

# The van Breemen Group and Chicago Mass Spectrometry Laboratory 2012 Newsletter

## Highlights of 2011

February, 2012  
Volume 1, Issue 1

This is the inaugural newsletter of the van Breemen research group. Highlights this year included the acquisition of an Orbitrap Velos mass spectrometer and a Shimadzu LCMS-8030

triple quadrupole. Three graduate students and one postdoctoral fellow completed their studies. Research funding was renewed from Hershey, PepsiCo and the NIH (for our Botanical Center). Dr.

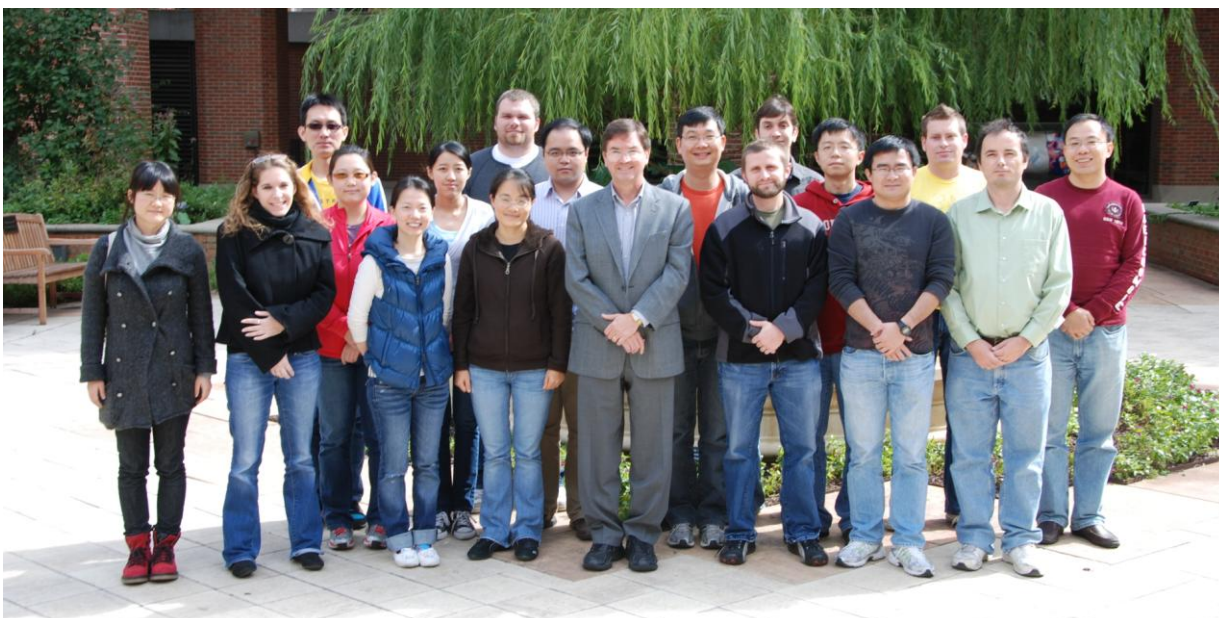
Farnsworth retired and I became the Botanical Center Director. Details of these achievements, lab publications and awards are provided below. Thanks for reading, Richard B. van Breemen

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**2011 van Breemen Research Group in the Dorothy Atkins Botanical Garden.** Front row: Guannan Li, Sigrid Baumgarten, Soyoun Ahn, Shunyan Mo, Richard van Breemen, Caleb Nienow, Yongchao Li, Dejan Nikolic. Middle row: Yang Yuan, Lian Chen, Rui Yu, Linlin Dong, Ke Huang, Kevin Krock, Zhiyuan Sun. Back row: Xi Qiu, Jerry White, and Andrew Newsome (Not pictured: Chenqi Hu, Rich Morrissy, Yang Song and Brian Wright)

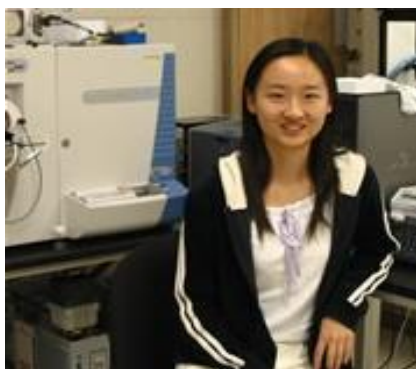
## New Instrumentation

Since relocating our laboratory from North Carolina to Chicago in 1994, we have been fortunate to acquire a new mass spectrometer almost every year. Using an instrument grant from the NIH, we purchased a Thermo Orbitrap Velos mass

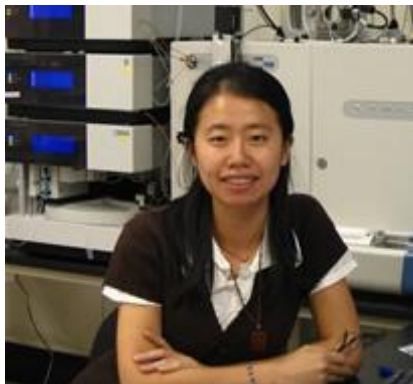
spectrometer. This new high resolution instrument has enhanced our proteomics and metabolomics efforts. We traded in the LCQ ion trap acquired back in 1996 as part of the deal. With support from Shimadzu, we installed an LCMS-8030 triple

quadrupole mass spectrometer equipped with a Nexera UHPLC system. Using this ultrafast system, we were able to show UHPLC-MS-MS data at the ASMS Conference just a few months later. Our lab is now equipped with almost every type of biomedical mass spectrometer.

## Lab Graduates of 2011



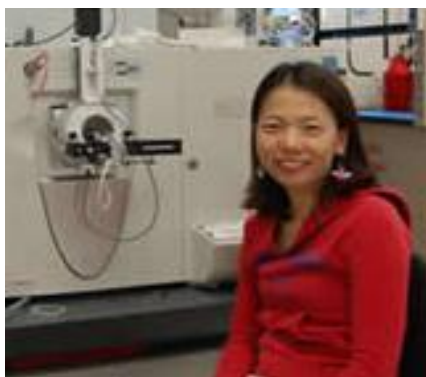
Chenqi Hu, a student in the Medicinal Chemistry Graduate Program, successfully defended her dissertation during 2011 which was entitled, "Analysis of Nrf2-Keap1 chemoprevention signaling using mass spectrometry." She moved to the Boston area and was offered a postdoctoral position in a proteomics laboratory at Harvard University and a job at Biogen-Idec., Chenqi chose to join Biogen-Idec and is working at their facility in Cambridge, MA.



Pharmacognosy graduate student Yang Song defended her dissertation and graduated in 2011. The title of Yang's dissertation was, "ADMEt evaluation of anti-tuberculosis compounds and new methodologies development." This study was a collaborative effort with the TB Institute. Prof. Scott Franzblau, who directs the TB Institute, served as Yang's co-advisor along with Prof. van Breemen.



Sigrid Baumgarten received her Ph.D. in 2009 working with Prof. Jean-Claude Tabet at the University of Paris/Pierre and Marie Curie in Paris, France. Then, she joined our laboratory in Chicago and was a postdoctoral fellow until November 2011. In Chicago, Sigrid developed an ultrafiltration-mass spectrometry assay for the discovery of ligands for the vitamin D receptor as leads for cancer chemoprevention. She also collaborated with radiologist Dr. Ron Gaba and used UHPLC-MS-MS to measure chemotherapeutic drugs in liver tissue. One manuscript from these studies has been published, one is in press and another is in preparation.



A student in the Pharmacognosy Graduate Program, Soyoun Ahn defended her dissertation in 2011, which was entitled, "In vitro studies of intestinal absorption and blood-brain barrier penetration of pharmacologically active compounds using cell monolayer models combined with HPLC-mass spectrometry." After staying in the group as a postdoctoral fellow for a few months, Soyoun is now a postdoctoral fellow in the mass spectrometry laboratory of Prof. Fred Stevens at Oregon State University.



Graduate student Zhiyuan Sun completed his M.S. degree in Medicinal Chemistry at the end of 2011. His thesis was entitled, "Mass spectrometric studies of Keap1-Nrf2 binding interactions." During the summer of 2011, Zhiyuan carried out a summer internship at Biogen-Idec. At the beginning of 2012, Zhiyuan joined the Genomics and Proteomics Core Laboratory of the University of Pittsburgh where he is applying his proteomics skills.

**As the laboratory grew to over 20 members during 2011, we also witnessed a record number of graduate students and postdoctoral fellows finishing their studies.**

## New Grants in 2011

The grant supporting our UIC/NIH Center for Botanical Dietary Supplements Research (P50 AT0155-12) was renewed for another five years at approximately \$1,000,000 per year. The new funding began at the end of 2010 and will extend until September 2015.

Founded in 1999, our Botanical Center is the oldest of its kind in the United States and was the first to be supported by the Office of Dietary Supplements and the National Center for Complementary and Alternative Medicine of the NIH. Founding Director Norman R. Farnsworth retired in 2011, and Prof. van Breemen became the new Director. We will miss Norm, who passed away in September.

The UIC Botanical Center remains focused on the evaluation of the

safety and efficacy of botanical dietary supplements used by women for the management of menopausal symptoms such as hot flashes.

The Analytical Core for the Botanical Center received a special supplemental award in 2011 of \$141,208 for the development and validation of UHPLC-MS-MS assays for the standardization and pharmacokinetics studies of the estrogenic constituents of hops. Hops contain prenylated flavonoids such as 8-prenylnaringenin that show estrogenic effects in

**“Our Botanical Center is the oldest of its kind and was the first to be supported by the National Institutes of Health.”**

bioassays. After validation of the method, we used this assay to measure the estrogenic hop constituents in serum from women who participated in our Phase I clinical trial during the summer of 2011.

During 2011, our Botanical Center published 12 research papers. Exactly half of these papers (6 of 12) originated from our group.

In another grant awarded during 2011, we were funded by PepsiCo to study natural pigments. We also received an instrument grant of \$600,000 from the NIH National Center for Research Resources (grant number 1 S10 RR025653) for the project entitled, “Orbitrap mass spectrometer for biomedical research.” Read more about this award in the “New Instrumentation” section.

## Awards

Pharmacognosy graduate student Andrew Newsome, who is working on our PepsiCo pigments project, received a 2011 American Foundation for Pharmaceutical Education (AFPE) Pre-doctoral Fellowship. This award is helping to offset his student fees and other expenses. Andrew also received honorable mention in the 2011



College of Pharmacy Images of Research competition for his entry, “Natural Blue Martini,” showing a

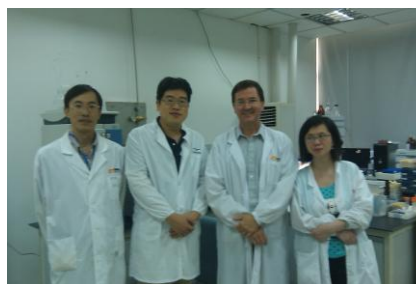
natural blue pigment that turns red upon acidification.

Medicinal chemistry graduate student Rui Yu, who is working on our prostaglandin project in collaboration with Dr. John Christman in Pulmonology, received a W. E. van Doren Scholar Award in 2011 from the College of Pharmacy.

## Meetings and travel

Most members of our group attended the ASMS conference in Denver CO during 2011, but we also made presentations at meetings of the International Carotenoid Society in Krakow Poland, the North American Phytochemical Society in Hawaii and a meeting sponsored by Shimadzu in Shanghai China. Prof. van Breemen met four of our lab graduates in Shanghai and one graduate from Dr. Bolton’s lab.

Linning Yu, Wenzhong Liang, Richard, & Yi Tao at ChemPartners, Shanghai



Xiaoying Xu (Novartis, Shanghai) and Yan Luo (Dow, Shanghai)



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## 2011 Publications

For more than ten years, we have been publishing between 10 and 20 peer-reviewed papers and book chapters each year. The list of our 2011 publications, 12 in all, is shown below. In addition to publications, our group presented over 20 posters and talks at national and international meetings which are too numerous to list.

For example, at the 2011 American Society for Mass Spectrometry and Allied Topics Conference in Denver, CO, our group presented 17 posters and talks. That was the second highest number of abstracts we have ever presented at a single meeting. Since the ASMS allows each author to present only once per meeting, we

sent 17 group members to Denver. Note, we presented 19 talks and posters at the 2010 ASMS conference in Salt Lake City, UT, which is our all-time record for presentations at a single meeting.

1. Cao H, Yu R, Tao Y, Nikolic D, van Breemen RB. Measurement of cyclooxygenase inhibition using liquid chromatography-tandem mass spectrometry. *J. Pharm. Biomed. Anal.* **54**, 230-235 (2011).
2. White AB, Galbiati F, Givogri MI, Lopez Rosas A, Qiu X, van Breemen R, Bongarzone ER. Persistence of psychosine in brain lipid rafts is a limiting factor in the therapeutic recovery of a mouse model for Krabbe disease. *J. Neurosci. Res.* **89**, 352-364 (2011).
3. Choi Y, Jermihov K, Nam S-J, Sturdy M, Maloney K, Qiu X, Chadwick LR, Main M, Chen S-N, Mesecar AD, Farnsworth NR, Pauli GF, Fenical W, Pezzuto JM, van Breemen RB. Screening natural products for inhibitors of quinone reductase-2 using ultrafiltration LC-MS. *Anal. Chem.* **83**, 1048-1052 (2011).
4. van Breemen RB, Tao Y, Li W. Cyclooxygenase-2 inhibitors in ginger (*Zingiber officinale*). *Fitoterapia*, **82**, 38-43 (2011). PubMed # 20837112; NIHMSID# 241578
5. Chen SN, Friesen JB, Webster D, Nikolić D, van Breemen RB, Wang ZJ, Fong HH, Farnsworth NR, Pauli GF. Phytoconstituents from *Vitex agnus-castus* fruits. *Fitoterapia*, **82**, 528-533 (2011).
6. Yang JH, Kondratyuk TP, Jermihov KC, Marler LE, Qiu X, Choi Y, Cao H, Yu R, Sturdy M, Huang R, Liu Y, Wang LQ, Mesecar AD, van Breemen RB, Pezzuto JM, Fong HH, Chen YG, Zhang HJ. Bioactive compounds from the fern *Lepisorus contortus*. *J. Nat. Prod.* **74**, 129-136 (2011).
7. Castelvetri LC, Givogri MI, Zhu H, Smith B, Lopez-Rosas A, Qiu X, van Breemen R, Bongarzone ER. Axonopathy is a compounding factor in the pathogenesis of Krabbe disease. *Acta Neuropathol.* **122**, 35-48 (2011).
8. Hu C, Egglar AL, Mesecar AD, van Breemen RB. Modification of Keap1 cysteine residues by sulforaphane. *Chem. Res. Toxicol.* **24**, 515-21 (2011).
9. van Breemen RB, Sharifi R, Viana M, Pajkovic N, Zhu D, Yuan L, Yang Y, Bowen PE, Stacewicz-Sapuntzakis M. Antioxidant effects of lycopene in African American men with prostate cancer or benign prostate hyperplasia: a randomized controlled trial. *Cancer Prev. Res. (Phila.)* **4**, 711-718 (2011).
10. Park EJ, Kondratyuk TP, Morrell A, Kiselev E, Conda-Sheridan M, Cushman M, Ahn S, Choi Y, White JJ, van Breemen RB, Pezzuto JM. Induction of retinoid X receptor activity and consequent upregulation of p21WAF1/CIP1 by indenoisoquinolines in MCF7 cells. *Cancer Prev. Res. (Phila.)* **4**, 592-607 (2011).
11. Kondratyuk TP, Park EJ, Marler LE, Ahn S, Yuan Y, Choi Y, Yu R, van Breemen RB, Sun B, Hoshino J, Cushman M, Jermihov KC, Mesecar AD, Grubbs CJ, Pezzuto JM. Resveratrol derivatives as promising chemopreventive agents with improved potency and selectivity. *Mol. Nutr. Food Res.* **55**, 1249-1265 (2011).
12. Yu R, Xiao L, Zhao G, Christman JW, van Breemen RB. Competitive enzymatic interactions determine the relative amounts of prostaglandins E<sub>2</sub> and D<sub>2</sub>. *J. Pharmacol. Exper. Ther.* **339**, 716-725 (2011).