
201. Computational and experimental approaches to understand a living biotic-abiotic interface using gold binding peptides. **M.C. Small**, D.A. Sarkes, H. Dong, D.N. Stratis-Cullum, M. Hurley

**SATURDAY MORNING**

UMBC
Lecture Hall 5

**Emerging Investigators: Early Career Organic Chemists**

Cosponsored by ORGN
W. Farrell, Organizer, Presiding

8:30 Introductory Remarks.

8:35 202. Mechanistic studies of Fe-catalyzed cross-coupling reactions as a platform for reaction discovery. **O. Gutierrez**

9:00 203. Alcohols coupling to alkenes via deoxygenative coupling. **A. Voutchkova**

9:25 204. Using electricity to amp up organic synthesis: Electrocatalytic alkene difunctionalization. **S. Lin**

9:50 Intermission.

10:00 205. New Directions in olefin metathesis and polyhomologation. **W. Farrell**

10:25 206. Poly(arylenevinylene)s through ring-opening metathesis polymerization of an unsymmetrical ‘electronically-ambiguous’ cyclophane. **E. Elacqua**

10:50 207. Chemoenzymatic strategies for optimizing bacterial glycosyltransferase activity for controlled carbohydrate synthesis. **P.C. McCarthy**


UMBC
Lecture Hall 8

**Humanizing Science: The Key Roles of Mentoring & Building Community**

E. Sesmero, Organizer, Presiding

8:30 Introductory Remarks.

8:35 209. Creating a motivating environment in your class: The courage of vulnerability. **E. Sesmero**

8:45 210. Building community and growing success in chemistry through a Learning Assistant program. **C.P. Schick**
9:05 211. Role of strong faculty mentorship in the development of effective learning assistants in chemistry courses. **V.L. Miller, N.N. Tahmazian**

9:25 212. The Pace Path experience: Running and managing an undergraduate research group. **E.E. Mojica**

9:45 Intermission.

9:55 213. Connecting with students in a large introductory course. **T.S. Carpenter**

10:15 214. The role of community in upper division teaching labs. **M.N. van Staveren**

10:35 215. You are a chemist, now what? A student centered approach to teach senior level laboratory courses. **L.A. Avila**

10:55 Panel Discussion- A. McRae, L. Anna S. Konath.

11:25 Discussion.

11:55 Concluding Remarks.

UMBC
Meyerhoff 120

**Optimization Methods in Chemistry**

C. B. Rinderspacher, *Organizer, Presiding*

8:30 216. Searching chemical compound space. **C.B. Rinderspacher**

8:50 Discussion.

9:00 217. Molecular crystal structure prediction with GAtoR and Genarris. **N. Marom**

9:20 Discussion.

9:30 Intermission.

9:50 218. Rapid screening of molecular materials using evolutionary algorithms: Seeking photovoltaics, capacitors, and piezoelectrics. **G. Hutchison**

10:10 Discussion.

10:20 219. Reduced-density-matrix based approaches to dynamical and nondynamical electron correlation. **A.E. DePrince**

10:40 Discussion.

10:50 Concluding Remarks.

UMBC
Lecture Hall 7
Physical Chemistry

B. Arnold, Organizer
B. M. Cullum, Presiding

8:30 Introductory Remarks.


9:50 Intermission.

10:10 223. Binding of BRACO19 to a telomeric G-quadruplex DNA probed by all-atom molecular dynamics simulations with explicit solvent. C. Wu, H. Sullivan, B. Machireddy

10:35 224. Transire: Software for automating the study of solid state, chemical interfaces. C. Carlin, C.B. Rinderspacher

11:00 225. Polyacrylamide in glycerol solutions: A molecular dynamics study. G. Gogovi, E. Weisel, E. Blaisten-Barojas


11:50 Concluding Remarks.

UMBC
Ballroom

Undergraduate Poster Session

P. J. Smith, Organizer

10:00 - 12:00

227. Development and study of an isothermal microcalorimeter. A. Frederick, A. Hussam


229. Structure activity relation studies of nucleotide reverse transcriptase inhibitor (NRTI) AZT (Zidovudine) analogs using Gaussian computational techniques. K. Quirk

231. Microwave synthesis of rhenium pentylcarbonato complexes. J. Akinbami, A.J. Winstead, S. Mandal


235. Ionic distribution of monovalent and divalent cations in aqueous reverse micelles. M. Hernandez, A. Sharma, C. Thuemer

236. Solvation properties of microhydrated environmentally sensitive anion clusters. V. Phuong, V. Ruan, A. Sharma

237. Detection of delayed fluorescence emission (αS₁) from aggregated carbon nanodots. E. Ra, R. Knoblauch, C.D. Geddes


239. Monitoring transverse relaxation times of kerosene-adulterated diesel using low-field nuclear magnetic resonance spectroscopy. T. Rumbaugh, A.M. Nagy, C. Santai

240. Using carbon quantum dots as a fluorescent DNA sensor. J.M. Hernandez

241. Raman spectroscopy for standoff detection of trace materials using single and multiple excitation wavelengths. S. Tahir, E. Bowman, B. Arnold


243. Calorimetric measurement of the xylose isomerase binding energetics – an instructional experiment for physical chemistry. W.N. Hoxie, M.N. van Staveren

244. Electrochemical oxidation of trinary metal carbides in aqueous solutions and morphology of porous carbonaceous products. S. Palumbo, A.T. Mazahra, B. Kleinhans, J. Hettinger, L. Yu

245. Photodegradation of sulfonamide antibiotics: Apparent reaction kinetics and identification of phototransformation products. L. Harris, M. Hopanna, L.M. Blaney

246. Cancer treatment: Naturally occurring compounds for telomerase inhibition. A. Mustafa

247. The advantages and limitations of quantum dot synthesis via microwave irradiation. E. Harazinska, M. Dands, D.N. Williams, Z. Rosenzweig


249. Synthesis of cis-platin: An advanced inorganic laboratory to explore chemistry and reactivity of dihalogenodiammineplatinum (II) complexes. E. Diessner, G. Paniconi

251. Green Chemistry Club at a community college. S. Serafin, S. DeSouza, C. Middlebrooks, C. Mullen

SATURDAY AFTERNOON

UMBC
Meyerhoff 120

Analytical Chemistry

B. Arnold, Organizer
M. Kyoung, Presiding

1:30 Introductory Remarks.

1:35 252. 4D spatiofunctional mapping of metabolic pathways in living cells. M. Kyoung

2:00 253. In situ synthesis of fluorescent gold nanoclusters in human embryonic kidney cells. K.J. Perry, P. Agarwal, R. Kumar, S.P. Karna, R. Gupta


2:50 Intermission.


4:00 257. Application of a radiotracer to evaluate extraction efficiency and test material degradation in a small-scale avian diet preparation. L. Lockard, K. Martin, L. Zhang

4:25 258. Inductive touch sensors as detectors for nanoparticles. B. Rapp, A. Hussam

4:50 Concluding Remarks.

UMBC
Lecture Hall 8

Organic & Medicinal Chemistry

Cosponsored by MEDI
T. Tsukamoto, Organizer
S. Zimmermann, Presiding

1:30 Introductory Remarks.

1:35 259. Pyridinium-functionalized hydroquinone. H. Arslan
2:00 260. Efficient copper catalyzed homocoupling and heterocoupling of terminal alkynes. L.K. Trigoura, M. Holganza, Y. Xing


2:50 262. Conformation dependent dual function of a 1,2-diketone for sensitized photooxidation and thermal binding. S. Belh, N. Walalawela, S. Lekhtman, A. Greer

3:15 Intermission.

3:25 263. Derivatives of (1H-imidazol-2-yl)phenol as inhibitors of neutral sphingomyelinase 2. O. Stepanek, N. Hin, A. Thomas, R. Rais, C. Rojas, B. Slusher, T. Tsukamoto


UMBC
Lecture Hall 7

Physical Chemistry

B. Arnold, Organizer
L. Kelly, Presiding

1:30 Introductory Remarks.

1:35 266. Biradical formation and reactivity in 1,4,5,8-naphthalene diimide-carboxylate conjugates. L. Kelly, S. Sova

2:00 267. Interaction of protoporphyrinIX (PPIX) and 5-amino levulinic acid (ALA) in nanoemulsion. M.O. Iwunze

2:25 268. Solid polymer-peroxide complexes for the detoxification of chemical warfare agent and fentanyl analogues. J. Landers, C.J. Karwacki

2:50 269. Polymer-guided synthesis of Au/Pt coaxial hollow nanotube with high photothermal stability. Q. Zhang, Z. Nie

3:15 Intermission.

3:35 270. Incorporation of a reactive metal-organic framework component into anisotropic laponite-polyethylene oxide composite membranes and effect on performance as a barrier material. M. Browe

4:00 271. Designed optically multi-adaptive materials. C.B. Rinderspacher, R.H. Lambeth


4:50 Concluding Remarks.
Undergraduate Poster Session

P. J. Smith, Organizer

1:30 - 3:30

273. Coarse-grained molecular dynamics simulations identify on/off rates of an atypical membrane-active peptide. **E. Kaufmann**, B. Mertz

274. Using real world images as visualization tools to convey chemical concepts. **S. DiStefano**, K.K. Bagga

275. Syt1 interaction with charged membrane lipids is key for triggered release of neurotransmitters. **N. Karandikar**

276. Validation of a fast-pulling protocol for quantifying the thermodynamics associated with the insertion of cell-penetrating peptides. **A.R. Clark**, B. Mertz

277. Using QuEChERS and LC-MS/MS analysis to investigate the effectiveness of washing strategies on pesticide removal from strawberries, apples, and grapes. **V. Tran**, J.A. Palkendo


279. Total synthesis of the phenolic natural product cinnamic A1. **C. Craescu**, A.Y. Nuriye

280. Styrene migration from food packaging into Ramen noodles. **B. Binkley**, H.N. Currie, K.L. Gares


286. Liquid-liquid extraction and analysis of the antioxidant, resveratrol, from various red, rose’ and white wines from local Lehigh Valley vineyards. **D.M. Simons, V. Asbrock, F.C. Mayville**

287. Green chemistry investigation of the esterification of vanillin isomers under acidic and basic conditions. **C. Richards, A. Eggleston**, K. Bhat, L. Bastin

288. Investigation of the release mechanism of naproxen sodium, acetaminophen and ibuprofen from tablet delivery systems. **J.A. Carrero, H.M. Fadel, F.C. Mayville**
289. Withdrawn


