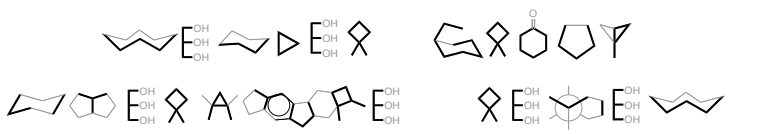

Lit Picks 2011-2012

This year's Lit Picks reflect the diversity of research and scientific interests within the group, especially with regard to our core enthusiasm for organic synthesis and improving human health.

Most Selected Papers
Multiple members of the group chose each the following papers; papers are listed in descending order of votes, then in alphabetical order by first author in the case of a tie.

---

4 Votes

Cohen, Myron S.; Chen, Ying Q.; McCauley, Marybeth; Gamble, Theresa; Hosseinipour, Mina C.; Kumarasamy, Nagalingeswaran; Hakim, James G.; Kumwenda, Johnstone; Grinsztejn, Beatriz; Pilotto, Jose; Godbole, Sheela V.; Mehendale, Sanjay; Chariyalertsak, Suwat; Santos, Breno R.; Mayer, Kenneth H.; Hoffman, Irving F.; Eshleman, Susan H.; Piwowar-Manning, Estelle; Wang, Lei; Makhema, Joseph; Mills, Lisa A.; de Bruyn, Guy; Sanne, Ian; Eron, Joseph; Gallant, Joel; Havlir, Diane; Swindells, Susan; Ribaudo, Heather; Elharrar, Vanessa; Burns, David; Taha, Taha E.; Nielsen-Saines, Karin; Celentano, David; Essex, Max; Fleming, Thomas R. "Prevention of HIV-1 Infection with Early Antiretroviral Therapy." *New England Journal of Medicine*, **2011**, 493-505.

"From a public health perspective, the results of this study are beginning to greatly affect treatment strategies for those living with HIV/AIDS, suggesting that earlier treatment can help control the pandemic by minimizing further disease transmission." – Brian L.

"The HPTN 052 trial has been called a "game changer" because it adds yet another tool in the fight against HIV/AIDS. When an HIV positive person is treated with HAART therapy early (before CD4 dropped below 250 cells per mL), the transmission rate to an uninfected partner dropped 96%." – Jen

"This could have significant impact in limiting the transmission of HIV!" – Katie

Leonard, Thomas H.; Rozycki, Bartsoz; Saldi, Layla F.; Hummer, Gerhard; Hurley, James H. "Crystal Structure and Allosteric Activation of Protein Kinase C βII." *Cell*, **2011**, 55-66.

"This is significant as it is the first structure (X-ray crystal AND NMR solution) of a full length PKC isoform, rather than just the C1b domain, and has direct relevance to our group as the target of many of our compounds." – Katie

"This paper gives us the crystal structure of PKC in a partially activated form. This gives us a significant amount of information about the mechanism of PKC activation, and gives a very helpful crystal structure upon which more binding and docking studies can be made." – Steven

---

3 Votes

Stang, E. M.; White, M. Christina "Molecular Complexity via C-H Activation: A Dehydrogenative Diels-Alder Reaction" *Journal of the American Chemical Society,* **2011**, 14892-14895.

"Utilizes a dehydrogenative Diels-Alder on a terminal olefin to rapidly construct complex molecular scaffolds." – Micah

"Diels-Alder reaction is one of the most powerful reactions to synthesize 6-membered rings but there is a problem that handling 1,3-dienes is not easy, especially in the case of synthesis of complex molecules. This method enables to escape using 1,3-dienes by C-H activation of terminal olefins, which are easy to handle and most of which are commercially available." – Yasayuki

Wolfe-Simon, F.; Blum, J.S.; Kulp, T.R.; Gordon, G.W.; Hoeft, S.E.; Pett-Ridge, J.; Stolz, J.F.; Webb, S.M.; Weber, P.K.; Davies, P.C.; Anbar, A.D.; Oremland, R.S. "A Bacterium That Can Grow by Using Arsenic Instead of Phosphorus." *Science,* **2011**, *332*, 1163-1166.

"This paper suggests that bacteria can continue to grow by incorporating arsenic into their DNA! It's looking like it's already been disproven, but what a crazy suggestion!" – Erika

---

2 Votes

Brantley, Johnathan N.; Wiggins, Kelly M.; Bielawski, Christopher W. "Unclicking the Click: Mechanically Facilitated 1,3-Dipolar Cycloreversions." *Science*, **2011**, 1606-1609.

"Mechanically-facilitated "retro-Click" reaction could lead to the development of triazoles and other cycloadducts as protecting groups in organic synthesis." – Micah

Cramer, P. E.; Cirrito, J. R.; Wesson, D. W.; Lee, C. Y. D.; Karlo, J. C.; Zinn, A. E.; Casali, B. T.; Restivo, J. L.; Goebel, W. D.; James, M. J.; Brunden, K. R.; Wilson, D. A.; Landreth, G. E. "ApoE-Directed Therapeutics Rapidly Clear β-Amyloid and Reverse Deficits in AD Mouse Models." *Science* **2012**, 1-4.

"Study out of Case Western that shows the efficacy of a clinically used anti-cancer agent (lymphoma) that results in enhanced clearance of soluble Aβ within hours and thus has great efficacy for treatment of Alzheimer's disease." – Alison

Fuechsle, M.; Miwa, J. A.; Mahapatra, S.; Ryu, H.; Lee, S.; Warschkow, O.; Hollenberg, L. C. L.; Klimeck, G.; Simmons, M. Y. "A single-atom transistor." *Nature Nanotechnology*, **2012**, ASAP.

"Moore's Law predicts microchips containing single atom transistors will arrive in 2020. This paper, presenting the first example of a reproducible method to produce a single atom transistor hints that this threshold may be reached sooner than predicted." – Liz

Jones, S. B.; Simmons, B.; Mastracchio, A.; MacMillan, D.W.C. "Collective Synthesis of Natural Products by Means of Organocascade Catalysis." *Nature*, **2011**, *475,* 183-188.

"This paper aimed to expedite the process of synthesizing large collections of biologically relevant molecules with similar scaffolds. This could be very useful in creating and testing many analogs of natural products." – Spencer

Kedei, N.; Lubart, E.; Lewin, N.; Telek, A.; Lim, L.; Mannan, P.; Garfield, S.; Kraft, M.; Keck, G.; Kolusheva, S.; Jelinek, R.; Blumberg, P. "Some Phorbol Esters Might Partially Resemble Bryostatin 1 in the Actions on LNCaP Prostate Cancer Cells and U937 Leukemia Cells." *ChemBioChem*. **2011**, 1242-1251.

"This paper involves the synthesis of a wide range of phorbol esters in a similar vein to the prostratin analogues that we synthesize in this lab. Their results in both cancer cells and leukemia cells give us more information about how a possible analogue strategy might work." – Steven

Lee, E.; Kamlet, A.S.; Powers, D.C.; Neumann, C.N.; Boursalian, G.B.; Furuya, T.; Choi, D.C.; Hooker, J. M.; Ritter, T. A Fluoride-Derived Electrophilic Late-Stage Fluorination Reagent for PET Imaging. *Science,* **2011***, 344,* 639-642.

"They fluorinate some pretty complex molecules late-stage for PET imaging. This method can allow molecules that would otherwise not be good PET candidates to be used for PET." – Erika

Lévesque, F.; Seeberger, P. H. "Continuous-Flow Synthesis of the Anti-Malaria Drug Artemisinin." *Angew. Chem. Int. Ed.* **2012**, *51*, 1706-1709.

"This report provides a high-yielding, scalable and low-cost continuous-flow process for the preparation of artemisinin from artemisinic acid, which can be prepared by fermentation in engineered yeast. Artemisinin is currently the most effective treatment for multidrug resistant malaria; however, current reliance on extraction from plant sources severely limits the supply of the drug, elevating costs for patients around the world." – Brian L.

Lu, Yu; Woo, Sang Kook; Krische, Michael J. "Total Synthesis of Bryostatin 7 via C-C Bond-Forming Hydrogenation." *J. Am. Chem. Soc.* **2011**, 13876-13879.

"This dramatic example of step economy furnishes a biologically active Bryostatin in half as many steps as the pervious synthesis of this molecule. I see this as a demonstration of how far organic synthesis has advanced over the last two decades, and a call to action for synthetic chemists to carefully select/design the molecules we synthesize for transformative applications." – Liz

Lustig, Robert H.; Schmidt, Laura A.; Brindis, Claire D. "Public Health: The Toxic Truth About Sugar." *Nature*, **2012**, 27-29.

"Chronic non-communicable diseases contribute to 35 million annual deaths. Sugar consumption is linked to a rise in these diseases, and the dissemination of these findings has the potential to address disease in a preventative manner." – Jessica

Martin, D. B. C.; Vanderwal, C. D. "A synthesis of strychnine by a longest linear sequence of six steps" *Chem. Sci.*, **2011**, 2, 649-651.

"Successive Brook rearrangement and intramolecular conjugate addition was highly impact process. I was really surprised about this short step synthesis." – Fuyuhiko

Mendoza, A.; Ishihara, Y.; Baran, P. S. "Scalable enantioselective total synthesis of taxanes" *Nat. Chem.* **2012**, 21-25.

"This is a practical method for construction of taxane skeleton." – Yasayuki

Michaudel, Q.; Thevenet, D.; Baran, P.S. "Intermolecular Ritter-Type C-H Amination of Unactivated sp3 Carbons". *J. Am. Chem. Soc.* **2011**, *134*, 2547-2550.

"Direct functionalization (amination) of saturated hydrocarbons (i.e. completely unactivated), allowing for a very large increase in value from many starting materials that are feedstocks." – Brian T.

Nagib, D. A.; MacMillan, W. C. "Trifluoromethylation of arenes and heteroarenes by means of photoredox catalysis" *Nature,* **2011**, 480, 224-228.

"Trifluoromethyl group is common in medicinal chemistry, but there are a few methods to introduce trifluoromethyl group. This method enables to introduce trifluormethyl group easily and doesn't need function group on the substrates." – Yasayuki

Shan, Y.; Kim, E. T.; Eastwood, M. P.; Dror, R. O.; Seeliger, M. A.; Shaw, D. E. "How Does a Drug Molecule Find Its Target?" *Journal of the American Chemical Society*, **2011**, 9181-9183.

"*By far, one of the most amazing articles read, Shan et al. developed a docking system for molecules without any initial parameterization of biasing. It is the closest method so far to mimic what naturally occurs in host-guest complexation*." – Brandon

---

1 Vote (Entries are formatted as submitted in alphabetical order by first author).

Ahuja, R.; Punji, B.; Findlater, M.; Supplee, C.; Schinski, W.; Brookhart, M.; Goldman, A. S. "Catalytic dehydroaromatization of *n*-alkanes by pincer-ligated iridium complexes" *Nat. Chem.* **2011**, *3*, 167–171.

Alabugin, I.; Gilmore, K.; Manoharan, M. "Rules for Anionic and Radical Ring Closure of Alkynes." *JACS*. **2011**, *133* (*32*), 12608-12623.

Bagnara, D.; Kaufman, M. S.; Calissano, C.; Marsilio, S.; Patten, P. E.; Simone, R.; Chum,P.; Yan, X. J.; Allen, S. L.; Kolitz, J. E.; Baskar, S.; Rader, C.; Mellstedt, H.; Rabbani, H.; Lee.; Gregersen, P. K.; Rai, K. R.; Chiorazzi, N. "A novel adoptive transfer model of chronic lymphocytic leukemia suggests a key role for T lymphocytes in the disease." *Blood* **2011**, 5463-5472.

Baran, Phil S.; Gaich, Tanja. Aiming for the Ideal Synthesis. *J. Org. Chem*. **2010**, 75, 4657–4673.

Budin, I.; Devaraj, N. K. Membrane Assembly Driven by a Biomimetic Coupling Reaction. *J. Am. Chem. Soc*. 2011, *134*, 751-753.

Burgett, A.W. G.; Poulsen, T.B.; Wangkanont, K.; Anderson, D.R.; Kikuchi, C.; Shimada, K.; Okubo, S.; Fortner, K.C.; Mimaki, Y.; Kuroda, M.; Murphy, J.P.; Schwalb, D.J.; Petrella, E.C.; Cornella-Taracdo, I.; Schirle, M.; Tallarico, J.A.; Shair, M. D. Natural Products Reveal Cancer Cell Dependence on Oxysterol-Binding Proteins. *Nat. Chem. Biol*. **2011**, *7,* 639-647.

Cronican, J.J.; Beier, K.T.; Davis, T.N.; Tseng, J.C.; Li, W.; Thompson, D.B.; Shih, A.F.; May, E.M.; Cepko, C.L.; Kung, A.L.; Zhou, Q.; Liu, D.R. Chemistry and Biology **2011**, 18, 833-838.

Devaraj, N. K.; Weissleder, R. Biomedical Applications of Tetrazine Cycloadditions. *Acc. Chem. Res*. **2011**, *44*, 816–827.

Dranoff, Glenn. "Experimental mouse tumour models: what can be learnt about human cancer immunology?" *Nat. Rev. Immunol*. **2012**, 61-66.

Ebalunode, Jerry O.; Zheng, Weifan; Tropsha, Alexander. "Application of QSAR and Shape Pharmacophore Modeling Approaches for Targeted Chemical Library Design." *Methods in Molecular Biology*, 111-133.

Esvelt, K. M.; Carlson, J. C.; Liu, D. R., "A system for the continuous directed evolution of biomolecules" *Nature,* **2011**, *472*, 499-503.

Gao, X.; Han, H.; Krische, M. J. "Direct Generation of Acyclic Polypropionate Stereopolyads *via* Double Diastereo- and Enantioselective Iridium-Catalyzed Crotylation of 1,3-Diols: Beyond Stepwise Carbonyl Addition in Polyketide Construction" *J. Am. Chem. Soc*. **2011**, *133*, 12795–12800.

He, Y.; Liu, D.R. A Sequential Strand-Displacement Strategy Enables Efficient Six-Step DNA-Templated Synthesis. *J. Am. Chem. Soc*. **2011**, *133*, 9972.

Hirai, Go; Ohkubo, Megumi; Tamura, Y; Sodeoka, Mikiko. "Design and synthesis of protein kinase Ca activators based on 'out of pocket' interactions." *Bioorganic & Medicinal Chemistry Letters*, 3587-3590.

Holland, D. J.; Bostock, M. J.; Gladden, L. F.; Nietlispach, D. Fast Multidimensional NMR Spectroscopy Using Compressed Sensing. *Angewandte Chemie International Edition* 2011, *50*, 6548-6551.

Haun, J. B.; Castro, C. M.; Wang, R.; Peterson, V. M.; Marinelli, B. S.; Lee, H.; Weissleder, R., "Micro-NMR for Rapid Molecular Analysis of Human Tumor Samples" *Sci. Transl. Med.*, **2011**, *3*, 71ra16.

Hoshimoto Yoichi, Ohashi Masato, and Ogoshi Sensuke, Nickel-Catalyzed Selective Conversion of Two Different Aldehydes to Cross-Coupled Esters, *J. Am. Chem. Soc.* **2011**, *133*, 4668-4671.

Huters, A. D.; Quasdorf, K. W.; Styduhar, E. D.; Garg, N. K., "Total Synthesis of (-)-N-Methylwelwitindolinone C Isothiocyanate" *J. Am. Chem. Soc.,* **2011**, *133*, 15797-15799.

Jain, Ajay N., Cleves, Ann E. "Does your model weigh the same as a Duck?" *J. Comput. Aided Mol. Des.*, 57-67.

Jordan, J. B.; Poppe, L.; Xia, X.; Cheng, A. C.; Sun, Y.; Michelsen, K.; Eastwood, H.; Schnier, P. D.; Nixey, T.; Zhong, W., "Fragment Based Drug Discovery: Practical Implementation Based on ^{19}F NMR Spectroscopy" *J. Med. Chem.* **2012**, *55*, 678-687.

Lancaster, Kyle M.; Roemelt, M.; Ettenhuber, P.; Hu, Y.; Ribbe, Markus W.; Neese, F.; Bergmann, Uwe; DeBeer, Serena. "X-Ray Emission Spectroscopy Evidences a Central Carbon in the Nitrogenase Iron-Molybdenum Cofactor" *Science*. **2011**, *334*, 974-977.

Li, Zhenwu; Nakashige, Mika; Chain, William J. A Brief Synthesis of (-)-Englerin A. *J. Am. Chem. Soc.* **2011**, 133, 6553–6556.

Meek, S. J.; O'Brien, R. V.; Llaveria, J.; Schrock, R. R.; Hoveyda, A. H. "Catalytic *Z*-selective olefin cross-metathesis for natural product synthesis" *Nature* **2011**, 471, 461-466.

Meng, W.; Breiner, B.; Rissanen, K.; Thoburn, J.D.; Clegg, J.K.; Nitschke, J.R. "A Self-Assembled M8L6 Cubic Cage that Selectively Encapsulates Large Aromatic Guests" *Angew. Chem. Int. Ed. Eng.* **2011**, *50*, 3479-3483.

Miki, K.; Kimura, A.; Oride, K.; Kuramochi, Y.; Matsuoka, H.; Harada, H.; Hiraoka, M.; Ohe, K. High-Contrast Fluorescence Imaging of Tumors In Vivo Using Nanoparticles of Amphiphilic Brush-Like Copolymers Produced by ROMP**.** *Angew. Chem. Int.* **2011**, *50*, 6567-6570.

Montgomery, J. High-Throughput Discovery of New Chemical Reactions. *Science* **2011**, *333*, 1387–1388.

Nadin, A.; Hattotuwagama, C.; Churcher, I. Lead-Oriented Synthesis: A New Opportunity for Synthetic Chemistry. *Angewandte Chemie International Edition* **2012**, *51*, 1114–1122.

Negishi, E. Magical Power of Transition Metals: Past, Present, and Future (Nobel Lecture).

Angewandte Chemie International Edition 2011, *50*, 6738-6764.

Nicolaou, K. C.; Vourloumis, D.; Winssinger, N.; and Phil S. Baran, Phil S. The art and science of total synthesis. *Angew. Chem. Int. Ed.* **2000**, 39, 44 – 122.

O'Brien, M.; Denton, R.; Ley, S. Lesser-Known Enabling Technologies for Organic Synthesis. *Synthesis* **2011**, *2011*, 1157–1192.

Paige E. Cramer, John R. Cirrito, Daniel W. *Wesson*, C. Y. Daniel Lee, J. Colleen Karlo, Adriana E. Zinn, Brad T. Casali, Jessica L. Restivo, Whitney D. Goebel, Michael J. James, Kurt R. Brunden, Donald A. Wilson, and Gary E. Landreth. "ApoE-Directed Therapeutics Rapidly Cleared β-Amyloid and Reverse Deficits in AD Mouse Models." *Science*. Published online 9 February 2012

Payandeh, J.; Scheuer, T.; Zheng, N.; Catterall, W. A. "The crystal structure of a voltage-gated sodium channel." *Nature*, **2011**, *475*, 353-358.

Peacock, Hayden; Kannan, Arunkumar; Beal, Peter; Burrows, Cynthia. Chemical Modification of siRNA Bases To Probe and Enhance RNA Interference. Bioconjugate Chemistry, 2011, 7295-7300.

Prendergas, George C. Why tumours eat tryptophan. *Nature* **2011**, 478, 192 – 193

Pronin, S. V.; Tabor, M. G.; Jansen, D. J.; Shenvi, R. A., "A Stereoselective Hydroamination Transform to Access Polysubstituted Indolizidines" *J. Am. Chem. Soc.* **2012**, *134*, 2012-2015.

Qi, Y.; Ma, S. "The Medicinal Potential of Promising Marine Macrolides with Anticancer Activity." *ChemMedChem*. **2011**, *6*, 399-409.

Raj, L.; Ide, T.; Gurkar, A.U.; Foley, M.; Schenone, M.; Li, X.; Tolliday, N.J.; Golub, T.R.; Carr, S.A.; Shamji, A..; Stern, A.M.; Mandinova, A.; Schreiber, S.L.; Lee, S.W.

Renault, M.; Tommassen-van Boxtel, R.; Bos, M. P.; Post, J. A.; Tommassen, J.; Baldus, M. Cellular solid-state nuclear magnetic resonance spectroscopy. *Proceedings of the National Academy of Sciences* 2012.

Rettig, G.R. & Behlke, M.A. "Progress Toward In Vivo Use of siRNAs." *Molecular Therapy*. **2011**, ASAP.

Robbins, D. W.; Hartwig J. F. A Simple, Multidimensional Approach to High-Throughput Discovery of Catalytic Reactions. *Science*. **2011**, *333*, 1423-1427.

Roche, S.; Porco, J. "Dearomatization Strategies in the Synthesis of Complex Natural Products." *Angew.* **2011**, *50*, 4068-4093.

Schreiber, S.L. "Organic Synthesis Toward Small Molecule Probes and Drugs." *Proc Natl Acad Sci*.**2011**, *108(17)*, 6699-6702.

Scott, L. T.; Jackson, E. A.; Zhang, Q.; Steinberg, B. D.; Bancu, M.; Li, B. A Short, Rigid, Structurally Pure Carbon Nanotube by Stepwise Chemical Synthesis. *J. Am. Chem. Soc.* **2011**, *134*, 107–110.

Sergeev, A.G.; Hartwig, J.F. "Selective, Nickel-Catalyzed Hydrogenolysis of Aryl Ethers" *Science* **2011**, 439-443.

Shimokawa Jun, Harada Takaaki, Yokoshima Satoshi, and Fukuyama Tohru, Total Synthesis of Gelsemoxonine, *J. Am. Chem. Soc.* **2011**, *133*, 17634-17637.

Tang, Pingping; Wang, Weike; Ritter, Tobias. "Deoxyfluorination of Phenols**"** *J. Am. Chem. Soc*.**, 2011,** *133***,** pp 11482–11484

Tondreau, A.M.; Atienza, C.C.; Weller, K.J.; Nye, S.A.; Lewis, K.M.; Delis, J.G.; Chirik, P.J. Iron Catalysts for Selective Anti-Markovnikov Alkene Hydrosilylation Using Tertiary Silanes. *Science* **2012**, *335*, 567.

Tyson, P.; Hassanzadeh, A.; Mordi, N.; Allison, D.; Marquez, V.; Barber, J. "Erythromycin B: conformational analysis and antibacterial activity." *Med Chem Comm*. **2011**, *2*, 331-336.

Wang Dong-Hui and Yu Jin-Quan, Highly Convergent Total Synthesis of (±)-Lithospermic Acid via a Late-Stage Intermolecular C-H Olefination, *J. Am. Chem. Soc.* **2011**, *133*, 5767-5769.

Wolschendorf, F.; Bosque, A.; Shihido, T.; Duverger, A.; Jones, J.; Planelles, V.; Kutsch, O. "Kinase control prevents HIV-1 reactivation in spite of high levels of induced NF-ϰB activity." *J. Virol*. **2012**, ASAP.

Wright, Chapman M.; Wright, R. Clay; Eshleman, James R.; Ostermeier, Marc. A protein therapeutic modality founded on molecular regulation. *PNAS* **2011**, 108, 39, 16206 - 16211

Yu Miao, Wang Chenbo, Kyle Andrew, Jakubec Pavol, Dixon Darren, Schrock Richard and Hoveyda Amir, Synthesis of macrocyclic natural products by catalyst-controlled stereoselective ring-closing metathesis, *Nature*, **2011**, *479*, 88-93.

Zhan, C.; Li, B.; Hu, L.; Wei, X.; Feng, L.; Fu, W.; Lu, W. "Micelle-Based Brain-Targeted Drug Delivery Enabled by a Nicotine Acetylcholine Receptor Ligand." *Angew. Chem. Int. Ed.* **2011**, *50*, 5482-5485.

Zhuang, T. Jap, BK, & Sanders, CR. "Solution NMR Approaches for Establishing Specificity of Weak Heterodimerization of Membrane Proteins." *J. Am. Chem. Soc.*, 2011, 133 (50), pp 20571–20580.