

The van Breemen Group and Chicago Mass Spectrometry Laboratory 2013 Newsletter

Highlights of 2012

February, 2013
Volume 2, Issue 2

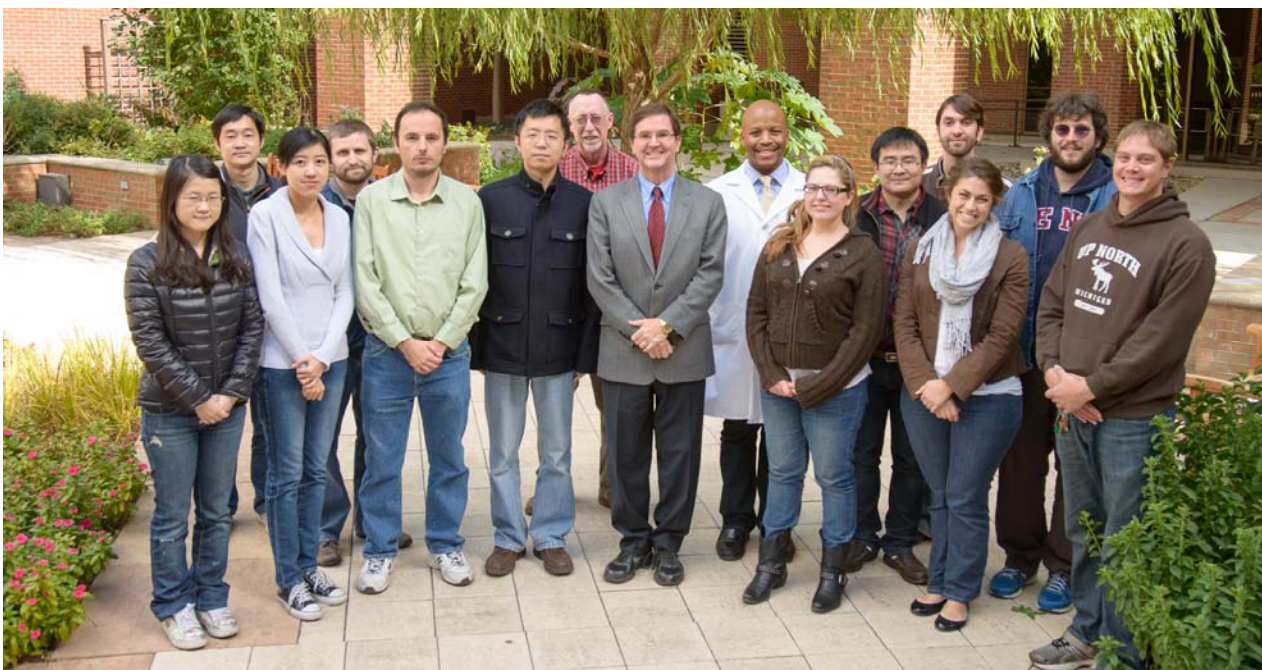
This is the second edition of the van Breemen research group newsletter. Highlights this year included the installation of a Shimadzu LCMS-8040 and LCMS-8080 triple quadrupole mass

spectrometers. **Five graduate students (this was a new single-year record)** and one postdoctoral fellow completed their studies. Research funding was renewed from Hershey

and the NIH (for our Botanical Center), and a new training grant was funded by the NIH to begin in 2013. Details of these achievements, lab publications and awards are provided below.

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2012 van Breemen Research Group in the Dorothy Atkins Botanical Garden. *Front row:* Guannan Li, Lian Chen, Dejan Nikolic, Ke Huang, Richard van Breemen, Elizabeth Martinez, Laura Gauthier, Zane Hauk. *Back row:* Jinbo Fang, Caleb Nienow, Rich Morrissy, Brian Wright, Yongchao Li, Andrew Newsome, Josh Henkin. (*Not pictured:* Linlin Dong and Kevin Krock)

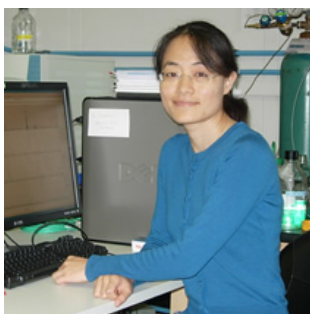
New Instrumentation

We continue to work closely with the Shimadzu Corporation. Jeff Dahl (PhD 2010) works for Shimadzu Scientific Instruments in Maryland and Kevin Krock (a Ph.D. candidate from our lab) already works for Shimadzu in

California. The Shimadzu LCMS-8030 mass spectrometer in our lab was replaced with the new LCMS-8040, which is more sensitive but equal in speed as the fastest triple quadrupole in the world. To enable quantitative

analysis with even better sensitivity, we were fortunate to install a Shimadzu LCMS-8080 triple quadrupole with a Nexera UHPLC system. We showed great data from both instruments at the 2012 ASMS conference.

Lab Graduates of 2012



Shunyan Mo, received her Pharmacognosy Ph.D. in 2009 working with Prof. Jimmy Orjala here at the University of Illinois College of Pharmacy. Then, she joined our laboratory as postdoctoral fellow until 2012. In our group, Shunyan worked on our project with the Hershey Company studying procyanidins in cocoa and human bioavailability and metabolism of epicatechin after drinking cocoa. One manuscript from these studies has been published, one is in press and another is in preparation.



Qiu Xi, a student in the Pharmacognosy Graduate Program and in the UIC/NIH Center for Botanical Dietary Supplements Research, received his Ph.D. after defending his dissertation in early 2012. The title of his dissertation was, "Chemoprevention studies of botanical dietary supplements by mass spectrometry." Xi's chemoprevention research included proteomics of lycopene and drug-botanical interactions of hops. He also continued our laboratory collaboration with the neuroscience group of Dr. Bongarzone by measuring psychosine in biological specimens. Xi was co-author on eight papers including a lycopene proteomics study currently in press in *Cancer Prevention Research*. Xi

is currently a postdoctoral fellow for Pfizer in Groton, CT.



A student in the Medicinal Chemistry Graduate Program, Yang Yuan defended her dissertation in mid-2012, which was entitled, "Quantitative analysis of estrogenic xenobiotics in humans using liquid chromatography-mass spectrometry." Yang was a member of the UIC Botanical Center and responsible for the quantitative analysis of botanical estrogens. She used our new Shimadzu LCMS-8030 and 8040 triple quadrupole instruments extensively in her work, and published a model paper on UPLC-MS-MS analysis of hop prenylated flavonoids in the *Journal of AOAC International*. Currently, Yang is a scientist at DuPont Crop Protection in Newark, DE.



Medicinal Chemistry graduate student Rui Yu received his Ph.D in mid-2012. The title of Rui's dissertation was, "Studies of cellular pathways and enzymatic modulations of prostanoids using mass spectrometry." These studies were part of our collaboration with the pulmonology group directed by Dr. John Christman. As in the past, this project was highly productive and enabled Rui to publish eight papers. Currently, Rui is currently a postdoctoral fellow with Dr. James Swenberg at the University of North



Lian Chen completed her Ph.D. in Pharmacognosy at the end of 2012. Her dissertation was entitled, "High throughput discovery, metabolism and disposition of chemopreventive agents using mass spectrometry," and focused on screening natural products for RXR ligands. These studies were part of our natural product drug discovery of chemoprevention agents collaboration with Dr. John Pezzuto. Lian carried out summer internships at Biogen-Idec (San Diego, CA) in 2009 and at Johnson & Johnson (Raritan, NJ) in 2010.



Jerry White received his Ph.D. in Medicinal Chemistry in 2012. His dissertation, "A high throughput LC-MS platform for the discovery of vitamin D receptor ligands," concerned the development of faster than ever ultrafiltration LCMS screening methods. Jerry received the Oscar Robert Olberg Prize in Medicinal Chemistry as a graduate student. Today, he works in the MS Laboratory of the UIC Research Resources Center.

In 2012, we set a new record for the most graduate students (5) finishing their studies in our laboratory during a single year.

Grants in 2012

We received a new grant that will support 6 graduate students and 3 postdoctoral fellows studying natural products in our department. I am the principal investigator, but not all of these trainees will be in our lab. Since this NIH T32 training grant begins on January 1, 2013, I will provide details in the next issue.

Our grant from Hershey was renewed, as was the UIC/NIH Center for Botanical Dietary Supplements Research (Year 13 of NIH grant P50 AT0155) which was refunded for \$1,450,247. Annual

renewals of this grant will continue through 2015. In 2012, the Center had 16 publications with our lab supplying over half.



2012 members of the UIC Botanical Center. I continue as Director with Judy Bolton and Guido Pauli as Project Leaders.

Awards

1. At the 3rd Annual College of Pharmacy Research Day last spring, Medicinal Chemistry graduate student Rui Yu received a W. E. van Doren Scholar Award for the second year in a row.



2. Yang Yuan, a graduate student in Medicinal Chemistry until graduating in mid-2012, received

the Charles Wesley Petranek Scholarship on Research Day.



3. Pharmacognosy graduate student Xi Qiu received a W. E. van Doren Scholar Award on Research Day 2012. Rui Yu, Yang Yuan and Xi Qiu graduated with Ph.D. degrees in 2012.

Alumni News

Congratulations to the following lab alumni (just a few highlights of many possible announcements)

Young-Geun Shin (postdoc 2001) is leaving Genentech for an associate professor position at Chungnam National University in DaeJeon, Korea. Email: shiny1027@gmail.com

Yongsoo Choi (postdoc 2010) left the FDA for a senior research scientist position at the Korean Institute of Science and Technology. Email: yongsoo.choi@kist.re.kr

Shunyan Mo (postdoc 2012) and Linlin Dong (Ph.D. 2013) welcomed the arrival of their son Ethan on August 28, 2012.



4. Finally, I was nominated by the American Society for Mass Spectrometry for Member at Large for Publications for the term 2013-2015. Although honored to be on the ballot, I did not win the election that was held in late 2012. Help me get out the vote next time!

Meetings

Our group presented 24 talks and posters at national and international meetings in 2012.

At the 60th ASMS Conference in Vancouver during May 2012, we presented 5 posters while I gave talks at the Shimadzu users' meeting and breakfast symposium. I also presided over a symposium on natural products and Traditional Chinese Medicine.

Pharmacognosy graduate student Andrew Newsome described his

research on natural blue pigments at the 244th American Chemical Society National Conference in Philadelphia in August 2012. This presentation was attended by our former group member Cathy Culver (PhD 1991) of PepsiCo, who was also responsible for initiating and funding this research.

I presented a talk and poster at the International Mass Spectrometry Conference in Kyoto, Japan in September 2012. I also helped Robert Cotter (my postdoctoral

advisor at Johns Hopkins University) sing his "Time-of-Flight" song for the last time at this conference. Bob died of heart failure in Baltimore on November 12, 2012. We will miss him.



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We're on the Web!
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2012 Publications

For more than 11 years, our laboratory has been publishing between 10 and 20 peer-reviewed papers and book chapters per year. In 2012, our group published 15 peer-reviewed papers, which exceeded our 2011 total of 12 papers and book chapters.

- Gödecke T, Yao P, Napolitano JG, Nikolić D, Dietz BM, Bolton JL, van Breemen RB, Farnsworth NR, Chen S-N, Lankin DC, Pauli GF. Integrated standardization concept for *Angelica* botanicals using quantitative NMR. *Fitoterapia* **83**, 18-32 (2012). PMC3380541
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