

Chemistry Research Day 2007 - List of Posters

No.	PRESENTERS	AUTHORS	TITLE
1	am Ende, Christopher	Christopher W. am Ende, Todd J. Sullivan, Nina Liu, Hua Xu, Sylvia Luckner, James J. Truglio, Francis Johnson, Howard Lu1, Kathleen Brostrom, Ann Lenaerts, Richard A. Slayden, Caroline Kisker, and Peter J. Tonge	High Affinity InhA Inhibitors with Activity against Drug-Resistant Strains of <i>Mycobacterium tuberculosis</i> and <i>Francisella tularensis</i>
2	Amarante, Daniel	Daniel Amarante and Stephen Koch	Chemistry of Ruthenium Carbonyl Cyanide Compounds
3	Baessler, Keith A.	Keith A. Baessler, Younjoo Lee, and Nicole S. Sampson	Probing the Mechanisms Behind Inhibition of Fertilization and Activation of Development by Fertilin-a Derived Oligopeptide Polymers
4	Balius, Trent E.	Trent E. Balius and Robert C. Rizzo	Computational Binding Models for Ligands with EGFR: Characterizing the Basis of Resistance
5	Banerjee, Partha	Partha Sarathi Banerjee and Issac Carrico	Viral Surface Remodeling Using Unnatural Substrates to Produce Novel Gene Therapy Vectors
6	Bergonzo, Christina	Christina Bergonzo, Kun Song, Arthur Campbell, and Carlos Simmerling	Finding the Right Path: A Computational Approach to DNA Base Eversion
7	Bi, Yuan	Yuan Bi, Jae-Hyun Cho, Eun-Young Kim, Bing Shan, Hermann Schindelin, and Daniel P. Raleigh	Rational Design, Structural and Thermodynamic Characterization of a Hyperstable Variant of the Villin Headpiece Helical Subdomain
8	Calder, Matthew	Matthew Calder, Peng Wang, and Kathlyn A. Parker	Deconstruction/Reconstruction of Oleandomycin Towards the Total Synthesis of Discodermolide pt. II
9	Calderone, Paul	Paul J. Calderone, Debasis Banerjee, Paul M. Forster, and John B. Parise	Ionothermal Synthesis: Novel Compounds at Ambient Conditions
10	Campbell, Arthur	Arthur Campbell, Kun Song, Angelo Guainazzi, Orlando Schärer, and Carlos Simmerling	The Structural Effects of Interstrand Crosslinks on DNA through Molecular Dynamic Simulations
11	Chen, Hailong	Hailong Chen, Lihua Zhang, and Clare P. Grey	Synthesis, characterization and high rate performance of LiCoO ₂ nanostructures as cathode for lithium ion batteries
12	Chen, Shuyi	Shuyi Chen, Jingyi Chen, Xianrui Zhao, Stanislaus S. Wong, and Iwao Ojima	Functionalized Single-walled Carbon Nanotubes as Rationally Designed Vehicles for Tumor-Targeted Drug Delivery
13	Cheng, Mark	Mark Cheng and Fernando O. Raineri	Studies on the Solvation of Meso-Substituted N-methylimidazolyl Zn-Porphyrins and their Dimers
14	Chionchio, Alicia	Alicia Chionchio, Xianrui Zhao, Shuyi Chen, Manisha Das, Seung-Yub Lee, and Iwao Ojima	Targeting the Cancer Cell: A Novel Double Ligand Guiding Conjugate Approach
15	Choi, Jun Yong	Jun Yong Choi, Elzbieta S. Selinger, Lisa M. Ballou, Richard Z. Lin, and Dale G. Drueckhammer	Rational Design, Synthesis, and Bioassay of Small Molecules for Inhibition of the mTOR Signaling Pathway

16	Christiansen, Matthew and Dai, Zhou	Matthew Christiansen, Zhou Dai, Stephanie Georgiou, Farook Taha, Taemee Pak, Ming Yang, and Elizabeth Boon	H-NOX: When NO means Yes - Determining the Molecular Basis of the H-NOX/NO Pathway in Bacteria
17	Connors, David	David Connors, Li Cui, Zachary E. Katsamanis, Lu Zhou, and Nancy S. Goroff	The Ongoing Synthesis of a Substituted [12]Cyclophenacene Using a 1,3,5-Substituted Benzene Scaffold
18	Cooper, Eric	Eric Cooper and Fernando O. Raineri	Solvation Energetics for Electron Transfer Reactions in Face to Face Porphyrin-Quinone Dyads
19	Das, Manisha	Manisha Das and Iwao Ojima	Design, Synthesis and Evaluation of Tumor-targeting Folate-Taxoid Conjugate
20	Denton, Richard	Richard Denton and Kathlyn A. Parker	Selective Hydrogenation of Propargylic Alcohols in the Presence of Vinyl Iodide
21	Ding, Fangyu	Fangyu Ding, Melinda Layten, and Carlos Simmerling	Study the Flexibility of the Flap Regions of HIV1-PR by Molecular Dynamics Simulation
22	Dogan, Fulya	Fulya Dogan, Hua Huo, and Clare P. Grey	Applications of Solid-State MAS NMR in Structural Characterization of Microporous and Mesoporous Molecular Sieve Basic Catalysts
23	Dufour, Antoine	Antoine Dufour, Stanley Zucker, and Jian Cao, and Nicole S. Sampson	Role of the Hemopexin Domain of Matrix Metalloproteinase-9 in Cell Migration
24	Fernando, Marian and Rajaram, Lakshmi	Marian Fernando, Lakshmi Rajaram, and Isaac Carrico	Metabolic Labeling of O-GlcNAcylated Proteins for Cancer Biomarker Discovery
25	Fujimoto, Yuki	Yuki K. Fujimoto, Ryan Terbush, and Vadim Patsalo, and David F. Green	Carbohydrate Recognition by Anti-Viral Cyanobacterial Proteins: Computational Approaches to Understanding and Design
26	Gao, Jin	Jin Gao and Nicole S. Sampson	Biofunction Exploration of choD (Rv3409c) from <i>M. tuberculosis</i>
27	Gegina, Yelizaveta	Yelizaveta Gegina, Christopher am Ende, Avinash Khanna, Peter J. Tonge	Synthesis of Potent Inhibitors of the Fatty Acid Biosynthesis Pathway in <i>Mycobacterium tuberculosis</i>
28	Ghang, Yoo-Jin	Yoo-Jin Ghang and Nicole S. Sampson	Investigating the Metabolic Pathway of Cholesterol by <i>Mycobacterium tuberculosis</i> Cytochrome P450s
29	Guainazzi, Angelo	Angelo Guainazzi, Todor Anguelov and Orlando Schärer	Exploring Structure and Biochemistry of Nitrogen Mustard Interstrand Crosslink Analogs
30	Gualbert, Jérôme	Jérôme Gualbert, Ludovic Gillet, and Orlando Schärer	New substrate for innovative investigations of the Nucleotide Excision Repair pathway
31	Gupta, Ruchi	Ruchi Gupta and Daniel P. Raleigh	Kinetics of Amyloid Formation by Human Islet Amyloid Polypeptide
32	Ho, Vinh The	The Vinh Ho, Milica Enoiu and Orlando Schärer	Transcription of Interstrand Crosslinked DNA Template
33	Holmes, Lesley	L. Holmes, Clare P. Grey, I. Heinmaa, E. Hellstrom, and D. Morgan	Analysis of Structural Characteristics and Dynamics of Lanthanum-Doped and Hydrated Samples of Ba ₂ In ₂ O ₅ Perovskite Materials via Ultra-High Field ¹⁷ O Solid State NMR
34	Hooker, Jacob M.	Jacob M. Hooker, Wynne Schiffer, Yuwen Xu, David Alexoff, Vinal Patel, Shiva Kothari, and Joanna Fowler	Pharmacokinetics and Pharmacodynamics of the Potent Hallucinogen, Salvinorin A

35	Huo, Hua	Hua Huo, Luming Peng, and Clare P. Grey	Multinuclear Solid state NMR Studies of Brønsted Acid Sites in Zeolite H-Mordenite
36	Kapilashrami, Kanishk	Kanishk Kapilashrami , Carl Machutta, Bela Ruzsicska, Francis Picart, and Peter J. Tonge	Targeting the FAS II Pathway in <i>m. tuberculosis</i> - Understanding InhA and KasA Inhibitor Binding
37	Key, Baris	Baris Key, Meng Jiang, Julien Breger, and Clare P. Grey	High Energy X-ray Scattering Studies as a Tool to Understand the Structural Changes that Occur upon Lithium Deintercalation of $\text{Li}[\text{Ni}_x\text{Li}_{(1/3-2x/3)}\text{Mn}_{(2/3-x/3)}]\text{O}_2$ ($0 \leq x \leq 1/2$)
38	Khanna, Avinash	Avinash Khanna, Chris am Ende, and Peter J. Tonge	Design of Bio-available InhA Inhibitors with Activity against Drug-Resistant Strains of <i>Mycobacterium tuberculosis</i>
39	Kil, Kun-Eek	Kun-Eek Kil, Anat Biegón, Yu-Shin Ding, Andre Fisher, Carolin Ehrlich, and Joanna S. Fowler	Synthesis and PET Imaging Study of [^{11}C]-Ietrozole
40	Kim, Keunsoo	Keunsoo Kim and Kathlyn A. Parker	Strategies for Asymmetric 8π , 6π Electrocyclization for Preparing Natural Products
41	Kim, Sung Won	Sung Won Kim, Yu-Shin Ding, David Alexoff, and Joanna S. Fowler	Synthesis and PET Studies of ^{11}C -Labeled GTS-21, a Partial $\alpha 7$ Nicotinic Cholinergic Agonist Drug
42	Kim, TaeSoo	TaeSoo Kim, Edward Melief, and Peter J. Tonge	Probing the Mechanism of Chromophore Formation; Refolding Circularly Permutated GFP
43	Kumar, Kunal	Kunal Kumar, Seung-Yub Lee ,Iaria Zanardi, Keita Morohashi, Bela Ruzsicska, Richard A. Slayden, Peter J. Tonge, and Iwao Ojima	Synthesis and Optimization of a Library of Novel Benzimidazole Leads for Antituberculosis Drug Discovery
44	Lee, Eunjung	Eunjung Lee and Nicole S. Sampson	Design and Synthesis of Multivalent Ligand in the Exploration of Receptor-Binding Inhibitor for Cholera Toxin
45	Lee, Younjoo	Younjoo Lee and Nicole S. Sampson	Nano-Engineered Multivalent Fertilin β and Cypitestin Mimics for Inhibition of Fertilization
46	Li, Huei Jiun	Huei Jiun Li and Peter J. Tonge	Characterization of the <i>trpE</i> Product from <i>M. tuberculosis</i> as a Chorismate-Utilizing Enzyme
47	Li, Xiaokai	Xiaokai Li, Huaning Zhang, and Peter J. Tonge	Synthesis of Stable Amide OSB-CoA Analogue and High-Throughput Screening for MenB Inhibitors
48	Li, Zhong	Zhong Li, Frank W. Fowler and Joseph W. Lauher	The Study of Aryl Diacetylenes supramolecular system for Topochemical Polymerization
49	Liu, Nina	Nina Liu, Christopher am Ende, Kathleen Brostrom, and Peter J. Tonge	Study of the Inhibition of FabI, the Enoyl-ACP Reductase from <i>Burkholderia Pseudomallei</i>
50	Lu, Hao	Hao Lu, Melissa Boyne, James Truglio, Chris amEnde, Sylvia Luckner, Kathleen Brostrom, Caroline Kisker, Richard, Slayden, and Peter J. Tonge	Inhibition of FabI, the Fatty Acid Biosynthesis Enoyl Reductase: Novel Chemotherapeutics Against <i>Francisella Tularensis</i>

51	Luo, Liang	Liang Luo, Aiwu Sun, Chris Wilhelm, Joseph W. Lauher, and Nancy S. Goroff	Designing Host-guest Co-crystals to Prepare Poly(diiododiacetylene), a Conjugated Polymer of Carbon and Iodine
52	Ma, Hongyang	Hongyang Ma, Lixia Rong, Kyunghwan Yoon, Benjamin S Hsiao, and Benjamin Chu	Structure and Property of High Flux Cellulose Membranes Fabricated by Ionic Liquid
53	Machutta, Carl	Carl Machutta, Kanishk Kapilashrami, Francis Picart, Bela Ruzsicska, Pilho Kim, Cynthia Dowd, Clifton Barry, and Peter Tonge	Slow Onset Inhibition of KasA by Thiolactomycin: Mechanistic Insights for Lead Optimization
54	Mao, Yimin	Yimin Mao, Feng Zuo, Jong Kahk Keum, and Benjamin S. Hsiao	Shear-induced crystallization: the influence of shear strain
55	Marai, Christopher N. J.	Christopher N. J. Marai, Jae-Hyun Cho, Daniel Raleigh and Jin Wang	Identification and Characterization of the Transition State Ensemble of the N-terminal Domain of L9
56	Marek, Peter	Peter Marek, Andisheh Abedini, BenBen Song, Mandakini Kanungo, Megan E. Johnson, Ruchi Gupta, Warda Zaman, Stanislaus S. Wong and Daniel P. Raleigh.	Aromatic Interactions Are Not Required For Amyloid Fibril Formation By Islet Amyloid Polypeptide But Do Influence the Rate of Fibril Formation
57	Melief, Edward	Edward H. Melief, TaeSoo Kim, and Peter J. Tonge	N/C Terminal Relocation, Truncation, and Native Chemical Ligation; Accessing the Chromophore of Green Fluorescent Protein
58	Meng, Fanling	Fanling Meng, Andisheh Abedini, Benben Song, and Daniel P. Raleigh	Amyloid Formation by pro-Islet Amyloid Polypeptide Processing Intermediates: Examination of the Role of Protein Heparan Sulfate Interactions and Implications for Islet Amyloid Formation in Type 2 Diabetes.
59	Meng, Wenli	Wenli Meng, Bing Shan and Daniel P. Raleigh	Are Unfolded Proteins Really Random Coils?
60	Mukherjee, Sudipto	Sudipto Mukherjee and Dr. Robert C. Rizzo	Improved Methods and Protocols in Docking
61	Muñoz-Espí, Rafael	Rafael Muñoz-Espí, Chirakkal V. Krishnan, Christian Burger, and Benjamin Chu	Polymer-Assisted Formation of Nanostructured Transition Metal Clusters and Crystals
62	Olajide, Adebanke	Adebanke Olajide, Ludovic Gillet, and Orlando Schärer	Analyzing Global Damage Recognition in Nucleotide Excision Repair by Photocrosslinking
63	Orelli, Barbara	Barbara Orelli, Oleg V. Tsodikov, Dmitri Ivanov, Ilana Shoshani, Lidiya Staresincic, Gerhard Wagner and Tom Ellenberger, Orlando D. Schärer	Biochemical and Structural Basis for the Interaction of ERCC1 and XPA in Human Nucleotide Excision Repair
64	Patsalo, Vadim	Vadim Patsalo, Dimitris Papamichail, Steven S. Skiena, and David F. Green	Design and Synthesis of Minimal and Persistent Protein Complexes.
65	Patterson, Melissa J.	Melissa J. Patterson, James M. Lightstone, and Michael G. White	Size Selected Deposition of Mo ₆ S ₈ ⁺ on Au (111)
66	Rafi, Salma	Salma B. Rafi, Peter J. Tonge, Carlos L. Simmerling	New ammunition against old enemy: Using computational structural biology tools to beat the world's most successful bug, <i>Mycobacterium tuberculosis</i>

67	Reid, Alicia	Alicia Reid, Colleen Shea, Youwen Xu, Phillip Christ, Carmine Leggett, and Joanna S. Fowler	Pharmacokinetics of [¹¹ C]-Labeled Aminoalkylindole Derivatives, for PET Imaging of Cannabinoid CB1 Receptors, in Baboons
68	Repala, Rohit	Rohit Repala, Jin Chen, and Iwao Ojima	Design, Synthesis and Mechanism Study of Taxane Based Tumor-targeting Anticancer Agents
69	Salerno, Rosemarie	Rosemarie Salerno, David M. Connors, Sarah J. Richards, Lu Zhou, and Nancy S. Goroff	The Ongoing Synthesis of a Tetrahedral Chromophore
70	Shan, Bing	Bing Shan, Ying Li, and Daniel P. Raleigh	The Cold Denatured State is Compact but Expands at Low Temperatures: Hydrodynamic Properties of the Cold Denatured State of the C-terminal Domain of L9'
71	Shi, Ce	Ce Shi, Stephen Chaterpaul, and Iwao Ojima	Development of Chiral Biphenol-Based Monodentate Phosphoramidite Ligands and Their Application to Asymmetric Allylic Substitution Reactions
72	Shrock, Christine and Shrock, Ellen	Christine Shrock, Ellen Shrock, and Carlos Simmerling	Investigating a Potential Allosteric Binding Site for the Development of New Drugs to Counter Multi-Drug-Resistant HIV-1 Protease
73	Song, Airong	Airong Song, Jaechul Lee, Younjoon Lee, Kathlyn Parker, and Nicole S. Sampson	Regio- and Stereocontrol of ROMP/ROM Reactions for 1-Substituted Cyclobutene Derivatives
74	Song, Benben	Benben Song, Burcu Anil, Daniel P. Raleigh	Stabilization of Proteins by Targeting Unfolded State Entropy
75	Sporleder, David	David Sporleder, Robert Beuhler, and Michael G. White	Photoinduced Desorption and Reaction of O ₂ from Rutile TiO ₂ (110) Surfaces
76	Stelling, Allison	Allison Stelling, Kate L. Ronayne, Jerome Nappa, and Peter J. Tonge, and Stephen R. Meech	Ultrafast Structural Dynamics in BLUF Domains: Transient Infrared Spectroscopy of AppA and its Mutants
77	Sun, Liang	Liang Sun, Carlos Simmerling, and Iwao Ojima	Structural and Computational Analysis Supports REDOR-Taxol as the Bioactive Conformation of Taxol
78	Szymanski, Paul	Paul Szymanski and Nicholas Camillone, III, Chemistry Department, Brookhaven National Laboratory	Ultrafast Surface Chemical Dynamics
79	Taskent, Humeyra	Humeyra Taskent, Jae-Hyun Cho, and Daniel P. Raleigh	Temperature Dependent Hammond Behavior in a Protein Folding Reaction: Analysis of Transition State Movement and Ground State Effects
80	Teng, Yu-Han Gary	Yu-Han Gary Teng, Joseph J. Kaloko, Wen Chen, and Iwao Ojima	Rh-catalyzed [2+2+2+1] and [2+2+2] cycloadditions: Construction of 5-7-5 and 5-6-5 Fused-Rings System from Triynes, Eneidyne, and Related Substrates
81	Thomas, Suzanne	Suzanne Thomas, Xinxin Yang, and Nicole S. Sampson	Preliminary Investigation of the Inhibition of <i>Mycobacterium tuberculosis</i> 3-beta Hydroxysteroid Dehydrogenase
82	Wang, Hui	Hui Wang and Nancy S. Goroff	Measuring the Equilibrium Constant of the Lewis acid-base interaction between 1-iodo-1-hexyne and Lewis bases by NMR
83	Wang, Zhong	Zhong Wang, Greg Hall, Yangsoo Kim, and Trevor Sears	Optical-Optical Double Resonance Spectroscopy of CH ₂
84	Wei, Jie	Jie Wei, Benjamin S. Hsiao and Benjamin Chu	UV curable top layer based on nanofibrous polyvinyl alcohol substrate

85	Wei, Rui	Rui Wei and Jianguyong Jia	Probe the properties of Quark Gluon Plasma via Elliptic Flow Measurement at Relativistic Heavy-Ion Collider
86	Wickstrom, Lauren	Lauren Wickstrom, Yuan Bi, Viktor Hornak, Daniel P. Raleigh, and Carlos Simmerling	To be Native or not to be Native, That is the Question: Studies of the Unfolded State Structure of the Villin Headpiece Helical Subdomain
87	Wilhelm, Christopher	Christopher Wilhelm, Stephen A. Boyd, Samrat Chawda, Frank W. Fowler, Nancy S. Goroff, Clare P. Grey, Gary Halada, Joseph P. Lauher, Liang Luo, C. Dave Martin, John. B. Parise, and Jeffery A. Webb	Pressure-Induced Polymerization of Diiododiacetylene to 1,4-Poly(Diiododiacetylene)
88	Wilson, Daniel	Daniel Wilson, David Sporleder, Michael G. White	Acetone and Butanone Photochemistry on Rutile TiO ₂ (110)
89	Xiao, Shifeng	Shifeng Xiao, Yuan Bi and Daniel P. Raleigh	What Defines a Protein Fold: Analysis of the Hydrophobic Core of a Miniature Protein
90	Yang, Xinxin	Xinxin Yang, Eugenie Dubnau, Issar Smith, Nicole S. Sampson	Rv1106c from <i>Mycobacterium tuberculosis</i> is a 3-beta hydroxysteroid dehydrogenase
91	Yeo, Jung-Eun	Jung-Eun Yeo, Ludovic C. J. Gillet, and Orlando D. Schärer	Sequence-Dependent Repair efficiency of dG-AAF and dG-AF substrates by Nucleotide Excision Repair
92	Yoon, Kyunghwan	Kyunghwan Yoon, Christopher Pang, Benjamin S. Hsiao, and Benjamin Chu	High Flux Nanofiltration Membranes based on Interfacially Polymerized Polyamide on Nanofibrous Scaffolds
93	Zhang, Fen	Fen Zhang, Yuanbing Mao, Tae-Jin Park, and Stanislaus S. Wong	Green Synthesis and Property Characterization of Single-Crystalline Perovskite Fluoride Nanorods
94	Zhang, Xujie	Xujie Zhang, Salma Rafi, Polina Novichenok, and Peter J. Tonge	Substrate Recognition by Bacterial Enoyl Reductases
95	Zhao, Xianrui	Xianrui Zhao, Shuyi Chen, Jin Chen, Jingyi Chen, and Iwao Ojima	Synthesis and Application of Fluorescence-Labeled Biotin-Taxoid Conjugate for the Investigation into Efficacious Tumor-Targeting Drug Delivery System
96	Zhou, Hongjun	Hongjun Zhou, Yuanbing Mao, and Stanislaus S. Wong	Shape Control and Probing Structure-Parameter Correlations in the Molten Salt Synthesis of BaZrO ₃ Perovskite Submicrometer-Sized Particles
97	Zhou, Jing	Jing Zhou and Michael G. White	Two-photon Photoemission on Au(111) Surface
98	Zhou, Rong	Rong Zhou and Peter J. Tonge	Comparative Structural and Biochemical Studies of Chorismate Binding Enzymes
99	Zhou, Zhou	Zhou Zhou and Kathlyn A. Parker	Progress Towards Total Synthesis of Bisabosqual A
100	Zuo, Feng	Feng Zuo, Yimin Mao, Jong Kahk Keum, Benjamin S Hsiao, Hongyu Chen, Debbie Chiu, and Shih-Yaw Lai	Shear-induced Crystallization of Olefin Block Copolymers via <i>in-situ</i> Synchrotron X-ray studies