Poster Session A:

1a Christopher R Brewer, The University of Florida – "Photochemical Reactions of Ru Precursors for Photoassisted Chemical Vapor Deposition"

Chemical vapor deposition (CVD) is a potentially attractive technique for the metallization of organic thin films. However, thermal CVD processes often require high temperatures, which are incompatible with organic substrates. Photochemistry provides an alternative means of initiating precursor decomposition without heating the substrate. Readily available Ru precursors, such as (allyl)$Ru(CO)_3X$ (X = Cl, Br, I), have been used to deposit Ru on functionalized self-assembled monolayers by means of photochemical CVD as a model system for deposition of metal on a thermally sensitive substrate. Identification of carbonyl loss as the primary photoprocess and determination of the quantum yields for ligand loss will be discussed in the context of precursor design for photochemical deposition techniques.

Authors: Christopher R. Brewer, Olivia M. Hawkins, Bryan Salazar, Amy V. Walker, Lisa McElwee-White

2a Devarapalli Venkatasai, Augusta University – "Design, synthesis and 3D pharmacophore studies of pyrazinoic acid-isoniazid hybrid conjugates as potential anti-tubercular agents"

Tuberculosis (TB) is a bacterial pathogen caused by Mycobacterium tuberculosis, which generally causes pulmonary infection and is extremely pervasive within the lungs and between subjects. Pyrazinamide (PZA) is a first-line anti-tuberculosis prodrug often used in combinational therapy with drugs like isoniazid, ethambutol, streptomycin and/or rifampicin. With prolonged administration of the recommended dose, harmful side effects have been reported: hepatitis, acute hypertension, thrombocytopenia, and gastrointestinal discomfort. To overcome the problem of toxicity and drug resistance, combination therapy has been used which utilizes the simultaneous administration of two or more antibiotics with independent modes of action and different biochemical targets in the bacteria. Recently, the concept of hybrid molecules has been introduced in anticipation that molecules of this type may overcome drug resistance. In hybrid molecules, two or more pharmacophores are linked together covalently, and it is believed that these compounds act by inhibiting two conventional targets simultaneously. This multiple target strategy led to the discovery of various bio-effective hybrid molecules.
Drug-amino acid conjugates are used because of increased tissue delivery, in which the amino acids act as effective carriers of these agents while maintaining, and even amplifying, their bioactive integrity. Amino acid conjugates can increase bioavailability and quantitatively decrease the required amount of active drug thus preventing toxic side effects. We have synthesized several pyrazinoic acid hybrid conjugates with isoniazid *via* amino acid linkers with retention of the chiral integrity of the desired products. All of the synthesized compounds were characterized by spectral studies. The synthesized conjugates are expected to have better anti-tubercular properties with fewer side effects.

Authors: Venkatasai Devarapalli, Will Littlefield and Siva S. Panda

3a Chris Evoniuk, Florida State University – "Coupling N-H deprotonation, C-H activation and oxidation: metal-free C(sp3)-H aminations with unprotected anilines"

An intramolecular oxidative C(sp3)-H amination from unprotected anilines and C(sp3)-H bonds readily occurs under mild conditions using *t*-BuOK, molecular oxygen and *N,N*-dimethylformamide (DMF). Success of this process, which requires mildly acidic N-H bonds and an activated C(sp3)-H bond (BDE = < 85 kcal/mol), stems from synergy between basic, radical and oxidizing species working together to promote a coordinated sequence of deprotonation; H-atom transfer and oxidation that forges a new C-N bond. This process is applicable for the synthesis of a wide variety of *N*-heterocycles, ranging from small molecules to extended aromatics without the need for transition-metals or strong oxidants. Computational results reveal the mechanistic details and energy landscape for the sequence of individual steps that comprise this reaction cascade. The importance of base in this process stems from the much greater acidity of transition state and product for the 2c,3e C-N bond formation relative to the reactant. In this scenario, selective deprotonation provides the driving force for the process. The process opens a quick access to the previously unknown classes of extended *N*-heterocycles.

C. J. Evoniuk, G. d. P. Gomes, S. P. Hill, F. Satoshi, K. Hanson, I. V. Alabugin, *J. Am. Chem. Soc.*, **2017**, *139*, 16210 – 16221.

Authors: Christopher J. Evoniuk, Gabriel dos Passos, Gomes, Igor V. Alabugin

4a Ehsan Fereyduni, The University of Florida – "A Simple Route to Access Aryl-6-7 Scaffolds."

Terpenoid natural products have drawn the interests of synthetic organic chemists for their biological and chemical properties, especially for their medicinal and therapeutic effects in fighting diseases. The goal of our research is to design a simple, scalable, and cost-effective synthetic route to access terpenoid cores from commercially available sources within two steps. First a one-pot Pd-catalyzed α-allylation/[3,3] Cope rearrangement produces a γ-allylated alkylidene malononitrile. Subsequent addition of an allylic electrophile provides a difunctionalized Knoevenagel adduct. Then, ring-closing metathesis furnishes the terpenoid core. This synthetic design allows for the functionalization of Knoevenagel adducts with both symmetrical and unsymmetrical electrophiles to generate complex terpenoid cores in an efficient fashion.

Authors: Fereyduni, E.; Gonzalez, G.; Grenning, A. J.

5a Gabriel Gomes, Florida State University – "Taming Peroxides with Stereoelectronic Effects: Stereoelectronic Control in the Ozone-Free Synthesis of Ozonides"

The unusual stability of bis-peroxides contradicts the conventional wisdom – some of them can melt without decomposition at temperatures exceeding 100 °C. In this work, we disclose a stabilizing stereoelectronic effect that two peroxide groups can exert on each other. This stabilization originates from strong anomeric interactions that are absent in mono-peroxides, but reintroduced in molecules where two peroxide moieties are separated by a CH_2 group. The two unstable peroxides are transformed into two acetals.
The value of stereoelectronic guidelines is illustrated by the discovery of a convenient, ozone-free synthesis of bridged secondary ozonides from 1,5-dicarbonyl compounds and H_2O_2. The expected tetraoxanes are not formed when the structural distortions imposed on the tetraoxacyclohexane subunit by a three-carbon bridge partially deactivate the anomeric effects. The ozone-free approach to ozonides is readily scalable to the gram scale.

Authors: Gabriel dos Passos Gomes, Ivan A. Yaremenko, Vera A. Vil, Alexander O. Terent'ev, Igor V. Alabugin

6a Edgar Gonzalez-Rodriguez, Florida State University – "Design of Polyaromatics by Regioselective Sn-radical Cyclizations

Annealing two armchair polyaromatic units via an alkyne demonstrates the ability of this functionality to serve as a "carbon-rich glue" that could potentially connect two carbon nanostructures.[1] The scope of this approach is continuously expanding. Specifically, formation of phenanthrenes by alkyne benzannulations at a biphenyl unit have been extensively studied. However, the available examples are limited to the extension at the armchair edge of polycyclic aromatics. In contrast, alkyne annulations at a zigzag edge of carbon-nanostructures remain remarkably scarce even when peri-cyclizations can serve as a potential strategy for terminating *exo*-dig cyclization cascades that transform oligoalkynes into extended polyaromatics.

This type of deceivingly simple cyclizations remained unknown until our recent discovery of a general approach to benzannulations at the peri-position of a variety of polyaromatic cores via Bu_3Sn-mediated radical cyclization of appropriately substituted propargylic ethers. Through this approach, we were able to accomplish the synthesis of functionalized phenalenes, benzanthrenes, and olympicene.[2]
Furthermore, we tested the feasibility of this approach while overcoming the need of an external oxidant by equipping an aromatic core with two alkyne moieties. In such cascades, the two vinyl radical attacks could converge in the central core to yield bistannyl-polyaromatics.

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2. N. P. Tsvetkov, E. Gonzalez-Rodriguez, A. Hughes, G. dos Passos Gomes, F. D. White, F. Kuriakose, I. V. Alabugin. *Angew. Chem. Int. Ed.*, under revision.

Authors: Edgar Gonzalez-Rodriguez, Nikolay P. Tsvetkov, Miguel M. Abdo, Gabriel dos Passos Gomes and Igor V. Alabugin*

7a Ying He, University of South Florida – "G-Quadruplex Formation from H8 Modified Guanosine Derivatives: From Structure to Function."

G-quadruplex (GQ) has been developed extensively over the past decades. It has been reported that GQs could be used in many directions of chemical, material and biological researches, including supramolecular hydrogel, molecular switch and ionophores. To form a controllable G-quadruplex, one general consideration of self-assembly process is the competition between H formed by hydrogen bonding and the S generated from formation of highly organized structure. It is reasonable to assume that structurally more rigid monomer will lead to the formation of more stable G-quartet due to the reduction of conformation flexibility. One general approach to achieve structurally rigid G-monomer is the modification of C-8 position by fixing the sugar syn/anti conformation. However, according to literature, the studies of C-8-modified G-quadruplexes are rare, mainly due to the challenges associated with the substrate synthesis.

Taking advantage of the electron deficiency of 1,2,3-triazole and electron rich guanosine, we designed a triazole-substituted guanosine and successfully achieved high fluorescent intensity, which can be used in the application of molecular switch. Herein, we report the new synthesis of 8-aryl guanosine and fluorescent active 8-triazole guanosine and their selfassembly property in solid state and in solution. Through cation templation (Mn+= Na+, K+, Ba2+, Pb2+, Sr2+, La3+), discrete self-assembled G-quartet structures were formed. Both structurally novel and functional enriched G-quartets are achieved using this new system. Potential applications in molecular sensing and biological target recognition are expected with this new system.

Authors: Ying He, Prof. Xiaodong Shi

8a Hitesh Honkanadavar, Augusta University – "Synthesis, Antibacterial Properties and 2D-QSAR Studies of Quinolone-triazole Hybrids"

Quinolones are one of the most important synthetic antibacterial agents have been widely used in the treatment of diverse infections including urinary tract, respiratory and bone joint infections as well as sexually transmitted diseases, prostatitis, pneumonia and acute bronchitis. However, quinolones resistance increases in almost all Gram-negative and Gram-positive species as well as tuberculosis. Molecular conjugation has been known for the rational design of new biologically active entities by fusion of compounds and/or pharmacophoric units recognized and derived from known bioactive molecules.

The present work deals with conjugation of quinolone antibiotics with triazole ring. Interest in the 1,2,3-triazole scaffold for developing novel bio-conjugates is due to the various pharmacological properties exhibited by 1,2,3-triazole containing compounds, Computational chemistry studies including 2D-QSAR (quantitative structure-activity relationship) modeling support the observed biological properties. The details of the study will be discuss in the conference.

Authors: Hitesh Honkanadavar and Siva S. Panda

9a Martin Iglesias-Arteaga, Universidad Nacional Autónoma de México – "Palladium-catalyzed generation of *o*-quinone methides. A three-component synthesis of dimeric steroid chroman ketals"

Ortho-quinone methides (o-QMs) are highly reactive intermediates that have received considerable attention. Their ability to participate in [4 + 2] cycloadditions with electron rich dienophiles confers o-QMs a significant importance as tools for the assembly of structures increased complexity.[1] Generation of o-QMs can be achieved by several methods that includes photochemistry or thermal initiation, as well as Lewis acid, base, or oxidative treatment of phenol derivatives.[2]

We have recently reported the synthesis of chromane ketals, by a three-component reaction that comprises a) generation of an enol ether by Pd-catalyzed cyclization of an alkynol; b) Pd-catalyzed generation of an o-QM from salicylaldehyde and trimethyl orthoformate, and c) a [4 + 2] cycloaddition between the an enol ether and the an o-QM.[3]

Here in we describe the synthesis of dimeric steroid chroman ketals by a Pd-catalyzed three-component reaction of 2-formylestradiol-17 monoacetate, trimethyl orthoformate and the alkynols.

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2. Singh, M.S.; Nagaraju, A.; Anad, N.; Chowdhury, S. *RSC Adv.*, **2014**, *4*, 55924.
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10a Farukh Jabeen, Laurentian University – "Fast and forward: In silico modeling and prediction for polymers, coating systems and drug like molecules."

Computerized models catalyze discoveries by crossing the boundaries between disciplines in addition to reducing the cost and time. Computational chemistry is the arsenal of tool boxes comprising techniques for speedy and reliable prediction. We utilized these tools for modeling and prediction of properties of polymers and polymer based coating systems in addition to molecular docking for prediction of binding energies and interaction of the drug like molecules with targets.

A Quantitative Structure Property Relationship (QSPR) has been a focus of interest for prediction of properties and activities of novel materials and compounds based on the 2D and 3D to multidimensional QSAR models.[1] We utilized this technique to predict the refractive indices of novel polymers. A predictive/validated QSAR model was generated from training set. A virtual library of the novel polymers has been designed and RI values has been predicted by using the developed model.

Mixture QSAR[3] approach was adopted for development of predictive models for polymer based coating systems with best anti-biofouling and fouling release properties.[2] The purpose of this QSAR modeling in relation to concentration of coating systems is our vision for the development of the field. Mixture descriptors were developed and predictive QSAR/QSPR models for 4 end points 18K-PDMS compositions of the coatings were generated. The developed models can be used for the prediction for properties of novel coating systems.

Molecular docking[3] was utilized to predict the binding energies and binding interaction to prioritize the compounds as useful urease inhibitors. Docking studies and experimental results were found in close agreement.

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[3]. *Molecular Modelling: Principles and Applications, 2nd Edition*, **2006** Leach, A. Publisher: Pearson Education Company, Upper Saddle River, New Jersey 07458, 1-477.

Authors: Farukh Jabeen, Philip Boudjoukc

11a Guangde Jiang, The University of Florida – "Production of herbicidal diketopiperazine thaxtomins in nonpathogenic Streptomyces strains"

Thaxtomins are virulence factors of most plant pathogenic Streptomyces strains and are active ingredients of EPA-approved bioherbicides. However, the low productivity of native producers and lengthy, costly, and environmentally damaging chemical synthesis limit the wide agricultural use of thaxtomins. Here we report the heterologous production of thaxtomins by expressing its gene cluster in multiple nonpathogenic Streptomyces hosts. The thaxtomin gene cluster comprising of 8 genes is located within a mobile pathogenicity island (PAI, >100 kb), called the toxicogenic region (TR). The transfer of PAI/TR from thaxtomin-producing *S. scabiei* and *S. turgidiscabies* into five non-pathogenic Streptomyces species created the strains that produced varying levels of thaxtomins, indicating the substantial effects of the host genetic backgrounds on the expression of the gene cluster. Furthermore, we cloned the thaxtomin gene cluster (~15 kb) and expressed it in *S. albus* J1074 that produced the highest amount of thaxtomin from PAI/TR. Screening different media, we achieved the yield of thaxtomin A at 170 mg/L, 20 times higher than the native producer. Furthermore, the versatility of the biosynthetic system in S. albus J1074 was capitalized to produce one unnatural fluorinated analog 5-F-thaxtomin A. Natural and unnatural thaxtomins demonstrated potent herbicidal activity in radish seedling assays. These results presented a new strategy to synthesize valuable, structurally complex natural products and suggested the broad use of *S. albus* J1074 for synthetic biology research.

Authors: Guangde Jiang, Yucheng Zhang, Magan Powell, Peilan Zhang, Ran Zuo, Yi Zhang, Dimitris Kallifidas, Albert M. Tieu, Isolde M. Francis, Hendrik Luesch, Rosemary Loria, Yousong Ding

12a Byeong-Seon Kim, Rice University – "Rapid and programmed synthesis of structurally diverse fused N-heterocycles via [3,3]-sigmatropic rearrangements."

Heterocycles, especially nitrogen-containing ring systems, are ubiquitous and appears as a building block in a large number of biologically active natural products, active pharmaceutical ingredients, agrochemicals, and functional materials. Despite their apparent abundance and importance, efficient synthetic approaches to quite a few of these heterocycles are lacking. As a result, there is an urgent need for the development of novel C-C and C-heteroatom bond-forming methods and reagents that expand the toolbox of synthetic organic chemists and enable the environmentally friendly construction of complex heterocyclic structures under mild conditions, while using the fewest number of chemical steps and generating the least amount waste. With *N*-aryl *O*-cyclopropyl hydroxylamine derivatives, we present a rapid and programmed synthesis of structurally diverse dihydroquinolines and quinolines as well as fused *N*-heterocycles *via* Brönsted acid and [3,3]-sigmatropic rearrangements. A great deal of flexibility is expected in terms of the substitution patterns on easily available *O*-cyclopropyl hydroxylamines that are set to couple with diaryliodonium salts.

Authors: Byeong-Seon Kim, Kaitlyn Lovato, Molly Hurley, László Kürti

13a Brittany M Klootwyk, Florida Gulf Coast University – "Synthesis of Heterofunctionalized Cyclopropenones and Investigation of their Reactivity."

Cyclopropenones are a unique class of compounds in that they possess very high levels of ring strain that is counterbalanced by a stabilizing aromatic character. Preliminary studies in our group have demonstrated that the substituents on the cyclopropenone substantially affect the reactivity of the ring. Using a variety of methodologies, several cyclopropenones have been synthesized with alkyl, aryl, alkoxy, and amino substituents. The differing behavior of these substrates is discussed in a Favorskii-type acrylate synthesis and in [3+2]-cycloadditions. A rationale for the disparity in reactivity is also provided.

Authors: Brittany M. Klootwyk, Gregory Boyce

14a Viktor Kolman, Institute of Organic Chemistry and Biochemistry – "Polysubstituted 2-aminopyrimidines as inhibitors of Nitic Oxide and Prostaglandin E2 production"

Over the course of last years we were concerned with polysubstituted 2-amino pyrimidines as inhibitors of nitric oxide (NO) and/or prostaglandin E2 (PGE2) production as the marker of anti-inflammatory properties of our coupounds. First we focused on 4,6-dichloropyrimidines and the influence of the C-5 alkyl substitution. Partial hydrolysis of the dimethylaminomethylene protecting group on C-2 amino position to formyl group was developed as well. As the next step we introduced substituted aryls and heteroaryls into positions C-4 and C-6 of the pyrimidine ring. The most in vivo promising compound 5-butyl-4-(4-methoxyphenyl)-6-phenylpyrimidin-2-amine was selected for further optimization and the synthetic route was steam lined as well. We also modified the amino group in C-2 position of the pyrimidine with series of substituted aryl derivatives. Later, we focused on the alkoxy moiety on the 4-(4-alkoxy)phenyl scaffold and discovered that derivatives bearing benzyloxy moiety increase the PGE2 inhibition up to 1000 fold. Finally, we modified the substituent in C-5 position of the pyrimidine ring in order to increase the solubility of studied molecules.

Authors: Viktor Kolman, Jansa Petr, Filip Kalčic, Ondřej Baszczyński, Zlatko Janeba

15a Tomohiro Kubo, The University of Florida – "Sequential, chemoselective post-polymerization modification strategy"

Post-polymerization modification techniques can allow for preparations of polymers with complex architectures and/or with various functions, thus extending the range of attainable, useful materials. Efficient and concise route to side-chain heterodifunctional polymers was developed using 2,4,6-trichloro-1,3,5-triazine (TCT). By leveraging TCT's controlled electrophilicity, which was corroborated through small molecule model studies, we demonstrated the straightforward synthesis of otherwise laboriously prepared polymers bearing multiple functionalities in each repeat unit. This TCT-based synthetic strategy was applied for the modular preparation of amphiphilic homopolymers, in which hydrophobic and hydrophilic groups were sequentially incorporated within side chains of polymers. Formation of self-assembled nanostructures was indicated via light

scattering measurements, while amphiphilic properties were demonstrated *via* fluorescence measurements of encapsulated hydrophobic dye and water-oil interfacial tension studies.

Authors: Tomohiro Kubo, C. Adrian Figg, Jeremy L. Swartz, Maxym Tansky, Kyle C. Bentz, Kristin C. Powell, Anuj Chauhan, Daniel A. Savin, Brent S. Sumerlin

16a Qingjiang Li, The University of Florida – "TBD"

Therapeutic cancer vaccines targeting overexpressed carbohydrate antigens on cancer cells have witnessed great progress recently until it was stalled by the intrinsic problems of autoimmunization and T-cell independency. Our appoach to tackle these two problems is to develop fully synthetic vaccines which would consist of cancer-specific antigens and immunostimulator, ligand of Toll-like receptor 4 Lipid A. KH-1 antigen is a nonasaccharide first isolated in adenocarcinoma cells, but has not been detected in normal cells. In addition to its potency in intiating immune response, the potential cancer-specificity of KH-1 may be a solution to autoimmunity of cancer vaccines Lipid A is the anchoring motif of lipopolysacchride that are widely present in bacteria. Monophosporylated Lipid A has been proved to be an exceptional vaccine carrier/adjuvant acting by binding Toll-like receptor 4 on dendritic cells and thereby initiate T-cell dependent, adaptive immune response.

Authors: Qingjiang Li and ZHongwu Guo

17a Simon E. Lopez D'Sola, The University of Florida – "Photoredox-Catalyzed Difluoroalkylation of C(sp2)-H α-Oxoketenedithioacetals"

α-Oxoketene *S,S*-acetals are 1,3-bielectrophilic synthons widely employed in the preparation of a diverse variety of substituted and fused aromatic and heterocyclic systems. Many of those methods include their reaction with nucleophiles such as Grignard,[1] Reformatsky,[2] organolithium,[3] and organocuprate reagents.[4] α-Halogenated oxoketene dithioacetals have been employed as synthons in metal catalyzed reactions.[5] The preparation and chemistry of α-oxoketene S,S-acetals have been reviewed.[6-10]

Due the high impact of organofluorine chemistry in the development of new drugs, agrochemicals and materials, the incorporation of fluorine itself or polyfluorinated groups into organic molecules is an increasing demand. ✔-Fluoro-α-oxoketene *S,S*-acetals have been prepared using selectfluorR as fluorinating agent.[11] Only few examples of ✔-trifluoromethyl-α-oxoketene *S,S*-acetals have been reported,[12-14] including CuII-catalyzed trifluoromethylation, electrophilic trifluoromethylation using "in situ" generated PhI+CF_3 and the nucleophilic trifluoromethylation of iodo-substituted α-oxoketene dithioacetals. Recently, our lab has successfully employed photoredox reactions for the difluoroalkylation of terminal olefins.[15] In this work we present interesting results about our explorations towards an efficient photoredox difluoroalkylation of internal alkenes, such as α-oxoketene *S,S*-acetals and its application to the preparation of fluorinated heterocycles, i.e. 4(1H)-quinolones.

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Authors: Simon E. Lopez, Nathaniel Schmidt, Ricardo Torres, Jordan Hamburger, Robert J. Gilliland and William R. Dolbier, Jr.

18a Jagadeesh Nagendra Manda, The University of Florida – "Synthesis and Biological Evaluation of Spirastrellolide A Analogues''

Spirastrellolide A is a marine macrolide first isolated by the Anderson group from the Caribbean marine sponge Spirastrella coccinea in 2003. Due to its novel antimitotic potency (IC50 = 100 ng/mL) and selective inhibition of protein phosphatase 2A (IC_{50} = 1 nM), Spirastrellolide A is potentially a lead compound for anti-cancer therapeutics; however, further evaluation of its biological potency was hindered by inadequate supplies. This issue could be circumvented by developing structurally simplified analogues of Spirastrellolide A that could retain the biological activity. A convergent synthesis of the southern hemisphere of spirastrellolide A, which involved two key intermediates including a tetrahydropyran and a [6,6]-spiroketal was designed. Two gold-catalyzed cyclization methods developed in our group were employed in the synthesis, namely 1) Gold-catalyzed dehydrative cyclization of monoallylic diols for the synthesis of the tetrahydropyran, and 2) Regioselective gold-catalyzed spiroketalization for the efficient generation of the [6,6]-spiroketal. Progress towards the synthesis of Spirastrellolide A analogues will be presented.

Authors: Jagadeesh Nagendra Manda, Barry B. Butler Jr, Aaron Aponick

19a Sourabh Mishra, The University of Florida – "Facile Tuning of Atropisomeric P,N-Ligands for Enantioselective Catalysis''

Asymmetric catalysis is an important tool in the assembly of chiral compounds and the development of new chiral ligands is essential for efficient asymmetric induction. In addition, catalyst design and ligand development often unveil new reactivity and the possibility of developing new methodologies. Utilizing the high modularity of 5-membered imidazole rings, a family of P,N-Ligands namely StackPhos was developed. In this vein, highly enantioselective conjugate alkynylation reactions of Meldrum's acid derived acceptors was achieved. Additionally, ligand accelerated serendipitous new reactivity was observed, leading to enantioselective synthesis of chiral dihydropyranone. Ligand design and development will be presented, as well as application towards enantioselective catalysis.

Authors: Sourabh Mishra, Ji Liu, Aaron Aponick

20a Alexander Nauth, Johannes Gutenberg-University Mainz – "Isoquinolinium Functionalized Titanium(IV)dioxide Nanoparticles as a Heterogeneous Catalyst in Photoredox Chemistry"

The recent resurgence of photoredox chemistry has resulted in a considerable number of transformations involving homogeneous and heterogeneous photocatalysts. A variety of such catalysts are already available to make use of UV and visible light for organic chemistry. Due to favorable reaction kinetics, most of the catalyst development focuses on homogenous systems. Nevertheless, in terms of stability and recoverability, heterogeneous catalysts are often superior. In 2014, Jain and coworkers used semiconductors like titanium(IV)dioxide functionalized with ruthenium complexes which could be excited with visual light for photoredox reactions. These ruthenium-polyazine-complex functionalized particles encouraged us to find an alternative devoid of expensive transition metals. In some organic catalysts big aromatic pi-system, as well as a positive charge, like in DAP 2+, can be found. Based on these characteristics we decided to functionalize the TiO_2 nanoparticles with an isoquinolinium linker. We tested the resulting nanoparticles in various photoredox reactions with visible light and were able to synthesize useful compounds such as alpha-am inonitriles and sulfones with their help. Based on the amine scope, we were able to show the applicability to arylic, aliphatic and complex substrates.

Authors: Alexander M. Nauth, Eugen Schechtel, Karsten Korschelt, Wolfgang Tremel and Till Opatz

21a Marco Nebe, Johannes Gutenberg-University Mainz – "Functionalization of Heteroaromatic Compounds via Photoaddition/Horner- Olefination Sequence"

Photoredox catalysis has emerged as a powerful tool in preparative organic chemistry over the past decade, enabling transformations involving highly reactive species under mild conditions.[1] Utilizing this method, useful synthetic transformations, e.g. carbon–carbon bond formations can be performed.[2]

In 2010, the Stephenson group reported the addition of 2-bromomalonate to pyrroles, indoles and furans employing photoredox-catalysis using $Ru(bpy)_3^{2+}$ as a photocatalyst.[3]

Inspired by this report, we have developed a method utilizing 2-bromophosphonoacetates for the addition to heteroaromatic indole systems. The reaction proceeds by irradiation with a white LED employing the organic dye Eosin Y as an inexpensive and non-toxic photoredox catalyst. In this fashion, a phosphonacetate group is introduced into the molecule, which can be employed for a subsequent Horner olefination. Both the photoaddition as well as the olefination run smoothly providing the respective products in generally high yields.

This reaction sequence could be applied in the total synthesis of complex natural products as well as for the late stage functionalization of existing heterocycles, e.g. with respect to the modification of tryptophan residues in peptide structures.

Authors: Marco M. Nebe and Till Opatz

22a Michelle M. Nolan, The University of Florida – "Synthesis and characterization of precursors for the deposition of tungsten carbonitride thin films"

The use of thin film materials in the electronics industry has motivated considerable research in chemical vapor deposition (CVD), a fabrication technique in which films are grown directly at a substrate surface through the reaction of vapor phase precursor compounds. The design of single source CVD precursors relies on the simultaneous optimization of compound properties, including volatility and thermal stability, and compound decomposition. Tungsten (VI) complexes with N-bound ligands, including nitrido, imido, amido, and guanidinato, were synthesized to serve as single source precursors for the CVD of tungsten carbonitride (WNxCy) thin films. Effects of ligand sets on precursor volatility were assessed, revealing that improved volatility was associated with the use of bulky ligands and low symmetry compounds. Mechanistic investigation of precursor thermal decomposition, including in situ Raman spectroscopy during CVD, was employed to refine precursor design for low temperature deposition. Synthesis, characterization, and film deposition results will be discussed.

Authors: Michelle M. Nolan, Alexander J. Touchton, Seo Young Kim, Timothy J. Anderson, Lisa McElwee-White

23a Aude Nyadanu, Ecole Polytechnique/ENS Paris – "$TiCl_4$-mediated Pseudo Thio-Passerini Reactions: Straightforward Synthesis of 4-Thio-isocoumarines and 3- Amido-benzothiophenones"

Through the years, sulfur-containing heterocycles have been identified as leading constituents of numerous pharmaceuticals. But simple synthetic methods are quite restricted. In this context, as part of our continuing interest in isocyanide based multicomponent reactions[1], we decided to study the straightforward access to thiophtalide derivatives.

By the formal extension of the Passerini reaction[2] to thiocarbonyl derivatives, the straightforward preparation of 4-thio-isocoumarines and 3-amido-benzothiophenones was developed. This method involves the intermediate formation of a sulfanyl-phthalide[3] followed by a titanium tetrachloride mediated isocyanide insertion reaction. In most cases, it results in the formation of 4-thio-isocoumarines. In the particular case of *tert*-butyl thiol, thanks to the deprotection of the *tert*-butyl group, a thiophthalide resulting from a 1,5-Mumm rearrangement is isolated. Owing to the multifaceted activity of $TiCl_4$, all steps may conveniently be performed in one pot, starting directly from 2-formylbenzoic acids, thiols, and isocyanides. This method constitutes the first example of a multicomponent reaction involving thiocarbonyl derivatives.

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2. Passerini, M. Gazz. *Chim. Ital.* **1921**, *51*, 126–129.
3. Mal, D.; Ray, S. *Euro. J. Org. Chem.*, **2008**, 3014-3020.

Authors: Aude Nyadanu, Sudipta Ponra, Laurent El Kaim, Laurence Grimaud, and Maxime Vitale

24a Siva S. Panda, Augusta University – "Curcumin Conjugates as Potential Nonsteroidal Anti-inflammatory Agents"

Phytochemical products constitute one of the basic resources for many human needs including food and medicines. Many clinically used drugs are either derived from medicinal plants or inspired by a chemical

scaffold of biologically active agents of plant origin. Curcumin, a component of turmeric (Curcuma longa), has been used as a remedy to treat a wide variety of ailments for centuries. A considerable amount of research is currently being conducted to determine its various biological abilities. Inflammation is associated with many pathological diseases such as rheumatoid arthritis, lupus, periodontitis, diabetes, chronic hepatitis, myocardial infarction (cardiovascular diseases), brain ischemic injuries such as stroke, cancer, pulmonary diseases or inflammatory bowel disease. Although many non-steroidal anti-inflammatory drugs (NSAIDs) (e.g. ibuprofen, naproxen, indomethacin, etc.) are in practice, gastrointestinal ulceration, bleeding, nephrotoxicity side effects including heart and kidney failure limit their long-term utilization. This research is concerned with synthesizing potential curcumin-based drug candidates that combat inflammation and overcome the limitations. The synthesized conjugates proved as potent anti-inflammatory agents as compared to current standard commercially available drugs. The details of chemistry and pharmacological studies will be discussed in the conference.

Authors: Siva S. Panda

25a: Mukesh Pappoppula, The University of Florida – "Enantioselective Nucleophilic Dearomatization of Nitrogen Heterocycles''

The tetrahydroquinoline (THQ) motif is an important structural construct found in a myriad of natural products and biologically active molecules. Among many substitution patterns found in THQ alkaloids, substitution at the α-position to nitrogen is particularly interesting. A highly enantioselective alkynylation of quinolinium salts is reported with the chiral imidazole-based biaryl P,N-ligand StackPhos and copper bromide as the catalytic system in high yields with excellent ee values of up to 98%. Encouraged by the success of StackPhos as a chiral ligand, we anticipated that the enantioselective addition of nucleophiles to other nitrogen heterocycles might be conceivable. The development of this methodology and its application will be described.

Authors: Mukesh Pappoppula, Kathryn. L. Olsen, Aaron Aponick

26a Taroshkumar S. Patel, Sardar Patel University – "Stereoselective synthesis of alanine linked quinazoline-4(3H)-one-sulphonamide hybrid molecules in imidazolium based ionic liquid as medium and catalyst"

Grimmel's method was optimized as well as modified leading to the cyclization and incorporation of L-Alanine linked sulphonamide in 4-quinazolin-(3H)-ones. Further, the generation of heterocyclic motif at position-3 of 4-quinazolinones was explored by synthesis of imines, which unfortunately led to an isomeric mixture of stereoisomers. The hurdle of diastereomers encountered on the path was eminently rectified by development of a new rapid and reproducible methodology involving the use of imidazolium-based ionic liquids as solvents as well as catalysts for cyclization as well as synthesis of imines in situ at position 3 leading to procurement of single E-isomers as the target hybrid heterocyclic molecules. The purity and presence of a single isomer was also confirmed by HPLC and spectroscopic techniques. Further, studies along the generation of fused heterocyclic motifs at position 3 are in continuation in our laboratory.

Authors: Taroshkumar S. Patel, Jaimin D. Bhatt, Ritu B. Dixit and Bharat C. Dixit

27a Victor W. Pike, National Institutes of Health – "New approaches to radiotrifluoromethylations"

Positron emission tomography (PET) is an increasingly important molecular imaging modality for disease diagnosis, biomedical research and drug development. The value of this technique derives from its use of biochemically specific radiotracers to report on specific proteins (e.g., neurotransmitter receptors, transporters, enzymes or plaques). These radiotracers are typically labeled with cyclotron-produced short-lived positron-emitters, such as carbon-11 (t1/2 = 20.4 min) of fluorine-18= (t1/2 = 110 min), utilizing for example [C-11]methane of [F-18]fluoride = as primary reagents. Labeling processes must be late-stage, rapid, efficient and conserve a high ratio of radioactivity to mass (molar activity). Here we describe our recent breathroughs in the rapid production of C-11 or F-18 labeled fluoroforms and in methods for their application to the rapid and efficient introduction of radiolabeled trifluoromethyl groups into various small and radiotracer like molecules. Molar activity is moderately conserved for F-18 and exceptionally well conserved for C-11.

Authors: Victor W. Pike, Bo-Yeun Yang, Mohammad B. Haskali, and Sanjay Telu

28a Shyam Samanta, Florida Atlantic University – "Synthesis of α,α-Disubstituted Amino Esters"

Bacterial resistance to marketed antibiotics has been a global health concern for many years. In fact, S. aureus accounts for 16% of the most common hospital-acquired infections, the highest number associated with a single pathogen, with MRSA being responsible for more than 50% of them. (–)-Fumimycin (1) displayed an important activity as a peptide deformylase (PDF) inhibitor (IC_{50} = 4.1 μM). In fact, 1 showed some inhibition of Staphylococcus aureus PDF, specifically two strains of methicillin-resistant S. aureus (MRSA) with a Minimum Inhibitory Concentration (MIC90 = 100 μM). Given its bioactivity profile against MRSA and its unique mode of action (PDF inhibitor), a methodology was developed to synthesize 1 and some analogues in a straightforward manner for an initial structure-activity-relationship study.
In order to synthesize these sterically congested α,α-disubstituted amino esters, a novel cascade transformation mediated by thionyl chloride and several other halogenating reagents was studied. Under optimized conditions, arene nucleophiles 4 have been crafted to obtain α,α-disubstituted amino esters 9 in one pot.. This method featured the formation of an enamide 7 via condensation between 2 and 3 in presence of a halogenating agent which traps the water from the condensation step in situ. Further tautomerization between enamide 7 /iminium 8 (promoted by Bronsted acids) was achieved to trigger the nucleophilic attack and the pivotal C-C bond formation toward the final α,α-disubstituted amino esters 9. Further variants of this work for an asymmetric synthesis of α,α-disubstituted amino esters will also be presented.

Authors: Shyam S. Samanta and Stéphane P. Roche

29a Brittany R. Smith, The University of Florida – "Towards the development of carbohydrate cancer vaccines"

Our laboratory focuses on the use of monophosphoryl lipid A (MPLA) as a self-adjuvanting carrier molecule in the development of carbohydrate conjugate vaccines. MPLA is a derivative of the immunostimulant, lipid A, expressed on the lipopolysaccharide (LPS) of bacteria such as E. coli. MPLA activates toll-like receptor 4 (TLR4) and lymphocyte antigen 96 (MD2) to trigger an immune response and is a self-adjuvanting carrier molecule. Carbohydrate conjugate vaccines containing MPLA attached to cancer-specific antigens can be used to educate the immune system to recognize and kill cancer cells, which are normally tolerated by the immune system.

Authors: Brittany R. Smith and Zhongwu Guo

30a James Siriwongsup, Rice University – "Practical Singly and Doubly Electrophilic Aminating Agents: A New, More Sustainable Platform for Carbon-Nitrogen Bond Formation"

Given the importance of amines in a large number of biologically active natural products, active pharmaceutical ingredients, agrochemicals, and functional materials, the development of efficient C–N bond-forming methods with wide substrate scope continues to be at the forefront of research in synthetic organic chemistry. We present a general and fundamentally new synthetic approach for the direct, transition-metal-free preparation of symmetrical and unsymmetrical diaryl-, arylalkyl-, and dialkylamines that relies on the facile single or double addition of readily available C-nucleophiles such as Grignard and organolithium reagents to the nitrogen atom of bench-stable electrophilic aminating agents. Practical single and double polarity reversal (i.e. umpolung) of the nitrogen atom is achieved using sterically and electronically tunable ketomalonate-derived imines and oximes. Overall, this novel approach represents an operationally simple, scalable, and environmentally friendly alternative to transition-metal-catalyzed C–N cross-coupling methods that are currently used to access structurally diverse secondary amines. At present, an extension to this work is now underway in which softer C-nucleophiles such as enolates are added to our newly developed aminating agents. These efforts have resulted in the development of robust methodologies for the enantioselective synthesis of multisubstituted α-amino γ-butyrolactones as well as the formation of brand new N-aryl donor-acceptor aziridines, the latter of which can be used as intermediates to access a variety of complex nitrogen-containing heterocycles.

Authors: Siriwongsup, Surached (James), Kattamuri, Padmanabha V., Kürti, László

31a Christian Stevens, University of Ghent – "Synthesis of polysubstituted pyrazoles via a tandem gold-catalyzed cyclization and 1,4-allyl migration."

Pyrazoles are an important class of heterocyclic compounds that are present in different pharmaceuticals and agrochemicals. Numerous methodologies to synthesize pyrazoles have been developed. Of these procedures, the most common approaches are: 1) reaction of alkynyl aldehydes or ketones with hydrazines, 2) reaction of 1,3-dicarbonyl compounds with hydrazines, and 3) 1,3-dipolar cycloaddition of diazoalkanes or nitrilimines with alkenes or alkynes. However, each of these approaches has its downsides and rarely results in regioselective polysubstituted pyrazoles.

In order to develop a methodology which results in regioselective polysubstituted pyrazoles, N-allyl-N-aryl/alkyl hydrazines were chosen. The advantage of a N,N-disubstituted hydrazine is that the imine formation always occurs regioselectively. For the synthesis of these polysubstituted pyrazoles, N-allyl-N-aryl/alkyl hydrazine oxalate and an alkynyl aldehyde or ketone were used. These pyrazoles were prepared by a one-pot procedure through a domino reaction which includes imine formation, a gold-catalyzed 5-endo-dig cyclization and a subsequent sigmatropic rearrangement. The present method can be used for both the synthesis of 1,4,5-tri– or 1,3,4,5-tetrasubstituted pyrazoless and allows for the efficient construction of functionalized pyrazoles with the possibility to vary at least three substituents. Furthermore, these pyrazole analogues proved to reduce oxidative stress in plants which indicates that they could be used as oxidative stress protecting agents.

Authors: Arno Verlee, Thomas Heugebaert, Tom van der Meer, Pavel Kerchev, Frank van Breusegem and Christian V. Stevens

32a Xianwei Sui, University of Central Florida – "A new method for the synthesis of L-allo-Enduracididine derivative"

Bacterial infection has been a threat to humanity for millennia. Discovery and development of new bioactive molecules are desired. In early 2015, teixobactin was discovered and exhibited anti-microbial properties with a new mode of action. Here, we present a new method for the synthesis of L-allo-Enduracididine derivative fragment, which is convenient for the synthesis of teixobactin and its analogue. Ester and amide were reduced in one step and the use of Bis-Boc-pyrazolocarboxamidine avoids the hydrogenation reaction that is not compatible with further synthesis.

Xianwei Sui, Yu Yuan

33a Jennifer C. Walters, Temple University – "(Poly)cationic Iodane (III) Mediated Oxidative Ring Expansion of Secondary Alcohols"

Medium-sized cyclic ethers are commonly encountered structural motifs in natural products, and as such, methods for their synthesis have been a long-standing pursuit. Although there are several approaches currently utilized to access these heterocycles, there were no methods to directly synthesize them from commonly encountered alcohols. Our lab has reported the transformation of benzylic, tertiary alcohol substrates into cyclic ethers, employing [bis(pyridinium)iodo]benzene ditriflate as the electrophilic activator. We now report the extension of this methodology to the oxidative rearrangement of a variety of alkyl, secondary alcohol substrates, which occurs with high chemoselectivity over direct oxidation of the alcohol. The utility of this methodology for late-stage natural product derivatization was also demonstrated, providing a new tool for diversity-oriented synthesis and complexity-to-diversity (CTD) efforts.

Authors: Jennifer C. Walters, Dr. Anthony F. Tierno, Aimee H. Dubin, and Prof. Dr. Sarah E. Wengryniuk

34a Kellie Weeks, Florida Gulf Coast University – "Progress towards the enantioselective synthesis of thujone"

Thujone is a bicyclo[3.1.0]hexanone monoterpene commonly found in sage, cedarleaf, and wormwood. Our efforts to develop an asymmetric variant of this synthesis are presented. The asymmetry of the strategy relies on an enantioselective crotylation of a propargyl aldehyde. The results of various asymmetric crotylation methods will be presented with the current optimal conditions using a chiral Brønsted acid to provide a quantitative yield in a 99:1 d.r. and a 68% ee. A key inquiry of this synthetic strategy is whether the stereochemical information from the crotylation can transfer to the new quaternary carbon stereocenter generated in the cycloisomerization to provide thujone. The optimization of the cycloisomerization to provide high stereochemical transfer will also be presented.

Authors: Kellie Weeks and Gregory Boyce

35a Hongfen Yang, The University of Florida – "Highly Potent Classes of Halogenated Phenazine Antibacterial and Biofilm-Eradicating Agents Accessed Through a Modular Wohl-Aue Synthesis"

Unlike individual, free-floating planktonic bacteria, biofilms are surface-attached communities of slow- or non-replicating bacteria encased within a protective extracellular polymeric matrix enabling persistent bacterial population to tolerate high concentrations of antibiotics. It is estimated that biofilm-related infections result in 17,000,000 infections and >500,000 deaths every year in the United States.[1] However, most currently-used antibiotics inhibit or kill rapidly-dividing planktonic cells through growth-dependent mechanisms and are ineffective in eradicating slow-growing and growth-arrested persistent biofilms.[2] Our group has reported series of novel Halogenated Phenazines (HPs) as effective biofilm eradication of MRSA, methicillin-resistant S. epidermidis (MRSE) and vancomycin-resistant Enterococcus faecium (VRE) biofilms. Here we discovered new methods accessing diverse HPs as potent antibacterial and biofilm-eradicating agents.

Authors: Hongfen Yang, Yasmeen Abouelhassan, Robert W. Huigens III

36a Zhe Zhou, Rice University – "Copper-mediated amination of highly-functionalized aryl- and hetero-arylmetals"

Introduction: Aryl- and heteroarylmetals are highly valuable carbon nucleophiles that are readily and inexpensively prepared from aryl halides or arenes and widely used on both laboratory and industrial scales. The focus of our research is to develop a method for the direct transfer of primary amino (–NH2) and secondary amino (–NHR) groups to arylmetals in an efficient and scalable fashion.

Method: A sterically-hindered and bench-stable N–H oxaziridine was prepared from a commercially available NH imine. Aryl- and heteroarylmetals were first transmetalated with Cu(I) salts before treated with slight excess of the oxaziridine. For secondary amination, bench-stable O-benzoyl hydroxylamines were used in place of the oxaziridine

Results: In the presence of Cu(I), the N-H oxaziridine acts as an exclusive nitrogen-transfer reagent when reacted with aryl- and heteroarylmetals at low temperature, generating highly-functionalized primary anilines from Grignard, organozinc and organolithium reagents. On the other hand, O-benzoyl hydroxylamines can effectively convert these arylmetals to their corresponding secondary anilines with the mediation of Cu(I). These reagents show remarkable chemoselectivity and functional group tolerance, and this method can be applied to the late stage functionalization of complex molecules.

Conclusion: we have developed a novel method for the direct electrophilic primary and secondary amination of aryl- and heteroarylmetals in the presence of Cu(I)-salts. This transformation offers a practical solution for a long-standing synthetic problem of aminating heteroarylmetals efficiently and it does not rely on the presence of ortho-directing groups and requires only equimolar amounts of the aminating reagent. It is anticipated that this general amination approach will find wide utility in the synthesis of structurally complex molecules such as active pharmaceutical ingredients and natural products.

Authors: Zhe Zhou, Zhiwei Ma, Nicole E. Behnke, Hongyin Gao and László Kürti

37a Zhengbo Zhu, The University of Florida – "Redox-Annulation of Cyclic Amines"

Redox-neutral methods for the C–H functionalization of amines are an attractive avenue for reaction development as they exclude the need for external oxidants or reductants. Intramolecular versions, also referred to as redox-annulations, provide a facile pathway to polycyclic structures. Specifically, aldehydes possessing a pendent (pro)nucleophile undergo condensation with cyclic amines in processes that combine reductive N-alkylation with concurrent oxidative α-C–H bond functionalization. These reactions involve the formation of azomethine ylides as key intermediates. Carboxylic acids play important roles as catalysts or promotors in most of these transformations.

Authors: Zhengbo Zhu and Daniel Seidel