THE REACTION TIMES

All the news that's fit to react to.

Published twice a year by the ACS Division of Medicinal Chemistry

Volume 14, Number 2 Winter Newsletter July, 2015

Abstracts for the Boston ACS Meeting Will Soon Be Available for Download

Abstracts for the upcoming Boston ACS meeting will soon be available on the Division web site. Follow the link below to download the MEDI abstracts for the Boston ACS meeting:

http://www.acsmedchem.org/?nd=nationalmeetings

Quick Reference Guide to Services

Division Web Site: http://www.acsmedchem.org

Division Hall of Fame:
http://www.acsmedchem.org/?nd=hof

Link to Division Newsletter Archive:
http://www.acsmedchem.org/?nd=newsletters

Link to Archived MEDI Meeting Abstracts:
http://www.acsmedchem.org/?nd=nationalmeetings

ACS Web Page
http://portal.acs.org

Journal of Medicinal Chemistry
http://pubs.acs.org/journal/jmcmar

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Contact information for all Division Officers appears at the end of this Newsletter.

Scientific Program for the 250th ACS Meeting, Boston (Aug 16-19, 2015)

(ACS Abstract system now closed for this meeting)

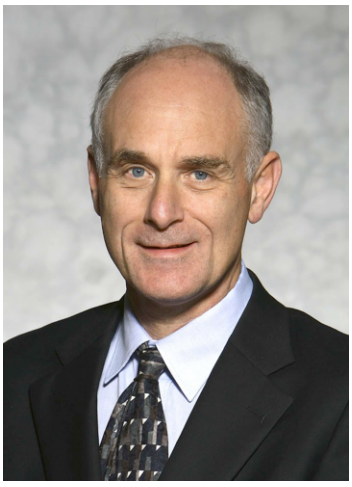
SUN AM	Neuroinflammation
SUN AM	Natural Products
SUN AM	General Oral Session I
SUN PM	Protein-Protein Interactions
SUN PM	Young Investigators Symposium
SUN PM	General Oral Session II
SUN EVE	Poster Session I and Social Hour
MON AM	Antibody Drug Conjugates
MON AM	Safety--In Silico Approaches
MON AM	Ophthalmic Drug Discovery
MON PM	Cancer Immunotherapy
MON PM	Safety--Case Studies
MON PM	Design of Allosteric Modulators
TUES AM	Med Chem Toolbox: Inducible pockets, water
TUES AM	MEDI Awards Symposium
TUES PM	Case Studies of Successful Drugs
TUES PM	Deuterated Drugs
WED AM	Recent Advances in Heart Failure
WED AM	Covalent Inhibitors Past Oncology
WED AM	General Oral Session III
WED PM	First Time Disclosures
WED PM	General Oral Session IV
WED EVE	Poster Session II

Scientific Program for the 251st ACS Meeting, San Diego (Mar 13-17, 2016)

(ACS Abstract system open soon, maps.acs.org)

SUN AM	Targeting Bromodomains
SUN AM	General Oral Session I
SUN PM	Med Chem Toolbox: Off-target Liabilities
SUN PM	General Oral Session II
SUN EVE	Poster Session I and Social Hour
MON AM	Neuroactive Steroids
MON AM	Countering Lethal Chemicals & Biologicals
MON AM	Young Investigators Symposium
MON PM	Med Chem Driven by Phenotypic Assays
MON PM	EFMC-sponsored symposium, TBD
MON PM	Ketamine as Antidepressant
TUES AM	Antibiotic Drug Resistance
TUES AM	MEDI Awards Symposium--Burger
TUES PM	Blood Brain Barrier in Drug Discovery
TUES PM	Type II Kinase Inhibitors
TUES PM	General Oral Session III
WED AM	First Time Disclosures
WED AM	Accelerating Med Chem by Trusting Genetics
WED PM	First Time Disclosures
WED PM	General Oral Session IV
WED EVE	Poster Session II

Nicholas Meanwell to Receive Portoghese Lectureship



The American Chemical Society's Division of Medicinal Chemistry and the *Journal of Medicinal Chemistry* are pleased to announce that **Nicholas A. Meanwell** has been selected as the 2015 recipient of the fifth Philip S. Portoghese Medicinal Chemistry Lectureship. This award is named in honor of Phil Portoghese, the long-standing Editor-in-Chief of the Journal of Medicinal Chemistry. The Lectureship is administered jointly by the Editor-in-Chief of the Journal and the ACS Division of Medicinal Chemistry. The objective of the lectureship is to honor the contributions of an individual who has had a major impact on medicinal chemistry research. The award is funded principally by the Journal of Medicinal Chemistry (ACS Publications Division) and the awardee is selected by a committee appointed jointly by the Journal and the Division of Medicinal Chemistry. Dr. Meanwell will receive the award and give the award address at the 250th National American Chemical Society Meeting in Boston, MA, on Tuesday, August 8.

Dr. Meanwell was awarded the B.Sc. with Special Honours in Chemistry, and the Ph.D. in Organic Chemistry, from the University of Sheffield. He carried out post-doctoral research with Prof. Carl R. Johnson at Wayne State University. Next, he joined Bristol-Myers Squibb Research and Development, where he is currently Executive Director of the Department of Discovery Chemistry. There, he has led teams that discovered the platelet aggregation inhibitor BMY-20844 which was advanced into clinical trials, and developed the early phase discovery chemistry around the potassium channel modulators that ultimately resulted in flindokalner (MaxiPost™) which was advanced into Phase 3 clinical trials for the treatment of stroke. Significant discoveries to emerge from the antiviral arena include a series of RSV fusion inhibitors and a series of HIV-1 attachment inhibitors. From this work, BMS-663068, a phosphonooxymethyl prodrug of BMS-626529, has just successfully completed Phase 2 clinical trials and entered Phase 3 studies in early 2015. More recently, the HIV-1 maturation inhibitor BMS-955176 has completed Phase 2a clinical trials with the results presented at an international meeting in February 2015.

Significant compounds in the HCV arena include daclatasvir (Daklinza™), the first-in-class NS5A inhibitor that established this viral protein as a clinically-relevant target, and the HCV NS3 protease inhibitor asunaprevir (Sunvepra™), which incorporates the cyclopropyl acylsulfonamide moiety that has been widely adopted, both of which have completed Phase 3 clinical trials. The combination of daclatasvir and asunaprevir in a clinical trial conducted in HCV-infected subjects who had not responded to or had failed pegylated-interferon-α and ribavirin established for the first time that an HCV infection could be cured by direct acting antiviral agents in the absence of immune stimulation. Daklinza™ and Sunvepra™ were approved for marketing in Japan in 2014 and Daklinza™ is approved for the treatment of HCV infection in Europe when used in conjunction with other agents. In addition, beclabuvir, a thumb site inhibitor of HCV NS5B polymerase, is currently in Phase 3 trials in combination with daclatasvir and asunaprevir.

Dr. Meanwell is a Member of the Connecticut Academy of Science and Engineering. He is a Fellow and a Chartered Chemist of the Royal Society of Chemistry, and a Chartered Scientist of the Science Council (UK), and a member of the American Chemical Society. He serves on the Editorial Advisory Boards of *The Journal of Medicinal Chemistry*, *ACS Infectious Diseases*, and *Drug Discovery Today*. Dr. Meanwell has co-authored more than 140 peer-reviewed publications, over 50 review articles and book chapters, over 160 meeting abstracts, and is inventor or co-inventor of over 110 U.S. Patents. He is co-recipient of a PhRMA Research and Hope Award for Biopharmaceutical Industry Research, 2014 for outstanding research in the area of HIV/AIDS associated with the development of the HIV-1 attachment inhibitor BMS-626529 and its prodrug BMS-663068.

Attending ACS - Fall in Boston?

Don't miss out on the Tetrahedron Prize for Creativity in Organic Chemistry Symposium

When:
Monday, August 17, 2015
1:00 PM - 5:10 PM

Location:
Ballroom East, Boston Convention Center, USA

Congratulations to **Professor Barry Trost** from Stanford University, USA who was joint winner* of the **2014 Tetrahedron Prize** for his outstanding contributions to Organic Chemistry. The prize will be presented to Professor Barry Trost during this event which will be presided by Stephen F. Martin, The University of Texas at Austin, USA.

Speakers include:

Michael Krische, *The University of Texas at Austin, USA*
Formation of C-C Bonds via Hydrogenation and Transfer Hydrogenation

Gary Molander, *University of Pennsylvania, USA*
A Novel Mechanistic Paradigm for Cross-Coupling

Dean Toste, *UC Berkeley, USA*
Enantioselective Catalysis with Cations and Anions

Barry Trost, *Stanford University, USA*
On the invention of PD catalyzed allylic alkylations for enabling chemical synthesis

**Note: The Tetrahedron Prize was shared this year with Professor Jiro Tsuji who was awarded with his prize at the Chemical Society of Japan meeting earlier this year.*

ELSEVIER

Three Students Selected to Receive ACSMEDI Predoctoral Fellowships

The Division of Medicinal Chemistry is pleased to announce that three graduate students have been selected to receive 2015-2016 Predoctoral Fellowships. The awards, consisting of a $26,000 stipend, are granted to predoctoral students in their third or fourth year of graduate study. Winners must be engaged in medicinal chemistry research in a Medicinal Chemistry, Pharmaceutical Chemistry, Biochemistry, or Chemistry department listed in the current ACS Directory of Graduate Research. Two of these awards are supported by the Medicinal Chemistry Division of ACS. One of the fellowships is supported through the generosity of Division members Thomas Perun. The awardees for the 2015-2016 academic year are:

Dana Klug, Northeastern University, Advisor: Michael Pollastri. Dana earned a B.S. in Chemistry from DePaul University in 2013, where her work in the laboratory of Dr. Caitlin Karver focused on the development of a small-molecule probe to aid in the discovery of caspase-1 inhibitors. She is currently pursuing her Ph.D. at Northeastern University in Dr. Michael Pollastri's group, where her research is centered on the development of small molecules that target the causative agents of such neglected diseases as human African trypanosomiasis and malaria via both target repurposing and HTS-based approaches.

Jonathan Tietz, University of Illinois, Advisor: Douglas A. Mitchell. Jonathan I. Tietz received a B.S. in chemistry (2011) with a minor in biology from Kent State University in Kent, OH, followed by an M.S. in organic chemistry (2012) at the same institution; there he worked for Dr. Alexander J. Seed and Dr. Paul Sampson studying the synthesis and characterization of low molecular-weight, electron-rich liquid crystals. In 2012, Jonathan joined Dr. Douglas A. Mitchell's lab at the University of Illinois at Urbana-Champaign. His current research focuses on genome-guided discovery of biologically active natural products via chemoselective methods as well as using genomics for natural product structure elucidation.

Kelsey Knewtson, University of Kansas, Advisor: Blake Peterson. Kelsey received a B.S. in Biochemistry from the University of Arkansas, where she worked in the lab of Dr. Bob Gawley. In 2012 she joined the lab of Blake Peterson in the Department of Medicinal Chemistry at the University of Kansas. Her current research focuses on improving the efficacy and decreasing the off-target effects of antibody-drug conjugates.

ACS Webinar Series on Drug Design and Delivery

2015 Drug Design and Delivery Symposium

MEET THE BEST AND BRIGHTEST MINDS IN MEDICINAL CHEMISTRY

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www.acs.org/content/acs/en/acs-webinars/drug-discovery.html

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Cresset posters:

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MEDI 90: Sunday August 16, 7:00pm

"Is this compound worth making?"
MEDI 92: Sunday August 16, 7:00pm

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"Data visualisation: New directions or just familiar routes"
CINF: Sunday August 16, 1:30pm

"Modeling ABC transporters as potential DILI targets
CINF: Wednesday August 19, 3:50pm

Meet us:

Satellite exposition: MEDI sessions

Get a free evaluation:

optibrium.com/stardrop

Meet us at exposition hall booth 417

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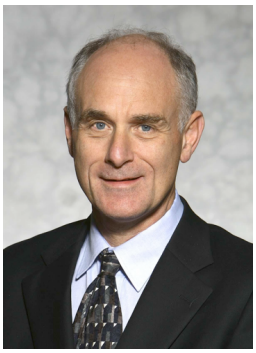
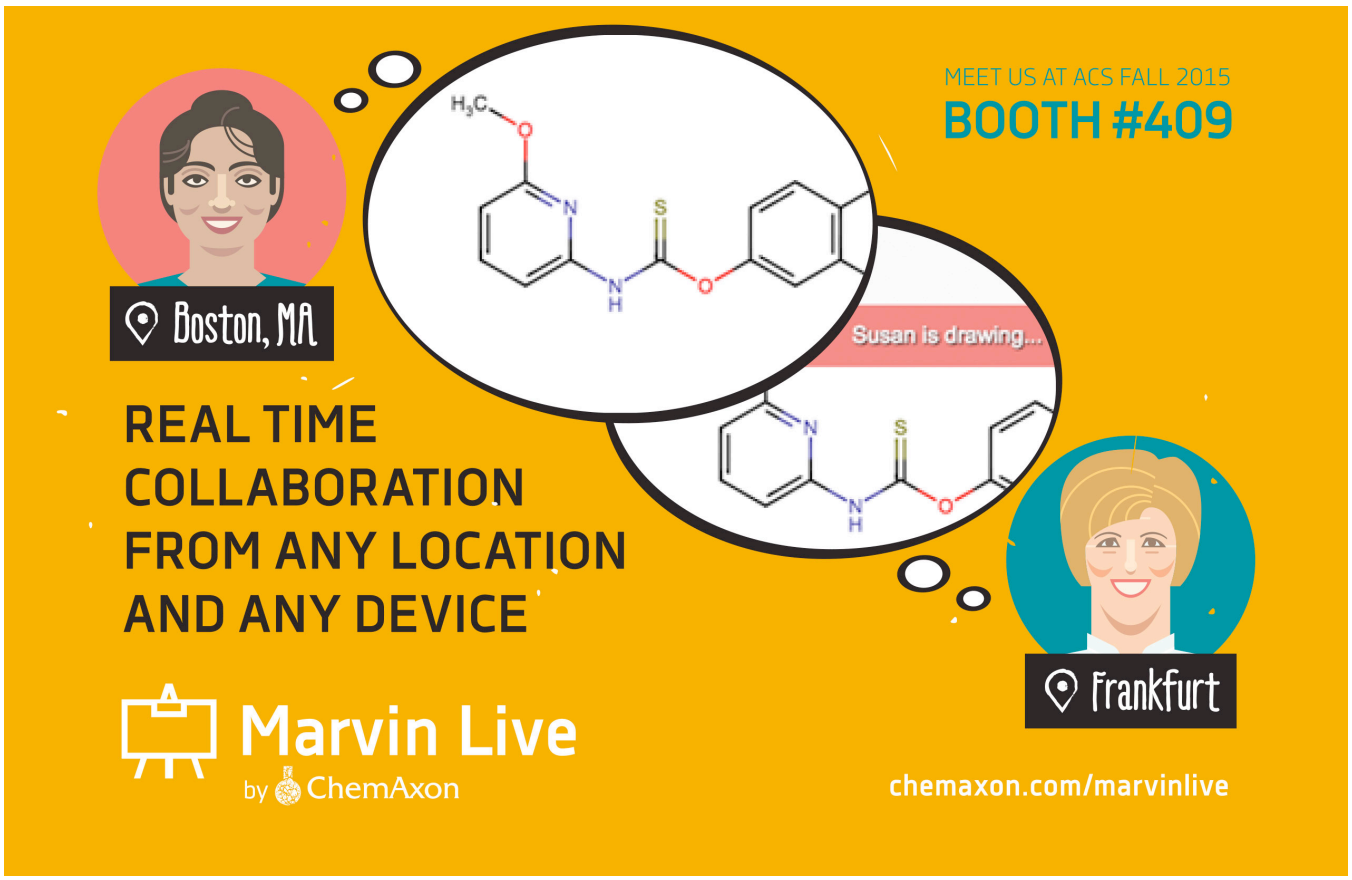
2015 Hall of Fame Inductees Announced

The Division is pleased to announce that **Nicholas A. Meanwell**, Executive Director of the Department of Discovery Chemistry at Bristol-Myers Squibb, will be inducted into the ACS Division of Medicinal Chemistry Hall of Fame at the Boston ACS meeting. His biographical information appears in the previous pages of this Newsletter. The Med Chem Hall of Fame Induction Ceremony will be held on Tuesday, August 18, at 5:30 p.m. in the Boston Convention and Exhibition Center, room 52AB. Dr. Richard Glennon and Dr. Ruth Wexler, who were elected to the Hall of Fame last year, were unable to travel to last year's meeting; they will be formally inducted at this ceremony as well. All MEDI members are cordially invited to attend.



Richard A. Glennon is Alfred and Frances Burger Distinguished Professor of Medicinal Chemistry at Virginia Commonwealth University. **Ruth R. Wexler** is Executive Director of Discovery Chemistry at Bristol-Myers Squibb Company in Hopewell, New Jersey.



Medicinal Chemistry Division Members named as ACS Fellows

The American Chemical Society Fellows Program recognizes members of ACS for outstanding achievements in and contributions to science, the profession, and society. Six distinguished medicinal chemists are among the 2015 Fellows.

Yusuf Abul-Hajj is Professor of Medicinal Chemistry, and former chair of the Department, at the University of Minnesota. He is also a Fellow of the American Association for the Advancement of Science.

Amjad Ali is Director of Discovery Chemistry at Merck, and is an Alternate Councilor of the MEDI Division.

Michael Appel is a Research Scientist at the USDA's Agricultural Research Service in Peoria, IL. He holds a Ph.D. from the Department of Medicinal Chemistry at the University of Illinois Chicago.

Bonnie A. Charpentier is Senior Vice President for Regulator and Quality at Cytokinetics, Inc., in the San Francisco Bay area.

Mark D. Frishberg is retired from Eastman Kodak Company, where he was a Senior Research Scientist, Director, and Business Development Executive.

Michael Singer is R&D Manager at Sigma Aldrich in the Boston area.

Call for Nominations:
2016 Division of Medicinal Chemistry Award

Nominations are now being accepted for the 2016 Division of Medicinal Chemistry Award. The Division of Medicinal Chemistry award consists of three thousand dollars, a plaque and travel expenses incidental to receiving the Award. The award will be presented as a part of a special session at the 2016 National Medicinal Chemistry Symposium held in Chicago, IL, June 26 - 29, 2016.

The Award shall be open to any scientist here or abroad, whose research has, directly or indirectly, had a significant effect on Medicinal Chemistry. Although other types of accomplishment (such as a new research tool or a biological discovery) shall not be excluded, emphasis shall be placed on (a) medicinal chemistry, (b) recent contributions, and (c) scientists whose accomplishments have not already been adequately recognized in the form of other honors. Research teams shall not be excluded as sharers of the Award.

Nominations must include a detailed letter describing the candidate's research accomplishments and contributions to medicinal chemistry, at least one seconding letter and a current curriculum vitae of the nominee(s). Materials must be submitted electronically by **September 1, 2015** to the Chair of the Division:

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See the website, www.acsmedchem.org/?nd=divisionaward, for further information and previous winners.

251st NATIONAL ACS MEETING
San Diego, CA, Mar 13-17, 2016
ACS Abstracts System to open soon

You are invited to submit an abstract for a research presentation at the 251st National Meeting of the American Chemical Society, to be held March 13-17, 2016, in San Diego, CA. All abstracts should be submitted online using the new ACS Abstract system, MAPS (http://maps.acs.org), which will open soon. The **deadline** for abstract submission will also be the deadline for submission of travel grant applications, as outlined elsewhere in this Newsletter. The MEDI scientific program and abstracts will be available for download 3-4 weeks prior to the meeting, and their availability will be announced by email. For more information on programming or abstract submission, contact the Program Chair, Wendy Young, at young.wendy@gene.com.

Sponsorship for Division of Medicinal Chemistry Symposia

Division of Medicinal Chemistry symposia at National Meetings are presented in part through the financial support of sponsor companies. Sponsorship opportunities are available for all upcoming Division of Medicinal Chemistry Symposia. Symposium sponsors for national ACS meetings are acknowledged with a prominent sign outside the meeting room, and by session chairs during the symposium. In addition, a table is provided where company representatives can interact with meeting attendees, and provide promotional materials. For more information on symposium sponsorship, contact the 2015 Program Chair, Wendy Young (young.wendy@gene.com), or the 2015 Division Chair, John Macor (john.macor@bms.com).

The Division would like to thank the generous sponsors of our Boston symposia!

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Invitation to Authors: *Journal of Medicinal Chemistry* Perspective Series

The Perspective series of the *Journal of Medicinal Chemistry* is designed to provide an enlightened appraisal of a field of research in which experts review the state-of-the-art for a given area or therapeutic target. Authors have editorial freedom to express their views on the strategic directions of the field of research. The Perspective series provides a forum with high visibility within the pharmaceutical industry and academia. We would like to identify a wide range of potential topics and authors to ensure that a Perspective article is published in every issue of the Journal. We would like the series to be useful to a broad range of scientists interested in the design, discovery and development of novel medicines. We invite you to submit an idea for a Perspective, along with a brief outline of what you will cover in the manuscript. We also welcome your input regarding potential topics of interest and authors for Perspective manuscripts. Please direct correspondence or calls regarding the series to:

William J. Greenlee
MedChem Discovery Consulting
115 Herrick Avenue
Teaneck, NJ 07666-4106
Phone (908)-463-5332
william@william-greenlee.com

See You in Chicago Next Summer!

Plan to come to Chicago next Summer for the National Medicinal Chemistry Symposium! The Medicinal Chemistry Division will be held June 26-29, 2016, at the Chicago Hilton Hotel on Michigan Avenue, within walking distance of the Art Institute of Chicago, the Field Museum of Natural History, the Adler Planetarium, and the Shedd Aquarium.

NMCS 2016 is the 35th in the series that was initiated in 1948, and the meeting continues to be a centerpiece conference sponsored by the ACS Division of Medicinal Chemistry. The scientific program for the NMCS will feature sessions covering the latest advances in medicinal chemistry. Session topic areas include:

- Transcription Factors as Drug Targets
- Open Innovation and External Partnership Platforms
- Challenges and Recent Advances in the Treatment of Neurodegenerative Disorders
- DMPK Concepts in Medicinal Chemistry--Case Studies
- Epigenetic Mechanisms of Action in the Treatment of Human Diseases
- Drugging the Undruggable
- Medicinal Chemistry Division Award Session

If you are interested in sponsorship or in being an exhibitor, please contact the Organizing Chairs:

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Division Travel Grants

The Division of Medicinal Chemistry makes 14 grants of $600 - $1000 available annually to aid young chemists in presenting papers at the ACS National Meetings. Applicants must be ACS regular or student members, and not have previously received a travel award. Each University department can have only one awardee. Application deadlines are the same as the abstract deadline for each meeting. In order of priority, the following individuals will be considered for awards: Graduate Student, Postdoctoral Fellow, individual with less than five years post-Ph.D. experience. The scientific merit of the paper to be presented will also be considered. Applications are to be submitted online at the ACS Med Chem website:

https://www.acsmedchem.org/?nd=travelgrants

Awardees will be notified in sufficient time so that they can pre-register for the meeting. **All travel grant recipients are required to acknowledge the Division in a slide or on their poster as a condition of accepting the award**. Awards are made at the Division business meeting, which is held at each national meeting immediately before the Sunday night poster session and mixer. Address info and a complete application appears on the following page.

Advertise in the ACSMEDI Newsletter

The ACSMEDI Newsletter is distributed twice a year to 10,500 medicinal and organic chemist members, and is freely accessible to all through the ACSMEDI homepage. In response to a number of inquiries, we have established the following advertising policy:

Full page:	$900.00
One-half page:	$500.00
One-quarter page:	$350.00

To place an ad or obtain more information, contact the editor at eric.walters@rosalindfranklin.edu

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Division Archives Available On-line

Division newsletters, scientific programs and abstract books dating to 2002 are archived online. These documents can be downloaded in pdf format through the Division WWW page:

http://www.acsmedchem.org

Annual Reports in Medicinal Chemistry

Changes in Delivery

One of the benefits of membership in the Medicinal Chemistry Division (MEDI) of the ACS is getting a free copy of *Annual Reports in Medicinal Chemistry*. The cost of producing and shipping the book presently is approximately $15 per book shipped in the US, and more than $30 for international delivery. Since the cost of the book shipped internationally is actually greater than the cost of MEDI membership, the Executive Committee of MEDI has decided to deliver *Annual Reports in Medicinal Chemistry* electronically to our non-US members to the e-mail address listed with the ACS. This change in delivery of Annual Reports in Medicinal Chemistry began with Volume 49.

Going forward, with Volume 50 in 2015, MEDI will deliver all copies of *Annual Reports in Medicinal Chemistry* electronically to all members of MEDI, US and international, with an option to print at additional cost. This is consistent with the practices in the publishing industry, and will allow MEDI to better utilize its limited resources. Thank you for your membership in MEDI and for your understanding in this change. Please address your comments and suggestions to John Macor (john.macor@bms.com) or Manoj Desai (manoj.desai@gilead.com).

Help Wanted: Social Media & Website Volunteers

The Division currently has only a limited presence in social media. Other Divisions (Organic, for instance) make good use of this avenue to engage their members and potential members. If you have ideas, suggestions, or time & energy to invest in this area, please contact the Division Secretary, Eric (not a social media guru) Walters, at eric.walters@rosalindfranklin.edu or secretary@acsmedchem.org. This can be a great way to get involved with the Division!

ACS Division of Medicinal Chemistry
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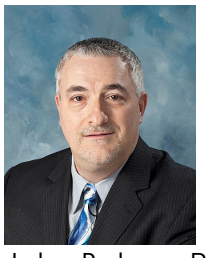

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