Chemistry

G. Li, Organizer, Presiding

1:30 41. Modeling photo-active TiO2-graphene interfaces. N.A. Deskins, B. Bukowski

1:50 42. Mechanism of CO2 reduction to CO and CH3OH on ceria surface: Density functional theory study. N. KUMARI, M. Haider, M. Agarwal, N. Sinha, S. Basu
2:10 43. Hybrid photocatalysts for solar energy conversion. T. Jin, B.D. Stewart, S.A. Pantovich, G. Li

2:30 44. Amidoxime-functionalized microcrystalline cellulose-mesoporous silica composites for high temperature carbon dioxide sorption. C. Gunathilake, R. Dassanayake, N. Abidi, M. Jaroniec

Hilton Portland & Executive Tower
Studio Suite

Conversion of Renewables: Catalysis, Methods and Technologies

K. Barta, P. Bruijnincx, Organizers, Presiding

1:30 45. A temperature controlled approach for the homogenously catalyzed conversion of oleocompounds in aqueous media. T. Gaide, J. Dreiman, J. Bianga, A. Behr, A. Vorholt

1:50 46. Synthesis of biobased building blocks from vegetable oils: A chemicals platform approach for polymer synthesis. S. Caillol

2:10 49. Catalyst structure-performance relations for supported Ru-catalysed hydrogenations of levulinic acid to gamma-valerolactone. E. Heeres

2:50 Intermission.


3:50 50. Conversion of cellulosic biomass by heterogeneous catalysts. A. Fukuoka

4:30 47. Withdrawn

Hilton Portland & Executive Tower
Broadway III/IV

Driving Waste toward Zero: The Importance of Superior Process Design

D. K. Leahy, Organizer
J. Yin, Presiding

1:30 51. A practical synthesis of ERK inhibitor GDC-0994 on multi-kilogram scale. X. Linghu
1:50 52. Chemical development of a novel antiviral at Merck: Greener chemistry through process innovation. M. McLaughlin

2:10 53. Development of a green and efficient Suzuki-Miyaura process for the triple reuptake inhibitor penultimate BMS-821754. B. Mudryk

2:30 54. Greener chemistry in research labs with higher-concentration reactions. L. Sun, Y. Yin, R. Ma

2:50 Intermission.

3:10 55. Efficient asymmetric synthesis of the Akt kinase inhibitor GDC-0068. F. Gosselin

3:30 56. Towards the zero waste commercial API process. G.R. Humphrey

3:50 57. Ligand-accelerated C-H activation reactions: Distance and geometry. J. Yu

Hilton Portland & Executive Tower Council Suite

Ensuring Commercial Success in Sustainable Technology Transfer by Design

Financially supported by ACS Green Chemistry Institute Formulators’ Roundtable
T. J. Burns, P. Silva, Organizers
C. K. Choy, Presiding

1:30 Introductory Remarks.

1:35 58. What is takes to make a dent: The development of a new-to-the-world metathesis-based surfactant which makes water work like an organic solvent. R. Slone

1:55 59. Finding new ways to catalyze innovation and achieve sustainability in additive manufacturing. T. McKeag, D. Danby

2:15 60. Value of GHG reductions and sports events in advancing low-carbon technologies into the market. A.M. Behr, M.H. Mazor, S. Phillips, J. Natalense

2:35 61. Economic and ecologic strategies for chemical manufacturing by means of continuous flow chemistry. D. Kirschneck

2:55 Intermission.

3:30 63. The commercial success of Polymeric FR: Market transformation driven by green chemistry. S. Hunter, C. Lukas

3:50 Panel Discussion.

Hilton Portland & Executive Tower
Directors Suite

Sustainable Strategies for Next Generation Biologics and Therapeutics

K. Budzinski, Organizer, Presiding

1:30 277. Green metrics for biologics manufacturing: Current collaborative effort and future direction. S.V. Ho, K. Budzinski


2:50 Intermission

3:10 279. Sharing learnings from Johnson & Johnson’s biologics life cycle assessment studies. P. Dahlin

3:30 280. Sustainable science in bioconjugate process development. R. Finn

4:10 281. Rational selection of alternative, environmentally compatible, surfactants for biotechnological production of pharmaceuticals - a step toward green biotechnology. R. Shearer

Hilton Portland & Executive Tower
Broadway I/II

Green Chemistry in the Semiconductor and Electronics Supply Chain

E. Gately, M. Kirschner, Organizers, Presiding

3:00 70. Green chemistry in 3D printing technology. T. McKeag, D. Danby


3:40 72. Opportunities and challenges for green chemistry in semiconductor technology. L.T. Kenny
4:00 73. Competing on green chemistry: Can the electronics industry do it? M. Kirschner

Hilton Portland & Executive Tower
Pavilion Ballroom East

GreenX
4:45pm-6:15pm

Hilton Portland & Executive Tower
TBA

Opening Reception
6:15pm-8:00pm

WEDNESDAY MORNING

Hilton Portland & Executive Tower
Plaza Foyer

7:30am-8:30am
Networking Breakfast

7:30am-5pm
Registration

7:30pm-5pm
Exhibits

Hilton Portland & Executive Tower
Pavilion Ballroom East
8:30am-9:30am

Keynote address presented by

Hilton Portland & Executive Tower
Plaza Foyer
9:30am-9:50am

Networking Break

Hilton Portland & Executive Tower
Broadway I/II

Alternatives Assessment & De Novo Design
9:50 74. On the design of safer chemicals: The path forward. S. DeVito


10:30 76. Computational model for Nrf2-ARE activation in human HepG2 cells based on whole-molecule chemical properties and mechanistic domains. F. Melnikov, A. Vouthkova, L. Shen, J. Kostal, J.B. Zimmerman, P.T. Anastas


11:10 78. Predicting chemical hazard with a big data approach. A. Maertens, T. Luechtedfeld, T. Hartung


11:50 80. The California safer consumer products regulations’ approach to alternatives assessment. E. Rodriguez

12:10 81. Understanding the unexpected or unanticipated consequences of a chemical over its life cycle is fundamental to eco-design. J. Fava, E. Mulholland

Hilton Portland & Executive Tower
Council Suite

**Design of New Strategies for the Conversion of Lignin**

K. Barta, P. Bruijnincx, Organizers, Presiding

9:50 25. On the activation parameters for model lignin linkages over a promising Cu-doped porous metal oxide catalyst. C.M. Bernt, H. Maneesuwan, M.A. Chui, K. Barta, P.C. Ford

10:10 82. Aromatic monomers by *in situ* conversion of reactive intermediates in the acid-catalyzed depolymerization of lignin. P.J. Deuss

10:30 83. Lignin valorization using biological funneling and chemical catalysis. G. Beckham

11:10 84. Sustainable energy materials for lithium sulfur batteries from lignosulfonate liquor. L. Li, N. Koratkar, T.J. Simmons
11:30 85. Electric insulating resin with high heat resistance derived from woody lignin obtained by steam-explosion. H. Kagawa, Y. Okabe, C. Sasaki, Y. Nakamura

11:50 86. Sustainable conversion of lignin to value-added chemicals, thermoplastics and fuels. M.M. Abu-Omar

Hilton Portland & Executive Tower
Studio Suite

Education Resources Designed to Share Sustainable Solutions to Plastics & Materials

Financially supported by NSF - Center for Sustainable Polymers (U of MN) Center for Bioplastics and Biocomposites (Iowa State University) ACS Division of Polymer Chemistry
J. E. Wissinger, Organizer, Presiding


10:50 89. Polymers experiments in the general chemistry laboratory curriculum at UC Berkeley. M.T. Robak, M.C. Douskey, L.B. Armstrong, G. Kerstiens, A.M. Baranger


11:30 91. Polymers for the planet: Engaging students in sustainable solutions. J.C. Levine


Hilton Portland & Executive Tower
Forum Suite

How to Get There From Here: Sustainably

S. G. Koenig, Organizer
C. Beaudry, Presiding

9:50 93. The impact of a novel organocatalytic dynamic kinetic asymmetric transformation (DyKAT) on the synthesis of a drug candidate. T. Benkovics
10:30 94. Development of a green manufacturing process. K.M. Maloney, G.R. Humphrey

11:10 95. The quest for efficiency in natural product synthesis. C. Beaudry

11:50 96. Synthetic strategy, chemical innovation and the context of an efficient synthesis. M.D. Eastgate

Hilton Portland & Executive Tower
Broadway III/IV

New Sustainable Synthetic Strategies through Photoredox Catalysis

D. K. Leahy, Organizer
N. Strotman, Presiding

9:50 97. Tandem lewis acid-photoredox catalysis for enantioselective photoreactions. T.P. Yoon

10:30 98. Application of photoredox catalysis to green manufacturing processes. D. DiRocco


11:50 100. Organocatalyzed photoredox atom transfer radical polymerization: Catalyst development and application in the design of degradable polymers from biomass. R.M. Pearson, G. Miyake

Hilton Portland & Executive Tower
Directors Suite

Sustainable Chemical Separations: Accelerating Industrial Application of Less-Energy Intensive Alternatives

E. Ponnusamy, A. Sehgal, Organizers, Presiding

9:50 101. Toward sustainable chemical separation processes. R. Giraud

10:30 102. ALTSEP: Initial steps on the road to low energy-intensity chemical separations. A. Sehgal

11:10 Discussion and Brainstorming.

Hilton Portland & Executive Tower
Senate

9:50am-12:30pm
Business Plan Competition

WEDNESDAY AFTERNOON

12:30pm-1:30pm
Lunch on your own

Hilton Portland & Executive Tower
Forum Suite

Bridging Green Solvent Design, Impacts & Application

A. M. Scurto, Organizer
L. Soh, Organizer, Presiding

1:30 103. Tailoring physicochemical solvent properties through CO$_2$ expanded liquids. E.E. Urena-Benavides, P. Pollet, C.A. Eckert, C.L. Liotta

1:50 104. Using liquid carbon dioxide in a new, novel “green” flash chromatography purification system. R. Schlake, M. Przybyciel, A. Kaziunas, K. Pearl

2:10 105. Fractionation of microalgae lipid and nutraceutical compounds with supercritical carbon dioxide. T.A. Kwan, J.B. Zimmerman

2:30 106. Novel series of diphenyl phosphate based ionic liquids for the dissolution and ecofriendly extraction of biomass at room temperature. R. MEDIMAGH, R. Zarrougui, H. Essadam

2:50 Intermission.


3:50 109. Solvent selection guides for pharmaceutical chemistry. D. PRAT

4:30 Panel Discussion.

Hilton Portland & Executive Tower
Broadway I/II

Design of New Strategies for the Conversion of Carbohydrates
K. Barta, P. Bruijnincx, Organizers, Presiding


2:10 112. Efficient, chemical-catalytic approaches to the production of renewable succinic, 3-hydroxypropanoic, and furandicarboxylic acids from biomass-derived 5-(chloromethyl)furfural. M. Mascal, L. Wu, S. Dutta

2:50 Intermission.


3:50 115. Catalytic processing of wood to pulp and their valorization. B.F. Sels

Hilton Portland & Executive Tower
Studio Suite

Exploring Opportunities for Green Chemistry Educators & Researchers as Change Agents
Addressing the Social and Environmental (In)Justices of Chemical Exposure

E. J. Brush, Organizer, Presiding

1:30 Introductory Remarks.

1:50 116. Pesticide impacts of banana cultivation: A disconnect between producing regions and consumers. A.A. Mendez, C. Ng, L. Castillo, C. Ruepert

2:10 117. Chemistry in a social justice context. M.M. Kirchhoff

2:30 118. Two decades of the Presidential Green Chemistry Challenge awards: Bringing about positive change for society, the environment and the economy. M.C. Cann

2:50 Intermission.
3:10 119. Exploring social and environmental justice through green chemistry education, research and outreach. **E.J. Brush**

3:30 120. Mainstreaming green chemistry: Sharing the twelve principals. **A. Lujan, M. Simpson, O. Krel**

3:50 Discussion.

4:10 Concluding Remarks.

Hilton Portland & Executive Tower
Broadway III/IV

**Green Chemistry & Medicinal Chemistry Are Miscible!**

S. G. Koenig, *Organizer*
D. T. Richter, *Presiding*

1:30 121. Green medicinal chemistry by design. **K. Freeman-Cook**

1:50 122. Progress towards embedding a culture of green into Amgen’s medicinal chemistry program. **A. Siegmund**

2:10 123. Putting spin on flow chemistry. **J. Britton, C. Raston, G. Weiss**

2:30 124. Microplate microreactor scaffolds: Making the most of existing lab infrastructure. **S.B. Corry, R. Parmenter**

2:50 Intermission.


3:30 126. Base-free and ligand-free Suzuki coupling reactions of basic nitrogen-containing substrates in water. **Z. Li, C. Gelbaum, J.S. Fisk, B. Holden, A. Jaganathan, P. Pollet, C.L. Liotta**

3:50 127. Novel direct arylation and amination reactions: Rapid synthesis of functionalized biaryls, a-arylated ketones, arylamines and heterocycles. **L. Kurti**

Hilton Portland & Executive Tower
Directors Suite

**Sustainable Strategies for Organic Synthesis Using Biocatalysis**
A. Goswami, *Organizer, Presiding*

1:30 128. Novel sustainable cyclopropanation biocatalysts. **J.D. Rozzell**

2:10 129. Biocatalytic synthesis of fluorescent polyphenols for sensing applications. **W. Kiratitanavit, F. Bruno, C. Doona, R. Nagarajan**

2:30 130. Computational design of new biocatalysts and retro-synthetic approaches. **A. Zanghellini**

2:50 Intermission.

3:10 131. (R)- and (S)-amines through amine dehydrogenase catalysis. **A.S. Bommarius, S.K. Au, B.B. Bommarius**

3:50 132. Efficient synthesis of chiral pharmaceutical intermediates using biocatalysis. **J.W. Wong**

Hilton Portland & Executive Tower
Council Suite

**Workshop on Data Uncertainty in Predictive Toxicology & Alternative Assessments**

J. Kostal, *Organizer, Presiding*

Hilton Portland & Executive Tower
Senate

1:30pm-4:30pm
Business Plan Competition

Hilton Portland & Executive Tower
Pavilion Ballroom

**Poster: Curriculum & Education**

J. E. Hutchison, A. Voutchkova, *Organizers*
S. van Bergen, *Student Poster Chair*

4:30 - 6:30
133. Green chemistry in the undergraduate curriculum. Y. Caballero, A. Navarro-Ocaña, L. Hernández-Vázquez, A. Arellano

134. Synthesis of aspirin in introductory chemistry courses using Nafion-H.P. Auburn

135. The graduate student's guide to designing a green chemistry course. R.A. Haley, H. Hopgood, K. Leahy, J. Ringo, A. Das, D.C. Waddell

269. The Greener Solutions Program: Client-based learning and a bioinspired systems approach to safer and more sustainable chemistry. T. McKeag

Hilton Portland & Executive Tower
Pavilion Ballroom

Poster: Designing More Sustainable Products

J. E. Hutchison, A. Voutchkova, Organizers

4:30 - 6:30

136. Chemical isolation and characterization of cellulose nanofibers to produce bionanocomposite films onto chitosan matrix for seafood packaging. B. Soni

137. A life cycle analysis of tandem perovskite solar cells: When are they warranted?.i. celik, Z. Song, M. Heben, D.S. Apul


139. Adsorption process simulation as strategy for greener separations design. I. Sáenz-Tavera, V. Rosas-García, R. Silvestre-de-León

140. Madder dye (CI natural red 8) chlorination products: Identification and toxicity. T.C. dos Santos, J.A. Vendemiatti, A. Caloto de Oliveira, G. de Aragao Umbuzeiro, H.S. Freeman

141. Application of recycled rare earth elements in dye-sensitized solar cells. W. Li, C. Su, C. Yang, S. Kathirvel, B. Yu, Y. Lin

142. Toughening thermosetting epoxy resins using renewable fatty acids modified epoxidized soybean oil. F. Hu, S. Yadav, G. Palmese

143. Inversion and hydrogen exchange in 1,2-cyclopentanediols: A geometrically constrained model for aqueous-phase "green" catalytic carbohydrate hydrogenolysis. D.E. Howell
144. The safety and efficacy of color pigments in commerce: Industry sustainability practices contrasted with environmental misconceptions. **M. Maxwell**


146. Comparative lifecycle assessment of nanofiltration, adsorption and ion exchange: An arsenic removal case study. **K.R. Chavan**

147. Withdrawn

148. Withdrawn


Hilton Portland & Executive Tower
Pavilion Ballroom

**Poster: Designing Safer Chemicals**

J. E. Hutchison, A. Voutchkova, *Organizers*

4:30 - 6:30

149. Effect of atmospheric pressure plasma (APP) on dyeing cotton fabrics with *Zataria multiflora Boiss* extracts. **S. Hajahmadi**

150. Comparative study of life cycle of green synthesis of magnetite nanoparticles. **W. Marimon Bolivar, E. Gonzalez Jimenes**

151. Data quality in skin permeation modelling: Tailoring the ToxRTool. **J. Machado, J. Kostal**

152. Mammalian cell toxicity studies of several proposed green plasticizers. **H. Erythropel, M. Maric, R.L. Leask, J.A. Nicell**

153. Predicting bioconcentration factor based on nuclear magnetic resonance spectroscopic data. **N. An, A. Voutchkova, J. Magliozzo**

154. What are the elements for considering exposure in alternative assessments?. **A.M. Mason, B.E. Howard**

156. Progressing from alternatives assessment to de novo green chemistry. H. Plugge, L. Shen

157. A coupled molecular design strategy against chemicals perturbing NRF2-ARE antioxidant pathway and inducing cytotoxicity. L. Shen, R. Judson, J. Roethle, J.B. Zimmerman, P.T. Anastas

158. A probabilistic diagram to guide chemical design with reduced potency to incur cytotoxicity. L. Shen, R. Judson, F. Melnikov, J. Roethle, J.B. Zimmerman, P.T. Anastas

159. De Novo design of molecular inhibitors of ubiquitin C-terminal hydrolases for Parkinson disease study. D. Kiao, J. An

160. Exploring the rate of surface microbial redevelopment after cleaning in schools: DNA-sequencing and ATP analysis. S.E. Kwan, E. Bar-Zeev, M. Elimelech


Hilton Portland & Executive Tower
Pavilion Ballroom

Poster: Design of Next Generation Catalysis

J. E. Hutchison, A. Voutchkova, Organizers

4:30 - 6:30


163. Catalytic urea synthesis utilizing methanol as the C1 feedstock. S. Kim, B. Kang, S. Hong


165. IR study of aromatic system physisorption on carbon-supported metal catalysts. J. Lindale, D.G. Kovacs

166. C-N oxidation by flavin mimic organocatalysts: An approach towards synthesis of polycyclic heterocycles. P. Thapa

167. Synthesis of pyridone ligands and iron precursors for the development of iron-based hydrogenation catalysts. B. Hanscam, L. Boisvert

169. Withdrawn

170. Continuous flow bio-transformations base on enzymes immobilized onto supported ionic liquid like phases (SILLPs). **S. Luis**, M. Burguete, P. Lozano, E. Garcia-Verdugo, B. Altava


172. Development of sulfated titania photocatalysts for degradation of organic pollutants. **S.F. Li**, X. Lin

173. Development of novel visible light responsive photocatalysts for water treatment. **S.K. Kansal**


327. Removal of impurities from n-Butane isomerization feedstock using sodalite cage of faujasite zeolites. **S. Singh**, N. Goyal, P. Kumar, R. Jasra

330. CeO$_2$/CNTs-CuO composite catalysts for preferential CO oxidation in excess H$_2$ stream. **S. Zeng**

Hilton Portland & Executive Tower
Pavilion Ballroom

**Poster: Green Chemistry for Society and Markets**

J. E. Hutchison, A. Voutchkova, *Organizers*

4:30 - 6:30

175. Synthesis and characterisation of ionic liquids incorporating benzimidazolate anions. **C. white**, J. Holbrey

176. Value added derivatives of bio derived 2,3-butanediol. **J. Toland**, M. Atkins, J. Holbrey

177. Chemical footprint project as a tool for moving markets to greener chemistry. **M. Rossi**, C. Peele

178. The business of sustainability. **M. Sanders**, **N. Pryde**, A.M. Noce
Poster: Moving towards more Sustainable Chemical Building Blocks

J. E. Hutchison, A. Voutchkova, Organizers

4:30 - 6:30

179. Mesoporous alumina with amidoxime groups for CO₂ sorption at ambient and elevated temperatures. C. Gunathilake, M. Jaroniec


181. Photo- and electrocatalytic CO₂ reduction promoted by non-innocent ligand Mn(I) and Re(I) catalysts. M.E. McKinnon, K.T. Ngo, D.C. Grills, J.J. Rochford

182. Towards a mechanistic understanding of copper-catalyzed reductive lignin depolymerization. L. Petitjean, E.S. Beach, P.T. Anastas

183. Isocyanate-free polyurethanes for safer foams, adhesives and other green materials. A.W. Myers, T. Dawsey, I.J. Javni, O. Bilic, N. Bilic

184. Synthesis of cardanol oil building blocks for polymer synthesis. S. Caillol

186. Catalytic pyrolysis of vegetable oil to fuels and chemicals in a novel continuous-flow reactor. Y. Shirazi, S. Viamajala, S. Varanasi


188. 1D nanocellulose to 2D and 3D functional materials. Y. Hsieh

189. A pectin biorefinery: Galactaric acid production from D-galacturonic acid with an enzymatic bioanode. R. Sakuta, K. Takeda, H. Ohno, N. Nakamura


192. Real-time determination of lignin conversion reactions in nanostructural self-assembly of lignin-ABA block copolymer in aqueous media by NMR. M. Azadfar, W.C. Hiscox, S. Chen

193. New platform of lignin based building blocks for polymers. S. Caillol
194. Lignin to liquid fuels and value-added products using fast pyrolysis and electrocatalytic upgrading. M. Garedew, J.E. Jackson, C.M. Saffron

328. Catalytic conversion of lignocellulose to lignin-derived phenolics and liquid fuels over Cu doped porous metal oxide. Z. Sun, K. Barta

Hilton Portland & Executive Tower
Pavilion Ballroom

Poster: State of the Art Green Chemistry and Engineering

J. E. Hutchison, A. Voutchkova, Organizers

4:30 - 6:30


196. Understanding molecular interactions to develop sustainable (green) synthesis of nanosilicas. J.R. Manning, S. Patwardhan

197. Synthesis of gold nanorods using C\textsubscript{12}EDMAB as a less toxic, alternative growth-directing agent. J.W. Stone, J. Allen, J. Xu, S. Canonico-May

198. Withdrawn

199. Industrial lignin-based thermoplastic elastomers: Solvent-free synthesis, processability, and tunable mechanical properties via nano-dispersed lignin blends. T. Bova, C.D. Tran, R. Boy, A.K. Naskar


Hilton Portland & Executive Tower
Pavilion Ballroom

Poster: Sustainable Materials

J. E. Hutchison, A. Voutchkova, Organizers

4:30 - 6:30

201. A green route to white-light emission. G. Guo, Y. Chen


204. Aminopolycarboxylate ionic liquids and their application for efficient synthesis of organic carbonate fuel additives. D. Tao, K. Huang, S. Dai


206. Making the synthesis of N-phenyl-5-aminovaleric acid more sustainable: Green Chemistry for robots. J. Husson, T. Vrlinic, C. Buron, S. Lakard, B. Lakard

207. A salen-Mn(V) catalyzed synthesis of poly(silylether)s from diols, dicarboxyls and hydrosilanes. S. Vijjamari

208. Bio-based thermoset polymers from waste vegetable oil. F. Cicaroni Fernandes, P. Wilson, K. Kirwan, S.R. Coles

209. Toward a green multi-layer, multi-functional water filtration unit. C. Fausey, J.B. Zimmerman

210. Orange peel conversion to carbon nanostructures for dye adsorption from wastewater. A.H. Pinto, S. Chen, A. Sharma, R. Penn

211. Enzymatic synthesis of polycardanol and their potential application in Industry. I. Sharma, D. Kim

212. Towards sustainable water treatment: Developing selective adsorbents for inorganic contaminants using nano-enabled biomaterials. L.N. Pincus, J. Yamani, J.B. Zimmerman

213. Informing sustainable design of multi-walled carbon nanotubes based on property-function-hazard relationships. M. Falinski, J.B. Zimmerman, L.M. Gilbertson

214. Systems-level evaluation of nano-enabled applications in the agricultural sector: Informing design to maximize net environmental and human health benefit. J. Yin, Y. Wang, L.M. Gilbertson

215. Design and synthesis of “green” oligomer with high bio-based content for UV-curable coating applications. O. AKDOGAN, S. Shendre, V.M. Mannari

216. Can we meet the new challenges of thermoresponsive non-isocyanates polyurethanes? S. Caillol
217. Syntheses of biobased hybrid poly(epoxy-hydroxyurethane) polymers. A. Cornille, S. Caillol


221. Using QM computations to predict the $^1$H-NMR spectra of metal hydroxo clusters. L. Wills, A.F. Oliveri, D.W. Johnson, P. Cheong

222. Precise size control and dopant incorporation of metal oxide nanocrystals via a greener, “living” growth synthesis. A.W. Jansons, b. crockett, L.K. Plummer, J.E. Hutchison


Hilton Portland & Executive Tower
Pavilion Ballroom

Poster: Synthetic Design in Green Chemistry

J. E. Hutchison, A. Voutchkova, Organizers

4:30 - 6:30

223. Solvent-free noncovalent functionalization of carbon nanotubes with phthalocyanines. V.A. Basiuk, L.J. Flores-Sánchez, V. Meza-Laguna, L. Bucio, J.O. Flores-Flores, E.V. Basiuk


225. Exploring keratin films as a substrate in the design of sustainable hair colorants. T.N. Williams, H.S. Freeman

226. Green synthesis of [1-(substituted-sulfonyl)-piperidin-4-yl]-(2,4-difluoro-phenyl)-methanone oximes and their biological activity. L. MALLESHA
227. Synthesis of new Ru (II) complexes with terpyridines and isothiocyanates ligands, using biomass-derived aldehydes, and their use in DSSCs. F. Charrier, J. Husson, L. Guyard

228. Advancement of magnetic field application on performance of Fe-Cu/MCM-41 catalysts in CO₂ hydrogenation reaction. S. Kiatphuengporn, M. Chareonpanich

229. Towards a green synthesis of glucosinolates. R. Hewitt

230. Sustainability metrics for the synthesis of active pharmaceutical ingredients (API): Application of FLASC and other mass metrics tools in the assessment of the synthesis of a HIV drug candidate. J. Guo, S. Xie

231. One-pot, four-component synthesis of medicinally privileged pyranopyrazoles. S. Huerta

232. Applying green chemistry principles to improve the efficiency and regioselectivity of the electrophilic addition of bromine to oxindole-3-acetic acid. N. Ivanowsky, E. J. Brush


234. Molecular iron complex catalyzed amination of alcohols through the borrowing hydrogen strategy. T. Yan, B. Feringa, K. Barta


237. University of Toronto's green chemistry initiative: Shining a green light on chemical research and education. I. Mallov

238. Vestaron's new SPEAR™ line of biopesticide products. B. Kennedy

239. Getting ready for 21st century photochemistry: Teaming up continuous flow and LED. C. R. Horn, C. Cerato Noyerie, O. Lobet, S. Gremetz

240. Sustainable chemical transformations based on the use of functional polymers under flow conditions. E. Garcia-Verdugo, S. Luis, M. Burguete, R. Porcar, E. Peris

Hilton Portland & Executive Tower
Galleria

ACS GCI 6th Annual Roundtable Poster Reception
6:30pm-8:30pm
Hilton Portland & Executive Tower
Forum Suite

ACS Careers Workshop
6:45pm-10:00pm

THURSDAY MORNING

Hilton Portland & Executive Tower
Plaza Foyer

7:30am-8:30am
Networking Breakfast

7:30am-3:00pm
Registration

7:30am-3:00pm
Exhibits

Hilton Portland & Executive Tower
Senate Suite

Designing Precursors for Functional Materials through Sustainable Chemistry

B. L. Maddux, Organizer
C. K. Perkins, Organizer, Presiding

8:30 241. Printing with clusters. D.A. Keszler

8:50 242. Metal oxide EUV photoresists: Novel materials in a mature industry. A. Telecky


9:30 244. Precise tuning of optoelectronic properties of Sn-doped In$_2$O$_3$ nanocrystals through size and dopant distribution, and their use as additive solution-processed materials in electronic devices. B. Crockett


Hilton Portland & Executive Tower
Forum Suite

Design of Heterogeneous Catalysis

A. Voutchkova, Organizer, Presiding

8:30 249. Multi-functional heterogeneous catalyst for the conversion of ethanol to C₄ chemical building block. C. Alvarez-Vasco, M. Gray, H. Job, K.K. Ramasamy

8:50 250. Protecting palladium: Balancing stability and reactivity in support-tether design. D. Paull

9:10 251. Designing the interface between nanoparticle catalysts and electrode materials for enhanced electrocatalysis. S.L. Young, J. Kellon, J.E. Hutchison

9:30 252. Selective hydrodeoxygenation of guaiacol over bifunctional Co/Al-MCM-41 catalyst. N.T. Tran, Y. Uemura, A. Ramli


10:30 255. Palladium-LDHs: Active and recyclable catalysts on decarbonylation of biomass-relevant substrates. N. An, A. Adeniyi, M. Finn, P. Pereira, A. Voutchkova

10:50 256. Inverse molecular design of green catalysts for converting biomass molecules into value-added chemicals. D. Xiao

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Broadway III/IV

Design of Processes for Cleaner Water

S. Shukla, Organizer, Presiding
8:30 257. Is there a way to clean drinking water for masses? An overview of the need and the quest of low cost low tech water treatment systems. S. Shukla, A. Shukla

8:50 258. Enhanced capacitive desalination performance with polysaccharide binders. R.D. Cusick

9:10 259. Withdrawn


9:30 262. Comparative sorption studies of 17-ß estradiol on raw bone powder, bone char and commercial hydroxyapatite. S. Patel, J. Han, W. Gao

10:10 263. Highly efficient and greener approach for fluorinating organic compounds. S. Dhingra

Design of State of the Art Green Chemistry Curricula

J. E. Hutchison, Organizer, Presiding

8:30 264. Green chemistry education roadmap: Overview and update. J.E. Hutchison

8:50 265. Infusing the concepts and tools of toxicology into the chemistry curriculum. A. Voutchkova

9:30 266. Green chemistry education roadmap: Embedding systems thinking in the chemistry curriculum. E.J. Beckman

10:10 267. Toxicology experiments in the general chemistry laboratory curriculum at UC Berkeley. L.B. Armstrong, M.C. Douskey, M.T. Robak, A.M. Baranger, C.W. Tam, P. Pande, G. Kerstiens

10:30 268. Teaching green chemistry and engineering principles through life cycle inventory analysis. M. Sabahi

8:30 Introductory Remarks.

8:40 271. Sustainable Design Strategies that Consumers Recognize in Polymers. K. Muenchinger


10:00 Intermission.


10:45 276. Methane recovery from the anaerobic digestion of food waste and pretreated bioplastic. S.R. Hobbs, A.E. Landis

11:05 Concluding Remarks.

Hilton Portland & Executive Tower
Broadway I/II

Sustainable Strategies for Next Generation Biologics and Therapeutics

Greener Approaches to Therapeutic Synthetic Polypeptides

K. Budzinski, Organizer
T. Benkovics, Presiding
8:30 322. Peptide API Manufacturing: A green chemists paradise or nightmare?. M.E. Kopach


9:50 324. Synthetic peptide process design and control strategy. A. Lower

10:30 325. Solid phase peptide synthesis as method to understand the molecular basis of protein function. P. Dawson

Hilton Portland & Executive Tower
Plaza Foyer

Networking Break
11:10am-11:30am

Hilton Portland & Executive Tower
Pavilion Ballroom East

Keynote address presented by Nathan Lewis
11:30am-12:30pm

THURSDAY AFTERNOON

Hilton Portland & Executive Tower
Council Suite

Design of Curricular Materials: Rapid Fire Session

J. E. Wissinger, Organizer, Presiding

2:00 282. Sewer science: A calibrated peer review (CPR) writing project for quantitative analysis lab. L.D. Margerum

2:10 283. The next generation of green scientists. D. Paull

2:20 284. Micro-scale synthesis of biofuels in undergraduate research at a community college. R.R. Klepper

2:40 286. Teaching inquiry and sustainability in introductory chemistry by inviting students as participants in the redesign of a green chemistry laboratory curriculum. V. Lykourinou, J. de la Parra, A. Rovira

2:50 Panel Discussion.

3:10 Intermission.

3:40 287. Green making and sustainable team design. T.A. Kwan, J.B. Zimmerman

3:50 288. Connecting green chemistry and toxicology concepts through a senior seminar course. E.J. Brush

4:00 289. Green metric workshop for the undergraduate organic chemistry lab. K.N. Goodwin


4:20 291. Introducing green chemistry through a research-based laboratory project. D.G. Kovacs

4:30 292. Oxone replacements of bleach in organic chemistry laboratory experiments. J.E. Wissinger, J.J. Palesch

4:40 Panel Discussion.

Hilton Portland & Executive Tower
Forum Suite

Design of Homogeneous Catalysis

A. Voutchkova, Organizer
C. H. Leung, Presiding

2:00 293. Catalytic isomerization of allyl functionalities in water by hexaaquaruthenium(II) tosylate. L.Y. Kuo


2:40 295. Regioselective cobalt-catalyzed hydroboration of 1,3-dienes. K. Dewese, T. RajanBabu
3:00 296. Ligand-assisted cleavage of dihydrogen in the design of new iron hydrogenation catalysts. L. Boisvert

3:20 Intermission.

3:40 297. Computational modeling to advance lignin valorization. L. Berstis, D. Vardon, T.J. Elder, M.F. Crowley, G. Beckham

4:00 298. Synthesis of dicaticionic main group Lewis acid catalysts using the naphthyl framework. I. Mallov, D.W. Stephan

4:20 299. C-C and C-N bond formation by organocatalytic mimics of flavoprotein oxidases. F.W. Foss, P. Thapa


Hilton Portland & Executive Tower
Directors Suite

Design Strategies to Maximize the Net Environmental and Human Health Benefit of Emerging Approaches to Environmental Challenges

L. M. Gilbertson, Organizer, Presiding

2:00 301. Designing with Okala metrics. P. White


3:00 303. Life cycle assessment of UV-curable biobased wood flooring coatings. M. Montazeri, M. Eckelman

3:20 Intermission.


4:00 305. Software guided design of safer chemicals. J.R. Vanderveen, P.T. Anastas, J.B. Zimmerman, P.G. Jessop

4:20 306. Difficult choices: Evaluating green decision-making in the regulatory domain. T. Malloy

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Broadway III/IV
Green Chemistry Design for a Rainbow of Colorants

L. Heine, S. van Bergen, Organizers
A. Nestler, Organizer, Presiding

2:00 307. Inadvertent PCB formation from a pigment chemistry perspective. R. Christie


2:35 309. The chemistry of color pigments: Engineering green chemistry solutions to achieve product stewardship goals. R. Mott

2:50 310. Textile colorants: Chemical properties and performance requirements. T. Schaefer

3:05 Discussion: Chemical properties and performance requirements of pigments and dyes: Innovation needs.

3:20 Intermission.

3:40 311. The rainbow of material health criteria to assess colorants: Comparing U.S. EPA Safer Choice, Cradle to Cradle Certified™, and GreenScreen® criteria. M.H. Whittaker, B. Reid, Z. Guerette

4:00 312. Industrial application of anthocyanins extracted from food waste. R.S. Blackburn, C.M. Rayner, M. Benohoud

4:20 313. Characterization of the mutagenicity of some phenylenediamine based bisazo dyes. H.S. Freeman, J.P. Clemmons, L.D. Claxton


Hilton Portland & Executive Tower
Senate Suite

Inorganic Thin-Films: From Sustainable Design to Advanced Functionalities

B. L. Maddux, Organizer
C. K. Perkins, Organizer, Presiding

2:00 315. Solution-cast oxide films from aqueous all-inorganic molecular precursors: Solution chemistry, design principles, and electronic applications. S.W. Boettcher, M. Kast, L.J. Enman, J. Wager, D.A. Keszler


3:20 Intermission.


Hilton Portland & Executive Tower
Broadway I/II

**New Directions in Green Synthetic Design**

D. K. Leahy, **Organizer, Presiding**


2:40 66. Poly(4-vinylpyridine) as a green solid support for acid catalysts and reagents. **T. Mathew**, S.G. Prakash, G.A. Olah

3:00 67. Abstract to be determined. **D.K. Leahy**

3:20 Intermission.

3:40 68. Highly efficient synthesis of HIV NNRTI doravirine. **D.R. Gauthier**
Unsymmetrical aryl(mesityl)iodonium salts as reagents for selective metal-free arylation reactions in organic synthesis. D. Stuart, S. Sundalam, A. Nilova